Full wwPDB EM Validation Report ⓘ

Dec 8, 2022 – 04:15 PM JST

PDB ID	:	7Y85
EMDB ID	:	EMD-33681
Title	:	CryoEM structure of type III-E CRISPR Craspase gRAMP-crRNA in complex with TPR-CHAT protease bound to self RNA target
Authors	:	Zhang, J.T.; Cui, N.; Huang, H.D.; Jia, N.
Deposited on	:	2022-06-22
Resolution	:	2.73 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:

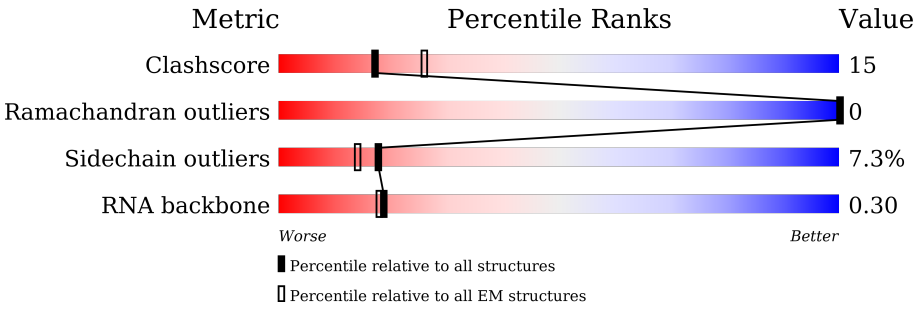
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.73 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
RNA backbone	4643	859

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	1728	7% 45% 25% 29%
2	B	110	7% 14% 11% 67%
3	C	56	7% 14% 16% 11% 59%
4	D	746	25% 51% 33% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16502 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 RAMP superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1232	Total	C	N	O	S	0	0
			9941	6333	1734	1843	31		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A0B0EGF3
A	-4	HIS	-	expression tag	UNP A0A0B0EGF3
A	-3	HIS	-	expression tag	UNP A0A0B0EGF3
A	-2	HIS	-	expression tag	UNP A0A0B0EGF3
A	-1	HIS	-	expression tag	UNP A0A0B0EGF3
A	0	HIS	-	expression tag	UNP A0A0B0EGF3
A	1	HIS	-	expression tag	UNP A0A0B0EGF3
A	2	LYS	-	expression tag	UNP A0A0B0EGF3
A	3	SER	-	expression tag	UNP A0A0B0EGF3
A	4	ASN	-	expression tag	UNP A0A0B0EGF3
A	5	ASP	-	expression tag	UNP A0A0B0EGF3

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	36	Total	C	N	O	P	0	0
			757	339	128	254	36		

- Molecule 3 is a RNA chain called Self RNA target.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	23	Total	C	N	O	P	0	0
			496	221	93	159	23		

- Molecule 4 is a protein called CHAT domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	652	Total	C	N	O	S	0	0
			5303	3391	907	980	25		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	717	GLY	-	expression tag	UNP A0A0B0EKL4
D	718	GLY	-	expression tag	UNP A0A0B0EKL4
D	719	SER	-	expression tag	UNP A0A0B0EKL4
D	720	GLY	-	expression tag	UNP A0A0B0EKL4
D	721	TRP	-	expression tag	UNP A0A0B0EKL4
D	722	SER	-	expression tag	UNP A0A0B0EKL4
D	723	HIS	-	expression tag	UNP A0A0B0EKL4
D	724	PRO	-	expression tag	UNP A0A0B0EKL4
D	725	GLN	-	expression tag	UNP A0A0B0EKL4
D	726	PHE	-	expression tag	UNP A0A0B0EKL4
D	727	GLU	-	expression tag	UNP A0A0B0EKL4
D	728	LYS	-	expression tag	UNP A0A0B0EKL4
D	729	GLY	-	expression tag	UNP A0A0B0EKL4
D	730	GLY	-	expression tag	UNP A0A0B0EKL4
D	731	GLY	-	expression tag	UNP A0A0B0EKL4
D	732	SER	-	expression tag	UNP A0A0B0EKL4
D	733	GLY	-	expression tag	UNP A0A0B0EKL4
D	734	GLY	-	expression tag	UNP A0A0B0EKL4
D	735	GLY	-	expression tag	UNP A0A0B0EKL4
D	736	SER	-	expression tag	UNP A0A0B0EKL4
D	737	GLY	-	expression tag	UNP A0A0B0EKL4
D	738	GLY	-	expression tag	UNP A0A0B0EKL4
D	739	TRP	-	expression tag	UNP A0A0B0EKL4
D	740	SER	-	expression tag	UNP A0A0B0EKL4
D	741	HIS	-	expression tag	UNP A0A0B0EKL4
D	742	PRO	-	expression tag	UNP A0A0B0EKL4
D	743	GLN	-	expression tag	UNP A0A0B0EKL4
D	744	PHE	-	expression tag	UNP A0A0B0EKL4
D	745	GLU	-	expression tag	UNP A0A0B0EKL4
D	746	LYS	-	expression tag	UNP A0A0B0EKL4

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	Zn	0
			4	4	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

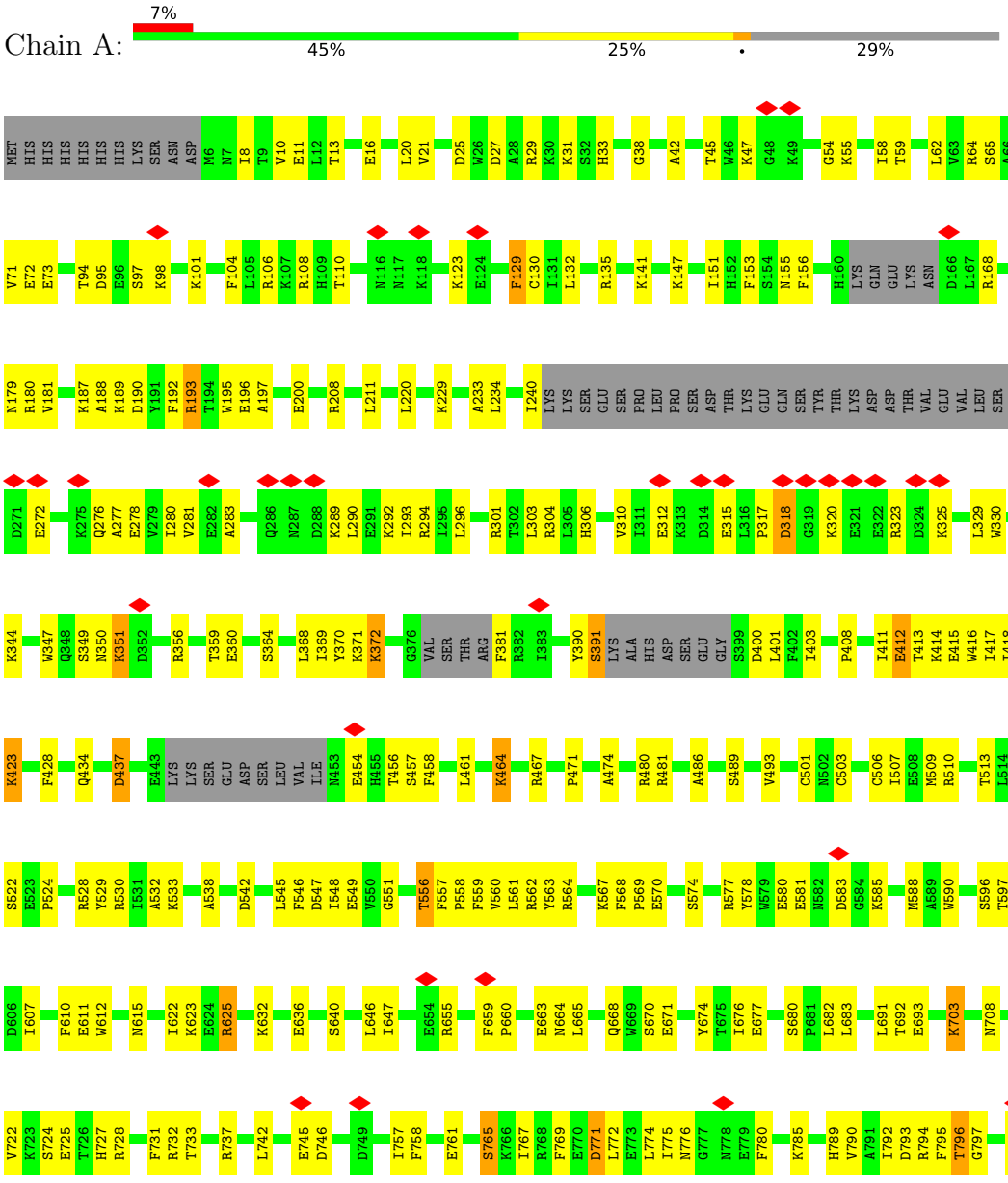
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

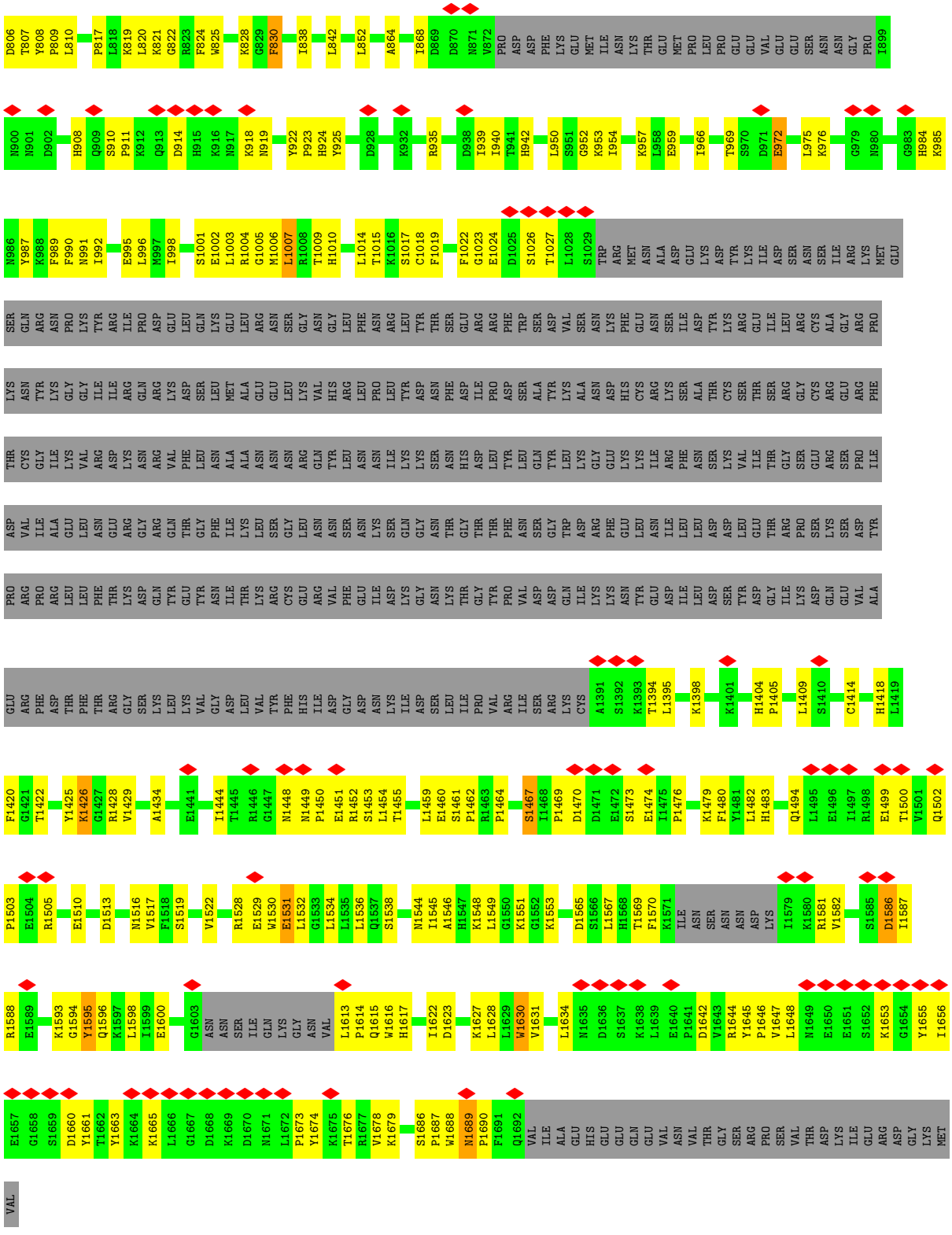
3 Residue-property plots (i)

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: RAMP superfamily protein

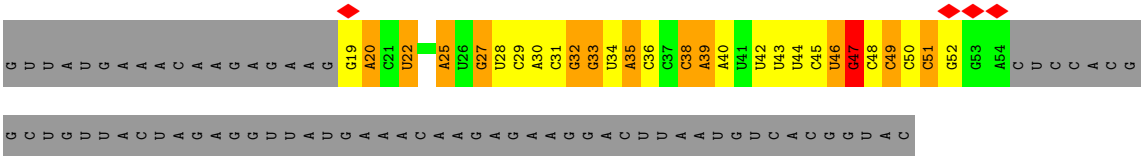
Chain A:





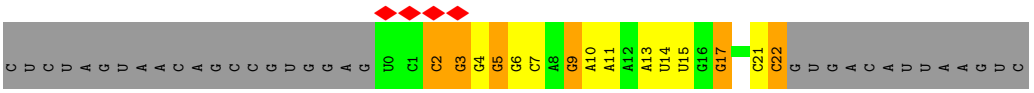
- Molecule 2: crRNA

Chain B: 7% 14% 11% 67%



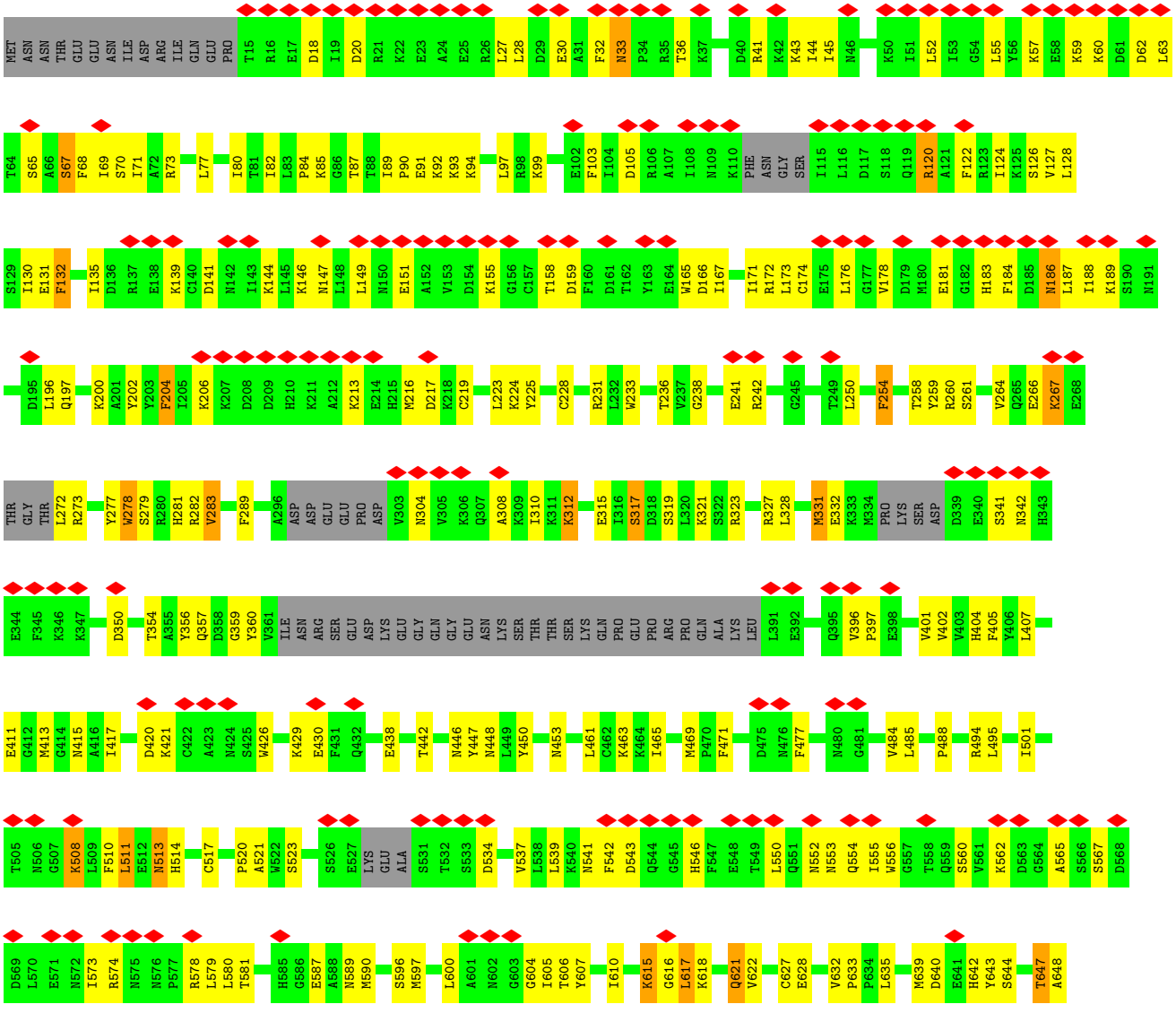
• Molecule 3: Self RNA target

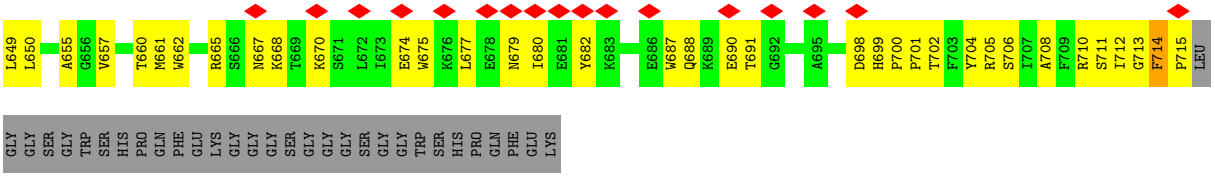
Chain C:



• Molecule 4: CHAT domain protein

Chain D:




L649 L650 A655 G656 V657 T660 M661 W662 R665 S666 N667 K668 T669 K670 S671 L672 I673 E674 W675 K676 L677 E678 N679 I680 E681 Y682 K683 E686 W687 Q688 K689 E690 T691 G692 A695 D698 H699 P700 P701 T702 F703 Y704 R705 S706 I707 A708 F709 R710 S711 I712 G713 F714 P715 LEU
GLY GLY SER GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.560	Depositor
Minimum map value	-6.045	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.218	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.29	0/10174	0.49	1/13710 (0.0%)
2	B	0.49	1/843 (0.1%)	0.91	2/1309 (0.2%)
3	C	0.30	0/555	0.82	0/864
4	D	0.26	0/5412	0.48	0/7287
All	All	0.29	1/16984 (0.0%)	0.54	3/23170 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	45	C	O3'-P	-5.81	1.54	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	47	G	O4'-C1'-N9	9.44	115.75	108.20
2	B	45	C	P-O3'-C3'	-6.72	111.64	119.70
1	A	437	ASP	CB-CG-OD1	5.30	123.07	118.30

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	9941	0	9818	308	0
2	B	757	0	387	44	0
3	C	496	0	250	15	0
4	D	5303	0	5299	175	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
All	All	16502	0	15754	494	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 15.

All (494) 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:1595:TYR:CD2	1:A:1614:PRO:HB3	1.44	1.52
1:A:1595:TYR:CD2	1:A:1614:PRO:CB	2.20	1.23
1:A:1595:TYR:HD2	1:A:1614:PRO:CB	1.57	1.13
1:A:1595:TYR:CE2	1:A:1614:PRO:HB3	2.02	0.95
1:A:1595:TYR:CE2	1:A:1614:PRO:CB	2.62	0.81
1:A:580:GLU:HG3	1:A:607:ILE:HD12	1.62	0.79
1:A:1595:TYR:HD2	1:A:1614:PRO:HB2	1.46	0.79
4:D:579:LEU:HD23	4:D:680:ILE:HD11	1.65	0.77
4:D:59:LYS:HB3	4:D:62:ASP:HB3	1.70	0.73
1:A:1026:SER:HB2	1:A:1395:LEU:HD22	1.71	0.72
4:D:494:ARG:NH1	4:D:633:PRO:O	2.17	0.71
4:D:69:ILE:HG21	4:D:120:ARG:HE	1.55	0.71
1:A:501:CYS:O	1:A:510:ARG:NH2	2.24	0.70
1:A:456:THR:HG21	1:A:549:GLU:HG3	1.75	0.69
1:A:772:LEU:HD23	1:A:822:GLY:HA3	1.74	0.69
1:A:401:LEU:HB3	4:D:438:GLU:HG3	1.73	0.69
1:A:785:LYS:NZ	1:A:991:ASN:O	2.25	0.69
1:A:674:TYR:OH	1:A:727:HIS:NE2	2.26	0.69
1:A:1004:ARG:NH1	1:A:1429:VAL:O	2.27	0.67
1:A:1644:ARG:HH12	1:A:1656:ILE:HD13	1.59	0.67
1:A:1689:ASN:HB3	1:A:1690:PRO:HD3	1.77	0.67
1:A:581:GLU:HB3	1:A:603:ALA:HB1	1.76	0.67
1:A:683:LEU:HB2	1:A:809:PRO:HB3	1.76	0.66
4:D:266:GLU:O	4:D:323:ARG:NH1	2.27	0.66
1:A:1595:TYR:CD2	1:A:1614:PRO:HB2	2.21	0.66
1:A:1426:LYS:HD3	2:B:43:U:H5”	1.77	0.66
1:A:728:ARG:HH22	1:A:765:SER:HB2	1.59	0.66
1:A:489:SER:HB3	4:D:587:GLU:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ARG:NH1	2:B:46:U:OP1	2.25	0.66
4:D:321:LYS:O	4:D:643:TYR:OH	2.14	0.66
1:A:757:ILE:HG21	1:A:838:ILE:HD11	1.77	0.65
1:A:1529:GLU:HB3	1:A:1593:LYS:HD3	1.77	0.65
1:A:417:ILE:HD13	1:A:562:ARG:HG2	1.77	0.65
1:A:304:ARG:NH1	1:A:360:GLU:OE2	2.30	0.65
1:A:757:ILE:HG23	1:A:830:PHE:HZ	1.60	0.65
1:A:1631:VAL:HB	1:A:1634:LEU:HB2	1.79	0.65
1:A:306:HIS:NE2	1:A:692:THR:OG1	2.31	0.64
1:A:16:GLU:OE2	2:B:31:C:N4	2.31	0.64
1:A:434:GLN:NE2	1:A:454:GLU:OE1	2.31	0.64
1:A:310:VAL:HA	1:A:315:GLU:HB2	1.79	0.64
4:D:665:ARG:HG2	4:D:705:ARG:HD3	1.79	0.64
1:A:1004:ARG:NH2	1:A:1420:PHE:O	2.32	0.63
1:A:296:LEU:HB2	1:A:329:LEU:HD11	1.80	0.63
4:D:272:LEU:HD11	4:D:341:SER:HB2	1.80	0.62
4:D:537:VAL:HG11	4:D:573:ILE:HG12	1.81	0.62
1:A:180:ARG:NH2	1:A:190:ASP:OD2	2.24	0.62
1:A:320:LYS:HB2	1:A:323:ARG:HB2	1.80	0.62
1:A:190:ASP:OD1	2:B:33:G:N2	2.33	0.62
1:A:400:ASP:HB2	2:B:27:G:H22	1.64	0.62
1:A:417:ILE:HD11	1:A:560:VAL:HG13	1.81	0.62
1:A:761:GLU:HG3	3:C:17:G:H21	1.63	0.62
1:A:975:LEU:HD21	1:A:1510:GLU:HG3	1.82	0.61
1:A:1647:VAL:HG21	1:A:1655:TYR:HB2	1.82	0.61
4:D:130:ILE:HG12	4:D:172:ARG:HG2	1.81	0.61
1:A:277:ALA:O	1:A:281:VAL:HG23	1.99	0.61
1:A:1444:ILE:HG23	1:A:1451:GLU:HB3	1.82	0.61
4:D:655:ALA:HB1	4:D:715:PRO:HG3	1.82	0.61
1:A:421:ARG:HE	1:A:556:THR:HB	1.66	0.61
3:C:5:G:H2'	3:C:6:G:H8	1.64	0.61
1:A:306:HIS:HE2	1:A:692:THR:HG1	1.39	0.61
4:D:687:TRP:O	4:D:691:THR:OG1	2.18	0.61
1:A:922:TYR:HH	1:A:1663:TYR:HH	1.46	0.60
1:A:47:LYS:H	1:A:54:GLY:HA2	1.66	0.60
1:A:408:PRO:HG2	1:A:411:ILE:HB	1.83	0.60
1:A:141:LYS:HD2	2:B:25:A:H5'	1.82	0.60
1:A:925:TYR:OH	1:A:1686:SER:O	2.19	0.60
1:A:925:TYR:HD2	1:A:1482:LEU:HD21	1.65	0.60
4:D:171:ILE:HD12	4:D:197:GLN:HE21	1.66	0.60
4:D:465:ILE:HG12	4:D:495:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:HG12	1:A:193:ARG:HG2	1.84	0.60
3:C:22:C:OP1	4:D:87:THR:N	2.32	0.59
1:A:312:GLU:OE2	1:A:351:LYS:NZ	2.35	0.59
1:A:461:LEU:HD23	1:A:471:PRO:HG3	1.85	0.59
1:A:515:LYS:HB2	1:A:560:VAL:HB	1.84	0.59
4:D:91:GLU:OE2	4:D:94:LYS:NZ	2.26	0.59
4:D:465:ILE:O	4:D:469:MET:HB2	2.02	0.59
4:D:622:VAL:HG11	4:D:649:LEU:HD13	1.84	0.59
4:D:661:MET:HG2	4:D:710:ARG:HD2	1.83	0.59
1:A:1598:LEU:HD13	1:A:1622:ILE:HD11	1.84	0.59
1:A:1660:ASP:HB3	1:A:1665:LYS:HD2	1.85	0.59
1:A:797:GLY:H	1:A:1479:LYS:HD2	1.67	0.59
1:A:391:SER:OG	2:B:30:A:N1	2.30	0.58
1:A:8:ILE:HG22	1:A:10:VAL:HG12	1.83	0.58
1:A:765:SER:OG	1:A:767:ILE:O	2.21	0.58
4:D:173:LEU:HD22	4:D:178:VAL:HG21	1.85	0.58
4:D:87:THR:HA	4:D:277:TYR:CE2	2.39	0.58
1:A:1615:GLN:HB3	1:A:1617:HIS:NE2	2.19	0.58
4:D:627:CYS:HA	4:D:660:THR:HG23	1.85	0.58
1:A:104:PHE:O	2:B:27:G:O2'	2.19	0.57
1:A:329:LEU:HD22	1:A:691:LEU:HD13	1.86	0.57
1:A:998:ILE:HB	1:A:1434:ALA:HB3	1.86	0.57
1:A:356:ARG:HD2	1:A:524:PRO:HG3	1.87	0.57
1:A:1426:LYS:HB2	2:B:43:U:H4'	1.86	0.57
4:D:635:LEU:HD21	4:D:640:ASP:HB2	1.86	0.57
4:D:139:LYS:O	4:D:144:LYS:NZ	2.35	0.57
1:A:173:ALA:HB1	1:A:195:TRP:HB3	1.86	0.57
1:A:731:PHE:HZ	1:A:842:LEU:HD13	1.68	0.57
4:D:27:LEU:HD22	4:D:44:ILE:HG23	1.86	0.57
4:D:223:LEU:HD11	4:D:236:THR:HG21	1.86	0.57
4:D:312:LYS:HA	4:D:315:GLU:HG3	1.86	0.57
1:A:708:ASN:HB2	1:A:715:GLU:HG2	1.87	0.56
1:A:676:ILE:HG21	1:A:852:LEU:HD11	1.87	0.56
2:B:42:U:H2'	2:B:43:U:H6	1.69	0.56
4:D:520:PRO:HG2	4:D:647:THR:HB	1.86	0.56
2:B:47:G:O2'	2:B:48:C:OP2	2.22	0.56
3:C:9:G:H2'	3:C:10:A:H8	1.71	0.56
4:D:675:TRP:CE2	4:D:687:TRP:HB2	2.40	0.56
4:D:159:ASP:N	4:D:166:ASP:OD2	2.38	0.56
4:D:643:TYR:HB3	4:D:647:THR:HG21	1.88	0.56
1:A:423:LYS:HB2	1:A:605:LYS:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ALA:HB3	1:A:1426:LYS:HB3	1.87	0.56
4:D:310:ILE:HG22	4:D:426:TRP:HB3	1.87	0.56
4:D:124:ILE:HA	4:D:127:VAL:HG22	1.89	0.55
1:A:72:GLU:OE2	1:A:106:ARG:NH2	2.39	0.55
1:A:728:ARG:NH2	1:A:758:PHE:O	2.40	0.55
1:A:1536:LEU:HD13	1:A:1587:ILE:HG23	1.87	0.55
4:D:442:THR:O	4:D:446:ASN:ND2	2.34	0.55
1:A:481:ARG:NH2	1:A:590:TRP:O	2.28	0.55
1:A:954:ILE:HG12	1:A:1567:LEU:HD12	1.88	0.55
4:D:158:THR:HG21	4:D:183:HIS:CE1	2.42	0.55
1:A:434:GLN:NE2	1:A:457:SER:O	2.40	0.54
2:B:35:A:H1'	2:B:36:C:C5	2.42	0.54
1:A:801:ASP:O	3:C:7:C:O2'	2.15	0.54
1:A:547:ASP:OD1	1:A:547:ASP:N	2.37	0.54
1:A:106:ARG:HB2	2:B:27:G:H1'	1.89	0.54
1:A:774:LEU:HD22	1:A:810:LEU:HD13	1.88	0.54
1:A:94:THR:HG23	2:B:27:G:N7	2.23	0.54
4:D:539:LEU:N	4:D:581:THR:O	2.34	0.54
4:D:264:VAL:HA	4:D:267:LYS:HE2	1.89	0.54
1:A:1500:THR:HG21	1:A:1653:LYS:HE2	1.89	0.54
1:A:1015:THR:HG1	1:A:1017:SER:HG	1.54	0.54
4:D:650:LEU:HD21	4:D:713:GLY:HA3	1.89	0.54
1:A:1642:ASP:OD2	1:A:1644:ARG:NH2	2.42	0.53
4:D:73:ARG:HG3	4:D:124:ILE:HD12	1.90	0.53
4:D:580:LEU:HD22	4:D:617:LEU:HD22	1.89	0.53
1:A:192:PHE:HB2	1:A:390:TYR:CE1	2.44	0.53
4:D:282:ARG:NH2	4:D:407:LEU:O	2.35	0.53
4:D:597:MET:HA	4:D:606:THR:HA	1.91	0.53
1:A:16:GLU:HG3	1:A:233:ALA:HB1	1.91	0.53
1:A:180:ARG:NH1	3:C:22:C:O2	2.36	0.53
1:A:317:PRO:O	1:A:340:ARG:NH2	2.26	0.53
1:A:1452:ARG:NE	1:A:1510:GLU:OE2	2.42	0.53
1:A:793:ASP:OD2	1:A:1023:GLY:N	2.41	0.53
1:A:984:HIS:ND1	1:A:1503:PRO:O	2.40	0.53
1:A:1598:LEU:HD12	1:A:1616:TRP:HZ3	1.73	0.53
1:A:604:LEU:HB3	1:A:607:ILE:HD11	1.90	0.53
1:A:1623:ASP:O	1:A:1627:LYS:HG2	2.08	0.53
1:A:1449:ASN:HB3	1:A:1450:PRO:HD3	1.90	0.52
1:A:940:ILE:HG13	1:A:1418:HIS:CE1	2.45	0.52
4:D:45:ILE:HD13	4:D:77:LEU:HB3	1.90	0.52
4:D:401:VAL:HG23	4:D:420:ASP:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:THR:O	1:A:1494:GLN:NE2	2.37	0.52
1:A:790:VAL:HG21	2:B:47:G:H21	1.74	0.52
4:D:120:ARG:HG3	4:D:120:ARG:HH11	1.75	0.52
4:D:213:LYS:HG3	4:D:250:LEU:HD11	1.92	0.52
1:A:954:ILE:HB	1:A:1522:VAL:HB	1.92	0.52
1:A:1544:ASN:HA	1:A:1634:LEU:HD23	1.92	0.52
4:D:200:LYS:HD2	4:D:204:PHE:HZ	1.74	0.52
2:B:42:U:H2'	2:B:43:U:C6	2.45	0.52
4:D:668:LYS:HG2	4:D:705:ARG:HB3	1.92	0.52
4:D:82:ILE:HD13	4:D:92:LYS:HG2	1.92	0.51
4:D:321:LYS:HB2	4:D:521:ALA:HB2	1.92	0.51
1:A:1002:GLU:HB3	1:A:1549:LEU:HD11	1.92	0.51
3:C:5:G:H2'	3:C:6:G:C8	2.43	0.51
4:D:679:ASN:HB3	4:D:682:TYR:CD2	2.45	0.51
1:A:596:SER:OG	2:B:38:C:OP1	2.23	0.51
1:A:181:VAL:HA	1:A:188:ALA:HA	1.91	0.51
1:A:1450:PRO:HB2	1:A:1453:SER:HB3	1.93	0.51
1:A:278:GLU:OE2	1:A:369:ILE:HG12	2.11	0.51
2:B:19:G:H3'	2:B:20:A:H8	1.75	0.51
1:A:418:ILE:HD12	1:A:561:LEU:HD22	1.93	0.51
1:A:1428:ARG:NH2	1:A:1531:GLU:OE1	2.43	0.51
1:A:922:TYR:OH	2:B:51:C:OP2	2.29	0.51
1:A:1513:ASP:O	1:A:1516:ASN:ND2	2.35	0.51
1:A:1616:TRP:HB3	1:A:1622:ILE:HG21	1.93	0.50
1:A:731:PHE:CZ	1:A:842:LEU:HD13	2.46	0.50
4:D:289:PHE:HE1	4:D:415:ASN:HD21	1.59	0.50
1:A:193:ARG:NH2	1:A:437:ASP:OD1	2.44	0.50
1:A:722:VAL:HB	1:A:772:LEU:HB2	1.93	0.50
4:D:513:ASN:OD1	4:D:513:ASN:N	2.44	0.50
4:D:661:MET:HG3	4:D:708:ALA:O	2.12	0.50
1:A:510:ARG:HA	2:B:32:G:OP2	2.11	0.50
1:A:1017:SER:HB3	1:A:1414:CYS:SG	2.52	0.50
4:D:127:VAL:HG11	4:D:165:TRP:HB3	1.92	0.50
4:D:607:TYR:CD2	4:D:648:ALA:HB2	2.47	0.50
1:A:959:GLU:HG3	1:A:1517:VAL:HG22	1.93	0.50
1:A:33:HIS:HB3	1:A:390:TYR:HB2	1.93	0.49
1:A:922:TYR:OH	1:A:1663:TYR:OH	2.19	0.49
1:A:155:ASN:HD22	2:B:22:U:H1'	1.76	0.49
1:A:674:TYR:HB3	1:A:868:ILE:HD13	1.94	0.49
1:A:1499:GLU:HG3	1:A:1500:THR:HG23	1.94	0.49
1:A:1596:GLN:O	1:A:1600:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LYS:HD3	1:A:292:LYS:HD2	1.94	0.49
1:A:294:ARG:NE	3:C:14:U:O2'	2.44	0.49
1:A:403:ILE:HG23	4:D:442:THR:HA	1.93	0.49
4:D:450:TYR:HB3	4:D:453:ASN:HB2	1.95	0.49
1:A:745:GLU:CD	1:A:745:GLU:H	2.15	0.49
4:D:513:ASN:HB2	4:D:514:HIS:CE1	2.46	0.49
4:D:553:ASN:OD1	4:D:554:GLN:N	2.46	0.49
1:A:312:GLU:HA	1:A:344:LYS:HE2	1.94	0.49
4:D:184:PHE:CE2	4:D:206:LYS:HD2	2.48	0.49
1:A:604:LEU:HD13	1:A:607:ILE:HD11	1.95	0.49
4:D:173:LEU:HA	4:D:176:LEU:HD12	1.93	0.49
1:A:176:ARG:NH2	1:A:196:GLU:OE2	2.45	0.49
4:D:550:LEU:HD23	4:D:674:GLU:HG2	1.94	0.49
4:D:657:VAL:N	4:D:712:ILE:O	2.42	0.49
1:A:998:ILE:HG21	1:A:1549:LEU:HD21	1.95	0.48
1:A:318:ASP:OD1	1:A:318:ASP:N	2.39	0.48
1:A:682:LEU:HD22	1:A:820:LEU:HD11	1.96	0.48
1:A:570:GLU:O	1:A:574:SER:OG	2.26	0.48
1:A:108:ARG:HB3	2:B:29:C:H5'	1.96	0.48
1:A:942:HIS:NE2	1:A:1426:LYS:O	2.46	0.48
1:A:1014:LEU:HD12	1:A:1622:ILE:HG12	1.95	0.48
4:D:231:ARG:HG2	4:D:359:GLY:HA3	1.94	0.48
1:A:1480:PHE:HB2	1:A:1628:LEU:HD13	1.95	0.48
2:B:48:C:H2'	2:B:49:C:C6	2.48	0.48
4:D:167:ILE:HD12	4:D:167:ILE:H	1.79	0.48
4:D:508:LYS:HE2	4:D:513:ASN:HD21	1.78	0.48
1:A:458:PHE:HB2	1:A:548:ILE:HG23	1.96	0.48
1:A:775:ILE:HD13	1:A:821:LYS:HB2	1.95	0.48
1:A:910:SER:HB2	1:A:911:PRO:HD3	1.95	0.48
4:D:141:ASP:H	4:D:144:LYS:HE3	1.79	0.48
4:D:310:ILE:CG2	4:D:426:TRP:HB3	2.43	0.48
1:A:151:ILE:HD13	1:A:211:LEU:HD13	1.95	0.48
1:A:369:ILE:HA	1:A:372:LYS:HE3	1.94	0.48
1:A:1459:LEU:HD22	2:B:49:C:H2'	1.96	0.48
1:A:179:ASN:HB3	2:B:34:U:H3'	1.95	0.48
1:A:418:ILE:HD11	1:A:568:PHE:HZ	1.78	0.48
4:D:85:LYS:HA	4:D:328:LEU:HB3	1.96	0.48
1:A:323:ARG:HH22	1:A:325:LYS:HZ3	1.61	0.48
4:D:33:ASN:O	4:D:41:ARG:NH2	2.47	0.48
4:D:238:GLY:HA2	4:D:241:GLU:HB2	1.95	0.48
1:A:132:LEU:HD21	1:A:220:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HE2	2:B:42:U:O2'	2.14	0.47
4:D:63:LEU:HG	4:D:67:SER:HB3	1.96	0.47
1:A:803:ALA:HA	3:C:9:G:H21	1.79	0.47
1:A:155:ASN:ND2	2:B:22:U:H1'	2.30	0.47
2:B:30:A:H4'	2:B:31:C:H5"	1.96	0.47
4:D:675:TRP:CZ2	4:D:682:TYR:HB3	2.49	0.47
4:D:397:PRO:HD2	4:D:714:PHE:HZ	1.78	0.47
4:D:579:LEU:HD23	4:D:680:ILE:CD1	2.41	0.47
4:D:605:ILE:HG12	4:D:610:ILE:HG13	1.95	0.47
1:A:20:LEU:HB3	1:A:195:TRP:HB2	1.95	0.47
1:A:276:GLN:O	1:A:280:ILE:HG13	2.15	0.47
1:A:950:LEU:HD13	1:A:1532:LEU:HD23	1.96	0.47
4:D:126:SER:HB2	4:D:149:LEU:HD22	1.96	0.47
4:D:171:ILE:HA	4:D:174:CYS:SG	2.54	0.47
4:D:317:SER:O	4:D:321:LYS:HG3	2.15	0.47
4:D:405:PHE:HB2	4:D:488:PRO:HA	1.96	0.47
4:D:589:ASN:O	4:D:642:HIS:NE2	2.45	0.47
4:D:701:PRO:HA	4:D:704:TYR:HB3	1.96	0.47
1:A:21:VAL:HG11	1:A:38:GLY:O	2.14	0.47
1:A:58:ILE:HG23	1:A:62:LEU:HD23	1.97	0.47
1:A:805:PHE:HB3	3:C:9:G:C4	2.50	0.47
1:A:1010:HIS:CE1	1:A:1538:SER:HA	2.49	0.47
4:D:429:LYS:HG3	4:D:477:PHE:CD2	2.50	0.47
1:A:272:GLU:OE1	1:A:350:ASN:ND2	2.48	0.47
1:A:733:THR:O	1:A:737:ARG:HG3	2.15	0.47
1:A:776:ASN:HB3	1:A:780:PHE:HE1	1.80	0.47
4:D:304:ASN:O	4:D:308:ALA:N	2.47	0.47
1:A:517:SER:HB2	1:A:557:PHE:HB3	1.97	0.47
4:D:447:TYR:CE1	4:D:662:TRP:HB2	2.50	0.47
1:A:732:ARG:CZ	2:B:39:A:H5"	2.45	0.46
4:D:402:VAL:HG13	4:D:485:LEU:HD23	1.97	0.46
1:A:168:ARG:HG3	1:A:168:ARG:HH11	1.80	0.46
4:D:94:LYS:HB2	4:D:94:LYS:HE3	1.73	0.46
4:D:188:ILE:HG13	4:D:189:LYS:N	2.29	0.46
4:D:224:LYS:HB2	4:D:224:LYS:HE2	1.67	0.46
4:D:628:GLU:O	4:D:632:VAL:HG22	2.15	0.46
1:A:94:THR:O	1:A:101:LYS:NZ	2.41	0.46
1:A:817:PRO:HG2	1:A:819:LYS:HE3	1.96	0.46
4:D:30:GLU:O	4:D:36:THR:OG1	2.33	0.46
4:D:122:PHE:HE2	4:D:151:GLU:HB2	1.79	0.46
4:D:700:PRO:N	4:D:701:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:HB2	1:A:240:ILE:HD13	1.98	0.46
1:A:1548:LYS:HB3	1:A:1553:LYS:HG2	1.96	0.46
1:A:347:TRP:CZ2	1:A:351:LYS:HD3	2.51	0.46
1:A:471:PRO:HD2	1:A:474:ALA:HB3	1.97	0.46
1:A:578:TYR:CZ	1:A:588:MET:HG2	2.50	0.46
1:A:1553:LYS:HE2	2:B:49:C:OP1	2.16	0.46
4:D:65:SER:O	4:D:69:ILE:N	2.45	0.46
4:D:84:PRO:HA	4:D:90:PRO:HG3	1.97	0.46
4:D:196:LEU:HB2	4:D:219:CYS:SG	2.56	0.46
4:D:404:HIS:N	4:D:417:ILE:O	2.44	0.46
1:A:180:ARG:O	1:A:189:LYS:N	2.45	0.46
1:A:1009:THR:HG21	2:B:46:U:C5	2.51	0.46
4:D:485:LEU:HD13	4:D:714:PHE:HB3	1.97	0.46
1:A:976:LYS:HA	1:A:976:LYS:HD3	1.63	0.46
4:D:350:ASP:O	4:D:354:THR:HG23	2.16	0.46
1:A:972:GLU:HG3	1:A:985:LYS:HG2	1.98	0.46
1:A:371:LYS:HD2	1:A:371:LYS:HA	1.70	0.46
1:A:795:PHE:CE1	1:A:1476:PRO:HD2	2.51	0.46
1:A:1582:VAL:HG12	1:A:1587:ILE:HG13	1.98	0.46
4:D:146:LYS:HA	4:D:176:LEU:HD13	1.97	0.46
4:D:228:CYS:HA	4:D:233:TRP:CD1	2.51	0.46
4:D:224:LYS:HG2	4:D:261:SER:HA	1.97	0.45
1:A:58:ILE:HB	1:A:156:PHE:HB2	1.98	0.45
1:A:200:GLU:OE1	1:A:467:ARG:NH2	2.49	0.45
1:A:187:LYS:HE2	1:A:187:LYS:HB3	1.60	0.45
1:A:1005:GLY:O	1:A:1009:THR:HG23	2.16	0.45
4:D:171:ILE:HD12	4:D:197:GLN:HB3	1.97	0.45
1:A:771:ASP:OD1	1:A:771:ASP:N	2.50	0.45
1:A:966:ILE:O	1:A:990:PHE:N	2.47	0.45
1:A:1027:THR:HG22	1:A:1394:THR:HG22	1.99	0.45
4:D:429:LYS:HG3	4:D:477:PHE:HD2	1.81	0.45
1:A:188:ALA:HB2	2:B:36:C:H1'	1.98	0.45
1:A:969:THR:HG1	2:B:47:G:H8	1.60	0.45
1:A:1469:PRO:HB2	1:A:1674:TYR:CD2	2.52	0.45
1:A:957:LYS:NZ	1:A:1565:ASP:OD2	2.40	0.45
1:A:1022:PHE:CZ	1:A:1395:LEU:HB3	2.51	0.45
1:A:1022:PHE:HD2	1:A:1024:GLU:HG3	1.82	0.45
1:A:1395:LEU:HD21	1:A:1464:PRO:HG2	1.99	0.45
1:A:1530:TRP:HB2	1:A:1594:GLY:HA2	1.98	0.45
1:A:1661:TYR:HE1	1:A:1688:TRP:HB3	1.81	0.45
4:D:94:LYS:HG2	4:D:132:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:228:CYS:HB3	4:D:278:TRP:NE1	2.31	0.45
1:A:415:GLU:OE1	1:A:564:ARG:NH1	2.50	0.45
1:A:612:TRP:CE2	1:A:646:LEU:HD13	2.52	0.45
4:D:600:LEU:H	4:D:604:GLY:HA2	1.82	0.45
1:A:632:LYS:O	1:A:636:GLU:HG2	2.17	0.45
1:A:939:ILE:HG13	1:A:1409:LEU:HB3	1.99	0.45
4:D:43:LYS:HE3	4:D:43:LYS:HB2	1.70	0.45
4:D:273:ARG:NH2	4:D:523:SER:HB2	2.32	0.45
4:D:665:ARG:HD2	4:D:667:ASN:HB2	1.98	0.45
1:A:20:LEU:N	1:A:195:TRP:O	2.44	0.45
1:A:20:LEU:HD12	1:A:42:ALA:HB3	1.98	0.44
1:A:130:CYS:SG	1:A:135:ARG:HD3	2.57	0.44
1:A:507:ILE:HD11	4:D:448:ASN:HB3	1.98	0.44
1:A:517:SER:HB3	1:A:558:PRO:O	2.17	0.44
1:A:577:ARG:NH1	1:A:580:GLU:OE1	2.38	0.44
1:A:585:LYS:HD2	1:A:655:ARG:CD	2.46	0.44
1:A:737:ARG:HD2	1:A:942:HIS:O	2.17	0.44
4:D:71:ILE:HG21	4:D:103:PHE:CD2	2.51	0.44
1:A:413:THR:N	1:A:615:ASN:OD1	2.49	0.44
1:A:793:ASP:HB3	1:A:796:THR:O	2.17	0.44
4:D:52:LEU:HD11	4:D:70:SER:OG	2.16	0.44
4:D:278:TRP:CE2	4:D:281:HIS:HB2	2.52	0.44
4:D:632:VAL:HG13	4:D:644:SER:HB3	1.99	0.44
1:A:64:ARG:HG3	1:A:153:PHE:CD1	2.51	0.44
1:A:428:PHE:CZ	1:A:551:GLY:HA3	2.53	0.44
1:A:952:GLY:HA2	1:A:1570:PHE:CE2	2.53	0.44
4:D:80:ILE:HG22	4:D:357:GLN:HG2	1.99	0.44
4:D:556:TRP:CH2	4:D:677:LEU:HD21	2.51	0.44
1:A:303:LEU:HD22	1:A:310:VAL:HG11	1.98	0.44
1:A:412:GLU:HG2	1:A:414:LYS:HE2	2.00	0.44
1:A:67:VAL:O	1:A:71:VAL:HG23	2.17	0.44
1:A:1448:ASN:ND2	1:A:1453:SER:O	2.46	0.44
4:D:565:ALA:HB3	4:D:600:LEU:HD22	2.00	0.44
4:D:579:LEU:HD22	4:D:621:GLN:O	2.18	0.44
1:A:47:LYS:HG3	1:A:55:LYS:HG3	2.00	0.44
1:A:989:PHE:HD2	1:A:996:LEU:HD22	1.81	0.44
4:D:411:GLU:O	4:D:413:MET:N	2.48	0.44
1:A:677:GLU:O	1:A:864:ALA:N	2.49	0.44
1:A:1582:VAL:HG13	1:A:1586:ASP:HB3	2.00	0.44
4:D:71:ILE:HD13	4:D:71:ILE:HA	1.87	0.44
1:A:200:GLU:OE1	1:A:464:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:HG13	1:A:293:ILE:HG13	2.00	0.44
4:D:643:TYR:HB3	4:D:647:THR:CG2	2.48	0.44
1:A:25:ASP:O	1:A:29:ARG:N	2.50	0.44
1:A:923:PRO:HG2	1:A:1645:TYR:CD2	2.53	0.44
4:D:463:LYS:HG2	4:D:501:ILE:HB	1.99	0.44
4:D:485:LEU:HD22	4:D:714:PHE:CD2	2.52	0.44
4:D:213:LYS:HA	4:D:254:PHE:CZ	2.53	0.43
4:D:241:GLU:OE2	4:D:283:VAL:HG11	2.18	0.43
4:D:555:ILE:HG21	4:D:677:LEU:HD22	2.00	0.43
1:A:179:ASN:O	2:B:33:G:O2'	2.22	0.43
1:A:364:SER:O	1:A:368:LEU:HG	2.18	0.43
1:A:597:THR:O	1:A:724:SER:OG	2.19	0.43
1:A:693:GLU:OE2	1:A:703:LYS:NZ	2.47	0.43
1:A:528:ARG:NH2	1:A:771:ASP:OD2	2.50	0.43
1:A:908:HIS:ND1	1:A:911:PRO:HD3	2.34	0.43
1:A:31:LYS:HA	1:A:31:LYS:HD3	1.94	0.43
1:A:98:LYS:HB2	1:A:98:LYS:HE2	1.63	0.43
4:D:120:ARG:HG3	4:D:120:ARG:NH1	2.33	0.43
4:D:213:LYS:HA	4:D:254:PHE:HZ	1.83	0.43
1:A:1470:ASP:OD1	1:A:1473:SER:OG	2.26	0.43
4:D:260:ARG:O	4:D:264:VAL:HG23	2.18	0.43
4:D:541:ASN:HB2	4:D:600:LEU:HD23	2.01	0.43
1:A:69:LYS:O	1:A:73:GLU:HG3	2.19	0.43
2:B:47:G:H1'	2:B:48:C:C6	2.53	0.43
4:D:543:ASP:HB3	4:D:546:HIS:ND1	2.33	0.43
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.84	0.43
1:A:532:ALA:HB2	2:B:39:A:H1'	2.00	0.43
1:A:728:ARG:HB2	1:A:769:PHE:HB2	2.01	0.43
4:D:471:PHE:HB2	4:D:477:PHE:CD2	2.54	0.43
1:A:1545:ILE:HG12	1:A:1630:TRP:HA	2.00	0.43
1:A:545:LEU:HD22	3:C:13:A:C2	2.53	0.43
4:D:80:ILE:HG23	4:D:360:TYR:CD2	2.53	0.43
3:C:10:A:H2'	3:C:11:A:H8	1.83	0.43
4:D:28:LEU:O	4:D:32:PHE:N	2.47	0.43
4:D:699:HIS:CD2	4:D:701:PRO:HG2	2.54	0.43
1:A:1018:CYS:SG	1:A:1405:PRO:HA	2.59	0.42
2:B:43:U:H2'	2:B:44:U:C6	2.54	0.42
4:D:328:LEU:O	4:D:332:GLU:HG2	2.19	0.42
1:A:683:LEU:HD22	1:A:807:THR:HB	2.01	0.42
1:A:176:ARG:NE	1:A:196:GLU:OE1	2.44	0.42
1:A:304:ARG:HB3	1:A:359:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ARG:HB2	1:A:509:MET:SD	2.59	0.42
1:A:493:VAL:HG11	2:B:33:G:H5'	2.01	0.42
4:D:541:ASN:ND2	4:D:541:ASN:O	2.52	0.42
4:D:556:TRP:HB2	4:D:562:LYS:HE2	2.01	0.42
1:A:1003:LEU:HD11	1:A:1434:ALA:HB2	2.01	0.42
1:A:1461:SER:HB3	3:C:5:G:H21	1.84	0.42
4:D:501:ILE:HD12	4:D:501:ILE:N	2.34	0.42
1:A:503:CYS:SG	1:A:506:CYS:HB2	2.59	0.42
1:A:660:PRO:O	1:A:664:ASN:HB2	2.19	0.42
1:A:1019:PHE:O	1:A:1405:PRO:HG3	2.19	0.42
4:D:97:LEU:HD23	4:D:132:PHE:HA	2.01	0.42
4:D:690:GLU:HG3	4:D:691:THR:HG23	2.00	0.42
4:D:71:ILE:HG21	4:D:103:PHE:CG	2.55	0.42
4:D:590:MET:HA	4:D:633:PRO:HG3	2.01	0.42
1:A:458:PHE:HD2	1:A:548:ILE:HG12	1.85	0.42
1:A:935:ARG:NH2	1:A:1404:HIS:O	2.53	0.42
1:A:1483:HIS:ND1	1:A:1631:VAL:HG22	2.35	0.42
1:A:64:ARG:HG3	1:A:153:PHE:CE1	2.55	0.42
1:A:301:ARG:NH2	1:A:529:TYR:OH	2.52	0.42
1:A:950:LEU:HD22	1:A:1569:THR:HG21	2.01	0.42
1:A:842:LEU:HD12	1:A:842:LEU:HA	1.90	0.42
1:A:992:ILE:O	1:A:995:GLU:HG2	2.20	0.42
1:A:1460:GLU:O	2:B:49:C:O2'	2.26	0.42
1:A:1022:PHE:CD2	1:A:1024:GLU:HG3	2.55	0.41
4:D:331:MET:H	4:D:331:MET:HG2	1.62	0.41
1:A:330:TRP:NE1	1:A:691:LEU:O	2.42	0.41
1:A:578:TYR:OH	1:A:588:MET:HG2	2.20	0.41
1:A:1015:THR:HG22	1:A:1534:LEU:HD13	2.01	0.41
4:D:120:ARG:O	4:D:124:ILE:HG22	2.20	0.41
1:A:173:ALA:HA	1:A:197:ALA:HA	2.01	0.41
4:D:89:ILE:HG13	4:D:90:PRO:HD2	2.02	0.41
1:A:283:ALA:HB1	1:A:334:VAL:HA	2.01	0.41
1:A:919:ASN:HB2	1:A:1687:PRO:HB3	2.02	0.41
4:D:327:ARG:O	4:D:331:MET:HG2	2.21	0.41
4:D:415:ASN:HB3	4:D:430:GLU:HG2	2.02	0.41
1:A:106:ARG:NH1	1:A:110:THR:OG1	2.46	0.41
3:C:3:G:H2'	3:C:4:G:C8	2.55	0.41
1:A:530:ARG:HB2	1:A:546:PHE:CZ	2.56	0.41
1:A:914:ASP:OD2	1:A:918:LYS:N	2.54	0.41
3:C:2:C:H4'	3:C:3:G:OP1	2.19	0.41
4:D:20:ASP:CG	4:D:55:LEU:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:537:VAL:HG13	4:D:560:SER:HB3	2.03	0.41
1:A:234:LEU:HD12	1:A:515:LYS:HG3	2.03	0.41
1:A:611:GLU:N	1:A:647:ILE:O	2.52	0.41
1:A:1462:PRO:HG3	2:B:49:C:O3'	2.21	0.41
4:D:484:VAL:HG21	4:D:510:PHE:HZ	1.85	0.41
1:A:737:ARG:HG2	1:A:742:LEU:HD22	2.01	0.41
1:A:72:GLU:HG3	1:A:129:PHE:HZ	1.86	0.41
1:A:293:ILE:HG22	1:A:370:TYR:HB2	2.03	0.41
1:A:417:ILE:CG2	1:A:610:PHE:HB2	2.51	0.41
1:A:530:ARG:CD	1:A:725:GLU:HG2	2.50	0.41
1:A:622:ILE:O	1:A:625:ARG:NH1	2.54	0.41
1:A:1483:HIS:HE1	1:A:1546:ALA:C	2.24	0.41
2:B:35:A:H1'	2:B:36:C:C6	2.56	0.41
4:D:147:ASN:O	4:D:151:GLU:HG3	2.20	0.41
4:D:461:LEU:HD11	4:D:495:LEU:HD22	2.02	0.41
4:D:573:ILE:O	4:D:616:GLY:HA3	2.21	0.41
4:D:590:MET:HA	4:D:633:PRO:CG	2.51	0.41
4:D:668:LYS:HA	4:D:668:LYS:HD2	1.81	0.41
1:A:272:GLU:OE2	1:A:349:SER:OG	2.39	0.41
1:A:671:GLU:HB3	1:A:825:TRP:CZ3	2.56	0.41
1:A:789:HIS:HA	2:B:47:G:O5'	2.20	0.41
4:D:80:ILE:HG23	4:D:360:TYR:HD2	1.86	0.41
4:D:254:PHE:O	4:D:258:THR:HG22	2.21	0.41
4:D:546:HIS:O	4:D:670:LYS:NZ	2.31	0.41
1:A:381:PHE:HB3	4:D:57:LYS:HD3	2.02	0.40
1:A:559:PHE:CD2	1:A:604:LEU:HD21	2.55	0.40
1:A:767:ILE:HD11	1:A:824:PHE:CD1	2.56	0.40
1:A:924:HIS:HB2	1:A:1479:LYS:HG3	2.03	0.40
1:A:1646:PRO:HD2	1:A:1663:TYR:CZ	2.56	0.40
1:A:1673:PRO:HG2	1:A:1676:THR:HG22	2.02	0.40
4:D:97:LEU:HD21	4:D:131:GLU:HB2	2.03	0.40
4:D:186:ASN:N	4:D:186:ASN:OD1	2.53	0.40
4:D:615:LYS:HG3	4:D:618:LYS:NZ	2.37	0.40
1:A:416:TRP:CE3	1:A:563:TYR:HD2	2.40	0.40
1:A:1646:PRO:HG3	1:A:1661:TYR:CE1	2.56	0.40
4:D:396:VAL:O	4:D:421:LYS:HE3	2.21	0.40
4:D:511:LEU:HD21	4:D:688:GLN:HB2	2.03	0.40
1:A:1502:GLN:HB2	1:A:1505:ARG:HB2	2.04	0.40
1:A:1674:TYR:O	1:A:1678:VAL:HG23	2.21	0.40
4:D:93:LYS:NZ	4:D:356:TYR:OH	2.32	0.40
4:D:223:LEU:HD22	4:D:233:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:494:ARG:NH2	4:D:640:ASP:OD1	2.48	0.40
1:A:59:THR:HA	1:A:155:ASN:OD1	2.22	0.40
1:A:486:ALA:HB2	1:A:665:LEU:HD11	2.03	0.40
1:A:663:GLU:O	1:A:828:LYS:NZ	2.53	0.40
1:A:1007:LEU:HA	1:A:1007:LEU:HD22	1.88	0.40
1:A:1409:LEU:HD21	1:A:1425:TYR:HB2	2.02	0.40
1:A:1467:SER:HB3	1:A:1476:PRO:HG2	2.03	0.40
1:A:1648:LEU:HD13	2:B:51:C:C2	2.57	0.40
4:D:714:PHE:HA	4:D:715:PRO:HD3	1.83	0.40
1:A:45:THR:OG1	2:B:22:U:OP1	2.35	0.40
1:A:461:LEU:CD2	1:A:471:PRO:HG3	2.49	0.40
1:A:563:TYR:CZ	1:A:569:PRO:HD3	2.57	0.40
1:A:668:GLN:O	1:A:828:LYS:N	2.54	0.40
4:D:89:ILE:HG12	4:D:135:ILE:HB	2.03	0.40
4:D:579:LEU:HD13	4:D:580:LEU:N	2.36	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	1212/1728 (70%)	1189 (98%)	23 (2%)	0	100	100
4	D	638/746 (86%)	619 (97%)	19 (3%)	0	100	100
All	All	1850/2474 (75%)	1808 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1073/1531 (70%)	1005 (94%)	68 (6%)	18 31
4	D	580/657 (88%)	528 (91%)	52 (9%)	9 18
All	All	1653/2188 (76%)	1533 (93%)	120 (7%)	18 25

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	27	ASP
1	A	65	SER
1	A	95	ASP
1	A	97	SER
1	A	123	LYS
1	A	129	PHE
1	A	147	LYS
1	A	193	ARG
1	A	208	ARG
1	A	229	LYS
1	A	290	LEU
1	A	318	ASP
1	A	351	LYS
1	A	372	LYS
1	A	391	SER
1	A	412	GLU
1	A	419	VAL
1	A	423	LYS
1	A	464	LYS
1	A	513	THR
1	A	515	LYS
1	A	517	SER
1	A	522	SER
1	A	542	ASP
1	A	556	THR
1	A	567	LYS
1	A	583	ASP
1	A	623	LYS
1	A	625	ARG
1	A	640	SER

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Mol	Chain	Res	Type
1	A	659	PHE
1	A	670	SER
1	A	680	SER
1	A	703	LYS
1	A	746	ASP
1	A	765	SER
1	A	771	ASP
1	A	792	ILE
1	A	796	THR
1	A	802	LYS
1	A	806	ASP
1	A	808	TYR
1	A	830	PHE
1	A	953	LYS
1	A	972	GLU
1	A	987	TYR
1	A	1001	SER
1	A	1006	MET
1	A	1007	LEU
1	A	1398	LYS
1	A	1422	THR
1	A	1426	LYS
1	A	1454	LEU
1	A	1467	SER
1	A	1474	GLU
1	A	1519	SER
1	A	1528	ARG
1	A	1531	GLU
1	A	1551	LYS
1	A	1581	ARG
1	A	1586	ASP
1	A	1588	ARG
1	A	1595	TYR
1	A	1613	LEU
1	A	1630	TRP
1	A	1679	LYS
1	A	1689	ASN
4	D	18	ASP
4	D	33	ASN
4	D	60	LYS
4	D	67	SER
4	D	68	PHE

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Mol	Chain	Res	Type
4	D	99	LYS
4	D	105	ASP
4	D	120	ARG
4	D	128	LEU
4	D	132	PHE
4	D	155	LYS
4	D	181	GLU
4	D	186	ASN
4	D	187	LEU
4	D	202	TYR
4	D	204	PHE
4	D	216	MET
4	D	217	ASP
4	D	225	TYR
4	D	242	ARG
4	D	254	PHE
4	D	259	TYR
4	D	267	LYS
4	D	278	TRP
4	D	279	SER
4	D	283	VAL
4	D	312	LYS
4	D	317	SER
4	D	319	SER
4	D	331	MET
4	D	342	ASN
4	D	508	LYS
4	D	511	LEU
4	D	513	ASN
4	D	517	CYS
4	D	534	ASP
4	D	542	PHE
4	D	552	ASN
4	D	567	SER
4	D	574	ARG
4	D	578	ARG
4	D	596	SER
4	D	615	LYS
4	D	617	LEU
4	D	621	GLN
4	D	639	MET
4	D	647	THR

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Mol	Chain	Res	Type
4	D	698	ASP
4	D	702	THR
4	D	706	SER
4	D	711	SER
4	D	714	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
1	A	1635	ASN
4	D	197	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	35/110 (31%)	17 (48%)	0
3	C	22/56 (39%)	8 (36%)	1 (4%)
All	All	57/166 (34%)	25 (43%)	1 (1%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	A
2	B	22	U
2	B	25	A
2	B	27	G
2	B	28	U
2	B	32	G
2	B	33	G
2	B	35	A
2	B	38	C
2	B	39	A
2	B	40	A
2	B	46	U
2	B	47	G
2	B	49	C
2	B	50	C
2	B	51	C
2	B	52	G

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Mol	Chain	Res	Type
3	C	2	C
3	C	3	G
3	C	5	G
3	C	9	G
3	C	15	U
3	C	17	G
3	C	21	C
3	C	22	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	2	C

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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 (i)

There are no chain breaks in this entry.

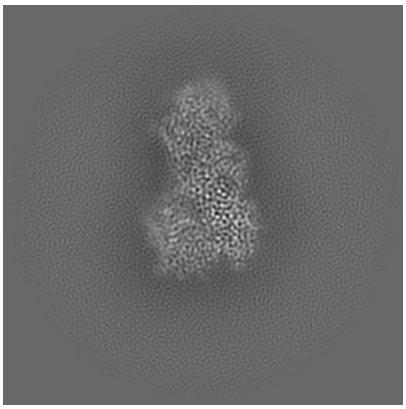
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33681. These allow visual inspection of the internal detail of the map and identification of artifacts.

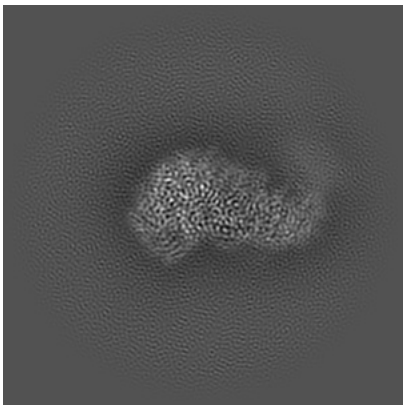
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

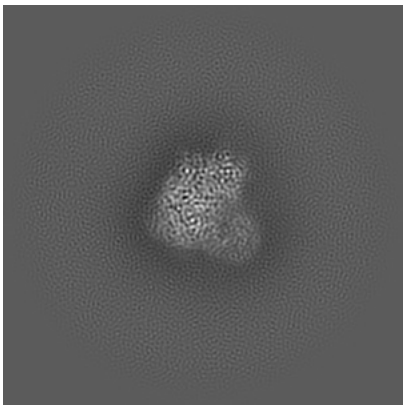
6.1.1 Primary map



X

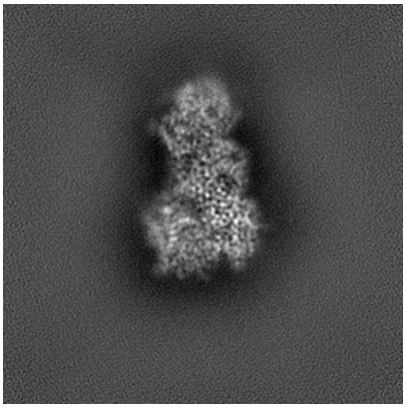


Y

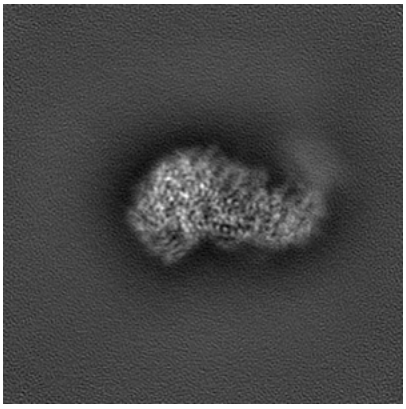


Z

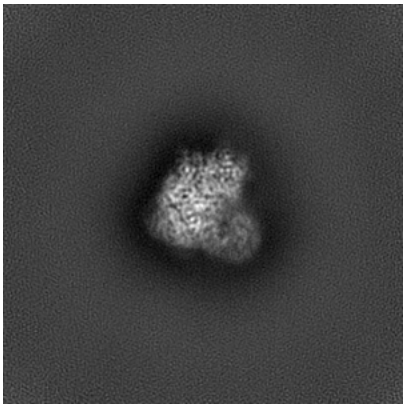
6.1.2 Raw map



X



Y

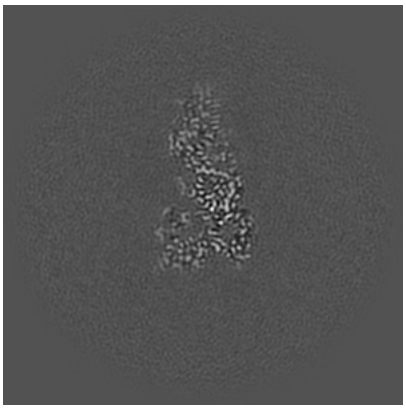


Z

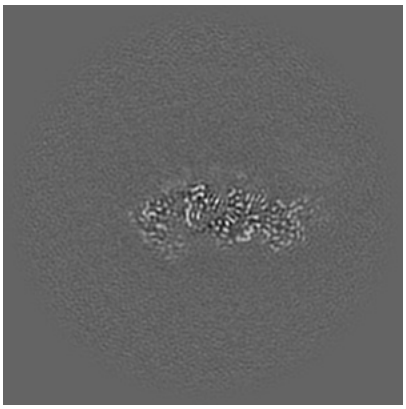
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

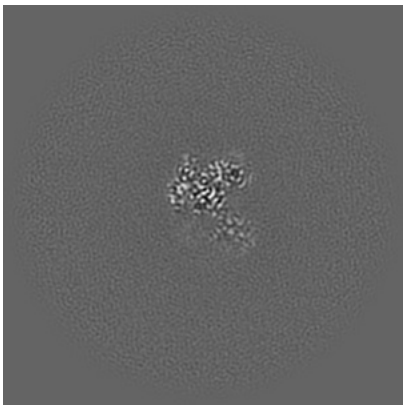
6.2.1 Primary map



X Index: 128

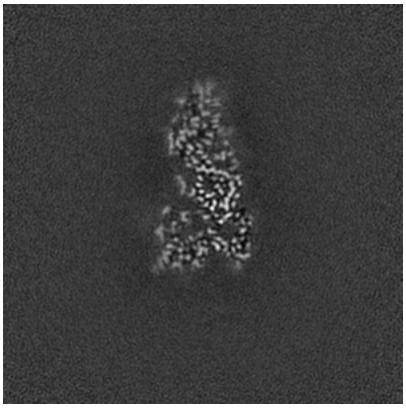


Y Index: 128

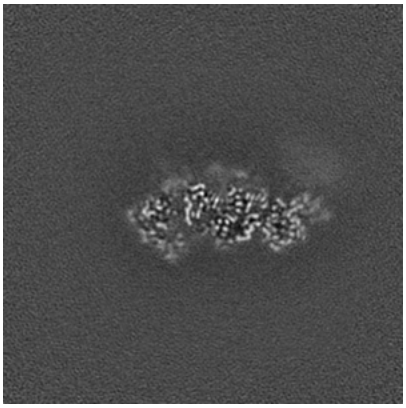


Z Index: 128

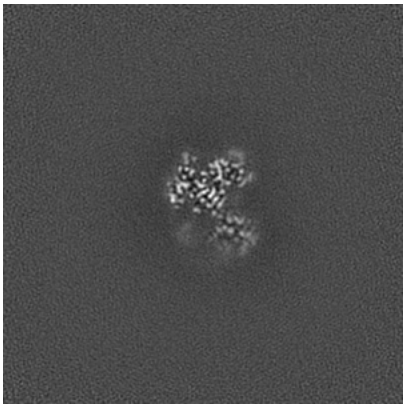
6.2.2 Raw map



X Index: 128



Y Index: 128

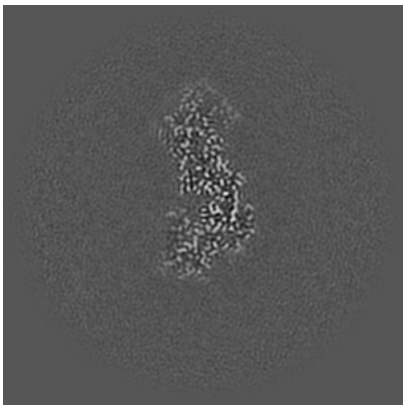


Z Index: 128

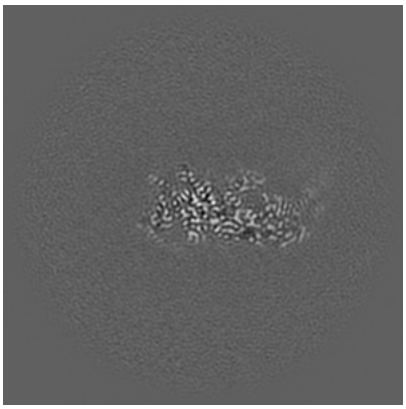
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

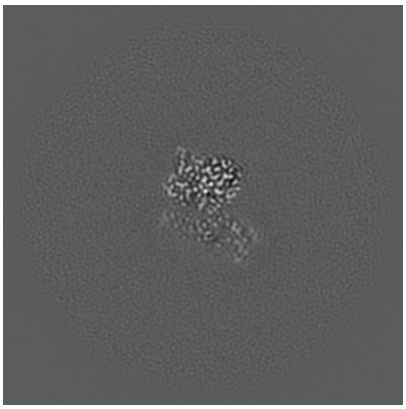
6.3.1 Primary map



X Index: 121

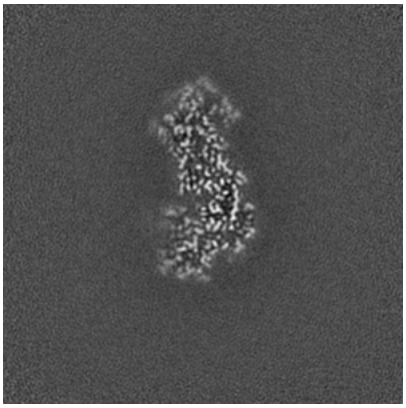


Y Index: 134

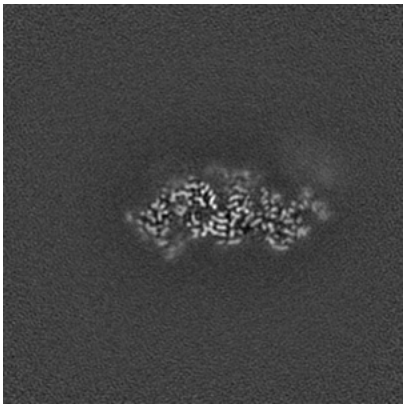


Z Index: 120

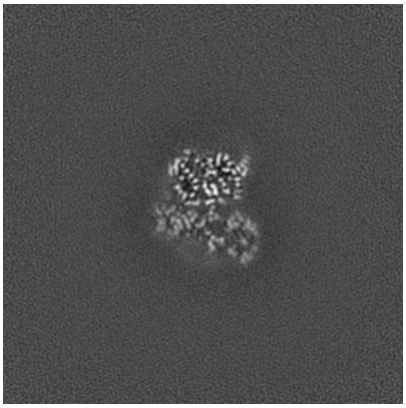
6.3.2 Raw map



X Index: 121



Y Index: 130



Z Index: 117

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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.

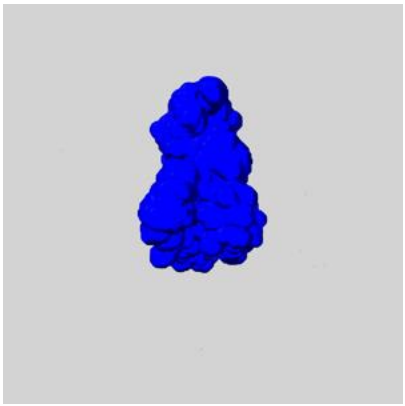
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

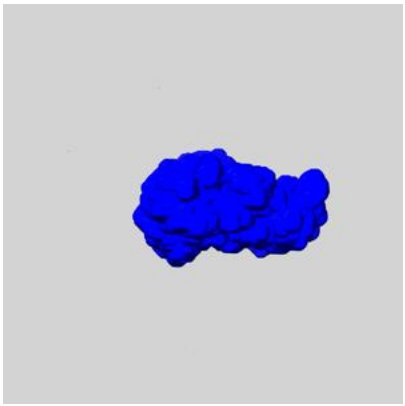
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

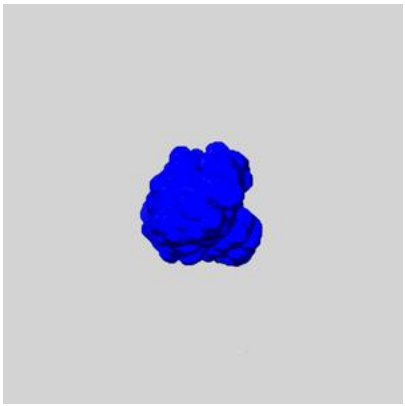
6.5.1 emd_33681_msk_1.map (i)



X



Y

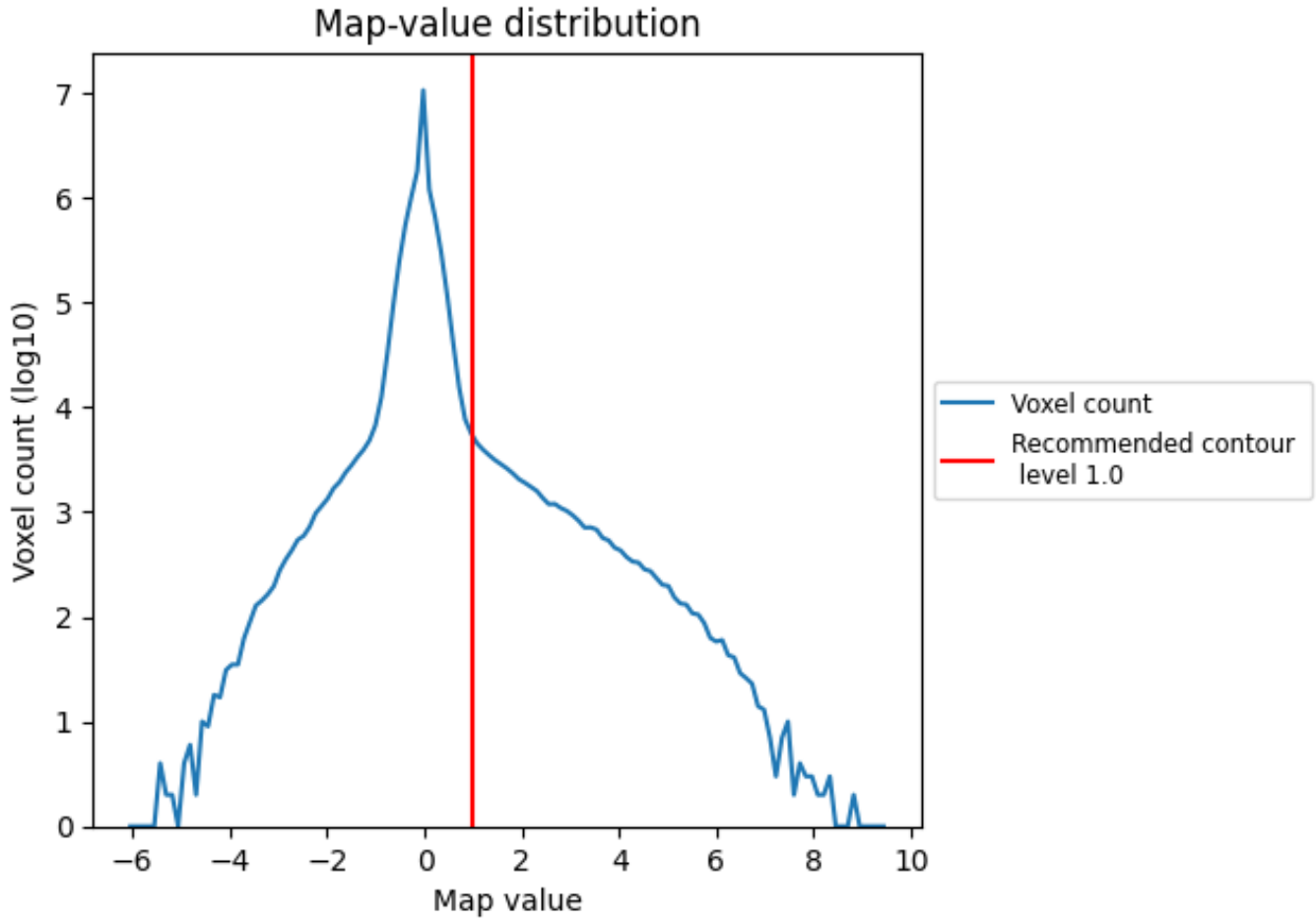


Z

7 Map analysis

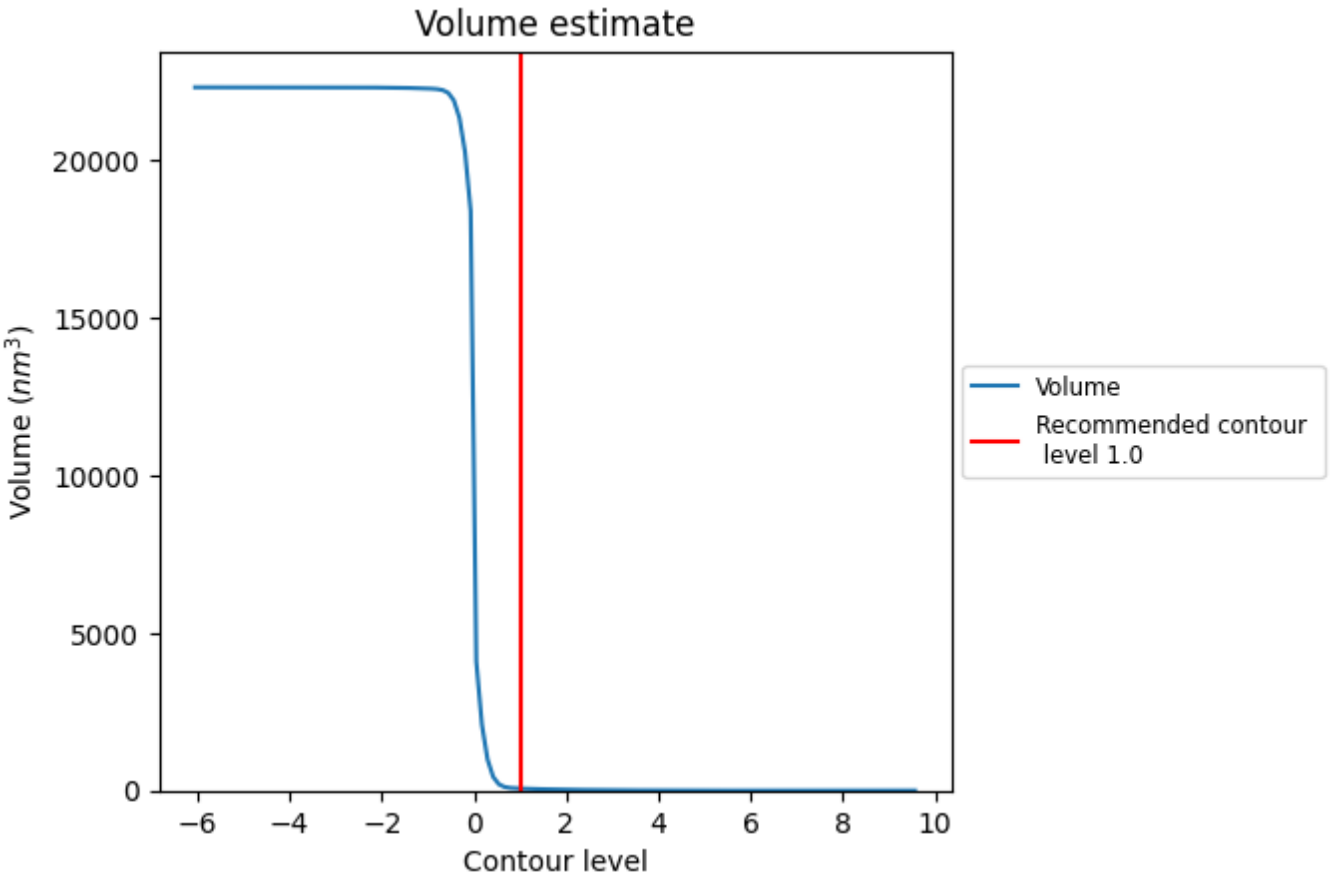
This section contains the results of statistical analysis of the map.

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.

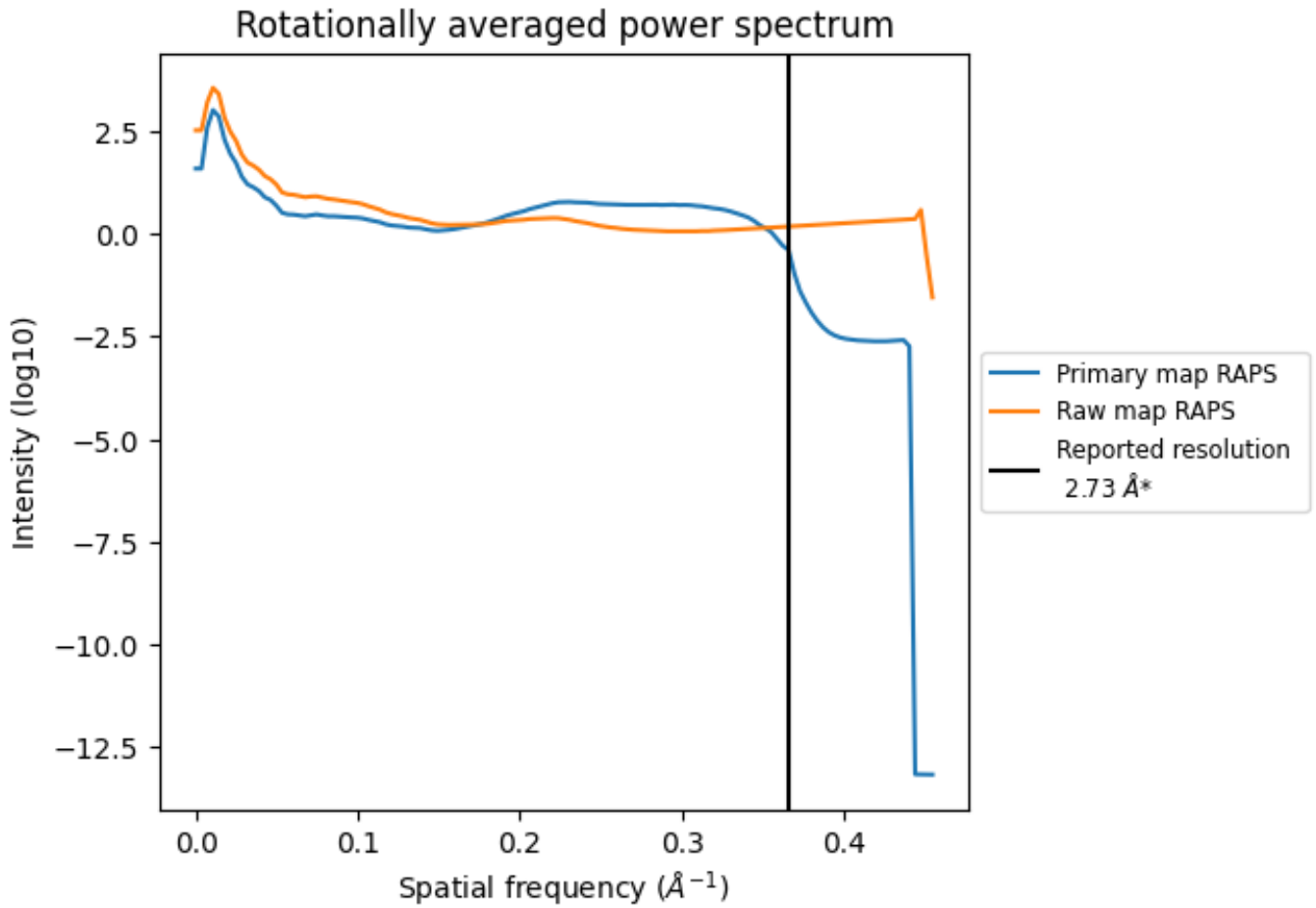
7.2 Volume estimate



The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 59 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)

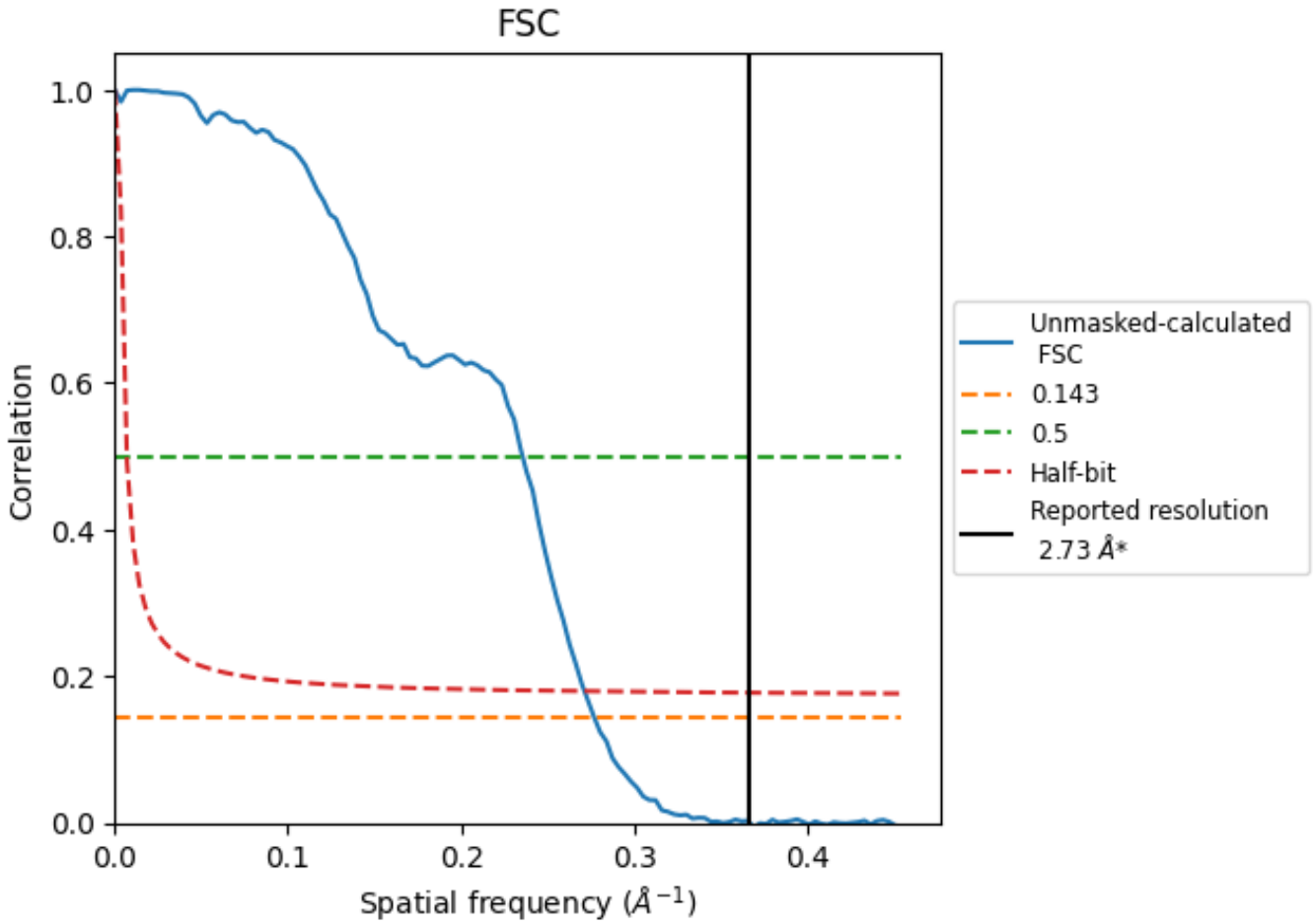


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8.2 Resolution estimates (i)

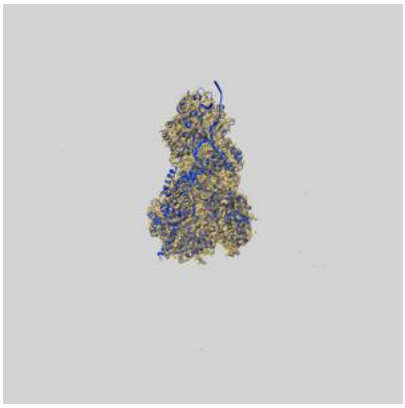
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.24	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.73 by more than 10 %

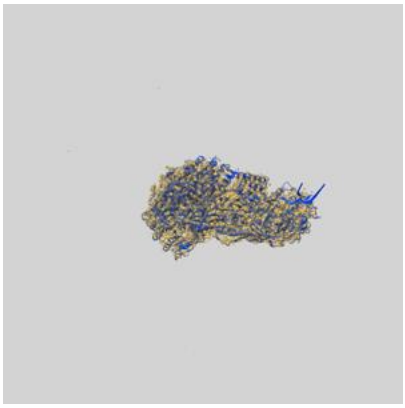
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33681 and PDB model 7Y85. Per-residue inclusion information can be found in section 3 on page 6.

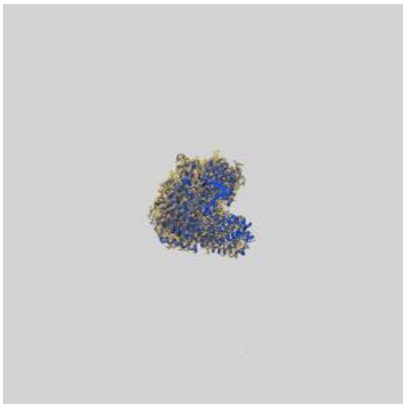
9.1 Map-model overlay



X



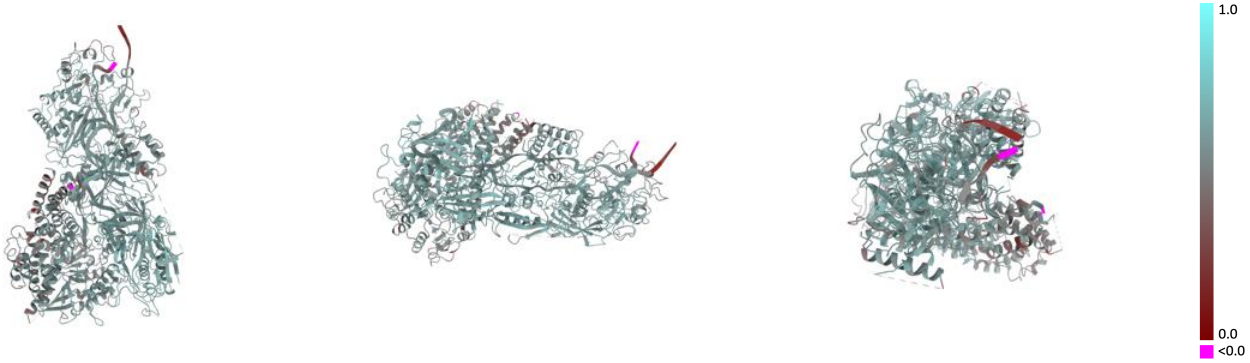
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

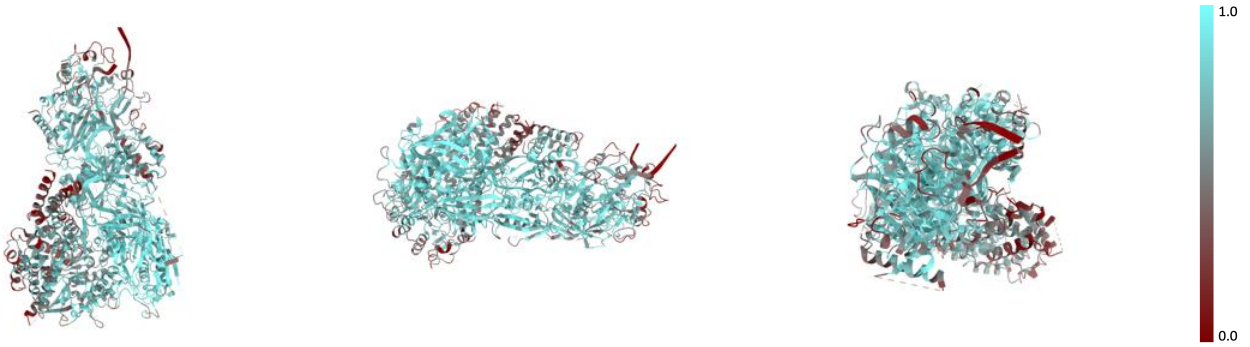
9.2 Q-score mapped to coordinate model (i)



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.

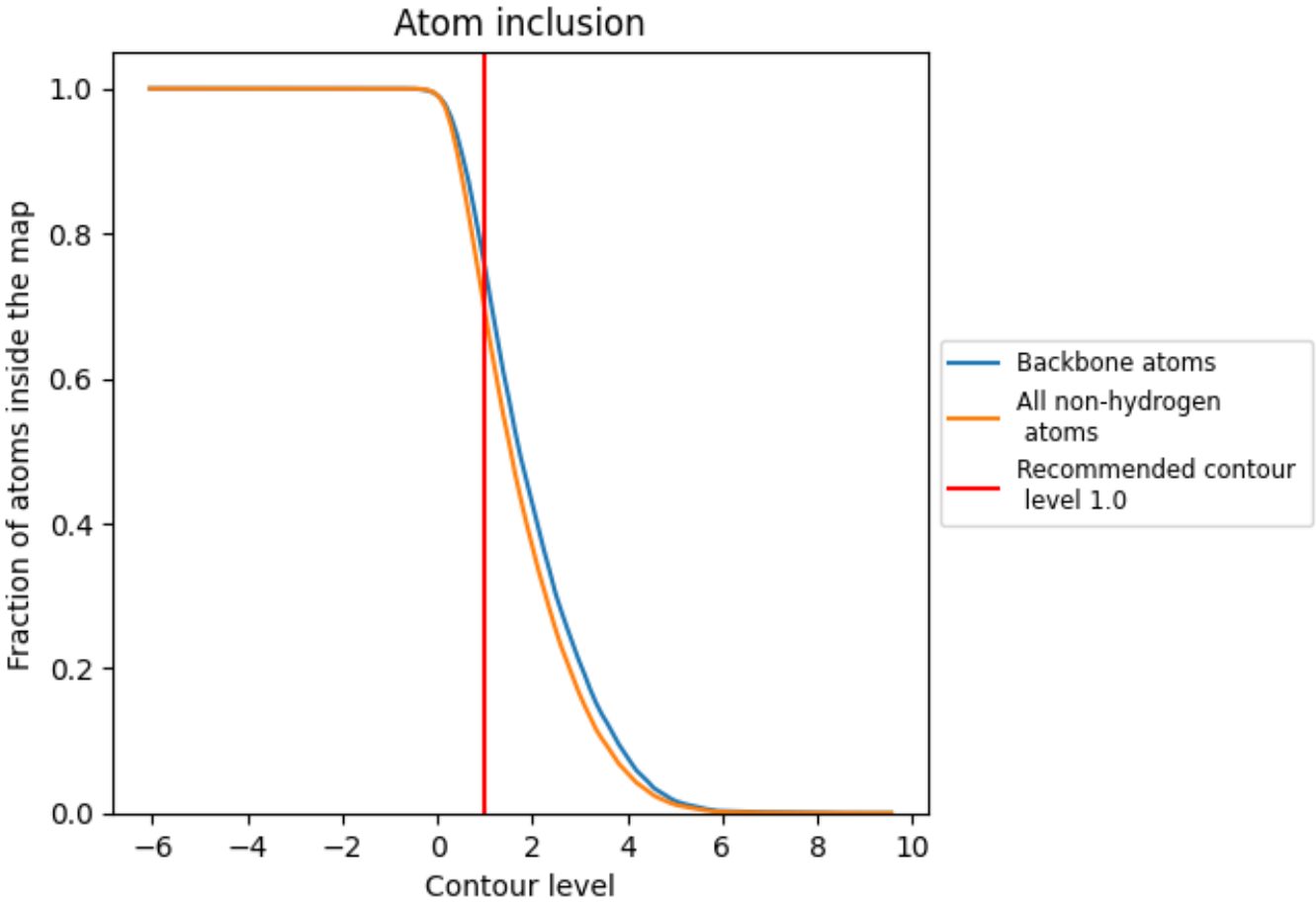
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6953	0.5700
A	0.7522	0.5910
B	0.8296	0.5700
C	0.6532	0.5100
D	0.5732	0.5360