



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:30 AM UTC

PDB ID : 8BJA / pdb_00008bj
EMDB ID : EMD-16087
Title : Structure of the human UBR5 Dimer.
Authors : Hodakova, Z.; Grishkovskaya, I.; Haselbach, D.
Deposited on : 2022-11-03
Resolution : 3.00 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

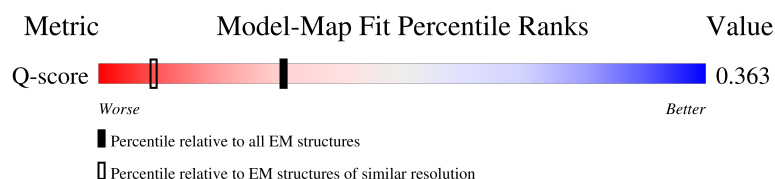
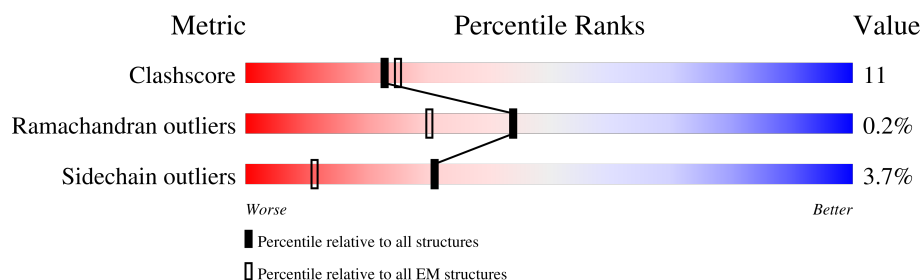
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	2830	9% 42% 13% • 45%
1	B	2830	11% 44% 13% • 42%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25204 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 E3 ubiquitin-protein ligase UBR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1638	Total	C	N	O	S	0	0
			12897	8178	2239	2384	96		
1	A	1563	Total	C	N	O	S	0	0
			12301	7806	2140	2265	90		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2799	VAL	-	expression tag	UNP O95071
B	2800	GLY	-	expression tag	UNP O95071
B	2801	SER	-	expression tag	UNP O95071
B	2802	ALA	-	expression tag	UNP O95071
B	2803	TRP	-	expression tag	UNP O95071
B	2804	SER	-	expression tag	UNP O95071
B	2805	HIS	-	expression tag	UNP O95071
B	2806	PRO	-	expression tag	UNP O95071
B	2807	GLN	-	expression tag	UNP O95071
B	2808	PHE	-	expression tag	UNP O95071
B	2809	GLU	-	expression tag	UNP O95071
B	2810	LYS	-	expression tag	UNP O95071
B	2811	GLY	-	expression tag	UNP O95071
B	2812	GLY	-	expression tag	UNP O95071
B	2813	GLY	-	expression tag	UNP O95071
B	2814	SER	-	expression tag	UNP O95071
B	2815	GLY	-	expression tag	UNP O95071
B	2816	GLY	-	expression tag	UNP O95071
B	2817	GLY	-	expression tag	UNP O95071
B	2818	SER	-	expression tag	UNP O95071
B	2819	GLY	-	expression tag	UNP O95071
B	2820	GLY	-	expression tag	UNP O95071
B	2821	SER	-	expression tag	UNP O95071
B	2822	ALA	-	expression tag	UNP O95071
B	2823	TRP	-	expression tag	UNP O95071
B	2824	SER	-	expression tag	UNP O95071

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2825	HIS	-	expression tag	UNP O95071
B	2826	PRO	-	expression tag	UNP O95071
B	2827	GLN	-	expression tag	UNP O95071
B	2828	PHE	-	expression tag	UNP O95071
B	2829	GLU	-	expression tag	UNP O95071
B	2830	LYS	-	expression tag	UNP O95071
A	2799	VAL	-	expression tag	UNP O95071
A	2800	GLY	-	expression tag	UNP O95071
A	2801	SER	-	expression tag	UNP O95071
A	2802	ALA	-	expression tag	UNP O95071
A	2803	TRP	-	expression tag	UNP O95071
A	2804	SER	-	expression tag	UNP O95071
A	2805	HIS	-	expression tag	UNP O95071
A	2806	PRO	-	expression tag	UNP O95071
A	2807	GLN	-	expression tag	UNP O95071
A	2808	PHE	-	expression tag	UNP O95071
A	2809	GLU	-	expression tag	UNP O95071
A	2810	LYS	-	expression tag	UNP O95071
A	2811	GLY	-	expression tag	UNP O95071
A	2812	GLY	-	expression tag	UNP O95071
A	2813	GLY	-	expression tag	UNP O95071
A	2814	SER	-	expression tag	UNP O95071
A	2815	GLY	-	expression tag	UNP O95071
A	2816	GLY	-	expression tag	UNP O95071
A	2817	GLY	-	expression tag	UNP O95071
A	2818	SER	-	expression tag	UNP O95071
A	2819	GLY	-	expression tag	UNP O95071
A	2820	GLY	-	expression tag	UNP O95071
A	2821	SER	-	expression tag	UNP O95071
A	2822	ALA	-	expression tag	UNP O95071
A	2823	TRP	-	expression tag	UNP O95071
A	2824	SER	-	expression tag	UNP O95071
A	2825	HIS	-	expression tag	UNP O95071
A	2826	PRO	-	expression tag	UNP O95071
A	2827	GLN	-	expression tag	UNP O95071
A	2828	PHE	-	expression tag	UNP O95071
A	2829	GLU	-	expression tag	UNP O95071
A	2830	LYS	-	expression tag	UNP O95071

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

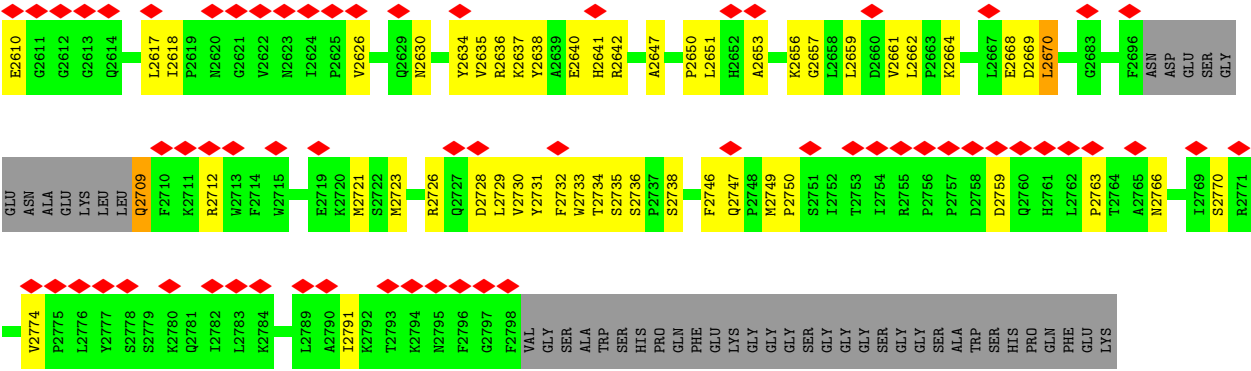
Mol	Chain	Residues	Atoms		AltConf
2	B	3	Total 3	Zn 3	0
2	A	3	Total 3	Zn 3	0











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288287	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.330	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0632	Depositor
Map size ($\text{\AA}$)	446.69998, 446.69998, 446.69998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.489, 1.489, 1.489	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/12550	0.42	1/17001 (0.0%)
1	B	0.19	0/13155	0.43	1/17813 (0.0%)
All	All	0.18	0/25705	0.42	2/34814 (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
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1369	VAL	N-CA-C	-5.49	104.01	110.21
1	B	2212	LEU	N-CA-C	-5.26	108.13	114.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2266	ARG	Sidechain
1	B	2246	ARG	Sidechain
1	B	2248	ARG	Sidechain

5.2 Too-close contacts

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	12301	0	12343	269	0
1	B	12897	0	12962	263	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	25204	0	25305	525	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 (525) 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:2656:LYS:HA	1:A:2659:LEU:HB2	1.54	0.89
1:A:2709:GLN:N	1:A:2709:GLN:HE21	1.71	0.88
1:B:1216:HIS:HD2	1:B:1219:HIS:ND1	1.72	0.85
1:B:2749:MET:HE3	1:B:2750:PRO:HD2	1.60	0.83
1:B:1961:MET:HG3	1:B:2171:PRO:HB3	1.60	0.83
1:A:387:LYS:HE2	1:A:387:LYS:H	1.45	0.81
1:A:2542:GLN:O	1:A:2543:ASN:ND2	2.17	0.78
1:A:2749:MET:HG3	1:A:2750:PRO:HD2	1.66	0.77
1:A:1870:HIS:HD2	1:A:1872:LEU:H	1.32	0.77
1:A:752:ASP:OD1	1:A:753:SER:N	2.19	0.76
1:B:1488:MET:HB3	1:A:1841:TRP:HE1	1.52	0.74
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.21	0.73
1:A:424:ILE:HG22	1:A:438:THR:HG22	1.70	0.73
1:A:1187:GLU:OE1	1:A:1187:GLU:N	2.22	0.72
1:B:2507:GLN:HB3	1:B:2511:ARG:HH22	1.54	0.71
1:B:1248:LYS:HZ1	1:B:1251:ARG:HD3	1.55	0.70
1:B:471:GLU:HB2	1:B:487:LEU:HD13	1.73	0.70
1:A:1199:CYS:SG	1:A:1216:HIS:HE1	2.11	0.70
1:A:909:GLN:OE1	1:A:909:GLN:N	2.21	0.70
1:B:2053:GLN:N	1:B:2053:GLN:OE1	2.25	0.69
1:A:2723:MET:SD	1:A:2723:MET:N	2.60	0.69
1:A:2202:GLU:N	1:A:2202:GLU:OE1	2.24	0.69
1:A:2046:GLU:N	1:A:2046:GLU:OE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:CYS:SG	1:B:480:ALA:N	2.65	0.69
1:B:2256:MET:HG2	1:B:2312:LEU:HD22	1.74	0.69
1:B:1176:ASN:O	1:B:1251:ARG:NH2	2.27	0.68
1:B:2219:GLU:OE1	1:B:2219:GLU:N	2.26	0.67
1:A:796:GLU:OE2	1:A:796:GLU:N	2.27	0.67
1:A:2661:VAL:HG12	1:A:2662:LEU:HD22	1.75	0.67
1:A:1326:GLN:OE1	1:A:1326:GLN:N	2.18	0.67
1:A:2182:HIS:ND1	1:A:2184:MET:SD	2.64	0.67
1:B:1822:GLN:N	1:B:1822:GLN:OE1	2.27	0.67
1:B:2277:VAL:HG21	1:B:2538:LEU:HD11	1.77	0.66
1:A:2653:ALA:HA	1:A:2656:LYS:NZ	2.09	0.66
1:B:2202:GLU:N	1:B:2202:GLU:OE2	2.27	0.66
1:A:822:MET:HE1	1:A:830:ILE:HG12	1.77	0.66
1:B:411:HIS:HB3	1:B:414:ALA:HB2	1.77	0.66
1:B:2575:MET:HE3	1:B:2575:MET:O	1.96	0.65
1:A:890:GLN:N	1:A:890:GLN:OE1	2.30	0.65
1:A:61:LEU:HD12	1:A:374:ILE:HG12	1.78	0.65
1:B:893:MET:HA	1:B:896:GLU:HB3	1.79	0.64
1:A:1188:HIS:HB3	1:A:1229:THR:HB	1.78	0.64
1:A:2747:GLN:N	1:A:2747:GLN:OE1	2.30	0.64
1:B:1:MET:SD	1:B:1:MET:N	2.71	0.64
1:B:2245:ASP:HB3	1:B:2282:LYS:HB2	1.80	0.64
1:A:916:CYS:SG	1:A:917:ASP:N	2.70	0.64
1:B:2221:LYS:HG2	1:B:2224:LYS:HZ1	1.62	0.64
1:A:2617:LEU:HD23	1:A:2641:HIS:HD2	1.63	0.64
1:A:1104:GLU:N	1:A:1104:GLU:OE2	2.30	0.63
1:A:1248:LYS:HE3	1:A:1248:LYS:HA	1.81	0.63
1:A:2669:ASP:OD1	1:A:2670:LEU:N	2.31	0.63
1:B:893:MET:H	1:B:893:MET:HE3	1.64	0.62
1:B:1265:VAL:O	1:B:1274:HIS:NE2	2.32	0.62
1:A:2730:VAL:HA	1:A:2733:TRP:HB2	1.82	0.62
1:A:1342:MET:HE2	1:A:1342:MET:HA	1.80	0.62
1:A:2606:LEU:HD13	1:A:2610:GLU:HG2	1.81	0.62
1:B:463:GLN:OE1	1:B:463:GLN:N	2.32	0.62
1:B:846:MET:HB3	1:B:867:ILE:HG23	1.82	0.62
1:A:765:TRP:O	1:A:767:ARG:NH1	2.32	0.62
1:A:2236:GLN:NE2	1:A:2273:ALA:O	2.32	0.62
1:B:1914:ARG:NH1	1:A:1505:ASP:OD1	2.31	0.61
1:A:2248:ARG:NE	1:A:2307:GLU:OE2	2.32	0.61
1:B:2:THR:HG22	1:B:872:GLU:HA	1.82	0.61
1:A:1213:ARG:HG3	1:A:1213:ARG:HH11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2219:GLU:N	1:A:2219:GLU:OE1	2.33	0.61
1:A:2636:ARG:HG3	1:A:2637:LYS:HD2	1.83	0.61
1:A:880:ILE:HG13	1:A:1088:ILE:HG21	1.83	0.61
1:A:2053:GLN:N	1:A:2053:GLN:OE1	2.33	0.61
1:B:2755:ARG:NH2	1:B:2762:LEU:O	2.33	0.61
1:A:779:GLU:OE1	1:A:779:GLU:N	2.25	0.61
1:B:2098:LEU:HD12	1:B:2099:PRO:HD2	1.82	0.61
1:A:1080:ASP:OD1	1:A:1081:ARG:N	2.33	0.61
1:A:2502:ALA:O	1:A:2525:ARG:NH2	2.33	0.61
1:B:1237:LYS:HE2	1:B:1237:LYS:H	1.66	0.60
1:B:1964:GLN:HB2	1:B:2171:PRO:HG2	1.83	0.60
1:B:2308:LYS:HA	1:B:2308:LYS:HE2	1.82	0.60
1:A:457:LYS:HE3	1:A:457:LYS:HA	1.83	0.60
1:A:440:ASN:OD1	1:A:440:ASN:N	2.35	0.60
1:A:2668:GLU:OE2	1:A:2668:GLU:N	2.23	0.60
1:A:1095:SER:O	1:A:1099:GLN:NE2	2.33	0.60
1:A:2557:VAL:HG11	1:A:2651:LEU:HG	1.82	0.60
1:A:1360:ILE:HG22	1:A:1363:LEU:HD12	1.83	0.59
1:B:2297:THR:HG21	1:B:2736:SER:HA	1.83	0.59
1:A:430:ASN:ND2	1:A:478:CYS:O	2.35	0.59
1:B:2229:MET:HE3	1:B:2229:MET:HA	1.84	0.59
1:A:2637:LYS:HE2	1:A:2637:LYS:HA	1.84	0.59
1:B:1818:LYS:HD3	1:B:1819:LEU:N	2.17	0.59
1:B:2509:GLY:O	1:B:2511:ARG:NH2	2.31	0.59
1:B:380:GLU:HA	1:B:394:LYS:HA	1.84	0.59
1:B:401:TYR:CE2	1:B:412:PRO:HD3	2.38	0.59
1:B:501:GLN:HA	1:B:504:LYS:HE3	1.84	0.59
1:B:1289:GLU:OE1	1:B:1289:GLU:N	2.34	0.58
1:A:2530:ARG:HH12	1:A:2534:ARG:CZ	2.16	0.58
1:B:1366:GLU:N	1:B:1366:GLU:OE1	2.36	0.58
1:B:1804:LYS:HE2	1:B:1804:LYS:N	2.18	0.58
1:B:2289:SER:OG	1:B:2768:CYS:O	2.21	0.58
1:B:2730:VAL:HA	1:B:2733:TRP:HB2	1.83	0.58
1:A:1920:TYR:HA	1:A:1938:VAL:HG21	1.84	0.58
1:B:2527:ASN:O	1:B:2531:ASN:N	2.34	0.58
1:B:399:GLU:OE2	1:B:402:ARG:HG3	2.02	0.58
1:B:393:TRP:NE1	1:B:398:SER:O	2.28	0.58
1:B:2304:LEU:HG	1:B:2514:TYR:CE2	2.39	0.58
1:A:1369:VAL:O	1:A:1370:TYR:HB2	2.03	0.58
1:B:2731:TYR:HD1	1:B:2735:SER:HA	1.69	0.58
1:A:1512:GLU:OE1	1:A:1512:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2502:ALA:O	1:B:2517:ARG:NH2	2.29	0.58
1:A:2656:LYS:H	1:A:2656:LYS:HD3	1.69	0.58
1:B:387:LYS:HE3	1:B:387:LYS:HA	1.86	0.57
1:B:1351:LYS:O	1:B:1351:LYS:NZ	2.31	0.57
1:A:18:LEU:HD11	1:A:811:ILE:HD11	1.86	0.57
1:B:480:ALA:HB2	1:B:806:GLN:HE22	1.70	0.57
1:A:741:PRO:HG2	1:A:744:THR:HG21	1.84	0.57
1:B:890:GLN:NE2	1:B:894:ASN:HD21	2.02	0.57
1:A:2579:LEU:HD21	1:A:2635:VAL:HG22	1.87	0.57
1:A:2276:ARG:NH1	1:A:2276:ARG:HB2	2.19	0.57
1:B:411:HIS:HD2	1:B:413:ARG:H	1.53	0.56
1:B:2244:VAL:O	1:B:2282:LYS:N	2.37	0.56
1:B:411:HIS:CD2	1:B:412:PRO:HD2	2.41	0.56
1:B:1392:THR:OG1	1:B:1393:ALA:N	2.36	0.56
1:B:2525:ARG:HG3	1:B:2525:ARG:HH11	1.70	0.56
1:B:2558:LEU:HA	1:B:2655:ARG:HD2	1.87	0.56
1:A:499:PHE:HA	1:A:502:ARG:HB2	1.87	0.56
1:B:1099:GLN:HB3	1:B:1100:PRO:HD3	1.88	0.56
1:A:825:ASP:OD1	1:A:829:GLY:N	2.38	0.56
1:B:411:HIS:CD2	1:B:413:ARG:H	2.24	0.56
1:A:1418:ARG:HG3	1:A:1418:ARG:HH11	1.71	0.56
1:B:397:GLU:N	1:B:397:GLU:OE1	2.37	0.56
1:B:1519:LEU:HD12	1:B:1520:PRO:HD2	1.88	0.56
1:B:1961:MET:HB3	1:B:2173:CYS:SG	2.45	0.56
1:B:900:VAL:HG23	1:B:901:LEU:HG	1.87	0.56
1:B:24:GLU:OE1	1:B:24:GLU:N	2.38	0.56
1:A:24:GLU:HA	1:A:27:GLU:HG3	1.88	0.55
1:A:827:MET:HE3	1:A:827:MET:HA	1.87	0.55
1:B:2558:LEU:HB3	1:B:2658:LEU:HD23	1.89	0.55
1:A:356:LEU:HD13	1:A:357:GLY:N	2.21	0.55
1:B:781:GLU:OE1	1:B:781:GLU:HA	2.07	0.55
1:A:765:TRP:CH2	1:A:767:ARG:HD3	2.41	0.55
1:A:1124:ARG:NE	1:A:1177:ASP:OD1	2.33	0.55
1:A:1334:GLN:HA	1:A:1404:THR:HG21	1.88	0.55
1:B:767:ARG:HD2	1:B:781:GLU:OE2	2.07	0.55
1:B:2174:SER:O	1:B:2174:SER:OG	2.23	0.55
1:A:2575:MET:HE1	1:A:2638:TYR:CZ	2.41	0.55
1:A:2721:MET:SD	1:A:2726:ARG:NH1	2.80	0.55
1:A:40:LEU:C	1:A:42:VAL:H	2.15	0.54
1:A:405:GLN:H	1:A:405:GLN:CD	2.16	0.54
1:B:52:VAL:HB	1:B:376:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1513:LEU:HD13	1:A:1922:LEU:HD22	1.89	0.54
1:A:1870:HIS:CD2	1:A:1872:LEU:H	2.19	0.54
1:B:499:PHE:O	1:B:503:LYS:N	2.40	0.54
1:B:907:MET:SD	1:B:907:MET:N	2.79	0.54
1:B:1399:ASP:OD1	1:B:1462:ARG:NH2	2.39	0.54
1:B:2779:SER:OG	1:B:2781:GLN:OE1	2.25	0.54
1:A:494:TRP:HD1	1:A:735:PRO:HA	1.71	0.54
1:B:780:GLN:N	1:B:780:GLN:OE1	2.41	0.54
1:B:2707:LEU:HD11	1:B:2754:ILE:HD13	1.88	0.54
1:B:889:ARG:HD3	1:B:890:GLN:N	2.23	0.54
1:A:898:ALA:O	1:A:904:ASN:ND2	2.41	0.54
1:A:1804:LYS:HE3	1:A:1804:LYS:HA	1.89	0.54
1:B:2296:TYR:CE2	1:B:2544:GLU:HG3	2.43	0.53
1:A:370:LYS:O	1:A:386:SER:N	2.39	0.53
1:A:461:THR:O	1:A:463:GLN:NE2	2.41	0.53
1:B:907:MET:HA	1:B:910:THR:HG22	1.90	0.53
1:A:844:LEU:HD13	1:A:869:MET:HB3	1.91	0.53
1:B:1108:ALA:O	1:B:1110:ASP:N	2.41	0.53
1:B:2218:PHE:CE1	1:B:2222:GLU:HB3	2.43	0.53
1:A:57:HIS:HB2	1:A:69:ARG:HH21	1.73	0.53
1:A:54:GLY:HA3	1:A:395:TRP:HZ2	1.73	0.53
1:A:2647:ALA:C	1:A:2650:PRO:HD2	2.34	0.53
1:B:874:GLN:HB3	1:B:877:MET:HB3	1.91	0.53
1:B:2676:ARG:NH1	1:B:2676:ARG:HB2	2.24	0.53
1:B:1444:ALA:HB2	1:B:1499:LEU:HB3	1.90	0.53
1:B:367:ASP:N	1:B:367:ASP:OD1	2.42	0.52
1:B:877:MET:HE3	1:B:877:MET:HA	1.91	0.52
1:B:2676:ARG:HB2	1:B:2676:ARG:HH11	1.74	0.52
1:B:893:MET:H	1:B:893:MET:CE	2.22	0.52
1:A:2239:ASP:N	1:A:2239:ASP:OD1	2.41	0.52
1:B:502:ARG:O	1:B:505:MET:HG3	2.10	0.52
1:B:2549:THR:HG22	1:B:2680:ASN:HD22	1.74	0.52
1:B:365:ASP:N	1:B:365:ASP:OD1	2.42	0.52
1:B:1290:HIS:CD2	1:B:1321:PRO:HB2	2.45	0.52
1:B:2211:ILE:HD12	1:B:2211:ILE:O	2.09	0.52
1:A:796:GLU:H	1:A:797:ARG:NH2	2.07	0.52
1:B:876:LEU:HD23	1:B:911:PHE:CE1	2.44	0.52
1:B:1236:GLU:HB2	1:B:1237:LYS:NZ	2.23	0.52
1:A:2533:GLY:HA3	1:A:2657:GLY:HA3	1.91	0.52
1:B:507:GLU:N	1:B:507:GLU:OE1	2.43	0.52
1:B:2610:GLU:OE1	1:B:2642:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2668:GLU:N	1:B:2668:GLU:OE1	2.42	0.52
1:A:2729:LEU:O	1:A:2733:TRP:N	2.40	0.52
1:B:498:PRO:HA	1:B:502:ARG:HB2	1.92	0.52
1:B:886:GLU:OE1	1:B:886:GLU:HA	2.10	0.52
1:A:18:LEU:HD22	1:A:809:PRO:HB2	1.91	0.52
1:A:1083:ALA:O	1:A:1086:HIS:ND1	2.28	0.52
1:B:401:TYR:HE2	1:B:412:PRO:HD3	1.75	0.52
1:B:2687:VAL:HG21	1:B:2719:GLU:HG2	1.91	0.51
1:B:1351:LYS:O	1:B:1521:PRO:HD3	2.10	0.51
1:A:2571:PHE:HE2	1:A:2642:ARG:HE	1.57	0.51
1:B:389:GLU:HG2	1:B:391:TYR:HE1	1.76	0.51
1:A:887:ALA:HA	1:A:890:GLN:HE22	1.74	0.51
1:B:1951:PHE:HE2	1:B:2193:LEU:HD21	1.75	0.51
1:B:2721:MET:SD	1:B:2721:MET:N	2.83	0.51
1:B:2114:MET:SD	1:B:2176:MET:HG2	2.51	0.51
1:B:2229:MET:HE1	1:B:2232:LEU:HD23	1.93	0.51
1:B:832:ASP:N	1:B:832:ASP:OD1	2.41	0.51
1:B:1152:ASP:OD1	1:B:1153:VAL:N	2.44	0.51
1:B:2591:ALA:O	1:B:2595:PHE:N	2.41	0.51
1:A:385:SER:OG	1:A:389:GLU:OE1	2.28	0.51
1:A:765:TRP:CZ2	1:A:767:ARG:HD3	2.46	0.51
1:A:2035:ILE:HG13	1:A:2037:PRO:HD2	1.91	0.51
1:A:2243:GLU:N	1:A:2258:GLN:OE1	2.43	0.51
1:A:2532:ILE:HG13	1:A:2535:ILE:HD11	1.92	0.51
1:B:370:LYS:O	1:B:386:SER:N	2.43	0.50
1:B:1233:ASP:O	1:B:1237:LYS:NZ	2.41	0.50
1:A:1331:ARG:O	1:A:1331:ARG:NH1	2.41	0.50
1:B:2600:LEU:O	1:B:2626:VAL:N	2.45	0.50
1:A:1124:ARG:HH21	1:A:1177:ASP:HA	1.75	0.50
1:B:2052:ASP:HB3	1:B:2053:GLN:OE1	2.11	0.50
1:B:2244:VAL:HA	1:B:2254:GLN:CD	2.37	0.50
1:A:880:ILE:H	1:A:880:ILE:HD12	1.76	0.50
1:A:435:THR:HG23	1:A:445:THR:HB	1.93	0.50
1:A:1836:ILE:O	1:A:1840:ASN:ND2	2.43	0.50
1:B:895:LEU:HD12	1:B:1097:VAL:HG21	1.93	0.50
1:A:2257:ARG:O	1:A:2261:ASN:ND2	2.45	0.50
1:B:916:CYS:SG	1:B:917:ASP:N	2.80	0.49
1:A:882:ARG:HH12	1:A:884:ASP:CG	2.18	0.49
1:A:1958:ILE:O	1:A:1962:ASN:ND2	2.45	0.49
1:A:2653:ALA:HA	1:A:2656:LYS:HZ2	1.75	0.49
1:A:2721:MET:HE1	1:A:2726:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2728:ASP:O	1:A:2732:PHE:N	2.35	0.49
1:B:2046:GLU:N	1:B:2046:GLU:OE1	2.45	0.49
1:B:2256:MET:HE1	1:B:2527:ASN:OD1	2.11	0.49
1:A:2251:LEU:O	1:A:2255:THR:OG1	2.25	0.49
1:A:2653:ALA:HA	1:A:2656:LYS:HZ3	1.74	0.49
1:B:468:LEU:HD13	1:B:473:ILE:HD11	1.93	0.49
1:B:2592:ASP:OD1	1:B:2593:ALA:N	2.45	0.49
1:A:2600:LEU:O	1:A:2626:VAL:N	2.35	0.49
1:B:2562:LYS:HD3	1:B:2562:LYS:C	2.37	0.49
1:A:905:LEU:HA	1:A:909:GLN:HE22	1.77	0.49
1:A:1240:CYS:SG	1:A:1242:THR:OG1	2.69	0.49
1:B:1860:ALA:HB2	1:B:1871:PRO:HG2	1.93	0.49
1:B:2542:GLN:HG2	1:B:2544:GLU:OE1	2.12	0.49
1:A:1080:ASP:O	1:A:1084:ASN:N	2.42	0.49
1:B:770:ILE:HD12	1:B:780:GLN:HE22	1.77	0.49
1:B:1394:ASP:O	1:B:1395:ILE:HD12	2.12	0.49
1:B:422:GLU:N	1:B:422:GLU:OE1	2.45	0.49
1:B:746:ILE:HD13	1:B:760:LEU:HD22	1.94	0.49
1:B:2530:ARG:NH1	1:B:2530:ARG:HB2	2.28	0.49
1:B:2728:ASP:HA	1:B:2731:TYR:HB3	1.94	0.49
1:A:2243:GLU:O	1:A:2258:GLN:NE2	2.45	0.49
1:A:359:ASP:OD1	1:A:360:LEU:N	2.46	0.49
1:A:2530:ARG:HD3	1:A:2656:LYS:HE2	1.95	0.49
1:A:798:ASN:O	1:A:813:ARG:NE	2.38	0.49
1:A:1406:VAL:HG23	1:A:1817:VAL:HG12	1.95	0.49
1:B:1796:SER:OG	1:B:1957:TRP:HD1	1.95	0.49
1:B:1392:THR:O	1:B:1459:LYS:NZ	2.44	0.48
1:A:367:ASP:OD1	1:A:367:ASP:N	2.34	0.48
1:A:1178:THR:HA	1:A:1242:THR:O	2.13	0.48
1:A:2575:MET:HE1	1:A:2638:TYR:CE1	2.48	0.48
1:B:68:CYS:SG	1:B:69:ARG:N	2.87	0.48
1:A:463:GLN:HB2	1:A:465:TYR:HE1	1.76	0.48
1:A:886:GLU:HB2	1:A:889:ARG:HH21	1.78	0.48
1:A:890:GLN:HA	1:A:893:MET:SD	2.54	0.48
1:A:2576:TYR:O	1:A:2580:ARG:N	2.46	0.48
1:B:1098:LEU:O	1:B:1099:GLN:C	2.56	0.48
1:A:390:LEU:HD23	1:A:411:HIS:CG	2.48	0.48
1:A:1124:ARG:NH2	1:A:1177:ASP:O	2.44	0.48
1:B:878:GLN:HE22	1:B:882:ARG:CZ	2.26	0.48
1:B:2529:PHE:O	1:B:2532:ILE:HG22	2.14	0.48
1:A:2238:ARG:NH2	1:A:2274:VAL:HG12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:THR:N	1:B:63:GLU:OE1	2.46	0.48
1:B:1248:LYS:HA	1:B:1248:LYS:HE3	1.94	0.48
1:A:761:LYS:NZ	1:A:763:GLY:O	2.41	0.48
1:A:893:MET:HA	1:A:896:GLU:HB3	1.95	0.48
1:B:898:ALA:HB1	1:B:907:MET:HE2	1.96	0.48
1:B:1203:GLU:CD	1:B:1204:SER:H	2.22	0.47
1:B:2504:LEU:HD23	1:B:2517:ARG:HH22	1.79	0.47
1:A:2311:ASN:OD1	1:A:2311:ASN:N	2.47	0.47
1:A:2746:PHE:CG	1:A:2750:PRO:HD3	2.49	0.47
1:B:426:LEU:HD23	1:B:437:ALA:HB3	1.95	0.47
1:B:1522:ARG:HA	1:A:1864:ASP:HB3	1.95	0.47
1:A:794:GLN:NE2	1:A:816:ASN:OD1	2.47	0.47
1:A:873:LYS:HA	1:A:873:LYS:HE2	1.95	0.47
1:A:494:TRP:HE3	1:A:495:GLY:H	1.63	0.47
1:B:2266:ARG:NH1	1:B:2271:PRO:O	2.47	0.47
1:A:1395:ILE:HG12	1:A:1395:ILE:O	2.15	0.47
1:A:1847:ASP:OD2	1:A:2188:ARG:NH2	2.48	0.47
1:A:2519:GLY:HA3	1:A:2525:ARG:NH1	2.29	0.47
1:B:2224:LYS:HD3	1:B:2225:PHE:N	2.30	0.47
1:B:2507:GLN:HB3	1:B:2511:ARG:NH2	2.26	0.47
1:A:38:PRO:N	1:A:39:PRO:HD2	2.29	0.47
1:A:893:MET:HE3	1:A:893:MET:H	1.78	0.47
1:A:936:LYS:O	1:A:936:LYS:HD3	2.14	0.47
1:A:24:GLU:H	1:A:24:GLU:CD	2.22	0.47
1:B:737:LYS:O	1:B:776:GLY:HA2	2.15	0.47
1:A:47:THR:OG1	1:A:63:GLU:OE1	2.28	0.47
1:A:463:GLN:HB2	1:A:465:TYR:CE1	2.50	0.47
1:A:1139:ILE:HD11	1:A:1157:MET:HE1	1.96	0.47
1:A:1195:GLU:HB3	1:A:1224:LYS:HZ2	1.80	0.47
1:A:2602:PHE:CD2	1:A:2618:ILE:HG12	2.50	0.47
1:A:2729:LEU:HD13	1:A:2791:ILE:HD11	1.96	0.47
1:B:1358:SER:OG	1:B:1359:ARG:N	2.41	0.46
1:A:2186:LEU:HD21	1:A:2215:LEU:HD21	1.96	0.46
1:A:2240:LEU:HD13	1:A:2241:SER:N	2.29	0.46
1:A:2276:ARG:HB2	1:A:2276:ARG:CZ	2.44	0.46
1:B:1205:LEU:HD13	1:B:1237:LYS:HD2	1.97	0.46
1:A:846:MET:HG3	1:A:867:ILE:HG12	1.97	0.46
1:A:862:LYS:C	1:A:862:LYS:HD2	2.40	0.46
1:B:876:LEU:HD22	1:B:891:TYR:CD1	2.50	0.46
1:B:912:ILE:HG13	1:B:1105:LEU:HD13	1.97	0.46
1:B:1961:MET:HE3	1:B:2171:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1961:MET:HG3	1:B:2171:PRO:CB	2.39	0.46
1:A:425:VAL:HG23	1:A:426:LEU:HG	1.97	0.46
1:A:1176:ASN:HB3	1:A:1210:GLU:CD	2.40	0.46
1:A:2529:PHE:CD2	1:A:2650:PRO:HB3	2.51	0.46
1:B:67:VAL:HG21	1:B:374:ILE:HD11	1.96	0.46
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.84	0.46
1:B:2195:LEU:O	1:B:2199:VAL:HG23	2.15	0.46
1:B:2598:MET:HE1	1:B:2600:LEU:HG	1.96	0.46
1:A:11:LEU:HD23	1:A:863:LYS:HB3	1.98	0.46
1:A:754:LYS:HD2	1:A:754:LYS:C	2.40	0.46
1:B:1216:HIS:CD2	1:B:1219:HIS:ND1	2.65	0.46
1:B:1345:PHE:O	1:B:1427:ARG:NH2	2.48	0.46
1:B:469:GLN:O	1:B:472:ARG:NH2	2.46	0.46
1:B:1197:ARG:HG2	1:B:1197:ARG:HH11	1.81	0.46
1:A:499:PHE:O	1:A:503:LYS:N	2.37	0.46
1:A:1213:ARG:HG3	1:A:1213:ARG:NH1	2.31	0.46
1:A:2519:GLY:HA3	1:A:2525:ARG:HH11	1.81	0.46
1:B:1951:PHE:CE2	1:B:2193:LEU:HD21	2.51	0.45
1:B:2107:ASN:O	1:B:2111:VAL:HG23	2.16	0.45
1:B:2792:LYS:O	1:B:2792:LYS:NZ	2.42	0.45
1:A:2234:ASN:OD1	1:A:2235:GLN:N	2.48	0.45
1:A:2602:PHE:HD1	1:A:2626:VAL:HG22	1.81	0.45
1:B:1182:THR:HB	1:B:1319:LEU:HB2	1.98	0.45
1:B:1318:ASP:OD1	1:B:1318:ASP:N	2.33	0.45
1:A:2749:MET:HE2	1:A:2749:MET:HB2	1.80	0.45
1:B:2239:ASP:OD1	1:B:2240:LEU:N	2.49	0.45
1:A:733:ARG:O	1:A:735:PRO:HD3	2.16	0.45
1:A:1197:ARG:HH21	1:A:1202:LEU:HD11	1.80	0.45
1:A:1803:PRO:HB2	1:A:1804:LYS:HD2	1.97	0.45
1:B:390:LEU:H	1:B:390:LEU:HD23	1.80	0.45
1:B:1320:GLU:OE1	1:B:1320:GLU:HA	2.16	0.45
1:A:2668:GLU:H	1:A:2668:GLU:CD	2.20	0.45
1:A:908:LEU:H	1:A:908:LEU:HD23	1.82	0.45
1:B:766:VAL:HG23	1:B:788:SER:HB2	1.98	0.45
1:B:876:LEU:HD12	1:B:879:HIS:HB2	1.99	0.45
1:B:893:MET:HE3	1:B:893:MET:N	2.30	0.45
1:B:1266:THR:HG23	1:B:1341:SER:HB2	1.99	0.45
1:B:2525:ARG:HG3	1:B:2525:ARG:NH1	2.31	0.45
1:A:476:LEU:HD23	1:A:485:ALA:HA	1.99	0.45
1:A:893:MET:H	1:A:893:MET:CE	2.29	0.45
1:A:2583:ILE:HD11	1:A:2635:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ILE:HD12	1:B:780:GLN:NE2	2.31	0.45
1:B:2510:LYS:HB2	1:B:2513:PHE:CD2	2.52	0.45
1:B:2721:MET:HG3	1:B:2725:GLU:OE1	2.16	0.45
1:A:1112:ARG:HG3	1:A:1114:MET:HG3	1.99	0.45
1:A:1348:GLN:O	1:A:1349:GLU:HB3	2.17	0.45
1:A:2182:HIS:CG	1:A:2183:ASP:H	2.35	0.45
1:B:1137:GLN:HG2	1:B:1154:PHE:CE1	2.52	0.45
1:B:2678:LEU:HD12	1:B:2678:LEU:HA	1.78	0.45
1:B:2723:MET:SD	1:B:2723:MET:N	2.89	0.45
1:A:19:ASN:O	1:A:23:ARG:HG3	2.17	0.45
1:A:892:LEU:HD23	1:A:892:LEU:HA	1.73	0.45
1:A:2759:ASP:OD1	1:A:2759:ASP:N	2.50	0.45
1:B:1094:ASP:OD1	1:B:1094:ASP:C	2.60	0.45
1:B:2308:LYS:NZ	1:B:2501:ASN:OD1	2.34	0.45
1:B:2505:PHE:HD2	1:B:2514:TYR:HD2	1.63	0.45
1:A:55:PRO:HD2	1:A:395:TRP:CZ2	2.51	0.45
1:A:2542:GLN:HB2	1:A:2544:GLU:OE1	2.17	0.44
1:A:821:PRO:HG2	1:A:833:PRO:HB3	2.00	0.44
1:A:479:CYS:HB3	1:A:751:VAL:HG22	2.00	0.44
1:A:2224:LYS:NZ	1:A:2224:LYS:HB3	2.32	0.44
1:B:25:VAL:HG23	1:B:838:LEU:HD21	2.00	0.44
1:B:2258:GLN:HA	1:B:2261:ASN:HD21	1.83	0.44
1:B:2680:ASN:N	1:B:2680:ASN:OD1	2.50	0.44
1:B:2296:TYR:HA	1:B:2299:ILE:HG22	2.00	0.44
1:A:804:ALA:HB3	1:A:808:SER:HB3	1.99	0.44
1:A:2259:LEU:HB2	1:A:2531:ASN:HD21	1.83	0.44
1:B:736:LYS:HG3	1:B:737:LYS:HG2	1.99	0.44
1:A:380:GLU:OE2	1:A:392:GLN:HA	2.17	0.44
1:A:394:LYS:HB3	1:A:397:GLU:OE1	2.16	0.44
1:A:480:ALA:C	1:A:481:LEU:HD23	2.43	0.44
1:B:2182:HIS:CD2	1:B:2182:HIS:H	2.35	0.44
1:B:2513:PHE:HB3	1:B:2551:ASN:HB3	2.00	0.44
1:B:2721:MET:HG2	1:B:2726:ARG:NH1	2.33	0.44
1:A:37:HIS:ND1	1:A:38:PRO:HD2	2.33	0.44
1:A:915:ARG:HD2	1:A:919:ASN:OD1	2.17	0.44
1:A:2297:THR:O	1:A:2301:GLN:HG2	2.18	0.44
1:B:759:VAL:HG12	1:B:801:ILE:HD11	2.00	0.44
1:A:1138:LYS:O	1:A:1141:LYS:NZ	2.51	0.44
1:A:2189:TRP:O	1:A:2193:LEU:HG	2.18	0.43
1:A:2733:TRP:HB3	1:A:2734:THR:HG23	1.99	0.43
1:B:430:ASN:HB2	1:B:478:CYS:SG	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1841:TRP:HZ3	1:B:1950:VAL:HG11	1.82	0.43
1:B:2526:LEU:HD13	1:B:2649:GLN:NE2	2.32	0.43
1:B:2714:PHE:O	1:B:2718:VAL:HG23	2.18	0.43
1:B:399:GLU:C	1:B:399:GLU:OE1	2.61	0.43
1:B:423:LYS:HE3	1:B:439:GLU:CD	2.43	0.43
1:B:2207:GLU:O	1:B:2210:SER:OG	2.30	0.43
1:B:2211:ILE:HA	1:B:2214:GLU:OE1	2.18	0.43
1:A:1444:ALA:HB2	1:A:1499:LEU:HB3	2.00	0.43
1:A:2709:GLN:N	1:A:2709:GLN:NE2	2.53	0.43
1:B:1147:SER:O	1:B:1147:SER:OG	2.33	0.43
1:A:862:LYS:HD2	1:A:863:LYS:HG3	2.01	0.43
1:A:1179:CYS:SG	1:A:1180:SER:N	2.92	0.43
1:A:1940:ASP:O	1:A:1943:SER:OG	2.35	0.43
1:A:904:ASN:HA	1:A:907:MET:HE1	2.01	0.43
1:B:385:SER:OG	1:B:386:SER:N	2.52	0.43
1:B:505:MET:HA	1:B:508:LYS:HE2	2.01	0.43
1:A:2664:LYS:HA	1:A:2664:LYS:HE3	2.00	0.43
1:B:38:PRO:N	1:B:39:PRO:HD2	2.34	0.43
1:B:1965:THR:HG22	1:B:2171:PRO:O	2.19	0.43
1:A:1381:ASP:OD1	1:A:1431:SER:OG	2.34	0.43
1:B:905:LEU:HB3	1:B:907:MET:SD	2.59	0.42
1:A:452:SER:HA	1:A:455:ALA:HB3	2.01	0.42
1:A:1186:ALA:N	1:A:1187:GLU:OE1	2.52	0.42
1:A:2308:LYS:HZ3	1:A:2501:ASN:C	2.27	0.42
1:A:2534:ARG:HD2	1:A:2657:GLY:HA2	2.00	0.42
1:B:504:LYS:HA	1:B:507:GLU:OE2	2.20	0.42
1:B:2788:LEU:HA	1:B:2791:ILE:HB	2.01	0.42
1:A:464:THR:OG1	1:A:469:GLN:NE2	2.48	0.42
1:A:851:LEU:H	1:A:851:LEU:HD12	1.84	0.42
1:A:16:ASP:OD1	1:A:16:ASP:N	2.51	0.42
1:B:379:SER:HB2	1:B:380:GLU:OE1	2.19	0.42
1:B:2252:ILE:HD12	1:B:2303:PHE:CE1	2.54	0.42
1:A:393:TRP:CD1	1:A:393:TRP:C	2.98	0.42
1:A:2240:LEU:HB3	1:A:2277:VAL:HG22	2.01	0.42
1:B:1442:GLU:HG3	1:A:1914:ARG:HD3	2.00	0.42
1:A:18:LEU:O	1:A:22:LEU:HG	2.20	0.42
1:B:1349:GLU:HB3	1:B:1355:SER:CB	2.49	0.42
1:A:421:ASN:OD1	1:A:421:ASN:N	2.44	0.42
1:A:2630:ASN:O	1:A:2634:TYR:N	2.45	0.42
1:B:2731:TYR:CD1	1:B:2735:SER:HA	2.51	0.42
1:A:377:LEU:HD23	1:A:382:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLU:OE1	1:A:389:GLU:N	2.53	0.42
1:A:1809:VAL:HG13	1:A:1813:ILE:HD12	2.00	0.42
1:A:2763:PRO:HG3	1:A:2774:VAL:HG13	2.02	0.42
1:B:70:ILE:HD12	1:B:70:ILE:HA	1.87	0.42
1:B:862:LYS:HA	1:B:862:LYS:HE2	2.01	0.42
1:A:387:LYS:HE2	1:A:387:LYS:N	2.25	0.42
1:B:499:PHE:HB3	1:B:500:SER:H	1.63	0.42
1:B:741:PRO:HG2	1:B:767:ARG:HH21	1.85	0.42
1:B:939:LYS:H	1:B:939:LYS:HD3	1.85	0.42
1:A:1331:ARG:HG3	1:A:1331:ARG:HH11	1.84	0.42
1:A:1348:GLN:C	1:A:1350:ASN:H	2.28	0.42
1:B:68:CYS:SG	1:B:360:LEU:HG	2.60	0.41
1:B:745:GLU:C	1:B:745:GLU:OE1	2.63	0.41
1:A:473:ILE:HD13	1:A:487:LEU:HD11	2.03	0.41
1:A:2035:ILE:CG1	1:A:2037:PRO:HD2	2.50	0.41
1:B:387:LYS:HA	1:B:387:LYS:CE	2.50	0.41
1:B:465:TYR:HB3	1:B:467:GLU:H	1.84	0.41
1:A:2552:ARG:HG2	1:A:2567:ASP:HB2	2.02	0.41
1:B:1239:LYS:NZ	1:B:1239:LYS:HB3	2.35	0.41
1:A:1873:HIS:CG	1:A:1874:ALA:N	2.89	0.41
1:A:2709:GLN:HA	1:A:2712:ARG:HG3	2.02	0.41
1:B:1859:LEU:HD23	1:B:1936:LEU:HD13	2.02	0.41
1:A:1331:ARG:NH1	1:A:1331:ARG:HG3	2.34	0.41
1:A:1959:LYS:HA	1:A:1959:LYS:HD2	1.82	0.41
1:A:2057:LEU:HD12	1:A:2057:LEU:HA	1.57	0.41
1:A:2229:MET:C	1:A:2229:MET:HE2	2.46	0.41
1:A:2640:GLU:OE2	1:A:2640:GLU:N	2.53	0.41
1:B:1511:GLU:OE1	1:B:1511:GLU:C	2.63	0.41
1:B:2534:ARG:H	1:B:2534:ARG:HG2	1.59	0.41
1:A:413:ARG:HB3	1:A:417:LEU:HD23	2.03	0.41
1:B:1284:ALA:O	1:B:1287:THR:HG22	2.20	0.41
1:B:2525:ARG:HD2	1:B:2525:ARG:C	2.45	0.41
1:B:2532:ILE:O	1:B:2536:LEU:HG	2.20	0.41
1:A:68:CYS:SG	1:A:360:LEU:HD21	2.60	0.41
1:A:465:TYR:O	1:A:469:GLN:NE2	2.53	0.41
1:A:2602:PHE:CD1	1:A:2626:VAL:HG22	2.56	0.41
1:B:432:ILE:HD11	1:B:480:ALA:O	2.21	0.41
1:B:877:MET:SD	1:B:916:CYS:HB2	2.61	0.41
1:B:2226:ARG:HB3	1:B:2227:ARG:HH12	1.84	0.41
1:B:2690:LEU:O	1:B:2694:THR:OG1	2.29	0.41
1:A:2731:TYR:HD1	1:A:2735:SER:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:LYS:NZ	1:B:770:ILE:HD13	2.36	0.41
1:B:760:LEU:HB2	1:B:767:ARG:CZ	2.51	0.41
1:B:876:LEU:HD23	1:B:911:PHE:HE1	1.84	0.41
1:B:904:ASN:OD1	1:B:904:ASN:N	2.54	0.41
1:B:1143:GLU:O	1:B:1145:SER:N	2.53	0.41
1:A:39:PRO:HG2	1:A:40:LEU:HD22	2.03	0.41
1:A:1274:HIS:HB3	1:A:1342:MET:CE	2.50	0.41
1:A:1343:ILE:HA	1:A:1380:LEU:HD13	2.02	0.41
1:B:480:ALA:HB2	1:B:806:GLN:NE2	2.36	0.41
1:B:1197:ARG:HG2	1:B:1197:ARG:NH1	2.36	0.41
1:B:2057:LEU:HD12	1:B:2057:LEU:HA	1.87	0.41
1:B:2557:VAL:HG21	1:B:2651:LEU:HD13	2.02	0.41
1:A:459:GLU:OE1	1:A:459:GLU:HA	2.21	0.41
1:A:761:LYS:C	1:A:767:ARG:HH22	2.28	0.41
1:A:802:PHE:CD2	1:A:844:LEU:HD23	2.56	0.41
1:A:876:LEU:HD23	1:A:911:PHE:CE1	2.56	0.41
1:A:920:ARG:HG2	1:A:924:HIS:HB3	2.02	0.41
1:A:2297:THR:HG21	1:A:2736:SER:HA	2.03	0.41
1:A:2540:LEU:HD23	1:A:2540:LEU:HA	1.86	0.41
1:A:2723:MET:HA	1:A:2726:ARG:HG3	2.03	0.41
1:B:1179:CYS:SG	1:B:1180:SER:N	2.94	0.41
1:B:2252:ILE:O	1:B:2256:MET:HB2	2.21	0.41
1:B:2293:ARG:NH2	1:B:2767:THR:O	2.54	0.41
1:A:886:GLU:O	1:A:889:ARG:HB3	2.21	0.41
1:A:2617:LEU:HD23	1:A:2641:HIS:CD2	2.49	0.41
1:B:2541:LEU:HB3	1:B:2542:GLN:OE1	2.20	0.40
1:A:1239:LYS:H	1:A:1239:LYS:HG2	1.77	0.40
1:A:1409:LEU:O	1:A:1418:ARG:NE	2.54	0.40
1:A:1511:GLU:OE1	1:A:1511:GLU:C	2.64	0.40
1:A:1867:HIS:HD2	1:A:1868:PRO:HD2	1.84	0.40
1:B:11:LEU:HD23	1:B:12:PRO:HA	2.02	0.40
1:B:1438:ILE:HG23	1:A:1918:LEU:HD13	2.03	0.40
1:B:1493:PRO:O	1:B:1780:SER:HB3	2.21	0.40
1:B:2212:LEU:HD23	1:B:2212:LEU:HA	1.88	0.40
1:B:2522:THR:O	1:B:2526:LEU:HG	2.21	0.40
1:B:2556:LYS:HG2	1:B:2561:ARG:HB3	2.02	0.40
1:A:1195:GLU:OE1	1:A:1197:ARG:HD2	2.21	0.40
1:A:2240:LEU:O	1:A:2277:VAL:HA	2.22	0.40
1:A:2766:ASN:O	1:A:2770:SER:N	2.55	0.40
1:B:745:GLU:OE1	1:B:747:LEU:HD22	2.21	0.40
1:B:2099:PRO:O	1:A:1370:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:ILE:HD12	1:A:880:ILE:N	2.36	0.40
1:A:882:ARG:O	1:A:1081:ARG:NH1	2.55	0.40
1:A:1468:LEU:HD22	1:A:1802:ILE:HD11	2.04	0.40
1:B:457:LYS:HD2	1:B:457:LYS:HA	1.91	0.40
1:A:2034:CYS:O	1:A:2036:PRO:HD3	2.21	0.40
1:A:2262:HIS:CE1	1:A:2266:ARG:HE	2.39	0.40
1:B:417:LEU:HD12	1:B:460:HIS:O	2.22	0.40
1:B:1833:GLU:C	1:B:1833:GLU:OE1	2.64	0.40
1:B:1962:ASN:ND2	1:B:2181:SER:HA	2.37	0.40
1:B:2753:THR:N	1:B:2772:LEU:O	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1533/2830 (54%)	1456 (95%)	75 (5%)	2 (0%)	48	80
1	B	1604/2830 (57%)	1506 (94%)	93 (6%)	5 (0%)	36	70
All	All	3137/5660 (55%)	2962 (94%)	168 (5%)	7 (0%)	44	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	462	ALA
1	B	499	PHE
1	B	873	LYS
1	A	41	ASN
1	A	2204	VAL
1	B	2178	MET
1	B	1395	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	1366/2439 (56%)	1317 (96%)	49 (4%)	31	65
1	B	1438/2439 (59%)	1384 (96%)	54 (4%)	29	63
All	All	2804/4878 (58%)	2701 (96%)	103 (4%)	31	64

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	THR
1	B	18	LEU
1	B	64	ASP
1	B	372	ILE
1	B	377	LEU
1	B	386	SER
1	B	415	THR
1	B	426	LEU
1	B	452	SER
1	B	479	CYS
1	B	500	SER
1	B	572	CYS
1	B	652	SER
1	B	653	LEU
1	B	759	VAL
1	B	803	THR
1	B	836	LEU
1	B	841	ILE
1	B	849	HIS
1	B	873	LYS
1	B	895	LEU
1	B	905	LEU
1	B	923	LEU
1	B	938	THR
1	B	939	LYS
1	B	1097	VAL
1	B	1157	MET

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Mol	Chain	Res	Type
1	B	1229	THR
1	B	1280	VAL
1	B	1354	LEU
1	B	1355	SER
1	B	1382	CYS
1	B	1392	THR
1	B	1404	THR
1	B	1441	VAL
1	B	1801	LEU
1	B	1838	THR
1	B	1861	SER
1	B	2167	THR
1	B	2172	GLN
1	B	2251	LEU
1	B	2294	SER
1	B	2304	LEU
1	B	2529	PHE
1	B	2535	ILE
1	B	2538	LEU
1	B	2541	LEU
1	B	2550	LEU
1	B	2586	SER
1	B	2635	VAL
1	B	2728	ASP
1	B	2733	TRP
1	B	2734	THR
1	B	2762	LEU
1	A	2	THR
1	A	37	HIS
1	A	40	LEU
1	A	367	ASP
1	A	395	TRP
1	A	440	ASN
1	A	447	VAL
1	A	464	THR
1	A	491	LEU
1	A	494	TRP
1	A	555	ILE
1	A	571	SER
1	A	572	CYS
1	A	576	LEU
1	A	787	SER

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Mol	Chain	Res	Type
1	A	788	SER
1	A	803	THR
1	A	818	THR
1	A	836	LEU
1	A	838	LEU
1	A	876	LEU
1	A	913	SER
1	A	1139	ILE
1	A	1179	CYS
1	A	1189	ILE
1	A	1192	ASP
1	A	1341	SER
1	A	1349	GLU
1	A	1355	SER
1	A	1404	THR
1	A	1411	ASN
1	A	1431	SER
1	A	1457	ILE
1	A	1776	SER
1	A	1779	THR
1	A	1819	LEU
1	A	1820	THR
1	A	2239	ASP
1	A	2280	THR
1	A	2507	GLN
1	A	2543	ASN
1	A	2575	MET
1	A	2579	LEU
1	A	2584	LEU
1	A	2600	LEU
1	A	2609	GLU
1	A	2670	LEU
1	A	2709	GLN
1	A	2738	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	ASN
1	B	405	GLN
1	B	411	HIS
1	B	486	GLN

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Mol	Chain	Res	Type
1	B	513	ASN
1	B	794	GLN
1	B	806	GLN
1	B	816	ASN
1	B	890	GLN
1	B	1290	HIS
1	B	1326	GLN
1	B	1374	GLN
1	B	1852	GLN
1	B	1869	ASN
1	B	2107	ASN
1	B	2110	ASN
1	B	2697	ASN
1	A	50	GLN
1	A	469	GLN
1	A	780	GLN
1	A	1350	ASN
1	A	1374	GLN
1	A	1962	ASN
1	A	2058	GLN
1	A	2641	HIS

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

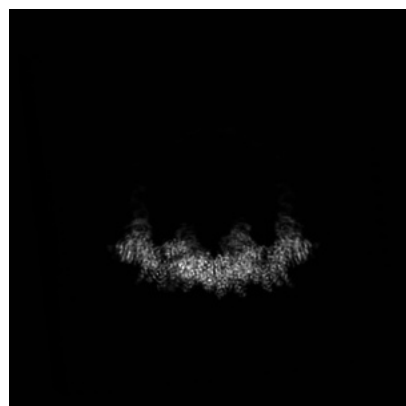
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16087. These allow visual inspection of the internal detail of the map and identification of artifacts.

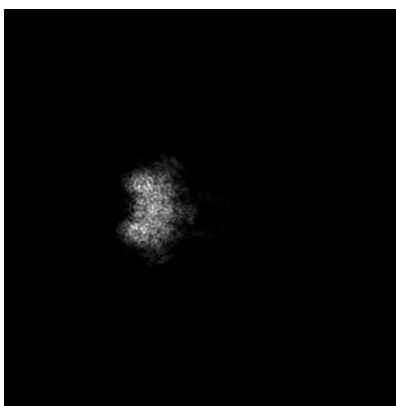
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

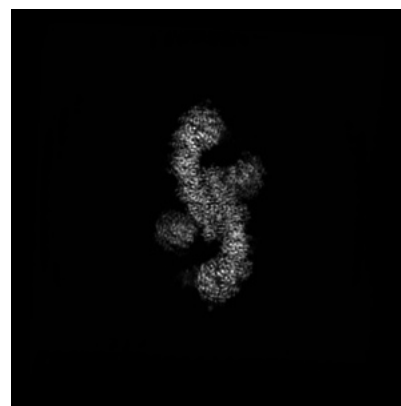
6.1.1 Primary map



X

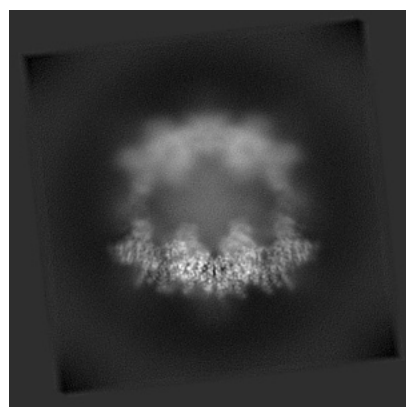


Y

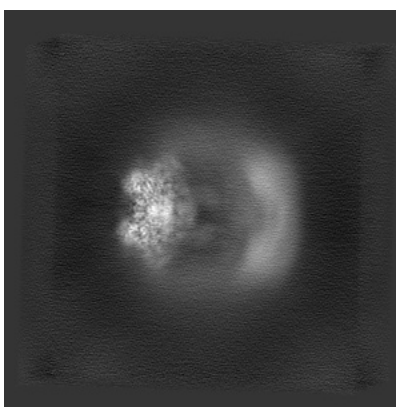


Z

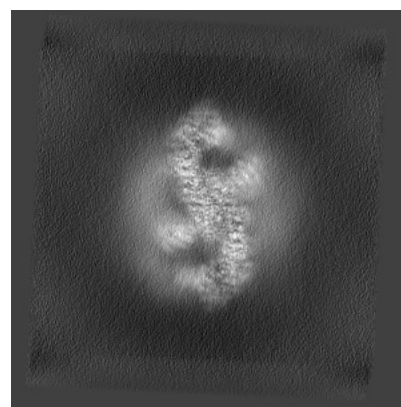
6.1.2 Raw map



X



Y

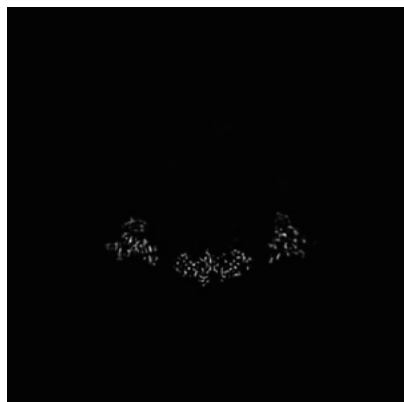


Z

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

6.2 Central slices [i](#)

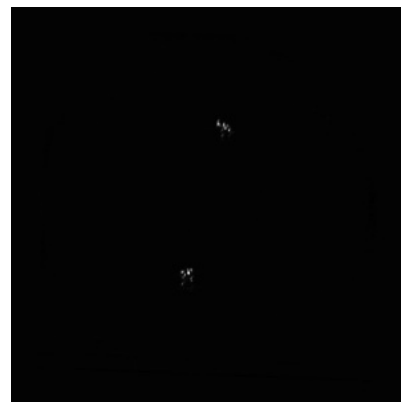
6.2.1 Primary map



X Index: 150

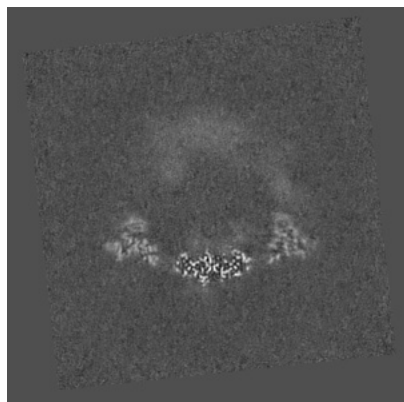


Y Index: 150

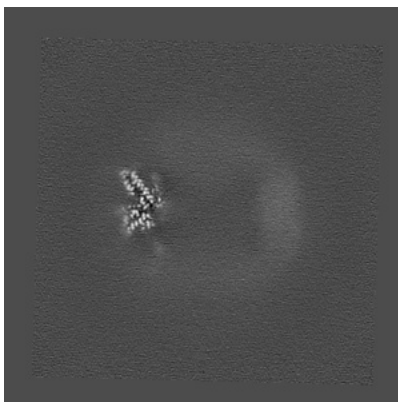


Z Index: 150

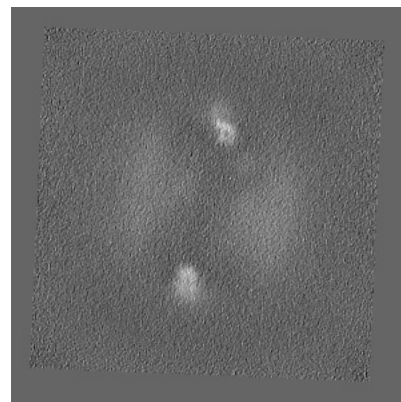
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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: 135

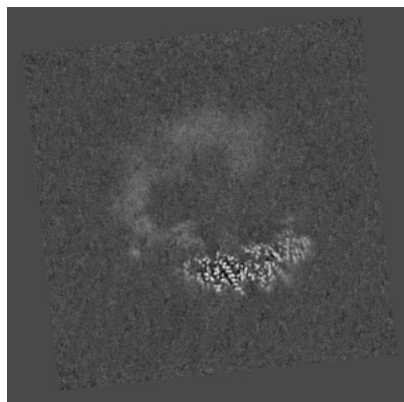


Y Index: 172

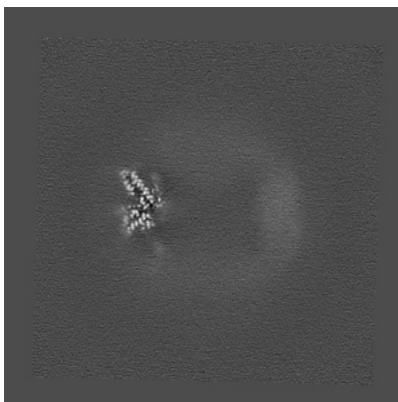


Z Index: 107

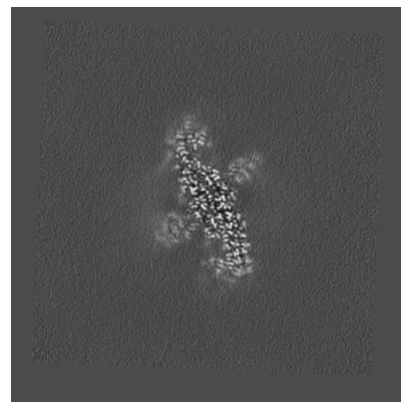
6.3.2 Raw map



X Index: 137



Y Index: 150

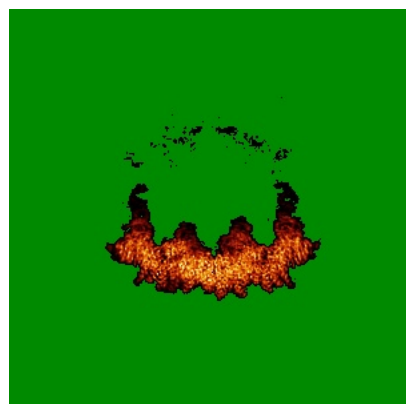


Z Index: 107

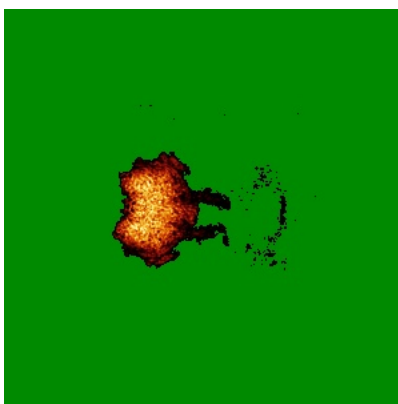
The images above show the largest variance slices of the map in three orthogonal directions.

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

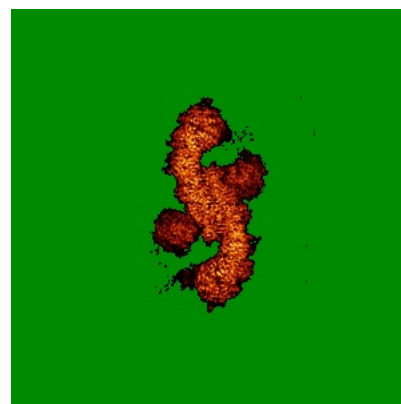
6.4.1 Primary map



X

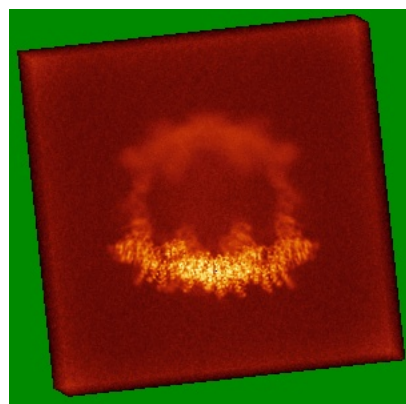


Y

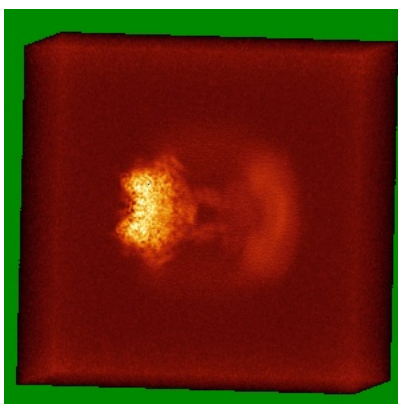


Z

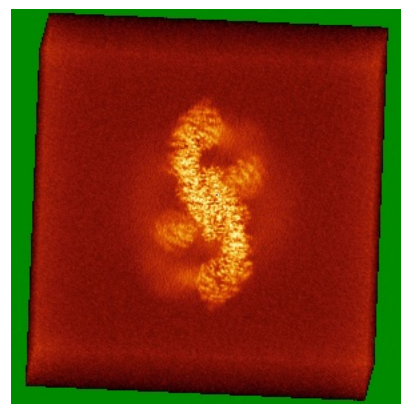
6.4.2 Raw map



X



Y

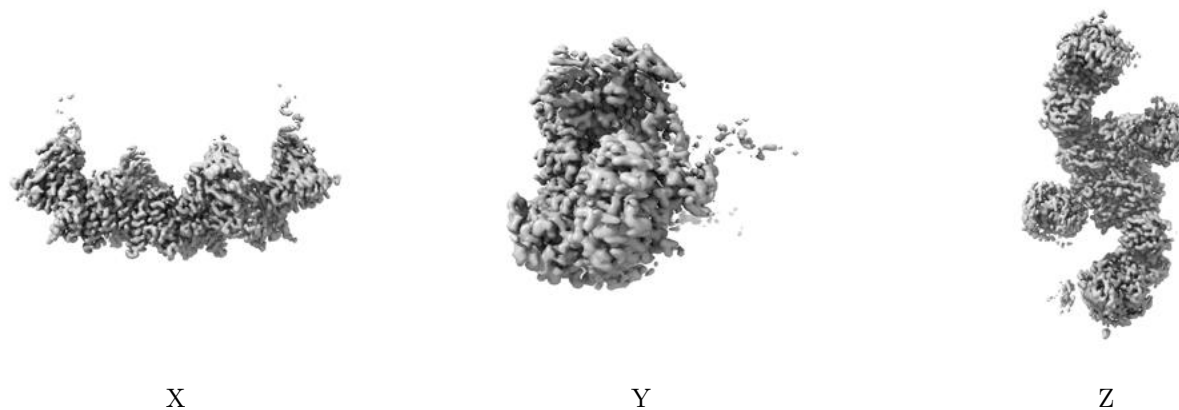


Z

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.

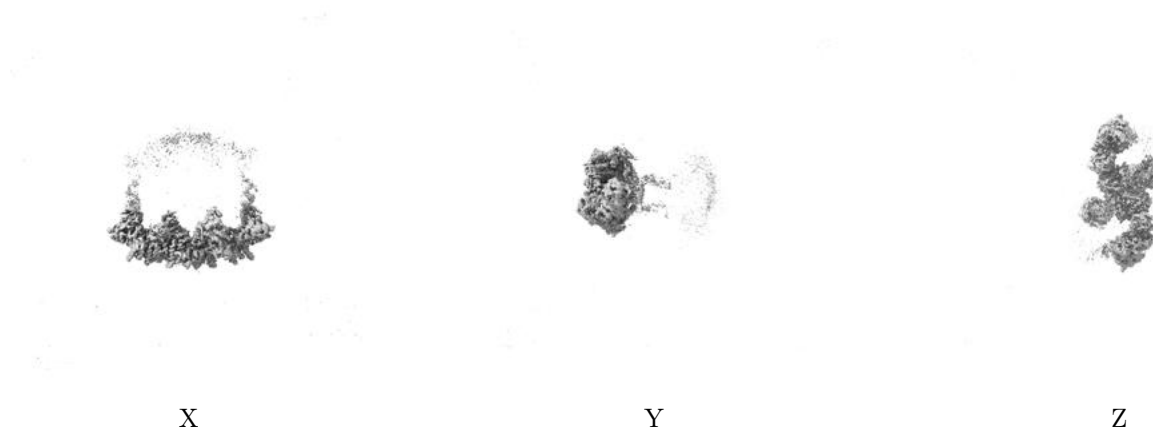
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0632. 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.

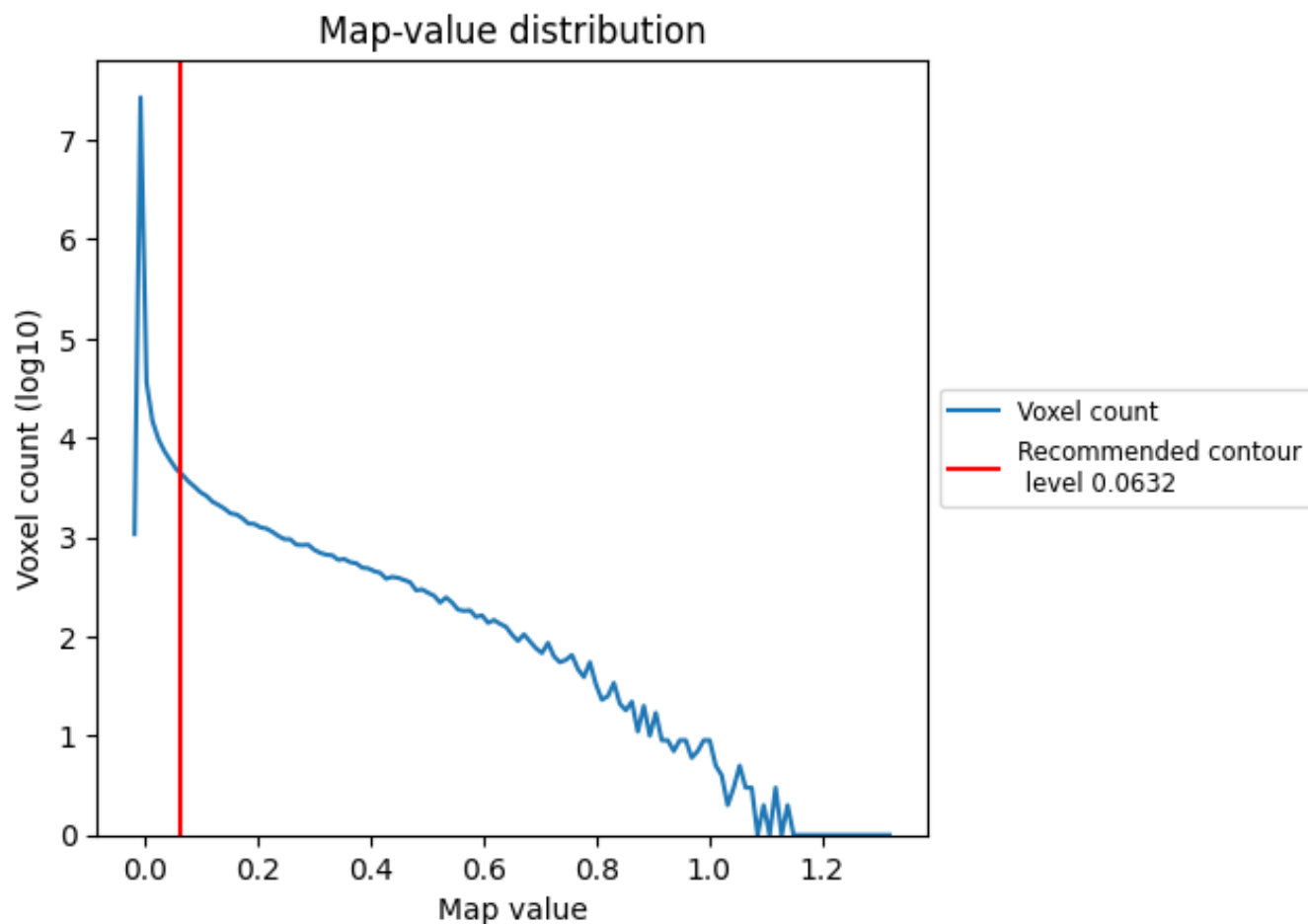
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

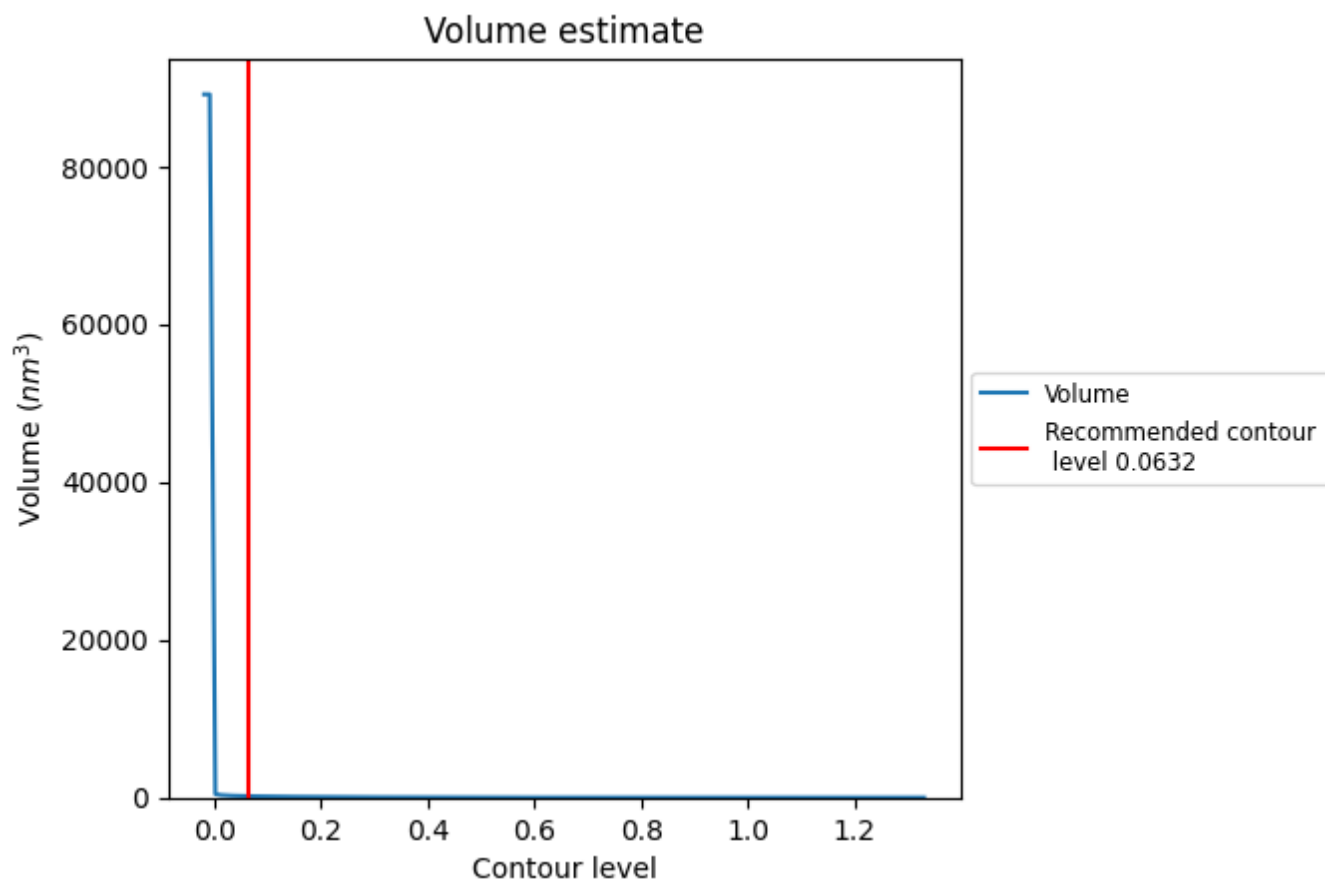
This section contains the results of statistical analysis of the map.

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.

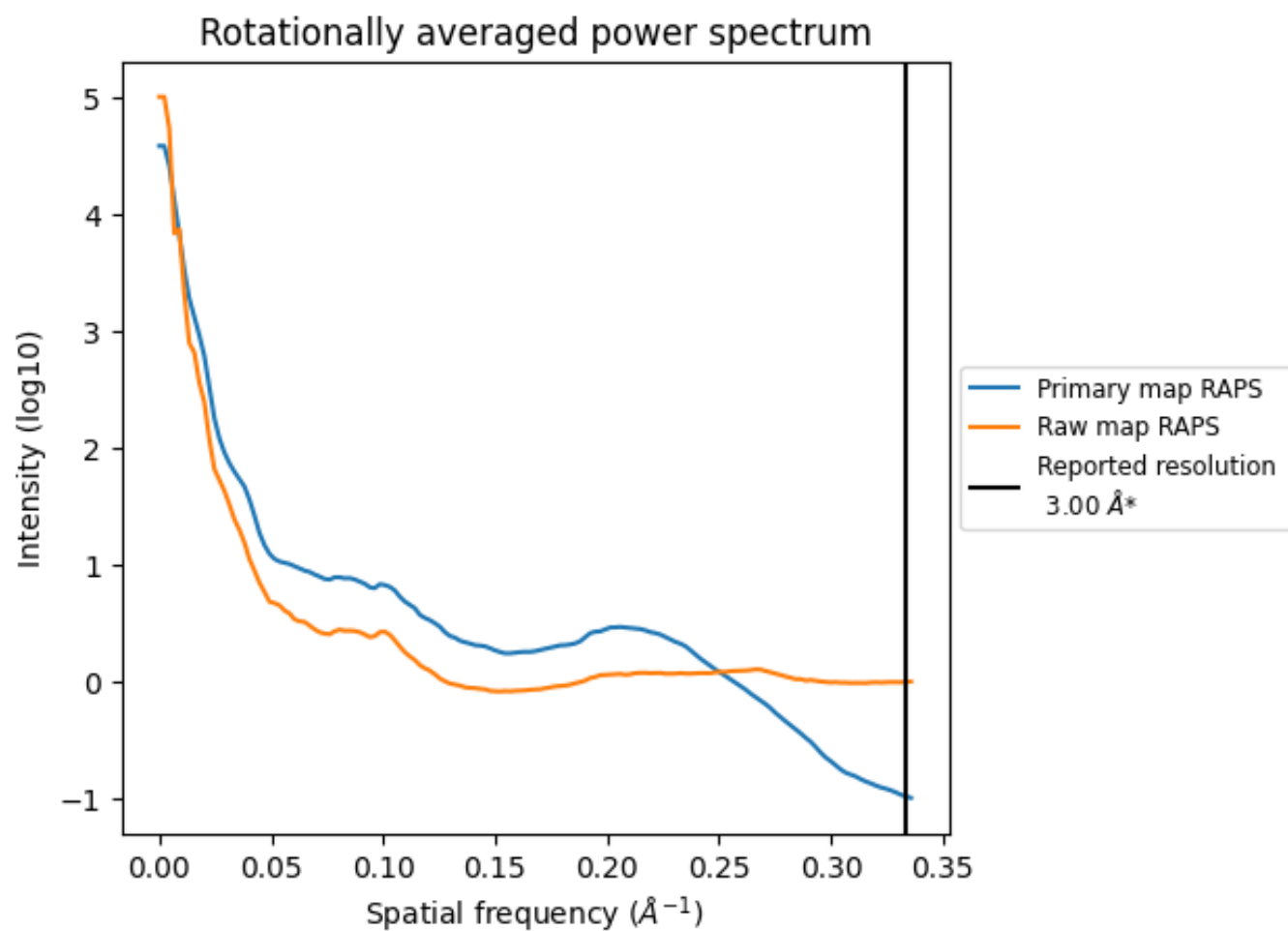
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 162 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 ⓘ

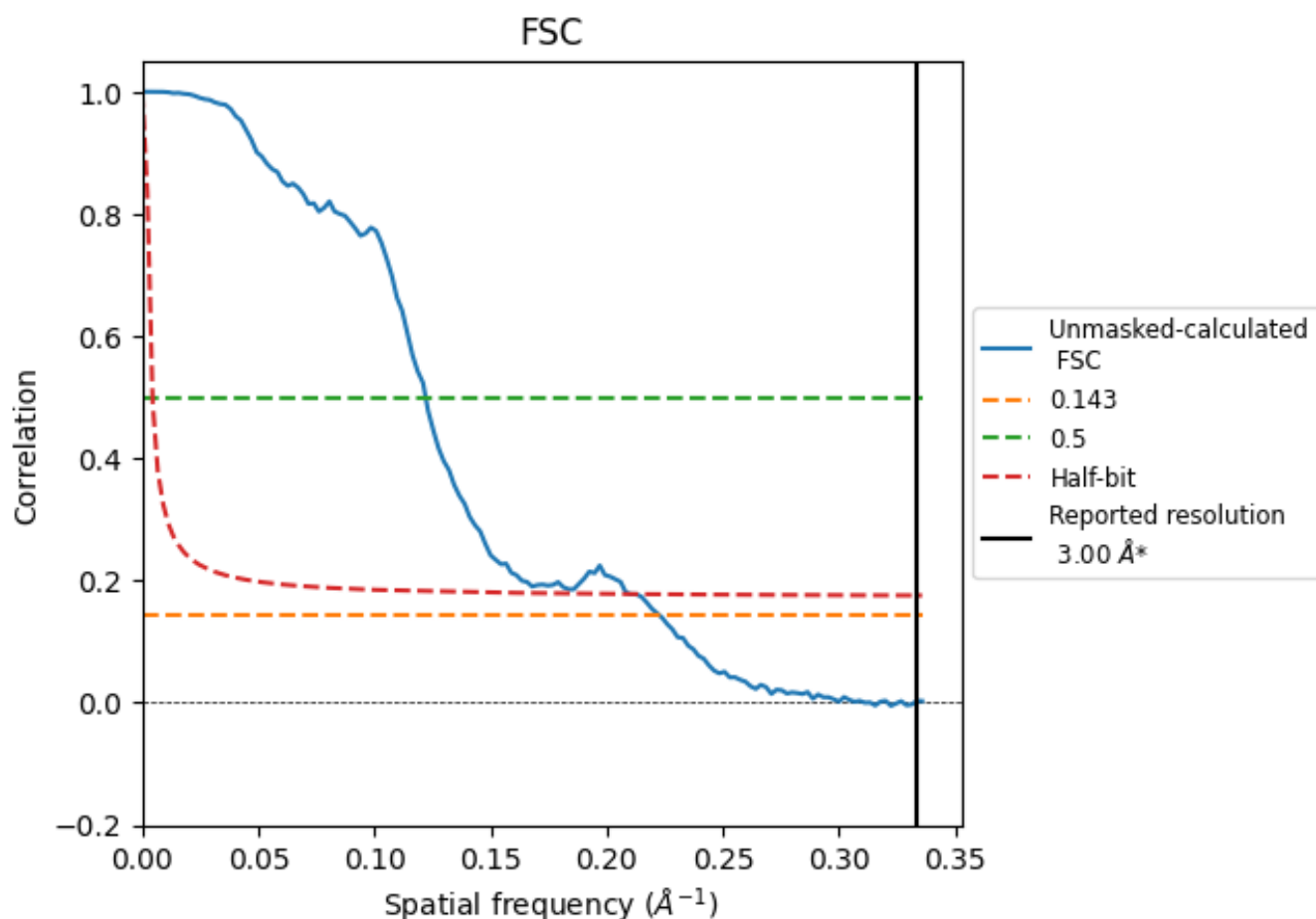


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

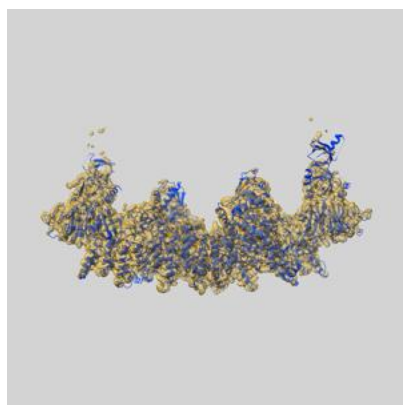
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.00	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	8.20	4.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 8.20 differs from the reported value 3.0 by more than 10 %

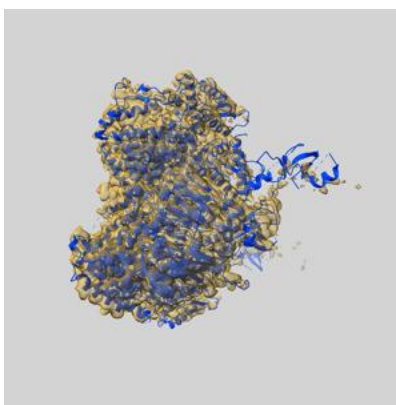
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16087 and PDB model 8BJA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

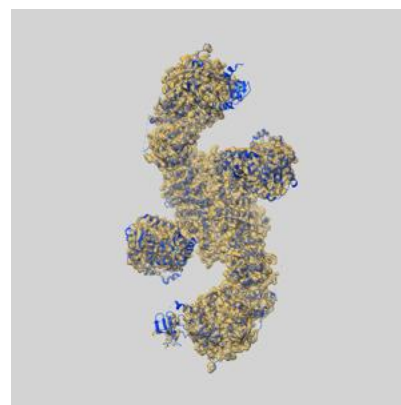
9.1 Map-model overlay [i](#)



X



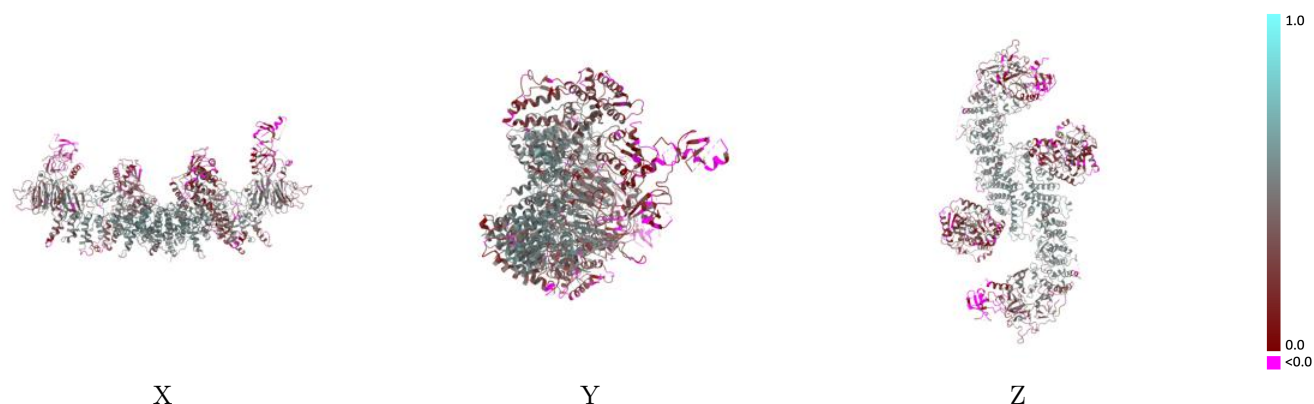
Y



Z

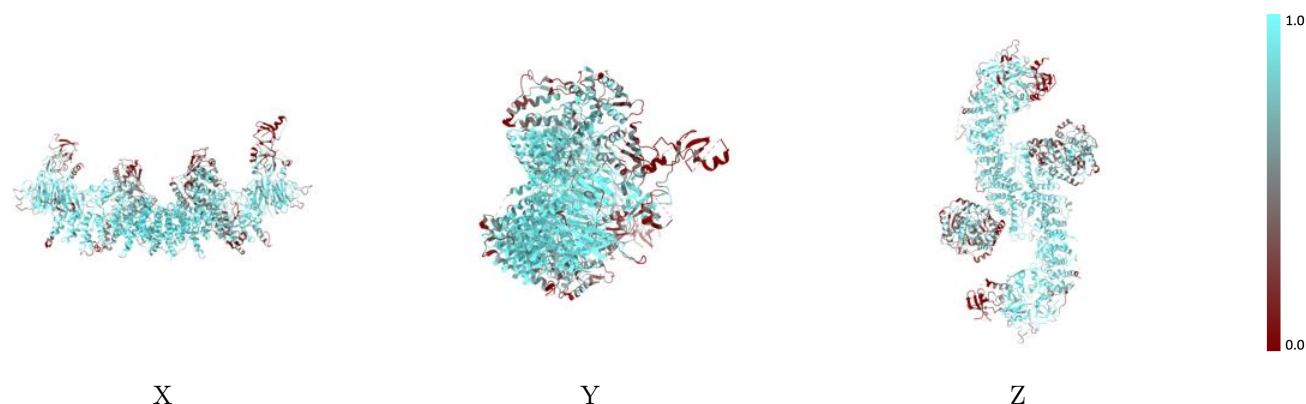
The images above show the 3D surface view of the map at the recommended contour level 0.0632 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



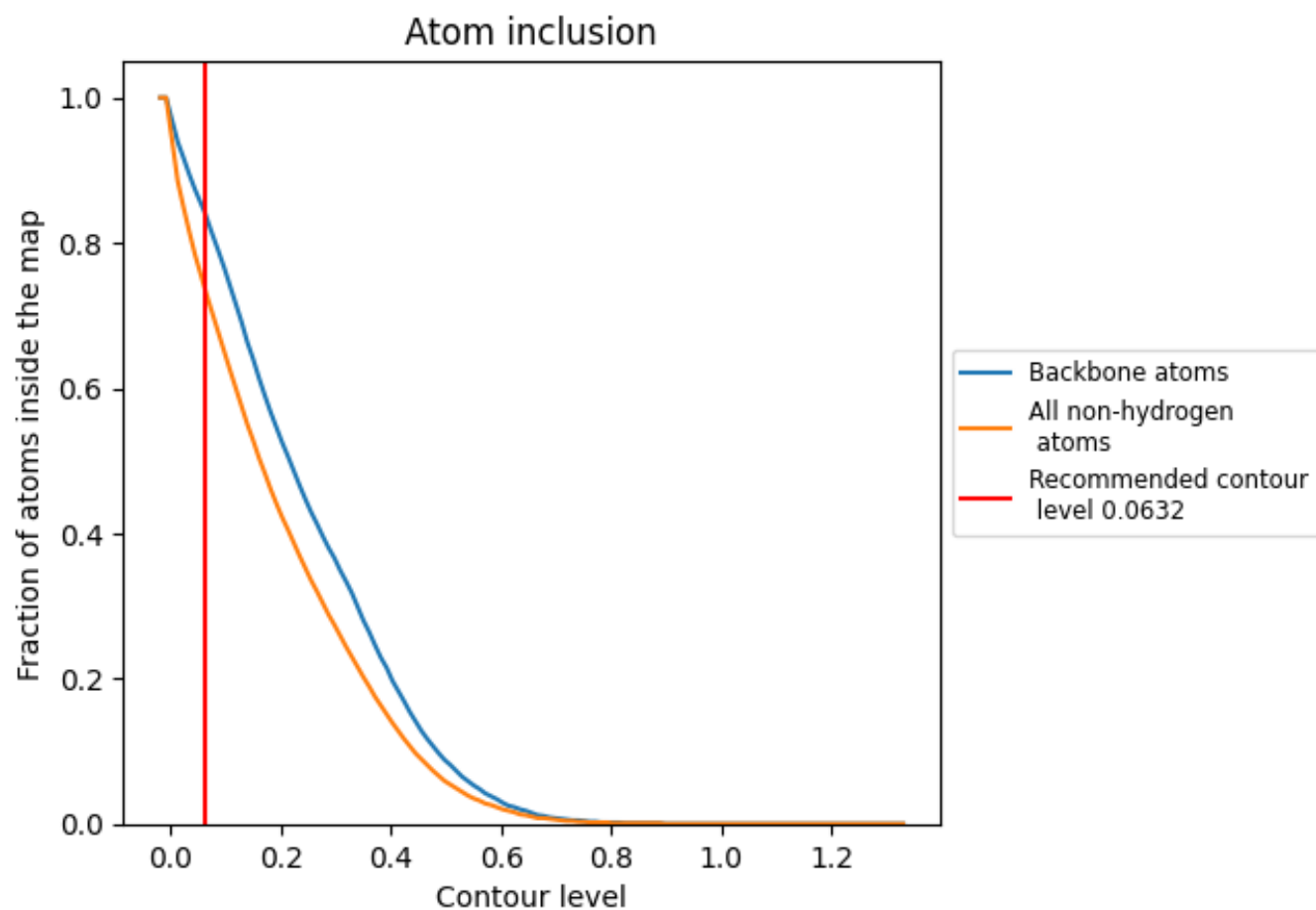
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0632).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0632) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.3630
A	0.7500	0.3700
B	0.7200	0.3570

