



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 11:19 pm BST

PDB ID : 9T5O / pdb_00009t5o
EMDB ID : EMD-55591
Title : Structure of heteromeric mouse LRRC8A/D Volume-Regulated Anion Channel
in complex with synthetic nanobody Sb1, Conformation 2
Authors : Lehmann, E.F.; Deneka, D.; Stierli, F.; Rutz, S.; Dutzler, R.
Deposited on : 2025-11-05
Resolution : 3.16 Å(reported)
Based on initial model : 7P5V

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:

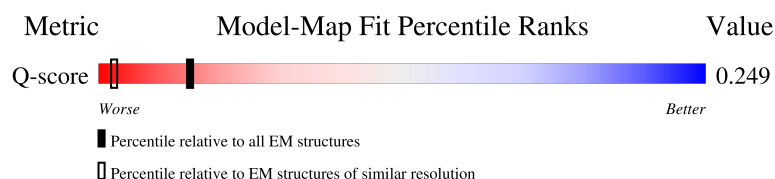
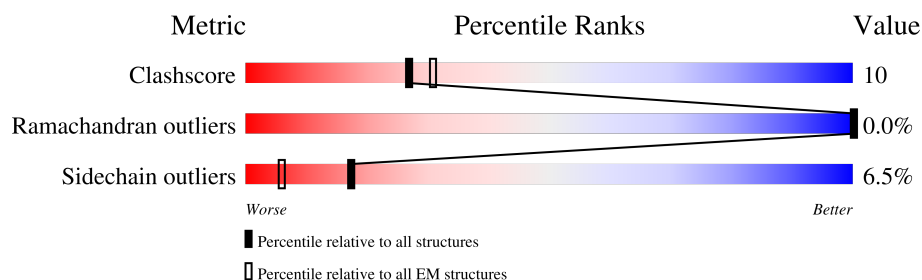
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.16 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	14474 (2.66 - 3.66)

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	A	818	 62% 23% • 12%
1	B	818	 58% 18% • 24%
1	C	818	 61% 24% • 12%
1	D	818	 65% 22% • 11%

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Mol	Chain	Length	Quality of chain
2	G	118	31%75%21%.
2	H	118	70%73%22%. .
2	I	118	.75%21%. .
2	J	118	.76%19%. .
3	E	924	.23%9%.67%
3	F	924	.22%10%.67%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31802 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 Volume-regulated anion channel subunit LRRC8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	718	Total	C	N	O	S	0	0
			5922	3853	997	1047	25		
1	B	624	Total	C	N	O	S	0	0
			5175	3381	860	912	22		
1	C	718	Total	C	N	O	S	0	0
			5922	3853	997	1047	25		
1	D	732	Total	C	N	O	S	0	0
			6030	3916	1018	1071	25		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q80WG5
A	1	SER	-	expression tag	UNP Q80WG5
A	811	ALA	-	expression tag	UNP Q80WG5
A	812	LEU	-	expression tag	UNP Q80WG5
A	813	GLU	-	expression tag	UNP Q80WG5
A	814	VAL	-	expression tag	UNP Q80WG5
A	815	LEU	-	expression tag	UNP Q80WG5
A	816	PHE	-	expression tag	UNP Q80WG5
A	817	GLN	-	expression tag	UNP Q80WG5
B	0	MET	-	initiating methionine	UNP Q80WG5
B	1	SER	-	expression tag	UNP Q80WG5
B	811	ALA	-	expression tag	UNP Q80WG5
B	812	LEU	-	expression tag	UNP Q80WG5
B	813	GLU	-	expression tag	UNP Q80WG5
B	814	VAL	-	expression tag	UNP Q80WG5
B	815	LEU	-	expression tag	UNP Q80WG5
B	816	PHE	-	expression tag	UNP Q80WG5
B	817	GLN	-	expression tag	UNP Q80WG5
C	0	MET	-	initiating methionine	UNP Q80WG5
C	1	SER	-	expression tag	UNP Q80WG5
C	811	ALA	-	expression tag	UNP Q80WG5
C	812	LEU	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	813	GLU	-	expression tag	UNP Q80WG5
C	814	VAL	-	expression tag	UNP Q80WG5
C	815	LEU	-	expression tag	UNP Q80WG5
C	816	PHE	-	expression tag	UNP Q80WG5
C	817	GLN	-	expression tag	UNP Q80WG5
D	0	MET	-	initiating methionine	UNP Q80WG5
D	1	SER	-	expression tag	UNP Q80WG5
D	811	ALA	-	expression tag	UNP Q80WG5
D	812	LEU	-	expression tag	UNP Q80WG5
D	813	GLU	-	expression tag	UNP Q80WG5
D	814	VAL	-	expression tag	UNP Q80WG5
D	815	LEU	-	expression tag	UNP Q80WG5
D	816	PHE	-	expression tag	UNP Q80WG5
D	817	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Synthetic Nanobody Sb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	114	Total	C	N	O	S	0	0
			903	575	152	172	4		
2	H	114	Total	C	N	O	S	0	0
			903	575	152	172	4		
2	I	114	Total	C	N	O	S	0	0
			903	575	152	172	4		
2	J	114	Total	C	N	O	S	0	0
			903	575	152	172	4		

- Molecule 3 is a protein called Volume-regulated anion channel subunit LRRC8D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	308	Total	C	N	O	S	0	0
			2567	1707	400	442	18		
3	F	309	Total	C	N	O	S	0	0
			2574	1712	401	443	18		

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP Q8BGR2
E	1	SER	-	expression tag	UNP Q8BGR2
E	60O	VAL	ILE	conflict	UNP Q8BGR2
E	62P	VAL	ALA	conflict	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	313	VAL	LEU	conflict	UNP Q8BGR2
E	347	ILE	THR	conflict	UNP Q8BGR2
E	859	ALA	-	expression tag	UNP Q8BGR2
E	860	LEU	-	expression tag	UNP Q8BGR2
E	861	GLU	-	expression tag	UNP Q8BGR2
E	862	VAL	-	expression tag	UNP Q8BGR2
E	863	LEU	-	expression tag	UNP Q8BGR2
E	864	PHE	-	expression tag	UNP Q8BGR2
E	865	GLN	-	expression tag	UNP Q8BGR2
E	866	GLY	-	expression tag	UNP Q8BGR2
E	867	PRO	-	expression tag	UNP Q8BGR2
E	868	GLN	-	expression tag	UNP Q8BGR2
E	869	GLY	-	expression tag	UNP Q8BGR2
E	870	THR	-	expression tag	UNP Q8BGR2
E	871	GLU	-	expression tag	UNP Q8BGR2
E	872	GLN	-	expression tag	UNP Q8BGR2
E	873	LYS	-	expression tag	UNP Q8BGR2
E	874	LEU	-	expression tag	UNP Q8BGR2
E	875	ILE	-	expression tag	UNP Q8BGR2
E	876	SER	-	expression tag	UNP Q8BGR2
E	877	GLU	-	expression tag	UNP Q8BGR2
E	878	GLU	-	expression tag	UNP Q8BGR2
E	879	ASP	-	expression tag	UNP Q8BGR2
E	880	LEU	-	expression tag	UNP Q8BGR2
E	881	ARG	-	expression tag	UNP Q8BGR2
E	882	GLY	-	expression tag	UNP Q8BGR2
E	883	ALA	-	expression tag	UNP Q8BGR2
E	884	SER	-	expression tag	UNP Q8BGR2
E	885	MET	-	expression tag	UNP Q8BGR2
E	886	ASP	-	expression tag	UNP Q8BGR2
E	887	GLU	-	expression tag	UNP Q8BGR2
E	888	LYS	-	expression tag	UNP Q8BGR2
E	889	THR	-	expression tag	UNP Q8BGR2
E	890	THR	-	expression tag	UNP Q8BGR2
E	891	GLY	-	expression tag	UNP Q8BGR2
E	892	TRP	-	expression tag	UNP Q8BGR2
E	893	ARG	-	expression tag	UNP Q8BGR2
E	894	GLY	-	expression tag	UNP Q8BGR2
E	895	GLY	-	expression tag	UNP Q8BGR2
E	896	HIS	-	expression tag	UNP Q8BGR2
E	897	VAL	-	expression tag	UNP Q8BGR2
E	898	VAL	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	899	GLU	-	expression tag	UNP Q8BGR2
E	900	GLY	-	expression tag	UNP Q8BGR2
E	901	LEU	-	expression tag	UNP Q8BGR2
E	902	ALA	-	expression tag	UNP Q8BGR2
E	903	GLY	-	expression tag	UNP Q8BGR2
E	904	GLU	-	expression tag	UNP Q8BGR2
E	905	LEU	-	expression tag	UNP Q8BGR2
E	906	GLU	-	expression tag	UNP Q8BGR2
E	907	GLN	-	expression tag	UNP Q8BGR2
E	908	LEU	-	expression tag	UNP Q8BGR2
E	909	ARG	-	expression tag	UNP Q8BGR2
E	910	ALA	-	expression tag	UNP Q8BGR2
E	911	ARG	-	expression tag	UNP Q8BGR2
E	912	LEU	-	expression tag	UNP Q8BGR2
E	913	GLU	-	expression tag	UNP Q8BGR2
E	914	HIS	-	expression tag	UNP Q8BGR2
E	915	HIS	-	expression tag	UNP Q8BGR2
E	916	PRO	-	expression tag	UNP Q8BGR2
E	917	GLN	-	expression tag	UNP Q8BGR2
E	918	GLY	-	expression tag	UNP Q8BGR2
E	919	GLN	-	expression tag	UNP Q8BGR2
E	920	ARG	-	expression tag	UNP Q8BGR2
E	921	GLU	-	expression tag	UNP Q8BGR2
E	922	PRO	-	expression tag	UNP Q8BGR2
F	0	MET	-	initiating methionine	UNP Q8BGR2
F	1	SER	-	expression tag	UNP Q8BGR2
F	61N	VAL	ILE	conflict	UNP Q8BGR2
F	63O	VAL	ALA	conflict	UNP Q8BGR2
F	313	VAL	LEU	conflict	UNP Q8BGR2
F	347	ILE	THR	conflict	UNP Q8BGR2
F	859	ALA	-	expression tag	UNP Q8BGR2
F	860	LEU	-	expression tag	UNP Q8BGR2
F	861	GLU	-	expression tag	UNP Q8BGR2
F	862	VAL	-	expression tag	UNP Q8BGR2
F	863	LEU	-	expression tag	UNP Q8BGR2
F	864	PHE	-	expression tag	UNP Q8BGR2
F	865	GLN	-	expression tag	UNP Q8BGR2
F	866	GLY	-	expression tag	UNP Q8BGR2
F	867	PRO	-	expression tag	UNP Q8BGR2
F	868	GLN	-	expression tag	UNP Q8BGR2
F	869	GLY	-	expression tag	UNP Q8BGR2
F	870	THR	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	871	GLU	-	expression tag	UNP Q8BGR2
F	872	GLN	-	expression tag	UNP Q8BGR2
F	873	LYS	-	expression tag	UNP Q8BGR2
F	874	LEU	-	expression tag	UNP Q8BGR2
F	875	ILE	-	expression tag	UNP Q8BGR2
F	876	SER	-	expression tag	UNP Q8BGR2
F	877	GLU	-	expression tag	UNP Q8BGR2
F	878	GLU	-	expression tag	UNP Q8BGR2
F	879	ASP	-	expression tag	UNP Q8BGR2
F	880	LEU	-	expression tag	UNP Q8BGR2
F	881	ARG	-	expression tag	UNP Q8BGR2
F	882	GLY	-	expression tag	UNP Q8BGR2
F	883	ALA	-	expression tag	UNP Q8BGR2
F	884	SER	-	expression tag	UNP Q8BGR2
F	885	MET	-	expression tag	UNP Q8BGR2
F	886	ASP	-	expression tag	UNP Q8BGR2
F	887	GLU	-	expression tag	UNP Q8BGR2
F	888	LYS	-	expression tag	UNP Q8BGR2
F	889	THR	-	expression tag	UNP Q8BGR2
F	890	THR	-	expression tag	UNP Q8BGR2
F	891	GLY	-	expression tag	UNP Q8BGR2
F	892	TRP	-	expression tag	UNP Q8BGR2
F	893	ARG	-	expression tag	UNP Q8BGR2
F	894	GLY	-	expression tag	UNP Q8BGR2
F	895	GLY	-	expression tag	UNP Q8BGR2
F	896	HIS	-	expression tag	UNP Q8BGR2
F	897	VAL	-	expression tag	UNP Q8BGR2
F	898	VAL	-	expression tag	UNP Q8BGR2
F	899	GLU	-	expression tag	UNP Q8BGR2
F	900	GLY	-	expression tag	UNP Q8BGR2
F	901	LEU	-	expression tag	UNP Q8BGR2
F	902	ALA	-	expression tag	UNP Q8BGR2
F	903	GLY	-	expression tag	UNP Q8BGR2
F	904	GLU	-	expression tag	UNP Q8BGR2
F	905	LEU	-	expression tag	UNP Q8BGR2
F	906	GLU	-	expression tag	UNP Q8BGR2
F	907	GLN	-	expression tag	UNP Q8BGR2
F	908	LEU	-	expression tag	UNP Q8BGR2
F	909	ARG	-	expression tag	UNP Q8BGR2
F	910	ALA	-	expression tag	UNP Q8BGR2
F	911	ARG	-	expression tag	UNP Q8BGR2
F	912	LEU	-	expression tag	UNP Q8BGR2

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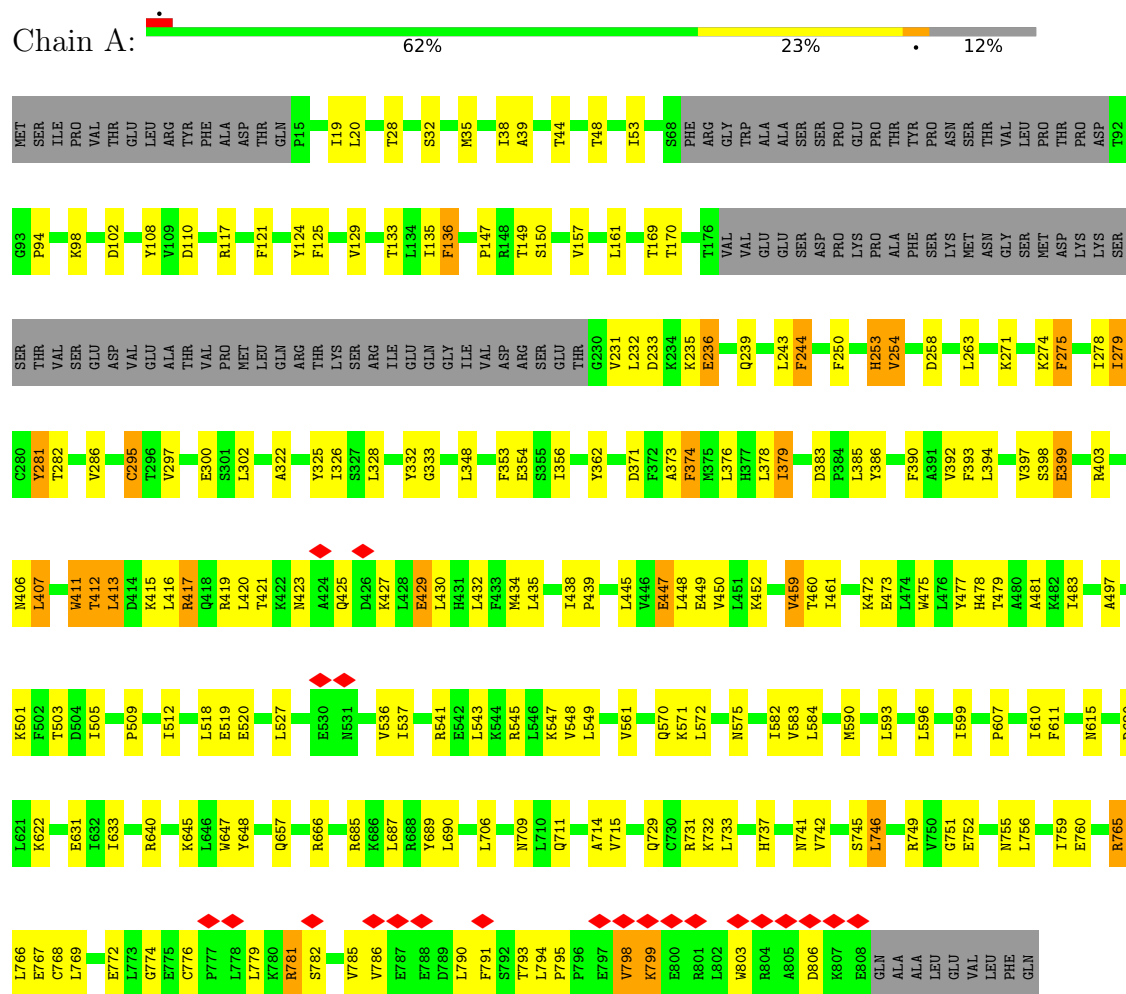
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Chain	Residue	Modelled	Actual	Comment	Reference
F	913	GLU	-	expression tag	UNP Q8BGR2
F	914	HIS	-	expression tag	UNP Q8BGR2
F	915	HIS	-	expression tag	UNP Q8BGR2
F	916	PRO	-	expression tag	UNP Q8BGR2
F	917	GLN	-	expression tag	UNP Q8BGR2
F	918	GLY	-	expression tag	UNP Q8BGR2
F	919	GLN	-	expression tag	UNP Q8BGR2
F	920	ARG	-	expression tag	UNP Q8BGR2
F	921	GLU	-	expression tag	UNP Q8BGR2
F	922	PRO	-	expression tag	UNP Q8BGR2

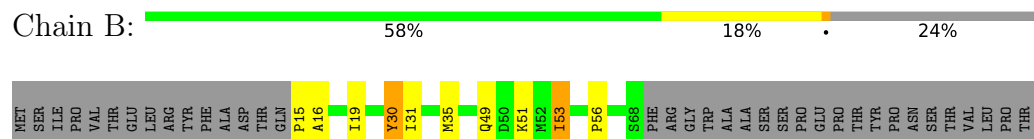
3 Residue-property plots

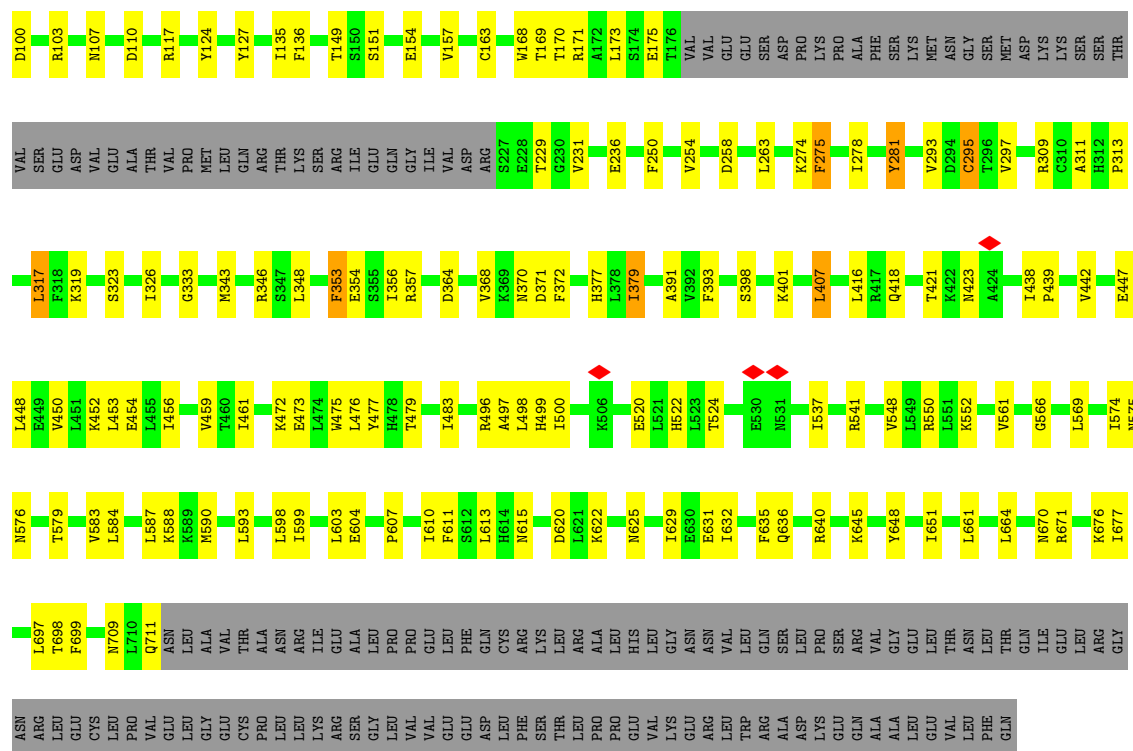
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Volume-regulated anion channel subunit LRRC8A



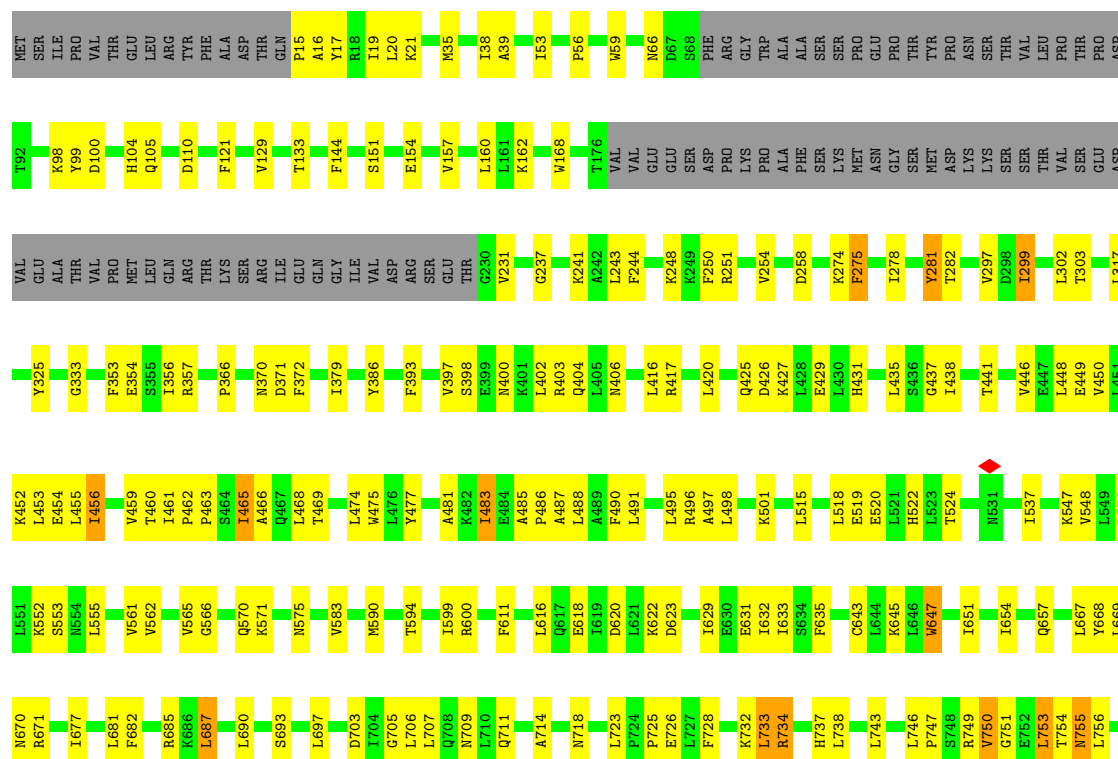
• Molecule 1: Volume-regulated anion channel subunit LRRC8A





• Molecule 1: Volume-regulated anion channel subunit LRRC8A

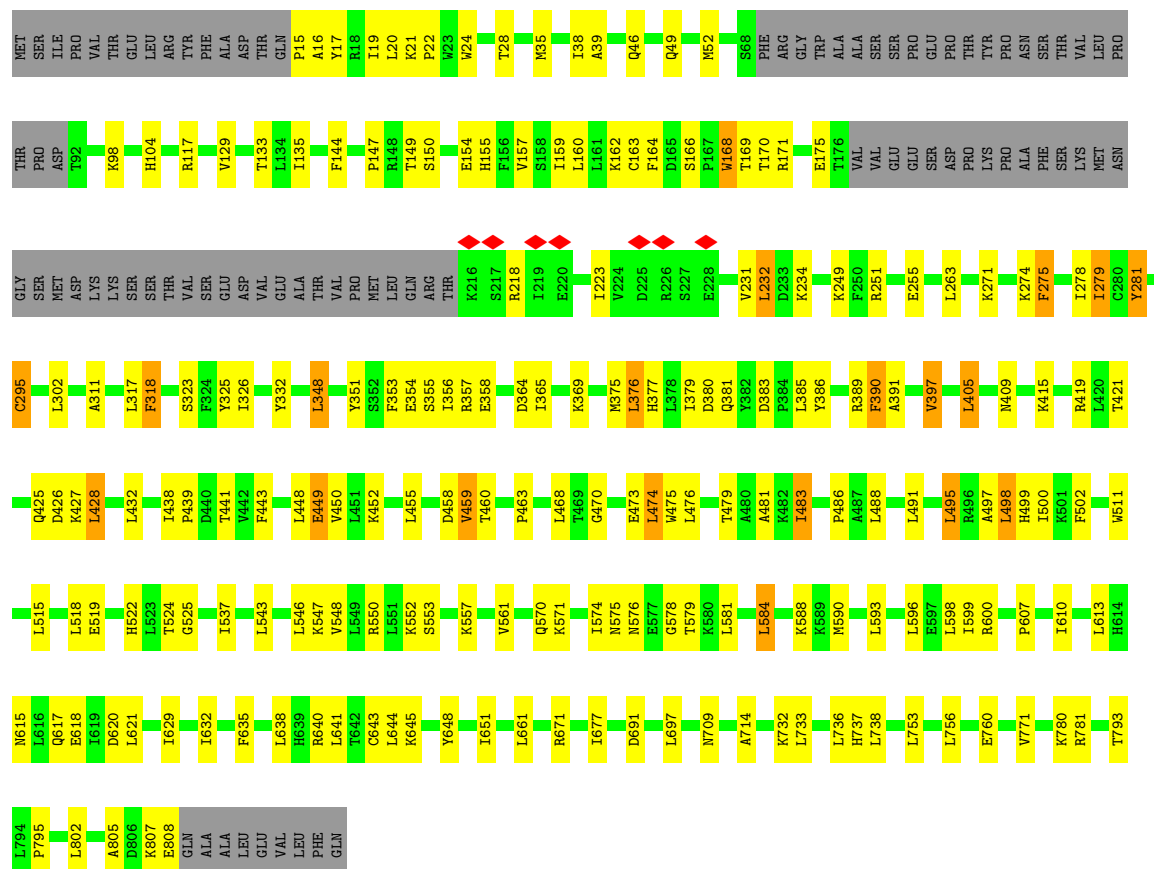
Chain C: 61% 24% 12%





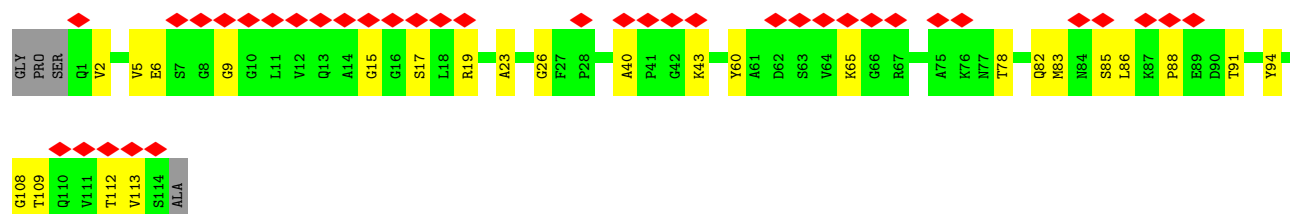
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain D: 65% 22% 11%



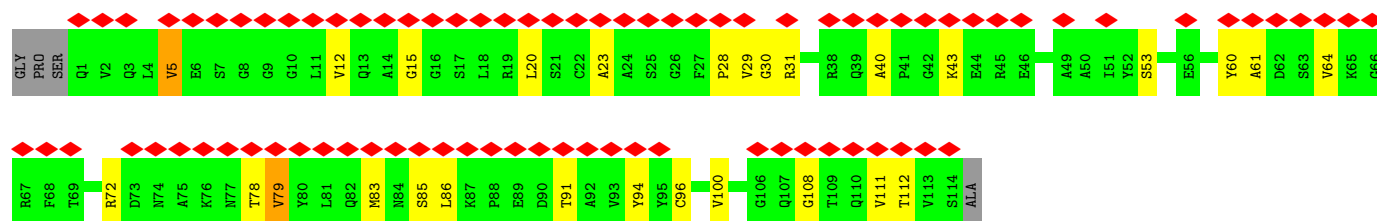
• Molecule 2: Synthetic Nanobody Sb1

Chain G: 31% 75% 21%

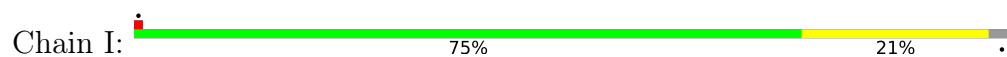


• Molecule 2: Synthetic Nanobody Sb1

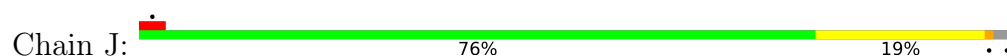
Chain H: 70% 73% 22%



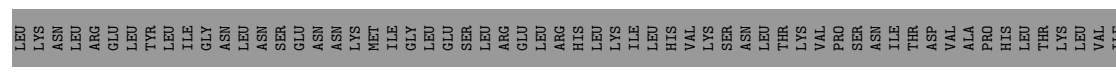
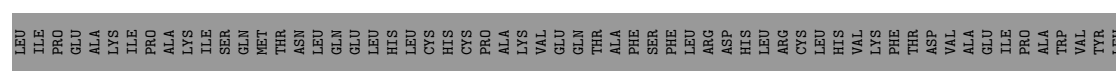
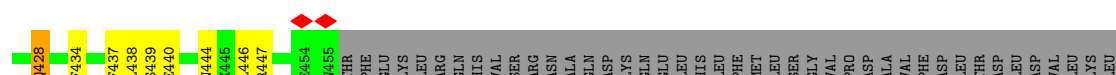
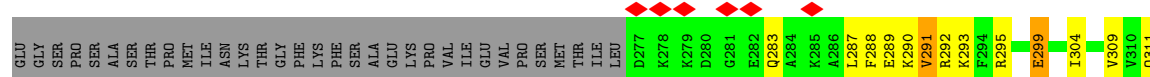
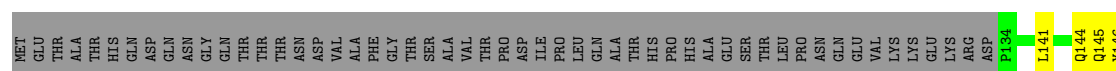
• Molecule 2: Synthetic Nanobody Sb1



• Molecule 2: Synthetic Nanobody Sb1



• Molecule 3: Volume-regulated anion channel subunit LRRC8D





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.03	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.416	Depositor
Minimum map value	-0.521	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0855	Depositor
Map size ($\text{\AA}$)	476.532, 476.532, 476.532	wwPDB
Map dimensions	366, 366, 366	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.302, 1.302, 1.302	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	A	0.13	0/6055	0.35	0/8207
1	B	0.11	0/5296	0.29	0/7177
1	C	0.13	0/6055	0.33	0/8207
1	D	0.12	0/6163	0.32	0/8352
2	G	0.08	0/927	0.25	0/1258
2	H	0.08	0/927	0.25	0/1258
2	I	0.08	0/927	0.25	0/1258
2	J	0.08	0/927	0.25	0/1258
3	E	0.11	0/2643	0.32	0/3579
3	F	0.12	0/2651	0.36	0/3591
All	All	0.12	0/32571	0.32	0/44145

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 [i](#)

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	A	5922	0	6081	128	0
1	B	5175	0	5298	88	0
1	C	5922	0	6081	140	0
1	D	6030	0	6184	127	0
2	G	903	0	852	16	0
2	H	903	0	852	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	903	0	852	16	0
2	J	903	0	852	14	0
3	E	2567	0	2564	56	0
3	F	2574	0	2571	55	0
All	All	31802	0	32187	635	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 10.

All (635) 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)
1:D:807:LYS:O	1:D:808:GLU:HG3	1.47	1.15
1:D:807:LYS:O	1:D:808:GLU:CG	2.13	0.96
2:I:94:TYR:O	2:I:108:GLY:HA2	1.76	0.85
2:G:17:SER:HA	2:G:83:MET:O	1.76	0.85
3:E:408:ASP:HB2	3:E:440:GLU:HG2	1.57	0.84
2:I:17:SER:HA	2:I:83:MET:O	1.78	0.84
1:B:522:HIS:HA	1:B:550:ARG:HB3	1.59	0.82
1:A:250:PHE:HA	1:A:253:HIS:HD2	1.45	0.82
2:G:94:TYR:O	2:G:108:GLY:HA2	1.80	0.81
2:H:94:TYR:O	2:H:108:GLY:HA2	1.82	0.80
1:A:459:VAL:HG23	1:A:481:ALA:HA	1.65	0.78
1:A:233:ASP:HB3	1:A:236:GLU:HB3	1.66	0.77
1:C:733:LEU:HB3	1:C:753:LEU:HD11	1.66	0.76
1:D:807:LYS:O	1:D:808:GLU:CB	2.34	0.76
2:J:94:TYR:O	2:J:108:GLY:HA2	1.85	0.74
1:C:251:ARG:HH22	1:C:366:PRO:HG2	1.53	0.74
1:A:714:ALA:HA	1:A:737:HIS:HB2	1.70	0.74
1:C:751:GLY:HA3	1:C:772:GLU:HB3	1.70	0.74
1:A:413:LEU:HG	1:A:417:ARG:HH12	1.52	0.73
3:E:397:PHE:HB3	3:E:409:ILE:HG21	1.70	0.73
3:E:149:ILE:HD11	3:E:347:ILE:HG13	1.71	0.73
1:B:499:HIS:HA	1:B:522:HIS:HB2	1.71	0.73
1:C:258:ASP:H	1:C:371:ASP:HB2	1.53	0.72
3:E:183:TRP:HB2	3:E:311:GLN:HE22	1.52	0.72
1:B:615:ASN:HA	1:B:640:ARG:HE	1.53	0.72
1:C:711:GLN:HE21	1:C:732:LYS:HB2	1.54	0.72
1:D:218:ARG:HG3	1:D:223:ILE:HD12	1.73	0.71
1:D:522:HIS:HA	1:D:550:ARG:HB3	1.73	0.71
1:D:463:PRO:HB3	1:D:486:PRO:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:PHE:HZ	1:A:631:GLU:HB3	1.56	0.70
2:H:20:LEU:HD11	2:H:83:MET:HE2	1.73	0.70
3:F:17:TYR:HB3	3:F:21:LYS:HE3	1.74	0.69
1:B:520:GLU:HA	1:B:548:VAL:HB	1.74	0.69
1:A:477:TYR:HA	1:A:501:LYS:HB3	1.74	0.68
1:C:515:LEU:HD13	1:C:518:LEU:HD13	1.75	0.68
1:C:429:GLU:HA	1:C:450:VAL:HB	1.74	0.68
1:D:781:ARG:HB2	1:D:802:LEU:HB3	1.74	0.68
3:F:397:PHE:HB3	3:F:400:VAL:HB	1.75	0.68
1:C:495:LEU:HD21	1:C:498:LEU:HD13	1.75	0.68
3:F:412:VAL:HB	3:F:416:PHE:HB3	1.76	0.68
1:D:278:ILE:HA	1:D:281:TYR:HD2	1.59	0.68
1:C:522:HIS:HA	1:C:550:ARG:HB3	1.76	0.67
1:B:258:ASP:H	1:B:371:ASP:HB2	1.58	0.67
1:A:411:TRP:HA	1:A:415:LYS:HD3	1.75	0.67
1:C:750:VAL:O	1:C:753:LEU:HB2	1.94	0.66
1:B:416:LEU:HD13	1:B:442:VAL:HA	1.78	0.65
2:J:20:LEU:HD11	2:J:83:MET:HE2	1.76	0.65
1:C:237:GLY:HA3	1:C:406:ASN:HD21	1.61	0.65
1:A:108:TYR:HA	1:B:53:ILE:HD13	1.79	0.65
1:A:711:GLN:HE21	1:A:732:LYS:HD3	1.62	0.65
1:B:354:GLU:HA	1:B:357:ARG:HE	1.60	0.65
1:D:459:VAL:O	1:D:481:ALA:HA	1.97	0.65
1:C:753:LEU:HD12	1:C:756:LEU:HB2	1.80	0.64
1:A:497:ALA:HA	1:A:520:GLU:HB2	1.78	0.64
1:C:354:GLU:HA	1:C:357:ARG:HG2	1.80	0.64
1:C:709:ASN:HA	1:C:732:LYS:HD2	1.79	0.64
1:D:632:ILE:O	1:D:635:PHE:HB2	1.98	0.64
3:E:350:GLU:HG3	3:E:351:VAL:HG23	1.79	0.63
1:A:751:GLY:HA3	1:A:772:GLU:HB3	1.80	0.63
1:B:632:ILE:O	1:B:635:PHE:HB2	1.98	0.63
1:C:711:GLN:HA	1:C:733:LEU:HA	1.81	0.63
1:C:781:ARG:H	1:C:806:ASP:HB2	1.63	0.63
3:F:400:VAL:HG13	3:F:432:LYS:HD3	1.79	0.63
1:A:794:LEU:HB2	1:A:799:LYS:HD3	1.79	0.63
1:D:498:LEU:HD23	1:D:500:ILE:HD11	1.80	0.63
1:D:302:LEU:HB3	3:E:55:LEU:HD23	1.80	0.63
3:F:192:LYS:HZ2	3:F:298:VAL:HG12	1.64	0.63
1:A:776:CYS:HB2	1:A:779:LEU:HB2	1.80	0.63
1:C:629:ILE:HD13	1:C:651:ILE:HD13	1.82	0.62
1:D:104:HIS:CE1	3:E:150:ASN:HD21	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:ILE:HD11	3:F:347:ILE:HG13	1.80	0.62
1:B:475:TRP:HA	1:B:499:HIS:HB2	1.82	0.61
1:C:459:VAL:HG23	1:C:481:ALA:HA	1.82	0.61
1:D:629:ILE:HD13	1:D:651:ILE:HD13	1.83	0.61
1:D:714:ALA:HA	1:D:737:HIS:HB2	1.83	0.61
1:D:511:TRP:HZ3	1:D:515:LEU:HD11	1.66	0.61
1:C:278:ILE:HA	1:C:281:TYR:HD2	1.65	0.61
1:B:438:ILE:HD11	1:B:453:LEU:HD11	1.81	0.61
1:A:278:ILE:HA	1:A:281:TYR:HD2	1.65	0.61
1:B:171:ARG:HH12	1:B:401:LYS:HE3	1.66	0.61
1:C:728:PHE:CD2	1:C:749:ARG:HB2	2.36	0.60
1:A:746:LEU:HB2	1:A:766:LEU:HD21	1.84	0.60
1:A:711:GLN:HA	1:A:733:LEU:HA	1.84	0.60
1:C:566:GLY:HA3	1:C:590:MET:HG2	1.84	0.60
1:B:278:ILE:HA	1:B:281:TYR:HD2	1.66	0.60
1:A:447:GLU:HG2	1:A:448:LEU:HD12	1.84	0.60
1:C:425:GLN:HB2	1:C:427:LYS:HD2	1.83	0.60
1:B:100:ASP:HB3	1:C:98:LYS:HE3	1.82	0.60
1:D:474:LEU:HD23	1:D:495:LEU:HD21	1.84	0.60
1:A:420:LEU:HD12	1:A:430:LEU:HD13	1.84	0.59
2:H:53:SER:HA	2:H:72:ARG:HH12	1.67	0.59
3:F:309:VAL:HG22	3:F:387:LEU:HD21	1.84	0.59
1:B:473:GLU:HA	1:B:497:ALA:HB3	1.84	0.59
1:B:620:ASP:HA	1:B:645:LYS:HB2	1.84	0.59
1:D:302:LEU:HD22	3:E:55:LEU:HB3	1.83	0.59
1:C:452:LYS:HG2	1:C:475:TRP:HB2	1.85	0.59
1:D:524:THR:HG23	1:D:552:LYS:HD3	1.84	0.59
1:A:407:LEU:HB3	1:A:439:PRO:HG3	1.85	0.59
1:B:461:ILE:HB	1:B:483:ILE:HG13	1.83	0.59
1:D:620:ASP:HA	1:D:645:LYS:HB2	1.85	0.59
1:D:677:ILE:HD11	1:D:697:LEU:HD13	1.85	0.58
2:I:23:ALA:HA	2:I:78:THR:HG22	1.86	0.58
1:A:53:ILE:HD13	3:F:147:VAL:HG23	1.86	0.58
1:D:255:GLU:HB2	1:D:369:LYS:HB2	1.84	0.58
3:F:294:PHE:HA	3:F:297:HIS:HB3	1.85	0.58
1:A:768:CYS:HA	1:A:790:LEU:HD11	1.86	0.58
3:E:32:ALA:HA	3:E:35:MET:HG2	1.85	0.58
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.86	0.58
1:A:250:PHE:O	1:A:254:VAL:HB	2.03	0.58
1:D:160:LEU:HD11	1:D:386:TYR:HB3	1.86	0.58
1:A:282:THR:O	1:A:286:VAL:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ARG:HH21	1:A:706:LEU:HD13	1.68	0.57
1:D:618:GLU:HG3	1:D:643:CYS:HB3	1.86	0.57
1:A:509:PRO:HB2	1:A:512:ILE:HG23	1.86	0.57
3:E:356:HIS:HB3	3:E:359:ALA:HB2	1.86	0.57
3:F:42:ALA:HB3	3:F:166:PRO:HB3	1.87	0.57
1:B:407:LEU:HD11	1:B:439:PRO:HG3	1.85	0.57
1:C:714:ALA:HA	1:C:737:HIS:HB2	1.85	0.57
3:E:144:GLN:HG3	3:F:146:TYR:CG	2.40	0.57
1:B:629:ILE:HD13	1:B:651:ILE:HD13	1.87	0.56
1:C:772:GLU:HA	1:C:775:GLU:HG2	1.86	0.56
3:F:279:LYS:HA	3:F:282:GLU:HG2	1.88	0.56
1:C:524:THR:HG23	1:C:552:LYS:HD3	1.88	0.56
1:B:611:PHE:HZ	1:B:631:GLU:HB3	1.71	0.56
1:C:501:LYS:HG3	1:C:524:THR:HB	1.87	0.56
2:J:40:ALA:HB3	2:J:43:LYS:HB3	1.88	0.56
1:C:456:ILE:HB	1:C:459:VAL:HG11	1.86	0.56
1:D:46:GLN:HB2	1:D:318:PHE:HZ	1.70	0.56
2:H:28:PRO:HG2	2:H:31:ARG:HB2	1.88	0.56
3:F:283:GLN:HE22	3:F:287:LEU:HD22	1.69	0.56
1:A:666:ARG:HG2	1:A:689:TYR:HB2	1.88	0.56
1:C:779:LEU:HG	1:C:802:LEU:HD11	1.88	0.56
1:D:21:LYS:HE2	1:D:144:PHE:HE2	1.70	0.56
1:C:105:GLN:HE22	1:C:303:THR:HG22	1.69	0.56
2:G:91:THR:HG23	2:G:112:THR:HA	1.88	0.56
1:A:250:PHE:HA	1:A:253:HIS:CD2	2.35	0.55
1:B:452:LYS:HG2	1:B:475:TRP:HB2	1.87	0.55
3:F:200:LEU:HA	3:F:203:CYS:HB2	1.88	0.55
1:A:420:LEU:HG	1:A:430:LEU:HB2	1.89	0.55
1:D:483:ILE:HG21	1:D:488:LEU:HD13	1.88	0.55
1:D:635:PHE:HB3	1:D:661:LEU:HD21	1.88	0.55
1:A:756:LEU:HD21	1:A:759:ILE:HB	1.87	0.55
2:H:40:ALA:HB3	2:H:43:LYS:HB3	1.87	0.55
1:C:491:LEU:HD22	1:C:495:LEU:HB2	1.87	0.55
1:A:411:TRP:HE3	1:A:415:LYS:HB3	1.72	0.55
1:D:164:PHE:CD1	1:D:389:ARG:HG3	2.41	0.55
2:H:12:VAL:HG11	2:H:86:LEU:HD22	1.88	0.55
2:H:83:MET:HE3	2:H:86:LEU:HD21	1.89	0.55
3:F:318:LYS:HG2	3:F:322:ILE:HG13	1.89	0.55
1:A:415:LYS:H	1:A:415:LYS:HD2	1.72	0.55
2:G:40:ALA:HB3	2:G:43:LYS:HB3	1.89	0.55
1:C:160:LEU:HD11	1:C:386:TYR:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:LEU:HD22	1:C:773:LEU:HD11	1.88	0.54
1:D:356:ILE:HG12	1:D:391:ALA:HB1	1.89	0.54
1:C:670:ASN:HD22	1:C:671:ARG:HG2	1.71	0.54
3:E:145:GLN:HE22	3:F:137:ARG:HB2	1.73	0.54
1:A:32:SER:HB2	1:A:332:TYR:HE2	1.71	0.54
1:A:620:ASP:HA	1:A:645:LYS:HB2	1.88	0.54
1:A:781:ARG:HG2	1:A:806:ASP:HB2	1.89	0.54
1:A:782:SER:HB2	1:A:806:ASP:OD1	2.07	0.54
1:A:459:VAL:HG21	1:A:479:THR:HG22	1.90	0.54
1:A:742:VAL:HA	1:A:765:ARG:HD3	1.90	0.54
1:B:541:ARG:HG3	1:B:561:VAL:HG23	1.90	0.54
1:B:524:THR:HG23	1:B:552:LYS:HD3	1.90	0.54
1:C:469:THR:HA	1:C:490:PHE:HZ	1.72	0.54
3:F:312:THR:HA	3:F:315:LYS:HE2	1.89	0.54
1:A:548:VAL:HG13	1:A:571:LYS:HD3	1.90	0.54
1:D:615:ASN:HA	1:D:640:ARG:HH21	1.73	0.54
2:I:98:VAL:HG12	2:I:104:TYR:HB2	1.89	0.54
1:A:374:PHE:CZ	1:A:378:LEU:HD11	2.43	0.54
1:D:166:SER:HB3	1:D:169:THR:HG23	1.90	0.54
2:I:94:TYR:O	2:I:108:GLY:CA	2.54	0.54
2:J:12:VAL:HG11	2:J:86:LEU:HD22	1.90	0.54
1:D:452:LYS:HG2	1:D:475:TRP:CG	2.42	0.54
3:E:390:ILE:HG13	3:E:391:PRO:HD2	1.89	0.54
2:I:91:THR:HG23	2:I:112:THR:HA	1.90	0.53
3:E:186:TYR:CG	3:E:187:PRO:HD2	2.43	0.53
1:A:769:LEU:HG	1:A:790:LEU:HG	1.90	0.53
1:C:620:ASP:HA	1:C:645:LYS:HB2	1.90	0.53
3:F:196:PHE:CE1	3:F:419:LEU:HB3	2.44	0.53
3:F:202:LYS:HA	3:F:205:GLU:HB2	1.90	0.53
2:I:53:SER:HA	2:I:72:ARG:HH12	1.73	0.53
2:I:83:MET:HB3	2:I:86:LEU:HD21	1.91	0.53
2:H:91:THR:HG23	2:H:112:THR:HA	1.90	0.53
1:B:107:ASN:HB3	1:C:53:ILE:HD13	1.91	0.53
1:B:453:LEU:HD22	1:B:456:ILE:HD12	1.90	0.53
1:B:453:LEU:HD12	1:B:476:LEU:HD22	1.91	0.53
3:F:356:HIS:HB3	3:F:359:ALA:HB2	1.91	0.53
2:J:91:THR:HG23	2:J:112:THR:HA	1.91	0.53
1:C:734:ARG:HA	1:C:755:ASN:HB2	1.90	0.53
1:D:39:ALA:HB2	1:D:129:VAL:HG12	1.89	0.53
1:A:135:ILE:HD13	1:A:274:LYS:HZ2	1.74	0.52
1:C:548:VAL:HG22	1:C:571:LYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LYS:O	1:A:803:TRP:HD1	1.91	0.52
1:C:496:ARG:HD2	1:C:519:GLU:HG3	1.92	0.52
1:C:769:LEU:HB3	1:C:773:LEU:HD22	1.91	0.52
1:D:35:MET:HE3	1:D:325:TYR:HE1	1.73	0.52
1:D:448:LEU:HD23	1:D:468:LEU:HD11	1.91	0.52
1:A:633:ILE:HB	1:A:657:GLN:HG2	1.90	0.52
1:B:598:LEU:HD13	1:B:603:LEU:HD11	1.91	0.52
1:D:753:LEU:HD12	1:D:756:LEU:HD22	1.92	0.52
1:A:117:ARG:HB2	1:A:295:CYS:HB3	1.92	0.52
1:C:761:LEU:HD13	1:C:766:LEU:HD22	1.91	0.52
1:A:615:ASN:HA	1:A:640:ARG:HE	1.74	0.52
3:E:36:LEU:HB2	3:E:173:THR:HG21	1.91	0.52
1:C:21:LYS:HE2	1:C:144:PHE:HE2	1.75	0.52
1:D:275:PHE:HA	1:D:278:ILE:HG12	1.91	0.52
1:D:483:ILE:HD11	1:D:491:LEU:HD12	1.91	0.52
2:G:9:GLY:HA3	2:G:109:THR:HB	1.92	0.52
1:A:709:ASN:HA	1:A:732:LYS:HD2	1.91	0.52
1:D:519:GLU:HA	1:D:546:LEU:HA	1.92	0.52
1:A:745:SER:HA	1:A:767:GLU:HG2	1.92	0.51
1:C:552:LYS:HG3	1:C:575:ASN:HB3	1.92	0.51
1:D:147:PRO:HA	1:D:150:SER:HB3	1.91	0.51
1:A:445:LEU:HD13	1:A:448:LEU:HD22	1.92	0.51
1:B:607:PRO:HG2	1:B:610:ILE:HG13	1.92	0.51
1:C:420:LEU:HD11	1:C:448:LEU:HD13	1.93	0.51
1:A:478:HIS:CE1	1:A:503:THR:HG23	2.45	0.51
1:D:638:LEU:HB3	1:D:641:LEU:HB2	1.91	0.51
1:C:633:ILE:HD13	1:C:657:GLN:HB3	1.92	0.51
1:D:547:LYS:HB3	1:D:570:GLN:HG3	1.92	0.51
1:A:452:LYS:HE3	1:A:475:TRP:CE2	2.46	0.51
2:G:19:ARG:HH11	2:G:82:GLN:HB2	1.75	0.51
1:C:254:VAL:O	1:C:371:ASP:HB3	2.10	0.51
3:E:16:THR:HA	3:E:197:VAL:HG11	1.93	0.51
3:F:337:HIS:HB2	3:F:354:CYS:HB2	1.93	0.51
1:C:465:ILE:HB	1:C:468:LEU:HD12	1.92	0.51
1:D:691:ASP:HA	1:D:714:ALA:HB3	1.92	0.51
2:J:83:MET:HE3	2:J:86:LEU:HD21	1.93	0.51
3:E:398:GLU:HA	3:E:401:ARG:HB3	1.92	0.51
1:A:411:TRP:HB3	1:A:415:LYS:HB2	1.91	0.50
1:D:385:LEU:O	1:D:389:ARG:HG2	2.11	0.50
1:A:423:ASN:ND2	1:A:429:GLU:HB2	2.25	0.50
1:B:51:LYS:HB3	1:B:313:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:ILE:O	1:C:635:PHE:HB2	2.11	0.50
3:E:299:GLU:HG3	3:E:413:LYS:HB2	1.92	0.50
1:C:491:LEU:HD22	1:C:495:LEU:HD13	1.93	0.50
1:C:491:LEU:HB3	1:C:495:LEU:HD22	1.92	0.50
3:F:439:SER:HB3	3:F:442:SER:HB3	1.94	0.50
1:A:737:HIS:HA	1:A:760:GLU:HB2	1.94	0.50
1:C:611:PHE:HZ	1:C:631:GLU:HB3	1.76	0.50
2:I:5:VAL:HG23	2:I:23:ALA:HB3	1.92	0.50
1:C:520:GLU:HG2	1:C:548:VAL:HB	1.93	0.50
1:C:647:TRP:CD1	1:C:647:TRP:H	2.30	0.50
1:D:537:ILE:HG13	1:D:561:VAL:HG11	1.93	0.50
1:D:557:LYS:HG3	1:D:584:LEU:HD21	1.94	0.50
2:H:29:VAL:HG22	2:H:72:ARG:HD2	1.94	0.50
3:E:54:CYS:HA	3:E:354:CYS:HA	1.94	0.50
1:B:250:PHE:CZ	1:B:254:VAL:HG21	2.47	0.50
1:C:599:ILE:HG22	1:C:600:ARG:HG3	1.94	0.50
2:H:15:GLY:HA2	2:H:85:SER:HA	1.94	0.50
3:E:312:THR:HA	3:E:315:LYS:HD3	1.94	0.50
1:B:323:SER:HA	1:B:326:ILE:HG12	1.94	0.49
1:B:450:VAL:HG22	1:B:473:GLU:HB2	1.94	0.49
1:B:661:LEU:HB3	1:B:664:LEU:HG	1.94	0.49
1:C:154:GLU:HA	1:C:157:VAL:HG12	1.93	0.49
1:C:438:ILE:HG12	1:C:453:LEU:HD22	1.94	0.49
2:G:23:ALA:HA	2:G:78:THR:HG22	1.94	0.49
1:A:348:LEU:HD12	1:A:348:LEU:H	1.77	0.49
1:D:129:VAL:O	1:D:133:THR:HG23	2.12	0.49
1:D:278:ILE:HA	1:D:281:TYR:CD2	2.44	0.49
2:J:83:MET:HE1	2:J:111:VAL:HG11	1.95	0.49
1:A:791:PHE:O	1:A:799:LYS:HD2	2.12	0.49
2:J:28:PRO:HG2	2:J:31:ARG:HB2	1.94	0.49
1:A:438:ILE:HG13	1:A:459:VAL:HG12	1.95	0.49
1:C:462:PRO:O	1:C:465:ILE:HG23	2.13	0.49
1:D:52:MET:HA	1:D:311:ALA:O	2.12	0.49
1:A:547:LYS:HD2	1:A:570:GLN:HG3	1.93	0.49
2:H:5:VAL:HG13	2:H:23:ALA:HB3	1.95	0.49
3:F:204:PHE:HD1	3:F:433:ARG:HD2	1.78	0.49
2:I:28:PRO:HG2	2:I:31:ARG:HG2	1.95	0.49
1:B:348:LEU:H	1:B:348:LEU:HD23	1.78	0.48
1:D:807:LYS:O	1:D:808:GLU:HB2	2.13	0.48
3:E:199:ILE:HG13	3:E:291:VAL:HG22	1.95	0.48
3:F:17:TYR:O	3:F:21:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASP:HA	1:A:371:ASP:HB2	1.95	0.48
1:C:244:PHE:O	1:C:248:LYS:HG3	2.14	0.48
1:C:299:ILE:HG22	1:C:302:LEU:HD12	1.95	0.48
3:F:165:PHE:CE1	3:F:326:THR:HG22	2.48	0.48
1:D:249:LYS:HG3	3:E:210:THR:HG22	1.95	0.48
2:I:40:ALA:HB3	2:I:43:LYS:HB3	1.95	0.48
3:E:393:LYS:H	3:E:393:LYS:HD2	1.79	0.48
1:C:725:PRO:HA	1:C:728:PHE:CD2	2.48	0.48
3:F:409:ILE:HD12	3:F:410:PRO:HD2	1.96	0.48
1:D:617:GLN:HA	1:D:641:LEU:HA	1.96	0.48
1:C:278:ILE:HA	1:C:281:TYR:CD2	2.46	0.48
1:D:807:LYS:C	1:D:808:GLU:HG3	2.30	0.48
1:A:423:ASN:HD22	1:A:429:GLU:HB2	1.79	0.48
1:C:416:LEU:HD11	1:C:441:THR:HG23	1.94	0.48
1:C:788:GLU:HA	1:C:791:PHE:HB3	1.95	0.48
1:C:804:ARG:HB2	1:C:804:ARG:HH11	1.78	0.48
1:A:527:LEU:HD22	1:A:537:ILE:HG21	1.95	0.47
1:A:537:ILE:HG13	1:A:561:VAL:HG11	1.96	0.47
1:A:715:VAL:HG23	1:A:741:ASN:HD21	1.79	0.47
3:F:390:ILE:HD12	3:F:391:PRO:HD2	1.96	0.47
1:C:437:GLY:HA2	1:C:459:VAL:HG12	1.96	0.47
3:E:295:ARG:O	3:E:299:GLU:HB2	2.14	0.47
1:C:618:GLU:HA	1:C:643:CYS:HB3	1.96	0.47
1:A:235:LYS:O	1:A:239:GLN:HG2	2.15	0.47
1:D:135:ILE:HG12	1:D:274:LYS:HZ3	1.80	0.47
3:E:444:ASN:HA	3:E:447:ARG:HH21	1.79	0.47
3:F:28:MET:HE1	3:F:376:TYR:HA	1.97	0.47
1:C:474:LEU:HD23	1:C:498:LEU:HD11	1.97	0.47
3:E:309:VAL:HG22	3:E:387:LEU:HD21	1.97	0.47
1:A:790:LEU:HD13	1:B:711:GLN:HE22	1.80	0.47
1:D:502:PHE:O	1:D:525:GLY:HA3	2.14	0.47
2:I:47:TRP:HE1	2:I:50:ALA:HB2	1.80	0.47
1:A:28:THR:HB	1:A:332:TYR:CZ	2.50	0.47
3:F:326:THR:HG21	3:F:369:TYR:HE2	1.79	0.47
1:C:19:ILE:HD11	1:C:157:VAL:HG23	1.97	0.47
1:D:575:ASN:HA	1:D:599:ILE:O	2.14	0.47
3:E:141:LEU:HD12	3:F:136:GLY:HA3	1.95	0.47
3:E:288:PHE:HA	3:E:437:PHE:HD2	1.79	0.47
1:B:698:THR:HG23	1:B:699:PHE:HD1	1.80	0.47
1:C:645:LYS:HA	1:C:668:TYR:HB2	1.97	0.47
3:E:292:ARG:HH22	3:E:295:ARG:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:HD13	1:B:391:ALA:HB3	1.97	0.46
1:B:171:ARG:NH2	1:B:229:THR:HG23	2.31	0.46
1:C:465:ILE:HD11	1:C:491:LEU:HD21	1.98	0.46
1:D:780:LYS:HD2	1:D:805:ALA:HB1	1.98	0.46
2:G:83:MET:HE2	2:G:86:LEU:HD21	1.96	0.46
1:A:379:ILE:HD13	1:A:379:ILE:HA	1.80	0.46
1:D:149:THR:HG21	1:D:263:LEU:HD12	1.98	0.46
1:C:537:ILE:HG13	1:C:561:VAL:HG11	1.97	0.46
1:D:476:LEU:HB3	1:D:479:THR:HB	1.97	0.46
1:D:590:MET:HE3	1:D:593:LEU:HD22	1.97	0.46
3:F:194:GLU:HA	3:F:197:VAL:HB	1.96	0.46
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.97	0.46
1:A:477:TYR:CD2	1:A:501:LYS:HD2	2.50	0.46
1:B:456:ILE:O	1:B:479:THR:HG23	2.15	0.46
2:J:94:TYR:O	2:J:108:GLY:CA	2.62	0.46
1:B:163:CYS:O	1:B:169:THR:HG21	2.15	0.46
1:B:343:MET:HG3	1:B:348:LEU:HD21	1.96	0.46
1:D:351:TYR:CE2	1:D:376:LEU:HB3	2.51	0.46
2:J:47:TRP:HE1	2:J:50:ALA:HB2	1.81	0.46
2:J:53:SER:HA	2:J:72:ARG:HH12	1.81	0.46
1:B:583:VAL:HG11	1:B:587:LEU:HD22	1.98	0.46
1:D:168:TRP:HE1	1:D:232:LEU:HG	1.81	0.46
2:G:2:VAL:HA	2:G:26:GLY:HA3	1.98	0.46
1:B:418:GLN:OE1	1:C:417:ARG:HD2	2.16	0.46
1:B:590:MET:HE3	1:B:593:LEU:HD22	1.98	0.46
1:C:297:VAL:HG23	1:C:299:ILE:HG12	1.96	0.46
1:C:682:PHE:CD2	1:C:703:ASP:HB2	2.50	0.46
1:B:448:LEU:HD11	1:B:450:VAL:O	2.16	0.45
1:A:94:PRO:HD2	3:F:59:PRO:HG3	1.99	0.45
1:A:374:PHE:O	1:A:378:LEU:HG	2.16	0.45
1:B:278:ILE:HA	1:B:281:TYR:CD2	2.50	0.45
1:D:354:GLU:O	1:D:358:GLU:HB2	2.15	0.45
1:D:511:TRP:CZ3	1:D:515:LEU:HD11	2.50	0.45
2:J:5:VAL:HG13	2:J:23:ALA:HB3	1.97	0.45
3:E:408:ASP:OD2	3:E:439:SER:HB3	2.17	0.45
1:A:575:ASN:HA	1:A:599:ILE:O	2.16	0.45
1:C:454:GLU:HG2	1:C:455:LEU:HG	1.97	0.45
2:G:15:GLY:HA2	2:G:85:SER:HA	1.98	0.45
1:A:774:GLY:HA3	1:A:798:VAL:HG13	1.98	0.45
1:D:231:VAL:HA	1:D:405:LEU:HD11	1.99	0.45
3:E:201:GLY:O	3:E:205:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:MET:HE2	1:A:593:LEU:HD13	1.99	0.45
1:B:154:GLU:HA	1:B:157:VAL:HG12	1.97	0.45
1:B:368:VAL:HG12	1:B:372:PHE:HB3	1.98	0.45
1:C:575:ASN:HD21	1:C:600:ARG:HE	1.64	0.45
1:D:499:HIS:HD2	1:D:522:HIS:CG	2.34	0.45
1:A:412:THR:HG23	1:A:413:LEU:H	1.82	0.45
1:A:769:LEU:HB2	1:A:794:LEU:HD21	1.98	0.45
1:D:35:MET:HE2	1:D:133:THR:HG22	1.99	0.45
1:D:473:GLU:HA	1:D:497:ALA:HB3	1.99	0.45
3:F:58:LEU:HD12	3:F:137:ARG:HH21	1.81	0.45
1:C:431:HIS:HA	1:C:452:LYS:HB2	1.99	0.45
1:C:705:GLY:CA	1:C:726:GLU:HB3	2.47	0.45
1:C:753:LEU:HB3	1:C:756:LEU:HB2	1.99	0.45
1:D:574:ILE:HG21	1:D:581:LEU:HD22	1.99	0.45
3:E:187:PRO:HD3	3:F:23:TRP:HB3	1.97	0.45
1:A:427:LYS:HB3	1:A:449:GLU:HB3	1.99	0.45
1:A:429:GLU:HA	1:A:450:VAL:O	2.17	0.45
1:A:445:LEU:HB3	1:A:448:LEU:HD13	1.98	0.45
1:C:461:ILE:HG22	1:C:487:ALA:HB1	1.99	0.45
1:C:463:PRO:HB3	1:C:486:PRO:HG2	1.98	0.45
1:C:547:LYS:HD2	1:C:570:GLN:HG3	1.98	0.45
2:H:83:MET:HE1	2:H:111:VAL:HG11	1.99	0.45
1:C:168:TRP:NE1	1:C:402:LEU:HD23	2.31	0.45
1:C:485:ALA:HB3	1:C:486:PRO:HD3	1.99	0.45
1:C:151:SER:O	1:C:154:GLU:HG3	2.16	0.45
2:J:15:GLY:HA2	2:J:85:SER:HA	1.98	0.45
1:A:541:ARG:HG3	1:A:561:VAL:HG23	1.99	0.44
1:A:599:ILE:HG23	1:A:622:LYS:HB3	1.98	0.44
1:C:682:PHE:HA	1:C:707:LEU:HD21	1.99	0.44
1:D:375:MET:O	1:D:379:ILE:HG12	2.16	0.44
3:F:144:GLN:HA	3:F:147:VAL:HG22	1.99	0.44
3:F:165:PHE:HZ	3:F:326:THR:HA	1.82	0.44
1:C:594:THR:HA	1:C:616:LEU:HA	1.98	0.44
1:D:353:PHE:HE1	1:D:391:ALA:HB2	1.83	0.44
2:G:88:PRO:HA	2:G:113:VAL:HB	2.00	0.44
3:F:322:ILE:HA	3:F:325:TYR:CE2	2.52	0.44
1:A:275:PHE:CD1	1:A:333:GLY:HA3	2.52	0.44
1:D:171:ARG:O	1:D:175:GLU:HG2	2.17	0.44
2:G:5:VAL:HG23	2:G:23:ALA:HB3	2.00	0.44
1:A:505:ILE:HD12	1:A:536:VAL:HG11	1.99	0.44
1:B:379:ILE:HD13	1:B:379:ILE:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:196:PHE:HE1	3:F:200:LEU:HD22	1.83	0.44
3:F:196:PHE:CG	3:F:419:LEU:HG	2.52	0.44
1:A:362:TYR:HD1	1:A:397:VAL:HB	1.81	0.44
1:A:390:PHE:HA	1:A:393:PHE:HD2	1.82	0.44
1:B:636:GLN:HE22	2:H:60:TYR:H	1.64	0.44
1:C:15:PRO:HB2	1:C:16:ALA:H	1.63	0.44
1:C:497:ALA:HA	1:C:520:GLU:O	2.18	0.44
1:D:449:GLU:HA	1:D:470:GLY:O	2.17	0.44
1:A:687:LEU:HD21	1:A:690:LEU:HD13	2.00	0.44
1:B:30:TYR:HD1	1:B:30:TYR:HA	1.68	0.44
1:B:275:PHE:CE1	1:B:333:GLY:HA3	2.52	0.44
1:B:677:ILE:HD11	1:B:697:LEU:HD13	1.99	0.44
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.79	0.44
3:F:283:GLN:NE2	3:F:287:LEU:HD22	2.33	0.44
1:B:19:ILE:HD11	1:B:157:VAL:HG23	1.99	0.44
1:C:160:LEU:HD21	1:C:386:TYR:HB3	2.00	0.44
1:D:576:ASN:HB3	1:D:579:THR:HB	1.98	0.44
1:D:598:LEU:HB2	1:D:621:LEU:HD23	1.99	0.44
1:A:124:TYR:CE1	1:B:317:LEU:HD23	2.53	0.44
1:A:279:ILE:HD13	1:A:279:ILE:HA	1.91	0.44
1:B:53:ILE:HD12	1:B:311:ALA:HB3	2.00	0.44
1:B:168:TRP:CZ3	1:B:398:SER:HB2	2.53	0.44
1:C:129:VAL:O	1:C:133:THR:HG23	2.18	0.44
1:C:622:LYS:HB2	1:C:647:TRP:HE1	1.83	0.44
1:C:17:TYR:HD1	1:C:20:LEU:HD23	1.83	0.44
1:C:17:TYR:HA	1:C:20:LEU:HD23	1.99	0.44
1:C:667:LEU:HG	1:C:669:LEU:HG	2.00	0.44
3:E:17:TYR:O	3:E:21:LYS:HG2	2.17	0.44
3:F:284:ALA:O	3:F:288:PHE:HB2	2.18	0.44
1:A:472:LYS:HD3	1:A:472:LYS:HA	1.82	0.43
1:A:549:LEU:HD23	1:A:572:LEU:HD13	2.00	0.43
1:B:171:ARG:O	1:B:175:GLU:HG2	2.18	0.43
1:D:491:LEU:O	1:D:495:LEU:HB2	2.18	0.43
1:D:737:HIS:HA	1:D:760:GLU:HB3	2.00	0.43
2:G:60:TYR:HB2	2:G:65:LYS:HG3	2.00	0.43
3:E:28:MET:HE3	3:E:28:MET:HB3	1.86	0.43
3:E:200:LEU:HD23	3:E:434:PHE:CZ	2.53	0.43
3:E:295:ARG:HH21	3:E:438:LEU:HD13	1.83	0.43
1:A:302:LEU:HD11	1:B:309:ARG:HD3	1.99	0.43
1:A:383:ASP:OD2	1:A:385:LEU:HB3	2.18	0.43
1:A:647:TRP:H	1:A:647:TRP:CD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:LEU:HD12	1:D:377:HIS:CB	2.48	0.43
2:H:61:ALA:HB3	2:H:64:VAL:HG22	1.99	0.43
1:A:607:PRO:HG2	1:A:610:ILE:HG13	1.99	0.43
1:C:370:ASN:C	1:C:372:PHE:H	2.26	0.43
1:C:553:SER:HB2	1:C:555:LEU:HG	2.00	0.43
1:D:415:LYS:O	1:D:419:ARG:HB2	2.19	0.43
1:D:548:VAL:HG22	1:D:571:LYS:HB3	1.99	0.43
1:D:550:ARG:HH12	1:D:575:ASN:HB2	1.84	0.43
1:D:736:LEU:HD22	1:D:738:LEU:HD21	2.00	0.43
2:G:83:MET:HB3	2:G:86:LEU:HD21	2.01	0.43
3:E:19:ILE:HD13	3:E:197:VAL:HG22	2.01	0.43
3:E:369:TYR:O	3:E:373:ILE:HG12	2.18	0.43
3:E:406:PHE:HB3	3:E:408:ASP:CG	2.44	0.43
1:B:56:PRO:HD2	1:B:99:TYR:CD2	2.53	0.43
1:B:258:ASP:N	1:B:371:ASP:HB2	2.29	0.43
1:C:600:ARG:HG2	1:C:623:ASP:HB3	2.00	0.43
1:D:452:LYS:HA	1:D:475:TRP:HB2	1.99	0.43
1:A:450:VAL:HA	1:A:473:GLU:HB2	2.00	0.43
1:D:543:LEU:HB3	1:D:546:LEU:HB2	2.01	0.43
2:H:30:GLY:HA2	2:H:72:ARG:CZ	2.48	0.43
2:J:61:ALA:HB3	2:J:64:VAL:HG22	1.99	0.43
3:F:339:CYS:SG	3:F:341:PRO:HG3	2.59	0.43
1:A:121:PHE:CZ	1:A:282:THR:HG23	2.53	0.43
1:B:472:LYS:HD2	1:B:496:ARG:HG2	1.99	0.43
1:D:17:TYR:HA	1:D:20:LEU:HD23	2.00	0.43
3:F:52:VAL:HG12	3:F:356:HIS:HA	2.00	0.43
1:B:498:LEU:HG	1:B:500:ILE:HG12	2.00	0.43
1:B:604:GLU:HG2	1:B:625:ASN:HB2	2.01	0.43
3:F:281:GLY:HA3	3:F:453:HIS:CD2	2.54	0.43
1:A:125:PHE:O	1:A:129:VAL:HG23	2.19	0.43
1:A:461:ILE:HB	1:A:483:ILE:HA	2.00	0.43
1:C:59:TRP:HB3	1:C:66:ASN:HB3	2.01	0.43
3:E:186:TYR:CD2	3:E:187:PRO:HD2	2.53	0.43
1:A:450:VAL:HG13	1:A:473:GLU:HB2	2.01	0.43
1:D:160:LEU:HD13	1:D:390:PHE:HD2	1.84	0.43
1:A:731:ARG:NH1	1:A:752:GLU:HB3	2.34	0.42
1:B:622:LYS:HG3	1:B:648:TYR:HB2	2.01	0.42
1:D:104:HIS:CD2	3:E:53:VAL:HG23	2.54	0.42
1:D:383:ASP:HB3	1:D:386:TYR:CE1	2.53	0.42
3:E:199:ILE:HD12	3:E:199:ILE:HA	1.85	0.42
1:A:622:LYS:HB2	1:A:647:TRP:NE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ARG:HB2	1:B:295:CYS:HB3	2.01	0.42
1:B:353:PHE:HD1	1:B:353:PHE:HA	1.71	0.42
1:C:685:ARG:HH21	1:C:706:LEU:HD13	1.84	0.42
1:D:19:ILE:HD11	1:D:157:VAL:HG23	2.00	0.42
1:D:28:THR:HB	1:D:332:TYR:CZ	2.53	0.42
1:A:518:LEU:HD23	1:A:543:LEU:HD13	2.02	0.42
1:B:31:ILE:HG22	1:B:35:MET:HE2	2.01	0.42
1:B:476:LEU:HB2	1:B:500:ILE:HD13	2.01	0.42
1:C:121:PHE:CZ	1:C:282:THR:HG23	2.54	0.42
1:D:369:LYS:HE3	1:D:369:LYS:HB3	1.88	0.42
1:D:607:PRO:HG2	1:D:610:ILE:HG13	2.01	0.42
3:E:412:VAL:HB	3:E:416:PHE:HB3	2.00	0.42
3:F:46:GLN:HG2	3:F:50:ASP:CG	2.43	0.42
3:F:196:PHE:CZ	3:F:419:LEU:HB3	2.54	0.42
3:F:413:LYS:HA	3:F:413:LYS:HD3	1.85	0.42
1:A:136:PHE:HE1	1:A:271:LYS:HG2	1.84	0.42
1:A:147:PRO:HA	1:A:150:SER:HB3	2.00	0.42
1:A:519:GLU:HG2	1:A:545:ARG:HG3	2.01	0.42
1:B:258:ASP:HB2	1:B:370:ASN:ND2	2.35	0.42
1:C:687:LEU:HD23	1:C:690:LEU:HD13	2.01	0.42
1:D:323:SER:HA	1:D:326:ILE:HG12	2.02	0.42
1:D:428:LEU:HD12	1:D:428:LEU:H	1.82	0.42
1:D:491:LEU:HD22	1:D:495:LEU:HD13	2.02	0.42
1:B:575:ASN:HA	1:B:599:ILE:O	2.20	0.42
1:B:611:PHE:CZ	1:B:631:GLU:HB3	2.53	0.42
1:B:670:ASN:HD22	1:B:671:ARG:HG2	1.85	0.42
1:C:35:MET:HE3	1:C:325:TYR:HE1	1.85	0.42
1:C:121:PHE:HZ	1:C:282:THR:HG23	1.85	0.42
1:C:491:LEU:O	1:C:495:LEU:HB3	2.19	0.42
1:D:154:GLU:HA	1:D:157:VAL:HG12	2.00	0.42
1:A:44:THR:O	1:A:48:THR:HG22	2.19	0.42
1:C:35:MET:HE3	1:C:325:TYR:CE1	2.54	0.42
1:C:466:ALA:HA	1:C:490:PHE:CG	2.54	0.42
1:C:770:PRO:HD2	1:C:773:LEU:HD13	2.02	0.42
1:D:117:ARG:HB2	1:D:295:CYS:HB3	2.01	0.42
1:D:733:LEU:HD21	1:D:736:LEU:HD21	2.00	0.42
3:F:366:LEU:HD12	3:F:366:LEU:HA	1.92	0.42
1:A:244:PHE:CE2	1:A:399:GLU:HG3	2.55	0.42
1:C:501:LYS:HE3	1:C:524:THR:HG21	2.01	0.42
1:C:693:SER:HA	1:C:718:ASN:HD21	1.84	0.42
2:H:23:ALA:HA	2:H:78:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:LYS:HA	3:E:185:LYS:HD2	1.93	0.42
3:E:196:PHE:HZ	3:E:420:LEU:HD12	1.84	0.42
3:F:373:ILE:HD13	3:F:373:ILE:HA	1.91	0.42
1:A:729:GLN:NE2	1:A:749:ARG:HH22	2.17	0.42
1:C:241:LYS:NZ	1:C:403:ARG:HD3	2.34	0.42
1:C:251:ARG:NH2	1:C:366:PRO:HG2	2.30	0.42
2:I:37:TYR:O	2:I:94:TYR:HA	2.20	0.42
1:A:572:LEU:O	1:A:596:LEU:HA	2.20	0.42
1:A:772:GLU:C	1:A:774:GLY:H	2.27	0.42
1:C:711:GLN:HA	1:C:733:LEU:HD12	2.01	0.42
1:D:154:GLU:HG3	1:D:155:HIS:N	2.34	0.42
3:E:325:TYR:HD2	3:E:329:PHE:HD2	1.67	0.42
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.89	0.42
1:A:795:PRO:HB2	1:A:798:VAL:HB	2.02	0.42
1:C:477:TYR:CD1	1:C:501:LYS:HB2	2.55	0.42
1:D:159:ILE:HA	1:D:162:LYS:HG2	2.02	0.42
1:D:377:HIS:O	1:D:381:GLN:HG2	2.20	0.42
3:E:141:LEU:HB3	3:E:146:TYR:CE2	2.55	0.42
3:F:148:PHE:CZ	3:F:346:LEU:HD23	2.55	0.42
1:B:135:ILE:HG12	1:B:274:LYS:HZ2	1.84	0.41
1:C:162:LYS:HG3	1:C:243:LEU:HD21	2.02	0.41
1:C:275:PHE:CE1	1:C:333:GLY:HA3	2.55	0.41
1:C:400:ASN:O	1:C:404:GLN:HG2	2.21	0.41
1:D:35:MET:HA	1:D:38:ILE:HG12	2.01	0.41
1:D:279:ILE:HD13	1:D:279:ILE:HA	1.95	0.41
1:A:149:THR:HG21	1:A:263:LEU:HD12	2.02	0.41
1:A:379:ILE:HG23	1:A:386:TYR:HB2	2.01	0.41
1:B:15:PRO:HB2	1:B:16:ALA:H	1.64	0.41
1:B:319:LYS:HE3	1:B:319:LYS:HB2	1.92	0.41
1:C:250:PHE:CZ	1:C:254:VAL:HG21	2.55	0.41
1:C:622:LYS:HB2	1:C:647:TRP:NE1	2.34	0.41
1:D:22:PRO:HG2	1:D:24:TRP:CZ2	2.54	0.41
1:A:622:LYS:HG3	1:A:648:TYR:HB2	2.02	0.41
1:B:576:ASN:HB3	1:B:579:THR:HB	2.02	0.41
1:D:357:ARG:HD3	1:D:365:ILE:O	2.20	0.41
3:E:292:ARG:HA	3:E:292:ARG:NH1	2.35	0.41
1:A:767:GLU:HA	1:B:709:ASN:HD21	1.86	0.41
1:C:677:ILE:HD11	1:C:697:LEU:HD13	2.02	0.41
1:D:427:LYS:NZ	1:D:449:GLU:HG2	2.35	0.41
1:D:476:LEU:HD13	1:D:481:ALA:HB3	2.02	0.41
1:D:578:GLY:H	1:D:600:ARG:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:ASN:HA	1:D:732:LYS:HD2	2.02	0.41
3:E:24:TRP:HE1	3:E:422:MET:HE3	1.85	0.41
3:E:416:PHE:HE2	3:E:438:LEU:HD11	1.85	0.41
1:A:35:MET:O	1:A:38:ILE:HG12	2.21	0.41
1:C:35:MET:HA	1:C:38:ILE:HG12	2.03	0.41
1:C:746:LEU:HD23	1:C:747:PRO:O	2.21	0.41
1:D:432:LEU:HD13	1:D:439:PRO:HD2	2.03	0.41
3:E:313:VAL:HA	3:E:316:THR:HG22	2.01	0.41
3:F:149:ILE:HD13	3:F:149:ILE:HA	1.89	0.41
1:B:588:LYS:HA	1:B:613:LEU:HD21	2.02	0.41
1:D:455:LEU:HD23	1:D:455:LEU:HA	1.95	0.41
1:D:543:LEU:HD12	1:D:546:LEU:HD22	2.03	0.41
1:D:588:LYS:HA	1:D:613:LEU:HD21	2.03	0.41
2:G:94:TYR:O	2:G:108:GLY:CA	2.62	0.41
2:I:67:ARG:HH21	2:I:86:LEU:HA	1.85	0.41
3:E:192:LYS:HE3	3:E:304:ILE:HD11	2.02	0.41
1:A:35:MET:HE2	1:A:133:THR:HG22	2.02	0.41
1:A:129:VAL:HG13	1:A:325:TYR:CE1	2.55	0.41
1:A:582:ILE:HG23	1:A:584:LEU:HG	2.03	0.41
1:C:56:PRO:HD2	1:C:99:TYR:CD2	2.56	0.41
1:C:483:ILE:HG12	1:C:488:LEU:HB2	2.02	0.41
1:D:427:LYS:HZ2	1:D:449:GLU:HG2	1.86	0.41
1:B:151:SER:O	1:B:154:GLU:HG3	2.21	0.41
1:B:346:ARG:HE	1:B:377:HIS:CD2	2.39	0.41
1:C:420:LEU:HD12	1:C:420:LEU:HA	1.92	0.41
1:C:562:VAL:HA	1:C:565:VAL:HG12	2.02	0.41
1:C:723:LEU:HD11	1:C:738:LEU:HD11	2.02	0.41
1:D:15:PRO:HB2	1:D:16:ALA:H	1.64	0.41
1:D:135:ILE:HD13	1:D:274:LYS:HD3	2.02	0.41
1:D:271:LYS:O	1:D:275:PHE:HB3	2.21	0.41
1:D:389:ARG:HA	1:D:389:ARG:HD3	1.88	0.41
1:D:593:LEU:HD21	1:D:596:LEU:HD13	2.03	0.41
2:I:9:GLY:HA3	2:I:109:THR:HB	2.01	0.41
2:I:83:MET:HE2	2:I:86:LEU:HD21	2.02	0.41
3:E:341:PRO:HG2	3:E:343:VAL:HG22	2.02	0.41
3:E:346:LEU:HD11	3:F:55:LEU:HB3	2.02	0.41
3:F:356:HIS:CD2	3:F:358:MET:H	2.39	0.41
3:F:395:TYR:OH	3:F:431:SER:HB2	2.20	0.41
1:A:19:ILE:HG13	1:A:20:LEU:HD22	2.04	0.41
1:B:149:THR:HG21	1:B:263:LEU:HD12	2.01	0.41
1:B:473:GLU:HB3	1:B:475:TRP:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLY:HA2	1:B:569:LEU:HD12	2.03	0.41
1:C:100:ASP:HB3	1:D:98:LYS:HE2	2.03	0.41
1:C:465:ILE:HA	1:C:468:LEU:HG	2.03	0.41
1:C:753:LEU:HD22	1:C:753:LEU:HA	1.86	0.41
3:E:428:GLN:HE21	3:E:428:GLN:HB3	1.65	0.41
1:A:295:CYS:HB2	1:A:297:VAL:HG13	2.03	0.40
1:A:35:MET:HG3	1:A:328:LEU:HD13	2.02	0.40
1:A:438:ILE:CG1	1:A:459:VAL:HG12	2.51	0.40
1:B:537:ILE:HG13	1:B:561:VAL:HG11	2.03	0.40
1:D:428:LEU:O	1:D:450:VAL:HB	2.21	0.40
1:A:39:ALA:HB2	1:A:129:VAL:CG1	2.52	0.40
1:A:322:ALA:O	1:A:326:ILE:HG23	2.21	0.40
1:C:168:TRP:HH2	1:C:398:SER:HB2	1.84	0.40
1:C:435:LEU:HD23	1:C:435:LEU:HA	1.96	0.40
1:C:654:ILE:HG21	1:C:681:LEU:HD12	2.03	0.40
1:C:753:LEU:HD12	1:C:756:LEU:CB	2.50	0.40
1:D:234:LYS:HB2	1:D:409:ASN:HB3	2.03	0.40
1:D:771:VAL:HG23	1:D:795:PRO:HG2	2.03	0.40
3:E:416:PHE:CE2	3:E:438:LEU:HD11	2.56	0.40
1:B:454:GLU:HA	1:B:477:TYR:O	2.22	0.40
1:D:364:ASP:OD2	1:D:397:VAL:HG23	2.20	0.40
1:D:648:TYR:CE2	1:D:671:ARG:HG3	2.56	0.40
2:G:6:GLU:HB3	2:G:109:THR:HG23	2.02	0.40
2:H:29:VAL:HG21	2:H:79:VAL:HG22	2.04	0.40
3:F:449:ILE:HD13	3:F:449:ILE:HA	1.97	0.40
1:A:373:ALA:HA	1:A:376:LEU:HD12	2.02	0.40
1:A:794:LEU:HB2	1:A:799:LYS:CD	2.49	0.40
1:B:124:TYR:HA	1:B:127:TYR:HD2	1.86	0.40
1:B:574:ILE:HB	1:B:598:LEU:HD23	2.04	0.40
1:C:452:LYS:HE2	1:C:475:TRP:CE3	2.57	0.40
1:C:751:GLY:CA	1:C:772:GLU:HB3	2.45	0.40
1:D:129:VAL:HG13	1:D:325:TYR:CE1	2.57	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	A	712/818 (87%)	681 (96%)	31 (4%)	0	100	100
1	B	618/818 (76%)	602 (97%)	16 (3%)	0	100	100
1	C	712/818 (87%)	688 (97%)	24 (3%)	0	100	100
1	D	726/818 (89%)	701 (97%)	25 (3%)	0	100	100
2	G	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
2	H	112/118 (95%)	112 (100%)	0	0	100	100
2	I	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
2	J	112/118 (95%)	112 (100%)	0	0	100	100
3	E	302/924 (33%)	292 (97%)	10 (3%)	0	100	100
3	F	303/924 (33%)	292 (96%)	10 (3%)	1 (0%)	36	64
All	All	3821/5592 (68%)	3700 (97%)	120 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	60	SER

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	A	666/756 (88%)	609 (91%)	57 (9%)	10	32
1	B	582/756 (77%)	555 (95%)	27 (5%)	24	53
1	C	666/756 (88%)	627 (94%)	39 (6%)	18	45
1	D	678/756 (90%)	639 (94%)	39 (6%)	18	46
2	G	92/94 (98%)	92 (100%)	0	100	100
2	H	92/94 (98%)	88 (96%)	4 (4%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	92/94 (98%)	91 (99%)	1 (1%)	65	75
2	J	92/94 (98%)	90 (98%)	2 (2%)	45	67
3	E	286/842 (34%)	255 (89%)	31 (11%)	6	23
3	F	287/842 (34%)	256 (89%)	31 (11%)	6	23
All	All	3533/5084 (70%)	3302 (94%)	231 (6%)	17	42

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LYS
1	A	102	ASP
1	A	110	ASP
1	A	136	PHE
1	A	157	VAL
1	A	161	LEU
1	A	169	THR
1	A	170	THR
1	A	231	VAL
1	A	232	LEU
1	A	236	GLU
1	A	243	LEU
1	A	244	PHE
1	A	253	HIS
1	A	254	VAL
1	A	275	PHE
1	A	279	ILE
1	A	281	TYR
1	A	295	CYS
1	A	300	GLU
1	A	353	PHE
1	A	354	GLU
1	A	356	ILE
1	A	374	PHE
1	A	379	ILE
1	A	392	VAL
1	A	394	LEU
1	A	398	SER
1	A	399	GLU
1	A	403	ARG
1	A	406	ASN
1	A	407	LEU

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Mol	Chain	Res	Type
1	A	411	TRP
1	A	412	THR
1	A	413	LEU
1	A	416	LEU
1	A	417	ARG
1	A	419	ARG
1	A	421	THR
1	A	425	GLN
1	A	429	GLU
1	A	432	LEU
1	A	434	MET
1	A	435	LEU
1	A	447	GLU
1	A	459	VAL
1	A	460	THR
1	A	583	VAL
1	A	746	LEU
1	A	755	ASN
1	A	765	ARG
1	A	781	ARG
1	A	785	VAL
1	A	786	VAL
1	A	793	THR
1	A	798	VAL
1	A	799	LYS
1	B	30	TYR
1	B	49	GLN
1	B	53	ILE
1	B	103	ARG
1	B	110	ASP
1	B	136	PHE
1	B	170	THR
1	B	173	LEU
1	B	231	VAL
1	B	236	GLU
1	B	275	PHE
1	B	281	TYR
1	B	293	VAL
1	B	295	CYS
1	B	297	VAL
1	B	317	LEU
1	B	353	PHE

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Mol	Chain	Res	Type
1	B	364	ASP
1	B	379	ILE
1	B	393	PHE
1	B	407	LEU
1	B	421	THR
1	B	423	ASN
1	B	447	GLU
1	B	459	VAL
1	B	584	LEU
1	B	676	LYS
1	C	104	HIS
1	C	110	ASP
1	C	231	VAL
1	C	275	PHE
1	C	281	TYR
1	C	299	ILE
1	C	317	LEU
1	C	353	PHE
1	C	356	ILE
1	C	379	ILE
1	C	393	PHE
1	C	397	VAL
1	C	426	ASP
1	C	446	VAL
1	C	449	GLU
1	C	456	ILE
1	C	460	THR
1	C	465	ILE
1	C	483	ILE
1	C	583	VAL
1	C	647	TRP
1	C	687	LEU
1	C	733	LEU
1	C	734	ARG
1	C	743	LEU
1	C	750	VAL
1	C	753	LEU
1	C	754	THR
1	C	755	ASN
1	C	760	GLU
1	C	761	LEU
1	C	769	LEU

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Mol	Chain	Res	Type
1	C	778	LEU
1	C	789	ASP
1	C	790	LEU
1	C	793	THR
1	C	799	LYS
1	C	802	LEU
1	C	804	ARG
1	D	49	GLN
1	D	163	CYS
1	D	168	TRP
1	D	170	THR
1	D	232	LEU
1	D	251	ARG
1	D	275	PHE
1	D	279	ILE
1	D	281	TYR
1	D	295	CYS
1	D	317	LEU
1	D	318	PHE
1	D	348	LEU
1	D	355	SER
1	D	376	LEU
1	D	380	ASP
1	D	390	PHE
1	D	397	VAL
1	D	405	LEU
1	D	421	THR
1	D	425	GLN
1	D	426	ASP
1	D	428	LEU
1	D	438	ILE
1	D	441	THR
1	D	443	PHE
1	D	449	GLU
1	D	458	ASP
1	D	459	VAL
1	D	460	THR
1	D	474	LEU
1	D	483	ILE
1	D	495	LEU
1	D	498	LEU
1	D	518	LEU

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Mol	Chain	Res	Type
1	D	553	SER
1	D	584	LEU
1	D	644	LEU
1	D	793	THR
2	H	5	VAL
2	H	79	VAL
2	H	96	CYS
2	H	100	VAL
2	I	12	VAL
2	J	5	VAL
2	J	100	VAL
3	E	19	ILE
3	E	49	LYS
3	E	54	CYS
3	E	55	LEU
3	E	151	GLN
3	E	165	PHE
3	E	170	LEU
3	E	185	LYS
3	E	199	ILE
3	E	208	TRP
3	E	283	GLN
3	E	287	LEU
3	E	289	GLU
3	E	290	LYS
3	E	291	VAL
3	E	293	LYS
3	E	299	GLU
3	E	337	HIS
3	E	355	THR
3	E	367	ILE
3	E	390	ILE
3	E	392	LEU
3	E	393	LYS
3	E	397	PHE
3	E	406	PHE
3	E	409	ILE
3	E	414	ASN
3	E	416	PHE
3	E	422	MET
3	E	428	GLN
3	E	446	LEU

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Mol	Chain	Res	Type
3	F	16	THR
3	F	20	LEU
3	F	165	PHE
3	F	175	ILE
3	F	178	VAL
3	F	199	ILE
3	F	213	LEU
3	F	282	GLU
3	F	292	ARG
3	F	293	LYS
3	F	295	ARG
3	F	330	VAL
3	F	366	LEU
3	F	373	ILE
3	F	390	ILE
3	F	406	PHE
3	F	408	ASP
3	F	419	LEU
3	F	420	LEU
3	F	421	HIS
3	F	422	MET
3	F	432	LYS
3	F	434	PHE
3	F	436	VAL
3	F	438	LEU
3	F	440	GLU
3	F	446	LEU
3	F	447	ARG
3	F	449	ILE
3	F	451	LEU
3	F	454	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	409	ASN
1	A	478	HIS
1	A	494	ASN
1	A	522	HIS
1	A	576	ASN
1	A	650	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	A	709	ASN
1	A	711	GLN
1	B	104	HIS
1	B	494	ASN
1	B	560	GLN
1	B	624	ASN
1	B	636	GLN
1	B	637	HIS
1	B	694	HIS
1	B	709	ASN
1	B	711	GLN
1	C	105	GLN
1	C	132	HIS
1	C	406	ASN
1	C	467	GLN
1	C	522	HIS
1	C	711	GLN
1	D	105	GLN
1	D	132	HIS
1	D	288	ASN
1	D	404	GLN
1	D	418	GLN
1	D	499	HIS
1	D	554	ASN
1	D	560	GLN
1	D	624	ASN
1	D	712	ASN
1	D	729	GLN
2	G	74	ASN
2	G	82	GLN
2	G	110	GLN
2	H	32	HIS
2	H	39	GLN
2	H	82	GLN
2	I	84	ASN
2	I	110	GLN
3	E	145	GLN
3	E	150	ASN
3	E	311	GLN
3	E	331	ASN
3	E	425	GLN
3	E	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	297	HIS
3	F	356	HIS
3	F	428	GLN
3	F	453	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

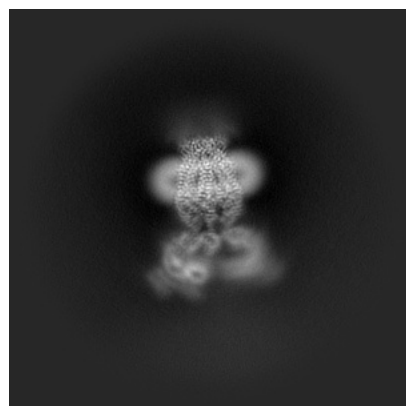
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55591. These allow visual inspection of the internal detail of the map and identification of artifacts.

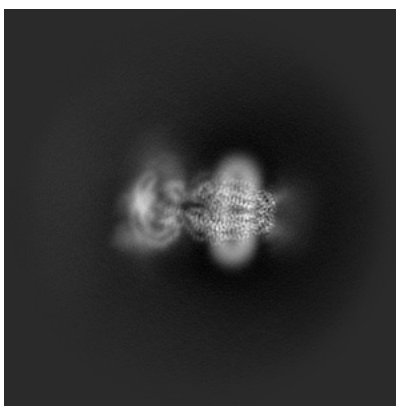
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

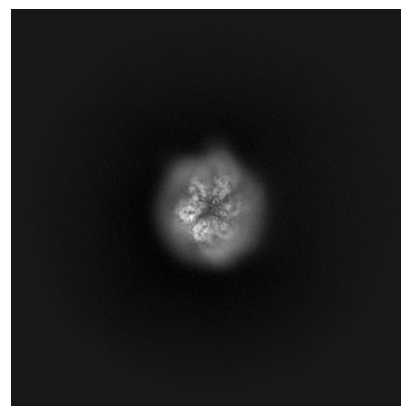
6.1.1 Primary map



X

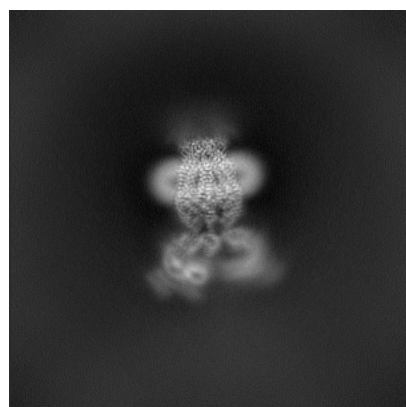


Y

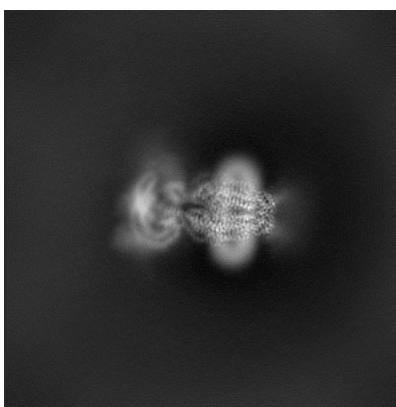


Z

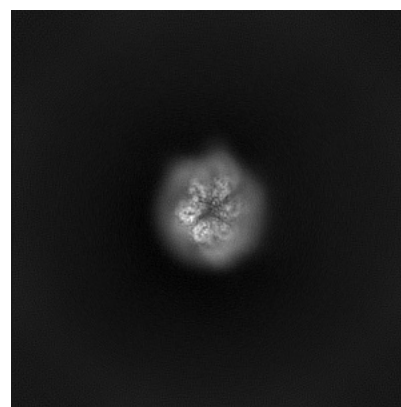
6.1.2 Raw map



X



Y

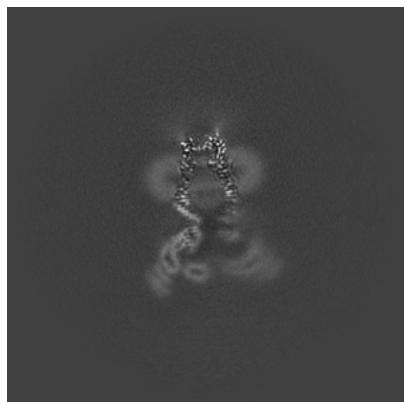


Z

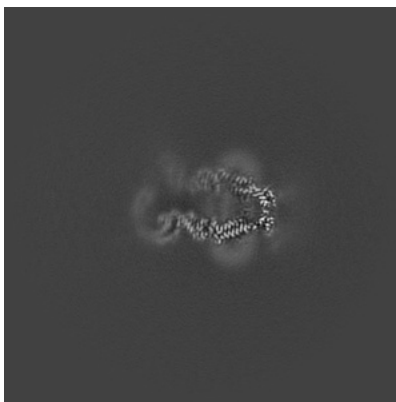
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

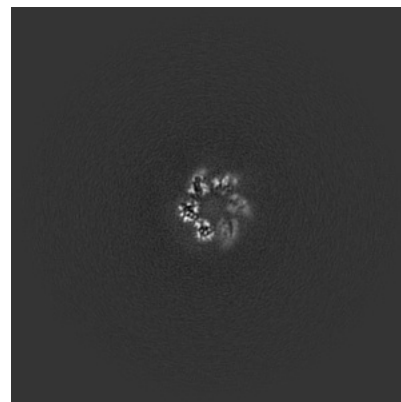
6.2.1 Primary map



X Index: 183

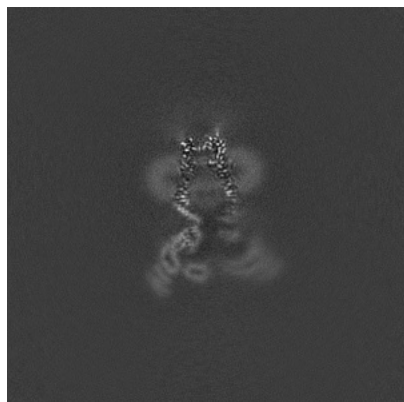


Y Index: 183

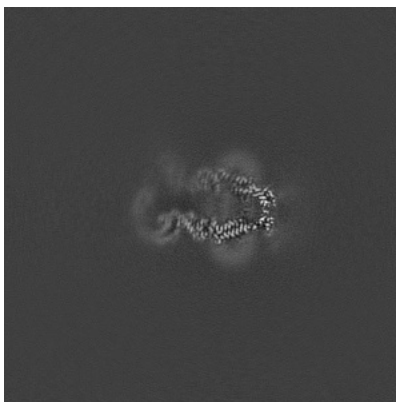


Z Index: 183

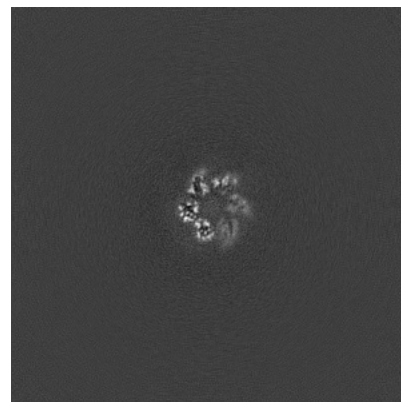
6.2.2 Raw map



X Index: 183



Y Index: 183

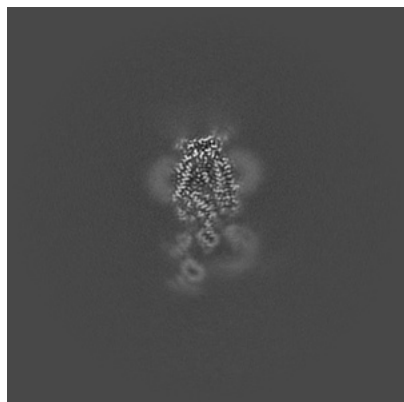


Z Index: 183

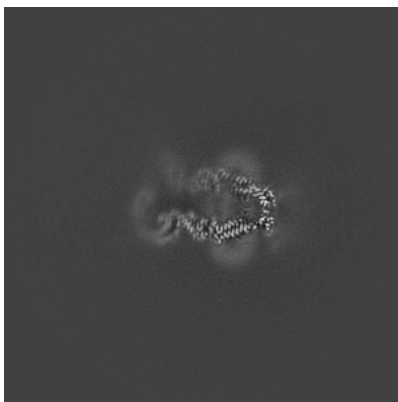
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

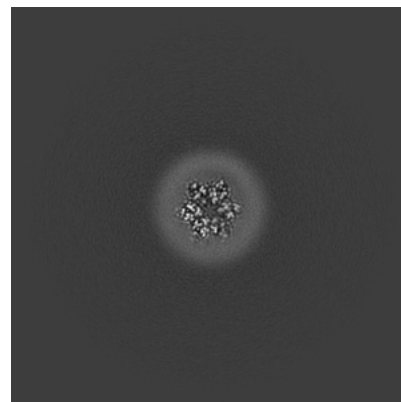
6.3.1 Primary map



X Index: 168

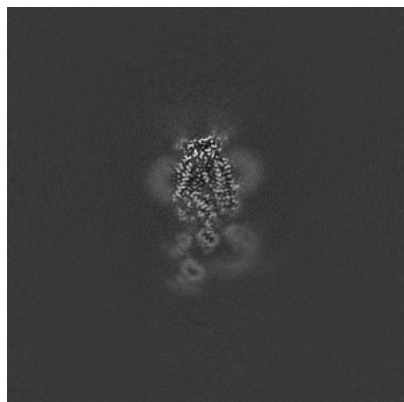


Y Index: 183

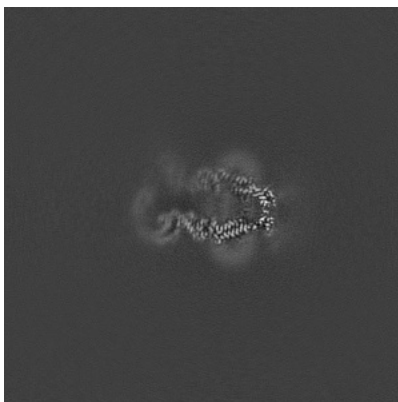


Z Index: 220

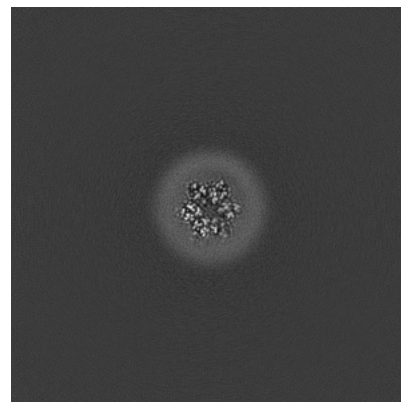
6.3.2 Raw map



X Index: 168



Y Index: 183



Z Index: 220

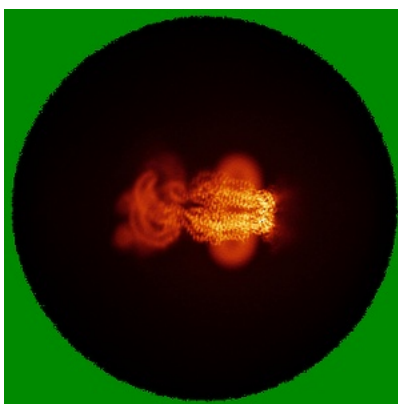
The images above show the largest variance slices of the map in three orthogonal directions.

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

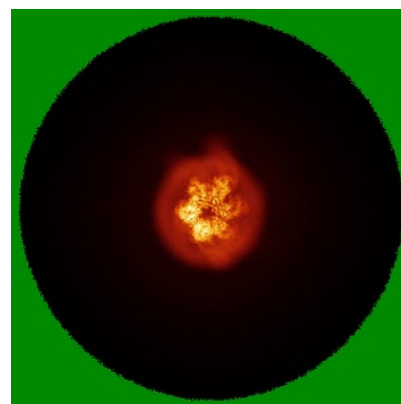
6.4.1 Primary map



X

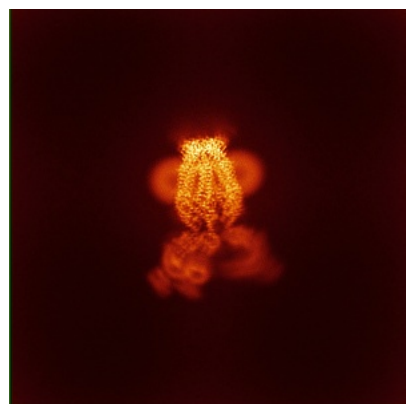


Y

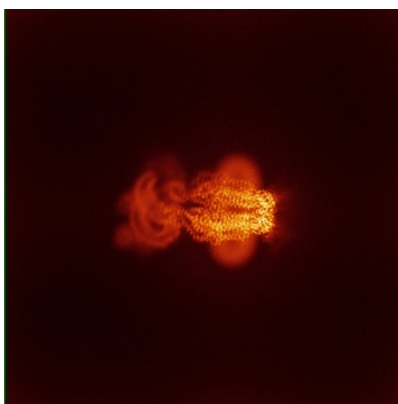


Z

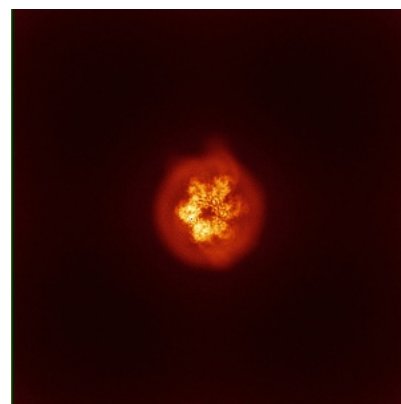
6.4.2 Raw map



X



Y



Z

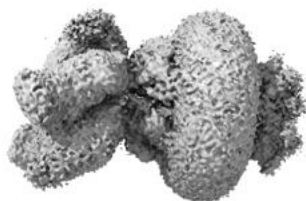
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

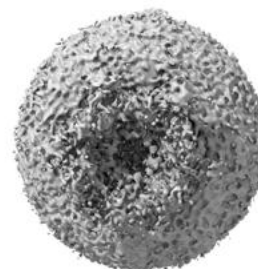
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0855. 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.

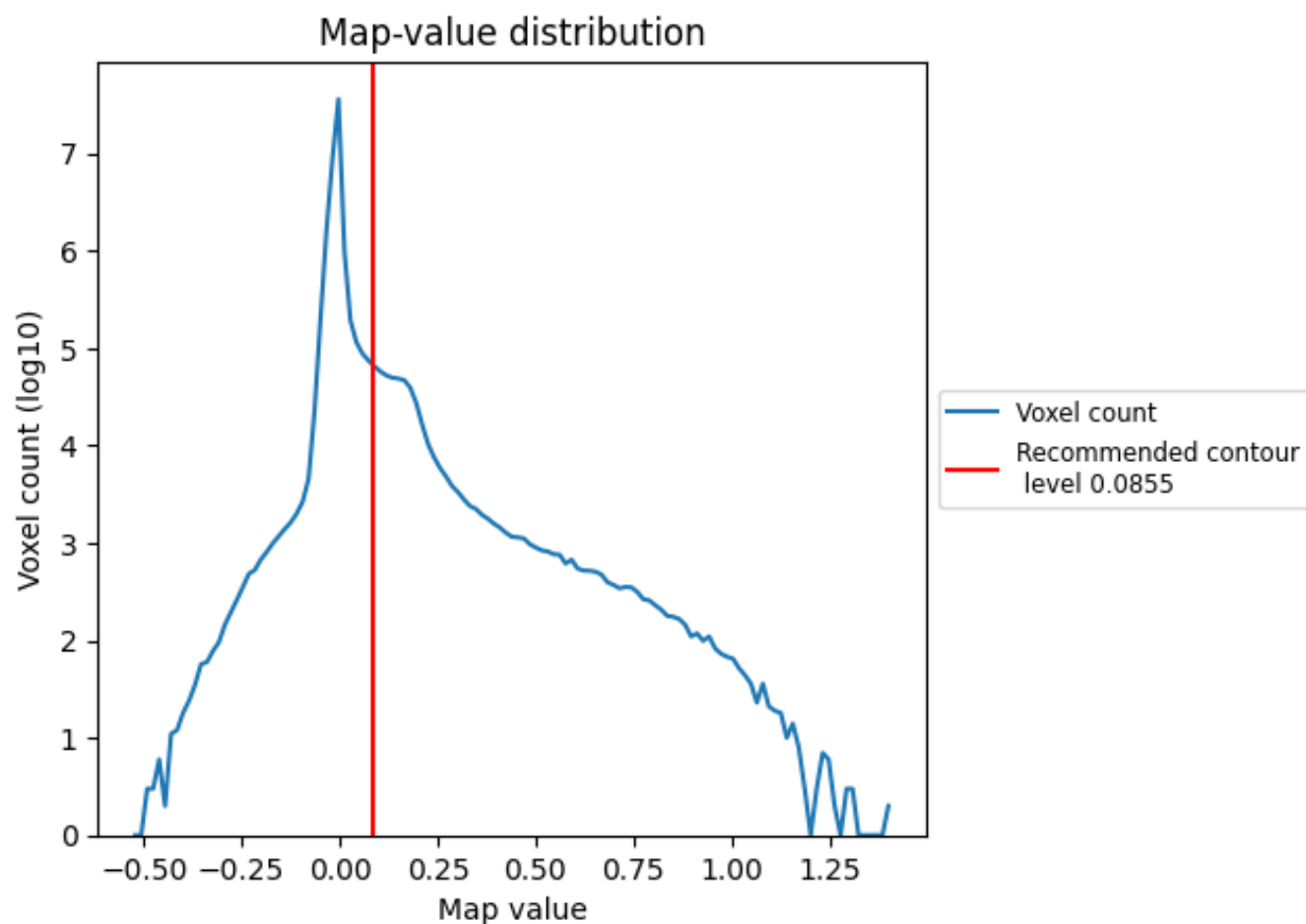
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

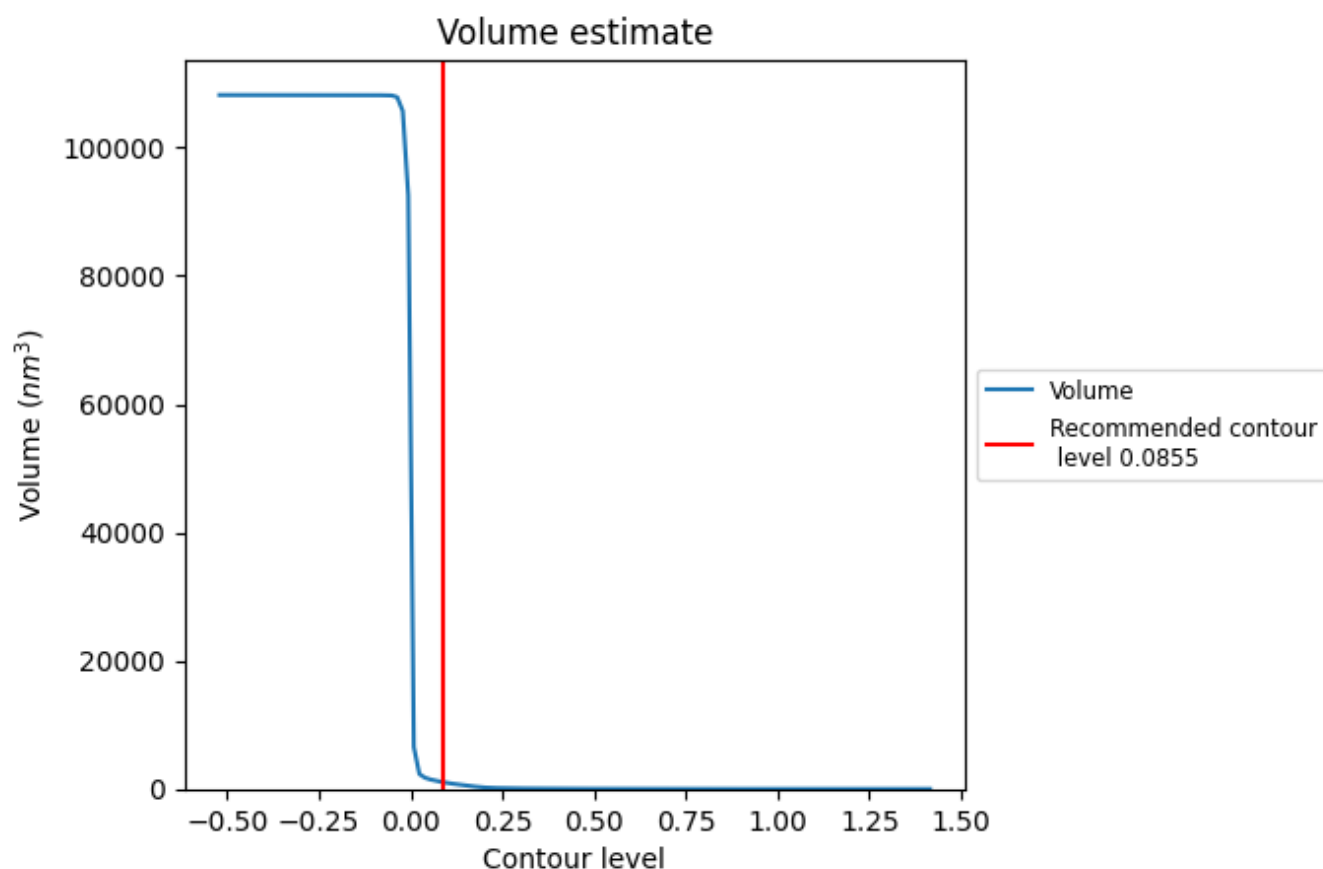
This section contains the results of statistical analysis of the map.

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.

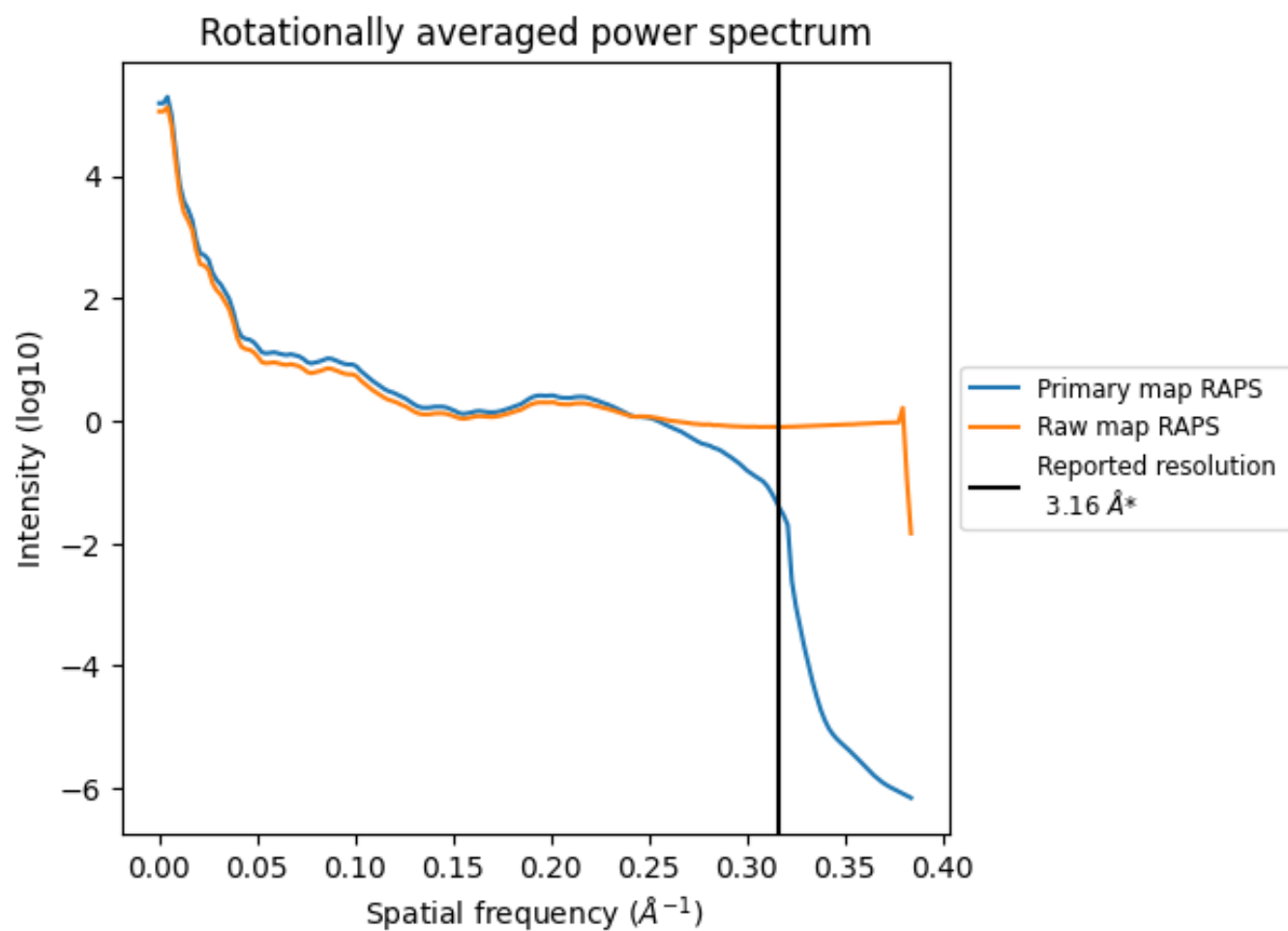
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1082 nm^3 ; this corresponds to an approximate mass of 977 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 ⓘ

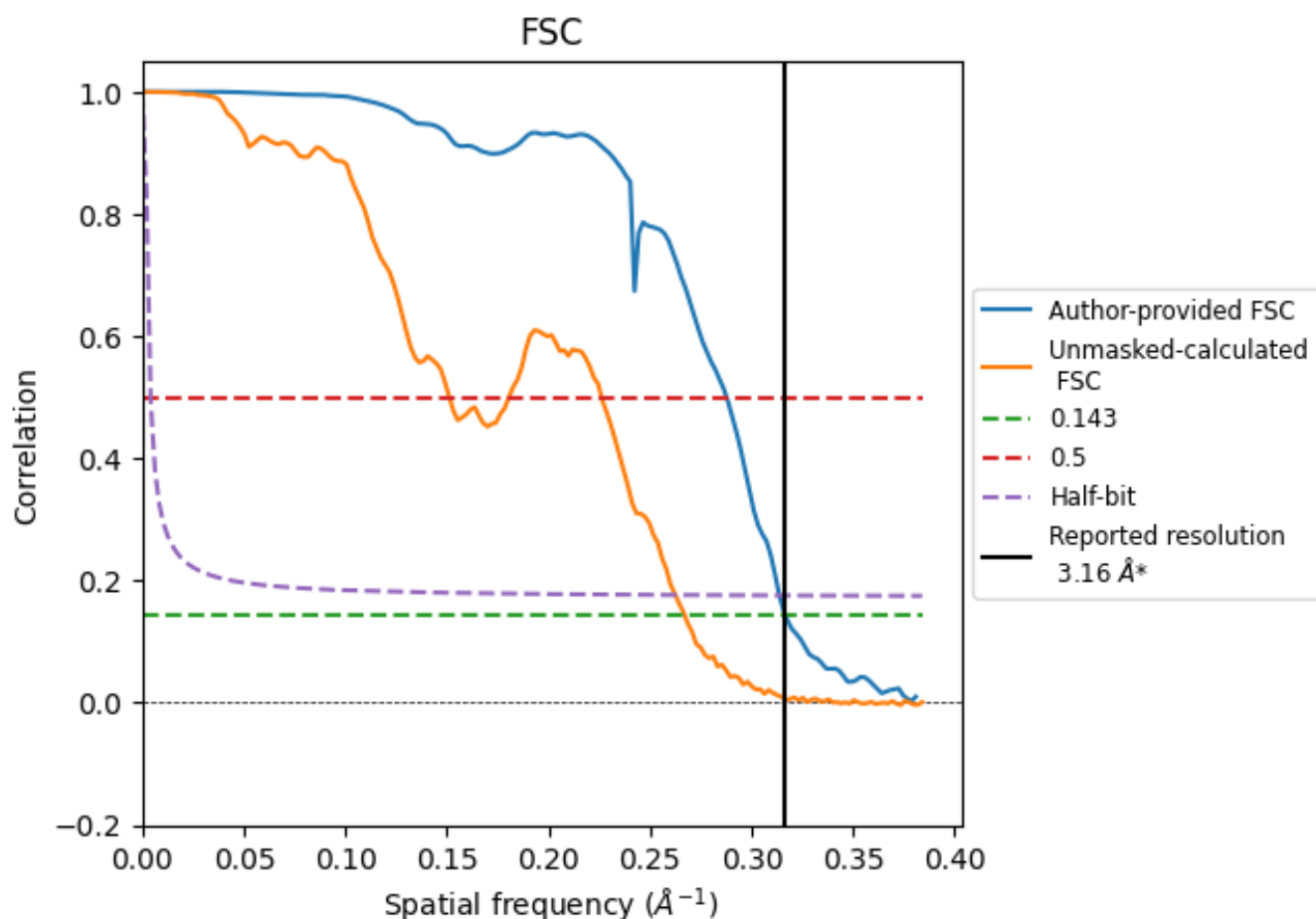


*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

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 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

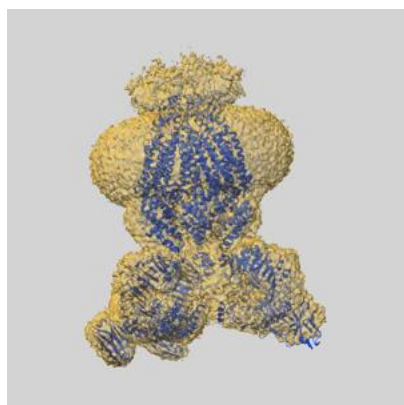
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.48	3.19
Unmasked-calculated*	3.74	6.61	3.81

*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 3.74 differs from the reported value 3.16 by more than 10 %

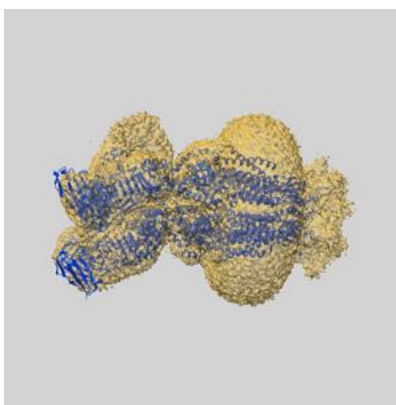
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55591 and PDB model 9T5O. Per-residue inclusion information can be found in section [3](#) on page [10](#).

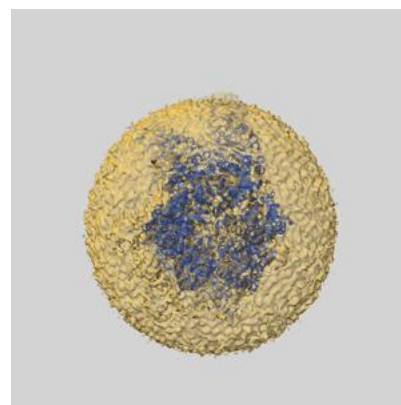
9.1 Map-model overlay [i](#)



X



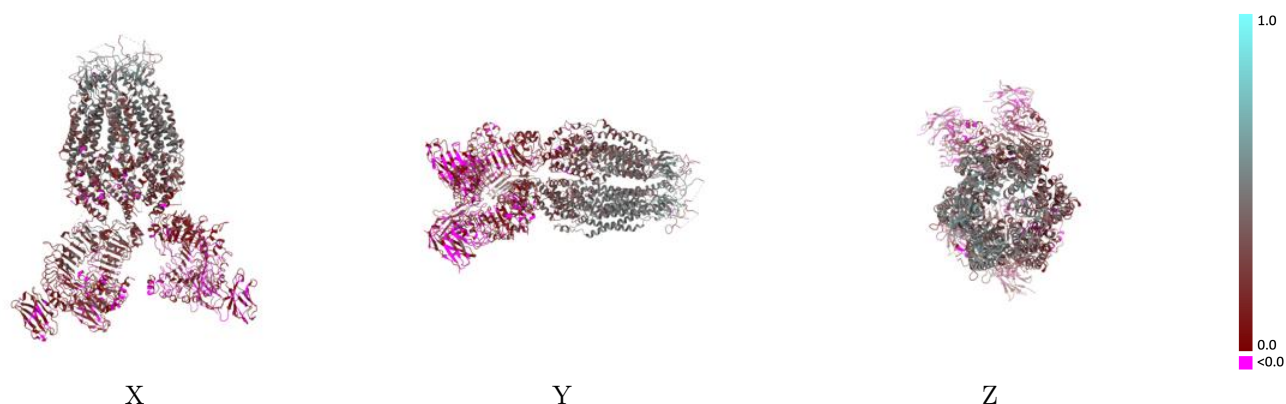
Y



Z

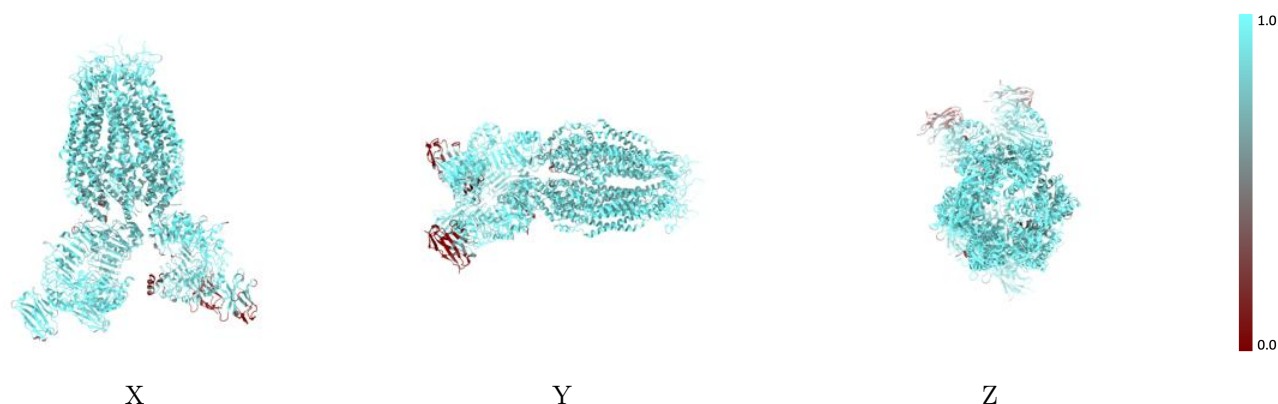
The images above show the 3D surface view of the map at the recommended contour level 0.0855 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



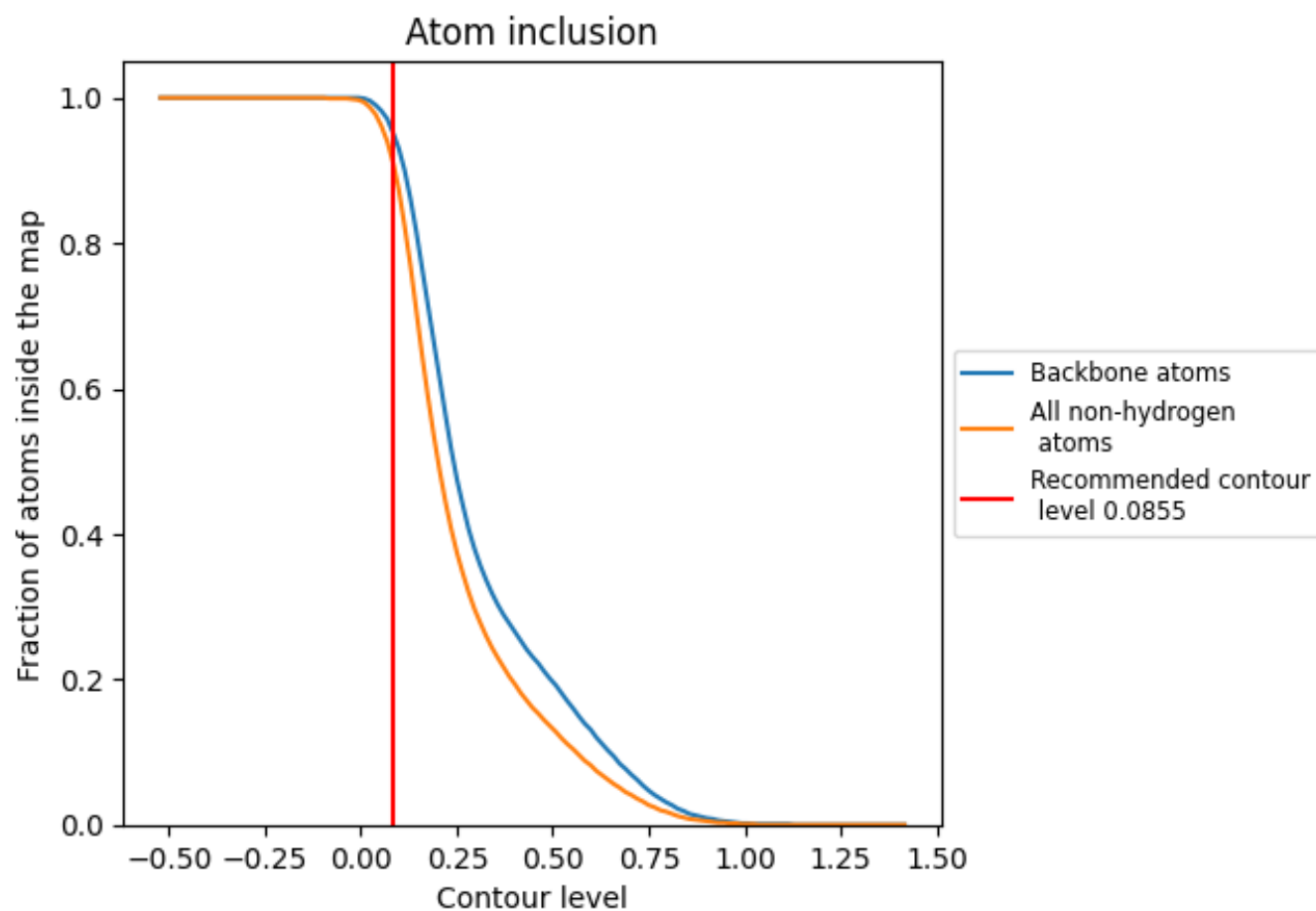
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0855).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.0855) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9080	0.2490
A	0.9220	0.2310
B	0.9360	0.2620
C	0.9520	0.2840
D	0.9460	0.2850
E	0.9060	0.2940
F	0.9140	0.3050
G	0.6450	0.0310
H	0.2630	0.0250
I	0.9660	0.1030
J	0.9580	0.1230

1.0

0.0

<0.0