



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 03:57 AM UTC

PDB ID : 6V9Q / pdb_00006v9q
EMDB ID : EMD-21126
Title : Cryo-EM structure of Cascade-TniQ binary complex
Authors : Jia, N.; Patel, D.J.
Deposited on : 2019-12-15
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

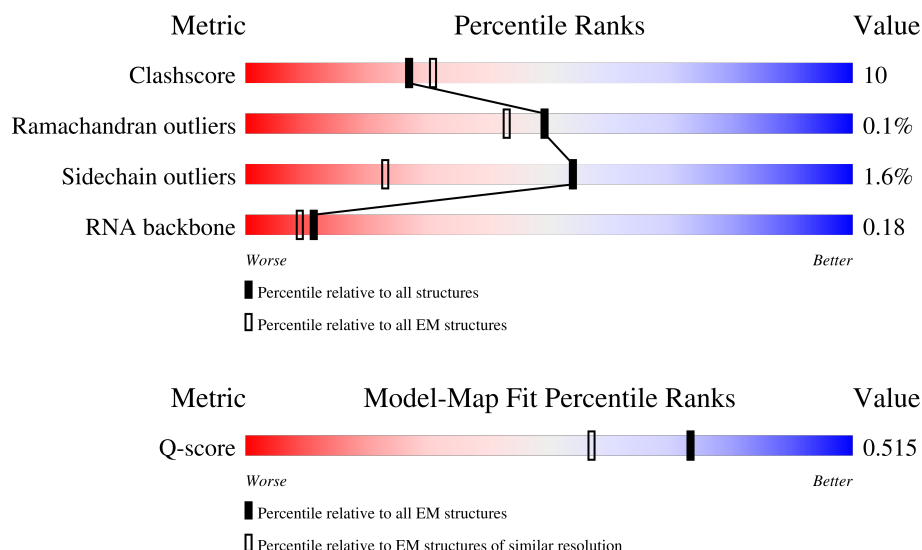
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	K	61	
2	A	640	
3	I	394	

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Mol	Chain	Length	Quality of chain
3	J	394	32% 85% 10% .
4	B	352	80% 16% . .
4	C	352	75% 20% . .
4	D	352	78% 17% . .
4	E	352	76% 18% . .
4	F	352	76% 19% . .
4	G	352	63% 22% . 14%
5	H	199	46% 21% . 32%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28090 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 RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	61	Total	C	N	O	P	0	0
			1275	569	219	427	60		

- Molecule 2 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	454	Total	C	N	O	S	0	0
			3573	2266	620	669	18		

- Molecule 3 is a protein called TniQ family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	378	Total	C	N	O	S	0	0
			3075	1975	526	555	19		
3	I	374	Total	C	N	O	S	0	0
			3050	1959	522	550	19		

- Molecule 4 is a protein called Type I-F CRISPR-associated protein Csy3.

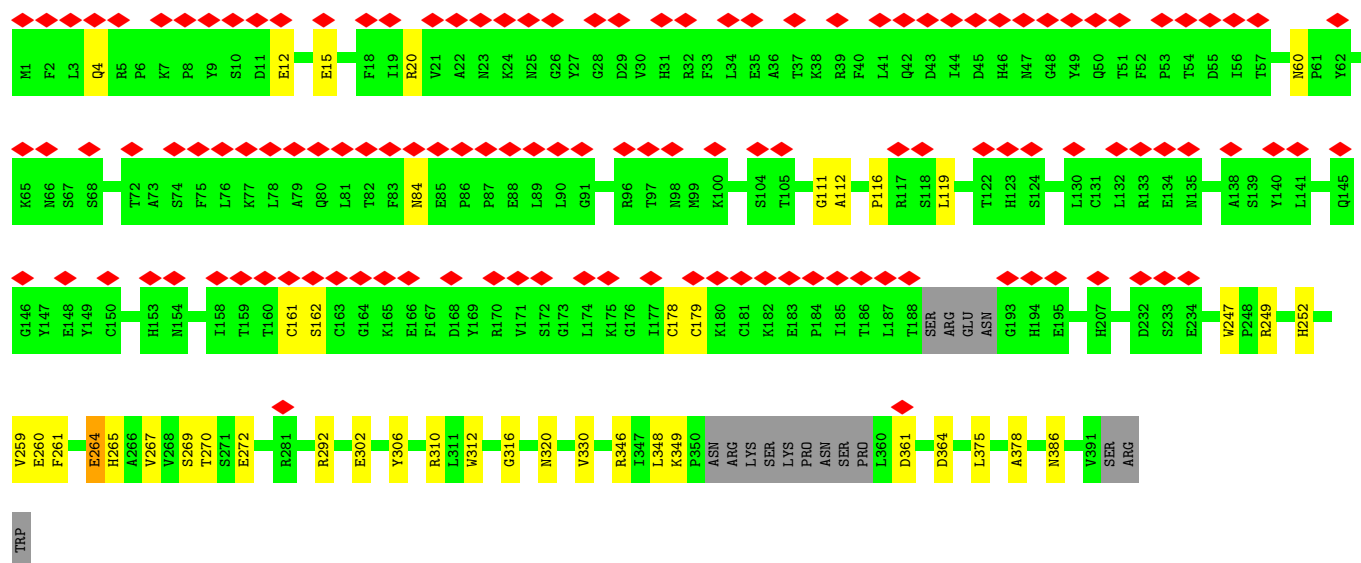
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	303	Total	C	N	O	S	0	0
			2453	1568	419	452	14		
4	B	341	Total	C	N	O	S	0	0
			2731	1737	469	510	15		
4	C	339	Total	C	N	O	S	0	0
			2713	1726	466	506	15		
4	D	338	Total	C	N	O	S	0	0
			2704	1721	465	503	15		
4	E	337	Total	C	N	O	S	0	0
			2695	1716	463	501	15		
4	F	338	Total	C	N	O	S	0	0
			2704	1721	464	504	15		

- Molecule 5 is a protein called Type I-F CRISPR-associated endoribonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	135	Total	C	N	O	S	0	0
			1113	712	203	192	6		

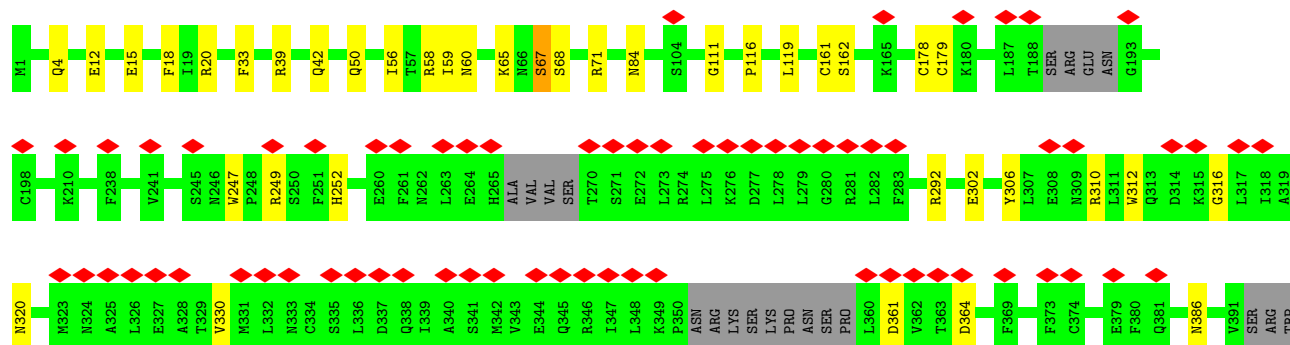
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	J	2	Total	Zn	0
			2	2	
6	I	2	Total	Zn	0
			2	2	



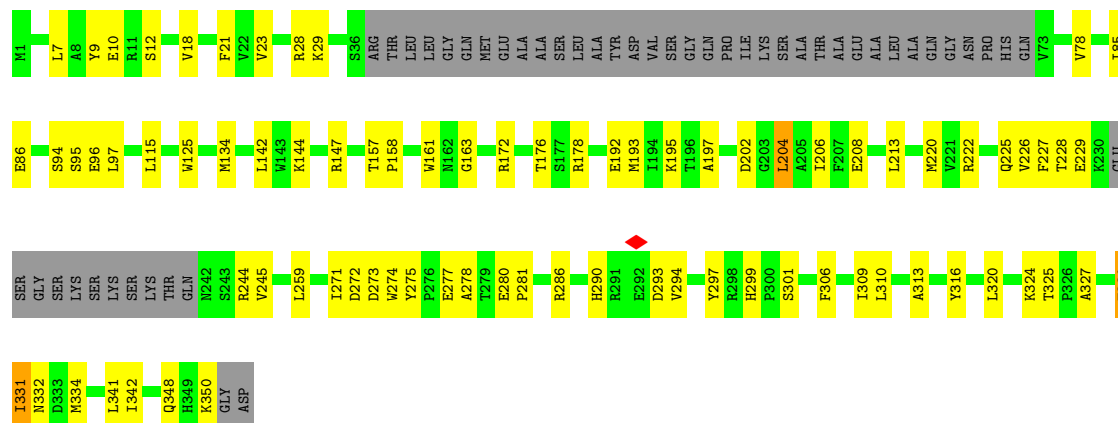
• Molecule 3: TniQ family protein

Chain I: 18% 85% 10% 5%



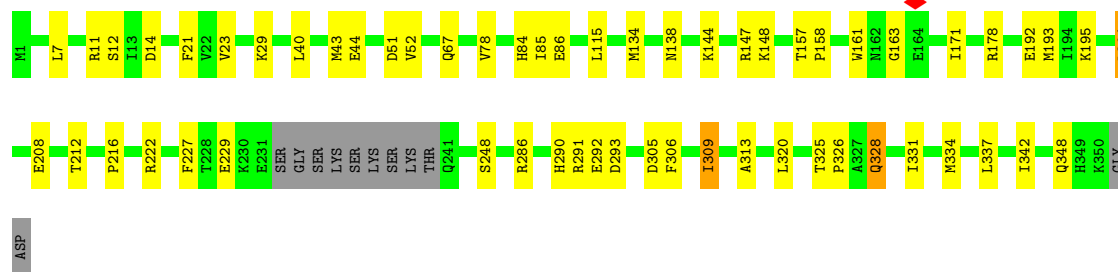
• Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain G: 63% 22% 14%



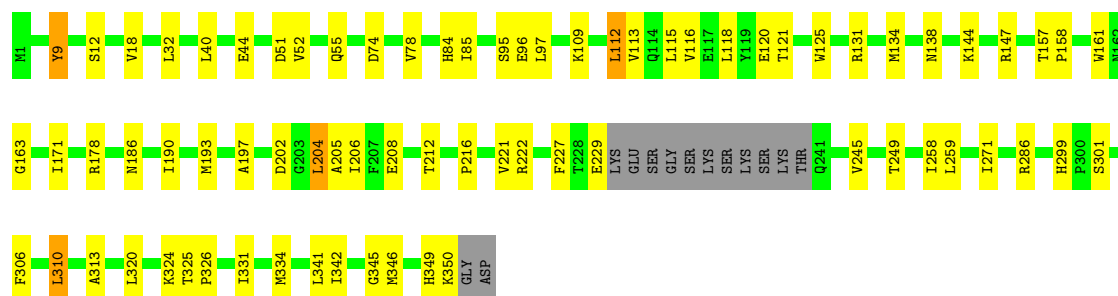
• Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain B:  80% 16% ..



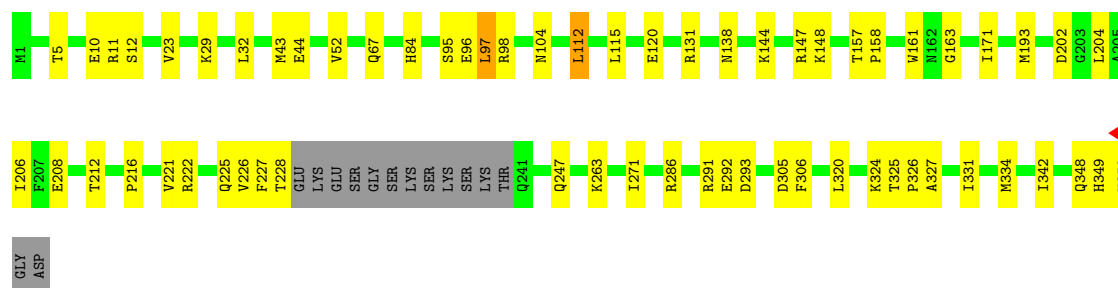
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain C:  75% 20% ..



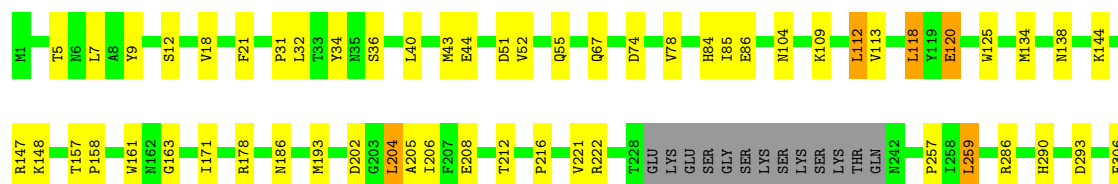
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain D:  78% 17% ..



- Molecule 4: Type I-F CRISPR-associated protein Csy3

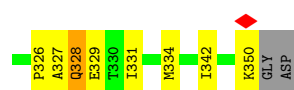
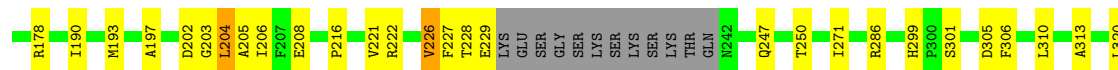
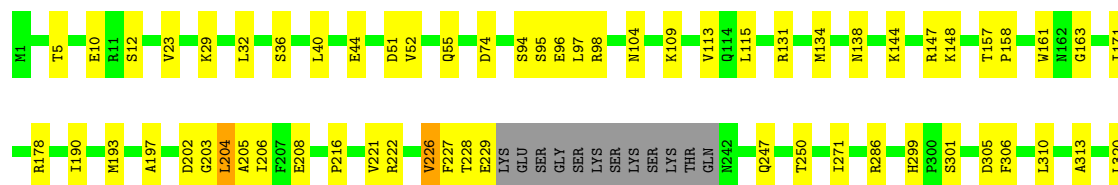
Chain E:  76% 18% ..





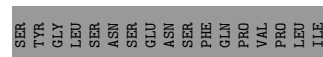
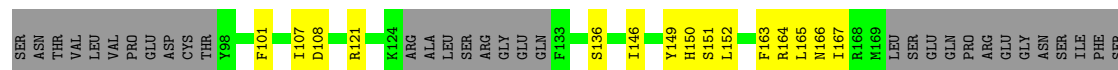
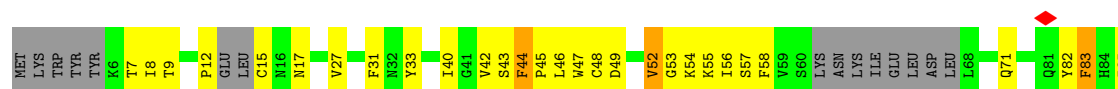
• Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain F: 76% 19% . .



• Molecule 5: Type I-F CRISPR-associated endoribonuclease Cas6/Csy4

Chain H: 46% 21% . 32%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.16	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	311.04, 311.04, 311.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	K	0.38	0/1423	0.69	1/2216 (0.0%)
2	A	0.47	0/3647	0.81	3/4942 (0.1%)
3	I	0.24	0/3134	0.46	0/4243
3	J	0.24	0/3160	0.45	0/4281
4	B	0.38	0/2802	0.66	1/3805 (0.0%)
4	C	0.46	0/2784	0.76	3/3782 (0.1%)
4	D	0.47	0/2775	0.74	0/3770
4	E	0.46	0/2766	0.73	1/3758 (0.0%)
4	F	0.45	0/2775	0.72	1/3770 (0.0%)
4	G	0.48	0/2519	0.76	0/3419
5	H	0.42	0/1135	0.77	0/1519
All	All	0.41	0/28920	0.69	10/39505 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	205	ALA	N-CA-C	6.33	118.93	111.02
4	C	205	ALA	N-CA-C	6.11	118.66	111.02
4	F	205	ALA	N-CA-C	5.85	118.33	111.02
4	C	96	GLU	CA-C-N	5.68	128.36	120.29
4	C	96	GLU	C-N-CA	5.68	128.36	120.29
2	A	564	MET	N-CA-C	5.67	117.55	110.91
1	K	21	U	C1'-C2'-O2'	-5.36	103.77	111.80
2	A	434	ARG	N-CA-C	5.33	117.15	110.91
2	A	540	LEU	N-CA-C	5.33	117.15	110.91
4	B	309	ILE	N-CA-C	-5.25	107.71	112.96

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	K	1275	0	642	42	0
2	A	3573	0	3556	117	0
3	I	3050	0	2958	39	0
3	J	3075	0	2992	39	0
4	B	2731	0	2664	45	0
4	C	2713	0	2645	62	0
4	D	2704	0	2639	56	0
4	E	2695	0	2631	47	0
4	F	2704	0	2637	56	0
4	G	2453	0	2393	77	0
5	H	1113	0	1113	73	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
All	All	28090	0	26870	542	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 10.

All (542) 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:A:101:GLN:HE22	2:A:118:PRO:CG	1.45	1.29
2:A:239:THR:HG22	2:A:473:TRP:HE1	1.00	1.15
5:H:31:PHE:HB2	5:H:71:GLN:HE22	1.05	1.11
2:A:239:THR:HG22	2:A:473:TRP:NE1	1.65	1.09
2:A:180:GLN:O	2:A:184:ILE:HG13	1.53	1.08
1:K:46:C:N4	5:H:163:PHE:HB2	1.67	1.07
3:J:260:GLU:O	3:J:264:GLU:HG2	1.54	1.06
5:H:151:SER:HA	5:H:165:LEU:O	1.53	1.05
2:A:239:THR:CG2	2:A:473:TRP:HE1	1.69	1.04
2:A:101:GLN:HE22	2:A:118:PRO:HG3	1.21	1.02
3:I:65:LYS:HB2	4:G:277:GLU:HG3	1.43	1.00
1:K:46:C:N4	5:H:163:PHE:CB	2.27	0.97
3:I:56:ILE:O	3:I:59:ILE:HG22	1.64	0.96
1:K:12:C:N4	4:C:346:MET:HE3	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:89:PHE:HB3	2:A:90:PRO:HD3	1.50	0.93
2:A:101:GLN:NE2	2:A:118:PRO:CG	2.31	0.93
2:A:449:LYS:HE3	2:A:471:ASP:OD2	1.69	0.92
2:A:206:SER:H	2:A:618:ASN:ND2	1.67	0.91
2:A:206:SER:H	2:A:618:ASN:HD22	0.96	0.91
5:H:31:PHE:HB2	5:H:71:GLN:NE2	1.86	0.91
5:H:12:PRO:HG2	5:H:15:CYS:SG	2.12	0.90
5:H:54:LYS:HG3	5:H:55:LYS:HE3	1.51	0.90
3:J:260:GLU:O	3:J:264:GLU:CG	2.20	0.89
5:H:151:SER:HB3	5:H:166:ASN:OD1	1.73	0.89
1:K:22:U:OP1	4:D:263:LYS:CE	2.22	0.88
1:K:22:U:OP1	4:D:263:LYS:HE3	1.73	0.87
4:C:40:LEU:HD12	4:D:227:PHE:CE1	2.09	0.87
5:H:152:LEU:HB2	5:H:165:LEU:HD12	1.57	0.87
2:A:194:ALA:HB3	2:A:195:PRO:HD3	1.56	0.86
1:K:44:A:O2'	1:K:45:A:P	2.33	0.86
3:J:267:VAL:HG12	5:H:15:CYS:SG	2.16	0.85
2:A:206:SER:N	2:A:618:ASN:HD22	1.75	0.85
3:J:267:VAL:CG1	5:H:15:CYS:SG	2.64	0.85
5:H:27:VAL:HG12	5:H:71:GLN:OE1	1.76	0.85
4:F:326:PRO:HB2	4:F:331:ILE:CG2	2.06	0.84
2:A:239:THR:CG2	2:A:473:TRP:NE1	2.34	0.84
2:A:101:GLN:NE2	2:A:118:PRO:HG3	1.93	0.82
3:I:65:LYS:HB2	4:G:277:GLU:CG	2.09	0.82
4:C:249:THR:HG23	4:C:258:ILE:HG21	1.62	0.82
1:K:46:C:C4	5:H:163:PHE:HB3	2.15	0.82
5:H:31:PHE:HD1	5:H:71:GLN:HE21	1.28	0.81
5:H:46:LEU:HD12	5:H:55:LYS:CG	2.12	0.80
2:A:101:GLN:HE22	2:A:118:PRO:HG2	1.42	0.80
5:H:52:VAL:HG23	5:H:150:HIS:CD2	2.16	0.79
2:A:433:PHE:CE1	2:A:485:THR:CG2	2.66	0.79
2:A:106:LEU:H	2:A:106:LEU:HD23	1.47	0.78
5:H:31:PHE:CD1	5:H:71:GLN:NE2	2.52	0.78
1:K:46:C:C4	5:H:163:PHE:CB	2.66	0.78
1:K:42:U:C6	4:G:220:MET:HE1	2.20	0.77
2:A:483:LEU:HD12	2:A:483:LEU:N	2.01	0.76
4:E:120:GLU:HG2	4:E:125:TRP:NE1	2.02	0.75
1:K:44:A:O2'	1:K:45:A:O5'	2.04	0.74
5:H:42:VAL:CG1	5:H:56:ILE:HD11	2.17	0.74
2:A:89:PHE:CB	2:A:90:PRO:HD3	2.18	0.73
2:A:103:LEU:C	2:A:103:LEU:HD23	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:97:LEU:CD1	4:G:341:LEU:HB2	2.17	0.73
1:K:42:U:H1'	1:K:44:A:H62	1.53	0.73
5:H:31:PHE:CB	5:H:71:GLN:HE22	1.94	0.73
4:B:44:GLU:HG2	4:C:286:ARG:HB2	1.70	0.72
5:H:46:LEU:HD12	5:H:55:LYS:HG2	1.72	0.72
3:I:65:LYS:CB	4:G:277:GLU:HG3	2.19	0.71
5:H:151:SER:HB2	5:H:164:ARG:HB3	1.73	0.71
3:I:65:LYS:HB2	4:G:277:GLU:CB	2.21	0.71
4:D:97:LEU:C	4:D:97:LEU:HD22	2.15	0.71
3:J:15:GLU:OE2	3:J:60:ASN:ND2	2.24	0.71
4:G:271:ILE:HG22	4:G:274:TRP:CH2	2.27	0.70
3:J:267:VAL:HG11	5:H:15:CYS:SG	2.30	0.70
2:A:239:THR:HG22	2:A:473:TRP:CD1	2.25	0.70
1:K:44:A:O2'	1:K:45:A:OP1	2.10	0.69
1:K:22:U:OP1	4:D:263:LYS:HE2	1.92	0.69
2:A:194:ALA:CB	2:A:195:PRO:HD3	2.22	0.69
3:I:15:GLU:OE2	3:I:60:ASN:ND2	2.24	0.69
3:J:267:VAL:HG11	5:H:12:PRO:HG3	1.76	0.68
2:A:103:LEU:HD23	2:A:103:LEU:O	1.93	0.68
4:C:44:GLU:HG2	4:D:286:ARG:HB2	1.76	0.68
2:A:102:ALA:HB1	2:A:571:HIS:CD2	2.29	0.67
2:A:101:GLN:HE22	2:A:118:PRO:CB	2.06	0.67
4:B:134:MET:HE1	4:B:178:ARG:HG3	1.77	0.67
4:D:44:GLU:HG2	4:E:286:ARG:HB2	1.77	0.67
2:A:194:ALA:HB3	2:A:195:PRO:CD	2.24	0.67
3:J:349:LYS:HE3	4:G:293:ASP:HB3	1.77	0.67
3:I:18:PHE:HD1	3:I:33:PHE:HE2	1.41	0.67
4:D:286:ARG:HG3	4:D:306:PHE:HB3	1.77	0.66
4:B:157:THR:HB	4:B:208:GLU:HB2	1.77	0.66
4:C:286:ARG:HG3	4:C:306:PHE:HB3	1.76	0.66
4:E:157:THR:HB	4:E:208:GLU:HB2	1.78	0.66
4:D:97:LEU:HD13	4:D:97:LEU:H	1.60	0.65
4:C:249:THR:CG2	4:C:258:ILE:HG21	2.25	0.65
4:F:97:LEU:HD23	4:F:97:LEU:H	1.60	0.65
2:A:433:PHE:CE1	2:A:485:THR:HG21	2.31	0.65
5:H:107:ILE:HD13	5:H:149:TYR:HB3	1.78	0.65
2:A:88:LYS:HG2	2:A:94:SER:O	1.97	0.65
4:G:157:THR:HB	4:G:208:GLU:HB2	1.79	0.65
4:G:95:SER:OG	4:G:95:SER:O	2.13	0.64
4:F:95:SER:O	4:F:95:SER:OG	2.13	0.64
1:K:12:C:C4	4:C:346:MET:HE3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:239:THR:CG2	2:A:473:TRP:CD1	2.80	0.64
2:A:433:PHE:CE1	2:A:485:THR:HG23	2.31	0.64
4:F:157:THR:HB	4:F:208:GLU:HB2	1.79	0.64
5:H:12:PRO:CG	5:H:15:CYS:SG	2.85	0.64
2:A:433:PHE:CZ	2:A:485:THR:HG23	2.33	0.63
4:F:286:ARG:HG3	4:F:306:PHE:HB3	1.79	0.63
2:A:453:THR:HG22	4:B:227:PHE:HD1	1.64	0.63
4:D:98:ARG:NH2	4:D:120:GLU:OE1	2.29	0.63
4:C:134:MET:HE1	4:C:178:ARG:HG3	1.81	0.62
4:G:327:ALA:O	4:G:331:ILE:HG23	1.99	0.62
4:D:157:THR:HB	4:D:208:GLU:HB2	1.81	0.62
4:E:134:MET:HE1	4:E:178:ARG:HG3	1.80	0.62
4:E:286:ARG:HG3	4:E:306:PHE:HB3	1.80	0.62
4:E:109:LYS:O	4:E:113:VAL:HG23	2.00	0.62
2:A:24:ARG:HD3	2:A:253:THR:HG22	1.82	0.61
2:A:433:PHE:O	2:A:486:ASN:HB3	2.01	0.61
4:F:134:MET:HE1	4:F:178:ARG:HG3	1.81	0.61
4:G:134:MET:HE1	4:G:178:ARG:HG3	1.81	0.61
3:I:65:LYS:NZ	4:G:297:TYR:CD1	2.63	0.60
5:H:151:SER:HA	5:H:165:LEU:C	2.23	0.60
2:A:481:LEU:CD1	2:A:483:LEU:HG	2.32	0.60
4:B:40:LEU:HD12	4:C:227:PHE:CE1	2.37	0.60
4:D:95:SER:O	4:D:95:SER:OG	2.15	0.60
4:G:192:GLU:OE2	4:G:195:LYS:NZ	2.25	0.60
2:A:481:LEU:HD12	2:A:483:LEU:HD11	1.84	0.60
2:A:601:ILE:HG22	2:A:603:PHE:H	1.66	0.60
4:D:97:LEU:H	4:D:97:LEU:CD1	2.15	0.60
2:A:82:ARG:HH22	2:A:139:GLU:HG2	1.66	0.60
2:A:106:LEU:HD23	2:A:106:LEU:N	2.15	0.59
4:G:286:ARG:HG3	4:G:306:PHE:HB3	1.83	0.59
2:A:538:ARG:NH1	2:A:562:GLN:OE1	2.35	0.59
3:I:252:HIS:NE2	3:I:302:GLU:OE2	2.35	0.59
4:G:274:TRP:HB3	4:G:332:ASN:HB3	1.84	0.59
2:A:237:ALA:HB2	2:A:262:LYS:HB2	1.85	0.59
2:A:134:ALA:O	2:A:138:ASN:ND2	2.35	0.59
3:J:267:VAL:HG12	5:H:15:CYS:CB	2.32	0.58
4:C:97:LEU:CD1	4:C:341:LEU:HB2	2.33	0.58
3:I:42:GLN:O	4:G:147:ARG:NH1	2.35	0.58
4:G:12:SER:HB2	4:G:342:ILE:HG23	1.86	0.58
2:A:469:THR:HB	4:B:229:GLU:OE2	2.03	0.58
4:E:309:ILE:HG22	4:E:337:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:327:ALA:HB3	4:E:330:THR:HG22	1.85	0.58
2:A:270:PRO:HD2	2:A:538:ARG:HE	1.69	0.58
4:C:40:LEU:HD12	4:D:227:PHE:CD1	2.39	0.58
1:K:60:G:OP1	5:H:33:TYR:OH	2.22	0.57
2:A:76:ILE:HD13	2:A:179:LYS:CD	2.34	0.57
3:I:39:ARG:HH21	4:G:176:THR:HG23	1.69	0.57
2:A:453:THR:HG22	4:B:227:PHE:CD1	2.40	0.57
3:J:267:VAL:CG2	5:H:82:TYR:CE2	2.87	0.57
3:I:161:CYS:SG	3:I:162:SER:N	2.78	0.57
4:C:161:TRP:NE1	4:C:163:GLY:O	2.38	0.57
5:H:27:VAL:CG1	5:H:71:GLN:OE1	2.49	0.57
4:B:115:LEU:HD11	4:B:313:ALA:HB1	1.85	0.57
3:J:161:CYS:SG	3:J:162:SER:N	2.78	0.57
4:F:161:TRP:NE1	4:F:163:GLY:O	2.38	0.57
3:J:267:VAL:HG12	5:H:15:CYS:HB3	1.86	0.57
4:G:277:GLU:OE1	4:G:277:GLU:HA	2.03	0.57
4:G:161:TRP:NE1	4:G:163:GLY:O	2.38	0.56
3:J:386:ASN:ND2	3:I:111:GLY:O	2.39	0.56
4:C:109:LYS:O	4:C:113:VAL:HG23	2.06	0.56
4:C:157:THR:HB	4:C:208:GLU:HB2	1.88	0.56
4:D:326:PRO:HB2	4:D:331:ILE:CG2	2.36	0.56
4:F:326:PRO:HB2	4:F:331:ILE:HG21	1.85	0.56
1:K:2:U:H5''	2:A:201:ILE:HG23	1.87	0.56
4:E:12:SER:HB2	4:E:342:ILE:HG23	1.87	0.56
3:J:252:HIS:NE2	3:J:302:GLU:OE2	2.35	0.56
4:C:144:LYS:O	4:C:222:ARG:NH2	2.39	0.56
1:K:46:C:C5	5:H:163:PHE:HA	2.41	0.56
4:C:320:LEU:HD11	4:C:334:MET:HE2	1.88	0.56
5:H:42:VAL:HG22	5:H:58:PHE:CD1	2.41	0.56
2:A:105:GLU:O	2:A:105:GLU:HG3	2.05	0.55
4:F:144:LYS:O	4:F:222:ARG:NH2	2.39	0.55
5:H:9:THR:HB	5:H:55:LYS:NZ	2.22	0.55
4:D:12:SER:HB2	4:D:342:ILE:HG23	1.88	0.55
4:E:18:VAL:HB	4:E:259:LEU:HB2	1.89	0.55
2:A:67:ARG:HB3	2:A:172:LYS:NZ	2.22	0.55
2:A:102:ALA:HB1	2:A:571:HIS:NE2	2.22	0.55
1:K:12:C:N4	4:C:346:MET:CE	2.63	0.55
4:B:320:LEU:HD11	4:B:334:MET:HE2	1.89	0.55
4:B:291:ARG:NH2	4:B:292:GLU:OE2	2.39	0.54
4:G:115:LEU:HD11	4:G:313:ALA:HB1	1.90	0.54
4:E:144:LYS:O	4:E:222:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:32:LEU:HD21	4:F:221:VAL:HG21	1.90	0.54
5:H:108:ASP:OD1	5:H:166:ASN:ND2	2.41	0.54
3:J:116:PRO:HG2	3:J:119:LEU:HB2	1.90	0.54
3:I:39:ARG:HH11	4:G:172:ARG:HG3	1.71	0.54
3:I:65:LYS:HD2	4:G:277:GLU:HB2	1.89	0.54
2:A:101:GLN:NE2	2:A:118:PRO:CB	2.68	0.54
2:A:418:PHE:HB2	2:A:504:LEU:HD23	1.90	0.54
3:J:4:GLN:OE1	3:J:84:ASN:ND2	2.41	0.54
3:I:4:GLN:OE1	3:I:84:ASN:ND2	2.41	0.54
4:D:32:LEU:HD21	4:D:221:VAL:HG21	1.89	0.54
4:D:226:VAL:HG23	4:D:228:THR:HG23	1.90	0.54
4:E:326:PRO:HB2	4:E:331:ILE:CG2	2.37	0.54
4:C:12:SER:HB2	4:C:342:ILE:HG23	1.89	0.54
4:C:95:SER:O	4:C:95:SER:OG	2.16	0.54
4:D:326:PRO:HB2	4:D:331:ILE:HG21	1.90	0.54
4:E:40:LEU:HD12	4:F:227:PHE:CE1	2.43	0.53
2:A:106:LEU:HD21	2:A:112:SER:OG	2.09	0.53
4:D:5:THR:OG1	4:D:104:ASN:ND2	2.40	0.53
3:J:261:PHE:O	3:J:265:HIS:ND1	2.41	0.53
3:J:292:ARG:NH2	3:J:330:VAL:O	2.40	0.53
4:E:161:TRP:NE1	4:E:163:GLY:O	2.41	0.53
4:D:144:LYS:O	4:D:222:ARG:NH2	2.42	0.53
4:C:52:VAL:HG13	4:D:350:LYS:HG2	1.90	0.52
4:E:5:THR:OG1	4:E:104:ASN:ND2	2.40	0.52
2:A:481:LEU:HD12	2:A:483:LEU:CD1	2.39	0.52
5:H:17:ASN:HB3	5:H:53:GLY:O	2.09	0.52
2:A:206:SER:N	2:A:618:ASN:ND2	2.43	0.52
2:A:211:ILE:HD11	2:A:623:LEU:HD11	1.91	0.52
4:G:244:ARG:O	4:G:244:ARG:HG3	2.09	0.52
4:C:326:PRO:HB2	4:C:331:ILE:CG2	2.39	0.52
4:F:327:ALA:O	4:F:331:ILE:HG23	2.10	0.52
5:H:42:VAL:HG22	5:H:58:PHE:CE1	2.44	0.52
5:H:146:ILE:HG21	5:H:149:TYR:CD1	2.44	0.52
4:B:148:LYS:HA	4:C:204:LEU:HD21	1.91	0.52
4:E:120:GLU:HG2	4:E:125:TRP:HE1	1.73	0.52
3:I:65:LYS:HZ3	4:G:297:TYR:HD1	1.48	0.52
4:G:202:ASP:OD1	4:F:147:ARG:NH1	2.42	0.52
4:G:320:LEU:HD11	4:G:334:MET:HE2	1.92	0.52
5:H:107:ILE:HD13	5:H:149:TYR:CB	2.40	0.52
4:G:97:LEU:CD1	4:G:341:LEU:CB	2.85	0.52
3:I:116:PRO:HG2	3:I:119:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:328:GLN:HE21	4:F:328:GLN:CA	2.22	0.52
2:A:83:GLN:NE2	2:A:96:GLY:O	2.42	0.52
3:J:267:VAL:CG1	5:H:12:PRO:HG3	2.39	0.52
4:G:272:ASP:O	4:G:281:PRO:HA	2.09	0.52
2:A:532:LEU:HD23	2:A:532:LEU:O	2.10	0.52
3:J:306:TYR:OH	3:J:310:ARG:NH1	2.44	0.52
3:I:56:ILE:O	3:I:59:ILE:CG2	2.47	0.52
3:I:59:ILE:O	3:I:71:ARG:NH2	2.42	0.52
3:I:292:ARG:NH2	3:I:330:VAL:O	2.40	0.51
4:G:227:PHE:C	4:G:227:PHE:CD2	2.87	0.51
3:I:65:LYS:HB2	4:G:277:GLU:HB3	1.93	0.51
4:G:275:TYR:CZ	4:G:278:ALA:HA	2.45	0.51
4:B:290:HIS:ND1	4:B:293:ASP:OD1	2.43	0.51
4:G:273:ASP:O	4:G:278:ALA:CB	2.59	0.51
1:K:11:A:C5	4:C:346:MET:HE2	2.46	0.51
3:I:306:TYR:OH	3:I:310:ARG:NH1	2.44	0.51
4:E:120:GLU:HG2	4:E:125:TRP:CD1	2.45	0.51
2:A:409:ILE:CG1	2:A:410:PRO:HD2	2.41	0.51
3:J:346:ARG:HH12	4:G:294:VAL:HB	1.75	0.51
4:C:249:THR:HG23	4:C:258:ILE:CG2	2.37	0.51
1:K:46:C:N4	5:H:163:PHE:HB3	2.10	0.51
4:B:7:LEU:H	4:B:348:GLN:HE21	1.56	0.51
4:F:138:ASN:HA	4:F:171:ILE:HD13	1.92	0.51
1:K:11:A:C6	4:C:346:MET:HE2	2.46	0.51
2:A:469:THR:CG2	4:B:229:GLU:OE2	2.58	0.51
4:C:97:LEU:HD13	4:C:341:LEU:HB2	1.92	0.51
4:F:320:LEU:HD11	4:F:334:MET:HE2	1.93	0.51
1:K:42:U:C5	4:G:220:MET:HE1	2.46	0.51
2:A:180:GLN:O	2:A:184:ILE:N	2.44	0.51
1:K:21:U:C6	4:D:227:PHE:CD1	2.98	0.50
2:A:106:LEU:HD22	2:A:571:HIS:CE1	2.45	0.50
2:A:622:TYR:HD2	2:A:624:VAL:HG23	1.76	0.50
4:D:161:TRP:NE1	4:D:163:GLY:O	2.45	0.50
4:E:327:ALA:O	4:E:331:ILE:HG23	2.11	0.50
3:I:50:GLN:HG3	4:G:280:GLU:OE1	2.11	0.50
4:F:328:GLN:HA	4:F:328:GLN:NE2	2.26	0.50
2:A:76:ILE:HD13	2:A:179:LYS:HD2	1.93	0.50
3:J:267:VAL:HG11	5:H:12:PRO:CG	2.40	0.50
4:C:51:ASP:OD2	4:C:55:GLN:NE2	2.44	0.50
4:F:23:VAL:HG22	4:F:29:LYS:HG2	1.93	0.50
3:J:267:VAL:HG22	5:H:82:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:291:ARG:NH2	4:D:292:GLU:OE2	2.45	0.50
4:D:115:LEU:HD22	4:D:334:MET:HE1	1.94	0.50
4:G:273:ASP:O	4:G:278:ALA:HB1	2.12	0.49
4:E:52:VAL:HG13	4:F:350:LYS:HG2	1.93	0.49
4:G:350:LYS:HG2	4:F:52:VAL:HG13	1.95	0.49
2:A:387:PHE:N	2:A:522:PHE:O	2.45	0.49
4:F:12:SER:HB2	4:F:342:ILE:HG23	1.94	0.49
4:F:326:PRO:HB2	4:F:331:ILE:HG22	1.90	0.49
4:D:324:LYS:HD3	4:D:325:THR:O	2.13	0.49
4:E:320:LEU:HD11	4:E:334:MET:HE2	1.94	0.49
4:C:97:LEU:HD21	4:C:125:TRP:HH2	1.77	0.49
4:D:52:VAL:HG13	4:E:350:LYS:HG2	1.95	0.49
4:C:147:ARG:NH1	4:D:202:ASP:OD1	2.46	0.49
5:H:31:PHE:CB	5:H:71:GLN:NE2	2.63	0.49
2:A:89:PHE:CB	2:A:90:PRO:CD	2.89	0.49
2:A:76:ILE:CD1	2:A:179:LYS:HD2	2.43	0.49
2:A:194:ALA:CB	2:A:195:PRO:CD	2.88	0.49
4:C:97:LEU:HD21	4:C:125:TRP:CH2	2.47	0.49
4:C:95:SER:HB2	4:C:197:ALA:O	2.13	0.48
4:C:227:PHE:HE2	4:C:229:GLU:HG3	1.76	0.48
2:A:437:SER:HB3	2:A:628:ARG:HH21	1.78	0.48
2:A:535:GLU:OE1	2:A:535:GLU:HA	2.13	0.48
4:G:97:LEU:HD12	4:G:341:LEU:CB	2.43	0.48
4:E:138:ASN:HA	4:E:171:ILE:HD13	1.95	0.48
3:J:267:VAL:HG12	3:J:267:VAL:O	2.12	0.48
4:G:225:GLN:HB2	4:G:245:VAL:O	2.13	0.48
4:C:78:VAL:HG22	4:C:85:ILE:HD11	1.95	0.48
4:D:23:VAL:HG22	4:D:29:LYS:HG2	1.95	0.48
4:D:97:LEU:HD13	4:D:97:LEU:N	2.27	0.48
1:K:45:A:N1	5:H:149:TYR:HE2	2.10	0.48
4:C:324:LYS:HD3	4:C:325:THR:O	2.13	0.48
4:B:138:ASN:HA	4:B:171:ILE:HD13	1.95	0.48
4:B:286:ARG:HG3	4:B:306:PHE:HB3	1.94	0.48
4:D:216:PRO:HG3	4:E:206:ILE:HD13	1.95	0.48
2:A:67:ARG:HB3	2:A:172:LYS:HZ3	1.78	0.48
2:A:103:LEU:C	2:A:103:LEU:CD2	2.85	0.48
2:A:133:SER:O	2:A:137:THR:OG1	2.26	0.48
3:I:67:SER:O	3:I:71:ARG:N	2.46	0.48
4:B:40:LEU:HD12	4:C:227:PHE:CD1	2.48	0.48
2:A:483:LEU:HD12	2:A:483:LEU:H	1.77	0.48
4:F:115:LEU:HD22	4:F:334:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:152:LEU:O	5:H:165:LEU:HG	2.13	0.48
2:A:486:ASN:HD22	2:A:486:ASN:C	2.20	0.48
3:I:65:LYS:HD2	4:G:277:GLU:CG	2.43	0.48
4:G:97:LEU:HD12	4:G:341:LEU:HB3	1.95	0.48
4:G:97:LEU:HD21	4:G:125:TRP:HH2	1.78	0.48
5:H:48:CYS:SG	5:H:49:ASP:N	2.87	0.48
3:J:260:GLU:O	3:J:264:GLU:CD	2.57	0.48
4:E:120:GLU:CG	4:E:125:TRP:HE1	2.26	0.48
4:G:158:PRO:HB2	4:G:193:MET:HE1	1.95	0.48
4:D:293:ASP:OD1	4:D:293:ASP:N	2.42	0.48
4:D:320:LEU:HD11	4:D:334:MET:HE2	1.96	0.48
1:K:33:C:C6	4:F:227:PHE:HA	2.48	0.47
4:G:97:LEU:HD21	4:G:125:TRP:CH2	2.48	0.47
1:K:39:A:N6	4:G:228:THR:O	2.46	0.47
3:I:65:LYS:CG	4:G:277:GLU:HG3	2.44	0.47
2:A:481:LEU:HD13	2:A:482:ILE:N	2.30	0.47
4:E:32:LEU:HD21	4:E:221:VAL:HG21	1.96	0.47
2:A:433:PHE:HE1	2:A:485:THR:HG21	1.79	0.47
4:G:271:ILE:CG2	4:G:274:TRP:CH2	2.95	0.47
4:B:78:VAL:HG22	4:B:85:ILE:HD11	1.96	0.47
4:B:12:SER:HB2	4:B:342:ILE:HG23	1.95	0.47
4:G:95:SER:HB2	4:G:197:ALA:O	2.13	0.47
4:C:32:LEU:HD21	4:C:221:VAL:HG21	1.95	0.47
4:C:138:ASN:HA	4:C:171:ILE:HD13	1.97	0.47
5:H:47:TRP:CZ3	5:H:52:VAL:HG22	2.49	0.47
2:A:67:ARG:CB	2:A:172:LYS:NZ	2.78	0.47
2:A:76:ILE:HD13	2:A:179:LYS:HD3	1.95	0.47
4:G:28:ARG:NH2	5:H:136:SER:OG	2.48	0.47
4:B:52:VAL:HG13	4:C:350:LYS:HG2	1.96	0.47
4:F:97:LEU:H	4:F:97:LEU:CD2	2.26	0.47
4:F:328:GLN:CA	4:F:328:GLN:NE2	2.78	0.47
2:A:486:ASN:C	2:A:486:ASN:ND2	2.73	0.47
3:J:269:SER:O	3:J:272:GLU:N	2.43	0.47
4:B:192:GLU:OE2	4:B:195:LYS:NZ	2.40	0.47
3:I:58:ARG:NH1	4:G:277:GLU:O	2.49	0.46
2:A:481:LEU:HD13	2:A:481:LEU:C	2.39	0.46
4:F:226:VAL:HG23	4:F:228:THR:HG23	1.96	0.46
2:A:529:ILE:O	2:A:532:LEU:CD2	2.63	0.46
3:J:269:SER:OG	3:J:272:GLU:HG2	2.15	0.46
3:J:378:ALA:HB1	3:I:68:SER:HB2	1.98	0.46
4:B:144:LYS:O	4:B:222:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:46:LEU:O	5:H:52:VAL:O	2.33	0.46
1:K:46:C:N3	5:H:163:PHE:HB3	2.31	0.46
2:A:433:PHE:O	2:A:486:ASN:CB	2.64	0.46
4:C:115:LEU:HD11	4:C:313:ALA:HB1	1.96	0.46
2:A:219:LEU:HD22	2:A:250:THR:HG21	1.96	0.46
2:A:483:LEU:N	2:A:483:LEU:CD1	2.73	0.46
4:G:330:THR:CG2	4:G:331:ILE:N	2.79	0.46
4:B:216:PRO:HG3	4:C:206:ILE:HD13	1.98	0.46
2:A:450:ARG:NH2	4:B:248:SER:O	2.49	0.46
2:A:43:LEU:HD22	2:A:138:ASN:HD22	1.81	0.46
1:K:41:G:H5'	1:K:42:U:H5''	1.98	0.46
4:E:78:VAL:HG22	4:E:85:ILE:HD11	1.97	0.46
4:F:51:ASP:OD2	4:F:55:GLN:NE2	2.49	0.46
2:A:89:PHE:HB3	2:A:90:PRO:CD	2.34	0.46
4:G:227:PHE:CE1	4:F:40:LEU:HD12	2.51	0.46
4:E:147:ARG:NH1	4:F:202:ASP:OD1	2.48	0.46
3:I:316:GLY:O	3:I:320:ASN:ND2	2.49	0.45
4:G:23:VAL:HG22	4:G:29:LYS:HG2	1.98	0.45
4:G:309:ILE:HG23	4:G:316:TYR:HE2	1.81	0.45
4:B:328:GLN:HA	4:B:331:ILE:HG12	1.99	0.45
4:C:158:PRO:HB2	4:C:193:MET:HE1	1.98	0.45
4:F:94:SER:O	4:F:96:GLU:OE2	2.34	0.45
4:F:227:PHE:CE2	4:F:229:GLU:HB2	2.51	0.45
5:H:31:PHE:CG	5:H:71:GLN:NE2	2.84	0.45
1:K:45:A:C8	5:H:164:ARG:NE	2.85	0.45
4:E:259:LEU:HD12	4:E:259:LEU:HA	1.74	0.45
4:F:10:GLU:O	4:F:96:GLU:HB2	2.16	0.45
1:K:48:G:N7	5:H:121:ARG:NH2	2.64	0.45
1:K:21:U:H2'	1:K:21:U:O2	2.15	0.45
3:I:65:LYS:NZ	4:G:297:TYR:HD1	2.09	0.45
4:C:116:VAL:O	4:C:120:GLU:HG2	2.17	0.45
5:H:152:LEU:HB2	5:H:165:LEU:CD1	2.38	0.45
1:K:46:C:H2'	1:K:47:U:C6	2.51	0.45
2:A:101:GLN:NE2	2:A:118:PRO:HG2	2.19	0.45
3:J:316:GLY:O	3:J:320:ASN:ND2	2.50	0.45
4:B:51:ASP:O	4:C:349:HIS:NE2	2.49	0.45
4:E:148:LYS:HA	4:F:204:LEU:HD21	1.99	0.45
4:F:5:THR:OG1	4:F:104:ASN:ND2	2.46	0.45
4:D:227:PHE:O	4:D:227:PHE:CD2	2.70	0.45
4:E:290:HIS:ND1	4:E:293:ASP:OD1	2.50	0.45
4:G:18:VAL:HB	4:G:259:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:94:SER:O	4:G:96:GLU:OE2	2.34	0.45
4:B:293:ASP:OD1	4:B:293:ASP:N	2.40	0.45
4:E:44:GLU:HG2	4:F:286:ARG:HB2	1.98	0.45
5:H:146:ILE:CG2	5:H:149:TYR:CD1	2.99	0.45
4:E:21:PHE:HB2	4:E:86:GLU:HB2	1.99	0.45
2:A:26:LEU:HD23	2:A:226:HIS:CD2	2.52	0.45
4:C:40:LEU:CD1	4:D:227:PHE:CE1	2.92	0.45
4:F:227:PHE:O	4:F:227:PHE:CD2	2.70	0.45
4:G:10:GLU:OE2	4:F:144:LYS:NZ	2.46	0.45
4:B:161:TRP:NE1	4:B:163:GLY:O	2.50	0.45
4:C:40:LEU:HD12	4:D:227:PHE:HE1	1.71	0.45
3:I:247:TRP:O	3:I:249:ARG:NH1	2.50	0.44
4:B:309:ILE:HG22	4:B:337:LEU:HD23	1.99	0.44
4:D:226:VAL:HG12	4:D:247:GLN:HG2	1.99	0.44
4:B:11:ARG:NH2	4:B:14:ASP:OD1	2.51	0.44
4:G:78:VAL:HG22	4:G:85:ILE:HD11	1.98	0.44
4:B:147:ARG:NH1	4:C:202:ASP:OD1	2.50	0.44
2:A:469:THR:CB	4:B:229:GLU:OE2	2.65	0.44
3:J:247:TRP:O	3:J:249:ARG:NH1	2.50	0.44
4:G:144:LYS:O	4:G:222:ARG:NH2	2.48	0.44
4:D:97:LEU:C	4:D:97:LEU:CD2	2.86	0.44
4:B:325:THR:HA	4:B:326:PRO:HD3	1.78	0.44
2:A:179:LYS:O	2:A:183:ASP:HB2	2.17	0.44
5:H:47:TRP:O	5:H:47:TRP:CD1	2.70	0.44
1:K:22:U:H3'	4:D:225:GLN:NE2	2.33	0.44
2:A:445:LEU:HD11	2:A:564:MET:HE3	2.00	0.44
2:A:498:THR:HG22	4:B:204:LEU:HG	2.00	0.44
4:G:286:ARG:HB2	4:F:44:GLU:HG2	2.00	0.44
4:G:290:HIS:ND1	4:G:293:ASP:OD1	2.51	0.44
4:E:216:PRO:HG3	4:F:206:ILE:HD13	2.00	0.44
5:H:8:ILE:HB	5:H:56:ILE:HG23	1.99	0.44
5:H:42:VAL:HG13	5:H:56:ILE:HD11	1.98	0.44
3:J:178:CYS:SG	3:J:179:CYS:N	2.91	0.43
2:A:622:TYR:CD2	2:A:624:VAL:HG23	2.52	0.43
1:K:3:G:OP1	2:A:411:SER:OG	2.37	0.43
1:K:46:C:H41	5:H:163:PHE:HB2	1.68	0.43
2:A:487:PHE:C	2:A:487:PHE:CD2	2.96	0.43
3:J:111:GLY:O	3:I:386:ASN:ND2	2.51	0.43
3:J:269:SER:OG	3:J:272:GLU:CG	2.66	0.43
3:I:178:CYS:SG	3:I:179:CYS:N	2.91	0.43
4:D:11:ARG:O	4:D:96:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:451:GLY:HA3	4:B:227:PHE:HB3	2.00	0.43
4:E:34:TYR:CD1	4:E:257:PRO:HG3	2.53	0.43
5:H:152:LEU:CD1	5:H:167:ILE:HD12	2.49	0.43
2:A:400:ALA:HB3	2:A:473:TRP:HB3	2.01	0.43
4:F:299:HIS:CD2	4:F:301:SER:H	2.37	0.43
4:F:329:GLU:HA	4:F:329:GLU:OE1	2.18	0.43
3:J:112:ALA:HA	3:I:386:ASN:HD21	1.83	0.43
2:A:86:ASN:HB2	2:A:219:LEU:HD21	2.01	0.43
4:G:226:VAL:HG22	4:G:245:VAL:HB	2.00	0.43
4:G:227:PHE:HE2	4:G:229:GLU:HG3	1.83	0.43
4:D:158:PRO:HB2	4:D:193:MET:HE1	2.00	0.43
4:E:43:MET:HE1	4:E:67:GLN:HB3	2.01	0.43
4:F:96:GLU:OE1	4:F:96:GLU:HA	2.19	0.43
2:A:102:ALA:HB3	2:A:114:SER:HB3	2.01	0.43
4:C:97:LEU:CD2	4:C:125:TRP:CH2	3.01	0.43
4:D:138:ASN:HA	4:D:171:ILE:HD13	2.01	0.43
1:K:49:C:H41	5:H:121:ARG:NH1	2.17	0.42
2:A:89:PHE:O	2:A:247:MET:HE1	2.20	0.42
4:G:299:HIS:CD2	4:G:301:SER:H	2.37	0.42
5:H:7:THR:HG22	5:H:57:SER:HB3	1.99	0.42
2:A:493:GLN:HE21	2:A:516:PHE:HB3	1.83	0.42
3:J:361:ASP:HB3	3:J:364:ASP:HB2	2.01	0.42
3:I:312:TRP:HA	3:I:316:GLY:HA2	2.02	0.42
3:I:361:ASP:HB3	3:I:364:ASP:HB2	2.01	0.42
4:C:84:HIS:CD2	4:C:212:THR:HG23	2.55	0.42
5:H:83:PHE:HD1	5:H:83:PHE:HA	1.74	0.42
3:J:312:TRP:HA	3:J:316:GLY:HA2	2.01	0.42
4:E:158:PRO:HB2	4:E:193:MET:HE1	2.00	0.42
2:A:409:ILE:HG12	2:A:410:PRO:HD2	2.01	0.42
4:B:227:PHE:C	4:B:227:PHE:CD2	2.97	0.42
4:C:97:LEU:CD1	4:C:341:LEU:CB	2.97	0.42
4:C:158:PRO:HG2	4:C:161:TRP:CG	2.55	0.42
4:C:216:PRO:HG3	4:D:206:ILE:HD13	2.02	0.42
4:D:43:MET:HE1	4:D:67:GLN:HB3	2.00	0.42
4:D:131:ARG:HB3	4:D:271:ILE:HG12	2.00	0.42
4:D:148:LYS:HA	4:E:204:LEU:HD21	2.00	0.42
4:E:118:LEU:HD13	4:E:118:LEU:HA	1.84	0.42
4:E:186:ASN:OD1	4:E:186:ASN:N	2.52	0.42
1:K:12:C:O2	1:K:12:C:H2'	2.20	0.42
2:A:481:LEU:HD11	2:A:483:LEU:HG	2.01	0.42
2:A:568:VAL:HG12	2:A:624:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:158:PRO:HB2	4:F:193:MET:HE1	2.01	0.42
2:A:469:THR:HG22	4:B:229:GLU:OE2	2.19	0.42
3:I:18:PHE:HD1	3:I:33:PHE:CE2	2.29	0.42
4:F:131:ARG:HB3	4:F:271:ILE:HG12	2.02	0.42
4:F:226:VAL:HG12	4:F:247:GLN:HG2	2.02	0.42
2:A:576:PRO:HB2	2:A:587:LYS:HB3	2.02	0.42
4:G:204:LEU:HD21	4:F:148:LYS:HA	2.02	0.42
4:G:227:PHE:CD1	4:F:40:LEU:HD12	2.55	0.42
4:B:43:MET:HE1	4:B:67:GLN:HB3	2.02	0.42
4:F:109:LYS:O	4:F:113:VAL:HG23	2.20	0.42
5:H:40:ILE:HD11	5:H:58:PHE:HB3	2.01	0.42
5:H:146:ILE:HG22	5:H:149:TYR:HD1	1.85	0.42
1:K:21:U:C6	4:D:227:PHE:CE1	3.08	0.42
2:A:110:LEU:O	2:A:115:LYS:NZ	2.39	0.42
4:C:74:ASP:OD2	4:C:245:VAL:HA	2.20	0.42
4:D:327:ALA:O	4:D:331:ILE:HG23	2.20	0.42
4:E:51:ASP:OD2	4:E:55:GLN:NE2	2.53	0.42
1:K:12:C:O4'	4:C:345:GLY:HA2	2.20	0.41
4:B:23:VAL:HG22	4:B:29:LYS:HG2	2.01	0.41
4:C:9:TYR:OH	4:C:112:LEU:HD23	2.20	0.41
4:D:305:ASP:OD1	4:D:305:ASP:N	2.52	0.41
5:H:8:ILE:HG12	5:H:85:ILE:HA	2.02	0.41
2:A:134:ALA:HB1	2:A:138:ASN:HD21	1.85	0.41
3:J:12:GLU:OE2	3:J:20:ARG:HD3	2.20	0.41
4:G:7:LEU:H	4:G:348:GLN:HG3	1.85	0.41
4:B:7:LEU:H	4:B:348:GLN:NE2	2.18	0.41
4:B:158:PRO:HB2	4:B:193:MET:HE1	2.03	0.41
4:F:197:ALA:HA	4:F:203:GLY:HA3	2.02	0.41
2:A:486:ASN:ND2	2:A:486:ASN:O	2.52	0.41
4:G:21:PHE:HB2	4:G:86:GLU:HB2	2.02	0.41
1:K:42:U:C6	4:G:220:MET:CE	2.99	0.41
4:E:84:HIS:CD2	4:E:212:THR:HG23	2.55	0.41
5:H:46:LEU:HG	5:H:55:LYS:HG3	2.02	0.41
4:G:142:LEU:HD13	4:G:213:LEU:HD21	2.02	0.41
5:H:43:SER:HB2	5:H:101:PHE:HE2	1.86	0.41
5:H:45:PRO:HG2	5:H:55:LYS:HB2	2.03	0.41
2:A:450:ARG:O	2:A:472:ASP:O	2.38	0.41
3:I:12:GLU:OE2	3:I:20:ARG:HD3	2.20	0.41
4:G:206:ILE:HD13	4:F:216:PRO:HG3	2.03	0.41
4:C:144:LYS:NZ	4:D:10:GLU:OE2	2.53	0.41
1:K:39:A:C8	4:G:227:PHE:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:46:C:O2	1:K:46:C:C2'	2.69	0.41
2:A:228:ARG:HB3	2:A:550:LEU:HD23	2.02	0.41
4:B:21:PHE:HB2	4:B:86:GLU:HB2	2.03	0.41
4:B:227:PHE:C	4:B:227:PHE:HD2	2.28	0.41
4:C:299:HIS:CD2	4:C:301:SER:H	2.38	0.41
4:D:84:HIS:CD2	4:D:212:THR:HG23	2.56	0.41
4:D:112:LEU:HD12	4:D:112:LEU:HA	1.83	0.41
4:D:348:GLN:HB3	4:D:349:HIS:H	1.73	0.41
4:E:7:LEU:H	4:E:348:GLN:HE21	1.69	0.41
4:E:36:SER:OG	4:E:74:ASP:OD1	2.34	0.41
5:H:152:LEU:H	5:H:165:LEU:HB2	1.86	0.41
4:B:305:ASP:OD1	4:B:305:ASP:N	2.54	0.41
4:C:310:LEU:HA	4:C:310:LEU:HD22	1.90	0.41
4:E:21:PHE:HD1	4:E:31:PRO:HA	1.84	0.41
4:E:293:ASP:OD1	4:E:293:ASP:N	2.39	0.41
4:F:115:LEU:HD11	4:F:313:ALA:HB1	2.02	0.41
2:A:241:PHE:CD1	2:A:470:ARG:HG2	2.56	0.40
2:A:543:TYR:HD1	2:A:599:ASN:HD21	1.68	0.40
4:B:84:HIS:CD2	4:B:212:THR:HG23	2.56	0.40
4:C:18:VAL:HB	4:C:259:LEU:HB3	2.03	0.40
4:C:186:ASN:OD1	4:C:186:ASN:N	2.53	0.40
4:F:305:ASP:OD1	4:F:305:ASP:N	2.53	0.40
3:J:348:LEU:HD13	3:J:375:LEU:HD22	2.03	0.40
4:C:131:ARG:HB3	4:C:271:ILE:HG12	2.04	0.40
4:C:227:PHE:CD2	4:C:227:PHE:C	2.98	0.40
4:E:112:LEU:HD12	4:E:112:LEU:HA	1.77	0.40
4:F:226:VAL:CG2	4:F:228:THR:HG23	2.51	0.40
4:G:158:PRO:HG2	4:G:161:TRP:CG	2.57	0.40
4:F:36:SER:OG	4:F:74:ASP:OD1	2.33	0.40
5:H:44:PHE:CD2	5:H:44:PHE:N	2.89	0.40
2:A:571:HIS:HB2	2:A:594:ILE:HD11	2.02	0.40
3:J:259:VAL:HG21	3:J:310:ARG:HH12	1.87	0.40
4:D:227:PHE:O	4:D:227:PHE:HD2	2.05	0.40
4:F:97:LEU:HD23	4:F:97:LEU:N	2.33	0.40
4:G:324:LYS:HD3	4:G:325:THR:N	2.36	0.40
4:D:147:ARG:NH1	4:E:202:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	436/640 (68%)	393 (90%)	40 (9%)	3 (1%)	18	48
3	I	366/394 (93%)	355 (97%)	11 (3%)	0	100	100
3	J	372/394 (94%)	359 (96%)	13 (4%)	0	100	100
4	B	337/352 (96%)	310 (92%)	26 (8%)	1 (0%)	36	65
4	C	335/352 (95%)	313 (93%)	22 (7%)	0	100	100
4	D	334/352 (95%)	310 (93%)	24 (7%)	0	100	100
4	E	333/352 (95%)	309 (93%)	24 (7%)	0	100	100
4	F	334/352 (95%)	307 (92%)	27 (8%)	0	100	100
4	G	297/352 (84%)	277 (93%)	20 (7%)	0	100	100
5	H	125/199 (63%)	120 (96%)	5 (4%)	0	100	100
All	All	3269/3739 (87%)	3053 (93%)	212 (6%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	195	PRO
4	B	328	GLN
2	A	89	PHE
2	A	194	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	404/573 (70%)	394 (98%)	10 (2%)	42	74
3	I	337/356 (95%)	336 (100%)	1 (0%)	86	96
3	J	340/356 (96%)	338 (99%)	2 (1%)	78	93
4	B	299/308 (97%)	298 (100%)	1 (0%)	86	96
4	C	297/308 (96%)	290 (98%)	7 (2%)	43	75
4	D	296/308 (96%)	293 (99%)	3 (1%)	68	89
4	E	295/308 (96%)	288 (98%)	7 (2%)	43	75
4	F	296/308 (96%)	289 (98%)	7 (2%)	43	75
4	G	271/308 (88%)	266 (98%)	5 (2%)	51	80
5	H	121/181 (67%)	118 (98%)	3 (2%)	42	74
All	All	2956/3314 (89%)	2910 (98%)	46 (2%)	54	83

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	103	LEU
2	A	106	LEU
2	A	205	ASP
2	A	207	ASP
2	A	471	ASP
2	A	472	ASP
2	A	477	VAL
2	A	483	LEU
2	A	532	LEU
2	A	563	LEU
3	J	264	GLU
3	J	270	THR
3	I	67	SER
4	G	9	TYR
4	G	204	LEU
4	G	310	LEU
4	G	330	THR
4	G	331	ILE
4	B	204	LEU
4	C	9	TYR
4	C	112	LEU
4	C	118	LEU
4	C	121	THR
4	C	190	ILE

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Mol	Chain	Res	Type
4	C	204	LEU
4	C	310	LEU
4	D	97	LEU
4	D	112	LEU
4	D	204	LEU
4	E	9	TYR
4	E	112	LEU
4	E	118	LEU
4	E	120	GLU
4	E	204	LEU
4	E	259	LEU
4	E	328	GLN
4	F	98	ARG
4	F	190	ILE
4	F	204	LEU
4	F	226	VAL
4	F	250	THR
4	F	310	LEU
4	F	328	GLN
5	H	44	PHE
5	H	52	VAL
5	H	83	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	83	GLN
2	A	101	GLN
2	A	120	HIS
2	A	138	ASN
2	A	200	GLN
2	A	226	HIS
2	A	272	HIS
2	A	486	ASN
2	A	493	GLN
2	A	599	ASN
2	A	618	ASN
3	J	66	ASN
3	J	154	ASN
3	J	194	HIS
3	J	237	HIS
3	J	262	ASN

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Mol	Chain	Res	Type
3	J	293	ASN
3	J	296	HIS
3	J	368	HIS
3	I	66	ASN
3	I	194	HIS
3	I	237	HIS
3	I	293	ASN
3	I	296	HIS
4	G	84	HIS
4	G	299	HIS
4	G	328	GLN
4	B	77	HIS
4	B	84	HIS
4	B	214	HIS
4	B	242	ASN
4	B	348	GLN
4	B	349	HIS
4	C	77	HIS
4	C	84	HIS
4	C	179	GLN
4	C	299	HIS
4	D	42	GLN
4	D	77	HIS
4	D	84	HIS
4	D	174	ASN
4	D	179	GLN
4	D	218	ASN
4	D	299	HIS
4	D	328	GLN
4	E	84	HIS
4	E	179	GLN
4	E	242	ASN
4	E	299	HIS
4	E	328	GLN
4	F	71	HIS
4	F	84	HIS
4	F	179	GLN
4	F	242	ASN
4	F	299	HIS
4	F	328	GLN
5	H	32	ASN
5	H	39	ASN

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Mol	Chain	Res	Type
5	H	71	GLN
5	H	150	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	K	59/61 (96%)	31 (52%)	11 (18%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	K	3	G
1	K	8	C
1	K	9	U
1	K	10	U
1	K	11	A
1	K	12	C
1	K	14	G
1	K	15	G
1	K	20	U
1	K	21	U
1	K	22	U
1	K	23	G
1	K	26	U
1	K	27	U
1	K	28	C
1	K	29	A
1	K	33	C
1	K	36	U
1	K	37	U
1	K	38	C
1	K	39	A
1	K	40	G
1	K	41	G
1	K	42	U
1	K	43	G
1	K	44	A
1	K	45	A
1	K	46	C
1	K	55	A
1	K	58	U

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Mol	Chain	Res	Type
1	K	59	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	K	12	C
1	K	20	U
1	K	21	U
1	K	22	U
1	K	37	U
1	K	38	C
1	K	41	G
1	K	42	U
1	K	43	G
1	K	44	A
1	K	45	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

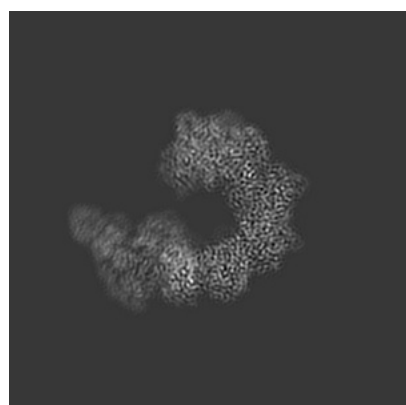
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21126. These allow visual inspection of the internal detail of the map and identification of artifacts.

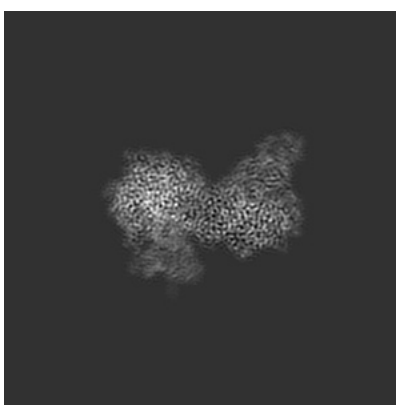
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

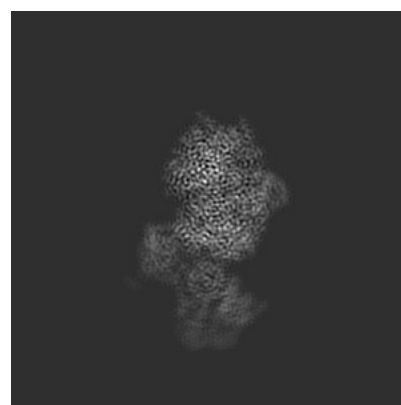
6.1.1 Primary map



X



Y



Z

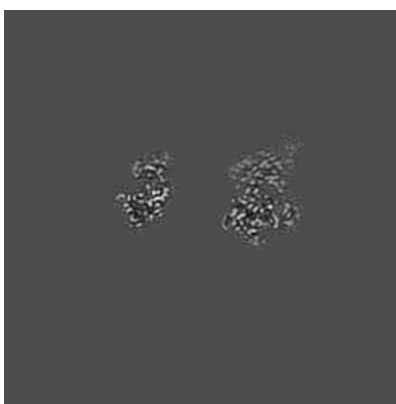
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

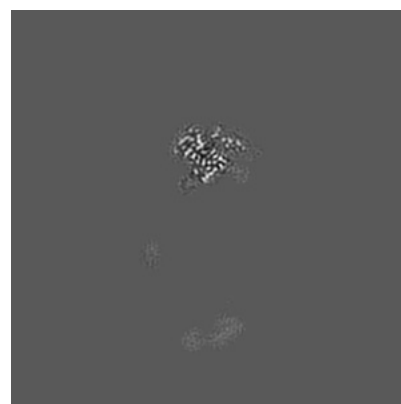
6.2.1 Primary map



X Index: 144



Y Index: 144

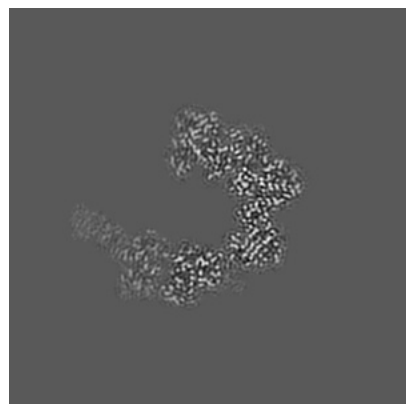


Z Index: 144

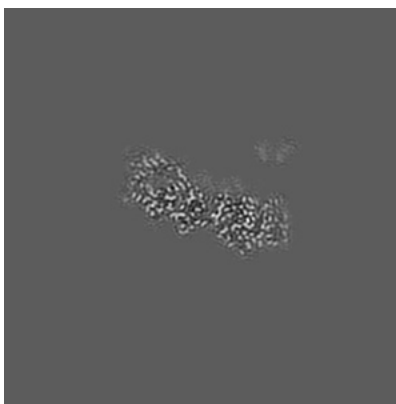
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

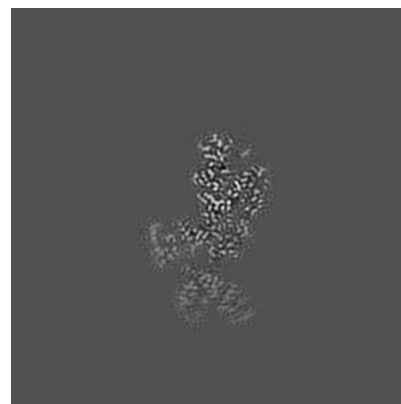
6.3.1 Primary map



X Index: 143



Y Index: 171

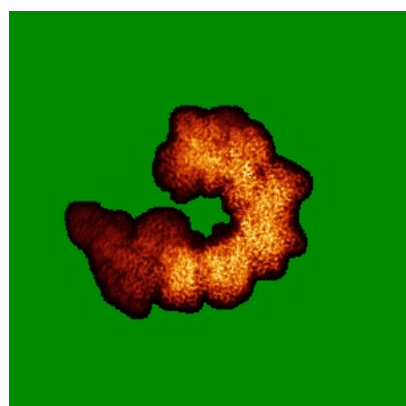


Z Index: 110

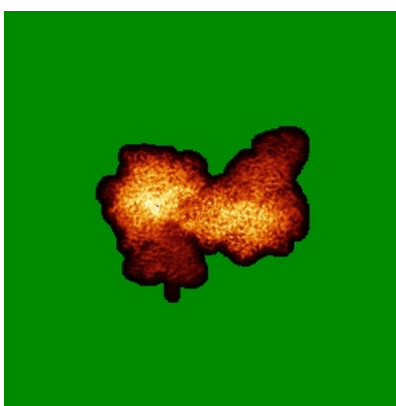
The images above show the largest variance slices of the map in three orthogonal directions.

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

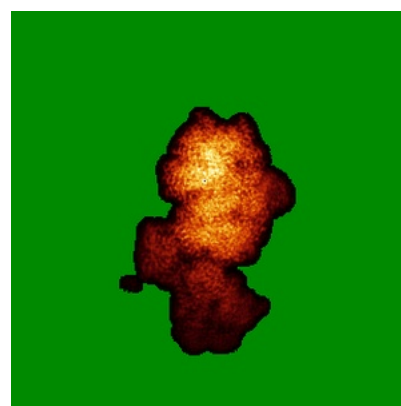
6.4.1 Primary map



X



Y

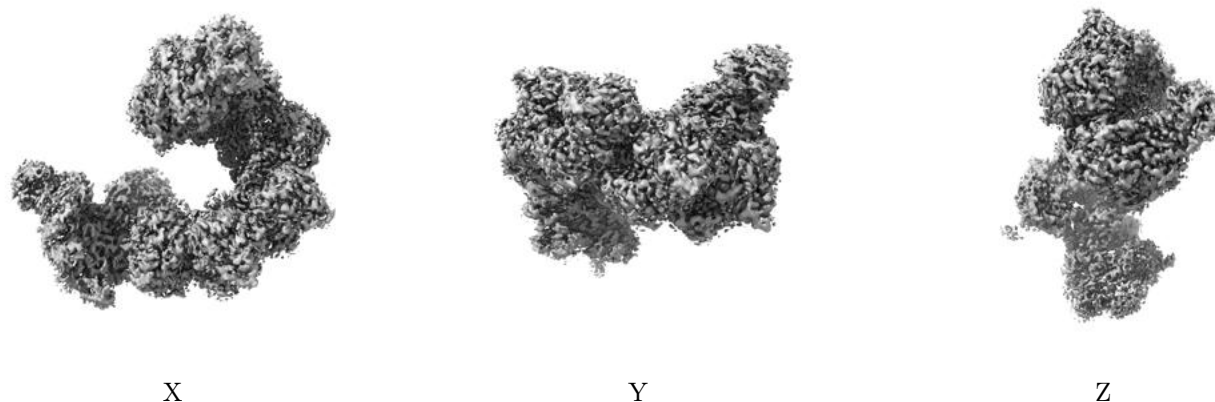


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

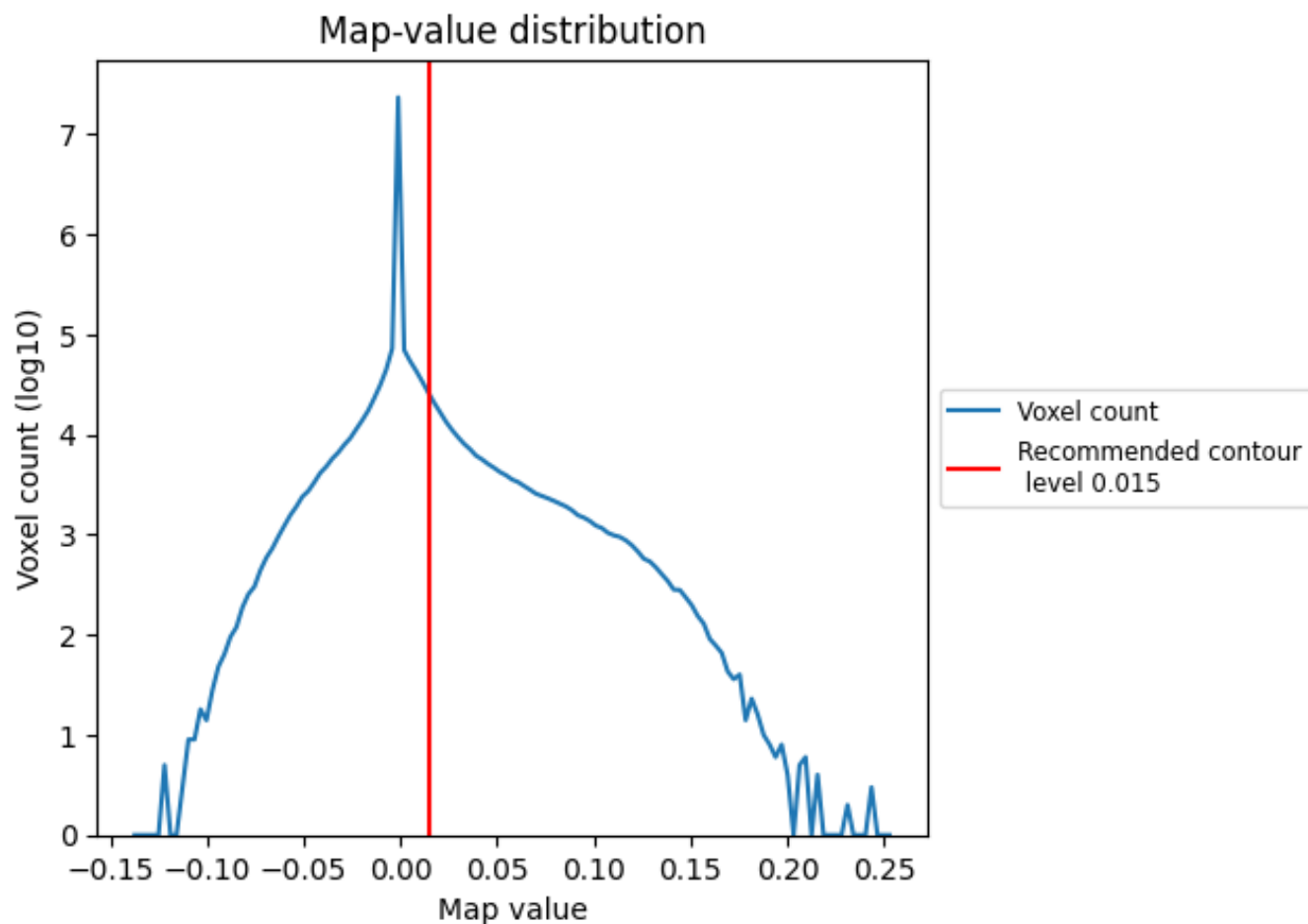
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

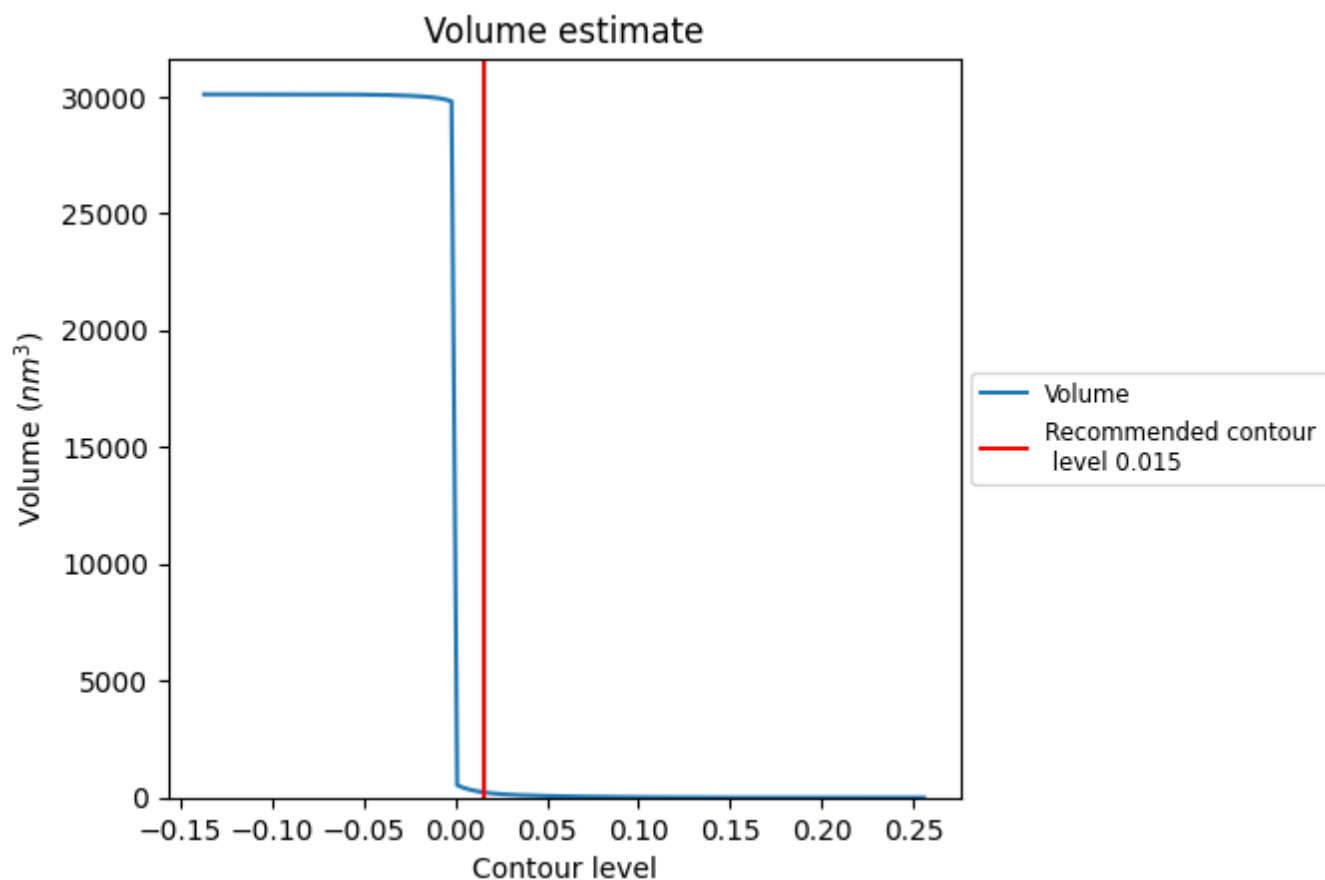
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

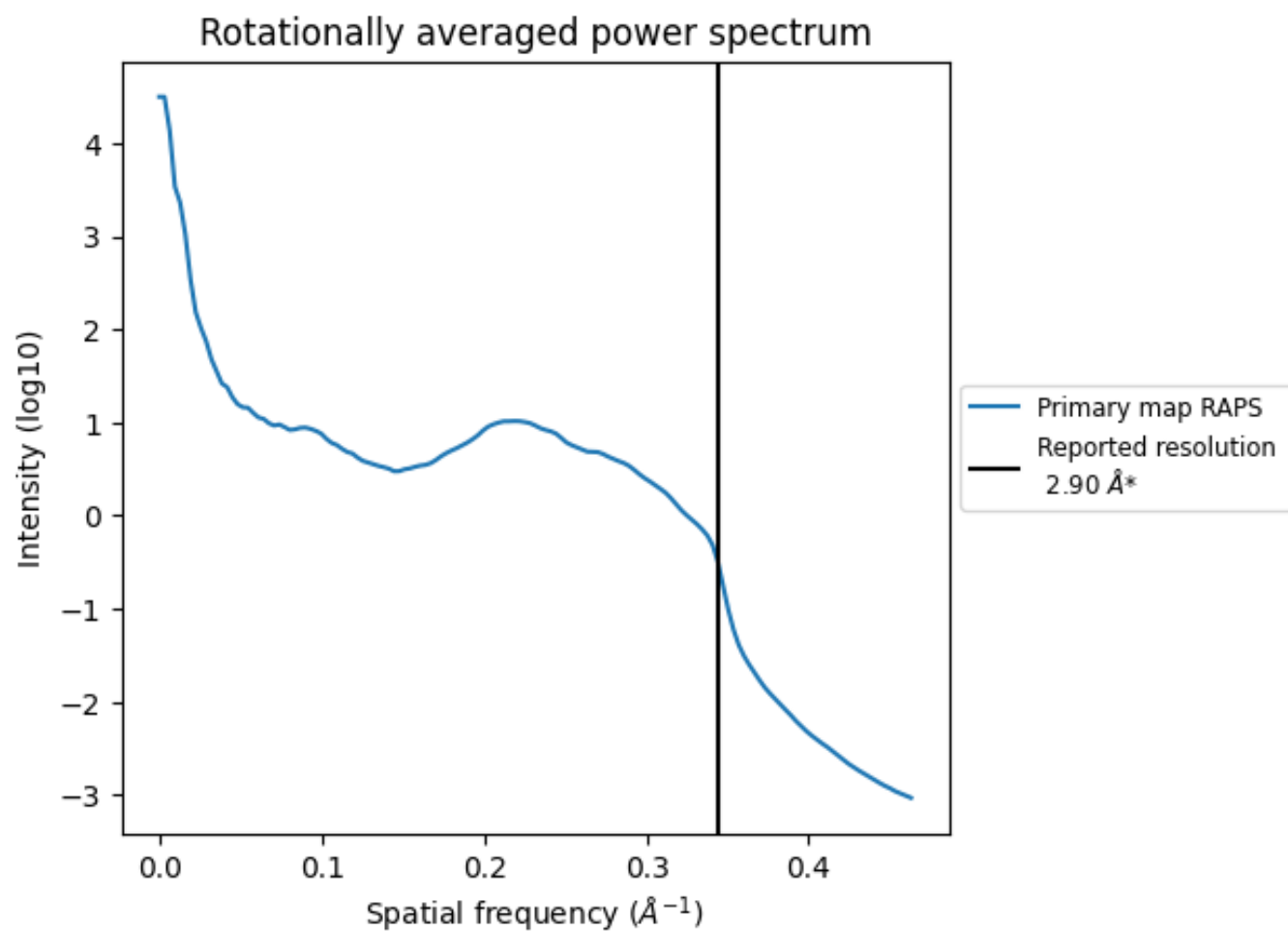
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm^3 ; this corresponds to an approximate mass of 206 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

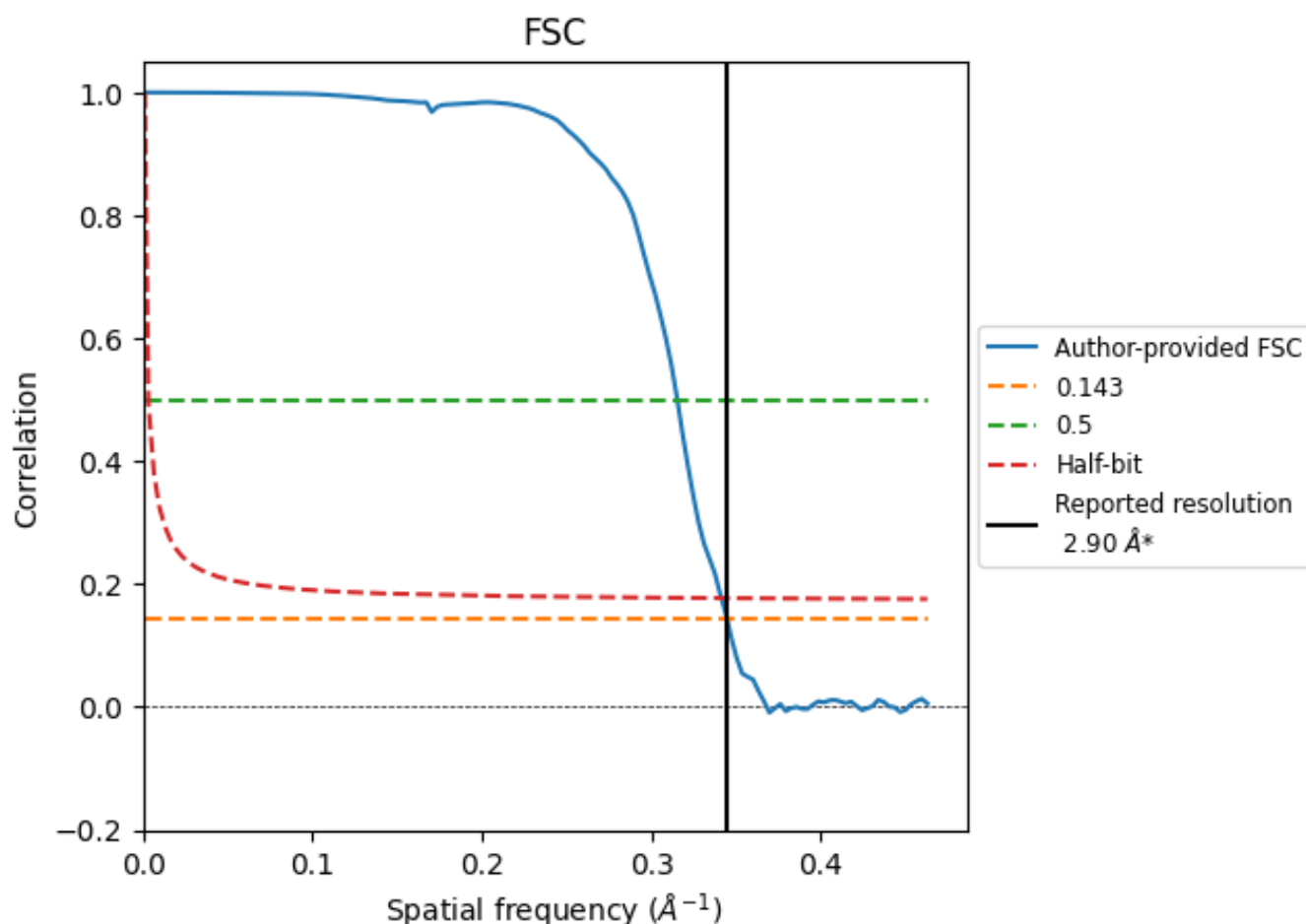


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

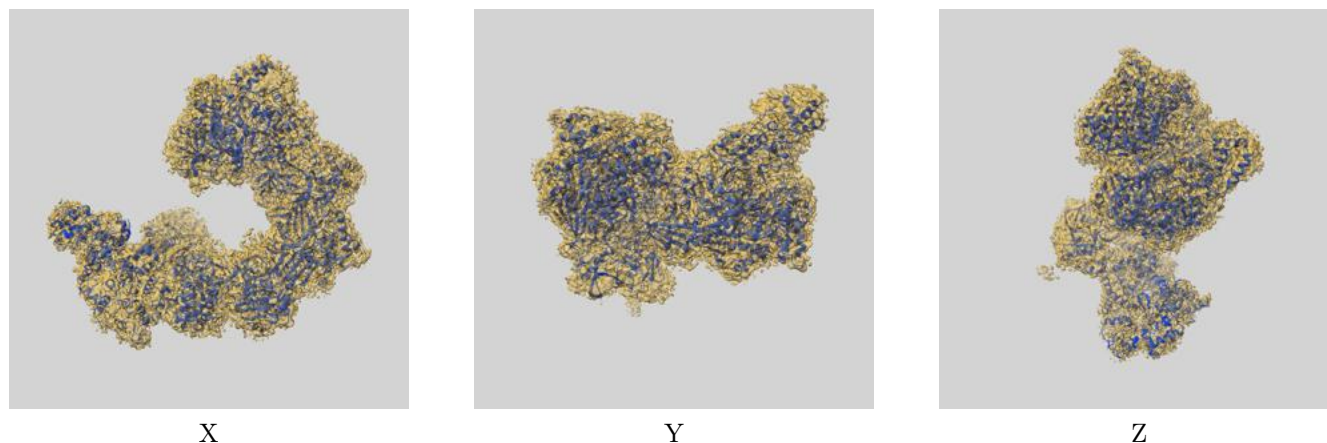
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.17	2.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

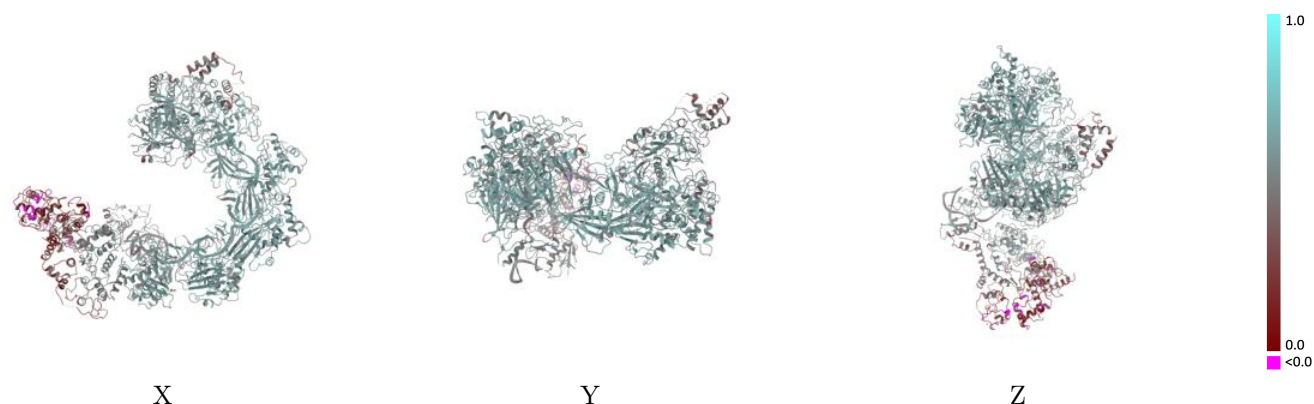
This section contains information regarding the fit between EMDB map EMD-21126 and PDB model 6V9Q. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



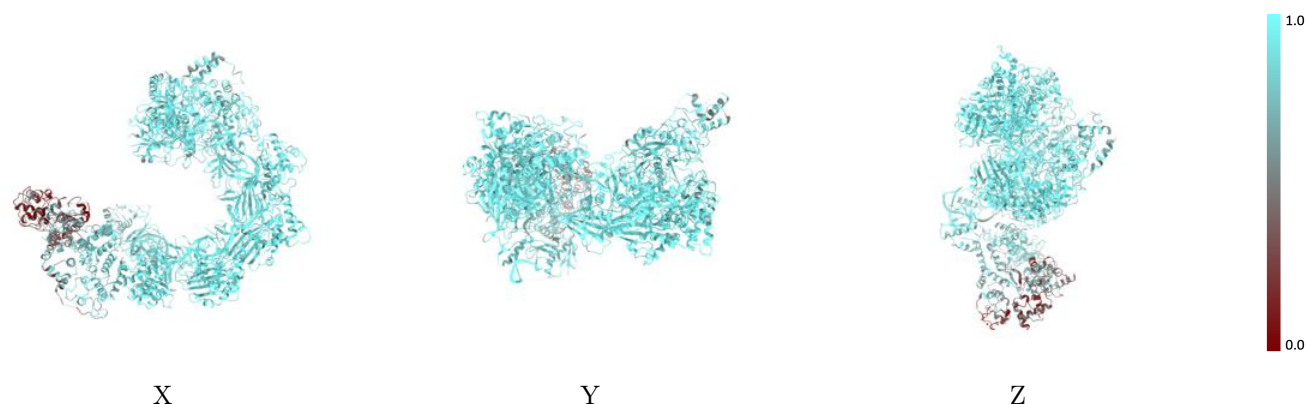
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



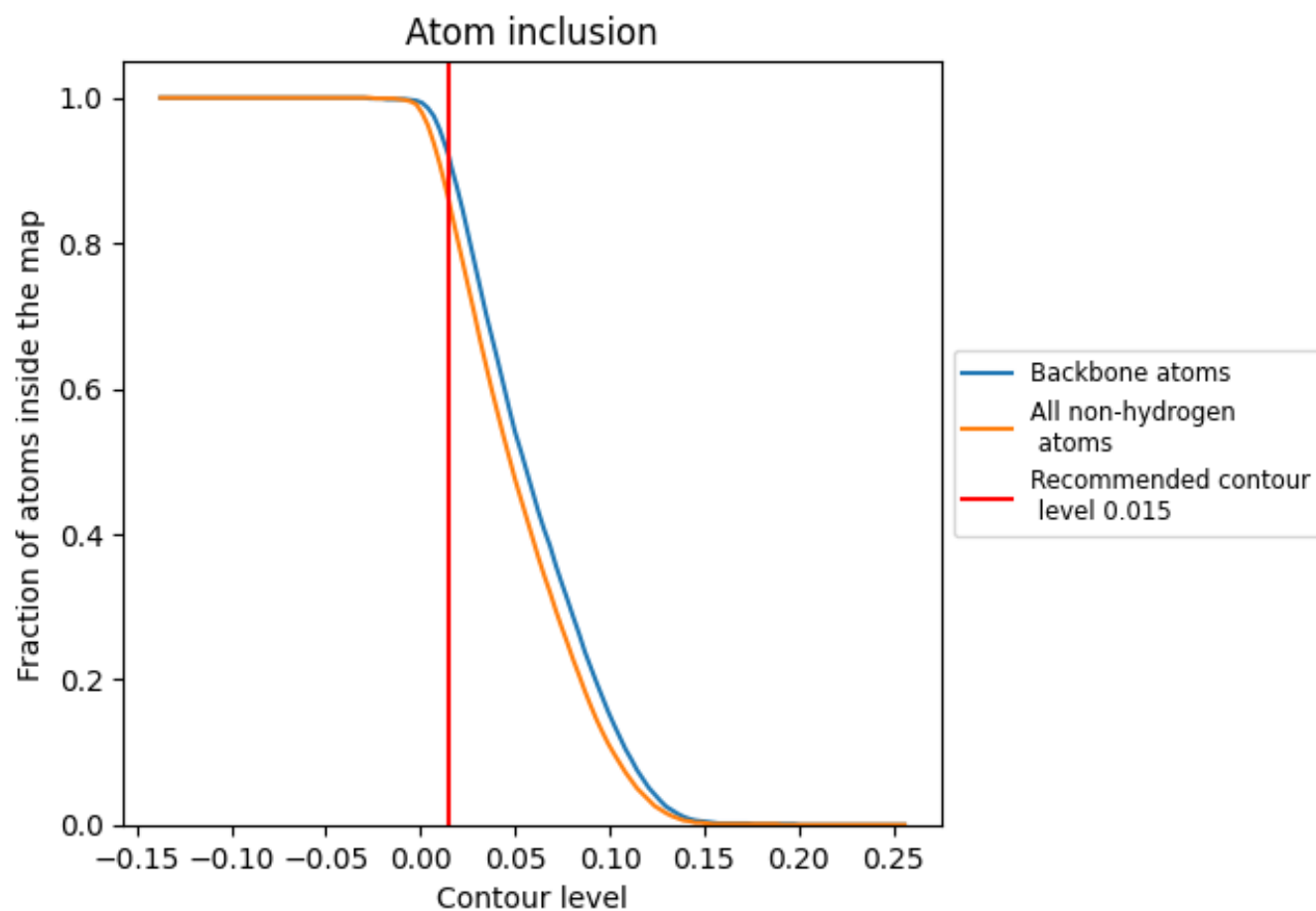
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.5150
A	0.8820	0.5170
B	0.9190	0.5580
C	0.9410	0.5820
D	0.9480	0.5880
E	0.9440	0.5850
F	0.9410	0.5810
G	0.9300	0.5660
H	0.8420	0.4620
I	0.6710	0.3680
J	0.5730	0.3320
K	0.9610	0.5680

1.0

0.0

<0.0