Full wwPDB EM Validation Report

Feb 24, 2024 – 06:39 PM EST

PDB ID	:	6XNY
EMDB ID	:	EMD-22273
Title	:	Structure of RAG1 (R848M/E649V)-RAG2-DNA Strand Transfer Complex (Paired-Form)
Authors	:	Zhang, Y.; Corbett, E.; Wu, S.; Schatz, D.G.
Deposited on	:	2020-07-05
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

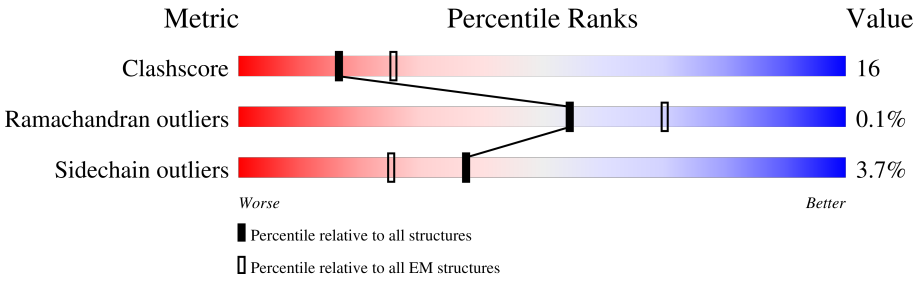
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	46% 26% • 27%
1	C	750	45% 27% • 27%
2	B	363	14% 61% 33% • 5%
2	D	363	15% 63% 31% • 5%
3	x	55	13% 64% 36%
4	y	66	8% 47% 53%
5	I	16	25% 56% 31% 12%
5	J	16	19% 50% 38% 12%

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Mol	Chain	Length	Quality of chain
6	L	45	
7	M	34	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16681 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	550	Total 4411	C 2783	N 771	O 824	S 33	0	0
1	C	548	Total 4398	C 2777	N 768	O 820	S 33	0	0

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	344	Total 2689	C 1719	N 457	O 494	S 19	0	0
2	D	345	Total 2694	C 1722	N 457	O 495	S 20	0	0

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 (55-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	x	35	Total	C	N	O	P	0	0
			704	336	123	211	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	31	Total	C	N	O	P	0	0
			627	299	112	186	30		

- Molecule 5 is a DNA chain called Flanking DNA top strand (16-mer).

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 DNA top strand (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 DNA top strand (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 (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

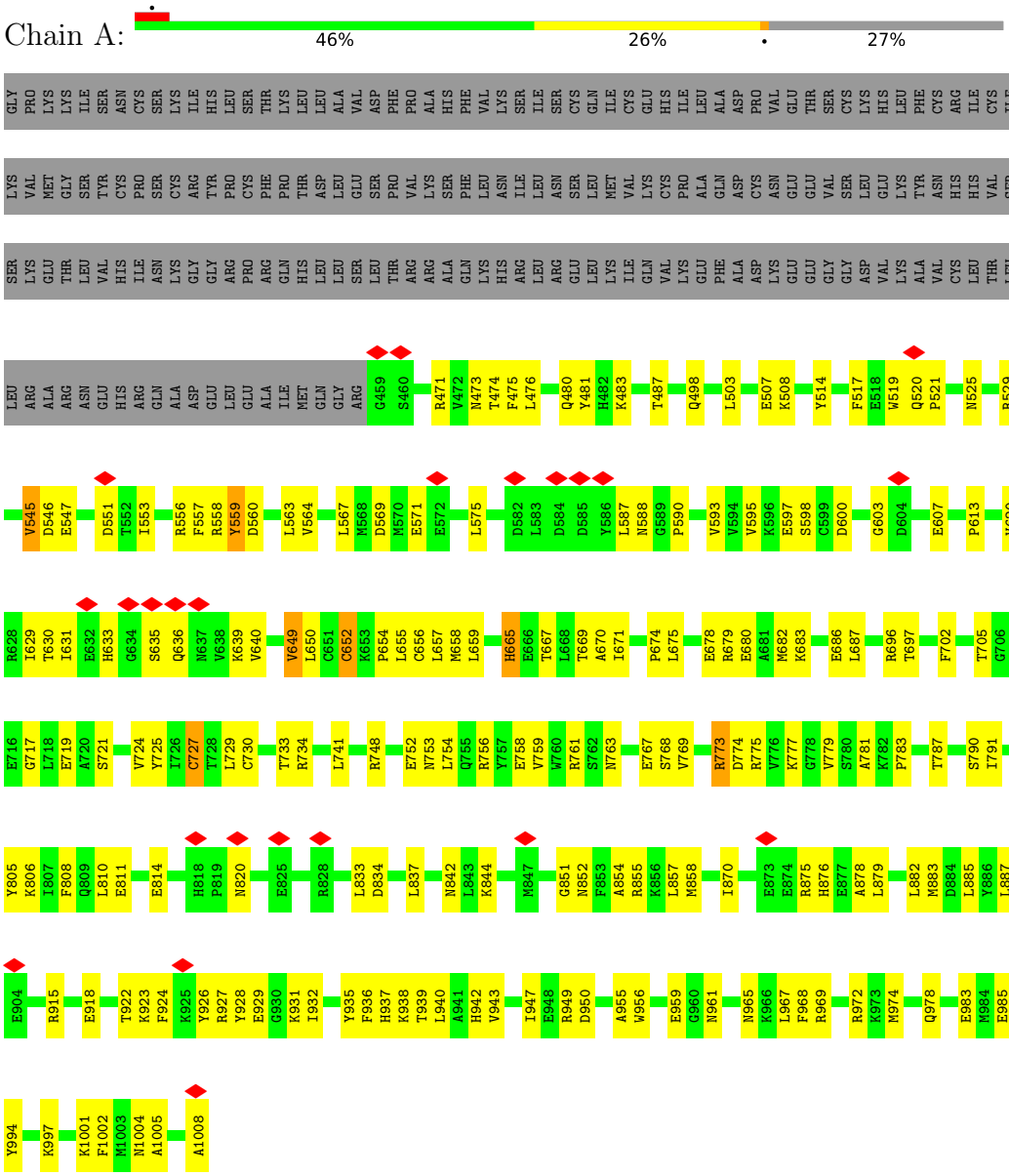
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total Zn 1 1	0
9	C	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

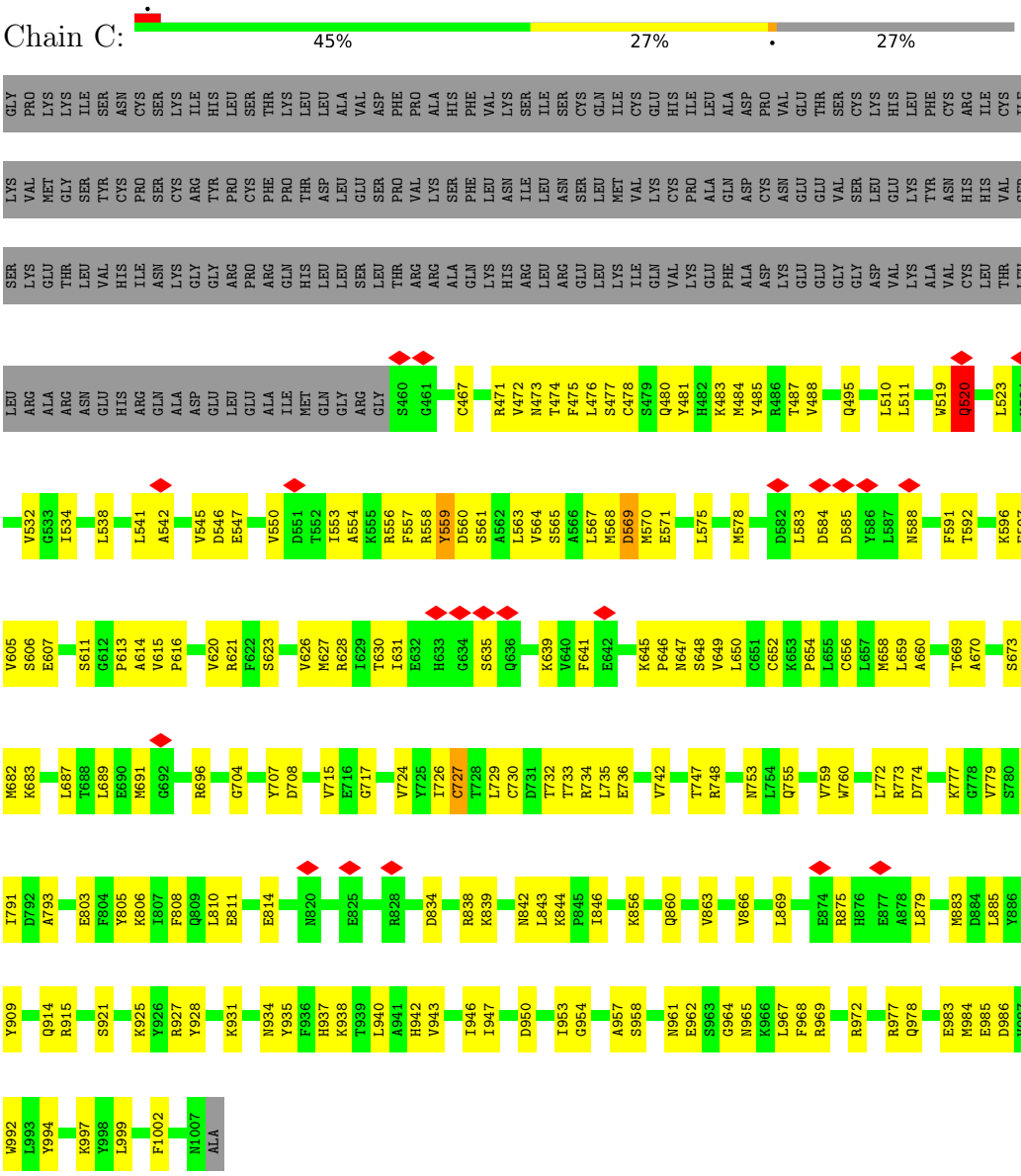
• Molecule 1: V(D)J recombination-activating protein 1

Chain A:



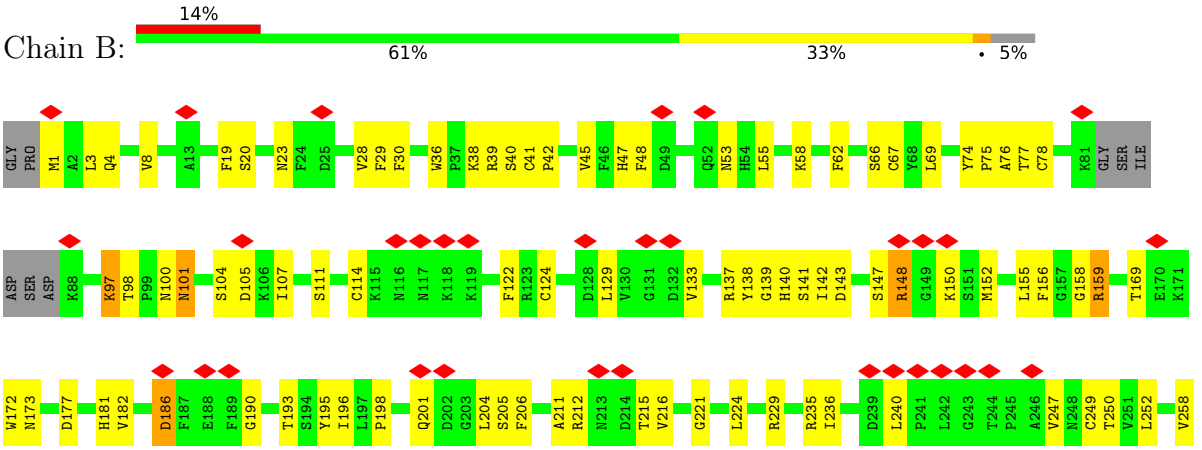
• Molecule 1: V(D)J recombination-activating protein 1

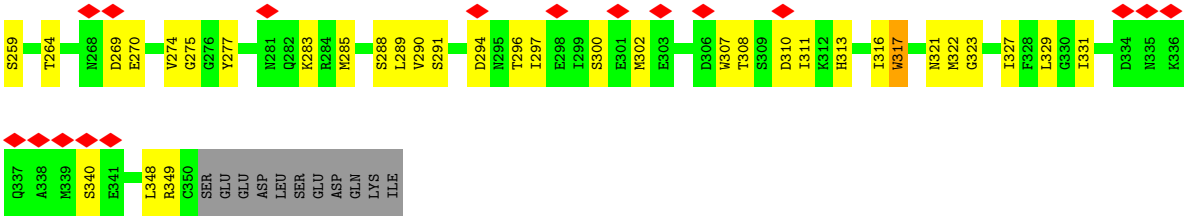
Chain C:



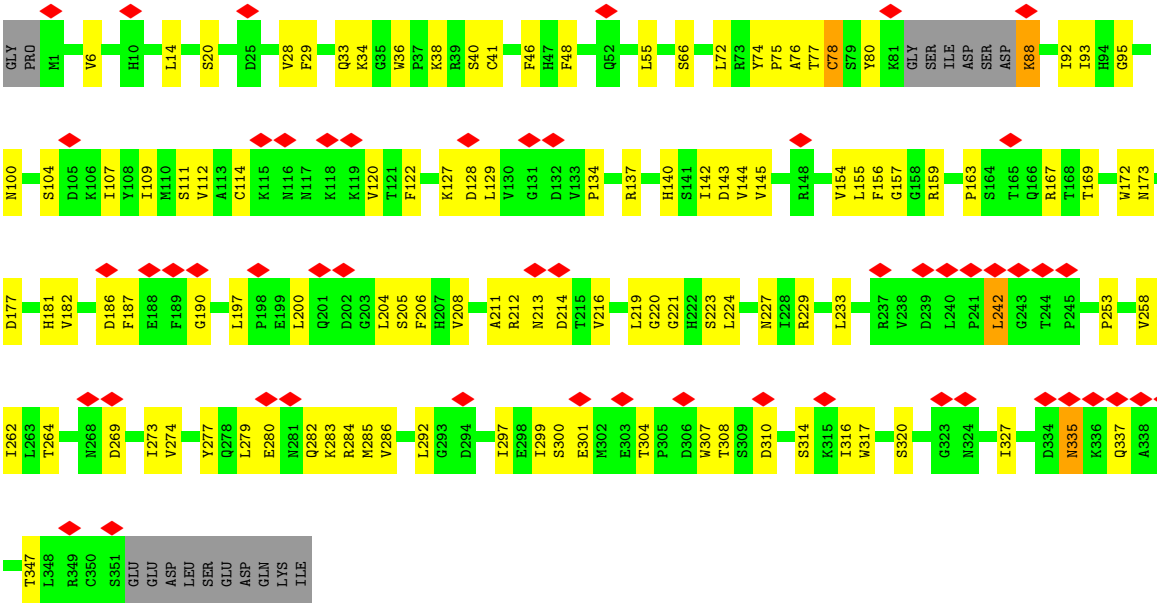
• Molecule 2: V(D)J recombination-activating protein 2

Chain B:

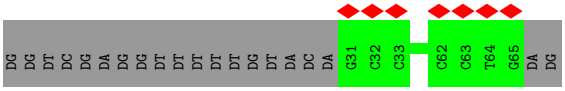




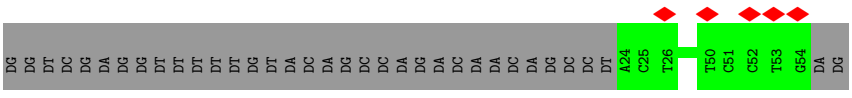
• Molecule 2: V(D)J recombination-activating protein 2



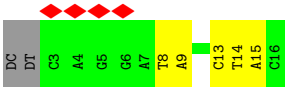
• Molecule 3: 12RSS integration strand (55-mer)



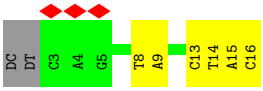
• Molecule 4: 23RSS integration strand (66-mer)



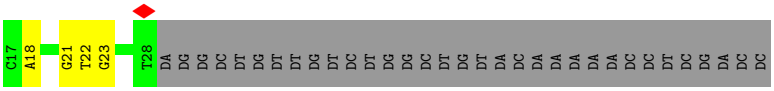
• Molecule 5: Flanking DNA top strand (16-mer)



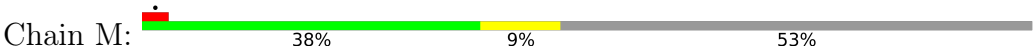
• Molecule 5: Flanking DNA top strand (16-mer)

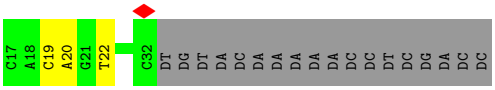


• Molecule 6: 23RSS signal DNA top strand (45-mer)



• Molecule 7: 12RSS signal DNA top strand (34-mer)





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44428	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 ($e^-/Å^2$)	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	0.171	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.031	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.53	0/4508	0.50	0/6079
1	C	0.54	0/4495	0.52	1/6063 (0.0%)
2	B	0.51	0/2757	0.53	0/3736
2	D	0.50	0/2762	0.53	0/3743
3	x	0.85	0/786	0.99	0/1209
4	y	0.82	0/701	1.00	0/1079
5	I	0.78	0/324	0.83	0/499
5	J	0.78	0/324	0.83	0/499
6	L	1.00	0/276	0.93	0/425
7	M	0.96	0/371	0.91	0/572
All	All	0.59	0/17304	0.62	1/23904 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	520	GLN	CB-CA-C	5.50	121.40	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	773	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4411	0	4366	155	0
1	C	4398	0	4354	160	0
2	B	2689	0	2652	91	0
2	D	2694	0	2652	86	0
3	x	704	0	395	0	0
4	y	627	0	350	0	0
5	I	288	0	158	4	0
5	J	288	0	158	6	0
6	L	246	0	137	6	0
7	M	330	0	181	3	0
8	A	2	0	0	0	0
8	C	2	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
All	All	16681	0	15403	464	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 16.

All (464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:MET:HG2	2:B:240:LEU:HD21	1.57	0.85
1:A:949:ARG:NH1	1:A:950:ASP:OD1	2.17	0.78
1:A:480:GLN:HB3	1:C:474:THR:HB	1.67	0.76
2:B:249:CYS:SG	2:B:250:THR:N	2.60	0.74
2:B:181:HIS:CE1	2:B:196:ILE:HD13	2.22	0.74
1:C:623:SER:OG	1:C:652:CYS:SG	2.47	0.73
1:C:656:CYS:HB2	1:C:675:LEU:HD11	1.71	0.72
1:C:962:GLU:OE2	1:C:965:ASN:ND2	2.22	0.72
1:A:546:ASP:OD1	2:B:229:ARG:NH1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:ASP:OD2	1:C:965:ASN:ND2	2.21	0.71
1:C:596:LYS:NZ	1:C:957:ALA:O	2.22	0.71
1:A:600:ASP:OD2	1:A:965:ASN:ND2	2.22	0.71
2:D:258:VAL:HG12	2:D:284:ARG:HD2	1.72	0.71
1:C:977:ARG:NH1	1:C:986:ASP:OD2	2.23	0.70
1:A:658:MET:CG	1:A:671:ILE:HG21	2.22	0.70
1:C:534:ILE:HG23	1:C:988:LEU:HD23	1.73	0.69
2:D:264:THR:HB	2:D:327:ILE:HD11	1.75	0.69
1:C:734:ARG:NH2	1:C:934:ASN:OD1	2.24	0.69
2:B:23:ASN:ND2	2:B:322:MET:O	2.26	0.68
1:C:585:ASP:O	1:C:696:ARG:NH2	2.27	0.68
1:C:603:GLY:O	1:C:969:ARG:NH2	2.25	0.68
1:C:597:GLU:OE1	1:C:679:ARG:NE	2.23	0.68
1:A:569:ASP:OD2	1:A:997:LYS:N	2.27	0.68
1:A:918:GLU:O	1:A:922:THR:HG23	1.94	0.68
1:A:858:MET:SD	1:A:858:MET:N	2.67	0.67
1:A:545:VAL:HG23	2:B:316:ILE:HG22	1.77	0.67
2:B:313:HIS:O	1:C:839:LYS:NZ	2.21	0.67
2:D:204:LEU:HD22	2:D:221:GLY:HA3	1.77	0.67
1:A:556:ARG:NH2	2:B:169:THR:O	2.29	0.65
2:D:142:ILE:HD13	2:D:155:LEU:HD12	1.79	0.65
1:A:607:GLU:OE2	1:C:838:ARG:NH2	2.29	0.65
1:A:929:GLU:OE1	1:A:929:GLU:N	2.30	0.65
1:C:556:ARG:NH2	2:D:169:THR:O	2.29	0.64
1:A:558:ARG:NH2	1:A:560:ASP:OD2	2.31	0.64
1:C:565:SER:HG	1:C:992:TRP:HE1	1.45	0.64
1:A:656:CYS:HB2	1:A:675:LEU:HD11	1.80	0.64
2:B:198:PRO:O	2:B:201:GLN:NE2	2.31	0.64
1:C:946:ILE:O	1:C:950:ASP:N	2.30	0.63
2:D:212:ARG:NH1	2:D:213:ASN:OD1	2.32	0.63
2:B:177:ASP:OD2	2:B:224:LEU:N	2.28	0.63
1:C:564:VAL:HG12	1:C:687:LEU:HD21	1.80	0.63
1:A:717:GLY:HA2	1:A:781:ALA:HB3	1.81	0.63
1:A:473:ASN:O	1:C:483:LYS:NZ	2.31	0.62
1:A:713:ARG:NH2	1:A:725:TYR:O	2.32	0.62
2:B:285:MET:O	2:B:307:TRP:NE1	2.28	0.62
2:D:335:ASN:OD1	2:D:335:ASN:N	2.28	0.62
1:A:678:GLU:HG3	2:B:169:THR:HG21	1.80	0.62
2:B:182:VAL:HG11	2:B:236:ILE:HD13	1.82	0.62
1:A:752:GLU:OE2	1:A:756:ARG:NH1	2.33	0.62
2:D:211:ALA:HB2	2:D:216:VAL:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ILE:HB	1:A:659:LEU:HD12	1.83	0.61
2:B:186:ASP:O	2:B:190:GLY:N	2.33	0.61
2:D:77:THR:HG22	2:D:93:ILE:HG12	1.83	0.61
1:A:727:CYS:SG	1:A:937:HIS:CD2	2.94	0.61
2:B:235:ARG:HB2	2:B:252:LEU:HD11	1.82	0.61
2:D:221:GLY:N	2:D:258:VAL:O	2.30	0.61
2:D:300:SER:OG	2:D:301:GLU:N	2.33	0.61
1:A:927:ARG:O	1:A:931:LYS:NZ	2.34	0.60
2:B:129:LEU:HB3	2:B:133:VAL:HG12	1.82	0.60
1:C:860:GLN:HA	1:C:863:VAL:HG12	1.83	0.60
2:D:177:ASP:OD2	2:D:224:LEU:N	2.35	0.60
1:A:870:ILE:O	1:A:876:HIS:NE2	2.31	0.60
2:D:6:VAL:HG21	2:D:347:THR:HG23	1.83	0.60
1:C:669:THR:HG21	2:D:100:ASN:HA	1.84	0.59
2:D:274:VAL:HG11	2:D:327:ILE:HG21	1.85	0.59
1:A:534:ILE:HG23	1:A:988:LEU:HD23	1.84	0.59
1:A:754:LEU:HD23	1:A:783:PRO:HD2	1.83	0.59
2:B:66:SER:OG	2:B:67:CYS:N	2.34	0.59
2:D:88:LYS:HZ3	2:D:88:LYS:N	2.01	0.59
1:A:474:THR:HB	1:C:480:GLN:HB3	1.85	0.59
1:A:657:LEU:HG	1:A:988:LEU:HD13	1.83	0.59
1:A:811:GLU:OE2	1:A:875:ARG:NH2	2.32	0.59
1:C:523:LEU:HD22	1:C:560:ASP:OD1	2.03	0.59
2:D:154:VAL:HG13	2:D:182:VAL:HG13	1.84	0.59
2:B:195:TYR:HB3	2:B:247:VAL:HG11	1.83	0.59
1:C:650:LEU:HD23	1:C:994:TYR:CE2	2.38	0.59
1:A:587:LEU:O	1:A:696:ARG:NE	2.36	0.59
1:C:645:LYS:NZ	7:M:20:DA:OP2	2.36	0.58
2:D:205:SER:HG	2:D:206:PHE:HD2	1.50	0.58
1:A:603:GLY:O	1:A:969:ARG:NH2	2.27	0.58
1:A:669:THR:HG21	2:B:100:ASN:HA	1.84	0.58
1:A:730:CYS:SG	1:A:937:HIS:CE1	2.95	0.58
1:C:525:ASN:O	2:D:169:THR:HG23	2.03	0.58
2:D:28:VAL:HG13	2:D:48:PHE:HB3	1.86	0.58
1:A:650:LEU:HD23	1:A:994:TYR:CE1	2.39	0.58
1:A:852:ASN:OD1	1:A:855:ARG:NH1	2.36	0.58
2:B:28:VAL:HG13	2:B:48:PHE:HB3	1.85	0.58
1:C:529:ARG:O	1:C:558:ARG:NH1	2.34	0.58
2:B:76:ALA:HB1	2:B:142:ILE:H	1.68	0.58
1:C:691:MET:O	1:C:696:ARG:NH1	2.36	0.58
1:A:563:LEU:HD11	1:A:702:PHE:HE1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:GLU:OE2	1:A:679:ARG:NE	2.36	0.58
1:A:670:ALA:O	2:B:173:ASN:ND2	2.31	0.57
2:D:154:VAL:HG11	2:D:216:VAL:HG21	1.86	0.57
2:B:317:TRP:CE3	2:B:329:LEU:HD21	2.38	0.57
1:C:600:ASP:HB3	1:C:961:ASN:ND2	2.20	0.57
2:D:223:SER:O	2:D:227:ASN:N	2.37	0.57
1:A:517:PHE:CG	1:A:564:VAL:HG21	2.40	0.57
1:A:590:PRO:HA	1:A:697:THR:HG23	1.87	0.57
2:D:286:VAL:HG12	2:D:304:THR:HG21	1.87	0.57
2:B:143:ASP:HB3	2:B:211:ALA:HB2	1.87	0.56
1:C:811:GLU:OE2	1:C:875:ARG:NH2	2.38	0.56
1:A:894:ARG:NH2	1:A:959:GLU:OE1	2.37	0.56
1:A:936:PHE:O	1:A:940:LEU:HG	2.05	0.56
1:C:568:MET:HG2	1:C:689:LEU:HD21	1.86	0.56
1:C:773:ARG:O	1:C:777:LYS:N	2.38	0.56
1:C:866:VAL:O	1:C:869:LEU:N	2.35	0.56
2:B:150:LYS:HD2	2:B:240:LEU:HD23	1.88	0.56
2:B:152:MET:CG	2:B:240:LEU:HD21	2.32	0.56
1:C:732:THR:OG1	1:C:736:GLU:OE1	2.23	0.56
1:C:927:ARG:O	1:C:931:LYS:NZ	2.34	0.56
1:A:707:TYR:CE2	1:A:787:THR:HG22	2.41	0.55
2:B:137:ARG:HD2	2:B:155:LEU:HD21	1.89	0.55
2:B:20:SER:HB3	2:B:77:THR:HG21	1.88	0.55
2:B:275:GLY:HA2	2:B:317:TRP:CZ2	2.40	0.55
1:C:553:ILE:HD11	1:C:613:PRO:HD2	1.88	0.55
2:B:283:LYS:NZ	2:B:311:ILE:O	2.40	0.55
1:A:483:LYS:NZ	1:C:473:ASN:O	2.40	0.55
1:A:588:ASN:O	1:A:697:THR:HG22	2.07	0.55
1:C:727:CYS:HB2	1:C:937:HIS:HE2	1.72	0.55
1:A:713:ARG:NE	1:A:719:GLU:O	2.37	0.55
1:A:475:PHE:HE1	1:A:967:LEU:HD22	1.71	0.54
2:D:14:LEU:HD23	2:D:46:PHE:CZ	2.42	0.54
1:C:546:ASP:OD2	2:D:229:ARG:NH2	2.38	0.54
2:D:78:CYS:HB3	2:D:142:ILE:HG23	1.88	0.54
1:C:715:VAL:O	1:C:784:PHE:N	2.34	0.54
2:B:147:SER:OG	2:B:240:LEU:HD22	2.08	0.54
2:D:285:MET:O	2:D:307:TRP:NE1	2.39	0.54
1:C:614:ALA:O	2:D:337:GLN:NE2	2.39	0.53
1:C:669:THR:HG21	2:D:100:ASN:CA	2.39	0.53
1:C:724:VAL:O	1:C:734:ARG:N	2.33	0.53
1:C:806:LYS:O	1:C:810:LEU:HG	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:ARG:HD2	2:B:205:SER:OG	2.09	0.53
1:C:753:ASN:O	1:C:779:VAL:HG11	2.07	0.53
1:C:570:MET:HE1	1:C:626:VAL:HG11	1.89	0.53
2:D:219:LEU:HD21	2:D:299:ILE:HD12	1.89	0.53
1:A:753:ASN:O	1:A:779:VAL:HG11	2.08	0.53
1:A:885:LEU:HD11	1:A:915:ARG:HG3	1.90	0.53
1:C:598:SER:O	1:C:961:ASN:ND2	2.41	0.53
1:A:517:PHE:CD1	1:A:564:VAL:HG21	2.44	0.53
1:A:631:ILE:HG22	1:A:640:VAL:CG1	2.39	0.53
1:A:724:VAL:HG12	1:A:773:ARG:HH12	1.74	0.53
1:C:808:PHE:HE1	1:C:879:LEU:HD22	1.73	0.53
2:D:159:ARG:NE	2:D:205:SER:OG	2.42	0.53
2:D:308:THR:HG22	2:D:310:ASP:H	1.74	0.53
1:A:621:ARG:NH1	1:A:961:ASN:O	2.41	0.53
1:A:759:VAL:O	1:A:763:ASN:N	2.38	0.53
2:D:107:ILE:HD12	2:D:129:LEU:HD21	1.90	0.53
2:D:314:SER:OG	2:D:316:ILE:O	2.23	0.53
1:C:658:MET:HG3	1:C:660:ALA:HB3	1.92	0.52
1:A:875:ARG:NH2	1:A:923:LYS:O	2.38	0.52
1:C:729:LEU:HD21	1:C:946:ILE:HD11	1.91	0.52
2:B:98:THR:O	2:B:101:ASN:N	2.43	0.52
2:D:36:TRP:NE1	2:D:100:ASN:OD1	2.38	0.52
1:C:511:LEU:HD21	1:C:989:LYS:HG2	1.90	0.52
1:C:717:GLY:HA2	1:C:781:ALA:HB3	1.90	0.52
1:C:803:GLU:OE2	1:C:927:ARG:NH1	2.43	0.52
1:A:625:THR:OG1	1:A:652:CYS:SG	2.65	0.52
2:B:105:ASP:OD1	2:B:105:ASP:N	2.40	0.51
1:A:773:ARG:HH21	2:B:39:ARG:HE	1.57	0.51
1:C:480:GLN:NE2	6:L:21:DG:OP1	2.36	0.51
2:D:186:ASP:O	2:D:190:GLY:N	2.41	0.51
1:A:665:HIS:O	1:A:669:THR:HG23	2.10	0.51
1:A:810:LEU:HD12	1:A:926:TYR:HE2	1.75	0.51
1:C:708:ASP:HB2	5:J:16:DC:O5'	2.10	0.51
1:A:1002:PHE:O	1:C:487:THR:HG23	2.10	0.51
1:C:484:MET:O	1:C:488:VAL:HG23	2.11	0.51
1:C:472:VAL:HG23	1:C:473:ASN:N	2.26	0.51
1:A:636:GLN:OE1	1:A:636:GLN:N	2.43	0.51
2:B:20:SER:CB	2:B:77:THR:HG21	2.40	0.51
2:B:235:ARG:NH1	2:B:250:THR:OG1	2.44	0.51
1:C:726:ILE:HD12	1:C:734:ARG:HE	1.76	0.51
2:D:242:LEU:HD23	2:D:242:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HG21	1:A:985:GLU:HG3	1.93	0.50
1:A:563:LEU:HD11	1:A:702:PHE:CE1	2.46	0.50
2:B:107:ILE:HD12	2:B:129:LEU:HD21	1.94	0.50
1:A:767:GLU:OE2	1:A:775:ARG:NE	2.38	0.50
2:B:67:CYS:N	2:B:124:CYS:O	2.45	0.50
1:C:627:MET:SD	1:C:646:PRO:HB3	2.51	0.50
1:A:855:ARG:NH1	6:L:18:DA:N7	2.58	0.50
1:A:520:GLN:HB2	1:A:521:PRO:HD3	1.93	0.50
1:A:564:VAL:HG22	1:A:687:LEU:HD21	1.94	0.50
2:D:262:ILE:HG21	2:D:327:ILE:HG23	1.94	0.50
1:C:553:ILE:HD11	1:C:613:PRO:CD	2.41	0.49
2:D:262:ILE:HG22	2:D:327:ILE:HD12	1.93	0.49
1:A:654:PRO:HB2	1:A:988:LEU:HD12	1.93	0.49
1:A:878:ALA:HB2	1:A:923:LYS:HD3	1.95	0.49
1:C:647:ASN:ND2	1:C:954:GLY:O	2.40	0.49
1:C:883:MET:O	1:C:887:LEU:HG	2.13	0.49
2:D:233:LEU:HD23	2:D:253:PRO:O	2.12	0.49
1:C:727:CYS:SG	1:C:942:HIS:CD2	3.05	0.49
2:D:76:ALA:HB1	2:D:142:ILE:H	1.78	0.49
2:D:212:ARG:NH2	2:D:269:ASP:OD1	2.45	0.49
2:B:148:ARG:NH2	2:B:148:ARG:HG3	2.26	0.49
2:B:4:GLN:NE2	2:B:53:ASN:OD1	2.46	0.48
2:B:150:LYS:CG	2:B:240:LEU:HD23	2.43	0.48
1:C:774:ASP:O	1:C:777:LYS:NZ	2.37	0.48
2:B:148:ARG:HG3	2:B:148:ARG:HH21	1.78	0.48
2:D:78:CYS:SG	2:D:144:VAL:HG13	2.53	0.48
2:D:219:LEU:HD22	2:D:273:ILE:CD1	2.43	0.48
1:A:658:MET:HG3	1:A:671:ILE:HG21	1.95	0.48
1:C:678:GLU:HG3	2:D:169:THR:HG21	1.93	0.48
1:A:790:SER:OG	1:A:791:ILE:N	2.45	0.48
2:B:78:CYS:HB3	2:B:142:ILE:HG23	1.93	0.48
2:D:95:GLY:HA2	2:D:104:SER:O	2.14	0.48
1:A:525:ASN:O	2:B:169:THR:HG23	2.14	0.48
2:B:229:ARG:NE	2:B:259:SER:OG	2.45	0.48
2:B:274:VAL:HG11	2:B:327:ILE:HD13	1.94	0.48
2:B:47:HIS:HB2	2:B:58:LYS:HB3	1.96	0.48
1:A:667:THR:O	1:A:671:ILE:HG12	2.13	0.48
2:D:197:LEU:HD12	2:D:200:LEU:HD12	1.95	0.48
5:J:13:DC:C2'	5:J:14:DT:H71	2.43	0.48
1:C:760:TRP:HA	1:C:772:LEU:HD11	1.95	0.48
2:B:4:GLN:OE1	2:B:349:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:628:ARG:HG2	1:C:630:THR:HG23	1.95	0.48
5:J:13:DC:H2'	5:J:14:DT:H71	1.96	0.47
1:C:621:ARG:HD2	1:C:968:PHE:HB2	1.96	0.47
5:I:13:DC:C2'	5:I:14:DT:H71	2.43	0.47
5:I:13:DC:H2'	5:I:14:DT:H71	1.96	0.47
1:A:471:ARG:HA	1:A:476:LEU:HB2	1.96	0.47
1:C:742:VAL:HG21	1:C:914:GLN:HA	1.96	0.47
1:A:727:CYS:SG	1:A:942:HIS:CD2	3.07	0.47
2:D:20:SER:HB3	2:D:77:THR:HG21	1.96	0.47
1:C:844:LYS:HE3	1:C:846:ILE:HG22	1.97	0.47
1:A:545:VAL:CG2	2:B:316:ILE:HG22	2.44	0.47
1:A:741:LEU:HD23	1:A:932:ILE:HD12	1.96	0.47
1:C:563:LEU:HD12	1:C:682:MET:SD	2.55	0.47
1:A:595:VAL:CG1	1:A:624:PHE:HB2	2.45	0.47
1:A:803:GLU:HG3	1:A:928:TYR:OH	2.15	0.47
1:C:567:LEU:O	1:C:571:GLU:N	2.48	0.47
1:C:921:SER:O	1:C:925:LYS:HB3	2.15	0.47
2:D:286:VAL:HG23	2:D:286:VAL:O	2.15	0.47
2:D:38:LYS:O	2:D:41:CYS:N	2.34	0.47
1:A:806:LYS:O	1:A:810:LEU:HG	2.15	0.47
1:A:875:ARG:NH1	1:A:923:LYS:O	2.48	0.47
1:C:558:ARG:O	1:C:561:SER:N	2.48	0.47
1:C:810:LEU:O	1:C:814:GLU:N	2.48	0.47
2:D:220:GLY:HA3	2:D:258:VAL:HG22	1.96	0.47
1:A:658:MET:HG2	1:A:671:ILE:HG21	1.96	0.47
1:A:758:GLU:OE2	1:A:761:ARG:NH2	2.45	0.47
2:B:74:TYR:N	2:B:75:PRO:CD	2.78	0.47
1:C:570:MET:HG2	1:C:997:LYS:HG3	1.96	0.47
1:A:474:THR:HA	1:C:480:GLN:OE1	2.15	0.46
1:C:478:CYS:N	6:L:23:DG:OP1	2.45	0.46
1:C:480:GLN:HG2	6:L:22:DT:OP2	2.15	0.46
1:C:983:GLU:HG3	1:C:984:MET:HE2	1.97	0.46
1:A:1001:LYS:O	1:A:1004:ASN:N	2.48	0.46
1:A:571:GLU:O	1:A:575:LEU:HG	2.15	0.46
1:A:621:ARG:HD2	1:A:968:PHE:HB2	1.97	0.46
1:C:554:ALA:HA	1:C:658:MET:HA	1.98	0.46
1:A:748:ARG:NH1	1:A:777:LYS:O	2.47	0.46
1:A:926:TYR:O	1:A:927:ARG:HB3	2.16	0.46
1:C:592:THR:N	1:C:630:THR:O	2.43	0.46
2:B:139:GLY:O	2:B:206:PHE:N	2.37	0.46
1:A:883:MET:O	1:A:887:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:MET:CE	1:A:955:ALA:HB1	2.45	0.46
1:A:717:GLY:O	1:A:779:VAL:HA	2.16	0.46
1:A:808:PHE:HE1	1:A:879:LEU:HD22	1.80	0.46
2:B:3:LEU:HD13	2:B:348:LEU:HD11	1.98	0.46
1:C:793:ALA:HB1	1:C:894:ARG:HD3	1.97	0.46
1:C:591:PHE:CZ	1:C:631:ILE:HD12	2.50	0.46
1:C:991:HIS:O	1:C:991:HIS:ND1	2.48	0.46
2:D:292:LEU:CD2	2:D:297:ILE:HD12	2.45	0.46
1:A:649:VAL:HG22	1:A:967:LEU:HD12	1.98	0.46
2:D:145:VAL:HB	2:D:214:ASP:HA	1.98	0.46
1:A:529:ARG:NH2	1:A:531:ASP:OD1	2.49	0.46
1:A:773:ARG:HD3	2:B:39:ARG:HE	1.81	0.46
1:C:510:LEU:HD11	1:C:999:LEU:HD21	1.97	0.46
2:B:158:GLY:N	2:B:204:LEU:O	2.41	0.45
2:D:211:ALA:CB	2:D:216:VAL:HG12	2.46	0.45
2:B:45:VAL:HG21	2:B:62:PHE:CE1	2.52	0.45
1:C:605:VAL:HG11	1:C:659:LEU:HD11	1.98	0.45
1:A:557:PHE:CE2	1:A:988:LEU:HG	2.51	0.45
1:C:547:GLU:HA	1:C:547:GLU:OE1	2.16	0.45
1:A:517:PHE:HB2	1:A:687:LEU:HD11	1.98	0.45
1:A:547:GLU:OE1	2:B:138:TYR:HE2	1.99	0.45
1:C:790:SER:OG	1:C:791:ILE:N	2.45	0.45
1:C:805:TYR:OH	1:C:834:ASP:OD1	2.35	0.45
1:A:545:VAL:HG13	2:B:277:TYR:CD2	2.52	0.45
1:A:560:ASP:N	1:A:560:ASP:OD1	2.43	0.45
2:B:169:THR:HA	2:B:172:TRP:HB2	1.98	0.45
1:A:547:GLU:OE1	2:B:138:TYR:CE2	2.69	0.45
1:A:563:LEU:HD12	1:A:682:MET:SD	2.57	0.45
1:A:620:VAL:HB	1:A:658:MET:HB2	1.99	0.45
1:A:924:PHE:O	1:A:926:TYR:O	2.35	0.45
1:C:810:LEU:HD11	1:C:927:ARG:HD3	1.98	0.45
2:B:156:PHE:HB2	2:B:182:VAL:HG12	1.98	0.45
1:C:972:ARG:NE	1:C:983:GLU:OE2	2.48	0.45
2:D:74:TYR:N	2:D:75:PRO:CD	2.80	0.45
2:D:169:THR:HA	2:D:172:TRP:HB2	1.98	0.45
1:A:974:MET:HA	7:M:22:DT:H5”	1.99	0.45
2:B:289:LEU:HB2	2:B:302:MET:HG3	1.99	0.45
1:C:475:PHE:HE1	1:C:967:LEU:HD22	1.82	0.45
1:A:894:ARG:NH1	1:A:959:GLU:OE1	2.50	0.45
1:C:534:ILE:HG21	1:C:985:GLU:HG3	1.98	0.44
5:I:8:DT:H1’	5:I:9:DA:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:ARG:HH12	6:L:18:DA:H62	1.64	0.44
1:C:620:VAL:HB	1:C:658:MET:HG2	1.99	0.44
1:C:621:ARG:HB3	1:C:621:ARG:CZ	2.47	0.44
1:C:648:SER:HA	7:M:19:DC:H4'	1.99	0.44
2:D:80:TYR:CE1	2:D:144:VAL:HG11	2.52	0.44
1:A:837:LEU:O	1:A:842:ASN:N	2.51	0.44
2:B:274:VAL:HG11	2:B:327:ILE:HG21	1.98	0.44
1:C:591:PHE:CE2	1:C:631:ILE:HD12	2.53	0.44
1:A:804:PHE:CE2	1:A:882:LEU:HD23	2.52	0.44
2:D:48:PHE:CE1	2:D:55:LEU:HD21	2.52	0.44
2:D:159:ARG:HD2	2:D:205:SER:CB	2.47	0.44
1:A:725:TYR:OH	1:A:774:ASP:HA	2.17	0.44
1:C:843:LEU:HD13	1:C:856:LYS:HB2	2.00	0.44
1:A:674:PRO:HG3	2:B:172:TRP:HB3	1.99	0.44
1:A:805:TYR:OH	1:A:834:ASP:OD1	2.34	0.44
1:C:519:TRP:CG	1:C:523:LEU:HD13	2.52	0.44
1:C:673:SER:N	1:C:674:PRO:CD	2.80	0.44
2:D:76:ALA:HB1	2:D:142:ILE:N	2.32	0.44
1:A:621:ARG:HB3	1:A:621:ARG:CZ	2.47	0.44
1:A:810:LEU:O	1:A:814:GLU:N	2.50	0.44
1:A:1005:ALA:HA	1:A:1008:ALA:HB3	1.98	0.44
2:B:204:LEU:HD22	2:B:221:GLY:HA3	1.99	0.44
2:B:19:PHE:HB2	2:B:30:PHE:CE1	2.53	0.44
2:B:97:LYS:HZ2	2:B:97:LYS:HB3	1.83	0.44
1:C:467:CYS:HB3	1:C:481:TYR:OH	2.18	0.44
1:C:480:GLN:OE1	1:C:483:LYS:NZ	2.30	0.44
1:C:569:ASP:OD1	1:C:997:LYS:N	2.50	0.44
1:A:551:ASP:OD1	1:A:551:ASP:N	2.47	0.44
1:A:630:THR:HG22	1:A:639:LYS:HG2	2.00	0.44
1:A:929:GLU:HG2	1:A:929:GLU:O	2.18	0.44
1:C:571:GLU:O	1:C:575:LEU:HG	2.17	0.44
5:J:8:DT:H1'	5:J:9:DA:C8	2.52	0.44
1:A:532:VAL:HG23	1:A:532:VAL:O	2.17	0.43
2:D:206:PHE:HB3	2:D:260:SER:H	1.83	0.43
1:A:503:LEU:O	1:A:507:GLU:HG3	2.18	0.43
1:C:532:VAL:HG23	1:C:532:VAL:O	2.18	0.43
2:D:72:LEU:HD13	2:D:95:GLY:O	2.19	0.43
1:A:680:GLU:OE2	1:A:683:LYS:NZ	2.51	0.43
1:C:616:PRO:HD2	1:C:659:LEU:O	2.18	0.43
1:C:938:LYS:HA	1:C:942:HIS:HD2	1.83	0.43
2:D:109:ILE:HD12	2:D:127:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:THR:OG1	1:A:956:TRP:HB3	2.18	0.43
1:A:810:LEU:HD12	1:A:926:TYR:CE2	2.54	0.43
2:B:212:ARG:O	2:B:215:THR:O	2.37	0.43
1:C:729:LEU:CD2	1:C:946:ILE:HD11	2.48	0.43
2:B:29:PHE:CD1	2:B:122:PHE:HZ	2.35	0.43
1:C:519:TRP:CH2	1:C:682:MET:SD	3.11	0.43
2:D:74:TYR:N	2:D:75:PRO:HD3	2.34	0.43
2:B:150:LYS:CD	2:B:240:LEU:HD23	2.47	0.43
1:C:935:TYR:OH	5:J:16:DC:OP1	2.33	0.43
2:B:142:ILE:HD13	2:B:155:LEU:HD12	2.01	0.43
1:C:565:SER:O	1:C:569:ASP:HB3	2.18	0.43
1:C:654:PRO:HG3	1:C:991:HIS:HB3	2.01	0.43
1:C:724:VAL:HG22	1:C:733:THR:CG2	2.48	0.43
1:C:838:ARG:O	1:C:842:ASN:HA	2.19	0.43
1:C:967:LEU:HD11	1:C:994:TYR:CE2	2.54	0.43
2:D:112:VAL:HG13	2:D:120:VAL:HG13	2.01	0.43
2:B:8:VAL:HG11	2:B:55:LEU:HD23	2.01	0.43
1:C:538:LEU:O	1:C:541:LEU:HB2	2.18	0.43
1:C:557:PHE:CE2	1:C:988:LEU:HG	2.54	0.43
1:A:820:ASN:OD1	1:A:820:ASN:N	2.51	0.43
1:C:471:ARG:HA	1:C:476:LEU:HB2	1.99	0.43
1:C:542:ALA:HB3	1:C:547:GLU:HG3	2.01	0.43
1:C:892:VAL:HG21	1:C:909:TYR:HD2	1.84	0.43
1:A:724:VAL:O	1:A:733:THR:HA	2.19	0.42
2:B:140:HIS:HB3	2:B:158:GLY:HA3	2.00	0.42
1:C:523:LEU:CD2	1:C:560:ASP:OD1	2.66	0.42
1:C:649:VAL:CG2	1:C:964:GLY:HA2	2.49	0.42
1:C:810:LEU:CD1	1:C:927:ARG:HD3	2.49	0.42
1:C:510:LEU:CD1	1:C:999:LEU:HD21	2.49	0.42
1:C:588:ASN:ND2	1:C:588:ASN:O	2.52	0.42
1:A:972:ARG:NE	1:A:983:GLU:OE1	2.52	0.42
2:B:296:THR:HG22	2:B:297:ILE:N	2.33	0.42
2:B:308:THR:HG22	2:B:310:ASP:H	1.85	0.42
2:D:14:LEU:O	2:D:34:LYS:N	2.44	0.42
2:D:279:LEU:HG	2:D:282:GLN:HB3	2.01	0.42
1:A:715:VAL:O	1:A:783:PRO:HA	2.20	0.42
1:A:844:LYS:NZ	1:C:607:GLU:O	2.28	0.42
2:D:159:ARG:CD	2:D:205:SER:OG	2.68	0.42
2:D:208:VAL:HG21	2:D:273:ILE:HD13	2.02	0.42
1:A:633:HIS:O	1:A:635:SER:N	2.48	0.42
1:A:508:LYS:O	1:A:514:TYR:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:CYS:SG	1:A:939:THR:OG1	2.77	0.42
1:A:851:GLY:O	1:A:855:ARG:HG2	2.19	0.42
2:B:36:TRP:NE1	2:B:100:ASN:OD1	2.46	0.42
2:D:143:ASP:HB3	2:D:211:ALA:HB2	2.02	0.42
5:I:14:DT:H2"	5:I:15:DA:O5'	2.20	0.42
1:A:532:VAL:HG21	1:A:558:ARG:HD3	2.01	0.42
1:A:559:TYR:HA	1:A:655:LEU:HD11	2.01	0.42
1:C:885:LEU:HD21	1:C:915:ARG:HG2	2.02	0.42
6:L:21:DG:H2'	6:L:22:DT:H72	2.01	0.42
1:A:481:TYR:OH	1:A:498:GLN:O	2.21	0.42
1:C:732:THR:HG23	1:C:733:THR:N	2.34	0.42
2:D:137:ARG:HH11	2:D:157:GLY:HA2	1.85	0.42
2:D:167:ARG:NH2	2:D:172:TRP:O	2.47	0.42
1:A:560:ASP:O	1:A:564:VAL:HG23	2.20	0.42
2:B:321:ASN:OD1	2:B:323:GLY:N	2.45	0.42
1:C:704:GLY:CA	1:C:707:TYR:HE1	2.32	0.42
2:D:163:PRO:O	2:D:167:ARG:N	2.50	0.42
1:A:480:GLN:OE1	1:C:474:THR:HA	2.20	0.41
1:A:487:THR:HG23	1:C:1002:PHE:O	2.20	0.41
1:A:796:CYS:HA	1:A:935:TYR:CG	2.54	0.41
2:B:48:PHE:CE1	2:B:55:LEU:HD21	2.55	0.41
2:B:310:ASP:O	2:B:331:ILE:HD12	2.20	0.41
1:C:621:ARG:NH1	1:C:961:ASN:O	2.52	0.41
1:A:551:ASP:HA	1:A:613:PRO:HB2	2.01	0.41
1:A:649:VAL:HG22	1:A:967:LEU:CD1	2.50	0.41
1:A:721:SER:O	1:A:734:ARG:NH1	2.52	0.41
1:A:943:VAL:O	1:A:947:ILE:HG12	2.20	0.41
2:B:316:ILE:HG13	2:B:317:TRP:N	2.34	0.41
1:C:545:VAL:HG11	2:D:280:GLU:O	2.19	0.41
2:D:297:ILE:HD11	2:D:299:ILE:HD11	2.02	0.41
1:A:598:SER:O	1:A:961:ASN:ND2	2.53	0.41
1:A:833:LEU:O	1:A:837:LEU:HG	2.21	0.41
2:B:29:PHE:HE1	2:B:47:HIS:CD2	2.38	0.41
1:C:545:VAL:HG12	2:D:316:ILE:HG22	2.01	0.41
1:C:559:TYR:HB2	1:C:678:GLU:OE1	2.20	0.41
1:C:669:THR:HG23	1:C:784:PHE:CE1	2.55	0.41
1:C:748:ARG:NH2	1:C:777:LYS:O	2.41	0.41
2:D:92:ILE:HG21	2:D:187:PHE:CZ	2.55	0.41
5:J:14:DT:H2"	5:J:15:DA:O5'	2.20	0.41
1:A:972:ARG:O	1:A:978:GLN:NE2	2.43	0.41
2:B:147:SER:OG	2:B:240:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:VAL:HG21	1:C:659:LEU:HD23	2.03	0.41
1:A:559:TYR:HB2	1:A:678:GLU:OE1	2.20	0.41
2:B:264:THR:OG1	2:B:327:ILE:HG13	2.20	0.41
1:C:972:ARG:O	1:C:978:GLN:NE2	2.52	0.41
2:D:29:PHE:CG	2:D:122:PHE:HZ	2.39	0.41
1:A:593:VAL:HG13	1:A:629:ILE:HG12	2.02	0.41
2:B:270:GLU:HA	2:B:290:VAL:O	2.21	0.41
1:C:475:PHE:CE1	1:C:967:LEU:HD22	2.56	0.41
1:C:606:SER:O	1:C:972:ARG:NH2	2.52	0.41
1:C:679:ARG:NH2	1:C:683:LYS:HD2	2.36	0.41
1:C:943:VAL:O	1:C:947:ILE:HG12	2.21	0.41
2:D:80:TYR:OH	2:D:187:PHE:CD1	2.72	0.41
1:A:769:VAL:HG21	2:B:42:PRO:CG	2.50	0.41
2:B:76:ALA:HB2	2:B:140:HIS:CD2	2.55	0.41
2:B:216:VAL:O	2:B:216:VAL:HG13	2.21	0.41
2:B:258:VAL:HG22	2:B:259:SER:N	2.36	0.41
1:C:519:TRP:O	1:C:520:GLN:C	2.58	0.41
1:C:550:VAL:HG23	1:C:550:VAL:O	2.20	0.41
1:C:670:ALA:O	2:D:173:ASN:ND2	2.40	0.41
1:C:989:LYS:HE3	1:C:989:LYS:HB3	1.93	0.41
2:D:112:VAL:HG22	2:D:120:VAL:HG11	2.02	0.41
1:A:519:TRP:HA	1:A:686:GLU:O	2.21	0.41
1:A:563:LEU:O	1:A:567:LEU:HG	2.21	0.41
1:C:563:LEU:O	1:C:567:LEU:HG	2.21	0.41
2:D:107:ILE:HG13	2:D:129:LEU:HD11	2.03	0.41
1:A:727:CYS:SG	1:A:729:LEU:HD13	2.61	0.40
2:B:38:LYS:O	2:B:41:CYS:N	2.54	0.40
1:C:893:TRP:HB3	1:C:953:ILE:HD12	2.03	0.40
1:C:570:MET:HE1	1:C:626:VAL:CG1	2.50	0.40
1:C:630:THR:HG22	1:C:639:LYS:HA	2.02	0.40
1:C:730:CYS:HB3	1:C:942:HIS:HE1	1.86	0.40
1:A:854:ALA:O	1:A:857:LEU:N	2.54	0.40
1:A:935:TYR:CD1	1:A:938:LYS:HD2	2.57	0.40
2:B:212:ARG:NE	2:B:269:ASP:OD1	2.54	0.40
1:C:600:ASP:OD2	1:C:965:ASN:OD1	2.38	0.40
1:C:623:SER:CB	1:C:652:CYS:HG	2.33	0.40
2:D:140:HIS:HB2	2:D:156:PHE:O	2.22	0.40
1:A:659:LEU:HD23	1:A:659:LEU:HA	1.90	0.40
1:C:578:MET:O	1:C:583:LEU:HB2	2.22	0.40
1:C:755:GLN:O	1:C:759:VAL:HG23	2.21	0.40
2:D:229:ARG:HE	2:D:259:SER:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ARG:NH1	2:B:294:ASP:HA	2.36	0.40
1:C:674:PRO:HG3	2:D:172:TRP:HB3	2.03	0.40
1:C:803:GLU:HG3	1:C:928:TYR:OH	2.21	0.40
2:D:277:TYR:HA	2:D:283:LYS:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	548/750 (73%)	499 (91%)	49 (9%)	0	100	100
1	C	546/750 (73%)	500 (92%)	46 (8%)	0	100	100
2	B	340/363 (94%)	305 (90%)	35 (10%)	0	100	100
2	D	341/363 (94%)	310 (91%)	30 (9%)	1 (0%)	41	71
All	All	1775/2226 (80%)	1614 (91%)	160 (9%)	1 (0%)	54	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	134	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	486/668 (73%)	477 (98%)	9 (2%)	57 84
1	C	485/668 (73%)	467 (96%)	18 (4%)	34 68
2	B	299/318 (94%)	281 (94%)	18 (6%)	19 49
2	D	299/318 (94%)	286 (96%)	13 (4%)	29 62
All	All	1569/1972 (80%)	1511 (96%)	58 (4%)	37 68

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545	VAL
1	A	559	TYR
1	A	649	VAL
1	A	652	CYS
1	A	665	HIS
1	A	708	ASP
1	A	727	CYS
1	A	768	SER
1	A	991	HIS
2	B	1	MET
2	B	40	SER
2	B	69	LEU
2	B	97	LYS
2	B	101	ASN
2	B	104	SER
2	B	111	SER
2	B	114	CYS
2	B	141	SER
2	B	148	ARG
2	B	159	ARG
2	B	186	ASP
2	B	193	THR
2	B	288	SER
2	B	291	SER
2	B	300	SER
2	B	317	TRP
2	B	340	SER
1	C	477	SER
1	C	485	TYR
1	C	495	GLN
1	C	520	GLN
1	C	527	SER
1	C	559	TYR

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Mol	Chain	Res	Type
1	C	569	ASP
1	C	584	ASP
1	C	598	SER
1	C	611	SER
1	C	635	SER
1	C	641	PHE
1	C	727	CYS
1	C	735	LEU
1	C	747	THR
1	C	940	LEU
1	C	958	SER
1	C	991	HIS
2	D	33	GLN
2	D	40	SER
2	D	66	SER
2	D	78	CYS
2	D	88	LYS
2	D	111	SER
2	D	114	CYS
2	D	128	ASP
2	D	181	HIS
2	D	242	LEU
2	D	317	TRP
2	D	320	SER
2	D	335	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	HIS
1	A	647	ASN
1	A	755	GLN
2	B	181	HIS
2	B	265	GLN
1	C	463	GLN
1	C	820	ASN
2	D	53	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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.

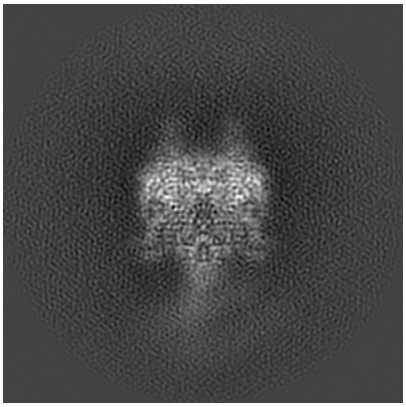
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22273. These allow visual inspection of the internal detail of the map and identification of artifacts.

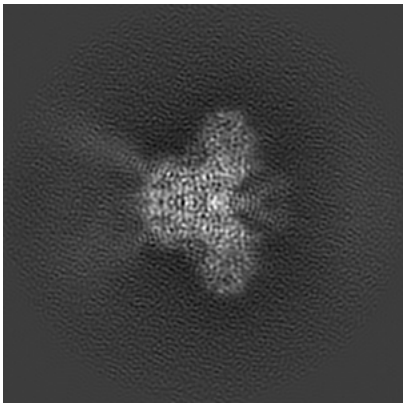
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

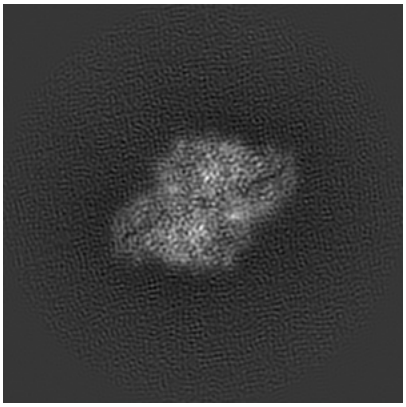
6.1.1 Primary map



X



Y

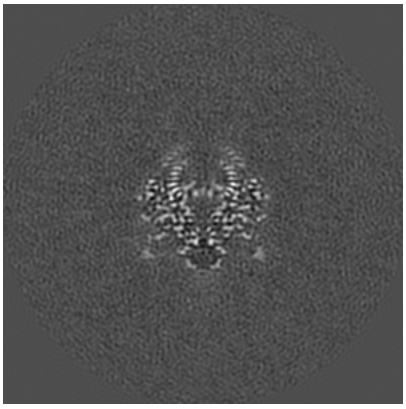


Z

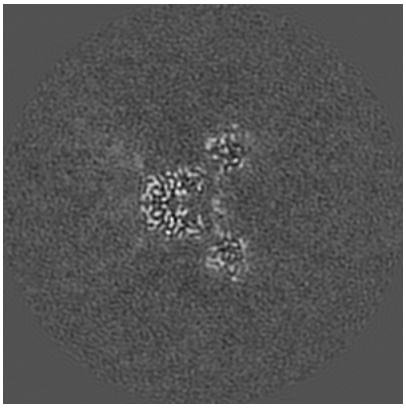
The images above show the map projected in three orthogonal directions.

6.2 Central slices

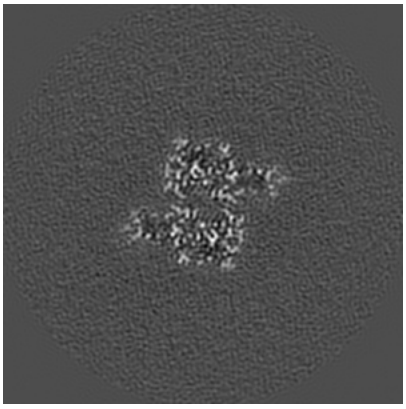
6.2.1 Primary map



X Index: 122



Y Index: 122

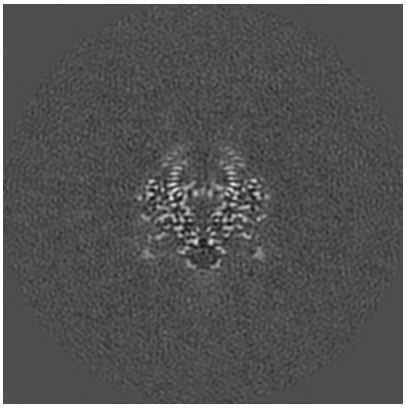


Z Index: 122

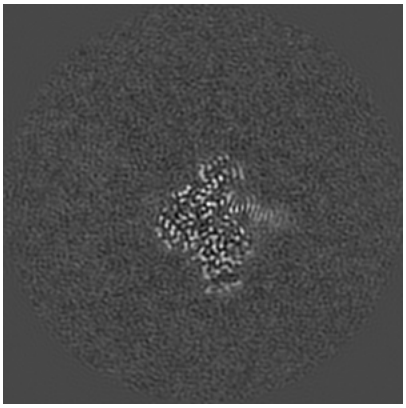
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

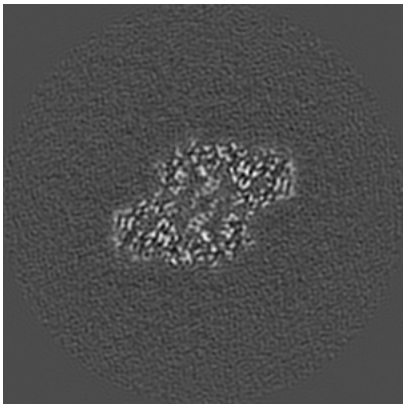
6.3.1 Primary map



X Index: 122



Y Index: 102

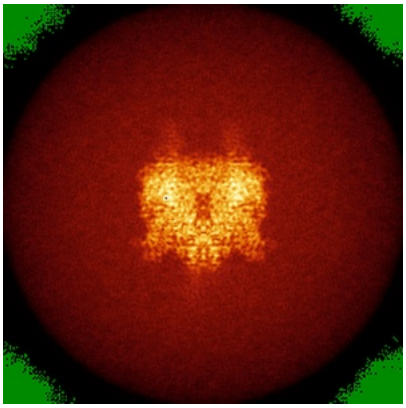


Z Index: 133

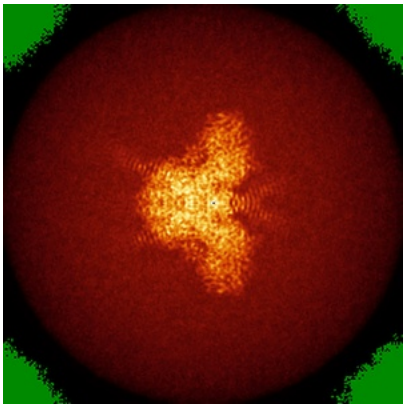
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

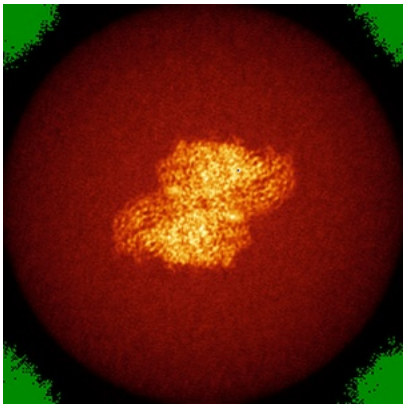
6.4.1 Primary map



X



Y

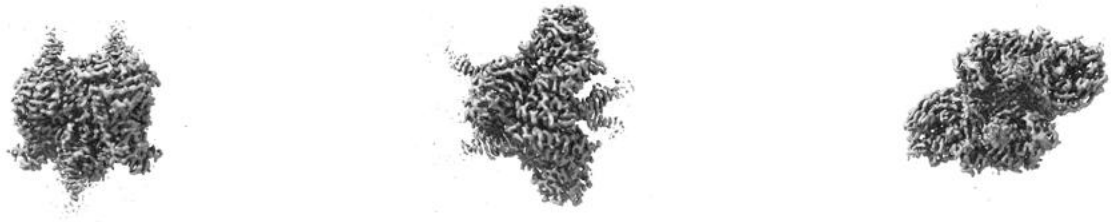


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

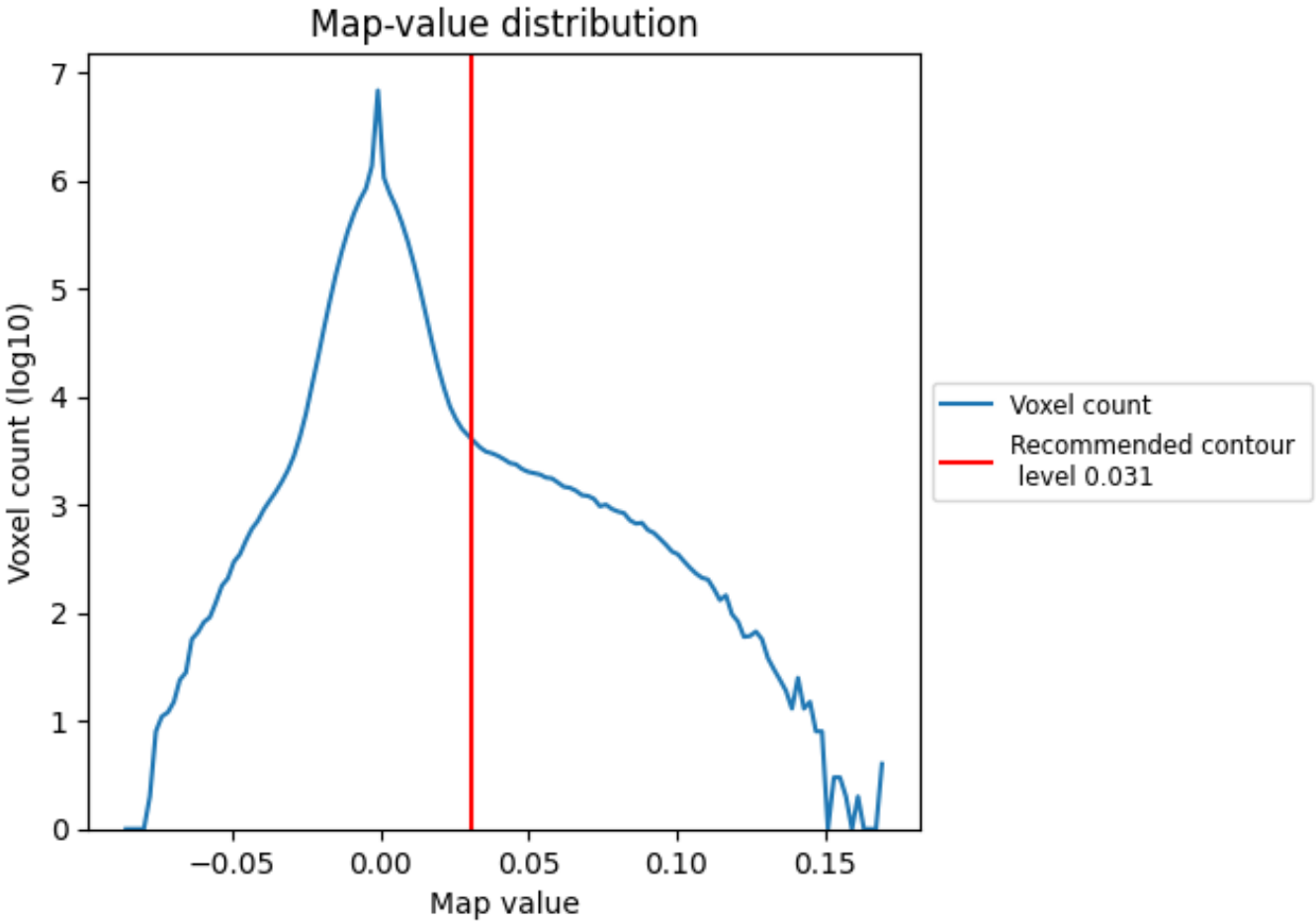
6.6 Mask visualisation (i)

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

7 Map analysis

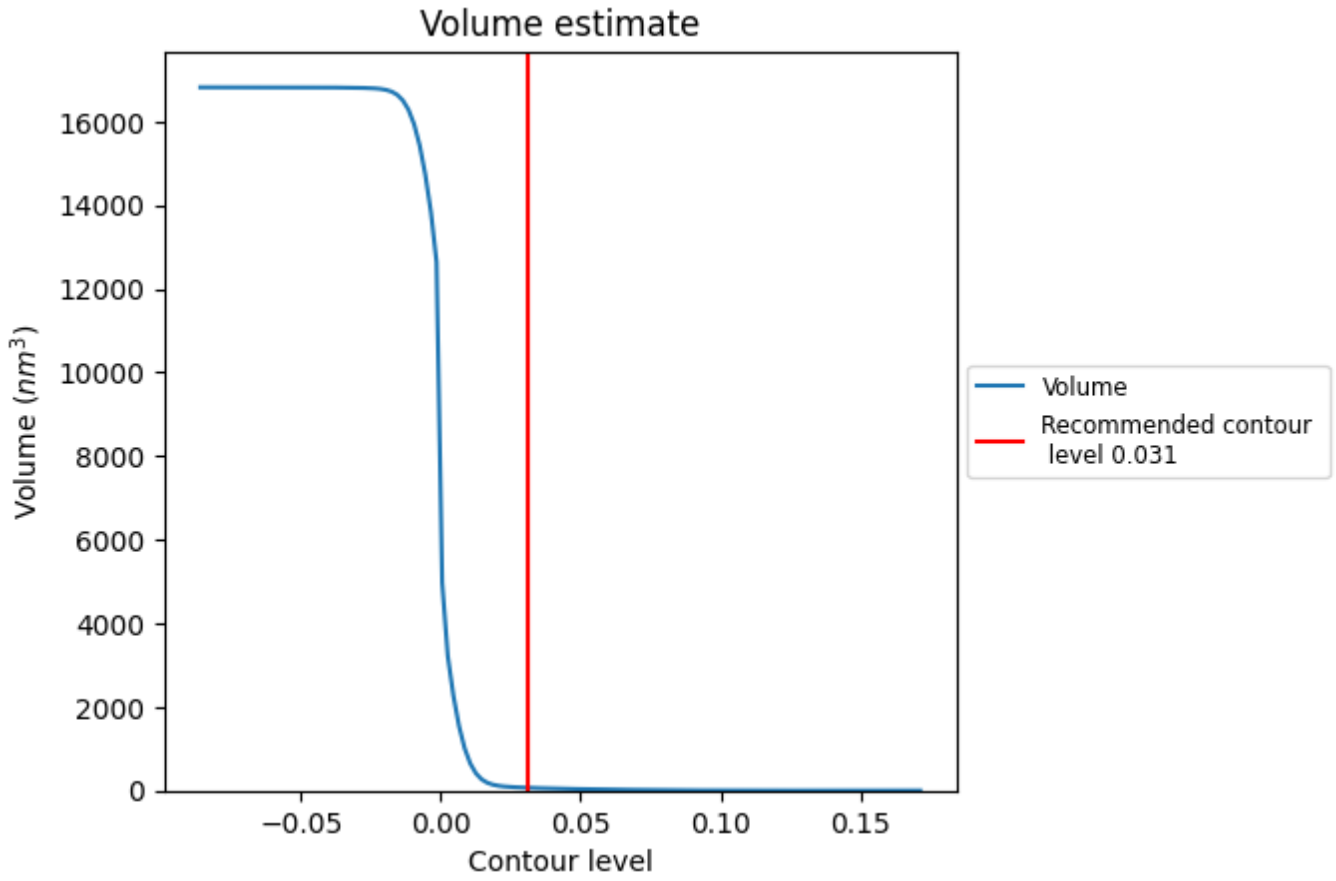
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

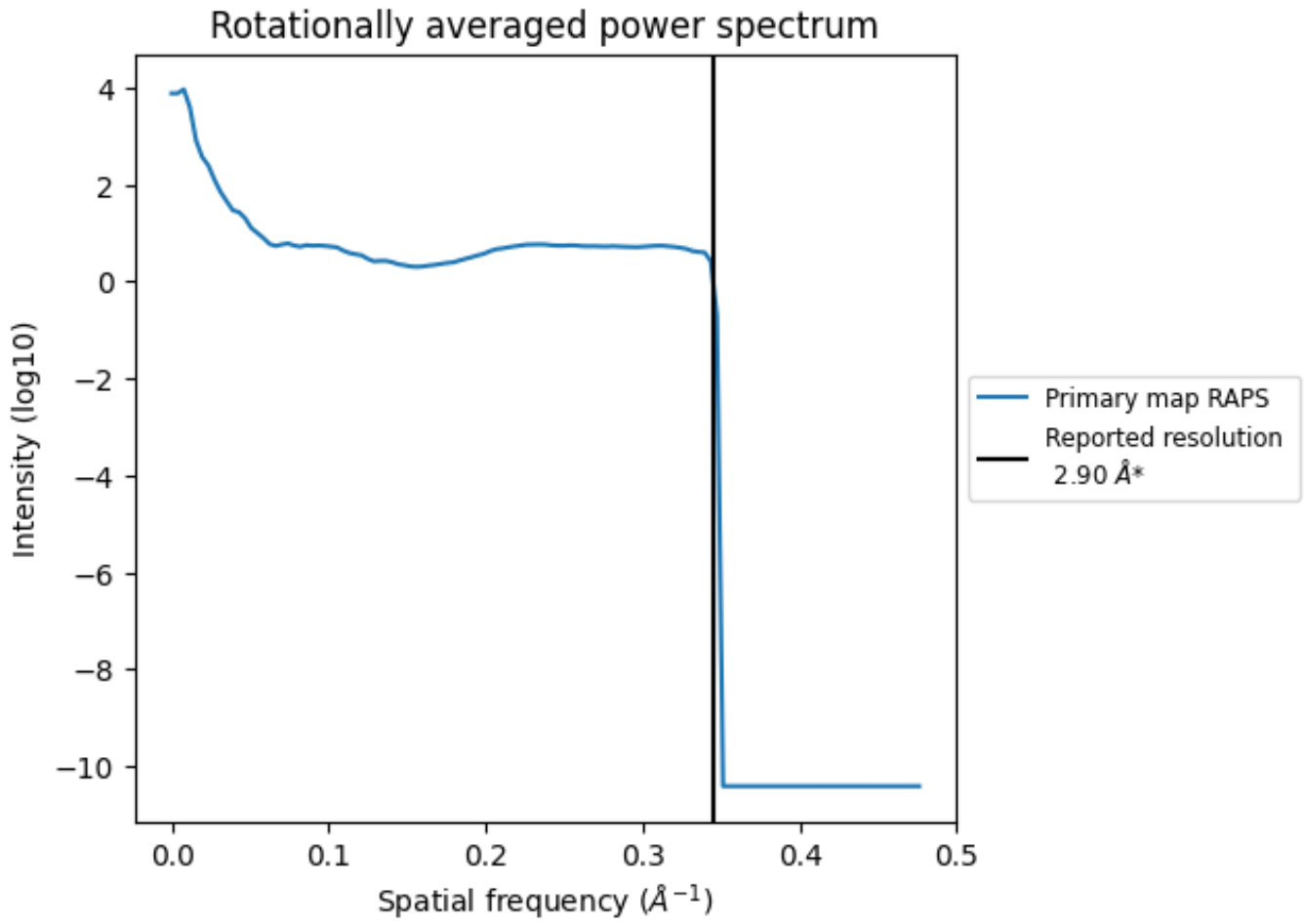
7.2 Volume estimate



The volume at the recommended contour level is 67 nm^3; this corresponds to an approximate mass of 60 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 (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

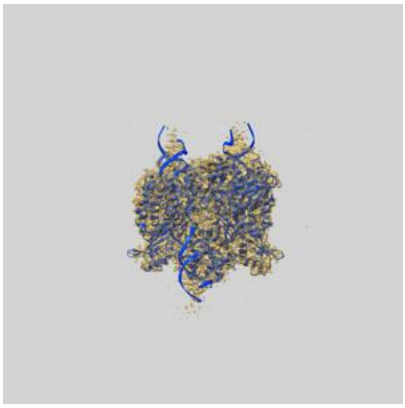
8 Fourier-Shell correlation (i)

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

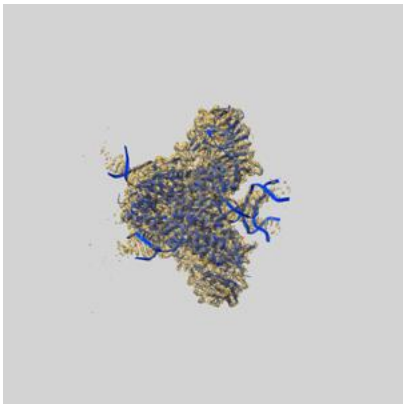
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22273 and PDB model 6XNY. Per-residue inclusion information can be found in section 3 on page 7.

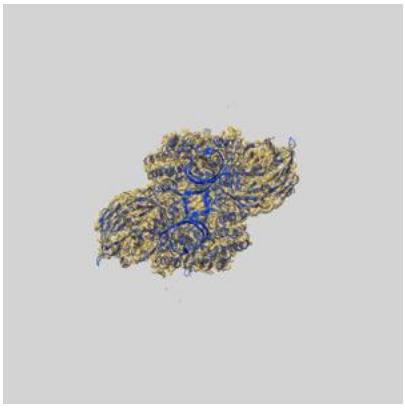
9.1 Map-model overlay



X



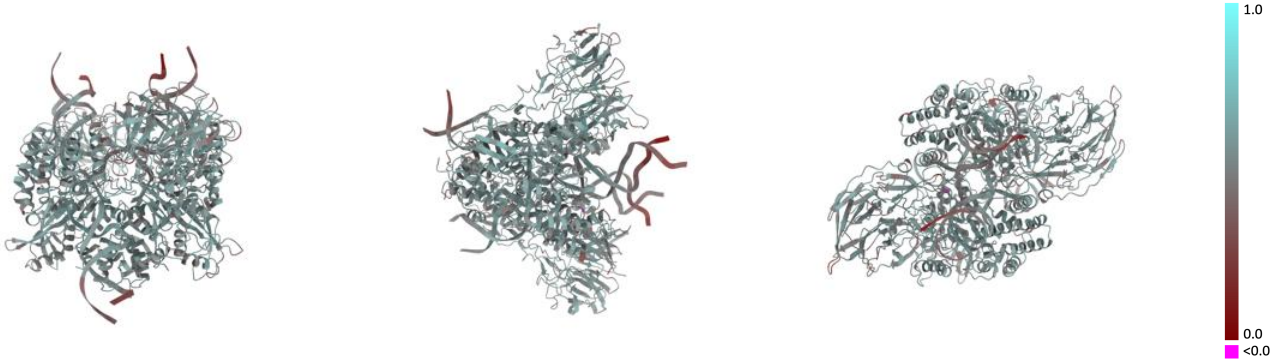
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.031 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.

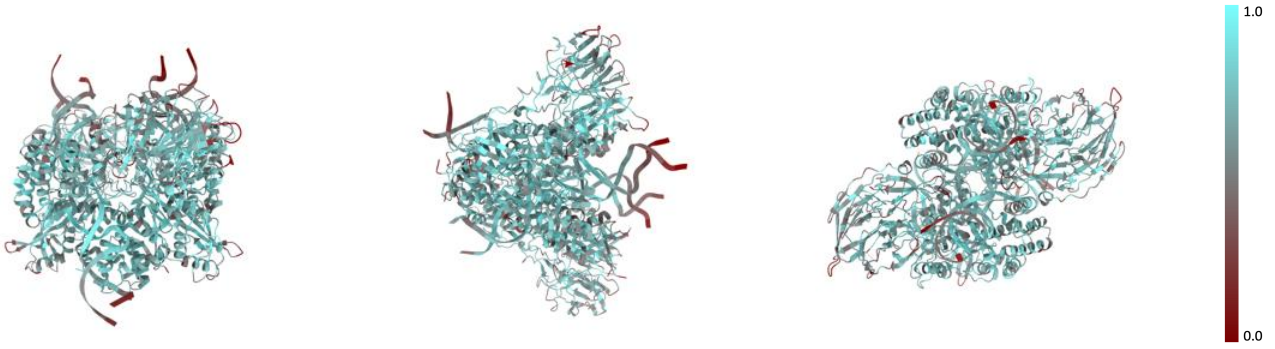
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

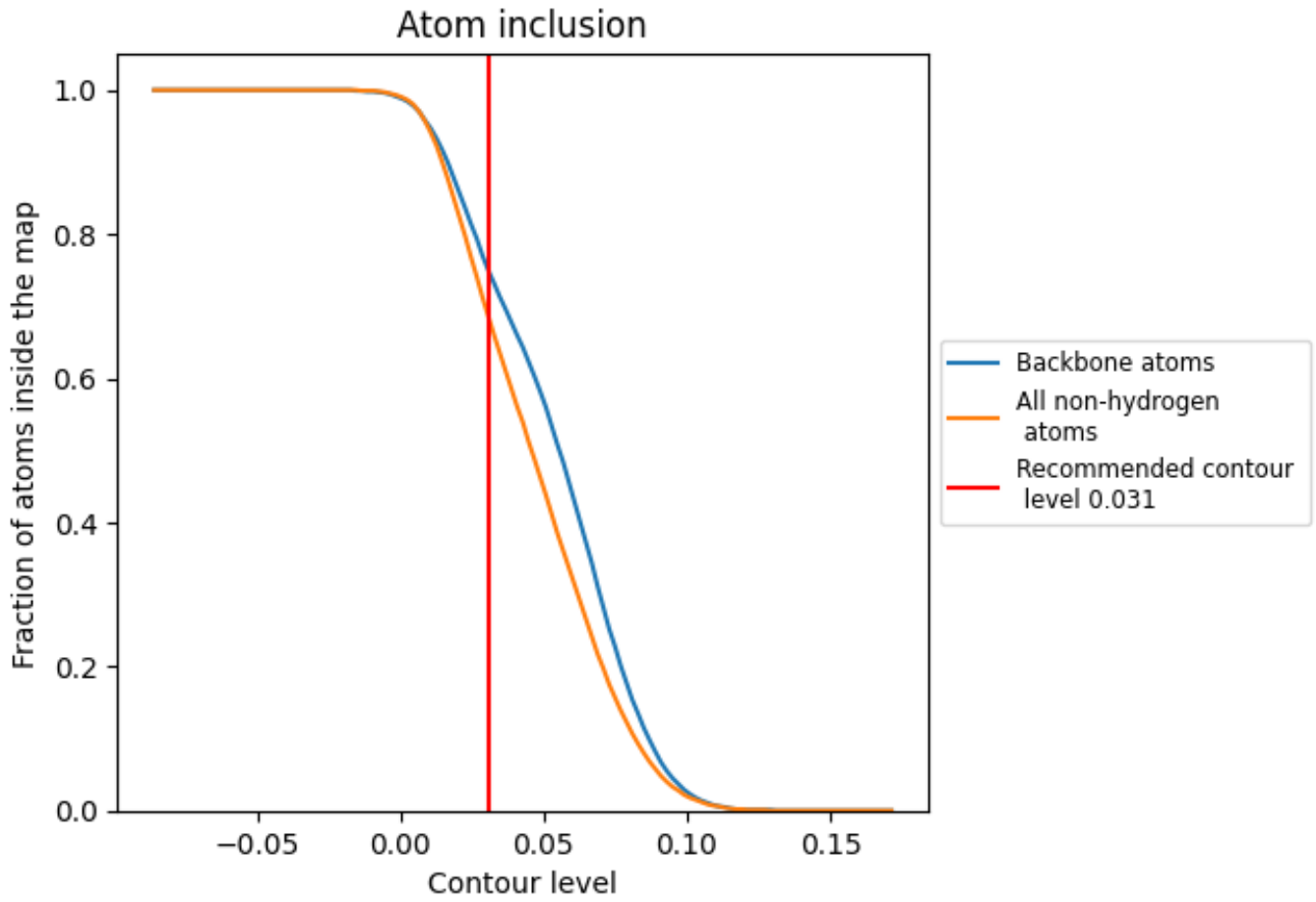
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.031).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.5340
A	0.7150	0.5500
B	0.6530	0.5330
C	0.7140	0.5500
D	0.6340	0.5240
I	0.5590	0.4500
J	0.5970	0.4720
L	0.7680	0.5640
M	0.7420	0.5310
x	0.6180	0.4630
y	0.6550	0.4850