



Full wwPDB EM Validation Report ⓘ

May 19, 2026 – 10:25 am BST

PDB ID : 8RZ9 / pdb_00008rz9
EMDB ID : EMD-19607
Title : MutSbeta-ATPgS with kinked MSH2 clamp
Authors : Lee, J.-H.; Thomsen, M.; Daub, H.; Steinbacher, S.; Sztyler, A.; Thieulin-Pardo, G.; Neudegger, T.; Plotnikov, N.; Iyer, R.R.; Wilkinson, H.; Montegudo, E.; Felsenfeld, D.P.; Haque, T.; Finley, M.; Dominguez, C.; Vogt, T.F.; Prasad, B.C.
Deposited on : 2024-02-12
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

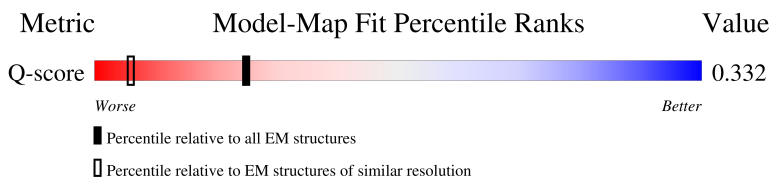
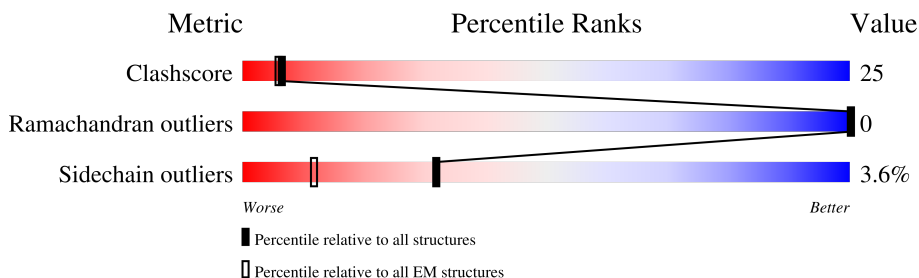
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

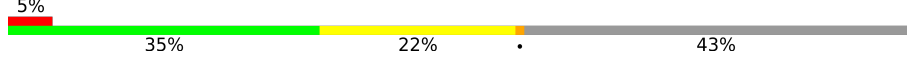
The reported resolution of this entry is 3.02 Å.

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	13913 (2.52 - 3.52)

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	934	
2	B	1137	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AGS	B	2001	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8571 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	534	Total	C	N	O	S	0	0
			4232	2684	720	804	24		

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	533	Total	C	N	O	S	0	0
			4275	2729	740	788	18		

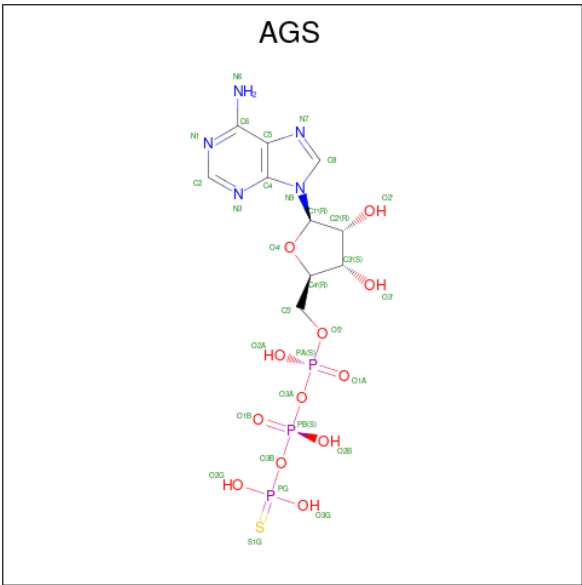
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	949	ARG	GLN	conflict	UNP P20585

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

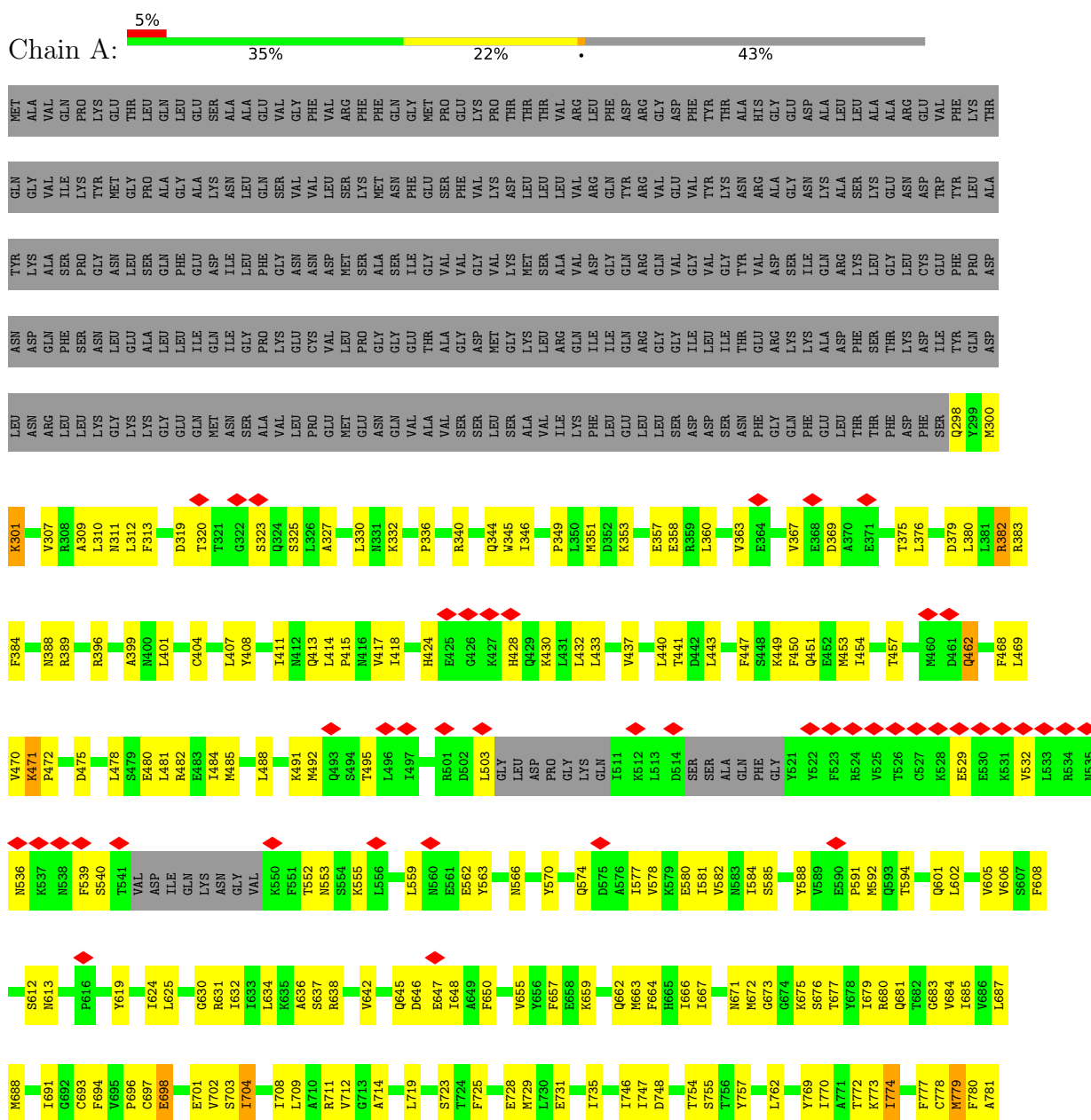


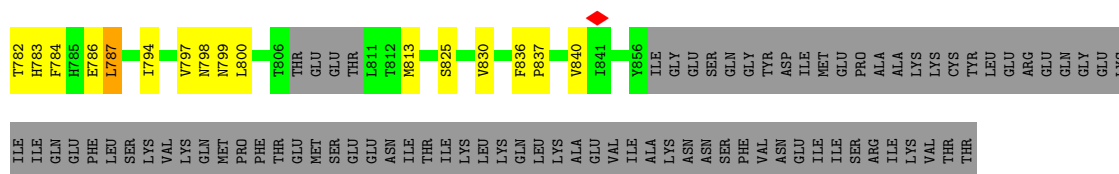
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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.

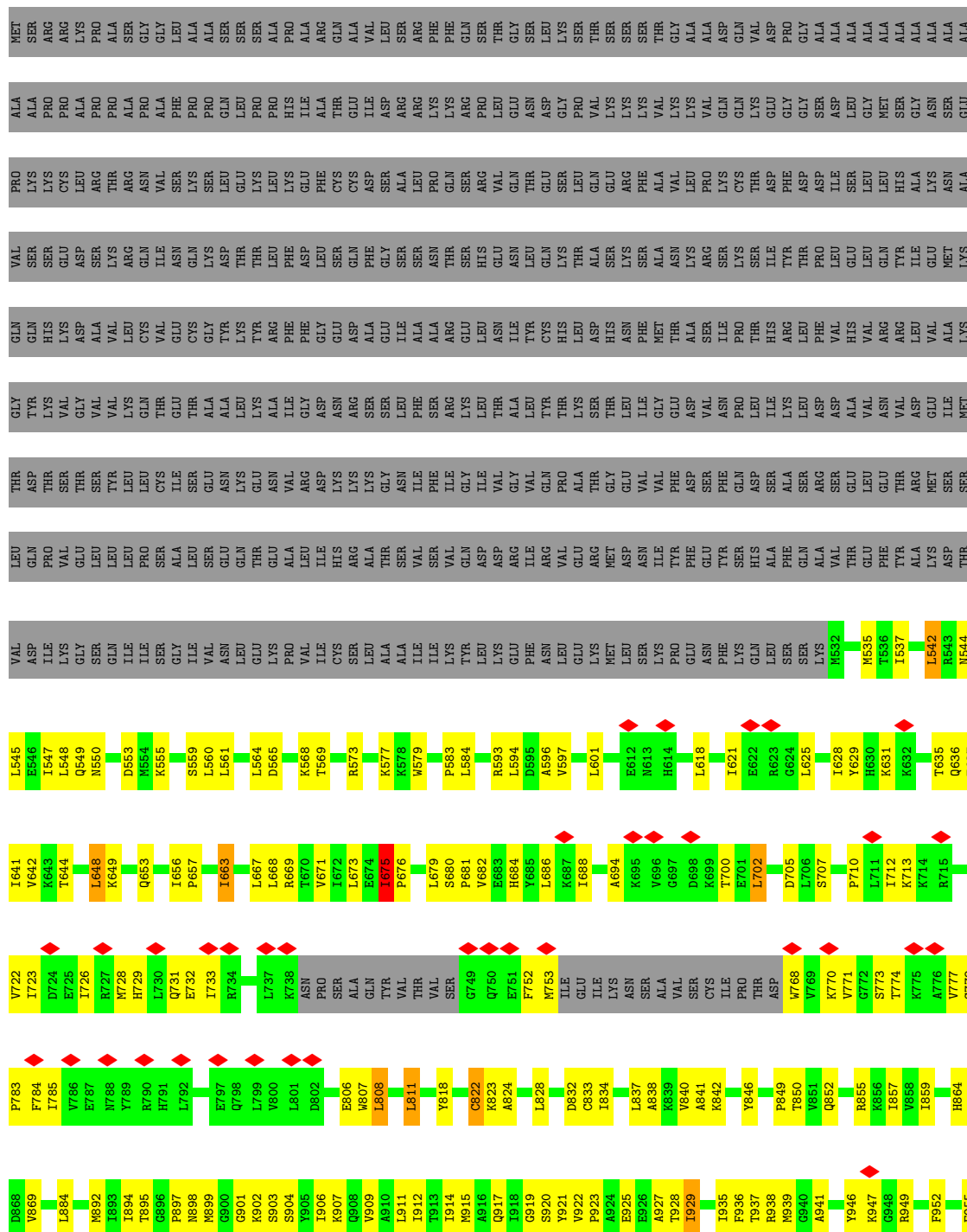
- Molecule 1: DNA mismatch repair protein Msh2





• Molecule 2: DNA mismatch repair protein Msh3

Chain B: 28% 18% 53%



L956	SER	LEU
T957	LYS	GLN
D958	LEU	GLN
T959	ASP	TRP
A960	PRO	THR
E961	GLY	GLU
T962	ALA	GLU
I963	ALA	PHE
R964	GLU	ASN
	GLN	MET
S968	VAL	GLU
	PRO	GLU
V972	D1051	THR
	F1052	GLN
D975		THR
G978	F1055	SER
		LEU
T981	I1059	LEU
	T1060	HIS
	R1061	
T987	G1062	
Y991	R1066	
A992	S1067	
T993	Y1068	
L994	G1069	
E995	L1070	
Y996	N1071	
F997	V1072	
	A1073	
R999		
D1000	P1079	
V1001	G1080	
K1002	E1081	
S1003	I1082	
L1004		
T1005	K1085	
L1006		
F1007	K1089	
	S1090	
V1008		
T1009	L1093	
Y1011		
H1010		
P1012	K1102	
P1013	R1103	
V1014	LEU	
C1015	LYS	
E1016	TYR	
L1017	PHE	
	ALA	
Y1028	LYS	
H1029	LEU	
	TRP	
	THR	
F1032	MET	
L1033	HIS	
V1034	ASN	
S1035	ALA	
GLU	GLN	
ASP	ASP	
GLU	ASP	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168225	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.98	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.151	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	292.544, 292.544, 292.544	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9142, 0.9142, 0.9142	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	9/4298 (0.2%)	0.82	1/5801 (0.0%)
2	B	0.61	6/4352 (0.1%)	0.88	3/5868 (0.1%)
All	All	0.61	15/8650 (0.2%)	0.85	4/11669 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	ARG	CD-NE	10.27	1.60	1.46
1	A	319	ASP	C-N	-9.72	1.19	1.33
2	B	1102	LYS	CA-CB	-9.09	1.39	1.53
2	B	1090	SER	CA-CB	-8.27	1.40	1.53
2	B	705	ASP	CA-CB	-7.77	1.43	1.52
1	A	323	SER	C-N	-7.43	1.24	1.33
1	A	389	ARG	CD-NE	-6.68	1.36	1.46
1	A	320	THR	C-N	-5.94	1.25	1.33
2	B	700	THR	CA-CB	-5.73	1.44	1.53
2	B	947	LYS	CA-CB	-5.65	1.44	1.53
1	A	646	ASP	CA-CB	-5.62	1.46	1.53
1	A	396	ARG	NE-CZ	5.39	1.39	1.33
2	B	707	SER	CB-OG	5.29	1.52	1.42
1	A	471	LYS	CA-CB	-5.22	1.45	1.53
1	A	428	HIS	CB-CG	-5.10	1.43	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	675	ILE	N-CA-CB	6.30	115.36	110.45
1	A	647	GLU	CB-CG-CD	5.75	122.37	112.60
2	B	1071	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	B	947	LYS	N-CA-CB	5.71	119.58	110.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ARG	Sidechain

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	4232	0	4262	180	0
2	B	4275	0	4362	224	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	19	0
All	All	8571	0	8648	388	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 25.

All (388) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:729:HIS:NE2	2:B:733:ILE:HD11	1.16	1.46
2:B:729:HIS:NE2	2:B:733:ILE:CD1	2.11	1.13
2:B:898:ASN:O	4:B:2001:AGS:O3B	1.68	1.10
2:B:731:GLN:HE21	2:B:732:GLU:CD	1.67	1.02
1:A:311:ASN:ND2	2:B:946:TYR:OH	1.93	1.02
2:B:729:HIS:CD2	2:B:733:ILE:HD11	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:904:SER:OG	4:B:2001:AGS:N7	1.97	0.97
2:B:1007:PHE:HE2	2:B:1009:THR:HB	1.29	0.94
1:A:723:SER:OG	4:B:2001:AGS:S1G	2.25	0.93
1:A:300:MET:HB3	1:A:349:PRO:HG2	1.53	0.90
1:A:369:ASP:OD2	1:A:424:HIS:ND1	2.06	0.89
1:A:330:LEU:HD13	1:A:608:PHE:CE1	2.08	0.88
2:B:729:HIS:HA	2:B:732:GLU:CD	2.01	0.85
2:B:675:ILE:HG23	2:B:676:PRO:HD3	1.59	0.84
2:B:1029:HIS:ND1	2:B:1062:GLY:O	2.10	0.84
2:B:731:GLN:NE2	2:B:732:GLU:CD	2.35	0.84
2:B:937:THR:HG23	2:B:939:MET:HE3	1.60	0.84
2:B:731:GLN:NE2	2:B:732:GLU:OE2	2.11	0.83
2:B:936:PHE:HB3	2:B:962:ILE:HG12	1.61	0.82
2:B:729:HIS:CD2	2:B:733:ILE:CD1	2.61	0.81
2:B:855:ARG:NH1	2:B:968:SER:O	2.14	0.81
2:B:773:SER:HA	2:B:778:SER:HA	1.61	0.81
1:A:383:ARG:HB2	1:A:413:GLN:HE22	1.48	0.78
2:B:865:PRO:HG3	2:B:923:PRO:HG3	1.65	0.78
1:A:578:VAL:HA	1:A:581:ILE:HG12	1.65	0.78
1:A:636:ALA:HB3	1:A:698:GLU:HB3	1.64	0.77
1:A:675:LYS:HE3	4:A:2001:AGS:O1B	1.84	0.77
2:B:997:PHE:HB3	2:B:1005:THR:HG21	1.66	0.77
1:A:725:PHE:HD2	2:B:1072:VAL:HG11	1.50	0.76
1:A:481:LEU:O	1:A:485:MET:HE3	1.86	0.75
1:A:311:ASN:ND2	2:B:946:TYR:CE2	2.55	0.75
2:B:728:MET:SD	2:B:732:GLU:OE1	2.45	0.74
2:B:542:LEU:HD12	2:B:548:LEU:HG	1.69	0.74
2:B:1007:PHE:CE2	2:B:1009:THR:HB	2.17	0.74
1:A:782:THR:HG21	1:A:787:LEU:HD12	1.70	0.74
2:B:663:ILE:HD11	2:B:669:ARG:HA	1.70	0.73
1:A:574:GLN:O	1:A:578:VAL:HG13	1.88	0.73
1:A:675:LYS:O	1:A:679:ILE:HG22	1.87	0.73
1:A:311:ASN:ND2	2:B:946:TYR:CZ	2.57	0.72
2:B:635:THR:HA	2:B:807:TRP:CH2	2.25	0.72
1:A:671:ASN:HB2	1:A:830:VAL:HG21	1.74	0.70
2:B:728:MET:O	2:B:732:GLU:OE2	2.08	0.69
1:A:424:HIS:O	1:A:430:LYS:NZ	2.25	0.69
2:B:628:ILE:HD11	2:B:641:ILE:HG21	1.75	0.69
2:B:902:LYS:NZ	4:B:2001:AGS:O1B	2.25	0.69
2:B:884:LEU:HB3	2:B:1004:LEU:HD22	1.76	0.68
2:B:729:HIS:CE1	2:B:785:ILE:HG23	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:LEU:O	2:B:915:MET:HG3	1.94	0.68
1:A:778:CYS:SG	1:A:779:MET:N	2.67	0.68
1:A:693:CYS:SG	1:A:694:PHE:N	2.67	0.68
1:A:330:LEU:HD13	1:A:608:PHE:HE1	1.58	0.67
1:A:729:MET:HA	1:A:729:MET:HE2	1.75	0.67
2:B:653:GLN:HA	2:B:656:ILE:HG13	1.75	0.67
2:B:937:THR:CG2	2:B:939:MET:HE3	2.24	0.67
2:B:649:LYS:CD	2:B:680:SER:HA	2.25	0.67
1:A:619:TYR:HB3	1:A:694:PHE:HB3	1.76	0.66
1:A:470:VAL:HG12	1:A:471:LYS:H	1.60	0.66
2:B:594:LEU:HD11	2:B:849:PRO:HD2	1.77	0.65
2:B:773:SER:HA	2:B:778:SER:CA	2.25	0.65
2:B:535:MET:HE2	2:B:583:PRO:HG2	1.77	0.65
2:B:653:GLN:HB2	2:B:676:PRO:HB3	1.78	0.65
1:A:688:MET:HA	1:A:691:ILE:HG12	1.79	0.65
2:B:679:LEU:HD11	2:B:824:ALA:HB1	1.79	0.65
1:A:481:LEU:HD21	1:A:570:TYR:HD1	1.61	0.64
1:A:481:LEU:O	1:A:485:MET:HG2	1.98	0.63
1:A:462:GLN:HE22	1:A:482:ARG:CZ	2.12	0.62
2:B:535:MET:SD	2:B:917:GLN:NE2	2.72	0.62
2:B:542:LEU:HD13	2:B:547:ILE:HB	1.80	0.62
1:A:457:THR:HB	1:A:470:VAL:HG13	1.83	0.61
1:A:659:LYS:HA	1:A:663:MET:HE1	1.81	0.61
2:B:628:ILE:HD12	2:B:641:ILE:HD13	1.83	0.61
2:B:771:VAL:HG23	2:B:781:HIS:HB2	1.81	0.61
1:A:540:SER:N	1:A:552:THR:O	2.33	0.61
2:B:545:LEU:HD11	2:B:935:ILE:HG21	1.83	0.61
2:B:857:ILE:HG22	2:B:859:ILE:HD11	1.83	0.61
1:A:311:ASN:HD21	2:B:946:TYR:HE2	1.45	0.60
1:A:725:PHE:CD2	2:B:1072:VAL:HG11	2.36	0.60
1:A:837:PRO:HD3	2:B:963:ILE:HG21	1.83	0.60
2:B:849:PRO:HD3	2:B:922:VAL:HG22	1.83	0.60
2:B:537:ILE:HG22	2:B:542:LEU:HD22	1.83	0.60
1:A:664:PHE:HE2	1:A:770:ILE:HB	1.65	0.60
2:B:864:HIS:ND1	2:B:867:ILE:HG13	2.15	0.60
1:A:344:GLN:OE1	1:A:345:TRP:HD1	1.85	0.59
2:B:597:VAL:HG13	2:B:838:ALA:HA	1.84	0.59
2:B:902:LYS:HG3	4:B:2001:AGS:O1B	2.03	0.59
1:A:536:ASN:ND2	1:A:539:PHE:O	2.35	0.59
2:B:771:VAL:CG2	2:B:781:HIS:HB2	2.33	0.59
2:B:906:ILE:HG22	2:B:1006:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:LEU:CD1	2:B:548:LEU:HG	2.34	0.58
1:A:327:ALA:HA	1:A:346:ILE:HD13	1.84	0.58
2:B:729:HIS:CE1	2:B:752:PHE:HE2	2.22	0.58
2:B:898:ASN:HA	4:B:2001:AGS:O3G	2.03	0.58
2:B:729:HIS:HA	2:B:732:GLU:OE2	2.03	0.57
1:A:330:LEU:HB3	1:A:608:PHE:HE1	1.70	0.57
1:A:401:LEU:HD12	1:A:404:CYS:HB2	1.85	0.57
1:A:659:LYS:HA	1:A:663:MET:CE	2.35	0.57
2:B:904:SER:CB	4:B:2001:AGS:N7	2.68	0.57
1:A:783:HIS:ND1	1:A:825:SER:OG	2.28	0.57
2:B:972:VAL:HG11	2:B:997:PHE:CE2	2.39	0.57
2:B:637:GLU:O	2:B:641:ILE:HG22	2.05	0.56
2:B:547:ILE:HD11	2:B:914:ILE:HD13	1.86	0.56
1:A:624:ILE:HD13	1:A:702:VAL:HG23	1.87	0.56
2:B:898:ASN:O	4:B:2001:AGS:PB	2.63	0.56
1:A:634:LEU:HB2	1:A:655:VAL:HB	1.87	0.56
2:B:564:LEU:HD23	2:B:840:VAL:HG21	1.88	0.56
2:B:857:ILE:HB	2:B:884:LEU:HB2	1.88	0.56
2:B:904:SER:CB	4:B:2001:AGS:C8	2.84	0.56
1:A:481:LEU:O	1:A:485:MET:CE	2.54	0.56
2:B:1007:PHE:CE2	2:B:1014:VAL:HG11	2.41	0.56
2:B:656:ILE:N	2:B:657:PRO:HD2	2.21	0.55
2:B:561:LEU:HD21	2:B:577:LYS:HD2	1.86	0.55
2:B:991:TYR:CE1	2:B:1014:VAL:HA	2.40	0.55
2:B:731:GLN:NE2	2:B:732:GLU:HG3	2.22	0.55
1:A:415:PRO:HA	1:A:418:ILE:HG22	1.89	0.55
1:A:357:GLU:HA	1:A:360:LEU:HD12	1.88	0.55
1:A:769:TYR:CE1	1:A:773:LYS:HE3	2.41	0.55
2:B:559:SER:OG	2:B:560:LEU:N	2.39	0.54
2:B:914:ILE:HG13	2:B:935:ILE:HD13	1.89	0.54
1:A:536:ASN:HB2	1:A:539:PHE:HB2	1.87	0.54
2:B:569:THR:OG1	2:B:832:ASP:OD2	2.23	0.54
2:B:729:HIS:HA	2:B:732:GLU:OE1	2.07	0.54
2:B:731:GLN:NE2	2:B:732:GLU:CG	2.70	0.54
2:B:904:SER:HB3	4:B:2001:AGS:C8	2.38	0.54
2:B:846:TYR:HB3	2:B:921:TYR:HB3	1.90	0.54
1:A:447:PHE:HE1	1:A:591:PRO:HB2	1.72	0.54
2:B:628:ILE:CD1	2:B:641:ILE:HG21	2.38	0.54
2:B:635:THR:HB	2:B:694:ALA:HA	1.89	0.54
1:A:676:SER:O	1:A:680:ARG:HG3	2.09	0.53
1:A:748:ASP:HA	1:A:781:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:902:LYS:NZ	4:B:2001:AGS:O3G	2.40	0.53
1:A:309:ALA:O	1:A:680:ARG:HD2	2.09	0.53
1:A:714:ALA:H	2:B:941:ALA:HB3	1.72	0.53
1:A:411:ILE:HG21	1:A:447:PHE:HB3	1.90	0.53
2:B:892:MET:HB2	2:B:1006:LEU:HD23	1.90	0.53
2:B:901:GLY:HA2	4:B:2001:AGS:PA	2.48	0.53
2:B:618:LEU:HD11	2:B:648:LEU:HD21	1.90	0.53
1:A:612:SER:HB3	1:A:619:TYR:HB2	1.91	0.53
1:A:769:TYR:CZ	1:A:773:LYS:HE3	2.44	0.53
1:A:677:THR:O	1:A:681:GLN:HB3	2.09	0.53
2:B:679:LEU:CD1	2:B:824:ALA:HB1	2.39	0.52
1:A:408:TYR:HB2	1:A:454:ILE:HG21	1.90	0.52
1:A:685:ILE:HG12	1:A:696:PRO:HD2	1.91	0.52
2:B:553:ASP:HB3	2:B:555:LYS:HG2	1.91	0.52
2:B:733:ILE:HD13	2:B:733:ILE:N	2.24	0.52
1:A:353:LYS:HE3	1:A:624:ILE:O	2.10	0.52
2:B:904:SER:HG	4:B:2001:AGS:C8	2.05	0.52
1:A:469:LEU:HA	1:A:570:TYR:HE2	1.75	0.52
2:B:768:TRP:HA	2:B:783:PRO:HD3	1.92	0.52
2:B:897:PRO:HB2	2:B:1055:PHE:HE1	1.75	0.52
1:A:307:VAL:HG13	1:A:312:LEU:HB2	1.91	0.52
1:A:310:LEU:HD11	1:A:708:ILE:HG21	1.92	0.52
1:A:470:VAL:HG12	1:A:471:LYS:N	2.24	0.52
2:B:1035:SER:HB3	2:B:1052:PHE:CE1	2.45	0.52
2:B:649:LYS:HD3	2:B:680:SER:HA	1.90	0.52
1:A:679:ILE:HD11	1:A:747:ILE:H	1.75	0.51
1:A:679:ILE:HD11	1:A:747:ILE:N	2.25	0.51
2:B:773:SER:HA	2:B:778:SER:H	1.74	0.51
1:A:485:MET:HE2	1:A:485:MET:N	2.25	0.51
2:B:573:ARG:O	2:B:577:LYS:HG2	2.10	0.51
2:B:621:ILE:HD11	2:B:644:THR:HG21	1.92	0.51
1:A:485:MET:HE1	1:A:566:ASN:HD22	1.75	0.51
1:A:401:LEU:HD23	1:A:468:PHE:CB	2.40	0.51
2:B:1079:PRO:HD2	2:B:1082:ILE:HD12	1.93	0.51
1:A:673:GLY:HA2	1:A:813:MET:SD	2.51	0.51
2:B:773:SER:HA	2:B:778:SER:N	2.26	0.51
2:B:912:ILE:HG12	2:B:923:PRO:HD2	1.93	0.51
2:B:1013:PRO:O	2:B:1016:GLU:HB2	2.10	0.51
1:A:642:VAL:O	1:A:648:ILE:HD11	2.11	0.51
1:A:645:GLN:HB2	1:A:648:ILE:HG12	1.93	0.51
1:A:757:TYR:HA	2:B:1093:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASN:ND2	2:B:946:TYR:HE2	2.01	0.50
1:A:681:GLN:HA	1:A:684:VAL:HG12	1.92	0.50
2:B:857:ILE:HG23	2:B:929:ILE:HG23	1.92	0.50
4:B:2001:AGS:O2G	4:B:2001:AGS:O2B	2.30	0.50
1:A:447:PHE:HZ	1:A:592:MET:HB2	1.77	0.50
1:A:667:ILE:HA	1:A:800:LEU:O	2.11	0.50
2:B:1001:VAL:HG12	2:B:1003:SER:HB3	1.94	0.50
2:B:729:HIS:CD2	2:B:729:HIS:O	2.65	0.50
2:B:901:GLY:O	2:B:904:SER:OG	2.29	0.50
1:A:634:LEU:HB3	1:A:637:SER:HB2	1.93	0.50
1:A:709:LEU:HB3	1:A:735:ILE:HG12	1.94	0.50
1:A:345:TRP:HE3	1:A:608:PHE:HE2	1.59	0.49
2:B:710:PRO:HA	2:B:713:LYS:HB2	1.94	0.49
2:B:995:GLU:CG	2:B:1017:LEU:HD21	2.43	0.49
1:A:754:THR:HG23	1:A:755:SER:H	1.77	0.49
2:B:642:VAL:HG13	2:B:682:VAL:HG13	1.93	0.49
1:A:747:ILE:HD12	1:A:780:PHE:CE2	2.46	0.49
2:B:675:ILE:CD1	2:B:828:LEU:HD21	2.42	0.49
2:B:579:TRP:CZ3	2:B:833:CYS:HB3	2.47	0.49
2:B:922:VAL:HG21	2:B:927:ALA:HB3	1.93	0.49
1:A:401:LEU:HD23	1:A:468:PHE:HB3	1.95	0.49
2:B:904:SER:HB3	4:B:2001:AGS:H8	1.95	0.49
1:A:719:LEU:HD13	2:B:550:ASN:ND2	2.29	0.48
1:A:632:ILE:HG23	1:A:702:VAL:HA	1.95	0.48
2:B:649:LYS:HD3	2:B:679:LEU:C	2.38	0.48
1:A:349:PRO:HG3	1:A:687:LEU:CD1	2.42	0.48
1:A:630:GLY:HA2	1:A:777:PHE:HZ	1.78	0.48
2:B:949:ARG:HD2	2:B:957:THR:HG21	1.95	0.48
2:B:857:ILE:HG22	2:B:859:ILE:CD1	2.42	0.48
2:B:544:ASN:HB2	2:B:937:THR:HG21	1.96	0.48
2:B:901:GLY:C	4:B:2001:AGS:O2A	2.57	0.48
1:A:762:LEU:HD11	2:B:1073:ALA:HB2	1.95	0.48
2:B:625:LEU:HG	2:B:818:TYR:CE1	2.48	0.48
2:B:628:ILE:HD11	2:B:641:ILE:CG2	2.42	0.48
1:A:503:LEU:HD11	1:A:536:ASN:HA	1.96	0.48
1:A:637:SER:HA	1:A:697:CYS:SG	2.53	0.48
2:B:635:THR:CA	2:B:807:TRP:CH2	2.96	0.48
2:B:903:SER:N	4:B:2001:AGS:O2A	2.47	0.48
2:B:994:LEU:O	2:B:997:PHE:N	2.47	0.48
2:B:991:TYR:CZ	2:B:1017:LEU:HG	2.49	0.48
2:B:1066:ARG:HD3	2:B:1068:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ILE:HG13	2:B:1004:LEU:HD13	1.95	0.48
1:A:358:GLU:HG3	1:A:432:LEU:HD21	1.96	0.47
2:B:731:GLN:HE22	2:B:732:GLU:HG3	1.79	0.47
2:B:968:SER:HA	2:B:1001:VAL:O	2.14	0.47
1:A:581:ILE:HG13	1:A:582:VAL:N	2.28	0.47
1:A:613:ASN:O	1:A:613:ASN:ND2	2.44	0.47
2:B:723:ILE:HA	2:B:726:ILE:HD12	1.96	0.47
1:A:313:PHE:N	1:A:325:SER:OG	2.48	0.47
1:A:449:LYS:O	1:A:453:MET:HG2	2.15	0.47
2:B:939:MET:HB3	2:B:975:ASP:HB3	1.95	0.47
1:A:840:VAL:HG13	2:B:992:ALA:HB1	1.96	0.47
2:B:1085:LYS:O	2:B:1089:LYS:HG2	2.14	0.47
2:B:841:ALA:HB1	2:B:921:TYR:CD2	2.50	0.47
1:A:475:ASP:HB2	1:A:478:LEU:HG	1.97	0.47
1:A:340:ARG:NH2	1:A:388:ASN:HD22	2.13	0.47
1:A:703:SER:OG	1:A:704:ILE:N	2.48	0.47
1:A:840:VAL:HG22	2:B:996:TYR:HB2	1.96	0.47
1:A:601:GLN:O	1:A:605:VAL:HG22	2.16	0.46
1:A:634:LEU:HD11	1:A:702:VAL:HG12	1.97	0.46
1:A:711:ARG:HG2	1:A:735:ILE:HD12	1.98	0.46
1:A:664:PHE:HB3	1:A:797:VAL:HG22	1.97	0.46
2:B:673:LEU:O	2:B:676:PRO:HD2	2.14	0.46
2:B:712:ILE:HD11	2:B:806:GLU:HB2	1.97	0.46
1:A:457:THR:HA	1:A:472:PRO:HD3	1.96	0.46
1:A:480:GLU:O	1:A:484:ILE:HG12	2.15	0.46
2:B:601:LEU:HD11	2:B:842:LYS:HB2	1.98	0.46
2:B:782:SER:C	2:B:784:PHE:N	2.72	0.46
1:A:679:ILE:CD1	1:A:746:ILE:HG23	2.46	0.46
2:B:635:THR:HA	2:B:807:TRP:HH2	1.77	0.46
2:B:753:MET:HB3	2:B:779:ARG:HG3	1.96	0.46
1:A:491:LYS:O	1:A:495:THR:HG23	2.16	0.46
1:A:344:GLN:OE1	1:A:345:TRP:CD1	2.68	0.45
1:A:379:ASP:OD1	1:A:380:LEU:N	2.48	0.45
2:B:564:LEU:HD23	2:B:564:LEU:HA	1.83	0.45
2:B:628:ILE:HG23	2:B:811:LEU:HD12	1.97	0.45
2:B:865:PRO:O	2:B:869:VAL:HG22	2.16	0.45
1:A:602:LEU:O	1:A:606:VAL:HG23	2.16	0.45
1:A:772:THR:HG22	1:A:794:ILE:HG12	1.98	0.45
2:B:568:LYS:HB2	2:B:568:LYS:HE2	1.80	0.45
2:B:864:HIS:HE2	2:B:907:LYS:HB3	1.82	0.45
1:A:539:PHE:HA	1:A:553:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:THR:HA	2:B:807:TRP:CZ3	2.51	0.45
2:B:1011:TYR:HB2	2:B:1014:VAL:HG23	1.98	0.45
2:B:991:TYR:HE1	2:B:1014:VAL:HA	1.82	0.45
2:B:995:GLU:HG2	2:B:1017:LEU:HD21	1.98	0.45
2:B:996:TYR:O	2:B:1000:ASP:HB2	2.16	0.45
2:B:1028:TYR:HB3	2:B:1059:ILE:HG13	1.99	0.45
1:A:414:LEU:O	1:A:417:VAL:HG12	2.16	0.45
1:A:443:LEU:HD11	1:A:594:THR:HG23	1.99	0.45
2:B:894:ILE:HG21	2:B:902:LYS:HB3	1.99	0.45
1:A:327:ALA:HA	1:A:346:ILE:CD1	2.47	0.45
1:A:475:ASP:O	1:A:478:LEU:N	2.50	0.44
2:B:549:GLN:HB2	2:B:555:LYS:O	2.17	0.44
2:B:1080:GLY:O	2:B:1081:GLU:C	2.60	0.44
2:B:596:ALA:HB1	2:B:834:ILE:HD13	2.00	0.44
2:B:631:LYS:HD2	2:B:808:LEU:HD12	1.98	0.44
1:A:401:LEU:HD13	1:A:581:ILE:HD11	2.00	0.44
1:A:450:PHE:CE1	1:A:585:SER:HB2	2.52	0.44
1:A:451:GLN:OE1	1:A:451:GLN:HA	2.16	0.44
2:B:675:ILE:HG13	2:B:679:LEU:HD13	1.99	0.44
2:B:729:HIS:ND1	2:B:752:PHE:HE2	2.16	0.44
1:A:638:ARG:HB2	1:A:650:PHE:CE1	2.53	0.44
1:A:675:LYS:NZ	1:A:783:HIS:CE1	2.86	0.44
2:B:729:HIS:HD2	2:B:732:GLU:HB2	1.83	0.44
2:B:822:CYS:C	2:B:824:ALA:N	2.74	0.44
1:A:625:LEU:HD13	1:A:631:ARG:HB2	2.00	0.44
2:B:579:TRP:CE2	2:B:593:ARG:NH2	2.86	0.44
1:A:383:ARG:O	1:A:413:GLN:NE2	2.51	0.44
1:A:642:VAL:HG22	2:B:946:TYR:HE1	1.83	0.44
2:B:719:ILE:HA	2:B:722:VAL:HG22	2.00	0.44
2:B:594:LEU:HD22	2:B:919:GLY:HA2	1.98	0.44
2:B:752:PHE:HD2	2:B:785:ILE:HG21	1.83	0.44
2:B:837:LEU:HD22	2:B:920:SER:HB2	2.00	0.44
1:A:630:GLY:HA2	1:A:777:PHE:CZ	2.53	0.43
1:A:470:VAL:HG11	1:A:581:ILE:HD13	1.99	0.43
1:A:529:GLU:O	1:A:532:VAL:HG12	2.17	0.43
1:A:553:ASN:ND2	1:A:555:LYS:HG2	2.34	0.43
2:B:770:LYS:HA	2:B:780:PHE:CD1	2.52	0.43
2:B:897:PRO:HG3	2:B:1032:PHE:HB3	2.01	0.43
2:B:902:LYS:HG3	2:B:902:LYS:H	1.64	0.43
1:A:664:PHE:HB3	1:A:797:VAL:HA	2.00	0.43
2:B:653:GLN:CB	2:B:676:PRO:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:CE1	1:A:451:GLN:NE2	2.87	0.43
1:A:642:VAL:HG22	2:B:946:TYR:CE1	2.54	0.43
1:A:407:LEU:O	1:A:411:ILE:HG12	2.18	0.43
1:A:662:GLN:OE1	1:A:798:ASN:HB3	2.19	0.43
2:B:584:LEU:HD13	2:B:593:ARG:HH12	1.83	0.43
2:B:771:VAL:HG23	2:B:781:HIS:H	1.84	0.43
1:A:488:LEU:HD12	1:A:488:LEU:O	2.18	0.43
2:B:680:SER:O	2:B:681:PRO:C	2.62	0.43
1:A:353:LYS:HD2	1:A:624:ILE:HG22	2.01	0.42
1:A:424:HIS:CD2	1:A:433:LEU:HD12	2.54	0.42
1:A:462:GLN:HE22	1:A:482:ARG:NH2	2.17	0.42
2:B:978:GLY:O	2:B:981:THR:HG22	2.19	0.42
2:B:1007:PHE:C	2:B:1007:PHE:CD2	2.97	0.42
1:A:679:ILE:HD11	1:A:746:ILE:HA	2.01	0.42
1:A:725:PHE:CB	4:B:2001:AGS:S1G	3.08	0.42
1:A:298:GLN:C	1:A:351:MET:HB2	2.43	0.42
1:A:418:ILE:HD11	1:A:441:THR:OG1	2.19	0.42
1:A:450:PHE:HB2	1:A:588:TYR:CE2	2.54	0.42
2:B:909:VAL:HG11	2:B:1006:LEU:HD11	2.01	0.42
2:B:962:ILE:HG21	2:B:972:VAL:HG13	2.00	0.42
1:A:408:TYR:CD1	1:A:451:GLN:OE1	2.72	0.42
1:A:577:ILE:O	1:A:581:ILE:HG23	2.18	0.42
1:A:632:ILE:HA	1:A:701:GLU:O	2.20	0.42
2:B:729:HIS:O	2:B:733:ILE:HG12	2.19	0.42
2:B:911:LEU:HD23	2:B:911:LEU:HA	1.87	0.42
1:A:363:VAL:HG13	1:A:694:PHE:CE1	2.54	0.42
2:B:564:LEU:CD2	2:B:840:VAL:HG21	2.49	0.42
2:B:952:PHE:CE2	2:B:956:LEU:HD11	2.55	0.42
1:A:437:VAL:O	1:A:440:LEU:N	2.53	0.42
1:A:345:TRP:CE3	1:A:608:PHE:HE2	2.37	0.42
1:A:787:LEU:HD23	1:A:787:LEU:HA	1.81	0.42
2:B:537:ILE:CG2	2:B:542:LEU:HD22	2.47	0.42
1:A:488:LEU:HD21	1:A:563:TYR:HB2	2.02	0.42
1:A:679:ILE:HG12	1:A:746:ILE:HG23	2.02	0.42
2:B:667:LEU:HD23	2:B:834:ILE:HD11	2.01	0.42
2:B:671:VAL:O	2:B:675:ILE:HG22	2.20	0.42
2:B:771:VAL:H	2:B:780:PHE:HA	1.84	0.42
2:B:852:GLN:HE22	2:B:928:THR:HG23	1.85	0.42
1:A:584:ILE:HD12	1:A:584:ILE:HA	1.91	0.42
2:B:811:LEU:HD13	2:B:811:LEU:HA	1.83	0.42
2:B:898:ASN:O	4:B:2001:AGS:PG	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:MET:HG2	2:B:1072:VAL:HG22	2.02	0.42
2:B:628:ILE:HG23	2:B:811:LEU:CD1	2.50	0.41
2:B:771:VAL:HB	2:B:779:ARG:O	2.20	0.41
2:B:938:ARG:HH11	2:B:958:ASP:HB2	1.85	0.41
2:B:601:LEU:CD1	2:B:842:LYS:HB2	2.49	0.41
2:B:635:THR:OG1	2:B:636:GLN:N	2.53	0.41
2:B:675:ILE:HD13	2:B:828:LEU:HD21	2.02	0.41
1:A:762:LEU:HA	1:A:762:LEU:HD23	1.80	0.41
2:B:773:SER:O	2:B:777:VAL:N	2.53	0.41
1:A:680:ARG:HD3	1:A:712:VAL:HG21	2.03	0.41
2:B:733:ILE:HG12	2:B:752:PHE:HZ	1.84	0.41
2:B:902:LYS:O	2:B:906:ILE:HG12	2.20	0.41
1:A:683:GLY:HA3	1:A:746:ILE:HD11	2.02	0.41
1:A:779:MET:HE2	1:A:779:MET:HB2	1.75	0.41
2:B:855:ARG:NH1	2:B:1002:LYS:O	2.54	0.41
1:A:301:LYS:HE2	1:A:301:LYS:HB2	1.96	0.41
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.77	0.41
1:A:774:ILE:HD12	1:A:774:ILE:HA	1.88	0.41
2:B:653:GLN:HG3	2:B:656:ILE:HD12	2.02	0.41
1:A:399:ALA:HB1	1:A:582:VAL:HB	2.01	0.41
1:A:488:LEU:O	1:A:492:MET:HG2	2.20	0.41
1:A:613:ASN:HD22	1:A:613:ASN:C	2.25	0.41
1:A:725:PHE:HA	1:A:728:GLU:HG3	2.03	0.41
2:B:561:LEU:O	2:B:565:ASP:N	2.31	0.41
2:B:694:ALA:HA	2:B:702:LEU:HD11	2.03	0.41
2:B:822:CYS:O	2:B:823:LYS:C	2.62	0.41
2:B:987:ILE:HD13	2:B:1013:PRO:HG2	2.03	0.41
1:A:401:LEU:HD23	1:A:468:PHE:HB2	2.02	0.41
2:B:752:PHE:CD2	2:B:785:ILE:HG21	2.56	0.41
2:B:960:ALA:O	2:B:964:ARG:HG3	2.21	0.41
1:A:332:LYS:HA	1:A:332:LYS:HD3	1.74	0.40
1:A:336:PRO:O	1:A:340:ARG:HG3	2.22	0.40
2:B:629:TYR:HB2	2:B:818:TYR:CE1	2.56	0.40
2:B:668:LEU:HA	2:B:671:VAL:HG22	2.04	0.40
2:B:782:SER:HB3	2:B:785:ILE:HG12	2.02	0.40
1:A:784:PHE:HB3	1:A:786:GLU:HG2	2.02	0.40
2:B:938:ARG:NH1	2:B:955:GLU:HA	2.37	0.40
1:A:578:VAL:C	1:A:580:GLU:N	2.78	0.40
2:B:601:LEU:HD22	2:B:841:ALA:HB1	2.02	0.40
2:B:894:ILE:CG2	2:B:902:LYS:HB3	2.51	0.40
1:A:478:LEU:HB3	1:A:570:TYR:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:ASN:CG	1:A:799:ASN:N	2.79	0.40
1:A:836:PHE:CZ	2:B:956:LEU:HD23	2.57	0.40
2:B:994:LEU:HA	2:B:994:LEU:HD12	1.76	0.40
2:B:1028:TYR:OH	2:B:1061:ARG:NH2	2.55	0.40
2:B:1035:SER:O	2:B:1051:ASP:HA	2.21	0.40
1:A:330:LEU:HD22	1:A:608:PHE:CD1	2.56	0.40
1:A:470:VAL:CG1	1:A:471:LYS:H	2.30	0.40
1:A:559:LEU:HA	1:A:562:GLU:OE1	2.22	0.40
1:A:632:ILE:HB	1:A:657:PHE:HB2	2.04	0.40
1:A:671:ASN:O	1:A:672:MET:HB2	2.21	0.40
1:A:675:LYS:N	4:A:2001:AGS:O1B	2.50	0.40
1:A:711:ARG:CD	1:A:731:GLU:HB3	2.52	0.40
2:B:728:MET:O	2:B:731:GLN:HG3	2.22	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	524/934 (56%)	491 (94%)	33 (6%)	0	100	100
2	B	525/1137 (46%)	495 (94%)	30 (6%)	0	100	100
All	All	1049/2071 (51%)	986 (94%)	63 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	467/808 (58%)	455 (97%)	12 (3%)	40	71
2	B	475/998 (48%)	453 (95%)	22 (5%)	24	57
All	All	942/1806 (52%)	908 (96%)	34 (4%)	32	64

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	LYS
1	A	367	VAL
1	A	375	THR
1	A	376	LEU
1	A	384	PHE
1	A	462	GLN
1	A	666	ILE
1	A	698	GLU
1	A	704	ILE
1	A	774	ILE
1	A	779	MET
1	A	787	LEU
2	B	542	LEU
2	B	648	LEU
2	B	663	ILE
2	B	675	ILE
2	B	684	HIS
2	B	686	LEU
2	B	688	ILE
2	B	702	LEU
2	B	719	ILE
2	B	774	THR
2	B	779	ARG
2	B	781	HIS
2	B	808	LEU
2	B	811	LEU
2	B	822	CYS
2	B	850	THR
2	B	895	THR
2	B	925	GLU
2	B	929	ILE
2	B	999	ARG
2	B	1033	LEU

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Mol	Chain	Res	Type
2	B	1070	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	388	ASN
1	A	413	GLN
1	A	462	GLN
1	A	645	GLN
2	B	549	GLN
2	B	731	GLN
2	B	827	HIS
2	B	944	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AGS	B	2001	3	29,33,33	0.51	0	39,52,52	0.87	1 (2%)
4	AGS	A	2001	3	29,33,33	0.50	0	39,52,52	0.82	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	B	2001	3	-	2/21/38/38	0/3/3/3
4	AGS	A	2001	3	-	2/21/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	AGS	PA-O3A-PB	-4.73	116.58	132.83
4	A	2001	AGS	PA-O3A-PB	-4.41	117.69	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	AGS	PA-O3A-PB-O1B
4	A	2001	AGS	PA-O3A-PB-O2B
4	B	2001	AGS	PA-O3A-PB-O1B
4	B	2001	AGS	PA-O3A-PB-O2B

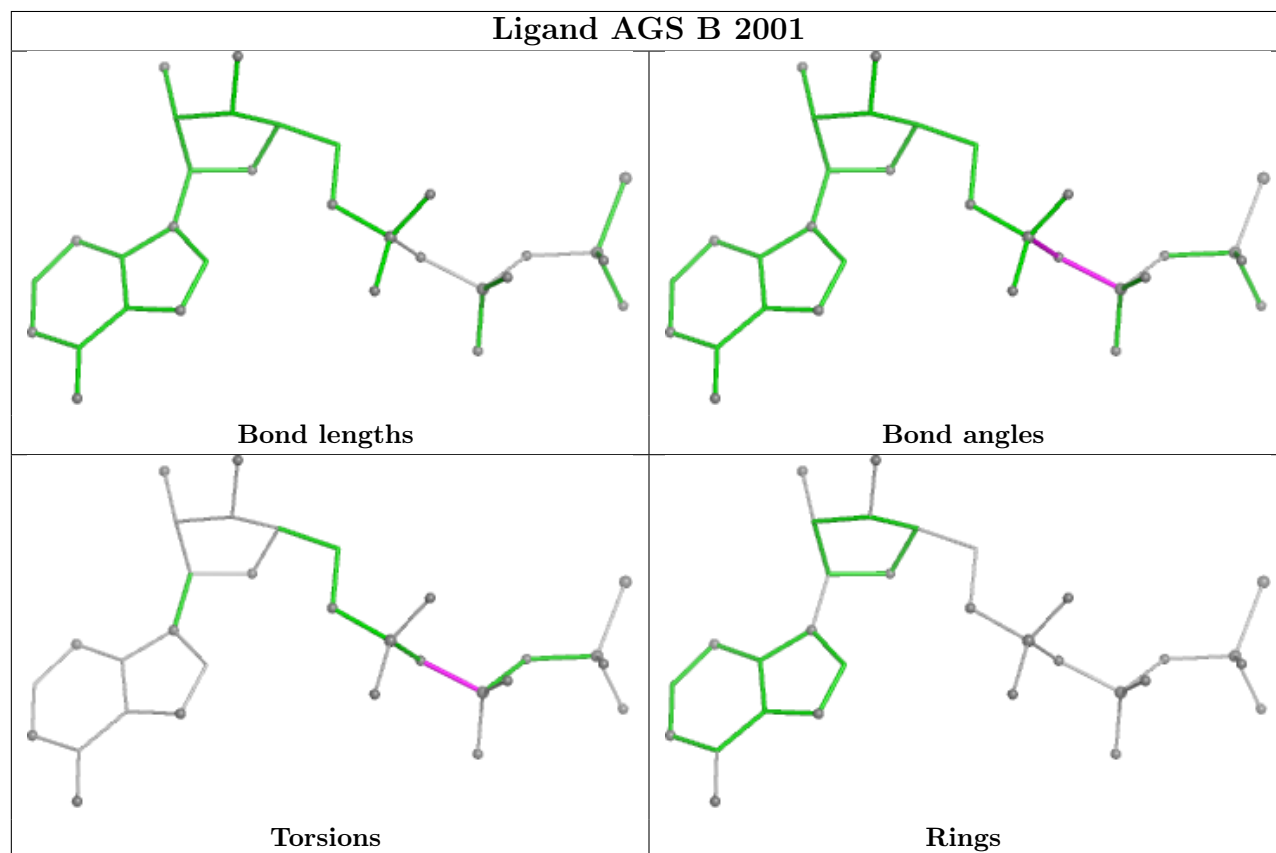
There are no ring outliers.

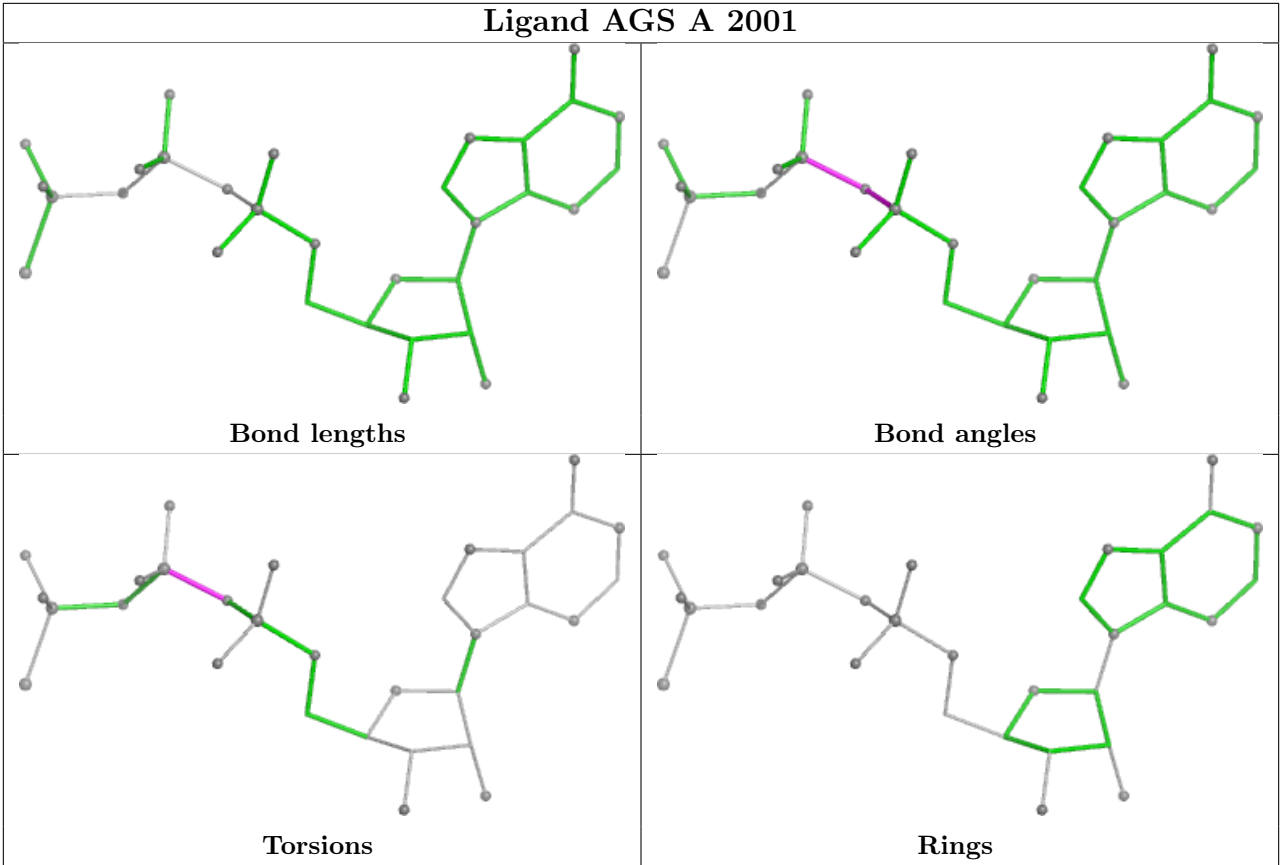
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	AGS	19	0
4	A	2001	AGS	2	0

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

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	319:ASP	C	320:THR	N	1.19

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19607. These allow visual inspection of the internal detail of the map and identification of artifacts.

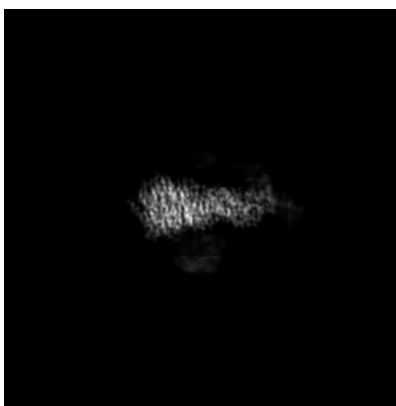
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

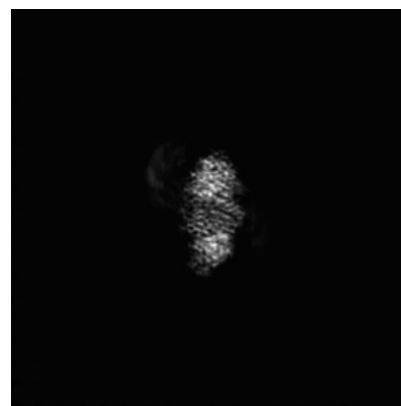
6.1.1 Primary map



X

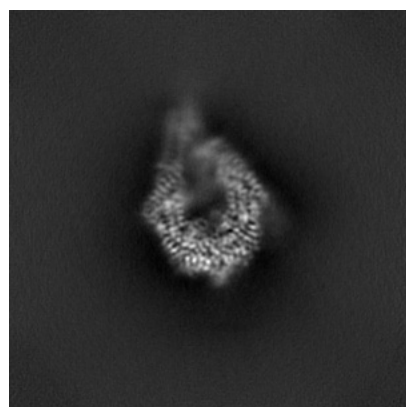


Y

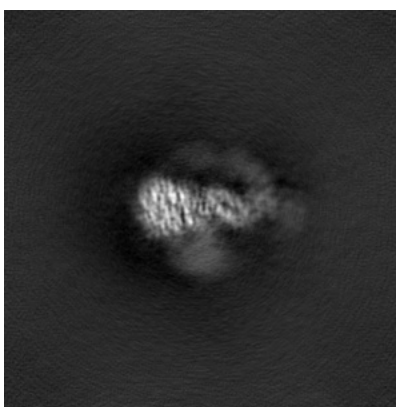


Z

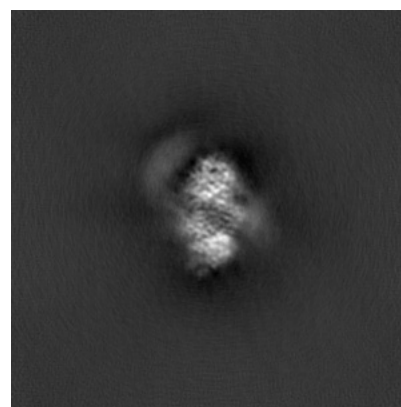
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

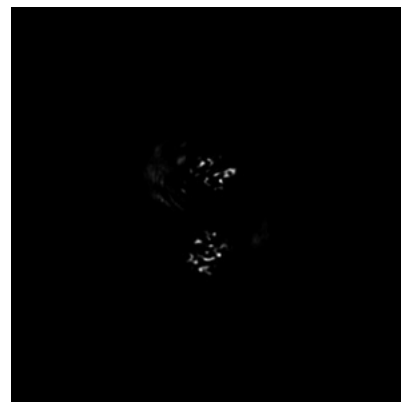
6.2.1 Primary map



X Index: 160

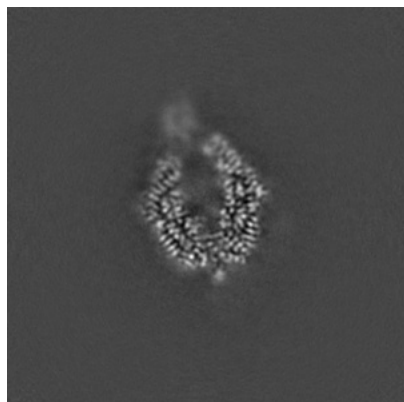


Y Index: 160

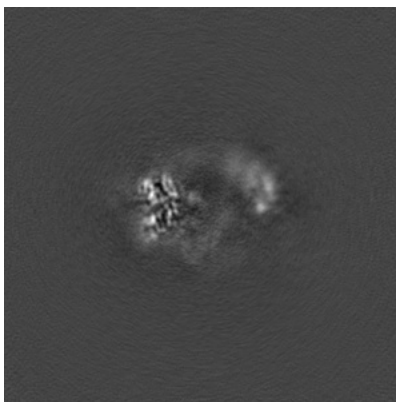


Z Index: 160

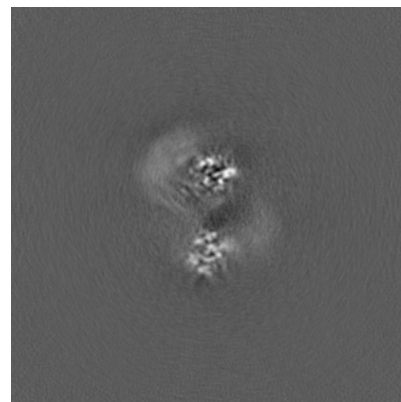
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 159

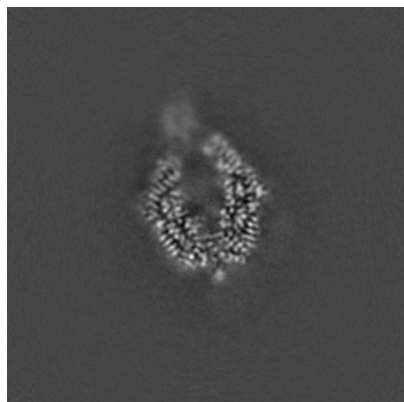


Y Index: 178

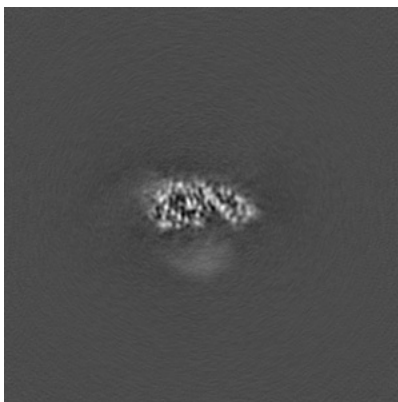


Z Index: 127

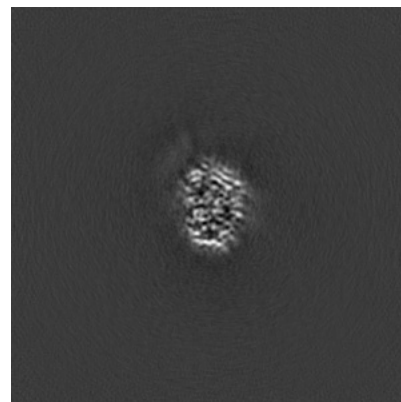
6.3.2 Raw map



X Index: 160



Y Index: 186



Z Index: 127

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

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

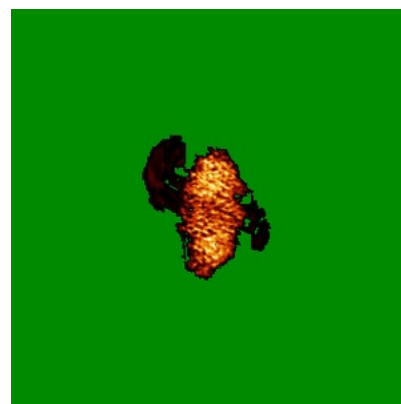
6.4.1 Primary map



X

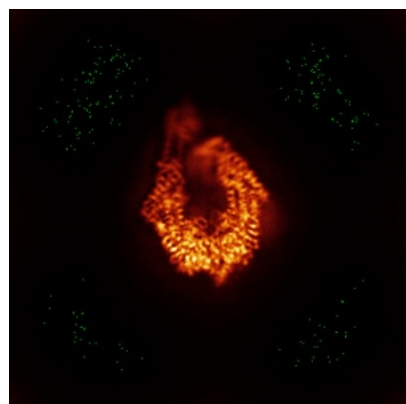


Y

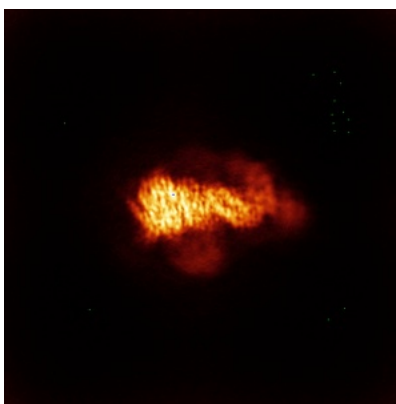


Z

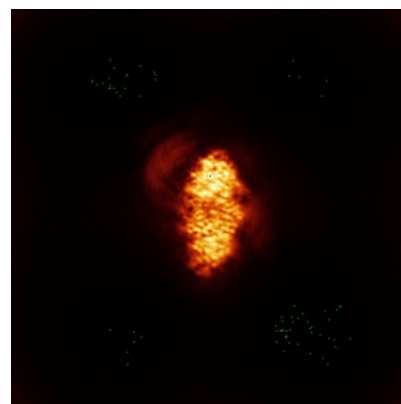
6.4.2 Raw map



X



Y

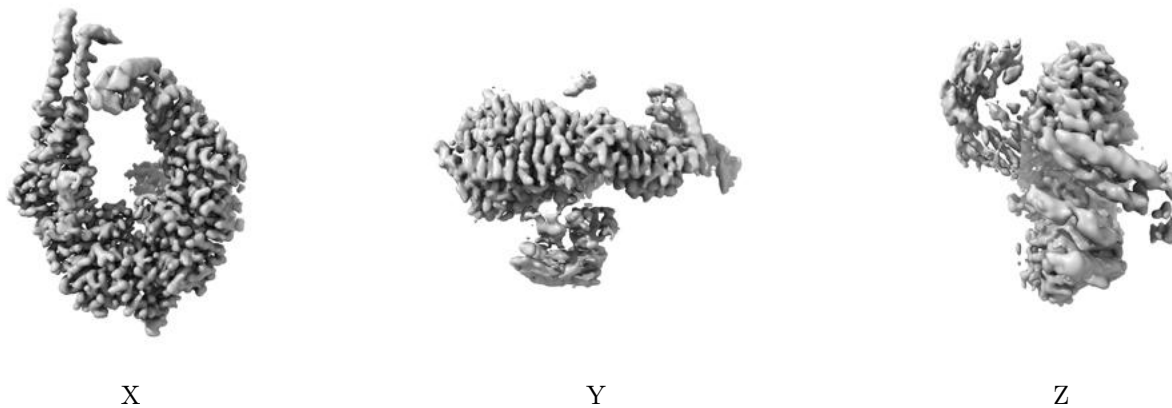


Z

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.

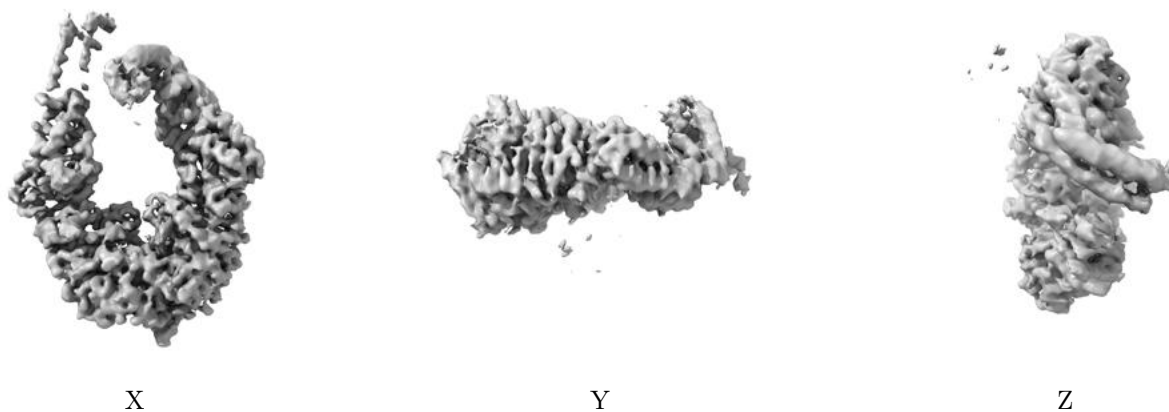
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

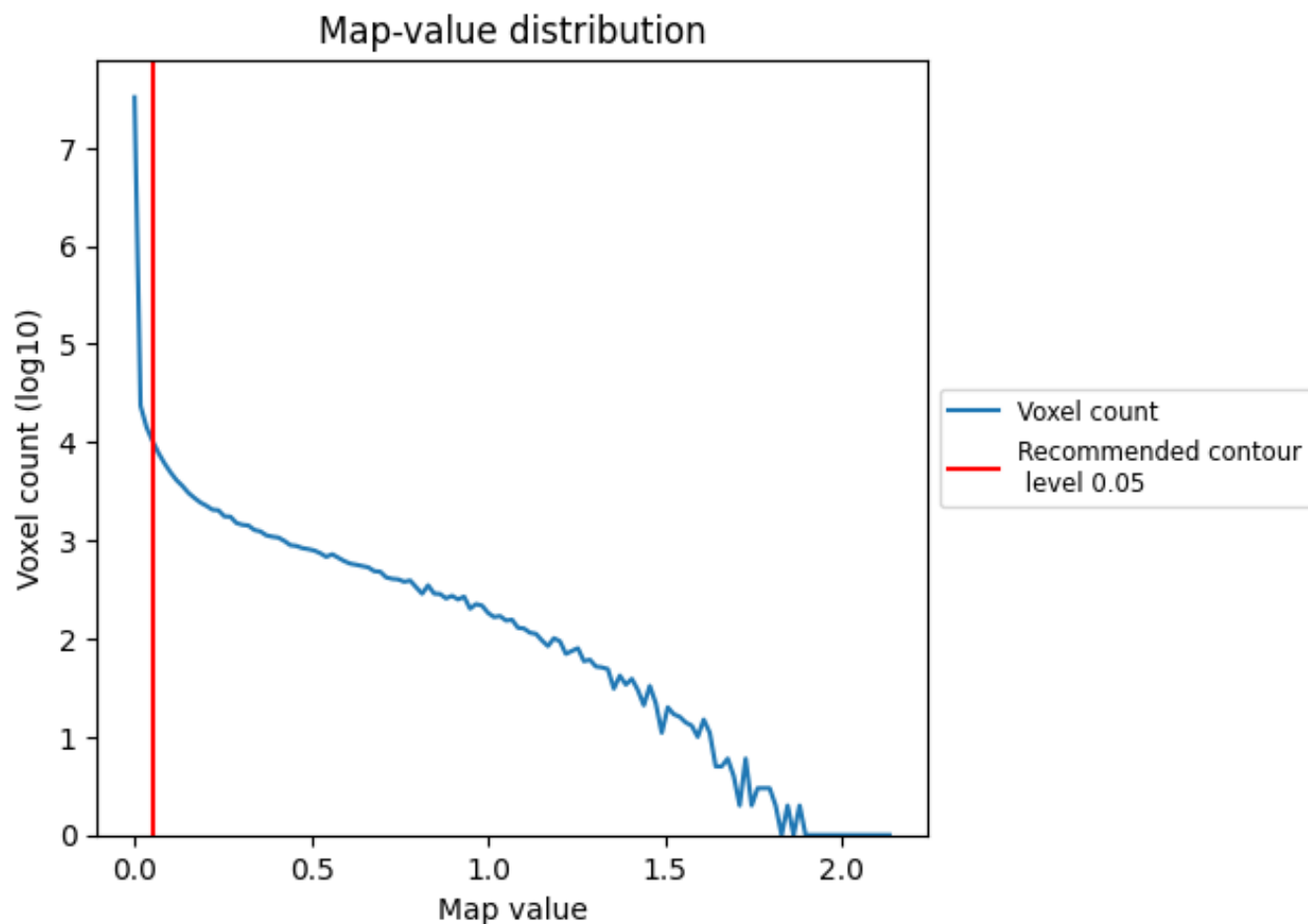
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

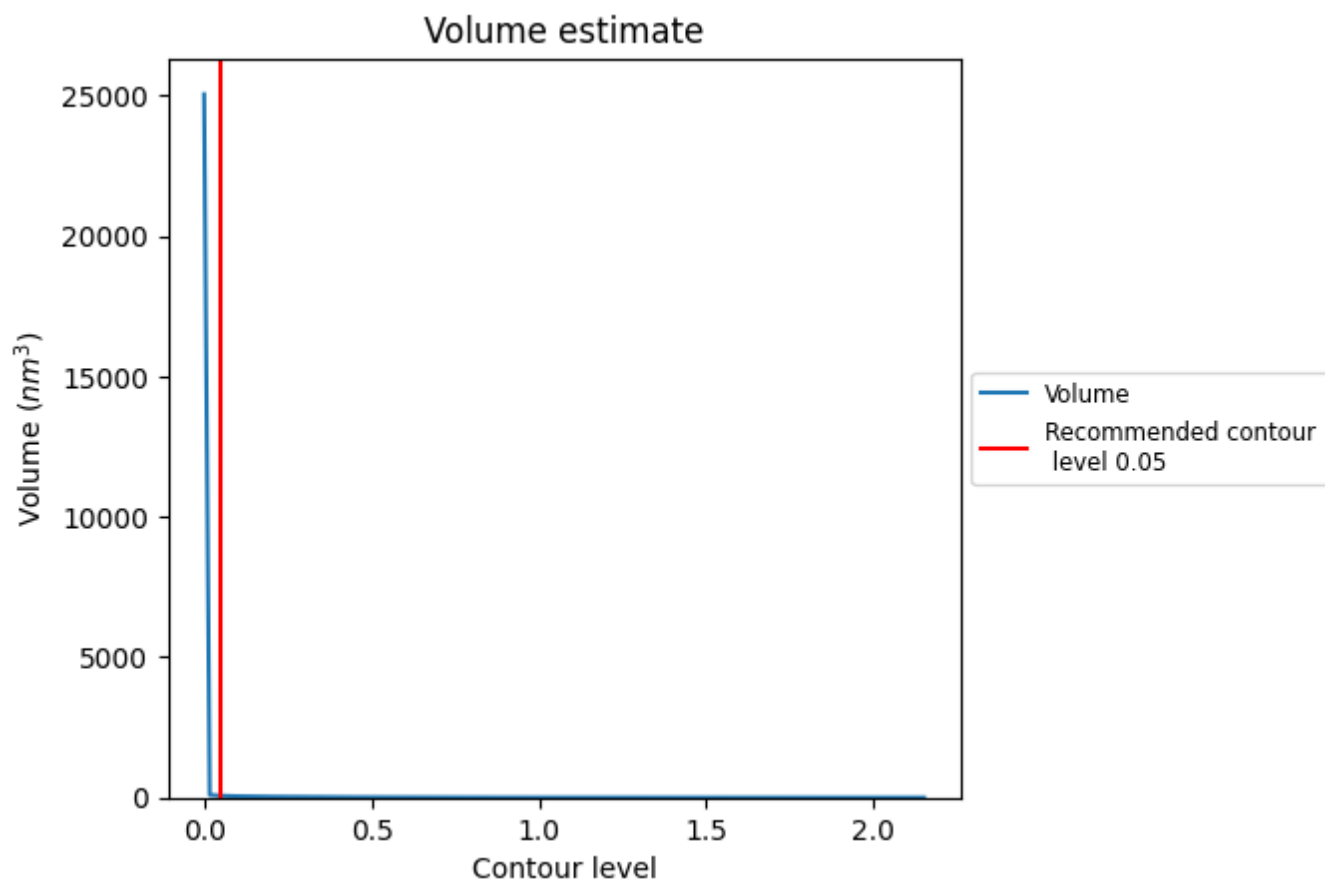
This section contains the results of statistical analysis of the map.

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.

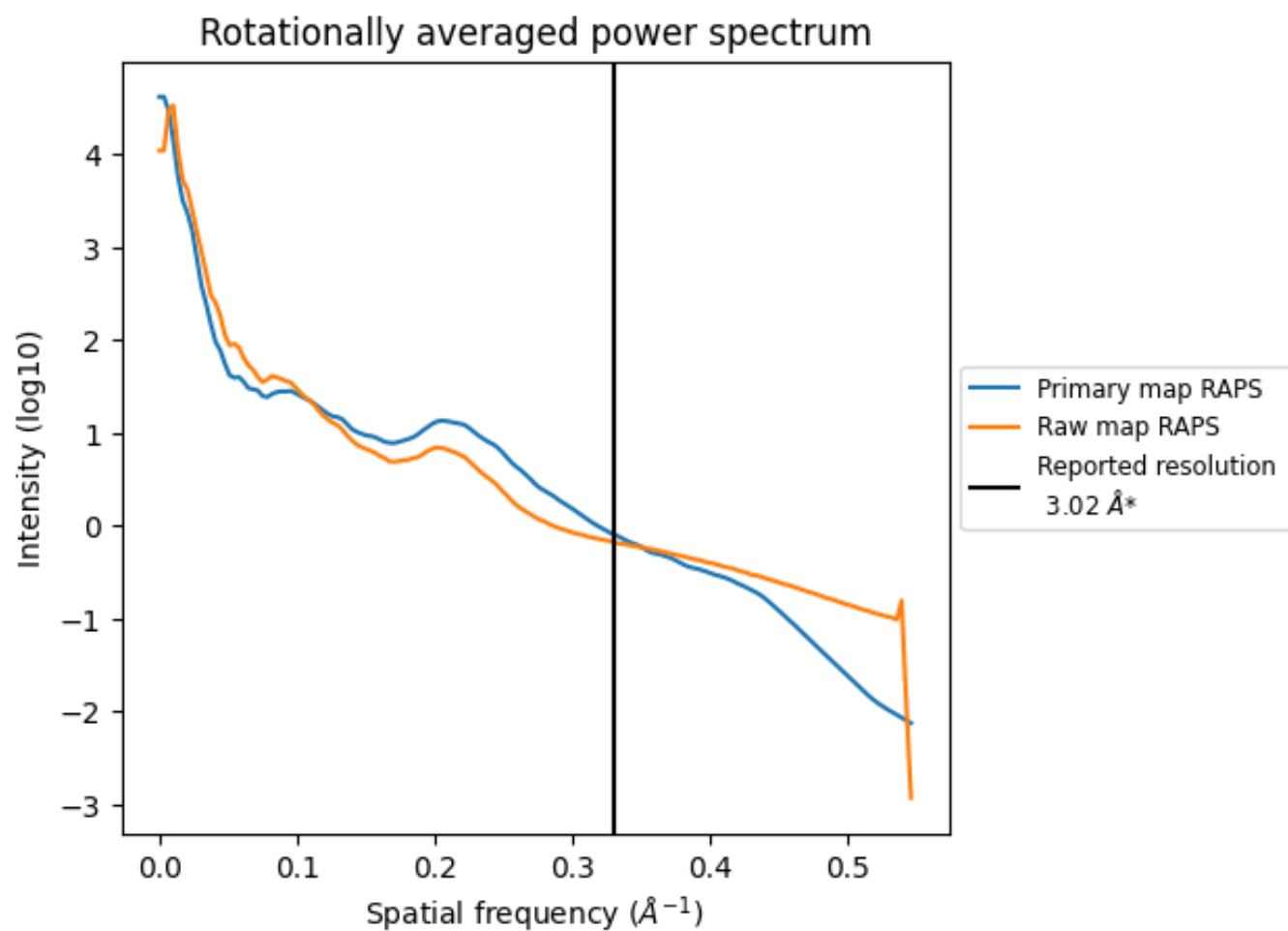
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 58 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 ⓘ

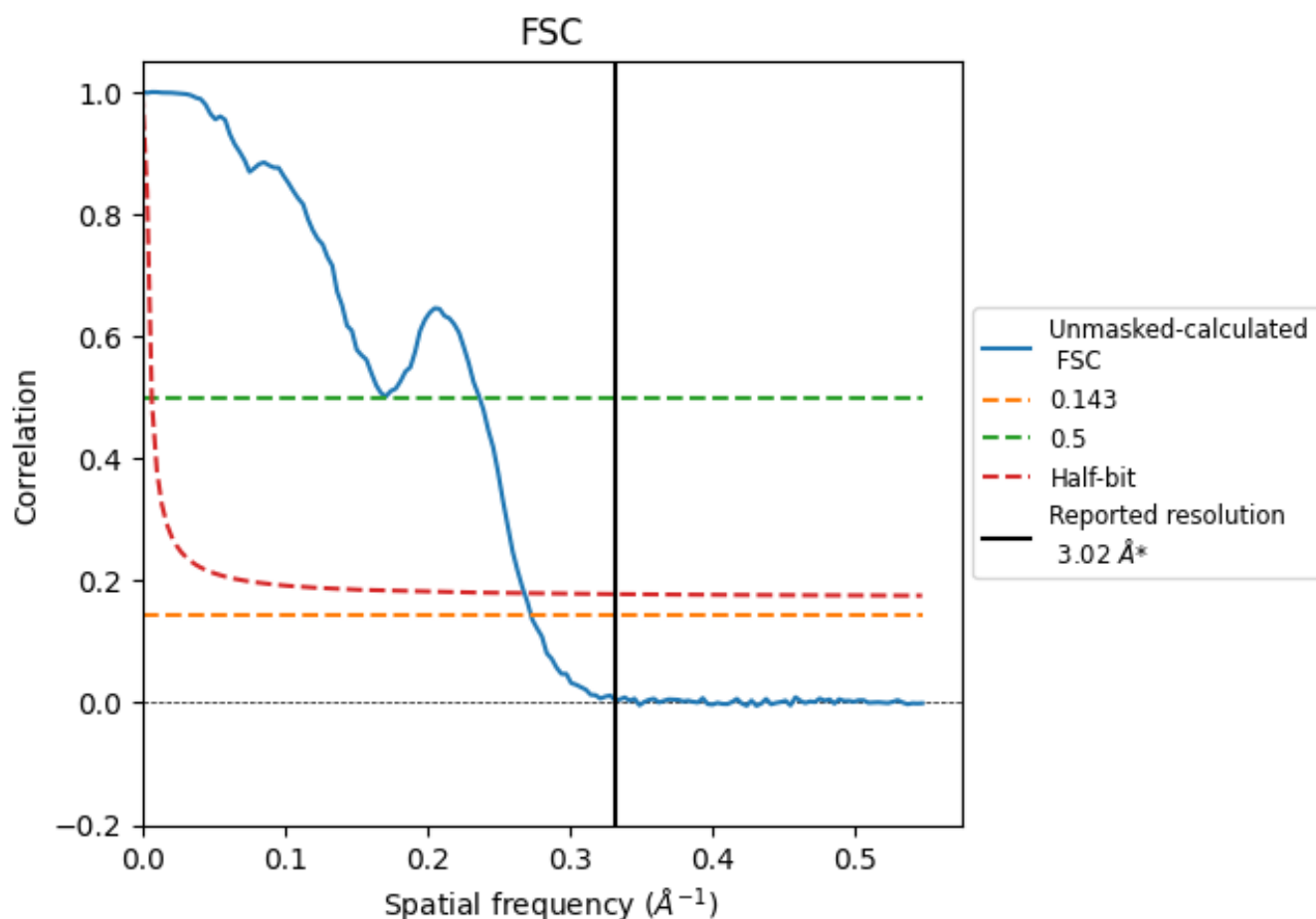


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

8.2 Resolution estimates [i](#)

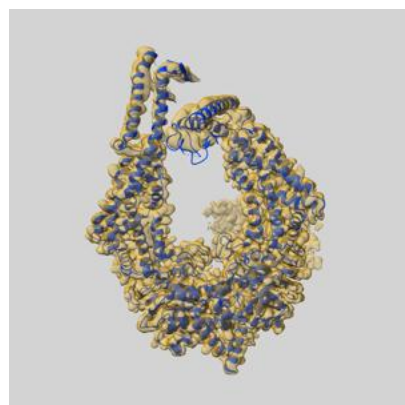
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.23	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 3.02 by more than 10 %

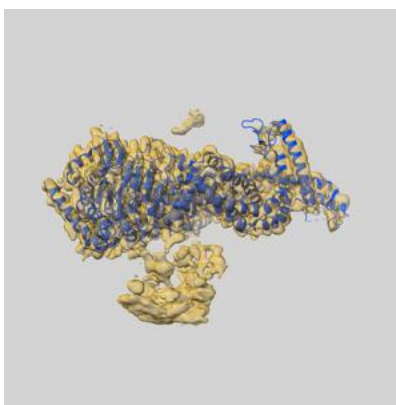
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19607 and PDB model 8RZ9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

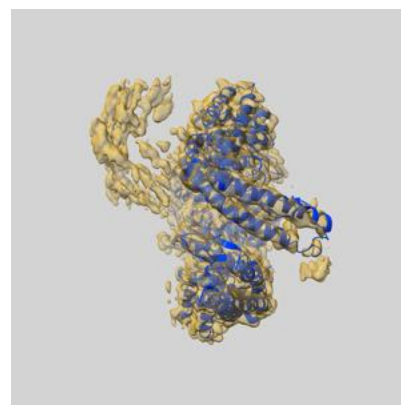
9.1 Map-model overlay [i](#)



X



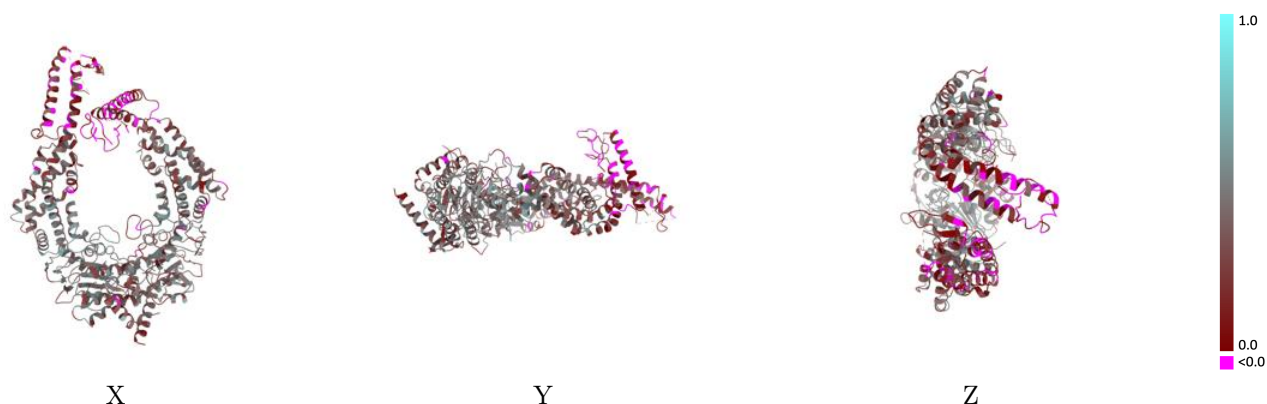
Y



Z

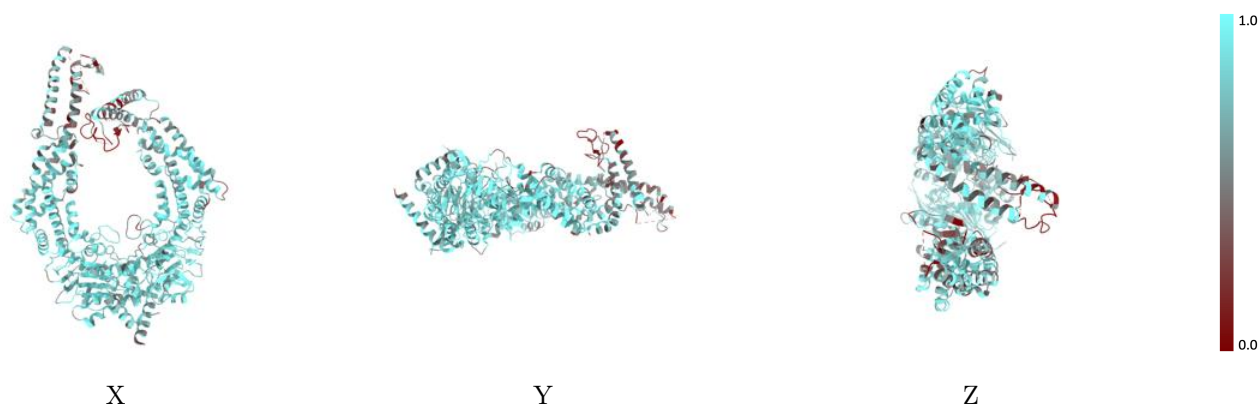
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



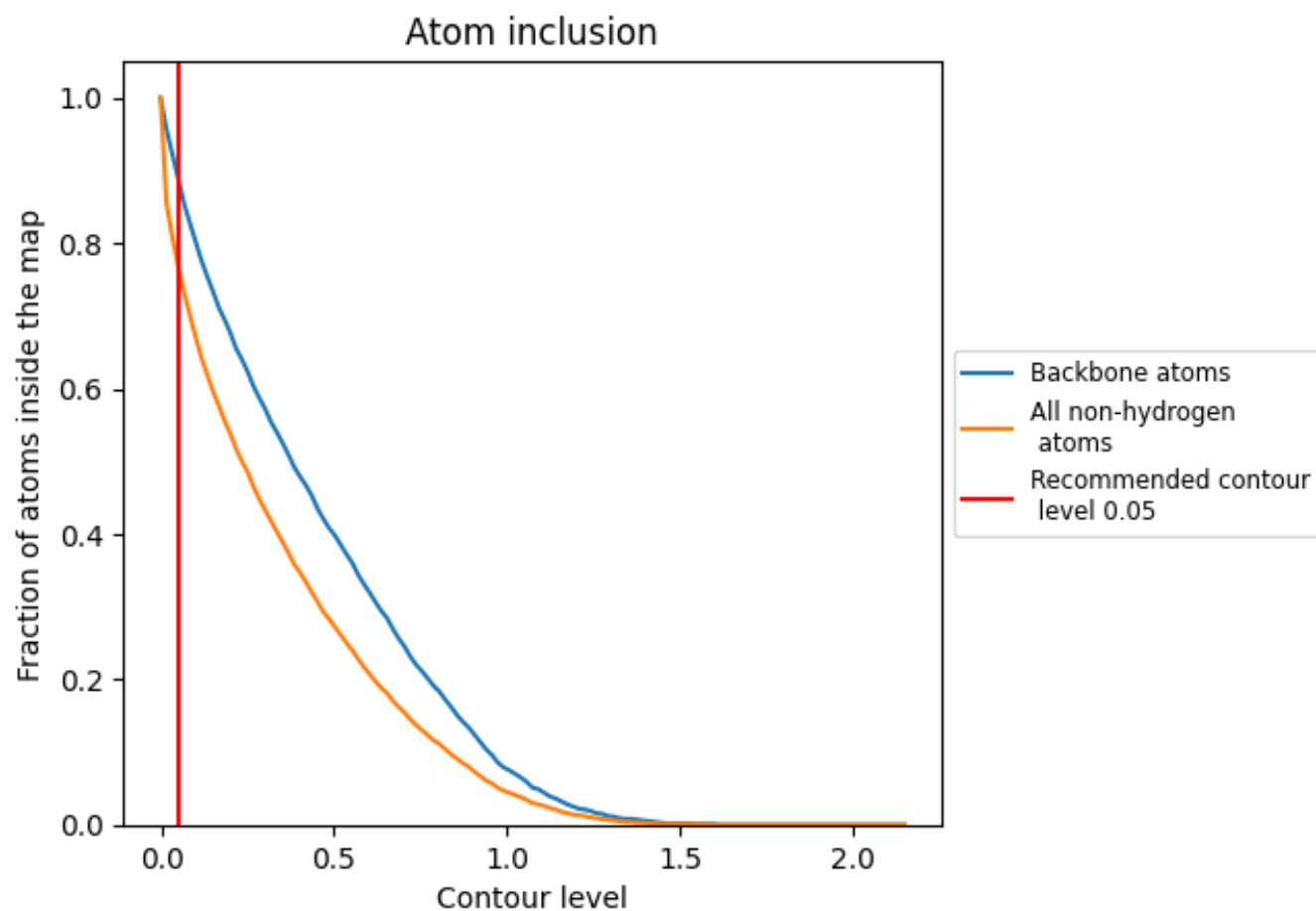
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 77% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.3320
A	0.7560	0.3170
B	0.7780	0.3470

