



## Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 01:35 pm BST

PDB ID : 9QU9 / pdb\_00009qu9  
EMDB ID : EMD-53375  
Title : Cryo-EM structure of Arabidopsis TIR-NLR WRR4A tetramer in complex with effector CCG40 (C2-symmetry)  
Authors : Zhao, H.; Lukyanova, N.; Selvaraj, M.; Jones, J.  
Deposited on : 2025-04-10  
Resolution : 3.50 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

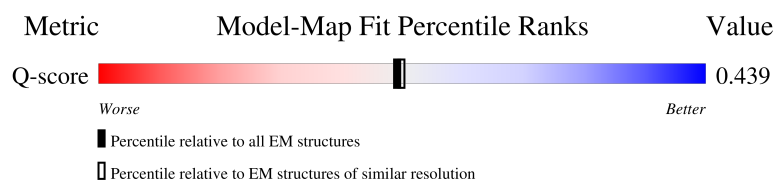
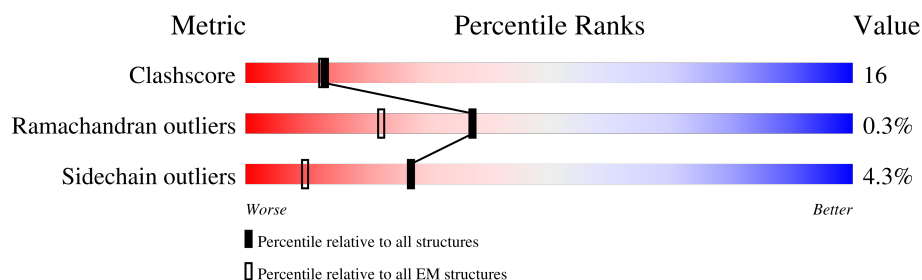
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 3.50 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	13950 ( 3.00 - 4.00 )

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  $\geq 3$ , 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	P	216	
1	Q	216	
1	R	216	
1	S	216	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	1007	<div><div></div><div>66%29%<div><div></div><div></div></div></div></div>
2	B	1007	<div><div></div><div>62%30%<div><div></div><div></div></div></div></div>
2	C	1007	<div><div></div><div>65%28%<div><div></div><div></div></div></div></div>
2	D	1007	<div><div></div><div>67%28%<div><div></div><div></div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33298 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.

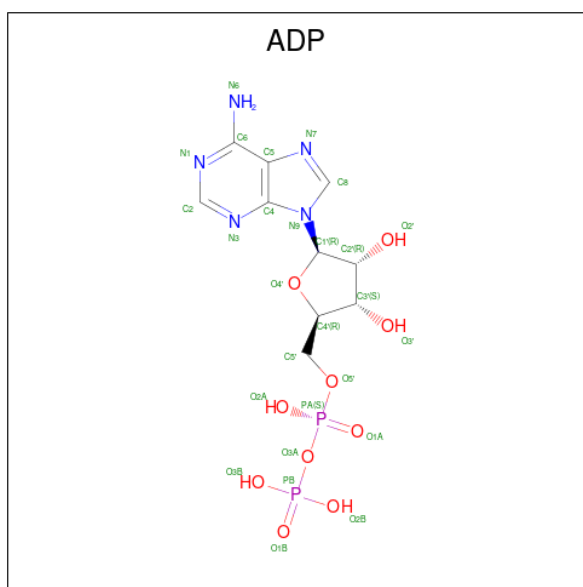
- Molecule 1 is a protein called CCG40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	74	Total	C	N	O	S	0	0
			565	350	98	112	5		
1	Q	76	Total	C	N	O	S	0	0
			576	357	100	114	5		
1	R	74	Total	C	N	O	S	0	0
			565	350	98	112	5		
1	S	73	Total	C	N	O	S	0	0
			558	345	97	111	5		

- Molecule 2 is a protein called Disease resistance protein ADR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	971	Total	C	N	O	S	0	0
			7722	4924	1314	1438	46		
2	B	974	Total	C	N	O	S	0	0
			7737	4933	1317	1441	46		
2	C	971	Total	C	N	O	S	0	0
			7722	4924	1314	1438	46		
2	D	974	Total	C	N	O	S	0	0
			7745	4938	1320	1441	46		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

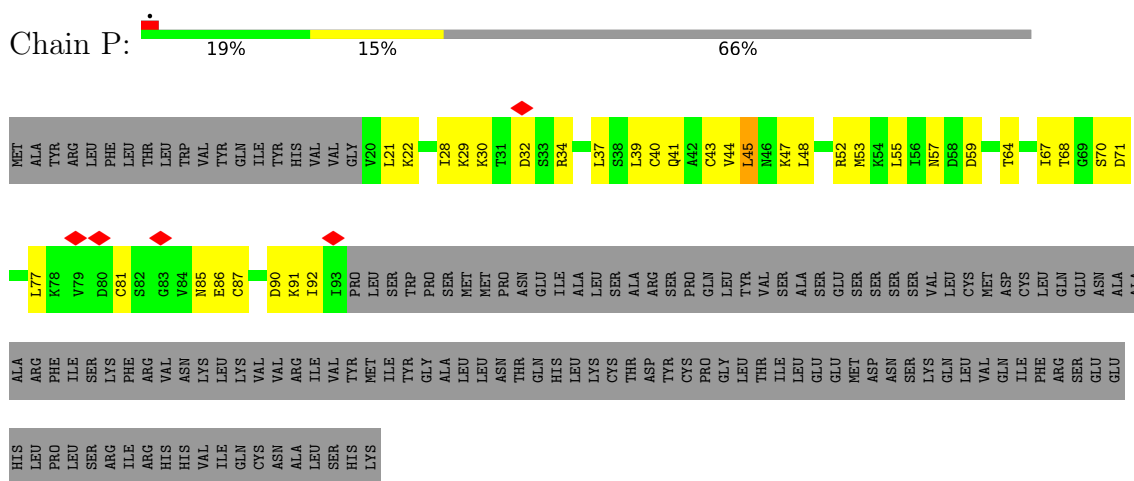


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0

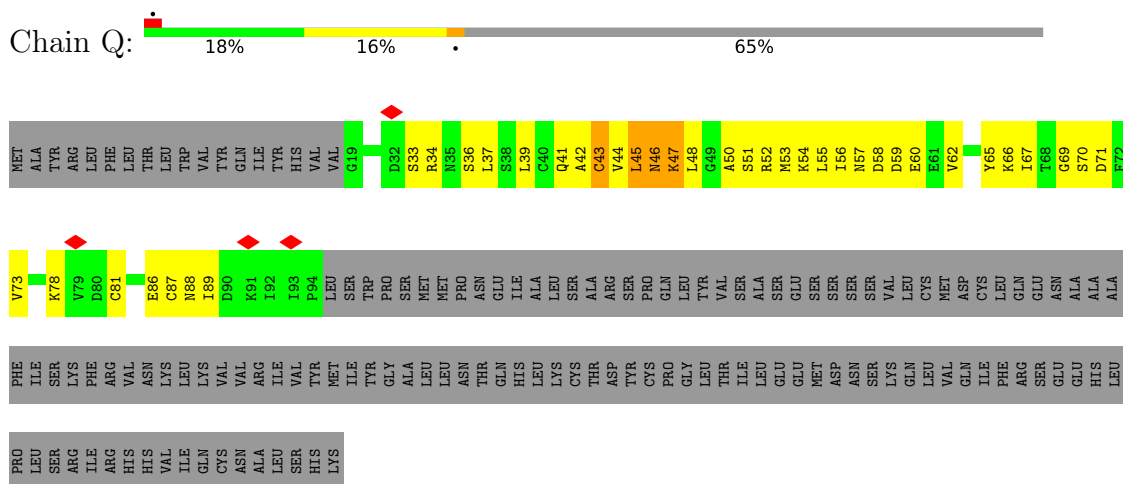
### 3 Residue-property plots

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: CCG40



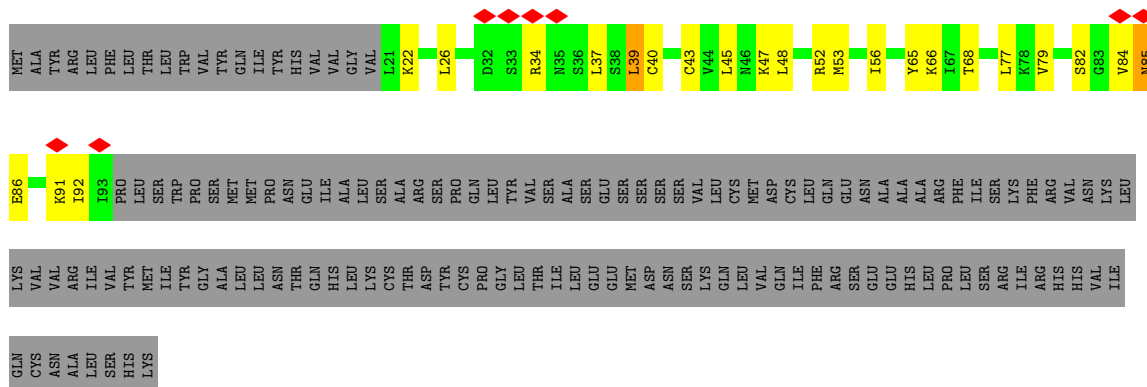
#### • Molecule 1: CCG40



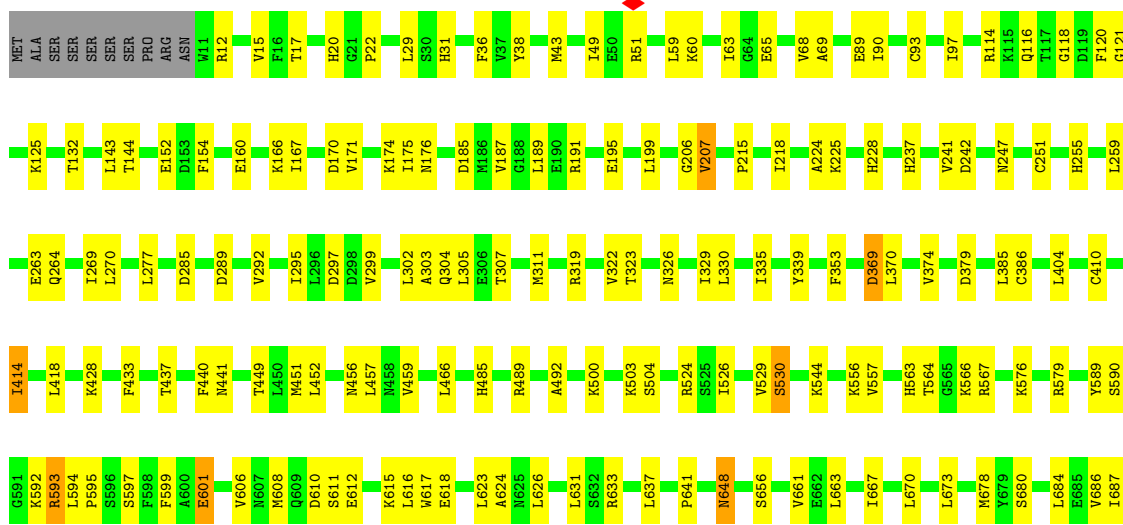
#### • Molecule 1: CCG40

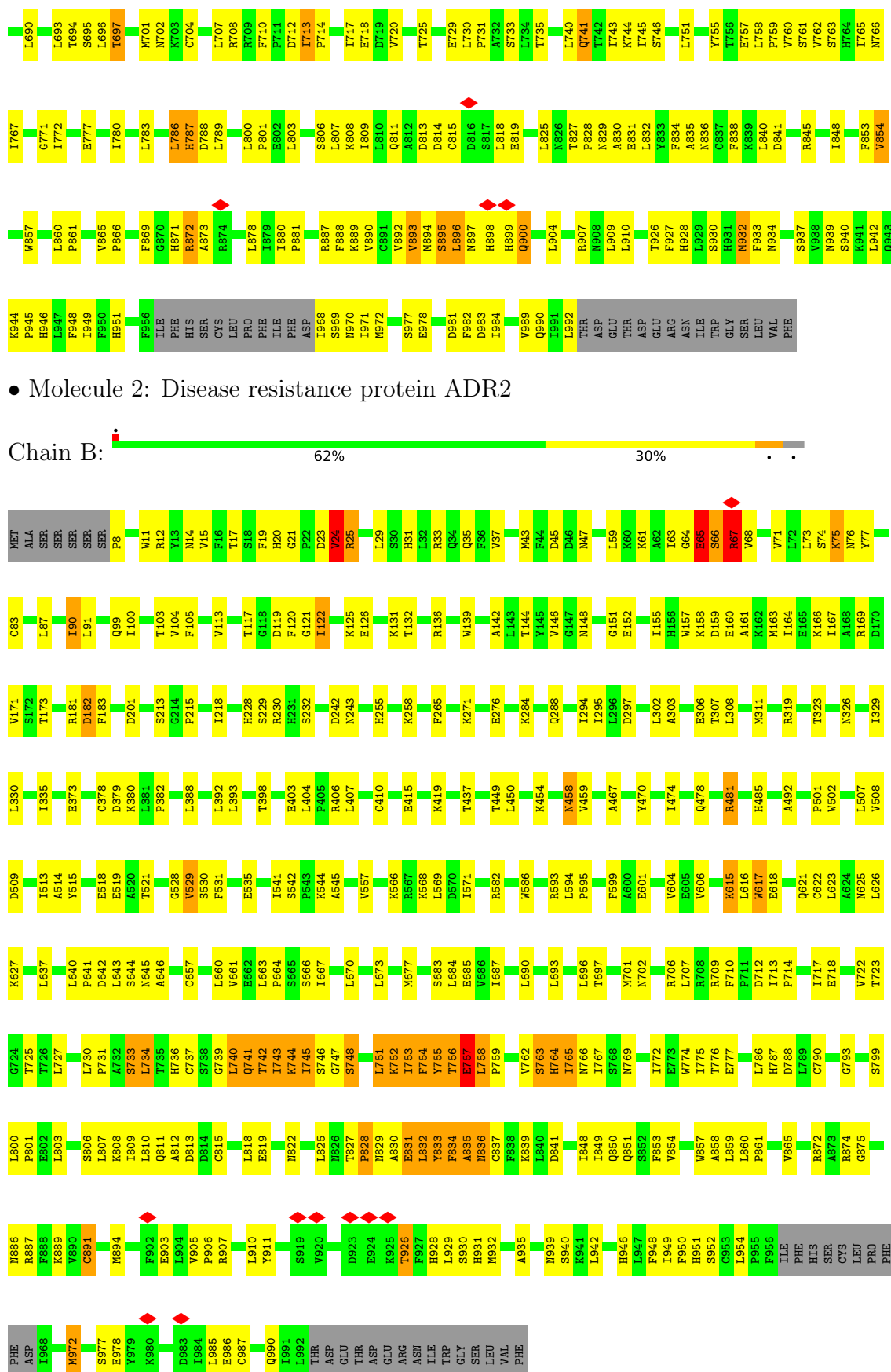


- Molecule 1: CCG40



- Molecule 2: Disease resistance protein ADR2











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	117347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	P	0.17	0/567	0.49	0/759
1	Q	0.35	0/579	0.69	0/776
1	R	0.25	0/568	0.51	0/761
1	S	0.19	0/560	0.52	0/749
2	A	0.27	3/7881 (0.0%)	0.48	3/10662 (0.0%)
2	B	0.36	3/7896 (0.0%)	0.60	12/10683 (0.1%)
2	C	0.31	4/7881 (0.1%)	0.54	8/10662 (0.1%)
2	D	0.27	0/7905	0.50	1/10694 (0.0%)
All	All	0.30	10/33837 (0.0%)	0.53	24/45746 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	529	VAL	C-O	-7.72	1.15	1.24
2	B	25	ARG	C-N	-7.11	1.24	1.33
2	B	25	ARG	C-O	-6.68	1.16	1.24
2	A	530	SER	C-N	-6.61	1.24	1.33
2	C	530	SER	C-O	-6.59	1.16	1.24
2	A	530	SER	C-O	-6.41	1.16	1.24
2	C	531	PHE	C-O	-5.89	1.17	1.24
2	B	755	TYR	C-N	-5.41	1.26	1.33
2	A	529	VAL	C-O	-5.39	1.18	1.24
2	C	531	PHE	C-N	-5.07	1.25	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	65	GLU	N-CA-C	-10.04	100.33	111.28
2	C	531	PHE	CA-CB-CG	9.04	122.84	113.80
2	B	65	GLU	N-CA-C	-8.92	100.41	111.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	741	GLN	CB-CA-C	-7.94	107.42	116.63
2	C	936	ASP	N-CA-C	-7.84	102.73	111.28
2	B	755	TYR	CA-C-N	-7.82	110.43	122.16
2	B	755	TYR	C-N-CA	-7.82	110.43	122.16
2	B	8	PRO	N-CA-CB	6.74	110.41	103.00
2	B	25	ARG	CB-CA-C	-6.03	100.43	110.68
2	C	932	MET	CA-C-N	-5.98	114.68	123.05
2	C	932	MET	C-N-CA	-5.98	114.68	123.05
2	C	851	GLN	CB-CA-C	-5.86	109.83	116.63
2	B	757	GLU	CA-C-O	-5.81	115.01	121.23
2	C	934	ASN	N-CA-C	-5.77	104.99	111.28
2	B	756	THR	N-CA-C	5.64	118.38	108.56
2	B	765	ILE	CA-C-O	-5.57	116.19	121.64
2	A	854	VAL	N-CA-C	-5.37	107.61	112.12
2	C	854	VAL	N-CA-C	-5.30	107.43	111.62
2	A	566	LYS	N-CA-C	-5.26	108.63	114.62
2	C	981	ASP	N-CA-C	-5.24	105.56	111.28
2	B	741	GLN	CB-CA-C	-5.16	110.64	116.63
2	B	835	ALA	CA-C-O	-5.06	115.50	121.16
2	B	67	ARG	N-CA-C	-5.04	100.06	110.80
2	B	765	ILE	N-CA-CB	-5.04	104.84	112.35

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	P	565	0	584	28	0
1	Q	576	0	596	39	0
1	R	565	0	584	30	0
1	S	558	0	573	22	0
2	A	7722	0	7761	239	0
2	B	7737	0	7767	297	0
2	C	7722	0	7761	240	0
2	D	7745	0	7784	253	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	2	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
All	All	33298	0	33458	1096	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 16.

All (1096) 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:A:895:SER:HA	2:A:982:PHE:HA	1.30	1.11
2:D:67:ARG:HB3	2:D:100:ILE:HD12	1.26	1.06
2:A:896:LEU:HB3	2:A:898:HIS:CE1	1.93	1.04
2:D:880:ILE:HD13	2:D:971:ILE:HD11	1.42	1.02
2:B:19:PHE:HZ	2:B:25:ARG:HG3	1.27	0.99
2:B:806:SER:HA	2:B:830:ALA:HB2	1.44	0.99
2:C:977:SER:HB3	2:C:980:LYS:HA	1.48	0.95
2:A:893:VAL:HB	2:A:945:PRO:HB2	1.53	0.91
2:D:11:TRP:CD1	2:D:64:GLY:HA2	2.05	0.90
1:Q:55:LEU:HD21	2:B:906:PRO:HB3	1.56	0.87
2:B:741:GLN:HA	2:B:762:VAL:HA	1.55	0.86
2:A:896:LEU:HB3	2:A:898:HIS:HE1	1.38	0.86
2:B:747:GLY:HA2	2:B:769:ASN:HB3	1.57	0.84
2:A:898:HIS:CE1	2:A:899:HIS:CD2	2.67	0.82
2:A:889:LYS:HG3	2:A:990:GLN:HG2	1.62	0.81
2:C:714:PRO:HD2	2:C:717:ILE:HB	1.60	0.80
2:A:733:SER:HB3	2:A:757:GLU:HB3	1.62	0.80
2:B:772:ILE:HD12	2:B:775:ILE:HD11	1.64	0.80
2:A:828:PRO:HB2	2:A:854:VAL:HG12	1.64	0.79
2:A:896:LEU:CB	2:A:898:HIS:CE1	2.65	0.79
1:S:34:ARG:HH21	1:S:37:LEU:HD11	1.48	0.79
2:B:790:CYS:HA	2:B:809:ILE:HG23	1.65	0.78
2:B:723:THR:HB	2:B:746:SER:HB2	1.65	0.78
1:P:53:MET:HB3	1:P:67:ILE:HD12	1.64	0.78
2:D:880:ILE:HB	2:D:971:ILE:HG12	1.64	0.78
2:A:789:LEU:HG	2:A:807:LEU:HD22	1.67	0.77
2:C:863:LEU:HG	2:C:864:GLU:HG2	1.67	0.77
2:D:66:SER:HB2	2:D:175:ILE:CD1	2.15	0.76
2:C:903:GLU:HB3	2:C:939:ASN:HD21	1.50	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:800:LEU:HG	2:A:818:LEU:HD11	1.68	0.76
2:B:730:LEU:HB3	2:B:755:TYR:HD1	1.51	0.76
2:C:196:MET:HG2	2:C:227:LEU:HD11	1.66	0.75
2:C:808:LYS:HB3	2:C:931:HIS:CE1	2.22	0.75
2:D:879:ILE:HB	2:D:970:ASN:HA	1.66	0.75
2:A:684:LEU:HD11	2:A:687:ILE:HG22	1.66	0.75
2:C:809:ILE:HD13	2:C:932:MET:HB3	1.68	0.75
2:B:730:LEU:HD21	2:B:751:LEU:HD22	1.68	0.75
2:B:65:GLU:HG3	2:C:288:GLN:HG3	1.67	0.75
2:A:898:HIS:NE2	2:A:899:HIS:CD2	2.55	0.74
2:B:831:GLU:HB3	2:B:857:TRP:H	1.50	0.74
2:D:742:THR:HA	2:D:764:HIS:O	1.88	0.73
2:A:900:GLN:HG2	2:A:981:ASP:HA	1.70	0.73
2:D:450:LEU:HD13	2:D:627:LYS:HD2	1.69	0.73
2:B:811:GLN:HA	2:B:834:PHE:HA	1.70	0.73
2:D:845:ARG:HG3	2:D:860:LEU:HD11	1.70	0.73
2:D:788:ASP:HB3	2:D:808:LYS:HB2	1.69	0.73
2:C:207:VAL:HG12	2:C:311:MET:HE2	1.70	0.73
2:D:63:ILE:HG22	2:D:99:GLN:OE1	1.89	0.73
2:A:758:LEU:HD12	2:A:759:PRO:HD2	1.71	0.72
2:C:808:LYS:CB	2:C:931:HIS:CE1	2.73	0.72
2:C:908:ASN:C	2:C:908:ASN:HD22	1.95	0.72
2:A:330:LEU:HD22	2:A:335:ILE:HD12	1.71	0.72
2:D:897:ASN:ND2	2:D:942:LEU:O	2.23	0.71
1:S:52:ARG:HB3	1:S:68:THR:HB	1.71	0.71
1:P:30:LYS:NZ	1:P:59:ASP:O	2.24	0.71
2:A:593:ARG:HA	2:A:615:LYS:O	1.91	0.71
2:B:972:MET:SD	2:B:972:MET:N	2.63	0.71
1:Q:54:LYS:HD3	1:Q:66:LYS:HE3	1.73	0.71
2:B:743:ILE:HD11	2:B:758:LEU:HD21	1.73	0.70
2:D:733:SER:HB3	2:D:757:GLU:HB3	1.72	0.70
1:Q:39:LEU:O	1:Q:43:CYS:HB3	1.92	0.70
2:A:783:LEU:HD22	2:A:786:LEU:HD12	1.73	0.70
2:D:873:ALA:HB2	2:D:878:LEU:HD22	1.73	0.69
2:A:896:LEU:CD2	2:A:898:HIS:HE1	2.05	0.69
2:A:897:ASN:HD21	2:A:942:LEU:H	1.39	0.69
2:B:849:ILE:O	2:B:889:LYS:NZ	2.26	0.69
1:S:45:LEU:HD11	1:S:53:MET:HE2	1.75	0.68
2:D:794:CYS:H	2:D:813:ASP:HA	1.59	0.68
2:D:723:THR:HB	2:D:746:SER:HB3	1.75	0.68
2:D:891:CYS:HB2	2:D:947:LEU:HD13	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:907:ARG:NH2	2:A:940:SER:OG	2.27	0.68
2:B:730:LEU:HB3	2:B:755:TYR:CD1	2.29	0.68
2:C:311:MET:HE3	2:C:311:MET:HA	1.76	0.68
2:D:869:PHE:O	2:D:872:ARG:NH1	2.26	0.68
2:B:454:LYS:HE2	2:B:582:ARG:HH21	1.58	0.68
2:B:617:TRP:CZ2	2:B:641:PRO:HB2	2.29	0.68
2:D:740:LEU:HD21	2:D:743:ILE:HG12	1.76	0.68
2:D:789:LEU:HB2	2:D:807:LEU:HD11	1.76	0.67
1:P:52:ARG:HH22	2:A:934:ASN:H	1.42	0.67
2:B:67:ARG:HG2	2:B:99:GLN:HA	1.75	0.67
2:C:258:LYS:HE3	2:C:307:THR:HG22	1.76	0.67
2:D:944:LYS:HD3	2:D:945:PRO:HD2	1.75	0.67
2:A:567:ARG:HH21	2:A:612:GLU:HG3	1.59	0.67
1:Q:52:ARG:HH12	2:B:809:ILE:HG21	1.60	0.67
2:B:747:GLY:CA	2:B:769:ASN:HB3	2.24	0.67
2:A:207:VAL:HB	2:A:311:MET:HE2	1.75	0.67
2:C:734:LEU:HG	2:C:757:GLU:HG2	1.75	0.67
1:S:84:VAL:O	1:S:85:ASN:ND2	2.27	0.67
1:S:56:ILE:HD12	1:S:56:ILE:H	1.60	0.66
2:B:874:ARG:HH11	2:B:875:GLY:H	1.44	0.66
2:D:777:GLU:OE1	2:D:822:ASN:ND2	2.28	0.66
2:A:741:GLN:O	2:A:743:ILE:HD12	1.95	0.66
2:B:690:LEU:HD22	2:B:693:LEU:HG	1.77	0.66
2:C:808:LYS:HB2	2:C:931:HIS:HE1	1.60	0.66
2:B:753:ILE:HD11	2:B:774:TRP:HE3	1.59	0.66
2:D:777:GLU:HA	2:D:801:PRO:HB3	1.77	0.66
2:C:766:ASN:HA	2:C:790:CYS:HB2	1.78	0.66
2:D:663:LEU:HD23	2:D:664:PRO:HD2	1.78	0.66
2:B:19:PHE:CZ	2:B:25:ARG:HG3	2.19	0.66
2:B:727:LEU:HB2	2:B:751:LEU:HD23	1.77	0.66
2:C:209:MET:HG3	2:C:311:MET:SD	2.36	0.66
2:D:68:VAL:HG11	2:D:171:VAL:HG13	1.77	0.66
2:A:777:GLU:HA	2:A:801:PRO:HB3	1.77	0.66
2:A:835:ALA:HB1	2:A:942:LEU:HD21	1.78	0.66
2:D:67:ARG:HD2	2:D:99:GLN:HA	1.77	0.66
2:A:895:SER:CA	2:A:982:PHE:HA	2.18	0.66
2:C:697:THR:HB	2:C:718:GLU:HG3	1.77	0.66
2:B:163:MET:HE2	2:B:167:ILE:HD11	1.76	0.66
2:B:865:VAL:HG11	2:B:872:ARG:HG2	1.78	0.65
2:C:699:LEU:HD21	2:C:701:MET:HE3	1.78	0.65
2:D:207:VAL:HG12	2:D:311:MET:HE2	1.77	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:739:GLY:O	2:D:740:LEU:HB3	1.96	0.65
2:A:648:ASN:OD1	2:A:648:ASN:N	2.28	0.65
2:A:873:ALA:HB2	2:A:878:LEU:HD13	1.79	0.65
2:A:894:MET:HE1	2:A:984:ILE:HA	1.79	0.65
2:B:832:LEU:O	2:B:858:ALA:HB1	1.97	0.65
2:B:745:ILE:HG23	2:B:767:ILE:HA	1.76	0.65
2:D:87:LEU:HD11	2:D:146:VAL:HG11	1.78	0.65
1:Q:44:VAL:HG22	1:Q:48:LEU:HD12	1.79	0.65
2:D:19:PHE:CE2	2:D:25:ARG:HB2	2.32	0.65
2:A:31:HIS:HE2	2:B:160:GLU:HG2	1.61	0.64
1:R:54:LYS:HE2	2:C:931:HIS:HB3	1.80	0.64
2:C:24:VAL:HG13	2:C:28:PHE:HB3	1.79	0.64
2:A:806:SER:HB3	2:A:808:LYS:HZ2	1.60	0.64
2:C:809:ILE:HD13	2:C:932:MET:CB	2.26	0.64
2:D:849:ILE:HD11	2:D:860:LEU:HD22	1.80	0.64
2:C:330:LEU:HD22	2:C:335:ILE:HD12	1.78	0.64
2:C:903:GLU:HB3	2:C:939:ASN:ND2	2.13	0.64
2:A:311:MET:HE3	2:A:311:MET:HA	1.79	0.63
2:C:247:ASN:ND2	2:C:264:GLN:OE1	2.31	0.63
2:D:907:ARG:HD3	2:D:929:LEU:HD23	1.78	0.63
2:A:740:LEU:HD12	2:A:761:SER:H	1.63	0.63
2:B:326:ASN:HB3	2:B:329:ILE:HD12	1.81	0.63
2:A:631:LEU:HD13	2:A:637:LEU:HD11	1.78	0.63
2:D:21:GLY:HA3	2:D:25:ARG:HH21	1.61	0.63
2:C:17:THR:HG1	2:C:19:PHE:HD1	1.45	0.63
2:D:209:MET:HE2	2:D:311:MET:HG2	1.80	0.63
2:C:31:HIS:HE2	2:D:160:GLU:HG2	1.63	0.63
2:C:840:LEU:O	2:C:845:ARG:NH1	2.31	0.63
2:D:63:ILE:HG21	2:D:97:ILE:HG21	1.79	0.63
2:D:894:MET:SD	2:D:982:PHE:HB2	2.39	0.63
2:B:663:LEU:HD23	2:B:664:PRO:HD2	1.81	0.63
2:A:840:LEU:HD23	2:A:861:PRO:HG2	1.80	0.63
2:A:896:LEU:CB	2:A:898:HIS:HE1	2.07	0.63
2:A:898:HIS:NE2	2:A:899:HIS:HD2	1.97	0.63
2:A:237:HIS:HB2	2:A:292:VAL:HG12	1.79	0.62
2:A:353:PHE:HB2	2:A:385:LEU:HD22	1.80	0.62
2:C:225:LYS:HE2	2:D:255:HIS:HB3	1.80	0.62
1:Q:44:VAL:CG2	1:Q:89:ILE:HD11	2.28	0.62
2:B:906:PRO:HB2	2:B:928:HIS:CE1	2.34	0.62
2:B:857:TRP:HB2	2:B:950:PHE:HA	1.82	0.62
2:B:910:LEU:HD11	2:B:978:GLU:HG2	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:848:ILE:HG21	2:C:860:LEU:HD21	1.80	0.62
2:B:722:VAL:O	2:B:745:ILE:HA	1.99	0.62
2:C:353:PHE:HB2	2:C:385:LEU:HD22	1.80	0.62
2:A:910:LEU:HD21	2:A:978:GLU:HG2	1.83	0.61
2:C:882:TYR:HB3	2:C:968:ILE:HB	1.82	0.61
1:Q:57:ASN:OD1	1:Q:58:ASP:N	2.32	0.61
2:A:892:VAL:HB	2:A:894:MET:SD	2.41	0.61
2:B:853:PHE:H	2:B:951:HIS:HD1	1.49	0.61
2:B:910:LEU:HD13	2:B:977:SER:HA	1.81	0.61
2:D:542:SER:HB2	2:D:545:ALA:HB2	1.82	0.61
2:A:215:PRO:HD2	2:A:218:ILE:HG13	1.81	0.61
2:B:77:TYR:CE1	2:B:83:CYS:HB3	2.36	0.61
2:D:12:ARG:H	2:D:61:LYS:HB3	1.65	0.61
2:A:896:LEU:HD11	2:A:983:ASP:HB3	1.81	0.61
2:B:542:SER:HB2	2:B:545:ALA:HB2	1.81	0.61
2:D:868:GLU:O	2:D:990:GLN:NE2	2.34	0.61
1:P:40:CYS:O	1:P:44:VAL:HG12	2.01	0.61
2:A:225:LYS:HE2	2:B:255:HIS:HB3	1.81	0.61
2:A:263:GLU:HG3	2:A:277:LEU:HB2	1.82	0.61
2:B:723:THR:HA	2:B:746:SER:H	1.65	0.61
2:B:741:GLN:HA	2:B:762:VAL:CA	2.30	0.61
2:B:741:GLN:N	2:B:762:VAL:HG12	2.15	0.61
2:D:14:ASN:O	2:D:68:VAL:HB	2.01	0.61
2:D:887:ARG:HH11	2:D:951:HIS:HE1	1.49	0.61
2:B:119:ASP:OD2	2:B:119:ASP:N	2.34	0.61
2:C:593:ARG:HG3	2:C:615:LYS:HG2	1.82	0.60
1:R:54:LYS:CE	2:C:931:HIS:HB3	2.31	0.60
1:S:77:LEU:HD13	1:S:92:ILE:HD12	1.82	0.60
2:D:970:ASN:O	2:D:971:ILE:HG23	2.02	0.60
2:C:218:ILE:HA	2:C:382:PRO:HD2	1.82	0.60
2:D:109:ASP:OD2	2:D:112:HIS:ND1	2.34	0.60
2:B:181:ARG:HD2	2:B:229:SER:HB3	1.83	0.60
2:B:19:PHE:CZ	2:B:29:LEU:HD22	2.35	0.60
2:D:63:ILE:CD1	2:D:97:ILE:HD13	2.32	0.60
2:A:696:LEU:HD13	2:A:714:PRO:HG3	1.84	0.60
2:A:17:THR:HG21	2:A:29:LEU:HD11	1.84	0.60
2:B:741:GLN:NE2	2:B:763:SER:HB2	2.17	0.60
2:C:24:VAL:HG12	2:C:29:LEU:HB2	1.84	0.60
2:D:64:GLY:H	2:D:67:ARG:HD3	1.65	0.60
2:C:116:GLN:N	2:C:116:GLN:OE1	2.35	0.60
2:A:247:ASN:ND2	2:A:264:GLN:OE1	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ARG:HH22	2:B:230:ARG:HH21	1.47	0.59
2:A:576:LYS:HE3	2:A:597:SER:HB3	1.85	0.59
2:A:12:ARG:NH1	2:A:65:GLU:OE1	2.35	0.59
2:B:663:LEU:HD22	2:B:667:ILE:HG12	1.84	0.59
2:B:894:MET:HB3	2:B:948:PHE:HE2	1.67	0.59
2:B:906:PRO:HB2	2:B:928:HIS:HE1	1.66	0.59
1:R:55:LEU:H	2:C:930:SER:CB	2.15	0.59
2:A:228:HIS:HB2	2:A:295:ILE:HD12	1.83	0.59
2:A:832:LEU:HB3	2:A:834:PHE:HE2	1.67	0.59
2:B:218:ILE:HA	2:B:382:PRO:HD2	1.85	0.59
2:B:808:LYS:NZ	2:B:830:ALA:HA	2.17	0.59
2:B:831:GLU:HB3	2:B:857:TRP:N	2.17	0.59
2:D:67:ARG:CB	2:D:100:ILE:HD12	2.18	0.59
2:D:67:ARG:CD	2:D:99:GLN:HA	2.33	0.59
2:C:777:GLU:HA	2:C:801:PRO:HB3	1.84	0.59
2:C:892:VAL:O	2:C:948:PHE:N	2.31	0.59
2:A:898:HIS:CE1	2:A:899:HIS:HD2	2.18	0.59
2:D:567:ARG:HH12	2:D:612:GLU:HB2	1.67	0.59
2:A:524:ARG:NH1	2:D:518:GLU:OE2	2.30	0.59
2:D:15:VAL:HG13	2:D:68:VAL:HG12	1.84	0.59
2:C:14:ASN:HB3	2:C:175:ILE:HD11	1.84	0.59
2:D:19:PHE:HB2	2:D:24:VAL:CG1	2.32	0.59
2:B:508:VAL:HG12	2:B:530:SER:HB3	1.85	0.59
2:C:697:THR:HA	2:C:717:ILE:HA	1.83	0.59
2:D:739:GLY:HA2	2:D:761:SER:HB2	1.83	0.59
2:B:806:SER:H	2:B:827:THR:HG21	1.67	0.58
2:C:808:LYS:HB2	2:C:931:HIS:CE1	2.37	0.58
2:C:889:LYS:HD2	2:C:951:HIS:CE1	2.38	0.58
2:C:395:LYS:HE3	2:D:332:GLN:HE21	1.69	0.58
2:D:20:HIS:O	2:D:24:VAL:HG12	2.03	0.58
2:D:66:SER:HB2	2:D:175:ILE:HD12	1.84	0.58
2:D:228:HIS:HB2	2:D:295:ILE:HD12	1.85	0.58
2:D:764:HIS:HB3	2:D:787:HIS:HB2	1.85	0.58
2:D:326:ASN:HB3	2:D:329:ILE:HD12	1.84	0.58
2:A:60:LYS:HA	2:A:63:ILE:HD12	1.85	0.58
2:B:182:ASP:OD1	2:C:255:HIS:NE2	2.31	0.58
2:A:667:ILE:HA	2:A:670:LEU:HG	1.84	0.58
2:B:745:ILE:CG2	2:B:767:ILE:HA	2.33	0.58
1:R:55:LEU:HB3	2:C:930:SER:HB3	1.85	0.58
2:A:766:ASN:ND2	2:A:934:ASN:OD1	2.37	0.58
2:B:819:GLU:HB3	2:B:839:LYS:HG2	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:PHE:CE1	2:B:29:LEU:HD22	2.39	0.58
1:S:39:LEU:HD13	1:S:86:GLU:HG3	1.84	0.58
2:B:87:LEU:HD11	2:B:146:VAL:HG11	1.85	0.58
2:B:696:LEU:HD23	2:B:714:PRO:HG2	1.86	0.58
2:B:742:THR:HG23	2:B:764:HIS:CD2	2.39	0.58
2:C:228:HIS:HB2	2:C:295:ILE:HD12	1.86	0.58
2:D:66:SER:HA	2:D:175:ILE:HD13	1.84	0.58
2:A:712:ASP:OD1	2:A:713:ILE:N	2.37	0.58
2:B:806:SER:CA	2:B:830:ALA:HB2	2.28	0.57
2:B:767:ILE:HG21	2:B:772:ILE:HD13	1.85	0.57
2:D:696:LEU:HD23	2:D:714:PRO:HG2	1.86	0.57
1:Q:51:SER:HB3	1:Q:69:GLY:HA2	1.86	0.57
2:B:458:ASN:N	2:B:458:ASN:OD1	2.37	0.57
2:B:730:LEU:CD2	2:B:751:LEU:HD22	2.33	0.57
2:A:302:LEU:HD21	2:D:393:LEU:HD23	1.86	0.57
2:C:907:ARG:HG2	2:C:929:LEU:HB2	1.85	0.57
2:A:269:ILE:HG22	2:A:270:LEU:HD23	1.85	0.57
2:B:77:TYR:HE1	2:B:83:CYS:HB3	1.70	0.57
2:B:713:ILE:HD12	2:B:736:HIS:HB3	1.86	0.57
2:C:887:ARG:HB2	2:C:992:LEU:HD22	1.87	0.57
1:R:32:ASP:O	1:R:34:ARG:NH1	2.38	0.56
2:A:326:ASN:HB3	2:A:329:ILE:HD12	1.88	0.56
2:B:11:TRP:CE3	2:B:63:ILE:HB	2.40	0.56
2:D:77:TYR:CE1	2:D:83:CYS:HB3	2.39	0.56
2:D:218:ILE:HA	2:D:382:PRO:HD2	1.86	0.56
1:Q:48:LEU:C	1:Q:73:VAL:HG13	2.30	0.56
2:B:518:GLU:OE2	2:C:524:ARG:NH1	2.36	0.56
2:B:886:ASN:ND2	2:B:954:LEU:O	2.39	0.56
2:D:874:ARG:HH12	2:D:986:GLU:HA	1.70	0.56
2:B:71:VAL:HB	2:B:103:THR:HG22	1.87	0.56
2:B:604:VAL:HA	2:B:626:LEU:HA	1.87	0.56
2:B:754:PHE:CD2	2:B:775:ILE:HD13	2.40	0.56
2:D:415:GLU:OE2	2:D:419:LYS:NZ	2.37	0.56
2:D:743:ILE:HB	2:D:765:ILE:HG23	1.87	0.56
2:A:289:ASP:OD2	2:D:65:GLU:HB3	2.05	0.56
2:A:809:ILE:HG13	2:A:811:GLN:HG3	1.86	0.56
2:A:972:MET:SD	2:A:972:MET:N	2.77	0.56
2:B:67:ARG:HB3	2:B:100:ILE:H	1.70	0.56
2:C:879:ILE:HB	2:C:970:ASN:HA	1.86	0.56
2:C:978:GLU:H	2:C:982:PHE:HE1	1.53	0.56
1:P:90:ASP:O	1:P:91:LYS:HG2	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:HIS:CD2	2:A:22:PRO:HD2	2.41	0.56
2:A:981:ASP:OD1	2:A:981:ASP:N	2.38	0.56
1:R:40:CYS:O	1:R:44:VAL:HG12	2.05	0.56
2:A:242:ASP:N	2:A:242:ASP:OD1	2.38	0.56
2:B:144:THR:O	2:B:148:ASN:ND2	2.39	0.56
2:C:63:ILE:HD11	2:C:86:GLU:OE2	2.06	0.56
2:C:178:THR:HG1	2:D:279:HIS:HE2	1.52	0.56
1:S:43:CYS:HA	1:S:47:LYS:NZ	2.21	0.56
2:A:615:LYS:HG2	2:A:616:LEU:H	1.71	0.56
2:B:415:GLU:OE2	2:B:419:LYS:NZ	2.33	0.56
2:C:567:ARG:NH1	2:C:612:GLU:HG2	2.21	0.56
2:C:710:PHE:HZ	2:C:713:ILE:HG23	1.69	0.56
2:A:299:VAL:HG21	2:A:322:VAL:HG13	1.88	0.55
2:B:911:TYR:HB3	2:B:926:THR:HA	1.88	0.55
2:C:594:LEU:HD23	2:C:613:LEU:HD21	1.88	0.55
2:C:610:ASP:OD2	2:C:633:ARG:NH2	2.39	0.55
2:B:265:PHE:HZ	2:B:294:ILE:HD12	1.71	0.55
2:B:617:TRP:CZ2	2:B:623:LEU:HD11	2.41	0.55
2:B:707:LEU:HD21	2:B:725:THR:HG23	1.89	0.55
2:D:11:TRP:CE3	2:D:63:ILE:HD11	2.41	0.55
1:Q:34:ARG:CZ	1:Q:34:ARG:HA	2.37	0.55
2:A:710:PHE:HB3	2:A:731:PRO:HD3	1.89	0.55
2:B:14:ASN:HA	2:B:66:SER:HB2	1.87	0.55
2:B:713:ILE:HD11	2:B:734:LEU:HD13	1.88	0.55
2:B:887:ARG:HH21	2:B:990:GLN:HB3	1.72	0.55
2:C:523:ASN:HB3	2:C:526:ILE:HG23	1.87	0.55
2:D:33:ARG:NE	2:D:45:ASP:OD2	2.40	0.55
2:B:748:SER:HB3	2:B:751:LEU:HD21	1.88	0.55
2:B:809:ILE:HG13	2:B:811:GLN:OE1	2.07	0.55
2:D:247:ASN:ND2	2:D:264:GLN:OE1	2.39	0.55
2:B:73:LEU:HD13	2:B:105:PHE:CD1	2.42	0.55
2:C:53:GLN:HG2	2:C:82:TRP:HE1	1.72	0.55
2:B:835:ALA:O	2:B:836:ASN:HB2	2.07	0.55
2:C:624:ALA:O	2:C:648:ASN:ND2	2.28	0.55
2:D:834:PHE:H	2:D:859:LEU:HB3	1.70	0.55
2:D:879:ILE:CB	2:D:970:ASN:HA	2.36	0.55
2:B:617:TRP:HD1	2:B:618:GLU:N	2.05	0.55
1:S:26:LEU:HB2	1:S:65:TYR:O	2.07	0.54
2:A:907:ARG:NH2	2:A:939:ASN:OD1	2.38	0.54
2:B:393:LEU:HD23	2:C:302:LEU:HD21	1.89	0.54
2:B:641:PRO:O	2:B:643:LEU:HG	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:ILE:HG13	2:B:860:LEU:HD23	1.89	0.54
2:D:663:LEU:HD22	2:D:667:ILE:HG12	1.90	0.54
2:B:181:ARG:NH2	2:B:230:ARG:HH21	2.05	0.54
2:C:730:LEU:HB2	2:C:753:ILE:HD11	1.89	0.54
1:Q:55:LEU:CD2	2:B:906:PRO:HB3	2.35	0.54
2:A:697:THR:HB	2:A:718:GLU:HG3	1.90	0.54
2:C:775:ILE:HB	2:C:801:PRO:HG2	1.89	0.54
2:D:64:GLY:O	2:D:67:ARG:HB2	2.08	0.54
2:A:615:LYS:NZ	2:A:618:GLU:HA	2.23	0.54
2:A:751:LEU:HD21	2:A:771:GLY:H	1.72	0.54
2:A:896:LEU:HD13	2:A:899:HIS:CG	2.42	0.54
2:D:509:ASP:O	2:D:513:ILE:HD12	2.08	0.54
2:C:914:THR:OG1	2:C:972:MET:O	2.24	0.54
2:A:735:THR:OG1	2:A:759:PRO:HB3	2.07	0.54
2:A:758:LEU:HD21	2:A:765:ILE:HG12	1.89	0.54
2:B:59:LEU:HD23	2:B:90:ILE:HG13	1.89	0.54
1:R:44:VAL:O	1:R:48:LEU:HB3	2.08	0.54
2:B:657:CYS:SG	2:B:660:LEU:HB2	2.48	0.54
2:C:53:GLN:HE21	2:C:82:TRP:HE1	1.56	0.54
2:C:692:ASN:OD1	2:C:692:ASN:N	2.41	0.54
2:D:200:LEU:HD12	2:D:210:VAL:HG21	1.89	0.54
2:D:907:ARG:HE	2:D:909:LEU:HG	1.73	0.54
2:A:663:LEU:HD11	2:A:678:MET:HE1	1.89	0.54
2:A:869:PHE:O	2:A:872:ARG:NH2	2.41	0.54
1:Q:44:VAL:HG23	1:Q:89:ILE:HD11	1.90	0.53
2:B:19:PHE:HD2	2:B:24:VAL:HG23	1.73	0.53
2:B:33:ARG:NE	2:B:45:ASP:OD1	2.39	0.53
2:C:62:ALA:O	2:C:66:SER:OG	2.25	0.53
2:D:11:TRP:HD1	2:D:64:GLY:HA2	1.68	0.53
1:S:34:ARG:NH2	1:S:37:LEU:HD11	2.21	0.53
2:A:116:GLN:N	2:A:116:GLN:OE1	2.42	0.53
2:B:714:PRO:HD2	2:B:717:ILE:HG21	1.89	0.53
2:B:907:ARG:NH2	2:B:940:SER:OG	2.41	0.53
2:C:754:PHE:HD1	2:C:776:THR:H	1.56	0.53
2:C:369:ASP:OD2	2:C:369:ASP:N	2.41	0.53
2:A:714:PRO:HG2	2:A:717:ILE:HB	1.91	0.53
2:C:714:PRO:HD2	2:C:717:ILE:CB	2.36	0.53
2:A:707:LEU:HB3	2:A:725:THR:HB	1.91	0.53
2:B:758:LEU:HD23	2:B:762:VAL:HG11	1.91	0.53
2:D:814:ASP:HB3	2:D:836:ASN:HB2	1.90	0.53
2:A:449:THR:HA	2:A:459:VAL:HG11	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:MET:O	2:B:722:VAL:HA	2.08	0.53
1:S:48:LEU:HG	1:S:79:VAL:HG11	1.90	0.53
2:A:896:LEU:HB3	2:A:898:HIS:ND1	2.22	0.53
2:D:215:PRO:HD2	2:D:218:ILE:HG12	1.91	0.53
2:D:836:ASN:O	2:D:943:GLN:NE2	2.40	0.53
2:B:64:GLY:N	2:B:66:SER:O	2.42	0.53
2:B:745:ILE:CG1	2:B:748:SER:HB2	2.39	0.53
2:A:740:LEU:CD1	2:A:761:SER:H	2.22	0.52
2:B:73:LEU:HD11	2:B:103:THR:HB	1.91	0.52
2:B:514:ALA:O	2:B:518:GLU:HG2	2.09	0.52
2:C:828:PRO:HA	2:C:853:PHE:HA	1.91	0.52
2:C:848:ILE:CG2	2:C:860:LEU:HD21	2.39	0.52
2:D:786:LEU:HD12	2:D:787:HIS:H	1.74	0.52
2:B:718:GLU:HA	2:B:739:GLY:O	2.09	0.52
2:C:781:LYS:HE2	2:C:802:GLU:HB3	1.91	0.52
2:A:191:ARG:O	2:A:195:GLU:HG2	2.09	0.52
2:C:563:HIS:CG	2:C:564:THR:H	2.27	0.52
2:D:528:GLY:O	2:D:529:VAL:HB	2.09	0.52
2:A:896:LEU:HD22	2:A:898:HIS:CE1	2.44	0.52
2:B:67:ARG:O	2:B:100:ILE:N	2.42	0.52
2:B:201:ASP:O	2:B:319:ARG:NH2	2.37	0.52
2:B:535:GLU:OE2	2:B:535:GLU:N	2.32	0.52
2:B:894:MET:HB3	2:B:948:PHE:CE2	2.44	0.52
1:Q:44:VAL:HG21	1:Q:89:ILE:HD11	1.91	0.52
2:A:806:SER:HA	2:A:830:ALA:HA	1.90	0.52
2:C:169:ARG:HH11	2:C:169:ARG:HG2	1.75	0.52
2:C:837:CYS:HB3	2:C:944:LYS:HG2	1.90	0.52
2:D:311:MET:HA	2:D:311:MET:HE3	1.92	0.52
2:B:887:ARG:HD2	2:B:951:HIS:CE1	2.45	0.52
2:B:740:LEU:HB3	2:B:759:PRO:CG	2.39	0.52
2:C:593:ARG:O	2:C:593:ARG:HG2	2.10	0.52
2:C:437:THR:HG21	2:C:492:ALA:HB3	1.92	0.52
2:D:64:GLY:H	2:D:67:ARG:CD	2.22	0.52
1:Q:44:VAL:HB	1:Q:87:CYS:SG	2.50	0.52
2:A:428:LYS:HE2	2:A:457:LEU:HD23	1.91	0.52
2:D:696:LEU:HD21	2:D:699:LEU:HB2	1.92	0.52
2:A:780:ILE:HD12	2:A:801:PRO:HB2	1.91	0.51
2:A:894:MET:HE3	2:A:982:PHE:HD1	1.74	0.51
2:B:741:GLN:CA	2:B:762:VAL:HA	2.35	0.51
2:D:983:ASP:HB2	2:D:985:LEU:HD23	1.91	0.51
2:B:215:PRO:HD2	2:B:218:ILE:HG12	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:707:LEU:HB3	2:C:725:THR:HG23	1.92	0.51
2:D:767:ILE:HB	2:D:791:LEU:HD13	1.92	0.51
1:P:57:ASN:O	1:P:64:THR:N	2.43	0.51
2:A:670:LEU:HD12	2:A:673:LEU:HD22	1.91	0.51
2:B:837:CYS:HG	2:B:946:HIS:CE1	2.24	0.51
2:D:9:ARG:HG3	2:D:10:ASN:N	2.25	0.51
1:S:56:ILE:HD11	1:S:66:LYS:H	1.74	0.51
2:A:686:VAL:HB	2:A:708:ARG:HH21	1.75	0.51
2:A:717:ILE:HG12	2:A:720:VAL:HG22	1.92	0.51
2:B:12:ARG:N	2:B:61:LYS:O	2.44	0.51
2:B:15:VAL:HB	2:B:43:MET:HG2	1.92	0.51
2:C:740:LEU:HD11	2:C:743:ILE:HG12	1.92	0.51
2:D:134:GLU:O	2:D:138:LYS:HG2	2.10	0.51
2:B:640:LEU:HG	2:B:660:LEU:HD11	1.92	0.51
2:A:563:HIS:ND1	2:A:564:THR:N	2.55	0.51
2:B:450:LEU:HG	2:B:627:LYS:HD2	1.92	0.51
2:B:743:ILE:O	2:B:766:ASN:N	2.43	0.51
2:D:242:ASP:OD2	2:D:243:ASN:N	2.41	0.51
2:A:896:LEU:CD2	2:A:898:HIS:CE1	2.91	0.51
2:B:449:THR:HA	2:B:459:VAL:HG11	1.93	0.51
2:C:49:ILE:HG23	2:C:51:ARG:H	1.75	0.51
2:C:908:ASN:C	2:C:908:ASN:ND2	2.67	0.51
2:D:710:PHE:HB3	2:D:731:PRO:HD3	1.93	0.51
1:P:70:SER:OG	1:P:71:ASP:N	2.44	0.51
2:B:228:HIS:HB2	2:B:295:ILE:HD12	1.91	0.51
2:D:163:MET:HE2	2:D:167:ILE:HD11	1.93	0.51
2:D:200:LEU:HD23	2:D:202:LEU:HD21	1.93	0.51
2:A:616:LEU:HD23	2:A:641:PRO:HG3	1.92	0.51
2:C:970:ASN:O	2:C:970:ASN:ND2	2.44	0.51
2:D:220:LYS:HB3	2:D:323:THR:HG23	1.93	0.51
2:D:740:LEU:HD23	2:D:762:VAL:HG12	1.93	0.51
1:P:52:ARG:HE	1:P:53:MET:H	1.59	0.50
1:Q:46:ASN:CG	2:B:702:ASN:HD22	2.19	0.50
1:S:53:MET:SD	1:S:53:MET:N	2.84	0.50
2:B:747:GLY:N	2:B:769:ASN:HB3	2.27	0.50
2:B:828:PRO:HB2	2:B:854:VAL:HG12	1.91	0.50
2:B:126:GLU:OE2	2:B:126:GLU:N	2.44	0.50
2:B:303:ALA:O	2:B:307:THR:HG23	2.11	0.50
2:A:456:ASN:ND2	2:D:535:GLU:OE1	2.44	0.50
2:B:437:THR:HG21	2:B:492:ALA:HB3	1.93	0.50
2:C:444:CYS:HA	2:C:481:ARG:HA	1.93	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:888:PHE:O	2:C:952:SER:HB3	2.11	0.50
2:D:20:HIS:ND1	2:D:22:PRO:HD2	2.25	0.50
1:R:41:GLN:HE22	2:C:938:VAL:HG23	1.75	0.50
2:B:15:VAL:HA	2:B:68:VAL:O	2.12	0.50
2:B:528:GLY:O	2:B:529:VAL:HB	2.10	0.50
2:B:764:HIS:C	2:B:765:ILE:HD12	2.37	0.50
2:C:12:ARG:NE	2:C:65:GLU:OE1	2.42	0.50
2:D:19:PHE:HB2	2:D:24:VAL:HG11	1.92	0.50
1:R:55:LEU:H	2:C:930:SER:HB3	1.77	0.50
2:A:437:THR:HG21	2:A:492:ALA:HB3	1.94	0.50
2:B:604:VAL:HG22	2:B:625:ASN:HB3	1.94	0.50
2:B:865:VAL:HG21	2:B:872:ARG:HE	1.76	0.50
2:D:77:TYR:HE1	2:D:83:CYS:HB3	1.77	0.50
2:D:297:ASP:HA	2:D:323:THR:HB	1.92	0.50
1:R:53:MET:HG3	1:R:65:TYR:CD2	2.47	0.50
2:A:767:ILE:HG21	2:A:772:ILE:HD13	1.93	0.50
2:D:67:ARG:O	2:D:100:ILE:HB	2.12	0.50
2:D:623:LEU:HB2	2:D:646:ALA:HB2	1.94	0.50
1:R:82:SER:HB3	2:C:633:ARG:NH2	2.27	0.50
2:A:787:HIS:ND1	2:A:787:HIS:C	2.69	0.50
2:C:294:ILE:HB	2:C:320:VAL:HG22	1.94	0.50
2:D:258:LYS:HE3	2:D:307:THR:HG22	1.93	0.50
2:D:265:PHE:HZ	2:D:294:ILE:HD12	1.77	0.50
1:P:52:ARG:NH2	1:P:53:MET:SD	2.63	0.50
1:P:55:LEU:HB3	2:A:928:HIS:NE2	2.27	0.50
2:A:452:LEU:HD12	2:A:457:LEU:HD12	1.94	0.50
2:B:747:GLY:H	2:B:769:ASN:HB3	1.76	0.50
2:B:857:TRP:CH2	2:B:929:LEU:HD21	2.47	0.50
2:C:248:TYR:OH	2:C:299:VAL:HG12	2.12	0.50
2:C:414:ILE:HG22	2:C:418:LEU:HG	1.94	0.50
2:C:536:ILE:O	2:C:568:LYS:NZ	2.44	0.50
2:C:887:ARG:HA	2:C:954:LEU:HD13	1.92	0.50
1:Q:48:LEU:HB3	1:Q:73:VAL:HG13	1.94	0.50
1:R:26:LEU:N	1:R:65:TYR:O	2.41	0.50
2:A:680:SER:N	2:A:702:ASN:O	2.43	0.50
2:A:853:PHE:HB2	2:A:951:HIS:HD1	1.77	0.50
2:B:853:PHE:HB2	2:B:951:HIS:HB2	1.93	0.50
2:C:303:ALA:O	2:C:307:THR:HG23	2.12	0.50
2:C:693:LEU:O	2:C:714:PRO:HB3	2.12	0.50
2:D:879:ILE:HA	2:D:970:ASN:HA	1.94	0.50
2:D:887:ARG:HH11	2:D:951:HIS:CE1	2.29	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:832:LEU:HB3	2:A:834:PHE:CE2	2.46	0.49
2:B:617:TRP:CD1	2:B:618:GLU:N	2.80	0.49
2:B:819:GLU:HG2	2:B:839:LYS:HZ3	1.77	0.49
2:D:730:LEU:HG	2:D:731:PRO:HD2	1.93	0.49
1:Q:59:ASP:OD1	1:Q:60:GLU:N	2.45	0.49
2:A:892:VAL:H	2:A:948:PHE:H	1.60	0.49
2:B:64:GLY:O	2:B:67:ARG:HD2	2.13	0.49
2:C:894:MET:HB3	2:C:946:HIS:CD2	2.47	0.49
2:D:682:GLU:N	2:D:682:GLU:OE1	2.45	0.49
2:A:594:LEU:HD22	2:A:616:LEU:HD12	1.95	0.49
2:A:809:ILE:HD12	2:A:932:MET:SD	2.52	0.49
2:A:909:LEU:HD23	2:A:927:PHE:HB2	1.94	0.49
2:B:684:LEU:HD12	2:B:687:ILE:HD11	1.94	0.49
2:C:906:PRO:HD2	2:C:979:TYR:CZ	2.47	0.49
2:D:23:ASP:O	2:D:24:VAL:HB	2.11	0.49
2:A:865:VAL:HG13	2:A:869:PHE:CD2	2.47	0.49
2:A:819:GLU:HB2	2:A:841:ASP:HB2	1.95	0.49
2:B:763:SER:O	2:B:786:LEU:HA	2.12	0.49
2:B:793:GLY:HA2	2:B:812:ALA:O	2.13	0.49
2:C:449:THR:HA	2:C:459:VAL:HG11	1.93	0.49
1:R:28:ILE:HG23	1:R:63:ALA:HB3	1.93	0.49
2:A:623:LEU:HD23	2:A:626:LEU:HD22	1.95	0.49
2:B:833:TYR:CE1	2:B:858:ALA:HA	2.48	0.49
2:C:523:ASN:OD1	2:C:524:ARG:N	2.46	0.49
2:D:303:ALA:O	2:D:307:THR:HG23	2.12	0.49
2:A:69:ALA:HB1	2:A:90:ILE:HD13	1.94	0.49
2:B:740:LEU:HD23	2:B:759:PRO:HD2	1.94	0.49
2:B:813:ASP:N	2:B:813:ASP:OD1	2.45	0.49
2:C:907:ARG:O	2:C:907:ARG:HG3	2.12	0.49
2:D:607:ASN:HA	2:D:630:ASP:HB3	1.95	0.49
2:A:713:ILE:HG13	2:A:717:ILE:HG21	1.94	0.49
2:B:73:LEU:HD22	2:B:113:VAL:HG11	1.95	0.49
2:C:246:GLU:OE2	2:C:246:GLU:HA	2.13	0.49
1:Q:34:ARG:HH22	1:Q:37:LEU:HD22	1.77	0.49
2:B:242:ASP:OD2	2:B:243:ASN:N	2.43	0.49
2:C:328:GLU:OE2	2:C:464:LYS:NZ	2.46	0.49
2:D:449:THR:HA	2:D:459:VAL:HG11	1.94	0.49
2:A:741:GLN:O	2:A:762:VAL:HG13	2.12	0.48
2:B:467:ALA:HB2	2:B:474:ILE:HD12	1.95	0.48
2:B:757:GLU:OE1	2:B:757:GLU:HA	2.12	0.48
2:C:682:GLU:OE1	2:C:682:GLU:N	2.42	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ILE:HA	2:D:67:ARG:HD3	1.95	0.48
2:D:64:GLY:N	2:D:67:ARG:HE	2.11	0.48
2:D:734:LEU:HB3	2:D:736:HIS:CE1	2.48	0.48
2:B:155:ILE:H	2:B:155:ILE:HD12	1.78	0.48
2:B:830:ALA:O	2:B:853:PHE:CE1	2.65	0.48
2:C:60:LYS:HA	2:C:63:ILE:HD12	1.95	0.48
2:D:887:ARG:HE	2:D:992:LEU:HB2	1.79	0.48
1:P:30:LYS:HE3	1:P:37:LEU:HD21	1.94	0.48
1:Q:33:SER:HB3	1:Q:36:SER:HB3	1.95	0.48
2:A:303:ALA:O	2:A:307:THR:HG23	2.13	0.48
2:A:831:GLU:HA	2:A:857:TRP:O	2.13	0.48
2:A:968:ILE:HG13	2:A:969:SER:H	1.78	0.48
2:C:70:ILE:HD11	2:C:171:VAL:HG21	1.95	0.48
2:C:896:LEU:HD13	2:C:942:LEU:HD21	1.94	0.48
2:D:379:ASP:HB3	2:D:485:HIS:CE1	2.48	0.48
2:B:531:PHE:HB3	2:B:557:VAL:HG12	1.95	0.48
2:B:836:ASN:O	2:B:837:CYS:C	2.55	0.48
2:C:714:PRO:O	2:C:717:ILE:HG22	2.13	0.48
2:D:531:PHE:HB3	2:D:557:VAL:HG12	1.95	0.48
1:Q:59:ASP:HB3	1:Q:62:VAL:O	2.13	0.48
2:C:863:LEU:HD23	2:C:863:LEU:H	1.78	0.48
2:D:493:ILE:O	2:D:497:THR:HG23	2.14	0.48
2:D:740:LEU:HG	2:D:740:LEU:O	2.13	0.48
2:A:933:PHE:O	2:A:937:SER:HB2	2.14	0.48
2:B:14:ASN:HA	2:B:66:SER:CB	2.43	0.48
2:B:758:LEU:CD2	2:B:762:VAL:HG11	2.44	0.48
2:D:66:SER:CA	2:D:175:ILE:HD13	2.43	0.48
2:D:685:GLU:HA	2:D:706:ARG:O	2.13	0.48
1:Q:48:LEU:O	1:Q:73:VAL:HG13	2.14	0.48
1:Q:53:MET:SD	1:Q:53:MET:N	2.82	0.48
2:C:295:ILE:HG12	2:C:321:ILE:HD12	1.96	0.48
2:C:348:GLU:O	2:C:352:ILE:HG13	2.14	0.48
2:D:63:ILE:HD12	2:D:97:ILE:HD13	1.95	0.48
2:A:848:ILE:HD12	2:A:860:LEU:HD12	1.96	0.48
2:A:898:HIS:CD2	2:A:899:HIS:HD2	2.32	0.48
2:C:181:ARG:NH2	2:D:285:ASP:OD1	2.46	0.48
2:C:526:ILE:HD11	2:C:549:MET:SD	2.53	0.48
2:D:330:LEU:HD22	2:D:335:ILE:HD12	1.96	0.48
2:D:879:ILE:CA	2:D:970:ASN:HA	2.44	0.48
2:B:297:ASP:HA	2:B:323:THR:HB	1.95	0.48
2:B:599:PHE:CE2	2:B:601:GLU:HB2	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:GLU:HB2	2:B:833:TYR:CE1	2.48	0.48
2:D:67:ARG:HD2	2:D:99:GLN:CA	2.44	0.48
2:D:437:THR:HG21	2:D:492:ALA:HB3	1.96	0.48
2:A:121:GLY:O	2:A:125:LYS:HG2	2.14	0.48
2:B:667:ILE:HA	2:B:670:LEU:HG	1.96	0.48
2:B:859:LEU:HG	2:B:948:PHE:CE1	2.48	0.48
2:C:374:VAL:HG22	2:C:404:LEU:HD21	1.94	0.48
2:C:754:PHE:HB2	2:C:772:ILE:HG21	1.96	0.48
2:D:874:ARG:CZ	2:D:874:ARG:HA	2.43	0.48
1:P:44:VAL:HG13	1:P:45:LEU:HD12	1.96	0.47
2:C:215:PRO:HD2	2:C:218:ILE:HG12	1.96	0.47
2:C:781:LYS:NZ	2:C:803:LEU:O	2.47	0.47
2:D:66:SER:O	2:D:68:VAL:HG23	2.14	0.47
1:R:45:LEU:HD12	1:R:53:MET:HE2	1.95	0.47
2:A:255:HIS:NE2	2:D:182:ASP:OD1	2.41	0.47
2:B:142:ALA:O	2:B:146:VAL:HG22	2.14	0.47
2:B:733:SER:HA	2:B:755:TYR:CD2	2.49	0.47
2:B:764:HIS:ND1	2:B:787:HIS:HB3	2.28	0.47
2:C:633:ARG:HA	2:C:656:SER:O	2.14	0.47
2:D:11:TRP:HB3	2:D:61:LYS:HA	1.94	0.47
2:D:874:ARG:HH22	2:D:986:GLU:HA	1.79	0.47
2:A:15:VAL:HA	2:A:68:VAL:O	2.14	0.47
2:D:859:LEU:HD23	2:D:860:LEU:N	2.28	0.47
1:Q:70:SER:HB2	1:Q:73:VAL:HG23	1.95	0.47
1:R:51:SER:HB3	2:C:764:HIS:CD2	2.49	0.47
2:A:814:ASP:HB2	2:A:838:PHE:CD2	2.49	0.47
2:B:228:HIS:O	2:B:232:SER:HB3	2.14	0.47
2:B:593:ARG:HG2	2:B:615:LYS:HE3	1.96	0.47
2:C:662:GLU:N	2:C:662:GLU:OE1	2.47	0.47
2:D:258:LYS:HG2	2:D:307:THR:CG2	2.45	0.47
2:D:703:LYS:HD2	2:D:703:LYS:N	2.30	0.47
2:D:779:CYS:SG	2:D:780:ILE:HG13	2.54	0.47
1:P:47:LYS:NZ	1:P:86:GLU:OE2	2.48	0.47
2:B:68:VAL:HG11	2:B:171:VAL:HG13	1.95	0.47
2:B:379:ASP:HB3	2:B:485:HIS:CE1	2.49	0.47
2:C:379:ASP:HB3	2:C:485:HIS:CE1	2.49	0.47
2:D:701:MET:HE3	2:D:701:MET:HB2	1.70	0.47
2:D:873:ALA:O	2:D:874:ARG:NH1	2.47	0.47
2:A:567:ARG:HD2	2:A:590:SER:HB3	1.95	0.47
2:B:152:GLU:OE2	2:B:166:LYS:NZ	2.41	0.47
2:B:157:TRP:CD1	2:B:163:MET:HG3	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:701:MET:HG3	2:D:704:CYS:SG	2.55	0.47
2:D:710:PHE:HE2	2:D:713:ILE:HD11	1.78	0.47
2:A:114:ARG:HA	2:A:144:THR:HA	1.97	0.47
2:A:500:LYS:HA	2:A:503:LYS:HG2	1.97	0.47
2:B:33:ARG:O	2:B:37:VAL:HG12	2.14	0.47
2:B:507:LEU:HB3	2:B:513:ILE:HG12	1.96	0.47
2:B:670:LEU:HD12	2:B:673:LEU:HD12	1.97	0.47
2:C:287:LEU:HD22	2:C:292:VAL:HG21	1.95	0.47
2:C:530:SER:HA	2:C:556:LYS:O	2.15	0.47
2:C:554:PHE:HA	2:C:583:LEU:HB3	1.97	0.47
2:C:934:ASN:O	2:C:935:ALA:HB3	2.15	0.47
2:C:946:HIS:CD2	2:C:946:HIS:H	2.33	0.47
2:D:11:TRP:CD1	2:D:64:GLY:CA	2.87	0.47
2:D:136:ARG:HH21	2:D:137:SER:HA	1.78	0.47
2:A:118:GLY:C	2:A:120:PHE:H	2.23	0.47
2:A:524:ARG:HD2	2:D:518:GLU:OE2	2.15	0.47
2:A:599:PHE:CZ	2:A:601:GLU:HG3	2.50	0.47
2:A:741:GLN:HA	2:A:763:SER:H	1.80	0.47
2:B:12:ARG:H	2:B:61:LYS:HB3	1.79	0.47
2:B:19:PHE:HE2	2:B:25:ARG:N	2.13	0.47
2:C:833:TYR:HE2	2:C:931:HIS:CD2	2.32	0.47
2:C:862:GLY:C	2:C:947:LEU:HD13	2.40	0.47
2:D:73:LEU:HD23	2:D:77:TYR:CD2	2.50	0.47
2:A:369:ASP:OD2	2:A:369:ASP:N	2.47	0.47
2:A:788:ASP:OD1	2:A:788:ASP:N	2.48	0.47
2:B:91:LEU:HD11	2:B:146:VAL:HG13	1.97	0.47
2:B:131:LYS:HG3	2:B:132:THR:H	1.80	0.47
2:B:169:ARG:O	2:B:173:THR:HG23	2.15	0.47
2:B:501:PRO:HG2	2:B:502:TRP:CE3	2.49	0.47
2:D:907:ARG:HH21	2:D:909:LEU:HG	1.79	0.47
2:C:242:ASP:OD1	2:C:242:ASP:N	2.48	0.47
2:C:906:PRO:HG2	2:C:979:TYR:OH	2.15	0.47
1:Q:78:LYS:HE2	2:B:481:ARG:HD2	1.97	0.46
1:R:25:GLU:HA	1:R:66:LYS:HA	1.98	0.46
2:A:441:ASN:OD1	2:A:489:ARG:NH1	2.49	0.46
2:A:854:VAL:HA	2:A:887:ARG:HH22	1.80	0.46
2:A:871:HIS:HD2	2:A:878:LEU:HD11	1.79	0.46
2:B:623:LEU:HB2	2:B:646:ALA:HB2	1.97	0.46
2:C:239:CYS:HB2	2:C:269:ILE:HG12	1.97	0.46
2:A:386:CYS:SG	3:A:1301:ADP:H1'	2.56	0.46
2:A:740:LEU:HD13	2:A:759:PRO:HB2	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:889:LYS:HD2	2:A:949:ILE:HB	1.96	0.46
2:A:904:LEU:H	2:A:904:LEU:HD23	1.80	0.46
2:A:933:PHE:O	2:A:934:ASN:HB2	2.15	0.46
2:B:403:GLU:HG2	2:C:461:LEU:HD21	1.98	0.46
2:C:893:VAL:HG23	2:C:947:LEU:HD12	1.97	0.46
2:A:370:LEU:O	2:A:374:VAL:HG23	2.16	0.46
2:A:615:LYS:HG2	2:A:616:LEU:N	2.30	0.46
2:B:213:SER:HG	2:B:470:TYR:HE2	1.63	0.46
2:B:258:LYS:HG2	2:B:307:THR:CG2	2.45	0.46
2:B:777:GLU:HG2	2:B:801:PRO:HA	1.96	0.46
2:C:370:LEU:O	2:C:374:VAL:HG23	2.15	0.46
2:D:15:VAL:HB	2:D:43:MET:HG2	1.97	0.46
2:A:828:PRO:HA	2:A:853:PHE:HA	1.98	0.46
2:C:780:ILE:HD12	2:C:801:PRO:HB2	1.98	0.46
2:D:682:GLU:HB3	2:D:706:ARG:HH21	1.81	0.46
1:R:43:CYS:HA	1:R:47:LYS:HG3	1.97	0.46
2:A:12:ARG:HB2	2:A:65:GLU:HB3	1.98	0.46
2:A:730:LEU:HD22	2:A:755:TYR:CD1	2.50	0.46
2:D:780:ILE:HD12	2:D:801:PRO:HG3	1.98	0.46
1:P:81:CYS:SG	1:P:86:GLU:HB2	2.56	0.46
2:A:759:PRO:HG2	2:A:762:VAL:HG21	1.98	0.46
2:B:677:MET:HE3	2:B:677:MET:HB2	1.84	0.46
2:B:713:ILE:HD11	2:B:734:LEU:HB3	1.96	0.46
2:B:727:LEU:CB	2:B:751:LEU:HD23	2.45	0.46
2:B:833:TYR:CD1	2:B:858:ALA:HA	2.50	0.46
2:C:326:ASN:HB3	2:C:329:ILE:HD12	1.96	0.46
2:C:690:LEU:HB3	2:C:693:LEU:HD12	1.98	0.46
2:C:851:GLN:HG3	2:C:853:PHE:CE2	2.51	0.46
2:C:894:MET:HB3	2:C:946:HIS:HD2	1.79	0.46
2:D:709:ARG:HG2	2:D:710:PHE:N	2.30	0.46
1:R:59:ASP:HB3	1:R:62:VAL:O	2.15	0.46
2:B:258:LYS:HE3	2:B:307:THR:HG22	1.97	0.46
2:C:616:LEU:HB2	2:C:641:PRO:HD3	1.97	0.46
2:B:302:LEU:HD23	2:B:306:GLU:HG3	1.98	0.46
2:B:709:ARG:HD3	2:B:710:PHE:N	2.30	0.46
2:D:19:PHE:HE2	2:D:25:ARG:HB2	1.79	0.46
2:D:199:LEU:HD22	2:D:339:TYR:HB2	1.98	0.46
2:D:788:ASP:OD1	2:D:788:ASP:N	2.49	0.46
1:P:91:LYS:HE3	1:P:91:LYS:HB3	1.63	0.46
2:B:181:ARG:HG3	2:B:183:PHE:HD2	1.80	0.46
2:C:557:VAL:HG22	2:C:586:TRP:HA	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:630:ASP:HA	2:C:653:TYR:HB2	1.97	0.46
1:Q:44:VAL:O	1:Q:48:LEU:HB2	2.15	0.45
2:B:515:TYR:O	2:B:519:GLU:HB2	2.15	0.45
2:B:740:LEU:HB3	2:B:759:PRO:HG2	1.98	0.45
2:B:874:ARG:HH11	2:B:875:GLY:N	2.11	0.45
2:C:713:ILE:H	2:C:713:ILE:HG13	1.54	0.45
2:D:51:ARG:HG2	2:D:54:ILE:HB	1.98	0.45
2:D:179:PRO:HA	2:D:181:ARG:HE	1.82	0.45
2:D:682:GLU:HB3	2:D:706:ARG:NH2	2.31	0.45
2:A:579:ARG:HB3	2:A:599:PHE:CD1	2.51	0.45
2:C:265:PHE:CZ	2:C:269:ILE:HD11	2.51	0.45
2:C:563:HIS:CG	2:C:564:THR:N	2.84	0.45
2:C:857:TRP:HB2	2:C:948:PHE:HE1	1.81	0.45
2:C:904:LEU:HD12	2:C:938:VAL:HG21	1.97	0.45
2:D:11:TRP:CD2	2:D:63:ILE:HD11	2.52	0.45
2:D:894:MET:C	2:D:945:PRO:HB3	2.42	0.45
1:R:30:LYS:HD3	1:R:37:LEU:HD13	1.97	0.45
2:A:187:VAL:O	3:A:1301:ADP:N6	2.49	0.45
2:A:251:CYS:HB3	2:A:304:GLN:HG2	1.99	0.45
2:B:478:GLN:OE1	2:B:481:ARG:NH1	2.49	0.45
2:B:903:GLU:O	2:B:939:ASN:ND2	2.49	0.45
2:C:797:LEU:HG	2:C:818:LEU:HD13	1.97	0.45
2:D:115:LYS:HB2	2:D:117:THR:HG23	1.99	0.45
1:P:85:ASN:OD1	1:P:85:ASN:O	2.35	0.45
2:B:73:LEU:HD12	2:B:104:VAL:O	2.16	0.45
2:B:541:ILE:HD11	2:B:569:LEU:HD12	1.98	0.45
2:B:661:VAL:HA	2:B:683:SER:O	2.16	0.45
2:C:194:LYS:HB2	2:C:194:LYS:HE3	1.67	0.45
2:C:889:LYS:O	2:C:989:VAL:HA	2.16	0.45
2:D:67:ARG:HG3	2:D:99:GLN:HA	1.98	0.45
1:S:91:LYS:HA	1:S:91:LYS:HD2	1.67	0.45
2:A:174:LYS:HE2	2:D:49:ILE:HG12	1.98	0.45
2:A:678:MET:HB3	2:A:678:MET:HE2	1.73	0.45
2:A:761:SER:O	2:A:761:SER:OG	2.32	0.45
2:A:887:ARG:HG3	2:A:992:LEU:HD11	1.98	0.45
2:B:808:LYS:HZ2	2:B:830:ALA:HA	1.78	0.45
2:D:142:ALA:O	2:D:146:VAL:HG22	2.16	0.45
2:B:744:LYS:HB2	2:B:744:LYS:HE2	1.62	0.45
2:D:501:PRO:HG2	2:D:502:TRP:CE3	2.51	0.45
2:D:621:GLN:HB2	2:D:623:LEU:HD21	1.99	0.45
2:D:880:ILE:HB	2:D:971:ILE:CG1	2.39	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:907:ARG:N	2:A:930:SER:OG	2.35	0.45
2:B:373:GLU:HG2	2:B:404:LEU:HD21	1.97	0.45
2:B:392:LEU:HD21	2:B:407:LEU:HD11	1.99	0.45
2:D:157:TRP:CD1	2:D:163:MET:HG3	2.52	0.45
2:D:933:PHE:HD1	2:D:937:SER:HB2	1.80	0.45
2:A:589:TYR:HB3	2:A:611:SER:HB2	1.98	0.45
2:A:610:ASP:OD2	2:A:633:ARG:NE	2.42	0.45
2:A:684:LEU:HG	2:A:684:LEU:O	2.16	0.45
2:A:895:SER:H	2:A:983:ASP:H	1.64	0.45
2:B:47:ASN:OD1	2:B:47:ASN:N	2.49	0.45
2:C:299:VAL:HG22	2:C:324:THR:HB	1.99	0.45
2:C:859:LEU:HD21	2:C:946:HIS:ND1	2.32	0.45
1:R:54:LYS:NZ	2:C:931:HIS:HB3	2.31	0.45
2:A:567:ARG:NH2	2:A:612:GLU:HG3	2.27	0.45
2:B:722:VAL:HG12	2:B:725:THR:OG1	2.17	0.45
2:D:606:VAL:O	2:D:630:ASP:N	2.46	0.45
1:P:77:LEU:HD12	1:P:77:LEU:HA	1.76	0.45
2:B:731:PRO:HD2	2:B:755:TYR:CE1	2.52	0.45
2:A:730:LEU:HD23	2:A:731:PRO:O	2.17	0.44
2:A:866:PRO:HD2	2:A:869:PHE:CE2	2.52	0.44
2:C:160:GLU:OE1	2:D:31:HIS:HE1	1.99	0.44
2:C:404:LEU:HD23	2:C:404:LEU:HA	1.80	0.44
2:C:807:LEU:O	2:C:808:LYS:HD3	2.18	0.44
2:D:220:LYS:HE2	2:D:220:LYS:HB2	1.49	0.44
2:D:783:LEU:HD23	2:D:783:LEU:HA	1.86	0.44
1:S:52:ARG:N	1:S:68:THR:O	2.45	0.44
2:A:504:SER:O	2:A:526:ILE:HG22	2.17	0.44
2:A:663:LEU:HD23	2:A:667:ILE:HD13	1.99	0.44
2:C:735:THR:HB	2:C:759:PRO:HD3	1.98	0.44
2:A:224:ALA:HB2	2:A:323:THR:HG21	1.97	0.44
2:A:813:ASP:OD1	2:A:813:ASP:N	2.47	0.44
2:A:944:LYS:HD3	2:A:944:LYS:HA	1.80	0.44
2:B:594:LEU:HD12	2:B:595:PRO:HD2	1.98	0.44
2:B:741:GLN:HE22	2:B:763:SER:CB	2.31	0.44
2:B:950:PHE:CD1	2:B:950:PHE:C	2.95	0.44
2:C:579:ARG:HG2	2:C:599:PHE:HD1	1.82	0.44
2:C:713:ILE:HD13	2:C:737:CYS:SG	2.57	0.44
2:C:789:LEU:HB3	2:C:807:LEU:CD1	2.47	0.44
2:C:809:ILE:CD1	2:C:932:MET:HB3	2.44	0.44
2:D:59:LEU:HD22	2:D:89:GLU:HB3	1.98	0.44
1:Q:36:SER:HB2	1:Q:88:ASN:HD22	1.82	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:93:CYS:O	2:A:97:ILE:HG22	2.17	0.44
2:A:680:SER:O	2:A:704:CYS:HA	2.17	0.44
2:A:814:ASP:HB3	2:A:836:ASN:ND2	2.32	0.44
2:B:121:GLY:O	2:B:125:LYS:HG2	2.18	0.44
2:B:406:ARG:NH2	2:C:461:LEU:HD23	2.33	0.44
2:B:697:THR:HB	2:B:718:GLU:HG3	1.99	0.44
2:C:872:ARG:HH21	2:C:874:ARG:HH22	1.65	0.44
2:D:740:LEU:HD21	2:D:743:ILE:CG1	2.46	0.44
2:D:803:LEU:HD12	2:D:807:LEU:HB3	2.00	0.44
1:R:41:GLN:NE2	2:C:938:VAL:HG23	2.32	0.44
2:A:744:LYS:C	2:A:745:ILE:HD13	2.42	0.44
2:A:896:LEU:HD22	2:A:899:HIS:CD2	2.53	0.44
2:B:74:SER:O	2:B:75:LYS:C	2.61	0.44
2:C:515:TYR:CE2	2:C:519:GLU:HG3	2.53	0.44
2:D:407:LEU:HA	2:D:410:CYS:HB3	1.99	0.44
2:D:620:THR:OG1	2:D:642:ASP:OD2	2.31	0.44
1:P:44:VAL:HA	1:P:48:LEU:HD12	2.00	0.44
1:Q:48:LEU:HB3	1:Q:73:VAL:CG1	2.48	0.44
1:S:43:CYS:HA	1:S:47:LYS:HZ3	1.82	0.44
2:A:49:ILE:HG13	2:A:51:ARG:HD3	1.99	0.44
2:A:171:VAL:O	2:A:175:ILE:HG13	2.17	0.44
2:A:894:MET:HE3	2:A:982:PHE:CD1	2.51	0.44
2:B:641:PRO:HG2	2:B:643:LEU:HD21	1.99	0.44
2:C:795:LYS:HG3	2:C:796:ARG:HD2	2.00	0.44
2:D:735:THR:HB	2:D:757:GLU:HG3	2.00	0.44
1:P:77:LEU:HD23	1:P:92:ILE:HG12	2.00	0.44
2:A:36:PHE:CD2	2:A:43:MET:HE3	2.53	0.44
2:B:59:LEU:CD2	2:B:90:ILE:HG13	2.47	0.44
1:P:43:CYS:HB3	1:P:87:CYS:SG	2.58	0.44
2:A:433:PHE:HB2	2:A:466:LEU:HD21	2.00	0.44
2:A:759:PRO:HG2	2:A:762:VAL:CG2	2.48	0.44
2:A:893:VAL:HA	2:A:946:HIS:O	2.17	0.44
2:B:258:LYS:HG2	2:B:307:THR:HG21	2.00	0.44
2:C:134:GLU:HG2	2:C:135:GLU:N	2.32	0.44
2:C:643:LEU:O	2:C:670:LEU:HD21	2.18	0.44
2:D:277:LEU:HG	2:D:282:VAL:HG21	1.99	0.44
2:D:305:LEU:HD23	2:D:305:LEU:HA	1.84	0.44
2:D:780:ILE:HD13	2:D:789:LEU:HD21	2.00	0.44
2:D:911:TYR:O	2:D:913:TRP:HD1	2.01	0.44
1:R:45:LEU:CD1	1:R:53:MET:HE2	2.48	0.44
2:A:59:LEU:O	2:A:63:ILE:HG13	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:544:LYS:HB2	2:A:544:LYS:HE2	1.59	0.44
2:A:895:SER:HA	2:A:982:PHE:CA	2.23	0.44
2:B:265:PHE:CZ	2:B:294:ILE:HD12	2.51	0.44
2:B:741:GLN:NE2	2:B:763:SER:CB	2.81	0.44
2:B:835:ALA:O	2:B:836:ASN:CB	2.66	0.44
2:C:251:CYS:HB3	2:C:304:GLN:HG2	2.00	0.44
2:D:134:GLU:HG2	2:D:135:GLU:N	2.33	0.44
2:D:876:ASN:N	2:D:876:ASN:HD22	2.16	0.44
1:P:21:LEU:HG	1:P:22:LYS:N	2.33	0.43
1:R:55:LEU:H	2:C:930:SER:HB2	1.83	0.43
2:A:63:ILE:HD13	2:A:89:GLU:HB3	2.00	0.43
2:A:176:ASN:HD22	2:A:176:ASN:HA	1.63	0.43
2:B:811:GLN:HG3	2:B:835:ALA:H	1.83	0.43
2:C:767:ILE:HG21	2:C:772:ILE:HD11	1.99	0.43
2:C:831:GLU:HA	2:C:857:TRP:O	2.18	0.43
2:C:911:TYR:HE1	2:C:973:LEU:HB3	1.83	0.43
1:P:32:ASP:O	1:P:34:ARG:NH1	2.52	0.43
1:P:41:GLN:HG3	1:P:45:LEU:HD13	2.00	0.43
2:A:189:LEU:HD12	2:A:189:LEU:HA	1.89	0.43
2:B:891:CYS:O	2:B:987:CYS:HA	2.18	0.43
2:C:166:LYS:NZ	2:C:170:ASP:OD2	2.50	0.43
2:C:811:GLN:HE21	2:C:932:MET:HE3	1.83	0.43
2:C:844:ALA:O	2:C:848:ILE:HG13	2.18	0.43
2:D:11:TRP:CH2	2:D:97:ILE:HD11	2.53	0.43
1:R:34:ARG:NE	1:R:34:ARG:HA	2.33	0.43
2:A:166:LYS:NZ	2:A:170:ASP:OD2	2.51	0.43
2:C:759:PRO:HG2	2:C:762:VAL:HG23	2.01	0.43
2:D:742:THR:HB	2:D:764:HIS:CE1	2.53	0.43
1:Q:39:LEU:HD23	1:Q:39:LEU:HA	1.88	0.43
2:C:38:TYR:CZ	2:D:271:LYS:HD2	2.52	0.43
2:D:284:LYS:O	2:D:288:GLN:HB2	2.18	0.43
2:B:330:LEU:HD22	2:B:335:ILE:HD12	2.00	0.43
2:B:571:ILE:HD11	2:B:586:TRP:CZ2	2.53	0.43
2:C:643:LEU:HB3	2:C:670:LEU:HD11	2.00	0.43
2:D:879:ILE:HB	2:D:970:ASN:CA	2.42	0.43
2:A:667:ILE:O	2:A:693:LEU:HD11	2.18	0.43
2:B:544:LYS:HE3	2:B:544:LYS:HB2	1.77	0.43
2:B:809:ILE:C	2:B:810:LEU:HD22	2.44	0.43
2:C:603:LEU:HD21	2:C:606:VAL:HB	2.00	0.43
1:Q:45:LEU:HB3	1:Q:50:ALA:HB2	1.99	0.43
2:C:803:LEU:HD11	2:C:807:LEU:HD22	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:911:TYR:HB2	2:C:975:PHE:HE1	1.83	0.43
2:C:913:TRP:CD1	2:C:913:TRP:N	2.85	0.43
1:R:29:LYS:HE3	1:R:61:GLU:OE1	2.19	0.43
2:A:199:LEU:HD22	2:A:339:TYR:HB2	2.01	0.43
2:A:206:GLY:O	2:A:319:ARG:NH1	2.52	0.43
2:B:713:ILE:CD1	2:B:736:HIS:HB3	2.49	0.43
2:C:381:LEU:HB3	2:C:384:ALA:HB3	2.00	0.43
1:Q:81:CYS:SG	1:Q:87:CYS:HB3	2.59	0.43
2:A:661:VAL:O	2:A:684:LEU:HA	2.19	0.43
2:A:880:ILE:HG22	2:A:971:ILE:HG21	2.00	0.43
2:B:985:LEU:HB3	2:B:986:GLU:H	1.63	0.43
2:C:36:PHE:CD2	2:C:43:MET:HE3	2.54	0.43
2:C:623:LEU:HD13	2:C:626:LEU:HD22	2.01	0.43
2:D:73:LEU:HD23	2:D:77:TYR:HD2	1.84	0.43
1:Q:55:LEU:HD12	1:Q:56:ILE:N	2.34	0.43
2:A:379:ASP:HB3	2:A:485:HIS:CE1	2.53	0.43
2:B:519:GLU:HB3	2:B:521:THR:HG23	2.01	0.43
2:B:644:SER:N	2:B:666:SER:HB3	2.34	0.43
2:B:851:GLN:HB3	2:B:951:HIS:CE1	2.54	0.43
2:C:299:VAL:CG2	2:C:324:THR:HB	2.49	0.43
2:C:723:THR:HA	2:C:746:SER:HB3	2.01	0.43
2:A:31:HIS:NE2	2:B:160:GLU:HG2	2.30	0.42
2:A:305:LEU:HD23	2:A:305:LEU:HA	1.87	0.42
2:A:530:SER:HA	2:A:556:LYS:O	2.18	0.42
2:A:694:THR:OG1	2:A:695:SER:N	2.51	0.42
2:A:717:ILE:HG13	2:A:718:GLU:N	2.33	0.42
2:B:19:PHE:CZ	2:B:21:GLY:HA2	2.54	0.42
2:B:103:THR:O	2:B:151:GLY:HA3	2.19	0.42
2:B:131:LYS:HE3	2:B:139:TRP:CH2	2.54	0.42
2:B:518:GLU:HG3	2:B:519:GLU:OE2	2.18	0.42
2:C:305:LEU:HD23	2:C:305:LEU:HA	1.82	0.42
2:C:728:GLU:HA	2:C:750:ASN:HB3	2.01	0.42
2:D:84:LEU:HD23	2:D:84:LEU:HA	1.88	0.42
2:D:791:LEU:HD23	2:D:810:LEU:HD23	2.00	0.42
2:B:131:LYS:HB2	2:B:131:LYS:HE2	1.74	0.42
2:B:837:CYS:SG	2:B:861:PRO:HB3	2.59	0.42
2:C:663:LEU:HD23	2:C:663:LEU:HA	1.89	0.42
2:C:693:LEU:HD23	2:C:693:LEU:HA	1.88	0.42
2:D:9:ARG:HB3	2:D:11:TRP:CZ2	2.54	0.42
2:D:756:THR:HG22	2:D:776:THR:HG21	2.00	0.42
2:A:38:TYR:CZ	2:B:271:LYS:HD2	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:762:VAL:HB	2:A:783:LEU:HD11	2.01	0.42
2:B:799:SER:HB2	2:B:822:ASN:ND2	2.34	0.42
2:C:536:ILE:HD13	2:C:536:ILE:HA	1.83	0.42
2:C:789:LEU:HB3	2:C:807:LEU:HD11	2.02	0.42
2:C:977:SER:CB	2:C:980:LYS:HA	2.36	0.42
2:D:540:MET:HE3	2:D:540:MET:HB3	1.92	0.42
1:Q:67:ILE:HD12	1:Q:67:ILE:HA	1.92	0.42
1:R:45:LEU:HD21	1:R:52:ARG:HA	2.00	0.42
2:A:160:GLU:OE1	2:B:31:HIS:HE1	2.01	0.42
2:A:815:CYS:HB3	2:A:818:LEU:H	1.83	0.42
2:B:718:GLU:O	2:B:741:GLN:HB2	2.19	0.42
2:B:799:SER:HB2	2:B:822:ASN:HD22	1.85	0.42
2:C:805:ARG:HA	2:C:827:THR:HB	2.00	0.42
2:C:807:LEU:HD21	2:C:810:LEU:HD21	2.01	0.42
1:Q:42:ALA:CB	2:B:935:ALA:HA	2.49	0.42
1:R:82:SER:HB3	2:C:633:ARG:HH22	1.84	0.42
1:S:79:VAL:H	1:S:82:SER:HB3	1.84	0.42
2:A:814:ASP:HB2	2:A:838:PHE:CG	2.55	0.42
2:B:640:LEU:HD23	2:B:640:LEU:HA	1.80	0.42
2:B:803:LEU:HB3	2:B:807:LEU:HD13	2.01	0.42
2:B:808:LYS:HZ3	2:B:830:ALA:HA	1.84	0.42
2:C:259:LEU:HD12	2:C:259:LEU:HA	1.90	0.42
2:C:791:LEU:HD13	2:C:791:LEU:HA	1.70	0.42
2:A:760:VAL:O	2:A:783:LEU:HG	2.19	0.42
2:B:742:THR:HA	2:B:764:HIS:O	2.19	0.42
2:C:19:PHE:HA	2:C:72:LEU:HB3	2.01	0.42
2:C:903:GLU:OE2	2:C:907:ARG:NH1	2.52	0.42
2:D:887:ARG:HG3	2:D:992:LEU:HD12	2.02	0.42
1:P:52:ARG:NH2	2:A:934:ASN:H	2.14	0.42
1:Q:55:LEU:HD13	1:Q:65:TYR:CZ	2.54	0.42
2:A:154:PHE:HE1	2:A:160:GLU:HG3	1.84	0.42
2:B:308:LEU:HD23	2:B:308:LEU:HA	1.91	0.42
2:B:806:SER:HA	2:B:830:ALA:CB	2.33	0.42
2:C:111:SER:OG	2:C:115:LYS:NZ	2.52	0.42
2:C:397:GLN:O	2:C:401:GLU:HG2	2.20	0.42
2:C:895:SER:O	2:C:895:SER:OG	2.28	0.42
2:D:800:LEU:HD11	2:D:810:LEU:HD22	2.01	0.42
1:P:67:ILE:HD12	1:P:67:ILE:HA	1.93	0.42
2:A:36:PHE:HD2	2:A:43:MET:HE3	1.84	0.42
2:A:259:LEU:HD12	2:A:259:LEU:HA	1.86	0.42
2:A:624:ALA:O	2:A:648:ASN:ND2	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:888:PHE:O	2:A:890:VAL:HG23	2.19	0.42
2:A:909:LEU:O	2:A:926:THR:OG1	2.32	0.42
2:B:752:LYS:HA	2:B:752:LYS:HD2	1.78	0.42
2:C:491:MET:HE3	2:C:491:MET:HB3	1.97	0.42
2:C:878:LEU:HD13	2:C:878:LEU:HA	1.89	0.42
2:D:269:ILE:HG23	2:D:270:LEU:HD13	2.01	0.42
1:R:81:CYS:SG	1:R:87:CYS:HB2	2.60	0.42
2:A:440:PHE:CZ	2:A:451:MET:HG2	2.55	0.42
2:A:890:VAL:H	2:A:989:VAL:HG12	1.83	0.42
2:B:65:GLU:H	2:B:65:GLU:HG2	1.41	0.42
2:B:380:LYS:HB2	2:B:380:LYS:HE2	1.77	0.42
2:C:862:GLY:HA3	2:C:947:LEU:HD22	2.00	0.42
2:D:41:ILE:H	2:D:41:ILE:HG13	1.67	0.42
2:D:207:VAL:HG22	2:D:316:PRO:HA	2.01	0.42
2:D:722:VAL:O	2:D:745:ILE:HA	2.20	0.42
1:Q:34:ARG:NH2	1:Q:37:LEU:HD22	2.35	0.42
1:R:54:LYS:HE2	2:C:931:HIS:CB	2.48	0.42
1:S:34:ARG:O	1:S:37:LEU:HD12	2.20	0.42
2:B:122:ILE:O	2:B:126:GLU:OE2	2.37	0.42
2:B:566:LYS:HD3	2:B:568:LYS:HB3	2.02	0.42
2:B:751:LEU:HD12	2:B:751:LEU:O	2.20	0.42
2:C:118:GLY:C	2:C:120:PHE:H	2.27	0.42
2:D:895:SER:HB3	2:D:945:PRO:HG3	2.02	0.42
1:P:29:LYS:HE2	1:P:30:LYS:O	2.20	0.41
2:A:745:ILE:O	2:A:767:ILE:HA	2.20	0.41
2:B:63:ILE:HD12	2:B:99:GLN:HB2	2.00	0.41
2:B:606:VAL:HG23	2:B:626:LEU:HD11	2.02	0.41
2:C:803:LEU:CD1	2:C:807:LEU:HD22	2.50	0.41
2:C:910:LEU:HD23	2:C:910:LEU:HA	1.84	0.41
2:A:969:SER:OG	2:A:970:ASN:N	2.53	0.41
2:B:509:ASP:O	2:B:513:ILE:HG13	2.20	0.41
2:B:637:LEU:HB3	2:B:657:CYS:SG	2.60	0.41
2:C:846:ARG:C	2:C:846:ARG:HH11	2.28	0.41
2:D:265:PHE:CZ	2:D:294:ILE:HD12	2.54	0.41
2:D:902:PHE:CE2	2:D:905:VAL:HG13	2.55	0.41
2:A:819:GLU:HA	2:A:840:LEU:HA	2.03	0.41
2:B:710:PHE:CD1	2:B:710:PHE:C	2.98	0.41
2:B:806:SER:H	2:B:827:THR:CG2	2.33	0.41
2:B:836:ASN:HD22	2:B:836:ASN:HA	1.77	0.41
2:C:611:SER:HB2	2:C:613:LEU:HD13	2.01	0.41
2:C:694:THR:OG1	2:C:695:SER:N	2.52	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:878:LEU:HD23	2:C:987:CYS:HB2	2.02	0.41
2:D:74:SER:OG	2:D:75:LYS:N	2.52	0.41
2:D:91:LEU:HD11	2:D:146:VAL:HG13	2.01	0.41
2:D:124:PHE:O	2:D:128:CYS:HB3	2.21	0.41
2:D:419:LYS:HE3	2:D:419:LYS:HB2	1.81	0.41
2:D:886:ASN:HB2	2:D:888:PHE:CE1	2.55	0.41
1:S:56:ILE:HD11	1:S:66:LYS:HB3	2.03	0.41
2:B:76:ASN:OD1	2:B:76:ASN:N	2.52	0.41
2:B:122:ILE:H	2:B:122:ILE:HG12	1.65	0.41
2:B:850:GLN:O	2:B:889:LYS:NZ	2.53	0.41
2:C:433:PHE:HB2	2:C:466:LEU:HD21	2.03	0.41
2:C:638:THR:HA	2:C:659:ALA:O	2.21	0.41
2:C:777:GLU:HG3	2:C:801:PRO:HB3	2.02	0.41
2:D:135:GLU:HA	2:D:138:LYS:CG	2.50	0.41
2:D:308:LEU:HD23	2:D:308:LEU:HA	1.90	0.41
2:D:894:MET:HB3	2:D:894:MET:HE3	1.74	0.41
2:A:825:LEU:HD23	2:A:825:LEU:H	1.85	0.41
2:B:693:LEU:HD12	2:B:696:LEU:HD22	2.01	0.41
2:B:733:SER:HB2	2:B:757:GLU:HB2	2.01	0.41
2:B:740:LEU:HD11	2:B:743:ILE:HG23	2.02	0.41
2:B:910:LEU:HD11	2:B:978:GLU:H	1.85	0.41
2:C:41:ILE:HG13	2:D:286:ARG:HH22	1.84	0.41
2:C:797:LEU:HD23	2:C:818:LEU:HD22	2.03	0.41
2:C:886:ASN:HB3	2:C:991:ILE:HD12	2.02	0.41
2:C:984:ILE:HG22	2:C:986:GLU:H	1.85	0.41
2:D:152:GLU:OE2	2:D:166:LYS:NZ	2.38	0.41
2:D:552:LEU:HD23	2:D:581:ILE:HG12	2.02	0.41
2:D:687:ILE:HD11	2:D:711:PRO:HB2	2.03	0.41
1:S:40:CYS:HA	1:S:43:CYS:HB2	2.03	0.41
2:A:414:ILE:HG22	2:A:418:LEU:HG	2.03	0.41
2:A:656:SER:HA	2:A:680:SER:OG	2.20	0.41
2:A:713:ILE:HD12	2:A:713:ILE:HA	1.87	0.41
2:B:601:GLU:OE2	2:B:622:CYS:N	2.48	0.41
2:C:754:PHE:HB2	2:C:772:ILE:CG2	2.49	0.41
2:D:754:PHE:HB2	2:D:775:ILE:HD13	2.03	0.41
2:D:859:LEU:HD21	2:D:946:HIS:CD2	2.55	0.41
1:Q:47:LYS:HE2	1:Q:47:LYS:HB2	1.28	0.41
1:Q:47:LYS:HZ1	1:Q:48:LEU:HG	1.86	0.41
1:Q:47:LYS:HD2	1:Q:86:GLU:O	2.20	0.41
2:A:31:HIS:HD2	2:B:161:ALA:HB2	1.85	0.41
2:A:845:ARG:HH21	2:A:861:PRO:HB2	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:880:ILE:HD12	2:A:881:PRO:HD2	2.03	0.41
2:B:754:PHE:HE2	2:B:776:THR:H	1.69	0.41
2:B:819:GLU:HB2	2:B:841:ASP:N	2.36	0.41
2:C:623:LEU:HD23	2:C:623:LEU:HA	1.95	0.41
2:C:767:ILE:HG22	2:C:770:SER:HB2	2.01	0.41
2:D:596:SER:HA	2:D:618:GLU:OE2	2.21	0.41
2:D:779:CYS:SG	2:D:780:ILE:N	2.93	0.41
2:D:825:LEU:HD11	2:D:832:LEU:HD11	2.02	0.41
2:D:837:CYS:HA	2:D:861:PRO:HB3	2.03	0.41
2:D:987:CYS:SG	2:D:988:GLY:N	2.94	0.41
2:B:311:MET:H	2:B:311:MET:HG2	1.74	0.41
2:B:685:GLU:HA	2:B:706:ARG:O	2.20	0.41
2:B:800:LEU:HD22	2:B:818:LEU:HD11	2.03	0.41
2:B:891:CYS:SG	2:B:949:ILE:HG22	2.60	0.41
2:D:353:PHE:HZ	2:D:400:TRP:HZ2	1.69	0.41
2:D:392:LEU:HD21	2:D:407:LEU:HD11	2.03	0.41
2:D:888:PHE:HZ	2:D:954:LEU:HB2	1.85	0.41
1:Q:47:LYS:H	1:Q:47:LYS:HG3	1.57	0.41
2:A:599:PHE:CE2	2:A:601:GLU:HG3	2.56	0.41
2:A:617:TRP:CD1	2:A:617:TRP:O	2.73	0.41
2:A:701:MET:HB3	2:A:704:CYS:SG	2.61	0.41
2:A:803:LEU:HG	2:A:807:LEU:HD11	2.03	0.41
2:B:17:THR:OG1	2:B:43:MET:SD	2.78	0.41
2:B:35:GLN:HG3	2:B:164:ILE:HG22	2.03	0.41
2:B:284:LYS:O	2:B:288:GLN:HB2	2.20	0.41
2:B:745:ILE:HD12	2:B:746:SER:N	2.36	0.41
2:B:930:SER:HA	2:B:932:MET:SD	2.61	0.41
2:C:20:HIS:O	2:C:20:HIS:ND1	2.49	0.41
2:C:218:ILE:HD13	2:C:341:VAL:HB	2.03	0.41
2:C:567:ARG:HG2	2:C:588:ALA:HB1	2.03	0.41
2:C:677:MET:HE2	2:C:677:MET:HB3	1.93	0.41
2:D:17:THR:OG1	2:D:43:MET:SD	2.74	0.41
2:D:24:VAL:CG2	2:D:28:PHE:HB3	2.51	0.41
2:D:64:GLY:H	2:D:67:ARG:NE	2.19	0.41
2:D:258:LYS:HG2	2:D:307:THR:HG21	2.03	0.41
2:D:454:LYS:HE2	2:D:582:ARG:HH21	1.86	0.41
2:D:533:THR:HG21	2:D:569:LEU:HD11	2.03	0.41
2:D:547:GLU:HB2	2:D:576:LYS:HB2	2.03	0.41
2:A:152:GLU:HG3	2:A:167:ILE:HG12	2.03	0.41
2:A:977:SER:HB2	2:A:982:PHE:CE2	2.56	0.41
2:B:622:CYS:HA	2:B:645:ASN:OD1	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:LEU:H	2:B:751:LEU:HG	1.69	0.41
2:C:604:VAL:HG22	2:C:625:ASN:HB3	2.02	0.41
2:D:297:ASP:OD1	2:D:298:ASP:N	2.54	0.41
2:D:328:GLU:HG3	2:D:468:ASN:OD1	2.21	0.41
1:S:22:LYS:H	1:S:22:LYS:HG2	1.71	0.40
2:B:20:HIS:HB3	2:B:23:ASP:CG	2.46	0.40
2:B:601:GLU:HA	2:B:622:CYS:O	2.21	0.40
2:B:815:CYS:CB	2:B:818:LEU:HB3	2.51	0.40
2:B:833:TYR:HE2	2:B:931:HIS:NE2	2.19	0.40
2:C:773:GLU:HB2	2:C:774:TRP:CD1	2.56	0.40
2:C:811:GLN:NE2	2:C:932:MET:HE3	2.36	0.40
2:D:544:LYS:HE3	2:D:544:LYS:HB2	1.76	0.40
1:S:84:VAL:HG13	1:S:85:ASN:HB3	2.02	0.40
2:A:594:LEU:HD12	2:A:594:LEU:HA	1.75	0.40
2:A:594:LEU:O	2:A:595:PRO:C	2.64	0.40
2:C:633:ARG:H	2:C:656:SER:HB3	1.85	0.40
2:D:746:SER:OG	2:D:747:GLY:N	2.54	0.40
1:P:81:CYS:SG	1:P:87:CYS:HB2	2.61	0.40
1:R:53:MET:HG2	2:C:933:PHE:CE2	2.56	0.40
2:A:297:ASP:OD1	2:A:323:THR:OG1	2.39	0.40
2:A:606:VAL:HG22	2:A:608:MET:HE2	2.03	0.40
2:C:169:ARG:HH21	2:D:274:GLY:H	1.68	0.40
2:D:71:VAL:HB	2:D:103:THR:HG22	2.04	0.40
2:D:786:LEU:HD12	2:D:787:HIS:N	2.37	0.40
2:A:887:ARG:HH21	2:A:951:HIS:HB3	1.86	0.40
2:B:744:LYS:HG3	2:B:766:ASN:HD22	1.86	0.40
2:B:788:ASP:HB2	2:B:809:ILE:HG22	2.03	0.40
2:C:679:TYR:HD1	2:C:679:TYR:H	1.69	0.40
2:D:21:GLY:N	2:D:22:PRO:CD	2.85	0.40
2:D:25:ARG:HA	2:D:29:LEU:HB3	2.02	0.40
2:D:665:SER:HA	2:D:688:PRO:HG2	2.03	0.40
2:D:780:ILE:O	2:D:783:LEU:HB2	2.21	0.40
1:P:39:LEU:HD12	1:P:39:LEU:HA	1.90	0.40
2:A:120:PHE:HE1	2:A:143:LEU:HD13	1.85	0.40
2:A:285:ASP:CG	2:D:178:THR:H	2.29	0.40
2:B:378:CYS:SG	2:B:388:LEU:HD12	2.61	0.40
2:C:831:GLU:HB3	2:C:833:TYR:CE1	2.56	0.40
2:D:19:PHE:CE2	2:D:29:LEU:HD22	2.57	0.40
2:D:67:ARG:HD3	2:D:67:ARG:HA	1.90	0.40
2:D:622:CYS:HA	2:D:645:ASN:OD1	2.21	0.40
2:D:724:GLY:HA2	2:D:747:GLY:HA3	2.04	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:946:HIS:CD2	2:D:946:HIS:C	2.99	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	P	72/216 (33%)	65 (90%)	7 (10%)	0	100	100
1	Q	74/216 (34%)	67 (90%)	6 (8%)	1 (1%)	9	38
1	R	72/216 (33%)	68 (94%)	4 (6%)	0	100	100
1	S	71/216 (33%)	67 (94%)	4 (6%)	0	100	100
2	A	967/1007 (96%)	903 (93%)	63 (6%)	1 (0%)	48	79
2	B	970/1007 (96%)	891 (92%)	74 (8%)	5 (0%)	24	57
2	C	967/1007 (96%)	905 (94%)	61 (6%)	1 (0%)	48	79
2	D	970/1007 (96%)	896 (92%)	70 (7%)	4 (0%)	30	62
All	All	4163/4892 (85%)	3862 (93%)	289 (7%)	12 (0%)	37	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	41	GLN
2	B	529	VAL
2	B	836	ASN
2	C	852	SER
2	D	24	VAL
2	D	529	VAL
2	D	753	ILE
2	D	971	ILE
2	B	24	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	67	ARG
2	B	828	PRO
2	A	895	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	P	66/196 (34%)	63 (96%)	3 (4%)	24	50
1	Q	67/196 (34%)	62 (92%)	5 (8%)	12	37
1	R	66/196 (34%)	65 (98%)	1 (2%)	57	71
1	S	65/196 (33%)	63 (97%)	2 (3%)	35	59
2	A	873/907 (96%)	846 (97%)	27 (3%)	35	59
2	B	873/907 (96%)	819 (94%)	54 (6%)	16	43
2	C	873/907 (96%)	836 (96%)	37 (4%)	26	52
2	D	875/907 (96%)	842 (96%)	33 (4%)	29	55
All	All	3758/4412 (85%)	3596 (96%)	162 (4%)	27	51

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	28	ILE
1	P	45	LEU
1	P	68	THR
1	Q	43	CYS
1	Q	45	LEU
1	Q	46	ASN
1	Q	47	LYS
1	Q	71	ASP
1	R	28	ILE
1	S	39	LEU
1	S	85	ASN
2	A	132	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	185	ASP
2	A	207	VAL
2	A	241	VAL
2	A	369	ASP
2	A	404	LEU
2	A	410	CYS
2	A	414	ILE
2	A	557	VAL
2	A	592	LYS
2	A	593	ARG
2	A	601	GLU
2	A	648	ASN
2	A	690	LEU
2	A	697	THR
2	A	713	ILE
2	A	729	GLU
2	A	746	SER
2	A	786	LEU
2	A	787	HIS
2	A	827	THR
2	A	829	ASN
2	A	872	ARG
2	A	893	VAL
2	A	896	LEU
2	A	900	GLN
2	A	932	MET
2	B	24	VAL
2	B	65	GLU
2	B	66	SER
2	B	67	ARG
2	B	75	LYS
2	B	90	ILE
2	B	117	THR
2	B	120	PHE
2	B	122	ILE
2	B	136	ARG
2	B	158	LYS
2	B	159	ASP
2	B	182	ASP
2	B	276	GLU
2	B	398	THR
2	B	410	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	458	ASN
2	B	481	ARG
2	B	615	LYS
2	B	616	LEU
2	B	617	TRP
2	B	621	GLN
2	B	642	ASP
2	B	712	ASP
2	B	733	SER
2	B	734	LEU
2	B	737	CYS
2	B	740	LEU
2	B	742	THR
2	B	743	ILE
2	B	744	LYS
2	B	745	ILE
2	B	748	SER
2	B	751	LEU
2	B	752	LYS
2	B	753	ILE
2	B	754	PHE
2	B	756	THR
2	B	757	GLU
2	B	758	LEU
2	B	763	SER
2	B	764	HIS
2	B	825	LEU
2	B	829	ASN
2	B	831	GLU
2	B	832	LEU
2	B	833	TYR
2	B	834	PHE
2	B	891	CYS
2	B	905	VAL
2	B	926	THR
2	B	942	LEU
2	B	952	SER
2	B	972	MET
2	C	79	SER
2	C	234	THR
2	C	362	SER
2	C	369	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	414	ILE
2	C	526	ILE
2	C	614	GLN
2	C	643	LEU
2	C	690	LEU
2	C	692	ASN
2	C	710	PHE
2	C	712	ASP
2	C	713	ILE
2	C	723	THR
2	C	783	LEU
2	C	787	HIS
2	C	788	ASP
2	C	789	LEU
2	C	791	LEU
2	C	827	THR
2	C	829	ASN
2	C	833	TYR
2	C	839	LYS
2	C	849	ILE
2	C	851	GLN
2	C	878	LEU
2	C	908	ASN
2	C	927	PHE
2	C	929	LEU
2	C	931	HIS
2	C	933	PHE
2	C	936	ASP
2	C	946	HIS
2	C	947	LEU
2	C	950	PHE
2	C	980	LYS
2	C	982	PHE
2	D	18	SER
2	D	23	ASP
2	D	25	ARG
2	D	27	LYS
2	D	41	ILE
2	D	61	LYS
2	D	63	ILE
2	D	65	GLU
2	D	67	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	70	ILE
2	D	74	SER
2	D	90	ILE
2	D	119	ASP
2	D	136	ARG
2	D	182	ASP
2	D	220	LYS
2	D	311	MET
2	D	414	ILE
2	D	580	THR
2	D	616	LEU
2	D	699	LEU
2	D	701	MET
2	D	717	ILE
2	D	740	LEU
2	D	742	THR
2	D	743	ILE
2	D	810	LEU
2	D	813	ASP
2	D	928	HIS
2	D	949	ILE
2	D	969	SER
2	D	971	ILE
2	D	985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	35	ASN
1	Q	85	ASN
2	A	237	HIS
2	A	279	HIS
2	A	288	GLN
2	A	409	ASN
2	A	456	ASN
2	A	645	ASN
2	A	675	HIS
2	A	897	ASN
2	A	898	HIS
2	A	899	HIS
2	A	970	ASN
2	B	148	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	156	HIS
2	B	231	HIS
2	B	237	HIS
2	B	468	ASN
2	B	476	HIS
2	B	702	ASN
2	B	721	GLN
2	B	741	GLN
2	B	822	ASN
2	B	829	ASN
2	B	871	HIS
2	C	53	GLN
2	C	148	ASN
2	C	237	HIS
2	C	272	GLN
2	C	333	HIS
2	C	585	HIS
2	C	602	ASN
2	C	609	GLN
2	C	671	HIS
2	C	811	GLN
2	C	908	ASN
2	C	946	HIS
2	C	951	HIS
2	D	31	HIS
2	D	237	HIS
2	D	476	HIS
2	D	766	ASN
2	D	785	ASN
2	D	951	HIS

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	D	1301	-	27,29,29	1.34	4 (14%)	42,45,45	1.91	10 (23%)
3	ADP	C	1301	-	27,29,29	1.35	4 (14%)	42,45,45	1.93	10 (23%)
3	ADP	B	1301	-	27,29,29	1.34	4 (14%)	42,45,45	1.93	10 (23%)
3	ADP	A	1301	-	27,29,29	1.36	4 (14%)	42,45,45	1.93	9 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	1301	-	-	0/16/32/32	0/3/3/3
3	ADP	C	1301	-	-	2/16/32/32	0/3/3/3
3	ADP	B	1301	-	-	3/16/32/32	0/3/3/3
3	ADP	A	1301	-	-	9/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	ADP	C5-C4	4.48	1.47	1.39
3	D	1301	ADP	C5-C4	4.39	1.47	1.39
3	C	1301	ADP	C5-C4	4.37	1.47	1.39
3	B	1301	ADP	C5-C4	4.37	1.47	1.39
3	A	1301	ADP	C5-C6	2.56	1.48	1.41
3	B	1301	ADP	C5-C6	2.53	1.48	1.41

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1301	ADP	C5-C6	2.53	1.48	1.41
3	D	1301	ADP	C5-C6	2.50	1.48	1.41
3	A	1301	ADP	C5-N7	-2.35	1.34	1.39
3	B	1301	ADP	C8-N7	2.35	1.36	1.31
3	D	1301	ADP	C8-N7	2.35	1.36	1.31
3	C	1301	ADP	C5-N7	-2.33	1.34	1.39
3	D	1301	ADP	C5-N7	-2.32	1.34	1.39
3	B	1301	ADP	C5-N7	-2.31	1.34	1.39
3	C	1301	ADP	C8-N7	2.30	1.35	1.31
3	A	1301	ADP	C8-N7	2.28	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	ADP	C5-C4-N3	-6.25	118.60	126.75
3	B	1301	ADP	C5-C4-N3	-6.21	118.64	126.75
3	D	1301	ADP	C5-C4-N3	-6.16	118.72	126.75
3	C	1301	ADP	C5-C4-N3	-6.11	118.78	126.75
3	A	1301	ADP	N3-C4-N9	4.91	135.17	127.08
3	C	1301	ADP	N3-C4-N9	4.87	135.10	127.08
3	B	1301	ADP	N3-C4-N9	4.86	135.09	127.08
3	D	1301	ADP	N3-C4-N9	4.82	135.02	127.08
3	A	1301	ADP	C2-N3-C4	3.82	120.77	111.75
3	B	1301	ADP	C2-N3-C4	3.82	120.76	111.75
3	D	1301	ADP	C2-N3-C4	3.81	120.74	111.75
3	C	1301	ADP	C2-N3-C4	3.79	120.70	111.75
3	A	1301	ADP	PA-O3A-PB	-3.71	120.10	132.83
3	B	1301	ADP	PA-O3A-PB	-3.39	121.20	132.83
3	C	1301	ADP	PA-O3A-PB	-3.28	121.58	132.83
3	D	1301	ADP	C4-C5-N7	-3.19	106.73	110.62
3	B	1301	ADP	C4-C5-N7	-3.16	106.77	110.62
3	D	1301	ADP	N3-C2-N1	-3.09	123.76	128.60
3	C	1301	ADP	C4-C5-N7	-3.09	106.86	110.62
3	C	1301	ADP	N3-C2-N1	-3.09	123.77	128.60
3	B	1301	ADP	N3-C2-N1	-3.08	123.79	128.60
3	A	1301	ADP	N3-C2-N1	-3.02	123.87	128.60
3	D	1301	ADP	PA-O3A-PB	-3.00	122.53	132.83
3	A	1301	ADP	C4-C5-N7	-3.00	106.97	110.62
3	C	1301	ADP	C4-N9-C8	2.68	108.64	105.73
3	D	1301	ADP	C5-N7-C8	2.67	107.30	103.51
3	B	1301	ADP	C5-N7-C8	2.62	107.23	103.51
3	C	1301	ADP	C5-N7-C8	2.59	107.19	103.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1301	ADP	C4-N9-C8	2.56	108.50	105.73
3	B	1301	ADP	C4-N9-C8	2.52	108.46	105.73
3	A	1301	ADP	C5-N7-C8	2.46	107.01	103.51
3	A	1301	ADP	C4-N9-C8	2.30	108.22	105.73
3	A	1301	ADP	O4'-C1'-N9	2.12	112.24	108.06
3	C	1301	ADP	C3'-C2'-C1'	2.08	105.37	101.43
3	D	1301	ADP	C6-C5-N7	2.07	135.88	132.02
3	B	1301	ADP	C3'-C2'-C1'	2.07	105.36	101.43
3	D	1301	ADP	C3'-C2'-C1'	2.05	105.31	101.43
3	C	1301	ADP	C6-C5-N7	2.02	135.78	132.02
3	B	1301	ADP	C6-C5-N7	2.00	135.75	132.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	ADP	C5'-O5'-PA-O1A
3	A	1301	ADP	C5'-O5'-PA-O2A
3	A	1301	ADP	C5'-O5'-PA-O3A
3	C	1301	ADP	O4'-C4'-C5'-O5'
3	A	1301	ADP	O4'-C4'-C5'-O5'
3	C	1301	ADP	C3'-C4'-C5'-O5'
3	A	1301	ADP	O4'-C1'-N9-C4
3	A	1301	ADP	C3'-C4'-C5'-O5'
3	A	1301	ADP	O4'-C1'-N9-C8
3	B	1301	ADP	PA-O3A-PB-O1B
3	B	1301	ADP	PA-O3A-PB-O2B
3	B	1301	ADP	PA-O3A-PB-O3B
3	A	1301	ADP	PB-O3A-PA-O1A
3	A	1301	ADP	PB-O3A-PA-O2A

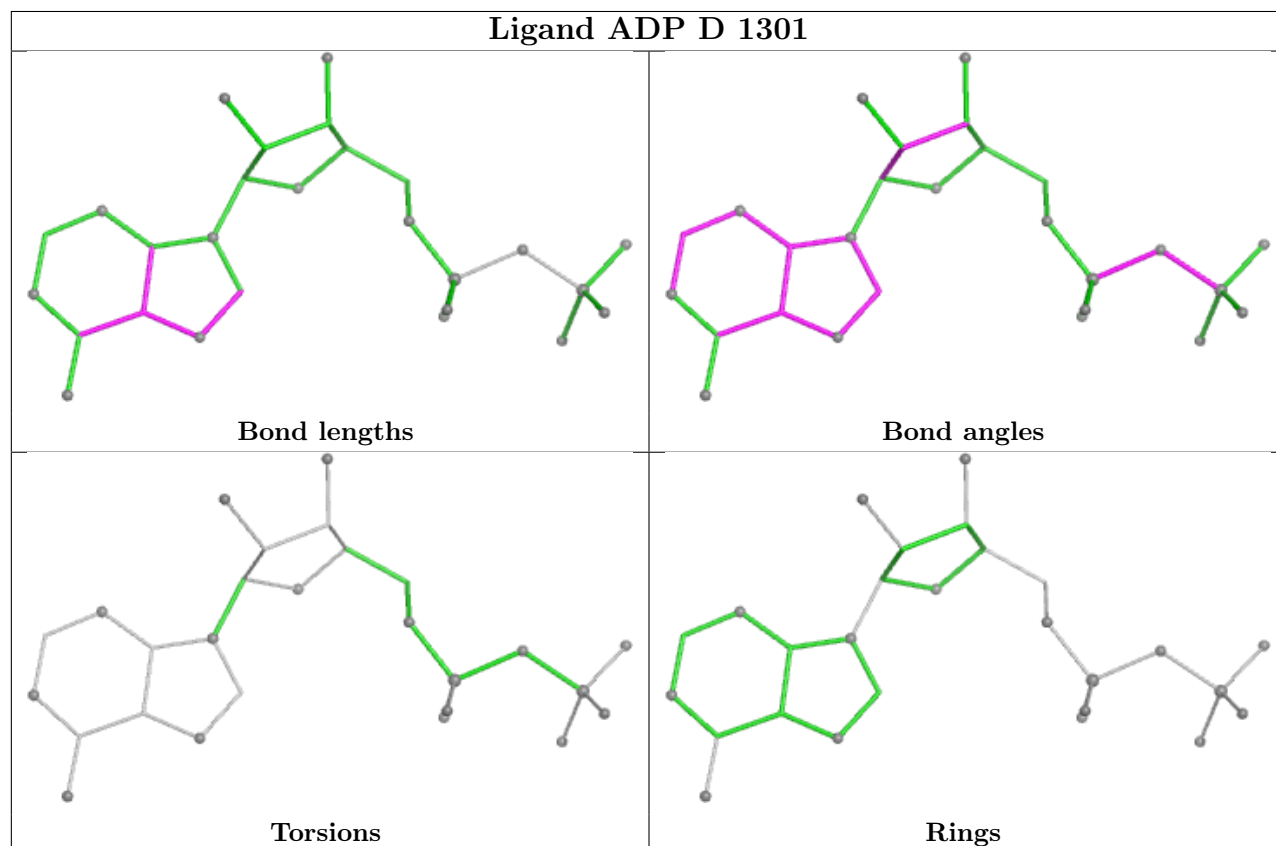
There are no ring outliers.

1 monomer is involved in 2 short contacts:

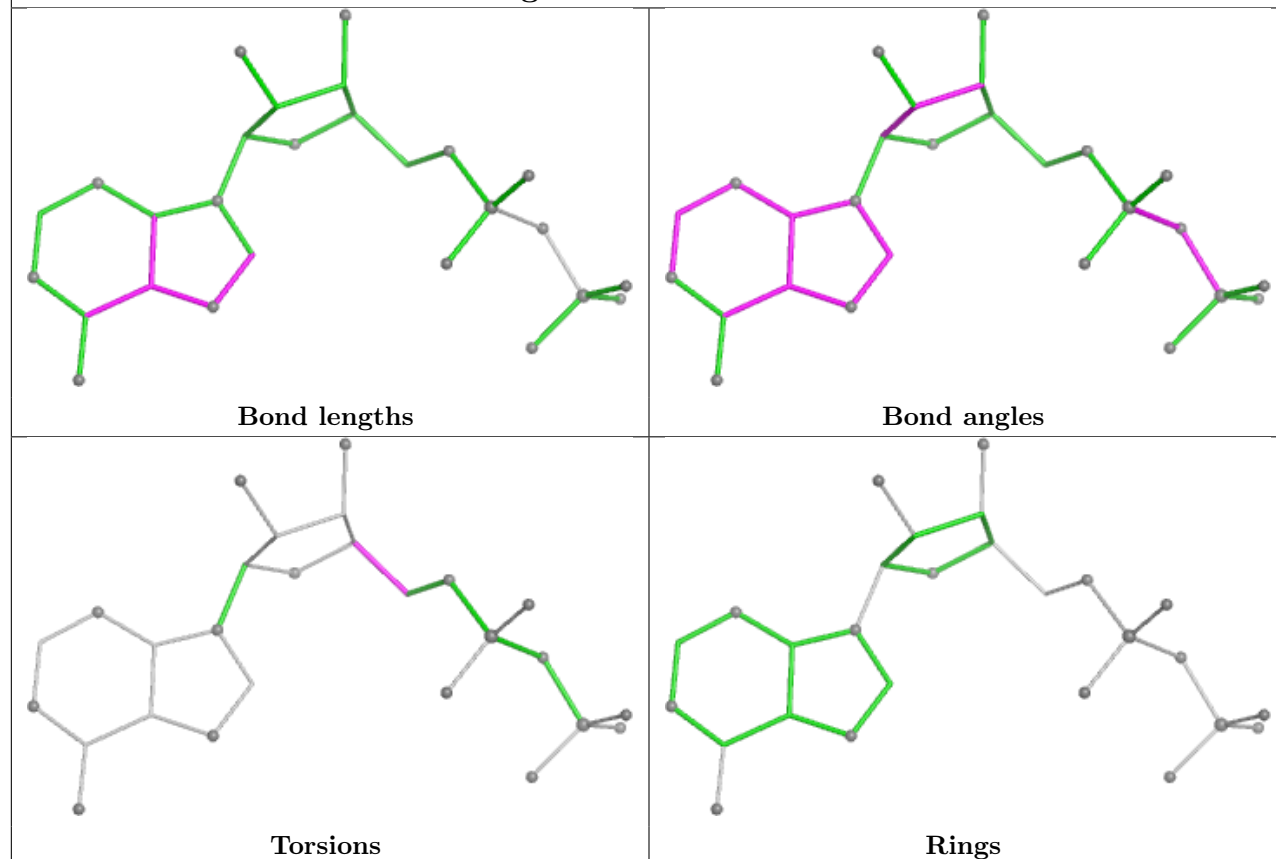
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

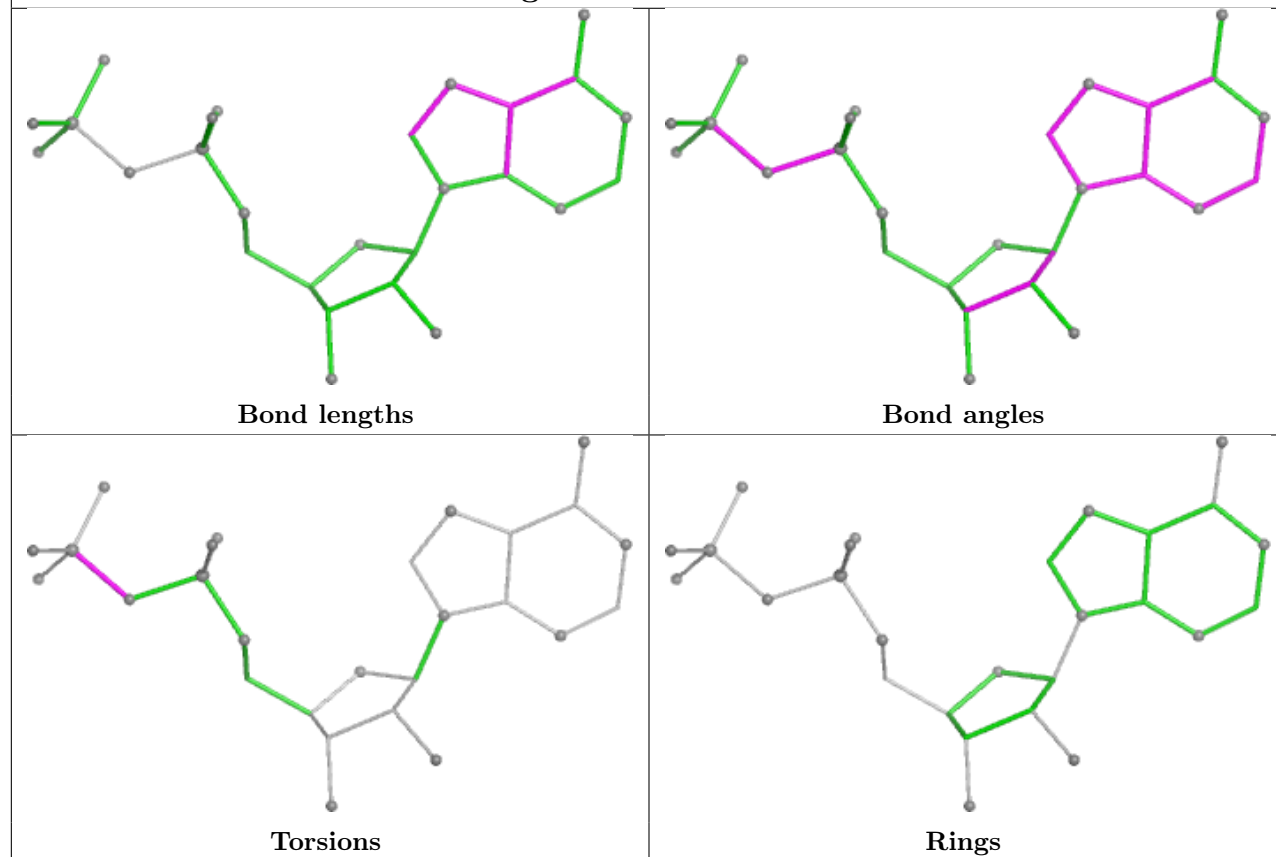
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

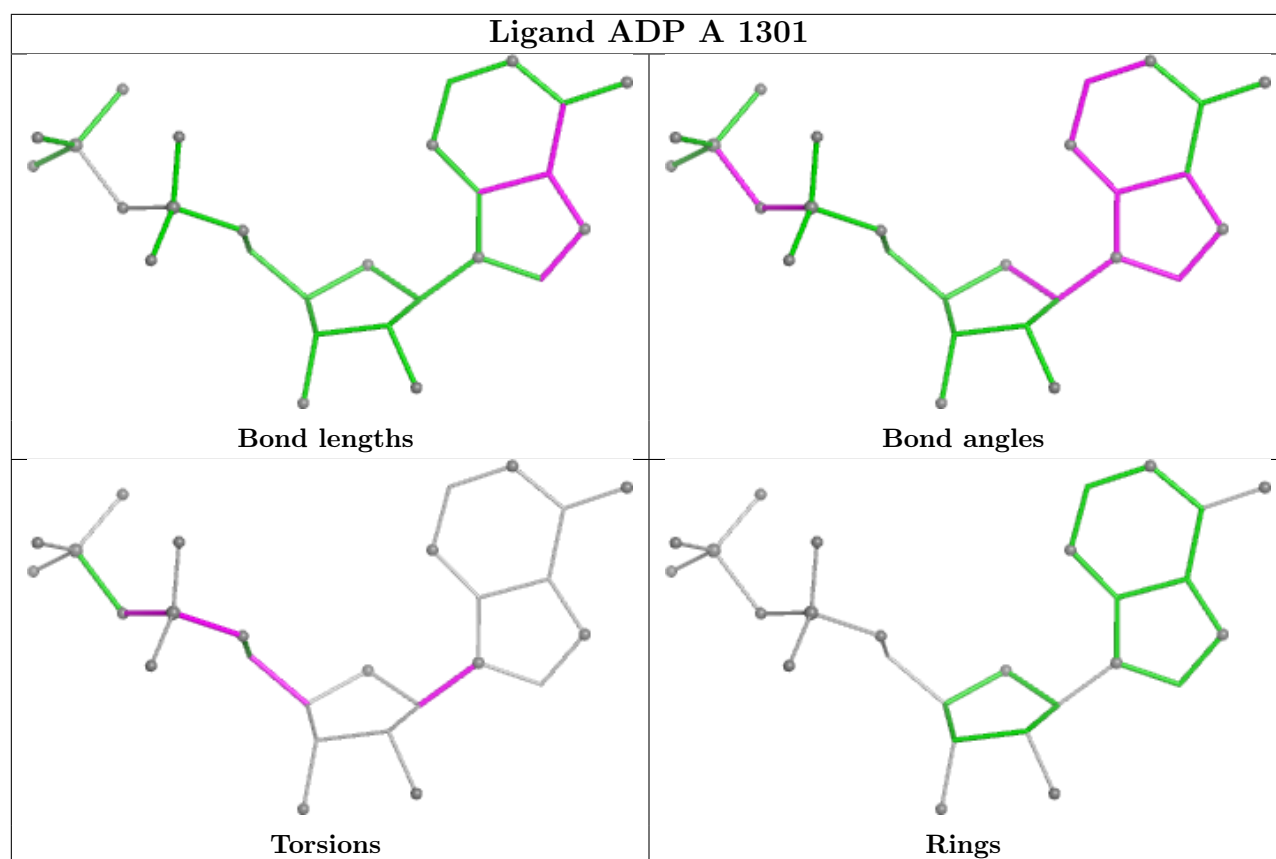


## Ligand ADP C 1301



## Ligand ADP B 1301





## 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.

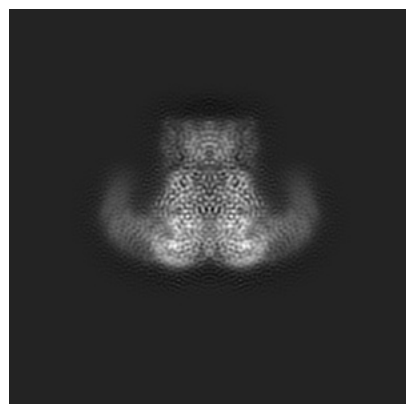
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53375. These allow visual inspection of the internal detail of the map and identification of artifacts.

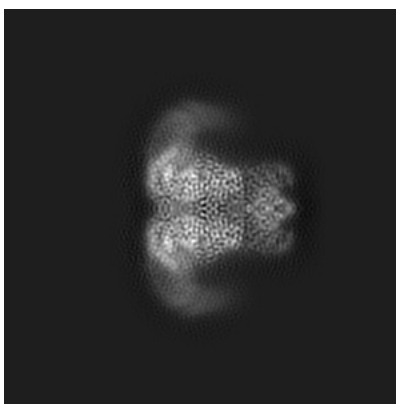
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

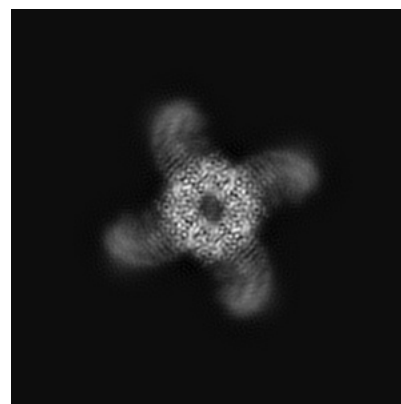
#### 6.1.1 Primary map



X

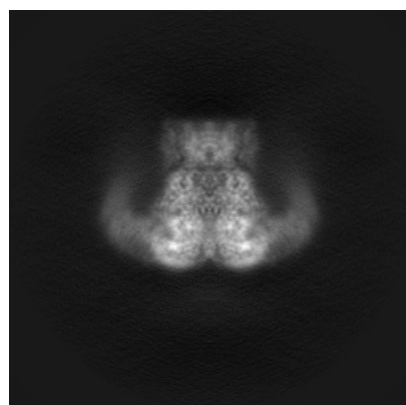


Y

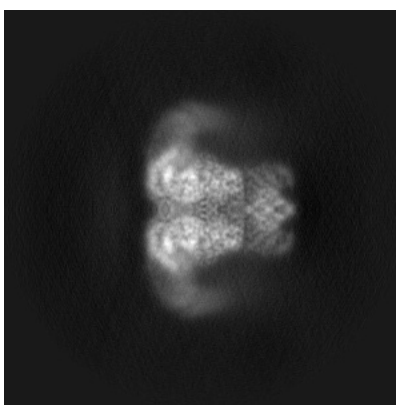


Z

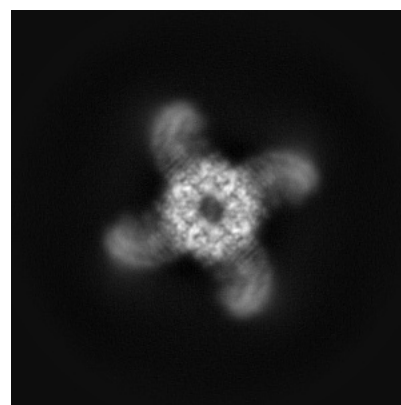
#### 6.1.2 Raw map



X



Y

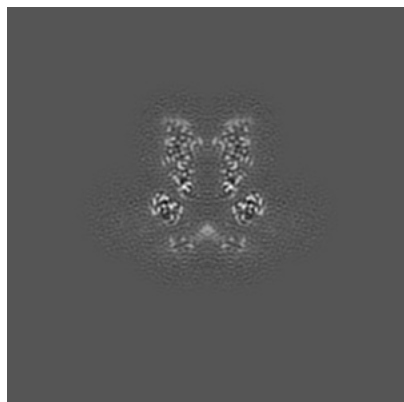


Z

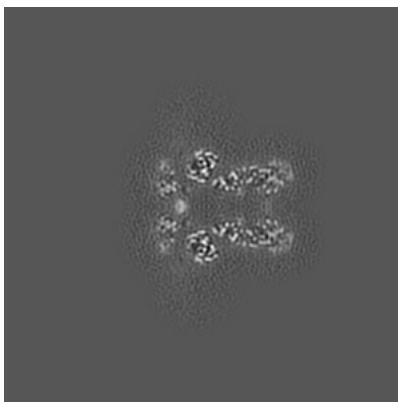
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

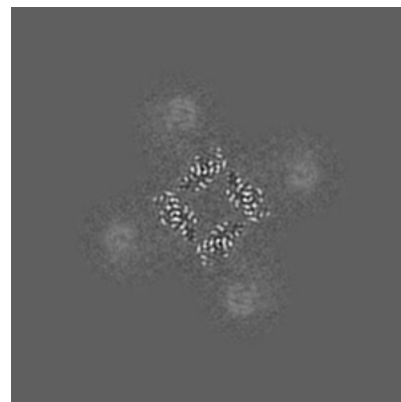
### 6.2.1 Primary map



X Index: 200

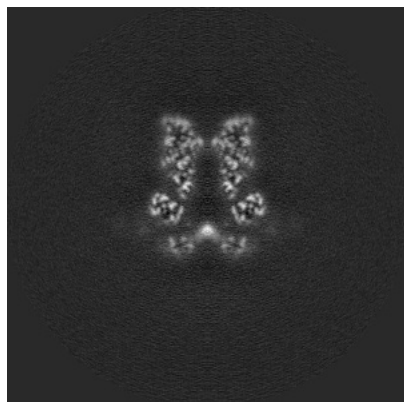


Y Index: 200

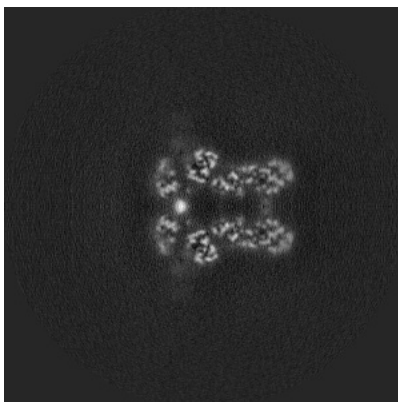


Z Index: 200

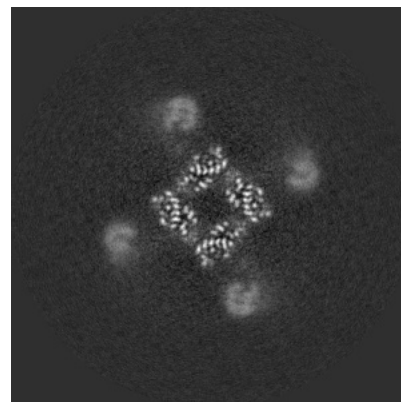
### 6.2.2 Raw map



X Index: 200



Y Index: 200

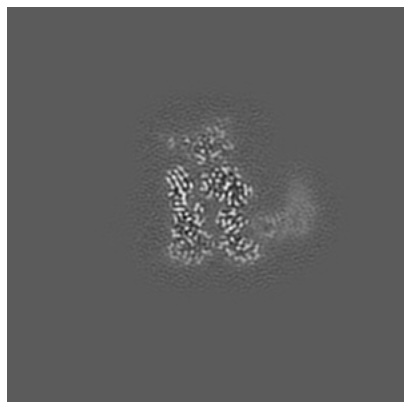


Z Index: 200

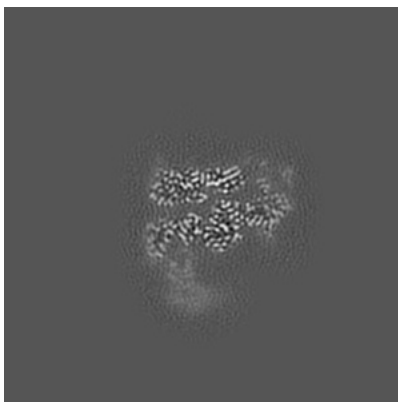
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

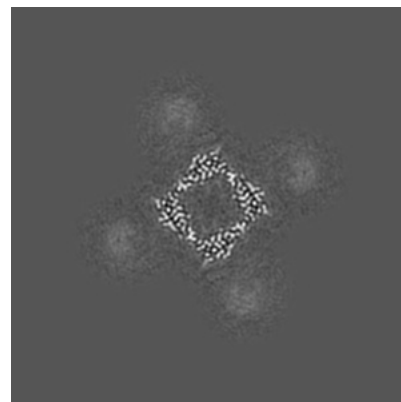
### 6.3.1 Primary map



X Index: 178

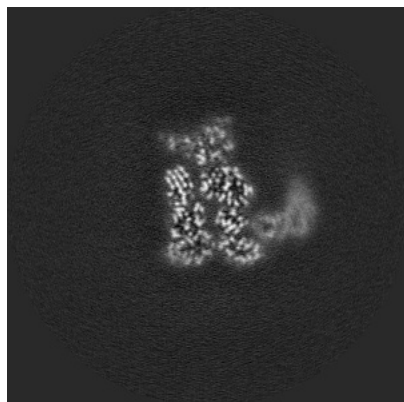


Y Index: 178

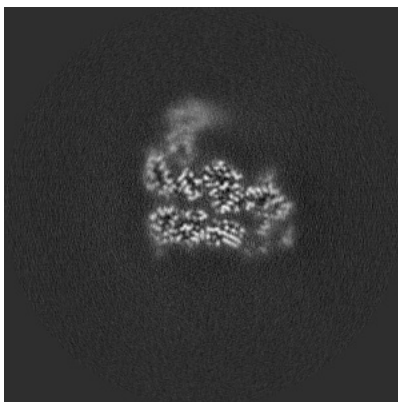


Z Index: 203

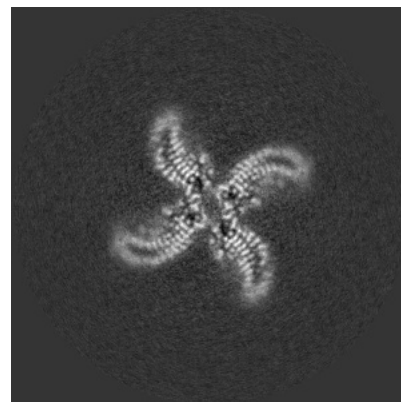
### 6.3.2 Raw map



X Index: 178



Y Index: 222



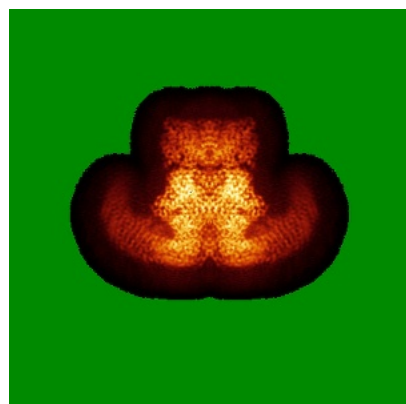
Z Index: 163

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

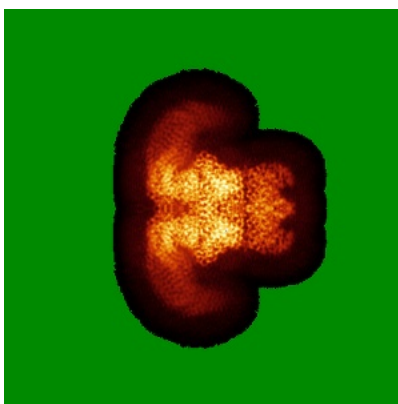


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

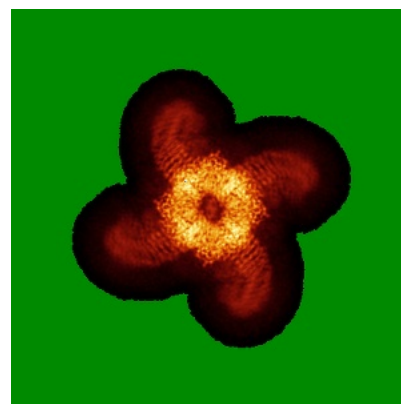
### 6.4.1 Primary map



X

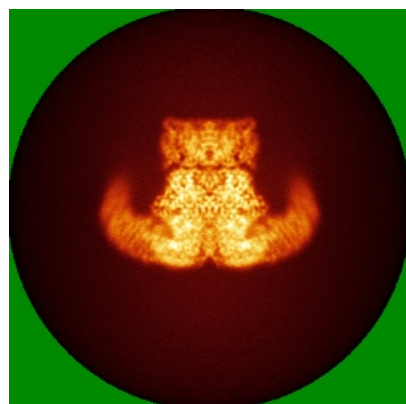


Y

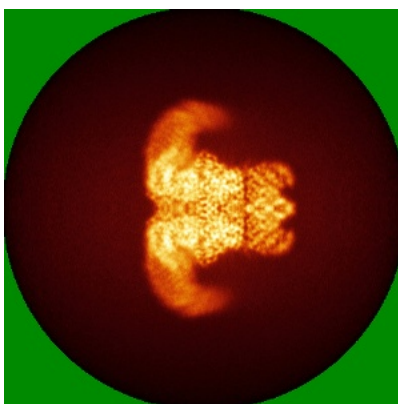


Z

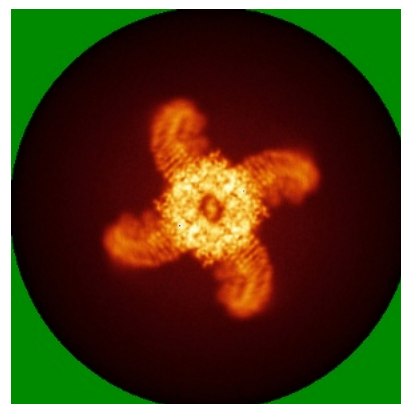
### 6.4.2 Raw map



X



Y

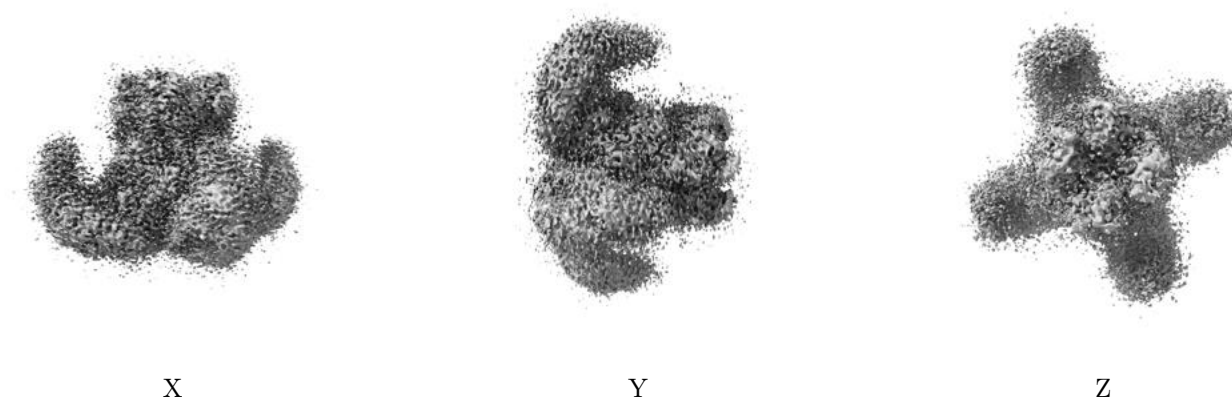


Z

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.

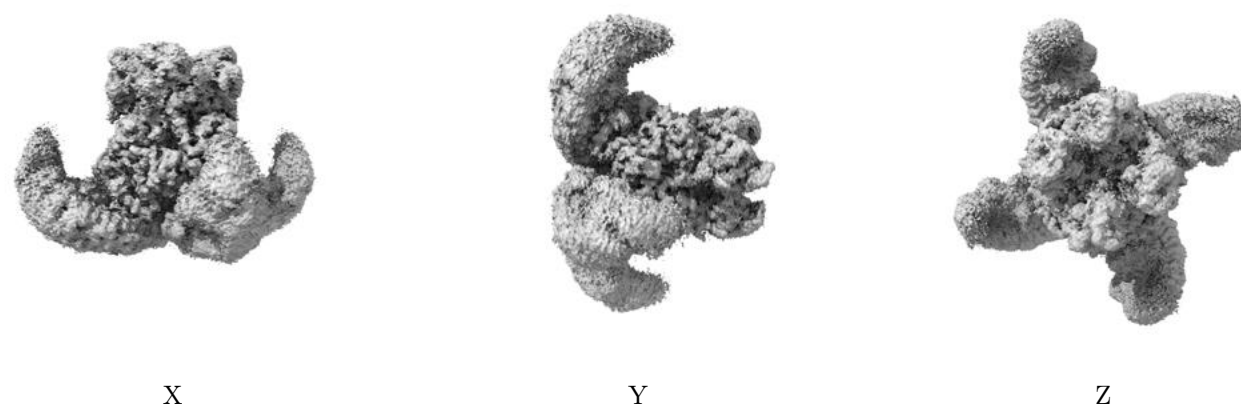
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



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.

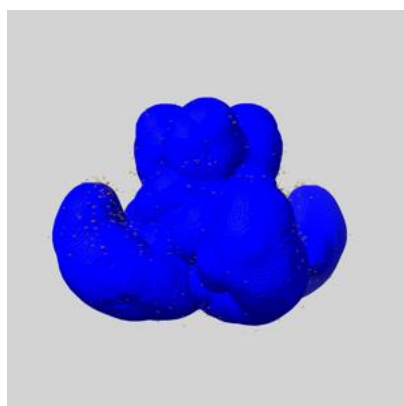
## 6.6 Mask visualisation [i](#)

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

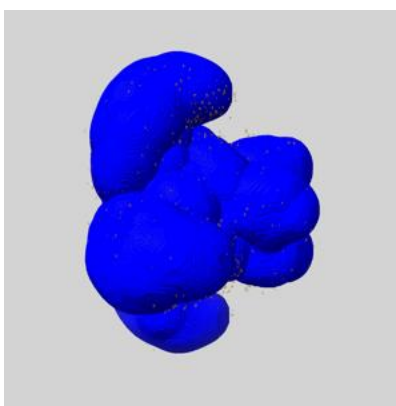
A mask typically either:

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

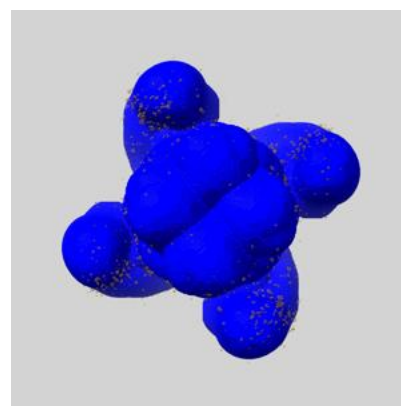
### 6.6.1 emd\_53375\_msk\_1.map [i](#)



X



Y

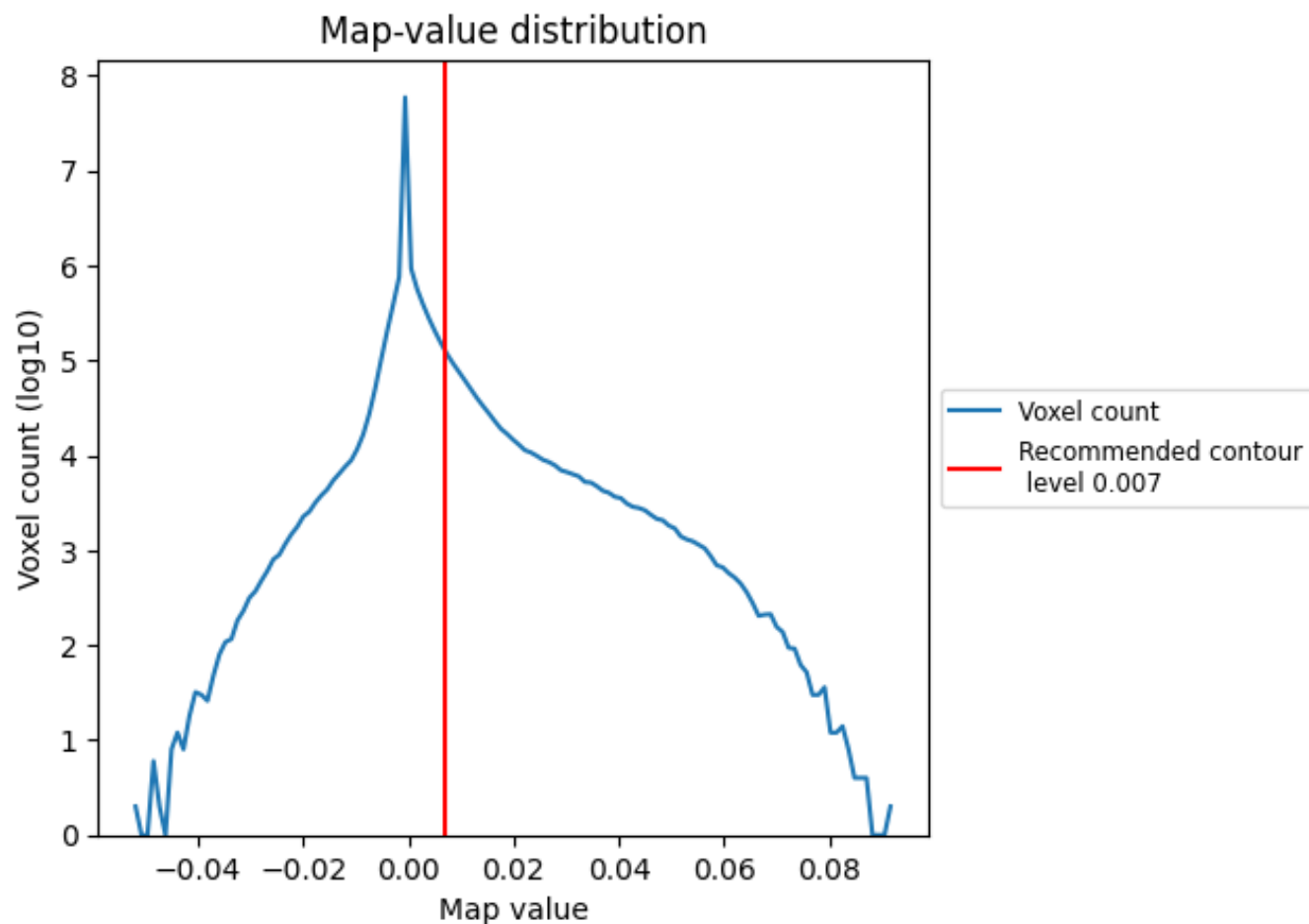


Z

## 7 Map analysis [i](#)

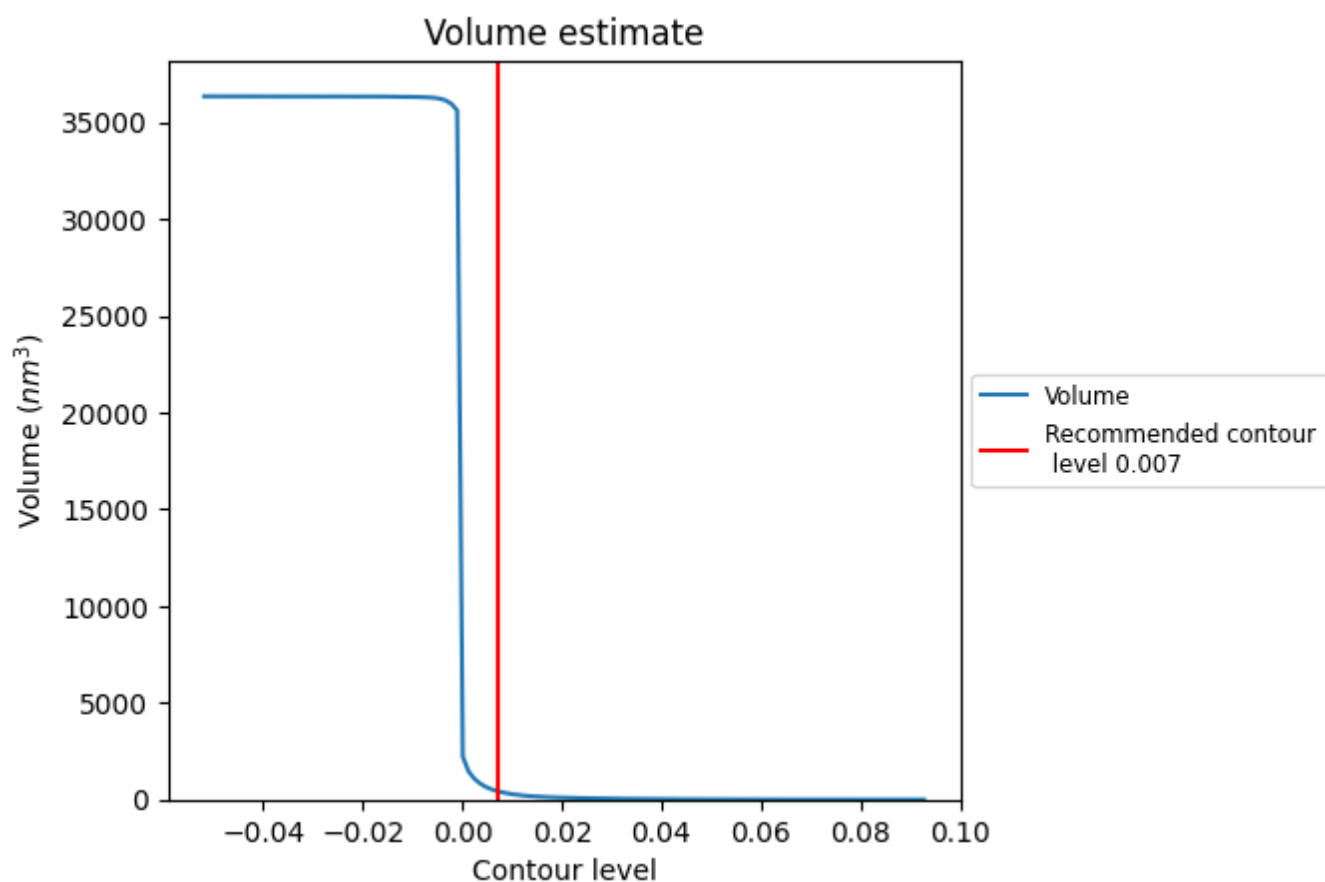
This section contains the results of statistical analysis of the map.

### 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.

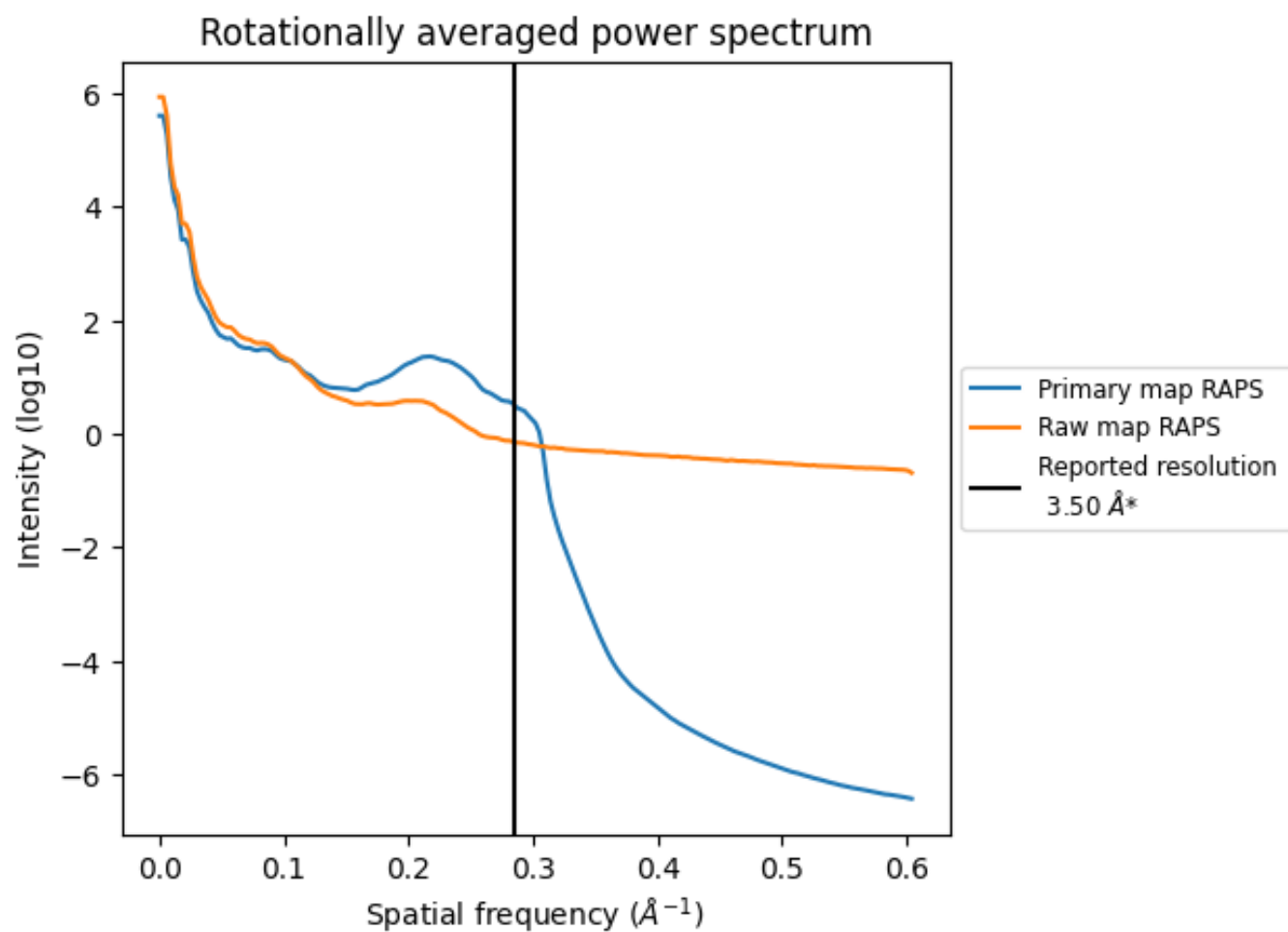
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439  $\text{nm}^3$ ; this corresponds to an approximate mass of 397 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 ⓘ

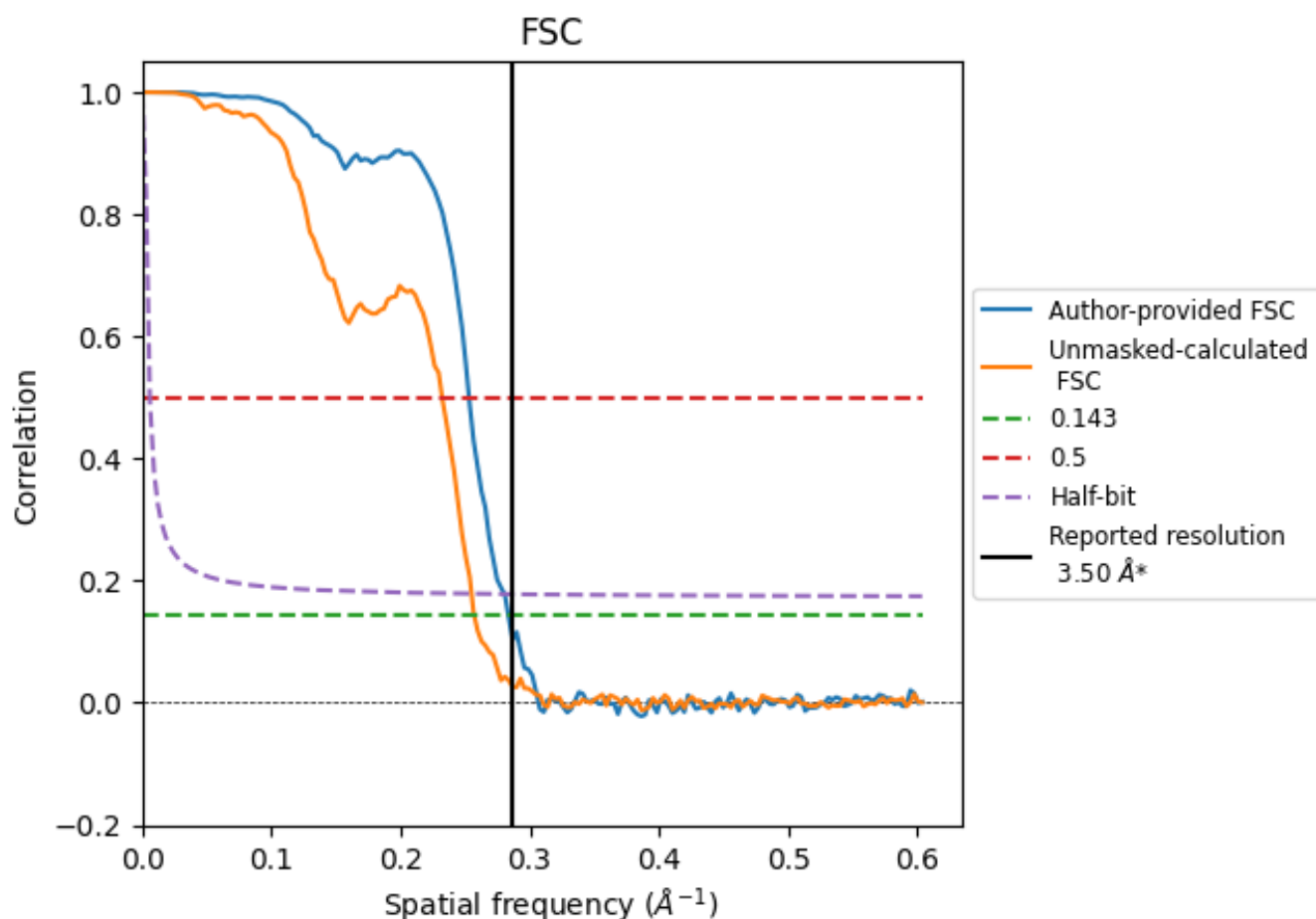


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	3.95	3.57
Unmasked-calculated*	3.89	4.31	3.92

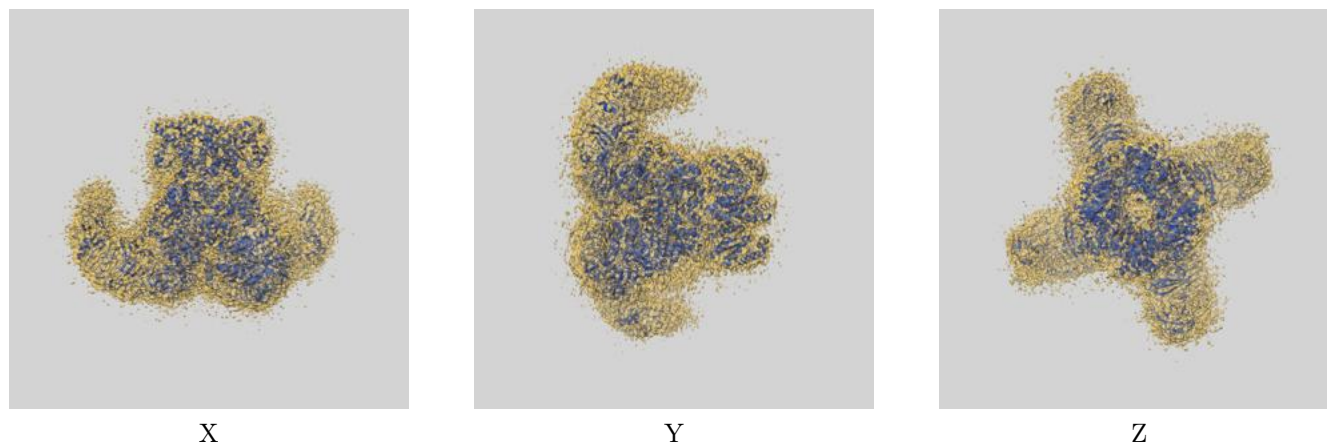
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.5 by more than 10 %



## 9 Map-model fit [i](#)

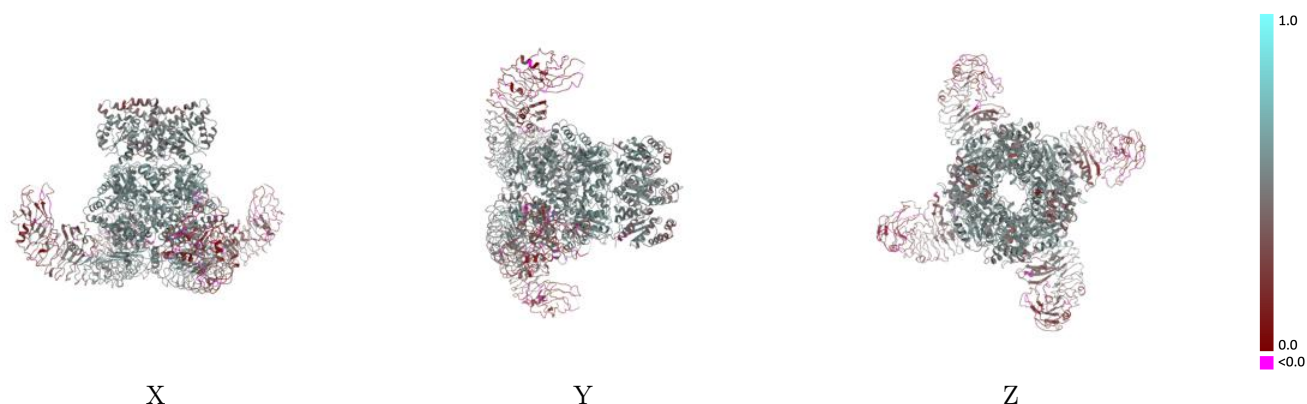
This section contains information regarding the fit between EMDB map EMD-53375 and PDB model 9QU9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



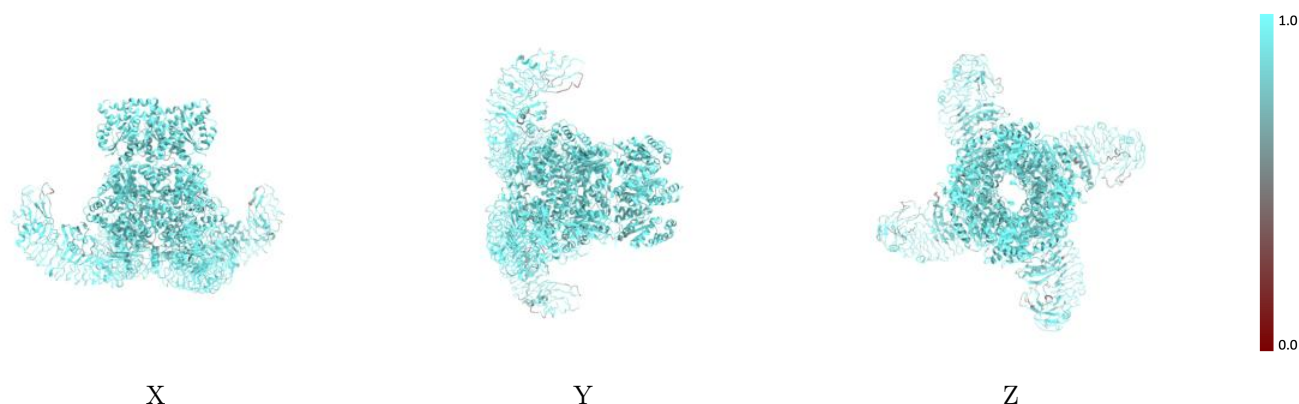
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



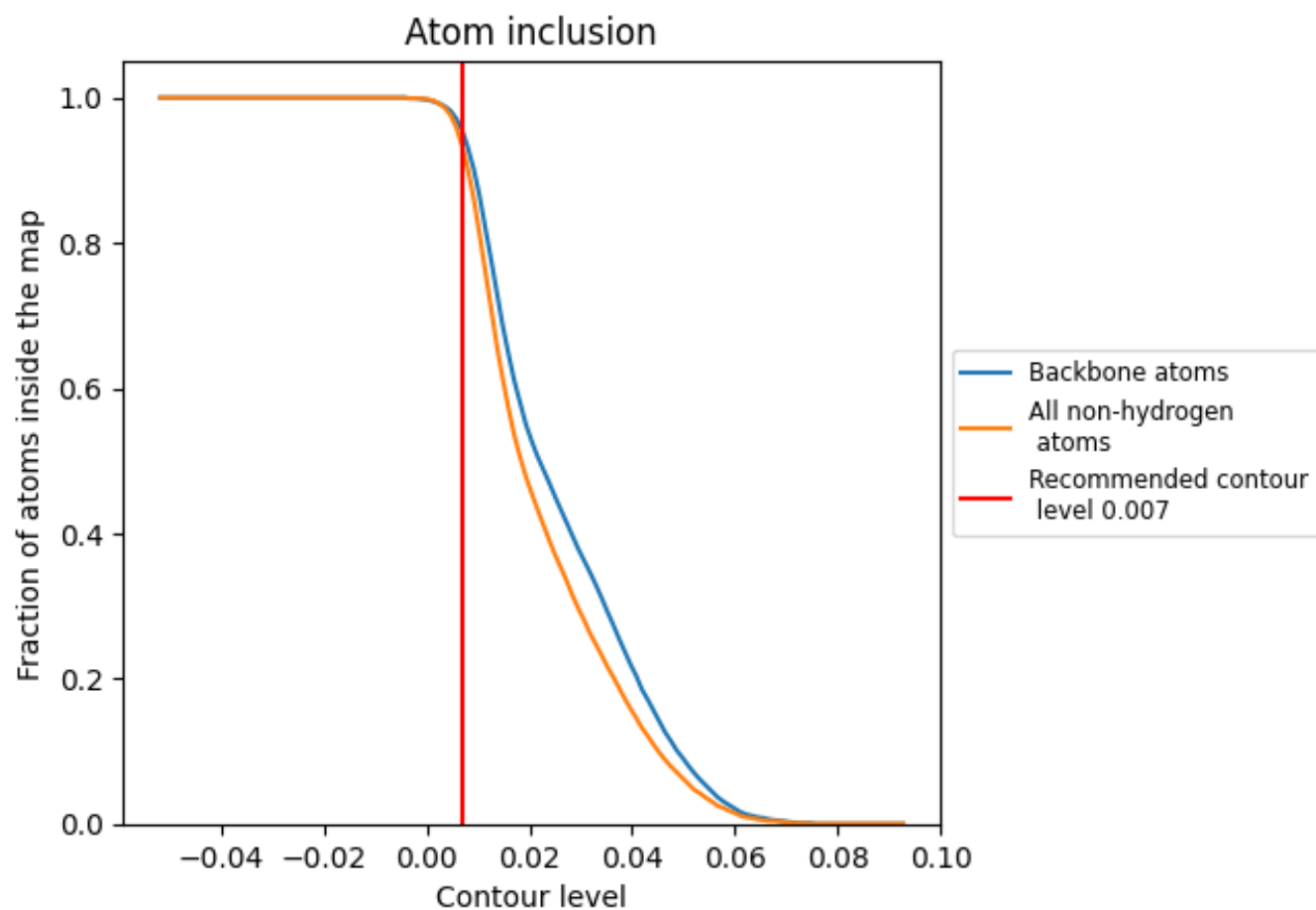
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9310	<div></div> 0.4390
A	<div></div> 0.9450	<div></div> 0.4620
B	<div></div> 0.9290	<div></div> 0.4330
C	<div></div> 0.9470	<div></div> 0.4640
D	<div></div> 0.9310	<div></div> 0.4380
P	<div></div> 0.8600	<div></div> 0.3210
Q	<div></div> 0.8310	<div></div> 0.2630
R	<div></div> 0.8870	<div></div> 0.3400
S	<div></div> 0.7950	<div></div> 0.2530

1.0

0.0

<0.0