



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 8I6P / pdb_00008i6p
EMDB ID : EMD-35202
Title : The cryo-EM structure of OsCyc1 tetramer state
Authors : Ma, X.L.; Xu, H.F.; Tong, Y.R.; Luo, Y.F.; Dong, Q.H.; Jiang, T.
Deposited on : 2023-01-29
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

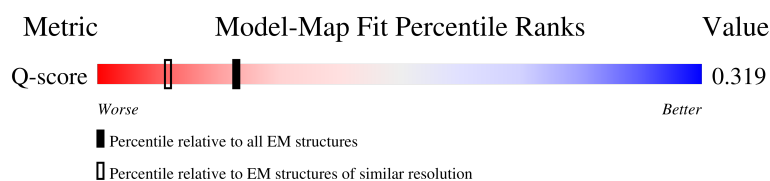
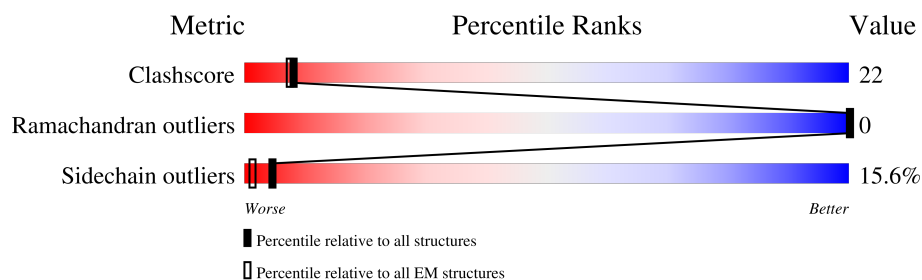
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	775	
1	B	775	
1	C	775	
1	D	775	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22016 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 Syn-copalyl diphosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		
1	C	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		
1	D	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		
1	A	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	768	GLU	-	expression tag	UNP Q0JF02
B	769	PHE	-	expression tag	UNP Q0JF02
B	770	HIS	-	expression tag	UNP Q0JF02
B	771	HIS	-	expression tag	UNP Q0JF02
B	772	HIS	-	expression tag	UNP Q0JF02
B	773	HIS	-	expression tag	UNP Q0JF02
B	774	HIS	-	expression tag	UNP Q0JF02
B	775	HIS	-	expression tag	UNP Q0JF02
C	768	GLU	-	expression tag	UNP Q0JF02
C	769	PHE	-	expression tag	UNP Q0JF02
C	770	HIS	-	expression tag	UNP Q0JF02
C	771	HIS	-	expression tag	UNP Q0JF02
C	772	HIS	-	expression tag	UNP Q0JF02
C	773	HIS	-	expression tag	UNP Q0JF02
C	774	HIS	-	expression tag	UNP Q0JF02
C	775	HIS	-	expression tag	UNP Q0JF02
D	768	GLU	-	expression tag	UNP Q0JF02
D	769	PHE	-	expression tag	UNP Q0JF02
D	770	HIS	-	expression tag	UNP Q0JF02
D	771	HIS	-	expression tag	UNP Q0JF02
D	772	HIS	-	expression tag	UNP Q0JF02
D	773	HIS	-	expression tag	UNP Q0JF02

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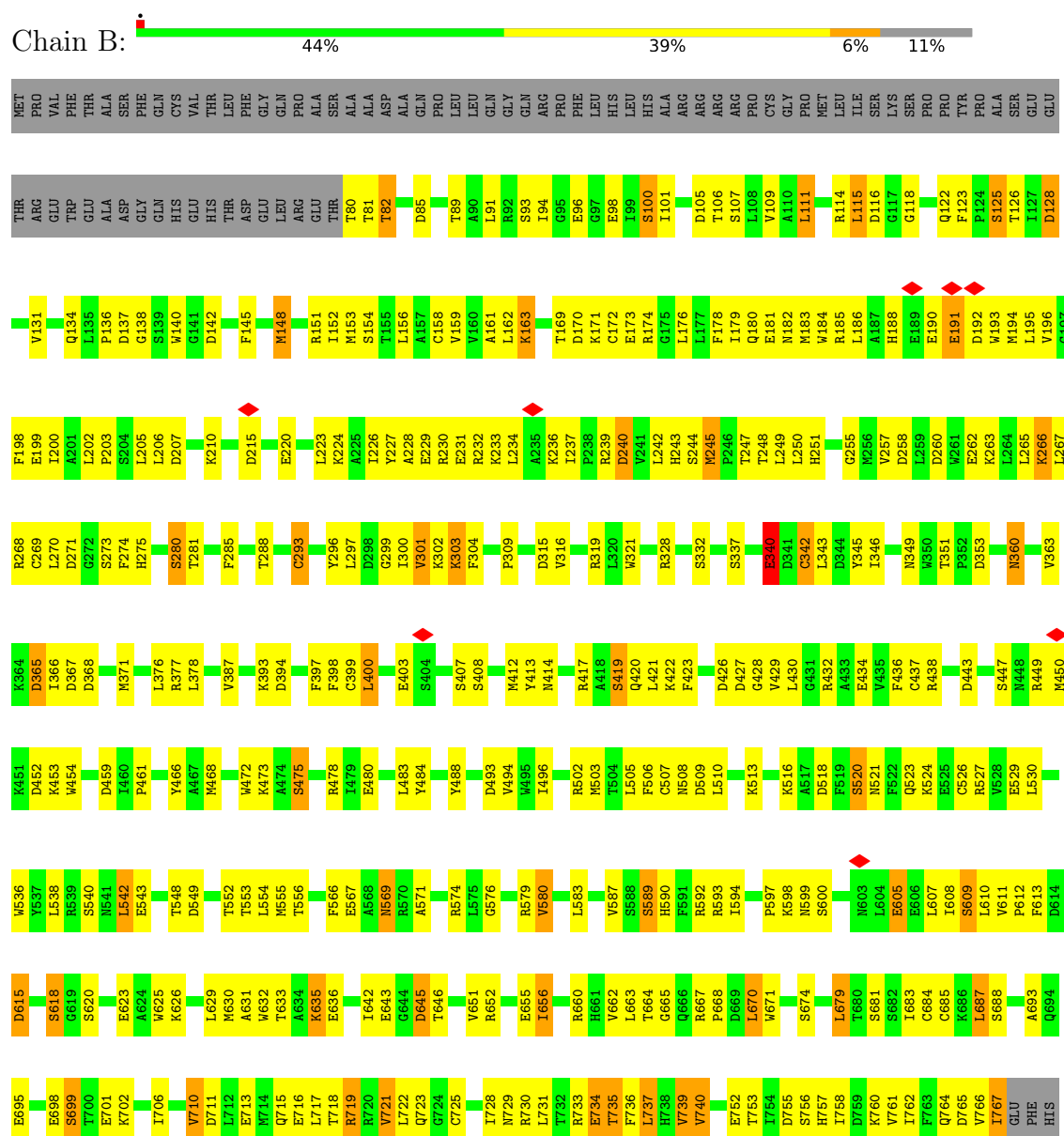
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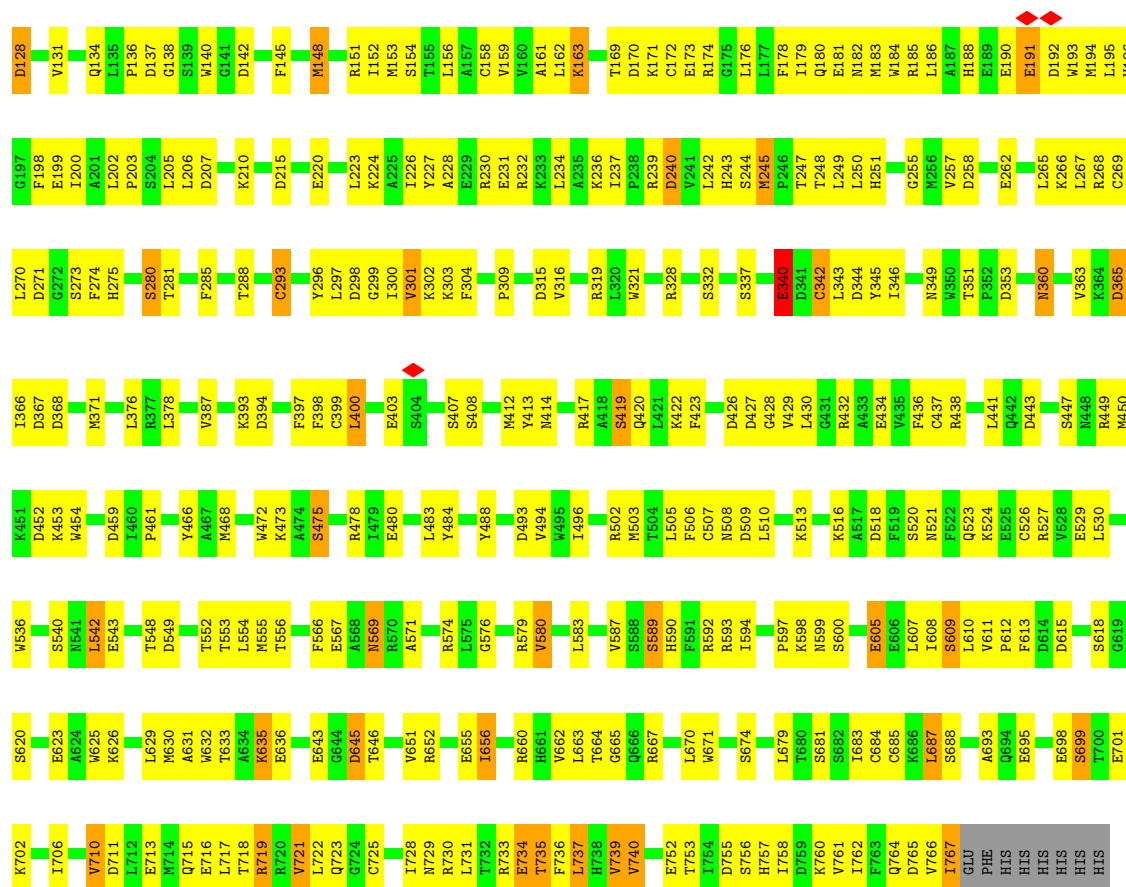
Chain	Residue	Modelled	Actual	Comment	Reference
D	774	HIS	-	expression tag	UNP Q0JF02
D	775	HIS	-	expression tag	UNP Q0JF02
A	768	GLU	-	expression tag	UNP Q0JF02
A	769	PHE	-	expression tag	UNP Q0JF02
A	770	HIS	-	expression tag	UNP Q0JF02
A	771	HIS	-	expression tag	UNP Q0JF02
A	772	HIS	-	expression tag	UNP Q0JF02
A	773	HIS	-	expression tag	UNP Q0JF02
A	774	HIS	-	expression tag	UNP Q0JF02
A	775	HIS	-	expression tag	UNP Q0JF02

3 Residue-property plots

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

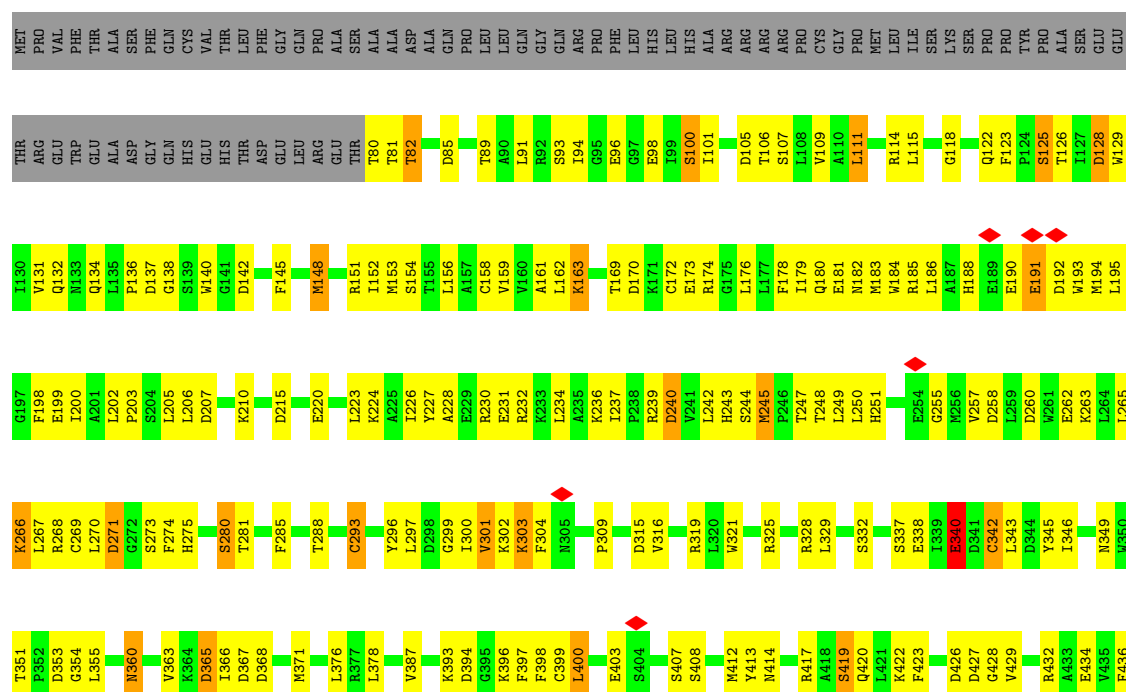
- Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic





• Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

Chain A: 43% 40% 6% 11%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149837	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0137	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/5627	0.45	1/7615 (0.0%)
1	B	0.28	0/5627	0.45	1/7615 (0.0%)
1	C	0.28	0/5627	0.45	1/7615 (0.0%)
1	D	0.28	0/5627	0.45	1/7615 (0.0%)
All	All	0.28	0/22508	0.45	4/30460 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	GLU	CA-CB-CG	5.50	125.10	114.10
1	C	340	GLU	CA-CB-CG	5.49	125.08	114.10
1	A	340	GLU	CA-CB-CG	5.49	125.08	114.10
1	D	340	GLU	CA-CB-CG	5.48	125.06	114.10

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	5504	0	5413	241	0
1	B	5504	0	5413	255	0
1	C	5504	0	5413	234	0
1	D	5504	0	5413	243	0
All	All	22016	0	21652	960	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 22.

All (960) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:LEU:O	1:D:301:VAL:CG1	1.94	1.16
1:D:297:LEU:O	1:D:301:VAL:HG12	1.44	1.11
1:D:631:ALA:C	1:D:635:LYS:HE2	1.77	1.10
1:A:631:ALA:C	1:A:635:LYS:HE2	1.82	1.03
1:B:631:ALA:O	1:B:635:LYS:HE3	1.67	0.93
1:D:631:ALA:O	1:D:635:LYS:HE2	1.68	0.93
1:B:297:LEU:O	1:B:301:VAL:HG13	1.70	0.91
1:C:635:LYS:HZ2	1:C:642:ILE:HG22	1.35	0.91
1:B:632:TRP:HA	1:B:635:LYS:CE	2.01	0.90
1:A:297:LEU:O	1:A:301:VAL:HG13	1.70	0.90
1:C:661:HIS:NE2	1:D:667:ARG:NH2	2.21	0.89
1:D:304:PHE:HE2	1:D:309:PRO:HD3	1.36	0.89
1:A:631:ALA:O	1:A:635:LYS:HE2	1.72	0.88
1:C:297:LEU:O	1:C:301:VAL:HG13	1.74	0.87
1:D:365:ASP:OD1	1:D:366:ILE:N	2.09	0.86
1:B:365:ASP:OD1	1:B:366:ILE:N	2.09	0.85
1:C:365:ASP:OD1	1:C:366:ILE:N	2.09	0.85
1:A:663:LEU:HD12	1:A:665:GLY:H	1.42	0.85
1:B:663:LEU:HD12	1:B:665:GLY:H	1.42	0.84
1:A:365:ASP:OD1	1:A:366:ILE:N	2.09	0.84
1:C:663:LEU:HD12	1:C:665:GLY:H	1.42	0.83
1:D:297:LEU:O	1:D:301:VAL:HG13	1.76	0.83
1:D:663:LEU:HD12	1:D:665:GLY:H	1.42	0.83
1:A:645:ASP:N	1:A:645:ASP:OD1	2.14	0.80
1:D:632:TRP:HA	1:D:635:LYS:CE	2.10	0.80
1:D:298:ASP:HA	1:D:301:VAL:HG13	1.63	0.80
1:A:632:TRP:HA	1:A:635:LYS:CE	2.12	0.79
1:C:297:LEU:O	1:C:301:VAL:CG1	2.30	0.79
1:C:645:ASP:N	1:C:645:ASP:OD1	2.14	0.79
1:D:645:ASP:OD1	1:D:645:ASP:N	2.14	0.78
1:D:632:TRP:N	1:D:635:LYS:HE2	1.98	0.78
1:B:297:LEU:O	1:B:301:VAL:CG1	2.32	0.78
1:C:635:LYS:NZ	1:C:642:ILE:HG22	1.98	0.78
1:A:297:LEU:O	1:A:301:VAL:CG1	2.32	0.77
1:B:645:ASP:OD1	1:B:645:ASP:N	2.14	0.76
1:B:191:GLU:OE1	1:B:191:GLU:N	2.18	0.76
1:D:298:ASP:CA	1:D:301:VAL:HG13	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:TRP:N	1:A:635:LYS:HE2	2.01	0.75
1:A:207:ASP:HA	1:A:210:LYS:HE3	1.69	0.75
1:D:304:PHE:CE2	1:D:309:PRO:HD3	2.21	0.74
1:C:207:ASP:HA	1:C:210:LYS:HE3	1.69	0.74
1:B:207:ASP:HA	1:B:210:LYS:HE3	1.69	0.74
1:A:191:GLU:OE1	1:A:191:GLU:N	2.18	0.73
1:D:207:ASP:HA	1:D:210:LYS:HE3	1.69	0.73
1:D:191:GLU:OE1	1:D:191:GLU:N	2.18	0.71
1:D:631:ALA:O	1:D:635:LYS:CE	2.38	0.71
1:B:631:ALA:O	1:B:635:LYS:CE	2.37	0.71
1:C:191:GLU:OE1	1:C:191:GLU:N	2.18	0.71
1:B:631:ALA:C	1:B:635:LYS:CE	2.64	0.70
1:D:148:MET:HE2	1:D:148:MET:HA	1.74	0.70
1:B:615:ASP:OD2	1:D:667:ARG:NH1	2.25	0.69
1:A:140:TRP:NE1	1:A:158:CYS:HG	1.89	0.69
1:C:148:MET:HE2	1:C:148:MET:HA	1.74	0.69
1:B:148:MET:HA	1:B:148:MET:HE2	1.74	0.69
1:D:203:PRO:HB3	1:D:227:TYR:HE1	1.58	0.69
1:C:203:PRO:HB3	1:C:227:TYR:HE1	1.58	0.68
1:A:148:MET:HE2	1:A:148:MET:HA	1.74	0.68
1:B:239:ARG:O	1:B:243:HIS:ND1	2.26	0.68
1:A:239:ARG:O	1:A:243:HIS:ND1	2.26	0.68
1:C:239:ARG:O	1:C:243:HIS:ND1	2.26	0.68
1:D:192:ASP:HB2	1:D:453:LYS:HG3	1.76	0.68
1:C:192:ASP:HB2	1:C:453:LYS:HG3	1.76	0.68
1:A:632:TRP:CA	1:A:635:LYS:HE2	2.23	0.68
1:D:632:TRP:CA	1:D:635:LYS:HE2	2.23	0.68
1:A:716:GLU:OE2	1:A:719:ARG:NH1	2.27	0.67
1:A:203:PRO:HB3	1:A:227:TYR:HE1	1.58	0.67
1:C:667:ARG:NH2	1:D:660:ARG:O	2.28	0.67
1:C:716:GLU:OE2	1:C:719:ARG:NH1	2.27	0.67
1:B:192:ASP:HB2	1:B:453:LYS:HG3	1.76	0.67
1:B:203:PRO:HB3	1:B:227:TYR:HE1	1.58	0.67
1:B:716:GLU:OE2	1:B:719:ARG:NH1	2.27	0.67
1:D:239:ARG:O	1:D:243:HIS:ND1	2.26	0.67
1:A:631:ALA:O	1:A:635:LYS:CE	2.43	0.67
1:A:632:TRP:HA	1:A:635:LYS:HE2	1.76	0.67
1:D:716:GLU:OE2	1:D:719:ARG:NH1	2.27	0.66
1:A:98:GLU:OE1	1:A:505:LEU:N	2.29	0.66
1:D:345:TYR:O	1:D:349:ASN:ND2	2.28	0.66
1:C:98:GLU:OE1	1:C:505:LEU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:THR:CG2	1:C:126:THR:HB	2.26	0.66
1:D:106:THR:CG2	1:D:126:THR:HB	2.26	0.66
1:D:713:GLU:N	1:D:713:GLU:OE2	2.29	0.66
1:A:192:ASP:HB2	1:A:453:LYS:HG3	1.76	0.66
1:B:106:THR:CG2	1:B:126:THR:HB	2.26	0.66
1:D:98:GLU:OE1	1:D:505:LEU:N	2.29	0.65
1:A:713:GLU:OE2	1:A:713:GLU:N	2.29	0.65
1:B:98:GLU:OE1	1:B:505:LEU:N	2.29	0.65
1:A:140:TRP:NE1	1:A:158:CYS:SG	2.69	0.65
1:C:443:ASP:OD1	1:C:443:ASP:N	2.29	0.65
1:D:729:ASN:OD1	1:D:730:ARG:N	2.30	0.65
1:C:140:TRP:NE1	1:C:158:CYS:SG	2.70	0.65
1:C:713:GLU:OE2	1:C:713:GLU:N	2.29	0.65
1:B:140:TRP:NE1	1:B:158:CYS:SG	2.69	0.65
1:C:304:PHE:HE2	1:C:309:PRO:HD3	1.60	0.65
1:B:632:TRP:CA	1:B:635:LYS:CE	2.74	0.65
1:D:140:TRP:NE1	1:D:158:CYS:SG	2.69	0.65
1:A:106:THR:CG2	1:A:126:THR:HB	2.26	0.65
1:A:345:TYR:O	1:A:349:ASN:ND2	2.28	0.65
1:B:729:ASN:OD1	1:B:730:ARG:N	2.30	0.64
1:A:761:VAL:HG13	1:A:762:ILE:HG13	1.79	0.64
1:C:761:VAL:HG13	1:C:762:ILE:HG13	1.79	0.64
1:B:761:VAL:HG13	1:B:762:ILE:HG13	1.79	0.64
1:A:594:ILE:O	1:A:599:ASN:ND2	2.27	0.64
1:B:443:ASP:OD1	1:B:443:ASP:N	2.29	0.64
1:B:632:TRP:HA	1:B:635:LYS:HE3	1.77	0.64
1:D:443:ASP:N	1:D:443:ASP:OD1	2.29	0.64
1:A:729:ASN:OD1	1:A:730:ARG:N	2.30	0.64
1:B:713:GLU:N	1:B:713:GLU:OE2	2.29	0.64
1:B:736:PHE:O	1:B:740:VAL:HG12	1.98	0.64
1:C:729:ASN:OD1	1:C:730:ARG:N	2.30	0.63
1:A:736:PHE:O	1:A:740:VAL:HG12	1.98	0.63
1:B:345:TYR:O	1:B:349:ASN:ND2	2.28	0.63
1:D:632:TRP:HA	1:D:635:LYS:HE2	1.79	0.63
1:D:297:LEU:HA	1:D:300:ILE:HG12	1.80	0.63
1:B:304:PHE:HE2	1:B:309:PRO:HD3	1.63	0.63
1:C:345:TYR:O	1:C:349:ASN:ND2	2.28	0.63
1:D:761:VAL:HG13	1:D:762:ILE:HG13	1.79	0.63
1:D:220:GLU:O	1:D:224:LYS:NZ	2.30	0.63
1:A:304:PHE:HE2	1:A:309:PRO:HD3	1.63	0.63
1:D:736:PHE:O	1:D:740:VAL:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:GLU:O	1:B:224:LYS:NZ	2.30	0.63
1:C:736:PHE:O	1:C:740:VAL:HG12	1.98	0.62
1:C:661:HIS:CD2	1:D:667:ARG:HH21	2.17	0.62
1:B:594:ILE:O	1:B:599:ASN:ND2	2.27	0.62
1:A:443:ASP:N	1:A:443:ASP:OD1	2.29	0.62
1:D:608:ILE:HD12	1:D:625:TRP:HB2	1.82	0.62
1:B:608:ILE:HD12	1:B:625:TRP:HB2	1.81	0.62
1:C:667:ARG:HB3	1:C:671:TRP:CZ2	2.35	0.62
1:C:181:GLU:O	1:C:184:TRP:NE1	2.33	0.62
1:D:181:GLU:O	1:D:184:TRP:NE1	2.33	0.62
1:D:297:LEU:C	1:D:301:VAL:CG1	2.71	0.62
1:A:181:GLU:O	1:A:184:TRP:NE1	2.33	0.62
1:B:667:ARG:CZ	1:A:656:ILE:HG13	2.30	0.61
1:A:667:ARG:HB3	1:A:671:TRP:CZ2	2.35	0.61
1:B:181:GLU:O	1:B:184:TRP:NE1	2.33	0.61
1:A:523:GLN:NE2	1:A:761:VAL:O	2.34	0.61
1:B:632:TRP:HA	1:B:635:LYS:NZ	2.14	0.61
1:B:667:ARG:HB3	1:B:671:TRP:CZ2	2.35	0.61
1:C:367:ASP:OD1	1:C:368:ASP:N	2.33	0.61
1:C:608:ILE:HD12	1:C:625:TRP:HB2	1.81	0.61
1:D:413:TYR:CZ	1:D:417:ARG:HD2	2.36	0.61
1:B:413:TYR:CZ	1:B:417:ARG:HD2	2.36	0.60
1:A:265:LEU:O	1:A:268:ARG:NH1	2.30	0.60
1:A:608:ILE:HD12	1:A:625:TRP:HB2	1.81	0.60
1:B:631:ALA:C	1:B:635:LYS:HE2	2.25	0.60
1:C:413:TYR:CZ	1:C:417:ARG:HD2	2.36	0.60
1:B:523:GLN:NE2	1:B:761:VAL:O	2.34	0.60
1:C:523:GLN:NE2	1:C:761:VAL:O	2.34	0.60
1:A:220:GLU:O	1:A:224:LYS:NZ	2.30	0.60
1:B:569:ASN:N	1:B:569:ASN:OD1	2.34	0.60
1:A:413:TYR:CZ	1:A:417:ARG:HD2	2.36	0.60
1:B:367:ASP:OD1	1:B:368:ASP:N	2.33	0.60
1:D:265:LEU:O	1:D:268:ARG:NH1	2.30	0.60
1:B:140:TRP:NE1	1:B:158:CYS:HG	2.00	0.60
1:B:408:SER:HB2	1:B:453:LYS:HE2	1.84	0.60
1:B:632:TRP:N	1:B:635:LYS:HE2	2.17	0.60
1:C:543:GLU:OE1	1:C:543:GLU:N	2.30	0.60
1:D:170:ASP:OD1	1:D:170:ASP:N	2.35	0.60
1:D:523:GLN:NE2	1:D:761:VAL:O	2.34	0.60
1:C:594:ILE:O	1:C:599:ASN:ND2	2.27	0.59
1:D:717:LEU:O	1:D:721:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:N	1:B:170:ASP:OD1	2.35	0.59
1:A:367:ASP:OD1	1:A:368:ASP:N	2.33	0.59
1:A:408:SER:HB2	1:A:453:LYS:HE2	1.84	0.59
1:C:408:SER:HB2	1:C:453:LYS:HE2	1.84	0.59
1:A:170:ASP:OD1	1:A:170:ASP:N	2.35	0.59
1:A:569:ASN:OD1	1:A:569:ASN:N	2.34	0.59
1:A:717:LEU:O	1:A:721:VAL:HG23	2.02	0.59
1:D:367:ASP:OD1	1:D:368:ASP:N	2.33	0.59
1:C:170:ASP:OD1	1:C:170:ASP:N	2.35	0.59
1:B:631:ALA:C	1:B:635:LYS:HE3	2.24	0.59
1:C:717:LEU:O	1:C:721:VAL:HG23	2.02	0.59
1:D:191:GLU:H	1:D:191:GLU:CD	2.11	0.59
1:D:419:SER:O	1:D:422:LYS:NZ	2.36	0.58
1:B:543:GLU:OE1	1:B:543:GLU:N	2.29	0.58
1:D:543:GLU:OE1	1:D:543:GLU:N	2.30	0.58
1:D:569:ASN:N	1:D:569:ASN:OD1	2.34	0.58
1:D:408:SER:HB2	1:D:453:LYS:HE2	1.84	0.58
1:D:105:ASP:O	1:D:109:VAL:HG23	2.04	0.58
1:C:605:GLU:CD	1:C:605:GLU:H	2.12	0.58
1:C:635:LYS:HZ2	1:C:642:ILE:CG2	2.13	0.58
1:D:667:ARG:HB3	1:D:671:TRP:CZ2	2.39	0.58
1:A:181:GLU:OE2	1:A:182:ASN:ND2	2.37	0.58
1:C:140:TRP:NE1	1:C:158:CYS:HG	2.02	0.58
1:C:181:GLU:OE2	1:C:182:ASN:ND2	2.37	0.58
1:A:105:ASP:O	1:A:109:VAL:HG23	2.04	0.57
1:A:605:GLU:CD	1:A:605:GLU:H	2.12	0.57
1:B:717:LEU:O	1:B:721:VAL:HG23	2.02	0.57
1:A:419:SER:O	1:A:422:LYS:NZ	2.36	0.57
1:A:509:ASP:O	1:A:513:LYS:NZ	2.37	0.57
1:B:632:TRP:CA	1:B:635:LYS:HE3	2.34	0.57
1:C:158:CYS:SG	1:C:159:VAL:N	2.78	0.57
1:C:661:HIS:CD2	1:D:667:ARG:NH2	2.72	0.57
1:B:105:ASP:O	1:B:109:VAL:HG23	2.04	0.57
1:B:605:GLU:H	1:B:605:GLU:CD	2.12	0.57
1:B:269:CYS:N	1:B:273:SER:O	2.32	0.57
1:B:419:SER:O	1:B:419:SER:OG	2.23	0.57
1:B:509:ASP:O	1:B:513:LYS:NZ	2.38	0.57
1:D:605:GLU:H	1:D:605:GLU:CD	2.12	0.57
1:D:423:PHE:CG	1:D:719:ARG:HG3	2.40	0.57
1:D:181:GLU:OE2	1:D:182:ASN:ND2	2.37	0.57
1:D:419:SER:O	1:D:419:SER:OG	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLU:OE2	1:B:182:ASN:ND2	2.37	0.57
1:C:509:ASP:O	1:C:513:LYS:NZ	2.38	0.57
1:D:158:CYS:SG	1:D:159:VAL:N	2.78	0.57
1:B:412:MET:HB3	1:B:437:CYS:SG	2.45	0.56
1:C:105:ASP:O	1:C:109:VAL:HG23	2.04	0.56
1:A:360:ASN:OD1	1:A:360:ASN:N	2.38	0.56
1:A:423:PHE:CG	1:A:719:ARG:HG3	2.40	0.56
1:C:265:LEU:O	1:C:268:ARG:NH1	2.30	0.56
1:A:158:CYS:SG	1:A:159:VAL:N	2.78	0.56
1:B:360:ASN:OD1	1:B:360:ASN:N	2.38	0.56
1:B:670:LEU:HD13	1:A:673:TYR:CE2	2.41	0.56
1:C:220:GLU:O	1:C:224:LYS:NZ	2.30	0.56
1:C:227:TYR:HD1	1:C:230:ARG:HD3	1.70	0.56
1:D:227:TYR:HD1	1:D:230:ARG:HD3	1.70	0.56
1:A:227:TYR:HD1	1:A:230:ARG:HD3	1.70	0.56
1:A:412:MET:HB3	1:A:437:CYS:SG	2.45	0.56
1:C:412:MET:HB3	1:C:437:CYS:SG	2.45	0.56
1:D:509:ASP:O	1:D:513:LYS:NZ	2.37	0.56
1:D:706:ILE:O	1:D:710:VAL:HG12	2.06	0.56
1:D:360:ASN:OD1	1:D:360:ASN:N	2.38	0.56
1:B:265:LEU:O	1:B:268:ARG:NH1	2.30	0.56
1:C:423:PHE:CG	1:C:719:ARG:HG3	2.40	0.56
1:C:450:MET:HG3	1:C:461:PRO:HG3	1.88	0.56
1:C:635:LYS:NZ	1:C:645:ASP:OD2	2.28	0.56
1:D:594:ILE:O	1:D:599:ASN:ND2	2.27	0.56
1:A:706:ILE:O	1:A:710:VAL:HG12	2.06	0.56
1:C:569:ASN:OD1	1:C:569:ASN:N	2.34	0.56
1:A:450:MET:HG3	1:A:461:PRO:HG3	1.88	0.56
1:B:423:PHE:CG	1:B:719:ARG:HG3	2.40	0.56
1:C:706:ILE:O	1:C:710:VAL:HG12	2.06	0.56
1:B:227:TYR:HD1	1:B:230:ARG:HD3	1.70	0.56
1:C:643:GLU:O	1:C:646:THR:OG1	2.23	0.56
1:D:752:GLU:OE1	1:D:752:GLU:N	2.37	0.56
1:A:576:GLY:O	1:A:580:VAL:HG13	2.06	0.56
1:D:450:MET:HG3	1:D:461:PRO:HG3	1.88	0.55
1:B:597:PRO:HD2	1:B:636:GLU:HG3	1.89	0.55
1:D:412:MET:HB3	1:D:437:CYS:SG	2.45	0.55
1:B:576:GLY:O	1:B:580:VAL:HG13	2.06	0.55
1:B:760:LYS:HA	1:B:764:GLN:HB3	1.89	0.55
1:C:100:SER:OG	1:C:502:ARG:O	2.25	0.55
1:B:158:CYS:SG	1:B:159:VAL:N	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ILE:O	1:B:710:VAL:HG12	2.06	0.55
1:C:191:GLU:H	1:C:191:GLU:CD	2.11	0.55
1:D:693:ALA:HB1	1:D:698:GLU:HG3	1.88	0.55
1:A:597:PRO:HD2	1:A:636:GLU:HG3	1.89	0.55
1:C:136:PRO:O	1:C:174:ARG:NH2	2.34	0.55
1:C:242:LEU:HD21	1:C:249:LEU:HD12	1.89	0.55
1:D:242:LEU:HD21	1:D:249:LEU:HD12	1.89	0.55
1:D:298:ASP:HA	1:D:301:VAL:CG1	2.33	0.55
1:D:597:PRO:HD2	1:D:636:GLU:HG3	1.89	0.55
1:A:630:MET:O	1:A:633:THR:OG1	2.21	0.55
1:B:368:ASP:N	1:B:368:ASP:OD1	2.40	0.55
1:C:419:SER:O	1:C:422:LYS:NZ	2.36	0.55
1:C:576:GLY:O	1:C:580:VAL:HG13	2.06	0.55
1:C:693:ALA:HB1	1:C:698:GLU:HG3	1.88	0.55
1:A:419:SER:O	1:A:419:SER:OG	2.23	0.55
1:A:760:LYS:HA	1:A:764:GLN:HB3	1.89	0.55
1:D:140:TRP:NE1	1:D:158:CYS:HG	2.05	0.54
1:B:195:LEU:HB2	1:B:198:PHE:HB2	1.89	0.54
1:C:368:ASP:N	1:C:368:ASP:OD1	2.39	0.54
1:C:597:PRO:HD2	1:C:636:GLU:HG3	1.89	0.54
1:D:368:ASP:N	1:D:368:ASP:OD1	2.39	0.54
1:A:100:SER:OG	1:A:502:ARG:O	2.25	0.54
1:A:145:PHE:O	1:A:151:ARG:NH2	2.29	0.54
1:A:543:GLU:OE1	1:A:543:GLU:N	2.29	0.54
1:D:576:GLY:O	1:D:580:VAL:HG13	2.06	0.54
1:A:452:ASP:OD1	1:A:454:TRP:N	2.36	0.54
1:A:693:ALA:HB1	1:A:698:GLU:HG3	1.88	0.54
1:B:100:SER:OG	1:B:502:ARG:O	2.25	0.54
1:C:269:CYS:N	1:C:273:SER:O	2.32	0.54
1:A:242:LEU:HD21	1:A:249:LEU:HD12	1.89	0.54
1:B:242:LEU:HD21	1:B:249:LEU:HD12	1.89	0.54
1:B:693:ALA:HB1	1:B:698:GLU:HG3	1.88	0.54
1:B:450:MET:HG3	1:B:461:PRO:HG3	1.88	0.54
1:D:195:LEU:HB2	1:D:198:PHE:HB2	1.89	0.54
1:A:136:PRO:O	1:A:174:ARG:NH2	2.34	0.54
1:C:195:LEU:HB2	1:C:198:PHE:HB2	1.89	0.54
1:D:298:ASP:C	1:D:301:VAL:HG13	2.33	0.54
1:A:752:GLU:OE1	1:A:752:GLU:N	2.37	0.54
1:C:609:SER:HA	1:C:613:PHE:CE2	2.43	0.54
1:C:760:LYS:HA	1:C:764:GLN:HB3	1.89	0.54
1:D:100:SER:OG	1:D:502:ARG:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:760:LYS:HA	1:D:764:GLN:HB3	1.89	0.54
1:A:191:GLU:H	1:A:191:GLU:CD	2.11	0.54
1:B:766:VAL:HG23	1:B:767:ILE:HG23	1.90	0.53
1:B:145:PHE:O	1:B:151:ARG:NH2	2.29	0.53
1:C:548:THR:OG1	1:C:549:ASP:N	2.41	0.53
1:A:527:ARG:NH1	1:A:762:ILE:O	2.42	0.53
1:A:548:THR:OG1	1:A:549:ASP:N	2.41	0.53
1:B:731:LEU:HA	1:B:734:GLU:CD	2.34	0.53
1:C:598:LYS:NZ	1:C:636:GLU:OE2	2.42	0.53
1:D:269:CYS:N	1:D:273:SER:O	2.32	0.53
1:D:643:GLU:O	1:D:646:THR:OG1	2.23	0.53
1:A:609:SER:HA	1:A:613:PHE:CE2	2.43	0.53
1:D:598:LYS:NZ	1:D:636:GLU:OE2	2.42	0.53
1:B:527:ARG:NH1	1:B:762:ILE:O	2.42	0.53
1:C:731:LEU:HA	1:C:734:GLU:CD	2.34	0.53
1:D:731:LEU:HA	1:D:734:GLU:CD	2.34	0.53
1:B:609:SER:HA	1:B:613:PHE:CE2	2.43	0.53
1:C:527:ARG:NH1	1:C:762:ILE:O	2.42	0.53
1:C:752:GLU:OE1	1:C:752:GLU:N	2.37	0.53
1:A:195:LEU:HB2	1:A:198:PHE:HB2	1.89	0.53
1:B:630:MET:O	1:B:633:THR:OG1	2.21	0.53
1:D:136:PRO:O	1:D:174:ARG:NH2	2.34	0.53
1:D:609:SER:HA	1:D:613:PHE:CE2	2.43	0.53
1:A:598:LYS:NZ	1:A:636:GLU:OE2	2.42	0.53
1:A:766:VAL:HG23	1:A:767:ILE:HG23	1.90	0.53
1:C:145:PHE:O	1:C:151:ARG:NH2	2.30	0.53
1:C:765:ASP:OD1	1:C:766:VAL:N	2.42	0.53
1:D:548:THR:OG1	1:D:549:ASP:N	2.41	0.53
1:D:527:ARG:NH1	1:D:762:ILE:O	2.42	0.53
1:A:605:GLU:HA	1:A:625:TRP:CD1	2.44	0.53
1:A:728:ILE:O	1:A:733:ARG:NH1	2.42	0.53
1:A:148:MET:O	1:A:152:ILE:HG12	2.10	0.52
1:A:731:LEU:HA	1:A:734:GLU:CD	2.34	0.52
1:B:296:TYR:O	1:B:300:ILE:HG23	2.09	0.52
1:C:605:GLU:HA	1:C:625:TRP:CD1	2.45	0.52
1:D:605:GLU:HA	1:D:625:TRP:CD1	2.44	0.52
1:D:148:MET:O	1:D:152:ILE:HG12	2.09	0.52
1:A:368:ASP:N	1:A:368:ASP:OD1	2.39	0.52
1:B:419:SER:O	1:B:422:LYS:NZ	2.36	0.52
1:C:148:MET:O	1:C:152:ILE:HG12	2.09	0.52
1:C:766:VAL:HG23	1:C:767:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:THR:OG1	1:B:549:ASP:N	2.41	0.52
1:D:134:GLN:HG3	1:D:138:GLY:HA2	1.92	0.52
1:D:766:VAL:HG23	1:D:767:ILE:HG23	1.90	0.52
1:A:106:THR:HG23	1:A:126:THR:HB	1.91	0.52
1:A:765:ASP:OD1	1:A:766:VAL:N	2.42	0.52
1:B:191:GLU:H	1:B:191:GLU:CD	2.11	0.52
1:B:518:ASP:HA	1:B:521:ASN:HD21	1.75	0.52
1:B:598:LYS:NZ	1:B:636:GLU:OE2	2.42	0.52
1:D:518:ASP:HA	1:D:521:ASN:HD21	1.75	0.52
1:C:106:THR:HG23	1:C:126:THR:HB	1.91	0.52
1:B:106:THR:HG23	1:B:126:THR:HB	1.91	0.52
1:B:148:MET:O	1:B:152:ILE:HG12	2.09	0.52
1:B:605:GLU:HA	1:B:625:TRP:CD1	2.45	0.52
1:C:134:GLN:HG3	1:C:138:GLY:HA2	1.92	0.52
1:C:447:SER:OG	1:C:449:ARG:NH1	2.43	0.52
1:D:106:THR:HG23	1:D:126:THR:HB	1.91	0.52
1:A:296:TYR:O	1:A:300:ILE:HG23	2.09	0.52
1:B:134:GLN:HG3	1:B:138:GLY:HA2	1.92	0.52
1:B:452:ASP:OD1	1:B:454:TRP:N	2.36	0.52
1:C:296:TYR:O	1:C:300:ILE:HG23	2.09	0.52
1:A:190:GLU:HB2	1:A:193:TRP:HB2	1.92	0.52
1:B:190:GLU:HB2	1:B:193:TRP:HB2	1.92	0.51
1:C:400:LEU:HD13	1:C:403:GLU:HB3	1.92	0.51
1:C:419:SER:O	1:C:419:SER:OG	2.23	0.51
1:C:518:ASP:HA	1:C:521:ASN:HD21	1.75	0.51
1:A:447:SER:OG	1:A:449:ARG:NH1	2.43	0.51
1:C:240:ASP:O	1:C:244:SER:N	2.43	0.51
1:C:190:GLU:HB2	1:C:193:TRP:HB2	1.92	0.51
1:D:765:ASP:OD1	1:D:766:VAL:N	2.42	0.51
1:A:316:VAL:HG13	1:A:346:ILE:HD12	1.93	0.51
1:A:643:GLU:O	1:A:646:THR:OG1	2.23	0.51
1:B:447:SER:OG	1:B:449:ARG:NH1	2.43	0.51
1:B:530:LEU:HD21	1:B:555:MET:HE1	1.93	0.51
1:A:269:CYS:N	1:A:273:SER:O	2.32	0.51
1:A:518:ASP:HA	1:A:521:ASN:HD21	1.75	0.51
1:A:240:ASP:O	1:A:244:SER:N	2.43	0.51
1:B:240:ASP:O	1:B:244:SER:N	2.43	0.51
1:D:116:ASP:OD1	1:D:116:ASP:N	2.44	0.51
1:A:508:ASN:OD1	1:A:509:ASP:N	2.44	0.51
1:D:316:VAL:HG13	1:D:346:ILE:HD12	1.93	0.51
1:A:478:ARG:HD3	1:A:566:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ARG:HD3	1:B:566:PHE:CD2	2.46	0.51
1:C:360:ASN:N	1:C:360:ASN:OD1	2.38	0.51
1:D:630:MET:O	1:D:633:THR:OG1	2.21	0.51
1:B:400:LEU:HD13	1:B:403:GLU:HB3	1.92	0.51
1:B:643:GLU:O	1:B:646:THR:OG1	2.23	0.51
1:B:765:ASP:OD1	1:B:766:VAL:N	2.42	0.51
1:C:478:ARG:HD3	1:C:566:PHE:CD2	2.46	0.51
1:D:190:GLU:HB2	1:D:193:TRP:HB2	1.92	0.51
1:D:400:LEU:HD13	1:D:403:GLU:HB3	1.92	0.51
1:A:134:GLN:HG3	1:A:138:GLY:HA2	1.92	0.51
1:A:611:VAL:HB	1:A:613:PHE:CE1	2.46	0.51
1:B:274:PHE:H	1:B:281:THR:HG22	1.76	0.50
1:B:567:GLU:H	1:B:567:GLU:CD	2.19	0.50
1:B:407:SER:C	1:B:453:LYS:HZ1	2.20	0.50
1:C:567:GLU:CD	1:C:567:GLU:H	2.19	0.50
1:D:240:ASP:O	1:D:244:SER:N	2.43	0.50
1:B:611:VAL:HB	1:B:613:PHE:CE1	2.46	0.50
1:C:274:PHE:H	1:C:281:THR:HG22	1.76	0.50
1:D:478:ARG:HD3	1:D:566:PHE:CD2	2.46	0.50
1:B:508:ASN:OD1	1:B:509:ASP:N	2.44	0.50
1:C:508:ASN:OD1	1:C:509:ASP:N	2.44	0.50
1:D:611:VAL:HB	1:D:613:PHE:CE1	2.46	0.50
1:A:274:PHE:H	1:A:281:THR:HG22	1.76	0.50
1:D:508:ASN:OD1	1:D:509:ASP:N	2.44	0.50
1:A:400:LEU:HD13	1:A:403:GLU:HB3	1.92	0.50
1:A:530:LEU:HD21	1:A:555:MET:HE1	1.93	0.50
1:A:567:GLU:CD	1:A:567:GLU:H	2.19	0.50
1:B:304:PHE:CE2	1:B:309:PRO:HD3	2.44	0.50
1:B:316:VAL:HG13	1:B:346:ILE:HD12	1.93	0.50
1:C:530:LEU:HD21	1:C:555:MET:HE1	1.93	0.50
1:D:296:TYR:O	1:D:300:ILE:HG23	2.11	0.50
1:A:315:ASP:OD1	1:A:315:ASP:N	2.43	0.50
1:C:316:VAL:HG13	1:C:346:ILE:HD12	1.93	0.50
1:D:530:LEU:HD21	1:D:555:MET:HE1	1.93	0.50
1:D:728:ILE:O	1:D:733:ARG:NH1	2.42	0.50
1:C:321:TRP:CE2	1:C:371:MET:HE1	2.47	0.50
1:C:728:ILE:O	1:C:733:ARG:NH1	2.42	0.50
1:A:407:SER:C	1:A:453:LYS:HZ1	2.19	0.50
1:D:274:PHE:H	1:D:281:THR:HG22	1.76	0.49
1:C:304:PHE:CE2	1:C:309:PRO:HD3	2.43	0.49
1:B:199:GLU:HB2	1:B:226:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:LYS:NZ	1:B:642:ILE:HG22	2.27	0.49
1:C:611:VAL:HB	1:C:613:PHE:CE1	2.46	0.49
1:D:452:ASP:OD1	1:D:454:TRP:N	2.36	0.49
1:B:321:TRP:CE2	1:B:371:MET:HE1	2.47	0.49
1:B:728:ILE:O	1:B:733:ARG:NH1	2.42	0.49
1:D:407:SER:C	1:D:453:LYS:HZ1	2.21	0.49
1:A:321:TRP:CE2	1:A:371:MET:HE1	2.47	0.49
1:C:199:GLU:HB2	1:C:226:ILE:HB	1.95	0.49
1:C:407:SER:C	1:C:453:LYS:HZ1	2.20	0.49
1:C:635:LYS:NZ	1:C:642:ILE:CG2	2.73	0.49
1:D:315:ASP:N	1:D:315:ASP:OD1	2.43	0.49
1:A:484:TYR:CE2	1:A:488:TYR:HB2	2.48	0.49
1:B:635:LYS:HZ3	1:B:642:ILE:HG22	1.77	0.49
1:C:484:TYR:CE2	1:C:488:TYR:HB2	2.48	0.49
1:D:589:SER:HA	1:D:592:ARG:HE	1.77	0.49
1:C:315:ASP:OD1	1:C:315:ASP:N	2.43	0.49
1:B:251:HIS:HB2	1:B:275:HIS:CG	2.48	0.49
1:B:315:ASP:N	1:B:315:ASP:OD1	2.43	0.49
1:B:670:LEU:HD13	1:A:673:TYR:HE2	1.77	0.49
1:C:438:ARG:NH2	1:C:468:MET:O	2.46	0.49
1:D:223:LEU:HB3	1:D:224:LYS:HZ2	1.78	0.49
1:D:484:TYR:CE2	1:D:488:TYR:HB2	2.48	0.49
1:D:567:GLU:CD	1:D:567:GLU:H	2.19	0.49
1:A:438:ARG:NH2	1:A:468:MET:O	2.46	0.49
1:D:321:TRP:CE2	1:D:371:MET:HE1	2.47	0.48
1:A:251:HIS:HB2	1:A:275:HIS:CG	2.48	0.48
1:B:484:TYR:CE2	1:B:488:TYR:HB2	2.48	0.48
1:C:176:LEU:HD21	1:C:215:ASP:OD1	2.13	0.48
1:C:427:ASP:OD1	1:C:428:GLY:N	2.46	0.48
1:D:251:HIS:HB2	1:D:275:HIS:CG	2.48	0.48
1:D:438:ARG:NH2	1:D:468:MET:O	2.46	0.48
1:A:199:GLU:HB2	1:A:226:ILE:HB	1.95	0.48
1:B:203:PRO:O	1:B:206:LEU:HG	2.13	0.48
1:C:116:ASP:OD1	1:C:116:ASP:N	2.44	0.48
1:D:145:PHE:O	1:D:151:ARG:NH2	2.30	0.48
1:A:605:GLU:CD	1:A:605:GLU:N	2.71	0.48
1:B:140:TRP:HB2	1:B:154:SER:HB2	1.96	0.48
1:B:605:GLU:CD	1:B:605:GLU:N	2.71	0.48
1:C:605:GLU:CD	1:C:605:GLU:N	2.71	0.48
1:D:199:GLU:HB2	1:D:226:ILE:HB	1.95	0.48
1:B:579:ARG:NH1	1:B:612:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:SER:HA	1:C:592:ARG:HE	1.78	0.48
1:A:203:PRO:O	1:A:206:LEU:HG	2.13	0.48
1:B:136:PRO:O	1:B:174:ARG:NH2	2.34	0.48
1:B:223:LEU:HB3	1:B:224:LYS:HZ2	1.78	0.48
1:B:438:ARG:NH2	1:B:468:MET:O	2.46	0.48
1:C:630:MET:O	1:C:633:THR:OG1	2.21	0.48
1:D:605:GLU:CD	1:D:605:GLU:N	2.71	0.48
1:A:176:LEU:HD21	1:A:215:ASP:OD1	2.13	0.48
1:B:176:LEU:HA	1:B:179:ILE:HD12	1.96	0.48
1:B:589:SER:HA	1:B:592:ARG:HE	1.78	0.48
1:D:427:ASP:OD1	1:D:428:GLY:N	2.46	0.48
1:D:447:SER:OG	1:D:449:ARG:NH1	2.43	0.48
1:A:140:TRP:HB2	1:A:154:SER:HB2	1.96	0.48
1:A:304:PHE:CE2	1:A:309:PRO:HD3	2.45	0.48
1:A:579:ARG:NH1	1:A:612:PRO:HD2	2.29	0.48
1:D:169:THR:HG22	1:D:173:GLU:OE2	2.14	0.48
1:D:203:PRO:O	1:D:206:LEU:HG	2.13	0.48
1:D:579:ARG:NH1	1:D:612:PRO:HD2	2.29	0.48
1:A:752:GLU:H	1:A:752:GLU:CD	2.22	0.48
1:B:169:THR:HG22	1:B:173:GLU:OE2	2.14	0.48
1:B:176:LEU:HD21	1:B:215:ASP:OD1	2.13	0.48
1:B:542:LEU:HD12	1:B:542:LEU:HA	1.70	0.48
1:C:236:LYS:HB3	1:C:236:LYS:HE3	1.56	0.48
1:A:285:PHE:HA	1:A:288:THR:O	2.14	0.48
1:B:427:ASP:OD1	1:B:428:GLY:N	2.47	0.48
1:D:236:LYS:HB3	1:D:236:LYS:HE3	1.56	0.48
1:A:427:ASP:OD1	1:A:428:GLY:N	2.46	0.48
1:A:715:GLN:O	1:A:718:THR:OG1	2.29	0.48
1:B:632:TRP:N	1:B:635:LYS:CE	2.77	0.47
1:C:176:LEU:HA	1:C:179:ILE:HD12	1.96	0.47
1:C:297:LEU:O	1:C:301:VAL:HG12	2.12	0.47
1:C:715:GLN:O	1:C:718:THR:OG1	2.29	0.47
1:A:122:GLN:HG3	1:A:123:PHE:HD2	1.79	0.47
1:C:251:HIS:HB2	1:C:275:HIS:CG	2.48	0.47
1:D:176:LEU:HA	1:D:179:ILE:HD12	1.96	0.47
1:C:148:MET:HA	1:C:148:MET:CE	2.44	0.47
1:C:169:THR:HG22	1:C:173:GLU:OE2	2.14	0.47
1:C:203:PRO:O	1:C:206:LEU:HG	2.13	0.47
1:C:452:ASP:OD1	1:C:454:TRP:N	2.36	0.47
1:D:122:GLN:HG3	1:D:123:PHE:HD2	1.79	0.47
1:A:169:THR:HG22	1:A:173:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:OE2	1:A:567:GLU:N	2.45	0.47
1:B:494:VAL:HG12	1:B:502:ARG:HD2	1.97	0.47
1:C:223:LEU:HB3	1:C:224:LYS:HZ2	1.79	0.47
1:C:285:PHE:HA	1:C:288:THR:O	2.14	0.47
1:C:579:ARG:NH1	1:C:612:PRO:HD2	2.29	0.47
1:C:122:GLN:HG3	1:C:123:PHE:HD2	1.80	0.47
1:D:635:LYS:HE3	1:D:635:LYS:HB2	1.40	0.47
1:D:735:THR:O	1:D:739:VAL:HG23	2.15	0.47
1:A:176:LEU:HA	1:A:179:ILE:HD12	1.96	0.47
1:B:605:GLU:HA	1:B:625:TRP:NE1	2.30	0.47
1:C:752:GLU:H	1:C:752:GLU:CD	2.22	0.47
1:D:176:LEU:HD21	1:D:215:ASP:OD1	2.14	0.47
1:D:605:GLU:HA	1:D:625:TRP:NE1	2.30	0.47
1:B:285:PHE:HA	1:B:288:THR:O	2.14	0.47
1:C:494:VAL:HG12	1:C:502:ARG:HD2	1.97	0.47
1:D:185:ARG:HA	1:D:188:HIS:CE1	2.50	0.47
1:D:393:LYS:HZ2	1:D:398:PHE:HB2	1.80	0.47
1:A:185:ARG:HA	1:A:188:HIS:CE1	2.50	0.47
1:A:230:ARG:NH1	1:A:231:GLU:OE2	2.48	0.47
1:A:494:VAL:HG12	1:A:502:ARG:HD2	1.97	0.47
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.76	0.47
1:B:185:ARG:HA	1:B:188:HIS:CE1	2.50	0.47
1:D:140:TRP:HB2	1:D:154:SER:HB2	1.96	0.47
1:D:230:ARG:NH1	1:D:231:GLU:OE2	2.48	0.47
1:A:589:SER:HA	1:A:592:ARG:HE	1.78	0.47
1:C:140:TRP:HB2	1:C:154:SER:HB2	1.96	0.47
1:C:620:SER:HA	1:C:623:GLU:OE2	2.15	0.47
1:D:152:ILE:HG13	1:D:153:MET:N	2.30	0.47
1:A:223:LEU:HB3	1:A:224:LYS:HZ2	1.79	0.47
1:A:236:LYS:HE3	1:A:236:LYS:HB3	1.56	0.47
1:B:228:ALA:O	1:B:232:ARG:HG3	2.15	0.47
1:C:230:ARG:NH1	1:C:231:GLU:OE2	2.48	0.47
1:C:605:GLU:HA	1:C:625:TRP:NE1	2.30	0.47
1:D:494:VAL:HG12	1:D:502:ARG:HD2	1.97	0.47
1:C:735:THR:O	1:C:739:VAL:HG23	2.15	0.46
1:D:163:LYS:HD3	1:D:169:THR:HG23	1.97	0.46
1:D:285:PHE:HA	1:D:288:THR:O	2.14	0.46
1:B:122:GLN:HG3	1:B:123:PHE:HD2	1.79	0.46
1:B:230:ARG:NH1	1:B:231:GLU:OE2	2.48	0.46
1:B:251:HIS:O	1:B:280:SER:OG	2.33	0.46
1:B:620:SER:HA	1:B:623:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:GLU:C	1:D:224:LYS:HZ3	2.21	0.46
1:B:752:GLU:OE1	1:B:752:GLU:N	2.37	0.46
1:C:210:LYS:HB3	1:C:210:LYS:HE2	1.61	0.46
1:C:299:GLY:O	1:C:302:LYS:HG2	2.16	0.46
1:D:240:ASP:HA	1:D:243:HIS:HB2	1.98	0.46
1:A:605:GLU:HA	1:A:625:TRP:NE1	2.30	0.46
1:B:735:THR:O	1:B:739:VAL:HG23	2.15	0.46
1:D:752:GLU:H	1:D:752:GLU:CD	2.22	0.46
1:A:152:ILE:HG13	1:A:153:MET:N	2.30	0.46
1:A:163:LYS:HD3	1:A:169:THR:HG23	1.97	0.46
1:A:452:ASP:OD1	1:A:453:LYS:N	2.49	0.46
1:A:529:GLU:OE2	1:A:558:TYR:OH	2.26	0.46
1:B:632:TRP:HA	1:B:635:LYS:HZ1	1.78	0.46
1:B:752:GLU:H	1:B:752:GLU:CD	2.22	0.46
1:C:163:LYS:HD3	1:C:169:THR:HG23	1.97	0.46
1:C:542:LEU:HD12	1:C:542:LEU:HA	1.70	0.46
1:D:419:SER:OG	1:D:434:GLU:HB2	2.16	0.46
1:A:620:SER:HA	1:A:623:GLU:OE2	2.15	0.46
1:B:397:PHE:HB2	1:B:436:PHE:CE2	2.51	0.46
1:C:452:ASP:OD1	1:C:453:LYS:N	2.49	0.46
1:D:737:LEU:HD23	1:D:737:LEU:HA	1.76	0.46
1:A:735:THR:O	1:A:739:VAL:HG23	2.15	0.46
1:B:220:GLU:C	1:B:224:LYS:HZ3	2.21	0.46
1:B:503:MET:SD	1:B:503:MET:N	2.89	0.46
1:C:719:ARG:O	1:C:723:GLN:HG2	2.16	0.46
1:D:620:SER:HA	1:D:623:GLU:OE2	2.15	0.46
1:D:719:ARG:O	1:D:723:GLN:HG2	2.16	0.46
1:A:419:SER:OG	1:A:434:GLU:HB2	2.16	0.46
1:B:419:SER:OG	1:B:434:GLU:HB2	2.16	0.46
1:B:719:ARG:O	1:B:723:GLN:HG2	2.16	0.46
1:D:397:PHE:HB2	1:D:436:PHE:CE2	2.51	0.46
1:A:240:ASP:HA	1:A:243:HIS:HB2	1.98	0.46
1:B:180:GLN:HA	1:B:183:MET:HG2	1.98	0.46
1:B:240:ASP:HA	1:B:243:HIS:HB2	1.98	0.46
1:B:393:LYS:HZ1	1:B:398:PHE:HB2	1.80	0.46
1:D:542:LEU:HA	1:D:542:LEU:HD12	1.70	0.46
1:D:632:TRP:HA	1:D:635:LYS:NZ	2.31	0.46
1:A:251:HIS:O	1:A:280:SER:OG	2.33	0.46
1:B:163:LYS:HD3	1:B:169:THR:HG23	1.97	0.46
1:C:180:GLN:HA	1:C:183:MET:HG2	1.98	0.46
1:C:240:ASP:HA	1:C:243:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:LYS:HZ2	1:C:642:ILE:HA	1.80	0.46
1:D:202:LEU:HA	1:D:205:LEU:HB2	1.98	0.46
1:D:228:ALA:O	1:D:232:ARG:HG3	2.16	0.46
1:D:667:ARG:HB3	1:D:671:TRP:CH2	2.51	0.46
1:A:393:LYS:NZ	1:A:400:LEU:O	2.49	0.46
1:A:503:MET:SD	1:A:503:MET:N	2.89	0.46
1:B:152:ILE:HG13	1:B:153:MET:N	2.30	0.45
1:B:202:LEU:HA	1:B:205:LEU:HB2	1.98	0.45
1:B:210:LYS:HB3	1:B:210:LYS:HE2	1.61	0.45
1:B:667:ARG:HH21	1:A:655:GLU:HG3	1.80	0.45
1:C:503:MET:SD	1:C:503:MET:N	2.89	0.45
1:C:185:ARG:HA	1:C:188:HIS:CE1	2.50	0.45
1:C:228:ALA:O	1:C:232:ARG:HG3	2.16	0.45
1:C:419:SER:OG	1:C:434:GLU:HB2	2.16	0.45
1:D:503:MET:SD	1:D:503:MET:N	2.89	0.45
1:A:202:LEU:HA	1:A:205:LEU:HB2	1.98	0.45
1:A:299:GLY:O	1:A:302:LYS:HG2	2.16	0.45
1:A:397:PHE:HB2	1:A:436:PHE:CE2	2.51	0.45
1:B:299:GLY:O	1:B:302:LYS:HG2	2.15	0.45
1:B:684:CYS:O	1:B:687:LEU:HD23	2.16	0.45
1:D:452:ASP:OD1	1:D:453:LYS:N	2.49	0.45
1:D:684:CYS:O	1:D:687:LEU:HD23	2.16	0.45
1:A:228:ALA:O	1:A:232:ARG:HG3	2.16	0.45
1:A:393:LYS:NZ	1:A:398:PHE:HB2	2.32	0.45
1:A:719:ARG:O	1:A:723:GLN:HG2	2.16	0.45
1:B:679:LEU:HD13	1:B:679:LEU:HA	1.73	0.45
1:C:376:LEU:HD12	1:C:376:LEU:HA	1.77	0.45
1:C:393:LYS:NZ	1:C:400:LEU:O	2.49	0.45
1:C:684:CYS:O	1:C:687:LEU:HD23	2.16	0.45
1:D:210:LYS:HE2	1:D:210:LYS:HB3	1.61	0.45
1:D:262:GLU:OE1	1:D:262:GLU:N	2.50	0.45
1:D:567:GLU:OE2	1:D:567:GLU:N	2.45	0.45
1:A:180:GLN:HA	1:A:183:MET:HG2	1.98	0.45
1:B:116:ASP:OD1	1:B:116:ASP:N	2.44	0.45
1:B:199:GLU:H	1:B:199:GLU:CD	2.25	0.45
1:B:452:ASP:OD1	1:B:453:LYS:N	2.49	0.45
1:C:342:CYS:O	1:C:346:ILE:HG12	2.17	0.45
1:D:152:ILE:HG21	1:D:186:LEU:HD21	1.99	0.45
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.73	0.45
1:B:111:LEU:HD21	1:B:161:ALA:HA	1.99	0.45
1:C:152:ILE:HG13	1:C:153:MET:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:PHE:HB2	1:C:436:PHE:CE2	2.51	0.45
1:C:629:LEU:O	1:C:633:THR:HG23	2.17	0.45
1:D:299:GLY:HA2	1:D:302:LYS:HG2	1.99	0.45
1:D:629:LEU:O	1:D:633:THR:HG23	2.17	0.45
1:D:111:LEU:HD21	1:D:161:ALA:HA	1.99	0.45
1:A:629:LEU:O	1:A:633:THR:HG23	2.17	0.45
1:B:152:ILE:HG21	1:B:186:LEU:HD21	1.99	0.45
1:B:170:ASP:CG	1:B:171:LYS:HZ3	2.21	0.45
1:C:541:ASN:C	1:C:544:LYS:HZ2	2.25	0.45
1:D:180:GLN:HA	1:D:183:MET:HG2	1.98	0.45
1:D:715:GLN:O	1:D:718:THR:OG1	2.29	0.45
1:A:199:GLU:H	1:A:199:GLU:CD	2.25	0.45
1:A:342:CYS:O	1:A:346:ILE:HG12	2.17	0.45
1:C:262:GLU:N	1:C:262:GLU:OE1	2.50	0.45
1:C:472:TRP:O	1:C:475:SER:OG	2.35	0.45
1:D:753:THR:O	1:D:756:SER:OG	2.25	0.45
1:A:162:LEU:HD11	1:A:172:CYS:HB2	1.98	0.45
1:B:342:CYS:O	1:B:346:ILE:HG12	2.17	0.44
1:B:393:LYS:NZ	1:B:398:PHE:HB2	2.32	0.44
1:B:655:GLU:OE2	1:B:660:ARG:HB2	2.17	0.44
1:B:667:ARG:N	1:B:668:PRO:HD2	2.33	0.44
1:A:684:CYS:O	1:A:687:LEU:HD23	2.16	0.44
1:C:251:HIS:O	1:C:280:SER:OG	2.33	0.44
1:D:571:ALA:HA	1:D:574:ARG:HB2	1.99	0.44
1:A:111:LEU:HD21	1:A:161:ALA:HA	1.99	0.44
1:A:262:GLU:N	1:A:262:GLU:OE1	2.50	0.44
1:A:472:TRP:O	1:A:475:SER:OG	2.35	0.44
1:B:262:GLU:OE1	1:B:262:GLU:N	2.50	0.44
1:C:162:LEU:HD11	1:C:172:CYS:HB2	1.99	0.44
1:C:667:ARG:N	1:C:668:PRO:HD2	2.32	0.44
1:A:667:ARG:N	1:A:668:PRO:HD2	2.33	0.44
1:B:266:LYS:HB3	1:B:266:LYS:HE3	1.84	0.44
1:B:571:ALA:HA	1:B:574:ARG:HB2	1.99	0.44
1:C:220:GLU:C	1:C:224:LYS:HZ3	2.22	0.44
1:D:626:LYS:HE2	1:D:626:LYS:HB3	1.77	0.44
1:A:571:ALA:HA	1:A:574:ARG:HB2	1.99	0.44
1:A:755:ASP:OD1	1:A:756:SER:N	2.51	0.44
1:C:111:LEU:HD21	1:C:161:ALA:HA	1.99	0.44
1:C:521:ASN:O	1:C:524:LYS:HG2	2.18	0.44
1:A:521:ASN:O	1:A:524:LYS:HG2	2.18	0.44
1:B:552:THR:O	1:B:556:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:LYS:NZ	1:C:398:PHE:HB2	2.32	0.44
1:C:428:GLY:O	1:C:432:ARG:HG3	2.18	0.44
1:C:635:LYS:HE3	1:C:635:LYS:HB2	1.36	0.44
1:D:552:THR:O	1:D:556:THR:HG23	2.18	0.44
1:A:220:GLU:H	1:A:224:LYS:NZ	2.16	0.44
1:A:428:GLY:O	1:A:432:ARG:HG3	2.18	0.44
1:B:321:TRP:HB3	1:B:506:PHE:CE2	2.53	0.44
1:B:629:LEU:O	1:B:633:THR:HG23	2.17	0.44
1:C:552:THR:O	1:C:556:THR:HG23	2.18	0.44
1:C:755:ASP:OD1	1:C:756:SER:N	2.51	0.44
1:D:342:CYS:O	1:D:346:ILE:HG12	2.17	0.44
1:B:162:LEU:HD11	1:B:172:CYS:HB2	1.99	0.44
1:B:567:GLU:OE2	1:B:567:GLU:N	2.45	0.44
1:B:618:SER:CB	1:C:619:GLY:HA3	2.47	0.44
1:C:266:LYS:HE3	1:C:266:LYS:HB3	1.84	0.44
1:D:162:LEU:HD11	1:D:172:CYS:HB2	1.99	0.44
1:D:199:GLU:H	1:D:199:GLU:CD	2.25	0.44
1:D:655:GLU:OE2	1:D:660:ARG:HB2	2.17	0.44
1:A:152:ILE:HG21	1:A:186:LEU:HD21	1.99	0.44
1:B:268:ARG:H	1:B:268:ARG:HG2	1.68	0.43
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.77	0.43
1:B:428:GLY:O	1:B:432:ARG:HG3	2.18	0.43
1:C:571:ALA:HA	1:C:574:ARG:HB2	1.99	0.43
1:C:722:LEU:HA	1:C:722:LEU:HD23	1.73	0.43
1:A:250:LEU:HD11	1:A:267:LEU:HD23	2.00	0.43
1:A:303:LYS:HZ3	1:A:303:LYS:HB2	1.82	0.43
1:B:340:GLU:HA	1:B:343:LEU:HB2	2.00	0.43
1:C:152:ILE:HG21	1:C:186:LEU:HD21	1.99	0.43
1:C:202:LEU:HA	1:C:205:LEU:HB2	1.99	0.43
1:C:699:SER:HB2	1:C:702:LYS:HE2	2.00	0.43
1:D:521:ASN:O	1:D:524:LYS:HG2	2.18	0.43
1:C:220:GLU:H	1:C:224:LYS:NZ	2.16	0.43
1:C:473:LYS:HE2	1:C:711:ASP:OD2	2.19	0.43
1:D:170:ASP:CG	1:D:171:LYS:HZ3	2.23	0.43
1:D:376:LEU:HD12	1:D:376:LEU:HA	1.77	0.43
1:D:428:GLY:O	1:D:432:ARG:HG3	2.18	0.43
1:D:472:TRP:O	1:D:475:SER:OG	2.35	0.43
1:D:755:ASP:OD1	1:D:756:SER:N	2.51	0.43
1:A:655:GLU:OE2	1:A:660:ARG:HB2	2.17	0.43
1:B:200:ILE:HG22	1:B:255:GLY:HA3	2.01	0.43
1:B:472:TRP:O	1:B:475:SER:OG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LEU:HD11	1:C:227:TYR:CZ	2.53	0.43
1:C:655:GLU:OE2	1:C:660:ARG:HB2	2.17	0.43
1:D:234:LEU:HD23	1:D:237:ILE:HD11	2.01	0.43
1:A:137:ASP:HB2	1:A:178:PHE:CE1	2.54	0.43
1:C:503:MET:O	1:C:507:CYS:HB2	2.19	0.43
1:D:200:ILE:HG22	1:D:255:GLY:HA3	2.01	0.43
1:D:220:GLU:H	1:D:224:LYS:NZ	2.16	0.43
1:D:503:MET:O	1:D:507:CYS:HB2	2.19	0.43
1:A:200:ILE:HG22	1:A:255:GLY:HA3	2.01	0.43
1:A:321:TRP:HB3	1:A:506:PHE:CE2	2.53	0.43
1:B:227:TYR:HD1	1:B:227:TYR:HA	1.72	0.43
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.85	0.43
1:C:589:SER:HB2	1:C:592:ARG:HH21	1.84	0.43
1:C:605:GLU:HB3	1:C:629:LEU:HD12	2.00	0.43
1:D:251:HIS:O	1:D:280:SER:OG	2.33	0.43
1:D:321:TRP:HB3	1:D:506:PHE:CE2	2.53	0.43
1:D:393:LYS:NZ	1:D:398:PHE:HB2	2.32	0.43
1:D:623:GLU:HA	1:D:626:LYS:HE3	2.01	0.43
1:D:699:SER:HB2	1:D:702:LYS:HE2	2.00	0.43
1:A:210:LYS:HB3	1:A:210:LYS:HE2	1.61	0.43
1:A:503:MET:O	1:A:507:CYS:HB2	2.19	0.43
1:A:552:THR:O	1:A:556:THR:HG23	2.18	0.43
1:C:125:SER:HA	1:C:128:ASP:OD2	2.19	0.43
1:A:223:LEU:HD11	1:A:227:TYR:CZ	2.54	0.43
1:A:340:GLU:HA	1:A:343:LEU:HB2	2.00	0.43
1:A:473:LYS:HE2	1:A:711:ASP:OD2	2.19	0.43
1:A:605:GLU:HB3	1:A:629:LEU:HD12	2.00	0.43
1:B:236:LYS:HB3	1:B:236:LYS:HE3	1.56	0.43
1:B:503:MET:O	1:B:507:CYS:HB2	2.19	0.43
1:C:178:PHE:O	1:C:182:ASN:ND2	2.39	0.43
1:C:321:TRP:HB3	1:C:506:PHE:CE2	2.53	0.43
1:C:567:GLU:OE2	1:C:567:GLU:N	2.45	0.43
1:C:701:GLU:H	1:C:701:GLU:HG3	1.61	0.43
1:A:266:LYS:HE3	1:A:266:LYS:HB3	1.84	0.43
1:B:220:GLU:H	1:B:224:LYS:NZ	2.16	0.43
1:B:223:LEU:HD11	1:B:227:TYR:CZ	2.54	0.43
1:B:719:ARG:HD2	1:B:723:GLN:HE21	1.84	0.43
1:C:325:ARG:O	1:C:329:LEU:N	2.47	0.43
1:D:701:GLU:H	1:D:701:GLU:HG3	1.61	0.43
1:B:671:TRP:CD1	1:A:652:ARG:NE	2.87	0.43
1:B:715:GLN:O	1:B:718:THR:OG1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ASP:OD1	1:B:756:SER:N	2.51	0.43
1:C:199:GLU:H	1:C:199:GLU:CD	2.25	0.43
1:C:200:ILE:HG22	1:C:255:GLY:HA3	2.01	0.43
1:D:340:GLU:HA	1:D:343:LEU:HB2	2.00	0.43
1:D:731:LEU:HA	1:D:734:GLU:OE1	2.19	0.43
1:A:699:SER:HB2	1:A:702:LYS:HE2	2.00	0.43
1:A:714:MET:HE2	1:A:714:MET:HB2	1.91	0.43
1:B:137:ASP:HB2	1:B:178:PHE:CE1	2.54	0.42
1:B:299:GLY:HA2	1:B:302:LYS:HG2	2.01	0.42
1:B:328:ARG:HD2	1:B:484:TYR:CD1	2.54	0.42
1:B:393:LYS:NZ	1:B:400:LEU:O	2.49	0.42
1:D:137:ASP:HB2	1:D:178:PHE:CE1	2.54	0.42
1:D:250:LEU:HD11	1:D:267:LEU:HD23	2.00	0.42
1:A:178:PHE:O	1:A:182:ASN:ND2	2.39	0.42
1:B:245:MET:O	1:B:247:THR:HG23	2.19	0.42
1:B:632:TRP:CA	1:B:635:LYS:HE2	2.48	0.42
1:B:699:SER:HB2	1:B:702:LYS:HE2	2.00	0.42
1:D:125:SER:HA	1:D:128:ASP:OD2	2.19	0.42
1:D:223:LEU:HD11	1:D:227:TYR:CZ	2.54	0.42
1:D:245:MET:O	1:D:247:THR:HG23	2.19	0.42
1:D:473:LYS:HE2	1:D:711:ASP:OD2	2.19	0.42
1:B:125:SER:HA	1:B:128:ASP:OD2	2.19	0.42
1:B:178:PHE:O	1:B:182:ASN:ND2	2.39	0.42
1:B:521:ASN:O	1:B:524:LYS:HG2	2.18	0.42
1:C:137:ASP:HB2	1:C:178:PHE:CE1	2.54	0.42
1:C:250:LEU:HD11	1:C:267:LEU:HD23	2.00	0.42
1:C:340:GLU:HA	1:C:343:LEU:HB2	2.00	0.42
1:C:510:LEU:HA	1:C:513:LYS:HG2	2.01	0.42
1:C:623:GLU:HA	1:C:626:LYS:HE3	2.01	0.42
1:A:753:THR:O	1:A:756:SER:OG	2.25	0.42
1:B:516:LYS:O	1:B:520:SER:OG	2.34	0.42
1:C:719:ARG:HD2	1:C:723:GLN:HE21	1.84	0.42
1:C:753:THR:O	1:C:756:SER:OG	2.25	0.42
1:D:148:MET:HA	1:D:148:MET:CE	2.44	0.42
1:D:605:GLU:HB3	1:D:629:LEU:HD12	2.00	0.42
1:A:485:LEU:HD23	1:A:485:LEU:HA	1.86	0.42
1:A:719:ARG:HD2	1:A:723:GLN:HE21	1.84	0.42
1:A:731:LEU:HA	1:A:734:GLU:OE1	2.19	0.42
1:B:623:GLU:HA	1:B:626:LYS:HE3	2.01	0.42
1:B:753:THR:O	1:B:756:SER:OG	2.25	0.42
1:C:472:TRP:HE1	1:C:718:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:CYS:HA	1:D:529:GLU:HG2	2.02	0.42
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.85	0.42
1:A:626:LYS:HB3	1:A:626:LYS:HE2	1.77	0.42
1:B:260:ASP:OD2	1:B:263:LYS:N	2.50	0.42
1:B:510:LEU:HA	1:B:513:LYS:HG2	2.01	0.42
1:B:526:CYS:HA	1:B:529:GLU:HG2	2.02	0.42
1:B:671:TRP:CH2	1:A:624:ALA:HB2	2.54	0.42
1:C:234:LEU:HD23	1:C:237:ILE:HD11	2.01	0.42
1:D:472:TRP:HE1	1:D:718:THR:HG21	1.85	0.42
1:A:234:LEU:HD23	1:A:237:ILE:HD11	2.01	0.42
1:A:328:ARG:HD2	1:A:484:TYR:CD1	2.54	0.42
1:A:623:GLU:HA	1:A:626:LYS:HE3	2.01	0.42
1:B:250:LEU:HD11	1:B:267:LEU:HD23	2.00	0.42
1:B:423:PHE:HB2	1:B:426:ASP:OD2	2.20	0.42
1:B:589:SER:HB2	1:B:592:ARG:HH21	1.84	0.42
1:B:605:GLU:HB3	1:B:629:LEU:HD12	2.00	0.42
1:D:510:LEU:HA	1:D:513:LYS:HG2	2.01	0.42
1:D:757:HIS:O	1:D:761:VAL:HG12	2.20	0.42
1:A:125:SER:HA	1:A:128:ASP:OD2	2.19	0.42
1:A:260:ASP:OD2	1:A:263:LYS:N	2.50	0.42
1:A:325:ARG:O	1:A:329:LEU:N	2.48	0.42
1:A:510:LEU:HA	1:A:513:LYS:HG2	2.01	0.42
1:B:393:LYS:C	1:B:394:ASP:OD1	2.63	0.42
1:B:473:LYS:HE2	1:B:711:ASP:OD2	2.19	0.42
1:C:328:ARG:HD2	1:C:484:TYR:CD1	2.54	0.42
1:C:393:LYS:C	1:C:394:ASP:OD1	2.63	0.42
1:C:494:VAL:HA	1:C:502:ARG:HG2	2.02	0.42
1:C:635:LYS:NZ	1:C:642:ILE:HA	2.34	0.42
1:D:178:PHE:O	1:D:182:ASN:ND2	2.39	0.42
1:D:589:SER:HB2	1:D:592:ARG:HH21	1.84	0.42
1:B:626:LYS:HB3	1:B:626:LYS:HE2	1.77	0.42
1:C:281:THR:HB	1:C:293:CYS:SG	2.60	0.42
1:C:423:PHE:HB2	1:C:426:ASP:OD2	2.20	0.42
1:C:526:CYS:HA	1:C:529:GLU:HG2	2.02	0.42
1:D:281:THR:HB	1:D:293:CYS:SG	2.60	0.42
1:A:80:THR:OG1	1:A:82:THR:HG23	2.20	0.42
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.70	0.42
1:A:589:SER:HB2	1:A:592:ARG:HH21	1.84	0.42
1:A:635:LYS:HB2	1:A:635:LYS:HE3	1.40	0.42
1:B:91:LEU:O	1:B:94:ILE:HG12	2.20	0.42
1:B:731:LEU:HA	1:B:734:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASP:O	1:C:89:THR:HG23	2.20	0.42
1:A:245:MET:O	1:A:247:THR:HG23	2.19	0.42
1:B:234:LEU:HD23	1:B:237:ILE:HD11	2.01	0.41
1:B:516:LYS:HE3	1:B:767:ILE:HG22	2.02	0.41
1:C:589:SER:HA	1:C:592:ARG:NE	2.35	0.41
1:C:731:LEU:HA	1:C:734:GLU:OE1	2.19	0.41
1:D:85:ASP:O	1:D:89:THR:HG23	2.20	0.41
1:A:393:LYS:C	1:A:394:ASP:OD1	2.63	0.41
1:A:454:TRP:HA	1:A:496:ILE:HB	2.03	0.41
1:A:472:TRP:HE1	1:A:718:THR:HG21	1.85	0.41
1:B:590:HIS:CE1	1:B:594:ILE:HD13	2.55	0.41
1:B:652:ARG:O	1:B:656:ILE:HD12	2.21	0.41
1:C:245:MET:O	1:C:247:THR:HG23	2.19	0.41
1:C:271:ASP:OD1	1:C:271:ASP:N	2.53	0.41
1:C:757:HIS:O	1:C:761:VAL:HG12	2.20	0.41
1:D:393:LYS:C	1:D:394:ASP:OD1	2.63	0.41
1:D:423:PHE:HB2	1:D:426:ASP:OD2	2.20	0.41
1:A:91:LEU:O	1:A:94:ILE:HG12	2.20	0.41
1:C:91:LEU:O	1:C:94:ILE:HG12	2.20	0.41
1:C:319:ARG:HD3	1:C:346:ILE:HD11	2.02	0.41
1:C:454:TRP:HA	1:C:496:ILE:HB	2.03	0.41
1:C:518:ASP:HA	1:C:521:ASN:ND2	2.35	0.41
1:D:454:TRP:HA	1:D:496:ILE:HB	2.03	0.41
1:D:719:ARG:HD2	1:D:723:GLN:HE21	1.84	0.41
1:A:281:THR:HB	1:A:293:CYS:SG	2.60	0.41
1:B:115:LEU:H	1:B:115:LEU:HG	1.45	0.41
1:B:281:THR:HB	1:B:293:CYS:SG	2.60	0.41
1:B:737:LEU:HD23	1:B:737:LEU:HA	1.76	0.41
1:C:632:TRP:HA	1:C:635:LYS:HE2	2.02	0.41
1:D:494:VAL:HA	1:D:502:ARG:HG2	2.02	0.41
1:D:590:HIS:CE1	1:D:594:ILE:HD13	2.55	0.41
1:A:590:HIS:CE1	1:A:594:ILE:HD13	2.55	0.41
1:C:605:GLU:HA	1:C:625:TRP:HE1	1.85	0.41
1:C:626:LYS:HB3	1:C:626:LYS:HE2	1.77	0.41
1:C:652:ARG:O	1:C:656:ILE:HD12	2.21	0.41
1:D:328:ARG:HD2	1:D:484:TYR:CD1	2.54	0.41
1:A:299:GLY:HA2	1:A:302:LYS:HG2	2.01	0.41
1:A:757:HIS:O	1:A:761:VAL:HG12	2.20	0.41
1:B:518:ASP:HA	1:B:521:ASN:ND2	2.35	0.41
1:D:298:ASP:O	1:D:302:LYS:N	2.53	0.41
1:D:652:ARG:O	1:D:656:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:O	1:A:89:THR:HG23	2.20	0.41
1:A:338:GLU:H	1:A:338:GLU:HG3	1.47	0.41
1:A:376:LEU:HA	1:A:376:LEU:HD12	1.77	0.41
1:A:589:SER:HA	1:A:592:ARG:NE	2.35	0.41
1:B:227:TYR:O	1:B:231:GLU:HG2	2.21	0.41
1:B:589:SER:HA	1:B:592:ARG:NE	2.35	0.41
1:B:605:GLU:HA	1:B:625:TRP:HE1	1.85	0.41
1:D:114:ARG:HB3	1:D:118:GLY:HA3	2.03	0.41
1:D:319:ARG:HD3	1:D:346:ILE:HD11	2.02	0.41
1:D:417:ARG:O	1:D:420:GLN:HG2	2.21	0.41
1:D:589:SER:HA	1:D:592:ARG:NE	2.35	0.41
1:A:114:ARG:HB3	1:A:118:GLY:HA3	2.03	0.41
1:A:423:PHE:HB2	1:A:426:ASP:OD2	2.20	0.41
1:A:516:LYS:HE3	1:A:767:ILE:HG22	2.02	0.41
1:B:80:THR:OG1	1:B:82:THR:HG23	2.20	0.41
1:B:85:ASP:O	1:B:89:THR:HG23	2.20	0.41
1:B:454:TRP:HA	1:B:496:ILE:HB	2.03	0.41
1:B:538:LEU:HD21	1:D:344:ASP:HB2	2.03	0.41
1:B:722:LEU:HD23	1:B:722:LEU:HA	1.73	0.41
1:D:80:THR:OG1	1:D:82:THR:HG23	2.20	0.41
1:D:466:TYR:CE2	1:D:480:GLU:HG3	2.56	0.41
1:D:518:ASP:HA	1:D:521:ASN:ND2	2.35	0.41
1:A:220:GLU:C	1:A:224:LYS:HZ3	2.21	0.41
1:A:526:CYS:HA	1:A:529:GLU:HG2	2.02	0.41
1:A:541:ASN:C	1:A:544:LYS:HZ2	2.25	0.41
1:B:114:ARG:HB3	1:B:118:GLY:HA3	2.03	0.41
1:B:242:LEU:HA	1:B:242:LEU:HD23	1.90	0.41
1:B:494:VAL:HA	1:B:502:ARG:HG2	2.02	0.41
1:B:549:ASP:O	1:B:553:THR:HG22	2.21	0.41
1:C:80:THR:OG1	1:C:82:THR:HG23	2.20	0.41
1:C:549:ASP:O	1:C:553:THR:HG22	2.21	0.41
1:D:227:TYR:O	1:D:231:GLU:HG2	2.21	0.41
1:D:441:LEU:HD23	1:D:441:LEU:HA	1.91	0.41
1:D:516:LYS:HE3	1:D:767:ILE:HG22	2.02	0.41
1:D:597:PRO:O	1:D:600:SER:HB3	2.21	0.41
1:A:140:TRP:HE1	1:A:158:CYS:HG	1.63	0.41
1:A:227:TYR:O	1:A:231:GLU:HG2	2.21	0.41
1:A:271:ASP:OD1	1:A:271:ASP:N	2.53	0.41
1:A:319:ARG:HD3	1:A:346:ILE:HD11	2.02	0.41
1:A:417:ARG:O	1:A:420:GLN:HG2	2.21	0.41
1:A:549:ASP:O	1:A:553:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HD13	1:A:679:LEU:HA	1.73	0.41
1:B:466:TYR:CE2	1:B:480:GLU:HG3	2.56	0.41
1:C:679:LEU:HD13	1:C:679:LEU:HA	1.73	0.41
1:D:419:SER:HA	1:D:430:LEU:HD22	2.03	0.41
1:D:536:TRP:HE1	1:D:612:PRO:HD3	1.86	0.41
1:D:549:ASP:O	1:D:553:THR:HG22	2.21	0.41
1:D:589:SER:HA	1:D:592:ARG:HH21	1.86	0.41
1:D:721:VAL:HG13	1:D:733:ARG:HB3	2.03	0.41
1:A:518:ASP:HA	1:A:521:ASN:ND2	2.35	0.41
1:B:417:ARG:O	1:B:420:GLN:HG2	2.21	0.40
1:B:757:HIS:O	1:B:761:VAL:HG12	2.20	0.40
1:C:245:MET:HA	1:C:245:MET:CE	2.52	0.40
1:C:590:HIS:CE1	1:C:594:ILE:HD13	2.55	0.40
1:C:597:PRO:O	1:C:600:SER:HB3	2.21	0.40
1:C:690:ARG:HB2	1:C:706:ILE:HG21	2.03	0.40
1:D:91:LEU:O	1:D:94:ILE:HG12	2.20	0.40
1:D:122:GLN:HG3	1:D:123:PHE:CD2	2.56	0.40
1:A:245:MET:CE	1:A:245:MET:HA	2.51	0.40
1:A:605:GLU:HA	1:A:625:TRP:HE1	1.85	0.40
1:B:319:ARG:HD3	1:B:346:ILE:HD11	2.03	0.40
1:C:122:GLN:HG3	1:C:123:PHE:CD2	2.56	0.40
1:C:203:PRO:HG3	1:C:230:ARG:NE	2.36	0.40
1:C:227:TYR:O	1:C:231:GLU:HG2	2.21	0.40
1:C:299:GLY:HA2	1:C:302:LYS:CD	2.51	0.40
1:C:721:VAL:HG13	1:C:733:ARG:HB3	2.03	0.40
1:D:328:ARG:HD2	1:D:484:TYR:CE1	2.57	0.40
1:B:229:GLU:HB3	1:B:233:LYS:NZ	2.37	0.40
1:B:303:LYS:HZ3	1:B:303:LYS:HB2	1.86	0.40
1:B:377:ARG:NH1	1:B:421:LEU:O	2.48	0.40
1:B:472:TRP:HE1	1:B:718:THR:HG21	1.85	0.40
1:B:721:VAL:HG13	1:B:733:ARG:HB3	2.03	0.40
1:C:129:TRP:HA	1:C:132:GLN:OE1	2.22	0.40
1:C:466:TYR:CE2	1:C:480:GLU:HG3	2.56	0.40
1:D:758:ILE:HG23	1:D:762:ILE:HD12	2.03	0.40
1:A:129:TRP:HA	1:A:132:GLN:OE1	2.22	0.40
1:A:494:VAL:HA	1:A:502:ARG:HG2	2.02	0.40
1:A:632:TRP:HA	1:A:635:LYS:NZ	2.37	0.40
1:A:652:ARG:O	1:A:656:ILE:HD12	2.21	0.40
1:A:690:ARG:HB2	1:A:706:ILE:HG21	2.04	0.40
1:B:245:MET:HA	1:B:245:MET:CE	2.51	0.40
1:B:297:LEU:O	1:B:301:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:O	1:B:300:ILE:HG12	2.21	0.40
1:B:328:ARG:HD2	1:B:484:TYR:CE1	2.57	0.40
1:B:597:PRO:O	1:B:600:SER:HB3	2.21	0.40
1:B:758:ILE:HG23	1:B:762:ILE:HD12	2.03	0.40
1:C:510:LEU:HA	1:C:510:LEU:HD13	1.93	0.40
1:C:589:SER:HA	1:C:592:ARG:HH21	1.86	0.40
1:D:245:MET:CE	1:D:245:MET:HA	2.51	0.40
1:A:393:LYS:O	1:A:396:LYS:N	2.54	0.40
1:A:670:LEU:H	1:A:670:LEU:HG	1.66	0.40
1:A:758:ILE:HG23	1:A:762:ILE:HD12	2.03	0.40
1:B:419:SER:HA	1:B:430:LEU:HD22	2.03	0.40
1:B:536:TRP:HE1	1:B:612:PRO:HD3	1.86	0.40
1:B:701:GLU:H	1:B:701:GLU:HG3	1.61	0.40
1:C:354:GLY:O	1:C:355:LEU:HD23	2.22	0.40
1:D:207:ASP:O	1:D:210:LYS:HG2	2.22	0.40
1:D:242:LEU:HD23	1:D:242:LEU:HA	1.89	0.40
1:D:605:GLU:HA	1:D:625:TRP:HE1	1.85	0.40
1:D:722:LEU:HA	1:D:722:LEU:HD23	1.73	0.40
1:A:354:GLY:O	1:A:355:LEU:HD23	2.22	0.40
1:A:466:TYR:CE2	1:A:480:GLU:HG3	2.56	0.40
1:A:589:SER:HA	1:A:592:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	686/775 (88%)	647 (94%)	39 (6%)	0	100	100
1	B	686/775 (88%)	647 (94%)	39 (6%)	0	100	100
1	C	686/775 (88%)	647 (94%)	39 (6%)	0	100	100
1	D	686/775 (88%)	646 (94%)	40 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2744/3100 (88%)	2587 (94%)	157 (6%)	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	597/672 (89%)	504 (84%)	93 (16%)	2	15
1	B	597/672 (89%)	504 (84%)	93 (16%)	2	15
1	C	597/672 (89%)	504 (84%)	93 (16%)	2	15
1	D	597/672 (89%)	504 (84%)	93 (16%)	2	15
All	All	2388/2688 (89%)	2016 (84%)	372 (16%)	4	15

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	THR
1	B	82	THR
1	B	93	SER
1	B	96	GLU
1	B	100	SER
1	B	101	ILE
1	B	107	SER
1	B	111	LEU
1	B	115	LEU
1	B	125	SER
1	B	128	ASP
1	B	131	VAL
1	B	142	ASP
1	B	148	MET
1	B	156	LEU
1	B	163	LYS
1	B	191	GLU

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Mol	Chain	Res	Type
1	B	194	MET
1	B	196	VAL
1	B	240	ASP
1	B	245	MET
1	B	248	THR
1	B	257	VAL
1	B	258	ASP
1	B	266	LYS
1	B	270	LEU
1	B	271	ASP
1	B	280	SER
1	B	293	CYS
1	B	301	VAL
1	B	303	LYS
1	B	332	SER
1	B	337	SER
1	B	340	GLU
1	B	342	CYS
1	B	351	THR
1	B	353	ASP
1	B	360	ASN
1	B	363	VAL
1	B	365	ASP
1	B	378	LEU
1	B	387	VAL
1	B	399	CYS
1	B	400	LEU
1	B	414	ASN
1	B	419	SER
1	B	429	VAL
1	B	459	ASP
1	B	475	SER
1	B	483	LEU
1	B	493	ASP
1	B	520	SER
1	B	540	SER
1	B	542	LEU
1	B	554	LEU
1	B	569	ASN
1	B	580	VAL
1	B	583	LEU
1	B	587	VAL

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Mol	Chain	Res	Type
1	B	589	SER
1	B	593	ARG
1	B	605	GLU
1	B	607	LEU
1	B	609	SER
1	B	610	LEU
1	B	615	ASP
1	B	618	SER
1	B	635	LYS
1	B	645	ASP
1	B	651	VAL
1	B	656	ILE
1	B	662	VAL
1	B	664	THR
1	B	670	LEU
1	B	674	SER
1	B	679	LEU
1	B	681	SER
1	B	683	ILE
1	B	685	CYS
1	B	687	LEU
1	B	688	SER
1	B	695	GLU
1	B	699	SER
1	B	710	VAL
1	B	719	ARG
1	B	721	VAL
1	B	725	CYS
1	B	734	GLU
1	B	735	THR
1	B	737	LEU
1	B	739	VAL
1	B	740	VAL
1	B	767	ILE
1	C	81	THR
1	C	82	THR
1	C	93	SER
1	C	96	GLU
1	C	100	SER
1	C	101	ILE
1	C	107	SER
1	C	111	LEU

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Mol	Chain	Res	Type
1	C	115	LEU
1	C	125	SER
1	C	128	ASP
1	C	131	VAL
1	C	142	ASP
1	C	148	MET
1	C	156	LEU
1	C	163	LYS
1	C	191	GLU
1	C	194	MET
1	C	196	VAL
1	C	240	ASP
1	C	245	MET
1	C	248	THR
1	C	257	VAL
1	C	258	ASP
1	C	266	LYS
1	C	270	LEU
1	C	271	ASP
1	C	280	SER
1	C	293	CYS
1	C	301	VAL
1	C	303	LYS
1	C	332	SER
1	C	337	SER
1	C	340	GLU
1	C	342	CYS
1	C	351	THR
1	C	353	ASP
1	C	360	ASN
1	C	363	VAL
1	C	365	ASP
1	C	378	LEU
1	C	387	VAL
1	C	399	CYS
1	C	400	LEU
1	C	414	ASN
1	C	419	SER
1	C	429	VAL
1	C	459	ASP
1	C	475	SER
1	C	483	LEU

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Mol	Chain	Res	Type
1	C	493	ASP
1	C	520	SER
1	C	540	SER
1	C	542	LEU
1	C	554	LEU
1	C	569	ASN
1	C	580	VAL
1	C	583	LEU
1	C	587	VAL
1	C	589	SER
1	C	593	ARG
1	C	605	GLU
1	C	607	LEU
1	C	609	SER
1	C	610	LEU
1	C	615	ASP
1	C	618	SER
1	C	635	LYS
1	C	645	ASP
1	C	651	VAL
1	C	656	ILE
1	C	662	VAL
1	C	664	THR
1	C	670	LEU
1	C	674	SER
1	C	679	LEU
1	C	681	SER
1	C	683	ILE
1	C	685	CYS
1	C	687	LEU
1	C	688	SER
1	C	695	GLU
1	C	699	SER
1	C	710	VAL
1	C	719	ARG
1	C	721	VAL
1	C	725	CYS
1	C	734	GLU
1	C	735	THR
1	C	737	LEU
1	C	739	VAL
1	C	740	VAL

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Mol	Chain	Res	Type
1	C	767	ILE
1	D	81	THR
1	D	82	THR
1	D	93	SER
1	D	96	GLU
1	D	100	SER
1	D	101	ILE
1	D	107	SER
1	D	111	LEU
1	D	115	LEU
1	D	125	SER
1	D	128	ASP
1	D	131	VAL
1	D	142	ASP
1	D	148	MET
1	D	156	LEU
1	D	163	LYS
1	D	191	GLU
1	D	194	MET
1	D	196	VAL
1	D	240	ASP
1	D	245	MET
1	D	248	THR
1	D	257	VAL
1	D	258	ASP
1	D	266	LYS
1	D	270	LEU
1	D	271	ASP
1	D	280	SER
1	D	293	CYS
1	D	301	VAL
1	D	303	LYS
1	D	332	SER
1	D	337	SER
1	D	340	GLU
1	D	342	CYS
1	D	351	THR
1	D	353	ASP
1	D	360	ASN
1	D	363	VAL
1	D	365	ASP
1	D	378	LEU

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Mol	Chain	Res	Type
1	D	387	VAL
1	D	399	CYS
1	D	400	LEU
1	D	414	ASN
1	D	419	SER
1	D	429	VAL
1	D	459	ASP
1	D	475	SER
1	D	483	LEU
1	D	493	ASP
1	D	520	SER
1	D	540	SER
1	D	542	LEU
1	D	554	LEU
1	D	569	ASN
1	D	580	VAL
1	D	583	LEU
1	D	587	VAL
1	D	589	SER
1	D	593	ARG
1	D	605	GLU
1	D	607	LEU
1	D	609	SER
1	D	610	LEU
1	D	615	ASP
1	D	618	SER
1	D	635	LYS
1	D	645	ASP
1	D	651	VAL
1	D	656	ILE
1	D	662	VAL
1	D	664	THR
1	D	670	LEU
1	D	674	SER
1	D	679	LEU
1	D	681	SER
1	D	683	ILE
1	D	685	CYS
1	D	687	LEU
1	D	688	SER
1	D	695	GLU
1	D	699	SER

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Mol	Chain	Res	Type
1	D	710	VAL
1	D	719	ARG
1	D	721	VAL
1	D	725	CYS
1	D	734	GLU
1	D	735	THR
1	D	737	LEU
1	D	739	VAL
1	D	740	VAL
1	D	767	ILE
1	A	81	THR
1	A	82	THR
1	A	93	SER
1	A	96	GLU
1	A	100	SER
1	A	101	ILE
1	A	107	SER
1	A	111	LEU
1	A	115	LEU
1	A	125	SER
1	A	128	ASP
1	A	131	VAL
1	A	142	ASP
1	A	148	MET
1	A	156	LEU
1	A	163	LYS
1	A	191	GLU
1	A	194	MET
1	A	196	VAL
1	A	240	ASP
1	A	245	MET
1	A	248	THR
1	A	257	VAL
1	A	258	ASP
1	A	266	LYS
1	A	270	LEU
1	A	271	ASP
1	A	280	SER
1	A	293	CYS
1	A	301	VAL
1	A	303	LYS
1	A	332	SER

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Mol	Chain	Res	Type
1	A	337	SER
1	A	340	GLU
1	A	342	CYS
1	A	351	THR
1	A	353	ASP
1	A	360	ASN
1	A	363	VAL
1	A	365	ASP
1	A	378	LEU
1	A	387	VAL
1	A	399	CYS
1	A	400	LEU
1	A	414	ASN
1	A	419	SER
1	A	429	VAL
1	A	459	ASP
1	A	475	SER
1	A	483	LEU
1	A	493	ASP
1	A	520	SER
1	A	540	SER
1	A	542	LEU
1	A	554	LEU
1	A	569	ASN
1	A	580	VAL
1	A	583	LEU
1	A	587	VAL
1	A	589	SER
1	A	593	ARG
1	A	605	GLU
1	A	607	LEU
1	A	609	SER
1	A	610	LEU
1	A	615	ASP
1	A	618	SER
1	A	635	LYS
1	A	645	ASP
1	A	651	VAL
1	A	656	ILE
1	A	662	VAL
1	A	664	THR
1	A	670	LEU

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Mol	Chain	Res	Type
1	A	674	SER
1	A	679	LEU
1	A	681	SER
1	A	683	ILE
1	A	685	CYS
1	A	687	LEU
1	A	688	SER
1	A	695	GLU
1	A	699	SER
1	A	710	VAL
1	A	719	ARG
1	A	721	VAL
1	A	725	CYS
1	A	734	GLU
1	A	735	THR
1	A	737	LEU
1	A	739	VAL
1	A	740	VAL
1	A	767	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	HIS
1	B	357	HIS
1	B	420	GLN
1	B	531	ASN
1	B	551	GLN
1	B	590	HIS
1	B	678	GLN
1	B	696	ASN
1	B	709	GLN
1	B	764	GLN
1	C	168	HIS
1	C	357	HIS
1	C	401	HIS
1	C	420	GLN
1	C	531	ASN
1	C	551	GLN
1	C	590	HIS
1	C	678	GLN
1	C	696	ASN

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Mol	Chain	Res	Type
1	C	709	GLN
1	C	764	GLN
1	D	168	HIS
1	D	357	HIS
1	D	420	GLN
1	D	531	ASN
1	D	551	GLN
1	D	590	HIS
1	D	675	GLN
1	D	678	GLN
1	D	696	ASN
1	D	709	GLN
1	D	764	GLN
1	A	168	HIS
1	A	357	HIS
1	A	420	GLN
1	A	531	ASN
1	A	551	GLN
1	A	590	HIS
1	A	678	GLN
1	A	696	ASN
1	A	709	GLN
1	A	764	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

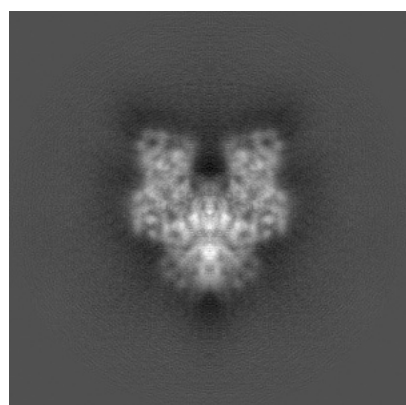
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35202. These allow visual inspection of the internal detail of the map and identification of artifacts.

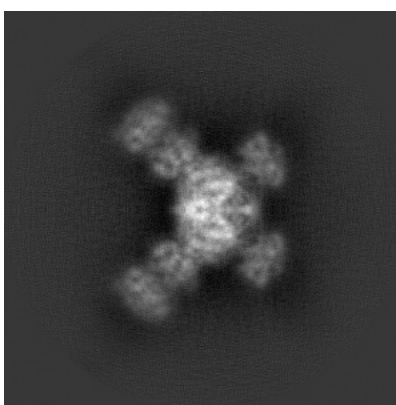
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

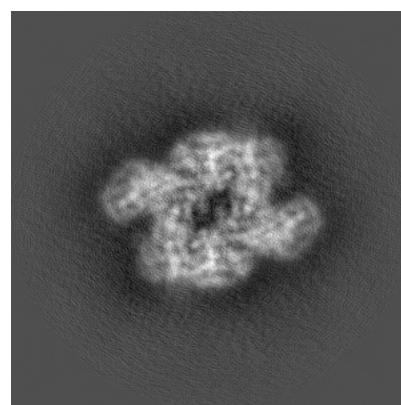
6.1.1 Primary map



X



Y

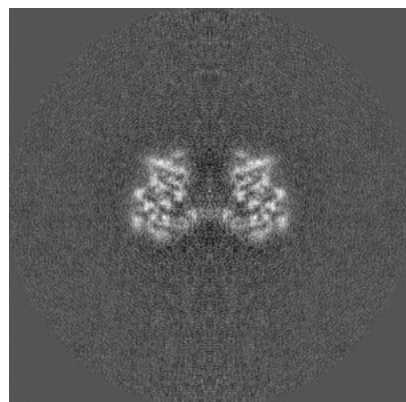


Z

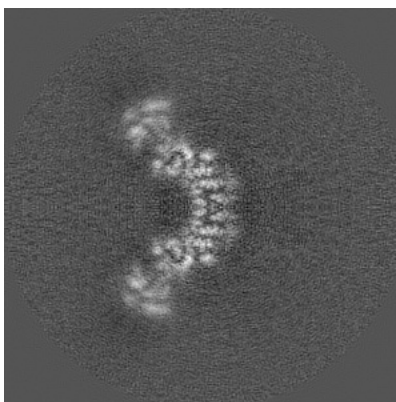
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

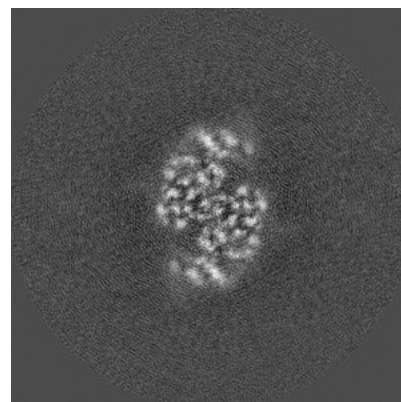
6.2.1 Primary map



X Index: 140



Y Index: 140

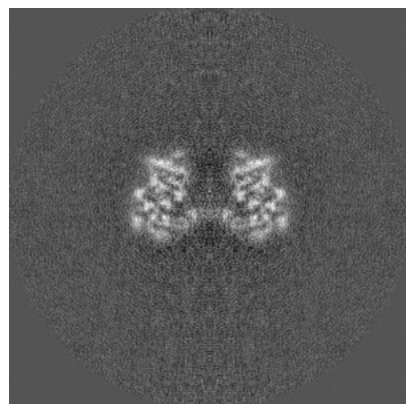


Z Index: 140

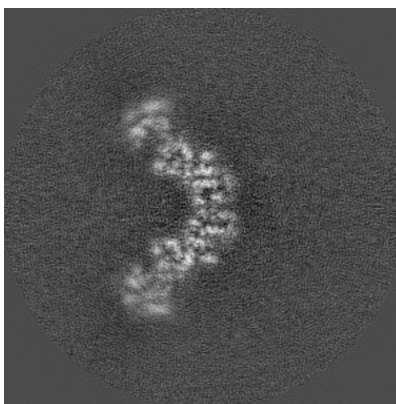
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

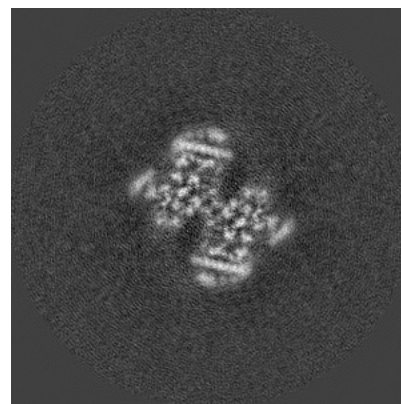
6.3.1 Primary map



X Index: 140



Y Index: 141

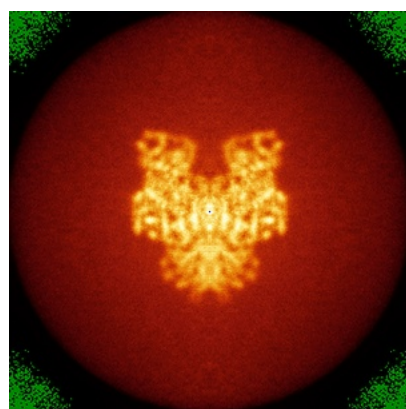


Z Index: 133

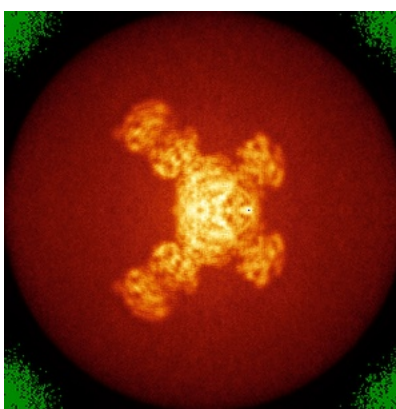
The images above show the largest variance slices of the map in three orthogonal directions.

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

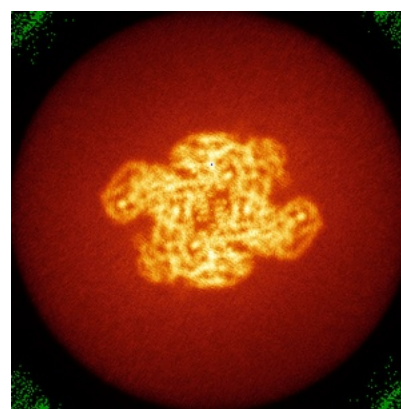
6.4.1 Primary map



X



Y

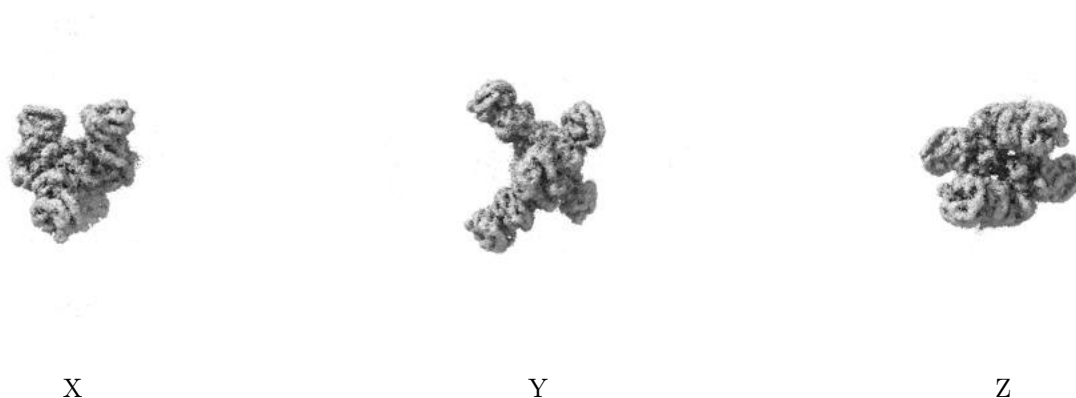


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0137. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

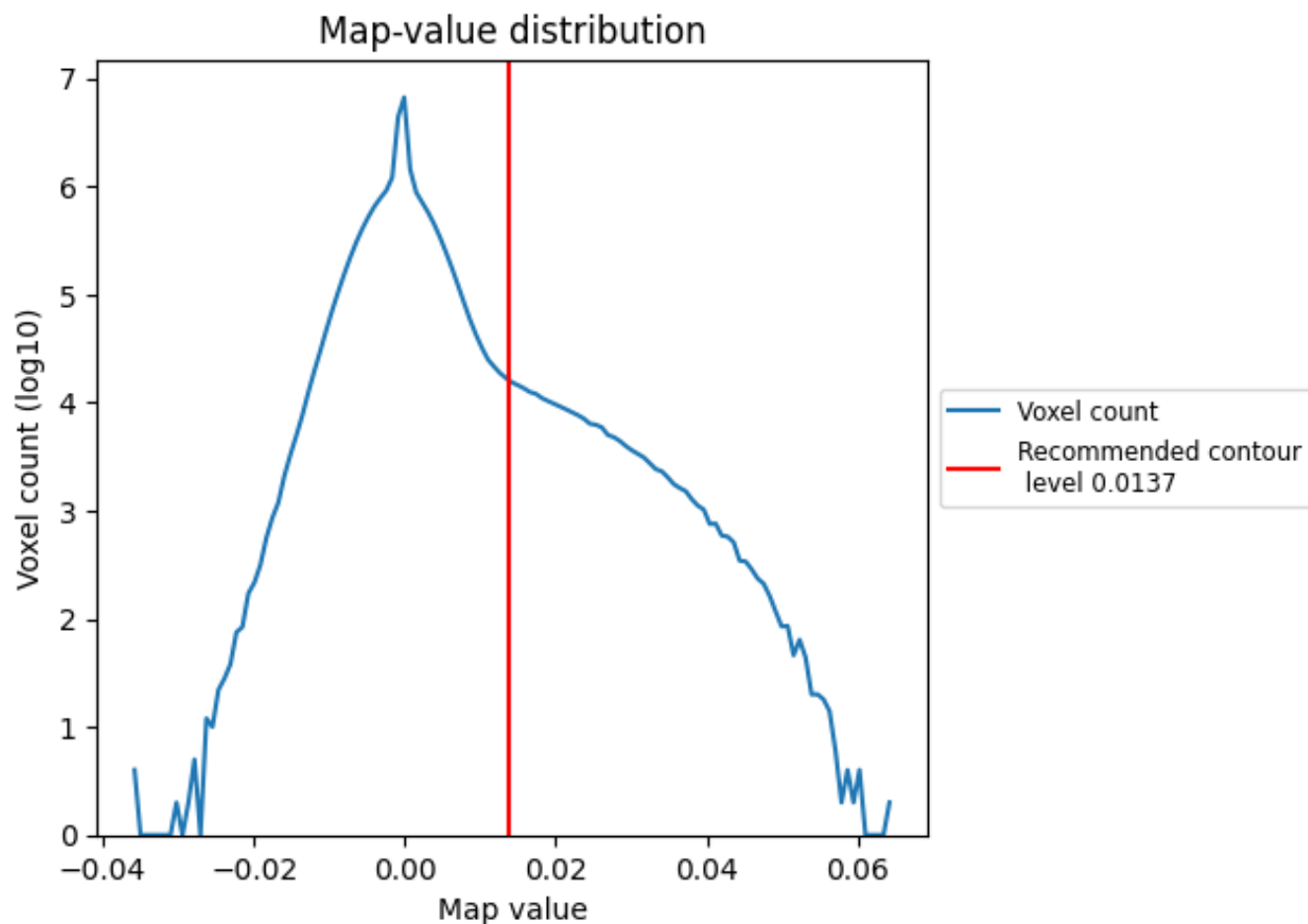
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

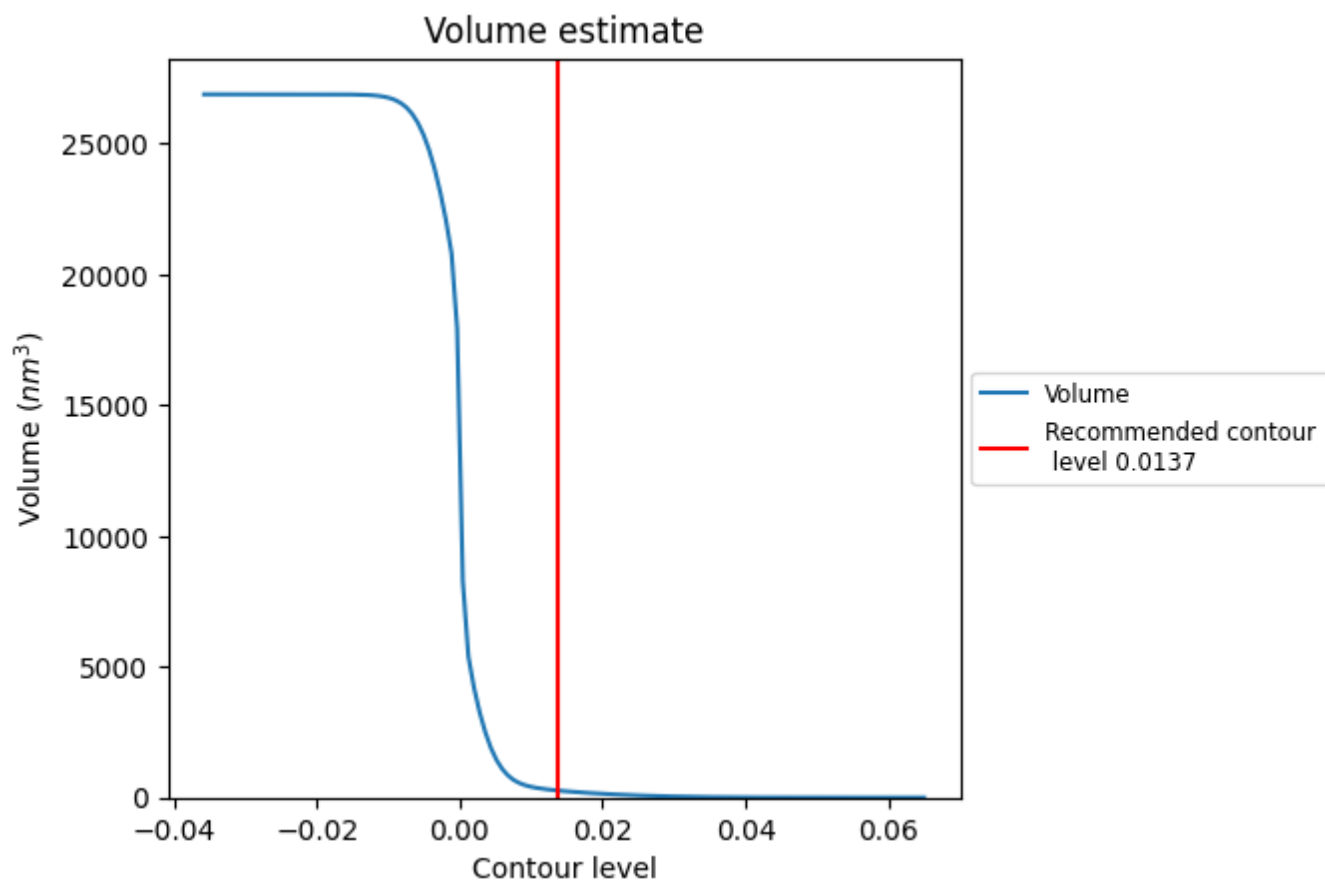
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

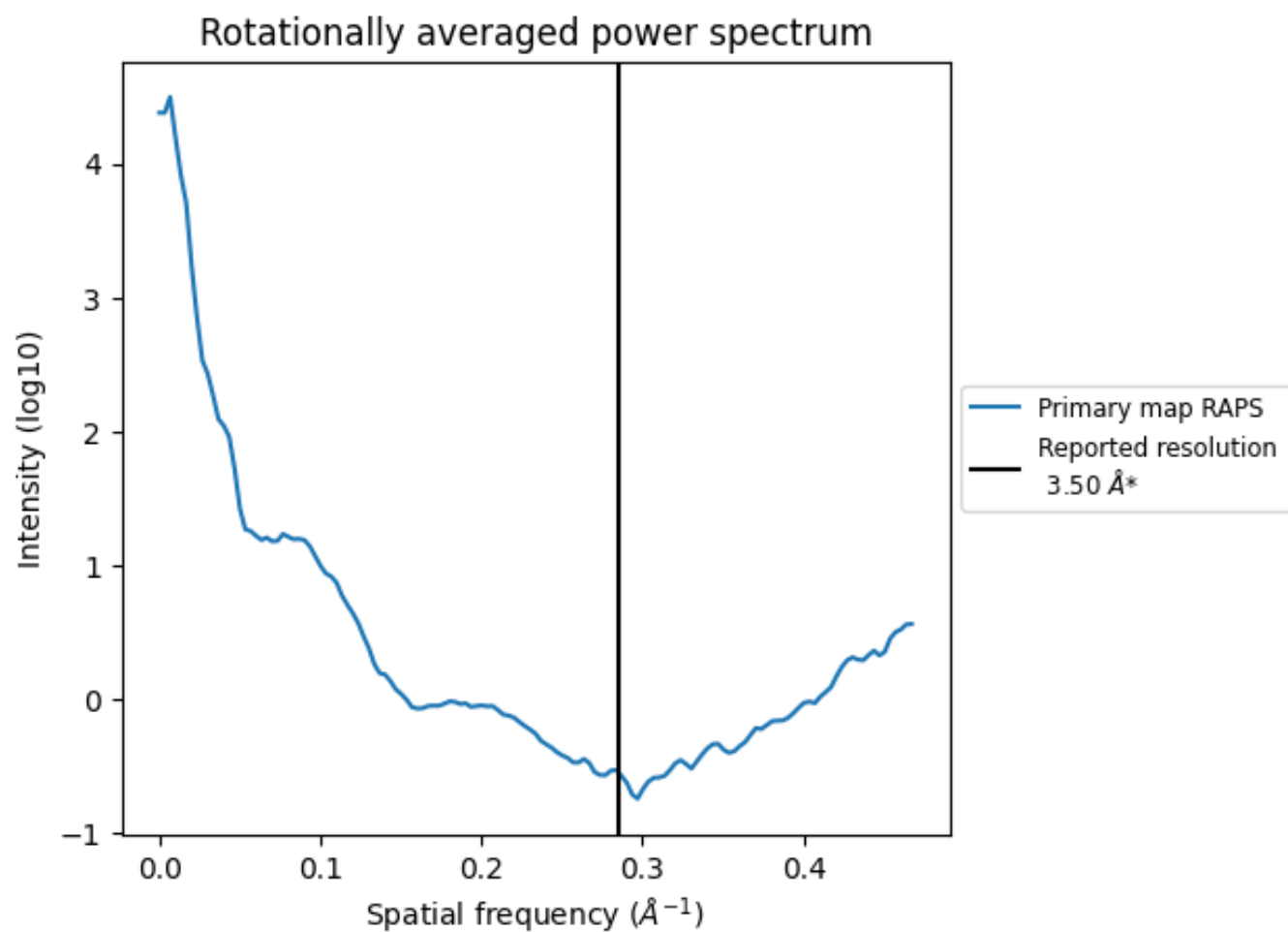
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

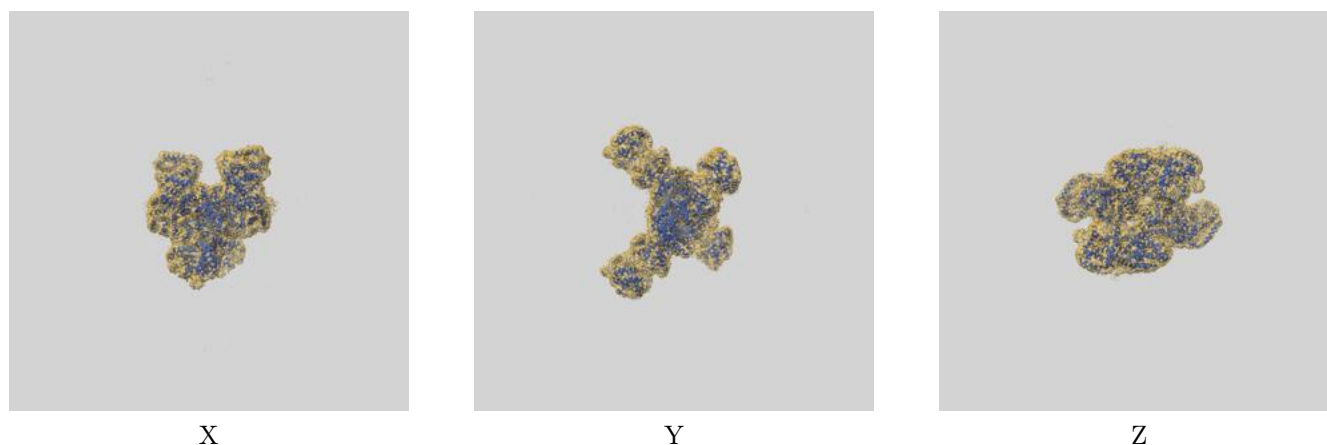
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

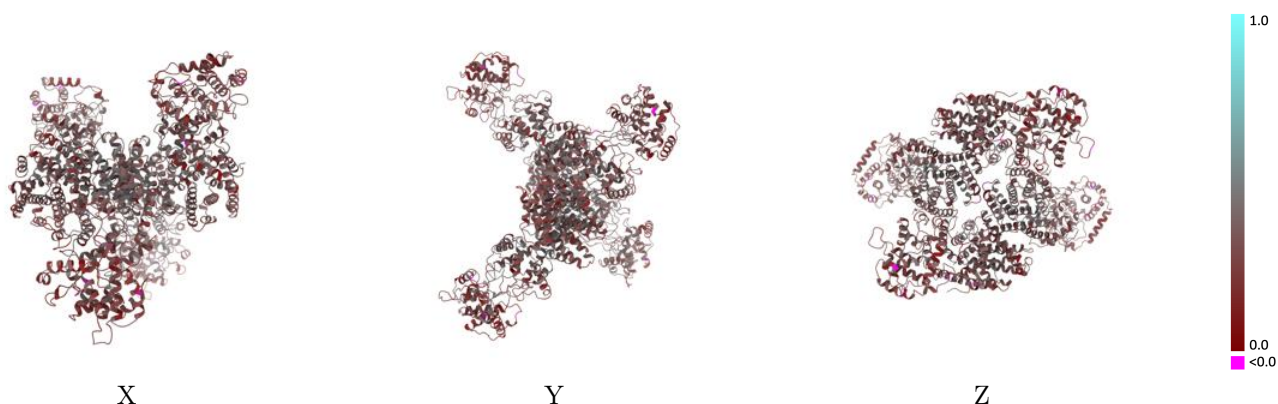
This section contains information regarding the fit between EMDB map EMD-35202 and PDB model 8I6P. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



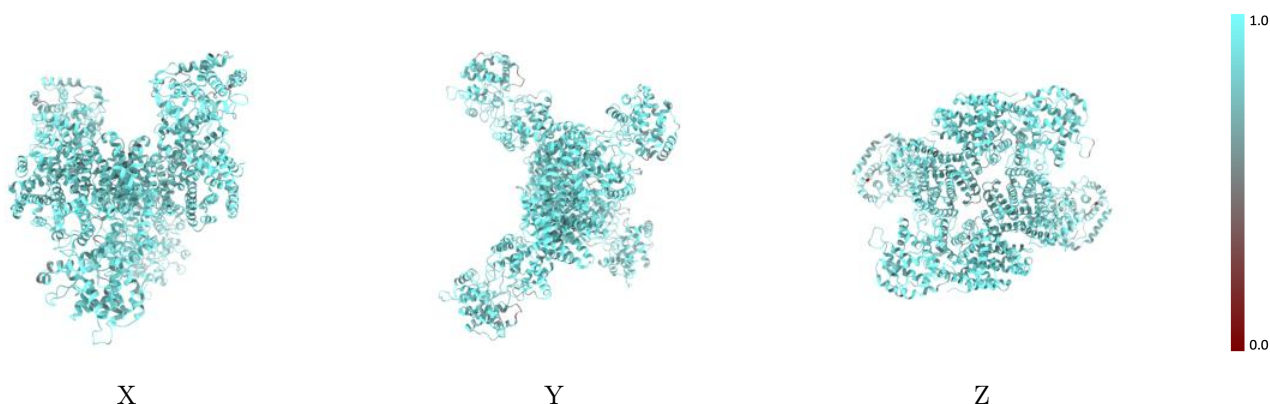
The images above show the 3D surface view of the map at the recommended contour level 0.0137 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



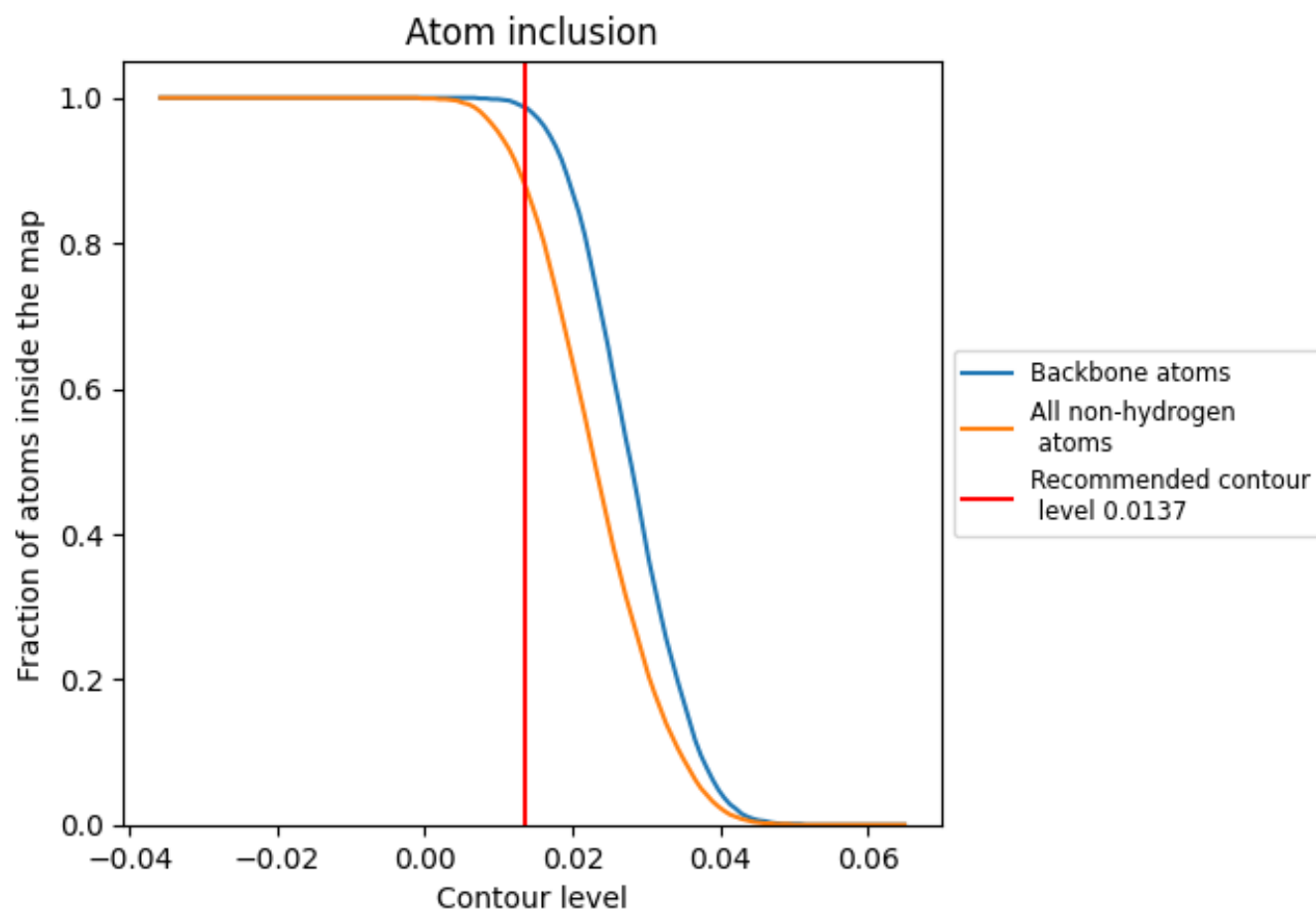
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0137).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 88% 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 (0.0137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.3190
A	0.8840	0.3140
B	0.8700	0.3210
C	0.8700	0.3270
D	0.8860	0.3130

