



Full wwPDB EM Validation Report ⓘ

Dec 28, 2024 – 02:39 PM EST

PDB ID : 7ELM
EMDB ID : EMD-31185
Title : Structure of Csy-AcrIF24
Authors : Zhang, L.; Feng, Y.
Deposited on : 2021-04-12
Resolution : 2.88 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

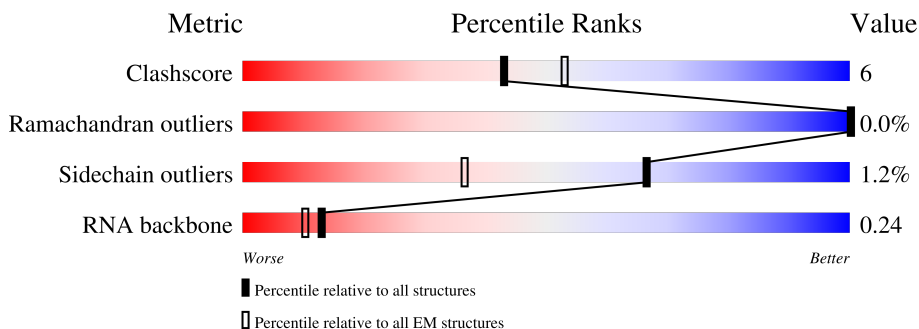
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	434	
1	K	434	
2	B	327	
2	L	327	
3	C	342	
3	D	342	
3	E	342	

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Mol	Chain	Length	Quality of chain
3	F	342	
3	G	342	
3	H	342	
3	M	342	
3	N	342	
3	O	342	
3	P	342	
3	Q	342	
3	R	342	
4	I	187	
4	S	187	
5	U	228	
5	V	228	
6	J	60	
6	T	60	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 47399 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 Type I-F CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	417	Total	C	N	O	0	0
			2015	1117	447	451		
1	K	424	Total	C	N	O	0	0
			2065	1144	461	460		

- Molecule 2 is a protein called CRISPR type I-F/YPEST-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	305	Total	C	N	O	S	0	0
			2204	1389	403	409	3		
2	L	305	Total	C	N	O	S	0	0
			2321	1471	431	414	5		

- Molecule 3 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	292	Total	C	N	O	S	0	0
			2139	1347	378	412	2		
3	D	334	Total	C	N	O	S	0	0
			2531	1590	454	485	2		
3	E	337	Total	C	N	O	S	0	0
			2590	1627	469	492	2		
3	F	335	Total	C	N	O	S	0	0
			2577	1619	470	486	2		
3	G	329	Total	C	N	O	S	0	0
			2517	1583	456	476	2		
3	H	332	Total	C	N	O	S	0	0
			2490	1556	453	479	2		
3	M	293	Total	C	N	O	S	0	0
			2227	1406	396	423	2		
3	N	335	Total	C	N	O	S	0	0
			2565	1610	465	488	2		
3	O	334	Total	C	N	O	S	0	0
			2562	1611	467	482	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	335	Total	C	N	O	S	0	0
			2581	1622	471	486	2		
3	Q	333	Total	C	N	O	S	0	0
			2552	1605	465	480	2		
3	R	333	Total	C	N	O	S	0	0
			2529	1588	461	479	1		

- Molecule 4 is a protein called type I-F CRISPR-associated endoribonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	187	Total	C	N	O	S	0	0
			1445	919	264	258	4		
4	S	187	Total	C	N	O	S	1	0
			1431	908	262	256	5		

- Molecule 5 is a protein called AcrIF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	227	Total	C	N	O	S	0	0
			1758	1124	308	323	3		
5	V	227	Total	C	N	O	S	0	0
			1758	1124	308	323	3		

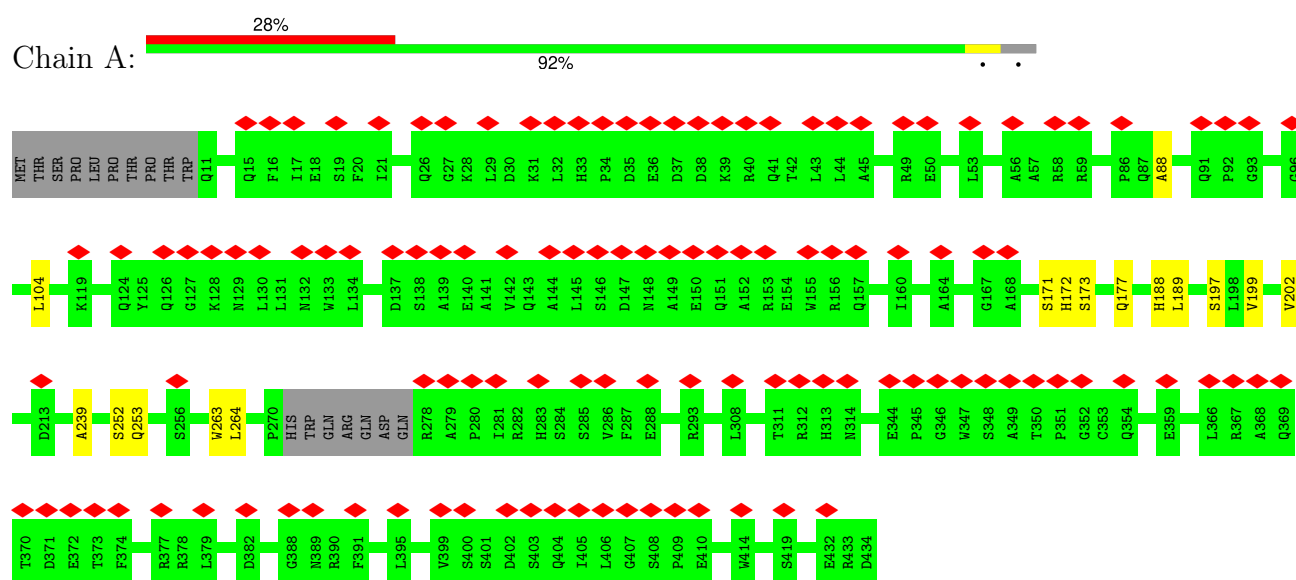
- Molecule 6 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		
6	T	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		

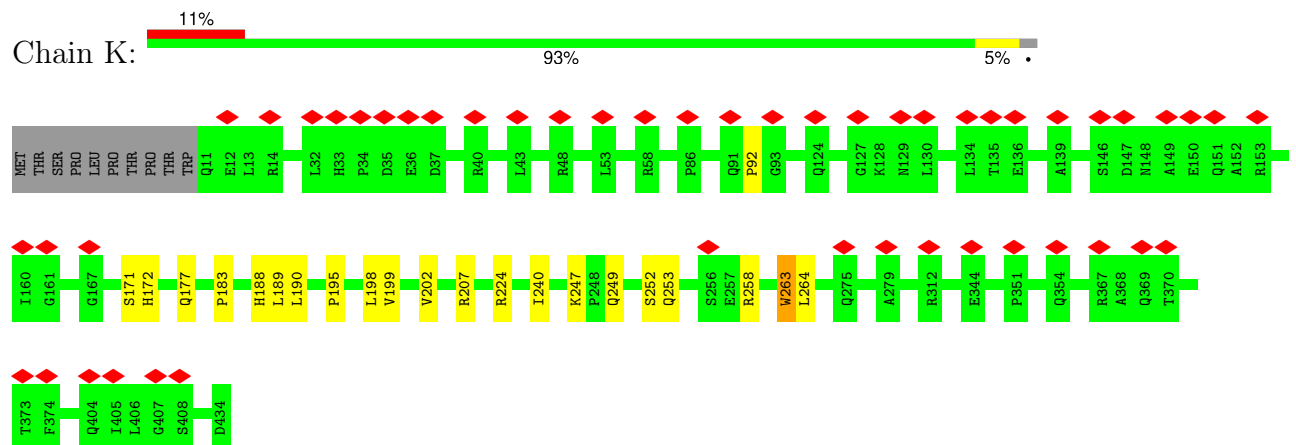
3 Residue-property plots

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.

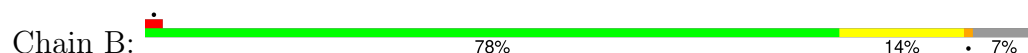
- Molecule 1: Type I-F CRISPR-associated protein Csy1

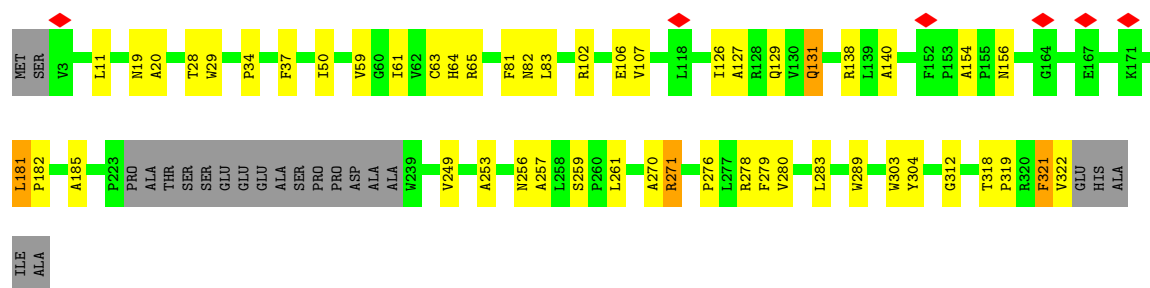


- Molecule 1: Type I-F CRISPR-associated protein Csy1



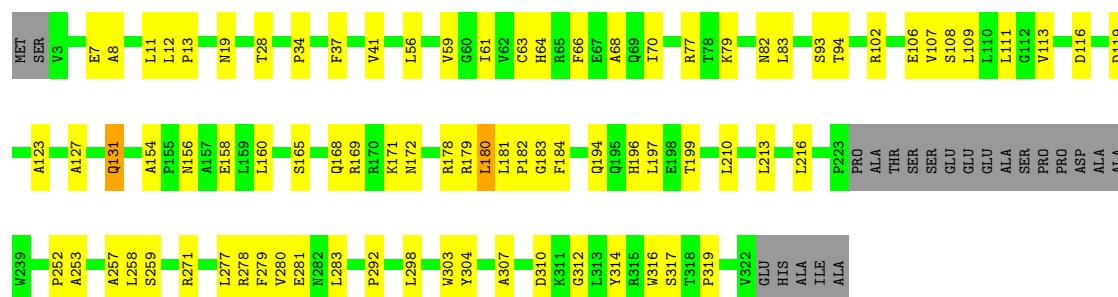
- Molecule 2: CRISPR type I-F/YPEST-associated protein Csy2





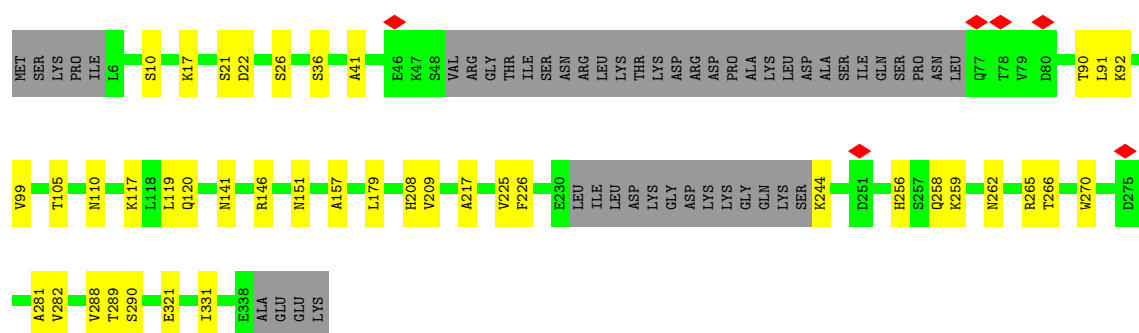
- Molecule 2: CRISPR type I-F/YPEST-associated protein Csy2

Chain L: 68% 24% 7%



- Molecule 3: CRISPR-associated protein Csy3

Chain C: 73% 12% 15%

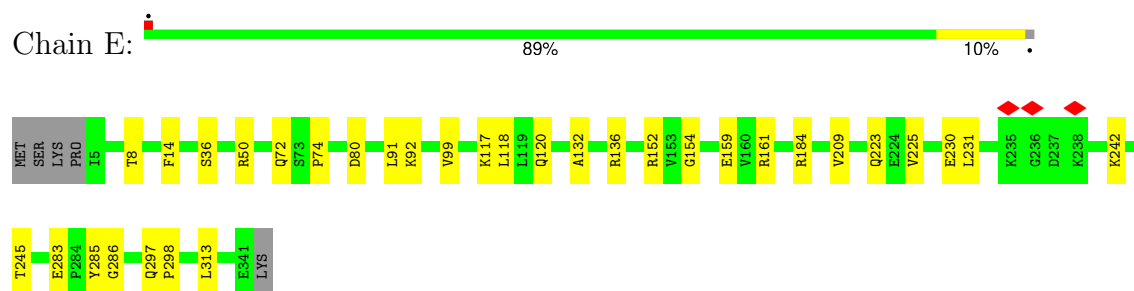


- Molecule 3: CRISPR-associated protein Csy3

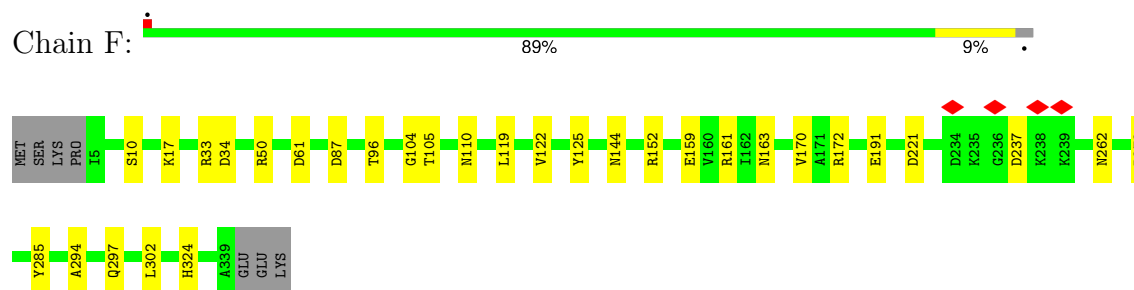
Chain D: 87% 11% 2%



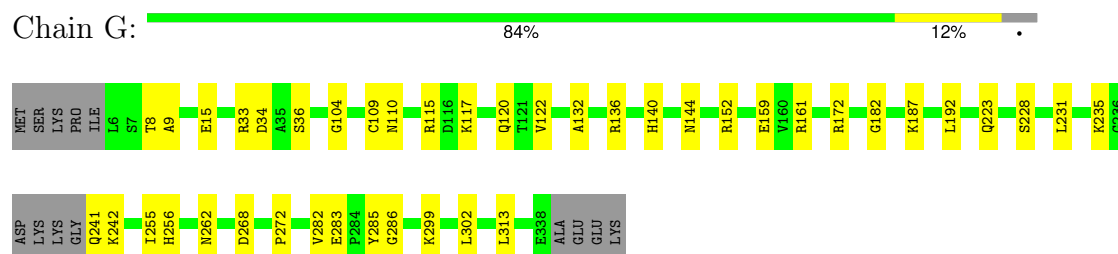
- Molecule 3: CRISPR-associated protein Csy3



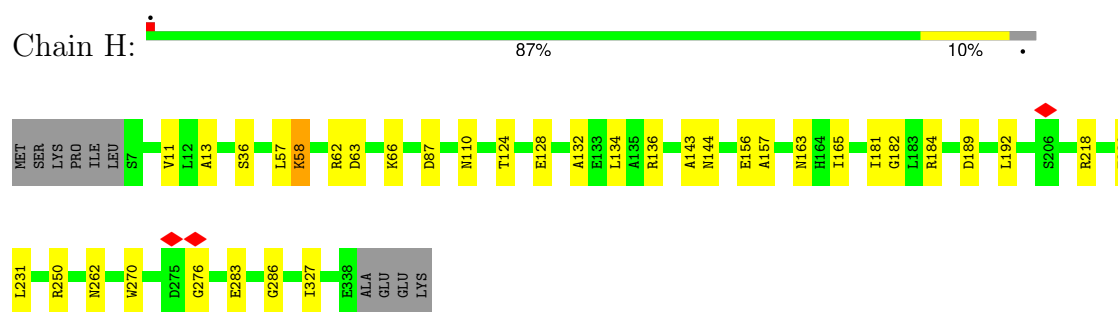
- Molecule 3: CRISPR-associated protein Csy3



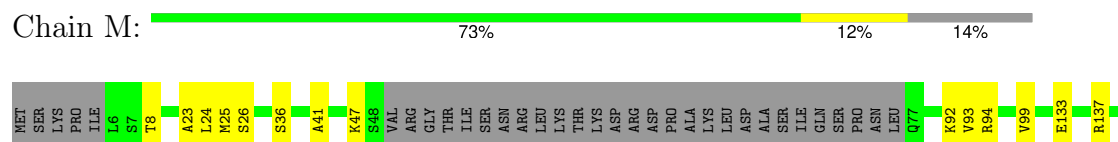
- Molecule 3: CRISPR-associated protein Csy3

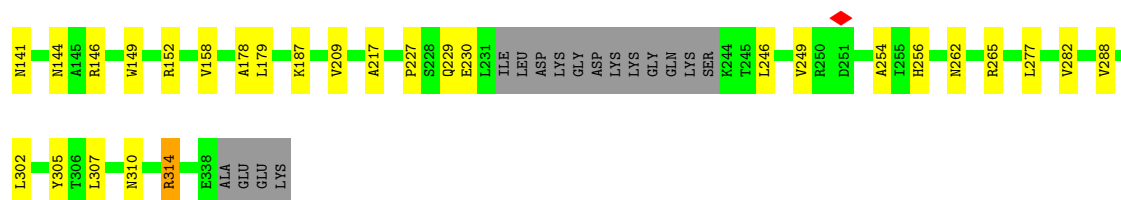


- Molecule 3: CRISPR-associated protein Csy3

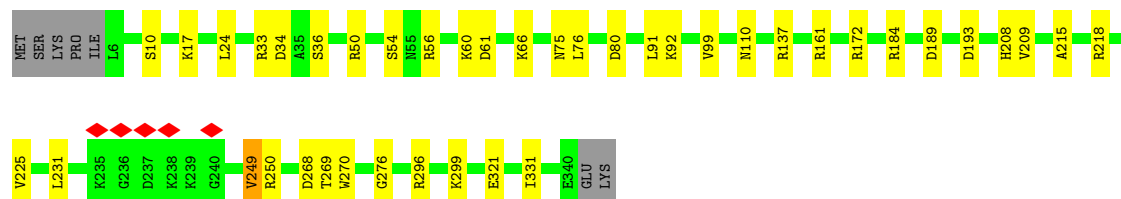
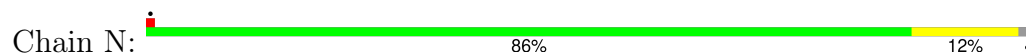


- Molecule 3: CRISPR-associated protein Csy3

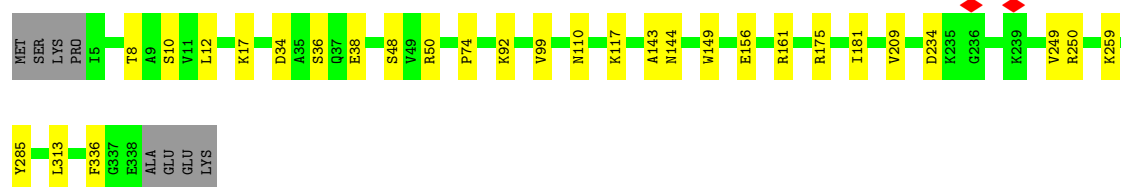
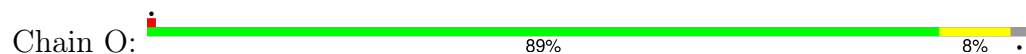




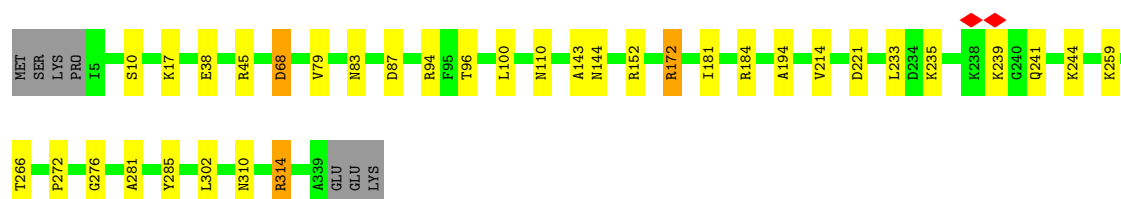
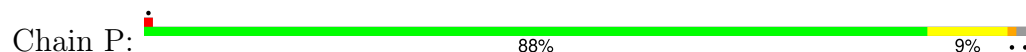
• Molecule 3: CRISPR-associated protein Csy3



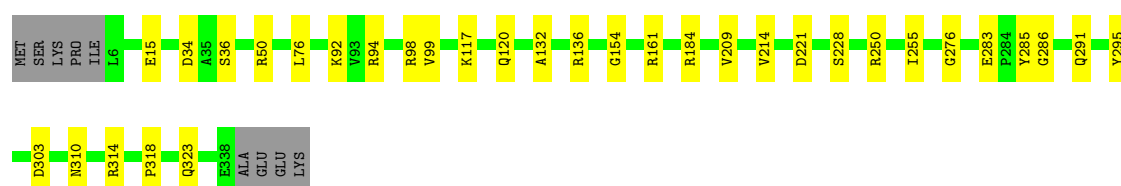
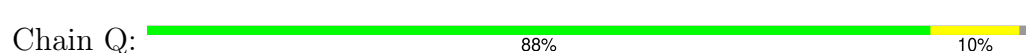
• Molecule 3: CRISPR-associated protein Csy3




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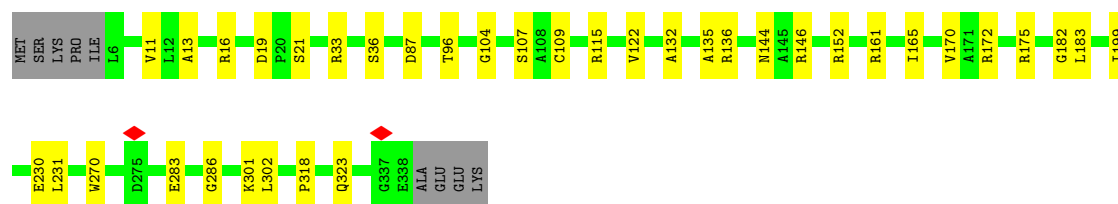


• Molecule 3: CRISPR-associated protein Csy3




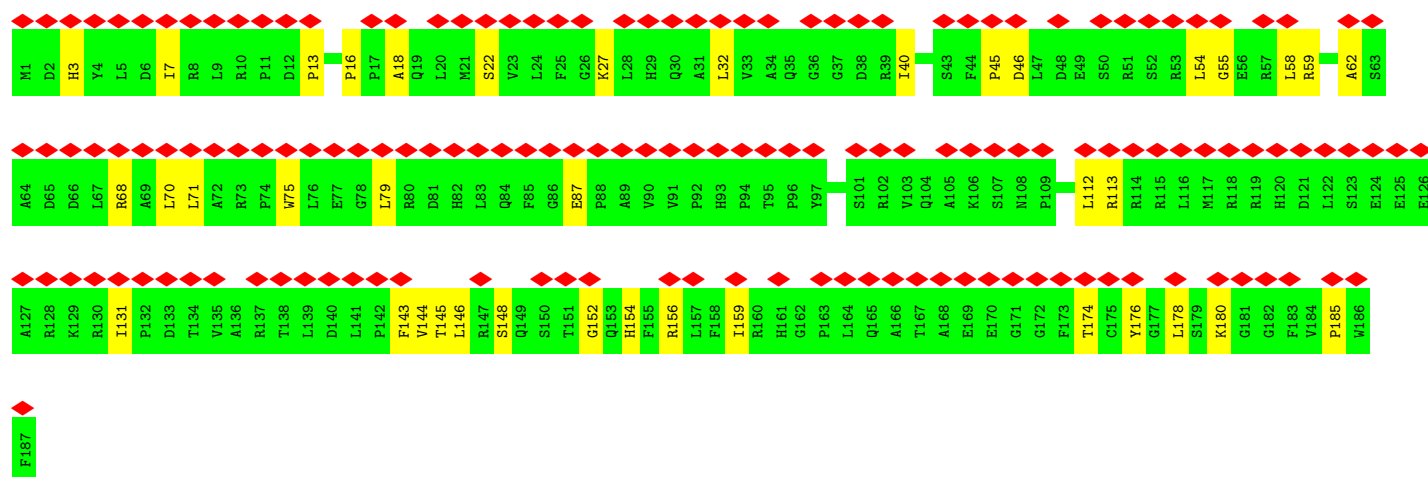
• Molecule 3: CRISPR-associated protein Csy3

Chain R: 



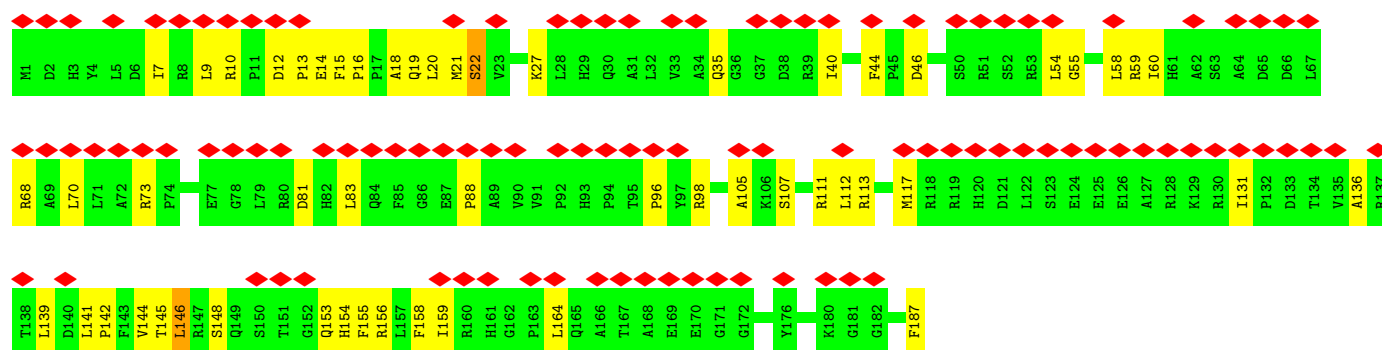
- Molecule 4: type I-F CRISPR-associated endoribonuclease Cas6/Csy4

Chain I: 




- Molecule 4: type I-F CRISPR-associated endoribonuclease Cas6/Csy4

Chain S: 



- Molecule 5: AcrIF24

Chain U: 

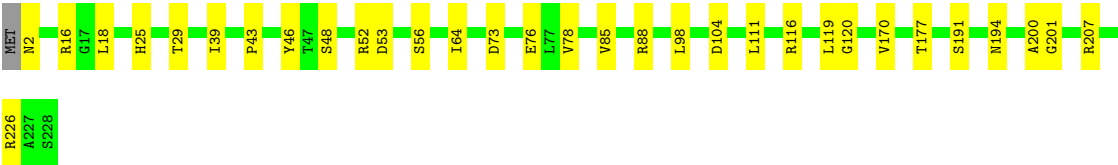


- Molecule 5: AcrIF24

Chain V:

86%

14%



● Molecule 6: RNA (60-MER)

Chain J:

30%

37%

30%

33%



● Molecule 6: RNA (60-MER)

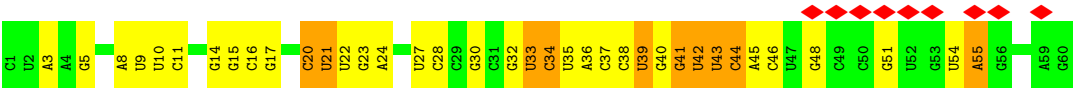
Chain T:

15%

38%

45%

17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	406065	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.130	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0075	Depositor
Map size (\AA)	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/2041	0.47	0/2643
1	K	0.25	0/2092	0.46	0/2710
2	B	0.28	0/2254	0.56	0/3084
2	L	0.30	0/2378	0.57	0/3246
3	C	0.27	0/2177	0.50	0/2970
3	D	0.32	0/2578	0.53	0/3507
3	E	0.34	0/2637	0.52	0/3579
3	F	0.34	0/2624	0.51	0/3561
3	G	0.32	0/2563	0.49	0/3481
3	H	0.29	0/2533	0.52	0/3444
3	M	0.28	0/2269	0.48	0/3087
3	N	0.35	0/2612	0.51	0/3548
3	O	0.37	0/2609	0.52	0/3542
3	P	0.36	0/2628	0.50	0/3565
3	Q	0.34	0/2599	0.50	0/3528
3	R	0.31	0/2576	0.51	0/3502
4	I	0.28	0/1484	0.58	0/2016
4	S	0.29	0/1472	0.56	0/2001
5	U	0.36	0/1809	0.50	0/2474
5	V	0.36	0/1809	0.51	0/2474
6	J	0.52	0/1419	0.93	0/2208
6	T	0.51	0/1419	0.89	0/2208
All	All	0.33	0/48582	0.55	0/66378

There are no bond length outliers.

There are no bond angle outliers.

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	2015	0	1028	19	0
1	K	2065	0	1089	19	0
2	B	2204	0	2028	52	0
2	L	2321	0	2248	70	0
3	C	2139	0	2024	33	0
3	D	2531	0	2464	35	0
3	E	2590	0	2565	24	0
3	F	2577	0	2562	20	0
3	G	2517	0	2481	28	0
3	H	2490	0	2409	28	0
3	M	2227	0	2167	31	0
3	N	2565	0	2526	25	0
3	O	2562	0	2540	16	0
3	P	2581	0	2573	19	0
3	Q	2552	0	2531	19	0
3	R	2529	0	2471	22	0
4	I	1445	0	1387	36	0
4	S	1431	0	1364	58	0
5	U	1758	0	1720	18	0
5	V	1758	0	1720	19	0
6	J	1271	0	647	76	0
6	T	1271	0	647	41	0
All	All	47399	0	43191	578	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 6.

All (578) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LEU:HD23	2:B:182:PRO:CD	1.17	1.63
2:B:181:LEU:CD2	2:B:182:PRO:HD3	0.99	1.44
2:B:181:LEU:HD23	2:B:182:PRO:N	1.43	1.33
6:J:40:G:O2'	6:J:41:G:H5''	1.14	1.27
2:B:181:LEU:CD2	2:B:182:PRO:CD	1.84	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:40:G:H1'	6:J:41:G:C8	1.75	1.22
2:B:303:TRP:CA	2:B:318:THR:HG22	1.69	1.21
6:T:39:U:C2'	6:T:40:G:H5''	1.73	1.18
6:T:39:U:H2'	6:T:40:G:H5''	1.19	1.15
2:B:303:TRP:HA	2:B:318:THR:CG2	1.78	1.13
2:L:179:ARG:O	2:L:180:LEU:HD12	1.49	1.12
2:B:181:LEU:HD22	2:B:182:PRO:HD3	1.16	1.11
6:J:40:G:H1'	6:J:41:G:H8	1.00	1.09
2:B:181:LEU:HD21	2:B:182:PRO:HD3	1.34	1.09
3:C:288:VAL:HG13	6:J:38:C:H41	1.18	1.07
4:S:146:LEU:HD13	4:S:155:PHE:CE2	1.91	1.05
2:B:303:TRP:CG	2:B:318:THR:CG2	2.41	1.04
3:E:297:GLN:NE2	3:E:298:PRO:HD2	1.76	1.01
4:S:16:PRO:HG3	6:T:41:G:O2'	1.63	0.99
6:J:40:G:O2'	6:J:41:G:C5'	2.10	0.99
2:B:303:TRP:CD1	2:B:318:THR:HG21	1.98	0.98
4:I:154:HIS:CG	6:J:44:C:H5	1.82	0.97
3:C:262:ASN:ND2	6:J:38:C:C6	2.32	0.97
2:L:181:LEU:N	2:L:182:PRO:HD2	1.80	0.96
4:I:154:HIS:CD2	6:J:44:C:H5	1.83	0.95
2:B:303:TRP:HA	2:B:318:THR:HG22	0.97	0.94
2:L:179:ARG:C	2:L:180:LEU:HD12	1.88	0.92
1:A:264:LEU:HD23	2:B:28:THR:O	1.68	0.92
4:I:154:HIS:HB2	6:J:44:C:C6	2.05	0.92
3:G:241:GLN:HG2	3:G:242:LYS:H	1.33	0.91
3:Q:50:ARG:HA	3:Q:76:LEU:HD23	1.52	0.90
4:S:16:PRO:CG	6:T:41:G:O2'	2.18	0.90
1:K:264:LEU:HD23	2:L:28:THR:O	1.71	0.90
3:C:288:VAL:HG13	6:J:38:C:N4	1.86	0.89
4:I:22:SER:HB2	4:I:145:THR:O	1.72	0.89
4:I:154:HIS:CG	6:J:44:C:C5	2.59	0.89
3:H:134:LEU:HD11	3:H:327:ILE:HG23	1.53	0.89
6:T:39:U:H2'	6:T:40:G:C5'	2.04	0.86
3:D:76:LEU:HD11	6:J:39:U:C2	2.11	0.86
3:D:49:VAL:HG11	6:J:37:C:N3	1.92	0.85
6:J:43:U:H4'	6:J:44:C:C5'	2.06	0.84
3:C:262:ASN:ND2	6:J:38:C:H6	1.74	0.84
2:B:303:TRP:CD2	2:B:318:THR:HG23	2.14	0.83
3:C:244:LYS:HG3	6:J:40:G:O6	1.78	0.82
2:L:181:LEU:H	2:L:182:PRO:HD2	1.40	0.82
4:S:156:ARG:HD3	4:S:158:PHE:CZ	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:24:LEU:HD21	3:N:249:VAL:HG21	1.61	0.81
6:J:41:G:H5'	6:J:42:U:H5''	1.63	0.80
5:V:48:SER:O	5:V:52:ARG:HG3	1.81	0.79
6:J:40:G:C1'	6:J:41:G:C8	2.63	0.79
2:L:179:ARG:C	2:L:180:LEU:CD1	2.52	0.78
6:T:42:U:H5'	6:T:43:U:OP2	1.83	0.78
3:D:51:GLY:HA3	6:J:37:C:O2'	1.83	0.78
3:N:75:ASN:OD1	3:N:75:ASN:O	2.00	0.77
2:L:181:LEU:N	2:L:182:PRO:CD	2.49	0.76
4:S:154:HIS:CE1	6:T:42:U:O3'	2.39	0.76
2:B:303:TRP:CG	2:B:318:THR:HG21	2.12	0.76
2:L:41:VAL:HG11	2:L:59:VAL:HG22	1.66	0.75
4:I:154:HIS:HB2	6:J:44:C:H6	1.51	0.74
3:G:241:GLN:HG2	3:G:242:LYS:N	2.03	0.74
4:S:14:GLU:N	4:S:14:GLU:OE2	2.20	0.74
6:T:41:G:H2'	6:T:41:G:N3	2.03	0.74
3:E:50:ARG:NH1	6:J:33:U:O2'	2.20	0.73
2:B:303:TRP:CG	2:B:318:THR:HG23	2.20	0.73
5:U:53:ASP:OD1	5:U:53:ASP:O	2.06	0.73
4:I:156:ARG:NH2	6:J:43:U:H6	1.85	0.73
2:B:303:TRP:CA	2:B:318:THR:CG2	2.52	0.73
3:N:76:LEU:HD11	6:T:39:U:C6	2.24	0.72
3:D:260:ILE:O	3:D:264:LEU:HG	1.90	0.72
6:T:39:U:O2'	6:T:40:G:H5''	1.88	0.71
3:F:34:ASP:OD1	3:F:161:ARG:NH1	2.23	0.71
4:I:146:LEU:HD12	4:I:146:LEU:O	1.90	0.70
2:L:178:ARG:O	2:L:181:LEU:CD2	2.40	0.70
3:D:76:LEU:HD21	6:J:39:U:C4	2.28	0.69
6:J:40:G:C1'	6:J:41:G:H8	1.92	0.69
4:I:154:HIS:CD2	6:J:44:C:C5	2.75	0.68
3:F:34:ASP:OD1	3:F:161:ARG:NH2	2.27	0.68
3:N:24:LEU:HD21	3:N:249:VAL:CG2	2.24	0.67
1:A:173:SER:HA	3:H:11:VAL:HG22	1.77	0.67
2:L:178:ARG:O	2:L:181:LEU:HD22	1.95	0.66
4:S:154:HIS:HB3	6:T:44:C:O2'	1.96	0.66
3:C:288:VAL:HG11	4:I:13:PRO:O	1.94	0.65
4:S:145:THR:HB	6:T:42:U:H1'	1.78	0.65
3:M:262:ASN:ND2	6:T:38:C:C2	2.65	0.65
3:R:135:ALA:HB1	3:R:199:ILE:HG23	1.79	0.65
1:A:173:SER:CA	3:H:11:VAL:HG22	2.27	0.64
2:L:181:LEU:H	2:L:182:PRO:CD	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:144:VAL:O	4:I:156:ARG:HA	1.97	0.64
4:S:35:GLN:HB3	4:S:73:ARG:HH12	1.63	0.64
5:U:201:GLY:H	5:U:207:ARG:HD2	1.63	0.64
5:V:111:LEU:O	5:V:120:GLY:HA2	1.98	0.64
4:S:154:HIS:HE1	6:T:42:U:O3'	1.79	0.63
5:V:201:GLY:H	5:V:207:ARG:HD2	1.63	0.63
6:T:39:U:C2'	6:T:40:G:C5'	2.64	0.63
5:U:111:LEU:O	5:U:120:GLY:HA2	1.98	0.63
2:L:131:GLN:NE2	2:L:154:ALA:O	2.32	0.63
3:Q:50:ARG:HA	3:Q:76:LEU:CD2	2.26	0.63
4:I:46:ASP:HB3	4:I:55:GLY:HA3	1.81	0.62
4:I:154:HIS:HB2	6:J:44:C:C5	2.33	0.62
2:B:303:TRP:CD2	2:B:318:THR:CG2	2.77	0.62
2:B:303:TRP:N	2:B:318:THR:HG22	2.14	0.62
2:B:270:ALA:O	3:H:110:ASN:ND2	2.33	0.62
3:R:144:ASN:HB2	3:R:152:ARG:HH12	1.64	0.62
3:E:297:GLN:HE21	3:E:298:PRO:HD2	1.60	0.62
4:S:148:SER:HB3	4:S:153:GLN:H	1.65	0.61
2:B:126:ILE:HA	2:B:129:GLN:HE21	1.64	0.61
3:F:144:ASN:HB2	3:F:152:ARG:HH12	1.64	0.61
4:I:148:SER:HB2	4:I:152:GLY:HA2	1.82	0.61
3:C:265:ARG:NH1	3:C:282:VAL:O	2.34	0.61
3:E:231:LEU:HD13	6:J:27:U:C4	2.36	0.61
3:D:76:LEU:CD1	6:J:39:U:C2	2.84	0.61
3:C:288:VAL:CG1	6:J:38:C:N4	2.64	0.60
4:I:59:ARG:NH2	4:I:185:PRO:O	2.34	0.60
2:B:181:LEU:HD23	2:B:181:LEU:C	2.14	0.60
2:L:127:ALA:HB1	2:L:156:ASN:HB2	1.84	0.60
3:G:144:ASN:HB2	3:G:152:ARG:HH12	1.67	0.60
3:Q:228:SER:OG	3:Q:255:ILE:HA	2.02	0.60
2:B:257:ALA:HA	2:B:280:VAL:HA	1.84	0.59
3:D:50:ARG:CB	6:J:39:U:H5''	2.32	0.59
1:A:104:LEU:HD12	1:A:197:SER:HB2	1.84	0.59
2:L:183:GLY:O	2:L:184:PHE:HD1	1.85	0.59
2:B:131:GLN:NE2	2:B:154:ALA:O	2.35	0.59
4:S:146:LEU:HD13	4:S:155:PHE:CD2	2.37	0.59
3:N:231:LEU:HG	3:O:48:SER:HB3	1.85	0.59
6:J:40:G:HO2'	6:J:41:G:H5''	1.56	0.59
4:S:139:LEU:HD23	4:S:141:LEU:HD12	1.85	0.59
3:C:99:VAL:HB	3:C:209:VAL:HB	1.83	0.59
3:R:283:GLU:HG2	3:R:286:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:HIS:ND1	2:L:314:TYR:OH	2.36	0.58
3:P:184:ARG:NH2	3:P:276:GLY:O	2.37	0.58
4:S:156:ARG:CD	4:S:158:PHE:CZ	2.86	0.58
3:D:265:ARG:NH2	6:J:32:G:OP2	2.37	0.58
2:L:12:LEU:HB2	2:L:109:LEU:HB2	1.83	0.58
3:M:99:VAL:HB	3:M:209:VAL:HB	1.86	0.58
3:M:256:HIS:ND1	6:T:39:U:OP1	2.29	0.58
4:S:145:THR:OG1	4:S:154:HIS:NE2	2.36	0.58
3:P:233:LEU:HB2	3:P:235:LYS:HZ3	1.68	0.58
6:J:44:C:H5'	6:J:45:A:OP2	2.04	0.58
3:C:151:ASN:HD21	3:C:226:PHE:H	1.51	0.57
3:H:134:LEU:HD11	3:H:327:ILE:CG2	2.29	0.57
3:D:184:ARG:NH2	3:D:276:GLY:O	2.37	0.57
2:L:213:LEU:HD23	2:L:216:LEU:HD21	1.86	0.57
3:C:256:HIS:ND1	6:J:39:U:OP1	2.38	0.57
2:B:65:ARG:HD2	3:H:250:ARG:HH21	1.69	0.57
2:L:253:ALA:N	2:L:283:LEU:O	2.37	0.57
6:J:43:U:H4'	6:J:44:C:H5''	1.86	0.57
4:I:146:LEU:HD12	4:I:146:LEU:C	2.25	0.57
2:L:181:LEU:HG	2:L:182:PRO:HD3	1.86	0.57
4:S:21:MET:CE	4:S:144:VAL:HG12	2.35	0.57
2:B:63:CYS:H	2:B:107:VAL:HG23	1.70	0.57
2:L:41:VAL:CG1	2:L:59:VAL:HG22	2.35	0.57
2:L:131:GLN:NE2	2:L:156:ASN:OD1	2.38	0.57
4:S:145:THR:HB	6:T:42:U:C1'	2.34	0.57
2:L:63:CYS:H	2:L:107:VAL:HG23	1.70	0.56
3:Q:76:LEU:HD11	6:T:21:U:C6	2.39	0.56
3:F:104:GLY:HA3	3:F:122:VAL:HG21	1.87	0.56
4:S:112:LEU:HD22	4:S:131:ILE:HG13	1.88	0.56
3:M:265:ARG:NH1	3:M:282:VAL:O	2.38	0.56
3:Q:184:ARG:NH2	3:Q:276:GLY:O	2.38	0.56
2:B:64:HIS:N	2:B:106:GLU:O	2.39	0.56
3:H:283:GLU:HG2	3:H:286:GLY:HA2	1.87	0.56
2:L:8:ALA:HB2	2:L:160:LEU:HD13	1.87	0.56
2:L:83:LEU:HB2	3:R:231:LEU:HD22	1.87	0.56
3:N:34:ASP:HA	3:N:161:ARG:HH12	1.69	0.56
3:R:161:ARG:HG2	3:R:175:ARG:HE	1.71	0.56
1:A:264:LEU:HD23	2:B:28:THR:C	2.26	0.56
3:F:34:ASP:OD1	3:F:161:ARG:CZ	2.54	0.55
2:L:64:HIS:NE2	2:L:108:SER:OG	2.39	0.55
3:M:262:ASN:ND2	6:T:38:C:N3	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:184:ARG:NH2	3:H:276:GLY:O	2.39	0.55
3:O:36:SER:O	3:O:92:LYS:NZ	2.39	0.55
4:S:16:PRO:HG3	6:T:41:G:C2'	2.36	0.55
2:B:34:PRO:HA	2:B:37:PHE:HD2	1.72	0.55
3:C:21:SER:OG	3:C:22:ASP:N	2.39	0.55
3:E:231:LEU:CD1	6:J:27:U:O4	2.55	0.55
3:D:99:VAL:HB	3:D:209:VAL:HB	1.89	0.55
3:G:262:ASN:ND2	6:J:14:G:OP2	2.39	0.54
4:I:3:HIS:HB2	4:I:62:ALA:O	2.07	0.54
6:J:43:U:H4'	6:J:44:C:O5'	2.01	0.54
3:E:36:SER:O	3:E:92:LYS:NZ	2.38	0.54
3:H:132:ALA:O	3:H:136:ARG:HB2	2.08	0.54
2:L:278:ARG:NH2	2:L:314:TYR:OH	2.41	0.54
4:I:154:HIS:CB	6:J:44:C:C5	2.90	0.54
5:U:200:ALA:HB3	5:U:207:ARG:HB2	1.90	0.54
5:V:29:THR:HG23	5:V:39:ILE:HG12	1.90	0.54
1:K:183:PRO:HD3	2:L:307:ALA:HB3	1.89	0.54
2:L:181:LEU:H	2:L:181:LEU:HD23	1.73	0.54
2:B:131:GLN:NE2	2:B:156:ASN:OD1	2.41	0.54
2:L:82:ASN:ND2	3:R:230:GLU:OE1	2.35	0.54
4:S:16:PRO:HG3	6:T:41:G:C1'	2.38	0.54
2:B:253:ALA:N	2:B:283:LEU:O	2.40	0.54
3:N:99:VAL:HB	3:N:209:VAL:HB	1.90	0.54
6:T:20:C:H2'	6:T:20:C:O2	2.08	0.54
2:L:34:PRO:HA	2:L:37:PHE:HD2	1.73	0.53
3:C:244:LYS:CG	6:J:40:G:O6	2.53	0.53
3:D:233:LEU:HG	3:D:235:LYS:H	1.74	0.53
1:K:177:GLN:O	2:L:271:ARG:NH1	2.40	0.53
6:T:33:U:C5	6:T:34:C:N4	2.77	0.53
3:M:149:TRP:O	4:S:15:PHE:HZ	1.90	0.53
2:L:183:GLY:O	2:L:184:PHE:CD1	2.61	0.53
4:S:12:ASP:OD1	4:S:14:GLU:OE2	2.26	0.53
5:V:78:VAL:HG12	5:V:85:VAL:HA	1.91	0.53
3:Q:310:ASN:OD1	3:Q:314:ARG:NH1	2.42	0.53
5:U:29:THR:HG23	5:U:39:ILE:HG12	1.90	0.53
1:K:171:SER:OG	1:K:172:HIS:N	2.42	0.53
4:S:107:SER:HA	4:S:136:ALA:HA	1.90	0.53
6:T:42:U:H3'	6:T:43:U:H5''	1.91	0.53
3:Q:291:GLN:NE2	3:Q:295:TYR:OH	2.40	0.53
2:B:82:ASN:ND2	3:H:230:GLU:OE1	2.42	0.52
2:B:181:LEU:CD2	2:B:182:PRO:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:290:SER:OG	4:I:13:PRO:O	2.28	0.52
3:F:237:ASP:OD1	3:F:237:ASP:N	2.43	0.52
2:L:64:HIS:N	2:L:106:GLU:O	2.42	0.52
5:U:53:ASP:HA	5:U:56:SER:HB3	1.91	0.52
5:U:76:GLU:HG2	5:U:88:ARG:HG2	1.91	0.52
5:U:78:VAL:HG12	5:U:85:VAL:HA	1.91	0.52
3:R:87:ASP:OD1	3:R:87:ASP:N	2.42	0.52
3:D:21:SER:OG	3:E:223:GLN:NE2	2.43	0.52
3:Q:132:ALA:O	3:Q:136:ARG:HB2	2.08	0.52
4:S:54:LEU:HG	4:S:142:PRO:HB2	1.91	0.52
5:V:200:ALA:HB3	5:V:207:ARG:HB2	1.90	0.52
3:C:259:LYS:HE3	6:J:38:C:O2'	2.09	0.52
6:J:20:C:H2'	6:J:20:C:O2	2.09	0.52
3:O:99:VAL:HB	3:O:209:VAL:HB	1.92	0.52
4:S:111:ARG:NH1	6:T:46:C:OP2	2.42	0.52
2:B:83:LEU:HB2	3:H:231:LEU:HD22	1.92	0.52
3:D:49:VAL:HG11	6:J:37:C:C4	2.44	0.52
4:I:27:LYS:HG3	4:I:79:LEU:HD11	1.92	0.52
3:G:104:GLY:HA3	3:G:122:VAL:HG21	1.91	0.52
4:I:112:LEU:HD11	6:J:54:U:H5'	1.91	0.52
3:C:208:HIS:NE2	3:D:154:GLY:O	2.43	0.51
1:K:247:LYS:HZ3	1:K:249:GLN:HG2	1.75	0.51
3:M:229:GLN:HE22	6:T:40:G:H3'	1.76	0.51
2:L:271:ARG:HA	3:R:11:VAL:HG21	1.92	0.51
5:V:76:GLU:HG2	5:V:88:ARG:HG2	1.91	0.51
3:F:10:SER:OG	5:U:16:ARG:NH2	2.44	0.51
3:G:117:LYS:HD2	3:G:120:GLN:HE21	1.75	0.51
5:V:53:ASP:HA	5:V:56:SER:HB3	1.92	0.51
3:M:310:ASN:OD1	3:M:314:ARG:NH2	2.44	0.51
2:B:19:ASN:OD1	2:B:102:ARG:NH1	2.42	0.51
3:N:10:SER:HB3	3:N:110:ASN:HD22	1.76	0.51
3:D:77:GLN:OE1	6:J:37:C:N4	2.43	0.51
3:D:140:HIS:CD2	3:D:192:LEU:HD21	2.46	0.51
3:D:296:ARG:NH1	3:D:322:GLN:OE1	2.38	0.51
3:G:15:GLU:HG2	6:J:11:C:H5''	1.93	0.51
3:H:87:ASP:OD1	3:H:87:ASP:N	2.43	0.51
4:S:105:ALA:HB2	4:S:139:LEU:HD11	1.91	0.51
3:P:259:LYS:HE3	6:T:20:C:H6	1.76	0.51
2:L:123:ALA:HB1	2:L:158:GLU:HB3	1.91	0.51
3:N:50:ARG:O	6:T:37:C:O2'	2.27	0.51
5:U:18:LEU:HD12	5:U:18:LEU:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:18:LEU:HD12	5:V:18:LEU:C	2.30	0.51
3:G:8:THR:HG23	3:G:313:LEU:HD11	1.93	0.50
4:I:32:LEU:HD13	4:I:40:ILE:HD12	1.93	0.50
3:C:290:SER:HB2	4:I:16:PRO:HD3	1.94	0.50
2:L:180:LEU:CD1	2:L:180:LEU:N	2.73	0.50
3:Q:34:ASP:OD2	3:Q:161:ARG:NH2	2.44	0.50
2:L:7:GLU:N	2:L:113:VAL:O	2.44	0.50
3:M:230:GLU:OE2	3:M:256:HIS:NE2	2.44	0.50
3:N:137:ARG:NH1	3:N:269:THR:OG1	2.41	0.50
3:E:50:ARG:HH21	3:E:74:PRO:HG3	1.76	0.50
4:I:156:ARG:NH2	6:J:43:U:C6	2.62	0.50
3:M:8:THR:HG21	3:N:56:ARG:HH12	1.76	0.50
3:P:10:SER:OG	5:V:16:ARG:NH2	2.45	0.50
1:A:172:HIS:O	1:A:177:GLN:NE2	2.44	0.50
3:G:283:GLU:HB2	3:G:286:GLY:HA2	1.94	0.50
3:D:51:GLY:HA3	6:J:37:C:HO2'	1.74	0.50
3:F:294:ALA:O	3:F:297:GLN:NE2	2.44	0.50
3:E:99:VAL:HB	3:E:209:VAL:HB	1.93	0.49
3:G:235:LYS:HD3	5:U:39:ILE:HD12	1.94	0.49
2:L:196:HIS:HA	2:L:199:THR:HG22	1.93	0.49
4:S:44:PHE:HE2	4:S:159:ILE:HG12	1.77	0.49
3:D:292:GLY:O	3:E:72:GLN:NE2	2.45	0.49
3:G:109:CYS:SG	3:G:115:ARG:HB3	2.53	0.49
3:G:228:SER:HB2	3:G:255:ILE:HA	1.94	0.49
3:C:17:LYS:HB2	3:C:331:ILE:HG23	1.93	0.49
1:A:173:SER:CB	3:H:11:VAL:HG22	2.42	0.49
2:L:258:LEU:CD1	2:L:281:GLU:HB2	2.43	0.49
3:G:159:GLU:OE2	3:G:161:ARG:NH1	2.45	0.49
2:B:261:LEU:HD13	2:B:278:ARG:HG3	1.94	0.49
3:C:259:LYS:HD2	6:J:38:C:H1'	1.95	0.49
2:L:180:LEU:O	2:L:292:PRO:HG2	2.12	0.49
2:B:127:ALA:HB1	2:B:156:ASN:HB2	1.93	0.49
3:M:158:VAL:HG22	3:M:179:LEU:HG	1.94	0.49
3:M:227:PRO:HG2	3:M:246:LEU:HD22	1.95	0.49
3:M:144:ASN:HB2	3:M:152:ARG:HH12	1.77	0.49
4:S:156:ARG:HD3	4:S:158:PHE:CE2	2.48	0.49
3:F:10:SER:HB3	3:F:110:ASN:HD22	1.77	0.49
5:U:98:LEU:HB3	5:U:119:LEU:HB3	1.95	0.49
6:J:37:C:O2'	6:J:38:C:OP1	2.22	0.49
6:T:51:G:H21	6:T:55:A:H62	1.61	0.49
3:F:163:ASN:HB3	3:F:170:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:61:ASP:OD1	3:N:61:ASP:N	2.46	0.48
2:L:168:GLN:O	2:L:172:ASN:ND2	2.47	0.48
3:P:310:ASN:OD1	3:P:314:ARG:NH2	2.43	0.48
2:B:303:TRP:CB	2:B:318:THR:CG2	2.90	0.48
3:E:8:THR:HG23	3:E:313:LEU:HD11	1.94	0.48
3:F:50:ARG:NH1	6:J:27:U:O2	2.46	0.48
2:L:165:SER:O	2:L:169:ARG:N	2.46	0.48
1:A:173:SER:OG	3:H:11:VAL:HG13	2.14	0.48
2:L:19:ASN:OD1	2:L:102:ARG:NH1	2.45	0.48
4:S:22:SER:OG	4:S:145:THR:O	2.19	0.48
5:V:98:LEU:HB3	5:V:119:LEU:HB3	1.95	0.48
3:D:140:HIS:NE2	3:D:192:LEU:HD21	2.28	0.48
3:P:144:ASN:HB2	3:P:152:ARG:HH12	1.78	0.48
1:A:173:SER:HA	3:H:11:VAL:CG2	2.42	0.48
3:R:21:SER:HG	3:R:96:THR:H	1.60	0.48
1:A:171:SER:OG	1:A:172:HIS:N	2.46	0.48
3:C:90:THR:HA	3:C:217:ALA:O	2.13	0.48
3:G:132:ALA:O	3:G:136:ARG:HB2	2.14	0.48
4:S:10:ARG:NH1	4:S:81:ASP:O	2.46	0.48
4:I:54:LEU:HD11	4:I:159:ILE:HD12	1.96	0.48
2:L:59:VAL:HG12	2:L:61:ILE:HG23	1.95	0.48
2:L:252:PRO:O	2:L:316:TRP:NE1	2.43	0.48
2:B:259:SER:HB2	2:B:279:PHE:HB2	1.94	0.47
3:D:51:GLY:HA2	6:J:38:C:OP1	2.14	0.47
3:G:140:HIS:CD2	3:G:192:LEU:HD11	2.49	0.47
3:H:157:ALA:H	3:H:218:ARG:HB2	1.79	0.47
3:C:91:LEU:HD13	3:C:225:VAL:HG11	1.95	0.47
1:K:253:GLN:O	1:K:258:ARG:NH1	2.45	0.47
5:V:104:ASP:OD1	5:V:104:ASP:N	2.47	0.47
4:S:70:LEU:HA	4:S:73:ARG:HD3	1.96	0.47
4:S:113:ARG:O	4:S:117:MET:HB2	2.15	0.47
3:E:230:GLU:HB2	3:E:245:THR:OG1	2.15	0.47
3:M:158:VAL:HG23	3:M:178:ALA:HB3	1.95	0.47
6:T:41:G:N3	6:T:41:G:C2'	2.75	0.47
4:I:70:LEU:O	4:I:75:TRP:NE1	2.40	0.47
4:S:112:LEU:HD13	4:S:131:ILE:HG21	1.96	0.47
3:F:262:ASN:ND2	6:J:20:C:OP2	2.45	0.47
3:M:36:SER:O	3:M:92:LYS:NZ	2.41	0.47
3:O:249:VAL:HG12	3:O:250:ARG:HG2	1.97	0.47
3:N:184:ARG:NH1	3:N:276:GLY:O	2.48	0.47
3:O:8:THR:HG23	3:O:313:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:94:ARG:HG3	3:P:214:VAL:HG22	1.96	0.47
3:P:100:LEU:HD22	3:Q:154:GLY:HA3	1.97	0.47
4:S:9:LEU:HB3	4:S:20:LEU:HD23	1.96	0.47
4:S:156:ARG:HH11	4:S:158:PHE:HZ	1.63	0.47
6:J:51:G:H21	6:J:55:A:H62	1.61	0.47
4:S:40:ILE:HD11	4:S:60:ILE:HD11	1.96	0.47
4:S:146:LEU:CD1	4:S:155:PHE:CE2	2.81	0.47
5:U:170:VAL:O	5:U:177:THR:OG1	2.30	0.47
3:C:105:THR:HG22	3:C:119:LEU:HD21	1.96	0.47
5:U:104:ASP:N	5:U:104:ASP:OD1	2.47	0.47
3:F:33:ARG:NE	3:F:159:GLU:OE1	2.48	0.47
3:M:229:GLN:NE2	6:T:40:G:H3'	2.31	0.46
3:N:33:ARG:HA	3:N:36:SER:HB3	1.97	0.46
3:R:144:ASN:ND2	3:R:182:GLY:O	2.48	0.46
2:B:321:PHE:HD1	2:B:322:VAL:HG23	1.81	0.46
4:I:113:ARG:HG3	4:I:131:ILE:HD11	1.97	0.46
3:P:79:VAL:HG13	3:P:244:LYS:HB3	1.97	0.46
3:D:87:ASP:OD1	3:D:87:ASP:N	2.46	0.46
3:D:100:LEU:HD22	3:E:154:GLY:HA3	1.97	0.46
3:F:61:ASP:OD1	3:F:61:ASP:N	2.48	0.46
2:B:20:ALA:HB1	2:B:140:ALA:HB3	1.97	0.46
3:D:314:ARG:NH2	5:U:105:ASP:OD1	2.48	0.46
3:H:36:SER:O	3:H:36:SER:OG	2.32	0.46
2:L:12:LEU:HD13	2:L:156:ASN:HD21	1.80	0.46
3:M:133:GLU:OE2	3:M:137:ARG:NE	2.41	0.46
3:Q:99:VAL:HB	3:Q:209:VAL:HB	1.98	0.46
1:K:199:VAL:HG23	1:K:258:ARG:HH22	1.81	0.46
1:K:252:SER:OG	1:K:253:GLN:N	2.48	0.46
1:A:104:LEU:HD12	1:A:197:SER:CB	2.46	0.46
3:P:239:LYS:HZ1	3:P:241:GLN:H	1.64	0.46
1:K:190:LEU:HD21	2:L:314:TYR:HD2	1.80	0.46
3:C:259:LYS:HE3	6:J:38:C:HO2'	1.81	0.45
2:L:303:TRP:HA	2:L:317:SER:O	2.16	0.45
3:O:50:ARG:HH21	3:O:74:PRO:HG3	1.81	0.45
6:T:41:G:H2'	6:T:42:U:OP1	2.14	0.45
3:F:96:THR:OG1	3:G:223:GLN:NE2	2.44	0.45
3:M:26:SER:HA	3:M:41:ALA:HA	1.99	0.45
6:T:42:U:C5'	6:T:43:U:OP2	2.61	0.45
3:R:16:ARG:NE	3:R:19:ASP:OD1	2.47	0.45
4:S:16:PRO:HG2	4:S:19:GLN:CB	2.46	0.45
3:D:13:ALA:HB1	6:J:29:C:HI'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:LEU:HD13	3:E:225:VAL:HG11	1.99	0.45
3:Q:15:GLU:HG2	6:T:11:C:H5''	1.98	0.45
4:S:96:PRO:HB2	4:S:164:LEU:HD22	1.97	0.45
3:F:172:ARG:NH2	3:F:191:GLU:OE1	2.49	0.45
3:R:104:GLY:HA3	3:R:122:VAL:HG11	1.99	0.45
3:H:144:ASN:ND2	3:H:182:GLY:O	2.47	0.45
3:M:187:LYS:HB2	3:M:187:LYS:HE2	1.77	0.45
2:L:258:LEU:HD11	2:L:281:GLU:HB2	1.99	0.45
3:N:299:LYS:HD3	3:N:299:LYS:HA	1.79	0.45
2:B:257:ALA:H	2:B:312:GLY:HA3	1.81	0.45
3:C:288:VAL:HG12	3:C:289:THR:N	2.32	0.45
4:I:143:PHE:CZ	6:J:42:U:N3	2.85	0.45
3:M:277:LEU:O	4:S:10:ARG:NH2	2.50	0.45
3:N:91:LEU:HD13	3:N:225:VAL:HG11	1.98	0.45
4:S:22:SER:OG	4:S:145:THR:HG23	2.17	0.45
5:V:170:VAL:O	5:V:177:THR:OG1	2.30	0.45
3:C:258:GLN:NE2	6:J:39:U:OP1	2.49	0.45
3:G:9:ALA:HB1	3:G:110:ASN:HB2	1.98	0.45
4:S:7:ILE:HD11	4:S:58:LEU:HD23	1.98	0.45
3:G:268:ASP:HB2	3:G:282:VAL:HG12	1.99	0.44
3:H:143:ALA:HB1	3:H:181:ILE:HD13	1.99	0.44
1:K:189:LEU:HD23	2:L:277:LEU:HD12	2.00	0.44
3:N:208:HIS:ND1	3:O:156:GLU:OE1	2.49	0.44
3:Q:318:PRO:O	3:Q:323:GLN:NE2	2.49	0.44
3:R:33:ARG:HA	3:R:36:SER:HB3	1.99	0.44
3:H:156:GLU:OE2	3:H:218:ARG:NH2	2.50	0.44
3:N:17:LYS:HB2	3:N:331:ILE:HG23	1.99	0.44
3:R:109:CYS:O	3:R:115:ARG:NH2	2.45	0.44
3:C:26:SER:HA	3:C:41:ALA:HA	2.00	0.44
1:K:195:PRO:HB2	1:K:198:LEU:HB3	1.98	0.44
1:K:240:ILE:HD13	1:K:263:TRP:HB3	2.00	0.44
2:L:179:ARG:C	2:L:180:LEU:HD13	2.37	0.44
3:Q:36:SER:O	3:Q:92:LYS:NZ	2.44	0.44
3:R:165:ILE:HG22	3:R:170:VAL:HA	1.97	0.44
3:D:76:LEU:CD2	6:J:39:U:C4	3.00	0.44
2:L:13:PRO:O	2:L:108:SER:OG	2.31	0.44
3:D:51:GLY:CA	6:J:37:C:HO2'	2.31	0.44
3:D:76:LEU:HD13	6:J:39:U:O4'	2.17	0.44
3:G:187:LYS:HD3	3:G:187:LYS:HA	1.73	0.44
3:F:125:TYR:OH	3:F:324:HIS:ND1	2.39	0.44
4:I:174:THR:HG23	4:I:180:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:45:PRO:HD3	4:I:59:ARG:HG3	2.00	0.44
2:L:70:ILE:HD12	2:L:79:LYS:HD3	1.98	0.44
2:L:259:SER:HB2	2:L:279:PHE:HB2	2.00	0.44
2:L:304:TYR:HD2	2:L:319:PRO:HD2	1.83	0.44
3:M:25:MET:HG2	3:M:93:VAL:HG12	1.99	0.44
3:P:143:ALA:HB1	3:P:181:ILE:HD13	2.00	0.44
3:R:132:ALA:O	3:R:136:ARG:HB2	2.17	0.44
4:S:59:ARG:NH1	4:S:187:PHE:OXT	2.44	0.44
4:S:146:LEU:HD12	4:S:155:PHE:O	2.17	0.44
3:M:305:TYR:OH	3:N:54:SER:O	2.34	0.43
3:R:301:LYS:HA	3:R:301:LYS:HD3	1.75	0.43
6:J:43:U:OP2	6:J:43:U:H3'	2.17	0.43
2:B:304:TYR:HD2	2:B:319:PRO:HD2	1.82	0.43
1:K:199:VAL:HA	1:K:202:VAL:HG22	1.99	0.43
1:K:224:ARG:HA	5:V:64:ILE:HD11	2.01	0.43
3:Q:283:GLU:HB2	3:Q:286:GLY:HA2	2.00	0.43
1:A:199:VAL:HA	1:A:202:VAL:HG22	2.00	0.43
3:G:144:ASN:ND2	3:G:182:GLY:O	2.49	0.43
4:I:176:TYR:HB3	4:I:178:LEU:HD23	1.99	0.43
2:L:11:LEU:HD13	2:L:180:LEU:HD21	2.00	0.43
3:N:92:LYS:HA	3:N:215:ALA:O	2.18	0.43
4:S:68:ARG:HH22	4:S:88:PRO:HD2	1.83	0.43
3:H:57:LEU:HD11	3:H:62:ARG:HA	2.00	0.43
3:O:234:ASP:OD1	3:O:234:ASP:N	2.42	0.43
3:G:231:LEU:HD13	6:J:15:G:N7	2.33	0.43
3:H:262:ASN:ND2	6:J:8:A:OP2	2.36	0.43
2:L:171:LYS:HD3	2:L:171:LYS:HA	1.82	0.43
2:L:310:ASP:N	2:L:310:ASP:OD1	2.51	0.43
3:M:141:ASN:OD1	3:M:146:ARG:NE	2.45	0.43
3:C:36:SER:O	3:C:92:LYS:NZ	2.39	0.43
1:K:92:PRO:O	2:L:194:GLN:NE2	2.52	0.43
3:P:272:PRO:HB3	3:P:302:LEU:HD12	2.00	0.43
4:S:18:ALA:HA	4:S:21:MET:HG2	2.00	0.43
4:S:154:HIS:CB	6:T:44:C:C6	3.01	0.43
6:J:33:U:C5	6:J:34:C:N4	2.86	0.43
3:G:34:ASP:OD1	3:G:161:ARG:NH2	2.51	0.43
3:M:24:LEU:HD21	3:M:249:VAL:HB	2.01	0.43
3:C:266:THR:HA	3:C:281:ALA:HA	2.00	0.43
3:G:231:LEU:CD1	6:J:15:G:N7	2.82	0.43
2:L:93:SER:OG	2:L:94:THR:N	2.52	0.43
3:P:68:ASP:OD1	3:P:68:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:13:ALA:O	3:R:107:SER:N	2.44	0.43
5:V:191:SER:OG	5:V:194:ASN:OD1	2.37	0.43
2:B:185:ALA:O	2:B:289:TRP:HA	2.18	0.43
3:C:270:TRP:NE1	3:C:321:GLU:OE2	2.51	0.43
3:D:141:ASN:OD1	3:D:146:ARG:NE	2.41	0.43
2:L:197:LEU:HB2	2:L:210:LEU:HD22	2.01	0.43
3:P:10:SER:HB3	3:P:110:ASN:HD22	1.83	0.43
4:S:154:HIS:HE1	6:T:42:U:O2'	2.02	0.43
3:M:158:VAL:HG12	3:M:217:ALA:HA	2.01	0.43
3:M:302:LEU:HD12	3:M:307:LEU:HD11	2.01	0.43
3:N:76:LEU:CD1	6:T:39:U:C6	2.99	0.43
3:C:157:ALA:HA	3:C:179:LEU:HD11	2.01	0.42
3:E:50:ARG:O	6:J:31:C:O2'	2.37	0.42
1:K:264:LEU:HD23	2:L:28:THR:C	2.39	0.42
2:L:257:ALA:H	2:L:312:GLY:HA3	1.84	0.42
3:N:189:ASP:O	3:N:193:ASP:N	2.44	0.42
4:S:21:MET:HE3	4:S:144:VAL:HG12	2.01	0.42
3:E:117:LYS:HD2	3:E:120:GLN:HE21	1.82	0.42
4:I:146:LEU:C	4:I:146:LEU:CD1	2.87	0.42
2:L:77:ARG:H	2:L:77:ARG:HG2	1.51	0.42
3:N:268:ASP:OD1	3:N:296:ARG:NH2	2.44	0.42
3:R:13:ALA:HB1	6:T:5:G:H1'	2.00	0.42
3:E:14:PHE:HZ	3:E:118:LEU:HD21	1.84	0.42
3:E:159:GLU:OE2	3:E:161:ARG:NE	2.46	0.42
3:H:58:LYS:HA	3:H:58:LYS:HD3	1.85	0.42
3:R:318:PRO:O	3:R:323:GLN:NE2	2.45	0.42
4:S:14:GLU:N	4:S:14:GLU:CD	2.73	0.42
4:S:46:ASP:HB3	4:S:55:GLY:HA3	2.01	0.42
5:V:73:ASP:OD1	5:V:73:ASP:N	2.52	0.42
3:E:132:ALA:O	3:E:136:ARG:HB2	2.20	0.42
2:L:181:LEU:HG	2:L:182:PRO:CD	2.48	0.42
5:V:226:ARG:HA	5:V:226:ARG:HD3	1.87	0.42
2:B:29:TRP:HB2	2:B:81:PHE:HZ	1.84	0.42
3:E:184:ARG:HE	3:E:184:ARG:HB3	1.70	0.42
3:E:231:LEU:CD1	6:J:27:U:C4	2.99	0.42
1:K:190:LEU:HD23	2:L:280:VAL:HG21	2.00	0.42
1:K:207:ARG:HE	1:K:207:ARG:HB3	1.74	0.42
2:L:116:ASP:HB3	2:L:119:ASP:HB2	2.01	0.42
3:N:36:SER:O	3:N:92:LYS:NZ	2.41	0.42
4:S:154:HIS:O	6:T:44:C:O2'	2.37	0.42
5:V:25:HIS:HA	5:V:43:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:CD2	2:B:276:PRO:HG2	2.55	0.42
2:B:50:ILE:HD12	2:B:50:ILE:HA	1.92	0.42
3:G:299:LYS:HA	3:G:299:LYS:HD3	1.85	0.42
3:P:87:ASP:OD1	3:P:87:ASP:N	2.52	0.42
2:B:11:LEU:O	2:B:156:ASN:ND2	2.44	0.42
3:E:297:GLN:HE21	3:E:298:PRO:CD	2.29	0.42
3:O:34:ASP:OD1	3:O:161:ARG:NH2	2.52	0.42
5:U:191:SER:OG	5:U:194:ASN:OD1	2.37	0.42
2:B:249:VAL:HG21	2:B:289:TRP:CD1	2.54	0.42
3:F:272:PRO:HB3	3:F:302:LEU:HD12	2.02	0.42
3:P:96:THR:HG21	3:Q:221:ASP:HB2	2.02	0.42
3:Q:94:ARG:HG3	3:Q:214:VAL:HG22	2.00	0.42
3:H:189:ASP:HB3	3:H:192:LEU:HB3	2.01	0.41
3:D:268:ASP:HB3	3:D:280:ILE:HG13	2.02	0.41
3:M:24:LEU:HD23	3:M:254:ALA:HB2	2.02	0.41
3:P:45:ARG:NH2	3:P:83:ASN:OD1	2.54	0.41
4:S:164:LEU:HD23	4:S:164:LEU:HA	1.95	0.41
6:J:44:C:C5'	6:J:45:A:OP2	2.67	0.41
3:H:63:ASP:HB3	3:H:66:LYS:HG2	2.02	0.41
2:L:298:LEU:HD12	2:L:298:LEU:HA	1.91	0.41
3:O:143:ALA:HB1	3:O:181:ILE:HD13	2.01	0.41
3:P:266:THR:HA	3:P:281:ALA:HA	2.02	0.41
4:S:7:ILE:HB	4:S:83:LEU:HD12	2.01	0.41
1:A:252:SER:OG	1:A:253:GLN:N	2.54	0.41
3:D:76:LEU:CD1	6:J:39:U:O4'	2.68	0.41
3:E:80:ASP:OD1	3:E:242:LYS:NZ	2.44	0.41
3:G:272:PRO:HB3	3:G:302:LEU:HD12	2.02	0.41
3:M:23:ALA:HA	3:M:94:ARG:O	2.20	0.41
4:I:68:ARG:HA	4:I:71:LEU:HD12	2.01	0.41
3:M:229:GLN:OE1	6:T:40:G:H2'	2.21	0.41
3:O:117:LYS:HD2	3:O:117:LYS:HA	1.90	0.41
3:Q:117:LYS:HA	3:Q:120:GLN:HE21	1.84	0.41
3:R:146:ARG:NH2	3:R:183:LEU:O	2.49	0.41
3:N:270:TRP:CD1	3:N:321:GLU:HB3	2.56	0.41
5:U:73:ASP:N	5:U:73:ASP:OD1	2.52	0.41
1:A:104:LEU:CD1	1:A:197:SER:OG	2.69	0.41
2:B:138:ARG:HH11	6:J:5:G:H5''	1.86	0.41
3:C:10:SER:HB3	3:C:110:ASN:HD22	1.86	0.41
5:U:25:HIS:HA	5:U:43:PRO:HA	2.01	0.41
1:A:104:LEU:CD1	1:A:197:SER:CB	2.98	0.41
2:B:59:VAL:HG12	2:B:61:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ASN:OD1	3:C:146:ARG:NE	2.40	0.41
3:G:228:SER:HG	3:G:256:HIS:CE1	2.37	0.41
4:I:146:LEU:O	4:I:154:HIS:HA	2.20	0.41
3:O:10:SER:HB3	3:O:110:ASN:HD22	1.86	0.41
3:O:144:ASN:HD22	3:O:181:ILE:HG22	1.86	0.41
3:Q:303:ASP:OD1	3:Q:303:ASP:N	2.51	0.41
4:S:98:ARG:HB3	4:S:164:LEU:HD23	2.02	0.41
1:A:88:ALA:O	2:B:256:ASN:ND2	2.53	0.41
3:D:136:ARG:O	3:D:140:HIS:ND1	2.54	0.41
3:M:24:LEU:O	3:M:93:VAL:HA	2.20	0.41
3:O:149:TRP:CE2	3:O:259:LYS:HE2	2.56	0.41
3:P:172:ARG:HH12	3:P:194:ALA:HB1	1.86	0.41
3:R:302:LEU:HA	3:R:302:LEU:HD23	1.88	0.41
4:S:44:PHE:CE2	4:S:159:ILE:HG12	2.55	0.41
6:T:41:G:C2'	6:T:42:U:OP1	2.69	0.41
1:A:189:LEU:HD21	2:B:271:ARG:H	1.86	0.41
6:J:36:A:O2'	6:J:37:C:O4'	2.34	0.41
3:D:50:ARG:O	6:J:38:C:H5''	2.20	0.40
3:F:105:THR:HG22	3:F:119:LEU:HD21	2.04	0.40
4:I:18:ALA:HB1	6:J:42:U:C6	2.56	0.40
3:O:161:ARG:HG2	3:O:175:ARG:HD3	2.02	0.40
4:S:156:ARG:O	4:S:156:ARG:HG3	2.21	0.40
3:C:117:LYS:HD2	3:C:120:GLN:HE21	1.86	0.40
3:D:132:ALA:O	3:D:136:ARG:HB2	2.21	0.40
3:E:283:GLU:HB2	3:E:286:GLY:HA2	2.03	0.40
3:H:13:ALA:HB1	6:J:5:G:H1'	2.03	0.40
2:L:66:PHE:HE1	2:L:68:ALA:HB2	1.87	0.40
3:O:12:LEU:HB3	3:O:336:PHE:O	2.22	0.40
3:F:87:ASP:OD1	3:F:87:ASP:N	2.52	0.40
3:G:302:LEU:HD23	3:G:302:LEU:HA	1.87	0.40
2:L:56:LEU:HD22	2:L:111:LEU:HD23	2.02	0.40
5:V:2:ASN:OD1	5:V:2:ASN:N	2.54	0.40
3:G:33:ARG:HA	3:G:36:SER:HB3	2.03	0.40
1:A:239:ALA:O	1:A:263:TRP:HA	2.20	0.40
3:D:91:LEU:HD13	3:D:225:VAL:HG11	2.04	0.40
3:H:124:THR:O	3:H:128:GLU:HG3	2.22	0.40
3:H:163:ASN:HB3	3:H:165:ILE:HD11	2.04	0.40
4:I:7:ILE:HD11	4:I:58:LEU:HD22	2.03	0.40
3:M:288:VAL:HG11	4:S:13:PRO:HB3	2.03	0.40
6:J:43:U:O2	6:J:43:U:C2'	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/434 (95%)	368 (89%)	45 (11%)	0	100	100
1	K	422/434 (97%)	370 (88%)	52 (12%)	0	100	100
2	B	301/327 (92%)	277 (92%)	24 (8%)	0	100	100
2	L	301/327 (92%)	275 (91%)	26 (9%)	0	100	100
3	C	286/342 (84%)	276 (96%)	10 (4%)	0	100	100
3	D	332/342 (97%)	316 (95%)	16 (5%)	0	100	100
3	E	335/342 (98%)	319 (95%)	16 (5%)	0	100	100
3	F	333/342 (97%)	317 (95%)	16 (5%)	0	100	100
3	G	325/342 (95%)	308 (95%)	17 (5%)	0	100	100
3	H	330/342 (96%)	310 (94%)	20 (6%)	0	100	100
3	M	287/342 (84%)	272 (95%)	15 (5%)	0	100	100
3	N	333/342 (97%)	313 (94%)	19 (6%)	1 (0%)	37	63
3	O	332/342 (97%)	317 (96%)	15 (4%)	0	100	100
3	P	333/342 (97%)	318 (96%)	15 (4%)	0	100	100
3	Q	331/342 (97%)	314 (95%)	16 (5%)	1 (0%)	37	63
3	R	331/342 (97%)	318 (96%)	13 (4%)	0	100	100
4	I	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
4	S	186/187 (100%)	179 (96%)	7 (4%)	0	100	100
5	U	225/228 (99%)	214 (95%)	11 (5%)	0	100	100
5	V	225/228 (99%)	214 (95%)	11 (5%)	0	100	100
All	All	6146/6456 (95%)	5772 (94%)	372 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	249	VAL

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Mol	Chain	Res	Type
3	Q	250	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	72/365 (20%)	72 (100%)	0	100	100
1	K	78/365 (21%)	77 (99%)	1 (1%)	65	86
2	B	204/270 (76%)	200 (98%)	4 (2%)	50	78
2	L	232/270 (86%)	230 (99%)	2 (1%)	75	91
3	C	202/274 (74%)	202 (100%)	0	100	100
3	D	253/274 (92%)	248 (98%)	5 (2%)	50	78
3	E	263/274 (96%)	261 (99%)	2 (1%)	79	92
3	F	262/274 (96%)	259 (99%)	3 (1%)	70	88
3	G	254/274 (93%)	252 (99%)	2 (1%)	79	92
3	H	245/274 (89%)	243 (99%)	2 (1%)	79	92
3	M	221/274 (81%)	219 (99%)	2 (1%)	75	91
3	N	259/274 (94%)	253 (98%)	6 (2%)	45	75
3	O	259/274 (94%)	256 (99%)	3 (1%)	67	87
3	P	263/274 (96%)	256 (97%)	7 (3%)	40	71
3	Q	258/274 (94%)	256 (99%)	2 (1%)	79	92
3	R	251/274 (92%)	249 (99%)	2 (1%)	79	92
4	I	145/160 (91%)	144 (99%)	1 (1%)	81	93
4	S	142/160 (89%)	139 (98%)	3 (2%)	48	76
5	U	181/182 (100%)	179 (99%)	2 (1%)	70	88
5	V	181/182 (100%)	179 (99%)	2 (1%)	70	88
All	All	4225/5242 (81%)	4174 (99%)	51 (1%)	66	87

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	GLN
2	B	181	LEU
2	B	271	ARG
2	B	321	PHE
3	D	38	GLU
3	D	60	LYS
3	D	66	LYS
3	D	234	ASP
3	D	285	TYR
3	E	152	ARG
3	E	285	TYR
3	F	17	LYS
3	F	221	ASP
3	F	285	TYR
3	G	172	ARG
3	G	285	TYR
3	H	58	LYS
3	H	270	TRP
1	K	263	TRP
4	I	87	GLU
2	L	131	GLN
2	L	180	LEU
3	M	47	LYS
3	M	314	ARG
3	N	60	LYS
3	N	66	LYS
3	N	80	ASP
3	N	172	ARG
3	N	218	ARG
3	N	250	ARG
3	O	17	LYS
3	O	38	GLU
3	O	285	TYR
3	P	17	LYS
3	P	38	GLU
3	P	68	ASP
3	P	172	ARG
3	P	221	ASP
3	P	285	TYR
3	P	314	ARG
3	Q	98	ARG
3	Q	285	TYR
3	R	172	ARG

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Mol	Chain	Res	Type
3	R	270	TRP
4	S	22	SER
4	S	27	LYS
4	S	146	LEU
5	U	46	TYR
5	U	116	ARG
5	V	46	TYR
5	V	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
2	B	129	GLN
2	B	131	GLN
3	C	77	GLN
3	C	127	ASN
3	C	151	ASN
3	D	75	ASN
3	D	110	ASN
3	D	208	HIS
3	E	72	GLN
3	E	120	GLN
3	E	223	GLN
3	E	297	GLN
3	G	127	ASN
3	H	127	ASN
4	I	120	HIS
4	I	161	HIS
2	L	172	ASN
3	M	291	GLN
3	O	144	ASN
3	O	223	GLN
3	P	120	GLN
3	Q	120	GLN
3	Q	241	GLN
3	Q	291	GLN
4	S	35	GLN
4	S	82	HIS
4	S	84	GLN
5	U	2	ASN
5	V	2	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	J	59/60 (98%)	33 (55%)	9 (15%)
6	T	59/60 (98%)	30 (50%)	3 (5%)
All	All	118/120 (98%)	63 (53%)	12 (10%)

All (63) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	J	3	A
6	J	8	A
6	J	9	U
6	J	10	U
6	J	14	G
6	J	15	G
6	J	16	C
6	J	17	G
6	J	20	C
6	J	21	U
6	J	22	U
6	J	23	G
6	J	24	A
6	J	27	U
6	J	28	C
6	J	30	G
6	J	32	G
6	J	33	U
6	J	34	C
6	J	35	U
6	J	36	A
6	J	37	C
6	J	38	C
6	J	39	U
6	J	40	G
6	J	41	G
6	J	42	U
6	J	43	U
6	J	44	C
6	J	45	A
6	J	48	G
6	J	54	U
6	J	55	A
6	T	3	A

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Mol	Chain	Res	Type
6	T	8	A
6	T	9	U
6	T	10	U
6	T	14	G
6	T	15	G
6	T	16	C
6	T	17	G
6	T	20	C
6	T	21	U
6	T	22	U
6	T	23	G
6	T	24	A
6	T	27	U
6	T	28	C
6	T	30	G
6	T	32	G
6	T	33	U
6	T	34	C
6	T	35	U
6	T	36	A
6	T	39	U
6	T	41	G
6	T	42	U
6	T	43	U
6	T	44	C
6	T	45	A
6	T	48	G
6	T	54	U
6	T	55	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	J	16	C
6	J	37	C
6	J	38	C
6	J	39	U
6	J	40	G
6	J	41	G
6	J	42	U
6	J	43	U
6	J	44	C

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Mol	Chain	Res	Type
6	T	16	C
6	T	43	U
6	T	44	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

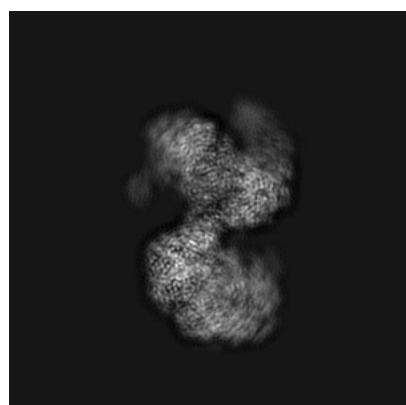
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31185. These allow visual inspection of the internal detail of the map and identification of artifacts.

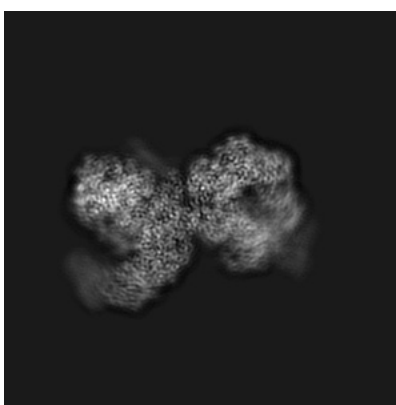
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

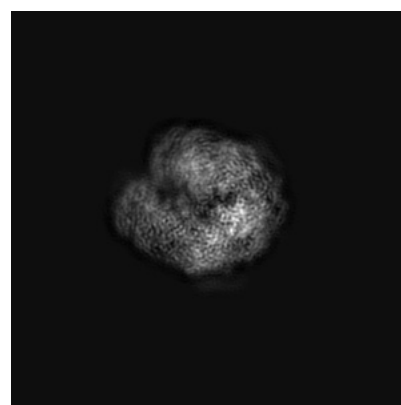
6.1.1 Primary map



X



Y

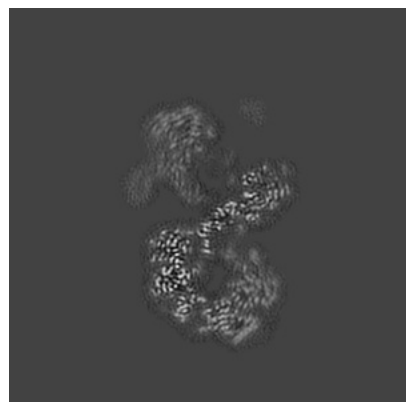


Z

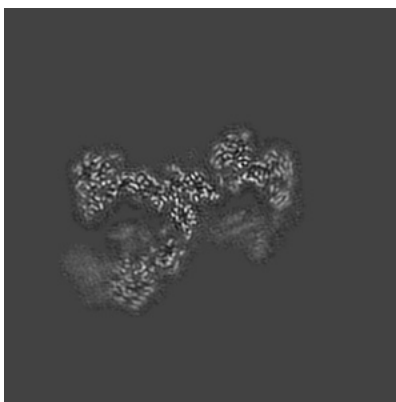
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

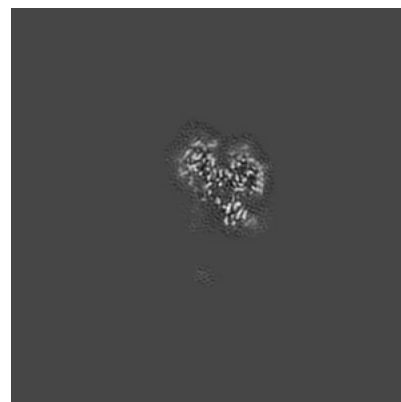
6.2.1 Primary map



X Index: 160



Y Index: 160

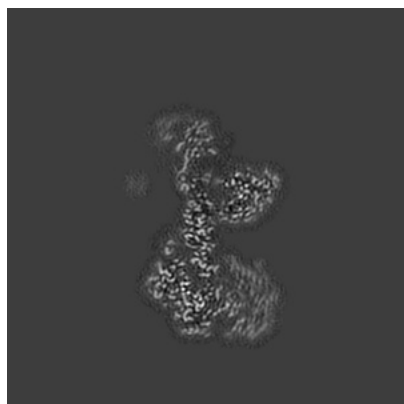


Z Index: 160

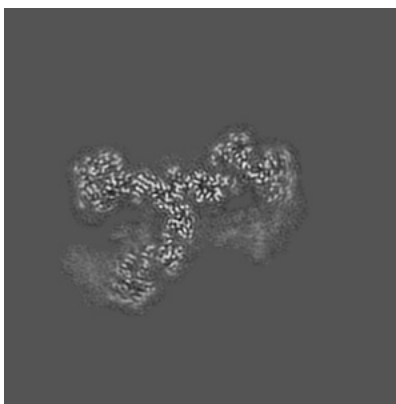
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

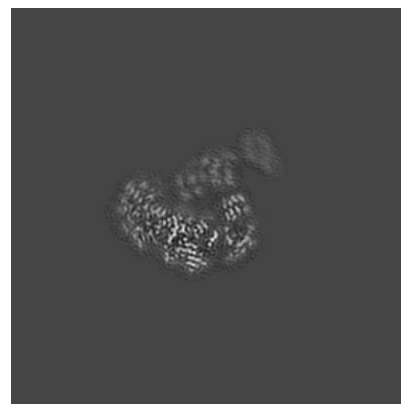
6.3.1 Primary map



X Index: 176



Y Index: 157

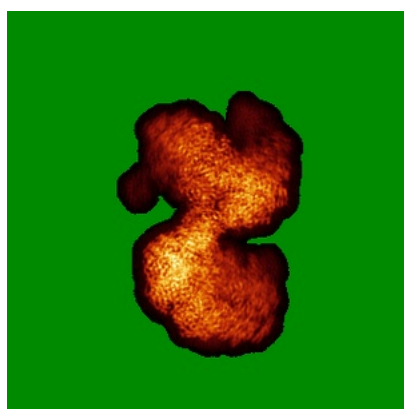


Z Index: 113

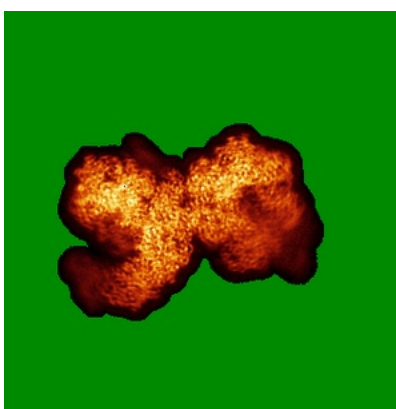
The images above show the largest variance slices of the map in three orthogonal directions.

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

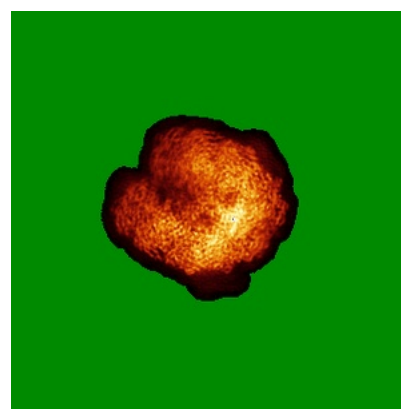
6.4.1 Primary map



X



Y



Z

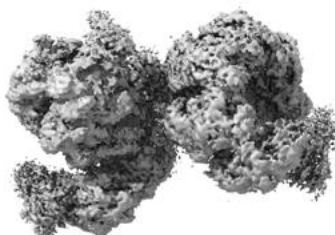
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

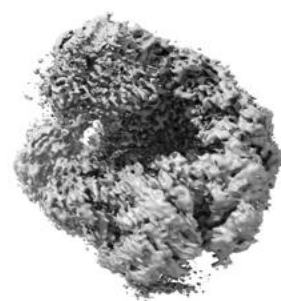
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

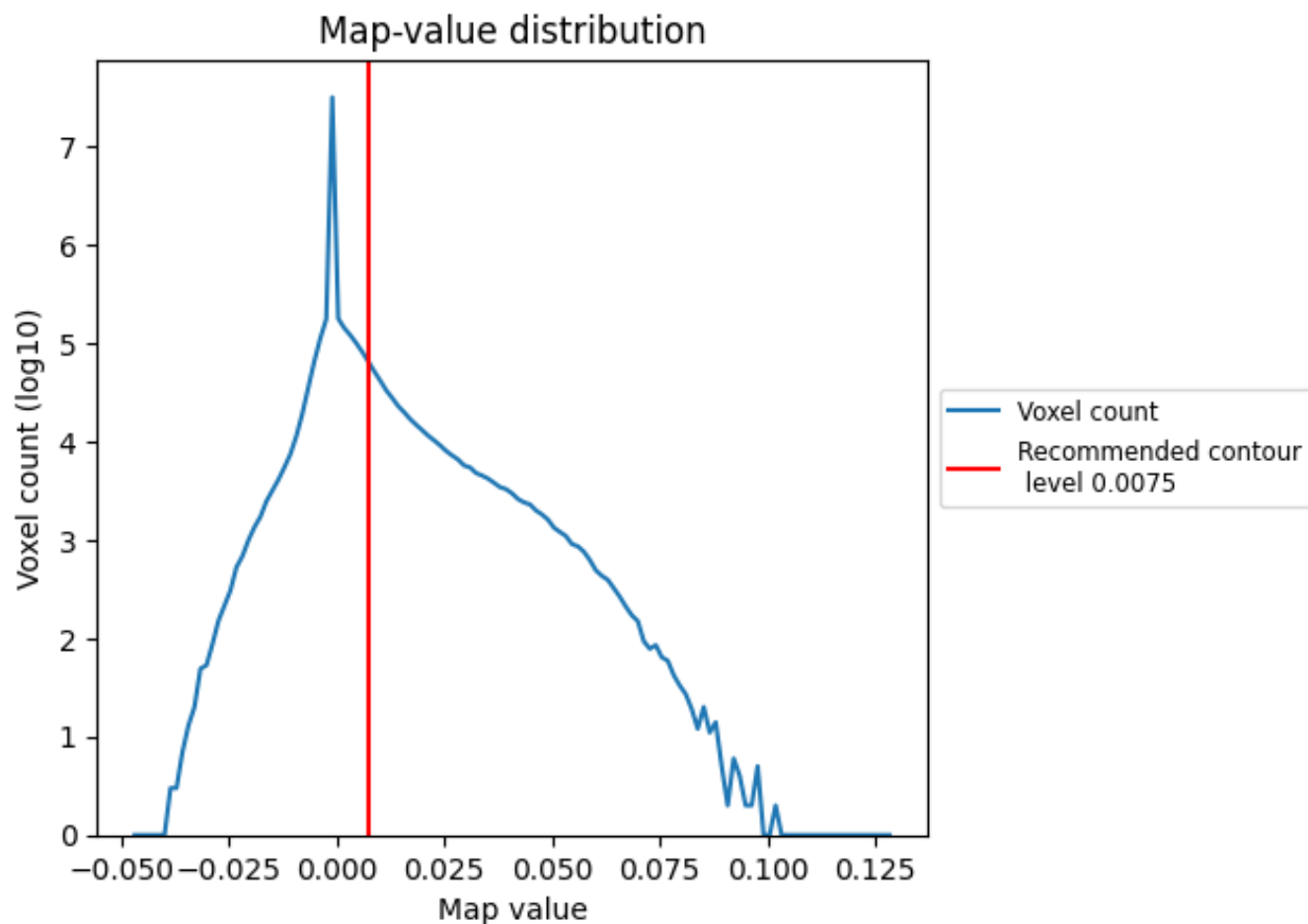
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

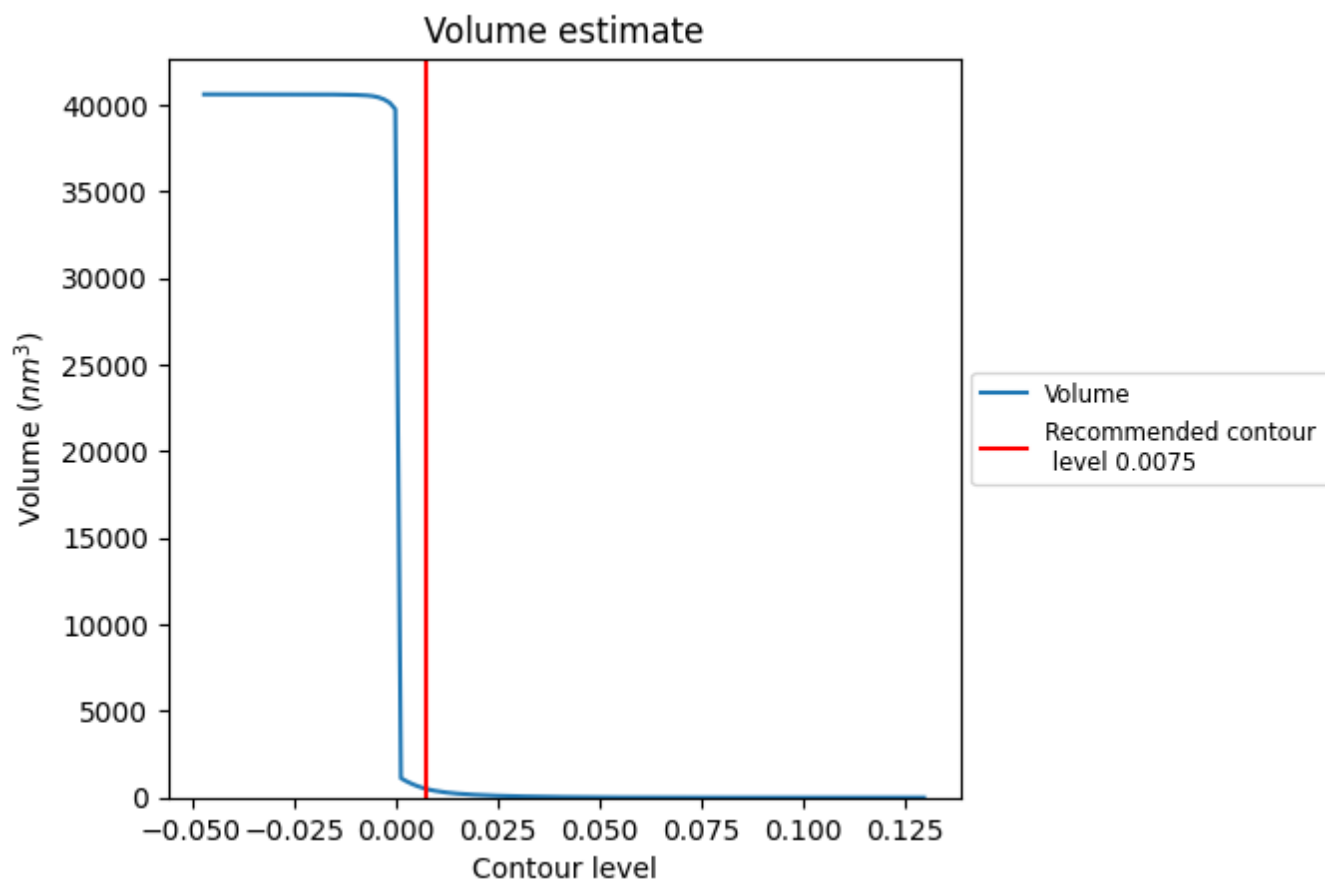
This section contains the results of statistical analysis of the map.

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.

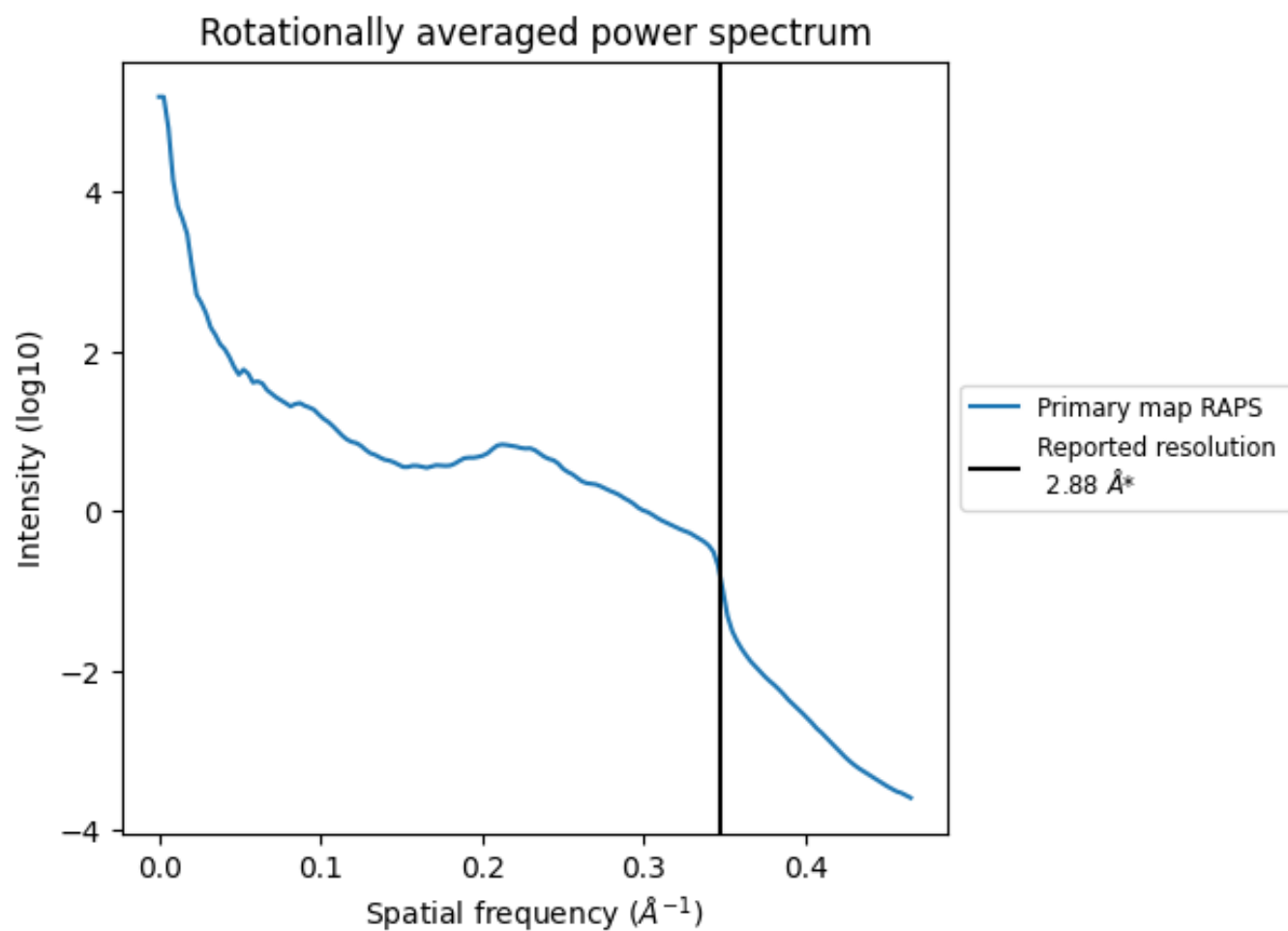
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 508 nm^3 ; this corresponds to an approximate mass of 459 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 ⓘ

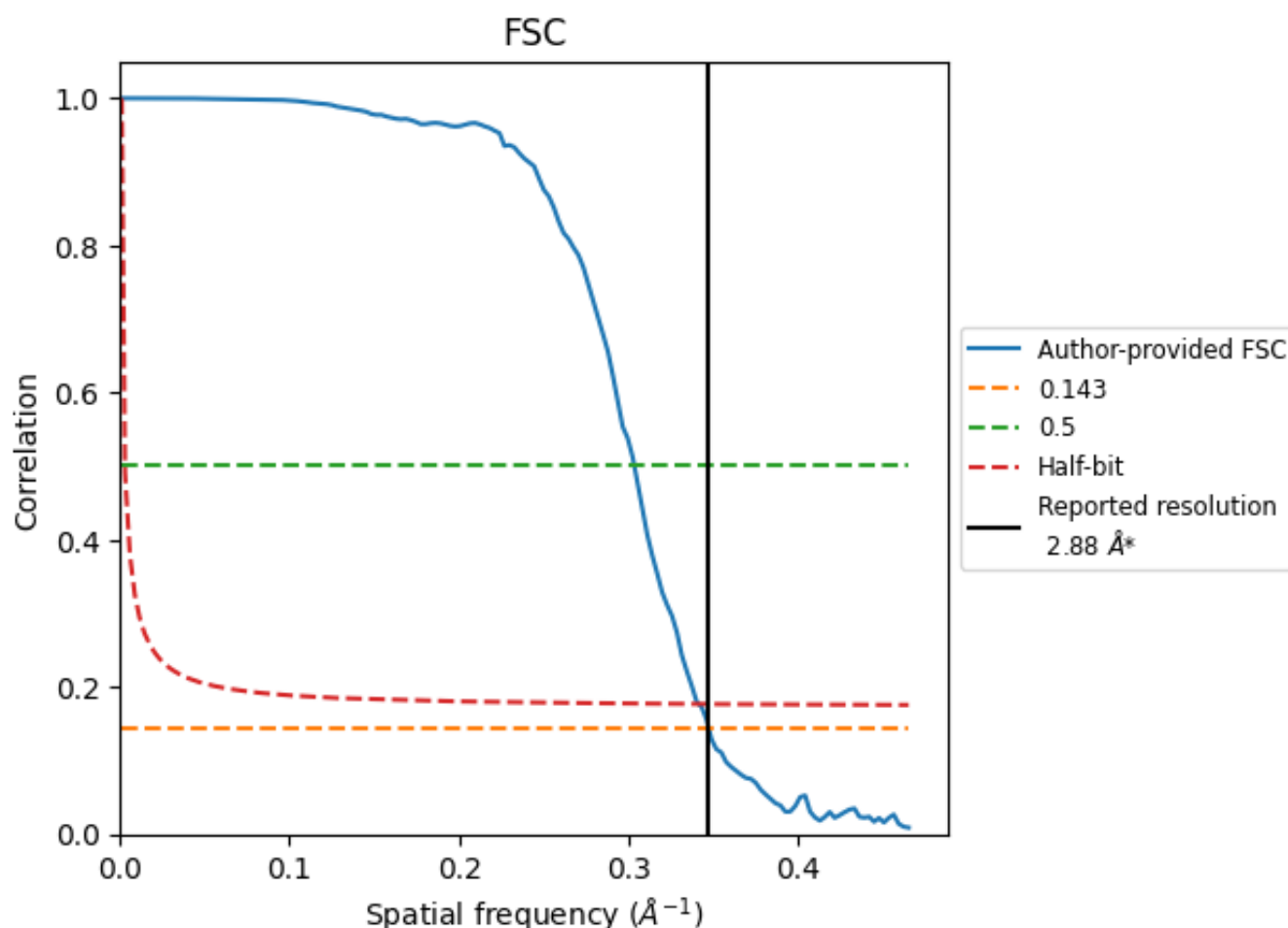


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

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 0.347 Å⁻¹

8.2 Resolution estimates [i](#)

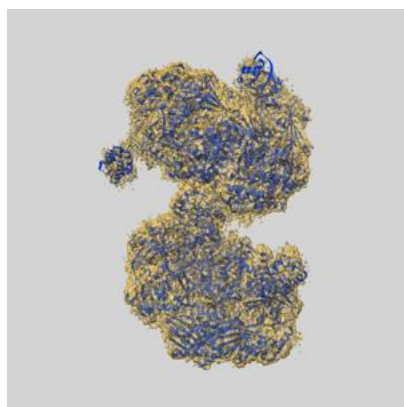
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.29	2.93
Unmasked-calculated*	-	-	-

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

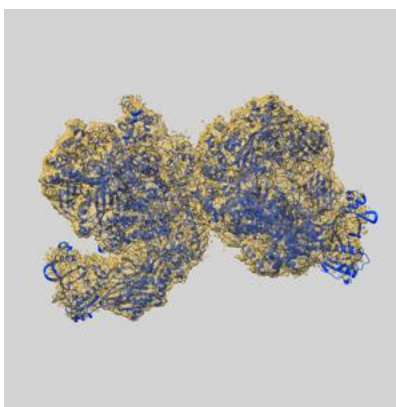
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31185 and PDB model 7ELM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

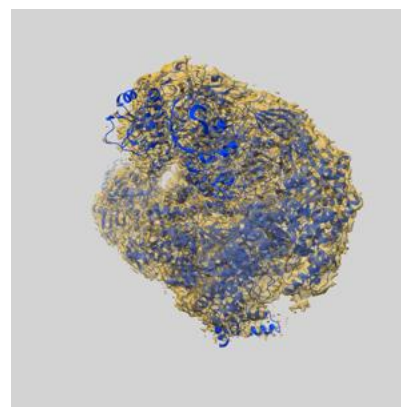
9.1 Map-model overlay [i](#)



X



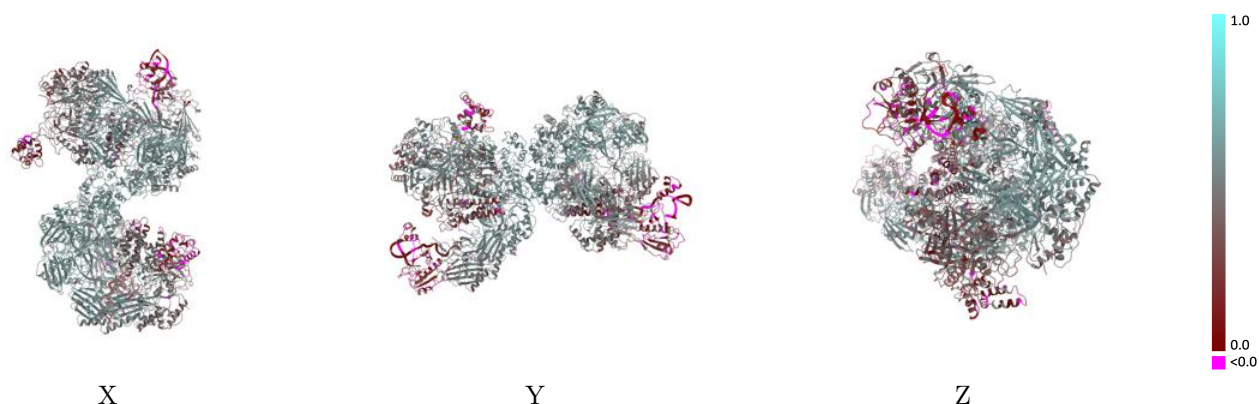
Y



Z

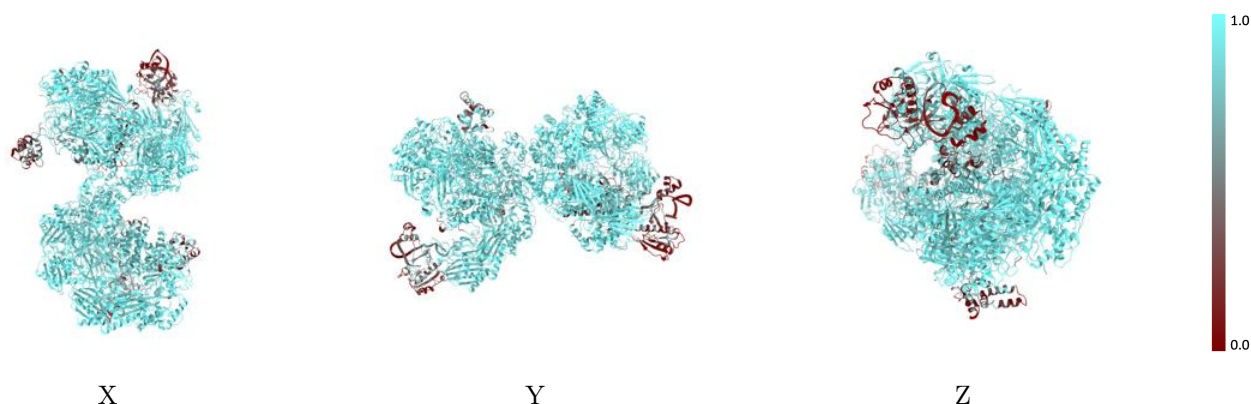
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



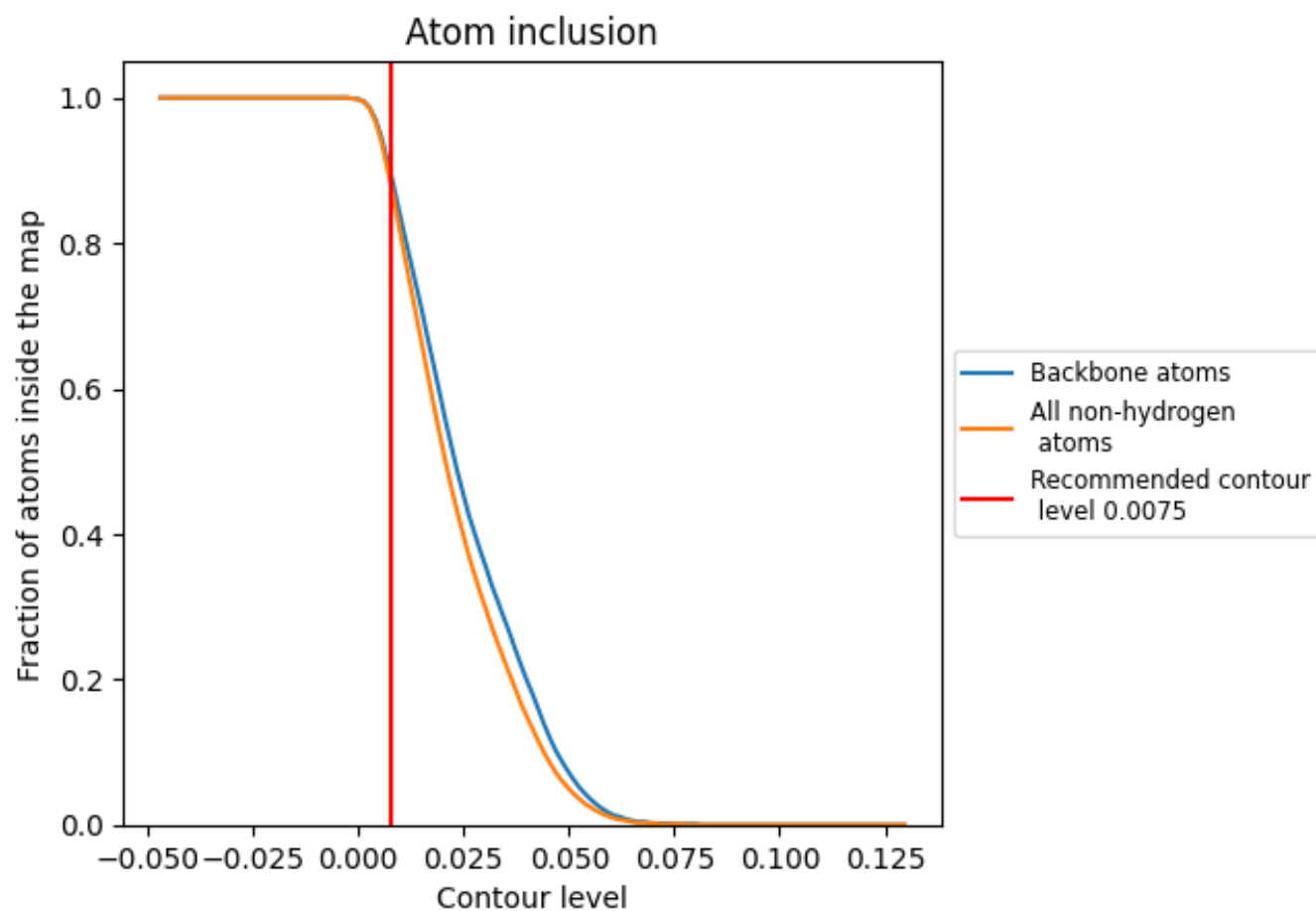
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).















































9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.4720
A	 0.6340	 0.3300
B	 0.8810	 0.3860
C	 0.9070	 0.4430
D	 0.9560	 0.5260
E	 0.9710	 0.5550
F	 0.9700	 0.5650
G	 0.9780	 0.5400
H	 0.9490	 0.4310
I	 0.2070	 0.1370
J	 0.7120	 0.3420
K	 0.8360	 0.3290
L	 0.9420	 0.4350
M	 0.9520	 0.4870
N	 0.9670	 0.5520
O	 0.9790	 0.5800
P	 0.9770	 0.5800
Q	 0.9800	 0.5670
R	 0.9690	 0.4980
S	 0.3950	 0.1570
T	 0.7950	 0.3930
U	 0.9740	 0.5700
V	 0.9740	 0.5800

