



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:52 PM UTC

PDB ID : 7WTA / pdb_00007wta
EMDB ID : EMD-32773
Title : Cryo-EM structure of human pyruvate carboxylase in apo state
Authors : Chai, P.; Lan, P.; Wu, J.; Lei, M.
Deposited on : 2022-02-04
Resolution : 3.90 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

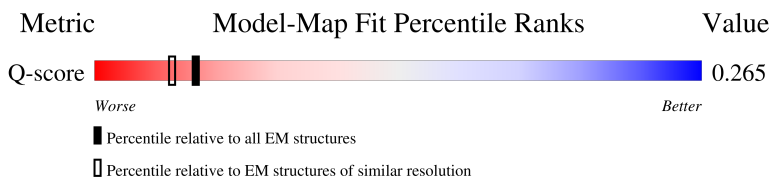
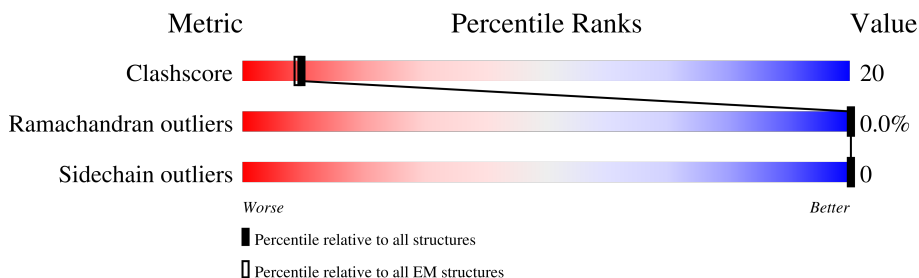
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

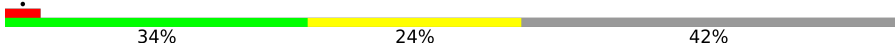
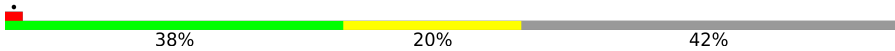
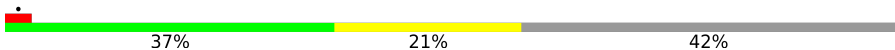
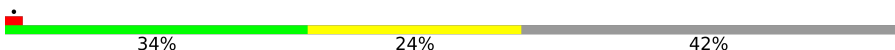
The reported resolution of this entry is 3.90 Å.

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	8855 (3.40 - 4.40)

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	1178	
1	B	1178	
1	C	1178	
1	D	1178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BTI	B	1900	-	-	X	-

2 Entry composition [i](#)

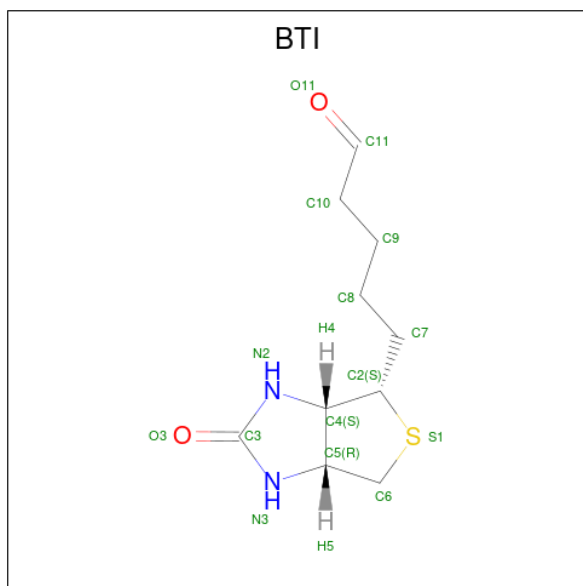
There are 2 unique types of molecules in this entry. The entry contains 21080 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		
1	B	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		
1	C	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		
1	D	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).

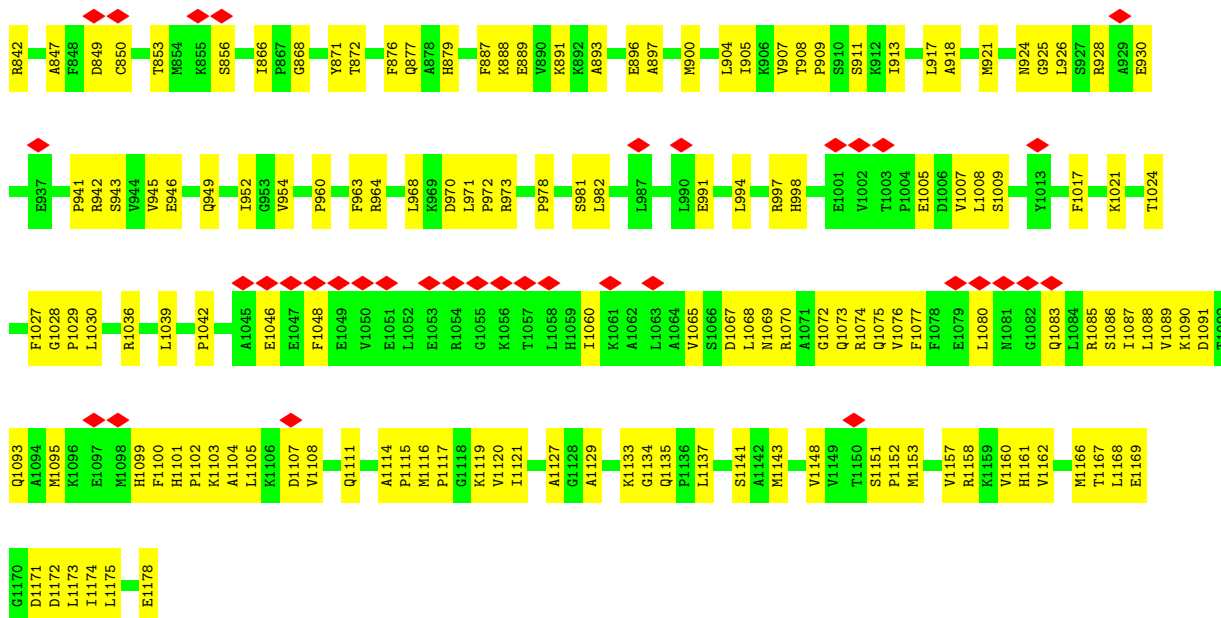


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	B	1	Total	C	N	O	S	0
			15	10	2	2	1	

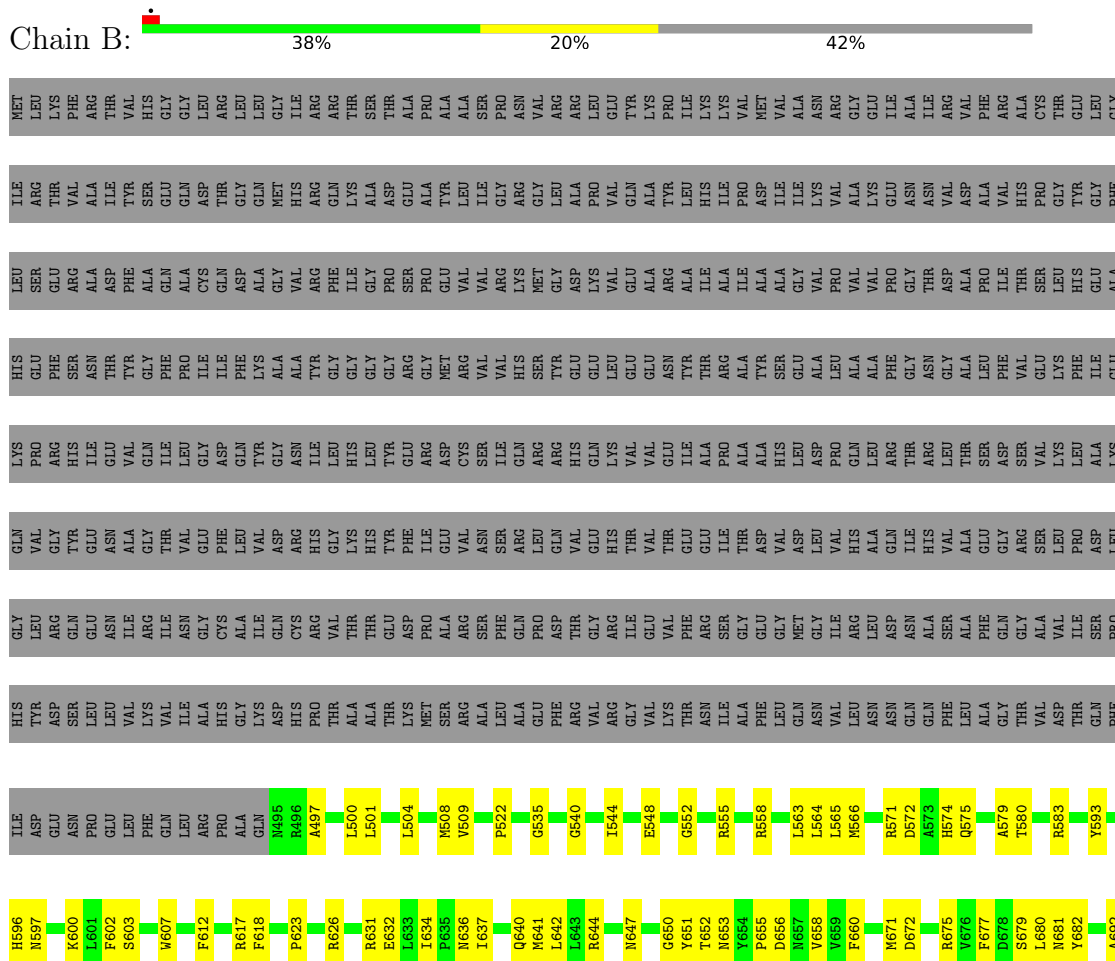
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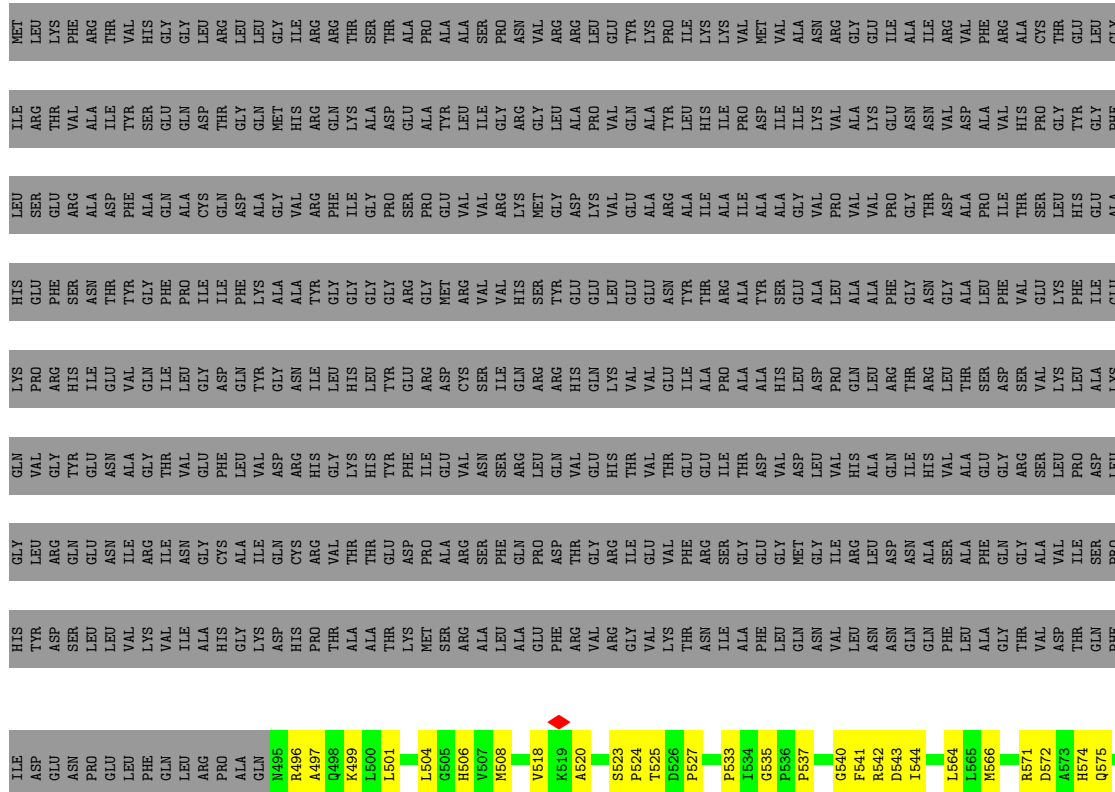
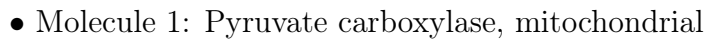
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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	D	1	Total	C	N	O	S	0
			15	10	2	2	1	

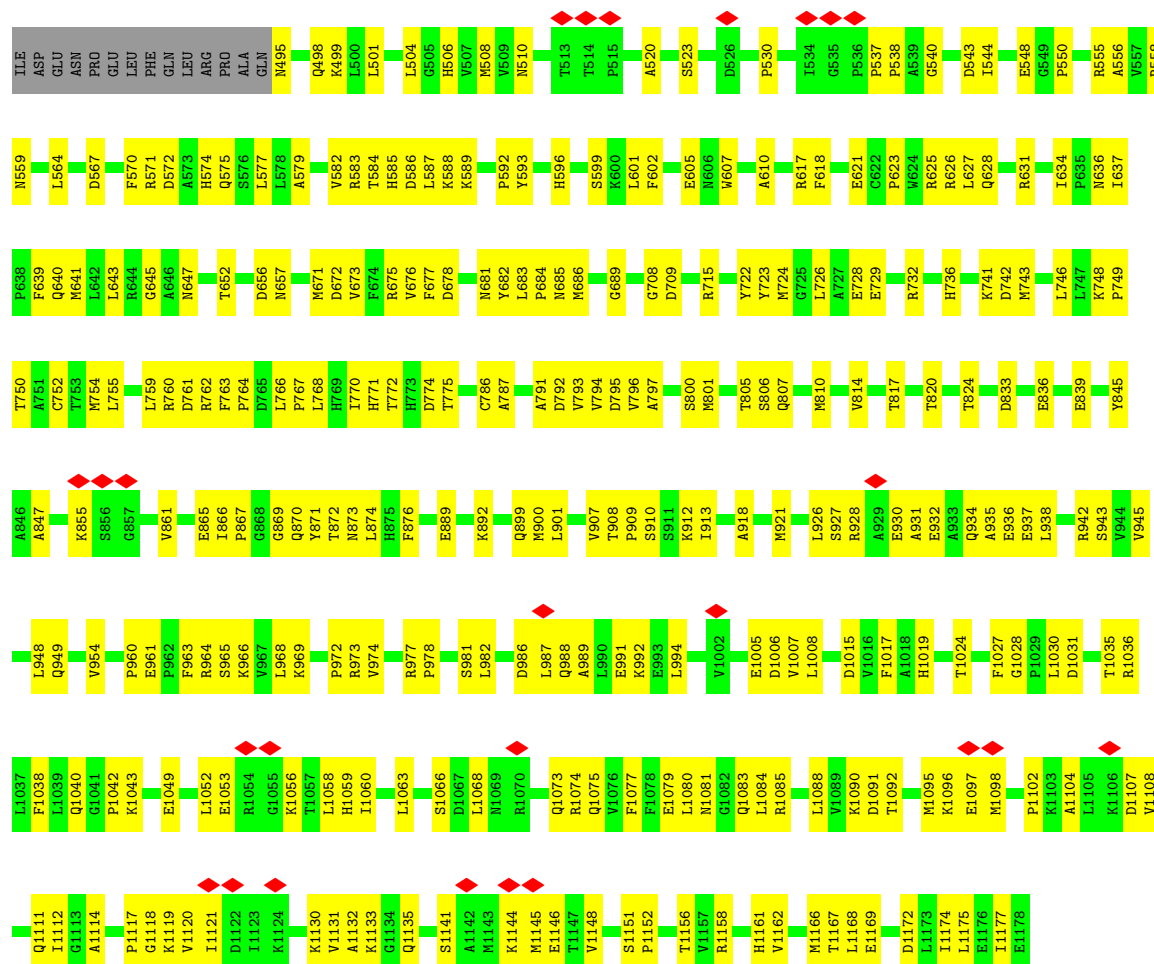


- Molecule 1: Pyruvate carboxylase, mitochondrial









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153965	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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: BTI

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	0.16	0/5373	0.38	0/7284
1	B	0.18	0/5373	0.37	0/7284
1	C	0.18	0/5373	0.37	0/7284
1	D	0.18	0/5373	0.40	0/7284
All	All	0.17	0/21492	0.38	0/29136

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	5255	0	5248	237	0
1	B	5255	0	5249	176	0
1	C	5255	0	5248	199	0
1	D	5255	0	5248	238	0
2	A	15	0	15	2	0
2	B	15	0	15	11	0
2	C	15	0	15	3	0
2	D	15	0	15	1	0
All	All	21080	0	21053	835	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 20.

All (835) 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:C:908:THR:CG2	1:C:909:PRO:HD3	1.63	1.28
1:D:908:THR:HG22	1:D:912:LYS:NZ	1.56	1.20
2:B:1900:BTI:N3	1:D:908:THR:CG2	2.07	1.18
2:B:1900:BTI:C3	1:D:908:THR:HG23	1.71	1.18
2:B:1900:BTI:HN3	1:D:908:THR:CG2	1.56	1.17
2:B:1900:BTI:HN3	1:D:908:THR:HG21	1.07	1.13
1:C:908:THR:HG22	1:C:909:PRO:HD3	1.21	1.12
1:C:908:THR:HG23	1:C:909:PRO:CD	1.80	1.10
2:B:1900:BTI:N3	1:D:908:THR:HG23	1.66	1.05
1:C:908:THR:CG2	1:C:909:PRO:CD	2.36	1.02
2:B:1900:BTI:O3	1:D:908:THR:HG23	1.63	0.98
1:A:739:CYS:HG	1:A:769:HIS:HD1	1.08	0.95
1:D:908:THR:HG22	1:D:912:LYS:HZ3	1.40	0.86
1:B:566:MET:HB3	1:B:795:ASP:HA	1.55	0.85
2:B:1900:BTI:C3	1:D:908:THR:CG2	2.55	0.85
1:A:653:ASN:HD21	1:A:952:ILE:HA	1.42	0.84
2:B:1900:BTI:N3	1:D:908:THR:HG21	1.77	0.81
1:A:708:GLY:HA2	1:A:715:ARG:HH11	1.47	0.80
1:A:978:PRO:HA	1:A:981:SER:HB3	1.65	0.79
1:C:924:ASN:HB2	1:C:926:LEU:HD22	1.62	0.78
1:D:918:ALA:HA	1:D:921:MET:HE2	1.66	0.78
1:D:908:THR:CG2	1:D:912:LYS:NZ	2.44	0.78
1:B:1061:LYS:HB3	1:B:1079:GLU:HB2	1.65	0.78
1:A:641:MET:HB2	1:A:671:MET:HE2	1.66	0.77
1:B:959:PHE:HE2	1:B:964:ARG:HD3	1.49	0.77
1:C:908:THR:HG23	1:C:909:PRO:CG	2.15	0.77
1:A:1075:GLN:NE2	1:A:1086:SER:OG	2.19	0.76
1:A:609:GLY:H	1:A:642:LEU:HD23	1.51	0.75
1:D:631:ARG:NH1	1:D:672:ASP:OD2	2.20	0.75
1:D:558:ARG:O	1:D:558:ARG:NH1	2.19	0.74
1:D:908:THR:HG22	1:D:912:LYS:HZ1	1.49	0.74
1:B:593:TYR:O	1:B:597:ASN:ND2	2.17	0.73
1:A:741:LYS:HA	1:A:771:HIS:HB3	1.68	0.73
1:D:520:ALA:HB3	1:D:847:ALA:HA	1.70	0.73
1:D:772:THR:O	1:D:807:GLN:NE2	2.19	0.73
1:B:617:ARG:HH12	1:D:1144:LYS:HE3	1.54	0.73
1:A:907:VAL:HG12	1:A:908:THR:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1156:THR:OG1	1:D:1158:ARG:NH2	2.22	0.72
1:A:678:ASP:HB3	1:A:686:MET:HE3	1.72	0.72
1:A:508:MET:HE3	1:A:1042:PRO:HD2	1.72	0.72
1:C:881:MET:HG3	1:C:883:LEU:HD13	1.71	0.72
1:B:1105:LEU:HD22	1:B:1108:VAL:HG23	1.71	0.72
1:C:1098:MET:HE3	1:C:1099:HIS:H	1.54	0.72
1:A:1075:GLN:NE2	1:A:1076:VAL:O	2.23	0.72
1:D:752:CYS:SG	1:D:786:CYS:N	2.63	0.71
1:B:631:ARG:NH1	1:B:672:ASP:OD2	2.22	0.71
1:A:639:PHE:H	1:A:672:ASP:HB2	1.56	0.71
1:C:566:MET:HB3	1:C:795:ASP:HA	1.73	0.70
1:C:644:ARG:NE	1:C:908:THR:HG21	2.06	0.70
1:C:535:GLY:O	1:C:596:HIS:NE2	2.23	0.70
1:C:908:THR:HG23	1:C:909:PRO:N	2.05	0.70
1:C:895:VAL:HG12	1:C:899:GLN:HE22	1.57	0.70
1:B:558:ARG:HB2	1:B:767:PRO:HG3	1.74	0.70
1:A:543:ASP:HB3	1:A:547:ARG:HH12	1.57	0.70
1:C:1124:LYS:HB2	1:C:1137:LEU:HA	1.74	0.69
1:B:1132:ALA:HA	1:B:1154:GLU:HG2	1.73	0.69
1:A:1075:GLN:HE22	1:A:1087:ILE:N	1.90	0.69
1:D:1090:LYS:NZ	1:D:1091:ASP:O	2.21	0.68
1:A:949:GLN:NE2	1:A:972:PRO:O	2.27	0.68
1:A:575:GLN:HA	1:A:580:THR:HB	1.76	0.68
1:C:597:ASN:O	1:C:830:ARG:NH1	2.27	0.68
1:C:1068:LEU:HD22	1:C:1072:GLY:HA2	1.76	0.68
1:A:643:LEU:HB3	1:A:676:VAL:HG22	1.76	0.67
1:A:897:ALA:HA	1:A:917:LEU:HD22	1.75	0.67
1:B:1101:HIS:NE2	1:B:1173:LEU:O	2.22	0.67
2:B:1900:BTI:H62	1:D:610:ALA:HB2	1.77	0.67
1:D:1080:LEU:HD22	1:D:1085:ARG:HD3	1.76	0.67
1:A:964:ARG:O	1:A:968:LEU:HB2	1.94	0.67
1:B:1047:GLU:HB2	1:B:1061:LYS:HD2	1.75	0.67
1:A:1090:LYS:NZ	1:A:1091:ASP:O	2.25	0.67
1:C:508:MET:HE1	1:C:1041:GLY:HA3	1.77	0.67
1:A:610:ALA:HB2	2:C:1900:BTI:H62	1.75	0.67
1:A:900:MET:HE1	1:A:928:ARG:HD2	1.77	0.67
1:B:597:ASN:O	1:B:830:ARG:NH1	2.28	0.67
1:C:827:PRO:HD2	1:C:830:ARG:HH21	1.60	0.67
1:D:978:PRO:HA	1:D:981:SER:HB3	1.77	0.67
1:A:631:ARG:NH2	1:A:634:ILE:O	2.23	0.66
1:D:583:ARG:HH21	1:D:1031:ASP:HA	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ARG:HD2	1:C:575:GLN:HE22	1.59	0.66
1:C:895:VAL:O	1:C:899:GLN:NE2	2.28	0.66
1:A:1091:ASP:OD1	1:A:1093:GLN:NE2	2.28	0.66
1:C:1022:ASP:OD1	1:C:1023:PHE:N	2.29	0.66
1:B:949:GLN:HE22	1:B:973:ARG:HA	1.60	0.66
2:B:1900:BTI:H73	1:D:912:LYS:HD3	1.78	0.66
1:B:572:ASP:OD1	1:B:575:GLN:NE2	2.29	0.66
1:C:520:ALA:HB3	1:C:847:ALA:HA	1.77	0.66
1:A:1103:LYS:NZ	1:A:1171:ASP:OD2	2.28	0.65
1:C:645:GLY:N	1:C:677:PHE:O	2.29	0.65
1:A:942:ARG:NH1	1:A:943:SER:OG	2.30	0.65
1:C:787:ALA:HA	1:C:791:ALA:HB3	1.77	0.65
1:D:1121:ILE:HG12	1:D:1141:SER:HB3	1.76	0.65
1:B:801:MET:HE1	1:B:838:TRP:HB3	1.78	0.65
1:A:921:MET:O	1:A:925:GLY:N	2.30	0.65
1:A:1135:GLN:HE22	1:A:1137:LEU:HB3	1.62	0.65
1:A:772:THR:O	1:A:807:GLN:NE2	2.23	0.65
1:B:949:GLN:NE2	1:B:972:PRO:O	2.30	0.65
1:B:1101:HIS:HE1	1:B:1161:HIS:HB3	1.62	0.65
1:D:537:PRO:HB2	1:D:636:ASN:HD21	1.62	0.65
1:D:796:VAL:HG13	1:D:810:MET:HE1	1.78	0.65
1:B:787:ALA:HA	1:B:791:ALA:HB3	1.80	0.64
1:D:538:PRO:O	1:D:636:ASN:ND2	2.30	0.64
1:B:535:GLY:O	1:B:596:HIS:NE2	2.30	0.64
1:B:641:MET:HB2	1:B:671:MET:HE2	1.79	0.64
1:D:750:THR:O	1:D:754:MET:HG3	1.98	0.64
1:A:1069:ASN:OD1	1:A:1070:ARG:N	2.29	0.64
1:C:994:LEU:HD13	1:C:997:ARG:HH12	1.62	0.64
1:A:577:LEU:HD11	1:A:806:SER:HB2	1.79	0.64
1:A:1095:MET:HE2	1:A:1095:MET:H	1.62	0.64
1:D:994:LEU:HD21	1:D:1007:VAL:HG22	1.78	0.64
1:C:501:LEU:HD22	1:C:1078:PHE:HD2	1.62	0.64
1:C:747:LEU:HD12	1:C:752:CYS:HB3	1.80	0.64
1:C:1066:SER:O	1:C:1074:ARG:NH1	2.31	0.64
1:C:566:MET:SD	1:C:603:SER:OG	2.55	0.63
1:C:641:MET:HG2	1:C:671:MET:HE2	1.80	0.63
1:C:1061:LYS:HB3	1:C:1079:GLU:HB2	1.80	0.63
1:B:1051:GLU:OE2	1:B:1054:ARG:NH2	2.31	0.63
1:C:908:THR:HG23	1:C:909:PRO:HG3	1.79	0.63
1:C:961:GLU:OE2	1:C:964:ARG:NH2	2.31	0.63
1:C:1034:ASN:HB3	1:C:1037:LEU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:MET:HE1	1:A:759:LEU:HD22	1.80	0.63
1:A:1135:GLN:HG3	1:A:1151:SER:HB2	1.81	0.63
1:C:1117:PRO:HG3	1:C:1170:GLY:H	1.62	0.63
1:D:741:LYS:HA	1:D:771:HIS:HB3	1.79	0.63
1:D:1130:LYS:NZ	1:D:1131:VAL:O	2.31	0.63
1:D:641:MET:HB3	1:D:671:MET:HE2	1.79	0.62
1:A:760:ARG:NH1	1:A:766:LEU:O	2.32	0.62
1:C:541:PHE:HA	1:C:544:ILE:HD12	1.82	0.62
1:C:653:ASN:ND2	1:C:951:TYR:O	2.32	0.62
1:A:570:PHE:O	1:A:574:HIS:NE2	2.25	0.62
1:B:631:ARG:NH2	1:B:637:ILE:O	2.26	0.62
1:B:1079:GLU:HA	1:B:1084:LEU:HD23	1.82	0.62
1:C:801:MET:HE1	1:C:842:ARG:HD2	1.81	0.62
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.28	0.62
1:B:959:PHE:CE2	1:B:964:ARG:HD3	2.33	0.62
1:D:682:TYR:HE1	1:D:954:VAL:HG12	1.65	0.61
1:D:558:ARG:HH21	1:D:760:ARG:NH2	1.98	0.61
1:A:600:LYS:NZ	1:A:825:GLU:O	2.27	0.61
1:A:1160:VAL:HG12	1:A:1175:LEU:HG	1.81	0.61
1:D:1096:LYS:HB3	1:D:1098:MET:HE2	1.82	0.61
1:A:641:MET:HE1	1:A:643:LEU:HB2	1.82	0.61
1:D:510:ASN:ND2	1:D:1090:LYS:O	2.33	0.61
1:B:923:GLN:NE2	1:B:924:ASN:OD1	2.33	0.61
1:D:722:TYR:CZ	1:D:726:LEU:HD11	2.36	0.61
1:C:644:ARG:HD3	1:C:908:THR:HG21	1.82	0.61
1:C:523:SER:O	1:C:1036:ARG:NH2	2.33	0.61
1:D:723:TYR:HA	1:D:726:LEU:HD12	1.83	0.61
1:A:800:SER:O	1:A:842:ARG:NH1	2.34	0.61
1:D:1024:THR:O	1:D:1028:GLY:N	2.33	0.61
1:B:552:GLY:HA2	1:B:555:ARG:HE	1.65	0.60
1:B:1039:LEU:HD12	1:B:1040:GLN:HG3	1.84	0.60
1:C:644:ARG:CD	1:C:908:THR:HG21	2.31	0.60
1:D:501:LEU:HD11	1:D:1060:ILE:HG21	1.82	0.60
1:A:613:ASP:OD2	1:A:651:TYR:OH	2.18	0.60
1:B:647:ASN:HD22	1:B:651:TYR:HA	1.64	0.60
1:A:624:TRP:HH2	1:A:1009:SER:HB2	1.66	0.60
1:A:1024:THR:O	1:A:1028:GLY:N	2.35	0.60
1:D:1068:LEU:HA	1:D:1074:ARG:HG2	1.83	0.60
1:A:1133:LYS:HD3	1:A:1153:MET:HA	1.84	0.60
1:D:949:GLN:HE22	1:D:974:VAL:HB	1.67	0.60
1:D:1066:SER:OG	1:D:1075:GLN:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:759:LEU:HD11	1:D:768:LEU:HD21	1.84	0.59
1:A:640:GLN:HA	1:A:673:VAL:HB	1.84	0.59
1:D:640:GLN:HG2	1:D:673:VAL:HB	1.83	0.59
1:A:548:GLU:HB3	1:A:552:GLY:HA3	1.82	0.59
1:A:1115:PRO:O	1:A:1116:MET:HE2	2.02	0.59
1:B:961:GLU:OE1	1:B:964:ARG:NH2	2.19	0.59
1:C:524:PRO:HA	1:C:1036:ARG:HH12	1.66	0.59
1:D:760:ARG:NH2	1:D:764:PRO:O	2.33	0.59
1:A:815:ALA:O	1:D:748:LYS:NZ	2.35	0.59
1:D:571:ARG:NH1	1:D:575:GLN:OE1	2.35	0.59
1:A:741:LYS:HE3	1:A:771:HIS:CD2	2.37	0.59
1:D:1083:GLN:NE2	1:D:1084:LEU:O	2.35	0.59
1:A:541:PHE:HB3	1:A:553:PHE:HE1	1.67	0.59
1:B:504:LEU:HD22	1:B:1042:PRO:HD3	1.85	0.59
1:C:597:ASN:HB3	1:C:830:ARG:HD2	1.84	0.59
1:D:866:ILE:HG21	1:D:871:TYR:HD1	1.68	0.58
1:D:1056:LYS:HZ2	1:D:1058:LEU:HB3	1.68	0.58
1:A:942:ARG:HH21	1:A:946:GLU:HG3	1.69	0.58
1:B:681:ASN:ND2	1:B:722:TYR:OH	2.36	0.58
1:B:852:ALA:O	1:B:855:LYS:NZ	2.34	0.58
1:D:729:GLU:HA	1:D:732:ARG:HG2	1.85	0.58
1:C:593:TYR:O	1:C:597:ASN:ND2	2.26	0.58
1:C:859:SER:OG	1:C:860:ASP:N	2.36	0.58
1:C:1053:GLU:HG3	1:C:1056:LYS:HB2	1.85	0.58
1:A:926:LEU:HB2	1:A:930:GLU:OE2	2.03	0.58
1:A:1143:MET:HE3	1:C:881:MET:HE2	1.86	0.58
1:A:538:PRO:HG2	1:A:599:SER:HB3	1.86	0.58
1:C:1156:THR:HG23	1:C:1158:ARG:HH12	1.69	0.58
1:D:770:ILE:HB	1:D:794:VAL:HG12	1.84	0.58
1:D:504:LEU:HD22	1:D:1042:PRO:HD3	1.86	0.58
1:C:728:GLU:HB3	1:C:762:ARG:HH22	1.68	0.58
1:A:907:VAL:O	1:A:911:SER:N	2.24	0.57
1:A:1119:LYS:HB2	1:A:1167:THR:HG22	1.86	0.57
1:C:720:LEU:HD22	1:C:754:MET:HE1	1.86	0.57
1:A:624:TRP:CE2	1:A:1005:GLU:HB2	2.39	0.57
1:A:647:ASN:ND2	1:A:650:GLY:O	2.36	0.57
1:B:565:LEU:HD23	1:B:566:MET:N	2.20	0.57
1:B:1139:VAL:HG22	1:B:1148:VAL:HG12	1.85	0.57
1:D:558:ARG:HB2	1:D:767:PRO:HG3	1.86	0.57
1:A:991:GLU:HG2	1:A:1007:VAL:HG21	1.86	0.57
1:B:677:PHE:HZ	1:B:705:SER:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:VAL:HG23	1:C:1076:VAL:HG22	1.84	0.57
1:C:1080:LEU:HG	1:C:1081:ASN:H	1.70	0.57
1:B:631:ARG:NH2	1:B:634:ILE:O	2.30	0.57
1:C:681:ASN:OD1	1:C:722:TYR:OH	2.22	0.57
1:B:1156:THR:O	1:B:1158:ARG:NH1	2.38	0.57
1:C:682:TYR:CE1	1:C:954:VAL:HG12	2.40	0.57
1:D:1169:GLU:N	1:D:1172:ASP:OD2	2.32	0.57
1:C:682:TYR:HE1	1:C:954:VAL:HG12	1.69	0.57
1:D:927:SER:OG	1:D:928:ARG:N	2.38	0.57
1:B:540:GLY:N	1:B:636:ASN:OD1	2.37	0.56
1:B:623:PRO:O	1:B:626:ARG:NH2	2.37	0.56
1:C:499:LYS:NZ	1:C:1025:ALA:O	2.37	0.56
1:B:741:LYS:HE3	1:B:743:MET:HE3	1.87	0.56
1:B:743:MET:HE1	1:B:771:HIS:HE1	1.70	0.56
1:C:949:GLN:HG3	1:C:973:ARG:HA	1.86	0.56
1:D:1152:PRO:HD2	1:D:1177:ILE:HG21	1.87	0.56
1:C:604:MET:HE1	1:C:606:ASN:HD22	1.69	0.56
1:D:742:ASP:N	1:D:771:HIS:O	2.34	0.56
1:A:1068:LEU:HD23	1:A:1074:ARG:HG3	1.87	0.56
1:C:968:LEU:HD13	1:C:973:ARG:HG2	1.87	0.56
1:D:1133:LYS:NZ	1:D:1151:SER:O	2.33	0.56
1:D:506:HIS:CE1	1:D:510:ASN:HD22	2.23	0.56
1:D:631:ARG:NH2	1:D:634:ILE:O	2.32	0.56
1:D:728:GLU:OE1	1:D:762:ARG:NH1	2.38	0.56
1:B:1151:SER:OG	1:B:1153:MET:O	2.22	0.56
1:C:1069:ASN:OD1	1:C:1070:ARG:N	2.33	0.56
1:A:1067:ASP:OD1	1:A:1068:LEU:N	2.32	0.56
1:D:761:ASP:OD1	1:D:762:ARG:N	2.39	0.56
1:A:571:ARG:NH1	1:A:575:GLN:OE1	2.39	0.56
1:A:888:LYS:NZ	1:A:889:GLU:OE2	2.24	0.56
1:C:542:ARG:NH1	1:C:634:ILE:O	2.39	0.56
1:D:908:THR:CG2	1:D:912:LYS:HZ3	2.14	0.56
1:A:1116:MET:HE3	1:C:920:PHE:HD1	1.70	0.55
1:A:499:LYS:HB3	1:A:1027:PHE:HA	1.88	0.55
1:A:1065:VAL:HG22	1:A:1076:VAL:HG23	1.88	0.55
1:A:608:GLY:HA2	1:A:642:LEU:HB3	1.88	0.55
1:A:1077:PHE:CE1	1:B:1063:LEU:HD23	2.42	0.55
1:C:926:LEU:HB2	1:C:930:GLU:OE2	2.06	0.55
1:A:742:ASP:HB3	1:A:772:THR:HA	1.88	0.55
1:B:898:ASN:O	1:B:902:GLY:N	2.40	0.55
1:B:936:GLU:OE2	1:B:966:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ARG:HE	1:C:908:THR:HG21	1.72	0.55
1:D:907:VAL:HG12	1:D:908:THR:H	1.72	0.55
1:A:558:ARG:HB2	1:A:767:PRO:HG3	1.89	0.55
1:A:907:VAL:HG12	1:A:908:THR:N	2.21	0.55
1:C:889:GLU:HA	1:C:892:LYS:HD3	1.87	0.55
1:D:540:GLY:H	1:D:636:ASN:HB2	1.72	0.55
1:B:558:ARG:HH22	1:B:760:ARG:CZ	2.20	0.55
1:B:574:HIS:HB3	1:B:580:THR:HA	1.89	0.55
1:B:710:VAL:HG21	1:B:755:LEU:HD21	1.89	0.55
1:D:592:PRO:O	1:D:596:HIS:ND1	2.31	0.55
1:D:743:MET:HE3	1:D:869:GLY:H	1.71	0.55
1:A:724:MET:SD	1:A:762:ARG:NH1	2.80	0.55
1:B:679:SER:OG	1:B:907:VAL:N	2.38	0.55
1:B:942:ARG:HB2	1:D:1146:GLU:O	2.07	0.55
1:A:761:ASP:OD1	1:A:762:ARG:N	2.40	0.55
1:B:778:ALA:HB2	1:C:812:ALA:HB1	1.89	0.55
1:D:583:ARG:HH12	1:D:1038:PHE:HB2	1.72	0.55
1:D:625:ARG:HH21	1:D:628:GLN:HE22	1.55	0.55
1:D:817:THR:HA	1:D:820:THR:HB	1.88	0.55
1:A:1148:VAL:O	1:C:939:SER:OG	2.24	0.54
1:B:1101:HIS:CE1	1:B:1161:HIS:HB3	2.42	0.54
1:A:741:LYS:HG2	1:A:771:HIS:HB3	1.89	0.54
1:D:631:ARG:NH2	1:D:637:ILE:O	2.34	0.54
1:D:931:ALA:HA	1:D:938:LEU:HD11	1.89	0.54
1:B:720:LEU:HD22	1:B:754:MET:HE1	1.90	0.54
1:D:499:LYS:HB3	1:D:1027:PHE:HA	1.89	0.54
1:D:550:PRO:HB2	1:D:736:HIS:NE2	2.22	0.54
1:A:543:ASP:HB3	1:A:547:ARG:NH1	2.21	0.54
1:A:1127:ALA:HB2	1:A:1160:VAL:HG22	1.89	0.54
1:C:1163:THR:H	1:C:1166:MET:HE2	1.72	0.54
1:D:900:MET:HE1	1:D:928:ARG:HA	1.88	0.54
1:D:1114:ALA:H	1:D:1172:ASP:H	1.56	0.54
1:B:1127:ALA:HB2	1:B:1160:VAL:HG13	1.90	0.54
1:C:501:LEU:HD22	1:C:1078:PHE:CD2	2.42	0.54
1:A:758:SER:O	1:A:762:ARG:NH1	2.40	0.54
1:B:909:PRO:O	1:B:913:ILE:HG12	2.07	0.54
1:A:594:VAL:HA	1:A:598:PHE:HD2	1.72	0.54
1:A:908:THR:HB	1:A:909:PRO:HD3	1.90	0.54
1:D:934:GLN:HB3	1:D:937:GLU:HB2	1.88	0.54
1:D:1030:LEU:HD21	1:D:1038:PHE:HE1	1.73	0.54
1:C:965:SER:HA	1:C:973:ARG:HH22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:GLU:OE1	1:D:675:ARG:NH2	2.40	0.54
1:D:771:HIS:ND1	1:D:795:ASP:OD2	2.36	0.54
1:D:1161:HIS:N	1:D:1174:ILE:O	2.40	0.54
1:A:994:LEU:HD13	1:A:997:ARG:HE	1.71	0.54
1:B:877:GLN:HE22	1:D:1145:MET:HE1	1.72	0.54
1:B:721:GLN:HA	1:B:724:MET:HB2	1.89	0.53
1:A:1105:LEU:HB3	1:A:1107:ASP:OD1	2.08	0.53
1:B:1034:ASN:O	1:B:1038:PHE:N	2.36	0.53
1:D:763:PHE:HB3	1:D:766:LEU:HD13	1.89	0.53
1:D:961:GLU:OE1	1:D:965:SER:OG	2.25	0.53
1:D:1073:GLN:HB3	1:D:1088:LEU:HD12	1.88	0.53
1:C:525:THR:N	1:C:1036:ARG:HH22	2.07	0.53
1:C:613:ASP:HB2	1:C:617:ARG:NH2	2.22	0.53
1:D:978:PRO:O	1:D:982:LEU:N	2.36	0.53
1:C:524:PRO:HA	1:C:1036:ARG:NH1	2.23	0.53
1:D:523:SER:O	1:D:1036:ARG:NH1	2.38	0.53
1:B:1108:VAL:HG12	1:B:1111:GLN:H	1.74	0.53
1:A:634:ILE:HB	1:A:639:PHE:HZ	1.74	0.53
1:B:994:LEU:HD11	1:B:1002:VAL:HG21	1.90	0.53
1:C:994:LEU:HD22	1:C:997:ARG:HH22	1.74	0.53
1:A:1077:PHE:HE1	1:B:1063:LEU:HD23	1.72	0.53
1:C:677:PHE:HZ	1:C:907:VAL:HG21	1.73	0.53
1:C:1117:PRO:HB3	1:C:1169:GLU:HA	1.91	0.53
1:D:901:LEU:HD23	1:D:960:PRO:HG2	1.91	0.53
1:D:948:LEU:HD13	1:D:964:ARG:HA	1.91	0.53
1:A:631:ARG:NH1	1:A:672:ASP:OD2	2.42	0.52
1:B:877:GLN:NE2	1:D:1145:MET:HE1	2.23	0.52
1:C:1033:LEU:HD11	1:C:1038:PHE:HA	1.92	0.52
1:D:989:ALA:HA	1:D:992:LYS:HE2	1.91	0.52
1:D:1145:MET:SD	1:D:1145:MET:N	2.82	0.52
1:D:1120:VAL:HG21	1:D:1162:VAL:HG11	1.91	0.52
1:A:725:GLY:O	1:A:728:GLU:HG3	2.09	0.52
1:A:1162:VAL:HG13	1:A:1166:MET:HE3	1.89	0.52
1:C:903:ASP:OD1	1:C:903:ASP:N	2.41	0.52
1:B:760:ARG:NH2	1:B:790:GLY:O	2.42	0.52
1:D:724:MET:O	1:D:728:GLU:HG2	2.08	0.52
1:D:1056:LYS:NZ	1:D:1058:LEU:HB3	2.24	0.52
1:A:570:PHE:HE1	1:A:838:TRP:HZ2	1.57	0.52
1:A:740:ILE:O	1:A:771:HIS:N	2.42	0.52
1:A:833:ASP:O	1:A:836:GLU:HG3	2.10	0.52
1:C:910:SER:HA	1:C:913:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:LEU:HB3	1:B:602:PHE:HB2	1.91	0.52
1:D:647:ASN:HB3	1:D:652:THR:O	2.10	0.52
1:D:908:THR:HG22	1:D:912:LYS:HZ2	1.66	0.52
1:D:796:VAL:HA	1:D:807:GLN:HB3	1.92	0.52
1:A:728:GLU:HA	1:A:731:VAL:HG12	1.91	0.52
1:A:729:GLU:HG2	1:A:732:ARG:HH22	1.75	0.52
1:D:544:ILE:O	1:D:548:GLU:N	2.35	0.52
1:D:1060:ILE:HG23	1:D:1085:ARG:HH22	1.74	0.52
1:A:570:PHE:HB2	1:A:604:MET:HE2	1.92	0.51
1:C:739:CYS:SG	1:C:769:HIS:ND1	2.79	0.51
1:D:775:THR:HA	1:D:805:THR:HA	1.92	0.51
1:D:867:PRO:HD2	1:D:870:GLN:HE21	1.74	0.51
1:C:890:VAL:HG22	1:C:922:VAL:HG11	1.91	0.51
1:D:579:ALA:HA	1:D:873:ASN:ND2	2.25	0.51
1:A:505:GLY:HA3	1:A:1089:VAL:HG21	1.93	0.51
1:B:833:ASP:O	1:B:836:GLU:HG3	2.11	0.51
1:D:678:ASP:HB3	1:D:681:ASN:HA	1.93	0.51
1:B:1072:GLY:O	1:B:1091:ASP:N	2.32	0.51
1:C:709:ASP:HB3	1:C:715:ARG:HG3	1.93	0.51
1:C:832:PHE:O	1:C:836:GLU:HG2	2.10	0.51
1:A:849:ASP:OD2	1:D:855:LYS:NZ	2.20	0.51
1:C:508:MET:HE3	1:C:1042:PRO:HD2	1.92	0.51
1:C:1132:ALA:O	1:C:1151:SER:OG	2.26	0.51
1:C:889:GLU:OE1	1:C:889:GLU:N	2.36	0.51
1:D:709:ASP:O	1:D:715:ARG:NH2	2.44	0.51
1:D:774:ASP:N	1:D:806:SER:O	2.39	0.51
1:A:523:SER:O	1:A:1036:ARG:NH2	2.37	0.51
1:A:1095:MET:HE2	1:A:1095:MET:N	2.26	0.51
1:B:728:GLU:HG3	1:B:762:ARG:HH12	1.75	0.51
1:C:683:LEU:HA	1:C:686:MET:HE2	1.93	0.51
1:C:738:LEU:HD11	1:C:768:LEU:HG	1.93	0.51
1:D:530:PRO:HG2	1:D:833:ASP:HB3	1.93	0.51
1:D:555:ARG:O	1:D:559:ASN:ND2	2.44	0.51
1:C:496:ARG:HH11	1:C:499:LYS:HD2	1.76	0.51
1:D:623:PRO:HA	1:D:626:ARG:NE	2.26	0.51
1:D:768:LEU:H	1:D:792:ASP:HB2	1.76	0.51
1:B:1080:LEU:HG	1:B:1081:ASN:H	1.76	0.51
1:A:641:MET:HE2	1:A:674:PHE:HD1	1.75	0.50
1:A:1121:ILE:HG12	1:A:1141:SER:HB3	1.94	0.50
1:A:747:LEU:HD11	1:A:752:CYS:HB2	1.93	0.50
1:C:624:TRP:CD1	1:C:1005:GLU:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:ASN:HB2	1:A:926:LEU:HD23	1.93	0.50
1:B:677:PHE:CZ	1:B:705:SER:HB3	2.46	0.50
1:B:680:LEU:HD23	1:B:682:TYR:HB2	1.94	0.50
1:B:949:GLN:NE2	1:B:973:ARG:HA	2.26	0.50
1:B:1013:TYR:HB3	1:B:1016:VAL:HG22	1.93	0.50
1:A:606:ASN:HD21	1:A:639:PHE:HB3	1.75	0.50
1:D:508:MET:HE2	1:D:508:MET:HA	1.93	0.50
1:C:1023:PHE:O	1:C:1026:THR:OG1	2.28	0.50
1:A:921:MET:HG2	1:A:926:LEU:HD11	1.92	0.50
1:C:993:GLU:HG2	1:C:997:ARG:NH2	2.27	0.50
1:D:899:GLN:HB2	1:D:928:ARG:NH2	2.27	0.50
1:A:836:GLU:HA	1:A:839:GLU:CD	2.36	0.50
1:A:571:ARG:HE	1:A:605:GLU:CD	2.20	0.50
1:B:864:ASN:OD1	1:B:865:GLU:N	2.45	0.50
1:C:613:ASP:OD1	1:C:613:ASP:N	2.44	0.50
1:C:1013:TYR:HB3	1:C:1016:VAL:HG12	1.94	0.50
1:D:814:VAL:HA	1:D:824:THR:HG21	1.94	0.50
1:D:907:VAL:N	1:D:910:SER:OG	2.43	0.50
1:B:987:LEU:H	1:B:987:LEU:HD23	1.77	0.49
1:C:583:ARG:HH21	1:C:1031:ASP:HA	1.78	0.49
1:D:845:TYR:CE1	1:D:1035:THR:HG21	2.47	0.49
1:C:641:MET:HE3	1:C:671:MET:SD	2.52	0.49
1:D:870:GLN:HG3	1:D:874:LEU:HD23	1.93	0.49
1:A:811:GLY:HA2	1:A:828:MET:HE1	1.94	0.49
1:B:607:TRP:NE1	1:B:626:ARG:HH22	2.11	0.49
1:D:1102:PRO:HG2	1:D:1161:HIS:CE1	2.48	0.49
1:D:1117:PRO:HB3	1:D:1169:GLU:HA	1.94	0.49
1:B:1063:LEU:HB2	1:B:1077:PHE:HB2	1.93	0.49
1:C:595:ALA:HB2	1:C:634:ILE:HG13	1.93	0.49
1:B:571:ARG:HH11	1:B:575:GLN:HE22	1.60	0.49
1:B:583:ARG:NH2	1:B:1033:LEU:O	2.45	0.49
1:C:496:ARG:HD2	1:C:1029:PRO:HD2	1.95	0.49
1:C:1132:ALA:HB3	1:C:1135:GLN:HB2	1.94	0.49
1:D:1030:LEU:HG	1:D:1031:ASP:H	1.77	0.49
1:C:607:TRP:HB2	1:C:641:MET:HE1	1.95	0.49
1:C:725:GLY:O	1:C:728:GLU:HG2	2.13	0.49
1:A:1137:LEU:HD13	1:A:1175:LEU:HD22	1.94	0.48
1:A:677:PHE:CE2	1:A:907:VAL:HG11	2.48	0.48
1:A:682:TYR:CE1	1:A:954:VAL:HG12	2.48	0.48
1:A:731:VAL:HG11	1:A:763:PHE:CE1	2.49	0.48
1:B:939:SER:OG	1:D:1148:VAL:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1059:HIS:N	1:B:1081:ASN:OD1	2.46	0.48
1:C:591:ALA:HB1	1:C:634:ILE:HD11	1.95	0.48
1:A:604:MET:O	1:A:640:GLN:N	2.45	0.48
1:B:799:ASP:O	1:B:802:SER:OG	2.29	0.48
1:C:1053:GLU:CD	1:C:1055:GLY:H	2.22	0.48
1:C:1094:ALA:HB1	1:C:1096:LYS:NZ	2.28	0.48
1:D:582:VAL:HA	1:D:845:TYR:CE2	2.48	0.48
1:A:909:PRO:O	1:A:913:ILE:HG12	2.14	0.48
1:B:978:PRO:HA	1:B:981:SER:HB3	1.94	0.48
1:C:1119:LYS:HA	1:C:1167:THR:HA	1.94	0.48
1:D:579:ALA:HB2	1:D:876:PHE:CD2	2.49	0.48
1:D:1059:HIS:CE1	1:D:1081:ASN:HA	2.48	0.48
1:A:577:LEU:O	1:A:872:THR:HG21	2.14	0.48
1:A:907:VAL:CG1	1:A:908:THR:H	2.23	0.48
1:A:1073:GLN:NE2	1:A:1088:LEU:HB3	2.28	0.48
1:B:680:LEU:HD11	1:B:955:PRO:HA	1.95	0.48
1:C:977:ARG:HG2	1:C:980:ALA:H	1.78	0.48
1:C:1061:LYS:O	1:C:1079:GLU:N	2.42	0.48
1:A:581:ARG:HH21	1:A:619:LEU:HG	1.78	0.48
1:A:817:THR:HG22	1:A:823:ASP:HA	1.96	0.48
1:C:760:ARG:NH1	1:C:766:LEU:O	2.35	0.48
1:D:556:ALA:HA	1:D:559:ASN:HD21	1.79	0.48
1:D:678:ASP:CG	1:D:682:TYR:H	2.20	0.48
1:A:581:ARG:NH2	1:A:618:PHE:HB3	2.29	0.48
1:A:593:TYR:O	1:A:597:ASN:ND2	2.39	0.48
1:B:924:ASN:HB3	1:B:926:LEU:HD13	1.95	0.48
1:C:755:LEU:O	1:C:758:SER:OG	2.26	0.48
1:A:607:TRP:HZ3	1:A:612:PHE:HB2	1.79	0.48
1:C:677:PHE:CZ	1:C:907:VAL:HG21	2.48	0.48
1:C:739:CYS:SG	1:C:740:ILE:N	2.87	0.48
1:C:1109:LYS:HD2	1:C:1153:MET:HE3	1.96	0.48
1:A:1169:GLU:HG3	1:A:1172:ASP:OD2	2.14	0.48
1:C:830:ARG:HA	1:C:833:ASP:OD2	2.13	0.48
1:C:1121:ILE:HD11	1:C:1141:SER:HB3	1.95	0.48
1:D:593:TYR:OH	1:D:833:ASP:OD2	2.30	0.48
1:D:617:ARG:HD2	1:D:618:PHE:CE2	2.49	0.48
1:A:836:GLU:HA	1:A:839:GLU:OE2	2.14	0.47
1:A:896:GLU:O	1:A:900:MET:HE2	2.14	0.47
1:C:967:VAL:O	1:C:969:LYS:NZ	2.34	0.47
1:D:585:HIS:O	1:D:589:LYS:HG2	2.14	0.47
1:D:640:GLN:HE21	1:D:675:ARG:HH21	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1058:LEU:HB2	1:D:1081:ASN:HD21	1.79	0.47
1:C:631:ARG:HD2	1:C:639:PHE:CE2	2.49	0.47
1:D:889:GLU:OE2	1:D:892:LYS:HD2	2.14	0.47
1:D:1080:LEU:HD21	1:D:1083:GLN:HB3	1.95	0.47
1:B:701:GLU:HG2	1:B:737:ILE:HB	1.95	0.47
1:B:746:LEU:HD22	1:B:862:TYR:CE1	2.48	0.47
1:B:779:GLY:O	1:B:783:MET:HG2	2.14	0.47
1:B:1059:HIS:ND1	1:B:1081:ASN:OD1	2.41	0.47
1:D:749:PRO:O	1:D:752:CYS:HB3	2.15	0.47
1:A:866:ILE:HD11	1:A:891:LYS:HB2	1.96	0.47
1:D:645:GLY:N	1:D:677:PHE:O	2.47	0.47
1:A:1048:PHE:HB2	1:A:1060:ILE:HG23	1.95	0.47
1:C:657:ASN:OD1	1:C:658:VAL:N	2.47	0.47
1:A:739:CYS:SG	1:A:769:HIS:ND1	2.60	0.47
1:A:1134:GLY:H	1:A:1151:SER:HB3	1.79	0.47
1:C:606:ASN:OD1	1:C:607:TRP:N	2.44	0.47
1:D:538:PRO:HG2	1:D:599:SER:HB2	1.97	0.47
1:D:935:ALA:HB3	1:D:966:LYS:HD3	1.96	0.47
1:D:1052:LEU:HD12	1:D:1053:GLU:N	2.29	0.47
1:A:571:ARG:HD3	1:A:608:GLY:HA3	1.95	0.47
1:A:604:MET:HE3	1:A:605:GLU:O	2.14	0.47
1:B:612:PHE:CD1	1:B:623:PRO:HG2	2.50	0.47
1:C:949:GLN:HE21	1:C:974:VAL:HG23	1.80	0.47
1:C:1070:ARG:NH1	1:C:1071:ALA:HB3	2.29	0.47
1:D:1015:ASP:OD1	1:D:1015:ASP:N	2.48	0.47
1:A:871:TYR:CZ	1:A:887:PHE:HE2	2.33	0.47
1:A:970:ASP:OD1	1:A:970:ASP:N	2.48	0.47
1:A:1099:HIS:O	1:A:1101:HIS:ND1	2.47	0.47
2:A:1900:BTI:HN3	1:C:908:THR:HA	1.80	0.47
1:C:936:GLU:HG2	1:C:966:LYS:HG2	1.97	0.47
1:D:800:SER:HB2	1:D:839:GLU:HB3	1.96	0.47
1:D:1118:GLY:O	1:D:1168:LEU:N	2.46	0.47
1:B:677:PHE:HB2	1:B:703:ALA:HB3	1.95	0.47
1:B:1069:ASN:HD21	1:B:1073:GLN:HB3	1.79	0.46
1:C:518:VAL:HB	1:C:847:ALA:O	2.16	0.46
1:C:1068:LEU:HD23	1:C:1074:ARG:HE	1.79	0.46
1:D:567:ASP:H	1:D:601:LEU:HD21	1.80	0.46
1:D:583:ARG:HG3	1:D:585:HIS:H	1.80	0.46
1:D:909:PRO:O	1:D:913:ILE:HG12	2.15	0.46
1:A:512:PRO:HB3	1:A:1039:LEU:O	2.15	0.46
1:A:647:ASN:HB3	1:A:652:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ASP:N	1:A:771:HIS:O	2.48	0.46
1:A:798:ALA:O	1:A:802:SER:N	2.48	0.46
1:A:1102:PRO:HB2	1:A:1173:LEU:HB3	1.98	0.46
1:D:1119:LYS:HD3	1:D:1167:THR:HG22	1.97	0.46
1:A:1104:ALA:HB2	1:A:1173:LEU:HA	1.98	0.46
1:B:783:MET:HE3	1:B:783:MET:HB3	1.79	0.46
1:C:643:LEU:HD11	1:C:662:PHE:HE2	1.79	0.46
1:D:987:LEU:H	1:D:987:LEU:HD23	1.79	0.46
1:A:945:VAL:O	1:A:949:GLN:HB2	2.14	0.46
1:C:881:MET:HE2	1:C:881:MET:HA	1.97	0.46
1:D:574:HIS:ND1	1:D:582:VAL:HG21	2.30	0.46
1:A:1119:LYS:HA	1:A:1167:THR:HA	1.96	0.46
1:B:653:ASN:ND2	1:B:951:TYR:O	2.20	0.46
1:B:704:ILE:HG13	1:B:738:LEU:HD11	1.98	0.46
1:B:806:SER:OG	1:B:807:GLN:N	2.48	0.46
1:B:1080:LEU:HD23	1:B:1083:GLN:HB2	1.96	0.46
1:C:801:MET:HE2	1:C:801:MET:HA	1.97	0.46
1:C:995:VAL:HA	1:C:999:GLY:HA3	1.97	0.46
1:C:1046:GLU:C	1:C:1061:LYS:HG3	2.41	0.46
1:D:572:ASP:OD2	1:D:771:HIS:NE2	2.49	0.46
1:A:896:GLU:HG2	1:A:921:MET:HE1	1.98	0.46
1:A:941:PRO:HA	1:C:1147:THR:HA	1.98	0.46
1:A:997:ARG:HD2	1:A:998:HIS:HB3	1.97	0.46
1:B:949:GLN:OE1	1:B:974:VAL:N	2.29	0.46
1:A:520:ALA:HB3	1:A:847:ALA:HA	1.96	0.46
1:A:642:LEU:HD13	1:A:675:ARG:CZ	2.45	0.46
1:B:571:ARG:NH1	1:B:575:GLN:HE22	2.13	0.46
1:C:1000:GLU:HG2	1:C:1001:GLU:OE1	2.16	0.46
1:B:1030:LEU:HG	1:B:1031:ASP:H	1.80	0.46
1:C:1114:ALA:H	1:C:1172:ASP:H	1.63	0.46
1:D:754:MET:SD	1:D:755:LEU:N	2.89	0.46
1:A:496:ARG:NH2	1:A:1029:PRO:O	2.49	0.46
1:A:529:VAL:HG22	1:A:837:TYR:HE1	1.80	0.46
1:A:739:CYS:HG	1:A:769:HIS:CE1	2.28	0.46
1:A:964:ARG:NH2	1:A:973:ARG:HB3	2.31	0.46
1:C:709:ASP:OD2	1:C:712:ASP:HB2	2.16	0.46
1:D:964:ARG:HG2	1:D:973:ARG:HH21	1.81	0.46
1:A:850:CYS:SG	1:A:853:THR:OG1	2.60	0.45
1:B:565:LEU:HD23	1:B:566:MET:H	1.81	0.45
1:B:647:ASN:ND2	1:B:650:GLY:O	2.49	0.45
1:D:530:PRO:HB2	1:D:593:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1063:LEU:HB2	1:D:1077:PHE:HB2	1.98	0.45
1:A:570:PHE:CE1	1:A:838:TRP:HZ2	2.34	0.45
1:A:595:ALA:HB2	1:A:634:ILE:HD13	1.97	0.45
1:C:804:MET:HE2	1:C:804:MET:HA	1.96	0.45
1:D:932:GLU:HA	1:D:963:PHE:HE2	1.81	0.45
1:D:1005:GLU:O	1:D:1008:LEU:HG	2.16	0.45
1:A:960:PRO:HB2	1:A:963:PHE:HB3	1.99	0.45
1:C:540:GLY:N	1:C:636:ASN:OD1	2.50	0.45
1:A:683:LEU:O	1:A:687:LEU:HG	2.17	0.45
1:A:1046:GLU:HB2	1:A:1048:PHE:CZ	2.51	0.45
1:B:642:LEU:HA	1:B:675:ARG:HB2	1.98	0.45
1:B:845:TYR:CE1	1:B:1035:THR:HG21	2.50	0.45
1:B:552:GLY:HA2	1:B:555:ARG:HH21	1.81	0.45
1:B:1137:LEU:N	1:B:1149:VAL:O	2.49	0.45
1:A:639:PHE:O	1:A:673:VAL:N	2.34	0.45
1:A:722:TYR:CZ	1:A:726:LEU:HD11	2.52	0.45
1:A:747:LEU:HD12	1:A:748:LYS:N	2.30	0.45
1:A:1133:LYS:NZ	1:A:1152:PRO:O	2.40	0.45
1:A:773:HIS:CD2	1:A:868:GLY:HA3	2.51	0.45
1:A:817:THR:HG21	1:A:822:LEU:HD12	1.98	0.45
1:C:742:ASP:HB3	1:C:772:THR:HA	1.99	0.45
1:C:1033:LEU:HB2	1:C:1037:LEU:HD23	1.98	0.45
1:D:495:ASN:O	1:D:498:GLN:NE2	2.50	0.45
1:D:501:LEU:HD13	1:D:504:LEU:HD12	1.99	0.45
1:A:828:MET:HE2	1:A:828:MET:HA	1.99	0.45
1:C:1105:LEU:N	1:C:1111:GLN:OE1	2.42	0.45
1:D:621:GLU:HG3	1:D:1031:ASP:OD2	2.17	0.45
1:D:865:GLU:OE2	1:D:865:GLU:N	2.50	0.45
1:B:920:PHE:HD2	1:B:921:MET:HE2	1.81	0.45
1:B:1124:LYS:HG3	1:B:1136:PRO:HB2	1.98	0.45
1:C:788:GLN:HG2	1:C:822:LEU:HD11	1.98	0.45
1:C:1051:GLU:HA	1:C:1057:THR:HA	1.99	0.45
1:A:551:GLU:HB3	1:A:555:ARG:HH12	1.81	0.45
1:A:797:ALA:O	1:A:809:SER:HA	2.17	0.45
1:B:769:HIS:NE2	1:B:795:ASP:OD1	2.50	0.45
1:B:1146:GLU:HB2	1:D:942:ARG:HG2	1.98	0.45
1:C:1067:ASP:HA	1:C:1074:ARG:CZ	2.47	0.45
1:D:501:LEU:HD21	1:D:1060:ILE:HG12	1.98	0.45
1:D:760:ARG:NH1	1:D:766:LEU:O	2.49	0.45
1:C:564:LEU:HB3	1:C:602:PHE:HB2	1.99	0.44
1:A:978:PRO:O	1:A:982:LEU:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:LYS:NZ	1:A:1120:VAL:O	2.50	0.44
1:B:1000:GLU:HG2	1:B:1001:GLU:N	2.32	0.44
1:D:636:ASN:OD1	1:D:637:ILE:HD12	2.16	0.44
1:D:676:VAL:HG11	1:D:689:GLY:HA3	2.00	0.44
1:A:850:CYS:HB2	1:A:872:THR:HG22	1.98	0.44
1:B:801:MET:SD	1:B:801:MET:N	2.90	0.44
1:C:898:ASN:O	1:C:902:GLY:N	2.50	0.44
1:D:932:GLU:HA	1:D:963:PHE:CE2	2.52	0.44
1:D:1049:GLU:CD	1:D:1059:HIS:HB3	2.41	0.44
1:D:1095:MET:O	1:D:1096:LYS:HE2	2.18	0.44
1:A:544:ILE:O	1:A:548:GLU:N	2.46	0.44
1:B:563:LEU:HD22	1:B:822:LEU:HB3	1.98	0.44
1:B:926:LEU:HB3	1:B:931:ALA:HB2	1.98	0.44
1:A:908:THR:HG23	2:C:1900:BTI:N3	2.33	0.44
1:B:1083:GLN:HB3	1:B:1085:ARG:HH12	1.81	0.44
1:D:907:VAL:HG12	1:D:908:THR:N	2.31	0.44
1:A:620:TYR:HB2	1:A:1030:LEU:HD12	1.99	0.44
1:A:804:MET:HE1	1:A:856:SER:HA	2.00	0.44
1:A:1129:ALA:H	1:A:1157:VAL:HG22	1.83	0.44
1:B:726:LEU:O	1:B:730:LEU:HD23	2.17	0.44
1:B:1084:LEU:O	1:B:1085:ARG:NH1	2.49	0.44
1:D:926:LEU:HD12	1:D:930:GLU:HB2	1.99	0.44
1:A:1107:ASP:OD1	1:A:1107:ASP:N	2.48	0.44
1:C:1069:ASN:OD1	1:C:1070:ARG:HD3	2.17	0.44
1:C:1141:SER:HB2	1:C:1146:GLU:HG2	2.00	0.44
1:A:617:ARG:HH11	1:C:1143:MET:HE3	1.83	0.44
1:B:896:GLU:OE1	1:B:896:GLU:N	2.44	0.44
1:B:961:GLU:N	1:B:962:PRO:HD2	2.32	0.44
1:D:742:ASP:HB3	1:D:772:THR:HA	1.99	0.44
1:D:836:GLU:O	1:D:839:GLU:HG3	2.18	0.44
1:A:560:HIS:HA	1:A:561:PRO:HD3	1.87	0.43
1:A:639:PHE:N	1:A:672:ASP:HB2	2.30	0.43
1:A:1021:LYS:HA	1:A:1021:LYS:HD2	1.80	0.43
1:B:640:GLN:HE21	1:B:675:ARG:HD2	1.83	0.43
1:B:900:MET:N	1:B:900:MET:HE2	2.33	0.43
1:B:908:THR:HB	1:B:909:PRO:HD3	2.00	0.43
1:B:1058:LEU:HB2	1:B:1081:ASN:HD21	1.82	0.43
1:C:964:ARG:NH1	1:C:973:ARG:HD3	2.32	0.43
1:D:564:LEU:HB3	1:D:602:PHE:HB2	2.00	0.43
1:D:709:ASP:OD1	1:D:709:ASP:N	2.51	0.43
1:C:584:THR:HG21	1:C:626:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ASP:OD1	1:C:656:ASP:N	2.50	0.43
1:C:968:LEU:HB2	1:C:973:ARG:HH21	1.83	0.43
1:C:1103:LYS:HD2	1:C:1172:ASP:OD1	2.18	0.43
1:D:986:ASP:CG	1:D:988:GLN:H	2.26	0.43
1:A:1093:GLN:HA	1:A:1095:MET:HE3	2.00	0.43
1:B:1067:ASP:HA	1:B:1074:ARG:NH1	2.33	0.43
1:B:1169:GLU:HG3	1:B:1172:ASP:OD2	2.18	0.43
1:C:1083:GLN:HG2	1:C:1085:ARG:CZ	2.48	0.43
1:D:708:GLY:HA3	1:D:715:ARG:HH12	1.83	0.43
1:D:833:ASP:O	1:D:836:GLU:HG3	2.18	0.43
1:D:1114:ALA:H	1:D:1172:ASP:N	2.16	0.43
1:B:859:SER:OG	1:B:860:ASP:N	2.52	0.43
1:B:1036:ARG:HG3	1:B:1037:LEU:N	2.33	0.43
1:D:1015:ASP:O	1:D:1019:HIS:ND1	2.51	0.43
1:A:525:THR:H	1:A:1036:ARG:HH22	1.65	0.43
1:A:799:ASP:OD1	1:A:809:SER:HB2	2.19	0.43
1:B:603:SER:OG	1:B:640:GLN:OE1	2.31	0.43
1:B:903:ASP:N	1:B:903:ASP:OD1	2.50	0.43
1:B:1042:PRO:HB3	1:B:1048:PHE:CE1	2.54	0.43
1:B:1141:SER:HB2	1:B:1146:GLU:OE1	2.18	0.43
1:C:771:HIS:HA	1:C:795:ASP:CG	2.43	0.43
1:D:797:ALA:HB2	1:D:807:GLN:HB2	2.01	0.43
1:D:945:VAL:O	1:D:949:GLN:HB2	2.18	0.43
1:D:1095:MET:HG3	1:D:1097:GLU:H	1.83	0.43
1:B:917:LEU:O	1:B:921:MET:HG2	2.18	0.43
1:C:590:ILE:HD11	1:C:837:TYR:CE1	2.53	0.43
1:D:583:ARG:NH2	1:D:1031:ASP:HA	2.30	0.43
1:D:1132:ALA:HB3	1:D:1135:GLN:NE2	2.34	0.43
1:B:632:GLU:OE1	1:B:632:GLU:N	2.46	0.43
1:B:952:ILE:HD12	1:B:952:ILE:H	1.83	0.43
1:C:574:HIS:HB3	1:C:580:THR:HA	2.01	0.43
1:D:543:ASP:OD1	1:D:544:ILE:N	2.52	0.43
1:D:641:MET:O	1:D:675:ARG:HG2	2.19	0.43
1:D:726:LEU:HA	1:D:729:GLU:OE2	2.19	0.43
1:D:1104:ALA:HB1	1:D:1111:GLN:HG3	2.01	0.43
1:B:863:GLU:OE1	1:B:863:GLU:N	2.52	0.43
1:A:1134:GLY:N	1:A:1151:SER:HB3	2.33	0.43
1:B:617:ARG:HD2	1:B:618:PHE:CZ	2.54	0.43
1:D:623:PRO:O	1:D:626:ARG:HD3	2.19	0.43
1:A:678:ASP:CB	1:A:686:MET:HE3	2.45	0.43
1:A:682:TYR:CD1	1:A:954:VAL:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:LEU:HD13	1:A:1085:ARG:HG3	2.00	0.43
1:A:1174:ILE:C	1:A:1175:LEU:HD12	2.44	0.43
1:B:964:ARG:HG3	1:B:968:LEU:HD12	2.01	0.43
1:B:995:VAL:HA	1:B:999:GLY:HA3	2.01	0.43
1:B:1066:SER:O	1:B:1074:ARG:NH1	2.52	0.43
1:C:543:ASP:OD1	1:C:543:ASP:N	2.49	0.43
1:C:657:ASN:O	1:C:661:LYS:HE3	2.19	0.43
1:C:681:ASN:O	1:C:683:LEU:HD12	2.19	0.43
1:D:913:ILE:HD12	1:D:943:SER:HB3	2.01	0.43
1:A:517:PRO:HA	1:A:879:HIS:CD2	2.54	0.42
1:A:686:MET:O	1:A:690:MET:HB2	2.19	0.42
1:A:720:LEU:HD11	1:A:724:MET:HE3	2.00	0.42
1:B:799:ASP:OD1	1:B:809:SER:HB2	2.19	0.42
1:B:867:PRO:O	1:B:870:GLN:NE2	2.29	0.42
1:B:906:LYS:HA	1:B:910:SER:OG	2.19	0.42
1:C:994:LEU:HD13	1:C:997:ARG:NH1	2.33	0.42
1:B:1130:LYS:HA	1:B:1156:THR:HA	2.01	0.42
1:D:641:MET:SD	1:D:643:LEU:HB2	2.60	0.42
1:D:1036:ARG:O	1:D:1040:GLN:HG3	2.20	0.42
1:D:1091:ASP:OD1	1:D:1092:THR:N	2.52	0.42
1:A:754:MET:SD	1:A:755:LEU:N	2.92	0.42
1:A:1100:PHE:CG	1:A:1101:HIS:N	2.87	0.42
1:C:527:PRO:HG3	1:C:840:GLY:C	2.45	0.42
1:D:558:ARG:HA	1:D:558:ARG:HD2	1.84	0.42
1:D:871:TYR:O	1:D:874:LEU:HG	2.19	0.42
1:D:1162:VAL:HG13	1:D:1166:MET:SD	2.59	0.42
1:A:662:PHE:HB2	1:A:1008:LEU:HD11	2.01	0.42
1:A:743:MET:N	1:A:743:MET:SD	2.93	0.42
1:A:1158:ARG:CZ	1:A:1178:GLU:HG3	2.49	0.42
1:B:1000:GLU:OE1	1:B:1000:GLU:N	2.52	0.42
1:B:1149:VAL:HG11	1:B:1174:ILE:HD11	2.01	0.42
1:C:571:ARG:NH1	1:C:572:ASP:OD1	2.53	0.42
1:C:775:THR:HA	1:C:804:MET:O	2.19	0.42
1:C:1043:LYS:HG3	1:C:1046:GLU:HG2	2.01	0.42
1:D:787:ALA:HA	1:D:791:ALA:HB3	2.02	0.42
1:D:800:SER:C	1:D:801:MET:HE2	2.44	0.42
1:D:949:GLN:NE2	1:D:974:VAL:H	2.18	0.42
1:D:1132:ALA:HB3	1:D:1135:GLN:CD	2.44	0.42
1:B:1137:LEU:HD11	1:B:1151:SER:HA	2.02	0.42
1:A:1129:ALA:H	1:A:1157:VAL:CG2	2.32	0.42
1:B:655:PRO:HB2	1:B:658:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:949:GLN:HG2	1:D:972:PRO:O	2.18	0.42
1:D:1112:ILE:HB	1:D:1175:LEU:O	2.19	0.42
1:C:537:PRO:HA	1:C:596:HIS:CD2	2.54	0.42
1:A:507:VAL:HG12	1:A:508:MET:HE2	2.02	0.42
1:A:918:ALA:HA	1:A:921:MET:CE	2.50	0.42
1:A:1114:ALA:H	1:A:1172:ASP:H	1.67	0.42
1:B:522:PRO:HB3	1:B:844:LEU:O	2.19	0.42
1:B:644:ARG:CZ	1:B:908:THR:HG21	2.50	0.42
1:C:586:ASP:OD1	1:C:586:ASP:N	2.51	0.42
1:D:1063:LEU:HD11	1:D:1079:GLU:HB2	2.01	0.42
1:A:529:VAL:HG22	1:A:837:TYR:CE1	2.54	0.42
1:A:1108:VAL:HG12	1:A:1111:GLN:H	1.85	0.42
1:B:600:LYS:NZ	1:B:825:GLU:O	2.47	0.42
1:B:1117:PRO:HA	1:B:1169:GLU:HA	2.02	0.42
1:C:751:ALA:O	1:C:754:MET:HG3	2.19	0.42
1:D:550:PRO:HB2	1:D:736:HIS:HE2	1.85	0.42
1:D:1043:LYS:HE2	1:D:1043:LYS:HA	2.02	0.42
1:A:630:LEU:HD23	1:A:630:LEU:HA	1.92	0.42
1:B:1047:GLU:OE2	1:B:1059:HIS:HB3	2.20	0.42
1:C:584:THR:C	1:C:588:LYS:HZ2	2.27	0.42
1:D:607:TRP:CE3	1:D:627:LEU:HD13	2.55	0.42
1:D:682:TYR:HD2	1:D:685:ASN:CG	2.28	0.42
1:D:741:LYS:HG3	1:D:771:HIS:CD2	2.55	0.42
1:A:726:LEU:O	1:A:730:LEU:HD23	2.20	0.41
1:B:1022:ASP:O	1:B:1026:THR:OG1	2.31	0.41
1:C:612:PHE:CE1	1:C:623:PRO:HB3	2.55	0.41
1:A:570:PHE:HB2	1:A:604:MET:CE	2.49	0.41
1:A:720:LEU:O	1:A:724:MET:HG2	2.19	0.41
1:A:904:LEU:H	1:A:904:LEU:HD23	1.85	0.41
1:A:1135:GLN:NE2	1:A:1137:LEU:HB3	2.33	0.41
1:A:1161:HIS:HD2	1:A:1174:ILE:C	2.28	0.41
1:C:533:PRO:HG2	1:C:596:HIS:CG	2.55	0.41
1:C:728:GLU:HA	1:C:731:VAL:HG12	2.02	0.41
1:C:926:LEU:HD23	1:C:926:LEU:H	1.85	0.41
1:C:994:LEU:HA	1:C:997:ARG:NH1	2.34	0.41
1:A:820:THR:HG22	1:A:822:LEU:H	1.85	0.41
1:A:893:ALA:HA	1:A:896:GLU:OE2	2.20	0.41
1:A:964:ARG:HH21	1:A:973:ARG:HB3	1.85	0.41
1:B:660:PHE:CE1	1:B:692:ALA:HA	2.55	0.41
1:C:537:PRO:HA	1:C:596:HIS:HD2	1.85	0.41
1:C:1127:ALA:HB1	1:C:1159:LYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:HIS:CD2	1:A:574:HIS:H	2.39	0.41
1:A:917:LEU:HD23	1:A:921:MET:HE2	2.03	0.41
1:A:918:ALA:HA	1:A:921:MET:HE3	2.01	0.41
2:C:1900:BTI:O11	2:C:1900:BTI:H72	2.20	0.41
1:A:604:MET:HE3	1:A:605:GLU:H	1.84	0.41
1:A:660:PHE:HZ	1:A:691:GLU:HG3	1.85	0.41
1:B:647:ASN:HB3	1:B:652:THR:O	2.21	0.41
1:B:810:MET:HE3	1:B:810:MET:HA	2.03	0.41
1:C:947:PHE:HD1	1:C:952:ILE:HD11	1.84	0.41
1:C:959:PHE:HE2	1:C:964:ARG:HE	1.68	0.41
1:C:1094:ALA:HB1	1:C:1096:LYS:HZ2	1.85	0.41
1:C:1101:HIS:CE1	1:C:1168:LEU:HD21	2.55	0.41
1:D:586:ASP:OD1	1:D:587:LEU:N	2.53	0.41
1:D:682:TYR:CD2	1:D:684:PRO:HD2	2.55	0.41
1:D:726:LEU:HA	1:D:729:GLU:CD	2.45	0.41
1:D:991:GLU:O	1:D:994:LEU:HG	2.21	0.41
1:D:1107:ASP:OD1	1:D:1108:VAL:N	2.52	0.41
1:A:1068:LEU:HD22	1:A:1072:GLY:HA2	2.03	0.41
1:B:728:GLU:OE1	1:B:762:ARG:NH1	2.54	0.41
1:B:767:PRO:HA	1:B:792:ASP:OD2	2.21	0.41
1:B:1144:LYS:HE3	1:D:617:ARG:NH2	2.36	0.41
1:C:828:MET:SD	1:C:828:MET:N	2.91	0.41
1:C:1068:LEU:CD2	1:C:1074:ARG:HE	2.33	0.41
1:D:760:ARG:HD3	1:D:768:LEU:HD13	2.03	0.41
1:A:499:LYS:HD3	1:A:1028:GLY:N	2.35	0.41
1:A:678:ASP:OD1	1:A:678:ASP:N	2.52	0.41
1:A:701:GLU:OE2	1:A:737:ILE:HB	2.21	0.41
1:A:888:LYS:HA	1:A:891:LYS:NZ	2.35	0.41
1:C:743:MET:SD	1:C:743:MET:N	2.93	0.41
1:C:796:VAL:HG13	1:C:810:MET:HE1	2.01	0.41
1:D:607:TRP:HB3	1:D:641:MET:HA	2.03	0.41
1:D:948:LEU:O	1:D:964:ARG:NE	2.54	0.41
1:A:709:ASP:OD1	1:A:709:ASP:N	2.54	0.41
1:A:799:ASP:HB2	1:A:835:SER:OG	2.21	0.41
1:B:908:THR:HA	2:D:1900:BTI:HN3	1.85	0.41
1:C:724:MET:HE1	1:C:759:LEU:HD22	2.03	0.41
1:C:1084:LEU:O	1:C:1085:ARG:HD3	2.21	0.41
1:D:936:GLU:HB2	1:D:969:LYS:HE2	2.02	0.41
1:A:723:TYR:HA	1:A:726:LEU:HD12	2.03	0.41
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.90	0.41
1:A:1117:PRO:HB3	1:A:1169:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1900:BTI:H93	2:A:1900:BTI:H2	1.83	0.41
1:B:501:LEU:HD22	1:B:1078:PHE:HD2	1.86	0.41
1:B:544:ILE:O	1:B:548:GLU:N	2.46	0.41
1:B:579:ALA:O	1:B:580:THR:OG1	2.35	0.41
1:B:656:ASP:OD1	1:B:656:ASP:N	2.52	0.41
1:B:725:GLY:O	1:B:729:GLU:HG3	2.21	0.41
1:B:1125:VAL:HG21	1:B:1131:VAL:HG22	2.03	0.41
2:B:1900:BTI:O3	1:D:908:THR:CG2	2.51	0.41
1:C:1075:GLN:HA	1:C:1087:ILE:O	2.21	0.41
1:D:577:LEU:O	1:D:872:THR:HG21	2.21	0.41
1:D:626:ARG:NH1	1:D:627:LEU:HB2	2.35	0.41
1:A:726:LEU:HA	1:A:729:GLU:OE1	2.21	0.41
1:A:970:ASP:O	1:A:971:LEU:HD12	2.21	0.41
1:A:1017:PHE:O	1:A:1021:LYS:HG2	2.21	0.41
1:D:709:ASP:H	1:D:715:ARG:HH22	1.69	0.41
1:A:905:ILE:HG22	1:A:907:VAL:HG23	2.02	0.40
1:A:1162:VAL:HG21	1:A:1168:LEU:HD21	2.03	0.40
1:B:508:MET:HE3	1:B:1042:PRO:HD2	2.03	0.40
1:B:565:LEU:HD21	1:B:810:MET:HE1	2.02	0.40
1:B:709:ASP:OD2	1:B:712:ASP:HB2	2.20	0.40
1:C:497:ALA:O	1:C:501:LEU:HG	2.20	0.40
1:C:629:GLU:O	1:C:633:LEU:HD23	2.21	0.40
1:D:639:PHE:H	1:D:672:ASP:HB2	1.85	0.40
1:D:683:LEU:HA	1:D:686:MET:HG3	2.01	0.40
1:D:1006:ASP:HB2	1:D:1017:PHE:CZ	2.56	0.40
1:A:657:ASN:O	1:A:661:LYS:HD3	2.21	0.40
1:B:1131:VAL:HG11	1:B:1137:LEU:HD21	2.02	0.40
1:C:504:LEU:HD23	1:C:504:LEU:HA	1.87	0.40
1:C:506:HIS:HA	1:C:1089:VAL:HG11	2.03	0.40
1:C:626:ARG:O	1:C:630:LEU:HD23	2.20	0.40
1:C:653:ASN:HD22	1:C:978:PRO:HB2	1.86	0.40
1:D:570:PHE:C	1:D:574:HIS:HD2	2.29	0.40
1:D:657:ASN:OD1	1:D:657:ASN:N	2.51	0.40
1:D:968:LEU:HB2	1:D:973:ARG:NH2	2.36	0.40
1:A:1080:LEU:N	1:A:1083:GLN:O	2.54	0.40
1:B:827:PRO:HD2	1:B:830:ARG:NH2	2.37	0.40
1:B:1095:MET:SD	1:B:1095:MET:N	2.95	0.40
1:C:499:LYS:HB3	1:C:1027:PHE:C	2.46	0.40
1:C:724:MET:HE1	1:C:759:LEU:CD2	2.51	0.40
1:C:804:MET:HE1	1:C:856:SER:C	2.47	0.40
1:D:607:TRP:CZ3	1:D:627:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:768:LEU:O	1:D:793:VAL:N	2.48	0.40
1:A:595:ALA:HB2	1:A:634:ILE:CD1	2.51	0.40
1:A:876:PHE:HD2	1:A:877:GLN:HE22	1.69	0.40
1:A:1067:ASP:HA	1:A:1074:ARG:CZ	2.51	0.40
1:B:509:VAL:HG21	1:B:1089:VAL:HB	2.04	0.40
1:B:881:MET:HA	1:B:881:MET:HE2	2.04	0.40
1:B:964:ARG:CG	1:B:968:LEU:HD12	2.51	0.40
1:B:1063:LEU:HD13	1:B:1077:PHE:C	2.46	0.40
1:C:581:ARG:NH1	1:C:618:PHE:HD2	2.19	0.40
1:D:746:LEU:HD21	1:D:861:VAL:HG12	2.03	0.40
1:D:899:GLN:HB2	1:D:928:ARG:HH22	1.86	0.40
1:A:558:ARG:NH2	1:A:764:PRO:O	2.49	0.40
1:A:835:SER:O	1:A:839:GLU:OE1	2.39	0.40
1:B:497:ALA:O	1:B:500:LEU:HG	2.22	0.40
1:C:906:LYS:HA	1:C:910:SER:OG	2.22	0.40
1:C:994:LEU:HA	1:C:997:ARG:HH12	1.87	0.40
1:C:1065:VAL:HG22	1:C:1066:SER:O	2.20	0.40
1:C:1095:MET:N	1:C:1095:MET:SD	2.94	0.40
1:D:584:THR:O	1:D:588:LYS:HG3	2.21	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	682/1178 (58%)	637 (93%)	45 (7%)	0	100	100
1	B	682/1178 (58%)	612 (90%)	70 (10%)	0	100	100
1	C	682/1178 (58%)	622 (91%)	59 (9%)	1 (0%)	48	80
1	D	682/1178 (58%)	632 (93%)	50 (7%)	0	100	100
All	All	2728/4712 (58%)	2503 (92%)	224 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	804	MET

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	564/968 (58%)	564 (100%)	0	100	100
1	B	564/968 (58%)	564 (100%)	0	100	100
1	C	564/968 (58%)	564 (100%)	0	100	100
1	D	564/968 (58%)	564 (100%)	0	100	100
All	All	2256/3872 (58%)	2256 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	653	ASN
1	A	669	ASN
1	A	877	GLN
1	A	923	GLN
1	A	924	ASN
1	A	1075	GLN
1	A	1135	GLN
1	B	575	GLN
1	B	998	HIS
1	C	510	ASN
1	C	574	HIS
1	C	575	GLN
1	C	653	ASN
1	C	721	GLN
1	C	899	GLN
1	C	1019	HIS
1	D	559	ASN

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Mol	Chain	Res	Type
1	D	574	HIS
1	D	870	GLN
1	D	934	GLN
1	D	949	GLN
1	D	1040	GLN
1	D	1059	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	BTI	B	1900	1	15,16,16	6.43	11 (73%)	20,21,21	3.01	7 (35%)
2	BTI	D	1900	1	15,16,16	6.43	11 (73%)	20,21,21	2.87	9 (45%)
2	BTI	C	1900	1	15,16,16	6.45	11 (73%)	20,21,21	3.23	11 (55%)
2	BTI	A	1900	1	15,16,16	6.45	11 (73%)	20,21,21	2.94	11 (55%)

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
2	BTI	B	1900	1	-	4/6/27/27	0/2/2/2
2	BTI	D	1900	1	-	3/6/27/27	0/2/2/2
2	BTI	C	1900	1	-	4/6/27/27	0/2/2/2
2	BTI	A	1900	1	-	4/6/27/27	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1900	BTI	C6-S1	-13.26	1.44	1.81
2	D	1900	BTI	C6-S1	-13.18	1.44	1.81
2	C	1900	BTI	C6-S1	-13.16	1.44	1.81
2	B	1900	BTI	C6-S1	-13.16	1.44	1.81
2	B	1900	BTI	C3-N3	12.48	1.58	1.35
2	D	1900	BTI	C3-N3	12.46	1.58	1.35
2	A	1900	BTI	C3-N3	12.42	1.58	1.35
2	C	1900	BTI	C3-N3	12.28	1.57	1.35
2	B	1900	BTI	C3-N2	8.80	1.51	1.35
2	A	1900	BTI	C3-N2	8.78	1.51	1.35
2	D	1900	BTI	C3-N2	8.78	1.51	1.35
2	C	1900	BTI	C3-N2	8.74	1.51	1.35
2	C	1900	BTI	C5-N3	-8.38	1.33	1.46
2	A	1900	BTI	C5-N3	-8.15	1.34	1.46
2	B	1900	BTI	C5-N3	-8.10	1.34	1.46
2	D	1900	BTI	C5-N3	-8.05	1.34	1.46
2	C	1900	BTI	C2-S1	-7.68	1.70	1.82
2	A	1900	BTI	C2-S1	-7.63	1.70	1.82
2	D	1900	BTI	C2-S1	-7.56	1.70	1.82
2	B	1900	BTI	C2-S1	-7.54	1.70	1.82
2	C	1900	BTI	C6-C5	5.62	1.65	1.53
2	A	1900	BTI	C6-C5	5.60	1.64	1.53
2	B	1900	BTI	C6-C5	5.59	1.64	1.53
2	D	1900	BTI	C6-C5	5.52	1.64	1.53
2	D	1900	BTI	C7-C2	3.83	1.62	1.52
2	D	1900	BTI	C4-N2	-3.82	1.38	1.45
2	A	1900	BTI	C4-N2	-3.81	1.38	1.45
2	B	1900	BTI	C7-C2	3.80	1.62	1.52
2	C	1900	BTI	C4-N2	-3.78	1.38	1.45
2	A	1900	BTI	C7-C2	3.74	1.62	1.52
2	A	1900	BTI	C2-C4	-3.70	1.43	1.53
2	C	1900	BTI	C7-C2	3.70	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1900	BTI	C2-C4	-3.68	1.43	1.53
2	B	1900	BTI	C4-N2	-3.67	1.39	1.45
2	B	1900	BTI	C2-C4	-3.63	1.43	1.53
2	D	1900	BTI	C2-C4	-3.63	1.43	1.53
2	D	1900	BTI	C5-C4	3.27	1.65	1.55
2	B	1900	BTI	C5-C4	3.25	1.65	1.55
2	C	1900	BTI	C5-C4	3.23	1.65	1.55
2	A	1900	BTI	C5-C4	3.20	1.64	1.55
2	C	1900	BTI	O3-C3	-2.32	1.18	1.23
2	A	1900	BTI	O3-C3	-2.20	1.18	1.23
2	D	1900	BTI	O3-C3	-2.20	1.18	1.23
2	B	1900	BTI	O3-C3	-2.18	1.18	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	BTI	C6-S1-C2	7.98	106.58	89.98
2	D	1900	BTI	C6-S1-C2	7.39	105.34	89.98
2	C	1900	BTI	C6-S1-C2	6.97	104.48	89.98
2	A	1900	BTI	C6-S1-C2	6.72	103.96	89.98
2	C	1900	BTI	C8-C7-C2	-5.88	100.52	114.04
2	C	1900	BTI	C4-C5-N3	5.36	108.38	102.43
2	D	1900	BTI	C4-C5-N3	5.33	108.35	102.43
2	A	1900	BTI	C4-C5-N3	5.14	108.13	102.43
2	B	1900	BTI	C4-C5-N3	5.06	108.05	102.43
2	A	1900	BTI	C5-C4-N2	4.93	108.25	102.68
2	B	1900	BTI	C5-C4-N2	4.92	108.23	102.68
2	C	1900	BTI	C5-C4-N2	4.80	108.09	102.68
2	D	1900	BTI	C5-C4-N2	4.76	108.05	102.68
2	C	1900	BTI	O11-C11-C10	-4.16	91.49	126.30
2	C	1900	BTI	C4-N2-C3	-4.04	107.55	112.56
2	B	1900	BTI	O11-C11-C10	-3.98	92.99	126.30
2	A	1900	BTI	C4-N2-C3	-3.89	107.72	112.56
2	B	1900	BTI	C4-N2-C3	-3.88	107.75	112.56
2	D	1900	BTI	C4-N2-C3	-3.81	107.83	112.56
2	A	1900	BTI	O11-C11-C10	-3.21	99.42	126.30
2	D	1900	BTI	C5-N3-C3	-3.13	107.78	112.38
2	C	1900	BTI	C5-N3-C3	-3.10	107.83	112.38
2	A	1900	BTI	C8-C7-C2	-3.05	107.03	114.04
2	D	1900	BTI	O11-C11-C10	-2.98	101.36	126.30
2	A	1900	BTI	C5-N3-C3	-2.95	108.04	112.38
2	C	1900	BTI	C6-C5-N3	-2.91	109.43	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	BTI	C5-N3-C3	-2.87	108.17	112.38
2	A	1900	BTI	C2-C4-C5	-2.71	105.58	108.89
2	C	1900	BTI	C2-C4-C5	-2.36	106.01	108.89
2	C	1900	BTI	C6-C5-C4	-2.29	105.44	109.06
2	A	1900	BTI	C6-C5-N3	-2.26	110.27	113.18
2	C	1900	BTI	C9-C8-C7	-2.24	105.19	113.62
2	D	1900	BTI	C2-C4-N2	-2.23	110.98	113.34
2	A	1900	BTI	C6-C5-C4	-2.20	105.58	109.06
2	B	1900	BTI	C4-C2-S1	2.12	107.44	105.03
2	D	1900	BTI	C6-C5-C4	-2.10	105.74	109.06
2	A	1900	BTI	C2-C4-N2	-2.06	111.16	113.34
2	D	1900	BTI	C2-C4-C5	-2.06	106.38	108.89

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1900	BTI	C9-C10-C11-O11
2	A	1900	BTI	S1-C2-C7-C8
2	A	1900	BTI	C4-C2-C7-C8
2	B	1900	BTI	C9-C10-C11-O11
2	B	1900	BTI	C4-C2-C7-C8
2	C	1900	BTI	C9-C10-C11-O11
2	C	1900	BTI	C7-C8-C9-C10
2	B	1900	BTI	S1-C2-C7-C8
2	C	1900	BTI	C4-C2-C7-C8
2	B	1900	BTI	C7-C8-C9-C10
2	D	1900	BTI	C2-C7-C8-C9
2	C	1900	BTI	C2-C7-C8-C9
2	A	1900	BTI	C7-C8-C9-C10
2	D	1900	BTI	C4-C2-C7-C8
2	D	1900	BTI	C11-C10-C9-C8

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1900	BTI	11	0
2	D	1900	BTI	1	0
2	C	1900	BTI	3	0
2	A	1900	BTI	2	0

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.

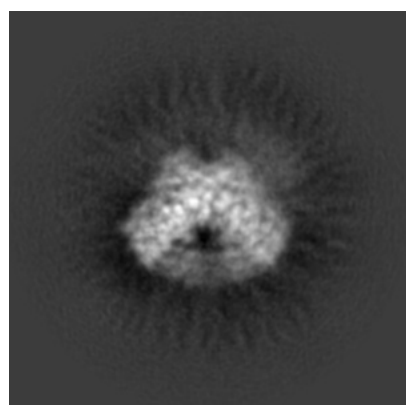
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32773. These allow visual inspection of the internal detail of the map and identification of artifacts.

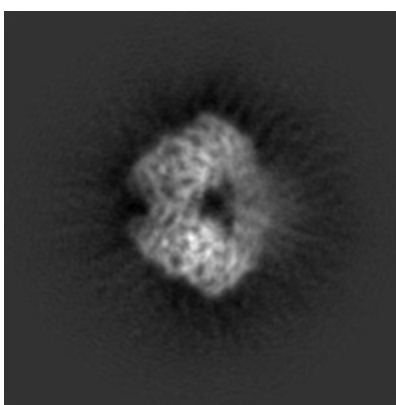
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

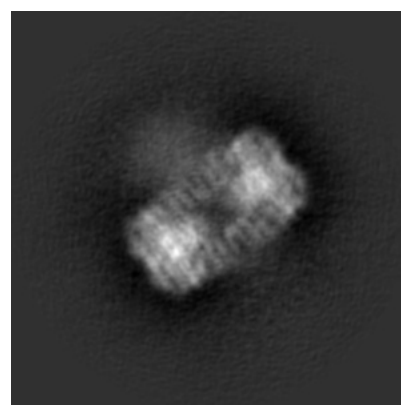
6.1.1 Primary map



X



Y

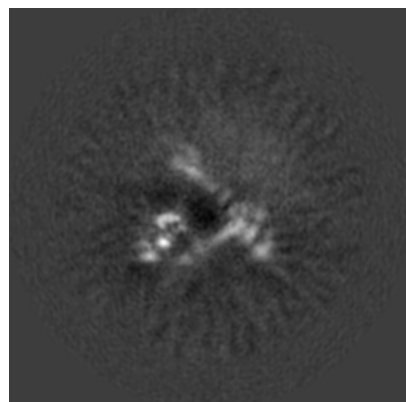


Z

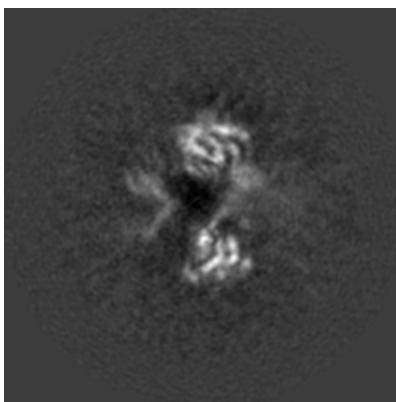
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

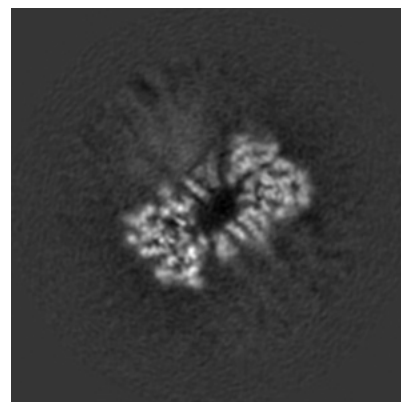
6.2.1 Primary map



X Index: 144



Y Index: 144

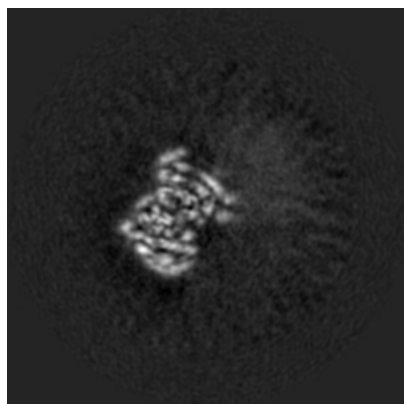


Z Index: 144

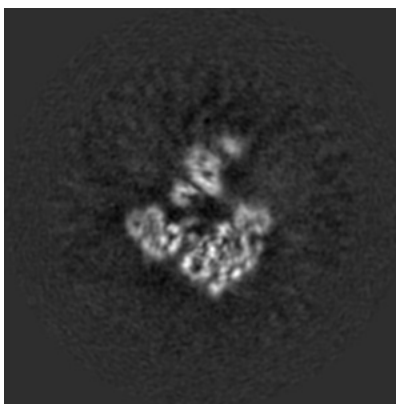
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

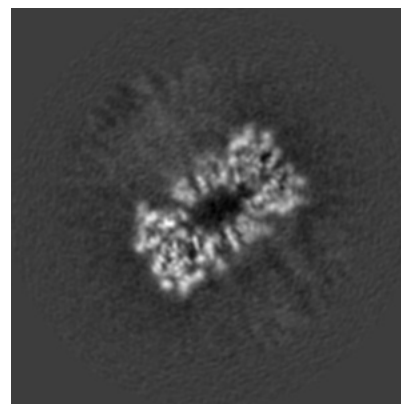
6.3.1 Primary map



X Index: 118



Y Index: 128

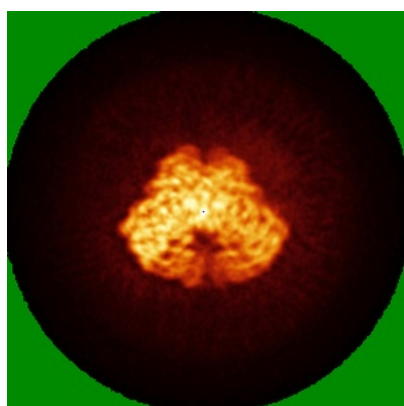


Z Index: 136

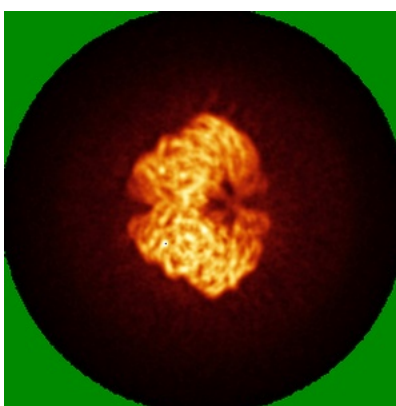
The images above show the largest variance slices of the map in three orthogonal directions.

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

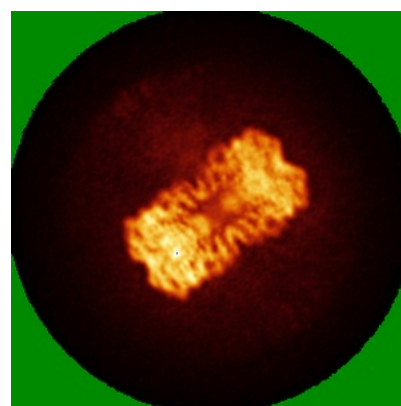
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

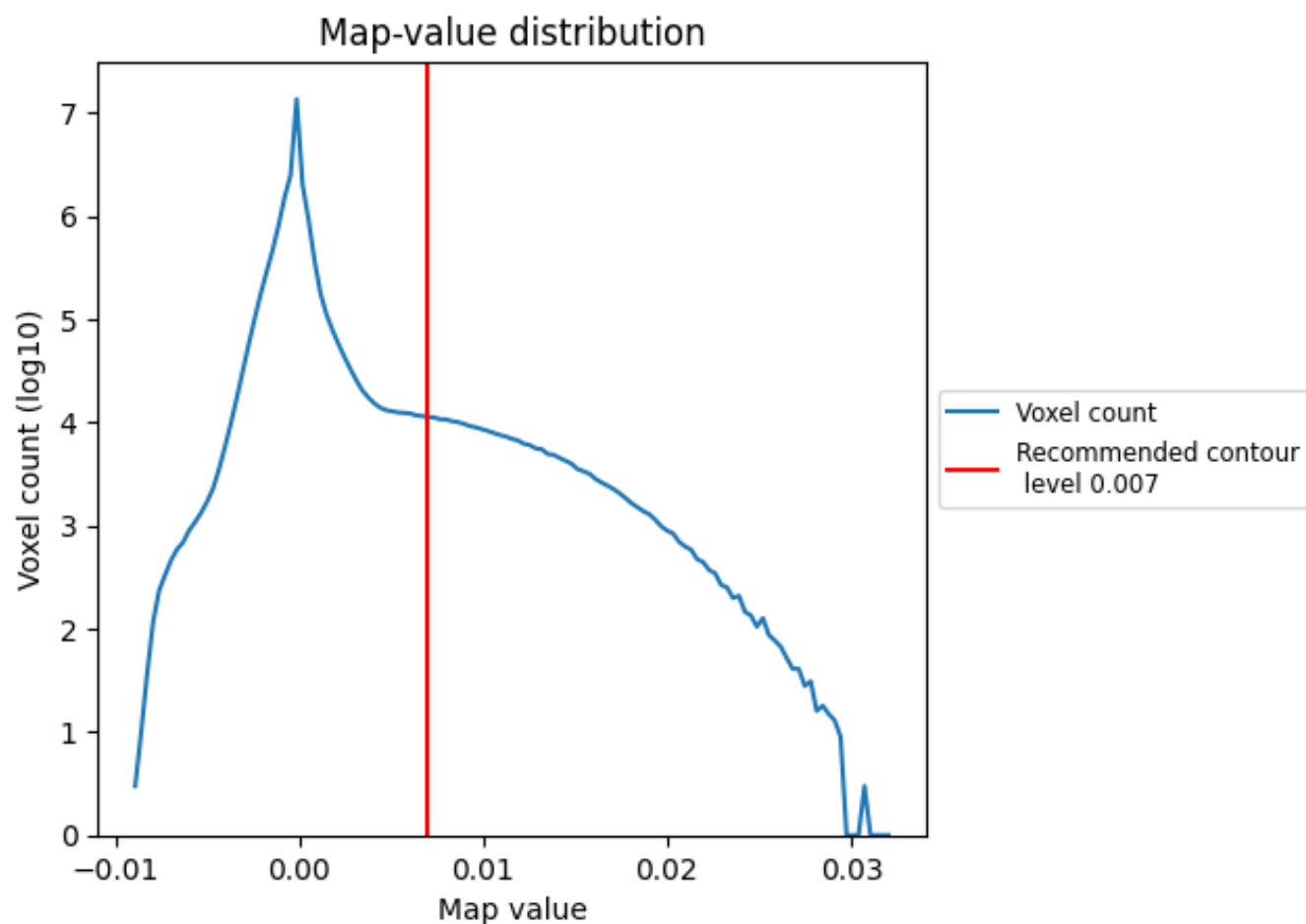
6.6 Mask visualisation

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

7 Map analysis [i](#)

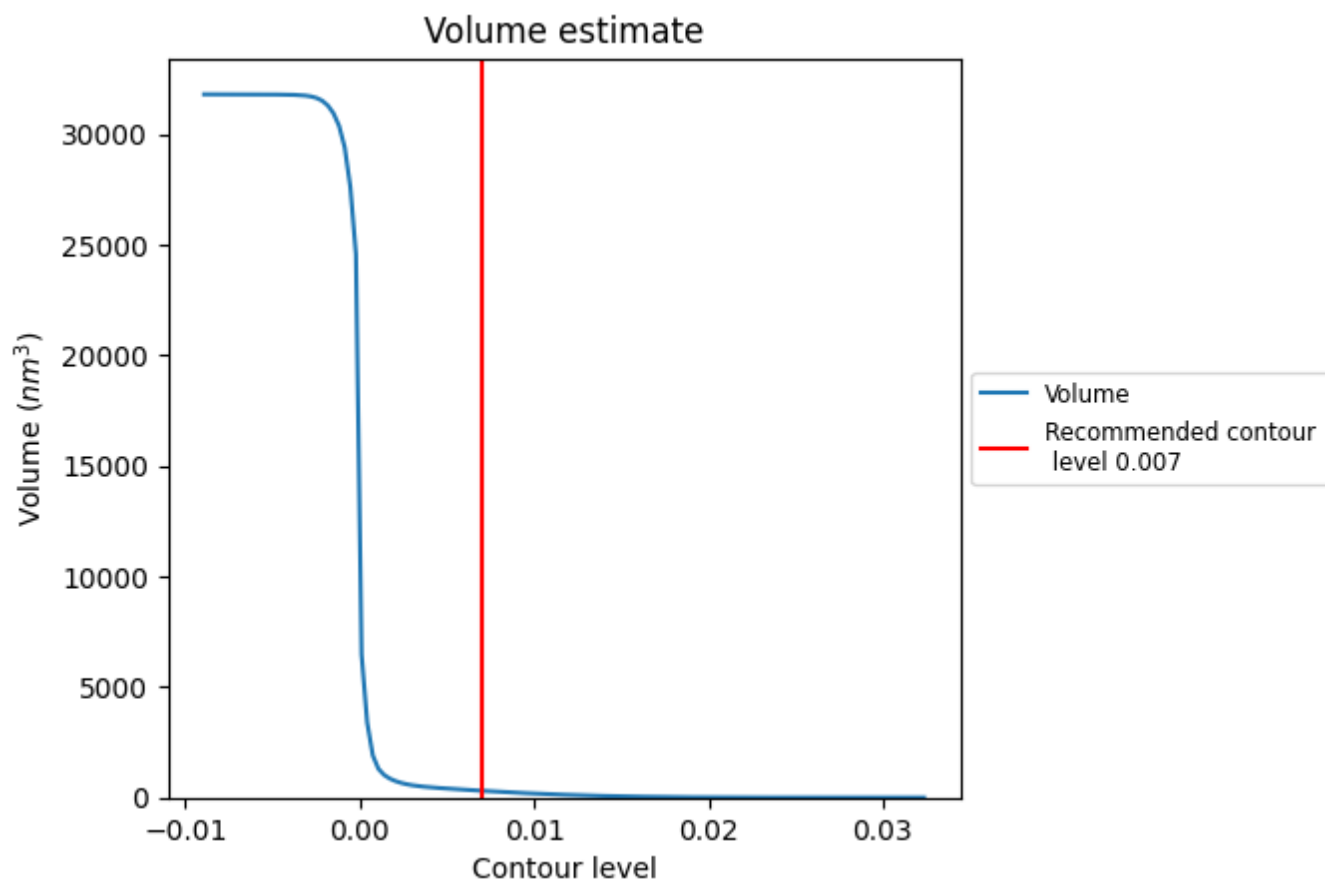
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

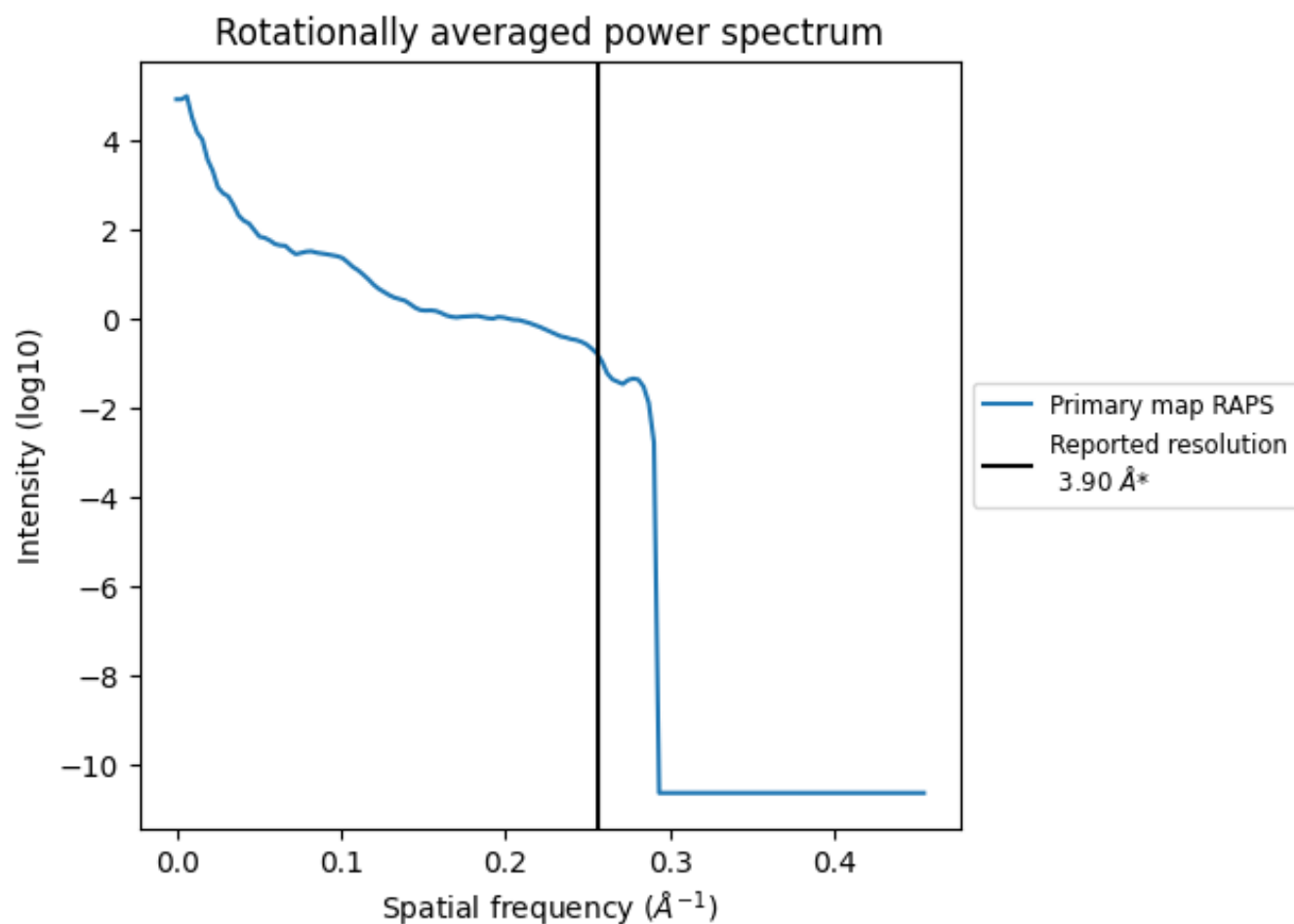
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 278 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 0.256 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

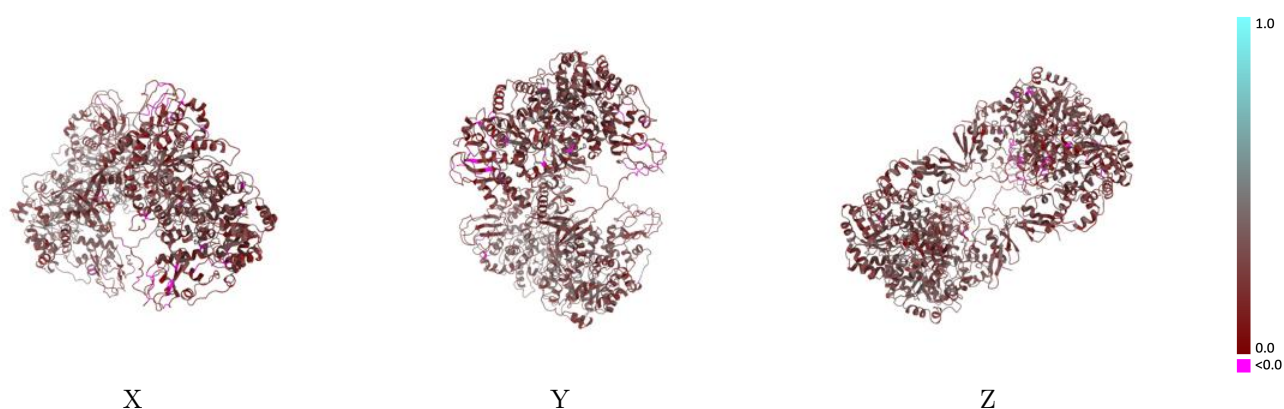
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32773 and PDB model 7WTA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

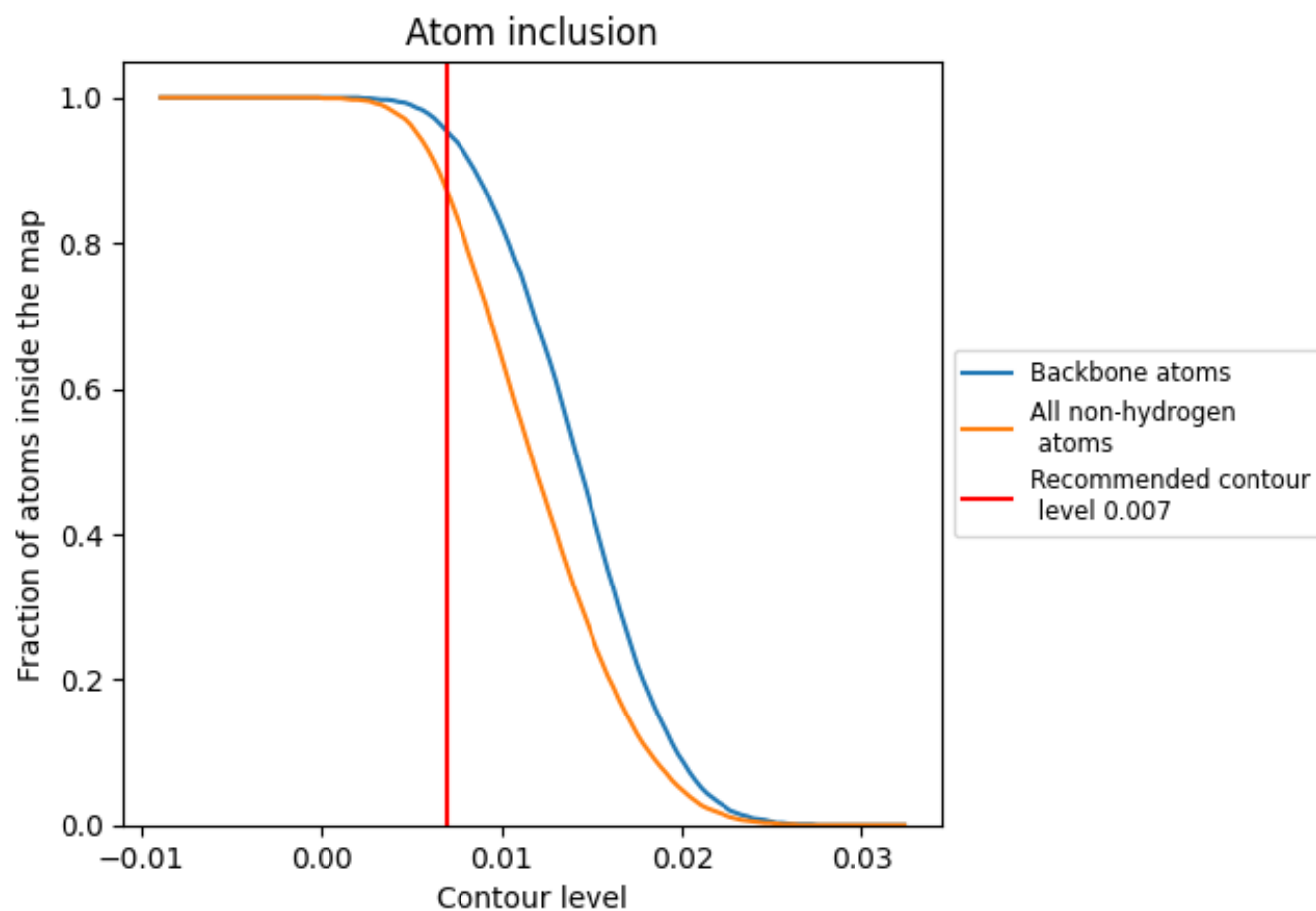


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% 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	0.8690	0.2650
A	0.8330	0.2460
B	0.8890	0.2780
C	0.8880	0.2900
D	0.8640	0.2450

