



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 6XNX / pdb_00006xnx
EMDB ID : EMD-22272
Title : Structure of RAG1 (R848M/E649V)-RAG2-DNA Strand Transfer Complex
(Dynamic-Form)
Authors : Zhang, Y.; Corbett, E.; Wu, S.; Schatz, D.G.
Deposited on : 2020-07-05
Resolution : 2.70 Å(reported)
Based on initial model : 5ZDZ

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

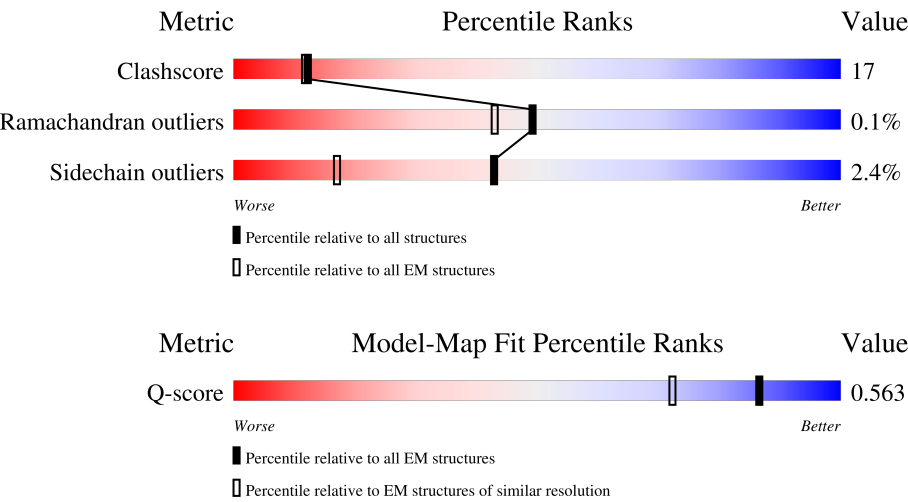
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	750	
1	C	750	
2	B	363	
2	D	363	

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Mol	Chain	Length	Quality of chain
3	x	55	15%22%36%42%
4	y	66	8%9%33%58%
5	I	16	31%31%56%12%
5	J	16	31%25%62%12%
6	L	45	16%11%73%
7	M	34	26%21%53%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16540 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	549	Total	C	N	O	S	0	0
			4407	2781	770	823	33		
1	C	548	Total	C	N	O	S	0	0
			4401	2778	769	821	33		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	GLY	-	expression tag	UNP P15919
A	260	PRO	-	expression tag	UNP P15919
A	649	VAL	GLU	engineered mutation	UNP P15919
A	848	MET	ARG	engineered mutation	UNP P15919
C	259	GLY	-	expression tag	UNP P15919
C	260	PRO	-	expression tag	UNP P15919
C	649	VAL	GLU	engineered mutation	UNP P15919
C	848	MET	ARG	engineered mutation	UNP P15919

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	342	Total	C	N	O	S	0	0
			2678	1712	454	492	20		
2	D	343	Total	C	N	O	S	0	0
			2688	1718	456	494	20		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P21784
B	0	PRO	-	expression tag	UNP P21784
B	1	MET	-	expression tag	UNP P21784
B	2	ALA	-	expression tag	UNP P21784
D	-1	GLY	-	expression tag	UNP P21784

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP P21784
D	1	MET	-	expression tag	UNP P21784
D	2	ALA	-	expression tag	UNP P21784

- Molecule 3 is a DNA chain called 12RSS integration strand DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	x	32	Total	C	N	O	P	0	0
			644	308	112	193	31		

- Molecule 4 is a DNA chain called 23RSS integration strand DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	28	Total	C	N	O	P	0	0
			564	270	99	168	27		

- Molecule 5 is a DNA chain called Flanking DNA top strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	14	Total	C	N	O	P	0	0
			288	137	58	80	13		
5	J	14	Total	C	N	O	P	0	0
			288	137	58	80	13		

- Molecule 6 is a DNA chain called 23RSS signal top strand DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	12	Total	C	N	O	P	0	0
			246	118	47	70	11		

- Molecule 7 is a DNA chain called 12RSS signal top strand DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	16	Total	C	N	O	P	0	0
			330	157	65	93	15		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

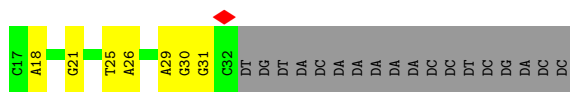
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total 2	Mg 2	0
8	C	1	Total 1	Mg 1	0
8	x	1	Total 1	Mg 1	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total 1	Zn 1	0
9	C	1	Total 1	Zn 1	0







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	106374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	256.19998, 256.19998, 256.19998	wwPDB
Map dimensions	244, 244, 244	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, MG

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	0.59	0/4504	0.47	2/6074 (0.0%)
1	C	0.59	1/4498 (0.0%)	0.45	0/6067
2	B	0.53	0/2745	0.44	0/3718
2	D	0.53	0/2755	0.45	0/3730
3	x	0.44	0/718	0.63	0/1102
4	y	0.45	0/629	0.61	0/965
5	I	0.35	0/324	0.38	0/499
5	J	0.36	0/324	0.38	0/499
6	L	0.55	0/276	0.46	0/425
7	M	0.54	0/371	0.46	0/572
All	All	0.55	1/17144 (0.0%)	0.47	2/23651 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	657	LEU	CA-CB	-5.01	1.46	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	ASP	CB-CA-C	-6.24	101.36	110.96
1	A	773	ARG	CG-CD-NE	-5.78	99.28	112.00

There are no chirality outliers.

There are no planarity outliers.

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	4407	0	4363	168	0
1	C	4401	0	4358	172	0
2	B	2678	0	2643	88	0
2	D	2688	0	2656	106	0
3	x	644	0	363	20	0
4	y	564	0	318	19	0
5	I	288	0	158	7	0
5	J	288	0	157	11	0
6	L	246	0	137	5	0
7	M	330	0	181	6	0
8	A	2	0	0	0	0
8	C	1	0	0	0	0
8	x	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
All	All	16540	0	15334	544	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 17.

All (544) 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:470:ILE:O	1:A:474:THR:HG23	1.70	0.90
2:B:152:MET:HG2	2:B:240:LEU:HD21	1.60	0.83
1:A:804:PHE:CD1	1:A:858:MET:HE1	2.14	0.83
2:D:212:ARG:NH1	2:D:213:ASN:OD1	2.13	0.81
1:C:470:ILE:O	1:C:474:THR:HG23	1.83	0.77
2:D:117:ASN:O	2:D:117:ASN:OD1	2.02	0.77
1:A:656:CYS:HB2	1:A:675:LEU:HD11	1.66	0.76
1:A:804:PHE:CG	1:A:858:MET:HE1	2.19	0.76
2:B:186:ASP:O	2:B:190:GLY:N	2.19	0.75
1:A:600:ASP:OD2	1:A:965:ASN:ND2	2.20	0.74
1:C:523:LEU:HD12	1:C:560:ASP:OD1	1.88	0.74
1:C:773:ARG:NH2	4:y:46:DC:OP1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:MET:HE1	2:D:110:MET:SD	2.28	0.74
2:B:6:VAL:HG21	2:B:347:THR:HG23	1.70	0.73
2:D:219:LEU:HD22	2:D:273:ILE:CD1	2.19	0.73
2:D:27:GLN:NE2	2:D:49:ASP:OD2	2.22	0.72
1:A:546:ASP:OD2	2:B:229:ARG:NH1	2.22	0.72
2:D:72:LEU:HD13	2:D:95:GLY:O	1.90	0.72
1:C:525:ASN:ND2	2:D:164:SER:O	2.23	0.72
1:C:656:CYS:HB2	1:C:675:LEU:HD11	1.72	0.71
1:A:664:ASP:OD1	2:B:34:LYS:NZ	2.23	0.71
2:D:146:TYR:N	2:D:213:ASN:O	2.24	0.71
1:A:556:ARG:NH2	2:B:169:THR:O	2.23	0.70
2:B:186:ASP:OD2	2:B:189:PHE:N	2.24	0.70
1:C:730:CYS:SG	1:C:937:HIS:CE1	2.84	0.70
1:C:949:ARG:NE	1:C:950:ASP:OD1	2.25	0.69
1:A:466:VAL:HG23	1:A:1002:PHE:HB3	1.75	0.69
1:A:713:ARG:NH2	1:A:725:TYR:O	2.25	0.69
1:C:840:ARG:NH1	1:C:868:GLU:OE1	2.26	0.69
2:D:63:SER:N	2:D:122:PHE:O	2.24	0.69
1:A:597:GLU:OE2	1:A:679:ARG:NE	2.26	0.69
1:C:694:ILE:HB	1:C:696:ARG:HH12	1.57	0.69
1:A:713:ARG:NE	1:A:719:GLU:O	2.24	0.68
1:A:670:ALA:O	2:B:173:ASN:ND2	2.24	0.68
1:C:570:MET:HE1	1:C:626:VAL:HG11	1.74	0.68
1:A:748:ARG:NH2	1:A:777:LYS:O	2.27	0.68
1:A:724:VAL:HG22	1:A:773:ARG:NH1	2.09	0.68
1:C:767:GLU:OE2	1:C:775:ARG:NE	2.26	0.67
2:D:23:ASN:O	2:D:89:HIS:NE2	2.27	0.67
2:D:116:ASN:O	2:D:119:LYS:N	2.27	0.67
2:D:14:LEU:HD22	2:D:33:GLN:HE21	1.58	0.67
1:C:797:ASP:OD2	1:C:894:ARG:NE	2.23	0.67
1:A:517:PHE:CG	1:A:564:VAL:HG21	2.30	0.67
4:y:32:DT:H2'	4:y:33:DG:C8	2.30	0.66
1:A:822:SER:O	1:A:824:GLU:N	2.29	0.66
2:B:340:SER:OG	2:B:341:GLU:OE1	2.13	0.66
2:B:25:ASP:OD2	2:B:115:LYS:NZ	2.24	0.66
2:B:182:VAL:HG21	2:B:247:VAL:HG11	1.76	0.66
1:A:974:MET:HE1	1:C:974:MET:HE1	1.77	0.66
1:C:670:ALA:O	2:D:173:ASN:ND2	2.24	0.65
2:B:177:ASP:OD2	2:B:224:LEU:N	2.27	0.65
1:C:569:ASP:OD2	1:C:997:LYS:N	2.30	0.65
1:A:740:ASN:ND2	1:A:743:PHE:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:y:41:DG:H3'	4:y:42:DT:H71	1.79	0.64
2:D:107:ILE:HD12	2:D:129:LEU:HD21	1.79	0.64
1:C:972:ARG:NE	1:C:983:GLU:OE2	2.28	0.64
1:C:773:ARG:O	1:C:777:LYS:N	2.29	0.64
1:A:488:VAL:CG1	1:A:496:ILE:HD12	2.27	0.64
2:D:317:TRP:HE3	2:D:329:LEU:HD21	1.63	0.64
2:D:204:LEU:HD22	2:D:221:GLY:HA3	1.78	0.64
2:D:117:ASN:HD22	5:J:6:DG:H4'	1.63	0.63
2:B:76:ALA:HB1	2:B:142:ILE:H	1.62	0.63
1:A:789:PRO:O	1:A:949:ARG:NH2	2.31	0.63
1:A:918:GLU:O	1:A:922:THR:HG23	1.99	0.63
1:A:547:GLU:OE2	2:B:159:ARG:NE	2.32	0.63
2:B:150:LYS:HB3	2:B:240:LEU:HD23	1.80	0.63
1:C:597:GLU:OE1	1:C:679:ARG:NE	2.30	0.63
1:A:552:THR:OG1	1:A:667:THR:HG21	1.99	0.62
1:C:657:LEU:HG	1:C:988:LEU:HD13	1.80	0.62
1:C:470:ILE:O	1:C:474:THR:CG2	2.46	0.62
1:C:621:ARG:NH1	1:C:961:ASN:O	2.32	0.62
1:A:849:MET:HE1	1:A:853:PHE:CD1	2.34	0.62
2:D:159:ARG:NE	2:D:205:SER:OG	2.33	0.62
2:D:117:ASN:ND2	5:J:6:DG:O3'	2.33	0.62
1:C:729:LEU:HD21	1:C:946:ILE:HD11	1.82	0.62
1:C:600:ASP:OD2	1:C:965:ASN:ND2	2.32	0.62
2:D:285:MET:HE3	2:D:307:TRP:CD1	2.35	0.61
1:A:621:ARG:NH1	1:A:961:ASN:O	2.32	0.61
1:A:676:ILE:HG21	1:A:784:PHE:O	2.01	0.61
1:A:590:PRO:HA	1:A:697:THR:HG23	1.82	0.61
1:C:804:PHE:CB	1:C:858:MET:HE1	2.31	0.61
1:A:730:CYS:SG	1:A:937:HIS:CE1	2.92	0.61
1:C:591:PHE:HE1	1:C:696:ARG:HG2	1.66	0.61
1:A:501:HIS:NE2	3:x:35:DA:OP2	2.31	0.61
1:A:735:LEU:HD12	1:A:930:GLY:HA2	1.82	0.60
2:D:138:TYR:O	2:D:159:ARG:N	2.32	0.60
2:D:285:MET:HE1	2:D:311:ILE:HG22	1.83	0.60
1:A:666:GLU:OE1	2:B:73:ARG:NE	2.33	0.60
1:A:669:THR:HG21	2:B:100:ASN:HA	1.83	0.60
2:B:274:VAL:HG21	2:B:327:ILE:HD13	1.82	0.60
2:D:80:TYR:HA	2:D:144:VAL:HG11	1.84	0.60
1:A:949:ARG:NH1	1:A:950:ASP:OD1	2.35	0.59
2:D:317:TRP:CE3	2:D:329:LEU:HD21	2.37	0.59
2:B:300:SER:OG	2:B:301:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:VAL:HG21	1:C:909:TYR:HD2	1.67	0.59
1:A:1002:PHE:O	1:C:487:THR:HG23	2.03	0.59
1:C:553:ILE:HD12	1:C:615:VAL:HG11	1.85	0.59
1:C:870:ILE:O	1:C:876:HIS:NE2	2.33	0.59
1:A:534:ILE:HG23	1:A:988:LEU:HD23	1.85	0.59
2:B:212:ARG:HB2	2:B:292:LEU:HD23	1.85	0.59
1:C:529:ARG:NH2	1:C:531:ASP:OD2	2.36	0.59
1:C:715:VAL:O	1:C:784:PHE:N	2.33	0.59
3:x:43:DT:H2'	3:x:44:DG:C8	2.37	0.59
1:A:569:ASP:OD2	1:A:997:LYS:N	2.32	0.58
1:A:615:VAL:HG21	1:A:659:LEU:HD23	1.84	0.58
2:D:285:MET:HE3	2:D:307:TRP:CG	2.38	0.58
1:A:972:ARG:NE	1:A:983:GLU:OE1	2.37	0.58
2:D:14:LEU:HD22	2:D:33:GLN:NE2	2.17	0.58
1:A:588:ASN:O	1:A:697:THR:HG22	2.03	0.58
1:A:591:PHE:CZ	1:A:631:ILE:HD12	2.38	0.58
1:C:875:ARG:NH2	1:C:923:LYS:O	2.36	0.58
2:D:275:GLY:HA2	2:D:317:TRP:CZ2	2.38	0.58
1:A:470:ILE:O	1:A:474:THR:CG2	2.48	0.58
1:C:591:PHE:CE1	1:C:696:ARG:HG2	2.38	0.58
2:D:20:SER:HB2	2:D:77:THR:HG21	1.84	0.57
1:A:875:ARG:NH2	1:A:923:LYS:O	2.34	0.57
2:D:283:LYS:HB2	2:D:317:TRP:NE1	2.18	0.57
1:A:727:CYS:SG	1:A:937:HIS:CD2	2.97	0.57
1:C:731:ASP:OD1	1:C:747:THR:OG1	2.21	0.57
2:D:285:MET:HE2	2:D:312:LYS:HA	1.87	0.57
2:D:148:ARG:NH2	2:D:239:ASP:OD1	2.38	0.57
1:A:568:MET:HG2	1:A:689:LEU:HD21	1.87	0.57
1:A:584:ASP:N	1:A:584:ASP:OD1	2.36	0.57
2:D:186:ASP:N	2:D:191:CYS:O	2.35	0.57
2:B:283:LYS:HD2	2:B:317:TRP:CD1	2.40	0.56
1:A:991:HIS:O	1:A:991:HIS:ND1	2.38	0.56
1:C:627:MET:HE1	1:C:955:ALA:HB1	1.87	0.56
2:D:283:LYS:HB2	2:D:317:TRP:HE1	1.70	0.56
2:B:27:GLN:NE2	2:B:49:ASP:OD1	2.37	0.56
2:D:223:SER:O	2:D:227:ASN:N	2.38	0.56
1:C:602:MET:HE1	1:C:968:PHE:CD1	2.40	0.56
2:D:273:ILE:HD12	2:D:290:VAL:HG21	1.88	0.56
1:A:852:ASN:OD1	1:A:855:ARG:NH1	2.38	0.56
2:B:43:THR:HG23	2:B:45:VAL:H	1.71	0.55
1:C:719:GLU:OE1	1:C:773:ARG:NE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:808:PHE:HE1	1:C:879:LEU:HD22	1.70	0.55
2:D:274:VAL:HG11	2:D:327:ILE:HG13	1.87	0.55
2:D:300:SER:OG	2:D:301:GLU:N	2.39	0.55
1:A:657:LEU:HG	1:A:988:LEU:HD13	1.89	0.55
1:C:774:ASP:O	1:C:777:LYS:NZ	2.26	0.55
1:C:891:PRO:O	1:C:895:SER:OG	2.23	0.55
1:A:750:HIS:NE2	1:A:754:LEU:HD11	2.22	0.54
1:A:852:ASN:ND2	4:y:33:DG:O6	2.33	0.54
2:D:6:VAL:HG21	2:D:347:THR:HG23	1.88	0.54
2:D:159:ARG:HD2	2:D:224:LEU:HD11	1.88	0.54
4:y:42:DT:H2'	4:y:43:DA:C8	2.42	0.54
1:A:656:CYS:CB	1:A:675:LEU:HD11	2.37	0.54
4:y:35:DG:H3'	4:y:36:DC:H5'	1.88	0.54
1:C:602:MET:HE1	1:C:968:PHE:HD1	1.71	0.54
1:A:715:VAL:HG12	1:A:784:PHE:CE1	2.42	0.54
2:B:28:VAL:HG13	2:B:48:PHE:HB3	1.89	0.54
1:A:591:PHE:CE1	1:A:696:ARG:HG3	2.42	0.54
1:C:807:ILE:HD11	1:C:928:TYR:OH	2.07	0.54
1:A:594:VAL:HG12	1:A:956:TRP:HH2	1.73	0.53
1:A:654:PRO:HB2	1:A:988:LEU:HD12	1.90	0.53
1:C:563:LEU:HD12	1:C:700:PHE:CE1	2.42	0.53
1:C:804:PHE:HB3	1:C:858:MET:HE1	1.91	0.53
2:D:78:CYS:HB3	2:D:142:ILE:HG23	1.89	0.53
1:A:909:TYR:OH	1:A:939:THR:O	2.20	0.53
1:C:603:GLY:O	1:C:969:ARG:NH2	2.28	0.53
1:C:615:VAL:HG21	1:C:659:LEU:HD23	1.89	0.53
2:D:334:ASP:OD1	2:D:335:ASN:N	2.41	0.53
1:A:678:GLU:HG3	2:B:169:THR:HG21	1.90	0.53
1:A:972:ARG:O	1:A:978:GLN:NE2	2.34	0.53
1:C:806:LYS:O	1:C:810:LEU:HG	2.08	0.53
1:A:636:GLN:OE1	1:A:636:GLN:N	2.41	0.53
2:B:321:ASN:OD1	2:B:323:GLY:N	2.42	0.53
2:B:76:ALA:HB2	2:B:140:HIS:CD2	2.43	0.53
1:C:600:ASP:OD1	1:C:961:ASN:ND2	2.42	0.53
1:C:805:TYR:OH	1:C:834:ASP:OD1	2.25	0.53
2:D:63:SER:OG	2:D:64:LYS:N	2.42	0.53
3:x:52:DG:H3'	3:x:53:DT:H71	1.90	0.53
1:A:483:LYS:HZ2	7:M:21:DG:P	2.32	0.52
3:x:33:DC:C6	3:x:34:DT:H72	2.43	0.52
1:C:666:GLU:OE2	2:D:35:GLY:N	2.37	0.52
1:A:517:PHE:CD1	1:A:564:VAL:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:PHE:O	1:C:699:LYS:N	2.42	0.52
2:D:207:HIS:ND1	2:D:218:ILE:HG23	2.24	0.52
1:C:729:LEU:CD2	1:C:946:ILE:HD11	2.39	0.52
1:C:669:THR:HG21	2:D:100:ASN:HA	1.91	0.52
1:A:495:GLN:NE2	3:x:35:DA:OP1	2.39	0.52
1:A:808:PHE:HE1	1:A:879:LEU:HD22	1.74	0.52
2:D:98:THR:O	2:D:101:ASN:N	2.41	0.52
1:A:858:MET:HE3	1:A:886:TYR:CE2	2.45	0.52
1:C:532:VAL:HG21	2:D:170:GLU:OE2	2.10	0.52
1:C:740:ASN:ND2	1:C:743:PHE:O	2.42	0.52
1:A:591:PHE:O	1:A:699:LYS:N	2.43	0.52
1:C:724:VAL:O	1:C:734:ARG:N	2.39	0.52
1:A:547:GLU:OE1	2:B:138:TYR:OH	2.21	0.52
1:A:734:ARG:NH2	1:A:934:ASN:OD1	2.35	0.52
1:A:806:LYS:O	1:A:810:LEU:HG	2.09	0.52
2:B:182:VAL:HG23	2:B:182:VAL:O	2.09	0.52
1:C:650:LEU:HD23	1:C:994:TYR:CE2	2.45	0.51
1:A:563:LEU:HD12	1:A:682:MET:SD	2.49	0.51
1:A:754:LEU:HD23	1:A:783:PRO:HD2	1.92	0.51
1:A:715:VAL:HG12	1:A:784:PHE:HE1	1.75	0.51
2:B:78:CYS:HB3	2:B:142:ILE:HG23	1.92	0.51
2:B:143:ASP:HB3	2:B:211:ALA:HB2	1.93	0.51
1:C:720:ALA:HB3	4:y:45:DC:H5''	1.92	0.51
1:C:830:GLN:O	1:C:834:ASP:OD2	2.29	0.51
1:A:870:ILE:O	1:A:876:HIS:NE2	2.38	0.51
1:A:567:LEU:O	1:A:571:GLU:N	2.44	0.51
1:A:627:MET:HE1	1:A:955:ALA:HB1	1.92	0.51
1:C:488:VAL:CG1	1:C:496:ILE:HD13	2.41	0.51
1:C:571:GLU:OE2	1:C:692:GLY:N	2.39	0.51
2:D:98:THR:HG22	2:D:100:ASN:H	1.75	0.51
1:A:815:VAL:HG13	1:A:819:PRO:HA	1.92	0.51
1:A:848:MET:HE2	3:x:52:DG:C2	2.46	0.51
1:C:557:PHE:CE2	1:C:988:LEU:HG	2.46	0.51
2:B:284:ARG:NH2	2:B:288:SER:OG	2.42	0.50
1:C:563:LEU:HD23	1:C:682:MET:HE1	1.93	0.50
3:x:63:DC:H2'	3:x:64:DT:H71	1.93	0.50
2:B:107:ILE:HD12	2:B:129:LEU:HD21	1.93	0.50
1:C:602:MET:HE3	1:C:965:ASN:HB3	1.94	0.50
1:C:793:ALA:HB1	1:C:894:ARG:HD3	1.93	0.50
1:A:537:GLY:N	1:A:554:ALA:O	2.38	0.50
1:A:807:ILE:HD11	1:A:928:TYR:OH	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:810:LEU:HD22	1:C:815:VAL:HG21	1.93	0.50
2:D:277:TYR:HA	2:D:283:LYS:HA	1.93	0.50
1:C:510:LEU:HD11	1:C:999:LEU:HD21	1.94	0.50
1:C:679:ARG:NH1	1:C:786:GLU:OE1	2.43	0.50
2:D:285:MET:O	2:D:307:TRP:NE1	2.35	0.50
1:A:473:ASN:O	1:C:483:LYS:NZ	2.44	0.50
2:B:322:MET:HB2	2:B:326:THR:HG23	1.92	0.50
2:B:143:ASP:OD2	2:B:209:SER:OG	2.21	0.50
1:C:563:LEU:HD12	1:C:700:PHE:HE1	1.77	0.50
2:D:31:PHE:CZ	2:D:69:LEU:HD11	2.47	0.50
1:A:883:MET:O	1:A:887:LEU:HG	2.12	0.50
1:C:662:GLU:HB2	1:C:711:LEU:HD13	1.94	0.49
2:D:7:THR:O	2:D:55:LEU:N	2.39	0.49
1:A:647:ASN:ND2	1:A:954:GLY:O	2.40	0.49
1:C:517:PHE:CD2	1:C:564:VAL:HG21	2.48	0.49
1:C:771:GLU:OE2	2:D:64:LYS:NZ	2.44	0.49
2:D:105:ASP:OD1	2:D:106:LYS:NZ	2.45	0.49
4:y:53:DT:H2'	4:y:54:DG:C5	2.47	0.49
1:C:472:VAL:HG23	1:C:473:ASN:N	2.27	0.49
2:B:339:MET:HE2	3:x:54:DA:OP1	2.12	0.49
2:D:197:LEU:HD12	2:D:200:LEU:HD12	1.94	0.49
1:A:622:PHE:CD1	1:A:655:LEU:HD23	2.47	0.49
1:A:759:VAL:O	1:A:763:ASN:N	2.42	0.49
2:D:33:GLN:OE1	2:D:44:GLY:HA2	2.12	0.49
1:C:570:MET:HE1	1:C:626:VAL:CG1	2.43	0.49
4:y:29:DC:H2'	4:y:30:DA:C8	2.47	0.49
2:B:98:THR:O	2:B:101:ASN:N	2.42	0.49
1:C:678:GLU:HG3	2:D:169:THR:HG21	1.94	0.49
1:C:691:MET:O	1:C:696:ARG:NH1	2.46	0.49
2:D:141:SER:HB3	2:D:207:HIS:CE1	2.48	0.49
1:A:718:LEU:HD23	1:A:779:VAL:HG22	1.95	0.48
1:A:649:VAL:HG22	1:A:967:LEU:HD12	1.96	0.48
1:A:848:MET:HE1	4:y:36:DC:H4'	1.95	0.48
2:B:129:LEU:HB2	2:B:133:VAL:HG23	1.95	0.48
2:B:163:PRO:O	2:B:167:ARG:N	2.45	0.48
1:A:844:LYS:HE2	1:A:846:ILE:HG22	1.94	0.48
1:C:550:VAL:HG13	1:C:550:VAL:O	2.12	0.48
1:C:620:VAL:HB	1:C:658:MET:HG2	1.95	0.48
1:C:691:MET:HE2	1:C:696:ARG:HD2	1.95	0.48
1:A:534:ILE:HG21	1:A:985:GLU:HG3	1.95	0.48
1:C:672:LEU:O	1:C:675:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:849:MET:HE1	1:C:853:PHE:CD1	2.49	0.48
1:A:936:PHE:O	1:A:940:LEU:HG	2.13	0.48
1:A:667:THR:O	1:A:671:ILE:HG12	2.14	0.48
1:C:694:ILE:HB	1:C:696:ARG:NH1	2.25	0.48
1:C:758:GLU:OE2	1:C:761:ARG:NH2	2.41	0.48
4:y:47:DC:H2'	4:y:48:DT:H71	1.96	0.48
1:A:822:SER:C	1:A:824:GLU:H	2.22	0.47
1:A:665:HIS:O	1:A:669:THR:HG23	2.13	0.47
1:A:727:CYS:SG	1:A:942:HIS:CD2	3.07	0.47
2:B:141:SER:OG	2:B:207:HIS:NE2	2.30	0.47
2:B:219:LEU:HD21	2:B:256:ILE:HG12	1.95	0.47
1:C:909:TYR:OH	1:C:939:THR:O	2.23	0.47
1:A:517:PHE:HB2	1:A:687:LEU:HD11	1.96	0.47
1:C:470:ILE:O	1:C:474:THR:OG1	2.32	0.47
2:D:98:THR:N	2:D:102:GLU:O	2.46	0.47
2:D:117:ASN:ND2	5:J:6:DG:H4'	2.29	0.47
1:A:466:VAL:HG21	1:C:491:ILE:HG13	1.96	0.47
2:B:219:LEU:HD22	2:B:273:ILE:HD13	1.96	0.47
1:C:477:SER:OG	6:L:22:DT:OP2	2.28	0.47
2:D:290:VAL:HG22	2:D:299:ILE:HD12	1.97	0.47
1:A:483:LYS:NZ	7:M:21:DG:OP1	2.46	0.47
1:C:790:SER:OG	1:C:791:ILE:N	2.43	0.47
1:A:557:PHE:CE2	1:A:988:LEU:HG	2.50	0.47
1:A:717:GLY:HA2	1:A:781:ALA:HB3	1.95	0.47
1:A:729:LEU:HD23	1:A:946:ILE:HD11	1.97	0.47
1:C:713:ARG:NH1	1:C:726:ILE:O	2.48	0.47
2:D:168:THR:O	2:D:172:TRP:N	2.48	0.47
2:B:137:ARG:HD2	2:B:155:LEU:HD21	1.96	0.47
1:C:717:GLY:HA2	1:C:781:ALA:HB3	1.97	0.47
1:C:541:LEU:HD23	1:C:550:VAL:HG21	1.97	0.47
1:C:460:SER:N	1:C:495:GLN:O	2.47	0.47
2:D:235:ARG:HD3	2:D:252:LEU:HD11	1.97	0.47
7:M:25:DT:H2''	7:M:26:DA:C8	2.50	0.47
2:D:314:SER:OG	2:D:331:ILE:HB	2.15	0.46
3:x:41:DA:H2''	3:x:42:DC:OP2	2.14	0.46
1:A:666:GLU:OE2	2:B:35:GLY:N	2.48	0.46
2:B:74:TYR:N	2:B:75:PRO:CD	2.79	0.46
3:x:32:DC:H2'	3:x:33:DC:C6	2.50	0.46
2:B:142:ILE:HD12	2:B:155:LEU:HB2	1.98	0.46
2:B:244:THR:HG23	2:B:244:THR:O	2.15	0.46
2:D:154:VAL:HG13	2:D:182:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:GLU:OE2	1:A:761:ARG:NH2	2.39	0.46
1:C:934:ASN:N	5:J:15:DA:OP1	2.48	0.46
1:A:621:ARG:HD2	1:A:968:PHE:HB2	1.98	0.46
1:C:708:ASP:HB2	5:J:16:DC:O5'	2.16	0.46
2:D:295:ASN:N	2:D:295:ASN:OD1	2.49	0.46
3:x:43:DT:H2''	3:x:44:DG:H5'	1.98	0.46
2:B:258:VAL:HG22	2:B:259:SER:N	2.30	0.46
1:C:571:GLU:O	1:C:575:LEU:HG	2.16	0.46
1:A:475:PHE:HE1	1:A:967:LEU:HD22	1.81	0.46
1:A:991:HIS:O	1:A:995:THR:HG23	2.16	0.46
1:A:708:ASP:O	1:A:711:LEU:N	2.48	0.46
1:A:722:GLY:O	3:x:56:DC:H4'	2.16	0.46
1:A:822:SER:OG	1:A:825:GLU:OE2	2.24	0.46
2:B:184:LEU:HD11	2:B:247:VAL:CG2	2.46	0.46
2:B:283:LYS:HD2	2:B:317:TRP:NE1	2.31	0.46
1:C:538:LEU:CD1	1:C:550:VAL:HG21	2.46	0.46
1:C:594:VAL:HG12	1:C:956:TRP:HH2	1.81	0.46
1:C:718:LEU:HD23	1:C:779:VAL:HG22	1.98	0.46
1:C:719:GLU:CD	1:C:773:ARG:HE	2.22	0.46
1:C:977:ARG:HH12	6:L:24:DG:H5'	1.81	0.46
1:A:621:ARG:NH1	1:A:961:ASN:OD1	2.48	0.46
2:B:98:THR:HG22	2:B:100:ASN:H	1.81	0.46
2:D:134:PRO:HA	2:D:183:PHE:CE2	2.51	0.46
2:D:273:ILE:CD1	2:D:290:VAL:HG21	2.46	0.46
1:A:810:LEU:HD22	1:A:815:VAL:HG21	1.98	0.46
1:A:833:LEU:O	1:A:837:LEU:HG	2.16	0.46
1:C:567:LEU:O	1:C:571:GLU:N	2.49	0.46
2:D:76:ALA:HB1	2:D:142:ILE:HG22	1.98	0.46
1:A:837:LEU:O	1:A:842:ASN:N	2.49	0.45
1:C:517:PHE:CG	1:C:564:VAL:HG21	2.50	0.45
2:D:74:TYR:N	2:D:75:PRO:CD	2.80	0.45
2:D:326:THR:HG23	2:D:349:ARG:HG2	1.97	0.45
2:D:19:PHE:HB2	2:D:30:PHE:CE1	2.51	0.45
1:A:658:MET:SD	1:A:660:ALA:HB3	2.56	0.45
1:A:753:ASN:O	1:A:779:VAL:HG11	2.17	0.45
2:D:137:ARG:HH11	2:D:157:GLY:HA2	1.82	0.45
1:C:725:TYR:OH	1:C:774:ASP:HA	2.17	0.45
2:D:15:ILE:HD11	2:D:57:LEU:HD21	1.98	0.45
1:A:893:TRP:NE1	1:A:939:THR:HG23	2.32	0.45
1:C:895:SER:O	1:C:952:SER:OG	2.34	0.45
1:C:554:ALA:HA	1:C:658:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:LEU:HD21	1:C:994:TYR:CE2	2.52	0.45
1:A:468:LEU:O	1:A:472:VAL:HG23	2.17	0.45
2:B:156:PHE:CE2	2:B:204:LEU:HB2	2.52	0.45
1:C:550:VAL:HG22	1:C:552:THR:HG22	1.98	0.45
1:C:882:LEU:HD11	1:C:920:LEU:HD13	1.99	0.45
2:B:258:VAL:HG23	2:B:284:ARG:HD2	1.98	0.45
1:C:943:VAL:O	1:C:947:ILE:HG12	2.17	0.45
2:D:221:GLY:N	2:D:258:VAL:O	2.40	0.45
1:A:627:MET:HE1	1:A:646:PRO:CB	2.47	0.44
2:B:184:LEU:HD12	2:B:245:PRO:HB2	1.98	0.44
1:C:665:HIS:NE2	2:D:100:ASN:OD1	2.48	0.44
2:D:334:ASP:OD1	2:D:336:LYS:N	2.50	0.44
1:A:674:PRO:HG3	2:B:172:TRP:HB3	1.99	0.44
1:A:803:GLU:HG3	1:A:928:TYR:OH	2.17	0.44
1:A:811:GLU:OE2	1:A:926:TYR:OH	2.20	0.44
1:A:892:VAL:HG21	1:A:909:TYR:HD2	1.82	0.44
2:B:38:LYS:O	2:B:41:CYS:N	2.48	0.44
1:C:875:ARG:NH1	1:C:923:LYS:O	2.49	0.44
2:D:78:CYS:SG	2:D:92:ILE:HB	2.57	0.44
2:D:182:VAL:HG11	2:D:247:VAL:HG21	1.99	0.44
1:A:630:THR:HA	1:A:639:LYS:HA	2.00	0.44
2:B:159:ARG:HD2	2:B:205:SER:OG	2.17	0.44
1:C:564:VAL:HG13	1:C:689:LEU:CD1	2.47	0.44
2:D:95:GLY:HA2	2:D:104:SER:O	2.18	0.44
2:D:20:SER:CB	2:D:77:THR:HG21	2.48	0.44
1:A:484:MET:O	1:A:488:VAL:HG23	2.17	0.44
1:C:794:LEU:O	1:C:798:ILE:HG12	2.17	0.44
1:A:934:ASN:N	5:I:15:DA:OP1	2.51	0.44
1:C:525:ASN:O	2:D:169:THR:HG23	2.18	0.44
1:C:525:ASN:HB3	2:D:172:TRP:HZ3	1.83	0.44
1:C:860:GLN:O	1:C:863:VAL:HG12	2.17	0.44
2:D:21:LEU:HG	2:D:320:SER:HB3	2.00	0.44
1:C:883:MET:O	1:C:887:LEU:HG	2.17	0.44
2:D:134:PRO:O	2:D:135:GLU:HB3	2.17	0.44
3:x:58:DC:H2'	3:x:59:DT:H71	2.00	0.44
1:A:602:MET:HG3	1:A:619:ALA:HB3	2.00	0.44
2:D:74:TYR:N	2:D:75:PRO:HD3	2.33	0.44
2:D:219:LEU:HD22	2:D:273:ILE:HD11	2.00	0.44
1:A:538:LEU:HD21	1:A:550:VAL:HG21	1.98	0.43
1:A:727:CYS:SG	1:A:729:LEU:HD13	2.58	0.43
2:B:152:MET:HE3	2:B:184:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:HIS:NE2	1:C:868:GLU:OE1	2.45	0.43
1:C:857:LEU:HA	1:C:862:THR:HG21	2.00	0.43
3:x:60:DA:H1'	3:x:61:DT:O5'	2.18	0.43
4:y:31:DC:H2''	4:y:32:DT:H5'	1.99	0.43
5:J:13:DC:C2'	5:J:14:DT:H71	2.48	0.43
1:A:570:MET:HE1	1:A:626:VAL:HB	2.01	0.43
1:A:724:VAL:O	1:A:733:THR:HA	2.18	0.43
1:A:769:VAL:HG21	2:B:42:PRO:CG	2.48	0.43
1:A:793:ALA:HB1	1:A:894:ARG:HD3	2.01	0.43
1:C:936:PHE:O	1:C:940:LEU:HG	2.18	0.43
1:A:538:LEU:CD2	1:A:550:VAL:HG21	2.49	0.43
1:C:667:THR:O	1:C:671:ILE:HG12	2.18	0.43
1:A:858:MET:SD	1:A:883:MET:HE1	2.58	0.43
2:B:229:ARG:NE	2:B:259:SER:OG	2.45	0.43
2:D:310:ASP:O	2:D:314:SER:HB2	2.18	0.43
5:I:13:DC:C2'	5:I:14:DT:H71	2.48	0.43
7:M:30:DG:H2'	7:M:31:DG:C8	2.54	0.43
1:A:849:MET:HE1	1:A:853:PHE:CE1	2.53	0.43
1:A:946:ILE:HB	1:A:953:ILE:HD11	2.00	0.43
3:x:52:DG:H2''	4:y:37:DG:N3	2.33	0.43
1:A:927:ARG:HD2	1:A:927:ARG:HA	1.74	0.43
2:B:168:THR:HG23	2:B:171:LYS:H	1.83	0.43
1:C:559:TYR:OH	1:C:597:GLU:HG2	2.18	0.43
3:x:53:DT:H2''	3:x:54:DA:H8	1.84	0.43
1:A:571:GLU:O	1:A:575:LEU:HG	2.18	0.43
2:B:226:SER:HB2	2:B:228:ILE:HG22	2.00	0.43
1:C:556:ARG:NH2	2:D:169:THR:O	2.52	0.43
1:C:991:HIS:O	1:C:991:HIS:ND1	2.38	0.43
1:A:471:ARG:HA	1:A:476:LEU:HB2	2.00	0.43
1:A:532:VAL:HG11	2:B:170:GLU:OE2	2.19	0.43
1:A:666:GLU:O	2:B:101:ASN:ND2	2.52	0.43
1:A:855:ARG:NH1	6:L:18:DA:H62	2.16	0.43
2:B:249:CYS:SG	2:B:250:THR:N	2.92	0.43
1:C:647:ASN:ND2	1:C:954:GLY:O	2.37	0.43
1:C:727:CYS:SG	1:C:729:LEU:HD13	2.59	0.43
1:A:504:ARG:O	1:A:508:LYS:HG2	2.19	0.43
2:B:95:GLY:HA2	2:B:104:SER:O	2.19	0.43
1:C:627:MET:HE3	1:C:627:MET:HB3	1.93	0.43
1:C:740:ASN:O	1:C:741:LEU:HB2	2.19	0.43
1:C:856:LYS:O	1:C:862:THR:OG1	2.35	0.43
2:B:159:ARG:NH2	2:B:224:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:848:MET:SD	3:x:47:DC:H1'	2.58	0.43
1:C:983:GLU:O	1:C:987:VAL:HG23	2.19	0.43
1:A:973:LYS:HE3	1:A:974:MET:HE3	2.01	0.42
2:B:219:LEU:HD13	2:B:273:ILE:HD11	2.00	0.42
1:C:471:ARG:O	1:C:476:LEU:N	2.51	0.42
1:C:734:ARG:HG2	1:C:931:LYS:HA	2.01	0.42
1:C:810:LEU:O	1:C:813:GLY:N	2.51	0.42
4:y:51:DC:H4'	4:y:52:DC:OP1	2.19	0.42
5:J:3:DC:H1'	5:J:4:DA:C5	2.54	0.42
1:A:553:ILE:HD12	1:A:615:VAL:HG11	2.00	0.42
2:B:289:LEU:O	2:B:300:SER:N	2.51	0.42
1:C:803:GLU:HG3	1:C:928:TYR:OH	2.20	0.42
1:C:878:ALA:O	1:C:919:LEU:HD21	2.19	0.42
1:C:621:ARG:NH1	1:C:961:ASN:OD1	2.51	0.42
1:A:519:TRP:CH2	1:A:682:MET:SD	3.12	0.42
1:A:943:VAL:O	1:A:947:ILE:HG12	2.20	0.42
2:B:272:VAL:HG12	2:B:274:VAL:HG23	2.01	0.42
5:I:3:DC:H1'	5:I:4:DA:C5	2.54	0.42
1:A:756:ARG:HB3	1:A:776:VAL:HB	2.01	0.42
2:B:98:THR:N	2:B:102:GLU:O	2.53	0.42
1:C:731:ASP:CG	1:C:747:THR:OG1	2.63	0.42
2:D:289:LEU:HB2	2:D:302:MET:HG3	2.02	0.42
3:x:60:DA:H2'	3:x:61:DT:H71	2.01	0.42
4:y:41:DG:C3'	4:y:42:DT:H71	2.49	0.42
5:I:8:DT:H2''	5:I:9:DA:C8	2.54	0.42
7:M:29:DA:H2'	7:M:30:DG:C8	2.54	0.42
2:B:19:PHE:HB2	2:B:30:PHE:CE1	2.55	0.42
2:D:208:VAL:HG23	2:D:219:LEU:HB2	2.02	0.42
2:D:259:SER:O	2:D:277:TYR:N	2.53	0.42
1:A:503:LEU:O	1:A:507:GLU:HG3	2.20	0.42
1:A:946:ILE:HD12	1:A:949:ARG:HH21	1.84	0.42
2:B:236:ILE:HG22	2:B:247:VAL:HG13	2.02	0.42
2:B:284:ARG:O	2:B:317:TRP:HZ2	2.01	0.42
2:D:258:VAL:CG2	2:D:284:ARG:HD2	2.49	0.42
4:y:31:DC:H2'	4:y:32:DT:C6	2.55	0.42
2:D:33:GLN:OE1	2:D:37:PRO:HA	2.20	0.42
4:y:46:DC:H2''	4:y:47:DC:C6	2.55	0.42
2:B:343:PHE:HB2	2:B:345:PHE:CZ	2.55	0.42
1:C:678:GLU:O	1:C:682:MET:SD	2.78	0.42
1:C:938:LYS:HA	1:C:942:HIS:HD2	1.85	0.42
1:C:968:PHE:CZ	1:C:984:MET:HE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:y:48:DT:H2''	4:y:49:DA:C8	2.55	0.42
5:J:13:DC:H2'	5:J:14:DT:H71	2.02	0.42
1:C:568:MET:SD	1:C:691:MET:HG3	2.60	0.42
5:J:8:DT:H2''	5:J:9:DA:C8	2.54	0.42
1:A:517:PHE:H	1:A:530:THR:HG21	1.85	0.41
1:C:654:PRO:HB2	1:C:988:LEU:HD12	2.02	0.41
2:D:212:ARG:HD2	2:D:292:LEU:HB2	2.02	0.41
1:A:563:LEU:HD11	1:A:702:PHE:HE1	1.85	0.41
1:A:694:ILE:HD12	1:A:694:ILE:N	2.35	0.41
1:A:885:LEU:HD11	1:A:915:ARG:HG3	2.02	0.41
1:C:682:MET:HE2	1:C:702:PHE:HZ	1.86	0.41
1:A:924:PHE:O	1:A:926:TYR:O	2.38	0.41
2:D:283:LYS:HG3	2:D:285:MET:SD	2.61	0.41
6:L:25:DT:H2''	6:L:26:DA:C8	2.55	0.41
1:A:851:GLY:O	1:A:855:ARG:HG2	2.21	0.41
1:C:665:HIS:O	1:C:669:THR:HG23	2.21	0.41
1:C:731:ASP:OD2	1:C:756:ARG:NH2	2.52	0.41
1:C:753:ASN:O	1:C:779:VAL:HG11	2.20	0.41
1:A:578:MET:HE1	1:A:696:ARG:HH11	1.85	0.41
2:B:25:ASP:C	2:B:27:GLN:H	2.28	0.41
2:B:31:PHE:CD1	2:B:31:PHE:C	2.99	0.41
2:B:220:GLY:O	2:B:258:VAL:O	2.38	0.41
2:B:275:GLY:HA2	2:B:317:TRP:CZ2	2.55	0.41
1:C:658:MET:HG3	1:C:660:ALA:HB3	2.02	0.41
2:B:25:ASP:CG	2:B:115:LYS:HZ1	2.19	0.41
2:B:47:HIS:HB2	2:B:58:LYS:HB2	2.03	0.41
1:C:564:VAL:HG22	1:C:687:LEU:HD21	2.01	0.41
1:C:627:MET:SD	1:C:646:PRO:HB3	2.60	0.41
1:C:679:ARG:NH1	1:C:786:GLU:O	2.53	0.41
1:C:893:TRP:HA	1:C:953:ILE:HB	2.03	0.41
2:D:272:VAL:HG22	2:D:302:MET:SD	2.61	0.41
5:J:6:DG:C2	5:J:7:DA:C4	3.08	0.41
1:A:481:TYR:CZ	1:A:503:LEU:HD11	2.55	0.41
1:C:598:SER:OG	1:C:961:ASN:HB2	2.20	0.41
1:C:601:GLY:HA2	1:C:619:ALA:O	2.21	0.41
1:A:852:ASN:OD1	6:L:18:DA:N6	2.45	0.41
1:C:852:ASN:OD1	7:M:18:DA:N6	2.45	0.41
2:D:18:GLY:HA2	2:D:74:TYR:CD1	2.56	0.41
2:D:117:ASN:HB3	2:D:119:LYS:HB3	2.03	0.41
1:A:578:MET:HE1	1:A:696:ARG:NH1	2.36	0.41
1:A:647:ASN:HB3	1:A:959:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:LYS:O	1:A:894:ARG:HB2	2.21	0.41
1:A:996:SER:OG	1:A:999:LEU:HG	2.21	0.41
2:B:308:THR:O	2:B:311:ILE:N	2.53	0.41
1:C:553:ILE:CD1	1:C:615:VAL:HG11	2.50	0.41
1:C:570:MET:HG2	1:C:997:LYS:HG3	2.02	0.41
1:C:759:VAL:O	1:C:763:ASN:N	2.53	0.41
1:C:962:GLU:O	3:x:45:DT:H2''	2.21	0.41
5:I:6:DG:C2	5:I:7:DA:C4	3.08	0.41
2:B:258:VAL:HG22	2:B:259:SER:H	1.84	0.41
1:C:704:GLY:CA	1:C:707:TYR:HE2	2.34	0.41
1:A:559:TYR:HB2	1:A:678:GLU:OE1	2.20	0.40
2:B:72:LEU:HD13	2:B:95:GLY:O	2.21	0.40
2:B:118:LYS:HB3	5:I:7:DA:OP1	2.21	0.40
2:D:46:PHE:CD1	2:D:46:PHE:N	2.89	0.40
2:D:229:ARG:HG2	2:D:259:SER:HB2	2.02	0.40
2:D:233:LEU:HD21	2:D:297:ILE:HD13	2.02	0.40
1:C:484:MET:O	1:C:488:VAL:HG23	2.21	0.40
1:C:596:LYS:HB2	1:C:627:MET:HG3	2.03	0.40
1:C:658:MET:HE1	1:C:672:LEU:HG	2.01	0.40
1:C:664:ASP:OD1	2:D:34:LYS:NZ	2.54	0.40
1:C:848:MET:SD	5:J:16:DC:N3	2.94	0.40
1:C:860:GLN:HA	1:C:863:VAL:HG12	2.03	0.40
4:y:25:DC:H2'	4:y:26:DT:H71	2.03	0.40
1:A:661:ASP:OD2	1:A:662:GLU:N	2.54	0.40
1:A:724:VAL:O	1:A:734:ARG:N	2.48	0.40
2:B:78:CYS:SG	2:B:144:VAL:HG23	2.62	0.40
1:C:471:ARG:HA	1:C:476:LEU:HB2	2.04	0.40
1:C:475:PHE:HZ	1:C:994:TYR:HH	1.65	0.40
5:I:13:DC:H2'	5:I:14:DT:H71	2.02	0.40
2:B:220:GLY:HA3	2:B:258:VAL:HG12	2.04	0.40
1:A:475:PHE:CE1	1:A:967:LEU:HD22	2.56	0.40
1:A:480:GLN:OE1	1:C:474:THR:HA	2.21	0.40
1:A:962:GLU:O	1:A:965:ASN:N	2.52	0.40
2:B:10:HIS:O	2:B:10:HIS:ND1	2.54	0.40
1:C:742:VAL:HG11	1:C:914:GLN:HA	2.03	0.40
1:C:989:LYS:O	1:C:993:LEU:HG	2.21	0.40
2:D:76:ALA:HB2	2:D:140:HIS:CD2	2.56	0.40
2:D:129:LEU:HD22	2:D:185:ILE:HG23	2.03	0.40
2:D:326:THR:HG22	2:D:327:ILE:H	1.86	0.40
3:x:42:DC:H2'	3:x:43:DT:C6	2.56	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	547/750 (73%)	513 (94%)	33 (6%)	1 (0%)	43	68
1	C	546/750 (73%)	520 (95%)	26 (5%)	0	100	100
2	B	336/363 (93%)	308 (92%)	28 (8%)	0	100	100
2	D	337/363 (93%)	305 (90%)	31 (9%)	1 (0%)	36	60
All	All	1766/2226 (79%)	1646 (93%)	118 (7%)	2 (0%)	49	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	823	LYS
2	D	134	PRO

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	486/668 (73%)	477 (98%)	9 (2%)	50	77
1	C	486/668 (73%)	472 (97%)	14 (3%)	37	67
2	B	299/318 (94%)	292 (98%)	7 (2%)	44	73
2	D	301/318 (95%)	294 (98%)	7 (2%)	44	73
All	All	1572/1972 (80%)	1535 (98%)	37 (2%)	43	72

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	561	SER
1	A	638	VAL
1	A	640	VAL
1	A	688	THR
1	A	724	VAL
1	A	768	SER
1	A	844	LYS
1	A	910	SER
1	A	950	ASP
2	B	1	MET
2	B	28	VAL
2	B	98	THR
2	B	111	SER
2	B	164	SER
2	B	326	THR
2	B	350	CYS
1	C	563	LEU
1	C	592	THR
1	C	659	LEU
1	C	723	SER
1	C	731	ASP
1	C	732	THR
1	C	738	SER
1	C	768	SER
1	C	780	SER
1	C	873	GLU
1	C	905	SER
1	C	910	SER
1	C	934	ASN
1	C	981	CYS
2	D	1	MET
2	D	111	SER
2	D	147	SER
2	D	174	SER
2	D	175	VAL
2	D	288	SER
2	D	347	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	HIS
1	A	744	HIS

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Mol	Chain	Res	Type
2	B	101	ASN
1	C	473	ASN
1	C	830	GLN
1	C	860	GLN
2	D	52	GLN
2	D	117	ASN
2	D	207	HIS
2	D	267	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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

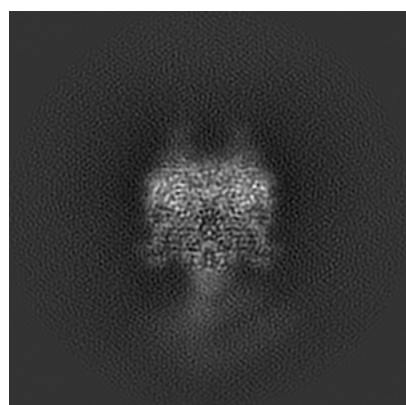
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22272. These allow visual inspection of the internal detail of the map and identification of artifacts.

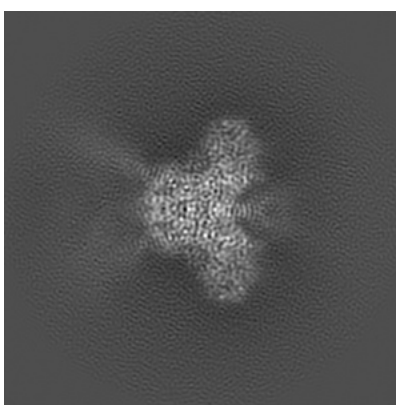
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

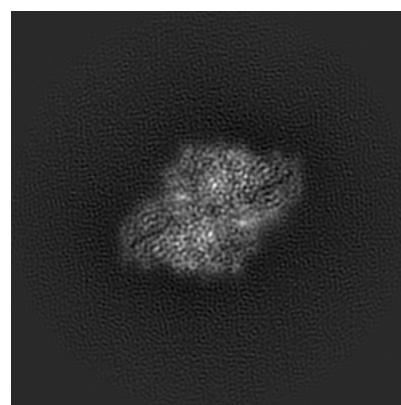
6.1.1 Primary map



X



Y

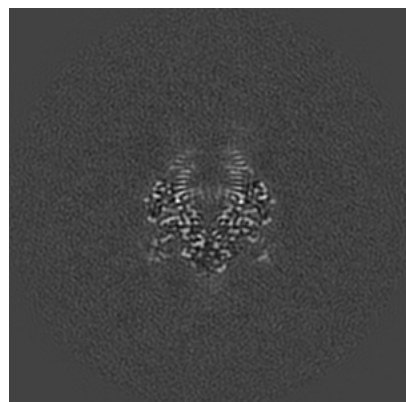


Z

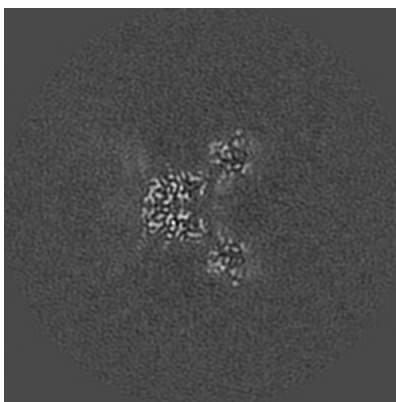
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

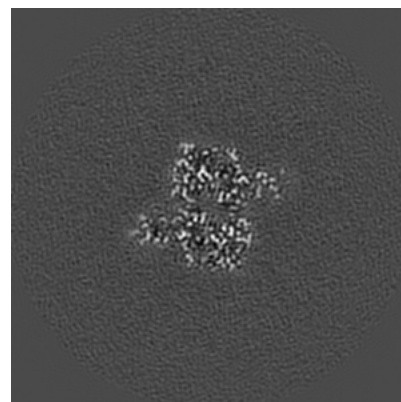
6.2.1 Primary map



X Index: 122



Y Index: 122

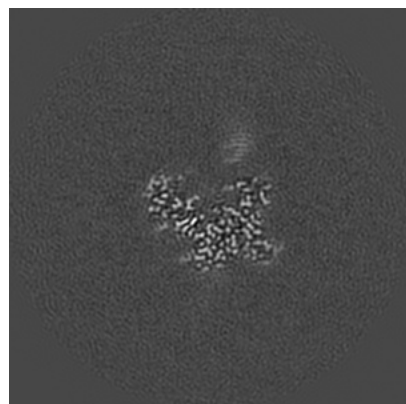


Z Index: 122

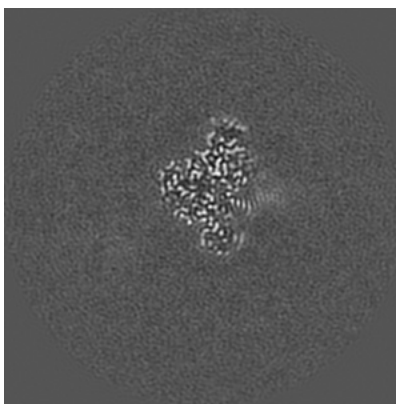
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

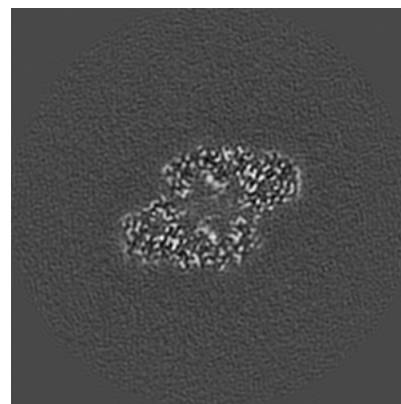
6.3.1 Primary map



X Index: 129



Y Index: 142

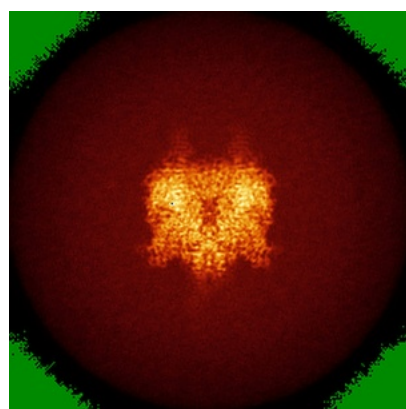


Z Index: 134

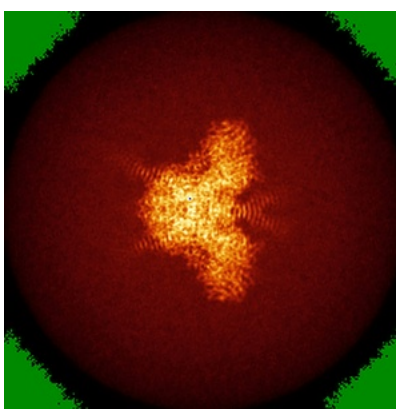
The images above show the largest variance slices of the map in three orthogonal directions.

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

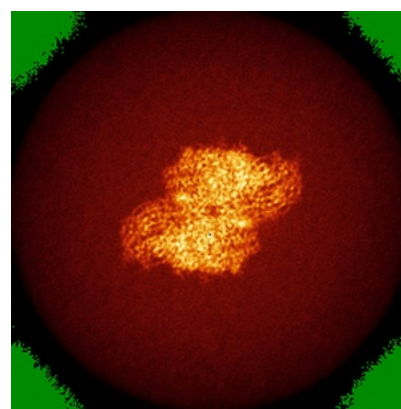
6.4.1 Primary map



X



Y

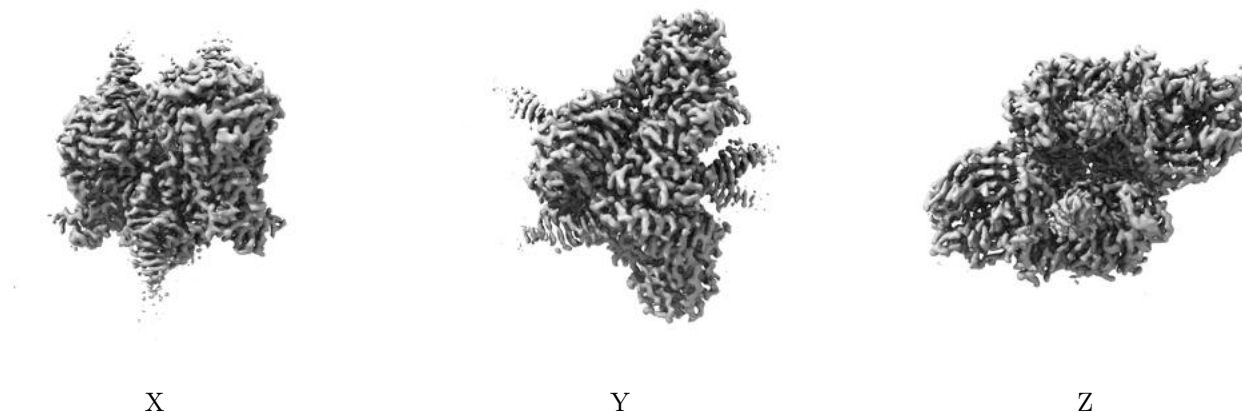


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

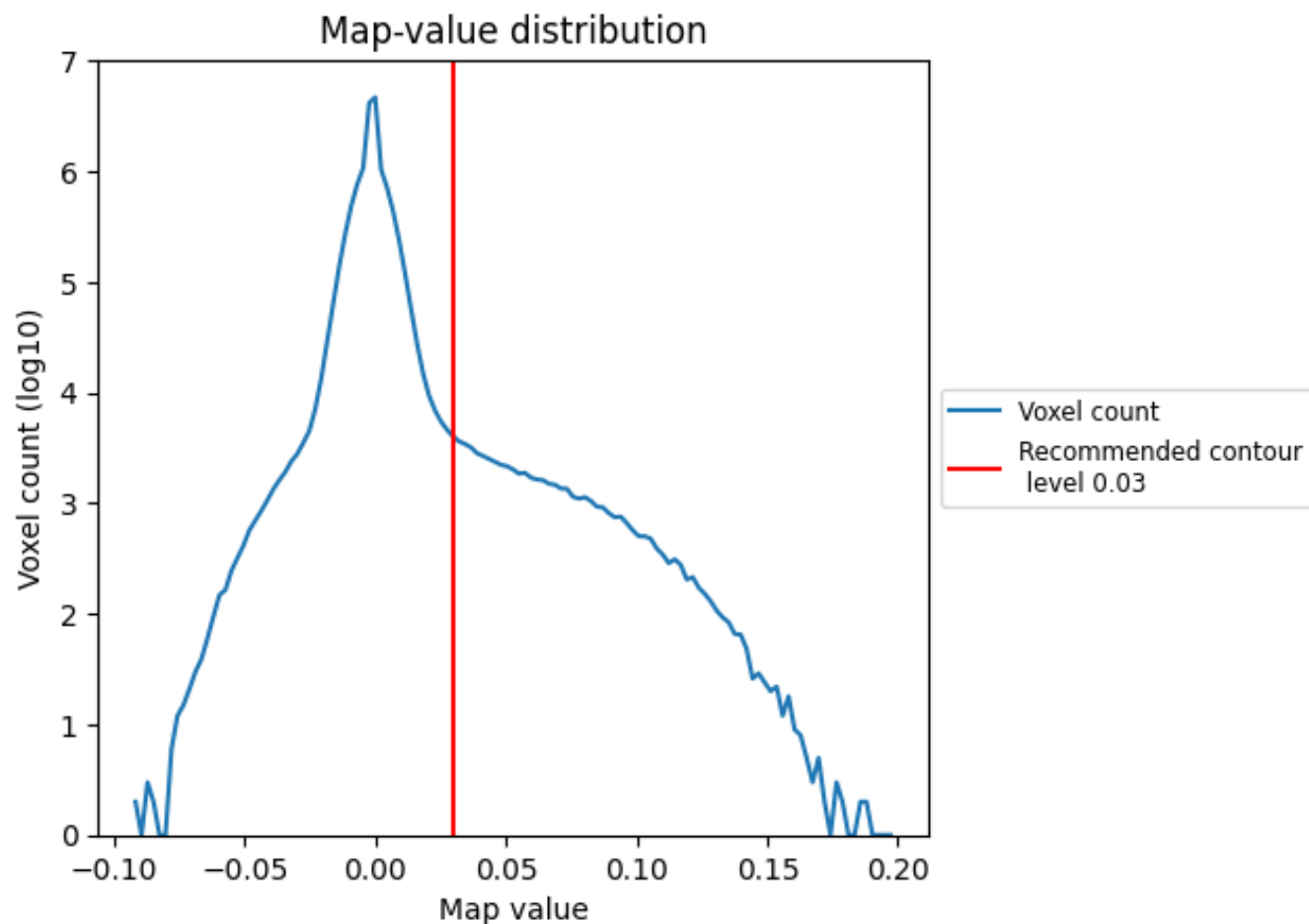
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

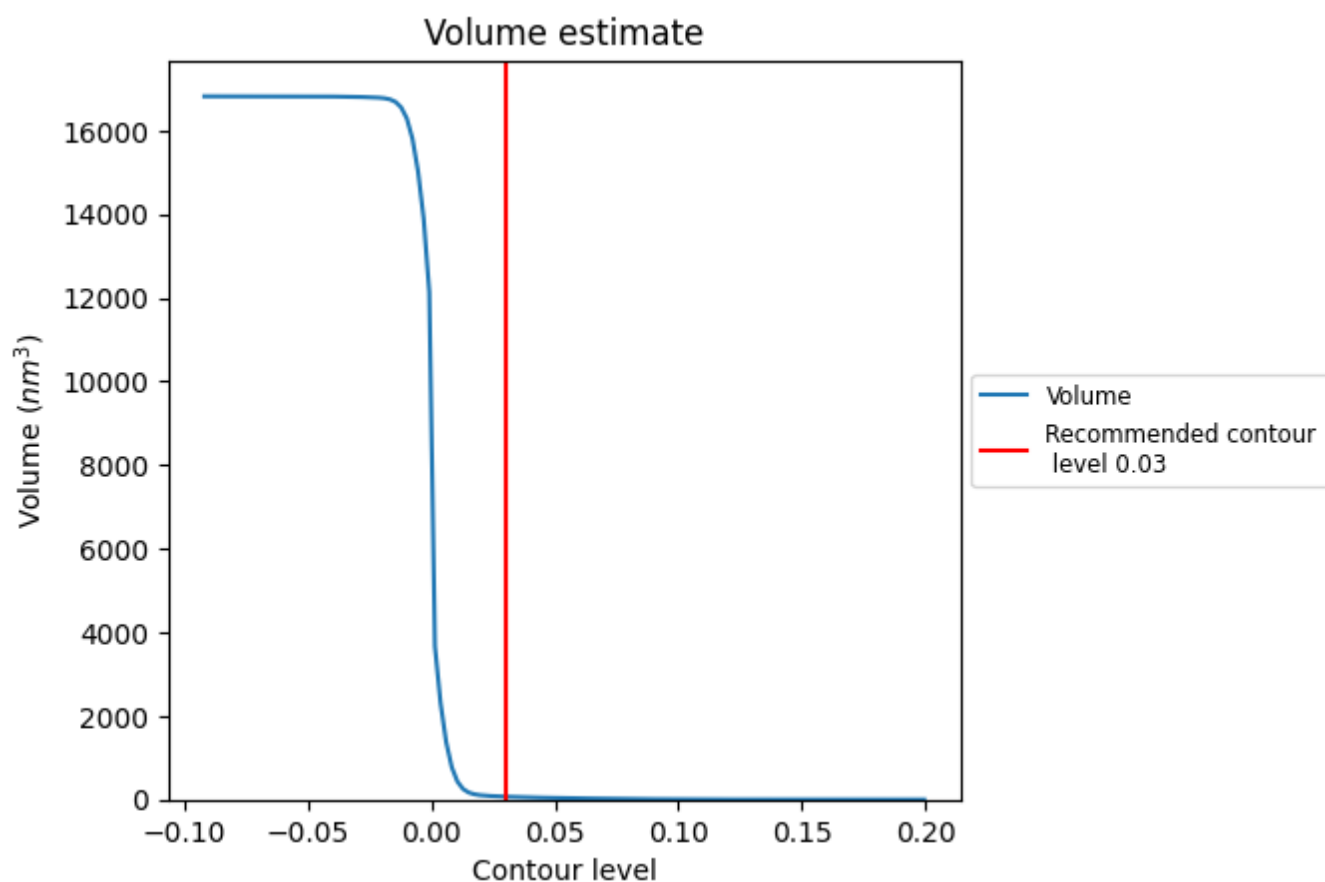
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

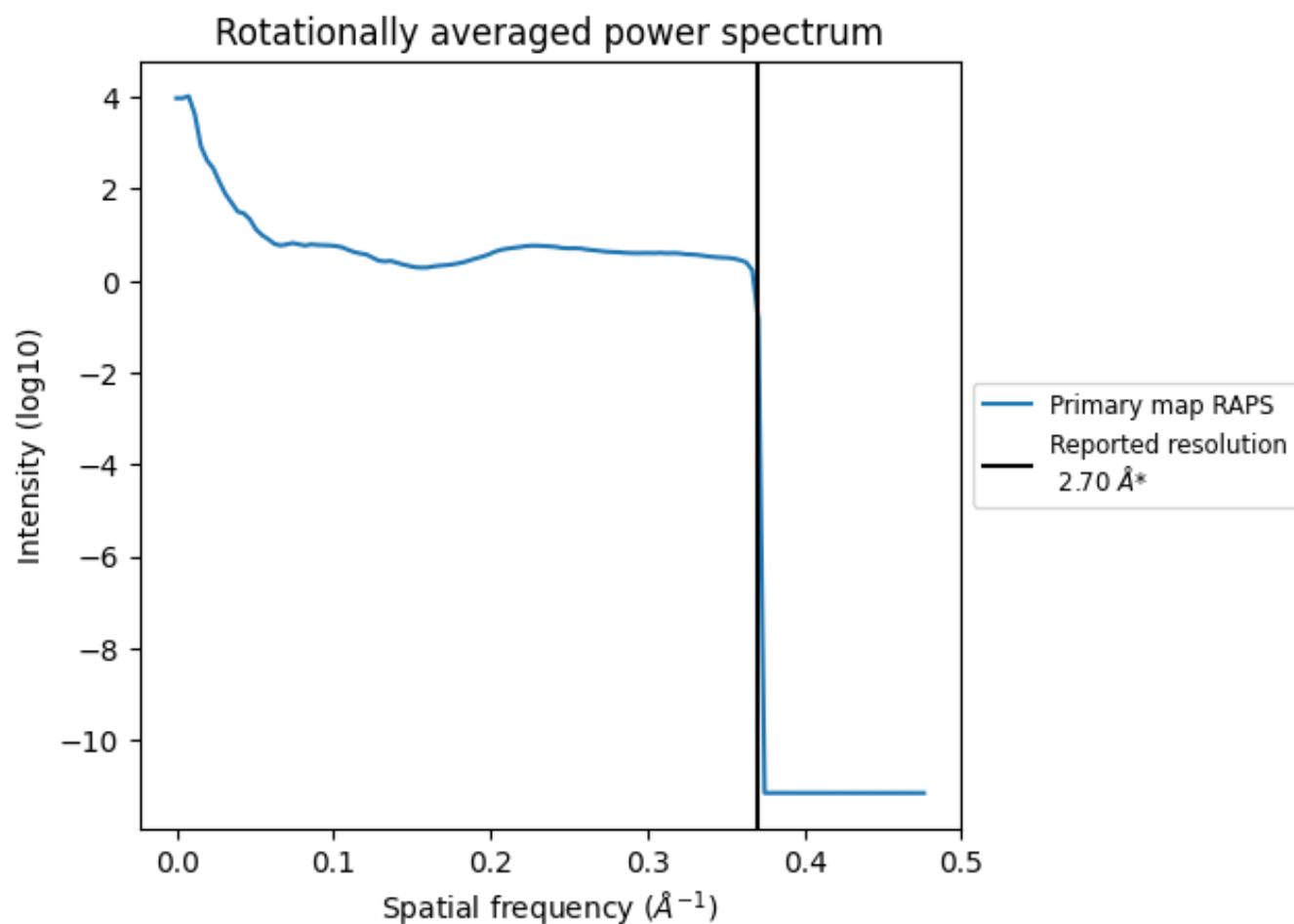
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm^3 ; this corresponds to an approximate mass of 62 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 0.370 Å⁻¹

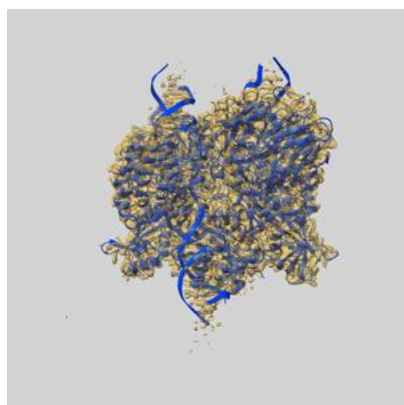
8 Fourier-Shell correlation

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

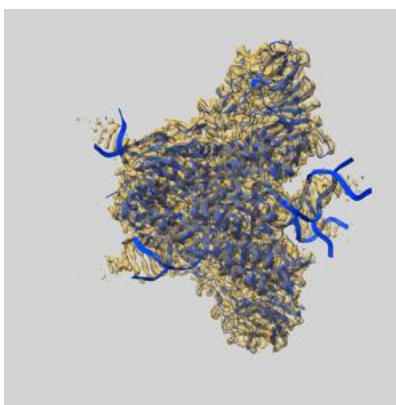
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22272 and PDB model 6XNX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

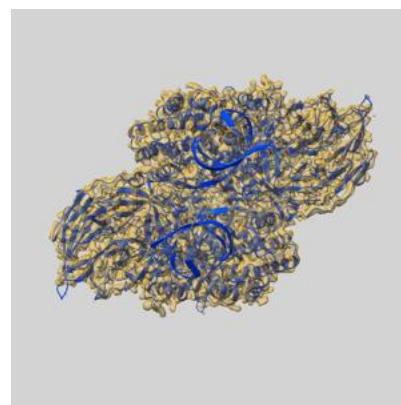
9.1 Map-model overlay [i](#)



X



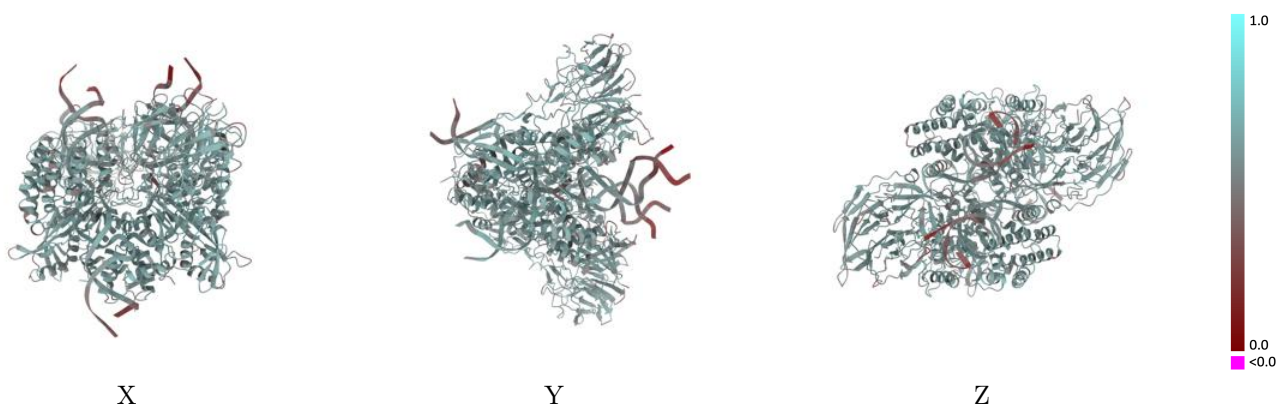
Y



Z

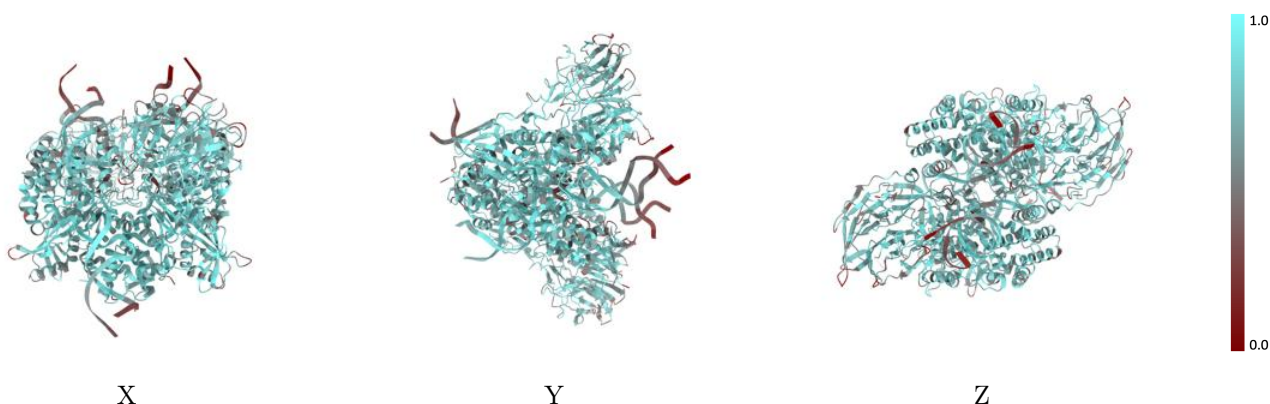
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



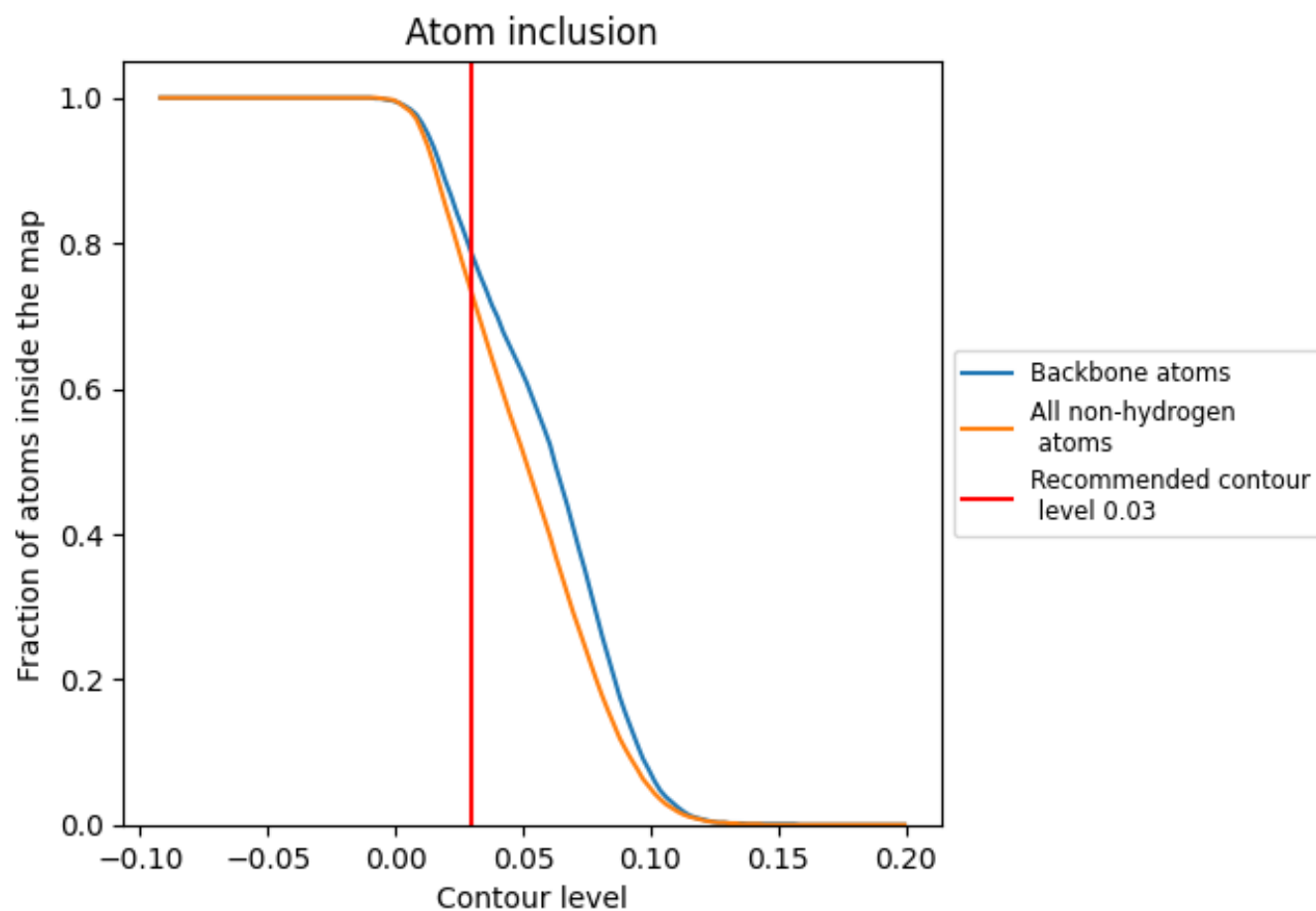
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.5630
A	0.7660	0.5830
B	0.7120	0.5600
C	0.7650	0.5820
D	0.7000	0.5570
I	0.5350	0.4320
J	0.5620	0.4550
L	0.8290	0.6010
M	0.7640	0.5470
x	0.6400	0.4990
y	0.6630	0.5040

1.0

0.0

<0.0