



Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 06:17 PM EDT

PDB ID : 9YDS / pdb_00009yds
EMDB ID : EMD-72833
Title : H-ring subunit FlgO and FlgP in Vibrio cholerae at assembled, opened state
Authors : Guo, W.; Yue, J.
Deposited on : 2025-09-23
Resolution : 3.45 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

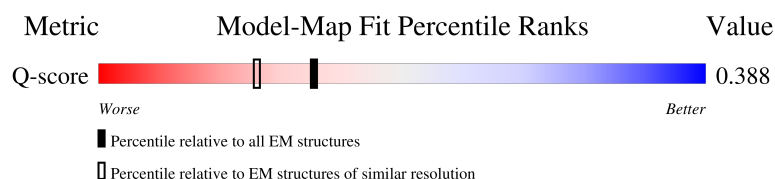
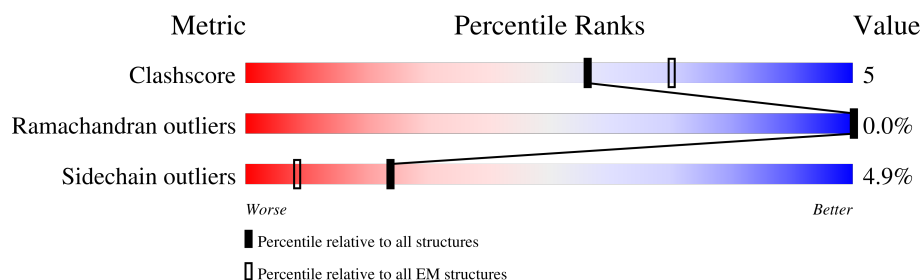
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















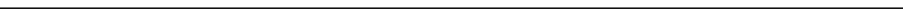











Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	104	87% 12% .
1	Ac	104	87% 13%
1	Ae	104	85% 15%
1	Ag	104	87% 12% .


























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Mol	Chain	Length	Quality of chain
1	Ai	104	 85% 13%
1	Ak	104	 88% 12%
1	Am	104	 88% 11%
1	Ao	104	 84% 16%
1	Aq	104	 88% 12%
1	As	104	 88% 12%
1	Au	104	 88% 12%
1	Aw	104	 87% 13%
1	Ay	104	 84% 16%
1	Ba	104	 84% 15%
1	Bc	104	 85% 14%
1	Be	104	 86% 13%
1	Bg	104	 86% 13%
1	Bi	104	 86% 14%
1	Bk	104	 87% 12%
1	Bm	104	 87% 12%
1	Bo	104	 86% 12%
1	Bq	104	 87% 12%
1	Bs	104	 86% 12%
1	Bu	104	 83% 15%
1	Bw	104	 90% 10%
1	By	104	 86% 13%
1	Ca	104	 88% 12%
1	Cc	104	 87% 12%
1	Ce	104	 85% 14%











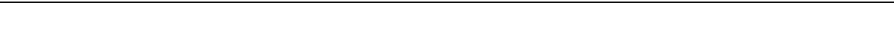

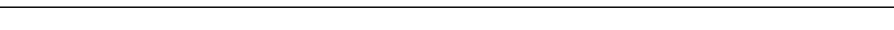
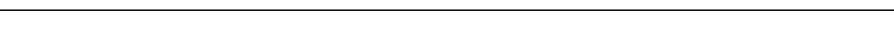











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Mol	Chain	Length	Quality of chain
1	Cg	104	 85% 14%
1	Ci	104	 83% 16%
1	Ck	104	 83% 16%
1	Cm	104	 87% 13%
1	Co	104	 87% 12%
1	Cq	104	 88% 11%
1	Cs	104	 88% 12%
1	Cu	104	 87% 13%
1	Cw	104	 88% 12%
1	Cy	104	 90% 10%
1	Da	104	 88% 12%
1	Dc	104	 85% 15%
1	De	104	 87% 12%
1	Dg	104	 86% 13%
1	Di	104	 87% 13%
1	Dk	104	 83% 16%
1	Dm	104	 85% 14%
1	Do	104	 89% 11%
1	Dq	104	 87% 12%
1	Ds	104	 84% 15%
1	Du	104	 84% 14%
1	Dw	104	 81% 19%
1	Dy	104	 85% 14%
1	Ea	104	 85% 13%
1	Ec	104	 87% 13%














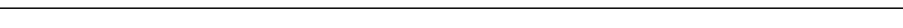











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Mol	Chain	Length	Quality of chain
1	Ee	104	 86% 14%
1	Eg	104	 87% 12% ..
1	Ei	104	 84% 16%
1	Ek	104	 85% 14% ..
2	Ab	192	 80% 18% ..
2	Ad	192	 80% 18% ..
2	Af	192	 85% 13% ..
2	Ah	192	 83% 15% ..
2	Aj	192	 82% 16% ..
2	Al	192	 80% 18% ..
2	An	192	 83% 15% ..
2	Ap	192	 83% 14% ..
2	Ar	192	 78% 19% ..
2	At	192	 78% 19% ..
2	Av	192	 80% 17% ..
2	Ax	192	 81% 17% ..
2	Az	192	 78% 20% ..
2	Bb	192	 83% 14% ..
2	Bd	192	 81% 16% ..
2	Bf	192	 81% 17% ..
2	Bh	192	 80% 17% ..
2	Bj	192	 84% 14% ..
2	Bl	192	 81% 17% ..
2	Bn	192	 80% 16% ..
2	Bp	192	 84% 14% ..




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Mol	Chain	Length	Quality of chain
2	Br	192	 81% 17% ..
2	Bt	192	 83% 15% ..
2	Bv	192	 78% 19% ..
2	Bx	192	 81% 17% ..
2	Bz	192	 83% 15% ..
2	Cb	192	 83% 15% ..
2	Cd	192	 81% 16% ..
2	Cf	192	 83% 15% ..
2	Ch	192	 82% 16% ..
2	Cj	192	 82% 16% ..
2	Cl	192	 84% 13% ..
2	Cn	192	 84% 14% ..
2	Cp	192	 81% 17% ..
2	Cr	192	 81% 17% ..
2	Ct	192	 82% 16% ..
2	Cv	192	 78% 20% ..
2	Cx	192	 79% 19% ..
2	Cz	192	 81% 17% ..
2	Db	192	 81% 17% ..
2	Dd	192	 83% 15% ..
2	Df	192	 80% 18% ..
2	Dh	192	 78% 20% ..
2	Dj	192	 80% 18% ..
2	Dl	192	 81% 17% ..
2	Dn	192	 82% 16% ..

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Mol	Chain	Length	Quality of chain
2	Dp	192	 82% 16% ..
2	Dr	192	 80% 18% ..
2	Dt	192	 81% 16% ..
2	Dv	192	 84% 14% ..
2	Dx	192	 80% 18% ..
2	Dz	192	 80% 18% ..
2	Eb	192	 79% 19% ..
2	Ed	192	 79% 19% ..
2	Ef	192	 80% 17% ..
2	Eh	192	 80% 17% ..
2	Ej	192	 82% 16% ..
2	El	192	 83% 15% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 133980 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ac	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ae	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ag	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ai	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ak	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Am	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ao	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Aq	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	As	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Au	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Aw	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ay	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ba	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bc	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Be	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bg	104	Total	C	N	O	S	0	0
			828	506	155	163	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bk	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bm	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bo	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bq	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bs	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bu	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Bw	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	By	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ca	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cc	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ce	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cg	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ci	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ck	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cm	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Co	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cq	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cs	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cu	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Cw	104	Total	C	N	O	S	0	0
			828	506	155	163	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Cy	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Da	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dc	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	De	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dg	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Di	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dk	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dm	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Do	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dq	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ds	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Du	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dw	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Dy	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ea	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ec	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ee	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Eg	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ei	104	Total	C	N	O	S	0	0
			828	506	155	163	4		
1	Ek	104	Total	C	N	O	S	0	0
			828	506	155	163	4		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	?	-	VAL	deletion	UNP Q9KQ01
Ac	?	-	VAL	deletion	UNP Q9KQ01
Ae	?	-	VAL	deletion	UNP Q9KQ01
Ag	?	-	VAL	deletion	UNP Q9KQ01
Ai	?	-	VAL	deletion	UNP Q9KQ01
Ak	?	-	VAL	deletion	UNP Q9KQ01
Am	?	-	VAL	deletion	UNP Q9KQ01
Ao	?	-	VAL	deletion	UNP Q9KQ01
Aq	?	-	VAL	deletion	UNP Q9KQ01
As	?	-	VAL	deletion	UNP Q9KQ01
Au	?	-	VAL	deletion	UNP Q9KQ01
Aw	?	-	VAL	deletion	UNP Q9KQ01
Ay	?	-	VAL	deletion	UNP Q9KQ01
Ba	?	-	VAL	deletion	UNP Q9KQ01
Bc	?	-	VAL	deletion	UNP Q9KQ01
Be	?	-	VAL	deletion	UNP Q9KQ01
Bg	?	-	VAL	deletion	UNP Q9KQ01
Bi	?	-	VAL	deletion	UNP Q9KQ01
Bk	?	-	VAL	deletion	UNP Q9KQ01
Bm	?	-	VAL	deletion	UNP Q9KQ01
Bo	?	-	VAL	deletion	UNP Q9KQ01
Bq	?	-	VAL	deletion	UNP Q9KQ01
Bs	?	-	VAL	deletion	UNP Q9KQ01
Bu	?	-	VAL	deletion	UNP Q9KQ01
Bw	?	-	VAL	deletion	UNP Q9KQ01
By	?	-	VAL	deletion	UNP Q9KQ01
Ca	?	-	VAL	deletion	UNP Q9KQ01
Cc	?	-	VAL	deletion	UNP Q9KQ01
Ce	?	-	VAL	deletion	UNP Q9KQ01
Cg	?	-	VAL	deletion	UNP Q9KQ01
Ci	?	-	VAL	deletion	UNP Q9KQ01
Ck	?	-	VAL	deletion	UNP Q9KQ01
Cm	?	-	VAL	deletion	UNP Q9KQ01
Co	?	-	VAL	deletion	UNP Q9KQ01
Cq	?	-	VAL	deletion	UNP Q9KQ01
Cs	?	-	VAL	deletion	UNP Q9KQ01
Cu	?	-	VAL	deletion	UNP Q9KQ01
Cw	?	-	VAL	deletion	UNP Q9KQ01
Cy	?	-	VAL	deletion	UNP Q9KQ01
Da	?	-	VAL	deletion	UNP Q9KQ01
Dc	?	-	VAL	deletion	UNP Q9KQ01
De	?	-	VAL	deletion	UNP Q9KQ01
Dg	?	-	VAL	deletion	UNP Q9KQ01

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Chain	Residue	Modelled	Actual	Comment	Reference
Di	?	-	VAL	deletion	UNP Q9KQ01
Dk	?	-	VAL	deletion	UNP Q9KQ01
Dm	?	-	VAL	deletion	UNP Q9KQ01
Do	?	-	VAL	deletion	UNP Q9KQ01
Dq	?	-	VAL	deletion	UNP Q9KQ01
Ds	?	-	VAL	deletion	UNP Q9KQ01
Du	?	-	VAL	deletion	UNP Q9KQ01
Dw	?	-	VAL	deletion	UNP Q9KQ01
Dy	?	-	VAL	deletion	UNP Q9KQ01
Ea	?	-	VAL	deletion	UNP Q9KQ01
Ec	?	-	VAL	deletion	UNP Q9KQ01
Ee	?	-	VAL	deletion	UNP Q9KQ01
Eg	?	-	VAL	deletion	UNP Q9KQ01
Ei	?	-	VAL	deletion	UNP Q9KQ01
Ek	?	-	VAL	deletion	UNP Q9KQ01

- Molecule 2 is a protein called FlgO domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ad	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Af	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ah	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Aj	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Al	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	An	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ap	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ar	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	At	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Av	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ax	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Az	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bb	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bd	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bf	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bh	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bj	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bl	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bn	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bp	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Br	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bt	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bv	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bx	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Bz	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cb	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cd	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cf	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ch	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cj	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cl	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cn	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cp	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cr	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ct	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cv	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cx	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Cz	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Db	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dd	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Df	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dh	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dj	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Di	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dn	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dp	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dr	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dt	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dv	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dx	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Dz	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Eb	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ed	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ef	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Eh	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	Ej	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		
2	El	190	Total	C	N	O	S	0	0
			1482	928	260	287	7		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lipoprotein

Chain Aa: 




- Molecule 1: Lipoprotein

Chain Ac: 




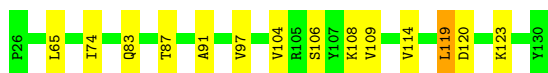
- Molecule 1: Lipoprotein

Chain Ae: 




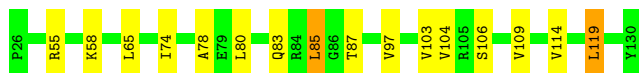
- Molecule 1: Lipoprotein

Chain Ag: 




- Molecule 1: Lipoprotein

Chain Ai: 



- Molecule 1: Lipoprotein

Chain Ak:  88% 12%




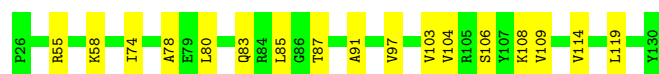
• Molecule 1: Lipoprotein

Chain Am:  88% 11%




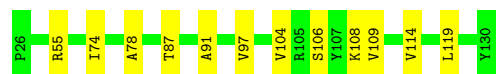
• Molecule 1: Lipoprotein

Chain Ao:  84% 16%




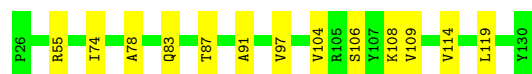
• Molecule 1: Lipoprotein

Chain Aq:  88% 12%




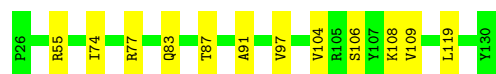
• Molecule 1: Lipoprotein

Chain As:  88% 12%




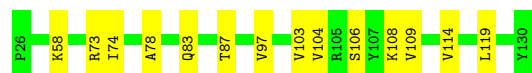
• Molecule 1: Lipoprotein

Chain Au:  88% 12%




• Molecule 1: Lipoprotein

Chain Aw:  87% 13%




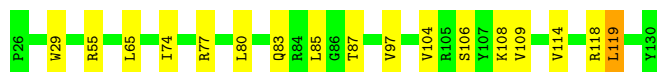
• Molecule 1: Lipoprotein

Chain Ay:  84% 16%




- Molecule 1: Lipoprotein

Chain Ba:  84% 15%




- Molecule 1: Lipoprotein

Chain Bc:  85% 14%




- Molecule 1: Lipoprotein

Chain Be:  86% 13%



- Molecule 1: Lipoprotein

Chain Bg:  86% 13%



- Molecule 1: Lipoprotein

Chain Bi:  86% 14%




- Molecule 1: Lipoprotein

Chain Bk:  87% 12%




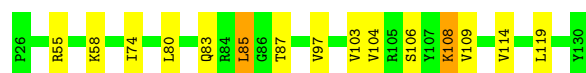
- Molecule 1: Lipoprotein

Chain Bm:  87% 12%




• Molecule 1: Lipoprotein

Chain Bo:  86% 12%




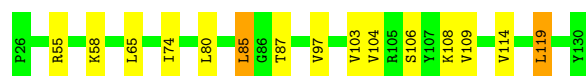
• Molecule 1: Lipoprotein

Chain Bq:  87% 12%




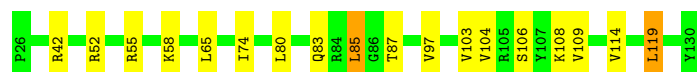
• Molecule 1: Lipoprotein

Chain Bs:  86% 12%



• Molecule 1: Lipoprotein

Chain Bu:  83% 15%




• Molecule 1: Lipoprotein

Chain Bw:  90% 10%




• Molecule 1: Lipoprotein

Chain By:  86% 13%




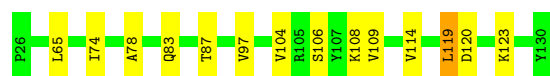
• Molecule 1: Lipoprotein

Chain Ca:  88% 12%




• Molecule 1: Lipoprotein

Chain Cc:  87% 12%




• Molecule 1: Lipoprotein

Chain Ce:  85% 14%




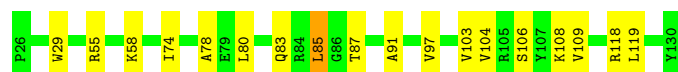
• Molecule 1: Lipoprotein

Chain Cg:  85% 14%




• Molecule 1: Lipoprotein

Chain Ci:  83% 16%



• Molecule 1: Lipoprotein

Chain Ck:  83% 16%




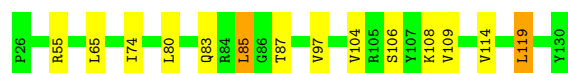
• Molecule 1: Lipoprotein

Chain Cm:  87% 13%




• Molecule 1: Lipoprotein

Chain Co:  87% 12% .




• Molecule 1: Lipoprotein

Chain Cq:  88% 11% .




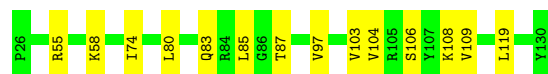
• Molecule 1: Lipoprotein

Chain Cs:  88% 12% .



• Molecule 1: Lipoprotein

Chain Cu:  87% 13% .



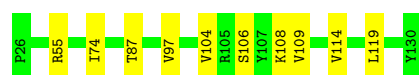
• Molecule 1: Lipoprotein

Chain Cw:  88% 12% .




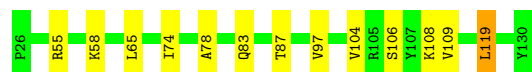
• Molecule 1: Lipoprotein

Chain Cy:  90% 10% .




• Molecule 1: Lipoprotein

Chain Da:  88% 12% .




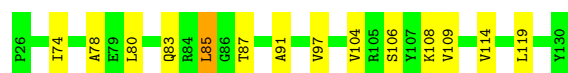
• Molecule 1: Lipoprotein

Chain Dc:  85% 15%




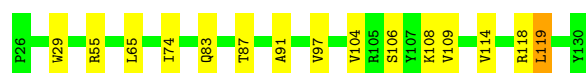
• Molecule 1: Lipoprotein

Chain De:  87% 12%




• Molecule 1: Lipoprotein

Chain Dg:  86% 13%




• Molecule 1: Lipoprotein

Chain Di:  87% 13%



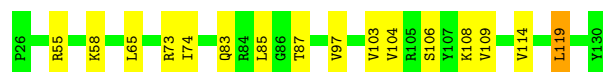
• Molecule 1: Lipoprotein

Chain Dk:  83% 16%



• Molecule 1: Lipoprotein

Chain Dm:  85% 14%




• Molecule 1: Lipoprotein

Chain Do:  89% 11%




• Molecule 1: Lipoprotein

Chain Dq:  87% 12%




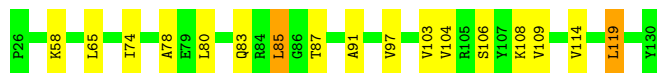
- Molecule 1: Lipoprotein

Chain Ds:  84% 15%




- Molecule 1: Lipoprotein

Chain Du:  84% 14%




- Molecule 1: Lipoprotein

Chain Dw:  81% 19%




- Molecule 1: Lipoprotein

Chain Dy:  85% 14%



- Molecule 1: Lipoprotein

Chain Ea:  85% 13%




- Molecule 1: Lipoprotein

Chain Ec:  87% 13%




- Molecule 1: Lipoprotein

Chain Ee:  86% 14%




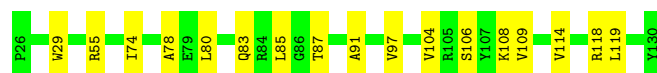
• Molecule 1: Lipoprotein

Chain Eg:  87% 12%




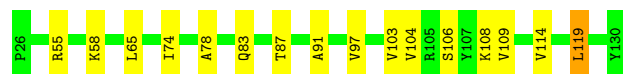
• Molecule 1: Lipoprotein

Chain Ei:  84% 16%




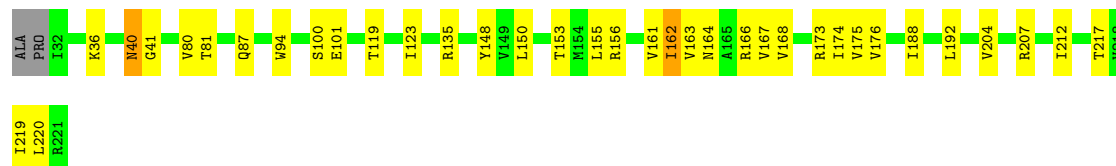
• Molecule 1: Lipoprotein

Chain Ek:  85% 14%




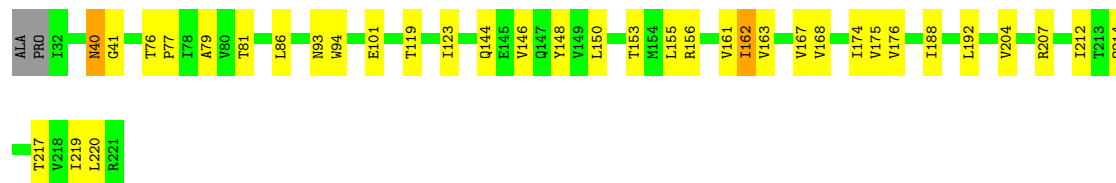
• Molecule 2: FlgO domain-containing protein

Chain Ab:  80% 18%




• Molecule 2: FlgO domain-containing protein

Chain Ad:  80% 18%

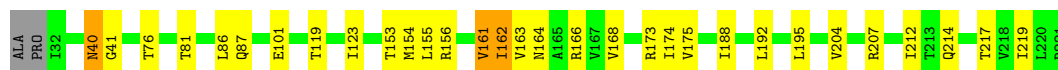
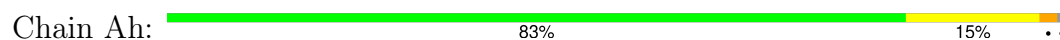


• Molecule 2: FlgO domain-containing protein

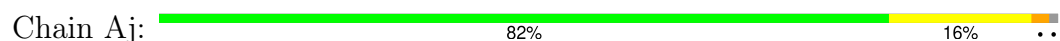
Chain Af:  85% 13%



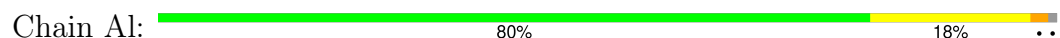
- Molecule 2: FlgO domain-containing protein



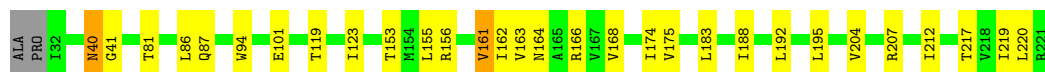
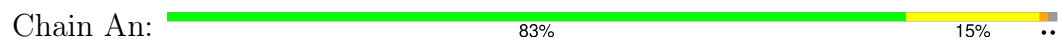
- Molecule 2: FlgO domain-containing protein



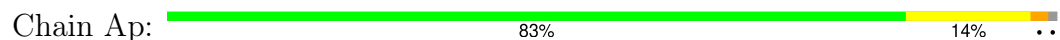
- Molecule 2: FlgO domain-containing protein



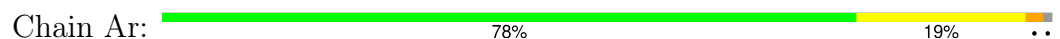
- Molecule 2: FlgO domain-containing protein

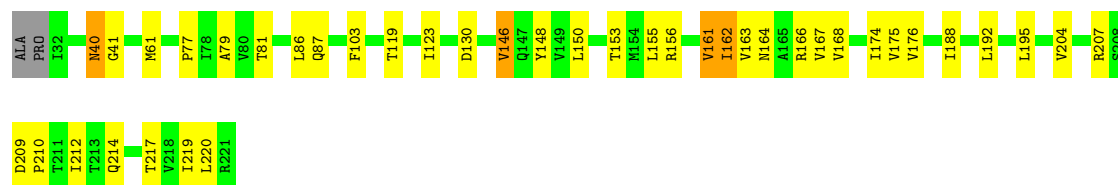


- Molecule 2: FlgO domain-containing protein



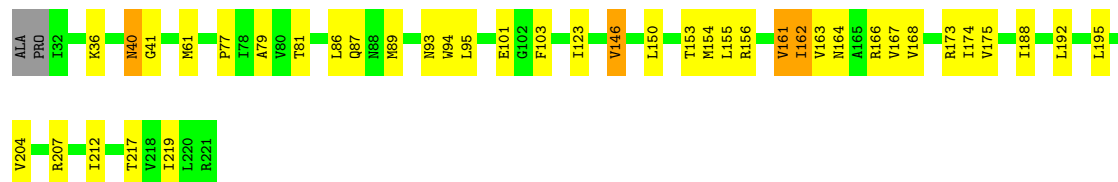
- Molecule 2: FlgO domain-containing protein





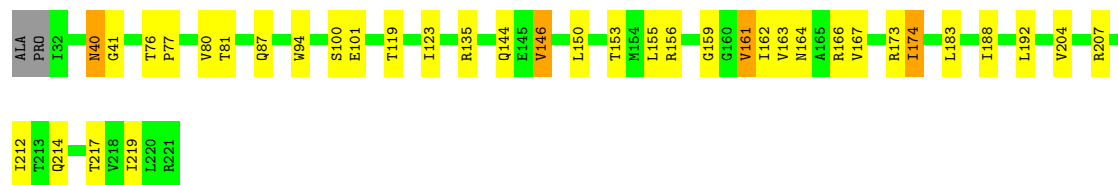
- Molecule 2: FlgO domain-containing protein

Chain At: 78% 19% ..



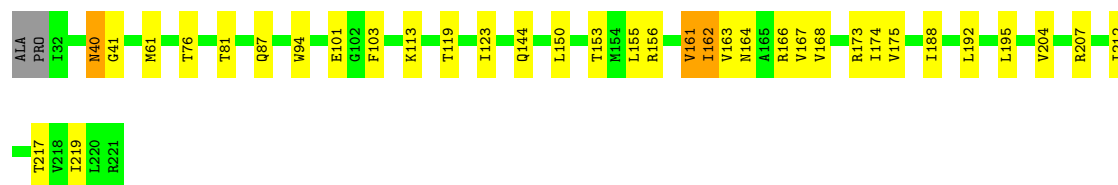
- Molecule 2: FlgO domain-containing protein

Chain Av: 80% 17% ..



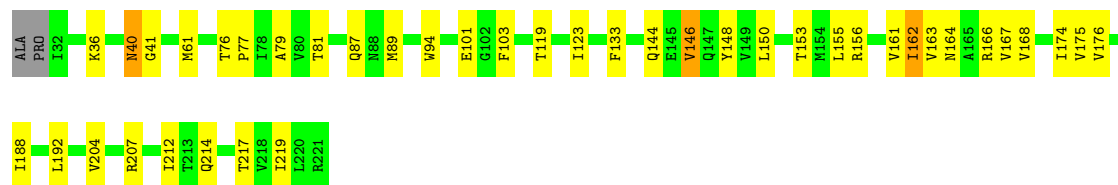
- Molecule 2: FlgO domain-containing protein

Chain Ax: 81% 17% ..



- Molecule 2: FlgO domain-containing protein

Chain Az: 78% 20% ..



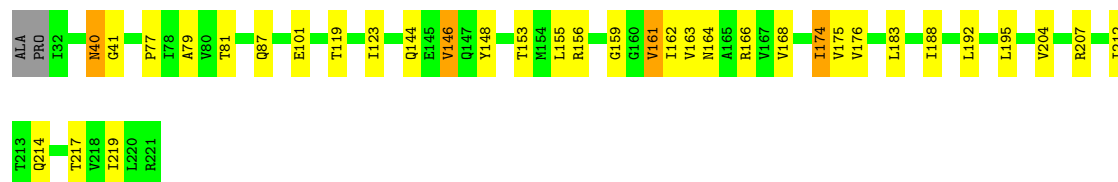
- Molecule 2: FlgO domain-containing protein

Chain Bb: 83% 14% ..



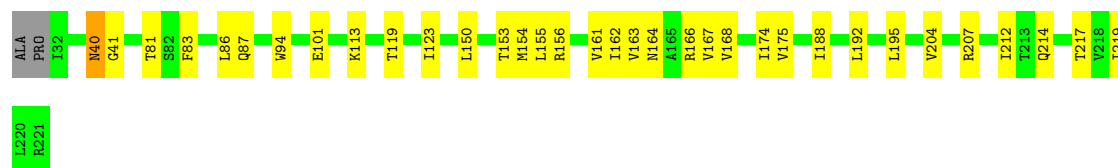
- Molecule 2: FlgO domain-containing protein

Chain Bd: 81% 16% ..



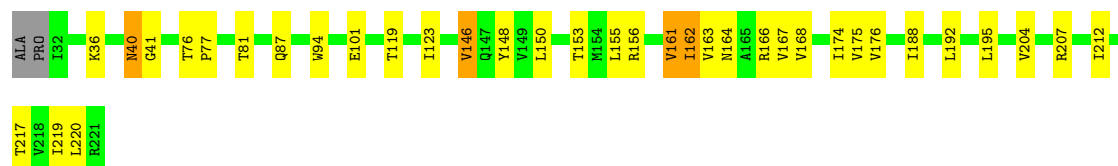
- Molecule 2: FlgO domain-containing protein

Chain Bf: 81% 17% ..



- Molecule 2: FlgO domain-containing protein

Chain Bh: 80% 17% ..



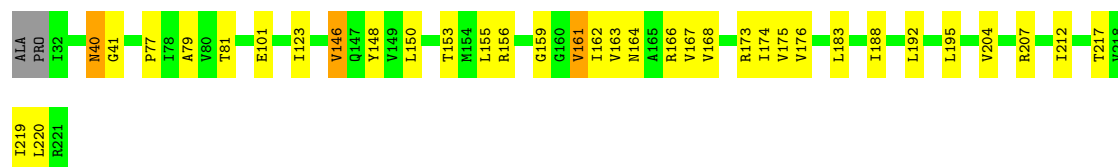
- Molecule 2: FlgO domain-containing protein

Chain Bj: 84% 14% ..

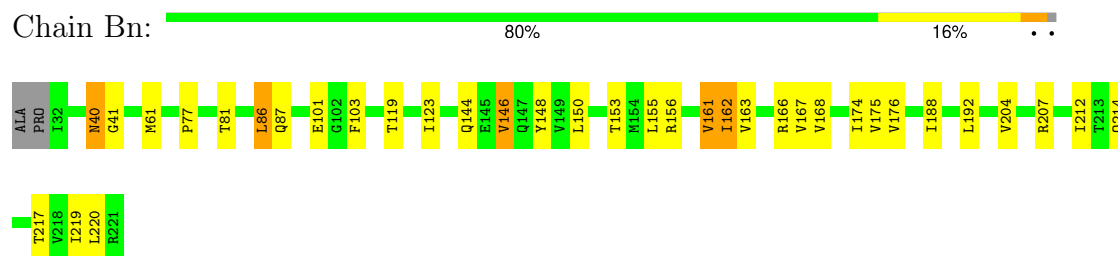


- Molecule 2: FlgO domain-containing protein

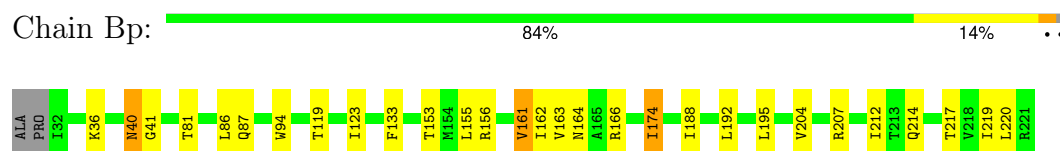
Chain Bl: 81% 17% ..



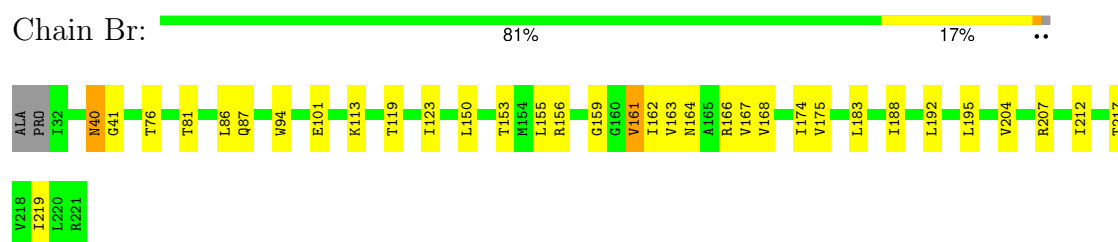
• Molecule 2: FlgO domain-containing protein



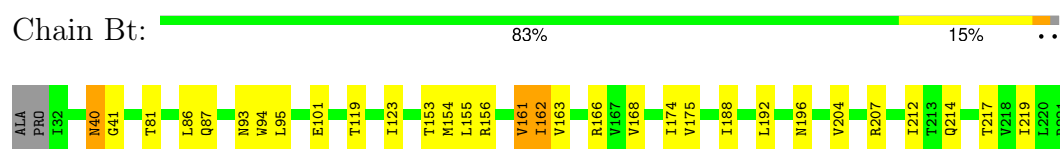
• Molecule 2: FlgO domain-containing protein



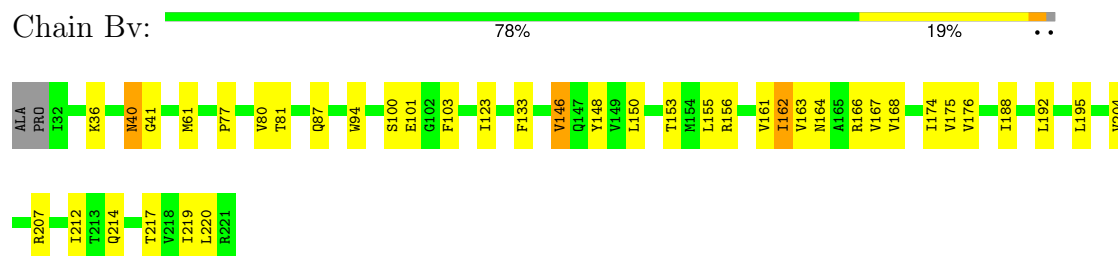
• Molecule 2: FlgO domain-containing protein



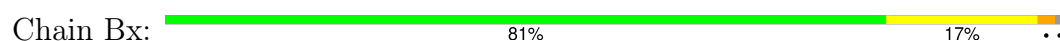
• Molecule 2: FlgO domain-containing protein

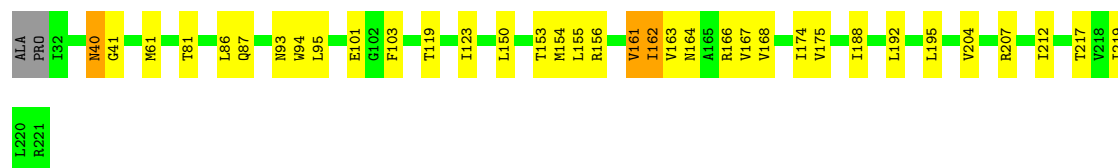


• Molecule 2: FlgO domain-containing protein



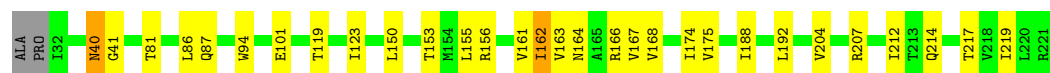
• Molecule 2: FlgO domain-containing protein





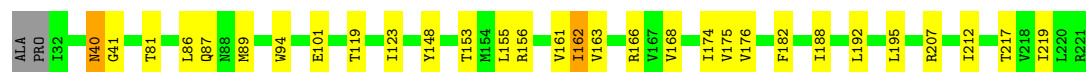
- Molecule 2: FlgO domain-containing protein

Chain Bz: 83% 15% ..



- Molecule 2: FlgO domain-containing protein

Chain Cb: 83% 15% ..



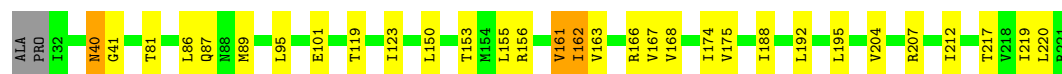
- Molecule 2: FlgO domain-containing protein

Chain Cd: 81% 16% ..



- Molecule 2: FlgO domain-containing protein

Chain Cf: 83% 15% ..



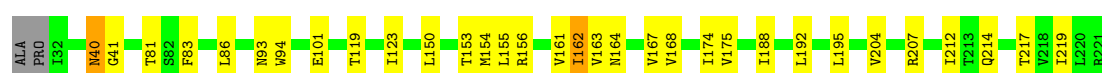
- Molecule 2: FlgO domain-containing protein

Chain Ch: 82% 16% ..



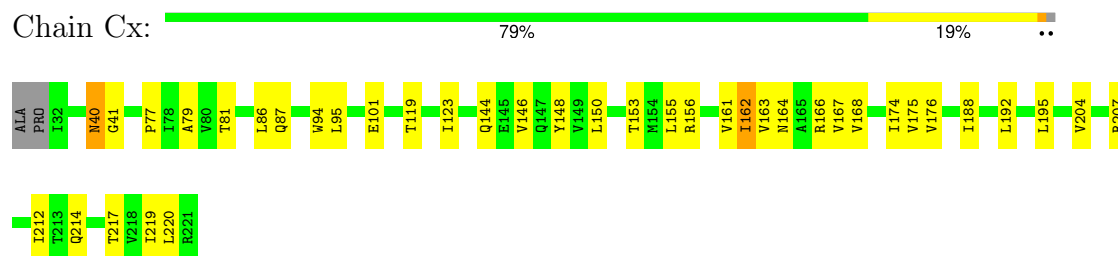
- Molecule 2: FlgO domain-containing protein

Chain Cj: 82% 16% ..

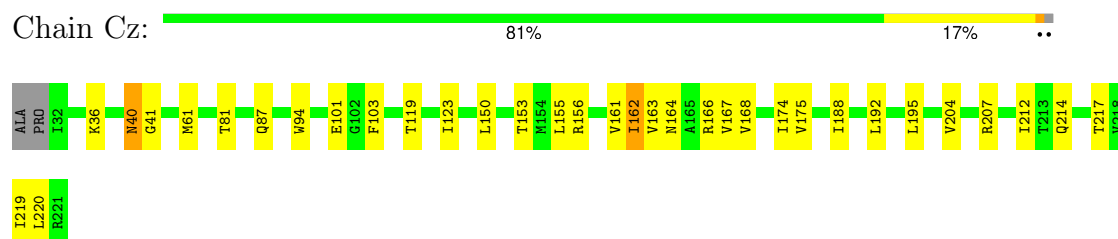


- [illegible]

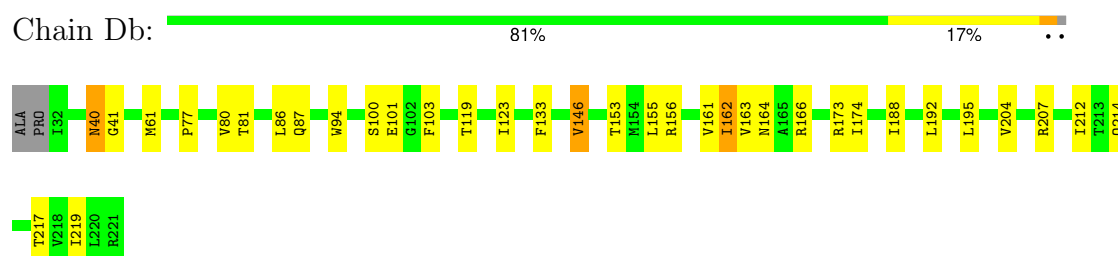
- Molecule 2: FlgO domain-containing protein



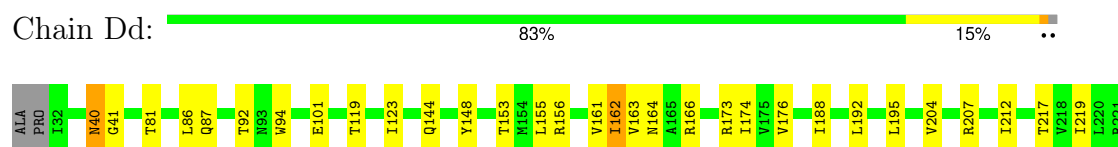
- Molecule 2: FlgO domain-containing protein



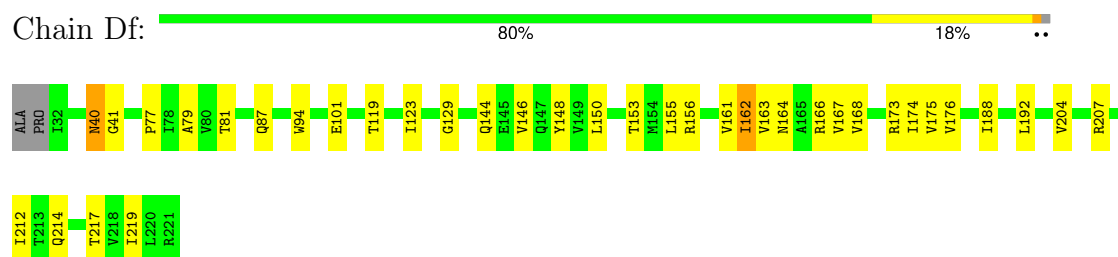
- Molecule 2: FlgO domain-containing protein



- Molecule 2: FlgO domain-containing protein

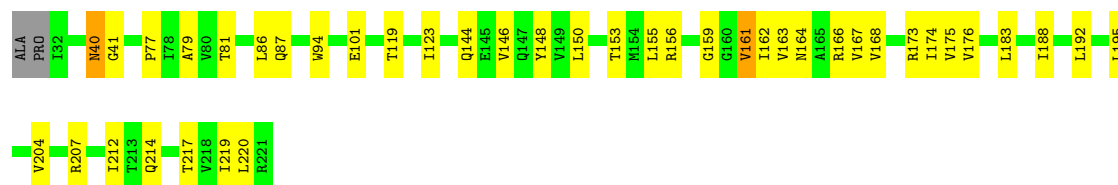


- Molecule 2: FlgO domain-containing protein

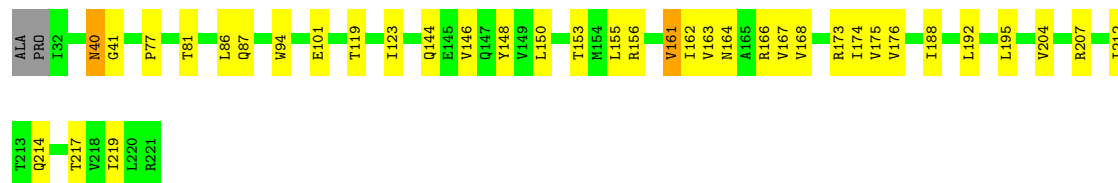
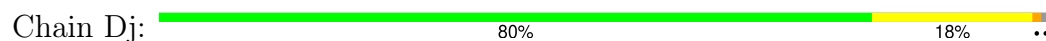


- Molecule 2: FlgO domain-containing protein

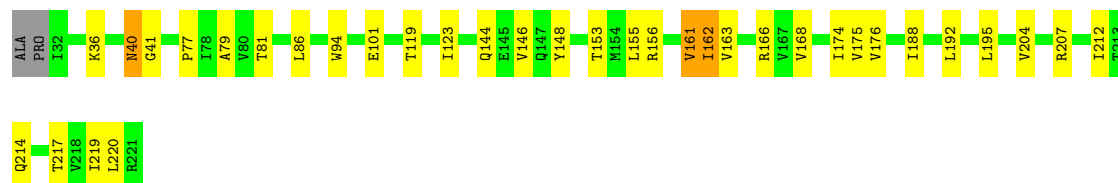
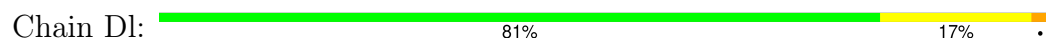




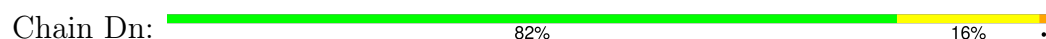
• Molecule 2: FlgO domain-containing protein



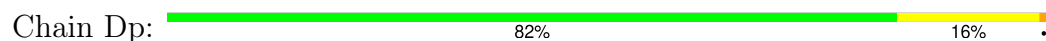
• Molecule 2: FlgO domain-containing protein



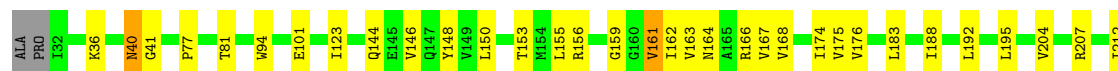
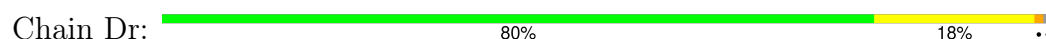
• Molecule 2: FlgO domain-containing protein



• Molecule 2: FlgO domain-containing protein



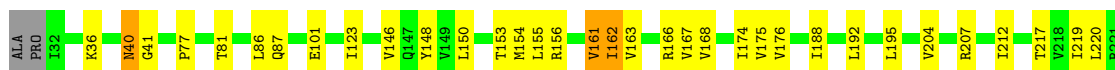
• Molecule 2: FlgO domain-containing protein





- Molecule 2: FlgO domain-containing protein

Chain Dt: 81% 16% ..



- Molecule 2: FlgO domain-containing protein

Chain Dv: 84% 14% ..



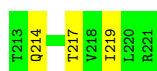
- Molecule 2: FlgO domain-containing protein

Chain Dx: 80% 18% ..



- Molecule 2: FlgO domain-containing protein

Chain Dz: 80% 18% ..




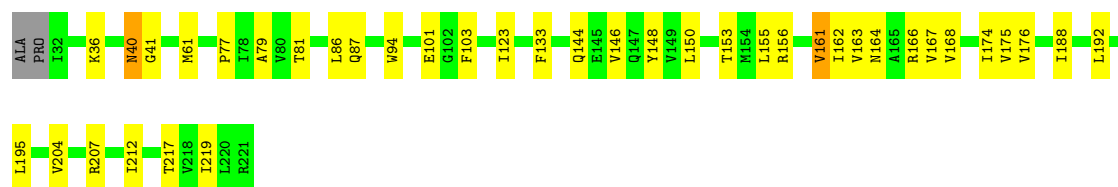
- Molecule 2: FlgO domain-containing protein

Chain Eb: 79% 19% ..




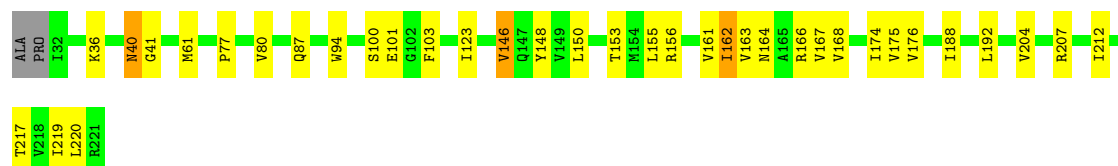
- Molecule 2: FlgO domain-containing protein

Chain Ed:  79% 19% ..




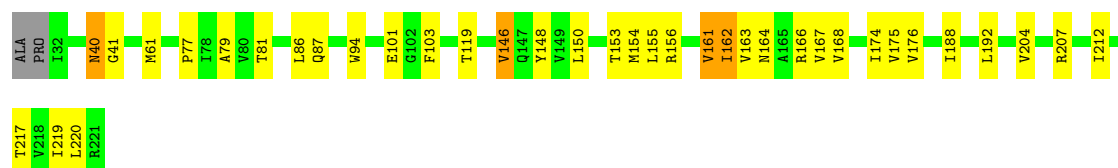
- Molecule 2: FlgO domain-containing protein

Chain Ef:  80% 17% ..




- Molecule 2: FlgO domain-containing protein

Chain Eh:  80% 17% ..




- Molecule 2: FlgO domain-containing protein

Chain Ej:  82% 16% ..



- Molecule 2: FlgO domain-containing protein

Chain El:  83% 15% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C58	Depositor
Number of particles used	35317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.630	Depositor
Minimum map value	-0.937	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	769.024, 769.024, 769.024	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.502, 1.502, 1.502	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Aa	0.14	0/836	0.38	0/1119
1	Ac	0.14	0/836	0.38	0/1119
1	Ae	0.14	0/836	0.36	0/1119
1	Ag	0.14	0/836	0.34	0/1119
1	Ai	0.14	0/836	0.37	0/1119
1	Ak	0.13	0/836	0.34	0/1119
1	Am	0.14	0/836	0.36	0/1119
1	Ao	0.15	0/836	0.36	0/1119
1	Aq	0.15	0/836	0.36	0/1119
1	As	0.14	0/836	0.36	0/1119
1	Au	0.14	0/836	0.36	0/1119
1	Aw	0.14	0/836	0.37	0/1119
1	Ay	0.15	0/836	0.37	0/1119
1	Ba	0.14	0/836	0.36	0/1119
1	Bc	0.15	0/836	0.36	0/1119
1	Be	0.15	0/836	0.37	0/1119
1	Bg	0.15	0/836	0.37	0/1119
1	Bi	0.15	0/836	0.36	0/1119
1	Bk	0.14	0/836	0.36	0/1119
1	Bm	0.14	0/836	0.38	0/1119
1	Bo	0.14	0/836	0.37	0/1119
1	Bq	0.15	0/836	0.37	0/1119
1	Bs	0.15	0/836	0.37	0/1119
1	Bu	0.15	0/836	0.37	0/1119
1	Bw	0.14	0/836	0.36	0/1119
1	By	0.15	0/836	0.37	0/1119
1	Ca	0.14	0/836	0.37	0/1119
1	Cc	0.14	0/836	0.36	0/1119
1	Ce	0.14	0/836	0.37	0/1119
1	Cg	0.14	0/836	0.37	0/1119
1	Ci	0.14	0/836	0.38	0/1119
1	Ck	0.14	0/836	0.35	0/1119
1	Cm	0.14	0/836	0.37	0/1119
1	Co	0.14	0/836	0.34	0/1119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Cq	0.14	0/836	0.33	0/1119
1	Cs	0.14	0/836	0.35	0/1119
1	Cu	0.14	0/836	0.36	0/1119
1	Cw	0.14	0/836	0.36	0/1119
1	Cy	0.14	0/836	0.36	0/1119
1	Da	0.14	0/836	0.36	0/1119
1	Dc	0.13	0/836	0.36	0/1119
1	De	0.14	0/836	0.37	0/1119
1	Dg	0.14	0/836	0.36	0/1119
1	Di	0.14	0/836	0.36	0/1119
1	Dk	0.14	0/836	0.37	0/1119
1	Dm	0.14	0/836	0.36	0/1119
1	Do	0.15	0/836	0.36	0/1119
1	Dq	0.14	0/836	0.36	0/1119
1	Ds	0.14	0/836	0.37	0/1119
1	Du	0.15	0/836	0.38	0/1119
1	Dw	0.14	0/836	0.36	0/1119
1	Dy	0.14	0/836	0.37	0/1119
1	Ea	0.15	0/836	0.33	0/1119
1	Ec	0.14	0/836	0.36	0/1119
1	Ee	0.15	0/836	0.38	0/1119
1	Eg	0.14	0/836	0.38	0/1119
1	Ei	0.14	0/836	0.36	0/1119
1	Ek	0.14	0/836	0.36	0/1119
2	Ab	0.15	0/1508	0.35	0/2045
2	Ad	0.15	0/1508	0.37	0/2045
2	Af	0.14	0/1508	0.36	0/2045
2	Ah	0.14	0/1508	0.36	0/2045
2	Aj	0.14	0/1508	0.35	0/2045
2	Al	0.14	0/1508	0.36	0/2045
2	An	0.13	0/1508	0.35	0/2045
2	Ap	0.14	0/1508	0.36	0/2045
2	Ar	0.14	0/1508	0.35	0/2045
2	At	0.14	0/1508	0.36	0/2045
2	Av	0.14	0/1508	0.35	0/2045
2	Ax	0.15	0/1508	0.36	0/2045
2	Az	0.15	0/1508	0.36	0/2045
2	Bb	0.14	0/1508	0.35	0/2045
2	Bd	0.14	0/1508	0.35	0/2045
2	Bf	0.14	0/1508	0.35	0/2045
2	Bh	0.14	0/1508	0.35	0/2045
2	Bj	0.14	0/1508	0.36	0/2045
2	Bl	0.15	0/1508	0.35	0/2045

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Bn	0.14	0/1508	0.36	0/2045
2	Bp	0.14	0/1508	0.36	0/2045
2	Br	0.14	0/1508	0.35	0/2045
2	Bt	0.15	0/1508	0.36	0/2045
2	Bv	0.15	0/1508	0.36	0/2045
2	Bx	0.15	0/1508	0.36	0/2045
2	Bz	0.14	0/1508	0.35	0/2045
2	Cb	0.15	0/1508	0.36	0/2045
2	Cd	0.15	0/1508	0.36	0/2045
2	Cf	0.14	0/1508	0.35	0/2045
2	Ch	0.14	0/1508	0.35	0/2045
2	Cj	0.14	0/1508	0.37	0/2045
2	Cl	0.14	0/1508	0.36	0/2045
2	Cn	0.14	0/1508	0.35	0/2045
2	Cp	0.15	0/1508	0.36	0/2045
2	Cr	0.14	0/1508	0.35	0/2045
2	Ct	0.14	0/1508	0.36	0/2045
2	Cv	0.14	0/1508	0.36	0/2045
2	Cx	0.15	0/1508	0.36	0/2045
2	Cz	0.14	0/1508	0.36	0/2045
2	Db	0.14	0/1508	0.36	0/2045
2	Dd	0.15	0/1508	0.36	0/2045
2	Df	0.14	0/1508	0.36	0/2045
2	Dh	0.14	0/1508	0.36	0/2045
2	Dj	0.15	0/1508	0.35	0/2045
2	Di	0.15	0/1508	0.34	0/2045
2	Dn	0.14	0/1508	0.34	0/2045
2	Dp	0.14	0/1508	0.36	0/2045
2	Dr	0.14	0/1508	0.35	0/2045
2	Dt	0.15	0/1508	0.36	0/2045
2	Dv	0.14	0/1508	0.35	0/2045
2	Dx	0.14	0/1508	0.35	0/2045
2	Dz	0.14	0/1508	0.36	0/2045
2	Eb	0.15	0/1508	0.36	0/2045
2	Ed	0.14	0/1508	0.35	0/2045
2	Ef	0.15	0/1508	0.36	0/2045
2	Ek	0.14	0/1508	0.35	0/2045
2	Ej	0.15	0/1508	0.37	0/2045
2	El	0.15	0/1508	0.36	0/2045
All	All	0.14	0/135952	0.36	0/183512

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	828	0	820	8	0
1	Ac	828	0	820	8	0
1	Ae	828	0	820	9	0
1	Ag	828	0	820	8	0
1	Ai	828	0	820	9	0
1	Ak	828	0	820	8	0
1	Am	828	0	820	8	0
1	Ao	828	0	820	10	0
1	Aq	828	0	820	7	0
1	As	828	0	820	8	0
1	Au	828	0	820	7	0
1	Aw	828	0	820	8	0
1	Ay	828	0	820	9	0
1	Ba	828	0	820	10	0
1	Bc	828	0	820	10	0
1	Be	828	0	820	8	0
1	Bg	828	0	820	9	0
1	Bi	828	0	820	9	0
1	Bk	828	0	820	8	0
1	Bm	828	0	820	9	0
1	Bo	828	0	820	8	0
1	Bq	828	0	820	7	0
1	Bs	828	0	820	8	0
1	Bu	828	0	820	10	0
1	Bw	828	0	820	5	0
1	By	828	0	820	9	0
1	Ca	828	0	820	8	0
1	Cc	828	0	820	8	0
1	Ce	828	0	820	10	0
1	Cg	828	0	820	10	0
1	Ci	828	0	820	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ck	828	0	820	11	0
1	Cm	828	0	820	8	0
1	Co	828	0	820	8	0
1	Cq	828	0	820	7	0
1	Cs	828	0	820	8	0
1	Cu	828	0	820	7	0
1	Cw	828	0	820	7	0
1	Cy	828	0	820	5	0
1	Da	828	0	820	8	0
1	Dc	828	0	820	9	0
1	De	828	0	820	8	0
1	Dg	828	0	820	9	0
1	Di	828	0	820	8	0
1	Dk	828	0	820	11	0
1	Dm	828	0	820	9	0
1	Do	828	0	820	5	0
1	Dq	828	0	820	10	0
1	Ds	828	0	820	10	0
1	Du	828	0	820	11	0
1	Dw	828	0	820	14	0
1	Dy	828	0	820	11	0
1	Ea	828	0	820	9	0
1	Ec	828	0	820	8	0
1	Ee	828	0	820	9	0
1	Eg	828	0	820	8	0
1	Ei	828	0	820	10	0
1	Ek	828	0	820	10	0
2	Ab	1482	0	1448	23	0
2	Ad	1482	0	1448	21	0
2	Af	1482	0	1448	18	0
2	Ah	1482	0	1448	22	0
2	Aj	1482	0	1448	22	0
2	Al	1482	0	1448	26	0
2	An	1482	0	1448	20	0
2	Ap	1482	0	1448	21	0
2	Ar	1482	0	1448	24	0
2	At	1482	0	1448	28	0
2	Av	1482	0	1448	26	0
2	Ax	1482	0	1448	24	0
2	Az	1482	0	1448	27	0
2	Bb	1482	0	1448	20	0
2	Bd	1482	0	1448	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bf	1482	0	1448	24	0
2	Bh	1482	0	1448	22	0
2	Bj	1482	0	1448	18	0
2	Bl	1482	0	1448	23	0
2	Bn	1482	0	1448	24	0
2	Bp	1482	0	1448	21	0
2	Br	1482	0	1448	24	0
2	Bt	1482	0	1448	23	0
2	Bv	1482	0	1448	26	0
2	Bx	1482	0	1448	24	0
2	Bz	1482	0	1448	20	0
2	Cb	1482	0	1448	21	0
2	Cd	1482	0	1448	22	0
2	Cf	1482	0	1448	20	0
2	Ch	1482	0	1448	21	0
2	Cj	1482	0	1448	20	0
2	Cl	1482	0	1448	18	0
2	Cn	1482	0	1448	19	0
2	Cp	1482	0	1448	25	0
2	Cr	1482	0	1448	25	0
2	Ct	1482	0	1448	22	0
2	Cv	1482	0	1448	28	0
2	Cx	1482	0	1448	26	0
2	Cz	1482	0	1448	23	0
2	Db	1482	0	1448	26	0
2	Dd	1482	0	1448	23	0
2	Df	1482	0	1448	25	0
2	Dh	1482	0	1448	29	0
2	Dj	1482	0	1448	26	0
2	Dl	1482	0	1448	24	0
2	Dn	1482	0	1448	20	0
2	Dp	1482	0	1448	23	0
2	Dr	1482	0	1448	25	0
2	Dt	1482	0	1448	23	0
2	Dv	1482	0	1448	21	0
2	Dx	1482	0	1448	27	0
2	Dz	1482	0	1448	26	0
2	Eb	1482	0	1448	28	0
2	Ed	1482	0	1448	27	0
2	Ef	1482	0	1448	22	0
2	Uh	1482	0	1448	22	0
2	Ej	1482	0	1448	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	El	1482	0	1448	21	0
All	All	133980	0	131544	1287	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1287) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bf:156:ARG:HE	2:Bf:192:LEU:HD13	1.60	0.67
2:Ap:156:ARG:HE	2:Ap:192:LEU:HD13	1.60	0.67
2:Dh:156:ARG:HE	2:Dh:192:LEU:HD13	1.60	0.66
2:Bz:156:ARG:HE	2:Bz:192:LEU:HD13	1.60	0.66
2:Dt:156:ARG:HE	2:Dt:192:LEU:HD13	1.60	0.66
2:Bn:156:ARG:HE	2:Bn:192:LEU:HD13	1.60	0.66
2:Bp:156:ARG:HE	2:Bp:192:LEU:HD13	1.61	0.66
2:Cb:156:ARG:HE	2:Cb:192:LEU:HD13	1.60	0.66
2:Cz:156:ARG:HE	2:Cz:192:LEU:HD13	1.61	0.66
2:Dv:156:ARG:HE	2:Dv:192:LEU:HD13	1.62	0.66
2:Dj:156:ARG:HE	2:Dj:192:LEU:HD13	1.61	0.65
2:Ej:156:ARG:HE	2:Ej:192:LEU:HD13	1.61	0.65
2:Bv:156:ARG:HE	2:Bv:192:LEU:HD13	1.61	0.65
1:By:106:SER:HB3	2:Bz:207:ARG:HB3	1.79	0.65
2:Dp:156:ARG:HE	2:Dp:192:LEU:HD13	1.61	0.65
2:Dl:156:ARG:HE	2:Dl:192:LEU:HD13	1.62	0.65
2:Dd:156:ARG:HE	2:Dd:192:LEU:HD13	1.61	0.65
2:Dn:156:ARG:HE	2:Dn:192:LEU:HD13	1.62	0.65
2:El:156:ARG:HE	2:El:192:LEU:HD13	1.62	0.65
2:Af:156:ARG:HE	2:Af:192:LEU:HD13	1.62	0.65
2:Al:156:ARG:HE	2:Al:192:LEU:HD13	1.62	0.64
2:Db:156:ARG:HE	2:Db:192:LEU:HD13	1.60	0.64
2:Aj:156:ARG:HE	2:Aj:192:LEU:HD13	1.63	0.64
2:Ax:156:ARG:HE	2:Ax:192:LEU:HD13	1.62	0.64
2:Dz:156:ARG:HE	2:Dz:192:LEU:HD13	1.62	0.64
2:Bj:156:ARG:HE	2:Bj:192:LEU:HD13	1.63	0.64
2:Dr:156:ARG:HE	2:Dr:192:LEU:HD13	1.62	0.64
2:Ed:156:ARG:HE	2:Ed:192:LEU:HD13	1.61	0.64
2:An:156:ARG:HE	2:An:192:LEU:HD13	1.63	0.64
2:Cf:156:ARG:HE	2:Cf:192:LEU:HD13	1.61	0.64
2:Ah:156:ARG:HE	2:Ah:192:LEU:HD13	1.62	0.64
2:Ab:156:ARG:HE	2:Ab:192:LEU:HD13	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:156:ARG:HE	2:Br:192:LEU:HD13	1.62	0.64
2:Bl:156:ARG:HE	2:Bl:192:LEU:HD13	1.63	0.64
2:Cx:156:ARG:HE	2:Cx:192:LEU:HD13	1.62	0.64
2:Dx:156:ARG:HE	2:Dx:192:LEU:HD13	1.63	0.64
2:Bb:156:ARG:HE	2:Bb:192:LEU:HD13	1.62	0.64
1:Bw:106:SER:HB3	2:Bx:207:ARG:HB3	1.80	0.64
2:Az:156:ARG:HE	2:Az:192:LEU:HD13	1.62	0.64
1:Ee:106:SER:HB3	2:Ef:207:ARG:HB3	1.80	0.64
2:Ch:156:ARG:HE	2:Ch:192:LEU:HD13	1.63	0.63
2:Cl:156:ARG:HE	2:Cl:192:LEU:HD13	1.61	0.63
2:Eb:156:ARG:HE	2:Eb:192:LEU:HD13	1.63	0.63
2:Ef:156:ARG:HE	2:Ef:192:LEU:HD13	1.62	0.63
2:Cp:156:ARG:HE	2:Cp:192:LEU:HD13	1.63	0.63
1:Dg:106:SER:HB3	2:Dh:207:ARG:HB3	1.81	0.63
2:Bh:156:ARG:HE	2:Bh:192:LEU:HD13	1.63	0.63
1:Ec:106:SER:HB3	2:Ed:207:ARG:HB3	1.81	0.62
2:Ar:156:ARG:HE	2:Ar:192:LEU:HD13	1.64	0.62
1:Bs:106:SER:HB3	2:Bt:207:ARG:HB3	1.82	0.62
2:Cr:156:ARG:HE	2:Cr:192:LEU:HD13	1.63	0.62
1:Cs:106:SER:HB3	2:Ct:207:ARG:HB3	1.81	0.62
1:Dk:106:SER:HB3	2:Dl:207:ARG:HB3	1.82	0.62
2:Bd:156:ARG:HE	2:Bd:192:LEU:HD13	1.65	0.62
2:Cd:156:ARG:HE	2:Cd:192:LEU:HD13	1.63	0.62
1:Aw:106:SER:HB3	2:Ax:207:ARG:HB3	1.82	0.62
1:Bg:106:SER:HB3	2:Bh:207:ARG:HB3	1.81	0.62
2:Cn:156:ARG:HE	2:Cn:192:LEU:HD13	1.65	0.62
2:Av:156:ARG:HE	2:Av:192:LEU:HD13	1.64	0.62
1:Ba:106:SER:HB3	2:Bb:207:ARG:HB3	1.82	0.62
1:Ae:106:SER:HB3	2:Af:207:ARG:HB3	1.82	0.62
1:Ce:106:SER:HB3	2:Cf:207:ARG:HB3	1.82	0.62
1:Co:106:SER:HB3	2:Cp:207:ARG:HB3	1.82	0.62
1:Dm:106:SER:HB3	2:Dn:207:ARG:HB3	1.83	0.61
1:Dq:106:SER:HB3	2:Dr:207:ARG:HB3	1.83	0.61
1:Ei:106:SER:HB3	2:Ej:207:ARG:HB3	1.83	0.61
1:As:106:SER:HB3	2:At:207:ARG:HB3	1.82	0.61
2:Bd:155:LEU:HD23	2:Bd:162:ILE:HD11	1.83	0.61
1:Am:106:SER:HB3	2:An:207:ARG:HB3	1.83	0.61
2:Db:166:ARG:HH22	2:Dd:101:GLU:HG2	1.64	0.61
1:De:106:SER:HB3	2:Df:207:ARG:HB3	1.83	0.61
1:Dy:106:SER:HB3	2:Dz:207:ARG:HB3	1.82	0.61
2:Eb:155:LEU:HD23	2:Eb:162:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ek:106:SER:HB3	2:El:207:ARG:HB3	1.83	0.61
1:Ay:106:SER:HB3	2:Az:207:ARG:HB3	1.82	0.61
1:Dc:106:SER:HB3	2:Dd:207:ARG:HB3	1.82	0.61
1:Be:106:SER:HB3	2:Bf:207:ARG:HB3	1.83	0.61
1:Aa:106:SER:HB3	2:Ab:207:ARG:HB3	1.83	0.61
1:Ai:106:SER:HB3	2:Aj:207:ARG:HB3	1.83	0.61
1:Bk:106:SER:HB3	2:Bl:207:ARG:HB3	1.83	0.61
1:Cc:106:SER:HB3	2:Cd:207:ARG:HB3	1.83	0.61
2:Cv:156:ARG:HE	2:Cv:192:LEU:HD13	1.65	0.61
1:Cy:106:SER:HB3	2:Cz:207:ARG:HB3	1.83	0.61
1:Ak:106:SER:HB3	2:Al:207:ARG:HB3	1.83	0.61
1:Ck:106:SER:HB3	2:Cl:207:ARG:HB3	1.82	0.61
2:An:155:LEU:HD23	2:An:162:ILE:HD11	1.83	0.60
1:Ac:106:SER:HB3	2:Ad:207:ARG:HB3	1.83	0.60
2:Df:156:ARG:HE	2:Df:192:LEU:HD13	1.66	0.60
1:Dw:106:SER:HB3	2:Dx:207:ARG:HB3	1.83	0.60
2:Ed:155:LEU:HD23	2:Ed:162:ILE:HD11	1.84	0.60
2:Av:155:LEU:HD23	2:Av:162:ILE:HD11	1.83	0.60
2:Dh:155:LEU:HD23	2:Dh:162:ILE:HD11	1.84	0.60
1:Ea:106:SER:HB3	2:Eb:207:ARG:HB3	1.83	0.60
2:Cr:155:LEU:HD23	2:Cr:162:ILE:HD11	1.83	0.60
1:Ao:106:SER:HB3	2:Ap:207:ARG:HB3	1.84	0.60
1:Cu:106:SER:HB3	2:Cv:207:ARG:HB3	1.83	0.60
2:Dd:166:ARG:HH22	2:Df:101:GLU:HG2	1.66	0.60
2:Dh:166:ARG:HH22	2:Dj:101:GLU:HG2	1.67	0.60
1:Aq:106:SER:HB3	2:Ar:207:ARG:HB3	1.83	0.60
1:Bq:106:SER:HB3	2:Br:207:ARG:HB3	1.84	0.60
2:Ch:155:LEU:HD23	2:Ch:162:ILE:HD11	1.83	0.60
1:Au:106:SER:HB3	2:Av:207:ARG:HB3	1.84	0.60
1:Cg:106:SER:HB3	2:Ch:207:ARG:HB3	1.84	0.60
1:Eg:106:SER:HB3	2:Eh:207:ARG:HB3	1.83	0.60
1:Cw:106:SER:HB3	2:Cx:207:ARG:HB3	1.83	0.60
1:Ag:106:SER:HB3	2:Ah:207:ARG:HB3	1.84	0.59
1:Bu:106:SER:HB3	2:Bv:207:ARG:HB3	1.84	0.59
1:Cq:106:SER:HB3	2:Cr:207:ARG:HB3	1.84	0.59
1:Ca:106:SER:HB3	2:Cb:207:ARG:HB3	1.84	0.59
1:Ds:106:SER:HB3	2:Dt:207:ARG:HB3	1.84	0.59
2:Cr:166:ARG:HH22	2:Ct:101:GLU:HG2	1.68	0.59
2:Dj:155:LEU:HD23	2:Dj:162:ILE:HD11	1.85	0.59
2:Cz:166:ARG:HH22	2:Db:101:GLU:HG2	1.65	0.59
2:Al:155:LEU:HD23	2:Al:162:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dn:155:LEU:HD23	2:Dn:162:ILE:HD11	1.85	0.59
2:Br:155:LEU:HD23	2:Br:162:ILE:HD11	1.85	0.59
2:El:155:LEU:HD23	2:El:162:ILE:HD11	1.84	0.59
1:Cm:106:SER:HB3	2:Cn:207:ARG:HB3	1.84	0.59
2:Dl:166:ARG:HH22	2:Dn:101:GLU:HG2	1.68	0.59
2:Ct:166:ARG:HH22	2:Cv:101:GLU:HG2	1.69	0.58
1:Bc:106:SER:HB3	2:Bd:207:ARG:HB3	1.85	0.58
1:Bo:106:SER:HB3	2:Bp:207:ARG:HB3	1.86	0.58
2:Dz:166:ARG:HH22	2:Eb:101:GLU:HG2	1.68	0.58
2:Bl:155:LEU:HD23	2:Bl:162:ILE:HD11	1.85	0.58
1:Di:106:SER:HB3	2:Dj:207:ARG:HB3	1.85	0.58
1:Do:106:SER:HB3	2:Dp:207:ARG:HB3	1.85	0.58
1:Du:106:SER:HB3	2:Dv:207:ARG:HB3	1.84	0.58
2:Cv:155:LEU:HD23	2:Cv:162:ILE:HD11	1.86	0.58
2:Dv:155:LEU:HD23	2:Dv:162:ILE:HD11	1.86	0.58
2:Ab:166:ARG:HH22	2:Ad:101:GLU:HG2	1.70	0.57
2:Df:166:ARG:HH22	2:Dh:101:GLU:HG2	1.69	0.57
1:Ci:106:SER:HB3	2:Cj:207:ARG:HB3	1.85	0.57
2:Ar:166:ARG:HH22	2:At:101:GLU:HG2	1.70	0.57
2:Bf:155:LEU:HD23	2:Bf:162:ILE:HD11	1.86	0.57
1:Bm:106:SER:HB3	2:Bn:207:ARG:HB3	1.87	0.57
1:Du:108:LYS:HE2	2:Dv:204:VAL:HG11	1.87	0.57
2:Dv:166:ARG:HH22	2:Dx:101:GLU:HG2	1.70	0.57
2:Ef:166:ARG:HH22	2:Eh:101:GLU:HG2	1.70	0.57
1:Dk:83:GLN:HE22	1:Dq:55:ARG:HH22	1.53	0.57
1:Bo:108:LYS:HE3	2:Bp:204:VAL:HG11	1.87	0.57
2:Dr:155:LEU:HD23	2:Dr:162:ILE:HD11	1.87	0.57
1:Bi:106:SER:HB3	2:Bj:207:ARG:HB3	1.87	0.56
2:Az:153:THR:HB	2:Az:164:ASN:H	1.70	0.56
1:Ac:55:ARG:HH22	1:Ei:83:GLN:HE22	1.53	0.56
1:Ba:108:LYS:HD2	2:Bb:204:VAL:HG11	1.87	0.56
1:Cc:104:VAL:HG12	2:Cd:212:ILE:HG13	1.88	0.56
1:Ca:104:VAL:HG12	2:Cb:212:ILE:HG13	1.87	0.56
2:Eh:154:MET:HB3	2:Eh:156:ARG:HH12	1.71	0.56
2:Dj:166:ARG:HH22	2:Dl:101:GLU:HG2	1.70	0.56
2:Ax:166:ARG:HH22	2:Az:101:GLU:HG2	1.71	0.56
2:Bt:166:ARG:HH22	2:Bv:101:GLU:HG2	1.71	0.56
1:Aw:108:LYS:HD2	2:Ax:204:VAL:HG11	1.89	0.55
2:Dn:166:ARG:HH22	2:Dp:101:GLU:HG2	1.72	0.55
1:Ag:83:GLN:HE22	1:Am:55:ARG:HH22	1.54	0.55
1:Bc:108:LYS:HD2	2:Bd:204:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cg:104:VAL:HG12	2:Ch:212:ILE:HG13	1.88	0.55
2:Dp:155:LEU:HD23	2:Dp:162:ILE:HD11	1.87	0.55
1:Cm:104:VAL:HG12	2:Cn:212:ILE:HG13	1.89	0.55
2:Dj:214:GLN:HG3	2:Dl:195:LEU:HD21	1.88	0.55
1:Ck:108:LYS:HD2	2:Cl:204:VAL:HG11	1.88	0.55
2:Bx:166:ARG:HH22	2:Bz:101:GLU:HG2	1.72	0.55
2:Ch:166:ARG:HH22	2:Cj:101:GLU:HG2	1.71	0.55
1:Da:106:SER:HB3	2:Db:207:ARG:HB3	1.87	0.55
1:Bm:83:GLN:HE22	1:Bs:55:ARG:HH22	1.55	0.55
1:Bu:104:VAL:HG12	2:Bv:212:ILE:HG13	1.88	0.55
2:Av:153:THR:HB	2:Av:164:ASN:H	1.72	0.55
1:Bo:104:VAL:HG12	2:Bp:212:ILE:HG13	1.88	0.55
2:Bv:166:ARG:HH22	2:Bx:101:GLU:HG2	1.71	0.55
2:Bd:166:ARG:HH22	2:Bf:101:GLU:HG2	1.72	0.55
2:Cj:214:GLN:HG3	2:Cl:195:LEU:HD21	1.89	0.55
1:Cw:104:VAL:HG12	2:Cx:212:ILE:HG13	1.89	0.55
2:Ab:153:THR:HB	2:Ab:164:ASN:H	1.72	0.54
2:Bp:155:LEU:HD23	2:Bp:162:ILE:HD11	1.90	0.54
2:Dl:214:GLN:HG3	2:Dn:195:LEU:HD21	1.89	0.54
1:Eg:104:VAL:HG12	2:Eh:212:ILE:HG13	1.88	0.54
2:An:166:ARG:HH22	2:Ap:101:GLU:HG2	1.72	0.54
1:As:108:LYS:HD2	2:At:204:VAL:HG11	1.89	0.54
2:Ab:36:LYS:HA	2:Ej:159:GLY:HA3	1.89	0.54
1:Aq:104:VAL:HG12	2:Ar:212:ILE:HG13	1.89	0.54
1:Ce:104:VAL:HG12	2:Cf:212:ILE:HG13	1.90	0.54
2:Bh:153:THR:HB	2:Bh:164:ASN:H	1.73	0.54
2:Eb:166:ARG:HH22	2:Ed:101:GLU:HG2	1.71	0.54
1:Ac:108:LYS:HD2	2:Ad:204:VAL:HG11	1.90	0.54
2:Ab:94:TRP:HB3	2:El:87:GLN:HE21	1.72	0.54
1:Cc:83:GLN:HE22	1:Ci:55:ARG:HH22	1.54	0.54
1:Cu:104:VAL:HG12	2:Cv:212:ILE:HG13	1.90	0.54
1:Aa:104:VAL:HG12	2:Ab:212:ILE:HG13	1.89	0.54
1:Ck:104:VAL:HG12	2:Cl:212:ILE:HG13	1.90	0.54
1:Dm:104:VAL:HG12	2:Dn:212:ILE:HG13	1.90	0.54
1:Bq:104:VAL:HG12	2:Br:212:ILE:HG13	1.90	0.54
1:Da:104:VAL:HG12	2:Db:212:ILE:HG13	1.90	0.54
2:Av:166:ARG:HH22	2:Ax:101:GLU:HG2	1.71	0.53
1:Aw:83:GLN:HE22	1:Bc:55:ARG:HH22	1.56	0.53
1:Ci:83:GLN:HE22	1:Co:55:ARG:HH22	1.56	0.53
2:Bd:153:THR:HB	2:Bd:164:ASN:H	1.73	0.53
1:Be:108:LYS:HD2	2:Bf:204:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:104:VAL:HG12	2:Bh:212:ILE:HG13	1.90	0.53
1:Bu:108:LYS:HD2	2:Bv:204:VAL:HG11	1.90	0.53
2:Cx:166:ARG:HH22	2:Cz:101:GLU:HG2	1.72	0.53
1:Cs:104:VAL:HG12	2:Ct:212:ILE:HG13	1.91	0.53
2:Df:153:THR:HB	2:Df:164:ASN:H	1.73	0.53
1:Aw:104:VAL:HG12	2:Ax:212:ILE:HG13	1.89	0.53
2:Al:153:THR:HB	2:Al:164:ASN:H	1.74	0.53
1:Dk:104:VAL:HG12	2:Dl:212:ILE:HG13	1.90	0.53
1:By:104:VAL:HG12	2:Bz:212:ILE:HG13	1.89	0.53
1:De:104:VAL:HG12	2:Df:212:ILE:HG13	1.90	0.53
1:Du:104:VAL:HG12	2:Dv:212:ILE:HG13	1.91	0.53
1:Ea:104:VAL:HG12	2:Eb:212:ILE:HG13	1.91	0.53
2:Eh:87:GLN:HE21	2:Ej:94:TRP:HB3	1.74	0.53
1:Ei:104:VAL:HG12	2:Ej:212:ILE:HG13	1.90	0.53
2:Ad:214:GLN:HG3	2:Af:195:LEU:HD21	1.91	0.53
1:Bg:108:LYS:HD2	2:Bh:204:VAL:HG11	1.89	0.53
2:Bl:219:ILE:HG23	2:Bn:192:LEU:HD12	1.91	0.53
1:Ci:104:VAL:HG12	2:Cj:212:ILE:HG13	1.90	0.53
1:Dg:104:VAL:HG12	2:Dh:212:ILE:HG13	1.91	0.53
2:Dx:155:LEU:HD23	2:Dx:162:ILE:HD11	1.89	0.53
1:As:104:VAL:HG12	2:At:212:ILE:HG13	1.91	0.52
2:Dn:153:THR:HB	2:Dn:164:ASN:H	1.73	0.52
2:Bb:155:LEU:HD23	2:Bb:162:ILE:HD11	1.90	0.52
1:Cy:108:LYS:HD2	2:Cz:204:VAL:HG11	1.92	0.52
1:Ao:104:VAL:HG12	2:Ap:212:ILE:HG13	1.89	0.52
1:Ao:108:LYS:HD2	2:Ap:204:VAL:HG11	1.92	0.52
2:Cd:153:THR:HB	2:Cd:164:ASN:H	1.74	0.52
1:Ci:108:LYS:HD2	2:Cj:204:VAL:HG11	1.92	0.52
2:Dx:87:GLN:HE21	2:Dz:94:TRP:HB3	1.73	0.52
1:Ee:104:VAL:HG12	2:Ef:212:ILE:HG13	1.90	0.52
1:Ac:104:VAL:HG12	2:Ad:212:ILE:HG13	1.90	0.52
1:Ao:83:GLN:HE22	1:Au:55:ARG:HH22	1.58	0.52
1:Cm:108:LYS:HD2	2:Cn:204:VAL:HG11	1.92	0.52
1:Aa:91:ALA:HB3	1:Ek:78:ALA:HB3	1.91	0.52
1:Ag:108:LYS:HD2	2:Ah:204:VAL:HG11	1.92	0.52
1:By:108:LYS:HD2	2:Bz:204:VAL:HG11	1.92	0.52
2:Cz:155:LEU:HD23	2:Cz:162:ILE:HD11	1.91	0.52
2:Dr:148:TYR:HE1	2:Dr:176:VAL:HG21	1.75	0.52
1:Dq:104:VAL:HG12	2:Dr:212:ILE:HG13	1.92	0.52
1:Ds:108:LYS:HD2	2:Dt:204:VAL:HG11	1.92	0.52
1:Dc:108:LYS:HD2	2:Dd:204:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:78:ALA:HB3	1:Ao:91:ALA:HB3	1.92	0.52
1:Ci:78:ALA:HB3	1:Ck:91:ALA:HB3	1.91	0.52
1:Cm:83:GLN:HE22	1:Cs:55:ARG:HH22	1.56	0.52
2:Ef:153:THR:HB	2:Ef:164:ASN:H	1.75	0.52
2:Ej:166:ARG:HH22	2:El:101:GLU:HG2	1.74	0.52
2:Dh:148:TYR:HE1	2:Dh:176:VAL:HG21	1.75	0.52
2:Ed:153:THR:HB	2:Ed:164:ASN:H	1.74	0.52
2:Ej:153:THR:HB	2:Ej:164:ASN:H	1.75	0.52
2:Aj:87:GLN:HE21	2:Al:94:TRP:HB3	1.75	0.52
2:At:155:LEU:HD23	2:At:162:ILE:HD11	1.92	0.52
2:Bd:219:ILE:HG23	2:Bf:192:LEU:HD12	1.92	0.52
1:Cy:104:VAL:HG12	2:Cz:212:ILE:HG13	1.91	0.52
1:Dg:108:LYS:HD2	2:Dh:204:VAL:HG11	1.92	0.52
1:Ds:104:VAL:HG12	2:Dt:212:ILE:HG13	1.91	0.52
2:Ax:153:THR:HB	2:Ax:164:ASN:H	1.76	0.51
1:Bw:104:VAL:HG12	2:Bx:212:ILE:HG13	1.91	0.51
1:Ae:108:LYS:HD2	2:Af:204:VAL:HG11	1.92	0.51
2:Bf:214:GLN:HG3	2:Bh:195:LEU:HD21	1.92	0.51
1:Bi:104:VAL:HG12	2:Bj:212:ILE:HG13	1.91	0.51
1:Co:108:LYS:HD2	2:Cp:204:VAL:HG11	1.92	0.51
2:Cr:161:VAL:HG12	2:Cr:188:ILE:HD11	1.92	0.51
2:Dx:86:LEU:HD13	2:Dx:153:THR:HG23	1.93	0.51
1:Bk:104:VAL:HG12	2:Bl:212:ILE:HG13	1.92	0.51
2:Al:161:VAL:HG12	2:Al:188:ILE:HD11	1.93	0.51
1:Ba:104:VAL:HG12	2:Bb:212:ILE:HG13	1.92	0.51
2:Bx:153:THR:HB	2:Bx:164:ASN:H	1.74	0.51
2:Cx:155:LEU:HD23	2:Cx:162:ILE:HD11	1.92	0.51
2:El:161:VAL:HG12	2:El:188:ILE:HD11	1.92	0.51
1:Ay:108:LYS:HD2	2:Az:204:VAL:HG11	1.91	0.51
1:Di:104:VAL:HG12	2:Dj:212:ILE:HG13	1.92	0.51
1:Ag:104:VAL:HG12	2:Ah:212:ILE:HG13	1.91	0.51
1:Ai:78:ALA:HB3	1:Ak:91:ALA:HB3	1.90	0.51
2:Bh:219:ILE:HG23	2:Bj:192:LEU:HD12	1.93	0.51
1:Bs:104:VAL:HG12	2:Bt:212:ILE:HG13	1.91	0.51
2:Ch:153:THR:HB	2:Ch:164:ASN:H	1.76	0.51
1:Cv:108:LYS:HD2	2:Cv:204:VAL:HG11	1.93	0.51
2:Br:86:LEU:HD13	2:Br:153:THR:HG23	1.93	0.51
2:Dn:161:VAL:HG12	2:Dn:188:ILE:HD11	1.92	0.51
2:Dv:153:THR:HB	2:Dv:164:ASN:H	1.76	0.51
2:Bb:161:VAL:HG12	2:Bb:188:ILE:HD11	1.93	0.51
2:Bz:161:VAL:HG12	2:Bz:188:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dx:161:VAL:HG12	2:Dx:188:ILE:HD11	1.93	0.51
1:Ee:108:LYS:HD2	2:Ef:204:VAL:HG11	1.92	0.51
1:Ae:78:ALA:HB3	1:Ag:91:ALA:HB3	1.92	0.51
1:Am:104:VAL:HG12	2:An:212:ILE:HG13	1.91	0.51
2:Av:161:VAL:HG12	2:Av:188:ILE:HD11	1.92	0.51
1:Bc:104:VAL:HG12	2:Bd:212:ILE:HG13	1.92	0.51
1:Be:104:VAL:HG12	2:Bf:212:ILE:HG13	1.92	0.51
2:Cx:214:GLN:HG3	2:Cz:195:LEU:HD21	1.93	0.51
1:Dw:83:GLN:HE22	1:Ec:55:ARG:HH22	1.58	0.51
2:Dz:77:PRO:HB2	2:Dz:146:VAL:HG13	1.93	0.51
1:Au:104:VAL:HG12	2:Av:212:ILE:HG13	1.93	0.51
2:Cj:93:ASN:HB2	2:Cj:156:ARG:HH22	1.75	0.51
1:Di:108:LYS:HD2	2:Dj:204:VAL:HG11	1.92	0.51
2:Dz:214:GLN:HG3	2:Eb:195:LEU:HD21	1.92	0.51
1:Ai:104:VAL:HG12	2:Aj:212:ILE:HG13	1.92	0.50
2:Ar:153:THR:HB	2:Ar:164:ASN:H	1.75	0.50
1:Bq:108:LYS:HD2	2:Br:204:VAL:HG11	1.92	0.50
1:Bw:108:LYS:HD2	2:Bx:204:VAL:HG11	1.93	0.50
1:Ce:83:GLN:HE22	1:Ck:55:ARG:HH22	1.59	0.50
2:Ct:155:LEU:HD23	2:Ct:162:ILE:HD11	1.92	0.50
1:Dm:108:LYS:HD2	2:Dn:204:VAL:HG11	1.91	0.50
2:Eb:153:THR:HB	2:Eb:164:ASN:H	1.76	0.50
2:Bb:153:THR:HB	2:Bb:164:ASN:H	1.75	0.50
2:Bf:83:PHE:HB3	2:Bf:154:MET:HG3	1.93	0.50
2:Ch:219:ILE:HG23	2:Cj:192:LEU:HD12	1.93	0.50
1:Cq:104:VAL:HG12	2:Cr:212:ILE:HG13	1.92	0.50
1:Cu:83:GLN:HE22	1:Da:55:ARG:HH22	1.58	0.50
2:Dd:155:LEU:HD23	2:Dd:162:ILE:HD11	1.93	0.50
2:Dp:214:GLN:HG3	2:Dr:195:LEU:HD21	1.93	0.50
2:Eh:161:VAL:HG12	2:Eh:188:ILE:HD11	1.93	0.50
2:Bf:153:THR:HB	2:Bf:164:ASN:H	1.77	0.50
2:Bn:219:ILE:HG23	2:Bp:192:LEU:HD12	1.92	0.50
2:Cj:161:VAL:HG12	2:Cj:188:ILE:HD11	1.93	0.50
2:Cv:166:ARG:HH22	2:Cx:101:GLU:HG2	1.75	0.50
2:Dh:161:VAL:HG12	2:Dh:188:ILE:HD11	1.92	0.50
2:An:153:THR:HB	2:An:164:ASN:H	1.76	0.50
2:At:153:THR:HB	2:At:164:ASN:H	1.76	0.50
2:Cf:219:ILE:HG23	2:Ch:192:LEU:HD12	1.93	0.50
2:Cn:86:LEU:HD13	2:Cn:153:THR:HG23	1.92	0.50
1:Ea:108:LYS:HD2	2:Eb:204:VAL:HG11	1.93	0.50
2:Bj:153:THR:HB	2:Bj:164:ASN:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bv:153:THR:HB	2:Bv:164:ASN:H	1.76	0.50
2:Cd:166:ARG:HH22	2:Cf:101:GLU:HG2	1.76	0.50
1:Co:104:VAL:HG12	2:Cp:212:ILE:HG13	1.93	0.50
2:Dj:153:THR:HB	2:Dj:164:ASN:H	1.77	0.50
2:Dr:153:THR:HB	2:Dr:164:ASN:H	1.77	0.50
2:Bx:161:VAL:HG12	2:Bx:188:ILE:HD11	1.92	0.50
2:Dx:77:PRO:HB2	2:Dx:146:VAL:HG13	1.94	0.50
2:Dz:148:TYR:HE1	2:Dz:176:VAL:HG21	1.76	0.50
2:Ej:155:LEU:HD23	2:Ej:162:ILE:HD11	1.94	0.50
2:Ah:166:ARG:HH22	2:Aj:101:GLU:HG2	1.76	0.50
2:Bj:166:ARG:HH22	2:Bl:101:GLU:HG2	1.77	0.50
2:Dr:161:VAL:HG12	2:Dr:188:ILE:HD11	1.94	0.50
2:Dt:219:ILE:HG23	2:Dv:192:LEU:HD12	1.94	0.50
2:Bl:153:THR:HB	2:Bl:164:ASN:H	1.76	0.50
2:Cx:87:GLN:HE21	2:Cz:94:TRP:HB3	1.77	0.50
1:Da:108:LYS:HD2	2:Db:204:VAL:HG11	1.93	0.50
1:Ae:104:VAL:HG12	2:Af:212:ILE:HG13	1.93	0.50
2:Bx:87:GLN:HE21	2:Bz:94:TRP:HB3	1.77	0.50
2:Cp:161:VAL:HG12	2:Cp:188:ILE:HD11	1.94	0.50
2:Cv:86:LEU:HD13	2:Cv:153:THR:HG23	1.94	0.50
2:Dp:161:VAL:HG12	2:Dp:188:ILE:HD11	1.93	0.50
2:Ef:161:VAL:HG12	2:Ef:188:ILE:HD11	1.94	0.50
2:Ab:192:LEU:HD12	2:El:219:ILE:HG23	1.94	0.49
2:Bf:161:VAL:HG12	2:Bf:188:ILE:HD11	1.94	0.49
1:Bs:108:LYS:HD2	2:Bt:204:VAL:HG11	1.95	0.49
2:Cr:153:THR:HB	2:Cr:164:ASN:H	1.77	0.49
2:Cx:161:VAL:HG12	2:Cx:188:ILE:HD11	1.94	0.49
1:Do:104:VAL:HG12	2:Dp:212:ILE:HG13	1.93	0.49
2:Eb:161:VAL:HG12	2:Eb:188:ILE:HD11	1.93	0.49
2:Eh:168:VAL:HG12	2:Eh:175:VAL:HA	1.94	0.49
2:Ab:161:VAL:HG12	2:Ab:188:ILE:HD11	1.94	0.49
2:Az:161:VAL:HG12	2:Az:188:ILE:HD11	1.95	0.49
2:Bd:161:VAL:HG12	2:Bd:188:ILE:HD11	1.93	0.49
2:Cn:161:VAL:HG12	2:Cn:188:ILE:HD11	1.94	0.49
2:Ct:161:VAL:HG12	2:Ct:188:ILE:HD11	1.94	0.49
2:Cv:87:GLN:HE21	2:Cx:94:TRP:HB3	1.77	0.49
2:Db:161:VAL:HG12	2:Db:188:ILE:HD11	1.94	0.49
2:Dh:40:ASN:HD22	2:Dh:41:GLY:H	1.59	0.49
1:Du:83:GLN:HE22	1:Ea:55:ARG:HH22	1.58	0.49
1:Dw:104:VAL:HG12	2:Dx:212:ILE:HG13	1.93	0.49
2:Ah:87:GLN:HE21	2:Aj:94:TRP:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:104:VAL:HG12	2:Al:212:ILE:HG13	1.94	0.49
2:Bn:161:VAL:HG12	2:Bn:188:ILE:HD11	1.95	0.49
2:Bt:161:VAL:HG12	2:Bt:188:ILE:HD11	1.95	0.49
2:Cl:161:VAL:HG12	2:Cl:188:ILE:HD11	1.95	0.49
2:Db:86:LEU:HD13	2:Db:153:THR:HG23	1.94	0.49
2:An:161:VAL:HG12	2:An:188:ILE:HD11	1.93	0.49
2:Cf:161:VAL:HG12	2:Cf:188:ILE:HD11	1.95	0.49
2:Cz:161:VAL:HG12	2:Cz:188:ILE:HD11	1.94	0.49
2:Dl:40:ASN:HD22	2:Dl:41:GLY:H	1.60	0.49
2:Al:166:ARG:HH22	2:An:101:GLU:HG2	1.77	0.49
1:Bm:104:VAL:HG12	2:Bn:212:ILE:HG13	1.93	0.49
2:Br:161:VAL:HG12	2:Br:188:ILE:HD11	1.93	0.49
2:Bz:155:LEU:HD23	2:Bz:162:ILE:HD11	1.93	0.49
2:Cp:214:GLN:HG3	2:Cr:195:LEU:HD21	1.93	0.49
2:Df:161:VAL:HG12	2:Df:188:ILE:HD11	1.94	0.49
1:Di:78:ALA:HB3	1:Dk:91:ALA:HB3	1.93	0.49
2:Dn:219:ILE:HG23	2:Dp:192:LEU:HD12	1.94	0.49
2:At:87:GLN:HE21	2:Av:94:TRP:HB3	1.78	0.49
2:At:161:VAL:HG12	2:At:188:ILE:HD11	1.93	0.49
1:Ay:83:GLN:HE22	1:Be:55:ARG:HH22	1.60	0.49
1:Cw:108:LYS:HD2	2:Cx:204:VAL:HG11	1.94	0.49
2:Dz:155:LEU:HD23	2:Dz:162:ILE:HD11	1.94	0.49
2:Ed:166:ARG:HH22	2:Ef:101:GLU:HG2	1.78	0.49
2:Ad:161:VAL:HG12	2:Ad:188:ILE:HD11	1.95	0.49
2:Bd:77:PRO:HB2	2:Bd:146:VAL:HG13	1.94	0.49
1:Bq:106:SER:HA	1:Bq:114:VAL:O	2.12	0.49
2:Bz:153:THR:HB	2:Bz:164:ASN:H	1.78	0.49
2:Cz:153:THR:HB	2:Cz:164:ASN:H	1.78	0.49
2:Ed:161:VAL:HG12	2:Ed:188:ILE:HD11	1.93	0.49
1:Eg:108:LYS:HD2	2:Eh:204:VAL:HG11	1.95	0.49
1:Bk:106:SER:HA	1:Bk:114:VAL:O	2.13	0.49
2:Bp:153:THR:HB	2:Bp:164:ASN:H	1.78	0.49
1:Dk:108:LYS:HD2	2:Dl:204:VAL:HG11	1.94	0.49
2:Dz:161:VAL:HG12	2:Dz:188:ILE:HD11	1.94	0.49
2:El:86:LEU:HD13	2:El:153:THR:HG23	1.95	0.49
2:Ah:86:LEU:HD13	2:Ah:153:THR:HG23	1.94	0.49
2:Aj:161:VAL:HG12	2:Aj:188:ILE:HD11	1.95	0.49
2:Ap:161:VAL:HG12	2:Ap:188:ILE:HD11	1.94	0.49
2:Av:219:ILE:HG23	2:Ax:192:LEU:HD12	1.95	0.49
2:Bj:161:VAL:HG12	2:Bj:188:ILE:HD11	1.95	0.49
2:Bt:214:GLN:HG3	2:Bv:195:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cb:168:VAL:HG12	2:Cb:175:VAL:HA	1.95	0.49
2:Cn:155:LEU:HD23	2:Cn:162:ILE:HD11	1.95	0.49
2:Cp:166:ARG:HH22	2:Cr:101:GLU:HG2	1.77	0.49
2:Dj:87:GLN:HE21	2:Dl:94:TRP:HB3	1.77	0.49
2:Dl:148:TYR:HE1	2:Dl:176:VAL:HG21	1.77	0.49
2:Ed:148:TYR:HE1	2:Ed:176:VAL:HG21	1.77	0.49
2:Eh:219:ILE:HG23	2:Ej:192:LEU:HD12	1.94	0.49
1:Ag:106:SER:HA	1:Ag:114:VAL:O	2.13	0.49
2:Bj:155:LEU:HD23	2:Bj:162:ILE:HD11	1.95	0.49
2:Bp:214:GLN:HG3	2:Br:195:LEU:HD21	1.95	0.49
2:Aj:219:ILE:HG23	2:Al:192:LEU:HD12	1.94	0.48
2:Ar:77:PRO:HB2	2:Ar:146:VAL:HG13	1.95	0.48
1:Bg:83:GLN:HE22	1:Bm:55:ARG:HH22	1.60	0.48
1:Bo:106:SER:HA	1:Bo:114:VAL:O	2.12	0.48
1:Cg:78:ALA:HB3	1:Ci:91:ALA:HB3	1.94	0.48
1:Dy:104:VAL:HG12	2:Dz:212:ILE:HG13	1.94	0.48
2:Dz:40:ASN:HD22	2:Dz:41:GLY:H	1.61	0.48
1:Ei:108:LYS:HD2	2:Ej:204:VAL:HG11	1.95	0.48
1:Ek:104:VAL:HG12	2:El:212:ILE:HG13	1.93	0.48
2:Af:219:ILE:HG23	2:Ah:192:LEU:HD12	1.95	0.48
2:Ar:155:LEU:HD23	2:Ar:162:ILE:HD11	1.94	0.48
2:Ar:161:VAL:HG12	2:Ar:188:ILE:HD11	1.95	0.48
2:At:166:ARG:HH22	2:Av:101:GLU:HG2	1.78	0.48
2:Bx:93:ASN:HB2	2:Bx:156:ARG:HH22	1.78	0.48
2:Cr:219:ILE:HG23	2:Ct:192:LEU:HD12	1.95	0.48
2:Ct:93:ASN:HB2	2:Ct:156:ARG:HH22	1.77	0.48
1:Dc:83:GLN:HE22	1:Di:55:ARG:HH22	1.59	0.48
1:Dc:104:VAL:HG12	2:Dd:212:ILE:HG13	1.95	0.48
1:Dy:108:LYS:HD2	2:Dz:204:VAL:HG11	1.95	0.48
2:El:153:THR:HB	2:El:164:ASN:H	1.79	0.48
1:Aa:55:ARG:HH22	1:Eg:83:GLN:HE22	1.59	0.48
2:Ab:219:ILE:HG23	2:Ad:192:LEU:HD12	1.94	0.48
2:Af:161:VAL:HG12	2:Af:188:ILE:HD11	1.96	0.48
2:Av:40:ASN:HD22	2:Av:41:GLY:H	1.60	0.48
2:Bb:40:ASN:HD22	2:Bb:41:GLY:H	1.59	0.48
2:Bj:214:GLN:HG3	2:Bl:195:LEU:HD21	1.96	0.48
2:Bx:155:LEU:HD23	2:Bx:162:ILE:HD11	1.94	0.48
2:Cv:161:VAL:HG12	2:Cv:188:ILE:HD11	1.94	0.48
2:Cx:153:THR:HB	2:Cx:164:ASN:H	1.77	0.48
2:Dj:161:VAL:HG12	2:Dj:188:ILE:HD11	1.94	0.48
2:Dn:159:GLY:HA3	2:Dr:36:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:173:ARG:HH21	2:Ad:144:GLN:HG2	1.77	0.48
2:At:93:ASN:HB2	2:At:156:ARG:HH22	1.79	0.48
1:Au:108:LYS:HD2	2:Av:204:VAL:HG11	1.94	0.48
2:Cd:161:VAL:HG12	2:Cd:188:ILE:HD11	1.95	0.48
2:Cd:219:ILE:HG23	2:Cf:192:LEU:HD12	1.95	0.48
1:De:108:LYS:HD2	2:Df:204:VAL:HG11	1.95	0.48
2:Dv:219:ILE:HG23	2:Dx:192:LEU:HD12	1.95	0.48
2:Dz:153:THR:HB	2:Dz:164:ASN:H	1.77	0.48
1:Aa:58:LYS:HZ2	1:Aa:103:VAL:HG21	1.78	0.48
2:Ad:93:ASN:HB2	2:Ad:156:ARG:HH22	1.79	0.48
2:Ax:161:VAL:HG12	2:Ax:188:ILE:HD11	1.96	0.48
1:Ay:104:VAL:HG12	2:Az:212:ILE:HG13	1.94	0.48
2:Bf:219:ILE:HG23	2:Bh:192:LEU:HD12	1.95	0.48
2:Bj:219:ILE:HG23	2:Bl:192:LEU:HD12	1.96	0.48
2:Cb:161:VAL:HG12	2:Cb:188:ILE:HD11	1.95	0.48
2:Db:40:ASN:HD22	2:Db:41:GLY:H	1.60	0.48
2:Dh:153:THR:HB	2:Dh:164:ASN:H	1.79	0.48
2:Dl:77:PRO:HB2	2:Dl:146:VAL:HG13	1.96	0.48
2:Dp:86:LEU:HD13	2:Dp:153:THR:HG23	1.96	0.48
2:Ad:77:PRO:HB2	2:Ad:146:VAL:HG13	1.96	0.48
1:Bk:108:LYS:HD2	2:Bl:204:VAL:HG11	1.95	0.48
2:Br:219:ILE:HG23	2:Bt:192:LEU:HD12	1.95	0.48
2:Bv:161:VAL:HG12	2:Bv:188:ILE:HD11	1.96	0.48
2:Ch:161:VAL:HG12	2:Ch:188:ILE:HD11	1.94	0.48
2:Dd:40:ASN:HD22	2:Dd:41:GLY:H	1.61	0.48
1:Du:106:SER:HA	1:Du:114:VAL:O	2.14	0.48
2:Bv:214:GLN:HG3	2:Bx:195:LEU:HD21	1.96	0.48
2:Cb:87:GLN:HE21	2:Cd:94:TRP:HB3	1.79	0.48
2:Ct:87:GLN:HE21	2:Cv:94:TRP:HB3	1.78	0.48
2:Dh:77:PRO:HB2	2:Dh:146:VAL:HG13	1.95	0.48
2:Dj:148:TYR:HE1	2:Dj:176:VAL:HG21	1.78	0.48
2:Dp:159:GLY:HA3	2:Dt:36:LYS:HA	1.95	0.48
2:Dt:161:VAL:HG12	2:Dt:188:ILE:HD11	1.95	0.48
2:Dx:150:LEU:HD13	2:Dx:167:VAL:HG22	1.96	0.48
2:Ef:155:LEU:HD23	2:Ef:162:ILE:HD11	1.95	0.48
2:Bf:40:ASN:HD22	2:Bf:41:GLY:H	1.61	0.48
1:Bu:106:SER:HA	1:Bu:114:VAL:O	2.13	0.48
2:Cf:166:ARG:HH22	2:Ch:101:GLU:HG2	1.77	0.48
2:Cp:219:ILE:HG23	2:Cr:192:LEU:HD12	1.96	0.48
2:Dd:161:VAL:HG12	2:Dd:188:ILE:HD11	1.96	0.48
1:Dm:83:GLN:HE22	1:Ds:55:ARG:HH22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dp:153:THR:HB	2:Dp:164:ASN:H	1.78	0.48
2:Dr:159:GLY:HA3	2:Dv:36:LYS:HA	1.95	0.48
2:Ed:77:PRO:HB2	2:Ed:146:VAL:HG13	1.96	0.48
1:Aa:78:ALA:HB3	1:Ac:91:ALA:HB3	1.96	0.48
2:Ah:155:LEU:HD23	2:Ah:162:ILE:HD11	1.95	0.48
1:Ai:83:GLN:HE22	1:Ao:55:ARG:HH22	1.62	0.48
2:Bj:40:ASN:HD22	2:Bj:41:GLY:H	1.61	0.48
2:Dh:219:ILE:HG23	2:Dj:192:LEU:HD12	1.96	0.48
2:Dr:77:PRO:HB2	2:Dr:146:VAL:HG13	1.96	0.48
2:Eb:87:GLN:HE21	2:Ed:94:TRP:HB3	1.78	0.48
1:Ak:108:LYS:HD2	2:Al:204:VAL:HG11	1.96	0.48
1:Ao:78:ALA:HB3	1:Aq:91:ALA:HB3	1.95	0.48
1:Aq:108:LYS:HD2	2:Ar:204:VAL:HG11	1.95	0.48
2:Az:219:ILE:HG23	2:Bb:192:LEU:HD12	1.95	0.48
2:Bl:161:VAL:HG12	2:Bl:188:ILE:HD11	1.95	0.48
1:Bm:108:LYS:HD2	2:Bn:204:VAL:HG11	1.95	0.48
1:Cs:108:LYS:HD2	2:Ct:204:VAL:HG11	1.96	0.48
1:Ec:104:VAL:HG12	2:Ed:212:ILE:HG13	1.94	0.48
2:Ed:150:LEU:HD13	2:Ed:167:VAL:HG22	1.96	0.48
2:Bl:168:VAL:HG12	2:Bl:175:VAL:HA	1.96	0.47
2:Bn:86:LEU:HD13	2:Bn:153:THR:HG23	1.95	0.47
1:Ce:78:ALA:HB3	1:Cg:91:ALA:HB3	1.96	0.47
1:Cq:108:LYS:HD2	2:Cr:204:VAL:HG11	1.97	0.47
1:Do:78:ALA:HB3	1:Dq:91:ALA:HB3	1.94	0.47
2:Az:168:VAL:HG12	2:Az:175:VAL:HA	1.96	0.47
1:Cs:83:GLN:HE22	1:Cy:55:ARG:HH22	1.61	0.47
1:Dq:108:LYS:HD2	2:Dr:204:VAL:HG11	1.96	0.47
2:Dt:150:LEU:HD13	2:Dt:167:VAL:HG22	1.97	0.47
2:Dv:40:ASN:HD22	2:Dv:41:GLY:H	1.62	0.47
2:Eh:77:PRO:HB2	2:Eh:146:VAL:HG13	1.96	0.47
1:Aa:108:LYS:HD2	2:Ab:204:VAL:HG11	1.95	0.47
2:Aj:155:LEU:HD23	2:Aj:162:ILE:HD11	1.96	0.47
2:Al:77:PRO:HB2	2:Al:146:VAL:HG13	1.96	0.47
2:Ar:168:VAL:HG12	2:Ar:175:VAL:HA	1.96	0.47
2:At:150:LEU:HD13	2:At:167:VAL:HG22	1.97	0.47
2:Av:174:ILE:HD12	2:Ax:113:LYS:HE3	1.96	0.47
2:Cj:168:VAL:HG12	2:Cj:175:VAL:HA	1.96	0.47
2:Dr:166:ARG:HH22	2:Dt:101:GLU:HG2	1.79	0.47
2:Ej:148:TYR:HE1	2:Ej:176:VAL:HG21	1.78	0.47
2:Ad:150:LEU:HD13	2:Ad:167:VAL:HG22	1.97	0.47
2:Ar:87:GLN:HE21	2:At:94:TRP:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ax:40:ASN:HD22	2:Ax:41:GLY:H	1.61	0.47
2:Bf:87:GLN:HE21	2:Bh:94:TRP:HB3	1.78	0.47
2:Bp:219:ILE:HG23	2:Br:192:LEU:HD12	1.95	0.47
2:Bx:219:ILE:HG23	2:Bz:192:LEU:HD12	1.95	0.47
2:Bz:168:VAL:HG12	2:Bz:175:VAL:HA	1.96	0.47
2:Cd:168:VAL:HG12	2:Cd:175:VAL:HA	1.96	0.47
1:Cm:106:SER:HA	1:Cm:114:VAL:O	2.15	0.47
2:Cr:214:GLN:HG3	2:Ct:195:LEU:HD21	1.96	0.47
2:Df:77:PRO:HB2	2:Df:146:VAL:HG13	1.96	0.47
2:Dp:166:ARG:HH22	2:Dr:101:GLU:HG2	1.80	0.47
1:Dy:58:LYS:HZ2	1:Dy:103:VAL:HG21	1.80	0.47
2:Al:40:ASN:HD22	2:Al:41:GLY:H	1.61	0.47
2:Cp:77:PRO:HB2	2:Cp:146:VAL:HG13	1.96	0.47
2:Cv:153:THR:HB	2:Cv:164:ASN:H	1.78	0.47
2:Cz:87:GLN:HE21	2:Db:94:TRP:HB3	1.79	0.47
2:Df:155:LEU:HD23	2:Df:162:ILE:HD11	1.97	0.47
1:Ek:106:SER:HA	1:Ek:114:VAL:O	2.13	0.47
2:Bh:161:VAL:HG12	2:Bh:188:ILE:HD11	1.96	0.47
1:Bi:78:ALA:HB3	1:Bk:91:ALA:HB3	1.96	0.47
1:Ca:106:SER:HA	1:Ca:114:VAL:O	2.14	0.47
2:Cv:40:ASN:HD22	2:Cv:41:GLY:H	1.60	0.47
2:Cz:214:GLN:HG3	2:Db:195:LEU:HD21	1.97	0.47
2:Ab:155:LEU:HD23	2:Ab:162:ILE:HD11	1.96	0.47
1:Ac:83:GLN:HE22	1:Ai:55:ARG:HH22	1.62	0.47
2:Az:77:PRO:HB2	2:Az:146:VAL:HG13	1.96	0.47
1:Bw:58:LYS:HZ2	1:Bw:103:VAL:HG21	1.80	0.47
2:Bz:166:ARG:HH22	2:Cb:101:GLU:HG2	1.78	0.47
1:Ci:58:LYS:HZ2	1:Ci:103:VAL:HG21	1.80	0.47
2:Cj:153:THR:HB	2:Cj:164:ASN:H	1.80	0.47
2:Cr:86:LEU:HD13	2:Cr:153:THR:HG23	1.96	0.47
2:Cv:214:GLN:HG3	2:Cx:195:LEU:HD21	1.96	0.47
2:Df:219:ILE:HG23	2:Dh:192:LEU:HD12	1.96	0.47
2:Dj:77:PRO:HB2	2:Dj:146:VAL:HG13	1.97	0.47
2:Dj:173:ARG:HH21	2:Dl:144:GLN:HG2	1.80	0.47
2:Dp:40:ASN:HD22	2:Dp:41:GLY:H	1.61	0.47
2:Dx:219:ILE:HG23	2:Dz:192:LEU:HD12	1.96	0.47
2:Ef:219:ILE:HD12	2:Eh:192:LEU:HD12	1.96	0.47
2:Eh:148:TYR:HE1	2:Eh:176:VAL:HG21	1.79	0.47
2:Ad:148:TYR:HE1	2:Ad:176:VAL:HG21	1.80	0.47
2:Af:86:LEU:HD13	2:Af:153:THR:HG23	1.96	0.47
1:Am:108:LYS:HD2	2:An:204:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:166:ARG:HH22	2:Bd:101:GLU:HG2	1.79	0.47
2:Bl:77:PRO:HB2	2:Bl:146:VAL:HG13	1.97	0.47
2:Cd:214:GLN:HG3	2:Cf:195:LEU:HD21	1.96	0.47
2:Cn:214:GLN:HG3	2:Cp:195:LEU:HD21	1.95	0.47
2:Dd:153:THR:HB	2:Dd:164:ASN:H	1.80	0.47
1:Dy:83:GLN:HE22	1:Ee:55:ARG:HH22	1.62	0.47
2:Bd:87:GLN:HE21	2:Bf:94:TRP:HB3	1.80	0.47
2:Bh:166:ARG:HH22	2:Bj:101:GLU:HG2	1.80	0.47
1:Cg:83:GLN:HE22	1:Cm:55:ARG:HH22	1.62	0.47
1:Ci:80:LEU:HD13	1:Ci:85:LEU:HD12	1.97	0.47
2:Cj:219:ILE:HG23	2:Cl:192:LEU:HD12	1.96	0.47
2:Cl:219:ILE:HG23	2:Cn:192:LEU:HD12	1.96	0.47
2:Ct:40:ASN:HD22	2:Ct:41:GLY:H	1.62	0.47
2:Dv:161:VAL:HG12	2:Dv:188:ILE:HD11	1.96	0.47
1:Ai:106:SER:HA	1:Ai:114:VAL:O	2.15	0.47
2:Al:219:ILE:HG23	2:An:192:LEU:HD12	1.96	0.47
2:Bb:219:ILE:HG23	2:Bd:192:LEU:HD12	1.97	0.47
2:Bt:93:ASN:HB2	2:Bt:156:ARG:HH22	1.80	0.47
1:Cc:106:SER:HA	1:Cc:114:VAL:O	2.14	0.47
2:Dl:155:LEU:HD23	2:Dl:162:ILE:HD11	1.97	0.47
2:Dr:40:ASN:HD22	2:Dr:41:GLY:H	1.62	0.47
2:Ah:161:VAL:HG12	2:Ah:188:ILE:HD11	1.97	0.46
2:Bd:174:ILE:HD12	2:Bf:113:LYS:HE3	1.96	0.46
2:Bv:219:ILE:HG23	2:Bx:192:LEU:HD12	1.97	0.46
1:Bw:106:SER:HA	1:Bw:114:VAL:O	2.15	0.46
1:Cy:106:SER:HA	1:Cy:114:VAL:O	2.15	0.46
1:Di:77:ARG:HH12	1:Dk:73:ARG:HH21	1.61	0.46
1:Do:106:SER:HA	1:Do:114:VAL:O	2.14	0.46
2:Dp:219:ILE:HG23	2:Dr:192:LEU:HD12	1.98	0.46
2:Dz:219:ILE:HG23	2:Eb:192:LEU:HD12	1.97	0.46
1:Ee:58:LYS:HZ2	1:Ee:103:VAL:HG21	1.79	0.46
2:Bh:155:LEU:HD23	2:Bh:162:ILE:HD11	1.96	0.46
1:Bo:83:GLN:HE22	1:Bu:55:ARG:HH22	1.61	0.46
2:Cr:87:GLN:HE21	2:Ct:94:TRP:HB3	1.81	0.46
2:Cv:159:GLY:HA3	2:Cz:36:LYS:HA	1.96	0.46
2:Eb:86:LEU:HD13	2:Eb:153:THR:HG23	1.96	0.46
1:Ec:108:LYS:HD2	2:Ed:204:VAL:HG11	1.97	0.46
2:Br:153:THR:HB	2:Br:164:ASN:H	1.81	0.46
1:Cc:78:ALA:HB3	1:Cc:91:ALA:HB3	1.97	0.46
1:Cc:108:LYS:HD2	2:Cd:204:VAL:HG11	1.96	0.46
2:Cd:77:PRO:HB2	2:Cd:146:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dj:219:ILE:HG23	2:Dl:192:LEU:HD12	1.96	0.46
2:Dl:161:VAL:HG12	2:Dl:188:ILE:HD11	1.97	0.46
2:Dz:87:GLN:HE21	2:Eb:94:TRP:HB3	1.79	0.46
2:Eh:40:ASN:HD22	2:Eh:41:GLY:H	1.63	0.46
1:Au:83:GLN:HE22	1:Ba:55:ARG:HH22	1.63	0.46
2:Az:40:ASN:HD22	2:Az:41:GLY:H	1.62	0.46
2:Az:166:ARG:HH22	2:Bb:101:GLU:HG2	1.79	0.46
1:Bc:77:ARG:HH12	1:Be:73:ARG:HH21	1.62	0.46
2:Bd:168:VAL:HG12	2:Bd:175:VAL:HA	1.98	0.46
2:Bj:150:LEU:HD13	2:Bj:167:VAL:HG22	1.98	0.46
2:Bn:155:LEU:HD23	2:Bn:162:ILE:HD11	1.97	0.46
1:Bq:58:LYS:HZ2	1:Bq:103:VAL:HG21	1.80	0.46
1:Bu:80:LEU:HD13	1:Bu:85:LEU:HD12	1.97	0.46
2:Cb:86:LEU:HD13	2:Cb:153:THR:HG23	1.97	0.46
1:Ci:29:TRP:HB3	1:Ci:118:ARG:HE	1.80	0.46
2:Cx:77:PRO:HB2	2:Cx:146:VAL:HG13	1.97	0.46
2:Dd:173:ARG:HH21	2:Df:144:GLN:HG2	1.81	0.46
2:Df:40:ASN:HD22	2:Df:41:GLY:H	1.61	0.46
2:Df:150:LEU:HD13	2:Df:167:VAL:HG22	1.98	0.46
2:Dp:150:LEU:HD13	2:Dp:167:VAL:HG22	1.98	0.46
1:Du:78:ALA:HB3	1:Dw:91:ALA:HB3	1.98	0.46
2:Dv:81:THR:HG21	2:Dx:123:ILE:HD12	1.98	0.46
2:Ab:101:GLU:HG2	2:El:166:ARG:HH22	1.81	0.46
2:Af:214:GLN:HG3	2:Ah:195:LEU:HD21	1.96	0.46
2:Ah:214:GLN:HG3	2:Aj:195:LEU:HD21	1.97	0.46
2:Ah:219:ILE:HG23	2:Aj:192:LEU:HD12	1.97	0.46
2:Bd:214:GLN:HG3	2:Bf:195:LEU:HD21	1.97	0.46
2:Bp:161:VAL:HG12	2:Bp:188:ILE:HD11	1.97	0.46
2:Bt:155:LEU:HD23	2:Bt:162:ILE:HD11	1.97	0.46
2:Cn:153:THR:HB	2:Cn:164:ASN:H	1.80	0.46
2:Cx:148:TYR:HE1	2:Cx:176:VAL:HG21	1.80	0.46
2:Dp:81:THR:HG21	2:Dr:123:ILE:HD12	1.97	0.46
1:Du:58:LYS:HZ2	1:Du:103:VAL:HG21	1.80	0.46
1:Dw:80:LEU:HD13	1:Dw:85:LEU:HD12	1.98	0.46
1:Bs:80:LEU:HD13	1:Bs:85:LEU:HD12	1.98	0.46
1:Bu:65:LEU:HD21	1:Bu:119:LEU:HB2	1.98	0.46
1:Cg:58:LYS:HZ2	1:Cg:103:VAL:HG21	1.80	0.46
2:Db:155:LEU:HD23	2:Db:162:ILE:HD11	1.98	0.46
1:Dm:106:SER:HA	1:Dm:114:VAL:O	2.16	0.46
2:Ef:148:TYR:HE1	2:Ef:176:VAL:HG21	1.80	0.46
1:Ei:78:ALA:HB3	1:Ek:91:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ah:153:THR:HB	2:Ah:164:ASN:H	1.80	0.46
2:Al:168:VAL:HG12	2:Al:175:VAL:HA	1.96	0.46
1:Aq:78:ALA:HB3	1:As:91:ALA:HB3	1.98	0.46
2:Ar:219:ILE:HG23	2:At:192:LEU:HD12	1.98	0.46
2:At:86:LEU:HD22	2:At:155:LEU:HB2	1.98	0.46
1:Ce:106:SER:HA	1:Ce:114:VAL:O	2.16	0.46
2:Cr:40:ASN:HD22	2:Cr:41:GLY:H	1.62	0.46
1:Dc:78:ALA:HB3	1:De:91:ALA:HB3	1.97	0.46
2:Dh:86:LEU:HD13	2:Dh:153:THR:HG23	1.97	0.46
1:Ac:58:LYS:HZ2	1:Ac:103:VAL:HG21	1.80	0.46
1:Am:106:SER:HA	1:Am:114:VAL:O	2.15	0.46
1:Bc:83:GLN:HE22	1:Bi:55:ARG:HH22	1.62	0.46
1:Bk:78:ALA:HB3	1:Bm:91:ALA:HB3	1.97	0.46
2:Bl:150:LEU:HD13	2:Bl:167:VAL:HG22	1.98	0.46
2:Cf:168:VAL:HG12	2:Cf:175:VAL:HA	1.98	0.46
1:Co:80:LEU:HD13	1:Co:85:LEU:HD12	1.98	0.46
2:Dd:86:LEU:HD13	2:Dd:153:THR:HG23	1.97	0.46
2:Dt:148:TYR:HE1	2:Dt:176:VAL:HG21	1.81	0.46
2:Dx:40:ASN:HD22	2:Dx:41:GLY:H	1.63	0.46
1:Ak:83:GLN:HE22	1:Aq:55:ARG:HH22	1.62	0.46
2:At:77:PRO:HB2	2:At:146:VAL:HG13	1.98	0.46
2:Br:87:GLN:HE21	2:Bt:94:TRP:HB3	1.81	0.46
2:Cl:155:LEU:HD23	2:Cl:162:ILE:HD11	1.98	0.46
2:Cn:40:ASN:HD22	2:Cn:41:GLY:H	1.63	0.46
2:Cv:168:VAL:HG12	2:Cv:175:VAL:HA	1.98	0.46
1:Dk:77:ARG:HH12	1:Dm:73:ARG:HH21	1.64	0.46
2:Ar:148:TYR:HE1	2:Ar:176:VAL:HG21	1.81	0.46
2:Av:77:PRO:HB2	2:Av:146:VAL:HG13	1.98	0.46
2:Ax:87:GLN:HE21	2:Az:94:TRP:HB3	1.81	0.46
2:Ax:173:ARG:HH21	2:Az:144:GLN:HG2	1.81	0.46
2:Bz:87:GLN:HE21	2:Cb:94:TRP:HB3	1.80	0.46
1:Cm:80:LEU:HD13	1:Cm:85:LEU:HD12	1.98	0.46
2:Cr:168:VAL:HG12	2:Cr:175:VAL:HA	1.98	0.46
2:Dl:81:THR:HG21	2:Dn:123:ILE:HD12	1.98	0.46
2:Dn:150:LEU:HD13	2:Dn:167:VAL:HG22	1.98	0.46
1:Dq:106:SER:HA	1:Dq:114:VAL:O	2.16	0.46
2:Dr:219:ILE:HG23	2:Dt:192:LEU:HD12	1.98	0.46
2:Ed:40:ASN:HD22	2:Ed:41:GLY:H	1.63	0.46
2:Eh:150:LEU:HD13	2:Eh:167:VAL:HG22	1.98	0.46
2:Eh:166:ARG:HH22	2:Ej:101:GLU:HG2	1.80	0.46
2:Ej:219:ILE:HG23	2:El:192:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:87:GLN:HE21	2:Ad:94:TRP:HB3	1.81	0.45
2:Cf:155:LEU:HD23	2:Cf:162:ILE:HD11	1.98	0.45
2:Dr:214:GLN:HG3	2:Dt:195:LEU:HD21	1.98	0.45
1:Du:80:LEU:HD23	1:Dw:89:LEU:HD22	1.98	0.45
2:Dx:148:TYR:HE1	2:Dx:176:VAL:HG21	1.82	0.45
1:Ea:80:LEU:HD13	1:Ea:85:LEU:HD12	1.98	0.45
1:Eg:58:LYS:HZ2	1:Eg:103:VAL:HG21	1.81	0.45
2:Al:87:GLN:HE21	2:An:94:TRP:HB3	1.81	0.45
2:At:86:LEU:HD13	2:At:153:THR:HG23	1.98	0.45
2:Az:81:THR:HG21	2:Bb:123:ILE:HD12	1.98	0.45
2:Bh:150:LEU:HD13	2:Bh:167:VAL:HG22	1.98	0.45
2:Cb:81:THR:HG21	2:Cd:123:ILE:HD12	1.99	0.45
2:Dl:168:VAL:HG12	2:Dl:175:VAL:HA	1.97	0.45
2:Dn:77:PRO:HB2	2:Dn:146:VAL:HG13	1.99	0.45
2:Ed:87:GLN:HE21	2:Ef:94:TRP:HB3	1.81	0.45
2:Ef:168:VAL:HG12	2:Ef:175:VAL:HA	1.96	0.45
2:Ab:168:VAL:HG12	2:Ab:175:VAL:HA	1.96	0.45
2:Ah:86:LEU:HD22	2:Ah:155:LEU:HB2	1.98	0.45
2:At:219:ILE:HG23	2:Av:192:LEU:HD12	1.97	0.45
1:Aw:78:ALA:HB3	1:Ay:91:ALA:HB3	1.98	0.45
2:Az:155:LEU:HD23	2:Az:162:ILE:HD11	1.97	0.45
2:Bt:86:LEU:HD13	2:Bt:153:THR:HG23	1.99	0.45
2:Bz:40:ASN:HD22	2:Bz:41:GLY:H	1.64	0.45
2:Bz:219:ILE:HG23	2:Cb:192:LEU:HD12	1.98	0.45
2:Cl:77:PRO:HB2	2:Cl:146:VAL:HG13	1.97	0.45
2:Cn:173:ARG:HH21	2:Cp:144:GLN:HG2	1.81	0.45
1:Cs:106:SER:HA	1:Cs:114:VAL:O	2.15	0.45
2:Dh:150:LEU:HD13	2:Dh:167:VAL:HG22	1.99	0.45
2:Dp:86:LEU:HD22	2:Dp:155:LEU:HB2	1.98	0.45
2:Eb:148:TYR:HE1	2:Eb:176:VAL:HG21	1.82	0.45
2:Eb:219:ILE:HG23	2:Ed:192:LEU:HD12	1.98	0.45
2:Ed:219:ILE:HG23	2:Ef:192:LEU:HD12	1.97	0.45
2:Ej:168:VAL:HG12	2:Ej:175:VAL:HA	1.97	0.45
2:Ad:219:ILE:HG23	2:Af:192:LEU:HD12	1.97	0.45
2:Ax:155:LEU:HD23	2:Ax:162:ILE:HD11	1.97	0.45
2:Bh:40:ASN:HD22	2:Bh:41:GLY:H	1.63	0.45
2:Br:86:LEU:HD22	2:Br:155:LEU:HB2	1.99	0.45
1:Ca:83:GLN:HE22	1:Cg:55:ARG:HH22	1.64	0.45
2:Cd:155:LEU:HD23	2:Cd:162:ILE:HD11	1.98	0.45
2:Cl:166:ARG:HH22	2:Cn:101:GLU:HG2	1.81	0.45
1:Co:83:GLN:HE22	1:Cu:55:ARG:HH22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cp:155:LEU:HD23	2:Cp:162:ILE:HD11	1.98	0.45
2:Cz:40:ASN:HD22	2:Cz:41:GLY:H	1.62	0.45
1:De:83:GLN:HE22	1:Dk:55:ARG:HH22	1.62	0.45
1:Ds:80:LEU:HD13	1:Ds:85:LEU:HD12	1.99	0.45
1:Ek:65:LEU:HD21	1:Ek:119:LEU:HB2	1.97	0.45
2:Ad:81:THR:HG21	2:Af:123:ILE:HD12	1.98	0.45
2:An:40:ASN:HD22	2:An:41:GLY:H	1.64	0.45
1:Bc:106:SER:HA	1:Bc:114:VAL:O	2.16	0.45
2:Cp:40:ASN:HD22	2:Cp:41:GLY:H	1.63	0.45
2:Cz:81:THR:HG21	2:Db:123:ILE:HD12	1.98	0.45
2:Db:77:PRO:HB2	2:Db:146:VAL:HG13	1.97	0.45
2:Db:219:ILE:HG23	2:Dd:192:LEU:HD12	1.98	0.45
2:Ef:77:PRO:HB2	2:Ef:146:VAL:HG13	1.99	0.45
1:Ek:108:LYS:HD2	2:El:204:VAL:HG11	1.99	0.45
2:Af:40:ASN:HD22	2:Af:41:GLY:H	1.62	0.45
1:Bg:106:SER:HA	1:Bg:114:VAL:O	2.16	0.45
2:Bp:81:THR:HG21	2:Br:123:ILE:HD12	1.97	0.45
2:Bz:81:THR:HG21	2:Cb:123:ILE:HD12	1.98	0.45
1:Ce:108:LYS:HD2	2:Cf:204:VAL:HG11	1.98	0.45
2:Cp:168:VAL:HG12	2:Cp:175:VAL:HA	1.99	0.45
2:Cv:81:THR:HG21	2:Cx:123:ILE:HD12	1.98	0.45
1:Dg:29:TRP:HB3	1:Dg:118:ARG:HE	1.81	0.45
2:Dr:168:VAL:HG12	2:Dr:175:VAL:HA	1.99	0.45
2:Dz:86:LEU:HD13	2:Dz:153:THR:HG23	1.98	0.45
1:Ec:106:SER:HA	1:Ec:114:VAL:O	2.16	0.45
2:Eh:155:LEU:HD23	2:Eh:162:ILE:HD11	1.99	0.45
1:Aq:106:SER:HA	1:Aq:114:VAL:O	2.16	0.45
2:Bb:168:VAL:HG12	2:Bb:175:VAL:HA	1.99	0.45
2:Br:166:ARG:HH22	2:Bt:101:GLU:HG2	1.82	0.45
2:Bv:40:ASN:HD22	2:Bv:41:GLY:H	1.64	0.45
2:Ch:81:THR:HG21	2:Cj:123:ILE:HD12	1.98	0.45
1:Co:106:SER:HA	1:Co:114:VAL:O	2.16	0.45
2:Cr:81:THR:HG21	2:Ct:123:ILE:HD12	1.98	0.45
2:Cz:219:ILE:HG23	2:Db:192:LEU:HD12	1.99	0.45
2:Dh:168:VAL:HG12	2:Dh:175:VAL:HA	1.98	0.45
2:El:168:VAL:HG12	2:El:175:VAL:HA	1.98	0.45
2:Ad:168:VAL:HG12	2:Ad:175:VAL:HA	1.98	0.45
2:Az:148:TYR:HE1	2:Az:176:VAL:HG21	1.82	0.45
2:Br:40:ASN:HD22	2:Br:41:GLY:H	1.65	0.45
1:Bs:65:LEU:HD21	1:Bs:119:LEU:HB2	1.99	0.45
2:Cb:166:ARG:HH22	2:Cd:101:GLU:HG2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cv:86:LEU:HD22	2:Cv:155:LEU:HB2	1.97	0.45
1:Dg:65:LEU:HD21	1:Dg:119:LEU:HB2	1.98	0.45
2:Dj:150:LEU:HD13	2:Dj:167:VAL:HG22	1.99	0.45
2:Dr:81:THR:HG21	2:Dt:123:ILE:HD12	1.99	0.45
2:Dx:153:THR:HB	2:Dx:164:ASN:H	1.81	0.45
2:Eb:40:ASN:HD22	2:Eb:41:GLY:H	1.64	0.45
2:Eh:81:THR:HG21	2:Ej:123:ILE:HD12	1.99	0.45
2:Ej:40:ASN:HD22	2:Ej:41:GLY:H	1.64	0.45
2:Al:86:LEU:HD13	2:Al:153:THR:HG23	1.98	0.45
1:Ba:65:LEU:HD21	1:Ba:119:LEU:HB2	1.98	0.45
2:Bh:77:PRO:HB2	2:Bh:146:VAL:HG13	1.99	0.45
2:Bl:159:GLY:HA3	2:Bp:36:LYS:HA	1.99	0.45
2:Bv:155:LEU:HD23	2:Bv:162:ILE:HD11	1.98	0.45
2:Bx:40:ASN:HD22	2:Bx:41:GLY:H	1.63	0.45
2:Cp:87:GLN:HE21	2:Cr:94:TRP:HB3	1.81	0.45
2:Dt:40:ASN:HD22	2:Dt:41:GLY:H	1.64	0.45
2:Eb:168:VAL:HG12	2:Eb:175:VAL:HA	1.97	0.45
1:Ae:83:GLN:HE22	1:Ak:55:ARG:HH22	1.64	0.45
2:Ah:40:ASN:HD22	2:Ah:41:GLY:H	1.63	0.45
1:Be:65:LEU:HD21	1:Be:119:LEU:HB2	1.99	0.45
2:Bf:86:LEU:HD13	2:Bf:153:THR:HG23	1.99	0.45
2:Bx:168:VAL:HG12	2:Bx:175:VAL:HA	1.99	0.45
2:Cb:219:ILE:HG23	2:Cd:192:LEU:HD12	1.97	0.45
2:Cj:155:LEU:HD23	2:Cj:162:ILE:HD11	1.99	0.45
1:Ds:78:ALA:HB3	1:Du:91:ALA:HB3	1.99	0.45
1:Dw:58:LYS:HZ2	1:Dw:103:VAL:HG21	1.81	0.45
1:Ea:106:SER:HA	1:Ea:114:VAL:O	2.17	0.45
2:Ed:168:VAL:HG12	2:Ed:175:VAL:HA	1.99	0.45
2:Ab:40:ASN:HD22	2:Ab:41:GLY:H	1.65	0.44
1:Ae:106:SER:HA	1:Ae:114:VAL:O	2.17	0.44
2:Ap:81:THR:HG21	2:Ar:123:ILE:HD12	1.99	0.44
1:As:83:GLN:HE22	1:Ay:55:ARG:HH22	1.64	0.44
1:Bc:58:LYS:HZ2	1:Bc:103:VAL:HG21	1.82	0.44
1:Bo:58:LYS:HZ2	1:Bo:103:VAL:HG21	1.82	0.44
1:Bu:58:LYS:HZ2	1:Bu:103:VAL:HG21	1.81	0.44
2:Bv:77:PRO:HB2	2:Bv:146:VAL:HG13	1.99	0.44
1:Cg:108:LYS:HD2	2:Ch:204:VAL:HG11	1.98	0.44
2:Ct:219:ILE:HG23	2:Cv:192:LEU:HD12	1.99	0.44
2:Cv:219:ILE:HG23	2:Cx:192:LEU:HD12	1.99	0.44
1:Dc:106:SER:HA	1:Dc:114:VAL:O	2.17	0.44
2:Dh:159:GLY:HA3	2:Dl:36:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dv:214:GLN:HG3	2:Dx:195:LEU:HD21	1.99	0.44
2:Dx:81:THR:HG21	2:Dz:123:ILE:HD12	1.99	0.44
2:Av:159:GLY:HA3	2:Az:36:LYS:HA	1.99	0.44
1:Bs:58:LYS:HZ2	1:Bs:103:VAL:HG21	1.82	0.44
2:Ch:87:GLN:HE21	2:Cj:94:TRP:HB3	1.82	0.44
2:Ch:168:VAL:HG12	2:Ch:175:VAL:HA	1.98	0.44
1:Ck:80:LEU:HD13	1:Ck:85:LEU:HD12	1.99	0.44
2:Cn:219:ILE:HG23	2:Cp:192:LEU:HD12	1.99	0.44
1:Co:65:LEU:HD21	1:Co:119:LEU:HB2	2.00	0.44
1:Cq:106:SER:HA	1:Cq:114:VAL:O	2.18	0.44
2:Db:87:GLN:HE21	2:Dd:94:TRP:HB3	1.82	0.44
2:Dt:166:ARG:HH11	2:Dv:133:PHE:HE2	1.64	0.44
1:Dy:80:LEU:HD13	1:Dy:85:LEU:HD12	1.99	0.44
2:Af:168:VAL:HG12	2:Af:175:VAL:HA	1.99	0.44
2:An:81:THR:HG21	2:Ap:123:ILE:HD12	2.00	0.44
2:Av:183:LEU:HG	2:Av:188:ILE:HG13	1.99	0.44
2:Bb:81:THR:HG21	2:Bd:123:ILE:HD12	1.99	0.44
2:Bl:81:THR:HG21	2:Bn:123:ILE:HD12	1.98	0.44
2:Br:81:THR:HG21	2:Bt:123:ILE:HD12	1.98	0.44
2:Cp:148:TYR:HE1	2:Cp:176:VAL:HG21	1.82	0.44
1:Cw:65:LEU:HD21	1:Cw:119:LEU:HB2	1.98	0.44
2:Cx:219:ILE:HG23	2:Cz:192:LEU:HD12	1.99	0.44
1:De:78:ALA:HB3	1:Dg:91:ALA:HB3	1.98	0.44
1:Di:29:TRP:HB3	1:Di:118:ARG:HE	1.83	0.44
2:Eb:77:PRO:HB2	2:Eb:146:VAL:HG13	1.99	0.44
1:Ai:80:LEU:HD13	1:Ai:85:LEU:HD12	1.99	0.44
2:Aj:40:ASN:HD22	2:Aj:41:GLY:H	1.63	0.44
1:Bg:65:LEU:HD21	1:Bg:119:LEU:HB2	2.00	0.44
2:Bl:40:ASN:HD22	2:Bl:41:GLY:H	1.65	0.44
2:Bt:87:GLN:HE21	2:Bv:94:TRP:HB3	1.81	0.44
2:Bv:168:VAL:HG12	2:Bv:175:VAL:HA	1.99	0.44
2:Dt:86:LEU:HD13	2:Dt:153:THR:HG23	1.98	0.44
2:Eb:81:THR:HG21	2:Ed:123:ILE:HD12	1.99	0.44
2:Af:155:LEU:HD23	2:Af:162:ILE:HD11	1.98	0.44
2:Aj:86:LEU:HD13	2:Aj:153:THR:HG23	2.00	0.44
2:Aj:168:VAL:HG12	2:Aj:175:VAL:HA	1.98	0.44
2:Ar:40:ASN:HD22	2:Ar:41:GLY:H	1.64	0.44
1:Be:80:LEU:HD13	1:Be:85:LEU:HD12	1.99	0.44
2:Bv:87:GLN:HE21	2:Bx:94:TRP:HB3	1.81	0.44
2:Ch:214:GLN:HG3	2:Cj:195:LEU:HD21	1.98	0.44
1:Cs:65:LEU:HD21	1:Cs:119:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dw:108:LYS:HD2	2:Dx:204:VAL:HG11	1.99	0.44
2:Ed:81:THR:HG21	2:Ef:123:ILE:HD12	2.00	0.44
1:Ee:106:SER:HA	1:Ee:114:VAL:O	2.18	0.44
1:Eg:78:ALA:HB3	1:Ei:91:ALA:HB3	1.99	0.44
2:Ad:40:ASN:HD22	2:Ad:41:GLY:H	1.65	0.44
1:As:106:SER:HA	1:As:114:VAL:O	2.17	0.44
2:Bf:81:THR:HG21	2:Bh:123:ILE:HD12	1.99	0.44
2:Bn:87:GLN:HE21	2:Bp:94:TRP:HB3	1.82	0.44
2:Cx:40:ASN:HD22	2:Cx:41:GLY:H	1.64	0.44
2:Dj:40:ASN:HD22	2:Dj:41:GLY:H	1.64	0.44
2:Dn:81:THR:HG21	2:Dp:123:ILE:HD12	1.99	0.44
2:Ar:81:THR:HG21	2:At:123:ILE:HD12	1.99	0.44
2:Ar:150:LEU:HD13	2:Ar:167:VAL:HG22	2.00	0.44
2:Bt:81:THR:HG21	2:Bv:123:ILE:HD12	1.99	0.44
2:Cf:86:LEU:HD13	2:Cf:153:THR:HG23	1.99	0.44
2:Cn:86:LEU:HD22	2:Cn:155:LEU:HB2	1.98	0.44
1:Ds:29:TRP:HB3	1:Ds:118:ARG:HE	1.83	0.44
2:Ad:86:LEU:HD13	2:Ad:153:THR:HG23	2.00	0.44
2:Ap:155:LEU:HD23	2:Ap:162:ILE:HD11	1.99	0.44
2:At:40:ASN:HD22	2:At:41:GLY:H	1.64	0.44
2:At:81:THR:HG21	2:Av:123:ILE:HD12	1.99	0.44
2:At:173:ARG:HH21	2:Av:144:GLN:HG2	1.83	0.44
2:Az:87:GLN:HE21	2:Bb:94:TRP:HB3	1.83	0.44
1:Be:29:TRP:HB3	1:Be:118:ARG:HE	1.83	0.44
2:Dj:86:LEU:HD13	2:Dj:153:THR:HG23	1.99	0.44
2:Al:81:THR:HG21	2:An:123:ILE:HD12	2.00	0.44
2:Av:87:GLN:HE21	2:Ax:94:TRP:HB3	1.83	0.44
2:Bj:81:THR:HG21	2:Bl:123:ILE:HD12	1.99	0.44
2:Bn:150:LEU:HD13	2:Bn:167:VAL:HG22	2.00	0.44
2:Bp:166:ARG:HH22	2:Br:101:GLU:HG2	1.82	0.44
1:By:83:GLN:HE22	1:Ce:55:ARG:HH22	1.63	0.44
1:Ca:58:LYS:HZ2	1:Ca:103:VAL:HG21	1.83	0.44
2:Ch:183:LEU:HG	2:Ch:188:ILE:HG13	2.00	0.44
1:Cw:83:GLN:HE22	1:Dc:55:ARG:HH22	1.66	0.44
1:Cw:106:SER:HA	1:Cw:114:VAL:O	2.18	0.44
2:Dd:87:GLN:HE21	2:Df:94:TRP:HB3	1.83	0.44
2:Dr:150:LEU:HD13	2:Dr:167:VAL:HG22	2.00	0.44
2:Dv:159:GLY:HA3	2:Dz:36:LYS:HA	1.99	0.44
1:Dw:106:SER:HA	1:Dw:114:VAL:O	2.18	0.44
1:Ee:83:GLN:HE22	1:Ek:55:ARG:HH22	1.66	0.44
2:Ab:81:THR:HG21	2:Ad:123:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Af:166:ARG:HH22	2:Ah:101:GLU:HG2	1.82	0.43
1:Ak:106:SER:HA	1:Ak:114:VAL:O	2.18	0.43
1:Ao:106:SER:HA	1:Ao:114:VAL:O	2.17	0.43
2:Bt:154:MET:HE2	2:Bt:154:MET:HB3	1.91	0.43
2:Cd:40:ASN:HD22	2:Cd:41:GLY:H	1.65	0.43
2:Dl:219:ILE:HG23	2:Dn:192:LEU:HD12	2.00	0.43
2:Al:214:GLN:HG3	2:An:195:LEU:HD21	1.99	0.43
2:Ap:40:ASN:HD22	2:Ap:41:GLY:H	1.65	0.43
2:Av:214:GLN:HG3	2:Ax:195:LEU:HD21	1.99	0.43
1:Aw:106:SER:HA	1:Aw:114:VAL:O	2.18	0.43
1:Ba:83:GLN:HE22	1:Bg:55:ARG:HH22	1.65	0.43
2:Bh:168:VAL:HG12	2:Bh:175:VAL:HA	1.99	0.43
2:Bn:40:ASN:HD22	2:Bn:41:GLY:H	1.66	0.43
2:Cn:168:VAL:HG12	2:Cn:175:VAL:HA	1.99	0.43
2:Ct:214:GLN:HG3	2:Cv:195:LEU:HD21	2.00	0.43
1:Di:106:SER:HA	1:Di:114:VAL:O	2.18	0.43
1:Du:80:LEU:HD13	1:Du:85:LEU:HD12	2.00	0.43
2:Ej:81:THR:HG21	2:El:123:ILE:HD12	1.99	0.43
2:Ah:81:THR:HG21	2:Aj:123:ILE:HD12	2.00	0.43
2:Ar:86:LEU:HD13	2:Ar:153:THR:HG23	2.00	0.43
2:Bf:86:LEU:HD22	2:Bf:155:LEU:HB2	2.00	0.43
2:Bt:86:LEU:HD22	2:Bt:155:LEU:HB2	2.00	0.43
2:Cx:81:THR:HG21	2:Cz:123:ILE:HD12	1.99	0.43
2:Db:214:GLN:HG3	2:Dd:195:LEU:HD21	1.99	0.43
2:Dd:148:TYR:HE1	2:Dd:176:VAL:HG21	1.83	0.43
2:Df:148:TYR:HE1	2:Df:176:VAL:HG21	1.83	0.43
1:Dg:106:SER:HA	1:Dg:114:VAL:O	2.18	0.43
1:Dq:80:LEU:HD23	1:Ds:89:LEU:HD22	2.00	0.43
2:Dt:155:LEU:HD23	2:Dt:162:ILE:HD11	2.00	0.43
2:Ej:77:PRO:HB2	2:Ej:146:VAL:HG13	1.99	0.43
2:Aj:81:THR:HG21	2:Al:123:ILE:HD12	2.00	0.43
2:Br:183:LEU:HG	2:Br:188:ILE:HG13	2.00	0.43
2:Cj:150:LEU:HD13	2:Cj:167:VAL:HG22	2.00	0.43
2:Cl:153:THR:HB	2:Cl:164:ASN:H	1.83	0.43
1:Cq:65:LEU:HD21	1:Cq:119:LEU:HB2	2.00	0.43
2:Cv:183:LEU:HG	2:Cv:188:ILE:HG13	2.00	0.43
1:Dk:29:TRP:HB3	1:Dk:118:ARG:HE	1.83	0.43
1:Dm:58:LYS:HZ2	1:Dm:103:VAL:HG21	1.82	0.43
1:Dw:80:LEU:HD23	1:Dy:89:LEU:HD22	2.00	0.43
1:Ei:29:TRP:HB3	1:Ei:118:ARG:HE	1.83	0.43
2:Ab:123:ILE:HD12	2:El:81:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:135:ARG:HG3	2:El:89:MET:HG3	2.00	0.43
2:Al:86:LEU:HD22	2:Al:155:LEU:HB2	2.00	0.43
2:Bd:79:ALA:HB2	2:Bd:146:VAL:HG11	2.01	0.43
1:Bi:106:SER:HA	1:Bi:114:VAL:O	2.17	0.43
2:Bp:86:LEU:HD13	2:Bp:153:THR:HG23	2.00	0.43
2:Ch:40:ASN:HD22	2:Ch:41:GLY:H	1.65	0.43
2:Cl:40:ASN:HD22	2:Cl:41:GLY:H	1.65	0.43
2:Ct:81:THR:HG21	2:Cv:123:ILE:HD12	1.99	0.43
2:Eb:150:LEU:HD13	2:Eb:167:VAL:HG22	2.00	0.43
2:Ad:155:LEU:HD23	2:Ad:162:ILE:HD11	2.00	0.43
2:Bd:148:TYR:HE1	2:Bd:176:VAL:HG21	1.84	0.43
1:Bk:65:LEU:HD21	1:Bk:119:LEU:HB2	2.01	0.43
1:Ck:65:LEU:HD21	1:Ck:119:LEU:HB2	2.00	0.43
2:Ct:86:LEU:HD13	2:Ct:153:THR:HG23	2.00	0.43
2:Dd:81:THR:HG21	2:Df:123:ILE:HD12	2.00	0.43
1:Dq:83:GLN:HE22	1:Dw:55:ARG:HH22	1.66	0.43
1:Ea:65:LEU:HD21	1:Ea:119:LEU:HB2	1.99	0.43
2:Af:81:THR:HG21	2:Ah:123:ILE:HD12	2.01	0.43
2:Ah:173:ARG:HH21	2:Aj:144:GLN:HG2	1.84	0.43
2:Av:81:THR:HG21	2:Ax:123:ILE:HD12	2.00	0.43
2:Az:61:MET:HE3	2:Az:103:PHE:HE1	1.83	0.43
2:Bd:40:ASN:HD22	2:Bd:41:GLY:H	1.65	0.43
2:Dl:86:LEU:HD13	2:Dl:153:THR:HG23	2.00	0.43
1:Am:83:GLN:HE22	1:As:55:ARG:HH22	1.65	0.43
2:Ap:150:LEU:HD13	2:Ap:167:VAL:HG22	2.01	0.43
2:Bp:40:ASN:HD22	2:Bp:41:GLY:H	1.66	0.43
2:Cb:155:LEU:HD23	2:Cb:162:ILE:HD11	2.00	0.43
2:Cl:79:ALA:HB2	2:Cl:146:VAL:HG11	2.01	0.43
2:Cn:81:THR:HG21	2:Cp:123:ILE:HD12	1.99	0.43
2:Cx:86:LEU:HD13	2:Cx:153:THR:HG23	2.00	0.43
2:Df:79:ALA:HB2	2:Df:146:VAL:HG11	2.01	0.43
2:Dj:81:THR:HG21	2:Dl:123:ILE:HD12	2.00	0.43
2:Dl:79:ALA:HB2	2:Dl:146:VAL:HG11	2.01	0.43
2:Dx:168:VAL:HG12	2:Dx:175:VAL:HA	2.00	0.43
2:Ef:40:ASN:HD22	2:Ef:41:GLY:H	1.66	0.43
2:Ar:79:ALA:HB2	2:Ar:146:VAL:HG11	2.01	0.43
2:Az:150:LEU:HD13	2:Az:167:VAL:HG22	2.01	0.43
1:By:58:LYS:HZ2	1:By:103:VAL:HG21	1.83	0.43
1:Da:83:GLN:HE22	1:Dg:55:ARG:HH22	1.66	0.43
2:Db:153:THR:HB	2:Db:164:ASN:H	1.84	0.43
1:Dm:65:LEU:HD21	1:Dm:119:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dt:81:THR:HG21	2:Dv:123:ILE:HD12	2.01	0.43
1:Ao:58:LYS:HZ2	1:Ao:103:VAL:HG21	1.83	0.43
1:Ay:106:SER:HA	1:Ay:114:VAL:O	2.18	0.43
2:Bf:168:VAL:HG12	2:Bf:175:VAL:HA	1.99	0.43
1:Bi:108:LYS:HD2	2:Bj:204:VAL:HG11	1.99	0.43
2:Bn:166:ARG:HH11	2:Bp:133:PHE:HE2	1.66	0.43
2:Br:150:LEU:HD13	2:Br:167:VAL:HG22	2.01	0.43
2:Bt:40:ASN:HD22	2:Bt:41:GLY:H	1.66	0.43
2:Cd:79:ALA:HB2	2:Cd:146:VAL:HG11	2.01	0.43
2:Cz:166:ARG:HH11	2:Db:133:PHE:HE2	1.67	0.43
2:Dx:183:LEU:HG	2:Dx:188:ILE:HG13	2.01	0.43
2:Eb:159:GLY:HA3	2:Ef:36:LYS:HA	2.00	0.43
2:An:183:LEU:HG	2:An:188:ILE:HG13	2.00	0.42
2:Ap:86:LEU:HD13	2:Ap:153:THR:HG23	2.01	0.42
2:Ap:86:LEU:HD22	2:Ap:155:LEU:HB2	1.99	0.42
1:Bm:65:LEU:HD21	1:Bm:119:LEU:HB2	2.00	0.42
2:Bp:87:GLN:HE21	2:Br:94:TRP:HB3	1.84	0.42
2:Bt:166:ARG:HH11	2:Bv:133:PHE:HE2	1.65	0.42
1:By:65:LEU:HD21	1:By:119:LEU:HB2	2.01	0.42
2:Cb:40:ASN:HD22	2:Cb:41:GLY:H	1.66	0.42
2:Cf:89:MET:HG3	2:Ch:135:ARG:HG3	2.01	0.42
2:Cr:86:LEU:HD22	2:Cr:155:LEU:HB2	2.00	0.42
2:Cr:159:GLY:HA3	2:Cv:36:LYS:HA	2.00	0.42
1:Da:78:ALA:HB3	1:Dc:91:ALA:HB3	2.00	0.42
2:Db:81:THR:HG21	2:Dd:123:ILE:HD12	2.00	0.42
1:Dk:58:LYS:HZ2	1:Dk:103:VAL:HG21	1.84	0.42
1:Dk:65:LEU:HD21	1:Dk:119:LEU:HB2	2.00	0.42
2:El:40:ASN:HD22	2:El:41:GLY:H	1.65	0.42
2:Ad:79:ALA:HB2	2:Ad:146:VAL:HG11	2.01	0.42
2:Az:79:ALA:HB2	2:Az:146:VAL:HG11	2.01	0.42
2:Bd:81:THR:HG21	2:Bf:123:ILE:HD12	2.00	0.42
2:Bd:183:LEU:HG	2:Bd:188:ILE:HG13	2.00	0.42
2:Bl:183:LEU:HG	2:Bl:188:ILE:HG13	2.01	0.42
1:Bq:107:TYR:CZ	2:Bt:196:ASN:HB3	2.55	0.42
2:Bx:86:LEU:HD13	2:Bx:153:THR:HG23	2.00	0.42
1:By:106:SER:HA	1:By:114:VAL:O	2.18	0.42
2:Bz:86:LEU:HD13	2:Bz:153:THR:HG23	2.00	0.42
2:Cd:81:THR:HG21	2:Cf:123:ILE:HD12	2.01	0.42
2:Cj:40:ASN:HD22	2:Cj:41:GLY:H	1.65	0.42
2:Cj:81:THR:HG21	2:Cl:123:ILE:HD12	2.00	0.42
1:Ck:78:ALA:HB3	1:Cm:91:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Df:81:THR:HG21	2:Dh:123:ILE:HD12	2.00	0.42
1:Dg:83:GLN:HE22	1:Dm:55:ARG:HH22	1.66	0.42
2:Dn:40:ASN:HD22	2:Dn:41:GLY:H	1.65	0.42
1:Dq:78:ALA:HB3	1:Ds:91:ALA:HB3	2.01	0.42
1:Dy:80:LEU:HD23	1:Ea:89:LEU:HD22	2.01	0.42
2:Eh:153:THR:HB	2:Eh:164:ASN:H	1.85	0.42
1:Ei:106:SER:HA	1:Ei:114:VAL:O	2.19	0.42
1:Ag:120:ASP:HB3	1:Ag:123:LYS:HB2	2.00	0.42
2:Ar:61:MET:HE3	2:Ar:103:PHE:HE1	1.85	0.42
1:Bg:80:LEU:HD23	1:Bi:89:LEU:HD22	2.01	0.42
2:Bx:81:THR:HG21	2:Bz:123:ILE:HD12	2.00	0.42
1:Ck:58:LYS:HZ2	1:Ck:103:VAL:HG21	1.83	0.42
2:Cp:153:THR:HB	2:Cp:164:ASN:H	1.84	0.42
2:Db:61:MET:HE3	2:Db:103:PHE:HE1	1.84	0.42
2:Dt:77:PRO:HB2	2:Dt:146:VAL:HG13	2.01	0.42
1:Ea:58:LYS:HZ2	1:Ea:103:VAL:HG21	1.83	0.42
2:Eb:173:ARG:HH21	2:Ed:144:GLN:HG2	1.84	0.42
2:Ed:86:LEU:HD13	2:Ed:153:THR:HG23	2.00	0.42
2:Bp:174:ILE:HD12	2:Br:113:LYS:HE3	2.01	0.42
2:Bt:168:VAL:HG12	2:Bt:175:VAL:HA	2.00	0.42
2:Cp:81:THR:HG21	2:Cr:123:ILE:HD12	2.01	0.42
2:Dn:183:LEU:HG	2:Dn:188:ILE:HG13	2.01	0.42
2:Dp:173:ARG:HH21	2:Dr:144:GLN:HG2	1.83	0.42
2:Dx:79:ALA:HB2	2:Dx:146:VAL:HG11	2.00	0.42
2:Dz:168:VAL:HG12	2:Dz:175:VAL:HA	2.01	0.42
2:Eh:79:ALA:HB2	2:Eh:146:VAL:HG11	2.01	0.42
2:Ah:168:VAL:HG12	2:Ah:175:VAL:HA	2.00	0.42
2:Al:150:LEU:HD13	2:Al:167:VAL:HG22	2.01	0.42
2:At:168:VAL:HG12	2:At:175:VAL:HA	2.00	0.42
2:Ax:81:THR:HG21	2:Az:123:ILE:HD12	2.00	0.42
1:Ba:80:LEU:HD13	1:Ba:85:LEU:HD12	2.01	0.42
2:Bb:173:ARG:HH21	2:Bd:144:GLN:HG2	1.85	0.42
2:Bt:219:ILE:HG23	2:Bv:192:LEU:HD12	2.00	0.42
2:Bx:150:LEU:HD13	2:Bx:167:VAL:HG22	2.01	0.42
2:Cd:148:TYR:HE1	2:Cd:176:VAL:HG21	1.84	0.42
2:Cl:86:LEU:HD13	2:Cl:153:THR:HG23	2.01	0.42
1:Cu:58:LYS:HZ2	1:Cu:103:VAL:HG21	1.84	0.42
2:Cv:173:ARG:HH21	2:Cx:144:GLN:HG2	1.85	0.42
2:Dj:168:VAL:HG12	2:Dj:175:VAL:HA	2.01	0.42
2:Eh:86:LEU:HD13	2:Eh:153:THR:HG23	2.02	0.42
2:Aj:150:LEU:HD13	2:Aj:167:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bo:80:LEU:HD13	1:Bo:85:LEU:HD12	2.01	0.42
1:Bq:80:LEU:HD13	1:Bq:85:LEU:HD12	2.00	0.42
1:Bu:42:ARG:HE	1:Bu:52:ARG:HH21	1.68	0.42
2:Bz:214:GLN:HG3	2:Cb:195:LEU:HD21	2.01	0.42
2:Cp:86:LEU:HD13	2:Cp:153:THR:HG23	2.01	0.42
2:Dx:159:GLY:HA3	2:Eb:36:LYS:HA	2.01	0.42
2:Ed:79:ALA:HB2	2:Ed:146:VAL:HG11	2.02	0.42
2:Bn:148:TYR:HE1	2:Bn:176:VAL:HG21	1.85	0.42
2:Ct:95:LEU:HB2	2:Ct:192:LEU:HD21	2.01	0.42
1:Ds:65:LEU:HD21	1:Ds:119:LEU:HB2	2.00	0.42
1:Ca:65:LEU:HD21	1:Ca:119:LEU:HB2	2.02	0.42
1:Ce:80:LEU:HD13	1:Ce:85:LEU:HD12	2.01	0.42
2:Dt:154:MET:HE2	2:Dt:154:MET:HB3	1.91	0.42
2:Dv:183:LEU:HG	2:Dv:188:ILE:HG13	2.01	0.42
2:Al:148:TYR:HE1	2:Al:176:VAL:HG21	1.85	0.42
2:Al:159:GLY:HA3	2:Ap:36:LYS:HA	2.02	0.42
1:Am:65:LEU:HD21	1:Am:119:LEU:HB2	2.00	0.42
2:An:86:LEU:HD13	2:An:153:THR:HG23	2.02	0.42
2:An:219:ILE:HG23	2:Ap:192:LEU:HD12	2.01	0.42
2:Ap:168:VAL:HG12	2:Ap:175:VAL:HA	2.00	0.42
1:Ba:29:TRP:HB3	1:Ba:118:ARG:HE	1.85	0.42
1:Bg:42:ARG:HE	1:Bg:52:ARG:HH21	1.68	0.42
2:Bx:86:LEU:HD22	2:Bx:155:LEU:HB2	2.00	0.42
2:Cb:86:LEU:HD22	2:Cb:155:LEU:HB2	2.01	0.42
1:Cg:106:SER:HA	1:Cg:114:VAL:O	2.20	0.42
2:Cj:83:PHE:HB3	2:Cj:154:MET:HG3	2.02	0.42
2:Cj:86:LEU:HD13	2:Cj:153:THR:HG23	2.01	0.42
2:Cn:95:LEU:HD23	2:Cn:154:MET:HE1	2.01	0.42
2:Cr:183:LEU:HG	2:Cr:188:ILE:HG13	2.02	0.42
1:Da:65:LEU:HD21	1:Da:119:LEU:HB2	2.01	0.42
2:Dd:219:ILE:HG23	2:Df:192:LEU:HD12	2.02	0.42
1:Dy:65:LEU:HD21	1:Dy:119:LEU:HB2	2.00	0.42
1:Ek:58:LYS:HZ2	1:Ek:103:VAL:HG21	1.85	0.42
1:Aa:65:LEU:HD21	1:Aa:119:LEU:HB2	2.02	0.42
2:Al:79:ALA:HB2	2:Al:146:VAL:HG11	2.02	0.42
2:Bj:168:VAL:HG12	2:Bj:175:VAL:HA	2.01	0.42
2:Bl:148:TYR:HE1	2:Bl:176:VAL:HG21	1.84	0.42
2:Bl:166:ARG:HH22	2:Bn:101:GLU:HG2	1.84	0.42
2:Bn:81:THR:HG21	2:Bp:123:ILE:HD12	2.02	0.42
1:Bs:106:SER:HA	1:Bs:114:VAL:O	2.19	0.42
2:Bx:95:LEU:HD23	2:Bx:154:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cf:87:GLN:HE21	2:Ch:94:TRP:HB3	1.84	0.42
2:Cv:150:LEU:HD13	2:Cv:167:VAL:HG22	2.02	0.42
2:Cz:168:VAL:HG12	2:Cz:175:VAL:HA	2.00	0.42
2:Df:214:GLN:HG3	2:Dh:195:LEU:HD21	2.01	0.42
2:Dh:79:ALA:HB2	2:Dh:146:VAL:HG11	2.02	0.42
2:Dn:168:VAL:HG12	2:Dn:175:VAL:HA	2.02	0.42
2:Dr:183:LEU:HG	2:Dr:188:ILE:HG13	2.02	0.42
1:Ae:29:TRP:HB3	1:Ae:118:ARG:HE	1.85	0.41
2:An:168:VAL:HG12	2:An:175:VAL:HA	2.02	0.41
2:Av:150:LEU:HD13	2:Av:167:VAL:HG22	2.02	0.41
2:Bx:95:LEU:HB2	2:Bx:192:LEU:HD21	2.02	0.41
1:Cc:120:ASP:HB3	1:Cc:123:LYS:HB2	2.02	0.41
1:Ce:65:LEU:HD21	1:Ce:119:LEU:HB2	2.02	0.41
1:Cg:65:LEU:HD21	1:Cg:119:LEU:HB2	2.01	0.41
2:Db:80:VAL:HG12	2:Db:100:SER:HB2	2.02	0.41
2:Dp:168:VAL:HG12	2:Dp:175:VAL:HA	2.00	0.41
1:Ae:55:ARG:HH22	1:Ek:83:GLN:HE22	1.67	0.41
2:Aj:209:ASP:HA	2:Aj:210:PRO:HD3	1.96	0.41
2:Bh:87:GLN:HE21	2:Bj:94:TRP:HB3	1.85	0.41
2:Cb:162:ILE:HG23	2:Cb:182:PHE:HD1	1.85	0.41
1:Ck:83:GLN:HE22	1:Cq:55:ARG:HH22	1.65	0.41
2:Ct:86:LEU:HD22	2:Ct:155:LEU:HB2	2.02	0.41
2:Cz:61:MET:HE3	2:Cz:103:PHE:HE1	1.85	0.41
1:Dw:107:TYR:CZ	2:Dz:196:ASN:HB3	2.55	0.41
1:Ee:35:TYR:HB3	1:Ee:114:VAL:HG22	2.02	0.41
2:Ej:86:LEU:HD13	2:Ej:153:THR:HG23	2.02	0.41
2:El:86:LEU:HD22	2:El:155:LEU:HB2	2.02	0.41
2:Ab:150:LEU:HD13	2:Ab:167:VAL:HG22	2.02	0.41
2:Af:86:LEU:HD22	2:Af:155:LEU:HB2	2.00	0.41
1:Ai:58:LYS:HZ2	1:Ai:103:VAL:HG21	1.84	0.41
1:As:78:ALA:HB3	1:Au:91:ALA:HB3	2.01	0.41
2:Bl:79:ALA:HB2	2:Bl:146:VAL:HG11	2.02	0.41
2:Cf:40:ASN:HD22	2:Cf:41:GLY:H	1.68	0.41
1:Cq:80:LEU:HD13	1:Cq:85:LEU:HD12	2.02	0.41
2:Cx:168:VAL:HG12	2:Cx:175:VAL:HA	2.01	0.41
2:Dh:81:THR:HG21	2:Dj:123:ILE:HD12	2.01	0.41
2:Dx:166:ARG:HH22	2:Dz:101:GLU:HG2	1.86	0.41
2:Ap:219:ILE:HG23	2:Ar:192:LEU:HD12	2.00	0.41
1:Ay:58:LYS:HZ2	1:Ay:103:VAL:HG21	1.84	0.41
2:Bl:173:ARG:HH21	2:Bn:144:GLN:HG2	1.85	0.41
2:Cd:80:VAL:HG12	2:Cd:100:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dh:183:LEU:HG	2:Dh:188:ILE:HG13	2.02	0.41
2:Dp:87:GLN:HE21	2:Dr:94:TRP:HB3	1.85	0.41
1:Ag:65:LEU:HD21	1:Ag:119:LEU:HB2	2.02	0.41
1:Ao:80:LEU:HD13	1:Ao:85:LEU:HD12	2.01	0.41
2:Ar:209:ASP:HA	2:Ar:210:PRO:HD3	1.95	0.41
1:Aw:58:LYS:HZ2	1:Aw:103:VAL:HG21	1.84	0.41
2:Bd:159:GLY:HA3	2:Bh:36:LYS:HA	2.01	0.41
2:Bh:81:THR:HG21	2:Bj:123:ILE:HD12	2.01	0.41
1:Bm:29:TRP:HB3	1:Bm:118:ARG:HE	1.85	0.41
2:Br:159:GLY:HA3	2:Bv:36:LYS:HA	2.02	0.41
2:Bv:80:VAL:HG12	2:Bv:100:SER:HB2	2.01	0.41
2:Db:173:ARG:HH21	2:Dd:144:GLN:HG2	1.85	0.41
1:De:106:SER:HA	1:De:114:VAL:O	2.21	0.41
2:Df:173:ARG:HH21	2:Dh:144:GLN:HG2	1.84	0.41
2:Dh:87:GLN:HE21	2:Dj:94:TRP:HB3	1.84	0.41
2:Di:86:LEU:HD22	2:Di:155:LEU:HB2	2.02	0.41
1:Du:65:LEU:HD21	1:Du:119:LEU:HB2	2.01	0.41
2:Dv:87:GLN:HE21	2:Dx:94:TRP:HB3	1.86	0.41
2:Dz:79:ALA:HB2	2:Dz:146:VAL:HG11	2.03	0.41
1:Bi:83:GLN:HE22	1:Bo:55:ARG:HH22	1.68	0.41
2:Bv:61:MET:HE3	2:Bv:103:PHE:HE1	1.86	0.41
2:Ct:150:LEU:HD13	2:Ct:167:VAL:HG22	2.03	0.41
1:Cu:80:LEU:HD13	1:Cu:85:LEU:HD12	2.03	0.41
2:Df:168:VAL:HG12	2:Df:175:VAL:HA	2.02	0.41
2:Dx:86:LEU:HD22	2:Dx:155:LEU:HB2	2.02	0.41
2:Ef:150:LEU:HD13	2:Ef:167:VAL:HG22	2.02	0.41
1:Bk:58:LYS:HZ2	1:Bk:103:VAL:HG21	1.84	0.41
2:Bv:81:THR:HG21	2:Bx:123:ILE:HD12	2.01	0.41
2:Cf:81:THR:HG21	2:Ch:123:ILE:HD12	2.01	0.41
1:Ck:106:SER:HA	1:Ck:114:VAL:O	2.20	0.41
2:Cl:81:THR:HG21	2:Cn:123:ILE:HD12	2.03	0.41
2:Cp:79:ALA:HB2	2:Cp:146:VAL:HG11	2.02	0.41
2:Dp:183:LEU:HG	2:Dp:188:ILE:HG13	2.01	0.41
2:Dz:86:LEU:HD22	2:Dz:155:LEU:HB2	2.01	0.41
2:Ef:87:GLN:HE21	2:Eh:94:TRP:HB3	1.86	0.41
1:Ak:65:LEU:HD21	1:Ak:119:LEU:HB2	2.02	0.41
2:At:79:ALA:HB2	2:At:146:VAL:HG11	2.03	0.41
2:Bf:166:ARG:HH22	2:Bh:101:GLU:HG2	1.84	0.41
2:Bh:148:TYR:HE1	2:Bh:176:VAL:HG21	1.85	0.41
2:Bn:214:GLN:HG3	2:Bp:195:LEU:HD21	2.02	0.41
1:De:80:LEU:HD13	1:De:85:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ef:61:MET:HE3	2:Ef:103:PHE:HE1	1.86	0.41
1:Eg:65:LEU:HD21	1:Eg:119:LEU:HB2	2.02	0.41
2:Eh:61:MET:HE3	2:Eh:103:PHE:HE1	1.86	0.41
1:Ai:65:LEU:HD21	1:Ai:119:LEU:HB2	2.01	0.41
2:Aj:92:THR:HG21	2:Al:129:GLY:HA3	2.02	0.41
2:Aj:214:GLN:HG3	2:Al:195:LEU:HD21	2.03	0.41
2:An:87:GLN:HE21	2:Ap:94:TRP:HB3	1.86	0.41
2:Ap:95:LEU:HB2	2:Ap:192:LEU:HD21	2.03	0.41
2:Ap:159:GLY:HA3	2:At:36:LYS:HA	2.03	0.41
2:Ap:214:GLN:HG3	2:Ar:195:LEU:HD21	2.03	0.41
2:Av:80:VAL:HG12	2:Av:100:SER:HB2	2.02	0.41
2:Ax:166:ARG:HH11	2:Az:133:PHE:HE2	1.67	0.41
2:Ax:219:ILE:HG23	2:Az:192:LEU:HD12	2.01	0.41
1:Ay:29:TRP:HB3	1:Ay:118:ARG:HE	1.86	0.41
2:Az:89:MET:HG3	2:Bb:135:ARG:HG3	2.03	0.41
1:Ba:77:ARG:HH12	1:Bc:73:ARG:HH21	1.69	0.41
1:Ba:106:SER:HA	1:Ba:114:VAL:O	2.20	0.41
2:Bb:214:GLN:HG3	2:Bd:195:LEU:HD21	2.02	0.41
1:Bc:65:LEU:HD21	1:Bc:119:LEU:HB2	2.02	0.41
2:Bf:150:LEU:HD13	2:Bf:167:VAL:HG22	2.03	0.41
1:Bm:106:SER:HA	1:Bm:114:VAL:O	2.20	0.41
2:Bn:168:VAL:HG12	2:Bn:175:VAL:HA	2.02	0.41
2:Br:168:VAL:HG12	2:Br:175:VAL:HA	2.02	0.41
1:Bu:83:GLN:HE22	1:Ca:55:ARG:HH22	1.67	0.41
2:Bx:61:MET:HE3	2:Bx:103:PHE:HE1	1.86	0.41
1:Cc:65:LEU:HD21	1:Cc:119:LEU:HB2	2.02	0.41
2:Cp:150:LEU:HD13	2:Cp:167:VAL:HG22	2.03	0.41
2:Cv:61:MET:HE3	2:Cv:103:PHE:HE1	1.86	0.41
1:Cw:80:LEU:HD13	1:Cw:85:LEU:HD12	2.03	0.41
2:Cx:79:ALA:HB2	2:Cx:146:VAL:HG11	2.03	0.41
2:Cx:150:LEU:HD13	2:Cx:167:VAL:HG22	2.03	0.41
2:Cz:150:LEU:HD13	2:Cz:167:VAL:HG22	2.03	0.41
2:Dh:214:GLN:HG3	2:Dj:195:LEU:HD21	2.03	0.41
2:Dj:86:LEU:HD22	2:Dj:155:LEU:HB2	2.02	0.41
1:Do:108:LYS:HD2	2:Dp:204:VAL:HG11	2.02	0.41
2:Dt:166:ARG:HH22	2:Dv:101:GLU:HG2	1.84	0.41
2:Dz:159:GLY:HA3	2:Ed:36:LYS:HA	2.01	0.41
2:Dz:173:ARG:HH21	2:Eb:144:GLN:HG2	1.86	0.41
2:Ed:61:MET:HE3	2:Ed:103:PHE:HE1	1.86	0.41
2:Ah:154:MET:HE3	2:Ah:154:MET:HB3	1.97	0.41
2:Av:173:ARG:HH21	2:Ax:144:GLN:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ax:168:VAL:HG12	2:Ax:175:VAL:HA	2.01	0.41
2:Bn:86:LEU:HD22	2:Bn:155:LEU:HB2	2.03	0.41
2:Bn:86:LEU:HD23	2:Bn:155:LEU:HD13	2.03	0.41
2:Bv:148:TYR:HE1	2:Bv:176:VAL:HG21	1.85	0.41
2:Bv:150:LEU:HD13	2:Bv:167:VAL:HG22	2.03	0.41
2:Cb:148:TYR:HE1	2:Cb:176:VAL:HG21	1.86	0.41
1:Ec:29:TRP:HB3	1:Ec:118:ARG:HE	1.86	0.41
1:Ec:78:ALA:HB3	1:Ee:91:ALA:HB3	2.03	0.41
1:Ei:80:LEU:HD13	1:Ei:85:LEU:HD12	2.02	0.41
2:Ab:80:VAL:HG12	2:Ab:100:SER:HB2	2.03	0.40
1:Ae:58:LYS:HZ2	1:Ae:103:VAL:HG21	1.86	0.40
2:Ar:214:GLN:HG3	2:At:195:LEU:HD21	2.03	0.40
2:Bn:77:PRO:HB2	2:Bn:146:VAL:HG13	2.03	0.40
2:Cl:168:VAL:HG12	2:Cl:175:VAL:HA	2.02	0.40
2:Cr:150:LEU:HD13	2:Cr:167:VAL:HG22	2.03	0.40
1:Dc:29:TRP:HB3	1:Dc:118:ARG:HE	1.85	0.40
2:Ab:148:TYR:HE1	2:Ab:176:VAL:HG21	1.86	0.40
2:Af:149:VAL:HG23	2:Af:170:MET:HB2	2.04	0.40
1:Au:77:ARG:HH12	1:Aw:73:ARG:HH21	1.69	0.40
2:Ax:150:LEU:HD13	2:Ax:167:VAL:HG22	2.03	0.40
1:Dq:65:LEU:HD21	1:Dq:119:LEU:HB2	2.01	0.40
2:Eb:214:GLN:HG3	2:Ed:195:LEU:HD21	2.03	0.40
1:Eg:106:SER:HA	1:Eg:114:VAL:O	2.20	0.40
2:Ej:87:GLN:HE21	2:El:94:TRP:HB3	1.85	0.40
2:Az:214:GLN:HG3	2:Bb:195:LEU:HD21	2.02	0.40
2:Bn:61:MET:HE3	2:Bn:103:PHE:HE1	1.86	0.40
2:Bt:95:LEU:HB2	2:Bt:192:LEU:HD21	2.03	0.40
2:Cb:89:MET:HG3	2:Cd:135:ARG:HG3	2.04	0.40
2:Cf:150:LEU:HD13	2:Cf:167:VAL:HG22	2.04	0.40
2:Cp:86:LEU:HD22	2:Cp:155:LEU:HB2	2.03	0.40
2:Cp:174:ILE:HD12	2:Cr:113:LYS:HE3	2.02	0.40
1:Cs:29:TRP:HB3	1:Cs:118:ARG:HE	1.86	0.40
1:Da:58:LYS:HZ1	2:Db:207:ARG:NH1	2.19	0.40
2:Db:86:LEU:HD22	2:Db:155:LEU:HB2	2.03	0.40
2:Dd:86:LEU:HD22	2:Dd:155:LEU:HB2	2.02	0.40
2:Dh:173:ARG:HH21	2:Dj:144:GLN:HG2	1.85	0.40
2:Dt:168:VAL:HG12	2:Dt:175:VAL:HA	2.02	0.40
1:Dw:80:LEU:HB3	1:Dy:89:LEU:HB2	2.02	0.40
2:Dx:72:ILE:HD12	2:Dx:72:ILE:HA	2.00	0.40
2:Eb:80:VAL:HG12	2:Eb:100:SER:HB2	2.02	0.40
1:Ac:106:SER:HA	1:Ac:114:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:At:89:MET:HG3	2:Av:135:ARG:HG3	2.04	0.40
1:By:35:TYR:HB3	1:By:114:VAL:HG22	2.04	0.40
1:By:78:ALA:HB3	1:Ca:91:ALA:HB3	2.03	0.40
2:Cv:148:TYR:HE1	2:Cv:176:VAL:HG21	1.85	0.40
2:Cx:95:LEU:HB2	2:Cx:192:LEU:HD21	2.02	0.40
2:Dd:92:THR:HG21	2:Df:129:GLY:HA3	2.03	0.40
2:Dh:86:LEU:HD22	2:Dh:155:LEU:HB2	2.03	0.40
1:Dw:29:TRP:HB3	1:Dw:118:ARG:HE	1.87	0.40
2:El:209:ASP:HA	2:El:210:PRO:HD3	1.95	0.40
2:Aj:86:LEU:HD22	2:Aj:155:LEU:HB2	2.03	0.40
2:At:61:MET:HE3	2:At:103:PHE:HE1	1.86	0.40
2:At:95:LEU:HD23	2:At:154:MET:HE1	2.04	0.40
2:Ax:61:MET:HE3	2:Ax:103:PHE:HE1	1.86	0.40
1:Bi:80:LEU:HD13	1:Bi:85:LEU:HD12	2.02	0.40
2:Bz:150:LEU:HD13	2:Bz:167:VAL:HG22	2.04	0.40
2:Cf:95:LEU:HB2	2:Cf:192:LEU:HD21	2.03	0.40
2:Ch:80:VAL:HG12	2:Ch:100:SER:HB2	2.03	0.40
2:Ct:80:VAL:HG12	2:Ct:100:SER:HB2	2.04	0.40
2:Df:87:GLN:HE21	2:Dh:94:TRP:HB3	1.87	0.40
2:Dt:87:GLN:HE21	2:Dv:94:TRP:HB3	1.86	0.40
1:Dy:106:SER:HA	1:Dy:114:VAL:O	2.22	0.40
2:Eb:166:ARG:HH11	2:Ed:133:PHE:HE2	1.68	0.40
1:Ec:83:GLN:HE22	1:Ei:55:ARG:HH22	1.68	0.40
2:Ef:80:VAL:HG12	2:Ef:100:SER:HB2	2.03	0.40
2:Ej:80:VAL:HG12	2:Ej:100:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	102/104 (98%)	96 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ac	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ae	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ag	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ai	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ak	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Am	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ao	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Aq	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	As	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Au	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Aw	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ay	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ba	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bc	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Be	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bg	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bi	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bk	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bm	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bo	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bq	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bs	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Bu	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
1	Bw	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	By	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ca	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cc	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ce	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cg	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ci	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ck	102/104 (98%)	96 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Cm	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Co	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cq	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cs	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cu	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cw	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Cy	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Da	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dc	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	De	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dg	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Di	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dk	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dm	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Do	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dq	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ds	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Du	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dw	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Dy	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ea	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ec	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ee	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Eg	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ei	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
1	Ek	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
2	Ab	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Ad	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Af	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Ah	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Aj	188/192 (98%)	181 (96%)	6 (3%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Al	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	An	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Ap	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Ar	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	At	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
2	Av	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Ax	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Az	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Bb	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Bd	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Bf	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Bh	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Bj	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Bl	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Bn	188/192 (98%)	181 (96%)	6 (3%)	1 (0%)	24	57
2	Bp	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Br	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Bt	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Bv	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Bx	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Bz	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
2	Cb	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Cd	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Cf	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Ch	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Cj	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Cl	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Cn	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Cp	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Cr	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Ct	188/192 (98%)	181 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Cv	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
2	Cx	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Cz	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
2	Db	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dd	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Df	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dh	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
2	Dj	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	DI	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dn	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dp	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Dr	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dt	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dv	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Dx	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
2	Dz	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Eb	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Ed	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
2	Ef	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
2	Eh	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
2	Ej	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
2	El	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
All	All	16820/17168 (98%)	16099 (96%)	719 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Aj	86	LEU
2	Bn	86	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ac	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ae	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ag	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ai	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Ak	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Am	84/84 (100%)	80 (95%)	4 (5%)	23	50
1	Ao	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Aq	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	As	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Au	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Aw	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ay	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Ba	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Bc	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Be	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Bg	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Bi	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Bk	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Bm	84/84 (100%)	80 (95%)	4 (5%)	23	50
1	Bo	84/84 (100%)	77 (92%)	7 (8%)	10	35
1	Bq	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Bs	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Bu	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Bw	84/84 (100%)	80 (95%)	4 (5%)	23	50
1	By	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ca	84/84 (100%)	80 (95%)	4 (5%)	23	50
1	Cc	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ce	84/84 (100%)	79 (94%)	5 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cg	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ci	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Ck	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Cm	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Co	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Cq	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Cs	84/84 (100%)	80 (95%)	4 (5%)	23	50
1	Cu	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Cw	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Cy	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Da	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Dc	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	De	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Dg	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Di	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Dk	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Dm	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Do	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Dq	84/84 (100%)	80 (95%)	4 (5%)	23	50
1	Ds	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Du	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Dw	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Dy	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ea	84/84 (100%)	78 (93%)	6 (7%)	13	40
1	Ec	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ee	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Eg	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ei	84/84 (100%)	79 (94%)	5 (6%)	17	45
1	Ek	84/84 (100%)	79 (94%)	5 (6%)	17	45
2	Ab	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Ad	165/170 (97%)	157 (95%)	8 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Af	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Ah	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Aj	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Al	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	An	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Ap	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Ar	165/170 (97%)	155 (94%)	10 (6%)	17	44
2	At	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Av	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Ax	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Az	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Bb	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Bd	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Bf	165/170 (97%)	160 (97%)	5 (3%)	36	61
2	Bh	165/170 (97%)	155 (94%)	10 (6%)	17	44
2	Bj	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Bl	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Bn	165/170 (97%)	156 (94%)	9 (6%)	19	47
2	Bp	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Br	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Bt	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Bv	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Bx	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Bz	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Cb	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Cd	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Cf	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Ch	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Cj	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Cl	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Cn	165/170 (97%)	159 (96%)	6 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Cp	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Cr	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Ct	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Cv	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Cx	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Cz	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Db	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Dd	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Df	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Dh	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Dj	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	DI	165/170 (97%)	157 (95%)	8 (5%)	23	50
2	Dn	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Dp	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Dr	165/170 (97%)	160 (97%)	5 (3%)	36	61
2	Dt	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Dv	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Dx	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Dz	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Eb	165/170 (97%)	159 (96%)	6 (4%)	31	58
2	Ed	165/170 (97%)	160 (97%)	5 (3%)	36	61
2	Ef	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	Eh	165/170 (97%)	156 (94%)	9 (6%)	19	47
2	Ej	165/170 (97%)	158 (96%)	7 (4%)	26	53
2	El	165/170 (97%)	159 (96%)	6 (4%)	31	58
All	All	14442/14732 (98%)	13741 (95%)	701 (5%)	24	50

All (701) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	74	ILE
1	Aa	87	THR
1	Aa	97	VAL

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Mol	Chain	Res	Type
1	Aa	109	VAL
1	Aa	119	LEU
2	Ab	40	ASN
2	Ab	119	THR
2	Ab	162	ILE
2	Ab	163	VAL
2	Ab	174	ILE
2	Ab	217	THR
2	Ab	220	LEU
1	Ac	74	ILE
1	Ac	87	THR
1	Ac	97	VAL
1	Ac	109	VAL
1	Ac	119	LEU
2	Ad	40	ASN
2	Ad	76	THR
2	Ad	119	THR
2	Ad	162	ILE
2	Ad	163	VAL
2	Ad	174	ILE
2	Ad	217	THR
2	Ad	220	LEU
1	Ae	74	ILE
1	Ae	87	THR
1	Ae	97	VAL
1	Ae	109	VAL
1	Ae	119	LEU
2	Af	40	ASN
2	Af	119	THR
2	Af	162	ILE
2	Af	163	VAL
2	Af	174	ILE
2	Af	217	THR
1	Ag	74	ILE
1	Ag	87	THR
1	Ag	97	VAL
1	Ag	109	VAL
1	Ag	119	LEU
2	Ah	40	ASN
2	Ah	76	THR
2	Ah	119	THR
2	Ah	161	VAL

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Mol	Chain	Res	Type
2	Ah	162	ILE
2	Ah	163	VAL
2	Ah	174	ILE
2	Ah	217	THR
1	Ai	74	ILE
1	Ai	85	LEU
1	Ai	87	THR
1	Ai	97	VAL
1	Ai	109	VAL
1	Ai	119	LEU
2	Aj	40	ASN
2	Aj	119	THR
2	Aj	162	ILE
2	Aj	163	VAL
2	Aj	174	ILE
2	Aj	217	THR
2	Aj	220	LEU
1	Ak	74	ILE
1	Ak	87	THR
1	Ak	97	VAL
1	Ak	109	VAL
1	Ak	119	LEU
2	Al	40	ASN
2	Al	119	THR
2	Al	146	VAL
2	Al	161	VAL
2	Al	163	VAL
2	Al	174	ILE
2	Al	217	THR
1	Am	74	ILE
1	Am	97	VAL
1	Am	109	VAL
1	Am	119	LEU
2	An	40	ASN
2	An	119	THR
2	An	161	VAL
2	An	163	VAL
2	An	174	ILE
2	An	217	THR
2	An	220	LEU
1	Ao	74	ILE
1	Ao	87	THR

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Mol	Chain	Res	Type
1	Ao	97	VAL
1	Ao	109	VAL
1	Ao	119	LEU
2	Ap	40	ASN
2	Ap	119	THR
2	Ap	161	VAL
2	Ap	162	ILE
2	Ap	163	VAL
2	Ap	174	ILE
2	Ap	217	THR
1	Aq	74	ILE
1	Aq	87	THR
1	Aq	97	VAL
1	Aq	109	VAL
1	Aq	119	LEU
2	Ar	40	ASN
2	Ar	119	THR
2	Ar	130	ASP
2	Ar	146	VAL
2	Ar	161	VAL
2	Ar	162	ILE
2	Ar	163	VAL
2	Ar	174	ILE
2	Ar	217	THR
2	Ar	220	LEU
1	As	74	ILE
1	As	87	THR
1	As	97	VAL
1	As	109	VAL
1	As	119	LEU
2	At	40	ASN
2	At	146	VAL
2	At	161	VAL
2	At	162	ILE
2	At	163	VAL
2	At	174	ILE
2	At	217	THR
1	Au	74	ILE
1	Au	87	THR
1	Au	97	VAL
1	Au	109	VAL
1	Au	119	LEU

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Mol	Chain	Res	Type
2	Av	40	ASN
2	Av	76	THR
2	Av	119	THR
2	Av	146	VAL
2	Av	161	VAL
2	Av	163	VAL
2	Av	174	ILE
2	Av	217	THR
1	Aw	74	ILE
1	Aw	87	THR
1	Aw	97	VAL
1	Aw	109	VAL
1	Aw	119	LEU
2	Ax	40	ASN
2	Ax	76	THR
2	Ax	119	THR
2	Ax	161	VAL
2	Ax	162	ILE
2	Ax	163	VAL
2	Ax	174	ILE
2	Ax	217	THR
1	Ay	74	ILE
1	Ay	85	LEU
1	Ay	87	THR
1	Ay	97	VAL
1	Ay	109	VAL
1	Ay	119	LEU
2	Az	40	ASN
2	Az	76	THR
2	Az	119	THR
2	Az	146	VAL
2	Az	162	ILE
2	Az	163	VAL
2	Az	174	ILE
2	Az	217	THR
1	Ba	74	ILE
1	Ba	87	THR
1	Ba	97	VAL
1	Ba	109	VAL
1	Ba	119	LEU
2	Bb	40	ASN
2	Bb	119	THR

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Mol	Chain	Res	Type
2	Bb	130	ASP
2	Bb	161	VAL
2	Bb	162	ILE
2	Bb	163	VAL
2	Bb	174	ILE
2	Bb	217	THR
1	Bc	74	ILE
1	Bc	87	THR
1	Bc	97	VAL
1	Bc	109	VAL
1	Bc	119	LEU
2	Bd	40	ASN
2	Bd	119	THR
2	Bd	146	VAL
2	Bd	161	VAL
2	Bd	163	VAL
2	Bd	174	ILE
2	Bd	217	THR
1	Be	74	ILE
1	Be	87	THR
1	Be	97	VAL
1	Be	109	VAL
1	Be	119	LEU
2	Bf	40	ASN
2	Bf	119	THR
2	Bf	163	VAL
2	Bf	174	ILE
2	Bf	217	THR
1	Bg	74	ILE
1	Bg	87	THR
1	Bg	97	VAL
1	Bg	109	VAL
1	Bg	119	LEU
2	Bh	40	ASN
2	Bh	76	THR
2	Bh	119	THR
2	Bh	146	VAL
2	Bh	161	VAL
2	Bh	162	ILE
2	Bh	163	VAL
2	Bh	174	ILE
2	Bh	217	THR

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Mol	Chain	Res	Type
2	Bh	220	LEU
1	Bi	74	ILE
1	Bi	87	THR
1	Bi	97	VAL
1	Bi	109	VAL
1	Bi	119	LEU
2	Bj	40	ASN
2	Bj	119	THR
2	Bj	162	ILE
2	Bj	163	VAL
2	Bj	174	ILE
2	Bj	217	THR
1	Bk	74	ILE
1	Bk	87	THR
1	Bk	97	VAL
1	Bk	109	VAL
1	Bk	119	LEU
2	Bl	40	ASN
2	Bl	146	VAL
2	Bl	161	VAL
2	Bl	163	VAL
2	Bl	174	ILE
2	Bl	217	THR
2	Bl	220	LEU
1	Bm	74	ILE
1	Bm	97	VAL
1	Bm	109	VAL
1	Bm	119	LEU
2	Bn	40	ASN
2	Bn	119	THR
2	Bn	146	VAL
2	Bn	161	VAL
2	Bn	162	ILE
2	Bn	163	VAL
2	Bn	174	ILE
2	Bn	217	THR
2	Bn	220	LEU
1	Bo	74	ILE
1	Bo	85	LEU
1	Bo	87	THR
1	Bo	97	VAL
1	Bo	108	LYS

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Mol	Chain	Res	Type
1	Bo	109	VAL
1	Bo	119	LEU
2	Bp	40	ASN
2	Bp	119	THR
2	Bp	161	VAL
2	Bp	163	VAL
2	Bp	174	ILE
2	Bp	217	THR
2	Bp	220	LEU
1	Bq	74	ILE
1	Bq	85	LEU
1	Bq	87	THR
1	Bq	97	VAL
1	Bq	109	VAL
1	Bq	119	LEU
2	Br	40	ASN
2	Br	76	THR
2	Br	119	THR
2	Br	161	VAL
2	Br	163	VAL
2	Br	174	ILE
2	Br	217	THR
1	Bs	74	ILE
1	Bs	85	LEU
1	Bs	87	THR
1	Bs	97	VAL
1	Bs	109	VAL
1	Bs	119	LEU
2	Bt	40	ASN
2	Bt	119	THR
2	Bt	161	VAL
2	Bt	162	ILE
2	Bt	163	VAL
2	Bt	174	ILE
2	Bt	217	THR
1	Bu	74	ILE
1	Bu	85	LEU
1	Bu	87	THR
1	Bu	97	VAL
1	Bu	109	VAL
1	Bu	119	LEU
2	Bv	40	ASN

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Mol	Chain	Res	Type
2	Bv	146	VAL
2	Bv	162	ILE
2	Bv	163	VAL
2	Bv	174	ILE
2	Bv	217	THR
2	Bv	220	LEU
1	Bw	74	ILE
1	Bw	97	VAL
1	Bw	109	VAL
1	Bw	119	LEU
2	Bx	40	ASN
2	Bx	119	THR
2	Bx	161	VAL
2	Bx	162	ILE
2	Bx	163	VAL
2	Bx	174	ILE
2	Bx	217	THR
1	By	74	ILE
1	By	87	THR
1	By	97	VAL
1	By	109	VAL
1	By	119	LEU
2	Bz	40	ASN
2	Bz	119	THR
2	Bz	162	ILE
2	Bz	163	VAL
2	Bz	174	ILE
2	Bz	217	THR
1	Ca	74	ILE
1	Ca	97	VAL
1	Ca	109	VAL
1	Ca	119	LEU
2	Cb	40	ASN
2	Cb	119	THR
2	Cb	162	ILE
2	Cb	163	VAL
2	Cb	174	ILE
2	Cb	217	THR
1	Cc	74	ILE
1	Cc	87	THR
1	Cc	97	VAL
1	Cc	109	VAL

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Mol	Chain	Res	Type
1	Cc	119	LEU
2	Cd	40	ASN
2	Cd	119	THR
2	Cd	146	VAL
2	Cd	162	ILE
2	Cd	163	VAL
2	Cd	174	ILE
2	Cd	217	THR
1	Ce	74	ILE
1	Ce	87	THR
1	Ce	97	VAL
1	Ce	109	VAL
1	Ce	119	LEU
2	Cf	40	ASN
2	Cf	119	THR
2	Cf	161	VAL
2	Cf	162	ILE
2	Cf	163	VAL
2	Cf	174	ILE
2	Cf	217	THR
2	Cf	220	LEU
1	Cg	74	ILE
1	Cg	87	THR
1	Cg	97	VAL
1	Cg	109	VAL
1	Cg	119	LEU
2	Ch	40	ASN
2	Ch	119	THR
2	Ch	161	VAL
2	Ch	163	VAL
2	Ch	174	ILE
2	Ch	217	THR
2	Ch	220	LEU
1	Ci	74	ILE
1	Ci	85	LEU
1	Ci	87	THR
1	Ci	97	VAL
1	Ci	109	VAL
1	Ci	119	LEU
2	Cj	40	ASN
2	Cj	119	THR
2	Cj	162	ILE

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Mol	Chain	Res	Type
2	Cj	163	VAL
2	Cj	174	ILE
2	Cj	217	THR
1	Ck	74	ILE
1	Ck	87	THR
1	Ck	97	VAL
1	Ck	109	VAL
1	Ck	119	LEU
2	Cl	40	ASN
2	Cl	119	THR
2	Cl	146	VAL
2	Cl	162	ILE
2	Cl	163	VAL
2	Cl	174	ILE
2	Cl	217	THR
1	Cm	74	ILE
1	Cm	87	THR
1	Cm	97	VAL
1	Cm	109	VAL
1	Cm	119	LEU
2	Cn	40	ASN
2	Cn	119	THR
2	Cn	162	ILE
2	Cn	163	VAL
2	Cn	174	ILE
2	Cn	217	THR
1	Co	74	ILE
1	Co	85	LEU
1	Co	87	THR
1	Co	97	VAL
1	Co	109	VAL
1	Co	119	LEU
2	Cp	40	ASN
2	Cp	119	THR
2	Cp	162	ILE
2	Cp	163	VAL
2	Cp	174	ILE
2	Cp	217	THR
1	Cq	74	ILE
1	Cq	85	LEU
1	Cq	87	THR
1	Cq	97	VAL

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Mol	Chain	Res	Type
1	Cq	109	VAL
1	Cq	119	LEU
2	Cr	40	ASN
2	Cr	119	THR
2	Cr	161	VAL
2	Cr	163	VAL
2	Cr	174	ILE
2	Cr	217	THR
1	Cs	74	ILE
1	Cs	97	VAL
1	Cs	109	VAL
1	Cs	119	LEU
2	Ct	40	ASN
2	Ct	119	THR
2	Ct	162	ILE
2	Ct	163	VAL
2	Ct	174	ILE
2	Ct	217	THR
2	Ct	220	LEU
1	Cu	74	ILE
1	Cu	87	THR
1	Cu	97	VAL
1	Cu	109	VAL
1	Cu	119	LEU
2	Cv	40	ASN
2	Cv	119	THR
2	Cv	151	THR
2	Cv	161	VAL
2	Cv	163	VAL
2	Cv	174	ILE
2	Cv	217	THR
1	Cw	74	ILE
1	Cw	87	THR
1	Cw	97	VAL
1	Cw	109	VAL
1	Cw	119	LEU
2	Cx	40	ASN
2	Cx	119	THR
2	Cx	162	ILE
2	Cx	163	VAL
2	Cx	174	ILE
2	Cx	217	THR

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Mol	Chain	Res	Type
2	Cx	220	LEU
1	Cy	74	ILE
1	Cy	87	THR
1	Cy	97	VAL
1	Cy	109	VAL
1	Cy	119	LEU
2	Cz	40	ASN
2	Cz	119	THR
2	Cz	162	ILE
2	Cz	163	VAL
2	Cz	174	ILE
2	Cz	217	THR
2	Cz	220	LEU
1	Da	74	ILE
1	Da	87	THR
1	Da	97	VAL
1	Da	109	VAL
1	Da	119	LEU
2	Db	40	ASN
2	Db	119	THR
2	Db	146	VAL
2	Db	162	ILE
2	Db	163	VAL
2	Db	174	ILE
2	Db	217	THR
1	Dc	74	ILE
1	Dc	85	LEU
1	Dc	87	THR
1	Dc	97	VAL
1	Dc	109	VAL
1	Dc	119	LEU
2	Dd	40	ASN
2	Dd	119	THR
2	Dd	162	ILE
2	Dd	163	VAL
2	Dd	174	ILE
2	Dd	217	THR
1	De	74	ILE
1	De	85	LEU
1	De	87	THR
1	De	97	VAL
1	De	109	VAL

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Mol	Chain	Res	Type
1	De	119	LEU
2	Df	40	ASN
2	Df	119	THR
2	Df	162	ILE
2	Df	163	VAL
2	Df	174	ILE
2	Df	217	THR
1	Dg	74	ILE
1	Dg	87	THR
1	Dg	97	VAL
1	Dg	109	VAL
1	Dg	119	LEU
2	Dh	40	ASN
2	Dh	119	THR
2	Dh	161	VAL
2	Dh	163	VAL
2	Dh	174	ILE
2	Dh	217	THR
2	Dh	220	LEU
1	Di	74	ILE
1	Di	85	LEU
1	Di	97	VAL
1	Di	109	VAL
1	Di	119	LEU
2	Dj	40	ASN
2	Dj	119	THR
2	Dj	161	VAL
2	Dj	163	VAL
2	Dj	174	ILE
2	Dj	217	THR
1	Dk	74	ILE
1	Dk	87	THR
1	Dk	97	VAL
1	Dk	109	VAL
1	Dk	119	LEU
2	Dl	40	ASN
2	Dl	119	THR
2	Dl	161	VAL
2	Dl	162	ILE
2	Dl	163	VAL
2	Dl	174	ILE
2	Dl	217	THR

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Mol	Chain	Res	Type
2	Dl	220	LEU
1	Dm	74	ILE
1	Dm	85	LEU
1	Dm	87	THR
1	Dm	97	VAL
1	Dm	109	VAL
1	Dm	119	LEU
2	Dn	40	ASN
2	Dn	119	THR
2	Dn	161	VAL
2	Dn	163	VAL
2	Dn	174	ILE
2	Dn	217	THR
2	Dn	220	LEU
1	Do	74	ILE
1	Do	85	LEU
1	Do	87	THR
1	Do	97	VAL
1	Do	109	VAL
1	Do	119	LEU
2	Dp	40	ASN
2	Dp	119	THR
2	Dp	161	VAL
2	Dp	163	VAL
2	Dp	174	ILE
2	Dp	217	THR
1	Dq	74	ILE
1	Dq	97	VAL
1	Dq	109	VAL
1	Dq	119	LEU
2	Dr	40	ASN
2	Dr	161	VAL
2	Dr	163	VAL
2	Dr	174	ILE
2	Dr	217	THR
1	Ds	74	ILE
1	Ds	87	THR
1	Ds	97	VAL
1	Ds	109	VAL
1	Ds	119	LEU
2	Dt	40	ASN
2	Dt	161	VAL

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Mol	Chain	Res	Type
2	Dt	162	ILE
2	Dt	163	VAL
2	Dt	174	ILE
2	Dt	217	THR
2	Dt	220	LEU
1	Du	74	ILE
1	Du	85	LEU
1	Du	87	THR
1	Du	97	VAL
1	Du	109	VAL
1	Du	119	LEU
2	Dv	40	ASN
2	Dv	119	THR
2	Dv	161	VAL
2	Dv	163	VAL
2	Dv	174	ILE
2	Dv	217	THR
1	Dw	74	ILE
1	Dw	87	THR
1	Dw	97	VAL
1	Dw	109	VAL
1	Dw	119	LEU
2	Dx	40	ASN
2	Dx	146	VAL
2	Dx	161	VAL
2	Dx	163	VAL
2	Dx	174	ILE
2	Dx	217	THR
1	Dy	74	ILE
1	Dy	87	THR
1	Dy	97	VAL
1	Dy	109	VAL
1	Dy	119	LEU
2	Dz	40	ASN
2	Dz	151	THR
2	Dz	162	ILE
2	Dz	163	VAL
2	Dz	174	ILE
2	Dz	217	THR
1	Ea	74	ILE
1	Ea	85	LEU
1	Ea	87	THR

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Mol	Chain	Res	Type
1	Ea	97	VAL
1	Ea	109	VAL
1	Ea	119	LEU
2	Eb	40	ASN
2	Eb	146	VAL
2	Eb	161	VAL
2	Eb	163	VAL
2	Eb	174	ILE
2	Eb	217	THR
1	Ec	74	ILE
1	Ec	85	LEU
1	Ec	97	VAL
1	Ec	109	VAL
1	Ec	119	LEU
2	Ed	40	ASN
2	Ed	161	VAL
2	Ed	163	VAL
2	Ed	174	ILE
2	Ed	217	THR
1	Ee	74	ILE
1	Ee	87	THR
1	Ee	97	VAL
1	Ee	109	VAL
1	Ee	119	LEU
2	Ef	40	ASN
2	Ef	146	VAL
2	Ef	162	ILE
2	Ef	163	VAL
2	Ef	174	ILE
2	Ef	217	THR
2	Ef	220	LEU
1	Eg	74	ILE
1	Eg	87	THR
1	Eg	97	VAL
1	Eg	109	VAL
1	Eg	119	LEU
2	Uh	40	ASN
2	Uh	119	THR
2	Uh	146	VAL
2	Uh	161	VAL
2	Uh	162	ILE
2	Uh	163	VAL

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Mol	Chain	Res	Type
2	Eh	174	ILE
2	Eh	217	THR
2	Eh	220	LEU
1	Ei	74	ILE
1	Ei	87	THR
1	Ei	97	VAL
1	Ei	109	VAL
1	Ei	119	LEU
2	Ej	40	ASN
2	Ej	119	THR
2	Ej	146	VAL
2	Ej	161	VAL
2	Ej	163	VAL
2	Ej	174	ILE
2	Ej	217	THR
1	Ek	74	ILE
1	Ek	87	THR
1	Ek	97	VAL
1	Ek	109	VAL
1	Ek	119	LEU
2	El	40	ASN
2	El	119	THR
2	El	161	VAL
2	El	163	VAL
2	El	174	ILE
2	El	217	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	83	GLN
2	Ab	40	ASN
2	Ab	97	ASN
2	Ab	171	HIS
1	Ac	37	ASN
2	Ad	40	ASN
2	Ad	97	ASN
2	Ad	105	HIS
2	Af	40	ASN
2	Af	105	HIS
2	Ah	40	ASN
2	Ah	105	HIS

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Mol	Chain	Res	Type
1	Ai	83	GLN
2	Aj	40	ASN
2	Aj	87	GLN
2	Aj	97	ASN
2	Aj	105	HIS
2	Al	40	ASN
2	Al	97	ASN
2	An	40	ASN
2	An	97	ASN
2	An	105	HIS
1	Ao	37	ASN
2	Ap	40	ASN
2	Ap	97	ASN
2	Ap	105	HIS
2	Ap	139	ASN
1	Aq	83	GLN
2	Ar	40	ASN
2	Ar	97	ASN
2	Ar	105	HIS
2	Ar	124	GLN
1	As	37	ASN
2	At	40	ASN
2	At	87	GLN
2	At	97	ASN
2	At	105	HIS
1	Au	37	ASN
1	Au	83	GLN
2	Av	40	ASN
2	Av	97	ASN
2	Av	105	HIS
2	Av	124	GLN
1	Aw	83	GLN
2	Ax	40	ASN
2	Ax	97	ASN
2	Ax	105	HIS
2	Ax	124	GLN
1	Ay	83	GLN
2	Az	40	ASN
2	Az	87	GLN
2	Az	97	ASN
1	Ba	83	GLN
2	Bb	40	ASN

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Mol	Chain	Res	Type
2	Bb	97	ASN
2	Bb	105	HIS
2	Bd	40	ASN
2	Bd	97	ASN
2	Bd	105	HIS
2	Bf	40	ASN
2	Bf	97	ASN
2	Bf	105	HIS
2	Bf	108	GLN
2	Bf	124	GLN
2	Bf	180	GLN
1	Bg	37	ASN
1	Bg	83	GLN
2	Bh	40	ASN
2	Bh	97	ASN
2	Bh	180	GLN
1	Bi	37	ASN
2	Bj	40	ASN
1	Bk	83	GLN
2	Bl	40	ASN
2	Bl	124	GLN
2	Bl	180	GLN
1	Bm	83	GLN
2	Bn	40	ASN
2	Bn	97	ASN
2	Bn	124	GLN
2	Bp	40	ASN
2	Bp	105	HIS
1	Bq	37	ASN
1	Bq	83	GLN
2	Br	40	ASN
2	Br	97	ASN
2	Br	105	HIS
2	Br	108	GLN
2	Bt	40	ASN
2	Bt	97	ASN
2	Bt	105	HIS
2	Bt	108	GLN
2	Bv	40	ASN
2	Bv	97	ASN
2	Bv	105	HIS
2	Bv	124	GLN

Continued on next page...

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Mol	Chain	Res	Type
2	Bx	40	ASN
2	Bx	97	ASN
2	Bx	105	HIS
1	By	37	ASN
1	By	83	GLN
2	Bz	40	ASN
2	Bz	97	ASN
2	Bz	105	HIS
1	Ca	37	ASN
1	Ca	83	GLN
2	Cb	40	ASN
2	Cb	97	ASN
2	Cb	105	HIS
2	Cb	124	GLN
1	Cc	83	GLN
2	Cd	40	ASN
2	Cd	97	ASN
2	Cd	105	HIS
1	Ce	37	ASN
1	Ce	83	GLN
2	Cf	40	ASN
2	Cf	97	ASN
2	Cf	105	HIS
1	Cg	83	GLN
2	Ch	40	ASN
2	Ch	97	ASN
2	Cj	40	ASN
2	Cj	97	ASN
2	Cj	105	HIS
2	Cl	40	ASN
2	Cl	97	ASN
2	Cl	105	HIS
2	Cl	124	GLN
1	Cm	83	GLN
2	Cn	40	ASN
2	Cn	105	HIS
1	Co	37	ASN
2	Cp	40	ASN
2	Cp	105	HIS
2	Cp	124	GLN
2	Cr	40	ASN
2	Cr	97	ASN

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Mol	Chain	Res	Type
2	Cr	105	HIS
2	Cr	124	GLN
2	Ct	40	ASN
2	Ct	97	ASN
2	Ct	105	HIS
2	Ct	124	GLN
1	Cu	37	ASN
1	Cu	83	GLN
2	Cv	40	ASN
2	Cv	97	ASN
2	Cv	124	GLN
2	Cv	139	ASN
1	Cw	83	GLN
2	Cx	40	ASN
2	Cx	97	ASN
2	Cx	105	HIS
2	Cx	124	GLN
2	Cz	40	ASN
2	Cz	97	ASN
2	Cz	105	HIS
2	Cz	124	GLN
1	Da	37	ASN
1	Da	83	GLN
2	Db	40	ASN
2	Db	97	ASN
2	Db	105	HIS
1	Dc	83	GLN
2	Dd	40	ASN
2	Dd	97	ASN
2	Dd	105	HIS
2	Dd	124	GLN
1	De	83	GLN
2	Df	40	ASN
2	Df	97	ASN
2	Df	105	HIS
2	Df	124	GLN
1	Dg	37	ASN
1	Dg	83	GLN
2	Dh	40	ASN
2	Dh	97	ASN
2	Dh	105	HIS
2	Dh	180	GLN

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Mol	Chain	Res	Type
1	Di	37	ASN
1	Di	83	GLN
2	Dj	40	ASN
2	Dj	97	ASN
2	Dj	124	GLN
1	Dk	37	ASN
1	Dk	83	GLN
2	Dl	40	ASN
2	Dl	97	ASN
2	Dl	105	HIS
2	Dl	124	GLN
2	Dn	40	ASN
2	Dn	97	ASN
2	Dn	105	HIS
2	Dn	180	GLN
1	Do	37	ASN
1	Do	83	GLN
2	Dp	40	ASN
2	Dp	97	ASN
1	Dq	83	GLN
2	Dr	40	ASN
2	Dr	97	ASN
2	Dr	180	GLN
1	Ds	83	GLN
2	Dt	40	ASN
2	Dt	97	ASN
2	Dt	180	GLN
1	Du	83	GLN
2	Dv	40	ASN
2	Dv	97	ASN
2	Dx	40	ASN
1	Dy	83	GLN
2	Dz	40	ASN
2	Dz	97	ASN
2	Dz	124	GLN
1	Ea	37	ASN
2	Eb	40	ASN
2	Eb	97	ASN
2	Eb	105	HIS
2	Eb	108	GLN
2	Eb	124	GLN
2	Eb	180	GLN

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Mol	Chain	Res	Type
1	Ec	83	GLN
2	Ed	40	ASN
2	Ed	97	ASN
1	Ee	37	ASN
1	Ee	83	GLN
2	Ef	40	ASN
2	Ef	97	ASN
2	Ef	105	HIS
2	Ef	180	GLN
1	Eg	83	GLN
2	Uh	40	ASN
2	Uh	97	ASN
2	Uh	124	GLN
2	Uh	180	GLN
1	Ei	83	GLN
2	Ej	40	ASN
1	Ek	83	GLN
2	El	40	ASN
2	El	97	ASN
2	El	105	HIS
2	El	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

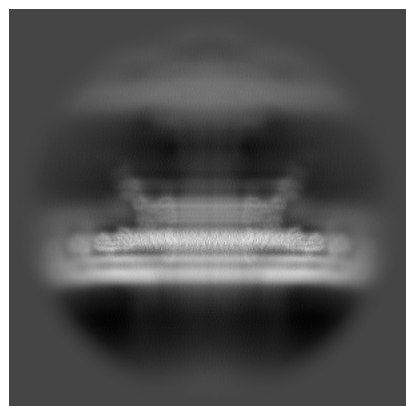
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72833. These allow visual inspection of the internal detail of the map and identification of artifacts.

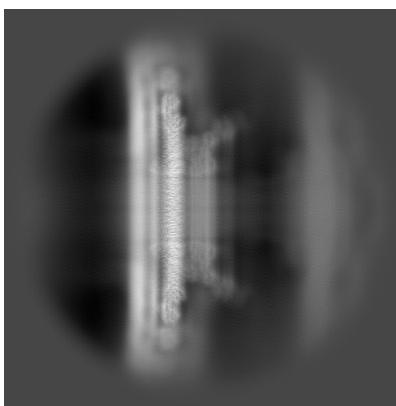
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

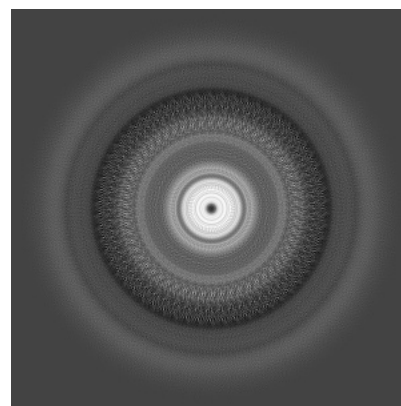
6.1.1 Primary map



X

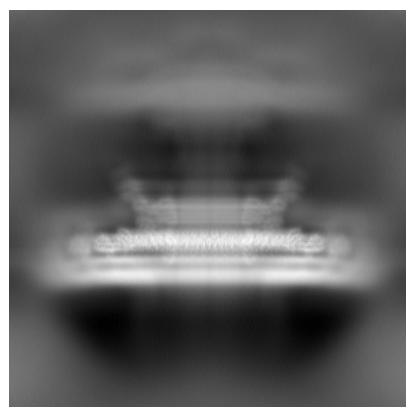


Y

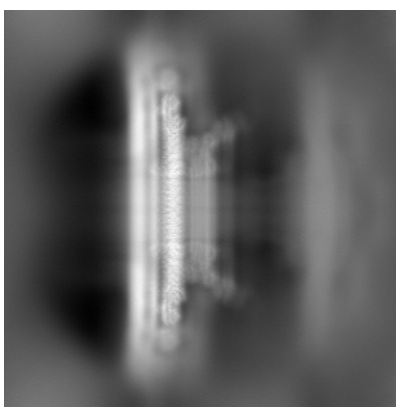


Z

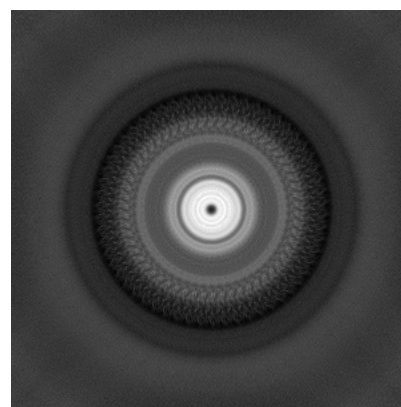
6.1.2 Raw map



X



Y

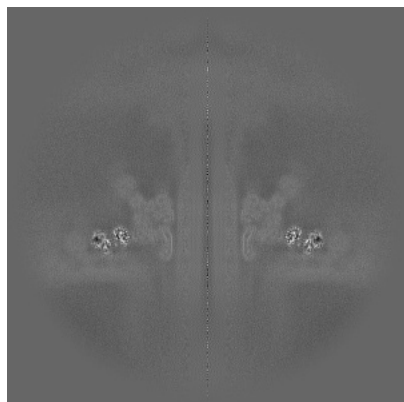


Z

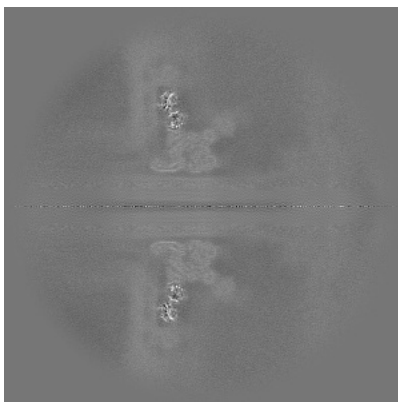
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

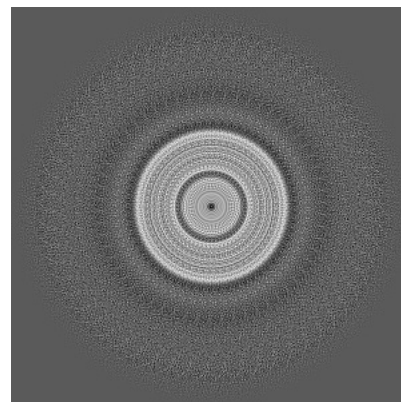
6.2.1 Primary map



X Index: 256

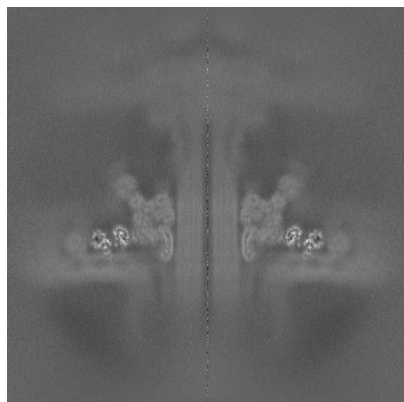


Y Index: 256

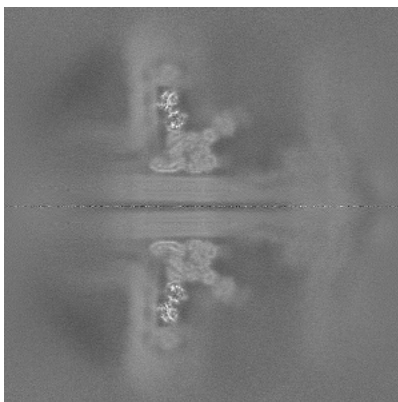


Z Index: 256

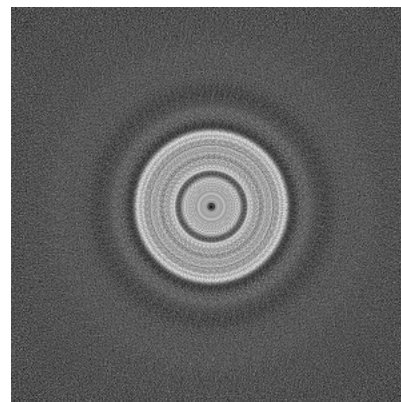
6.2.2 Raw map



X Index: 256



Y Index: 256

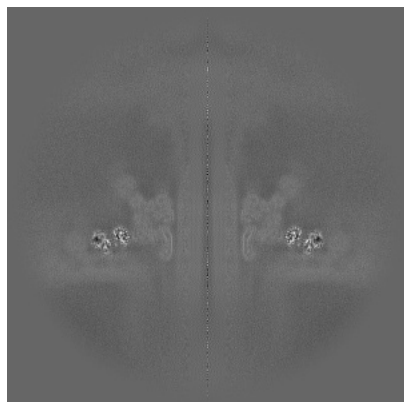


Z Index: 256

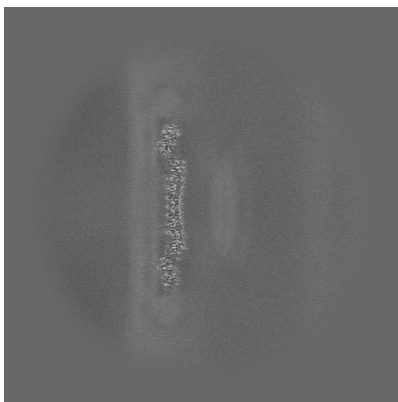
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

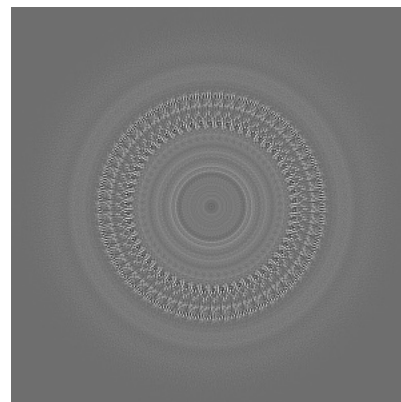
6.3.1 Primary map



X Index: 256

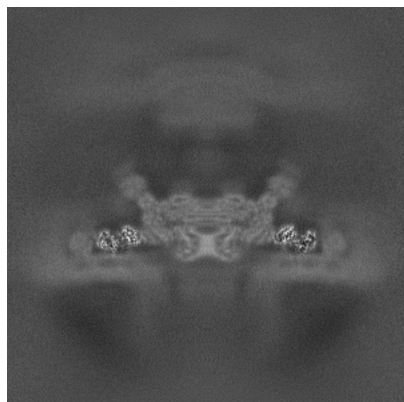


Y Index: 152

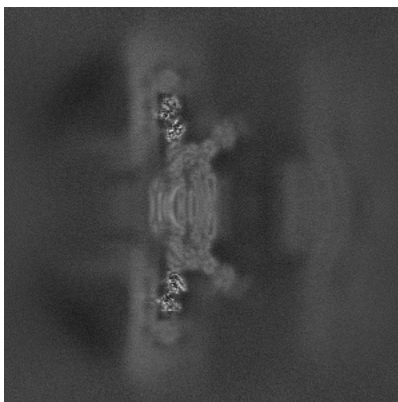


Z Index: 214

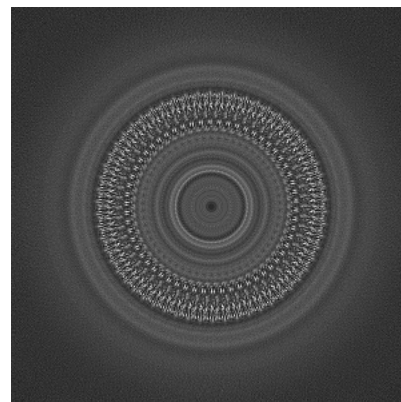
6.3.2 Raw map



X Index: 210



Y Index: 205

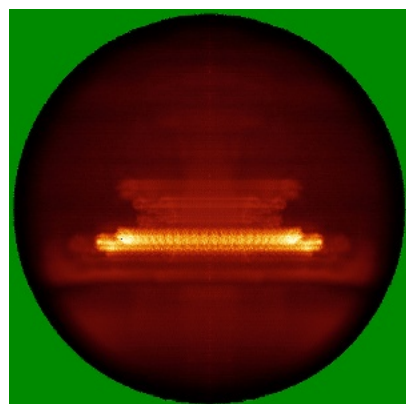


Z Index: 212

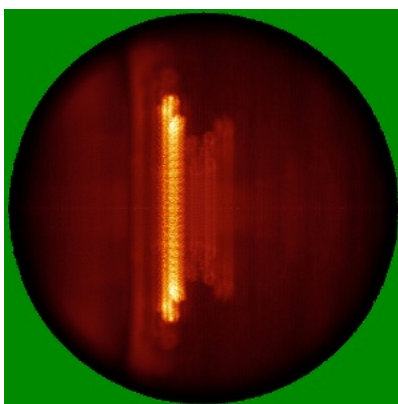
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

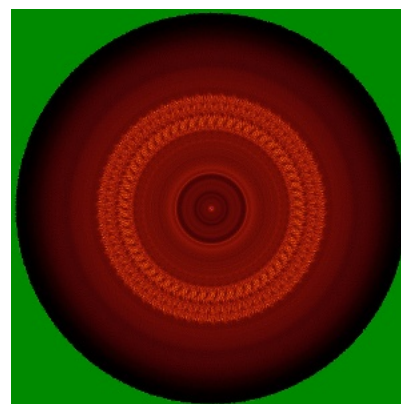
6.4.1 Primary map



X

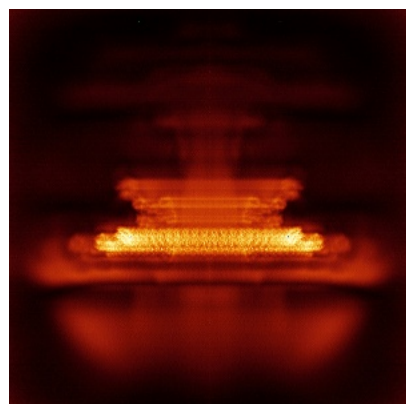


Y

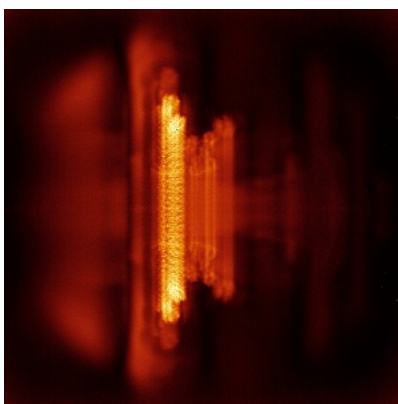


Z

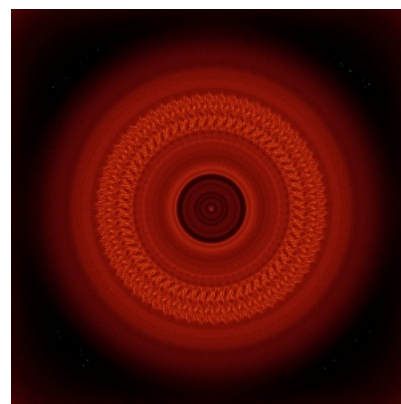
6.4.2 Raw map



X



Y



Z

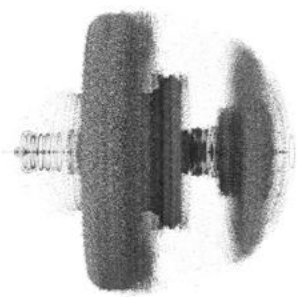
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

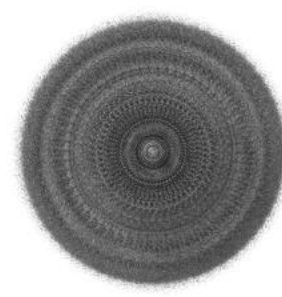
6.5.1 Primary map



X



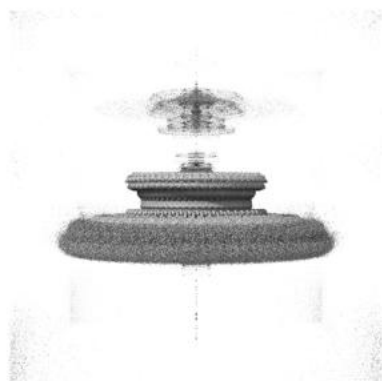
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

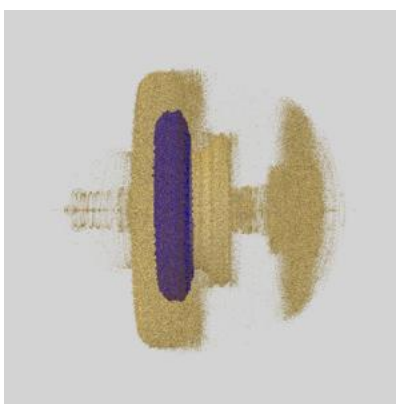
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

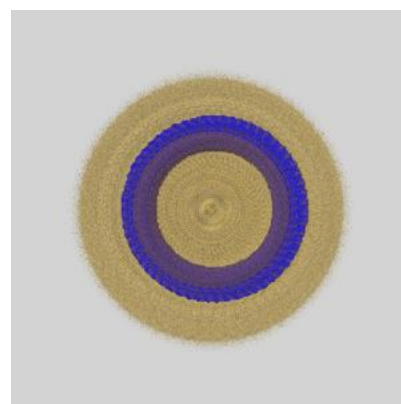
6.6.1 emd_72833_msk_1.map [i](#)



X



Y

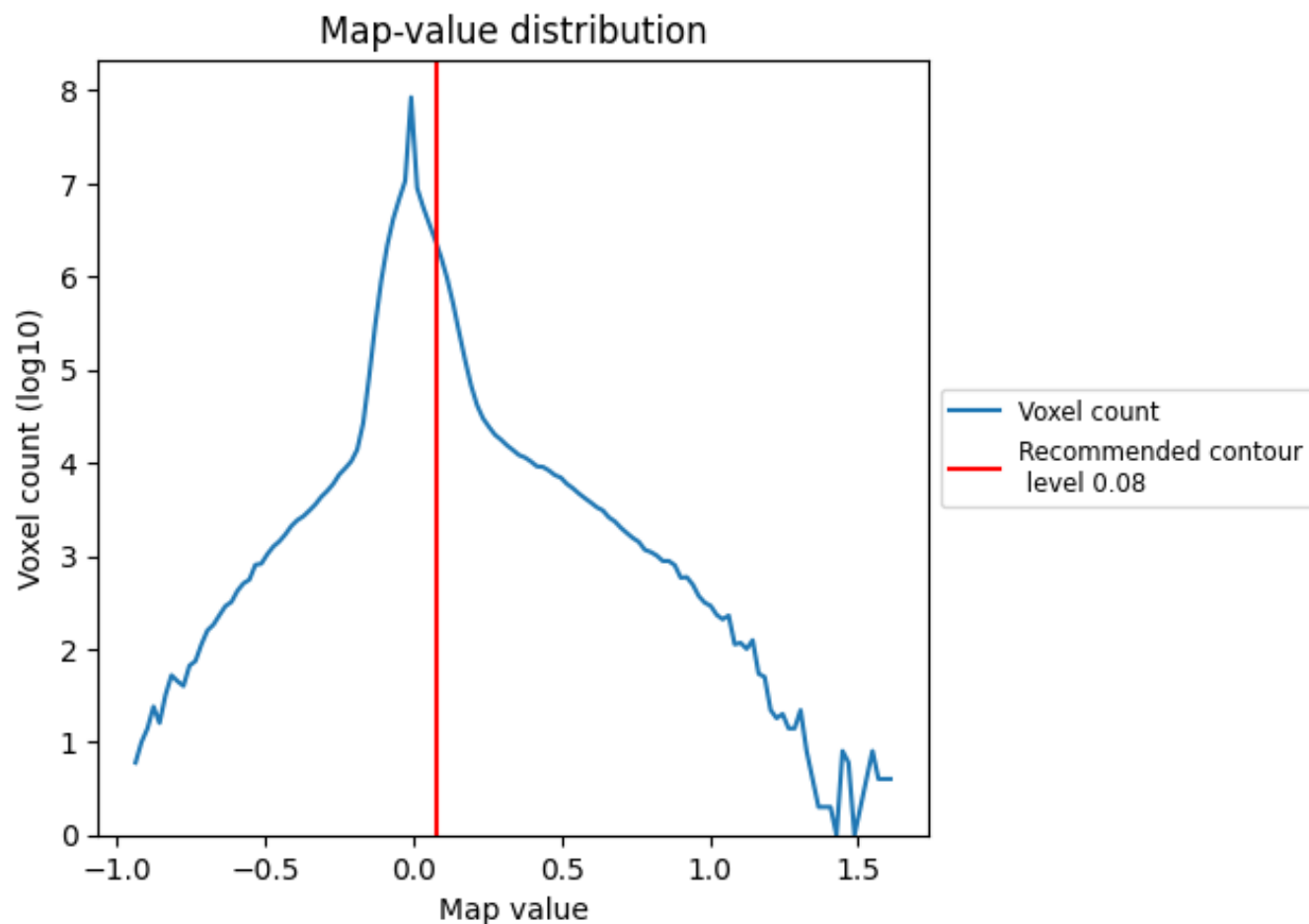


Z

7 Map analysis [i](#)

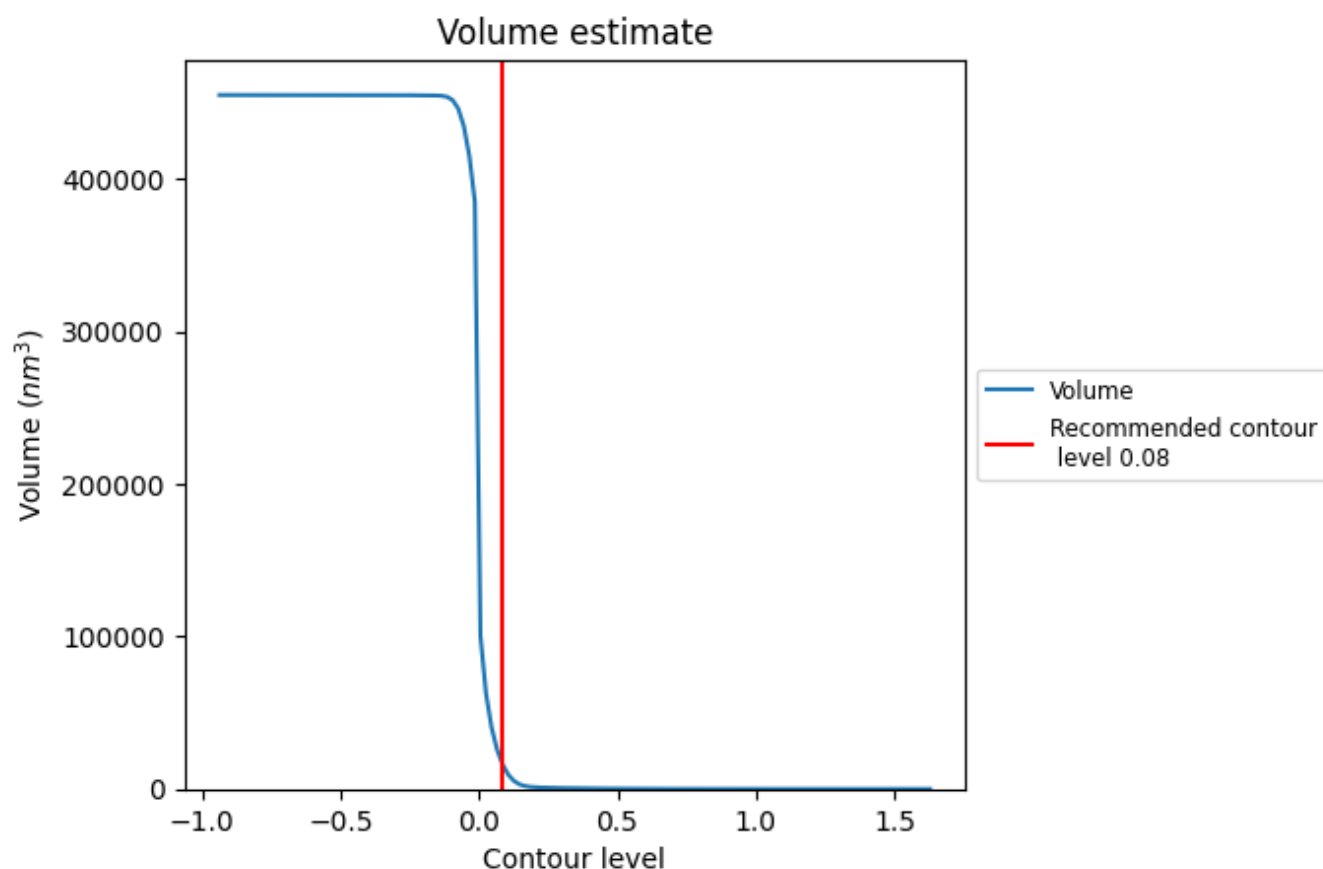
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

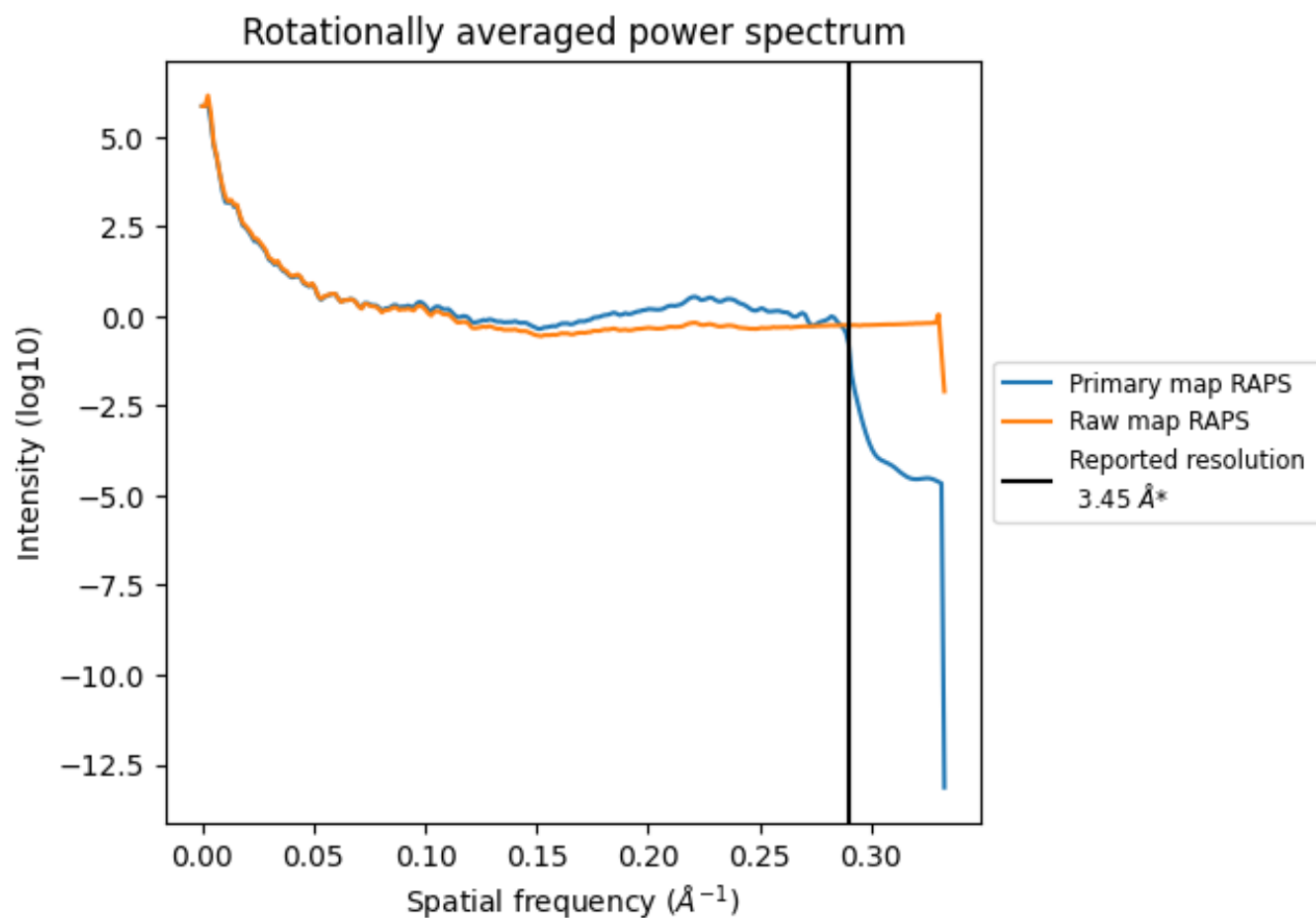
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18540 nm^3 ; this corresponds to an approximate mass of 16747 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

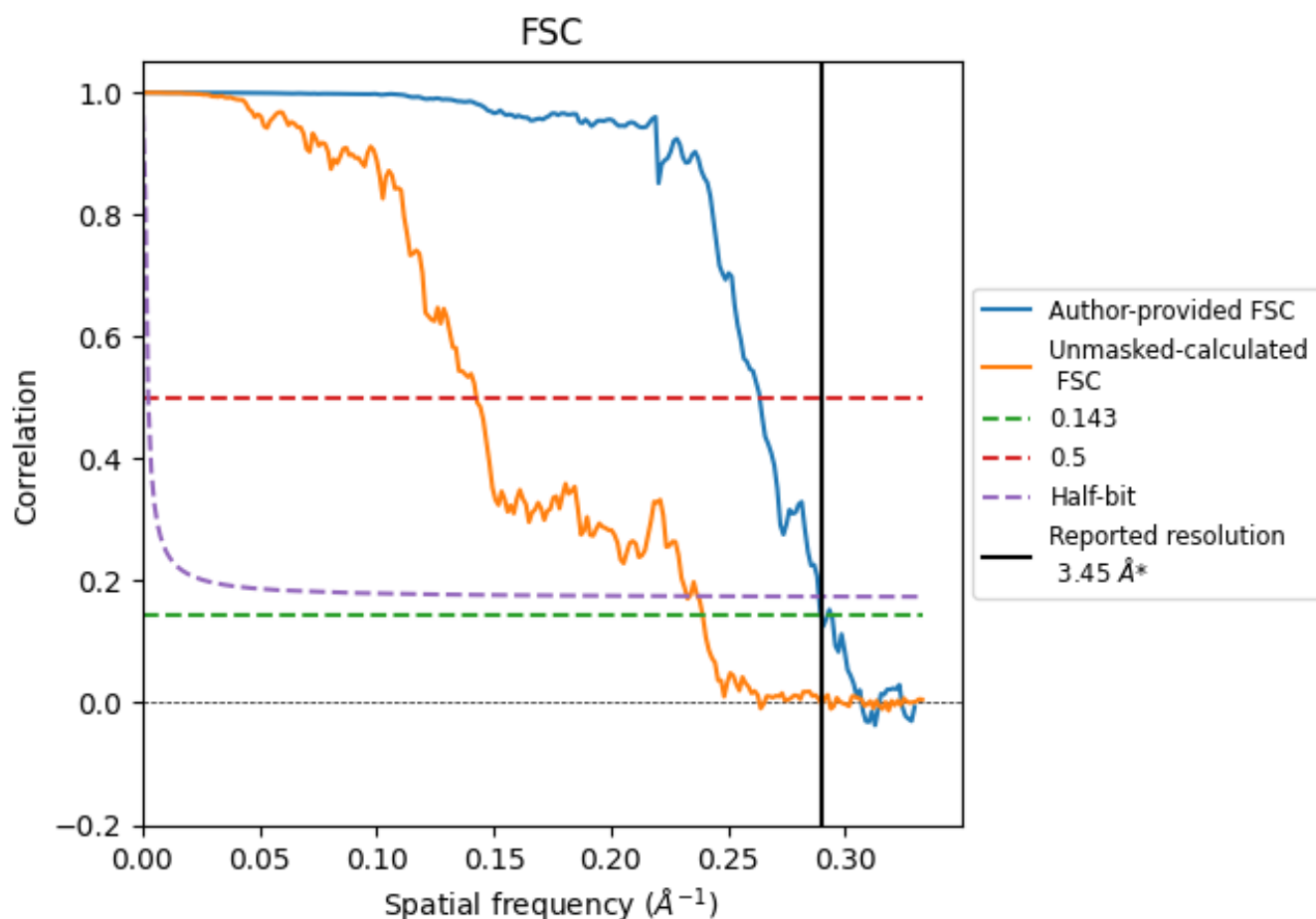


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.45	3.79	3.46
Unmasked-calculated*	4.18	7.01	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.45 by more than 10 %

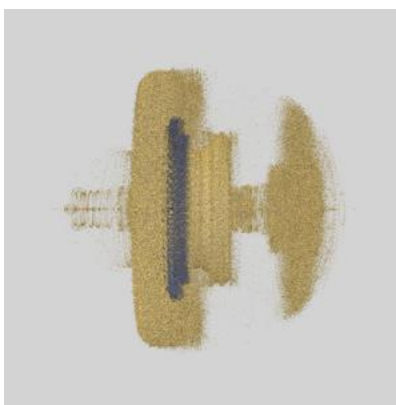
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72833 and PDB model 9YDS. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



X



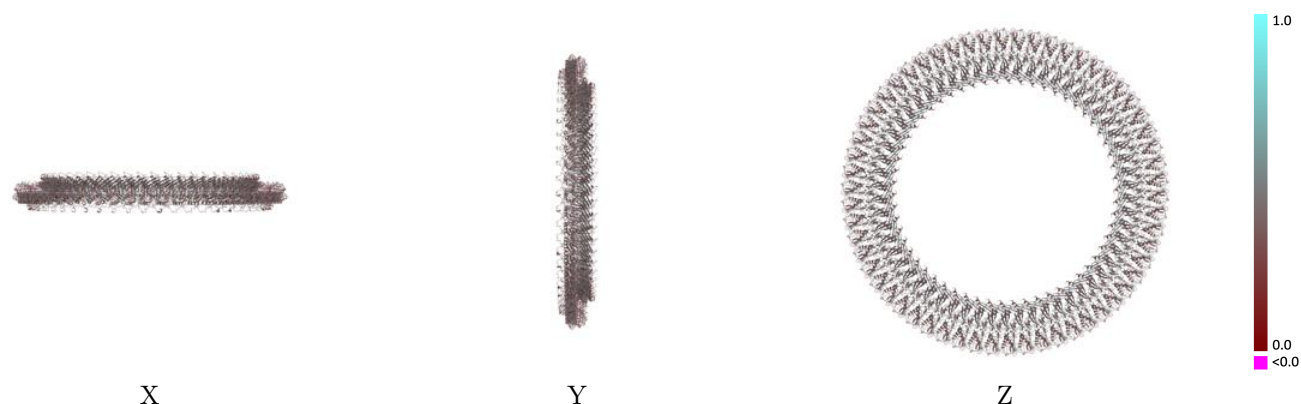
Y



Z

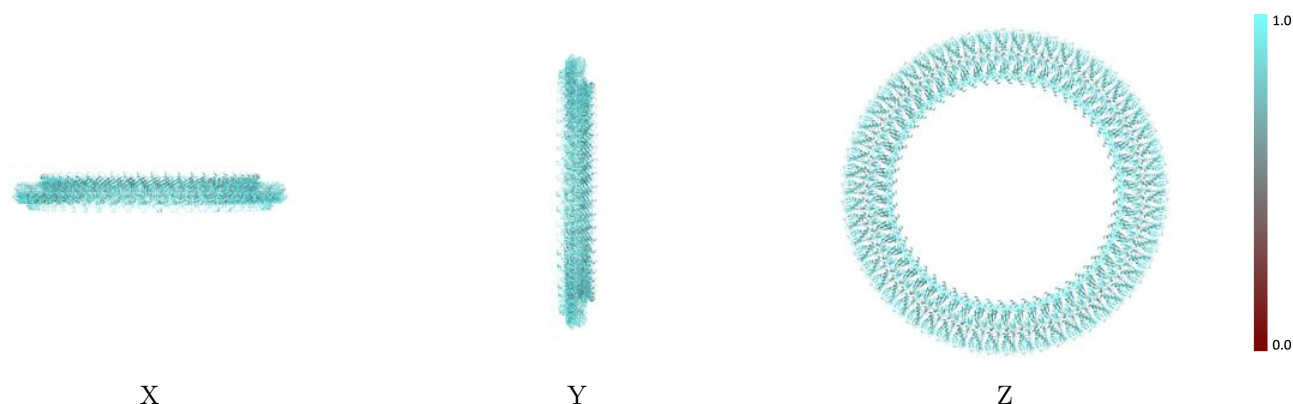
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



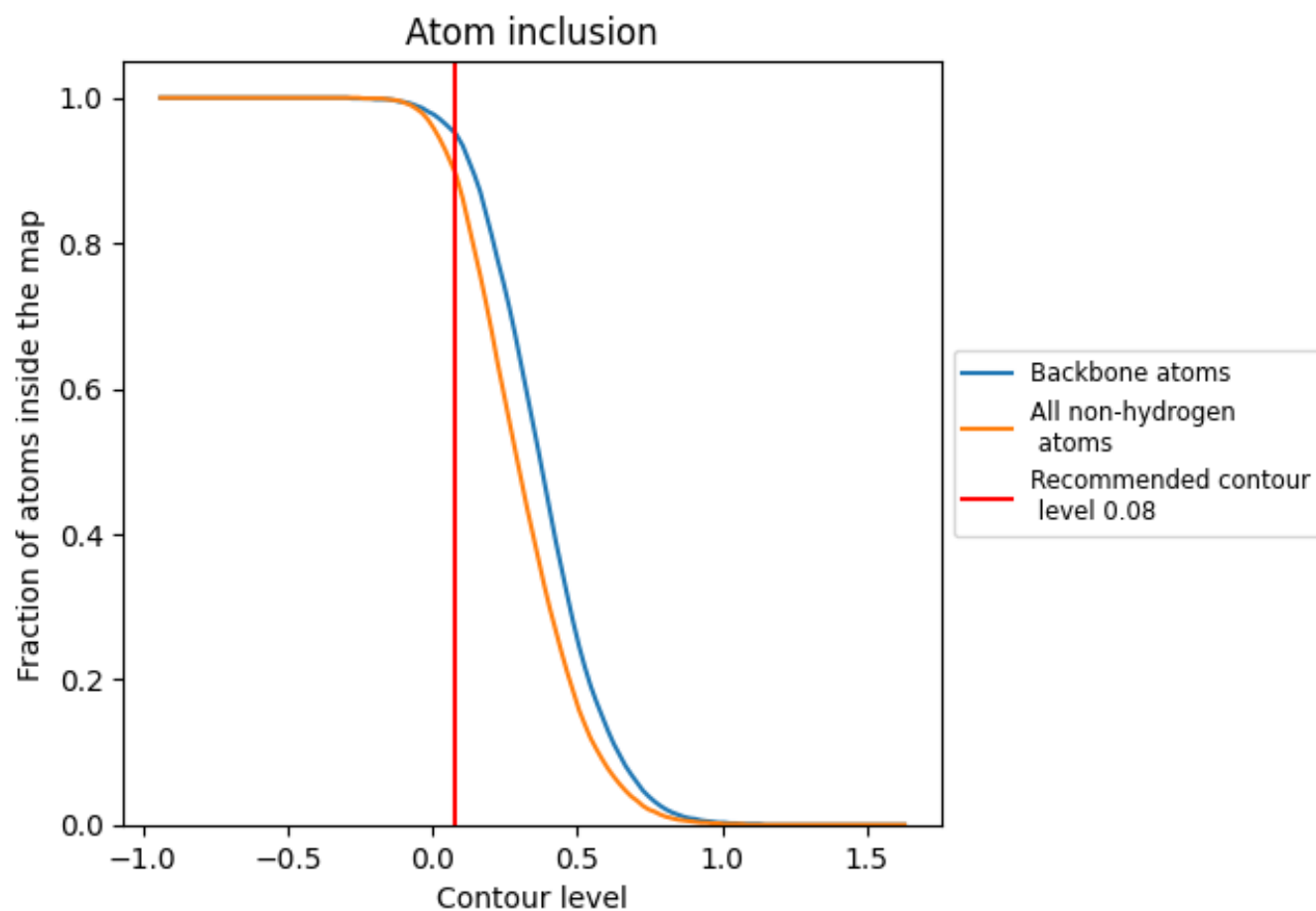
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.3880
Aa	 0.9040	 0.4160
Ab	 0.8900	 0.3710
Ac	 0.9140	 0.4120
Ad	 0.8910	 0.3700
Ae	 0.9070	 0.4140
Af	 0.8850	 0.3710
Ag	 0.9060	 0.4120
Ah	 0.8910	 0.3700
Ai	 0.9020	 0.4090
Aj	 0.8880	 0.3720
Ak	 0.9090	 0.4140
Al	 0.8880	 0.3720
Am	 0.9110	 0.4110
An	 0.8880	 0.3730
Ao	 0.9070	 0.4130
Ap	 0.8840	 0.3730
Aq	 0.9020	 0.4110
Ar	 0.8840	 0.3720
As	 0.9090	 0.4110
At	 0.8860	 0.3740
Au	 0.9110	 0.4130
Av	 0.8970	 0.3740
Aw	 0.9010	 0.4150
Ax	 0.8910	 0.3730
Ay	 0.9080	 0.4140
Az	 0.8880	 0.3740
Ba	 0.9060	 0.4120
Bb	 0.8950	 0.3800
Bc	 0.9010	 0.4100
Bd	 0.8950	 0.3730
Be	 0.9030	 0.4120
Bf	 0.8920	 0.3750
Bg	 0.9080	 0.4140
Bh	 0.8910	 0.3750



















































































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Chain	Atom inclusion	Q-score
Bi	 0.9090	 0.4120
Bj	 0.8920	 0.3720
Bk	 0.9080	 0.4160
Bl	 0.8890	 0.3750
Bm	 0.9130	 0.4140
Bn	 0.8860	 0.3760
Bo	 0.9070	 0.4130
Bp	 0.8830	 0.3740
Bq	 0.9070	 0.4110
Br	 0.8970	 0.3760
Bs	 0.9080	 0.4150
Bt	 0.8920	 0.3740
Bu	 0.9040	 0.4130
Bv	 0.8950	 0.3750
Bw	 0.9170	 0.4120
Bx	 0.8890	 0.3780
By	 0.9040	 0.4080
Bz	 0.8880	 0.3740
Ca	 0.9040	 0.4110
Cb	 0.8890	 0.3720
Cc	 0.9040	 0.4130
Cd	 0.8930	 0.3760
Ce	 0.9060	 0.4050
Cf	 0.8910	 0.3730
Cg	 0.9090	 0.4190
Ch	 0.8880	 0.3750
Ci	 0.9090	 0.4120
Cj	 0.8920	 0.3740
Ck	 0.9060	 0.4160
Cl	 0.8880	 0.3740
Cm	 0.9110	 0.4120
Cn	 0.8890	 0.3720
Co	 0.9040	 0.4110
Cp	 0.8920	 0.3730
Cq	 0.9110	 0.4130
Cr	 0.8850	 0.3750
Cs	 0.9070	 0.4130
Ct	 0.8850	 0.3740
Cu	 0.9080	 0.4150
Cv	 0.8860	 0.3750
Cw	 0.9010	 0.4130
Cx	 0.8880	 0.3740

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Chain	Atom inclusion	Q-score
Cy	 0.9060	 0.4130
Cz	 0.8860	 0.3760
Da	 0.9070	 0.4120
Db	 0.8910	 0.3750
Dc	 0.9020	 0.4150
Dd	 0.8910	 0.3720
De	 0.9080	 0.4140
Df	 0.8880	 0.3740
Dg	 0.9070	 0.4120
Dh	 0.8930	 0.3780
Di	 0.9060	 0.4090
Dj	 0.8930	 0.3720
Dk	 0.9030	 0.4110
Dl	 0.8890	 0.3710
Dm	 0.9060	 0.4140
Dn	 0.8880	 0.3740
Do	 0.9070	 0.4130
Dp	 0.8880	 0.3740
Dq	 0.9070	 0.4150
Dr	 0.8900	 0.3740
Ds	 0.9080	 0.4150
Dt	 0.8870	 0.3760
Du	 0.9060	 0.4100
Dv	 0.8870	 0.3740
Dw	 0.9030	 0.4070
Dx	 0.8970	 0.3740
Dy	 0.9040	 0.4140
Dz	 0.8930	 0.3730
Ea	 0.9070	 0.4140
Eb	 0.8950	 0.3750
Ec	 0.9140	 0.4130
Ed	 0.8960	 0.3760
Ee	 0.9060	 0.4090
Ef	 0.8870	 0.3730
Eg	 0.9070	 0.4120
Eh	 0.8870	 0.3690
Ei	 0.9080	 0.4150
Ej	 0.8950	 0.3750
Ek	 0.9070	 0.4050
El	 0.8860	 0.3720