



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:10 PM UTC

PDB ID : 8W56 / pdb_00008w56
EMDB ID : EMD-37272
Title : Cryo-EM structure of DSR2-DSAD1 state 1
Authors : Zhang, H.; Li, Z.; Li, X.Z.
Deposited on : 2023-08-25
Resolution : 3.59 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:

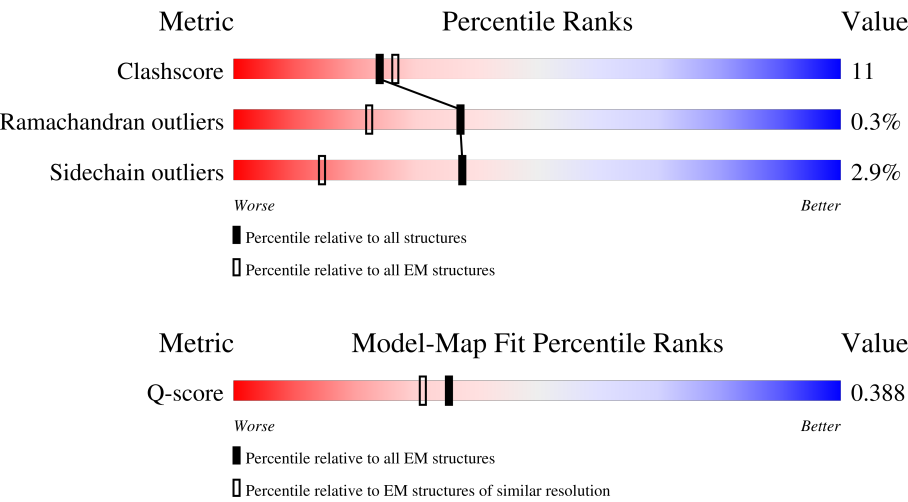
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.59 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	12565 (3.09 - 4.09)

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	1005	18% 69% 26% ..
1	B	1005	26% 73% 23% .
1	C	1005	5% 74% 22% ..
1	D	1005	73% 24% ..

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Mol	Chain	Length	Quality of chain
2	E	120	61% 42% 43% 6% 8%
2	F	120	9% 71% 22% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34051 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 SIR2-like domain-containing protein.

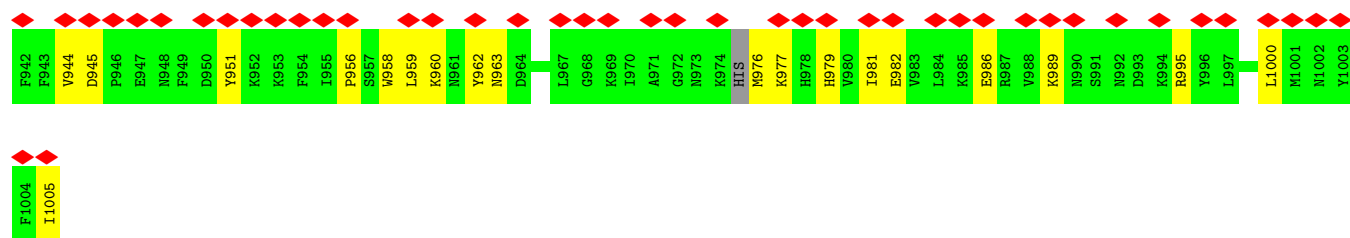
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	973	Total	C	N	O	S	0	0
			8076	5231	1302	1514	29		
1	B	972	Total	C	N	O	S	0	0
			8059	5211	1301	1516	31		
1	C	972	Total	C	N	O	S	0	0
			8095	5237	1309	1518	31		
1	D	973	Total	C	N	O	S	0	0
			8113	5253	1315	1514	31		

There are 4 discrepancies between the modelled and reference sequences:

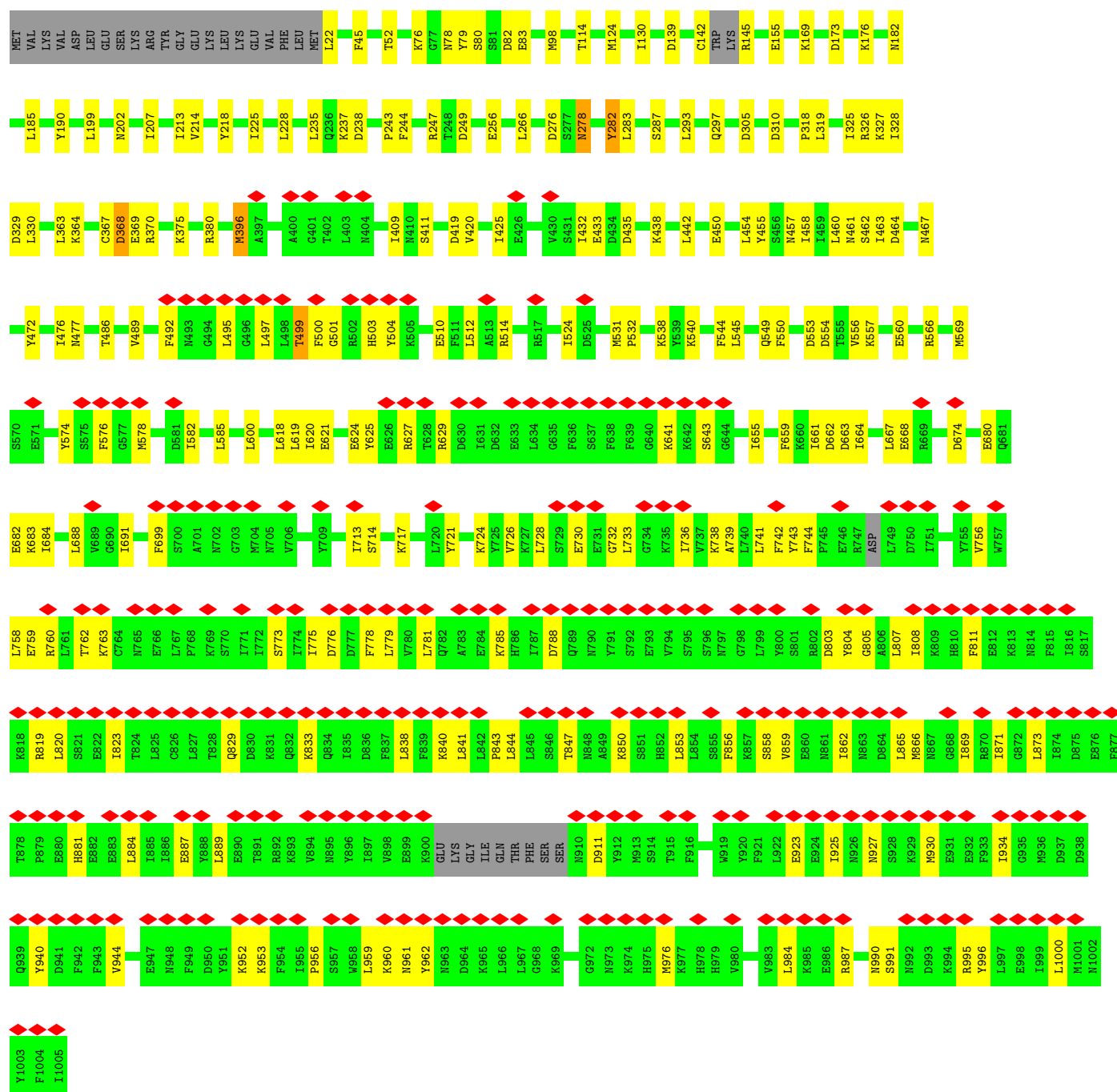
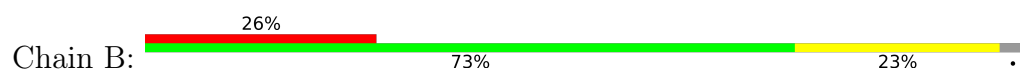
Chain	Residue	Modelled	Actual	Comment	Reference
A	643	SER	LEU	conflict	UNP A0A162TTM4
B	643	SER	LEU	conflict	UNP A0A162TTM4
C	643	SER	LEU	conflict	UNP A0A162TTM4
D	643	SER	LEU	conflict	UNP A0A162TTM4

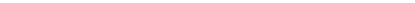
- Molecule 2 is a protein called SPbeta prophage-derived uncharacterized protein YotI.

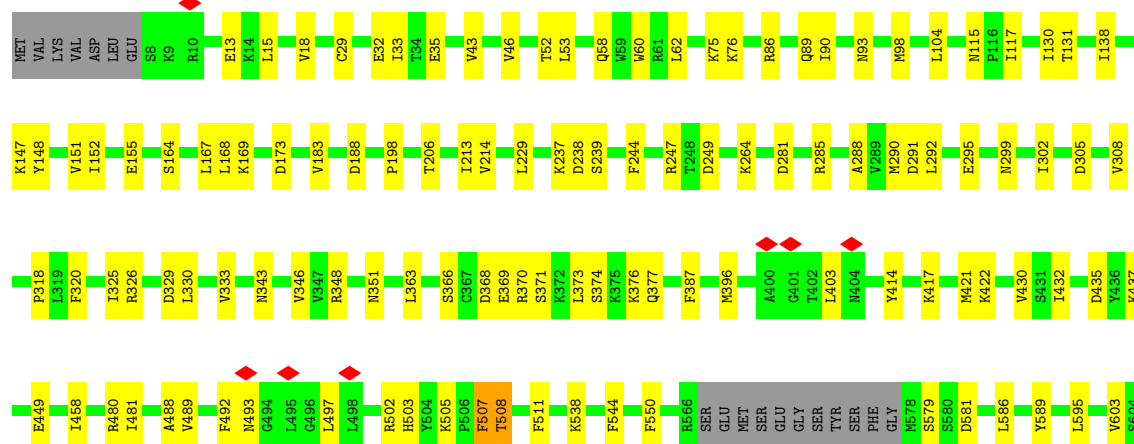
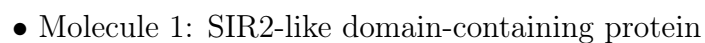
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	111	Total	C	N	O	S	0	0
			854	552	138	161	3		
2	F	111	Total	C	N	O	S	0	0
			854	552	138	161	3		

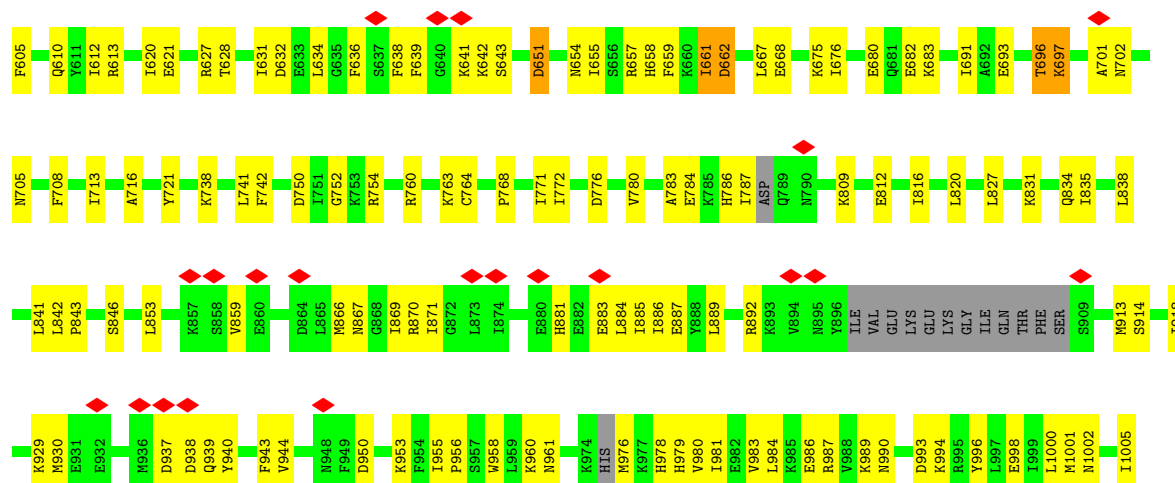


• Molecule 1: SIR2-like domain-containing protein

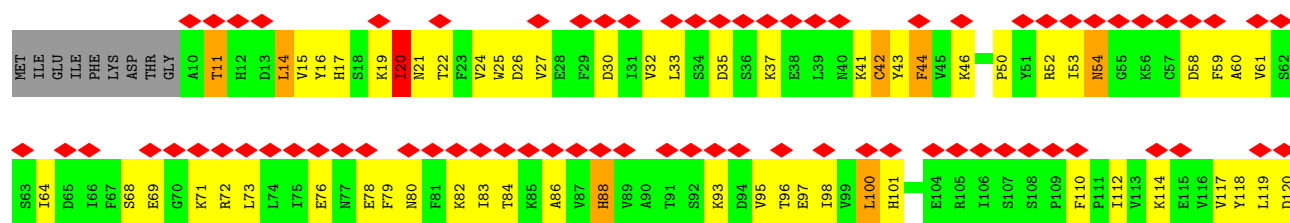


- Chain C:  5% 74% 22% ..

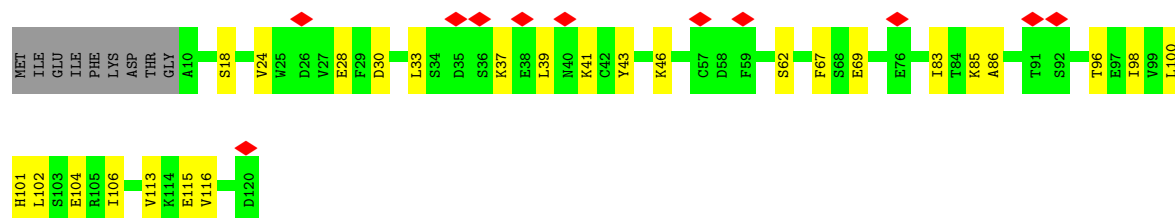




• Molecule 2: SPbeta prophage-derived uncharacterized protein YotI



• Molecule 2: SPbeta prophage-derived uncharacterized protein YotI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.583	Depositor
Minimum map value	-0.905	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.266	Depositor
Map size ($\text{\AA}$)	425.0, 425.0, 425.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	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	0.34	0/8261	0.53	1/11129 (0.0%)
1	B	0.29	1/8243 (0.0%)	0.46	0/11107
1	C	0.10	0/8281	0.28	0/11152
1	D	0.13	0/8298	0.32	0/11171
2	E	1.03	0/873	1.17	1/1188 (0.1%)
2	F	0.14	0/873	0.41	0/1188
All	All	0.28	1/34829 (0.0%)	0.45	2/46935 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	819	ARG	C-N	-7.34	1.22	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	20	ILE	N-CA-C	-5.74	107.53	113.10
1	A	10	ARG	N-CA-C	-5.41	106.68	113.72

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	8076	0	7887	198	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8059	0	7864	168	0
1	C	8095	0	7926	159	0
1	D	8113	0	7965	156	0
2	E	854	0	806	58	0
2	F	854	0	806	20	0
All	All	34051	0	33254	728	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 11.

All (728) 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:A:498:LEU:HA	1:A:503:HIS:CE1	2.09	0.86
1:D:930:MET:HE3	1:D:930:MET:H	1.42	0.85
2:E:30:ASP:HB2	2:E:41:LYS:HE3	1.60	0.83
1:B:499:THR:HB	1:B:503:HIS:HB2	1.61	0.82
1:A:739:ALA:HA	1:A:743:TYR:H	1.42	0.82
1:D:493:ASN:HA	1:D:503:HIS:CD2	2.15	0.81
1:A:488:ALA:HA	1:A:491:GLN:HE21	1.45	0.80
1:D:493:ASN:HA	1:D:503:HIS:HD2	1.47	0.80
1:A:963:ASN:HA	2:E:61:VAL:HG13	1.65	0.79
1:C:913:MET:N	1:C:913:MET:SD	2.56	0.78
1:C:985:LYS:HD2	1:D:1001:MET:HE1	1.67	0.77
1:A:868:GLY:O	1:A:872:GLY:N	2.18	0.76
1:C:284:GLU:OE1	1:C:284:GLU:N	2.19	0.76
2:E:68:SER:HB3	2:E:73:LEU:HB2	1.69	0.75
1:A:868:GLY:HA2	1:A:871:ILE:HG22	1.69	0.74
1:A:816:ILE:HD11	1:A:821:SER:HB2	1.70	0.73
1:D:488:ALA:O	1:D:492:PHE:HB3	1.89	0.73
2:E:26:ASP:HB3	2:E:88:HIS:CE1	2.24	0.73
1:C:662:ASP:OD1	1:C:662:ASP:N	2.24	0.71
1:C:753:LYS:HA	1:C:756:VAL:HG12	1.71	0.71
1:D:98:MET:HE3	1:D:98:MET:HA	1.72	0.71
1:A:797:ASN:HB3	2:E:117:VAL:HG11	1.74	0.70
1:A:986:GLU:HA	1:A:989:LYS:HD2	1.74	0.69
1:B:76:LYS:O	1:B:76:LYS:NZ	2.20	0.69
1:D:1001:MET:HA	1:D:1001:MET:HE2	1.74	0.69
1:C:787:ILE:HG12	1:C:834:GLN:HE21	1.58	0.68
2:E:11:THR:HA	2:E:25:TRP:CH2	2.29	0.68
2:E:27:VAL:HG11	2:E:86:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:SER:OG	1:C:176:LYS:NZ	2.28	0.67
1:A:674:ASP:C	1:A:676:ILE:H	2.02	0.67
1:A:120:LYS:NZ	1:A:287:SER:OG	2.29	0.66
1:C:981:ILE:O	1:C:985:LYS:HG2	1.96	0.66
1:D:955:ILE:HD12	1:D:956:PRO:HD2	1.78	0.66
1:B:841:LEU:HD11	1:B:844:LEU:HD12	1.78	0.66
2:E:52:ARG:HE	2:E:53:ILE:H	1.43	0.66
1:A:437:LYS:O	1:A:441:PHE:HB2	1.96	0.66
1:A:871:ILE:HG23	1:A:873:LEU:HD23	1.77	0.66
1:A:739:ALA:HB2	1:A:743:TYR:HD2	1.60	0.66
1:D:492:PHE:O	1:D:503:HIS:NE2	2.27	0.66
1:A:778:PHE:HA	1:A:781:LEU:HD12	1.77	0.66
1:D:343:ASN:HB2	1:D:403:LEU:HG	1.77	0.65
1:A:739:ALA:H	1:A:742:PHE:HB2	1.62	0.65
1:B:680:GLU:HB3	1:B:683:LYS:HD2	1.79	0.65
1:B:741:LEU:HD21	1:B:758:LEU:HD21	1.79	0.65
1:D:976:MET:SD	1:D:976:MET:N	2.69	0.65
1:B:788:ASP:O	1:B:833:LYS:NZ	2.27	0.65
1:D:373:LEU:HB3	1:D:377:GLN:HB2	1.78	0.65
2:E:30:ASP:O	2:E:84:THR:HA	1.98	0.64
1:D:396:MET:N	1:D:396:MET:HE2	2.12	0.64
1:A:527:LEU:HD23	1:A:531:MET:HE3	1.77	0.64
2:E:88:HIS:HB2	2:E:93:LYS:H	1.63	0.64
1:C:649:TYR:HA	1:C:684:ILE:HD11	1.80	0.64
1:C:787:ILE:O	1:C:831:LYS:NZ	2.31	0.64
1:D:783:ALA:O	1:D:786:HIS:HB2	1.98	0.64
1:A:838:LEU:HD23	1:A:853:LEU:HD12	1.80	0.63
1:D:831:LYS:HE2	1:D:834:GLN:H	1.63	0.63
2:E:53:ILE:O	2:E:54:ASN:C	2.41	0.63
1:B:805:GLY:C	1:B:807:LEU:N	2.53	0.63
1:C:98:MET:HE2	1:C:98:MET:HA	1.79	0.63
1:D:867:ASN:HA	1:D:870:ARG:HD3	1.80	0.63
2:F:96:THR:HG22	2:F:100:LEU:HD23	1.81	0.63
1:B:838:LEU:HD23	1:B:841:LEU:HD23	1.81	0.62
1:A:498:LEU:HA	1:A:503:HIS:HE1	1.62	0.62
1:D:950:ASP:HB3	1:D:953:LYS:HE3	1.81	0.62
1:B:364:LYS:O	1:B:370:ARG:NH2	2.32	0.62
2:E:50:PRO:HD2	2:E:120:ASP:HA	1.82	0.62
1:D:58:GLN:HB2	1:D:60:TRP:HD1	1.63	0.62
1:A:494:GLY:HA2	1:A:505:LYS:HD2	1.82	0.62
1:A:755:TYR:HB2	1:A:804:TYR:HE1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PHE:O	1:A:497:LEU:HB2	1.99	0.62
2:E:52:ARG:HG3	2:E:54:ASN:H	1.65	0.61
1:C:82:ASP:OD2	1:C:86:ARG:NH2	2.33	0.61
1:A:554:ASP:OD1	1:A:587:ARG:NH1	2.33	0.61
1:B:684:ILE:HD12	1:B:684:ILE:H	1.64	0.61
1:B:730:GLU:HA	1:B:733:LEU:HD12	1.83	0.61
1:D:435:ASP:HB2	1:D:458:ILE:HD11	1.81	0.61
1:D:721:TYR:O	1:D:760:ARG:NH1	2.31	0.61
1:B:98:MET:HE3	1:B:98:MET:HA	1.81	0.61
1:B:728:LEU:HD11	1:B:732:GLY:HA3	1.83	0.61
1:B:862:ILE:HG23	1:B:866:MET:HE3	1.82	0.61
2:E:11:THR:HA	2:E:25:TRP:HH2	1.65	0.61
1:A:635:GLY:HA3	1:A:638:PHE:HB3	1.81	0.61
1:A:828:THR:OG1	1:A:830:ASP:OD1	2.19	0.61
2:F:98:ILE:HA	2:F:101:HIS:CE1	2.35	0.61
1:C:327:LYS:NZ	1:C:391:ASN:O	2.32	0.60
1:A:668:GLU:HG2	1:A:673:ILE:HD11	1.82	0.60
1:B:641:LYS:NZ	1:B:643:SER:O	2.34	0.60
1:B:925:ILE:HD12	1:B:927:ASN:H	1.66	0.60
1:B:976:MET:SD	1:B:976:MET:N	2.75	0.60
1:A:565:VAL:HA	1:B:662:ASP:OD2	2.01	0.60
1:B:442:LEU:HD13	1:B:450:GLU:HG3	1.83	0.60
1:A:669:ARG:HH22	1:B:566:ARG:HB3	1.66	0.60
1:D:691:ILE:HD11	1:D:716:ALA:HA	1.83	0.60
2:E:50:PRO:HA	2:E:61:VAL:HB	1.83	0.60
1:B:124:MET:HE3	1:B:124:MET:O	2.01	0.60
1:C:975:HIS:CD2	1:C:976:MET:HE2	2.37	0.60
1:A:143:TRP:CZ2	1:B:463:ILE:HA	2.36	0.59
1:A:579:SER:O	1:A:582:ILE:HG22	2.00	0.59
1:B:682:GLU:OE2	1:B:683:LYS:NZ	2.33	0.59
2:F:30:ASP:HB3	2:F:85:LYS:HB2	1.83	0.59
1:C:755:TYR:HE2	1:C:799:LEU:HD13	1.67	0.59
1:A:739:ALA:HA	1:A:743:TYR:N	2.15	0.59
1:B:838:LEU:HB3	1:B:853:LEU:HD21	1.84	0.59
1:C:865:LEU:HD12	1:C:881:HIS:HB3	1.83	0.59
1:D:579:SER:OG	1:D:581:ASP:OD1	2.18	0.59
1:B:889:LEU:HD12	1:B:930:MET:HE1	1.84	0.59
1:C:824:THR:HG22	1:C:838:LEU:HD22	1.84	0.59
1:D:589:TYR:OH	1:D:651:ASP:OD1	2.19	0.59
1:A:409:ILE:HG12	1:A:593:ARG:HG3	1.84	0.59
1:D:886:ILE:HG12	1:D:929:LYS:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASP:OD2	1:B:991:SER:OG	2.14	0.59
1:A:368:ASP:N	1:A:368:ASP:OD1	2.35	0.58
1:D:914:SER:O	1:D:918:ILE:HG12	2.02	0.58
1:D:889:LEU:HB3	1:D:892:ARG:HH21	1.69	0.58
1:B:923:GLU:N	1:B:923:GLU:OE1	2.37	0.58
1:C:290:MET:HE3	1:C:290:MET:HA	1.85	0.58
1:C:359:ARG:NH2	1:C:369:GLU:OE1	2.37	0.58
1:C:80:SER:OG	1:C:82:ASP:OD1	2.20	0.58
1:C:963:ASN:OD1	1:C:965:LYS:NZ	2.35	0.58
1:C:749:LEU:HD12	1:C:753:LYS:HG3	1.84	0.58
1:B:176:LYS:HE2	1:B:182:ASN:HD21	1.69	0.58
1:C:104:LEU:O	1:C:108:PHE:HB2	2.04	0.58
1:A:913:MET:HA	1:A:916:PHE:HD2	1.69	0.57
1:A:318:PRO:HB3	1:A:538:LYS:HD3	1.86	0.57
1:B:492:PHE:CE2	1:B:503:HIS:HB3	2.38	0.57
1:A:956:PRO:HA	1:A:959:LEU:HD23	1.85	0.57
1:B:310:ASP:OD1	1:B:380:ARG:NH1	2.38	0.57
1:A:508:THR:HG23	1:A:511:PHE:HB2	1.85	0.57
1:A:620:ILE:HD12	1:A:667:LEU:HD11	1.85	0.57
1:A:960:LYS:HB3	1:A:995:ARG:HH22	1.68	0.57
2:F:33:LEU:HB3	2:F:37:LYS:HB2	1.85	0.57
1:B:214:VAL:HG22	1:B:244:PHE:HB2	1.86	0.57
1:A:641:LYS:O	1:A:675:LYS:NZ	2.36	0.57
1:A:671:CYS:O	1:A:672:SER:C	2.47	0.57
1:A:678:PHE:CE1	1:A:726:VAL:HG12	2.40	0.57
1:A:766:GLU:CD	1:A:767:LEU:H	2.13	0.57
1:B:805:GLY:C	1:B:807:LEU:H	2.12	0.57
1:C:761:LEU:O	1:C:765:ASN:ND2	2.38	0.57
1:D:396:MET:HE2	1:D:396:MET:H	1.69	0.57
1:B:425:ILE:HG22	1:B:438:LYS:HG2	1.86	0.57
1:A:145:ARG:NH1	1:A:145:ARG:O	2.38	0.57
1:A:488:ALA:HA	1:A:491:GLN:NE2	2.19	0.57
1:C:858:SER:OG	1:C:859:VAL:N	2.37	0.57
1:B:247:ARG:NH1	1:B:249:ASP:OD2	2.38	0.56
1:B:858:SER:OG	1:B:859:VAL:N	2.38	0.56
1:C:863:ASN:HA	1:C:866:MET:HE3	1.86	0.56
1:D:281:ASP:O	1:D:285:ARG:NH2	2.37	0.56
1:D:914:SER:HA	1:D:939:GLN:HE22	1.68	0.56
1:A:674:ASP:C	1:A:676:ILE:N	2.62	0.56
1:C:45:PHE:HD2	1:C:213:ILE:HD11	1.70	0.56
1:C:151:VAL:HG12	1:C:167:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:GLN:HG3	1:D:613:ARG:HH21	1.70	0.56
1:D:290:MET:HE3	1:D:290:MET:HA	1.87	0.56
1:C:813:LYS:H	1:C:813:LYS:HD2	1.70	0.56
1:A:799:LEU:HD11	2:E:119:LEU:HD22	1.87	0.56
1:B:419:ASP:OD1	1:B:420:VAL:N	2.39	0.56
2:E:42:CYS:SG	2:E:43:TYR:N	2.79	0.56
1:D:13:GLU:OE1	1:D:13:GLU:N	2.31	0.56
1:D:89:GLN:NE2	1:D:93:ASN:OD1	2.38	0.56
1:A:348:ARG:HE	1:A:351:ASN:HB3	1.71	0.56
1:D:502:ARG:HD2	1:D:503:HIS:H	1.71	0.56
1:A:817:SER:HB2	1:A:820:LEU:HB3	1.87	0.56
1:A:678:PHE:HB3	1:A:681:GLN:HE22	1.70	0.55
1:A:755:TYR:HB2	1:A:804:TYR:CE1	2.41	0.55
1:B:45:PHE:HD2	1:B:213:ILE:HD11	1.71	0.55
1:C:911:ASP:OD1	1:C:911:ASP:N	2.39	0.55
1:D:368:ASP:N	1:D:368:ASP:OD1	2.39	0.55
1:C:987:ARG:NH1	1:D:632:ASP:OD1	2.37	0.55
1:A:755:TYR:HA	1:A:758:LEU:HG	1.88	0.55
1:A:521:ASN:HD21	1:B:297:GLN:HG2	1.72	0.55
1:C:310:ASP:OD1	1:C:380:ARG:NH1	2.39	0.55
1:A:202:ASN:ND2	1:B:202:ASN:OD1	2.34	0.55
1:A:487:GLN:O	1:A:491:GLN:HG3	2.07	0.55
1:C:554:ASP:OD2	1:C:591:ASN:ND2	2.26	0.55
1:D:827:LEU:HD11	1:D:835:ILE:HG22	1.89	0.55
1:A:151:VAL:HG12	1:A:167:LEU:HD23	1.89	0.55
1:A:806:ALA:HB1	2:E:53:ILE:HG21	1.88	0.55
1:D:595:LEU:HB3	1:D:603:VAL:HG12	1.89	0.55
1:D:866:MET:HE2	1:D:866:MET:HA	1.87	0.55
1:B:576:PHE:HB2	2:E:14:LEU:HD21	1.88	0.55
1:C:744:PHE:O	1:C:754:ARG:NH2	2.39	0.54
1:A:775:ILE:HD12	1:A:776:ASP:N	2.23	0.54
1:C:771:ILE:O	1:C:775:ILE:HG13	2.07	0.54
1:C:913:MET:HB3	1:C:940:TYR:CE2	2.42	0.54
1:C:214:VAL:HG22	1:C:244:PHE:HB2	1.89	0.54
1:D:885:ILE:O	1:D:889:LEU:HG	2.08	0.54
2:F:98:ILE:O	2:F:102:LEU:HB2	2.07	0.54
1:D:325:ILE:HD11	1:D:329:ASP:HB2	1.90	0.54
1:A:580:SER:HA	1:A:583:VAL:HG12	1.90	0.54
1:B:775:ILE:HB	1:B:804:TYR:HE1	1.72	0.54
1:B:820:LEU:HD13	1:B:823:ILE:HD12	1.89	0.53
1:D:631:ILE:HG13	1:D:636:PHE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:GLU:OE2	1:B:627:ARG:NH2	2.37	0.53
1:C:780:VAL:HG11	1:C:819:ARG:HD2	1.89	0.53
1:D:507:PHE:HB3	1:D:511:PHE:HD2	1.73	0.53
1:A:995:ARG:NH2	2:E:19:LYS:O	2.41	0.53
1:C:247:ARG:NH1	1:C:251:SER:O	2.39	0.53
1:A:173:ASP:OD2	1:A:175:ARG:NH1	2.41	0.53
1:A:358:GLU:HG3	1:A:396:MET:HE2	1.90	0.53
1:B:463:ILE:HG23	1:B:464:ASP:H	1.72	0.53
1:B:668:GLU:OE2	1:B:760:ARG:NH2	2.42	0.53
1:B:805:GLY:HA2	1:B:808:ILE:HG12	1.91	0.53
1:B:960:LYS:HD3	1:B:995:ARG:NH2	2.22	0.53
1:B:80:SER:H	1:B:83:GLU:HG3	1.74	0.53
1:D:53:LEU:HB2	1:D:115:ASN:ND2	2.24	0.53
1:A:931:GLU:C	1:A:933:PHE:H	2.15	0.52
2:E:119:LEU:O	2:E:120:ASP:C	2.51	0.52
2:F:69:GLU:N	2:F:69:GLU:OE1	2.41	0.52
1:C:531:MET:HG3	1:C:532:PRO:HD2	1.91	0.52
2:E:52:ARG:HH21	2:E:53:ILE:HD13	1.73	0.52
1:C:414:TYR:O	1:C:657:ARG:NH2	2.42	0.52
1:B:911:ASP:OD1	1:B:911:ASP:N	2.38	0.52
2:E:22:THR:HG21	2:E:46:LYS:HD3	1.91	0.52
1:A:842:LEU:HG	1:A:843:PRO:HD3	1.90	0.52
1:B:629:ARG:HH22	1:B:643:SER:HB2	1.73	0.52
1:C:783:ALA:O	1:C:786:HIS:ND1	2.43	0.52
1:A:679:GLY:O	1:A:680:GLU:C	2.53	0.52
1:C:839:PHE:HZ	1:C:864:ASP:HA	1.75	0.52
1:C:964:ASP:OD1	1:C:965:LYS:N	2.43	0.52
1:D:884:LEU:O	1:D:887:GLU:HG3	2.09	0.52
1:D:655:ILE:O	1:D:659:PHE:HB2	2.10	0.52
1:C:771:ILE:HD12	1:C:771:ILE:H	1.74	0.52
1:C:783:ALA:HA	1:C:786:HIS:HD1	1.75	0.52
1:C:866:MET:HA	1:C:869:ILE:HG12	1.90	0.52
1:B:283:LEU:O	1:B:287:SER:OG	2.25	0.52
2:F:98:ILE:HA	2:F:101:HIS:HE1	1.73	0.51
1:A:963:ASN:HB3	2:E:60:ALA:C	2.35	0.51
1:B:278:ASN:OD1	1:B:278:ASN:N	2.43	0.51
1:B:820:LEU:HG	1:B:841:LEU:HD21	1.93	0.51
1:C:666:ASN:HD22	1:C:669:ARG:HH21	1.58	0.51
1:B:454:LEU:O	1:B:458:ILE:HG13	2.09	0.51
1:B:724:LYS:HE2	1:B:763:LYS:HD3	1.93	0.51
1:C:608:PHE:O	1:C:612:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:LEU:HD13	1:A:962:TYR:HE2	1.76	0.51
1:B:455:TYR:OH	1:B:477:ASN:ND2	2.44	0.51
1:B:866:MET:HA	1:B:869:ILE:HG22	1.92	0.51
1:A:243:PRO:HG2	1:A:266:LEU:HD23	1.93	0.51
1:A:455:TYR:HB3	1:A:478:ARG:HG3	1.92	0.51
1:B:560:GLU:OE2	1:B:560:GLU:N	2.43	0.51
1:B:990:ASN:OD1	1:B:991:SER:N	2.42	0.51
1:D:913:MET:HE2	1:D:937:ASP:HB3	1.92	0.51
1:D:620:ILE:HD12	1:D:667:LEU:HD11	1.92	0.51
2:E:17:HIS:O	2:E:21:ASN:N	2.44	0.51
1:B:739:ALA:HA	1:B:743:TYR:HD1	1.74	0.51
1:D:842:LEU:HG	1:D:843:PRO:HD3	1.92	0.51
1:C:989:LYS:NZ	1:D:998:GLU:OE1	2.44	0.51
1:D:750:ASP:OD1	1:D:752:GLY:N	2.41	0.51
1:D:780:VAL:HG12	1:D:820:LEU:CD2	2.40	0.51
1:A:839:PHE:HD1	1:A:853:LEU:HD11	1.75	0.50
1:C:771:ILE:HA	1:C:774:ILE:HG12	1.92	0.50
1:D:46:VAL:HG11	1:D:138:ILE:HD11	1.93	0.50
2:E:41:LYS:HB2	2:E:69:GLU:OE1	2.10	0.50
1:A:523:ASN:HB3	1:A:526:ASP:OD1	2.10	0.50
1:A:704:MET:SD	1:A:704:MET:N	2.83	0.50
1:B:319:LEU:HB3	1:B:325:ILE:CD1	2.41	0.50
1:A:512:LEU:O	1:A:516:GLU:HG2	2.11	0.50
1:D:784:GLU:C	1:D:786:HIS:N	2.67	0.50
1:A:236:GLN:O	1:A:239:SER:OG	2.28	0.50
1:C:977:LYS:O	1:C:981:ILE:HB	2.11	0.50
1:A:36:SER:OG	1:A:41:LYS:O	2.30	0.50
1:B:476:ILE:HD13	1:B:524:ILE:HD11	1.92	0.50
1:B:368:ASP:C	1:B:370:ARG:N	2.68	0.50
1:C:302:ILE:HG22	1:C:307:GLU:HB3	1.92	0.50
2:E:97:GLU:O	2:E:100:LEU:HG	2.12	0.50
1:A:621:GLU:HG2	1:A:671:CYS:SG	2.52	0.50
1:C:881:HIS:HA	1:C:884:LEU:HD12	1.93	0.50
1:B:741:LEU:HD11	1:B:758:LEU:HD11	1.93	0.50
1:C:37:SER:HB2	1:C:42:LEU:HD13	1.93	0.50
1:D:643:SER:HB2	1:D:676:ILE:HD13	1.93	0.50
1:B:987:ARG:HD3	1:B:996:TYR:HE2	1.76	0.50
1:B:582:ILE:HD13	1:B:585:LEU:HD23	1.93	0.49
1:B:432:ILE:HD12	1:B:433:GLU:N	2.26	0.49
1:D:414:TYR:OH	1:D:654:ASN:OD1	2.27	0.49
2:E:100:LEU:O	2:E:101:HIS:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:CYS:HA	1:A:370:ARG:HE	1.76	0.49
1:B:847:THR:HA	1:B:850:LYS:HG2	1.94	0.49
1:C:373:LEU:HB3	1:C:377:GLN:HB2	1.94	0.49
1:D:130:ILE:HG23	1:D:168:LEU:HB3	1.94	0.49
1:D:662:ASP:OD1	1:D:662:ASP:N	2.46	0.49
2:E:27:VAL:HG21	2:E:95:VAL:HG21	1.94	0.49
1:A:695:ILE:HG13	1:A:698:GLN:HE21	1.78	0.49
1:A:808:ILE:O	1:A:812:GLU:N	2.45	0.49
1:A:827:LEU:HD22	1:A:838:LEU:HD22	1.93	0.49
1:A:867:ASN:HD21	2:E:76:GLU:C	2.20	0.49
2:E:15:VAL:HB	2:E:24:VAL:HB	1.94	0.49
1:A:304:LYS:HG2	1:A:306:ASP:HB3	1.94	0.49
1:B:327:LYS:O	1:B:330:LEU:HB2	2.12	0.49
1:C:318:PRO:HG3	1:C:538:LYS:HG2	1.93	0.49
1:B:318:PRO:HB3	1:B:538:LYS:HD3	1.95	0.49
1:C:817:SER:HB3	1:C:844:LEU:HD11	1.93	0.49
1:B:80:SER:OG	1:B:82:ASP:OD1	2.29	0.49
1:B:432:ILE:HA	1:B:435:ASP:OD2	2.13	0.49
2:F:28:GLU:OE2	2:F:28:GLU:HA	2.13	0.49
2:F:104:GLU:OE1	2:F:104:GLU:N	2.39	0.49
1:A:199:LEU:HG	1:B:235:LEU:HD11	1.95	0.49
1:A:276:ASP:OD1	1:A:276:ASP:N	2.44	0.49
1:D:164:SER:O	1:D:164:SER:OG	2.31	0.49
1:B:501:GLY:HA2	1:B:504:TYR:CE1	2.48	0.49
1:C:888:TYR:O	1:C:892:ARG:HG2	2.13	0.49
1:D:741:LEU:O	1:D:754:ARG:NH1	2.46	0.49
1:D:784:GLU:C	1:D:786:HIS:H	2.21	0.49
1:A:419:ASP:N	1:A:419:ASP:OD1	2.46	0.49
1:B:367:CYS:O	1:B:370:ARG:HB2	2.12	0.49
1:B:714:SER:HA	1:B:717:LYS:HE3	1.94	0.49
1:B:829:GLN:NE2	1:B:856:PHE:O	2.37	0.49
2:E:27:VAL:HG22	2:E:88:HIS:HA	1.95	0.49
1:D:32:GLU:O	1:D:35:GLU:HG3	2.13	0.48
2:F:28:GLU:HG3	2:F:41:LYS:HB3	1.95	0.48
1:A:544:PHE:HD2	1:A:550:PHE:HB2	1.77	0.48
1:B:574:TYR:HB2	2:E:16:TYR:HB3	1.96	0.48
1:D:497:LEU:HB3	1:D:503:HIS:HE1	1.78	0.48
1:A:867:ASN:ND2	2:E:76:GLU:O	2.42	0.48
1:B:940:TYR:O	1:B:944:VAL:HG22	2.14	0.48
1:D:247:ARG:NH1	1:D:249:ASP:OD2	2.46	0.48
1:C:883:GLU:HA	1:C:886:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LYS:O	1:A:426:GLU:HG2	2.14	0.48
1:B:953:LYS:HA	1:B:953:LYS:HD3	1.71	0.48
2:E:52:ARG:HE	2:E:53:ILE:N	2.09	0.48
1:A:758:LEU:HD21	1:A:804:TYR:CE1	2.49	0.48
1:B:472:TYR:HD2	1:B:531:MET:HE2	1.78	0.48
1:C:370:ARG:HB3	1:C:378:TYR:HE1	1.78	0.48
1:C:425:ILE:HG12	1:C:442:LEU:HD12	1.96	0.48
1:C:807:LEU:O	1:C:810:HIS:ND1	2.33	0.48
1:C:310:ASP:OD2	1:C:377:GLN:NE2	2.47	0.48
1:C:442:LEU:HD21	1:C:450:GLU:HB3	1.95	0.48
1:D:318:PRO:HB3	1:D:538:LYS:HD3	1.94	0.48
1:D:768:PRO:HD2	1:D:771:ILE:HD11	1.96	0.48
1:B:775:ILE:HB	1:B:804:TYR:CE1	2.49	0.48
1:C:304:LYS:HE2	1:C:306:ASP:HB2	1.95	0.48
1:B:578:MET:HE1	1:B:582:ILE:HB	1.96	0.48
1:B:738:LYS:O	1:B:742:PHE:HB2	2.13	0.48
1:C:671:CYS:SG	1:C:672:SER:N	2.87	0.48
1:C:780:VAL:HG22	1:C:820:LEU:HD21	1.96	0.48
1:D:155:GLU:OE2	1:D:198:PRO:HD2	2.14	0.48
1:D:366:SER:OG	1:D:369:GLU:OE1	2.27	0.48
1:D:502:ARG:HH11	1:D:503:HIS:H	1.59	0.48
1:A:910:ASN:ND2	2:E:79:PHE:H	2.11	0.48
1:C:169:LYS:HD3	1:C:173:ASP:HB3	1.95	0.48
1:C:771:ILE:HG23	1:C:774:ILE:HD11	1.96	0.47
1:B:457:ASN:O	1:B:460:LEU:HG	2.14	0.47
1:B:641:LYS:HA	1:B:641:LYS:HD2	1.63	0.47
1:D:771:ILE:HD12	1:D:772:ILE:N	2.29	0.47
1:D:776:ASP:O	1:D:780:VAL:HG13	2.14	0.47
1:A:761:LEU:HD12	1:A:762:THR:HG23	1.97	0.47
1:B:544:PHE:HB3	1:B:550:PHE:HB3	1.96	0.47
1:C:761:LEU:HD23	1:C:765:ASN:HD22	1.78	0.47
1:C:951:TYR:OH	1:C:976:MET:SD	2.68	0.47
1:A:920:TYR:CD2	1:A:944:VAL:HG22	2.50	0.47
1:B:176:LYS:HB2	1:B:182:ASN:HD21	1.79	0.47
1:B:243:PRO:HG2	1:B:266:LEU:HD23	1.97	0.47
1:B:409:ILE:HG22	1:B:411:SER:H	1.80	0.47
1:B:620:ILE:HG21	1:B:667:LEU:HD21	1.95	0.47
1:C:1005:ILE:HG12	1:D:1005:ILE:HD11	1.95	0.47
1:A:632:ASP:OD2	1:B:987:ARG:NE	2.48	0.47
1:B:688:LEU:HD23	1:B:691:ILE:HD11	1.95	0.47
2:E:25:TRP:HA	2:E:25:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:GLU:C	1:A:933:PHE:N	2.71	0.47
1:B:674:ASP:OD1	1:B:674:ASP:N	2.47	0.47
1:B:959:LEU:HD13	1:B:984:LEU:HD21	1.96	0.47
1:C:877:PHE:CE2	1:C:924:GLU:HB3	2.50	0.47
1:D:705:ASN:HB2	1:D:708:PHE:HB3	1.97	0.47
1:A:124:MET:HE3	1:A:124:MET:O	2.15	0.47
1:C:886:ILE:HG12	1:C:929:LYS:HZ2	1.80	0.47
1:A:686:GLU:HA	1:A:689:VAL:HG12	1.97	0.47
1:B:489:VAL:HG21	1:B:512:LEU:HD21	1.97	0.47
1:C:499:THR:O	1:C:747:ARG:NE	2.48	0.47
1:C:820:LEU:O	1:C:824:THR:HG23	2.14	0.47
1:A:98:MET:HE2	1:A:98:MET:HA	1.97	0.47
1:A:810:HIS:HD2	2:E:53:ILE:HG13	1.80	0.47
1:B:305:ASP:HB2	1:B:363:LEU:HD11	1.96	0.47
1:B:396:MET:HE3	1:B:396:MET:HB3	1.69	0.47
1:D:437:LYS:HE2	1:D:437:LYS:HB3	1.72	0.47
1:B:569:MET:HG3	1:B:625:TYR:CD2	2.50	0.46
1:B:773:SER:HA	1:B:776:ASP:OD2	2.15	0.46
1:C:31:LYS:HE2	1:C:301:PHE:HD2	1.80	0.46
1:D:188:ASP:OD1	1:D:188:ASP:N	2.48	0.46
1:D:883:GLU:HA	1:D:886:ILE:HD12	1.97	0.46
2:E:71:LYS:HE3	2:E:72:ARG:H	1.79	0.46
2:F:115:GLU:N	2:F:115:GLU:OE1	2.48	0.46
1:A:452:TYR:HE1	1:A:478:ARG:HG2	1.80	0.46
1:A:486:THR:O	1:A:490:THR:HG22	2.16	0.46
1:B:510:GLU:OE2	1:B:514:ARG:NH2	2.43	0.46
1:B:618:LEU:O	1:B:621:GLU:HG2	2.15	0.46
1:C:704:MET:HE3	1:C:705:ASN:N	2.31	0.46
1:B:733:LEU:HA	1:B:736:ILE:HG12	1.97	0.46
1:B:884:LEU:O	1:B:887:GLU:HG3	2.15	0.46
1:C:799:LEU:HD23	1:C:799:LEU:HA	1.78	0.46
1:D:363:LEU:O	1:D:370:ARG:NH1	2.31	0.46
1:A:283:LEU:O	1:A:287:SER:HB2	2.15	0.46
1:B:256:GLU:CD	1:B:256:GLU:H	2.23	0.46
1:C:769:LYS:HA	1:C:772:ILE:HD12	1.98	0.46
1:A:637:SER:O	1:A:638:PHE:C	2.58	0.46
1:C:959:LEU:HD12	1:C:984:LEU:HD21	1.97	0.46
1:D:638:PHE:CD1	1:D:638:PHE:C	2.93	0.46
1:A:511:PHE:HE1	1:A:514:ARG:HH21	1.64	0.46
1:B:756:VAL:O	1:B:759:GLU:HG3	2.14	0.46
1:C:655:ILE:O	1:C:659:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:LEU:O	1:C:785:LYS:HG2	2.16	0.46
1:D:229:LEU:HD12	1:D:264:LYS:HD3	1.98	0.46
1:B:569:MET:HE2	1:B:625:TYR:HB2	1.98	0.46
2:F:30:ASP:HB2	2:F:41:LYS:HZ2	1.80	0.46
1:A:89:GLN:HE22	1:A:188:ASP:CG	2.24	0.46
1:A:959:LEU:HA	1:A:962:TYR:CE2	2.51	0.46
1:B:319:LEU:HB3	1:B:325:ILE:HD11	1.98	0.46
1:C:668:GLU:OE2	1:C:760:ARG:NH2	2.49	0.46
1:C:801:SER:O	1:C:804:TYR:HB2	2.16	0.46
1:C:842:LEU:HB2	1:C:871:ILE:HD13	1.97	0.46
2:E:68:SER:O	2:E:69:GLU:C	2.59	0.46
2:F:28:GLU:HG3	2:F:41:LYS:HE2	1.98	0.46
1:A:452:TYR:CE1	1:A:478:ARG:HG2	2.51	0.46
1:A:817:SER:O	1:A:818:LYS:C	2.59	0.46
1:A:930:MET:O	1:A:933:PHE:HD2	1.98	0.46
1:C:76:LYS:O	1:C:76:LYS:NZ	2.41	0.46
1:C:749:LEU:HA	1:C:753:LYS:HD2	1.97	0.46
1:C:786:HIS:NE2	1:C:834:GLN:HA	2.31	0.46
1:D:299:ASN:HB3	1:D:302:ILE:HD11	1.98	0.46
1:A:732:GLY:O	1:A:736:ILE:HG12	2.16	0.46
1:C:307:GLU:OE1	1:C:307:GLU:N	2.46	0.46
1:C:920:TYR:HE1	1:C:930:MET:HB2	1.81	0.46
1:D:986:GLU:O	1:D:989:LYS:HG2	2.16	0.46
2:E:97:GLU:HG2	2:E:98:ILE:N	2.31	0.46
1:A:493:ASN:OD1	1:A:503:HIS:HA	2.15	0.45
1:B:840:LYS:HB2	1:B:840:LYS:HE3	1.67	0.45
1:D:417:LYS:O	1:D:421:MET:HG2	2.15	0.45
2:E:27:VAL:HA	2:E:88:HIS:HA	1.97	0.45
1:A:1000:LEU:O	1:A:1005:ILE:HG13	2.16	0.45
1:B:45:PHE:HD1	1:B:218:TYR:HE2	1.63	0.45
1:C:809:LYS:HD3	1:C:815:PHE:HE1	1.81	0.45
1:D:305:ASP:HA	1:D:308:VAL:HG12	1.98	0.45
1:D:505:LYS:HD2	1:D:508:THR:HA	1.99	0.45
1:B:472:TYR:CD2	1:B:531:MET:HE2	2.52	0.45
1:C:328:ILE:HG13	1:C:329:ASP:N	2.32	0.45
1:D:680:GLU:OE1	1:D:683:LYS:N	2.40	0.45
1:D:831:LYS:HG2	1:D:834:GLN:HB3	1.99	0.45
1:A:865:LEU:O	1:A:869:ILE:HD12	2.16	0.45
1:B:169:LYS:HD3	1:B:173:ASP:HB3	1.98	0.45
1:B:305:ASP:OD1	1:B:305:ASP:N	2.50	0.45
1:B:713:ILE:HD11	1:B:744:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TYR:HE1	1:C:599:CYS:HB2	1.80	0.45
2:E:54:ASN:HB2	2:E:58:ASP:HB2	1.98	0.45
1:A:683:LYS:O	1:A:686:GLU:HG2	2.16	0.45
1:D:348:ARG:NH2	1:D:351:ASN:O	2.50	0.45
1:D:955:ILE:HD12	1:D:956:PRO:CD	2.44	0.45
1:A:46:VAL:HA	1:A:216:ILE:HG22	1.99	0.45
1:A:785:LYS:HE2	1:A:785:LYS:HB2	1.80	0.45
1:D:838:LEU:HB3	1:D:853:LEU:HD11	1.98	0.45
2:E:64:ILE:HG12	2:E:110:PHE:CE1	2.52	0.45
1:A:636:PHE:CZ	1:B:956:PRO:HG3	2.51	0.45
1:B:218:TYR:CG	1:B:225:ILE:HD11	2.52	0.45
1:B:960:LYS:HD2	1:B:996:TYR:HE1	1.81	0.45
1:C:998:GLU:O	1:C:1002:ASN:HB2	2.17	0.45
2:E:95:VAL:O	2:E:96:THR:C	2.59	0.45
1:A:407:ILE:HG12	1:A:589:TYR:HB3	1.99	0.45
1:A:673:ILE:H	1:A:673:ILE:HG13	1.46	0.45
1:A:412:LEU:HD22	1:A:441:PHE:CZ	2.52	0.45
1:A:914:SER:O	1:A:918:ILE:HD13	2.17	0.45
1:B:655:ILE:O	1:B:659:PHE:HB2	2.17	0.45
1:C:99:ALA:O	1:C:103:ILE:HG12	2.17	0.45
1:C:834:GLN:O	1:C:838:LEU:HD12	2.16	0.45
1:B:139:ASP:OD2	1:B:169:LYS:NZ	2.39	0.44
1:B:576:PHE:HB2	2:E:14:LEU:HD11	1.99	0.44
1:A:14:LYS:HB2	1:A:14:LYS:HE3	1.73	0.44
1:A:676:ILE:HD12	1:A:676:ILE:C	2.42	0.44
1:A:723:ALA:O	1:A:726:VAL:HG22	2.17	0.44
1:A:739:ALA:O	1:A:740:LEU:C	2.60	0.44
1:A:951:TYR:OH	1:A:976:MET:SD	2.69	0.44
1:A:977:LYS:HE2	1:A:981:ILE:HD11	1.99	0.44
1:D:86:ARG:O	1:D:90:ILE:HG12	2.17	0.44
1:D:480:ARG:HD2	1:D:605:PHE:HE2	1.81	0.44
1:D:642:LYS:HD3	1:D:642:LYS:HA	1.79	0.44
1:A:370:ARG:HB3	1:A:378:TYR:HE1	1.82	0.44
1:C:236:GLN:HB2	1:C:239:SER:HB3	2.00	0.44
1:C:829:GLN:HA	1:C:835:ILE:HD11	1.99	0.44
1:A:717:LYS:HD2	1:A:757:TRP:HH2	1.81	0.44
1:C:641:LYS:HB2	1:C:641:LYS:HE2	1.74	0.44
1:D:370:ARG:O	1:D:371:SER:OG	2.31	0.44
1:A:56:TYR:HA	1:A:112:LYS:HZ3	1.83	0.44
1:A:345:THR:HB	1:A:397:ALA:HA	2.00	0.44
1:A:755:TYR:O	1:A:756:VAL:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:SER:CB	1:A:820:LEU:HB3	2.48	0.44
1:B:545:LEU:HD13	1:B:600:LEU:HD21	1.99	0.44
1:C:462:SER:O	1:C:462:SER:OG	2.25	0.44
1:A:675:LYS:HB3	1:A:675:LYS:HE3	1.40	0.44
1:A:692:ALA:O	1:A:695:ILE:HG22	2.16	0.44
1:A:772:ILE:HD13	1:A:812:GLU:HG3	2.00	0.44
1:D:960:LYS:HE3	1:D:996:TYR:CZ	2.52	0.44
2:E:20:ILE:O	2:E:22:THR:HG23	2.18	0.44
1:A:449:GLU:H	1:A:449:GLU:CD	2.25	0.44
1:B:326:ARG:HG3	1:B:329:ASP:HB2	2.00	0.44
1:C:531:MET:HG2	1:C:535:PHE:CD2	2.53	0.44
1:D:763:LYS:HD2	1:D:764:CYS:HB2	2.00	0.44
2:F:43:TYR:CE1	2:F:67:PHE:HB2	2.53	0.44
1:A:979:HIS:HA	1:A:982:GLU:HG3	1.98	0.44
1:B:499:THR:O	1:B:500:PHE:HB2	2.18	0.44
1:B:557:LYS:HB2	1:B:557:LYS:HE2	1.70	0.44
1:C:150:SER:HG	1:C:163:SER:HG	1.59	0.44
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.87	0.44
1:C:422:LYS:O	1:C:425:ILE:HG22	2.17	0.44
1:C:480:ARG:HD2	1:C:605:PHE:HZ	1.83	0.44
1:C:772:ILE:HA	1:C:775:ILE:HD11	2.00	0.44
1:D:320:PHE:HE1	1:D:387:PHE:HB2	1.82	0.44
1:A:99:ALA:O	1:A:103:ILE:HG12	2.17	0.43
1:A:329:ASP:O	1:A:333:VAL:HG23	2.18	0.43
1:B:326:ARG:H	1:B:326:ARG:HG2	1.68	0.43
1:D:237:LYS:HZ2	1:D:238:ASP:HB2	1.83	0.43
1:D:325:ILE:HD12	1:D:326:ARG:H	1.83	0.43
2:F:24:VAL:HA	2:F:113:VAL:O	2.18	0.43
1:A:476:ILE:HD13	1:A:524:ILE:HD11	2.00	0.43
1:A:718:ALA:O	1:A:721:TYR:N	2.51	0.43
1:B:22:LEU:HD12	1:B:22:LEU:HA	1.90	0.43
1:B:155:GLU:OE1	1:B:199:LEU:HB2	2.18	0.43
1:C:421:MET:HE3	1:C:441:PHE:CD2	2.54	0.43
1:C:772:ILE:O	1:C:775:ILE:HD12	2.17	0.43
1:C:949:PHE:HZ	1:C:954:PHE:HB2	1.83	0.43
1:D:169:LYS:HD2	1:D:173:ASP:HB2	2.00	0.43
1:D:374:SER:O	1:D:376:LYS:N	2.49	0.43
2:E:44:PHE:HB3	2:E:64:ILE:HD11	2.00	0.43
1:A:718:ALA:O	1:A:719:ALA:C	2.61	0.43
1:C:589:TYR:OH	1:C:651:ASP:OD2	2.37	0.43
1:C:950:ASP:HB3	1:C:953:LYS:NZ	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:866:MET:O	1:D:869:ILE:HG13	2.18	0.43
1:A:471:TYR:HE2	1:A:531:MET:HE1	1.83	0.43
1:A:827:LEU:HD21	1:A:835:ILE:HG13	2.00	0.43
1:B:454:LEU:HA	1:B:457:ASN:HD22	1.83	0.43
1:B:881:HIS:HA	1:B:884:LEU:HD12	2.01	0.43
1:D:239:SER:O	1:D:239:SER:OG	2.32	0.43
1:D:784:GLU:O	1:D:786:HIS:N	2.52	0.43
2:E:64:ILE:HG12	2:E:110:PHE:CZ	2.54	0.43
1:C:642:LYS:HE2	1:C:642:LYS:HB3	1.80	0.43
1:B:540:LYS:HE2	1:B:540:LYS:HB2	1.74	0.43
1:C:477:ASN:ND2	1:C:601:TRP:H	2.16	0.43
1:A:148:TYR:CG	1:B:532:PRO:HD3	2.53	0.43
1:A:418:TYR:O	1:A:421:MET:HB3	2.19	0.43
1:D:502:ARG:NH1	1:D:503:HIS:HB2	2.33	0.43
1:D:816:ILE:HD13	1:D:816:ILE:HA	1.88	0.43
2:F:86:ALA:HB3	2:F:96:THR:HA	2.00	0.43
1:A:579:SER:O	1:A:580:SER:C	2.62	0.43
1:A:868:GLY:HA3	1:A:874:ILE:HD12	2.00	0.43
1:C:532:PRO:HG3	1:D:148:TYR:CZ	2.53	0.43
1:D:612:ILE:HG21	1:D:658:HIS:CD2	2.53	0.43
1:D:980:VAL:HA	1:D:983:VAL:HG12	2.00	0.43
1:D:987:ARG:HA	1:D:987:ARG:NH1	2.34	0.43
2:F:46:LYS:HB3	2:F:116:VAL:HG12	2.00	0.43
1:A:208:ILE:HD13	1:A:228:LEU:HD11	1.99	0.43
1:B:237:LYS:NZ	1:B:238:ASP:OD1	2.51	0.43
1:D:422:LYS:HB2	1:D:422:LYS:HE3	1.90	0.43
1:D:544:PHE:HD2	1:D:550:PHE:HB2	1.84	0.43
1:A:565:VAL:O	1:A:566:ARG:C	2.62	0.42
1:C:294:ILE:O	1:C:297:GLN:HG2	2.19	0.42
1:A:693:GLU:O	1:A:696:THR:HG22	2.19	0.42
1:C:762:THR:HA	1:C:765:ASN:HB2	2.01	0.42
1:C:998:GLU:HA	1:C:1001:MET:SD	2.59	0.42
1:D:291:ASP:O	1:D:295:GLU:HG2	2.18	0.42
1:D:984:LEU:HD11	1:D:1000:LEU:HB2	2.01	0.42
1:D:994:LYS:HD3	1:D:994:LYS:HA	1.80	0.42
1:A:554:ASP:OD2	1:A:591:ASN:ND2	2.51	0.42
1:B:759:GLU:HA	1:B:762:THR:HG22	2.01	0.42
1:B:811:PHE:CD1	1:B:811:PHE:N	2.87	0.42
1:C:326:ARG:NH1	1:C:328:ILE:HD11	2.34	0.42
1:C:767:LEU:HD22	1:C:771:ILE:HB	2.01	0.42
2:E:33:LEU:HA	2:E:80:ASN:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:114:LYS:HA	2:E:114:LYS:HD2	1.85	0.42
1:A:816:ILE:HD13	1:A:846:SER:N	2.35	0.42
1:B:585:LEU:HD13	1:B:619:LEU:HD21	2.02	0.42
1:C:755:TYR:HB2	1:C:804:TYR:CE1	2.54	0.42
1:C:839:PHE:CZ	1:C:864:ASP:HA	2.54	0.42
2:F:106:ILE:HD12	2:F:106:ILE:HA	1.88	0.42
1:A:308:VAL:O	1:A:312:ILE:HG22	2.18	0.42
1:A:328:ILE:HD11	1:A:587:ARG:HD2	2.01	0.42
1:A:423:LYS:HE3	1:A:423:LYS:HA	2.01	0.42
1:A:666:ASN:HA	1:A:669:ARG:HG3	1.99	0.42
1:B:744:PHE:C	1:B:744:PHE:CD1	2.98	0.42
1:D:214:VAL:HG22	1:D:244:PHE:HB2	2.01	0.42
1:D:693:GLU:O	1:D:696:THR:HG22	2.18	0.42
1:D:713:ILE:HD12	1:D:713:ILE:HA	1.83	0.42
1:A:357:MET:HB3	1:A:396:MET:HE1	2.02	0.42
1:A:361:PHE:CE2	1:A:395:CYS:HA	2.55	0.42
1:A:655:ILE:O	1:A:659:PHE:HB2	2.19	0.42
1:B:492:PHE:CZ	1:B:503:HIS:HB3	2.54	0.42
1:B:776:ASP:HA	1:B:779:LEU:HG	2.02	0.42
1:C:213:ILE:HG23	1:C:243:PRO:HB3	2.02	0.42
1:D:639:PHE:HE1	1:D:641:LYS:HA	1.84	0.42
1:A:442:LEU:HD21	1:A:447:ARG:HB2	2.02	0.42
1:A:526:ASP:OD1	1:A:526:ASP:N	2.53	0.42
1:B:553:ASP:OD1	1:B:554:ASP:N	2.52	0.42
1:B:553:ASP:O	1:B:556:VAL:HG12	2.19	0.42
1:B:699:PHE:HB2	1:B:743:TYR:HB3	2.01	0.42
1:C:768:PRO:HD2	1:C:771:ILE:HD13	2.02	0.42
1:C:836:ASP:O	1:C:840:LYS:HG2	2.19	0.42
1:D:75:LYS:O	1:D:76:LYS:HG2	2.20	0.42
1:A:8:SER:C	1:A:10:ARG:H	2.27	0.42
1:B:363:LEU:HD22	1:B:369:GLU:HB3	2.02	0.42
1:C:755:TYR:HB2	1:C:804:TYR:HE1	1.85	0.42
1:C:861:ASN:HA	1:C:888:TYR:OH	2.20	0.42
1:D:117:ILE:HD13	1:D:117:ILE:HA	1.91	0.42
1:D:414:TYR:O	1:D:657:ARG:NH2	2.53	0.42
1:D:628:THR:HA	1:D:631:ILE:HG22	2.02	0.42
1:D:738:LYS:O	1:D:742:PHE:HB2	2.20	0.42
1:D:783:ALA:HA	1:D:786:HIS:HD2	1.84	0.42
1:B:142:CYS:O	1:B:145:ARG:N	2.53	0.42
1:B:282:TYR:O	1:B:283:LEU:C	2.59	0.42
1:B:486:THR:O	1:B:489:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:GLY:O	1:B:807:LEU:N	2.53	0.42
1:C:278:ASN:OD1	1:C:281:ASP:HB2	2.20	0.42
1:C:467:ASN:OD1	1:C:468:GLY:N	2.53	0.42
1:C:479:TYR:HB2	1:C:522:PHE:HE2	1.84	0.42
1:C:629:ARG:NH1	1:C:643:SER:OG	2.52	0.42
1:C:981:ILE:HD13	1:C:981:ILE:HA	1.93	0.42
1:D:627:ARG:HH12	1:D:675:LYS:HG3	1.84	0.42
1:A:442:LEU:CD2	1:A:447:ARG:HB2	2.49	0.41
1:A:526:ASP:O	1:A:527:LEU:C	2.63	0.41
1:C:206:THR:HG21	1:D:206:THR:HG21	2.01	0.41
1:D:151:VAL:HA	1:D:167:LEU:HB3	2.02	0.41
1:A:699:PHE:CD2	1:A:743:TYR:HB3	2.55	0.41
1:B:661:ILE:HG12	1:B:717:LYS:NZ	2.35	0.41
1:B:663:ASP:OD1	1:B:664:ILE:N	2.52	0.41
1:B:742:PHE:HE1	1:B:778:PHE:HB2	1.84	0.41
1:C:122:LEU:HD23	1:C:122:LEU:HA	1.86	0.41
1:C:921:PHE:O	1:C:969:LYS:NZ	2.53	0.41
1:C:937:ASP:HB3	1:C:939:GLN:HG3	2.03	0.41
1:C:973:ASN:HB3	1:C:975:HIS:CE1	2.56	0.41
1:D:147:LYS:HA	1:D:147:LYS:HD3	1.91	0.41
1:D:958:TRP:HA	1:D:961:ASN:HD21	1.86	0.41
1:D:993:ASP:HB2	1:D:996:TYR:HD2	1.84	0.41
2:E:20:ILE:HD11	2:E:118:TYR:CE1	2.55	0.41
1:A:345:THR:HB	1:A:397:ALA:CA	2.50	0.41
1:A:348:ARG:NH2	1:A:353:GLY:O	2.53	0.41
1:A:405:THR:HG21	1:A:586:LEU:HD21	2.02	0.41
1:A:678:PHE:HB3	1:A:681:GLN:NE2	2.33	0.41
1:A:738:LYS:O	1:A:739:ALA:HB3	2.20	0.41
1:B:461:ASN:OD1	1:B:462:SER:N	2.54	0.41
1:C:624:GLU:HG3	1:C:671:CYS:SG	2.60	0.41
1:D:432:ILE:HD13	1:D:432:ILE:HA	1.88	0.41
1:D:682:GLU:OE1	1:D:682:GLU:N	2.45	0.41
1:D:841:LEU:HD12	1:D:841:LEU:HA	1.93	0.41
2:F:28:GLU:HG3	2:F:41:LYS:CE	2.51	0.41
1:A:322:LEU:HD12	1:A:325:ILE:HD11	2.03	0.41
1:A:578:MET:O	1:A:579:SER:C	2.63	0.41
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.86	0.41
1:D:634:LEU:HB2	1:D:638:PHE:CE2	2.55	0.41
1:D:668:GLU:OE2	1:D:760:ARG:NH2	2.53	0.41
1:A:118:HIS:O	1:A:121:ILE:HG22	2.21	0.41
1:A:374:SER:OG	1:A:375:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:GLN:H	1:A:681:GLN:HG2	1.71	0.41
1:A:941:ASP:OD1	1:A:945:ASP:HB3	2.20	0.41
1:B:811:PHE:N	1:B:811:PHE:HD1	2.19	0.41
1:B:843:PRO:HD3	1:B:871:ILE:HD13	2.03	0.41
1:C:304:LYS:HG2	1:C:305:ASP:H	1.85	0.41
1:C:402:THR:O	1:C:402:THR:HG23	2.21	0.41
1:C:831:LYS:HA	1:C:831:LYS:HD2	1.88	0.41
1:C:866:MET:SD	1:C:867:ASN:N	2.93	0.41
1:D:697:LYS:HB3	1:D:697:LYS:HE2	1.62	0.41
1:D:938:ASP:OD1	1:D:938:ASP:N	2.53	0.41
1:D:979:HIS:O	1:D:983:VAL:HG12	2.20	0.41
1:A:11:TYR:HD1	1:A:11:TYR:HA	1.74	0.41
1:B:721:TYR:O	1:B:760:ARG:NH1	2.43	0.41
1:A:37:SER:HB2	1:A:42:LEU:HD22	2.02	0.41
1:A:728:LEU:HD12	1:A:733:LEU:HD23	2.03	0.41
1:A:755:TYR:O	1:A:758:LEU:HG	2.21	0.41
1:A:913:MET:SD	1:A:913:MET:C	3.04	0.41
1:D:104:LEU:HD12	1:D:104:LEU:HA	1.95	0.41
1:D:787:ILE:HG12	1:D:834:GLN:OE1	2.21	0.41
1:D:987:ARG:NH1	1:D:990:ASN:HD22	2.19	0.41
1:D:990:ASN:OD1	1:D:990:ASN:C	2.64	0.41
1:B:781:LEU:O	1:B:785:LYS:HG3	2.20	0.41
1:C:495:LEU:O	1:C:499:THR:HG22	2.20	0.41
1:D:780:VAL:HG12	1:D:820:LEU:HD21	2.02	0.41
1:A:21:MET:C	1:A:21:MET:HE3	2.45	0.41
1:A:73:SER:N	1:A:74:PRO:HD3	2.36	0.41
1:A:179:LYS:HE2	1:A:179:LYS:HB2	1.89	0.41
1:A:412:LEU:HD11	1:A:420:VAL:HB	2.03	0.41
1:A:716:ALA:O	1:A:717:LYS:C	2.64	0.41
1:A:867:ASN:ND2	2:E:76:GLU:HA	2.35	0.41
1:B:78:ASN:O	1:B:79:TYR:HD1	2.03	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.85	0.41
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.93	0.41
1:B:889:LEU:HD23	1:B:889:LEU:HA	1.78	0.41
1:C:720:LEU:HD13	1:C:720:LEU:HA	1.93	0.41
1:C:732:GLY:O	1:C:736:ILE:HG12	2.20	0.41
1:C:869:ILE:HG13	1:C:870:ARG:N	2.35	0.41
1:C:889:LEU:HD11	1:C:933:PHE:CG	2.55	0.41
1:D:661:ILE:HD13	1:D:661:ILE:HA	1.83	0.41
1:D:940:TYR:O	1:D:944:VAL:HB	2.20	0.41
2:F:85:LYS:HA	2:F:85:LYS:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.86	0.41
1:B:873:LEU:HD23	1:B:873:LEU:HA	1.91	0.41
1:B:1000:LEU:HD23	1:B:1000:LEU:HA	1.88	0.41
1:C:423:LYS:HE3	1:C:423:LYS:HB3	1.98	0.41
1:C:592:LEU:HA	1:C:592:LEU:HD23	1.85	0.41
1:C:730:GLU:CD	1:C:730:GLU:H	2.29	0.41
1:A:397:ALA:O	1:A:398:LYS:C	2.64	0.40
1:A:738:LYS:HE3	1:A:738:LYS:HB3	1.97	0.40
1:A:910:ASN:HD22	2:E:79:PHE:N	2.19	0.40
1:A:1000:LEU:HD12	1:A:1005:ILE:HD11	2.03	0.40
1:B:368:ASP:C	1:B:370:ARG:H	2.28	0.40
1:B:952:LYS:HA	1:B:952:LYS:HD3	1.97	0.40
1:C:254:GLU:OE1	1:C:254:GLU:N	2.54	0.40
1:C:1005:ILE:HD12	1:C:1005:ILE:HA	1.96	0.40
1:D:15:LEU:O	1:D:18:VAL:HG12	2.21	0.40
2:E:11:THR:HB	2:E:14:LEU:HD22	2.02	0.40
2:E:32:VAL:HB	2:E:82:LYS:CB	2.51	0.40
1:A:105:LYS:O	1:A:109:GLN:HB2	2.20	0.40
1:B:130:ILE:HD11	1:B:207:ILE:HG21	2.03	0.40
1:C:678:PHE:HB3	1:C:681:GLN:HE22	1.86	0.40
1:D:288:ALA:O	1:D:292:LEU:HB2	2.21	0.40
1:D:330:LEU:HD23	1:D:330:LEU:HA	1.88	0.40
1:D:809:LYS:HD3	1:D:809:LYS:HA	1.80	0.40
1:D:987:ARG:HA	1:D:987:ARG:HH11	1.86	0.40
1:A:502:ARG:O	1:A:504:TYR:CD2	2.74	0.40
1:A:836:ASP:O	1:A:840:LYS:HG3	2.21	0.40
1:B:959:LEU:HA	1:B:962:TYR:CD2	2.57	0.40
1:C:987:ARG:NE	1:C:987:ARG:HA	2.37	0.40
1:D:62:LEU:HA	1:D:62:LEU:HD23	1.83	0.40
1:D:152:ILE:HB	1:D:168:LEU:HD12	2.03	0.40
1:D:701:ALA:O	1:D:702:ASN:ND2	2.55	0.40
1:B:865:LEU:HD21	1:B:881:HIS:HB3	2.04	0.40
1:C:114:THR:HG22	1:C:115:ASN:N	2.36	0.40
1:C:220:LEU:HD21	1:C:268:ILE:HD11	2.03	0.40
1:C:1002:ASN:HB3	1:C:1003:TYR:HD1	1.87	0.40
1:D:978:HIS:O	1:D:981:ILE:HG22	2.21	0.40
2:E:54:ASN:CB	2:E:58:ASP:HB2	2.51	0.40
1:B:419:ASP:OD1	1:B:420:VAL:HG23	2.20	0.40
1:B:544:PHE:HD1	1:B:549:GLN:HE21	1.70	0.40
1:B:987:ARG:HD3	1:B:996:TYR:CE2	2.56	0.40
1:C:744:PHE:CD1	1:C:749:LEU:HD23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:CYS:O	1:D:33:ILE:HG22	2.22	0.40
1:D:859:VAL:HG11	1:D:881:HIS:HE2	1.85	0.40
2:E:35:ASP:HB2	2:E:37:LYS:HE3	2.04	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	963/1005 (96%)	900 (94%)	57 (6%)	6 (1%)	21	54
1	B	964/1005 (96%)	924 (96%)	40 (4%)	0	100	100
1	C	964/1005 (96%)	939 (97%)	25 (3%)	0	100	100
1	D	963/1005 (96%)	928 (96%)	34 (4%)	1 (0%)	48	79
2	E	109/120 (91%)	87 (80%)	19 (17%)	3 (3%)	4	26
2	F	109/120 (91%)	100 (92%)	8 (7%)	1 (1%)	14	46
All	All	4072/4260 (96%)	3878 (95%)	183 (4%)	11 (0%)	37	65

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	83	ILE
1	A	680	GLU
2	E	54	ASN
1	A	403	LEU
1	A	495	LEU
1	A	672	SER
1	A	492	PHE
2	E	78	GLU
1	A	675	LYS

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Mol	Chain	Res	Type
1	D	507	PHE
2	E	83	ILE

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	885/923 (96%)	850 (96%)	35 (4%)	28	54
1	B	885/923 (96%)	866 (98%)	19 (2%)	47	65
1	C	892/923 (97%)	873 (98%)	19 (2%)	47	65
1	D	893/923 (97%)	869 (97%)	24 (3%)	39	61
2	E	92/113 (81%)	83 (90%)	9 (10%)	7	31
2	F	92/113 (81%)	89 (97%)	3 (3%)	33	58
All	All	3739/3918 (95%)	3630 (97%)	109 (3%)	38	60

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	14	LYS
1	A	17	GLU
1	A	160	ASN
1	A	276	ASP
1	A	396	MET
1	A	489	VAL
1	A	493	ASN
1	A	495	LEU
1	A	510	GLU
1	A	515	ILE
1	A	520	THR
1	A	525	ASP
1	A	526	ASP
1	A	527	LEU
1	A	584	VAL

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Mol	Chain	Res	Type
1	A	662	ASP
1	A	670	SER
1	A	673	ILE
1	A	675	LYS
1	A	678	PHE
1	A	680	GLU
1	A	714	SER
1	A	717	LYS
1	A	741	LEU
1	A	753	LYS
1	A	765	ASN
1	A	774	ILE
1	A	816	ILE
1	A	889	LEU
1	A	926	ASN
1	A	929	LYS
1	A	931	GLU
1	A	932	GLU
1	A	958	TRP
1	B	52	THR
1	B	114	THR
1	B	190	TYR
1	B	228	LEU
1	B	276	ASP
1	B	278	ASN
1	B	282	TYR
1	B	328	ILE
1	B	368	ASP
1	B	375	LYS
1	B	396	MET
1	B	467	ASN
1	B	495	LEU
1	B	497	LEU
1	B	499	THR
1	B	726	VAL
1	B	803	ASP
1	B	934	ILE
1	B	961	ASN
1	C	110	VAL
1	C	131	THR
1	C	160	ASN
1	C	213	ILE

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Mol	Chain	Res	Type
1	C	232	VAL
1	C	268	ILE
1	C	325	ILE
1	C	346	VAL
1	C	474	SER
1	C	490	THR
1	C	573	SER
1	C	662	ASP
1	C	722	PHE
1	C	810	HIS
1	C	955	ILE
1	C	975	HIS
1	C	981	ILE
1	C	984	LEU
1	C	988	VAL
1	D	43	VAL
1	D	52	THR
1	D	131	THR
1	D	183	VAL
1	D	213	ILE
1	D	333	VAL
1	D	346	VAL
1	D	430	VAL
1	D	449	GLU
1	D	481	ILE
1	D	489	VAL
1	D	508	THR
1	D	586	LEU
1	D	621	GLU
1	D	651	ASP
1	D	661	ILE
1	D	662	ASP
1	D	696	THR
1	D	697	LYS
1	D	812	GLU
1	D	846	SER
1	D	871	ILE
1	D	943	PHE
1	D	1002	ASN
2	E	11	THR
2	E	14	LEU
2	E	20	ILE

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Mol	Chain	Res	Type
2	E	42	CYS
2	E	44	PHE
2	E	59	PHE
2	E	88	HIS
2	E	100	LEU
2	E	112	ILE
2	F	18	SER
2	F	39	LEU
2	F	62	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	160	ASN
1	A	195	GLN
1	A	475	GLN
1	A	477	ASN
1	A	491	GLN
1	A	503	HIS
1	A	521	ASN
1	A	698	GLN
1	A	786	HIS
1	A	832	GLN
1	A	867	ASN
1	A	910	ASN
1	A	1002	ASN
1	B	109	GLN
1	B	182	ASN
1	B	297	GLN
1	B	339	HIS
1	B	404	ASN
1	B	457	ASN
1	B	493	ASN
1	B	614	ASN
1	B	789	GLN
1	B	926	ASN
1	B	975	HIS
1	B	978	HIS
1	B	979	HIS
1	B	1002	ASN
1	C	89	GLN

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Mol	Chain	Res	Type
1	C	93	ASN
1	C	297	GLN
1	C	382	ASN
1	C	457	ASN
1	C	477	ASN
1	C	503	HIS
1	C	666	ASN
1	C	681	GLN
1	C	698	GLN
1	C	711	GLN
1	C	782	GLN
1	C	834	GLN
1	C	848	ASN
1	C	990	ASN
1	D	89	GLN
1	D	93	ASN
1	D	118	HIS
1	D	136	ASN
1	D	192	ASN
1	D	211	HIS
1	D	339	HIS
1	D	391	ASN
1	D	477	ASN
1	D	609	HIS
1	D	658	HIS
1	D	786	HIS
1	D	810	HIS
1	D	961	ASN
1	D	978	HIS
1	D	979	HIS
2	E	40	ASN
2	E	49	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

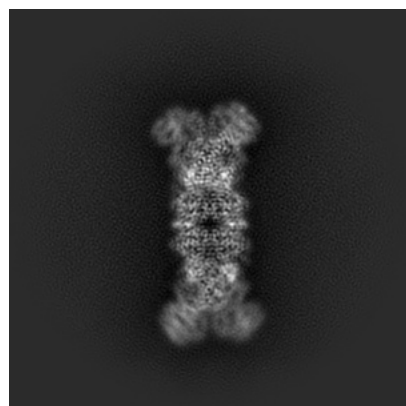
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37272. These allow visual inspection of the internal detail of the map and identification of artifacts.

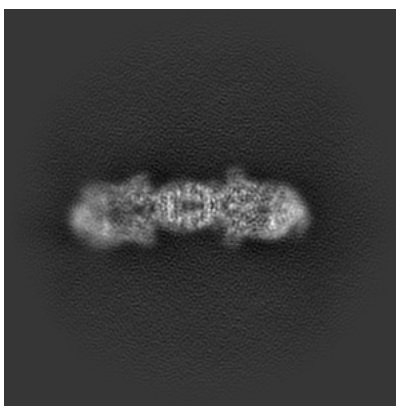
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

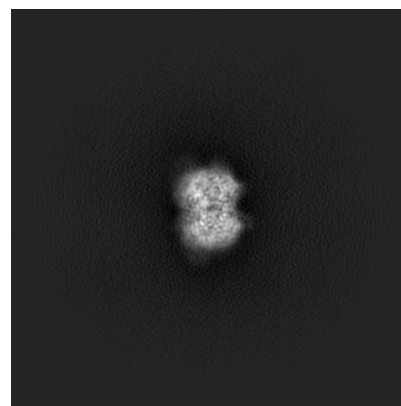
6.1.1 Primary map



X

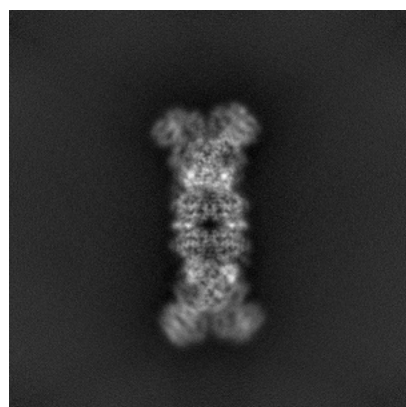


Y

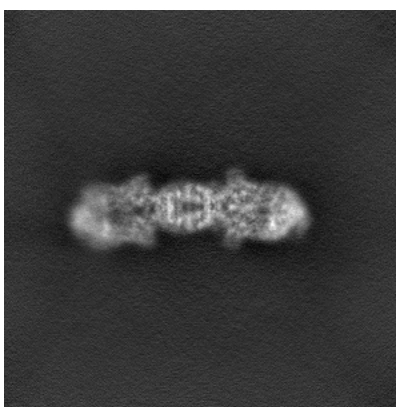


Z

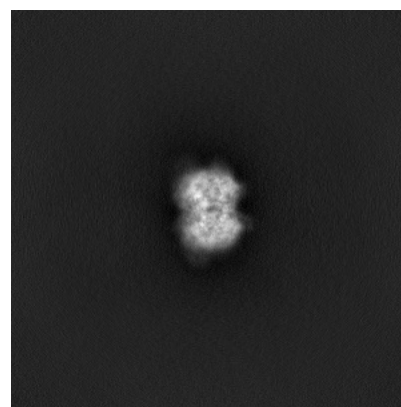
6.1.2 Raw map



X



Y

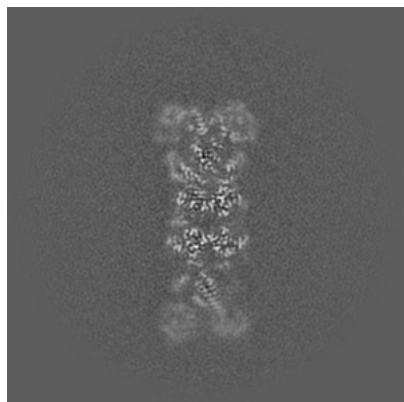


Z

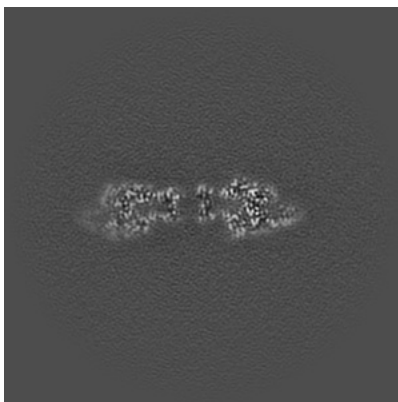
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

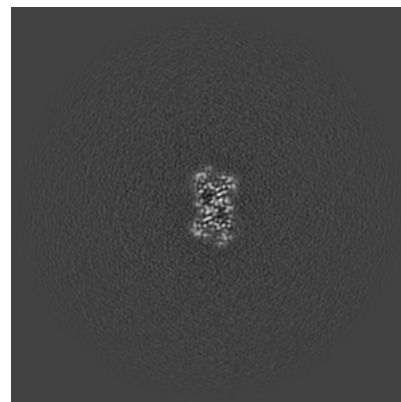
6.2.1 Primary map



X Index: 250

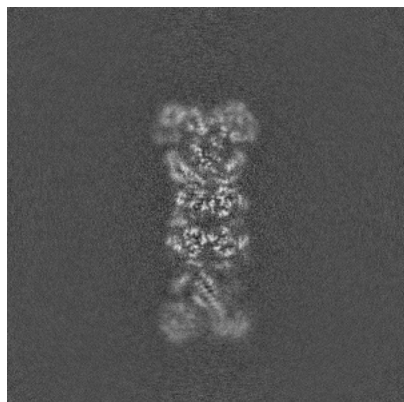


Y Index: 250

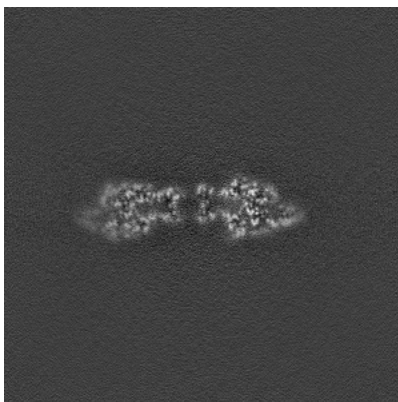


Z Index: 250

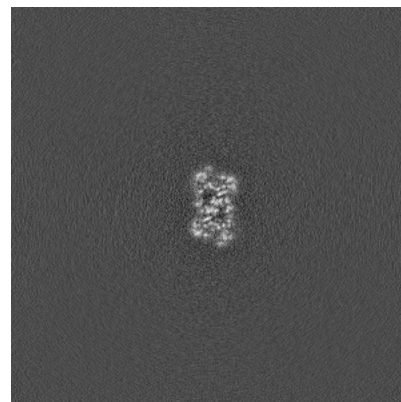
6.2.2 Raw map



X Index: 250



Y Index: 250

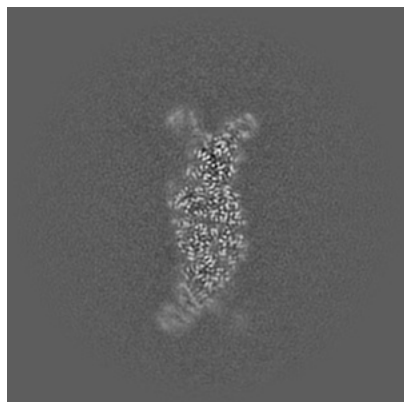


Z Index: 250

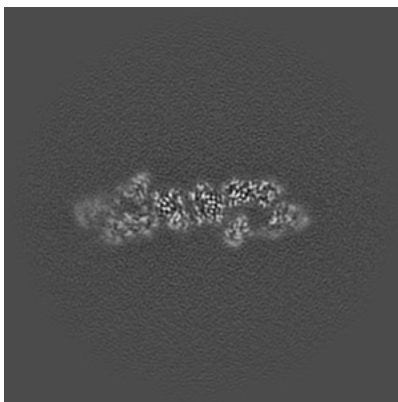
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

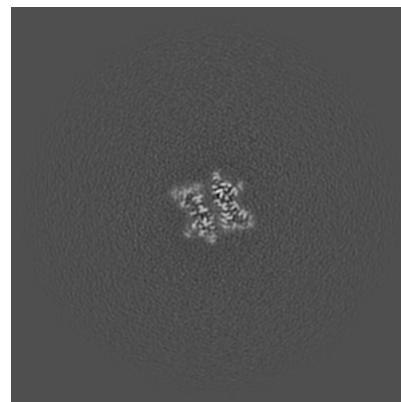
6.3.1 Primary map



X Index: 265

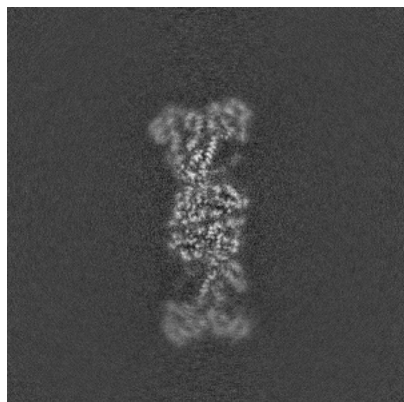


Y Index: 267

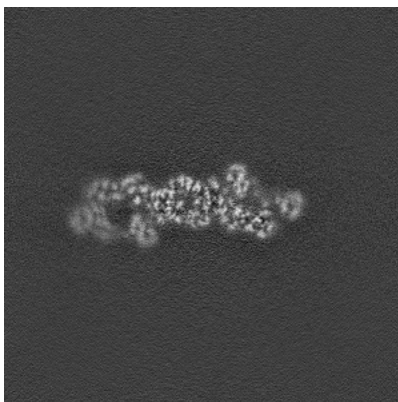


Z Index: 290

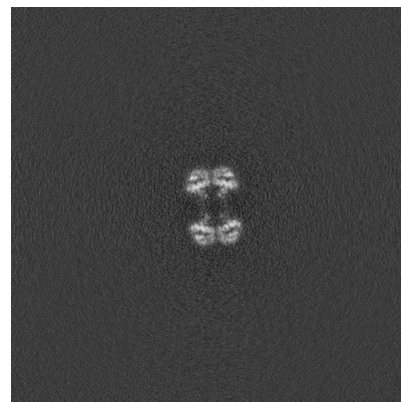
6.3.2 Raw map



X Index: 242



Y Index: 229

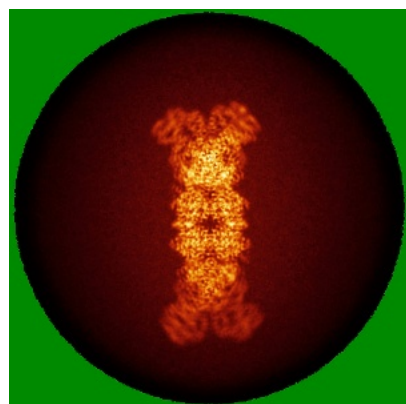


Z Index: 231

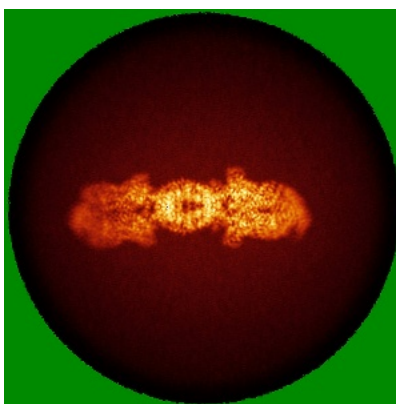
The images above show the largest variance slices of the map in three orthogonal directions.

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

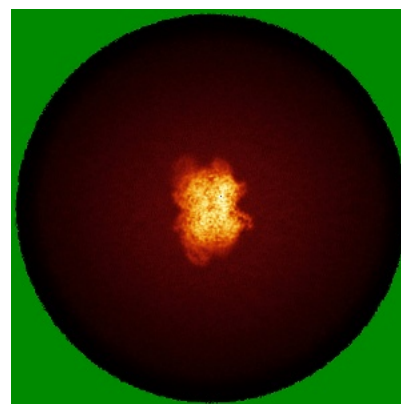
6.4.1 Primary map



X

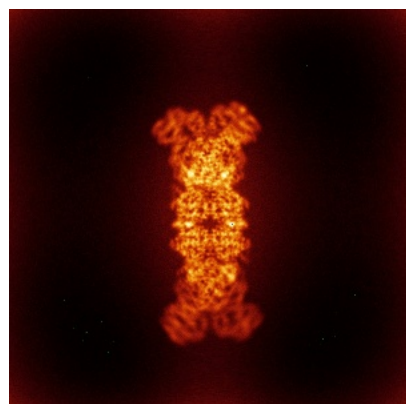


Y

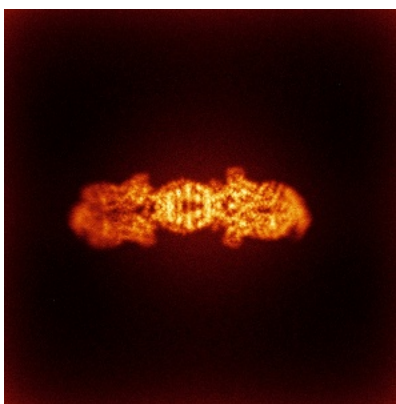


Z

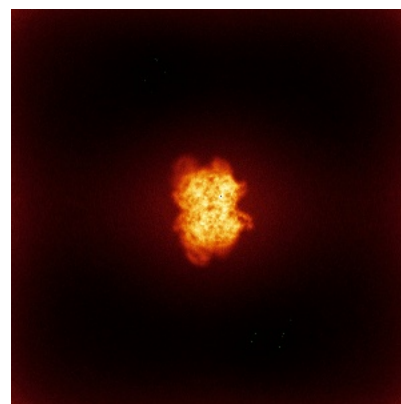
6.4.2 Raw map



X



Y

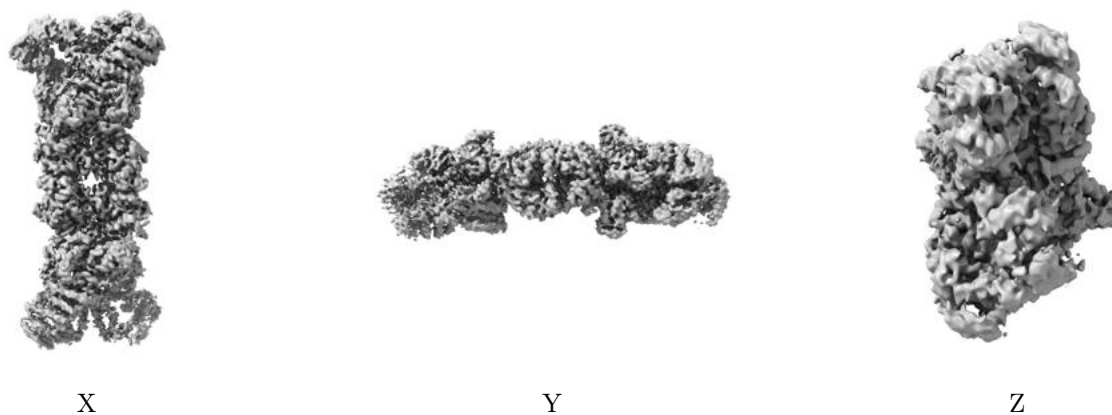


Z

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

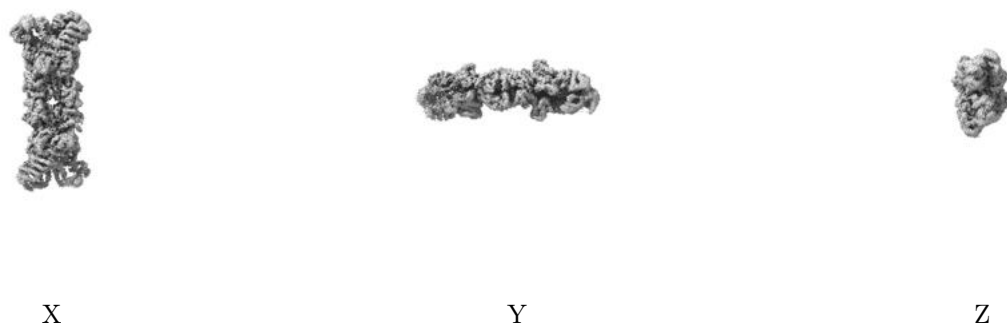
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.266. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

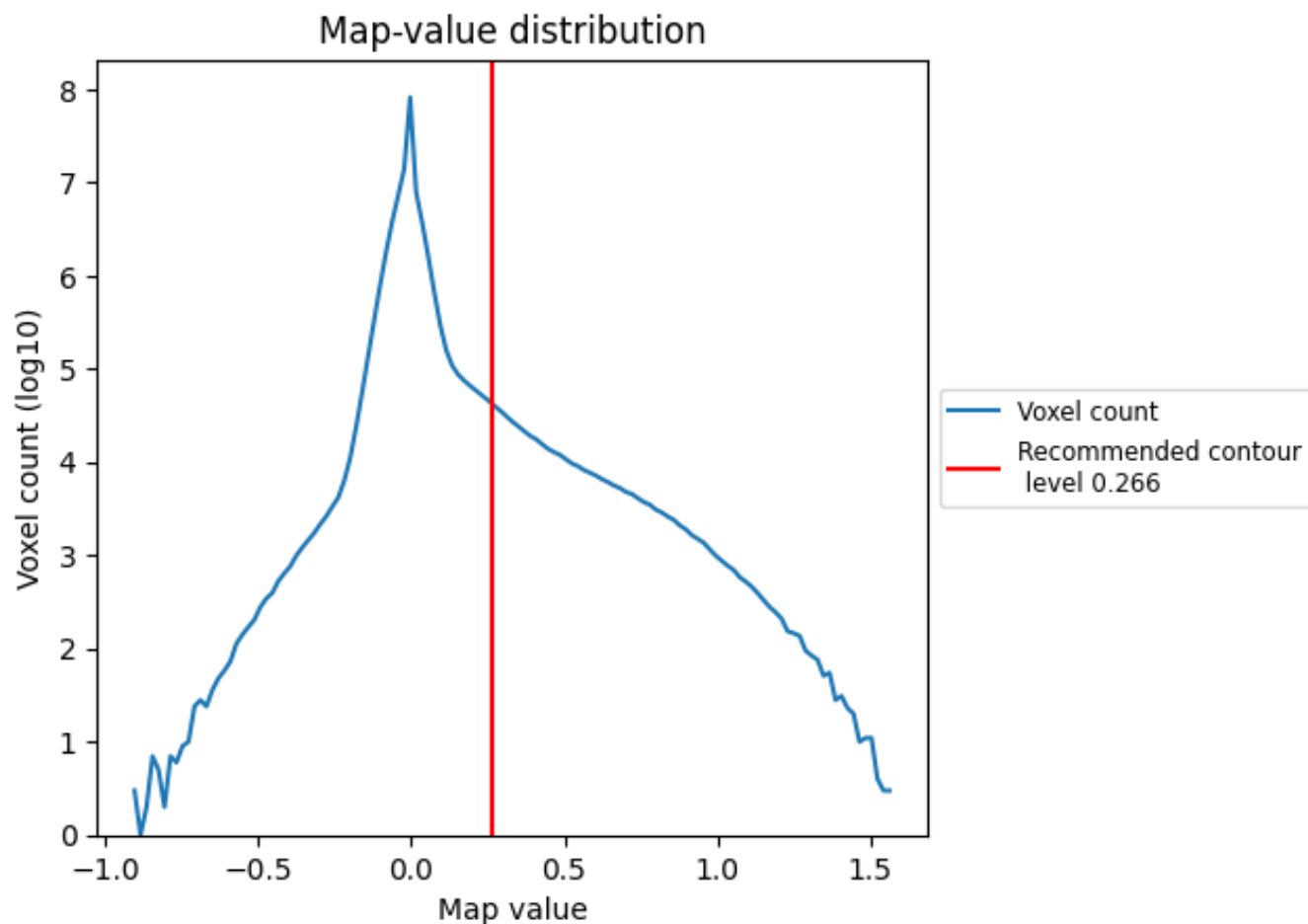
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

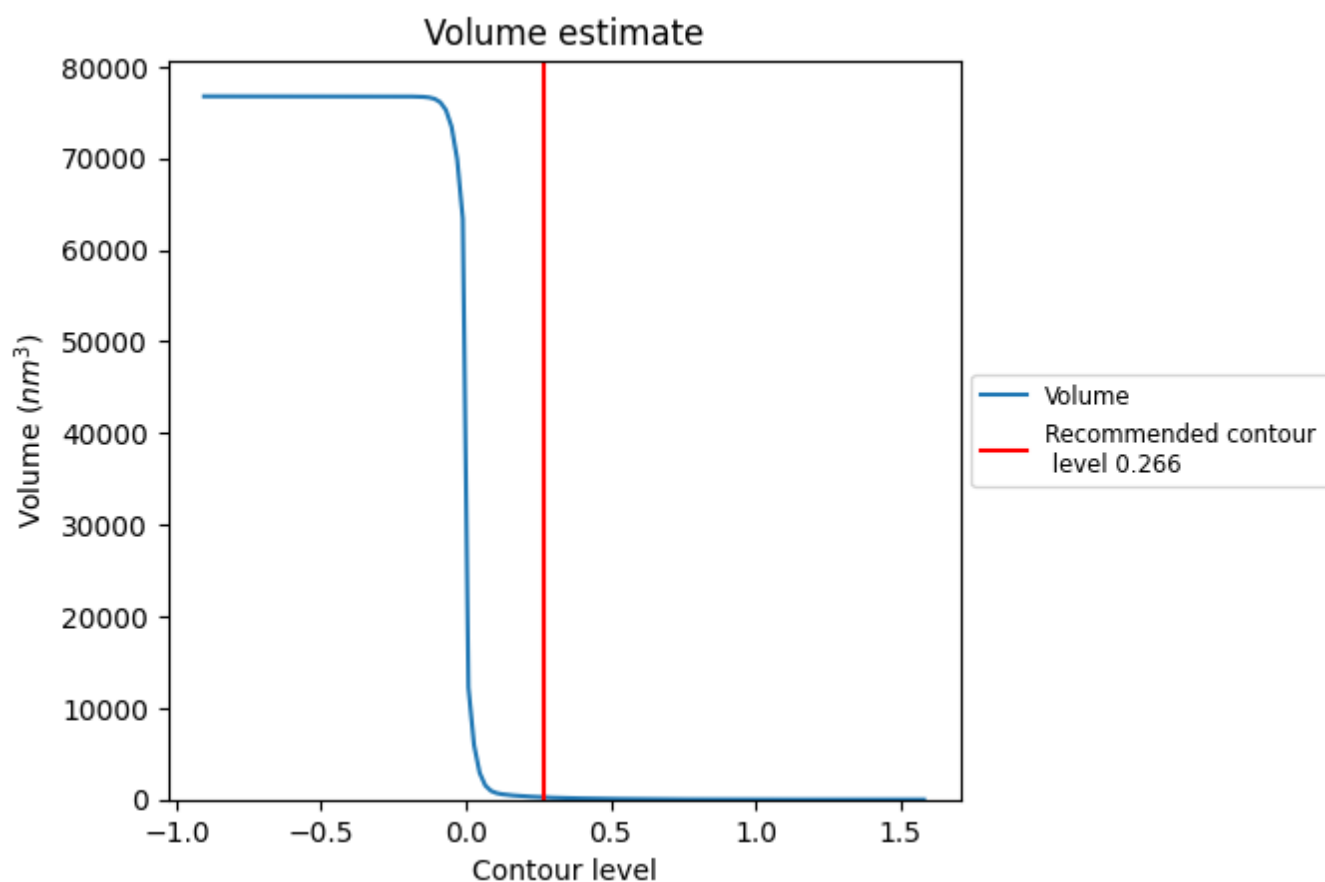
This section contains the results of statistical analysis of the map.

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.

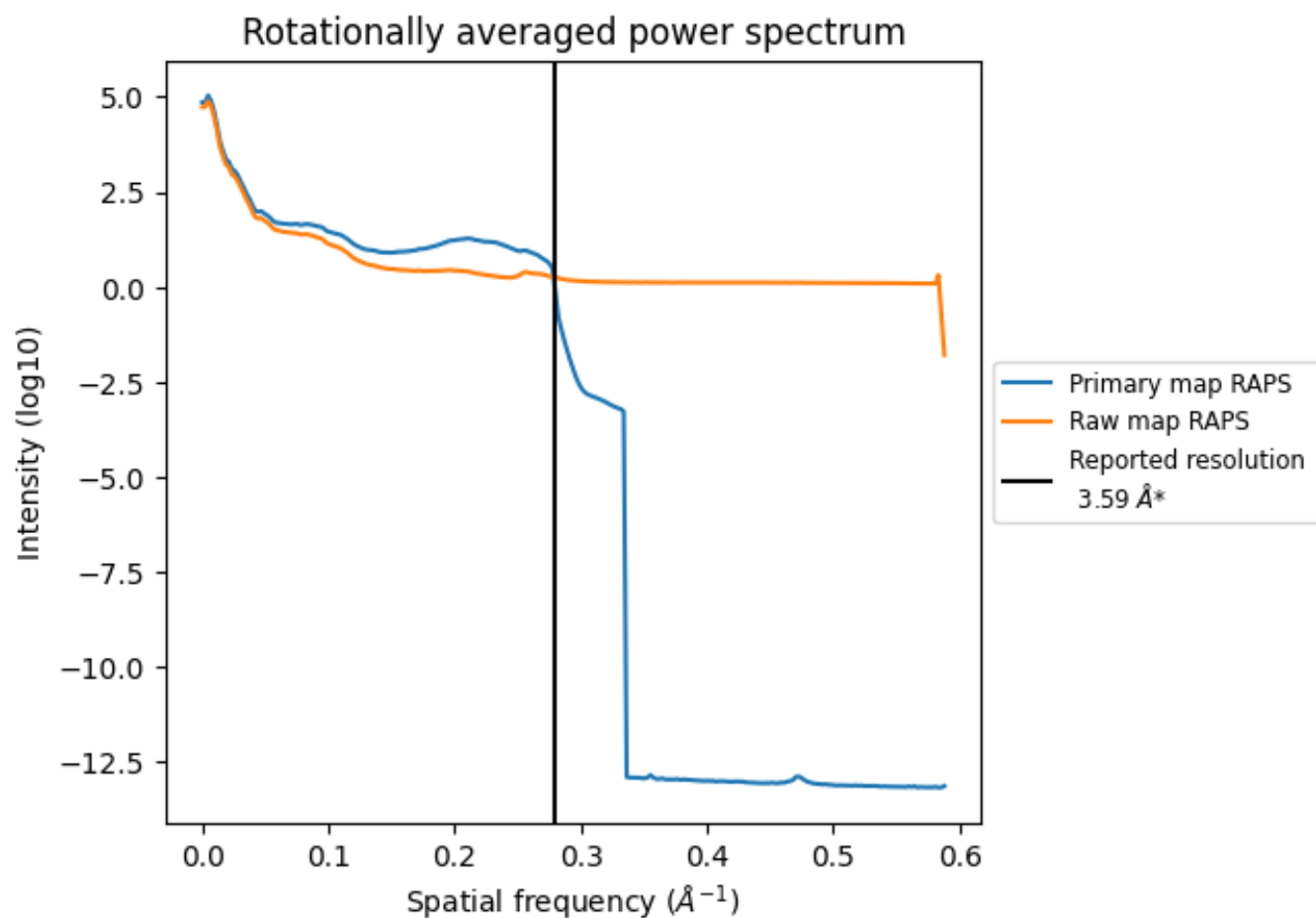
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 226 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 ⓘ

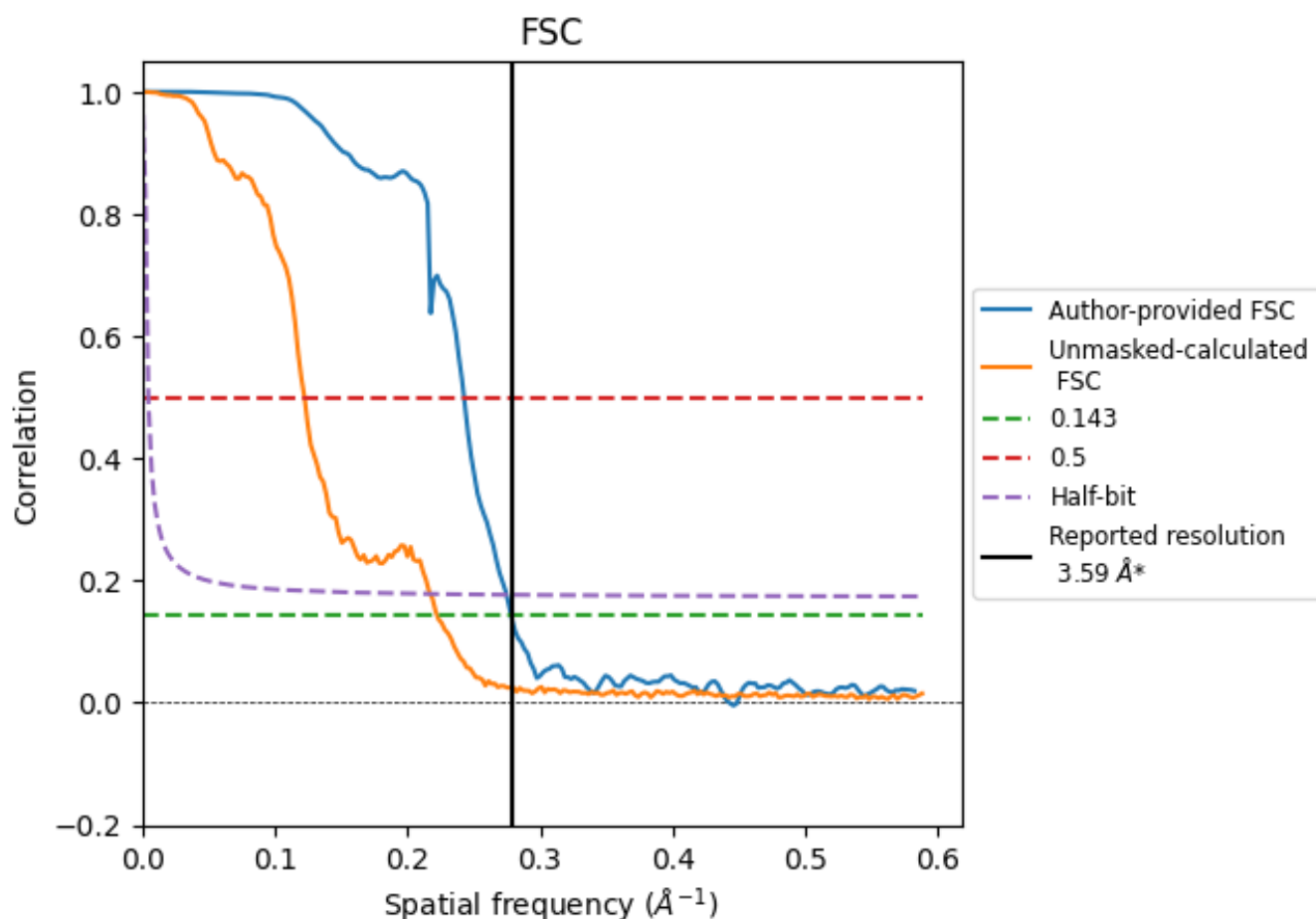


*Reported resolution corresponds to spatial frequency of 0.279 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

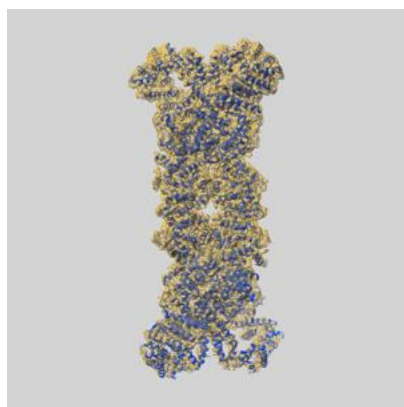
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	3.59	4.12	3.64
Unmasked-calculated*	4.50	8.18	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.59 by more than 10 %

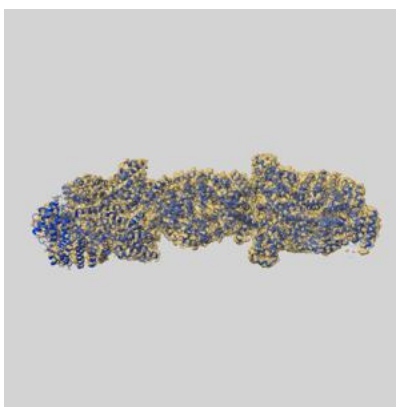
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37272 and PDB model 8W56. Per-residue inclusion information can be found in section 3 on page 5.

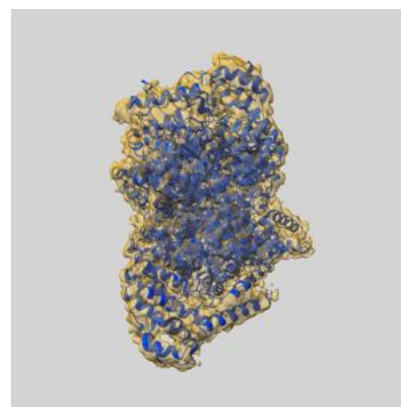
9.1 Map-model overlay [i](#)



X



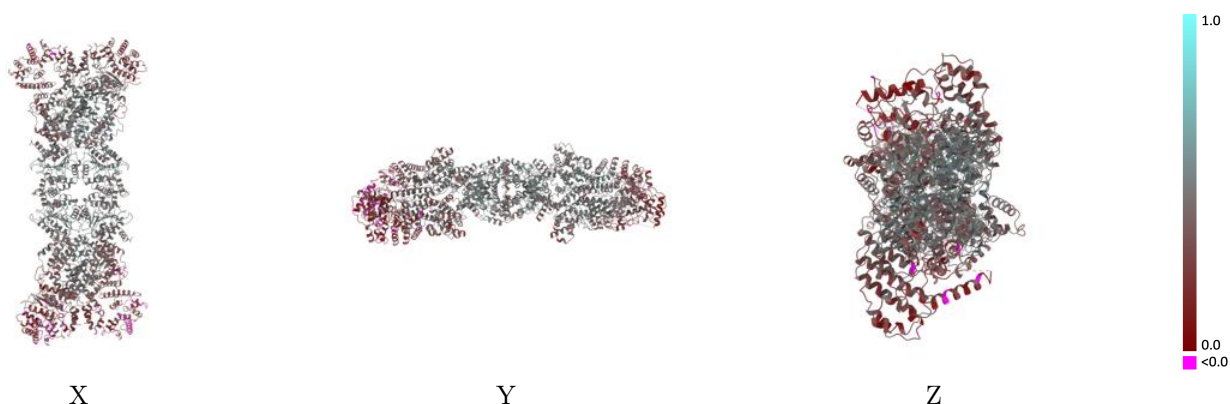
Y



Z

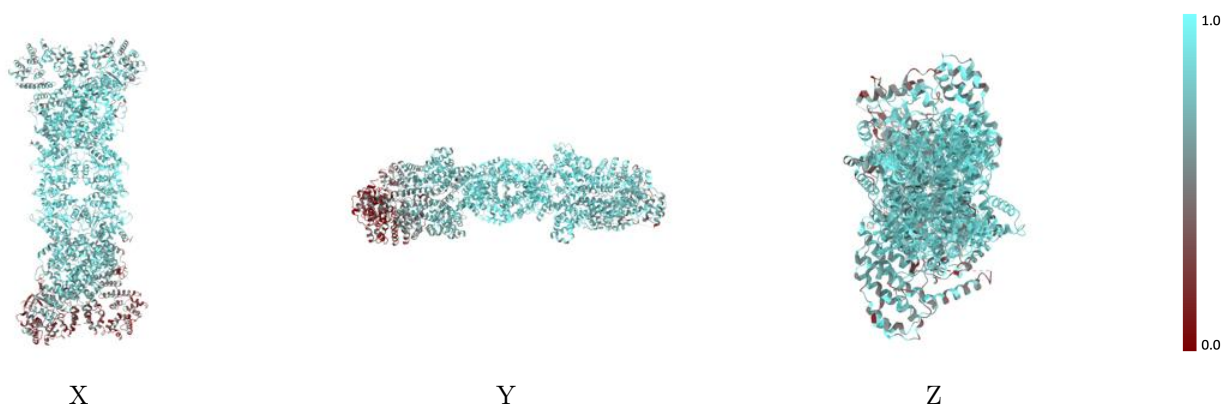
The images above show the 3D surface view of the map at the recommended contour level 0.266 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



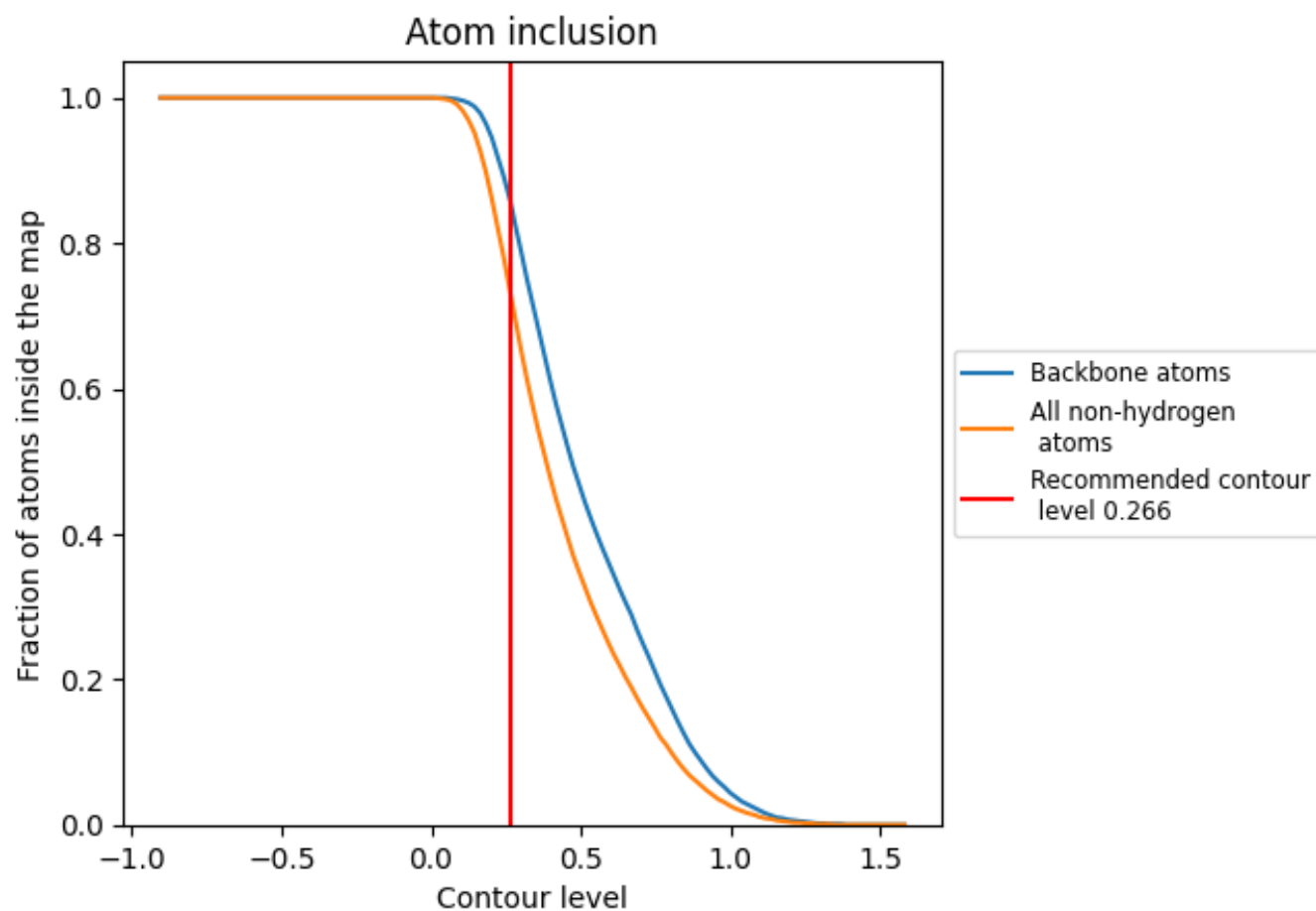
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.266).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7290	0.3880
A	0.6790	0.3730
B	0.6230	0.3500
C	0.8160	0.4100
D	0.8400	0.4290
E	0.3410	0.3130
F	0.7330	0.3580

1.0

0.0

<0.0