



Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 07:17 PM EST

PDB ID : 7VQO
EMDB ID : EMD-32091
Title : Cryo-EM structure of Ams1 bound to the FW domain of Nbr1
Authors : Zhang, J.; Ye, K.
Deposited on : 2021-10-20
Resolution : 2.19 Å (reported)
Based on initial model : 6LZ1

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

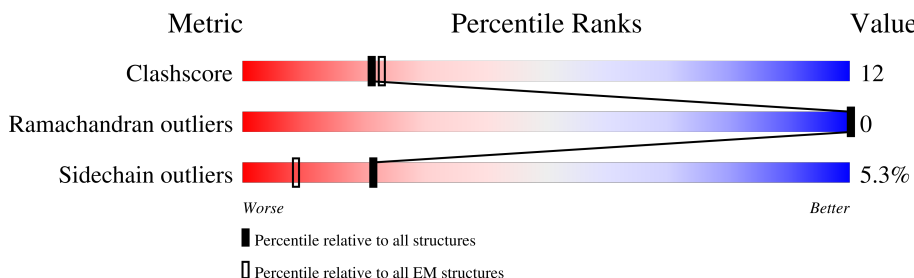
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.19 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1616	
1	B	1616	
1	C	1616	
1	D	1616	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38640 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 Ams1, Nbr1 and malE fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		
1	B	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		
1	C	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		
1	D	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1080	GLY	-	linker	UNP G0SGP6
A	1081	GLY	-	linker	UNP G0SGP6
A	1082	GLY	-	linker	UNP G0SGP6
A	1083	GLY	-	linker	UNP G0SGP6
A	1084	SER	-	linker	UNP G0SGP6
A	1085	GLY	-	linker	UNP G0SGP6
A	1086	GLY	-	linker	UNP G0SGP6
A	1087	GLY	-	linker	UNP G0SGP6
A	1088	PHE	-	linker	UNP G0SGP6
A	1089	LYS	-	linker	UNP G0SGP6
A	1090	LYS	-	linker	UNP G0SGP6
A	1091	ALA	-	linker	UNP G0SGP6
A	1092	SER	-	linker	UNP G0SGP6
A	1093	SER	-	linker	UNP G0SGP6
A	1094	SER	-	linker	UNP G0SGP6
A	1095	ASP	-	linker	UNP G0SGP6
A	1096	ASN	-	linker	UNP G0SGP6
A	1097	LYS	-	linker	UNP G0SGP6
A	1098	GLU	-	linker	UNP G0SGP6
A	1099	GLN	-	linker	UNP G0SGP6
A	1100	GLY	-	linker	UNP G0SGP6
A	1101	GLY	-	linker	UNP G0SGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	GLY	-	linker	UNP G0SGP6
A	1103	GLY	-	linker	UNP G0SGP6
A	1104	SER	-	linker	UNP G0SGP6
A	1105	GLY	-	linker	UNP G0SGP6
A	1106	GLY	-	linker	UNP G0SGP6
A	1107	GLY	-	linker	UNP G0SGP6
A	1108	SER	-	linker	UNP G0SGP6
A	1109	GLY	-	linker	UNP G0SGP6
B	1080	GLY	-	linker	UNP G0SGP6
B	1081	GLY	-	linker	UNP G0SGP6
B	1082	GLY	-	linker	UNP G0SGP6
B	1083	GLY	-	linker	UNP G0SGP6
B	1084	SER	-	linker	UNP G0SGP6
B	1085	GLY	-	linker	UNP G0SGP6
B	1086	GLY	-	linker	UNP G0SGP6
B	1087	GLY	-	linker	UNP G0SGP6
B	1088	PHE	-	linker	UNP G0SGP6
B	1089	LYS	-	linker	UNP G0SGP6
B	1090	LYS	-	linker	UNP G0SGP6
B	1091	ALA	-	linker	UNP G0SGP6
B	1092	SER	-	linker	UNP G0SGP6
B	1093	SER	-	linker	UNP G0SGP6
B	1094	SER	-	linker	UNP G0SGP6
B	1095	ASP	-	linker	UNP G0SGP6
B	1096	ASN	-	linker	UNP G0SGP6
B	1097	LYS	-	linker	UNP G0SGP6
B	1098	GLU	-	linker	UNP G0SGP6
B	1099	GLN	-	linker	UNP G0SGP6
B	1100	GLY	-	linker	UNP G0SGP6
B	1101	GLY	-	linker	UNP G0SGP6
B	1102	GLY	-	linker	UNP G0SGP6
B	1103	GLY	-	linker	UNP G0SGP6
B	1104	SER	-	linker	UNP G0SGP6
B	1105	GLY	-	linker	UNP G0SGP6
B	1106	GLY	-	linker	UNP G0SGP6
B	1107	GLY	-	linker	UNP G0SGP6
B	1108	SER	-	linker	UNP G0SGP6
B	1109	GLY	-	linker	UNP G0SGP6
C	1080	GLY	-	linker	UNP G0SGP6
C	1081	GLY	-	linker	UNP G0SGP6
C	1082	GLY	-	linker	UNP G0SGP6
C	1083	GLY	-	linker	UNP G0SGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1084	SER	-	linker	UNP G0SGP6
C	1085	GLY	-	linker	UNP G0SGP6
C	1086	GLY	-	linker	UNP G0SGP6
C	1087	GLY	-	linker	UNP G0SGP6
C	1088	PHE	-	linker	UNP G0SGP6
C	1089	LYS	-	linker	UNP G0SGP6
C	1090	LYS	-	linker	UNP G0SGP6
C	1091	ALA	-	linker	UNP G0SGP6
C	1092	SER	-	linker	UNP G0SGP6
C	1093	SER	-	linker	UNP G0SGP6
C	1094	SER	-	linker	UNP G0SGP6
C	1095	ASP	-	linker	UNP G0SGP6
C	1096	ASN	-	linker	UNP G0SGP6
C	1097	LYS	-	linker	UNP G0SGP6
C	1098	GLU	-	linker	UNP G0SGP6
C	1099	GLN	-	linker	UNP G0SGP6
C	1100	GLY	-	linker	UNP G0SGP6
C	1101	GLY	-	linker	UNP G0SGP6
C	1102	GLY	-	linker	UNP G0SGP6
C	1103	GLY	-	linker	UNP G0SGP6
C	1104	SER	-	linker	UNP G0SGP6
C	1105	GLY	-	linker	UNP G0SGP6
C	1106	GLY	-	linker	UNP G0SGP6
C	1107	GLY	-	linker	UNP G0SGP6
C	1108	SER	-	linker	UNP G0SGP6
C	1109	GLY	-	linker	UNP G0SGP6
D	1080	GLY	-	linker	UNP G0SGP6
D	1081	GLY	-	linker	UNP G0SGP6
D	1082	GLY	-	linker	UNP G0SGP6
D	1083	GLY	-	linker	UNP G0SGP6
D	1084	SER	-	linker	UNP G0SGP6
D	1085	GLY	-	linker	UNP G0SGP6
D	1086	GLY	-	linker	UNP G0SGP6
D	1087	GLY	-	linker	UNP G0SGP6
D	1088	PHE	-	linker	UNP G0SGP6
D	1089	LYS	-	linker	UNP G0SGP6
D	1090	LYS	-	linker	UNP G0SGP6
D	1091	ALA	-	linker	UNP G0SGP6
D	1092	SER	-	linker	UNP G0SGP6
D	1093	SER	-	linker	UNP G0SGP6
D	1094	SER	-	linker	UNP G0SGP6
D	1095	ASP	-	linker	UNP G0SGP6

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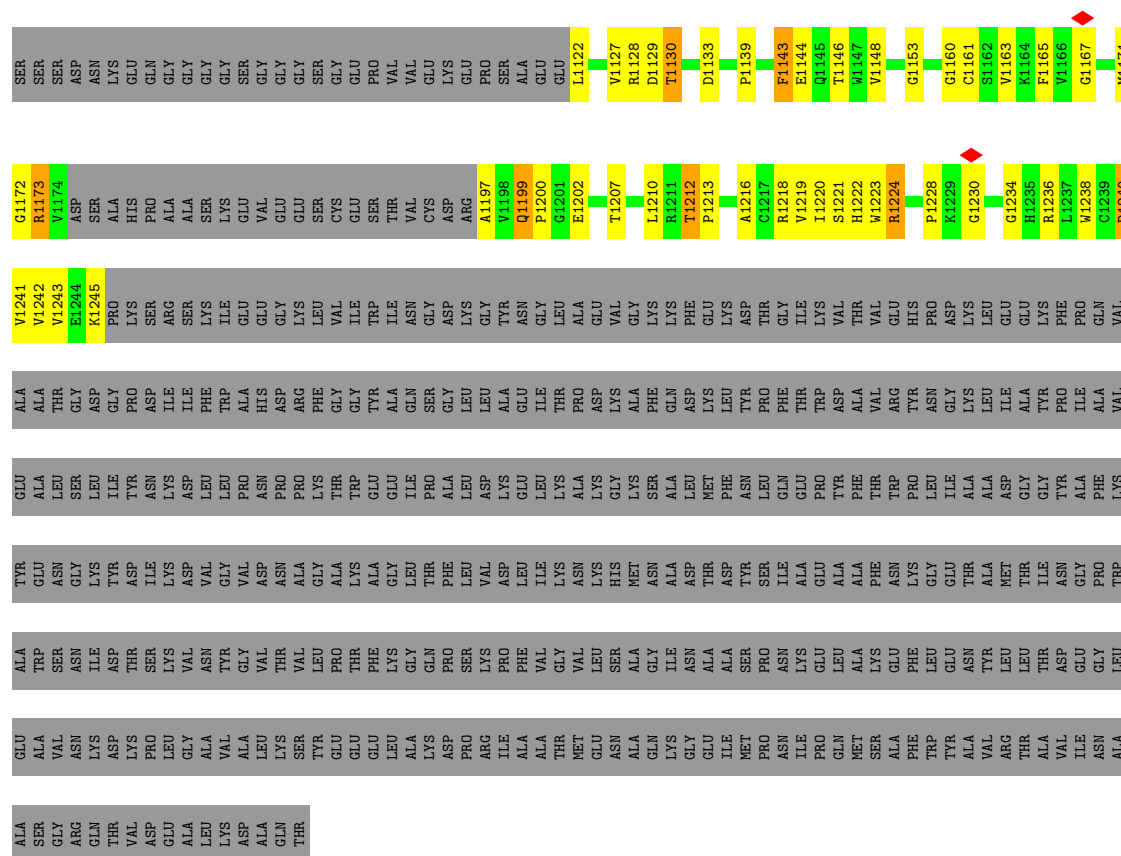
Chain	Residue	Modelled	Actual	Comment	Reference
D	1096	ASN	-	linker	UNP G0SGP6
D	1097	LYS	-	linker	UNP G0SGP6
D	1098	GLU	-	linker	UNP G0SGP6
D	1099	GLN	-	linker	UNP G0SGP6
D	1100	GLY	-	linker	UNP G0SGP6
D	1101	GLY	-	linker	UNP G0SGP6
D	1102	GLY	-	linker	UNP G0SGP6
D	1103	GLY	-	linker	UNP G0SGP6
D	1104	SER	-	linker	UNP G0SGP6
D	1105	GLY	-	linker	UNP G0SGP6
D	1106	GLY	-	linker	UNP G0SGP6
D	1107	GLY	-	linker	UNP G0SGP6
D	1108	SER	-	linker	UNP G0SGP6
D	1109	GLY	-	linker	UNP G0SGP6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0

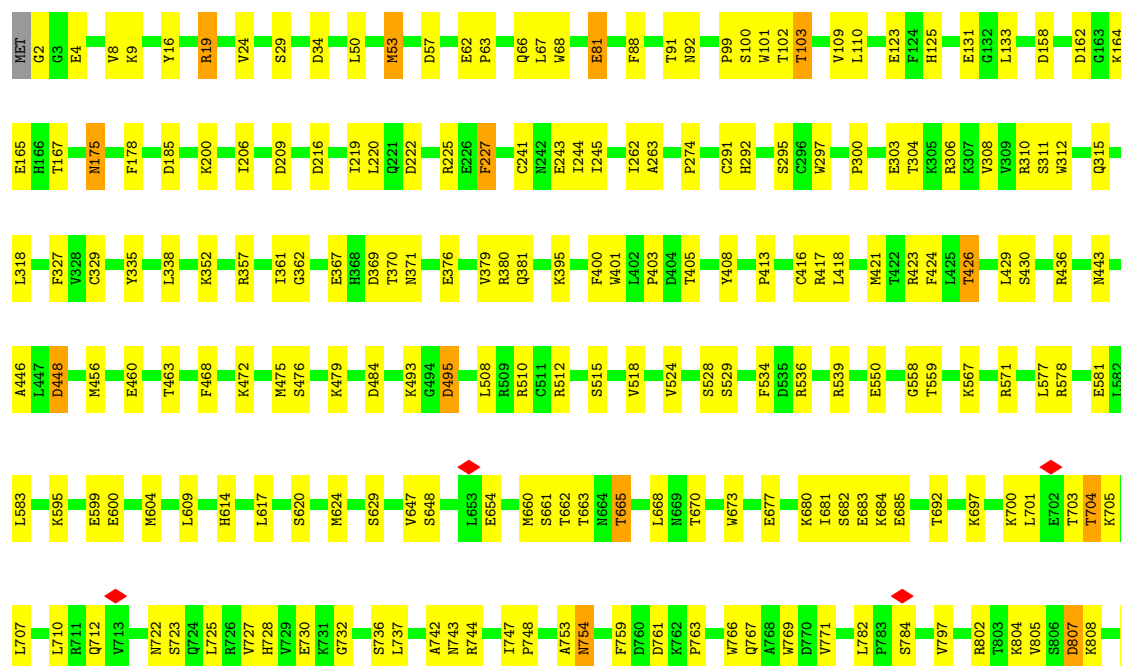
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	A	167	Total O 167 167	0
3	B	174	Total O 174 174	0
3	C	173	Total O 173 173	0
3	D	174	Total O 174 174	0



- Molecule 1: Ams1, Nbr1 and malE fusion protein

Chain C: 53% 18% 27%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	692409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.628	Depositor
Minimum map value	-38.771	Depositor
Average map value	0.052	Depositor
Map value standard deviation	2.444	Depositor
Recommended contour level	10	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/9750	0.50	0/13244
1	B	0.45	0/9750	0.50	0/13244
1	C	0.45	0/9750	0.50	0/13244
1	D	0.45	0/9750	0.50	0/13244
All	All	0.45	0/39000	0.50	0/52976

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	9487	0	9246	223	0
1	B	9487	0	9246	221	0
1	C	9487	0	9246	220	0
1	D	9487	0	9246	221	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	167	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	174	0	0	18	0
3	C	173	0	0	18	0
3	D	174	0	0	20	0
All	All	38640	0	36984	869	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 12.

All (869) 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:B:1161:CYS:H	1:B:1228:PRO:HD3	1.44	0.83
1:A:1161:CYS:H	1:A:1228:PRO:HD3	1.44	0.83
1:D:1161:CYS:H	1:D:1228:PRO:HD3	1.44	0.83
1:C:1161:CYS:H	1:C:1228:PRO:HD3	1.44	0.82
1:B:742:ALA:HB2	1:B:944:GLN:HE21	1.44	0.82
1:A:742:ALA:HB2	1:A:944:GLN:HE21	1.44	0.82
1:C:754:ASN:O	1:C:754:ASN:ND2	2.13	0.82
1:D:754:ASN:O	1:D:754:ASN:ND2	2.13	0.82
1:C:329:CYS:HG	1:C:335:TYR:HH	1.27	0.82
1:C:742:ALA:HB2	1:C:944:GLN:HE21	1.44	0.82
1:D:742:ALA:HB2	1:D:944:GLN:HE21	1.44	0.81
1:D:986:SER:HB2	1:D:1031:GLY:HA2	1.64	0.80
1:C:986:SER:HB2	1:C:1031:GLY:HA2	1.64	0.80
1:A:754:ASN:O	1:A:754:ASN:ND2	2.13	0.80
1:B:754:ASN:ND2	1:B:754:ASN:O	2.13	0.80
1:A:986:SER:HB2	1:A:1031:GLY:HA2	1.64	0.79
1:B:986:SER:HB2	1:B:1031:GLY:HA2	1.64	0.79
1:D:677:GLU:OE1	1:D:962:THR:CG2	2.30	0.79
1:D:329:CYS:HG	1:D:335:TYR:HH	1.30	0.78
1:A:703:THR:HG22	1:A:704:THR:H	1.50	0.76
1:B:703:THR:HG22	1:B:704:THR:H	1.50	0.76
1:D:703:THR:HG22	1:D:704:THR:H	1.50	0.75
1:C:703:THR:HG22	1:C:704:THR:H	1.50	0.75
1:C:761:ASP:OD2	1:C:920:ARG:NH1	2.21	0.74
1:D:761:ASP:OD2	1:D:920:ARG:NH1	2.21	0.74
1:B:761:ASP:OD2	1:B:920:ARG:NH1	2.21	0.74
1:A:761:ASP:OD2	1:A:920:ARG:NH1	2.21	0.73
1:C:380:ARG:NH2	1:C:581:GLU:OE2	2.21	0.73
1:D:380:ARG:NH2	1:D:581:GLU:OE2	2.21	0.73
1:A:380:ARG:NH2	1:A:581:GLU:OE2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:NH2	1:B:581:GLU:OE2	2.21	0.72
1:B:416:CYS:SG	3:B:1961:HOH:O	2.48	0.72
1:B:728:HIS:HB2	1:B:736:SER:HB3	1.72	0.71
1:A:728:HIS:HB2	1:A:736:SER:HB3	1.72	0.71
1:A:416:CYS:SG	3:A:1954:HOH:O	2.48	0.71
1:D:728:HIS:HB2	1:D:736:SER:HB3	1.72	0.71
1:C:728:HIS:HB2	1:C:736:SER:HB3	1.72	0.71
1:D:416:CYS:SG	3:D:1960:HOH:O	2.48	0.70
1:A:436:ARG:HH21	1:A:436:ARG:HG3	1.56	0.70
1:B:436:ARG:HG3	1:B:436:ARG:HH21	1.56	0.70
1:B:125:HIS:ND1	3:B:1808:HOH:O	2.24	0.70
1:C:125:HIS:ND1	3:C:1809:HOH:O	2.25	0.70
1:C:416:CYS:SG	3:C:1959:HOH:O	2.49	0.70
1:D:436:ARG:HH21	1:D:436:ARG:HG3	1.56	0.70
1:D:125:HIS:ND1	3:D:1809:HOH:O	2.25	0.70
1:C:436:ARG:HH21	1:C:436:ARG:HG3	1.56	0.69
1:A:1199:GLN:N	1:A:1202:GLU:OE2	2.25	0.69
1:B:1199:GLN:N	1:B:1202:GLU:OE2	2.25	0.69
1:B:329:CYS:SG	1:B:335:TYR:OH	2.50	0.69
1:C:1127:VAL:HB	1:C:1148:VAL:HG23	1.75	0.69
1:D:1127:VAL:HB	1:D:1148:VAL:HG23	1.75	0.69
1:A:329:CYS:SG	1:A:335:TYR:OH	2.50	0.69
1:C:980:VAL:HG22	1:C:1035:THR:HG22	1.76	0.68
1:D:980:VAL:HG22	1:D:1035:THR:HG22	1.76	0.68
1:C:1199:GLN:N	1:C:1202:GLU:OE2	2.25	0.68
1:D:1199:GLN:N	1:D:1202:GLU:OE2	2.26	0.68
1:B:1218:ARG:NE	3:B:1815:HOH:O	2.27	0.68
1:A:1127:VAL:HB	1:A:1148:VAL:HG23	1.75	0.68
1:B:1127:VAL:HB	1:B:1148:VAL:HG23	1.75	0.68
1:D:1218:ARG:NE	3:D:1814:HOH:O	2.27	0.68
1:A:1218:ARG:NE	3:A:1812:HOH:O	2.27	0.67
1:C:53:MET:SD	3:C:1861:HOH:O	2.52	0.67
1:A:53:MET:SD	3:A:1856:HOH:O	2.52	0.67
1:C:578:ARG:NH1	1:C:670:THR:O	2.28	0.67
1:D:578:ARG:NH1	1:D:670:THR:O	2.28	0.67
1:A:578:ARG:NH1	1:A:670:THR:O	2.28	0.67
1:A:980:VAL:HG22	1:A:1035:THR:HG22	1.76	0.67
1:B:980:VAL:HG22	1:B:1035:THR:HG22	1.76	0.67
1:B:53:MET:SD	3:B:1859:HOH:O	2.53	0.66
1:B:578:ARG:NH1	1:B:670:THR:O	2.28	0.66
1:A:110:LEU:O	1:A:165:GLU:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:O	1:B:165:GLU:HA	1.96	0.66
1:B:1197:ALA:N	3:B:1817:HOH:O	2.29	0.66
1:B:707:LEU:HD23	1:B:819:GLY:HA2	1.77	0.65
1:A:707:LEU:HD23	1:A:819:GLY:HA2	1.77	0.65
1:A:1197:ALA:N	3:A:1816:HOH:O	2.29	0.65
1:C:1197:ALA:N	3:C:1819:HOH:O	2.29	0.65
1:D:707:LEU:HD23	1:D:819:GLY:HA2	1.77	0.65
1:C:707:LEU:HD23	1:C:819:GLY:HA2	1.77	0.65
1:D:1197:ALA:N	3:D:1817:HOH:O	2.29	0.65
1:A:9:LYS:N	1:A:9:LYS:HE2	2.12	0.65
1:B:9:LYS:HE2	1:B:9:LYS:N	2.12	0.65
1:C:707:LEU:HD11	1:C:817:LEU:HB3	1.78	0.65
1:B:705:LYS:N	1:B:705:LYS:HE2	2.12	0.65
1:A:705:LYS:HE2	1:A:705:LYS:N	2.12	0.64
1:D:707:LEU:HD11	1:D:817:LEU:HB3	1.78	0.64
1:A:583:LEU:HD11	1:A:668:LEU:HD21	1.79	0.64
1:A:707:LEU:HD11	1:A:817:LEU:HB3	1.78	0.64
1:C:705:LYS:N	1:C:705:LYS:HE2	2.12	0.64
1:D:110:LEU:O	1:D:165:GLU:HA	1.96	0.64
1:D:705:LYS:HE2	1:D:705:LYS:N	2.12	0.64
1:B:707:LEU:HD11	1:B:817:LEU:HB3	1.78	0.64
1:B:583:LEU:HD11	1:B:668:LEU:HD21	1.79	0.64
1:C:110:LEU:O	1:C:165:GLU:HA	1.96	0.64
1:C:9:LYS:N	1:C:9:LYS:HE2	2.12	0.64
1:C:700:LYS:O	1:C:700:LYS:NZ	2.31	0.64
1:D:9:LYS:HE2	1:D:9:LYS:N	2.12	0.64
1:D:700:LYS:O	1:D:700:LYS:NZ	2.31	0.64
1:C:583:LEU:HD11	1:C:668:LEU:HD21	1.79	0.63
1:D:68:TRP:HB3	1:D:88:PHE:HB3	1.79	0.63
1:C:68:TRP:HB3	1:C:88:PHE:HB3	1.80	0.63
1:D:583:LEU:HD11	1:D:668:LEU:HD21	1.79	0.63
1:A:68:TRP:HB3	1:A:88:PHE:HB3	1.79	0.63
1:B:68:TRP:HB3	1:B:88:PHE:HB3	1.80	0.63
1:B:175:ASN:HA	1:B:180:ASN:HD21	1.63	0.63
1:D:677:GLU:OE1	1:D:962:THR:HG23	1.96	0.63
1:A:175:ASN:HA	1:A:180:ASN:HD21	1.63	0.62
1:A:2:GLY:N	3:A:1819:HOH:O	2.32	0.62
1:A:550:GLU:OE1	1:A:867:ARG:NH2	2.28	0.62
1:B:550:GLU:OE1	1:B:867:ARG:NH2	2.28	0.62
1:B:1122:LEU:N	3:B:1821:HOH:O	2.32	0.62
1:C:677:GLU:OE1	1:C:962:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:LEU:N	3:A:1822:HOH:O	2.33	0.62
1:A:743:ASN:O	1:B:1030:ARG:NH2	2.31	0.61
1:A:700:LYS:O	1:A:700:LYS:NZ	2.31	0.61
1:D:1122:LEU:N	3:D:1824:HOH:O	2.33	0.61
1:B:700:LYS:O	1:B:700:LYS:NZ	2.31	0.61
1:C:175:ASN:ND2	3:C:1824:HOH:O	2.33	0.61
1:A:1030:ARG:NH2	1:B:743:ASN:O	2.32	0.61
1:B:216:ASP:OD1	1:B:510:ARG:NE	2.28	0.61
1:B:484:ASP:OD1	1:B:536:ARG:NH2	2.34	0.61
1:C:216:ASP:OD1	1:C:510:ARG:NE	2.28	0.61
1:D:216:ASP:OD1	1:D:510:ARG:NE	2.28	0.61
1:D:371:ASN:O	1:D:885:HIS:NE2	2.32	0.61
1:A:216:ASP:OD1	1:A:510:ARG:NE	2.28	0.60
1:A:484:ASP:OD1	1:A:536:ARG:NH2	2.34	0.60
1:C:484:ASP:OD1	1:C:536:ARG:NH2	2.34	0.60
1:D:484:ASP:OD1	1:D:536:ARG:NH2	2.34	0.60
1:B:371:ASN:O	1:B:885:HIS:NE2	2.32	0.60
1:C:371:ASN:O	1:C:885:HIS:NE2	2.32	0.60
1:A:371:ASN:O	1:A:885:HIS:NE2	2.32	0.60
1:C:165:GLU:O	1:C:165:GLU:HG3	2.01	0.60
1:D:165:GLU:O	1:D:165:GLU:HG3	2.01	0.60
1:A:244:ILE:HD11	1:A:263:ALA:HB2	1.84	0.60
1:A:165:GLU:O	1:A:165:GLU:HG3	2.01	0.60
1:B:165:GLU:HG3	1:B:165:GLU:O	2.01	0.60
1:B:244:ILE:HD11	1:B:263:ALA:HB2	1.84	0.60
1:A:924:ALA:HB3	1:A:925:PRO:HD3	1.84	0.60
1:B:924:ALA:HB3	1:B:925:PRO:HD3	1.84	0.60
1:C:1030:ARG:NH2	1:D:743:ASN:O	2.32	0.59
1:D:244:ILE:HD11	1:D:263:ALA:HB2	1.84	0.59
1:C:244:ILE:HD11	1:C:263:ALA:HB2	1.84	0.59
1:C:1130:THR:OG1	1:C:1146:THR:OG1	2.20	0.59
1:C:743:ASN:O	1:D:1030:ARG:NH2	2.31	0.59
1:C:924:ALA:HB3	1:C:925:PRO:HD3	1.84	0.59
1:C:600:GLU:O	1:C:604:MET:HG3	2.02	0.59
1:D:600:GLU:O	1:D:604:MET:HG3	2.02	0.59
1:D:924:ALA:HB3	1:D:925:PRO:HD3	1.84	0.59
1:D:1213:PRO:HG3	1:D:1219:VAL:HG11	1.85	0.59
1:C:1213:PRO:HG3	1:C:1219:VAL:HG11	1.85	0.59
1:A:744:ARG:NH2	1:A:892:GLU:OE2	2.35	0.59
1:B:744:ARG:NH2	1:B:892:GLU:OE2	2.35	0.59
1:A:1213:PRO:HG3	1:A:1219:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ARG:HD2	1:B:1218:ARG:O	2.03	0.59
1:B:1213:PRO:HG3	1:B:1219:VAL:HG11	1.85	0.59
1:A:539:ARG:HD2	1:A:1218:ARG:O	2.03	0.59
1:C:821:VAL:HG23	1:C:824:GLU:HB2	1.85	0.58
1:D:821:VAL:HG23	1:D:824:GLU:HB2	1.85	0.58
1:A:1160:GLY:H	1:A:1228:PRO:HG3	1.67	0.58
1:B:1160:GLY:H	1:B:1228:PRO:HG3	1.67	0.58
1:C:682:SER:O	1:C:685:GLU:N	2.34	0.58
1:C:1160:GLY:H	1:C:1228:PRO:HG3	1.67	0.58
1:D:53:MET:SD	3:D:1866:HOH:O	2.57	0.58
1:A:1224:ARG:NH1	1:A:1234:GLY:O	2.36	0.58
1:B:600:GLU:O	1:B:604:MET:HG3	2.02	0.58
1:B:1130:THR:OG1	1:B:1146:THR:OG1	2.20	0.58
1:A:600:GLU:O	1:A:604:MET:HG3	2.02	0.58
1:B:1224:ARG:NH1	1:B:1234:GLY:O	2.36	0.58
1:C:744:ARG:HD3	1:C:895:TYR:CD2	2.39	0.58
1:C:1224:ARG:NH1	1:C:1234:GLY:O	2.36	0.58
1:D:682:SER:O	1:D:685:GLU:N	2.34	0.58
1:D:744:ARG:HD3	1:D:895:TYR:CD2	2.39	0.58
1:D:1160:GLY:H	1:D:1228:PRO:HG3	1.67	0.58
1:A:357:ARG:NE	3:A:1821:HOH:O	2.32	0.58
1:C:550:GLU:OE1	1:C:867:ARG:NH2	2.28	0.58
1:D:1224:ARG:NH1	1:D:1234:GLY:O	2.36	0.58
1:B:329:CYS:HG	1:B:335:TYR:HH	1.42	0.58
1:B:357:ARG:NE	3:B:1820:HOH:O	2.31	0.58
1:B:744:ARG:HD3	1:B:895:TYR:CD2	2.39	0.58
1:C:578:ARG:NH2	1:C:993:ASP:O	2.37	0.58
1:D:550:GLU:OE1	1:D:867:ARG:NH2	2.28	0.58
1:D:578:ARG:NH2	1:D:993:ASP:O	2.37	0.58
1:D:677:GLU:OE1	1:D:962:THR:HG21	2.03	0.58
1:B:821:VAL:HG23	1:B:824:GLU:HB2	1.85	0.58
1:A:744:ARG:HD3	1:A:895:TYR:CD2	2.39	0.57
1:A:821:VAL:HG23	1:A:824:GLU:HB2	1.85	0.57
1:D:1030:ARG:HG3	1:D:1030:ARG:HH11	1.69	0.57
1:B:677:GLU:OE1	1:B:962:THR:HG23	2.05	0.57
1:C:1030:ARG:HG3	1:C:1030:ARG:HH11	1.69	0.57
1:D:329:CYS:SG	1:D:335:TYR:OH	2.50	0.57
1:B:1030:ARG:HG3	1:B:1030:ARG:HH11	1.69	0.57
1:A:1030:ARG:HG3	1:A:1030:ARG:HH11	1.69	0.57
1:D:1130:THR:OG1	1:D:1146:THR:OG1	2.20	0.57
1:B:369:ASP:OD1	1:B:371:ASN:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASP:OD2	1:B:162:ASP:N	2.37	0.57
1:A:369:ASP:OD1	1:A:371:ASN:N	2.36	0.57
1:C:329:CYS:SG	1:C:335:TYR:OH	2.50	0.57
1:D:162:ASP:OD2	1:D:162:ASP:N	2.37	0.57
1:A:162:ASP:N	1:A:162:ASP:OD2	2.37	0.57
1:C:162:ASP:OD2	1:C:162:ASP:N	2.37	0.57
1:C:539:ARG:HD2	1:C:1218:ARG:O	2.03	0.57
1:D:1020:ARG:NH2	3:D:1835:HOH:O	2.38	0.57
1:C:744:ARG:NH2	1:C:892:GLU:OE2	2.35	0.57
1:D:175:ASN:ND2	3:D:1832:HOH:O	2.37	0.57
1:D:369:ASP:OD1	1:D:371:ASN:N	2.36	0.57
1:D:539:ARG:HD2	1:D:1218:ARG:O	2.03	0.57
1:C:369:ASP:OD1	1:C:371:ASN:N	2.36	0.56
1:D:744:ARG:NH2	1:D:892:GLU:OE2	2.35	0.56
1:D:297:TRP:HE1	1:D:769:TRP:HZ2	1.53	0.56
1:C:297:TRP:HE1	1:C:769:TRP:HZ2	1.53	0.56
1:C:571:ARG:NH2	1:C:885:HIS:O	2.38	0.56
1:D:571:ARG:NH2	1:D:885:HIS:O	2.38	0.56
1:A:578:ARG:NH2	1:A:993:ASP:O	2.37	0.56
1:B:578:ARG:NH2	1:B:993:ASP:O	2.37	0.56
1:B:175:ASN:ND2	3:B:1835:HOH:O	2.38	0.56
1:A:571:ARG:NH2	1:A:885:HIS:O	2.38	0.56
1:C:753:ALA:HA	1:C:848:PRO:HD2	1.87	0.56
1:C:1020:ARG:NH2	3:C:1830:HOH:O	2.39	0.56
1:A:753:ALA:HA	1:A:848:PRO:HD2	1.87	0.56
1:B:571:ARG:NH2	1:B:885:HIS:O	2.38	0.56
1:B:753:ALA:HA	1:B:848:PRO:HD2	1.87	0.56
1:D:753:ALA:HA	1:D:848:PRO:HD2	1.86	0.56
1:A:297:TRP:HE1	1:A:769:TRP:HZ2	1.53	0.55
1:B:297:TRP:HE1	1:B:769:TRP:HZ2	1.53	0.55
1:C:1129:ASP:OD1	1:C:1129:ASP:N	2.39	0.55
1:D:1129:ASP:N	1:D:1129:ASP:OD1	2.38	0.55
1:C:225:ARG:NH2	3:C:1836:HOH:O	2.39	0.55
1:A:329:CYS:HG	1:A:335:TYR:HH	1.44	0.55
1:B:225:ARG:NH2	3:B:1834:HOH:O	2.38	0.55
1:D:1015:GLN:NE2	3:D:1823:HOH:O	2.32	0.55
1:A:673:TRP:CD2	1:A:953:ARG:HD3	2.42	0.55
1:B:673:TRP:CD2	1:B:953:ARG:HD3	2.42	0.55
1:C:1015:GLN:NE2	3:C:1822:HOH:O	2.31	0.55
1:C:1218:ARG:HG3	1:C:1242:VAL:HG22	1.88	0.55
1:D:1218:ARG:HG3	1:D:1242:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:SER:O	1:A:685:GLU:N	2.34	0.55
1:B:682:SER:O	1:B:685:GLU:N	2.34	0.55
1:D:225:ARG:NH2	3:D:1837:HOH:O	2.39	0.55
1:A:1219:VAL:HG23	1:A:1241:VAL:HG23	1.89	0.55
1:A:225:ARG:NH2	3:A:1828:HOH:O	2.38	0.55
1:B:1219:VAL:HG23	1:B:1241:VAL:HG23	1.89	0.55
1:B:1129:ASP:OD1	1:B:1129:ASP:N	2.38	0.54
1:A:1129:ASP:OD1	1:A:1129:ASP:N	2.39	0.54
1:A:99:PRO:O	1:A:102:THR:OG1	2.25	0.54
1:A:1218:ARG:HG3	1:A:1242:VAL:HG22	1.88	0.54
1:B:99:PRO:O	1:B:102:THR:OG1	2.25	0.54
1:C:703:THR:HG22	1:C:704:THR:HG22	1.89	0.54
1:D:703:THR:HG22	1:D:704:THR:HG22	1.89	0.54
1:C:673:TRP:CD2	1:C:953:ARG:HD3	2.42	0.54
1:B:1218:ARG:HG3	1:B:1242:VAL:HG22	1.88	0.54
1:C:91:THR:OG1	1:C:92:ASN:N	2.41	0.54
1:D:91:THR:OG1	1:D:92:ASN:N	2.41	0.54
1:D:673:TRP:CD2	1:D:953:ARG:HD3	2.42	0.54
1:A:241:CYS:O	1:A:245:ILE:HG12	2.07	0.54
1:C:677:GLU:OE1	1:C:962:THR:CG2	2.56	0.54
1:B:91:THR:OG1	1:B:92:ASN:N	2.41	0.54
1:B:1020:ARG:NH2	3:B:1831:HOH:O	2.40	0.54
1:A:91:THR:OG1	1:A:92:ASN:N	2.41	0.54
1:B:241:CYS:O	1:B:245:ILE:HG12	2.07	0.54
1:C:241:CYS:O	1:C:245:ILE:HG12	2.07	0.54
1:D:241:CYS:O	1:D:245:ILE:HG12	2.07	0.54
1:C:418:LEU:O	1:C:1046:ASN:HB2	2.08	0.53
1:D:418:LEU:O	1:D:1046:ASN:HB2	2.08	0.53
1:A:418:LEU:O	1:A:1046:ASN:HB2	2.08	0.53
1:B:418:LEU:O	1:B:1046:ASN:HB2	2.08	0.53
1:B:703:THR:HG22	1:B:704:THR:HG22	1.89	0.53
1:A:703:THR:HG22	1:A:704:THR:HG22	1.89	0.53
1:C:1219:VAL:HG23	1:C:1241:VAL:HG23	1.89	0.53
1:D:274:PRO:HG2	1:D:1230:GLY:HA3	1.91	0.53
1:D:1219:VAL:HG23	1:D:1241:VAL:HG23	1.89	0.53
1:B:1015:GLN:NE2	3:B:1822:HOH:O	2.32	0.53
1:C:274:PRO:HG2	1:C:1230:GLY:HA3	1.91	0.53
1:B:274:PRO:HG2	1:B:1230:GLY:HA3	1.91	0.53
1:A:274:PRO:HG2	1:A:1230:GLY:HA3	1.91	0.53
1:A:1020:ARG:NH2	3:A:1833:HOH:O	2.42	0.53
1:B:822:GLU:OE2	1:B:822:GLU:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1130:THR:HG1	1:C:1146:THR:HG1	1.48	0.52
1:A:600:GLU:N	1:A:600:GLU:OE2	2.42	0.52
1:B:600:GLU:OE2	1:B:600:GLU:N	2.42	0.52
1:B:703:THR:HG22	1:B:704:THR:N	2.23	0.52
1:C:831:GLN:NE2	3:C:1838:HOH:O	2.42	0.52
1:D:357:ARG:NE	3:D:1822:HOH:O	2.30	0.52
1:A:703:THR:HG22	1:A:704:THR:N	2.23	0.52
1:A:822:GLU:OE2	1:A:822:GLU:N	2.38	0.52
1:B:831:GLN:NE2	3:B:1843:HOH:O	2.42	0.52
1:A:34:ASP:OD1	1:A:225:ARG:NH1	2.43	0.52
1:A:680:LYS:NZ	1:A:683:GLU:HG2	2.25	0.52
1:B:34:ASP:OD1	1:B:225:ARG:NH1	2.43	0.52
1:D:1130:THR:HG1	1:D:1146:THR:HG1	1.49	0.52
1:A:243:GLU:HG2	1:A:262:ILE:HD13	1.92	0.52
1:B:680:LYS:NZ	1:B:683:GLU:HG2	2.25	0.52
1:D:131:GLU:OE2	1:D:175:ASN:ND2	2.34	0.52
1:B:243:GLU:HG2	1:B:262:ILE:HD13	1.92	0.52
1:C:131:GLU:OE2	1:C:175:ASN:ND2	2.34	0.52
1:C:357:ARG:NE	3:C:1821:HOH:O	2.31	0.52
1:C:66:GLN:HG3	1:C:109:VAL:HB	1.92	0.52
1:D:66:GLN:HG3	1:D:109:VAL:HB	1.92	0.52
1:D:600:GLU:N	1:D:600:GLU:OE2	2.42	0.52
1:D:822:GLU:OE2	1:D:822:GLU:N	2.38	0.52
1:D:867:ARG:HD3	1:D:882:VAL:HG11	1.92	0.52
1:C:600:GLU:OE2	1:C:600:GLU:N	2.42	0.51
1:C:867:ARG:HD3	1:C:882:VAL:HG11	1.92	0.51
1:D:831:GLN:NE2	3:D:1843:HOH:O	2.43	0.51
1:C:103:THR:HB	1:C:306:ARG:HH12	1.76	0.51
1:C:1165:PHE:HB2	1:C:1223:TRP:CZ3	2.45	0.51
1:D:243:GLU:HG2	1:D:262:ILE:HD13	1.92	0.51
1:D:1165:PHE:HB2	1:D:1223:TRP:CZ3	2.45	0.51
1:A:103:THR:HB	1:A:306:ARG:HH12	1.76	0.51
1:A:831:GLN:NE2	3:A:1834:HOH:O	2.43	0.51
1:C:99:PRO:O	1:C:102:THR:OG1	2.25	0.51
1:C:822:GLU:OE2	1:C:822:GLU:N	2.38	0.51
1:D:103:THR:HB	1:D:306:ARG:HH12	1.76	0.51
1:D:680:LYS:NZ	1:D:683:GLU:HG2	2.25	0.51
1:B:131:GLU:OE2	1:B:175:ASN:ND2	2.34	0.51
1:C:243:GLU:HG2	1:C:262:ILE:HD13	1.92	0.51
1:C:680:LYS:NZ	1:C:683:GLU:HG2	2.25	0.51
1:D:34:ASP:OD1	1:D:225:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:HB	1:B:306:ARG:HH12	1.76	0.51
1:C:436:ARG:HG3	1:C:436:ARG:NH2	2.23	0.51
1:D:99:PRO:O	1:D:102:THR:OG1	2.25	0.51
1:D:436:ARG:HG3	1:D:436:ARG:NH2	2.23	0.51
1:A:131:GLU:OE2	1:A:175:ASN:ND2	2.34	0.51
1:A:436:ARG:HG3	1:A:436:ARG:NH2	2.23	0.51
1:B:1216:ALA:HA	1:B:1243:VAL:HB	1.93	0.51
1:C:34:ASP:OD1	1:C:225:ARG:NH1	2.43	0.51
1:C:802:ARG:HB3	1:C:802:ARG:HH11	1.76	0.51
1:A:8:VAL:C	1:A:9:LYS:HE2	2.32	0.51
1:A:1216:ALA:HA	1:A:1243:VAL:HB	1.93	0.51
1:B:436:ARG:HG3	1:B:436:ARG:NH2	2.23	0.51
1:B:742:ALA:O	1:B:744:ARG:N	2.44	0.51
1:A:867:ARG:HD3	1:A:882:VAL:HG11	1.92	0.51
1:B:8:VAL:C	1:B:9:LYS:HE2	2.32	0.51
1:C:8:VAL:C	1:C:9:LYS:HE2	2.32	0.51
1:C:380:ARG:NH2	1:C:996:LYS:HD3	2.26	0.51
1:D:8:VAL:C	1:D:9:LYS:HE2	2.32	0.51
1:D:380:ARG:NH2	1:D:996:LYS:HD3	2.26	0.51
1:D:802:ARG:HH11	1:D:802:ARG:HB3	1.76	0.51
1:A:66:GLN:HG3	1:A:109:VAL:HB	1.92	0.50
1:A:742:ALA:O	1:A:744:ARG:N	2.44	0.50
1:B:66:GLN:HG3	1:B:109:VAL:HB	1.92	0.50
1:B:867:ARG:HD3	1:B:882:VAL:HG11	1.92	0.50
1:A:654:GLU:HB3	1:A:965:TYR:HB3	1.94	0.50
1:A:380:ARG:NH2	1:A:996:LYS:HD3	2.26	0.50
1:B:654:GLU:HB3	1:B:965:TYR:HB3	1.94	0.50
1:A:682:SER:O	1:A:684:LYS:N	2.44	0.50
1:A:1165:PHE:HB2	1:A:1223:TRP:CZ3	2.45	0.50
1:B:1165:PHE:HB2	1:B:1223:TRP:CZ3	2.45	0.50
1:D:682:SER:O	1:D:684:LYS:N	2.44	0.50
1:B:380:ARG:NH2	1:B:996:LYS:HD3	2.26	0.50
1:B:846:GLU:HG2	1:B:915:ARG:HG3	1.93	0.50
1:C:682:SER:O	1:C:684:LYS:N	2.44	0.50
1:B:682:SER:O	1:B:684:LYS:N	2.44	0.50
1:C:722:ASN:OD1	1:C:723:SER:N	2.44	0.50
1:D:722:ASN:OD1	1:D:723:SER:N	2.44	0.50
1:A:846:GLU:HG2	1:A:915:ARG:HG3	1.93	0.50
1:B:759:PHE:CE2	1:B:844:LYS:HD2	2.47	0.49
1:A:759:PHE:CE2	1:A:844:LYS:HD2	2.47	0.49
1:B:662:THR:O	1:B:662:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:OE1	1:A:206:ILE:HG13	2.12	0.49
1:B:123:GLU:OE1	1:B:206:ILE:HG13	2.12	0.49
1:C:742:ALA:O	1:C:744:ARG:N	2.44	0.49
1:D:742:ALA:O	1:D:744:ARG:N	2.44	0.49
1:D:654:GLU:HB3	1:D:965:TYR:HB3	1.94	0.49
1:D:730:GLU:O	1:D:732:GLY:N	2.45	0.49
1:D:1212:THR:HG22	1:D:1213:PRO:HD2	1.94	0.49
1:A:101:TRP:O	3:A:1801:HOH:O	2.20	0.49
1:B:802:ARG:HH11	1:B:802:ARG:HB3	1.76	0.49
1:C:730:GLU:O	1:C:732:GLY:N	2.45	0.49
1:A:802:ARG:HH11	1:A:802:ARG:HB3	1.76	0.49
1:C:361:ILE:HD11	1:C:401:TRP:CE3	2.48	0.49
1:C:759:PHE:CE2	1:C:844:LYS:HD2	2.47	0.49
1:D:361:ILE:HD11	1:D:401:TRP:CE3	2.48	0.49
1:D:1216:ALA:HA	1:D:1243:VAL:HB	1.93	0.49
1:C:654:GLU:HB3	1:C:965:TYR:HB3	1.94	0.49
1:C:1212:THR:HG22	1:C:1213:PRO:HD2	1.94	0.49
1:C:1216:ALA:HA	1:C:1243:VAL:HB	1.93	0.49
1:D:759:PHE:CE2	1:D:844:LYS:HD2	2.47	0.49
1:C:62:GLU:N	1:C:63:PRO:HD2	2.28	0.49
1:D:62:GLU:N	1:D:63:PRO:HD2	2.28	0.49
1:C:123:GLU:OE1	1:C:206:ILE:HG13	2.12	0.49
1:C:512:ARG:HG3	1:C:524:VAL:O	2.13	0.49
1:C:681:ILE:O	1:C:681:ILE:HD12	2.13	0.49
1:C:697:LYS:HB3	1:C:974:VAL:HG11	1.95	0.49
1:D:512:ARG:HG3	1:D:524:VAL:O	2.13	0.49
1:D:807:ASP:O	1:D:808:LYS:HG2	2.13	0.49
1:B:807:ASP:O	1:B:808:LYS:HG2	2.13	0.48
1:B:839:THR:HG23	1:B:923:LYS:HE3	1.95	0.48
1:C:807:ASP:O	1:C:808:LYS:HG2	2.13	0.48
1:D:681:ILE:HD12	1:D:681:ILE:O	2.13	0.48
1:D:697:LYS:HB3	1:D:974:VAL:HG11	1.95	0.48
1:D:846:GLU:HG2	1:D:915:ARG:HG3	1.93	0.48
1:A:807:ASP:O	1:A:808:LYS:HG2	2.13	0.48
1:B:443:ASN:OD1	1:D:16:TYR:OH	2.30	0.48
1:C:846:GLU:HG2	1:C:915:ARG:HG3	1.93	0.48
1:D:101:TRP:O	3:D:1801:HOH:O	2.20	0.48
1:D:123:GLU:OE1	1:D:206:ILE:HG13	2.12	0.48
1:A:697:LYS:HB3	1:A:974:VAL:HG11	1.95	0.48
1:D:703:THR:HG22	1:D:704:THR:N	2.23	0.48
1:A:381:GLN:HG2	1:A:609:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:THR:HG23	1:A:923:LYS:HE3	1.96	0.48
1:B:528:SER:OG	1:B:529:SER:N	2.47	0.48
1:B:697:LYS:HB3	1:B:974:VAL:HG11	1.95	0.48
1:C:101:TRP:O	3:C:1801:HOH:O	2.20	0.48
1:C:222:ASP:HB3	1:C:468:PHE:HB3	1.95	0.48
1:C:703:THR:HG22	1:C:704:THR:N	2.23	0.48
1:D:222:ASP:HB3	1:D:468:PHE:HB3	1.95	0.48
1:A:463:THR:O	1:A:463:THR:OG1	2.26	0.48
1:A:528:SER:OG	1:A:529:SER:N	2.47	0.48
1:B:62:GLU:N	1:B:63:PRO:HD2	2.28	0.48
1:B:361:ILE:HD11	1:B:401:TRP:CE3	2.48	0.48
1:B:381:GLN:HG2	1:B:609:LEU:HD22	1.95	0.48
1:D:381:GLN:HG2	1:D:609:LEU:HD22	1.95	0.48
1:A:62:GLU:N	1:A:63:PRO:HD2	2.28	0.48
1:A:222:ASP:HB3	1:A:468:PHE:HB3	1.95	0.48
1:B:1212:THR:HG22	1:B:1213:PRO:HD2	1.94	0.48
1:C:381:GLN:HG2	1:C:609:LEU:HD22	1.95	0.48
1:A:300:PRO:HG3	1:A:624:MET:HE2	1.94	0.48
1:B:222:ASP:HB3	1:B:468:PHE:HB3	1.95	0.48
1:D:162:ASP:O	1:D:164:LYS:N	2.45	0.48
1:A:361:ILE:HD11	1:A:401:TRP:CE3	2.48	0.48
1:A:512:ARG:HG3	1:A:524:VAL:O	2.13	0.48
1:A:1212:THR:HG22	1:A:1213:PRO:HD2	1.94	0.48
1:B:463:THR:O	1:B:463:THR:OG1	2.27	0.48
1:B:996:LYS:NZ	1:B:1049:GLU:OE2	2.46	0.48
1:A:996:LYS:NZ	1:A:1049:GLU:OE2	2.46	0.48
1:A:1130:THR:OG1	1:A:1146:THR:OG1	2.20	0.48
1:B:300:PRO:HG3	1:B:624:MET:HE2	1.94	0.48
1:D:424:PHE:CE2	1:D:426:THR:CG2	2.96	0.48
1:A:443:ASN:OD1	1:C:16:TYR:OH	2.30	0.48
1:B:512:ARG:HG3	1:B:524:VAL:O	2.13	0.48
1:C:162:ASP:O	1:C:164:LYS:N	2.45	0.48
1:A:802:ARG:HB3	1:A:802:ARG:NH1	2.29	0.47
1:B:424:PHE:CE2	1:B:426:THR:CG2	2.96	0.47
1:B:668:LEU:HD12	1:B:668:LEU:HA	1.71	0.47
1:A:681:ILE:O	1:A:681:ILE:HD12	2.13	0.47
1:B:681:ILE:HD12	1:B:681:ILE:O	2.13	0.47
1:B:802:ARG:HB3	1:B:802:ARG:NH1	2.29	0.47
1:B:1172:GLY:N	3:B:1832:HOH:O	2.46	0.47
1:C:291:CYS:HB3	1:C:327:PHE:HZ	1.80	0.47
1:C:424:PHE:CE2	1:C:426:THR:CG2	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:O	1:C:463:THR:OG1	2.27	0.47
1:D:367:GLU:OE2	1:D:403:PRO:HD2	2.15	0.47
1:A:668:LEU:HD12	1:A:668:LEU:HA	1.71	0.47
1:C:367:GLU:OE2	1:C:403:PRO:HD2	2.15	0.47
1:D:291:CYS:HB3	1:D:327:PHE:HZ	1.80	0.47
1:D:1172:GLY:N	3:D:1834:HOH:O	2.47	0.47
1:A:424:PHE:CE2	1:A:426:THR:CG2	2.97	0.47
1:A:722:ASN:OD1	1:A:723:SER:N	2.44	0.47
1:C:429:LEU:HD22	1:C:456:MET:HE1	1.96	0.47
1:D:429:LEU:HD22	1:D:456:MET:HE1	1.96	0.47
1:D:463:THR:O	1:D:463:THR:OG1	2.27	0.47
1:A:367:GLU:OE2	1:A:403:PRO:HD2	2.15	0.47
1:B:367:GLU:OE2	1:B:403:PRO:HD2	2.15	0.47
1:B:722:ASN:OD1	1:B:723:SER:N	2.44	0.47
1:B:1030:ARG:HG3	1:B:1030:ARG:NH1	2.29	0.47
1:C:528:SER:OG	1:C:529:SER:N	2.47	0.47
1:C:766:TRP:HB3	1:C:769:TRP:CE3	2.50	0.47
1:C:839:THR:HG23	1:C:923:LYS:HE3	1.96	0.47
1:D:766:TRP:HB3	1:D:769:TRP:CE3	2.50	0.47
1:D:839:THR:HG23	1:D:923:LYS:HE3	1.95	0.47
1:A:1030:ARG:HG3	1:A:1030:ARG:NH1	2.29	0.47
1:B:730:GLU:O	1:B:732:GLY:N	2.45	0.47
1:C:802:ARG:HB3	1:C:802:ARG:NH1	2.29	0.47
1:D:528:SER:OG	1:D:529:SER:N	2.47	0.47
1:D:802:ARG:HB3	1:D:802:ARG:NH1	2.29	0.47
1:A:730:GLU:O	1:A:732:GLY:N	2.45	0.47
1:C:620:SER:HB2	1:C:769:TRP:CE2	2.50	0.47
1:D:220:LEU:HB3	1:D:241:CYS:SG	2.55	0.47
1:A:220:LEU:HB3	1:A:241:CYS:SG	2.55	0.46
1:A:1030:ARG:NE	1:A:1065:GLU:OE1	2.35	0.46
1:B:220:LEU:HB3	1:B:241:CYS:SG	2.55	0.46
1:B:1030:ARG:NE	1:B:1065:GLU:OE1	2.35	0.46
1:D:620:SER:HB2	1:D:769:TRP:CE2	2.50	0.46
1:A:291:CYS:HB3	1:A:327:PHE:HZ	1.80	0.46
1:A:620:SER:HB2	1:A:769:TRP:CE2	2.50	0.46
1:B:620:SER:HB2	1:B:769:TRP:CE2	2.50	0.46
1:C:220:LEU:HB3	1:C:241:CYS:SG	2.56	0.46
1:C:763:PRO:HG2	1:C:767:GLN:HA	1.97	0.46
1:C:996:LYS:NZ	1:C:1049:GLU:OE2	2.46	0.46
1:C:1172:GLY:N	3:C:1831:HOH:O	2.48	0.46
1:D:763:PRO:HG2	1:D:767:GLN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:996:LYS:NZ	1:D:1049:GLU:OE2	2.46	0.46
1:A:429:LEU:HD22	1:A:456:MET:HE1	1.96	0.46
1:B:291:CYS:HB3	1:B:327:PHE:HZ	1.80	0.46
1:D:668:LEU:HA	1:D:668:LEU:HD12	1.71	0.46
1:A:1172:GLY:N	3:A:1830:HOH:O	2.48	0.46
1:B:362:GLY:HA2	1:B:401:TRP:H	1.81	0.46
1:B:429:LEU:HD22	1:B:456:MET:HE1	1.96	0.46
1:B:766:TRP:HB3	1:B:769:TRP:CE3	2.50	0.46
1:C:19:ARG:NH1	3:C:1844:HOH:O	2.47	0.46
1:A:362:GLY:HA2	1:A:401:TRP:H	1.81	0.46
1:A:662:THR:O	1:A:662:THR:OG1	2.30	0.46
1:A:766:TRP:HB3	1:A:769:TRP:CE3	2.50	0.46
1:C:300:PRO:HG3	1:C:624:MET:HE2	1.98	0.46
1:C:417:ARG:HD2	1:C:417:ARG:HA	1.72	0.46
1:D:1144:GLU:OE2	1:D:1144:GLU:N	2.48	0.46
1:A:33:LYS:O	3:A:1802:HOH:O	2.20	0.46
1:B:577:LEU:HD21	1:B:604:MET:HE2	1.97	0.46
1:C:668:LEU:HD12	1:C:668:LEU:HA	1.71	0.46
1:C:1030:ARG:NE	1:C:1065:GLU:OE1	2.35	0.46
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.48	0.46
1:D:1030:ARG:NE	1:D:1065:GLU:OE1	2.35	0.46
1:A:599:GLU:OE2	1:A:1006:ARG:NH1	2.49	0.46
1:B:599:GLU:OE2	1:B:1006:ARG:NH1	2.49	0.46
1:C:436:ARG:HD3	1:C:479:LYS:HE2	1.96	0.46
1:D:300:PRO:HG3	1:D:624:MET:HE2	1.98	0.46
1:D:436:ARG:HD3	1:D:479:LYS:HE2	1.96	0.46
1:D:599:GLU:OE2	1:D:1006:ARG:NH1	2.49	0.46
1:B:436:ARG:HD3	1:B:479:LYS:HE2	1.96	0.46
1:C:577:LEU:HD21	1:C:604:MET:HE2	1.98	0.46
1:C:599:GLU:OE2	1:C:1006:ARG:NH1	2.49	0.46
1:A:682:SER:O	1:A:682:SER:OG	2.34	0.45
1:A:1143:PHE:CE1	1:A:1210:LEU:HB2	2.52	0.45
1:B:1143:PHE:CE1	1:B:1210:LEU:HB2	2.52	0.45
1:A:436:ARG:HD3	1:A:479:LYS:HE2	1.96	0.45
1:A:567:LYS:NZ	1:A:617:LEU:O	2.49	0.45
1:B:682:SER:O	1:B:682:SER:OG	2.34	0.45
1:B:954:LYS:HA	1:B:954:LYS:HD3	1.64	0.45
1:C:518:VAL:HG23	1:C:518:VAL:O	2.17	0.45
1:D:518:VAL:HG23	1:D:518:VAL:O	2.17	0.45
1:C:430:SER:HB2	1:C:460:GLU:HG2	1.99	0.45
1:D:430:SER:HB2	1:D:460:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:LYS:NZ	1:B:617:LEU:O	2.49	0.45
1:B:1171:MET:HB2	1:B:1210:LEU:HD22	1.99	0.45
1:A:308:VAL:HG12	1:A:338:LEU:HD13	1.98	0.45
1:A:754:ASN:ND2	1:A:754:ASN:C	2.70	0.45
1:A:1171:MET:HB2	1:A:1210:LEU:HD22	1.99	0.45
1:A:1173:ARG:NH1	1:A:1173:ARG:HB3	2.32	0.45
1:B:308:VAL:HG12	1:B:338:LEU:HD13	1.98	0.45
1:B:1173:ARG:HB3	1:B:1173:ARG:NH1	2.32	0.45
1:D:417:ARG:HA	1:D:417:ARG:HD2	1.72	0.45
1:A:292:HIS:CE1	1:A:614:HIS:HE1	2.35	0.45
1:A:1051:ASP:OD2	1:A:1051:ASP:N	2.50	0.45
1:B:754:ASN:ND2	1:B:754:ASN:C	2.70	0.45
1:B:1051:ASP:OD2	1:B:1051:ASP:N	2.50	0.45
1:C:567:LYS:NZ	1:C:617:LEU:O	2.49	0.45
1:B:162:ASP:O	1:B:164:LYS:N	2.45	0.45
1:B:292:HIS:CE1	1:B:614:HIS:HE1	2.35	0.45
1:C:1143:PHE:CE1	1:C:1210:LEU:HB2	2.51	0.45
1:D:567:LYS:NZ	1:D:617:LEU:O	2.49	0.45
1:D:1143:PHE:CE1	1:D:1210:LEU:HB2	2.52	0.45
1:A:954:LYS:HA	1:A:954:LYS:HD3	1.64	0.45
1:B:704:THR:HA	1:B:705:LYS:HE2	1.99	0.45
1:B:1146:THR:HG22	1:B:1207:THR:OG1	2.16	0.45
1:B:1167:GLY:HA3	1:B:1222:HIS:HB2	1.98	0.45
1:C:1030:ARG:HG3	1:C:1030:ARG:NH1	2.29	0.45
1:C:1173:ARG:HB3	1:C:1173:ARG:NH1	2.32	0.45
1:D:577:LEU:HD21	1:D:604:MET:HE2	1.99	0.45
1:D:1030:ARG:HG3	1:D:1030:ARG:NH1	2.29	0.45
1:D:1171:MET:HB2	1:D:1210:LEU:HD22	1.99	0.45
1:A:430:SER:HB2	1:A:460:GLU:HG2	1.99	0.45
1:A:1034:VAL:HG22	1:A:1061:ARG:HG2	1.99	0.45
1:A:1167:GLY:HA3	1:A:1222:HIS:HB2	1.98	0.45
1:B:430:SER:HB2	1:B:460:GLU:HG2	1.99	0.45
1:D:308:VAL:HG12	1:D:338:LEU:HD13	1.98	0.45
1:D:1173:ARG:NH1	1:D:1173:ARG:HB3	2.32	0.45
1:A:162:ASP:O	1:A:164:LYS:N	2.45	0.44
1:A:261:LYS:HE2	1:A:261:LYS:HB2	1.89	0.44
1:A:704:THR:HA	1:A:705:LYS:HE2	2.00	0.44
1:A:763:PRO:HG2	1:A:767:GLN:HA	1.97	0.44
1:A:1146:THR:HG22	1:A:1207:THR:OG1	2.16	0.44
1:B:677:GLU:OE1	1:B:962:THR:CG2	2.65	0.44
1:B:1034:VAL:HG22	1:B:1061:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:SER:HG	1:C:804:LYS:H	1.57	0.44
1:C:1146:THR:HG22	1:C:1207:THR:OG1	2.16	0.44
1:C:1171:MET:HB2	1:C:1210:LEU:HD22	1.99	0.44
1:D:1146:THR:HG22	1:D:1207:THR:OG1	2.16	0.44
1:A:379:VAL:HG13	1:A:1047:LEU:HD13	1.99	0.44
1:B:178:PHE:HE2	1:B:495:ASP:HB2	1.82	0.44
1:B:379:VAL:HG13	1:B:1047:LEU:HD13	1.99	0.44
1:B:763:PRO:HG2	1:B:767:GLN:HA	1.97	0.44
1:C:292:HIS:CE1	1:C:614:HIS:HE1	2.35	0.44
1:C:308:VAL:HG12	1:C:338:LEU:HD13	1.98	0.44
1:C:357:ARG:NH1	3:C:1832:HOH:O	2.50	0.44
1:C:362:GLY:HA2	1:C:401:TRP:H	1.81	0.44
1:C:475:MET:HE2	1:C:475:MET:HB2	1.88	0.44
1:C:1051:ASP:N	1:C:1051:ASP:OD2	2.50	0.44
1:D:292:HIS:CE1	1:D:614:HIS:HE1	2.35	0.44
1:D:662:THR:O	1:D:662:THR:OG1	2.30	0.44
1:D:1051:ASP:OD2	1:D:1051:ASP:N	2.50	0.44
1:A:178:PHE:HE2	1:A:495:ASP:HB2	1.83	0.44
1:A:577:LEU:HD21	1:A:604:MET:HE2	1.98	0.44
1:B:518:VAL:HG23	1:B:518:VAL:O	2.17	0.44
1:C:379:VAL:HG13	1:C:1047:LEU:HD13	1.99	0.44
1:D:379:VAL:HG13	1:D:1047:LEU:HD13	1.99	0.44
1:A:15:ASP:OD1	1:A:15:ASP:N	2.46	0.44
1:A:518:VAL:O	1:A:518:VAL:HG23	2.17	0.44
1:A:1139:PRO:HA	1:A:1243:VAL:CG1	2.48	0.44
1:B:15:ASP:OD1	1:B:15:ASP:N	2.46	0.44
1:B:1139:PRO:HA	1:B:1243:VAL:CG1	2.48	0.44
1:D:357:ARG:NH1	3:D:1836:HOH:O	2.50	0.44
1:D:362:GLY:HA2	1:D:401:TRP:H	1.81	0.44
1:C:662:THR:O	1:C:662:THR:OG1	2.30	0.44
1:D:295:SER:O	1:D:304:THR:OG1	2.29	0.44
1:D:475:MET:HE2	1:D:475:MET:HB2	1.87	0.44
1:C:1221:SER:O	1:C:1238:TRP:HA	2.17	0.44
1:A:219:ILE:HG13	1:A:510:ARG:HB2	2.00	0.44
1:A:361:ILE:HG12	3:A:1809:HOH:O	2.18	0.44
1:B:219:ILE:HG13	1:B:510:ARG:HB2	2.00	0.44
1:B:413:PRO:HB2	1:B:446:ALA:HB2	2.00	0.44
1:C:1139:PRO:HA	1:C:1243:VAL:CG1	2.48	0.44
1:C:1167:GLY:HA3	1:C:1222:HIS:HB2	1.98	0.44
1:D:1139:PRO:HA	1:D:1243:VAL:CG1	2.48	0.44
1:D:1167:GLY:HA3	1:D:1222:HIS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:GLU:OE2	1:A:1144:GLU:N	2.48	0.44
1:A:1221:SER:O	1:A:1238:TRP:HA	2.17	0.44
1:C:704:THR:HA	1:C:705:LYS:HE2	1.99	0.44
1:C:782:LEU:HD13	1:C:805:VAL:HG22	2.00	0.44
1:D:400:PHE:HB2	1:D:421:MET:HE3	1.99	0.44
1:D:704:THR:HA	1:D:705:LYS:HE2	1.99	0.44
1:D:782:LEU:HD13	1:D:805:VAL:HG22	2.00	0.44
1:D:1221:SER:O	1:D:1238:TRP:HA	2.17	0.44
1:A:413:PRO:HB2	1:A:446:ALA:HB2	2.00	0.44
1:B:1144:GLU:OE2	1:B:1144:GLU:N	2.48	0.44
1:C:178:PHE:HE2	1:C:495:ASP:HB2	1.82	0.44
1:C:295:SER:O	1:C:304:THR:OG1	2.29	0.44
1:C:493:LYS:NZ	3:C:1839:HOH:O	2.43	0.44
1:D:178:PHE:HE2	1:D:495:ASP:HB2	1.82	0.44
1:A:782:LEU:HD13	1:A:805:VAL:HG22	2.00	0.43
1:A:1220:ILE:HG13	3:A:1812:HOH:O	2.17	0.43
1:B:782:LEU:HD13	1:B:805:VAL:HG22	2.00	0.43
1:B:1221:SER:O	1:B:1238:TRP:HA	2.17	0.43
1:C:1034:VAL:HG22	1:C:1061:ARG:HG2	1.99	0.43
1:C:1153:GLY:O	1:C:1200:PRO:HB3	2.18	0.43
1:D:493:LYS:NZ	3:D:1844:HOH:O	2.44	0.43
1:A:754:ASN:C	1:A:754:ASN:HD22	2.15	0.43
1:B:361:ILE:HG12	3:B:1811:HOH:O	2.18	0.43
1:C:292:HIS:HE1	1:C:614:HIS:HE1	1.65	0.43
1:D:292:HIS:HE1	1:D:614:HIS:HE1	1.65	0.43
1:D:1034:VAL:HG22	1:D:1061:ARG:HG2	1.99	0.43
1:D:1153:GLY:O	1:D:1200:PRO:HB3	2.18	0.43
1:B:292:HIS:HE1	1:B:614:HIS:HE1	1.65	0.43
1:C:1001:ASP:OD1	1:C:1016:SER:N	2.49	0.43
1:D:1001:ASP:OD1	1:D:1016:SER:N	2.49	0.43
1:A:292:HIS:HE1	1:A:614:HIS:HE1	1.65	0.43
1:B:558:GLY:N	1:B:771:VAL:HG12	2.33	0.43
1:C:1058:GLU:OE2	1:C:1058:GLU:HA	2.19	0.43
1:A:423:ARG:HG2	1:A:534:PHE:CG	2.53	0.43
1:A:558:GLY:N	1:A:771:VAL:HG12	2.33	0.43
1:A:661:SER:O	1:A:663:THR:HG22	2.18	0.43
1:A:748:PRO:HG3	1:A:850:ASP:HB2	2.01	0.43
1:B:357:ARG:NH1	3:B:1837:HOH:O	2.51	0.43
1:B:423:ARG:HG2	1:B:534:PHE:CG	2.53	0.43
1:B:661:SER:O	1:B:663:THR:HG22	2.18	0.43
1:B:748:PRO:HG3	1:B:850:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASP:OD2	3:C:1802:HOH:O	2.21	0.43
1:C:318:LEU:HD23	1:C:318:LEU:HA	1.78	0.43
1:C:1139:PRO:HG3	1:C:1245:LYS:HA	2.00	0.43
1:D:1058:GLU:OE2	1:D:1058:GLU:HA	2.19	0.43
1:A:1058:GLU:HA	1:A:1058:GLU:OE2	2.19	0.43
1:B:401:TRP:CD1	1:B:403:PRO:HD3	2.54	0.43
1:B:1220:ILE:HG13	3:B:1815:HOH:O	2.18	0.43
1:C:219:ILE:HG13	1:C:510:ARG:HB2	2.00	0.43
1:C:767:GLN:HB2	1:C:924:ALA:HB2	2.01	0.43
1:C:1049:GLU:HB3	1:C:1075:ARG:NH1	2.32	0.43
1:D:1049:GLU:HB3	1:D:1075:ARG:NH1	2.32	0.43
1:A:401:TRP:CD1	1:A:403:PRO:HD3	2.54	0.43
1:A:1049:GLU:HB3	1:A:1075:ARG:NH1	2.32	0.43
1:B:1049:GLU:HB3	1:B:1075:ARG:NH1	2.32	0.43
1:B:1058:GLU:OE2	1:B:1058:GLU:HA	2.19	0.43
1:C:748:PRO:HG3	1:C:850:ASP:HB2	2.01	0.43
1:C:864:ILE:HD13	1:C:947:LEU:HD21	2.01	0.43
1:D:754:ASN:ND2	1:D:754:ASN:C	2.70	0.43
1:D:767:GLN:HB2	1:D:924:ALA:HB2	2.01	0.43
1:D:1139:PRO:HG3	1:D:1245:LYS:HA	2.00	0.43
1:A:448:ASP:OD1	1:A:450:SER:N	2.37	0.43
1:A:1153:GLY:O	1:A:1200:PRO:HB3	2.18	0.43
1:B:1153:GLY:O	1:B:1200:PRO:HB3	2.18	0.43
1:D:219:ILE:HG13	1:D:510:ARG:HB2	2.00	0.43
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.78	0.43
1:D:748:PRO:HG3	1:D:850:ASP:HB2	2.01	0.43
1:D:864:ILE:HD13	1:D:947:LEU:HD21	2.01	0.43
1:B:767:GLN:HB2	1:B:924:ALA:HB2	2.01	0.43
1:A:767:GLN:HB2	1:A:924:ALA:HB2	2.01	0.43
1:A:1139:PRO:HG3	1:A:1245:LYS:HA	2.00	0.43
1:B:101:TRP:O	3:B:1801:HOH:O	2.21	0.43
1:C:1133:ASP:HA	1:C:1240:ASP:HB3	2.01	0.43
1:D:423:ARG:HG2	1:D:534:PHE:CG	2.53	0.43
1:D:1133:ASP:HA	1:D:1240:ASP:HB3	2.01	0.43
1:B:598:LYS:HD2	1:B:598:LYS:HA	1.87	0.42
1:C:423:ARG:HG2	1:C:534:PHE:CG	2.53	0.42
1:C:558:GLY:N	1:C:771:VAL:HG12	2.33	0.42
1:D:558:GLY:N	1:D:771:VAL:HG12	2.33	0.42
1:D:1220:ILE:HG13	3:D:1814:HOH:O	2.18	0.42
1:B:1139:PRO:HG3	1:B:1245:LYS:HA	2.00	0.42
1:C:413:PRO:HB2	1:C:446:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HB3	1:A:1047:LEU:HG	2.01	0.42
1:A:811:ILE:HG12	1:A:834:VAL:HG13	2.01	0.42
1:B:16:TYR:OH	1:D:443:ASN:OD1	2.30	0.42
1:D:413:PRO:HB2	1:D:446:ALA:HB2	2.00	0.42
1:D:661:SER:O	1:D:663:THR:HG22	2.19	0.42
1:B:418:LEU:HB3	1:B:1047:LEU:HG	2.01	0.42
1:C:312:TRP:CE3	1:C:338:LEU:HD22	2.55	0.42
1:C:661:SER:O	1:C:663:THR:HG22	2.18	0.42
1:C:811:ILE:HG12	1:C:834:VAL:HG13	2.02	0.42
1:D:227:PHE:HD2	1:D:227:PHE:HA	1.73	0.42
1:D:811:ILE:HG12	1:D:834:VAL:HG13	2.02	0.42
1:B:87:GLN:OE1	3:B:1803:HOH:O	2.22	0.42
1:B:680:LYS:HZ2	1:B:683:GLU:HG2	1.83	0.42
1:B:811:ILE:HG12	1:B:834:VAL:HG13	2.02	0.42
1:C:859:GLU:HB2	1:C:887:TRP:CE2	2.54	0.42
1:D:312:TRP:CE3	1:D:338:LEU:HD22	2.55	0.42
1:A:864:ILE:HD13	1:A:947:LEU:HD21	2.00	0.42
1:A:1133:ASP:HA	1:A:1240:ASP:HB3	2.01	0.42
1:B:859:GLU:HB2	1:B:887:TRP:CE2	2.55	0.42
1:C:227:PHE:HD2	1:C:227:PHE:HA	1.72	0.42
1:C:824:GLU:OE1	1:C:954:LYS:NZ	2.32	0.42
1:D:50:LEU:HD12	1:D:50:LEU:HA	1.88	0.42
1:D:424:PHE:CE2	1:D:426:THR:HG21	2.54	0.42
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.87	0.42
1:A:680:LYS:HZ2	1:A:683:GLU:HG2	1.83	0.42
1:A:859:GLU:HB2	1:A:887:TRP:CE2	2.55	0.42
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.88	0.42
1:C:361:ILE:HG12	3:C:1811:HOH:O	2.18	0.42
1:C:859:GLU:OE1	1:C:886:ARG:NH2	2.53	0.42
1:D:401:TRP:CD1	1:D:403:PRO:HD3	2.54	0.42
1:D:859:GLU:HB2	1:D:887:TRP:CE2	2.55	0.42
1:D:859:GLU:OE1	1:D:886:ARG:NH2	2.53	0.42
1:A:16:TYR:OH	1:C:443:ASN:OD1	2.30	0.42
1:A:423:ARG:HG2	1:A:534:PHE:CD1	2.55	0.42
1:A:475:MET:HE3	1:A:522:PRO:HB3	2.01	0.42
1:B:424:PHE:CE2	1:B:426:THR:HG21	2.54	0.42
1:B:624:MET:H	1:B:624:MET:HG3	1.60	0.42
1:B:1133:ASP:HA	1:B:1240:ASP:HB3	2.01	0.42
1:C:424:PHE:CE2	1:C:426:THR:HG21	2.54	0.42
1:D:87:GLN:OE1	3:D:1802:HOH:O	2.22	0.42
1:A:448:ASP:OD1	1:A:448:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.88	0.42
1:B:423:ARG:HG2	1:B:534:PHE:CD1	2.55	0.42
1:B:448:ASP:OD1	1:B:448:ASP:C	2.58	0.42
1:B:864:ILE:HD13	1:B:947:LEU:HD21	2.01	0.42
1:C:369:ASP:HA	1:C:405:THR:HG23	2.02	0.42
1:C:401:TRP:CD1	1:C:403:PRO:HD3	2.54	0.42
1:C:423:ARG:HG2	1:C:534:PHE:CD1	2.55	0.42
1:C:727:VAL:HG22	1:C:737:LEU:HD13	2.02	0.42
1:C:742:ALA:O	1:C:744:ARG:HG2	2.20	0.42
1:D:727:VAL:HG22	1:D:737:LEU:HD13	2.02	0.42
1:D:742:ALA:O	1:D:744:ARG:HG2	2.20	0.42
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.88	0.41
1:A:376:GLU:O	1:A:380:ARG:HG2	2.20	0.41
1:B:859:GLU:OE1	1:B:886:ARG:HB2	2.21	0.41
1:D:361:ILE:HG12	3:D:1810:HOH:O	2.18	0.41
1:D:423:ARG:HG2	1:D:534:PHE:CD1	2.55	0.41
1:D:508:LEU:HD23	1:D:508:LEU:HA	1.93	0.41
1:D:767:GLN:HB2	1:D:924:ALA:CB	2.50	0.41
1:A:859:GLU:OE1	1:A:886:ARG:HB2	2.21	0.41
1:A:1129:ASP:OD2	1:C:2:GLY:HA3	2.20	0.41
1:B:376:GLU:O	1:B:380:ARG:HG2	2.20	0.41
1:B:583:LEU:HD23	1:B:583:LEU:HA	1.87	0.41
1:C:767:GLN:HB2	1:C:924:ALA:CB	2.50	0.41
1:C:918:LEU:HD22	1:C:936:ILE:HG21	2.02	0.41
1:D:369:ASP:HA	1:D:405:THR:HG23	2.02	0.41
1:D:918:LEU:HD22	1:D:936:ILE:HG21	2.02	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.78	0.41
1:A:624:MET:H	1:A:624:MET:HG3	1.60	0.41
1:A:707:LEU:HD12	1:A:797:VAL:HG22	2.02	0.41
1:A:1001:ASP:OD1	1:A:1016:SER:N	2.49	0.41
1:B:707:LEU:HD12	1:B:797:VAL:HG22	2.02	0.41
1:B:1001:ASP:OD1	1:B:1016:SER:N	2.49	0.41
1:C:418:LEU:HB3	1:C:1047:LEU:HG	2.01	0.41
1:C:742:ALA:HB3	1:C:895:TYR:HE2	1.85	0.41
1:D:418:LEU:HB3	1:D:1047:LEU:HG	2.01	0.41
1:A:312:TRP:CE3	1:A:338:LEU:HD22	2.55	0.41
1:A:424:PHE:CE2	1:A:426:THR:HG21	2.55	0.41
1:A:859:GLU:OE1	1:A:886:ARG:NH2	2.53	0.41
1:B:312:TRP:CE3	1:B:338:LEU:HD22	2.55	0.41
1:B:859:GLU:OE1	1:B:886:ARG:NH2	2.53	0.41
1:C:448:ASP:OD1	1:C:448:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:742:ALA:HB3	1:D:895:TYR:HE2	1.85	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.78	0.41
1:B:1236:ARG:NH2	1:D:4:GLU:OE2	2.54	0.41
1:C:303:GLU:OE1	3:C:1803:HOH:O	2.22	0.41
1:C:400:PHE:HB2	1:C:421:MET:HE3	2.02	0.41
1:C:859:GLU:OE1	1:C:886:ARG:HB2	2.20	0.41
1:D:164:LYS:HA	1:D:164:LYS:HD2	1.93	0.41
1:D:448:ASP:OD1	1:D:448:ASP:C	2.58	0.41
1:A:2:GLY:HA3	1:C:1129:ASP:OD2	2.21	0.41
1:A:539:ARG:CZ	1:A:1220:ILE:HB	2.51	0.41
1:A:722:ASN:HB3	1:A:725:LEU:H	1.86	0.41
1:B:4:GLU:OE2	1:D:1236:ARG:NH2	2.54	0.41
1:B:539:ARG:CZ	1:B:1220:ILE:HB	2.51	0.41
1:B:722:ASN:HB3	1:B:725:LEU:H	1.86	0.41
1:C:508:LEU:HD23	1:C:508:LEU:HA	1.93	0.41
1:D:424:PHE:CE2	1:D:426:THR:HG22	2.55	0.41
1:D:660:MET:HG3	1:D:665:THR:HG21	2.03	0.41
1:A:742:ALA:HB3	1:A:895:TYR:HE2	1.85	0.41
1:B:2:GLY:HA3	1:D:1129:ASP:OD2	2.21	0.41
1:B:227:PHE:HD2	1:B:227:PHE:HA	1.73	0.41
1:B:424:PHE:CE2	1:B:426:THR:HG22	2.55	0.41
1:C:315:GLN:HG3	1:C:327:PHE:CE1	2.56	0.41
1:C:660:MET:HG3	1:C:665:THR:HG21	2.03	0.41
1:C:817:LEU:HD12	1:C:817:LEU:HA	1.88	0.41
1:D:315:GLN:HG3	1:D:327:PHE:CE1	2.56	0.41
1:D:859:GLU:OE1	1:D:886:ARG:HB2	2.21	0.41
1:B:742:ALA:HB3	1:B:895:TYR:HE2	1.85	0.41
1:D:352:LYS:HA	1:D:352:LYS:HD3	1.86	0.41
1:D:370:THR:OG1	1:D:408:TYR:HA	2.21	0.41
1:D:707:LEU:HD12	1:D:797:VAL:HG22	2.02	0.41
1:D:1001:ASP:C	1:D:1003:ASP:H	2.24	0.41
1:D:1199:GLN:N	1:D:1199:GLN:CD	2.74	0.41
1:A:4:GLU:OE2	1:C:1236:ARG:NH2	2.54	0.41
1:A:369:ASP:HA	1:A:405:THR:HG23	2.02	0.41
1:A:678:LEU:HD23	1:A:678:LEU:HA	1.93	0.41
1:A:853:ASN:ND2	1:A:855:GLU:HG3	2.36	0.41
1:A:1001:ASP:C	1:A:1003:ASP:H	2.24	0.41
1:B:678:LEU:HD23	1:B:678:LEU:HA	1.93	0.41
1:B:853:ASN:ND2	1:B:855:GLU:HG3	2.36	0.41
1:B:1001:ASP:C	1:B:1003:ASP:H	2.24	0.41
1:B:1129:ASP:OD2	1:D:2:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:LYS:HA	1:C:352:LYS:HD3	1.86	0.41
1:C:370:THR:OG1	1:C:408:TYR:HA	2.21	0.41
1:C:424:PHE:CE2	1:C:426:THR:HG22	2.55	0.41
1:C:707:LEU:HD12	1:C:797:VAL:HG22	2.02	0.41
1:C:754:ASN:ND2	1:C:754:ASN:C	2.70	0.41
1:C:853:ASN:ND2	1:C:855:GLU:HG3	2.36	0.41
1:C:1001:ASP:C	1:C:1003:ASP:H	2.24	0.41
1:C:1199:GLN:N	1:C:1199:GLN:CD	2.74	0.41
1:D:376:GLU:O	1:D:380:ARG:HG2	2.20	0.41
1:A:227:PHE:HD2	1:A:227:PHE:HA	1.72	0.41
1:A:400:PHE:HB2	1:A:421:MET:HE3	2.04	0.41
1:A:417:ARG:HA	1:A:417:ARG:HD2	1.72	0.41
1:A:424:PHE:CE2	1:A:426:THR:HG22	2.56	0.41
1:A:855:GLU:OE2	1:A:866:ARG:HG2	2.21	0.41
1:B:369:ASP:HA	1:B:405:THR:HG23	2.02	0.41
1:B:855:GLU:OE2	1:B:866:ARG:HG2	2.21	0.41
1:C:376:GLU:O	1:C:380:ARG:HG2	2.20	0.41
1:C:423:ARG:HG2	1:C:534:PHE:HB3	2.02	0.41
1:D:303:GLU:OE1	3:D:1803:HOH:O	2.22	0.41
1:D:853:ASN:ND2	1:D:855:GLU:HG3	2.36	0.41
1:D:423:ARG:HG2	1:D:534:PHE:HB3	2.02	0.40
1:A:660:MET:HG3	1:A:665:THR:HG21	2.03	0.40
1:A:662:THR:N	3:A:1849:HOH:O	2.54	0.40
1:B:370:THR:OG1	1:B:408:TYR:HA	2.21	0.40
1:B:660:MET:HG3	1:B:665:THR:HG21	2.03	0.40
1:D:747:ILE:HD12	1:D:753:ALA:HB2	2.04	0.40
1:A:81:GLU:HA	1:A:81:GLU:OE2	2.21	0.40
1:A:457:PRO:HA	1:A:458:PRO:HD3	1.97	0.40
1:A:1236:ARG:NH2	1:C:4:GLU:OE2	2.54	0.40
1:B:81:GLU:HA	1:B:81:GLU:OE2	2.21	0.40
1:B:423:ARG:HG2	1:B:534:PHE:HB3	2.02	0.40
1:B:918:LEU:HD22	1:B:936:ILE:HG21	2.02	0.40
1:C:747:ILE:HD12	1:C:753:ALA:HB2	2.04	0.40
1:D:81:GLU:HA	1:D:81:GLU:OE2	2.21	0.40
1:A:315:GLN:HG3	1:A:327:PHE:CE1	2.56	0.40
1:A:370:THR:OG1	1:A:408:TYR:HA	2.21	0.40
1:A:681:ILE:HG22	1:A:964:LEU:HD13	2.02	0.40
1:A:727:VAL:HG22	1:A:737:LEU:HD13	2.02	0.40
1:B:417:ARG:HA	1:B:417:ARG:HD2	1.72	0.40
1:C:81:GLU:HA	1:C:81:GLU:OE2	2.21	0.40
1:C:722:ASN:HB3	1:C:725:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD13	1:D:310:ARG:HA	2.03	0.40
1:D:722:ASN:HB3	1:D:725:LEU:H	1.86	0.40
1:A:303:GLU:OE1	3:A:1804:HOH:O	2.22	0.40
1:A:423:ARG:HG2	1:A:534:PHE:HB3	2.02	0.40
1:A:747:ILE:HD12	1:A:753:ALA:HB2	2.04	0.40
1:A:767:GLN:HB2	1:A:924:ALA:CB	2.50	0.40
1:A:918:LEU:HD22	1:A:936:ILE:HG21	2.02	0.40
1:A:1128:ARG:HG2	1:A:1148:VAL:CG2	2.52	0.40
1:A:1216:ALA:HB2	1:A:1245:LYS:HB2	2.04	0.40
1:B:315:GLN:HG3	1:B:327:PHE:CE1	2.56	0.40
1:B:457:PRO:HA	1:B:458:PRO:HD3	1.97	0.40
1:B:727:VAL:HG22	1:B:737:LEU:HD13	2.02	0.40
1:B:747:ILE:HD12	1:B:753:ALA:HB2	2.04	0.40
1:B:767:GLN:HB2	1:B:924:ALA:CB	2.50	0.40
1:B:1128:ARG:HG2	1:B:1148:VAL:CG2	2.52	0.40
1:B:1216:ALA:HB2	1:B:1245:LYS:HB2	2.04	0.40
1:C:133:LEU:HD13	1:C:310:ARG:HA	2.03	0.40
1:C:681:ILE:HG22	1:C:964:LEU:HD13	2.02	0.40
1:D:681:ILE:HG22	1:D:964:LEU:HD13	2.02	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	1174/1616 (73%)	1066 (91%)	108 (9%)	0	100	100
1	B	1174/1616 (73%)	1065 (91%)	109 (9%)	0	100	100
1	C	1174/1616 (73%)	1064 (91%)	110 (9%)	0	100	100
1	D	1174/1616 (73%)	1065 (91%)	109 (9%)	0	100	100
All	All	4696/6464 (73%)	4260 (91%)	436 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	1023/1368 (75%)	970 (95%)	53 (5%)	19	24
1	B	1023/1368 (75%)	969 (95%)	54 (5%)	19	24
1	C	1023/1368 (75%)	968 (95%)	55 (5%)	18	23
1	D	1023/1368 (75%)	969 (95%)	54 (5%)	19	24
All	All	4092/5472 (75%)	3876 (95%)	216 (5%)	21	24

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	29	SER
1	A	53	MET
1	A	57	ASP
1	A	67	LEU
1	A	81	GLU
1	A	100	SER
1	A	103	THR
1	A	158	ASP
1	A	167	THR
1	A	175	ASN
1	A	185	ASP
1	A	200	LYS
1	A	209	ASP
1	A	227	PHE
1	A	311	SER
1	A	395	LYS
1	A	426	THR
1	A	448	ASP
1	A	472	LYS
1	A	476	SER
1	A	495	ASP

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Mol	Chain	Res	Type
1	A	515	SER
1	A	559	THR
1	A	595	LYS
1	A	629	SER
1	A	647	VAL
1	A	648	SER
1	A	665	THR
1	A	692	THR
1	A	701	LEU
1	A	704	THR
1	A	710	LEU
1	A	712	GLN
1	A	754	ASN
1	A	807	ASP
1	A	842	PHE
1	A	855	GLU
1	A	866	ARG
1	A	881	GLU
1	A	931	MET
1	A	935	HIS
1	A	999	GLU
1	A	1001	ASP
1	A	1051	ASP
1	A	1130	THR
1	A	1143	PHE
1	A	1163	VAL
1	A	1173	ARG
1	A	1199	GLN
1	A	1212	THR
1	A	1224	ARG
1	A	1240	ASP
1	B	19	ARG
1	B	24	VAL
1	B	29	SER
1	B	53	MET
1	B	57	ASP
1	B	67	LEU
1	B	81	GLU
1	B	100	SER
1	B	103	THR
1	B	158	ASP
1	B	167	THR

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Mol	Chain	Res	Type
1	B	175	ASN
1	B	185	ASP
1	B	200	LYS
1	B	209	ASP
1	B	227	PHE
1	B	311	SER
1	B	395	LYS
1	B	426	THR
1	B	448	ASP
1	B	472	LYS
1	B	476	SER
1	B	495	ASP
1	B	515	SER
1	B	559	THR
1	B	595	LYS
1	B	629	SER
1	B	647	VAL
1	B	648	SER
1	B	665	THR
1	B	692	THR
1	B	701	LEU
1	B	704	THR
1	B	710	LEU
1	B	712	GLN
1	B	754	ASN
1	B	807	ASP
1	B	842	PHE
1	B	855	GLU
1	B	866	ARG
1	B	881	GLU
1	B	931	MET
1	B	935	HIS
1	B	999	GLU
1	B	1001	ASP
1	B	1051	ASP
1	B	1130	THR
1	B	1143	PHE
1	B	1163	VAL
1	B	1173	ARG
1	B	1199	GLN
1	B	1212	THR
1	B	1224	ARG

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Mol	Chain	Res	Type
1	B	1240	ASP
1	C	19	ARG
1	C	24	VAL
1	C	29	SER
1	C	53	MET
1	C	57	ASP
1	C	67	LEU
1	C	81	GLU
1	C	100	SER
1	C	103	THR
1	C	158	ASP
1	C	167	THR
1	C	175	ASN
1	C	185	ASP
1	C	200	LYS
1	C	209	ASP
1	C	227	PHE
1	C	311	SER
1	C	395	LYS
1	C	426	THR
1	C	448	ASP
1	C	472	LYS
1	C	476	SER
1	C	495	ASP
1	C	515	SER
1	C	559	THR
1	C	595	LYS
1	C	629	SER
1	C	647	VAL
1	C	648	SER
1	C	665	THR
1	C	692	THR
1	C	701	LEU
1	C	704	THR
1	C	710	LEU
1	C	712	GLN
1	C	754	ASN
1	C	807	ASP
1	C	842	PHE
1	C	855	GLU
1	C	866	ARG
1	C	881	GLU

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Mol	Chain	Res	Type
1	C	931	MET
1	C	935	HIS
1	C	999	GLU
1	C	1001	ASP
1	C	1051	ASP
1	C	1130	THR
1	C	1143	PHE
1	C	1163	VAL
1	C	1173	ARG
1	C	1199	GLN
1	C	1212	THR
1	C	1224	ARG
1	C	1240	ASP
1	C	1241	VAL
1	D	19	ARG
1	D	24	VAL
1	D	29	SER
1	D	53	MET
1	D	57	ASP
1	D	67	LEU
1	D	81	GLU
1	D	100	SER
1	D	103	THR
1	D	158	ASP
1	D	167	THR
1	D	175	ASN
1	D	185	ASP
1	D	200	LYS
1	D	209	ASP
1	D	227	PHE
1	D	311	SER
1	D	395	LYS
1	D	426	THR
1	D	448	ASP
1	D	472	LYS
1	D	476	SER
1	D	495	ASP
1	D	515	SER
1	D	559	THR
1	D	595	LYS
1	D	629	SER
1	D	647	VAL

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Mol	Chain	Res	Type
1	D	648	SER
1	D	665	THR
1	D	692	THR
1	D	701	LEU
1	D	704	THR
1	D	710	LEU
1	D	712	GLN
1	D	754	ASN
1	D	807	ASP
1	D	842	PHE
1	D	855	GLU
1	D	866	ARG
1	D	881	GLU
1	D	931	MET
1	D	935	HIS
1	D	999	GLU
1	D	1001	ASP
1	D	1051	ASP
1	D	1130	THR
1	D	1143	PHE
1	D	1163	VAL
1	D	1173	ARG
1	D	1199	GLN
1	D	1212	THR
1	D	1224	ARG
1	D	1240	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	944	GLN
1	B	180	ASN
1	B	944	GLN
1	C	944	GLN
1	D	944	GLN

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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-32091. 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

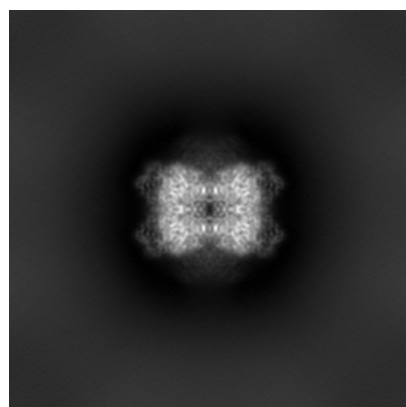


Y

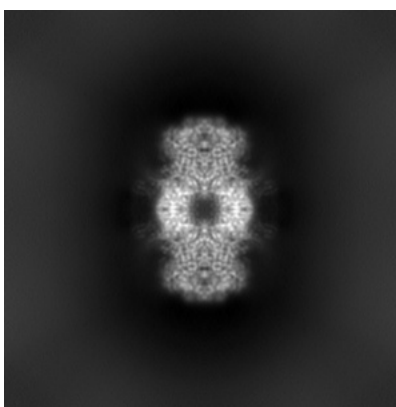


Z

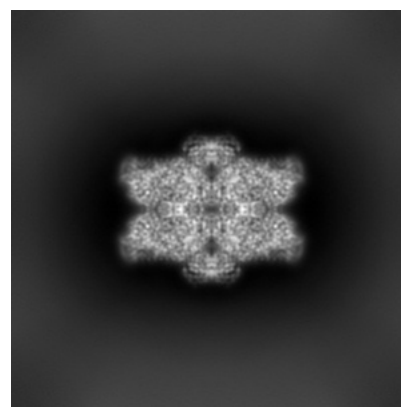
6.1.2 Raw map



X



Y



Z

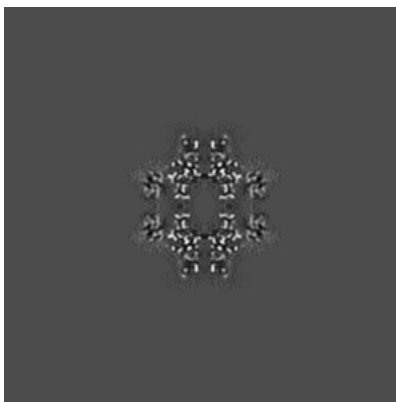
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

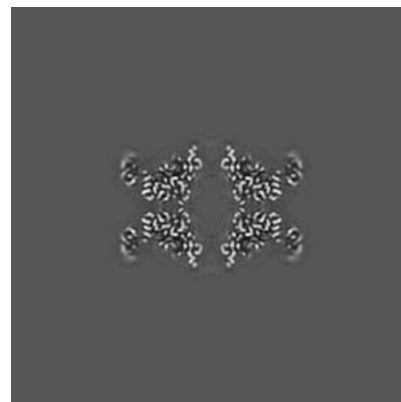
6.2.1 Primary map



X Index: 160

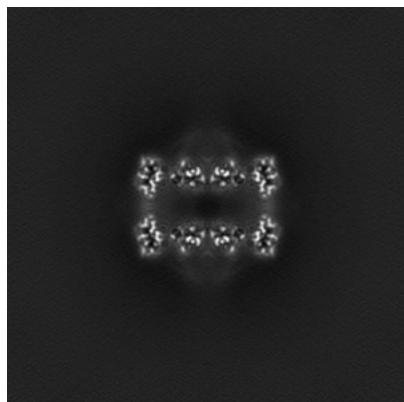


Y Index: 160

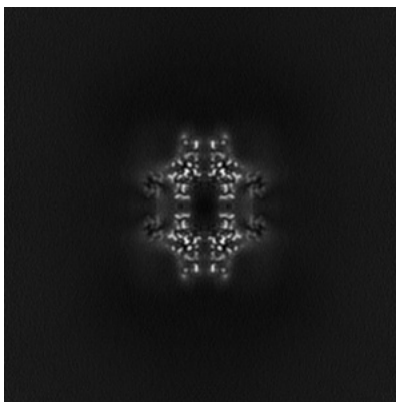


Z Index: 160

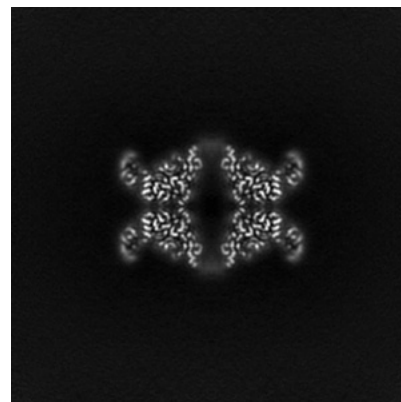
6.2.2 Raw map



X Index: 160



Y Index: 160

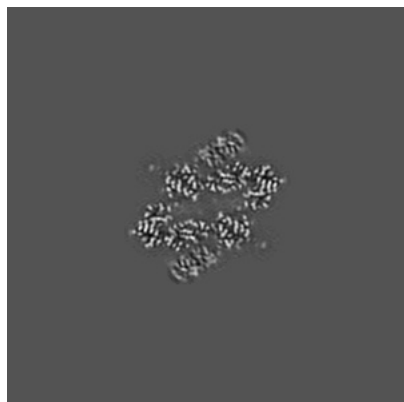


Z Index: 160

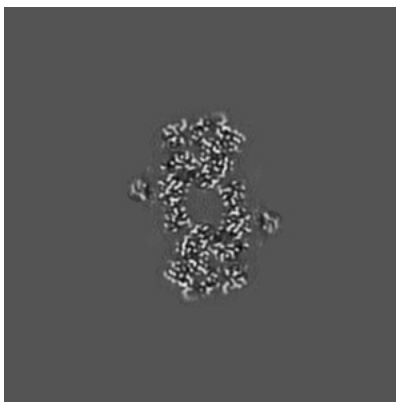
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

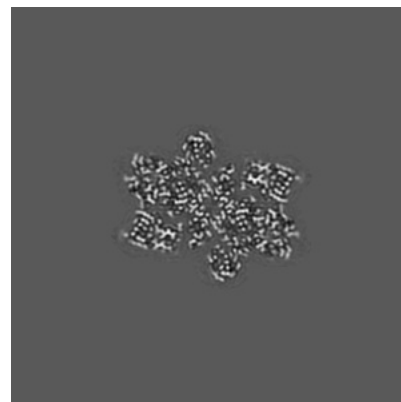
6.3.1 Primary map



X Index: 173

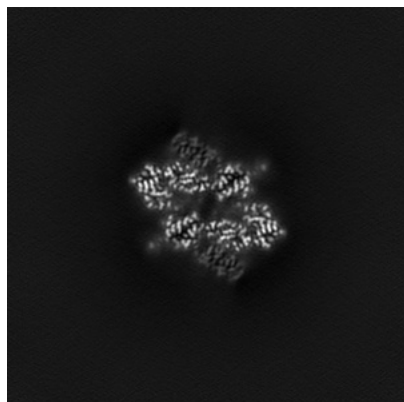


Y Index: 138

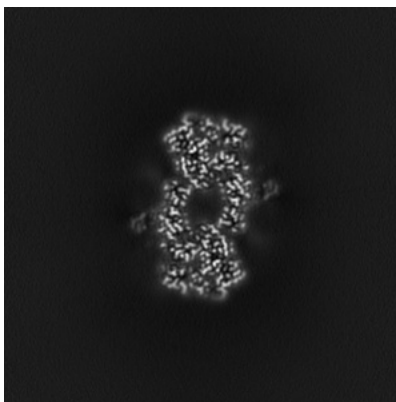


Z Index: 143

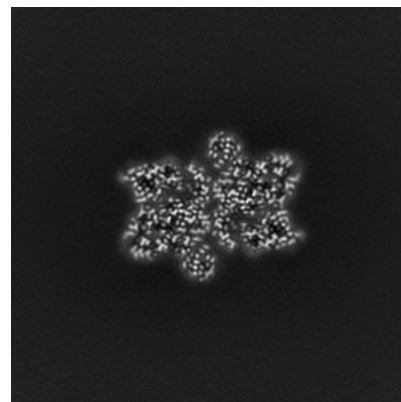
6.3.2 Raw map



X Index: 147



Y Index: 182

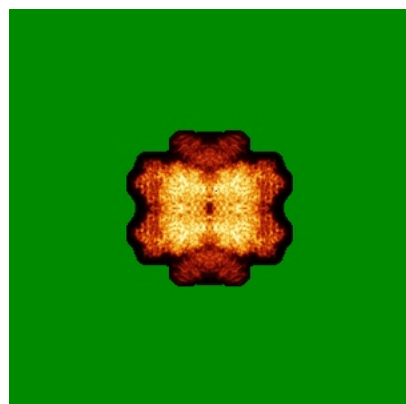


Z Index: 176

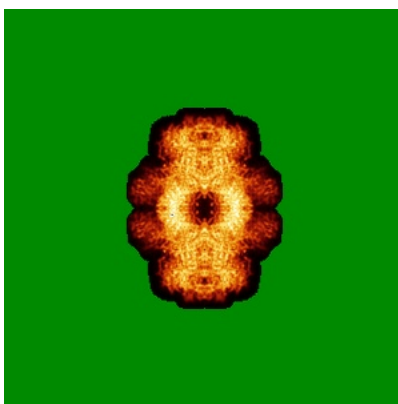
The images above show the largest variance slices of the map in three orthogonal directions.

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

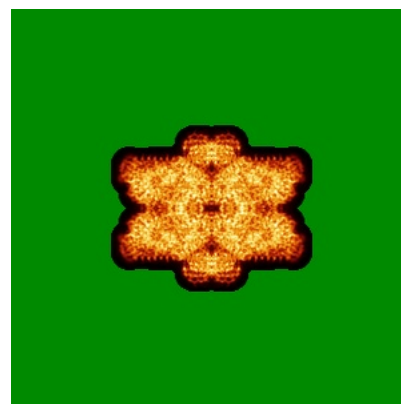
6.4.1 Primary map



X

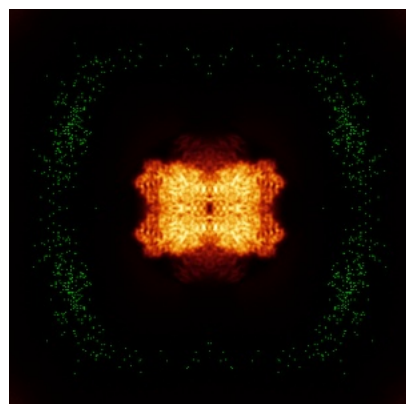


Y

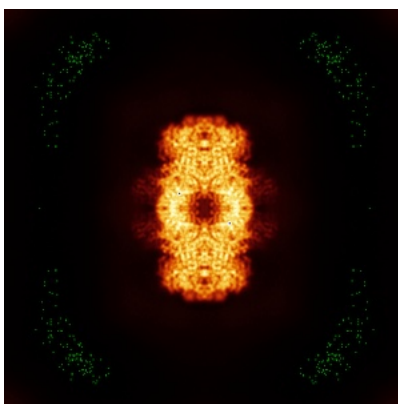


Z

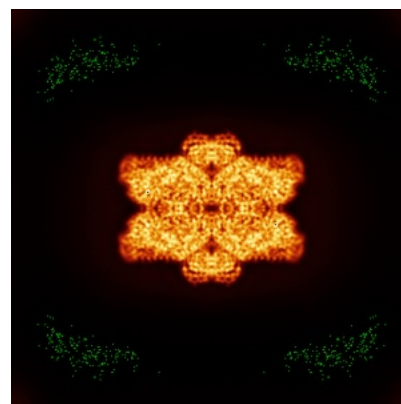
6.4.2 Raw map



X



Y

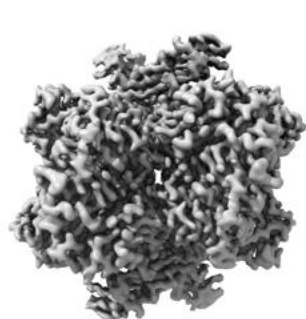


Z

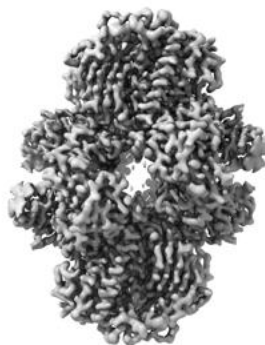
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



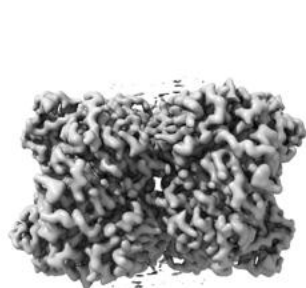
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

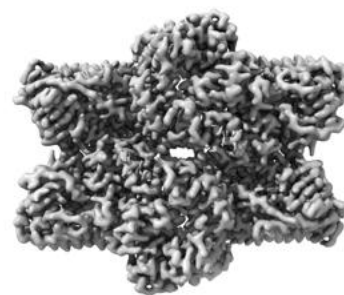
6.5.2 Raw map



X



Y



Z

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

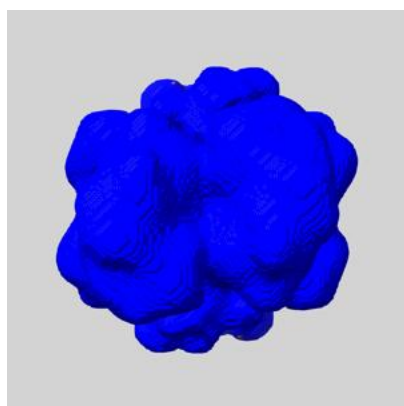
6.6 Mask visualisation [i](#)

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

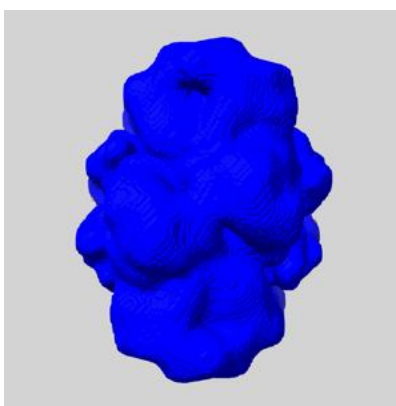
A mask typically either:

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

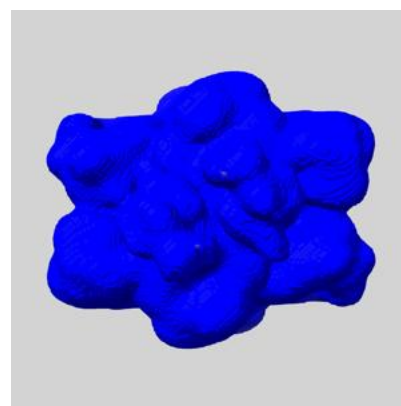
6.6.1 emd_32091_msk_1.map [i](#)



X



Y

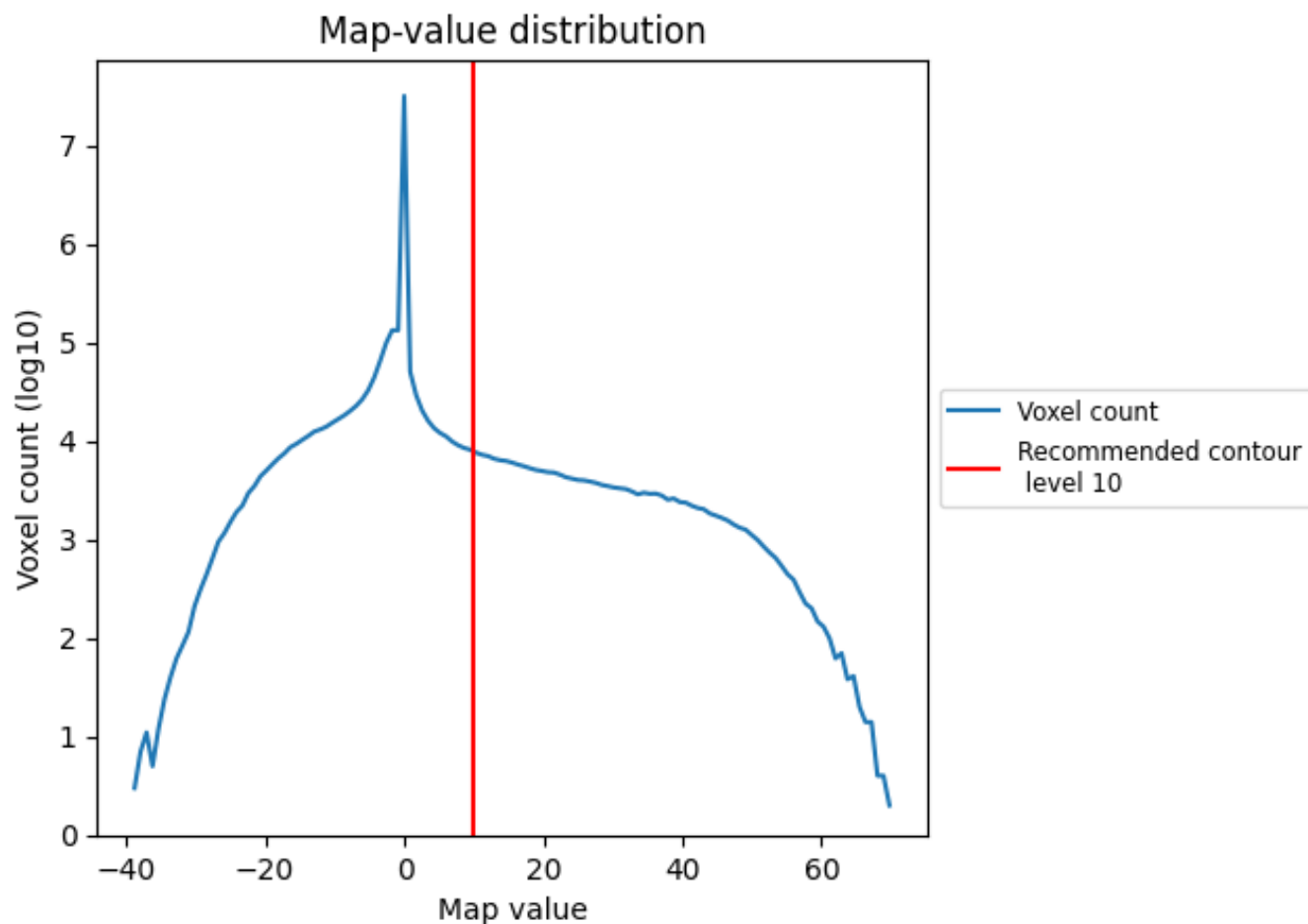


Z

7 Map analysis [i](#)

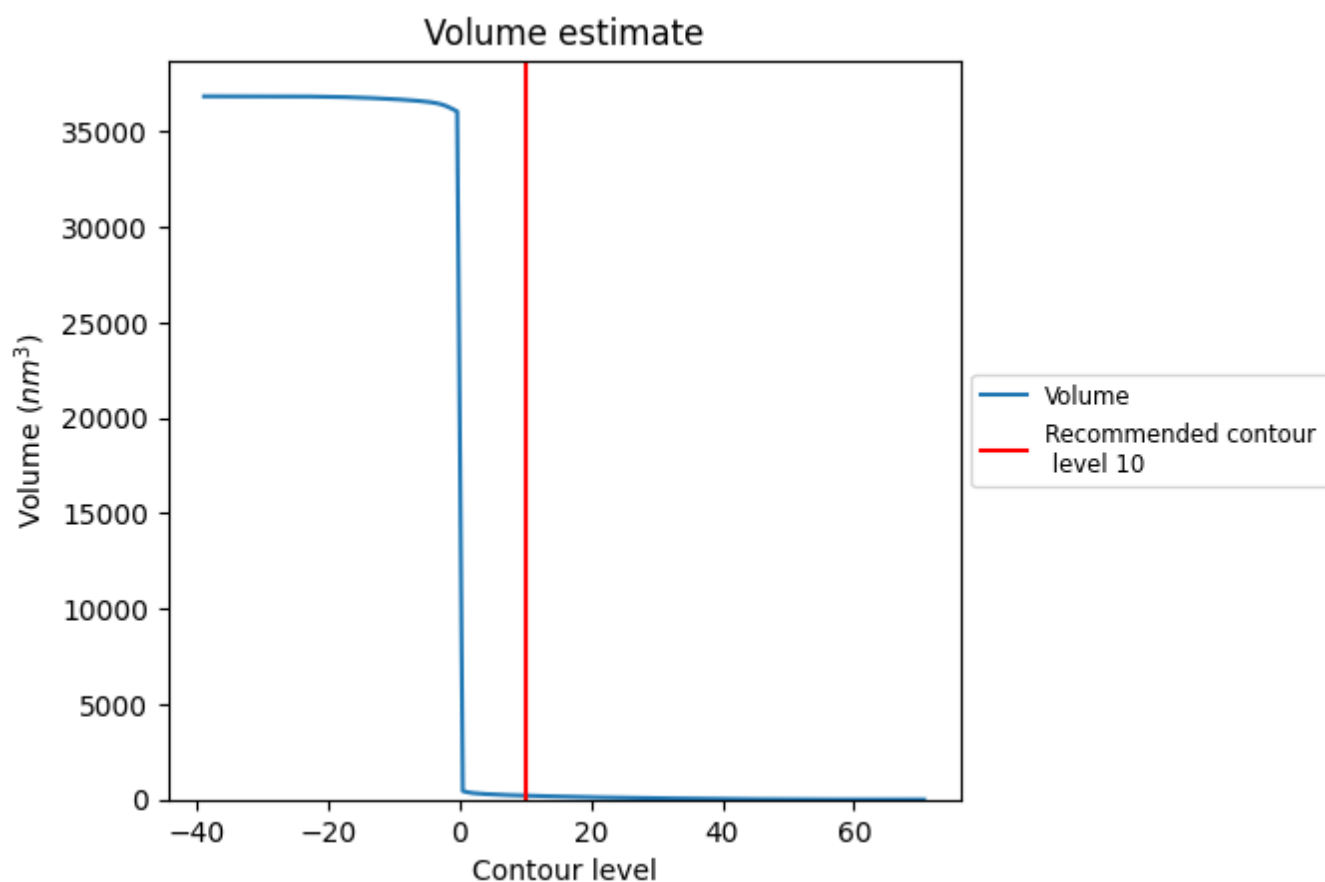
This section contains the results of statistical analysis of the map.

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.

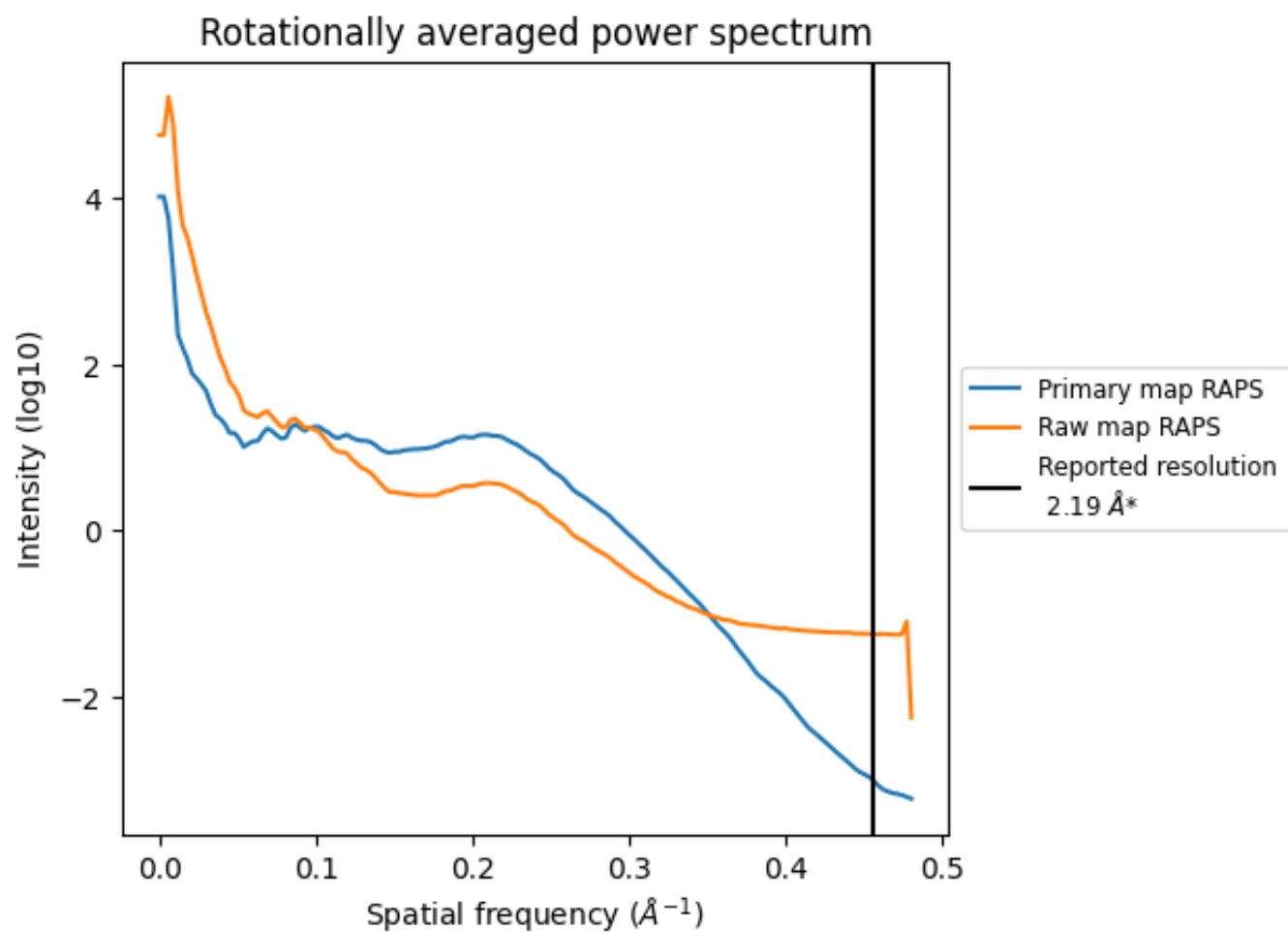
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 ⓘ

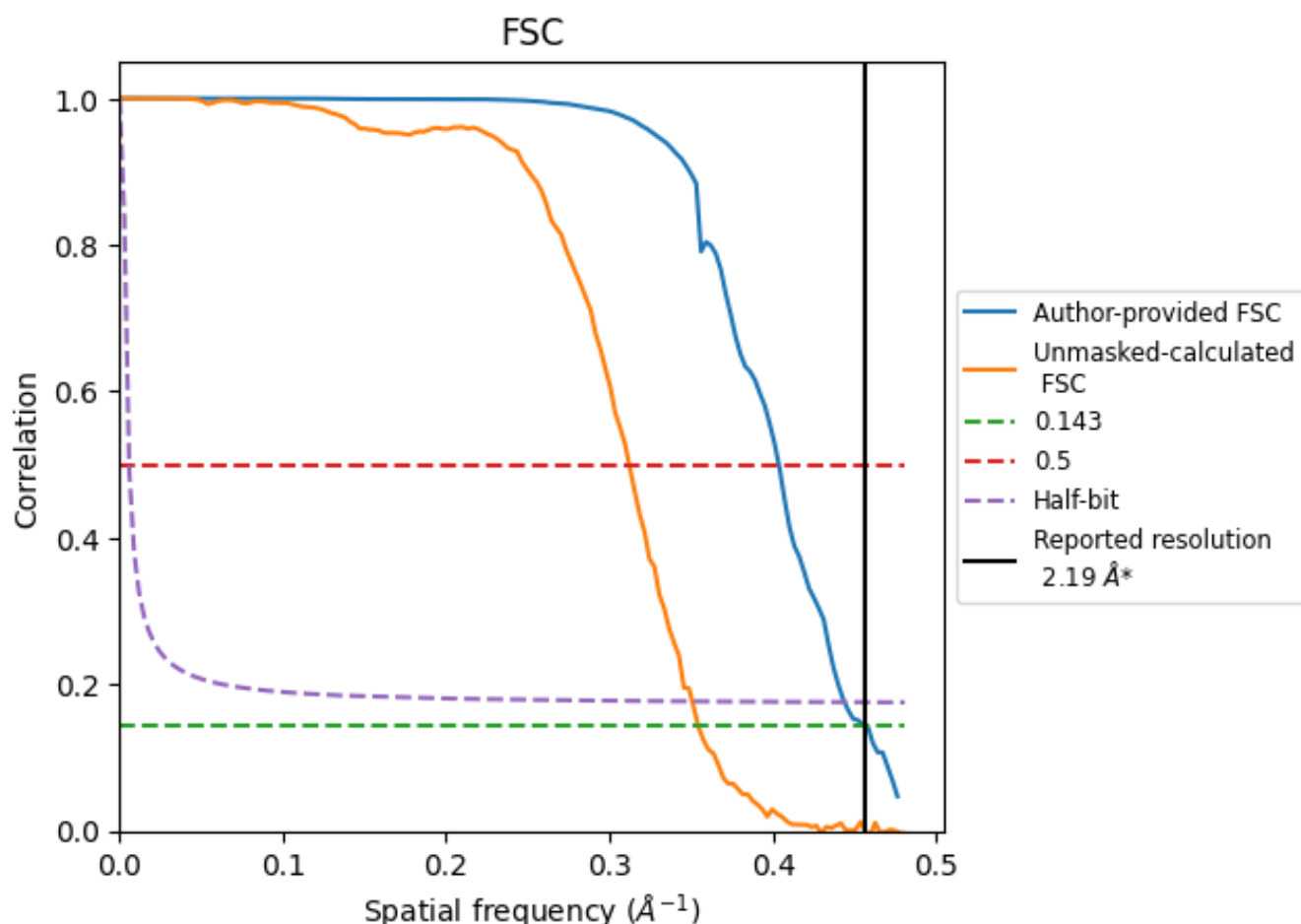


*Reported resolution corresponds to spatial frequency of 0.457 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.457 Å⁻¹

8.2 Resolution estimates [i](#)

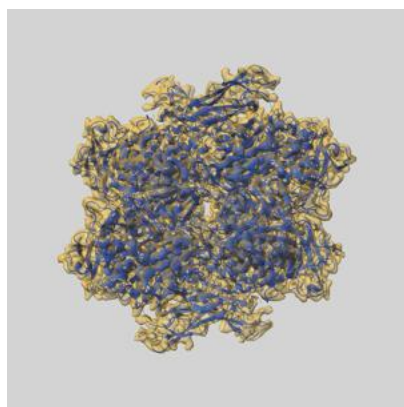
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.48	2.25
Unmasked-calculated*	2.82	3.20	2.85

*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 2.82 differs from the reported value 2.19 by more than 10 %

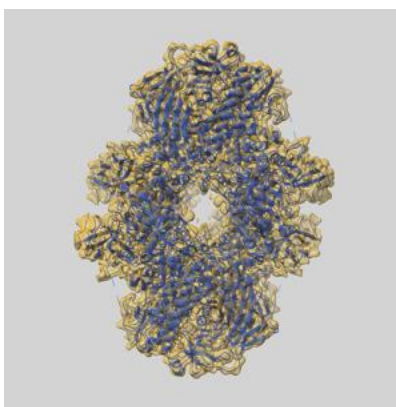
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32091 and PDB model 7VQO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

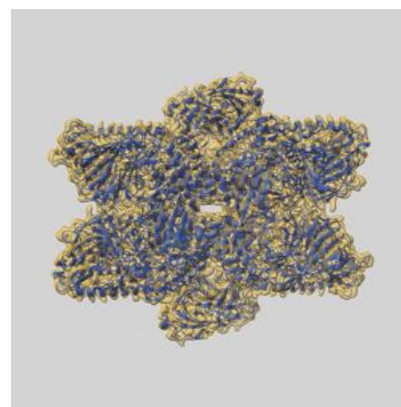
9.1 Map-model overlay [i](#)



X



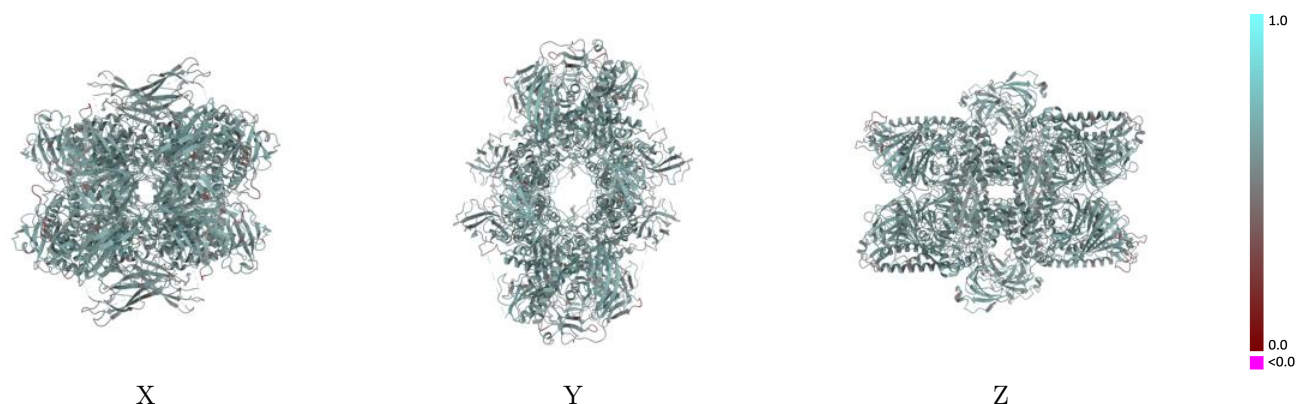
Y



Z

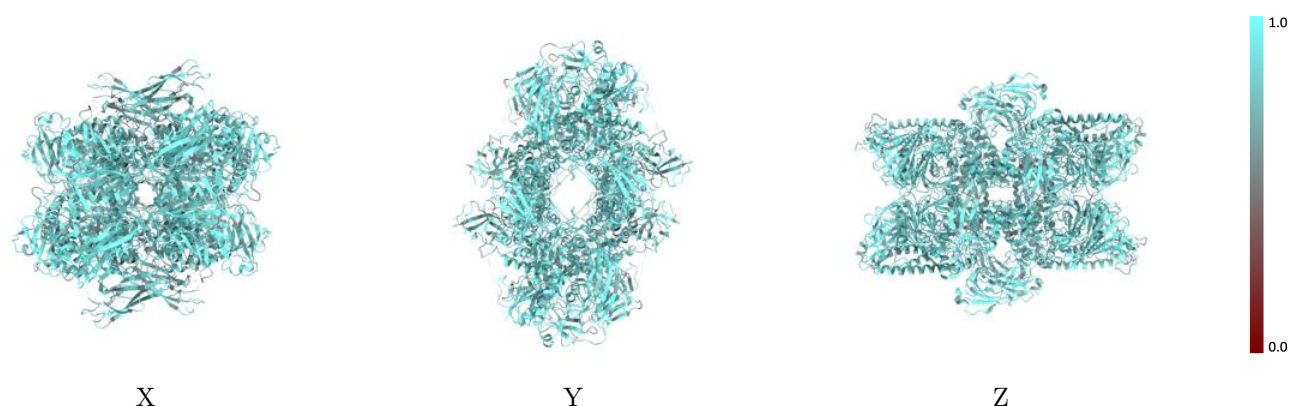
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



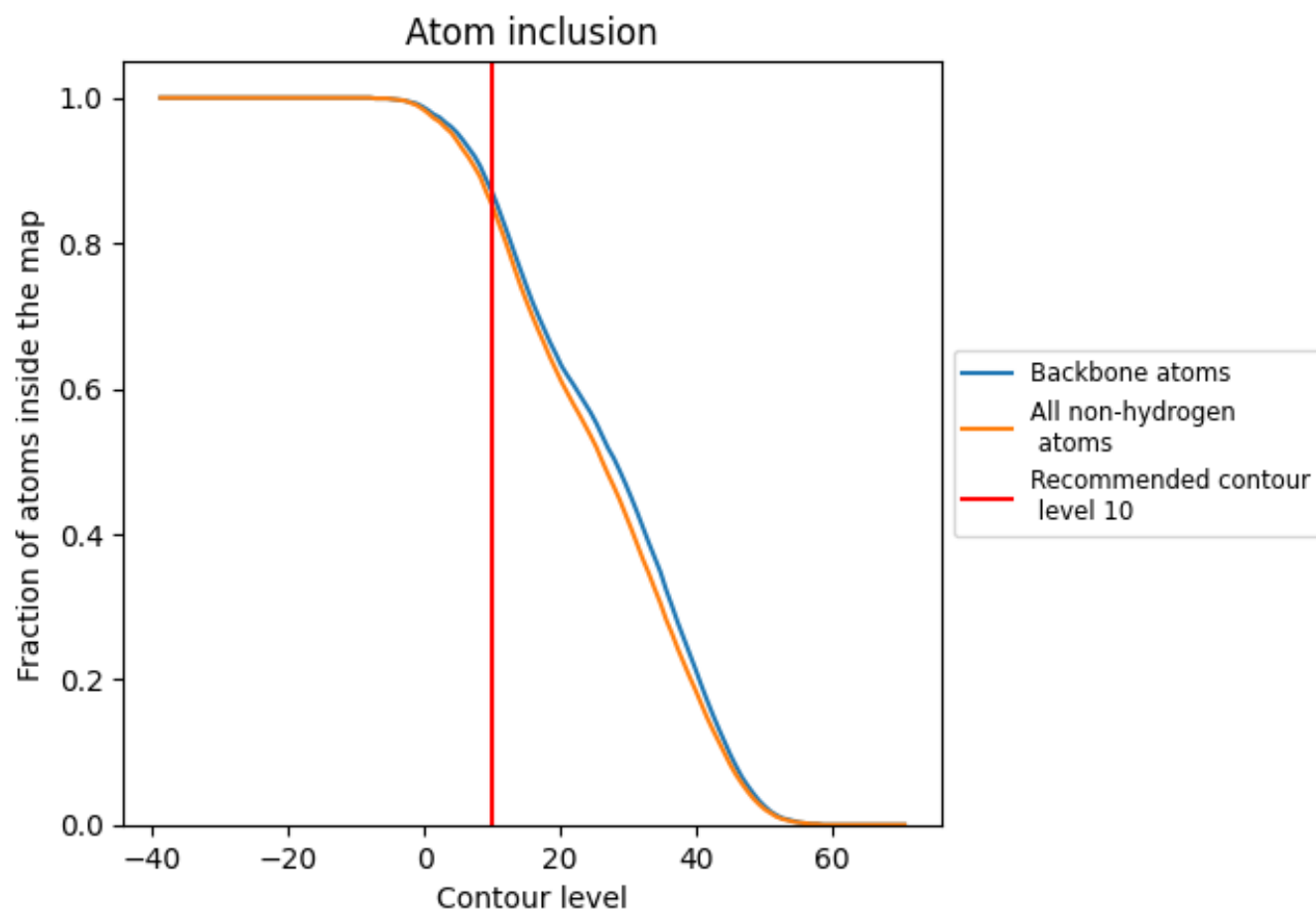
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8520	<div><div></div></div> 0.5830
A	<div><div></div></div> 0.8550	<div><div></div></div> 0.5840
B	<div><div></div></div> 0.8580	<div><div></div></div> 0.5840
C	<div><div></div></div> 0.8540	<div><div></div></div> 0.5830
D	<div><div></div></div> 0.8580	<div><div></div></div> 0.5830

