Full wwPDB EM Validation Report ⓘ

Nov 19, 2023 – 07:14 am GMT

PDB ID	:	8Q6O
EMDB ID	:	EMD-18191
Title	:	X. laevis CMG dimer bound to dimeric DONSON - without ATPase
Authors	:	Butryn, A.; Cvetkovic, M.A.; Costa, A.
Deposited on	:	2023-08-14
Resolution	:	3.14 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:

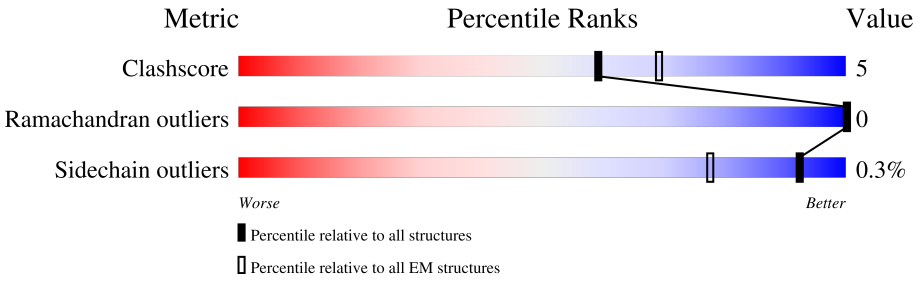
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	2	886	26% 5% 70%
1	A	886	26% 70%
2	3	807	29% 68%
2	B	807	30% 68%
3	4	863	24% 5% 70%
3	C	863	25% 5% 70%
4	5	735	31% 65%
4	D	735	31% 65%

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Mol	Chain	Length	Quality of chain
5	6	821	26% 5% 70%
5	E	821	26% 5% 70%
6	7	720	31% 7% 62%
6	F	720	30% 8% 62%
7	G	196	82% 18%
7	M	196	82% 18%
8	H	185	84% 10% 5%
8	N	185	84% 10% 5%
9	I	210	89% 8%
9	O	210	89% 8%
10	J	567	81% 11% 8%
10	P	567	80% 12% 8%
11	K	221	81% 10% 8%
11	Q	221	80% 12% 8%
12	L	579	55% 7% 38%
12	R	579	55% 7% 38%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 51983 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 DNA replication licensing factor mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total	C	N	O	S	0	0
			2141	1358	374	395	14		
1	2	267	Total	C	N	O	S	0	0
			2141	1358	374	395	14		

- Molecule 2 is a protein called Maternal DNA replication licensing factor mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	262	Total	C	N	O	S	0	0
			2066	1292	361	403	10		
2	3	262	Total	C	N	O	S	0	0
			2066	1292	361	403	10		

- Molecule 3 is a protein called DNA replication licensing factor mcm4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2112	1331	378	387	16		
3	4	258	Total	C	N	O	S	0	0
			2112	1331	378	387	16		

- Molecule 4 is a protein called DNA replication licensing factor mcm5-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	256	Total	C	N	O	S	0	0
			2059	1297	369	379	14		
4	5	256	Total	C	N	O	S	0	0
			2059	1297	369	379	14		

- Molecule 5 is a protein called Maternal DNA replication licensing factor mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	249	Total	C	N	O	S	0	0
			1997	1260	352	373	12		
5	6	249	Total	C	N	O	S	0	0
			1997	1260	352	373	12		

- Molecule 6 is a protein called DNA replication licensing factor mcm7-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	275	Total	C	N	O	S	0	0
			2227	1405	391	413	18		
6	7	275	Total	C	N	O	S	0	0
			2227	1405	391	413	18		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	196	Total	C	N	O	S	0	0
			1622	1023	290	297	12		
7	G	196	Total	C	N	O	S	0	0
			1623	1023	290	298	12		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	175	Total	C	N	O	S	0	0
			1418	907	237	267	7		
8	H	175	Total	C	N	O	S	0	0
			1418	907	237	267	7		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	202	Total	C	N	O	S	0	0
			1621	1026	284	304	7		
9	I	202	Total	C	N	O	S	0	0
			1621	1026	284	304	7		

- Molecule 10 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	523	Total	C	N	O	S	0	0
			4233	2700	701	799	33		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	523	Total	C	N	O	S	0	0
			4233	2700	701	799	33		

- Molecule 11 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	203	Total	C	N	O	S	0	0
			1655	1055	280	311	9		
11	K	203	Total	C	N	O	S	0	0
			1655	1055	280	311	9		

- Molecule 12 is a protein called Protein downstream neighbor of son homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	361	Total	C	N	O	S	0	0
			2835	1818	488	513	16		
12	L	361	Total	C	N	O	S	0	0
			2835	1818	488	513	16		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

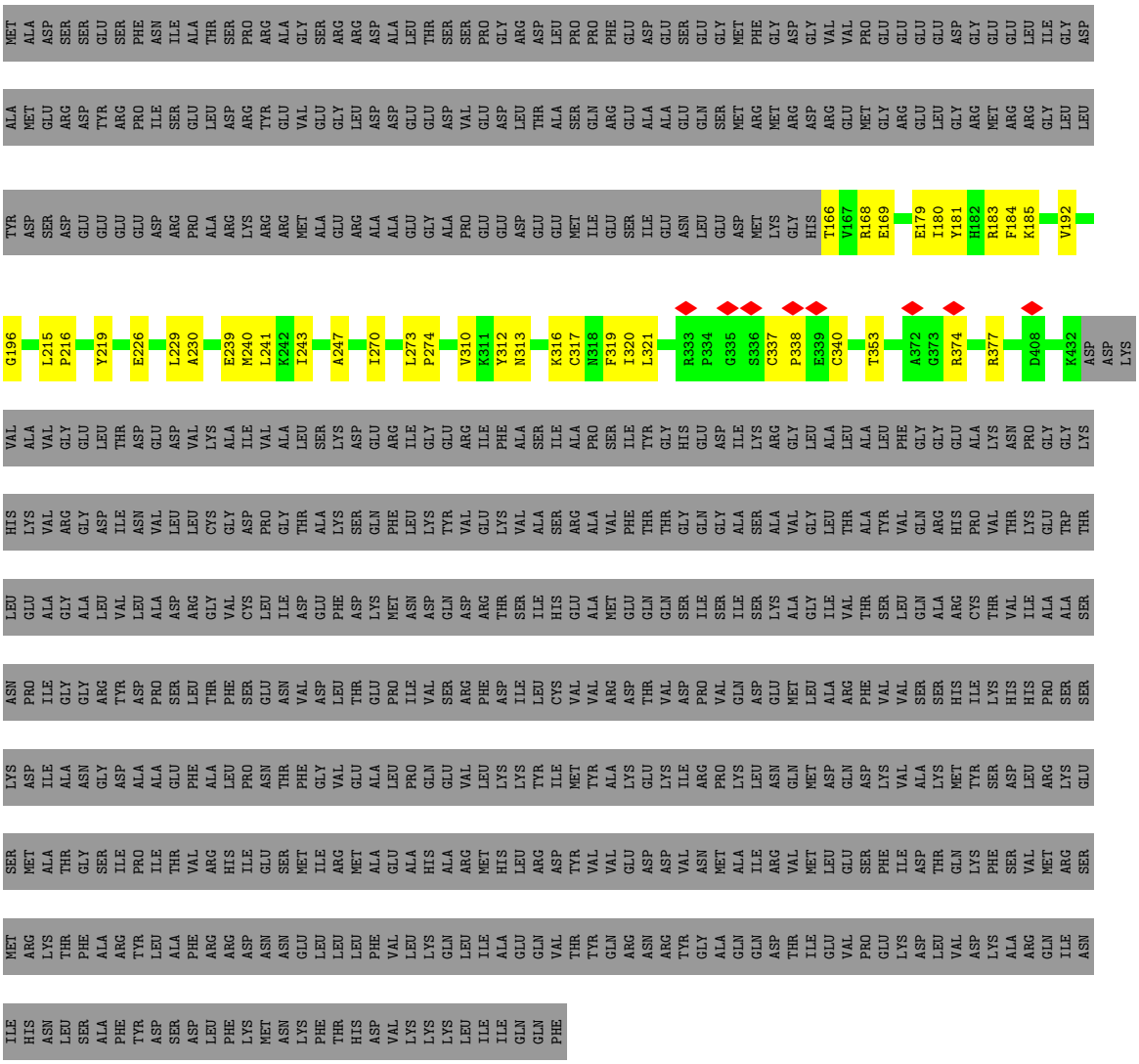
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Zn	0
			1	1	
13	C	1	Total	Zn	0
			1	1	
13	D	1	Total	Zn	0
			1	1	
13	E	1	Total	Zn	0
			1	1	
13	F	1	Total	Zn	0
			1	1	
13	2	1	Total	Zn	0
			1	1	
13	4	1	Total	Zn	0
			1	1	
13	5	1	Total	Zn	0
			1	1	
13	6	1	Total	Zn	0
			1	1	
13	7	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

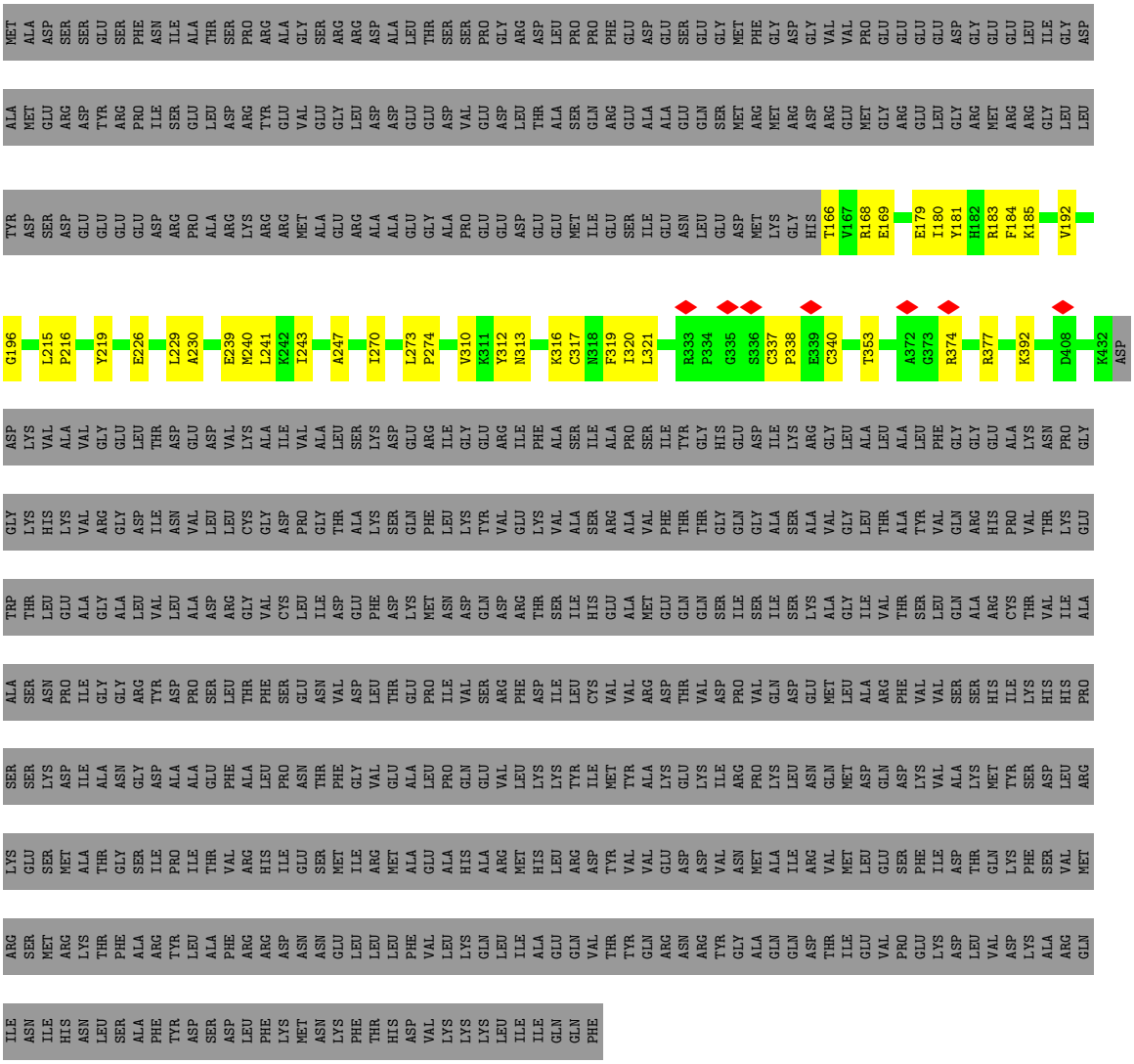
• Molecule 1: DNA replication licensing factor mcm2

Chain A:



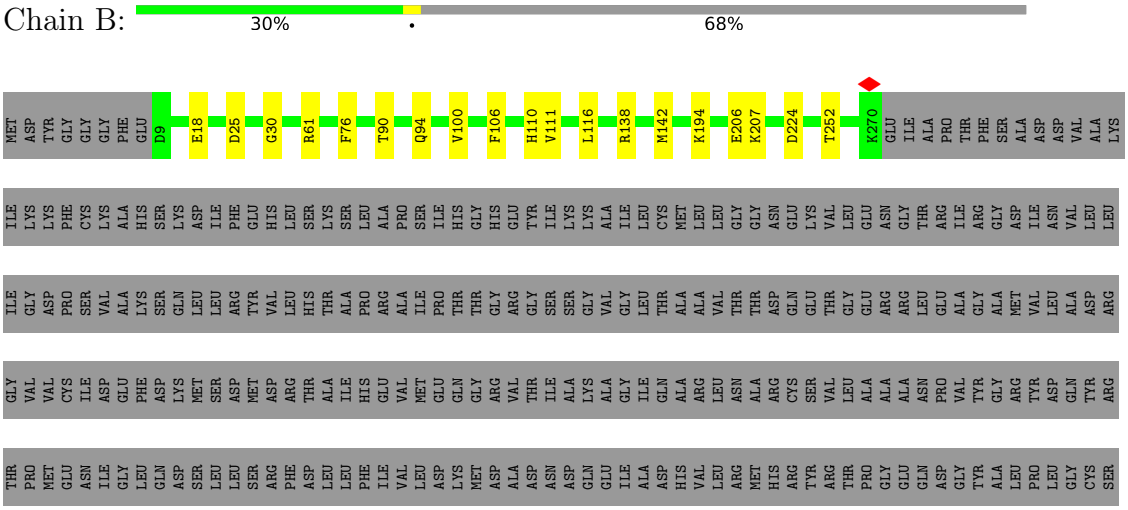
• Molecule 1: DNA replication licensing factor mcm2

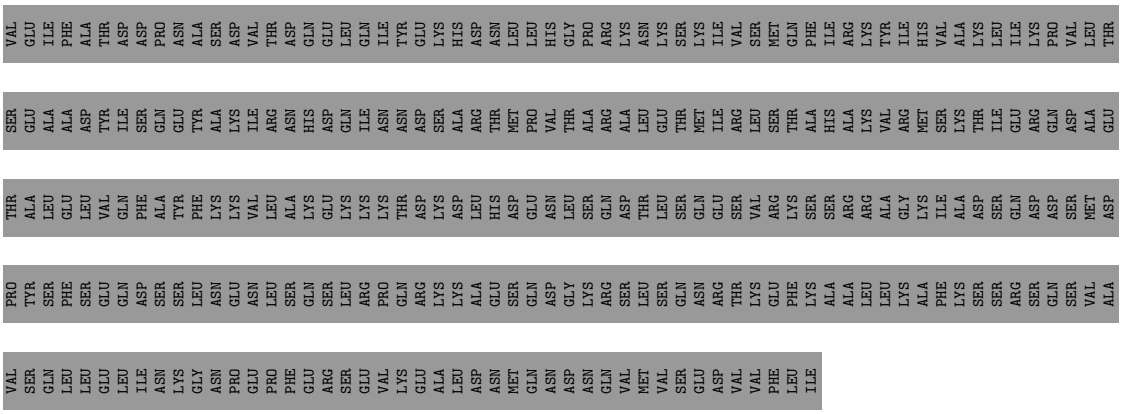
Chain 2:



• Molecule 2: Maternal DNA replication licensing factor mcm3

Chain B:



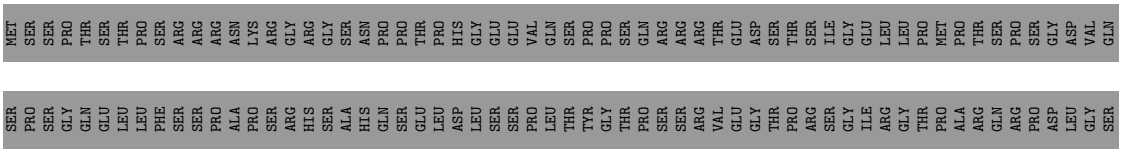


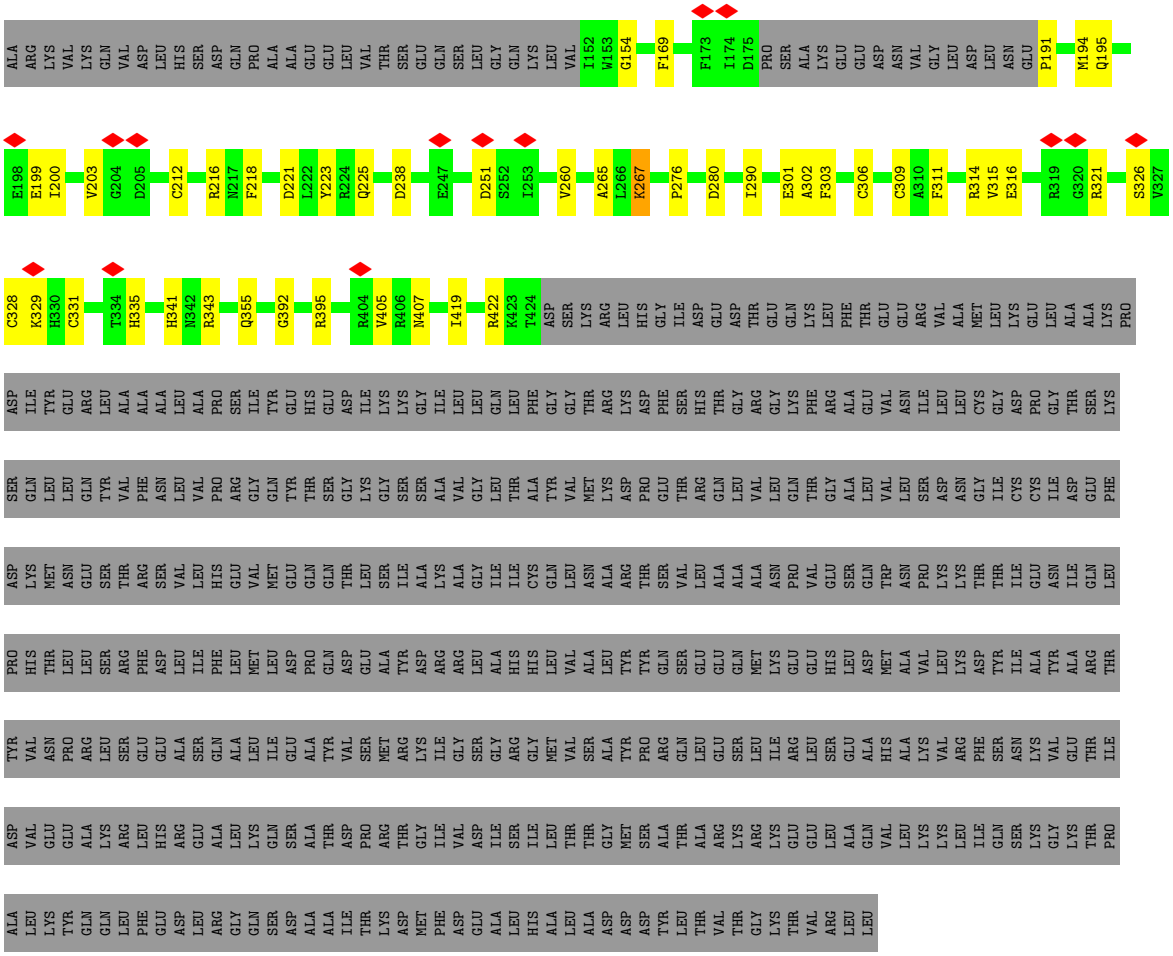
• Molecule 2: Maternal DNA replication licensing factor mcm3

Chain 3:

• Molecule 3: DNA replication licensing factor mcm4-B

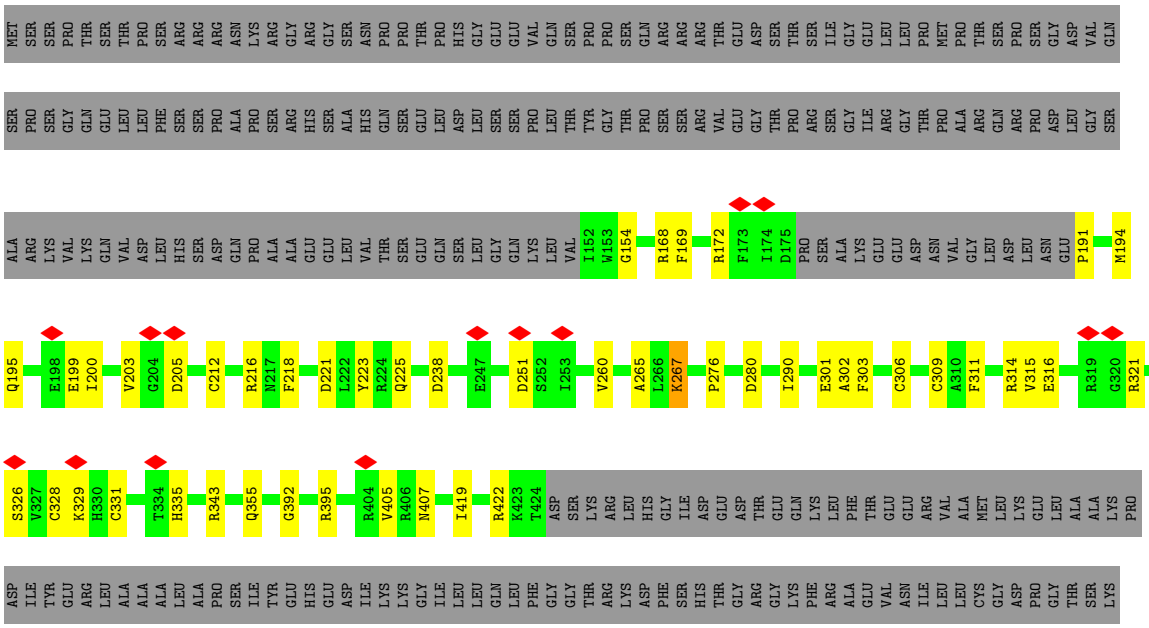
Chain C:

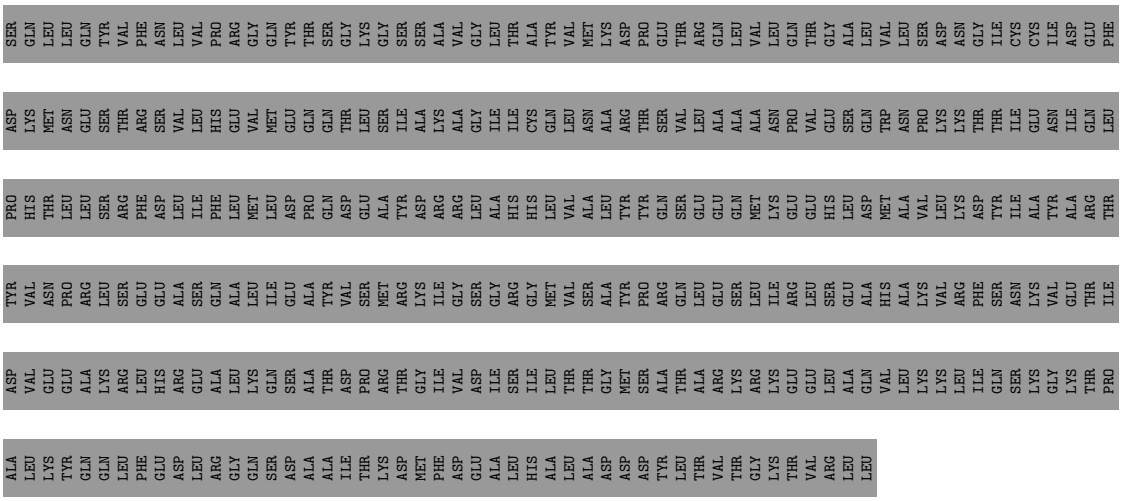




• Molecule 3: DNA replication licensing factor mcm4-B

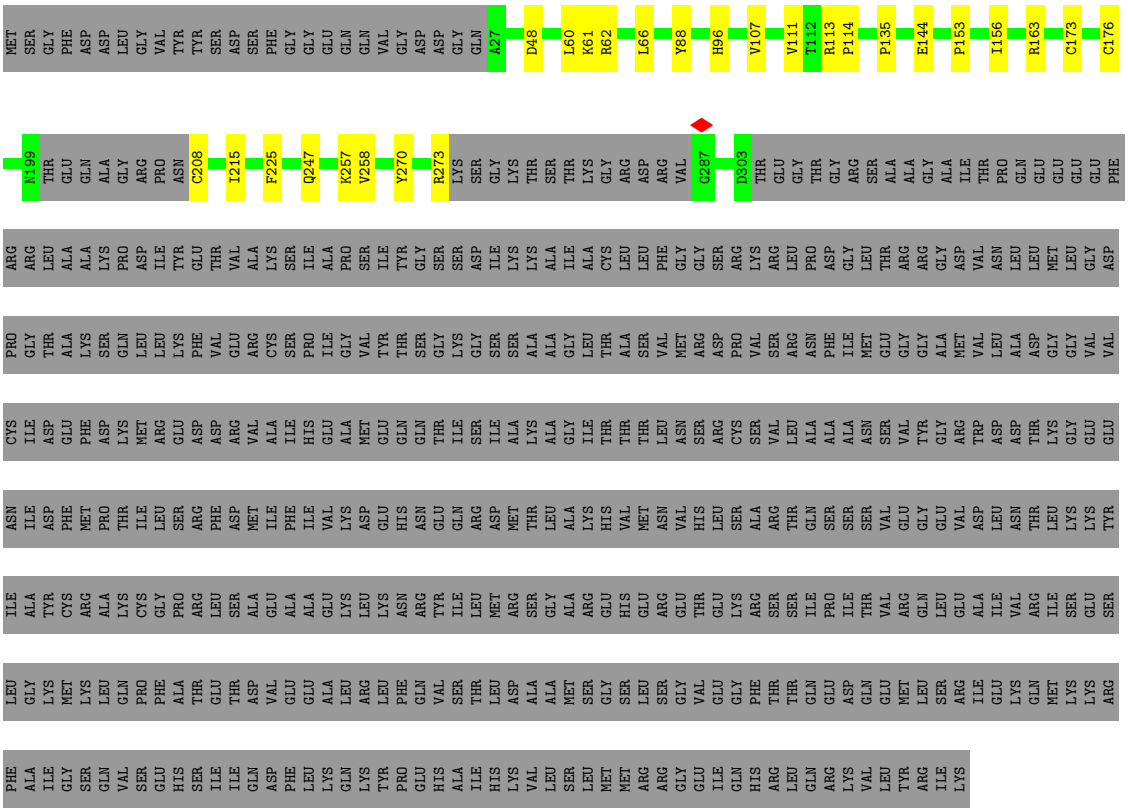
Chain 4:





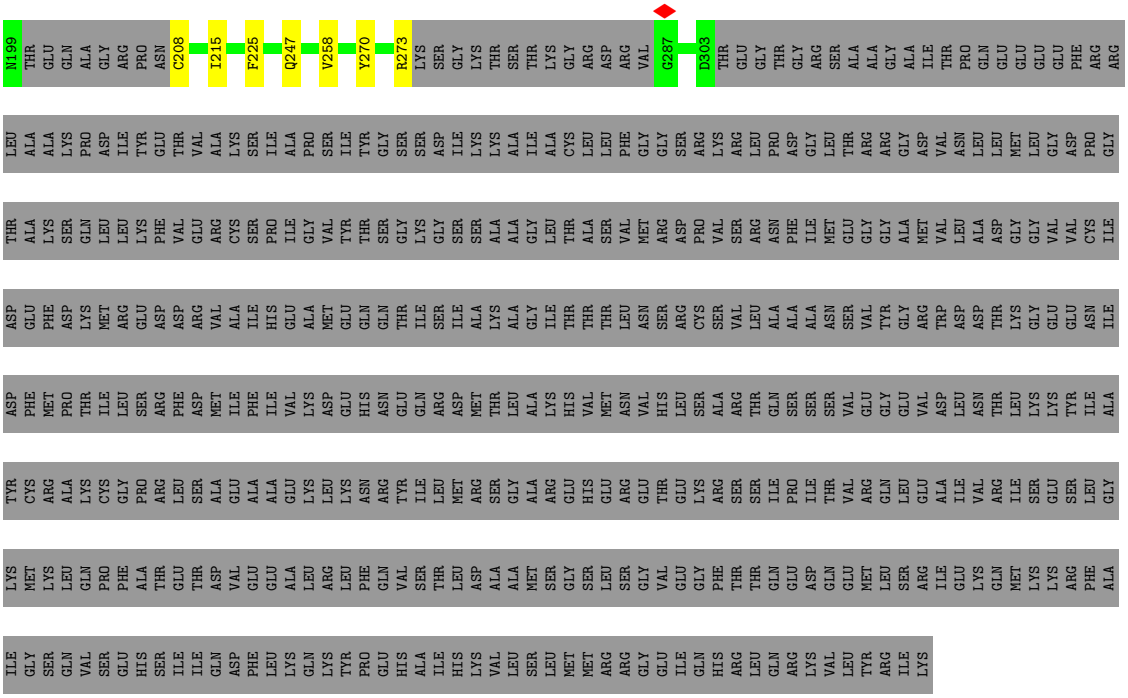
• Molecule 4: DNA replication licensing factor mcm5-A

Chain D:



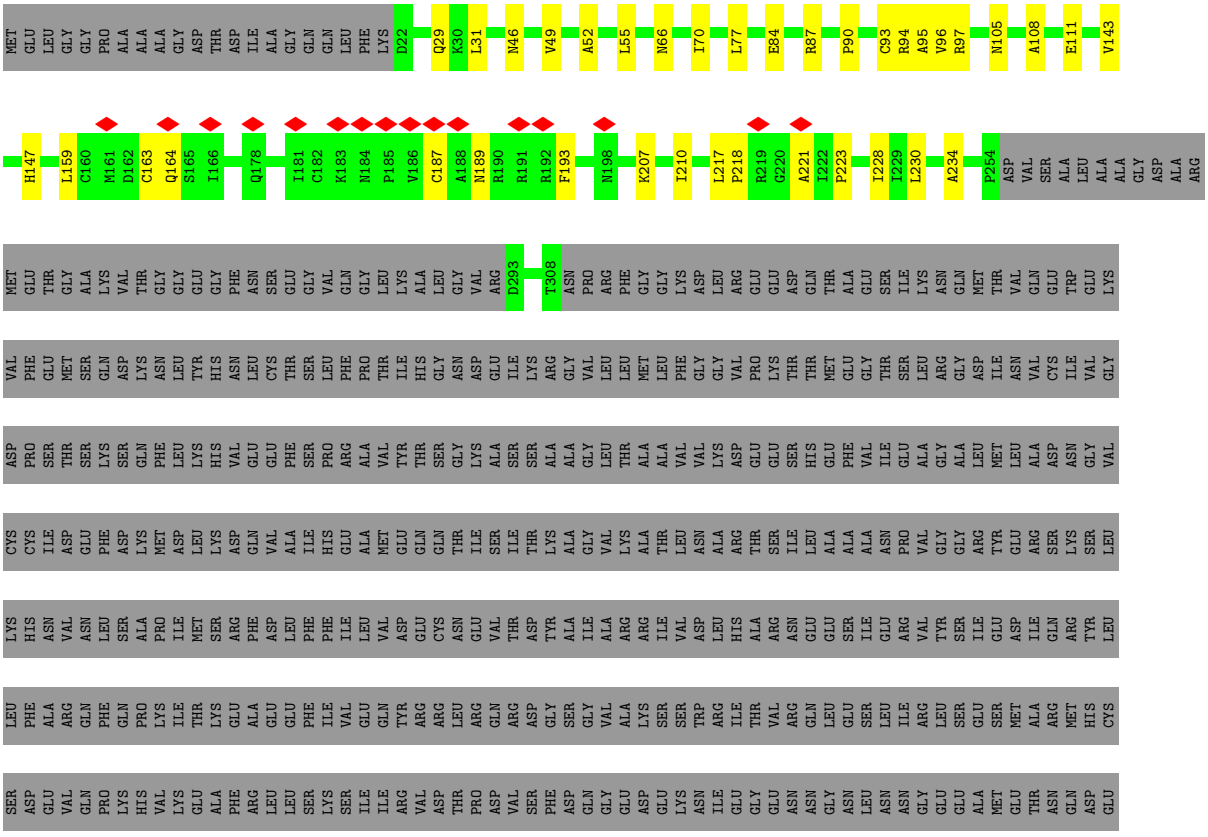
• Molecule 4: DNA replication licensing factor mcm5-A

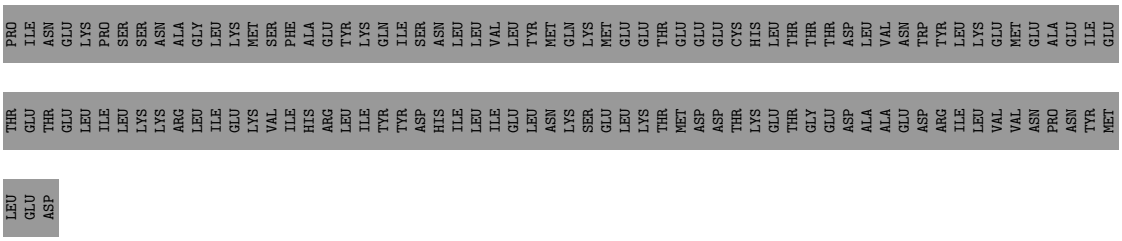
Chain 5:



• Molecule 5: Maternal DNA replication licensing factor mcm6

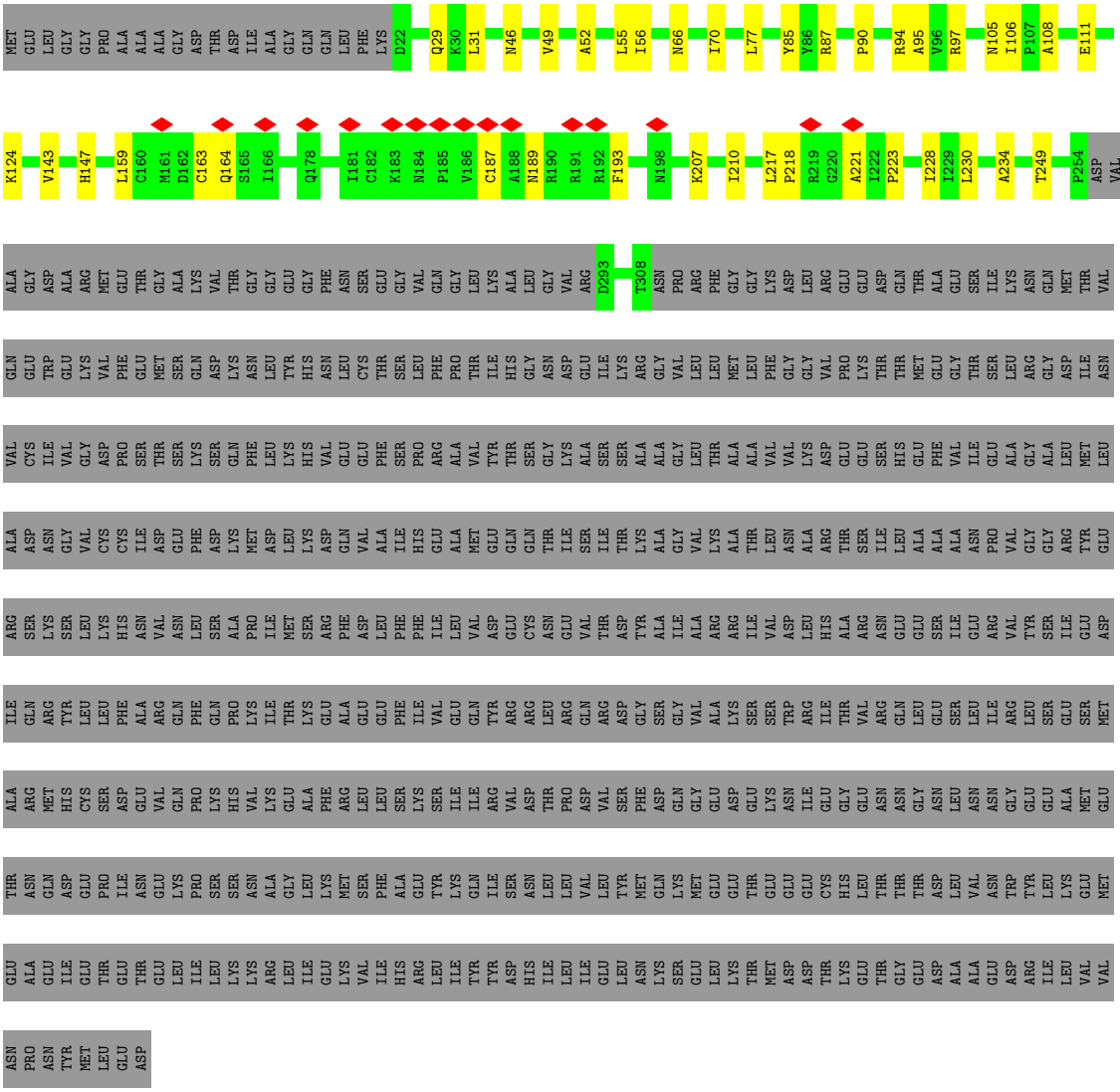
Chain E:





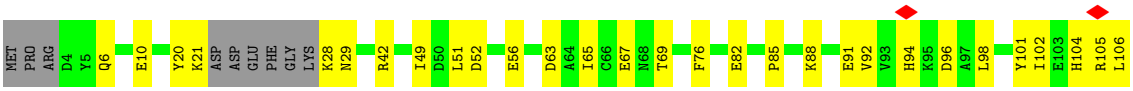
• Molecule 5: Maternal DNA replication licensing factor mcm6

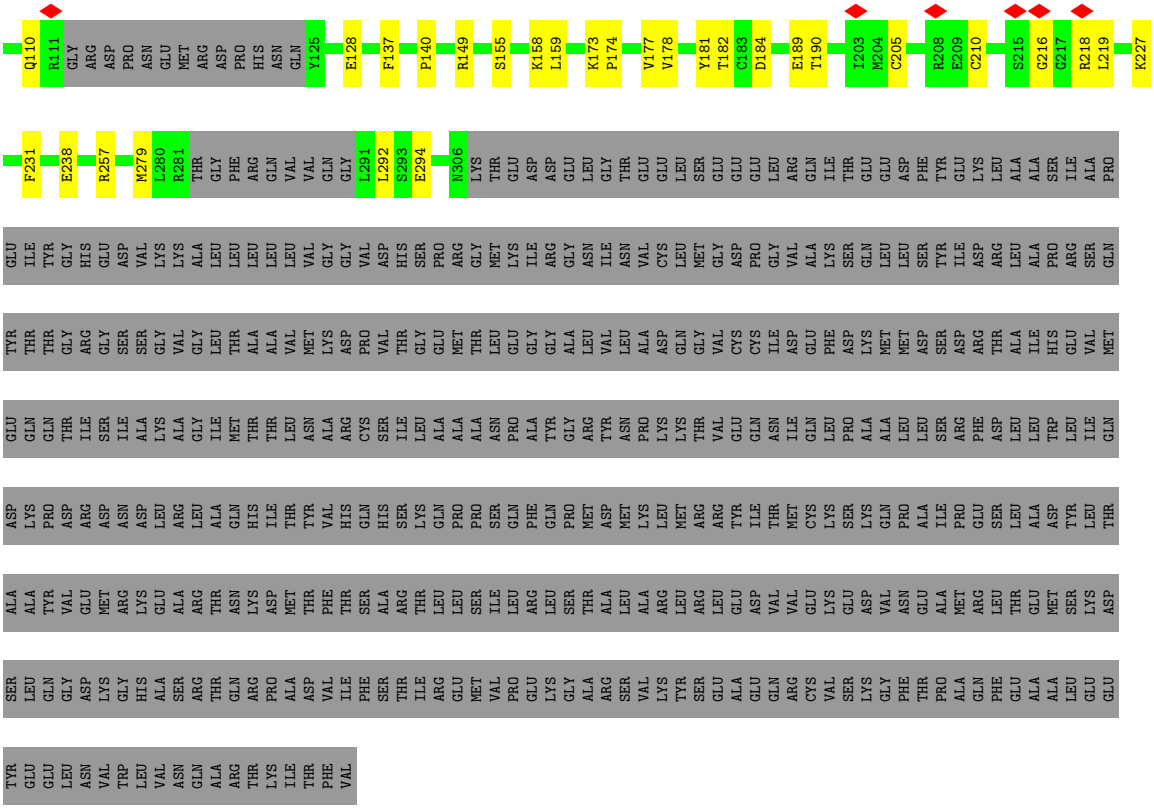
Chain 6:



• Molecule 6: DNA replication licensing factor mcm7-B

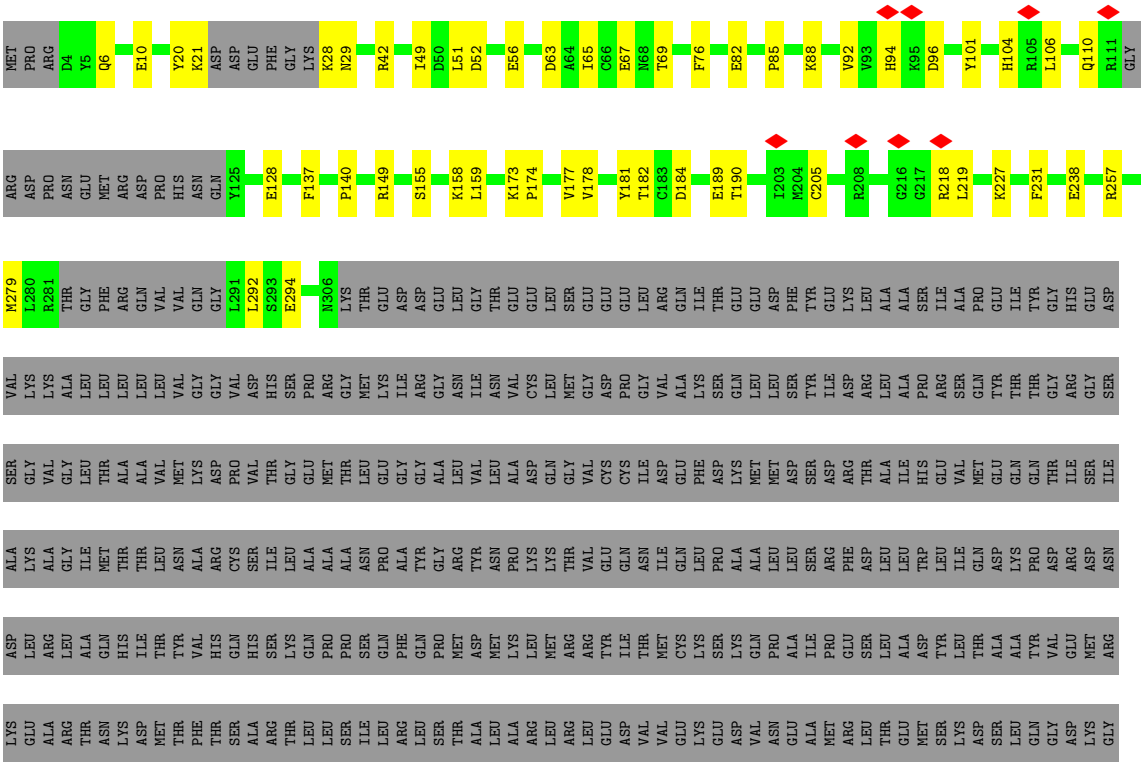
Chain F:

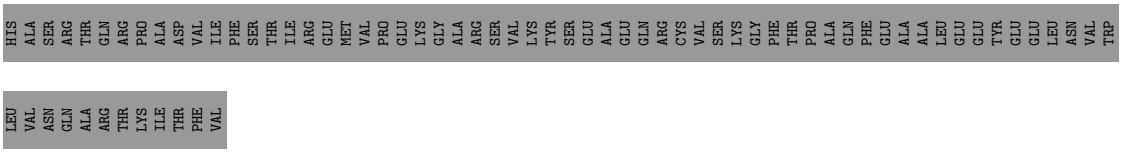




• Molecule 6: DNA replication licensing factor mcm7-B

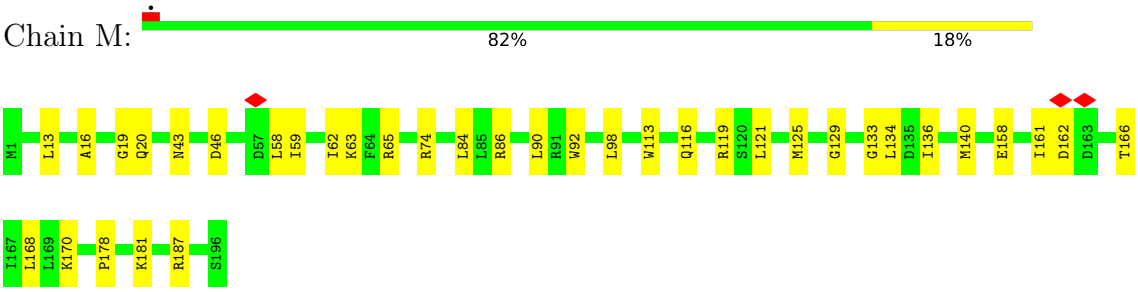
Chain 7:





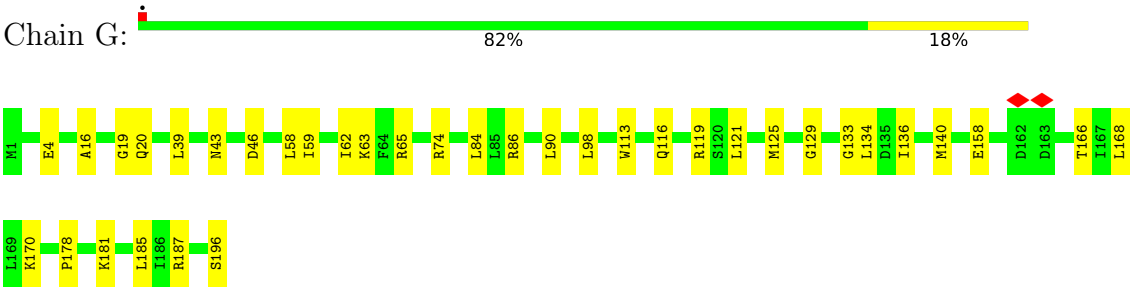
• Molecule 7: DNA replication complex GINS protein PSF1

Chain M:



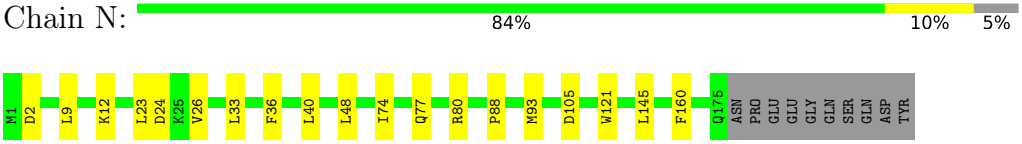
• Molecule 7: DNA replication complex GINS protein PSF1

Chain G:



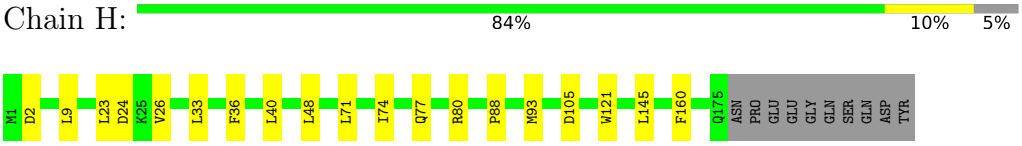
• Molecule 8: DNA replication complex GINS protein PSF2

Chain N:



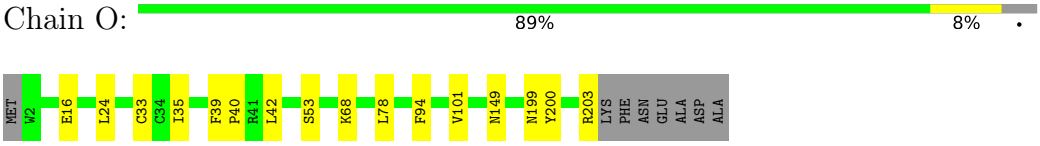
• Molecule 8: DNA replication complex GINS protein PSF2

Chain H:



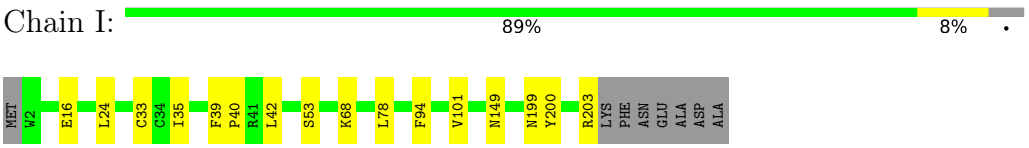
• Molecule 9: DNA replication complex GINS protein PSF3

Chain O:



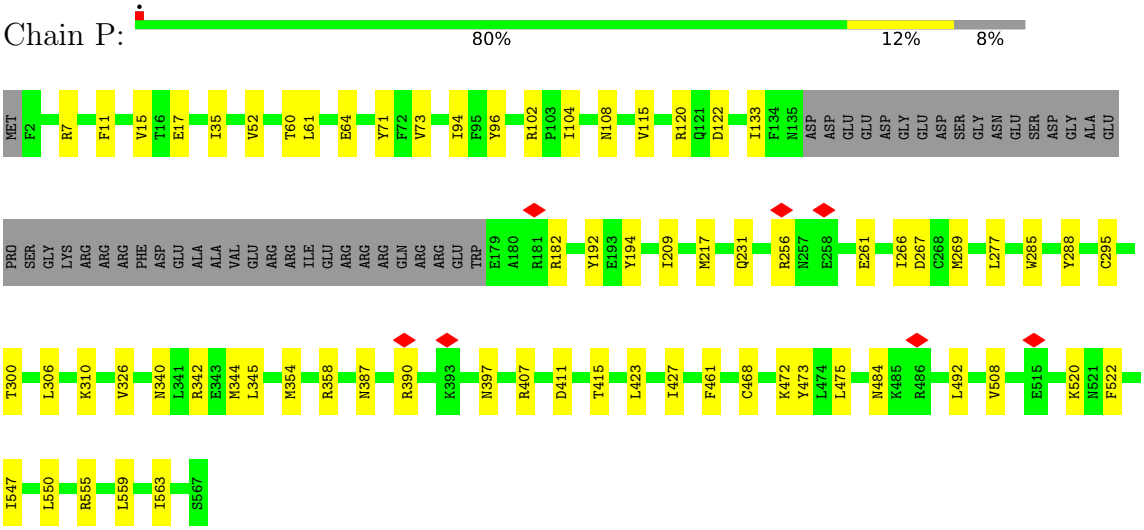
• Molecule 9: DNA replication complex GINS protein PSF3

Chain I:



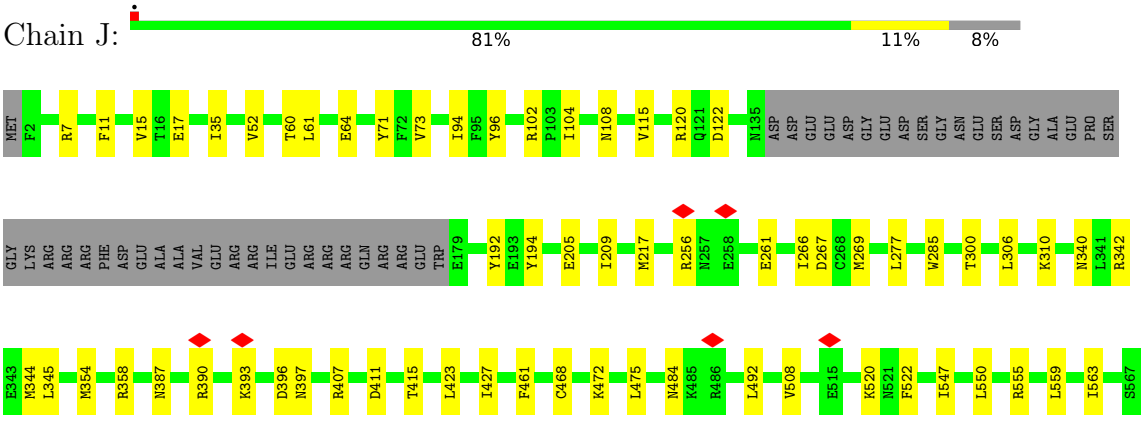
• Molecule 10: Cell division control protein 45 homolog

Chain P:



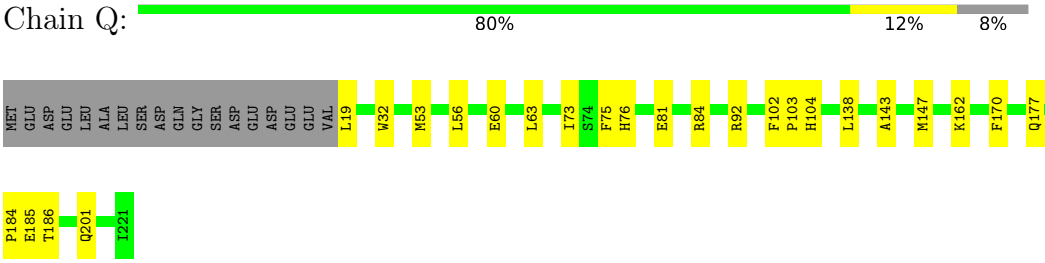
• Molecule 10: Cell division control protein 45 homolog

Chain J:



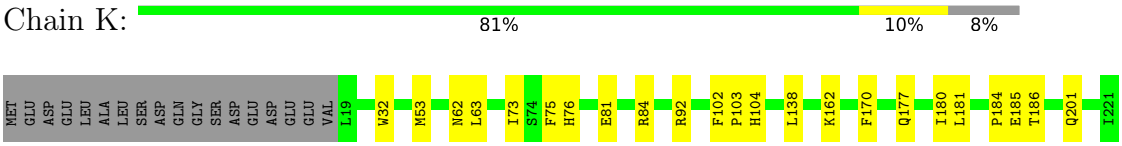
• Molecule 11: DNA replication complex GINS protein SLD5

Chain Q:



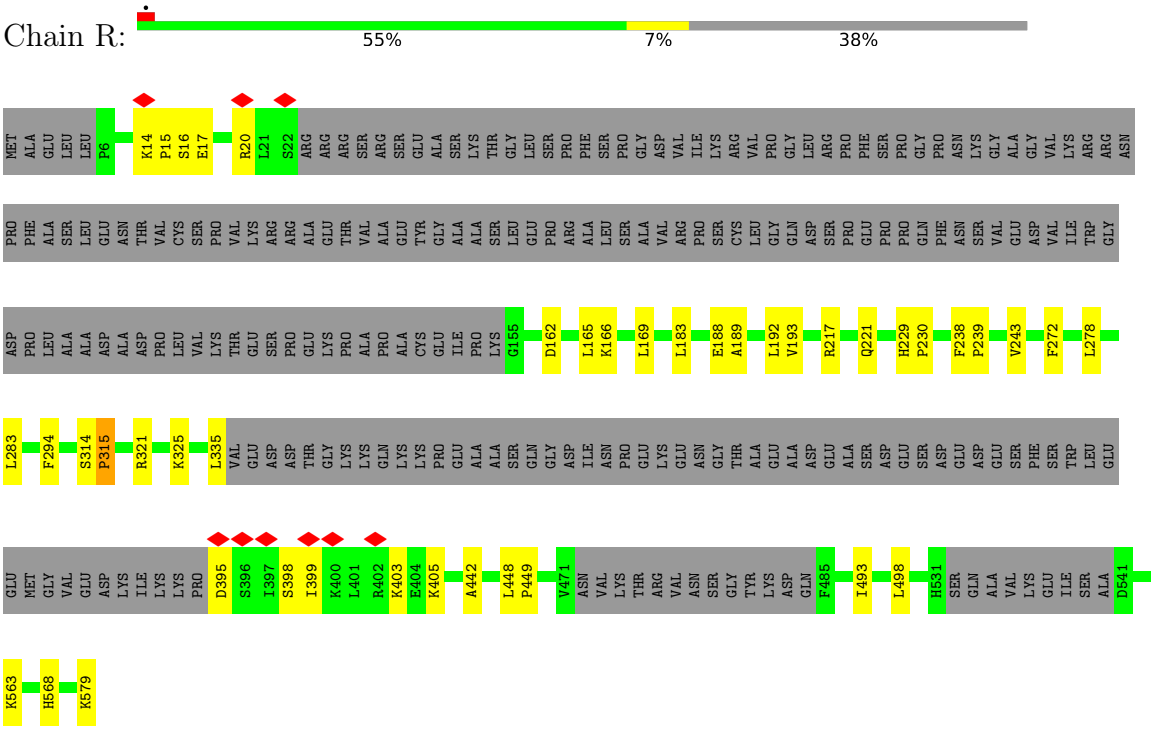
• Molecule 11: DNA replication complex GINS protein SLD5

Chain K:



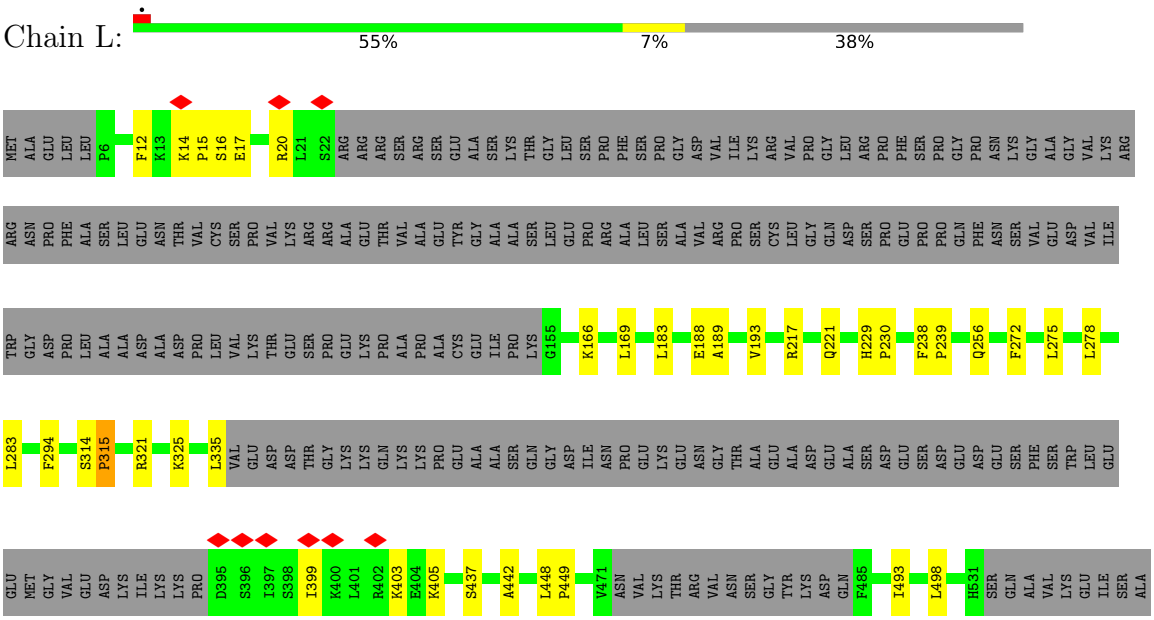
• Molecule 12: Protein downstream neighbor of son homolog

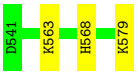
Chain R:



• Molecule 12: Protein downstream neighbor of son homolog

Chain L:




D541
K563
H568
K579

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	33.0	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.750	Depositor
Minimum map value	-1.490	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

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	2	0.25	0/2188	0.48	0/2963
1	A	0.25	0/2188	0.48	0/2963
2	3	0.25	0/2101	0.49	0/2834
2	B	0.25	0/2101	0.49	0/2834
3	4	0.24	0/2157	0.48	0/2921
3	C	0.24	0/2157	0.48	0/2921
4	5	0.27	0/2096	0.51	0/2825
4	D	0.26	0/2096	0.51	0/2825
5	6	0.24	0/2033	0.50	0/2747
5	E	0.24	0/2033	0.50	0/2747
6	7	0.24	0/2266	0.48	0/3053
6	F	0.24	0/2266	0.49	0/3053
7	G	0.24	0/1653	0.48	0/2221
7	M	0.24	0/1652	0.48	0/2221
8	H	0.25	0/1448	0.45	0/1964
8	N	0.25	0/1448	0.45	0/1964
9	I	0.25	0/1658	0.47	0/2236
9	O	0.25	0/1658	0.47	0/2236
10	J	0.24	0/4314	0.44	0/5823
10	P	0.24	0/4314	0.44	0/5823
11	K	0.25	0/1690	0.44	0/2280
11	Q	0.25	0/1690	0.44	0/2280
12	L	0.24	0/2904	0.45	0/3938
12	R	0.24	0/2904	0.45	0/3938
All	All	0.25	0/53015	0.47	0/71610

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2141	0	2124	22	0
1	A	2141	0	2124	22	0
2	3	2066	0	2059	18	0
2	B	2066	0	2059	13	0
3	4	2112	0	2090	31	0
3	C	2112	0	2090	30	0
4	5	2059	0	2074	15	0
4	D	2059	0	2074	15	0
5	6	1997	0	1987	22	0
5	E	1997	0	1987	21	0
6	7	2227	0	2232	33	0
6	F	2227	0	2232	38	0
7	G	1623	0	1623	27	0
7	M	1622	0	1623	25	0
8	H	1418	0	1433	15	0
8	N	1418	0	1433	14	0
9	I	1621	0	1589	10	0
9	O	1621	0	1589	11	0
10	J	4233	0	4211	37	0
10	P	4233	0	4211	38	0
11	K	1655	0	1669	19	0
11	Q	1655	0	1669	20	0
12	L	2835	0	2861	27	0
12	R	2835	0	2861	28	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
All	All	51983	0	51904	497	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 5.

All (497) 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)
11:Q:63:LEU:HD11	11:Q:73:ILE:HA	1.65	0.79
11:K:63:LEU:HD11	11:K:73:ILE:HA	1.66	0.77
3:4:306:CYS:HB3	3:4:311:PHE:H	1.52	0.75
3:C:306:CYS:HB3	3:C:311:PHE:H	1.52	0.74
3:C:276:PRO:HB3	6:F:174:PRO:HB3	1.72	0.72
3:4:276:PRO:HB3	6:7:174:PRO:HB3	1.72	0.72
6:F:205:CYS:HB2	6:F:219:LEU:HB3	1.77	0.67
6:F:21:LYS:HB3	6:F:29:ASN:HB3	1.77	0.66
6:7:21:LYS:HB3	6:7:29:ASN:HB3	1.77	0.66
6:7:205:CYS:HB2	6:7:219:LEU:HB3	1.77	0.66
5:6:56:ILE:HA	5:6:106:ILE:HD11	1.78	0.64
10:P:288:TYR:HB2	10:P:326:VAL:HG12	1.80	0.62
2:B:18:GLU:HG2	12:R:442:ALA:HB1	1.81	0.62
10:J:475:LEU:HD13	10:J:492:LEU:HB2	1.81	0.62
1:2:310:VAL:HA	1:2:353:THR:HG23	1.82	0.62
2:3:18:GLU:HG2	12:L:442:ALA:HB1	1.83	0.61
4:5:144:GLU:OE1	4:5:144:GLU:N	2.33	0.61
6:7:51:LEU:HD12	6:7:140:PRO:HD3	1.84	0.60
12:L:314:SER:HB3	12:L:315:PRO:HD3	1.84	0.60
5:6:163:CYS:HB3	5:6:187:CYS:SG	2.42	0.60
6:F:51:LEU:HD12	6:F:140:PRO:HD3	1.83	0.59
5:E:163:CYS:HB3	5:E:187:CYS:SG	2.42	0.59
10:J:407:ARG:NH2	4:5:48:ASP:OD1	2.36	0.59
12:R:239:PRO:HB2	12:R:243:VAL:HG21	1.83	0.58
12:R:314:SER:HB3	12:R:315:PRO:HD3	1.84	0.58
4:D:48:ASP:OD1	10:P:407:ARG:NH2	2.36	0.58
7:G:19:GLY:O	7:G:86:ARG:NH1	2.37	0.58
7:G:196:SER:O	4:5:49:ARG:NH1	2.36	0.58
7:M:19:GLY:O	7:M:86:ARG:NH1	2.36	0.58
4:D:144:GLU:N	4:D:144:GLU:OE1	2.33	0.57
1:A:316:LYS:HG2	1:A:340:CYS:HB2	1.86	0.57
2:B:206:GLU:HG3	2:B:207:LYS:HG3	1.86	0.57
6:7:92:VAL:HB	6:7:94:HIS:HD2	1.70	0.56
10:J:300:THR:HG21	10:J:354:MET:HG3	1.88	0.56
5:6:210:ILE:HG12	5:6:228:ILE:HD11	1.87	0.56
12:R:283:LEU:HD13	12:L:193:VAL:HG21	1.86	0.56
12:R:448:LEU:HD12	12:R:449:PRO:HD2	1.86	0.56
2:3:206:GLU:HG3	2:3:207:LYS:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:193:VAL:HG21	12:L:283:LEU:HD13	1.86	0.56
11:K:177:GLN:HB2	11:K:180:ILE:HD11	1.87	0.56
6:F:92:VAL:HB	6:F:94:HIS:HD2	1.70	0.56
10:P:300:THR:HG21	10:P:354:MET:HG3	1.88	0.56
1:A:310:VAL:HA	1:A:353:THR:HG23	1.88	0.55
1:2:316:LYS:HG2	1:2:340:CYS:HB2	1.87	0.55
6:7:42:ARG:NH1	6:7:96:ASP:OD2	2.39	0.55
1:A:241:LEU:HD21	1:A:270:ILE:HD11	1.89	0.55
9:I:16:GLU:OE2	9:I:68:LYS:NZ	2.40	0.55
1:2:241:LEU:HD21	1:2:270:ILE:HD11	1.88	0.55
5:E:210:ILE:HG12	5:E:228:ILE:HD11	1.88	0.55
11:Q:177:GLN:HB2	11:Q:180:ILE:HD11	1.88	0.55
6:7:69:THR:HG21	6:7:159:LEU:HB2	1.89	0.55
6:F:42:ARG:NH1	6:F:96:ASP:OD2	2.39	0.55
9:O:16:GLU:OE2	9:O:68:LYS:NZ	2.40	0.54
10:P:120:ARG:HG2	10:P:122:ASP:H	1.71	0.54
10:J:120:ARG:HG2	10:J:122:ASP:H	1.71	0.54
12:R:183:LEU:HA	12:R:217:ARG:HH21	1.73	0.54
1:2:166:THR:HB	1:2:169:GLU:HG3	1.90	0.54
12:L:294:PHE:HB2	12:L:315:PRO:HD2	1.90	0.54
12:L:183:LEU:HA	12:L:217:ARG:HH21	1.73	0.54
5:E:143:VAL:HA	5:E:210:ILE:HG22	1.90	0.53
3:4:216:ARG:HG2	3:4:223:TYR:CG	2.43	0.53
6:F:184:ASP:N	6:F:184:ASP:OD1	2.40	0.53
3:4:154:GLY:HA3	6:7:101:TYR:HD1	1.74	0.53
5:E:230:LEU:HB3	5:E:234:ALA:O	2.09	0.53
5:6:230:LEU:HB3	5:6:234:ALA:O	2.09	0.53
10:P:194:TYR:HB3	10:P:520:LYS:HG2	1.89	0.53
7:G:129:GLY:HA3	11:K:53:MET:HE2	1.90	0.53
5:6:143:VAL:HA	5:6:210:ILE:HG22	1.90	0.53
6:F:69:THR:HG21	6:F:159:LEU:HB2	1.90	0.53
1:A:166:THR:HB	1:A:169:GLU:HG3	1.90	0.52
4:5:163:ARG:HB2	4:5:225:PHE:HD2	1.74	0.52
3:C:154:GLY:HA3	6:F:101:TYR:HD1	1.74	0.52
12:R:294:PHE:HB2	12:R:315:PRO:HD2	1.90	0.52
3:C:216:ARG:HG2	3:C:223:TYR:CG	2.43	0.52
6:F:181:TYR:HB2	6:F:190:THR:HB	1.90	0.52
10:P:427:ILE:HG22	10:P:461:PHE:HE1	1.74	0.52
3:C:392:GLY:HA2	3:C:419:ILE:HG12	1.92	0.52
10:J:550:LEU:HD21	10:J:555:ARG:HA	1.92	0.52
11:Q:63:LEU:HD13	11:Q:76:HIS:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:LEU:HB3	7:G:98:LEU:HD21	1.92	0.52
7:M:46:ASP:HB3	7:M:58:LEU:HD13	1.92	0.52
7:G:46:ASP:HB3	7:G:58:LEU:HD13	1.92	0.52
4:D:163:ARG:HB2	4:D:225:PHE:HD2	1.74	0.52
5:E:97:ARG:NH2	5:E:111:GLU:OE2	2.42	0.52
3:4:191:PRO:HB2	3:4:194:MET:HB2	1.91	0.52
6:7:184:ASP:N	6:7:184:ASP:OD1	2.40	0.52
3:C:405:VAL:HG12	3:C:407:ASN:H	1.75	0.51
10:P:256:ARG:HA	10:P:261:GLU:HG3	1.91	0.51
10:P:550:LEU:HD21	10:P:555:ARG:HA	1.91	0.51
11:K:63:LEU:HD13	11:K:76:HIS:HB2	1.92	0.51
3:C:265:ALA:O	3:C:422:ARG:NH1	2.44	0.51
12:R:399:ILE:O	12:R:403:LYS:HG2	2.10	0.51
3:4:405:VAL:HG12	3:4:407:ASN:H	1.75	0.51
5:6:97:ARG:NH2	5:6:111:GLU:OE2	2.43	0.51
1:2:181:TYR:CZ	1:2:185:LYS:HD2	2.46	0.51
6:7:181:TYR:HB2	6:7:190:THR:HB	1.90	0.51
12:L:399:ILE:O	12:L:403:LYS:HG2	2.10	0.51
2:B:252:THR:HG21	4:D:215:ILE:HD11	1.93	0.51
8:H:105:ASP:OD1	8:H:105:ASP:N	2.44	0.51
10:J:427:ILE:HG22	10:J:461:PHE:HE1	1.74	0.51
9:I:149:ASN:HB3	4:5:62:ARG:HG3	1.93	0.51
10:J:194:TYR:HB3	10:J:520:LYS:HG2	1.91	0.51
1:A:179:GLU:O	1:A:183:ARG:HG3	2.11	0.51
6:F:182:THR:HG22	6:F:189:GLU:HG2	1.93	0.50
10:J:256:ARG:HA	10:J:261:GLU:HG3	1.91	0.50
3:4:392:GLY:HA2	3:4:419:ILE:HG12	1.93	0.50
7:M:74:ARG:HH11	9:O:24:LEU:HD13	1.76	0.50
7:M:90:LEU:HB3	7:M:98:LEU:HD21	1.93	0.50
9:O:33:CYS:HB3	9:O:78:LEU:HD11	1.93	0.50
4:D:62:ARG:HG3	9:O:149:ASN:HB3	1.93	0.50
2:3:252:THR:HG21	4:5:215:ILE:HD11	1.93	0.50
1:A:181:TYR:CZ	1:A:185:LYS:HD2	2.46	0.50
11:Q:185:GLU:HG2	11:Q:186:THR:HG23	1.94	0.50
11:K:185:GLU:HG2	11:K:186:THR:HG23	1.94	0.50
1:2:179:GLU:O	1:2:183:ARG:HG3	2.12	0.50
8:N:145:LEU:HD12	11:Q:170:PHE:HE1	1.76	0.50
6:F:20:TYR:HA	6:F:28:LYS:HA	1.93	0.50
3:4:154:GLY:HA3	6:7:101:TYR:CD1	2.47	0.50
3:C:191:PRO:HB2	3:C:194:MET:HB2	1.92	0.50
9:O:35:ILE:HD12	9:O:39:PHE:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:74:ARG:HH11	9:I:24:LEU:HD13	1.77	0.50
10:J:390:ARG:HH12	10:J:397:ASN:HA	1.77	0.50
6:7:182:THR:HG22	6:7:189:GLU:HG2	1.92	0.50
9:I:33:CYS:HB3	9:I:78:LEU:HD11	1.93	0.49
3:C:321:ARG:HH22	6:F:218:ARG:HD3	1.77	0.49
5:6:29:GLN:HG3	5:6:95:ALA:HB2	1.94	0.49
12:L:568:HIS:HB3	12:L:579:LYS:HB3	1.94	0.49
12:R:568:HIS:HB3	12:R:579:LYS:HB3	1.94	0.49
10:J:277:LEU:HD13	10:J:345:LEU:HD22	1.95	0.49
6:7:20:TYR:HA	6:7:28:LYS:HA	1.93	0.49
7:G:113:TRP:HB2	11:K:138:LEU:HD13	1.95	0.49
1:2:166:THR:HG22	1:2:168:ARG:H	1.77	0.49
3:4:321:ARG:HH22	6:7:218:ARG:HD3	1.77	0.49
9:I:39:PHE:HB3	9:I:42:LEU:HD12	1.94	0.49
1:A:313:ASN:HA	1:A:320:ILE:HA	1.94	0.49
5:E:46:ASN:O	5:E:49:VAL:HG12	2.13	0.49
5:E:218:PRO:HG2	5:E:221:ALA:HB3	1.95	0.49
9:I:35:ILE:HD12	9:I:39:PHE:HE2	1.77	0.49
3:4:265:ALA:O	3:4:422:ARG:NH1	2.45	0.49
3:4:169:PHE:HB2	3:4:218:PHE:CD2	2.48	0.49
5:6:46:ASN:O	5:6:49:VAL:HG12	2.13	0.49
12:L:188:GLU:HA	12:L:221:GLN:HG2	1.95	0.49
1:A:192:VAL:HB	1:A:196:GLY:HA2	1.95	0.49
3:C:169:PHE:HB2	3:C:218:PHE:CD2	2.48	0.49
3:C:301:GLU:HA	3:C:316:GLU:HA	1.95	0.49
11:K:170:PHE:HE1	8:H:145:LEU:HD12	1.77	0.49
1:2:313:ASN:HA	1:2:320:ILE:HA	1.95	0.49
12:L:448:LEU:HD12	12:L:449:PRO:HD2	1.95	0.49
3:C:154:GLY:HA3	6:F:101:TYR:CD1	2.47	0.48
3:C:212:CYS:O	3:C:216:ARG:HG3	2.13	0.48
10:P:390:ARG:HH12	10:P:397:ASN:HA	1.78	0.48
9:I:94:PHE:HE1	9:I:101:VAL:HG21	1.78	0.48
1:A:166:THR:HG22	1:A:168:ARG:H	1.77	0.48
9:O:39:PHE:HB3	9:O:42:LEU:HD12	1.93	0.48
3:4:212:CYS:O	3:4:216:ARG:HG3	2.13	0.48
5:E:29:GLN:HG3	5:E:95:ALA:HB2	1.94	0.48
7:M:113:TRP:HB2	11:Q:138:LEU:HD13	1.95	0.48
7:M:125:MET:O	7:M:133:GLY:HA3	2.13	0.48
11:K:75:PHE:CE1	8:H:48:LEU:HD11	2.49	0.48
10:J:52:VAL:HG12	10:J:61:LEU:HD12	1.96	0.48
8:N:2:ASP:N	8:N:2:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:94:PHE:HE1	9:O:101:VAL:HG21	1.78	0.48
10:P:192:TYR:CG	10:P:520:LYS:HB3	2.48	0.48
1:2:219:TYR:OH	1:2:230:ALA:O	2.23	0.48
3:4:303:PHE:HD2	3:4:314:ARG:HH11	1.61	0.48
12:L:17:GLU:HA	12:L:20:ARG:HD2	1.96	0.48
3:C:303:PHE:HD2	3:C:314:ARG:HH11	1.61	0.48
12:R:188:GLU:HA	12:R:221:GLN:HG2	1.95	0.48
2:3:111:VAL:HG21	2:3:116:LEU:HD13	1.95	0.48
5:6:218:PRO:HG2	5:6:221:ALA:HB3	1.95	0.48
7:G:125:MET:O	7:G:133:GLY:HA3	2.13	0.48
10:J:192:TYR:CG	10:J:520:LYS:HB3	2.48	0.48
3:4:301:GLU:HA	3:4:316:GLU:HA	1.95	0.48
4:D:113:ARG:HB3	4:D:114:PRO:HD3	1.96	0.48
10:P:277:LEU:HD13	10:P:345:LEU:HD22	1.95	0.48
11:Q:181:LEU:HD23	11:Q:184:PRO:HB3	1.96	0.48
4:D:156:ILE:HG13	4:D:258:VAL:HG11	1.95	0.48
10:P:52:VAL:HG12	10:P:61:LEU:HD12	1.96	0.47
1:2:192:VAL:HB	1:2:196:GLY:HA2	1.95	0.47
4:5:156:ILE:HG13	4:5:258:VAL:HG11	1.95	0.47
3:C:195:GLN:O	3:C:199:GLU:HG2	2.15	0.47
11:Q:102:PHE:CG	11:Q:103:PRO:HD3	2.49	0.47
11:K:102:PHE:CG	11:K:103:PRO:HD3	2.49	0.47
4:5:113:ARG:HB3	4:5:114:PRO:HD3	1.96	0.47
5:E:90:PRO:O	5:E:94:ARG:HG2	2.14	0.47
12:R:162:ASP:OD2	12:R:166:LYS:NZ	2.38	0.47
4:5:247:GLN:OE1	4:5:273:ARG:NH2	2.47	0.47
2:B:224:ASP:OD1	2:B:224:ASP:N	2.46	0.47
2:B:111:VAL:HG21	2:B:116:LEU:HD13	1.95	0.47
10:P:17:GLU:HG2	10:P:71:TYR:CE2	2.50	0.47
7:G:158:GLU:HB3	7:G:166:THR:HB	1.96	0.47
10:J:423:LEU:O	10:J:427:ILE:HG23	2.15	0.47
1:2:273:LEU:HD12	1:2:274:PRO:HD2	1.96	0.47
2:3:76:PHE:HD2	2:3:100:VAL:HG21	1.80	0.47
5:6:159:LEU:HD21	5:6:164:GLN:HG3	1.97	0.47
5:6:189:ASN:HB3	5:6:193:PHE:CE2	2.50	0.47
8:N:24:ASP:OD1	8:N:24:ASP:N	2.35	0.47
8:N:48:LEU:HD11	11:Q:75:PHE:CE1	2.49	0.47
10:P:423:LEU:O	10:P:427:ILE:HG23	2.15	0.47
12:R:17:GLU:HA	12:R:20:ARG:HD2	1.95	0.47
1:2:312:TYR:O	1:2:321:LEU:N	2.44	0.47
10:P:342:ARG:HB3	10:P:358:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:16:SER:O	12:L:20:ARG:HG3	2.15	0.47
7:M:116:GLN:OE1	7:M:119:ARG:NH2	2.48	0.47
7:G:178:PRO:HD2	7:G:181:LYS:HD2	1.97	0.47
11:K:181:LEU:HD23	11:K:184:PRO:HB3	1.96	0.47
2:3:224:ASP:OD1	2:3:224:ASP:N	2.47	0.47
2:B:76:PHE:HD2	2:B:100:VAL:HG21	1.80	0.46
4:D:135:PRO:HB2	4:D:153:PRO:HD3	1.96	0.46
7:M:158:GLU:HB3	7:M:166:THR:HB	1.97	0.46
7:G:121:LEU:O	7:G:125:MET:HG2	2.15	0.46
10:J:342:ARG:HB3	10:J:358:ARG:HH21	1.79	0.46
4:D:247:GLN:OE1	4:D:273:ARG:NH2	2.48	0.46
5:E:52:ALA:HA	5:E:55:LEU:HB2	1.97	0.46
6:F:65:ILE:HD11	6:F:137:PHE:CZ	2.50	0.46
7:M:121:LEU:O	7:M:125:MET:HG2	2.15	0.46
7:G:116:GLN:OE1	7:G:119:ARG:NH2	2.48	0.46
3:4:195:GLN:O	3:4:199:GLU:HG2	2.14	0.46
6:7:6:GLN:O	6:7:10:GLU:HG2	2.15	0.46
5:E:189:ASN:HB3	5:E:193:PHE:CE2	2.49	0.46
8:N:77:GLN:HG3	8:N:80:ARG:HH21	1.80	0.46
10:P:269:MET:HG3	10:P:407:ARG:HH11	1.80	0.46
10:P:427:ILE:HG22	10:P:461:PHE:CE1	2.50	0.46
8:H:77:GLN:HG3	8:H:80:ARG:HH21	1.80	0.46
4:5:135:PRO:HB2	4:5:153:PRO:HD3	1.96	0.46
5:6:97:ARG:NH1	5:6:108:ALA:O	2.48	0.46
10:P:340:ASN:O	10:P:344:MET:HG2	2.16	0.46
3:4:326:SER:HB2	3:4:335:HIS:H	1.80	0.46
7:M:59:ILE:HG22	7:M:63:LYS:HE3	1.98	0.46
8:H:2:ASP:OD1	8:H:2:ASP:N	2.47	0.46
1:A:273:LEU:HD12	1:A:274:PRO:HD2	1.96	0.46
6:F:177:VAL:HG12	6:F:178:VAL:HG13	1.98	0.46
6:7:65:ILE:HD11	6:7:137:PHE:CZ	2.50	0.46
6:F:63:ASP:O	6:F:67:GLU:HG2	2.16	0.46
11:K:81:GLU:HG2	11:K:84:ARG:HH22	1.80	0.46
3:4:267:LYS:H	3:4:267:LYS:HD2	1.81	0.46
8:H:93:MET:HG3	8:H:121:TRP:CE3	2.51	0.46
3:4:221:ASP:O	3:4:225:GLN:HG3	2.16	0.46
6:F:6:GLN:O	6:F:10:GLU:HG2	2.15	0.45
8:N:93:MET:HG3	8:N:121:TRP:CE3	2.51	0.45
5:6:90:PRO:O	5:6:94:ARG:HG2	2.15	0.45
3:C:311:PHE:HE2	3:C:329:LYS:HD2	1.81	0.45
5:E:159:LEU:HD21	5:E:164:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:269:MET:HG3	10:J:407:ARG:HH11	1.81	0.45
10:J:427:ILE:HG22	10:J:461:PHE:CE1	2.51	0.45
3:4:311:PHE:HE2	3:4:329:LYS:HD2	1.81	0.45
5:6:105:ASN:OD1	5:6:105:ASN:N	2.49	0.45
6:7:63:ASP:O	6:7:67:GLU:HG2	2.17	0.45
1:A:312:TYR:O	1:A:321:LEU:N	2.43	0.45
1:A:317:CYS:SG	1:A:319:PHE:HB3	2.56	0.45
8:N:40:LEU:HD23	8:N:40:LEU:HA	1.84	0.45
11:Q:81:GLU:HG2	11:Q:84:ARG:HH22	1.80	0.45
12:R:169:LEU:HD21	12:R:498:LEU:HD13	1.99	0.45
8:H:40:LEU:HD23	8:H:40:LEU:HA	1.84	0.45
6:F:155:SER:HA	6:F:158:LYS:HG3	1.99	0.45
8:N:105:ASP:OD1	8:N:105:ASP:N	2.43	0.45
8:H:23:LEU:HB3	8:H:36:PHE:HD2	1.82	0.45
5:6:31:LEU:HB3	5:6:77:LEU:HD22	1.98	0.45
10:J:7:ARG:HD2	10:J:209:ILE:HG22	1.98	0.45
10:J:340:ASN:O	10:J:344:MET:HG2	2.16	0.45
1:2:226:GLU:HG3	1:2:229:LEU:HB2	1.99	0.45
1:2:317:CYS:SG	1:2:319:PHE:HB3	2.56	0.45
1:A:226:GLU:HG3	1:A:229:LEU:HB2	1.99	0.45
3:C:200:ILE:HA	3:C:203:VAL:HB	1.99	0.45
5:E:31:LEU:HB3	5:E:77:LEU:HD22	1.98	0.45
7:M:129:GLY:HA3	11:Q:53:MET:HE2	1.97	0.45
7:M:134:LEU:HD11	11:Q:84:ARG:HG3	1.98	0.45
12:R:16:SER:O	12:R:20:ARG:HG3	2.16	0.45
6:7:155:SER:HA	6:7:158:LYS:HG3	1.99	0.45
3:C:267:LYS:H	3:C:267:LYS:HD2	1.81	0.45
3:C:280:ASP:OD1	3:C:395:ARG:NH1	2.50	0.45
3:C:309:CYS:HB3	3:C:331:CYS:HB3	1.99	0.45
12:R:189:ALA:HB1	12:L:278:LEU:HD23	1.99	0.45
8:H:24:ASP:OD1	8:H:24:ASP:N	2.35	0.45
10:J:17:GLU:HG2	10:J:71:TYR:CE2	2.52	0.45
3:4:343:ARG:HD3	5:6:87:ARG:HD2	1.99	0.45
10:P:7:ARG:HD2	10:P:209:ILE:HG22	1.98	0.45
10:P:102:ARG:O	10:P:104:ILE:HG13	2.17	0.45
12:R:238:PHE:HB3	12:R:239:PRO:HD3	1.99	0.45
2:3:27:GLN:HG3	12:L:437:SER:HB3	1.99	0.45
3:4:309:CYS:HB3	3:4:331:CYS:HB3	1.99	0.45
6:F:279:MET:HE2	6:F:294:GLU:HB2	1.98	0.45
10:J:108:ASN:HB3	10:J:115:VAL:HG11	1.99	0.45
3:4:280:ASP:OD1	3:4:395:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:23:LEU:HB3	8:N:36:PHE:HD2	1.82	0.44
7:G:59:ILE:HG22	7:G:63:LYS:HE3	1.98	0.44
12:L:169:LEU:HD21	12:L:498:LEU:HD13	1.99	0.44
12:L:335:LEU:HD13	12:L:563:LYS:HE2	1.98	0.44
3:C:326:SER:HB2	3:C:335:HIS:H	1.82	0.44
7:M:178:PRO:HD2	7:M:181:LYS:HD2	1.98	0.44
6:7:177:VAL:HG12	6:7:178:VAL:HG13	1.98	0.44
2:B:25:ASP:O	2:B:30:GLY:HA2	2.17	0.44
10:P:508:VAL:HG23	10:P:547:ILE:HG12	1.98	0.44
7:G:134:LEU:HD11	11:K:84:ARG:HG3	1.99	0.44
3:C:221:ASP:O	3:C:225:GLN:HG3	2.16	0.44
6:F:106:LEU:O	6:F:110:GLN:HG2	2.18	0.44
10:P:192:TYR:HE1	10:P:522:PHE:HD2	1.65	0.44
10:J:508:VAL:HG23	10:J:547:ILE:HG12	1.99	0.44
5:6:52:ALA:HA	5:6:55:LEU:HB2	1.97	0.44
12:L:405:LYS:HD3	12:L:405:LYS:HA	1.69	0.44
12:R:278:LEU:HD23	12:L:189:ALA:HB1	1.99	0.44
10:J:102:ARG:O	10:J:104:ILE:HG13	2.17	0.44
7:G:16:ALA:O	7:G:86:ARG:NH2	2.51	0.44
2:3:61:ARG:HA	2:3:61:ARG:HD3	1.67	0.44
12:R:165:LEU:HD23	12:R:165:LEU:HA	1.87	0.44
10:J:306:LEU:HG	10:J:310:LYS:HE3	2.00	0.44
3:4:168:ARG:O	3:4:172:ARG:N	2.40	0.44
1:A:337:CYS:SG	1:A:338:PRO:HD2	2.58	0.44
6:F:82:GLU:O	6:F:85:PRO:HD2	2.18	0.44
10:P:108:ASN:HB3	10:P:115:VAL:HG11	1.99	0.44
12:R:335:LEU:HD13	12:R:563:LYS:HE2	1.98	0.43
7:G:168:LEU:HG	7:G:170:LYS:HG3	2.00	0.43
6:7:279:MET:HE2	6:7:294:GLU:HB2	1.99	0.43
10:P:306:LEU:HG	10:P:310:LYS:HE3	2.00	0.43
10:P:475:LEU:HD13	10:P:492:LEU:HB2	1.99	0.43
2:B:106:PHE:HB2	2:B:110:HIS:CD2	2.53	0.43
3:C:238:ASP:OD1	3:C:260:VAL:HG12	2.19	0.43
6:F:128:GLU:O	6:F:227:LYS:NZ	2.47	0.43
10:J:559:LEU:O	10:J:563:ILE:HG13	2.19	0.43
2:3:106:PHE:HB2	2:3:110:HIS:CD2	2.53	0.43
7:M:13:LEU:HD23	7:M:13:LEU:HA	1.83	0.43
10:J:266:ILE:HG22	10:J:267:ASP:H	1.83	0.43
3:4:328:CYS:SG	3:4:329:LYS:N	2.91	0.43
3:C:343:ARG:HD3	5:E:87:ARG:HD2	1.99	0.43
6:F:88:LYS:HE3	6:F:92:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:231:GLN:O	10:P:472:LYS:NZ	2.38	0.43
4:D:66:LEU:HD23	4:D:66:LEU:HA	1.78	0.43
10:P:73:VAL:HG22	10:P:96:TYR:HB2	2.00	0.43
7:G:98:LEU:HD23	7:G:98:LEU:HA	1.84	0.43
1:2:337:CYS:SG	1:2:338:PRO:HD2	2.58	0.43
4:5:88:TYR:HB3	4:5:96:HIS:NE2	2.33	0.43
3:C:328:CYS:SG	3:C:329:LYS:N	2.92	0.43
6:F:231:PHE:HD1	6:F:257:ARG:HG2	1.84	0.43
10:P:35:ILE:HG23	10:P:217:MET:HG2	2.00	0.43
10:J:73:VAL:HG22	10:J:96:TYR:HB2	2.00	0.43
3:4:238:ASP:OD1	3:4:260:VAL:HG12	2.18	0.43
6:7:82:GLU:O	6:7:85:PRO:HD2	2.18	0.43
6:7:106:LEU:O	6:7:110:GLN:HG2	2.18	0.43
7:M:16:ALA:O	7:M:86:ARG:NH2	2.51	0.43
3:4:200:ILE:HA	3:4:203:VAL:HB	2.00	0.43
6:F:49:ILE:HG21	6:F:76:PHE:CE2	2.54	0.43
7:M:46:ASP:OD2	7:M:65:ARG:NH1	2.52	0.43
6:7:49:ILE:HG21	6:7:76:PHE:CE2	2.53	0.43
7:M:136:ILE:O	11:Q:92:ARG:NH1	2.52	0.43
10:P:133:ILE:HA	10:P:182:ARG:HD3	2.00	0.43
8:H:74:ILE:HD13	8:H:88:PRO:HD3	2.01	0.43
10:J:11:PHE:O	10:J:15:VAL:HG23	2.19	0.43
10:J:468:CYS:O	10:J:472:LYS:HG3	2.18	0.43
3:4:290:ILE:HG13	3:4:355:GLN:HG3	2.01	0.43
1:A:219:TYR:OH	1:A:230:ALA:O	2.23	0.42
3:C:290:ILE:HG13	3:C:355:GLN:HG3	2.01	0.42
10:P:559:LEU:O	10:P:563:ILE:HG13	2.19	0.42
7:G:84:LEU:HD21	11:K:138:LEU:HD22	2.01	0.42
4:5:176:CYS:HB3	4:5:208:CYS:SG	2.59	0.42
3:C:251:ASP:N	3:C:251:ASP:OD1	2.52	0.42
1:2:374:ARG:HH11	1:2:377:ARG:HH21	1.68	0.42
7:M:20:GLN:NE2	9:O:199:ASN:HB3	2.34	0.42
7:G:20:GLN:NE2	9:I:199:ASN:HB3	2.34	0.42
7:G:39:LEU:HD23	7:G:39:LEU:HA	1.85	0.42
7:G:46:ASP:OD2	7:G:65:ARG:NH1	2.52	0.42
1:2:180:ILE:HG23	1:2:229:LEU:HD21	2.01	0.42
2:3:138:ARG:HD2	6:7:292:LEU:HD21	2.01	0.42
6:7:52:ASP:O	6:7:56:GLU:HG3	2.20	0.42
6:7:128:GLU:O	6:7:227:LYS:NZ	2.47	0.42
6:7:231:PHE:HD1	6:7:257:ARG:HG2	1.84	0.42
1:A:239:GLU:O	1:A:243:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:TYR:HB3	4:D:96:HIS:NE2	2.34	0.42
9:O:200:TYR:HA	9:O:203:ARG:HD3	2.01	0.42
10:P:266:ILE:HG22	10:P:267:ASP:H	1.83	0.42
10:P:468:CYS:O	10:P:472:LYS:HG3	2.19	0.42
10:J:35:ILE:HG23	10:J:217:MET:HG2	2.01	0.42
10:J:387:ASN:HD22	10:J:390:ARG:HE	1.66	0.42
12:R:395:ASP:O	12:R:398:SER:OG	2.25	0.42
5:E:66:ASN:O	5:E:70:ILE:HG13	2.19	0.42
5:E:105:ASN:OD1	5:E:105:ASN:N	2.52	0.42
12:L:229:HIS:HB3	12:L:230:PRO:HD3	2.02	0.42
7:M:84:LEU:HD21	11:Q:138:LEU:HD22	2.01	0.42
11:K:201:GLN:HB2	8:H:145:LEU:O	2.19	0.42
1:2:184:PHE:HD2	1:2:247:ALA:HB3	1.85	0.42
1:A:180:ILE:HG23	1:A:229:LEU:HD21	2.01	0.42
6:F:52:ASP:O	6:F:56:GLU:HG3	2.19	0.42
10:J:60:THR:O	10:J:64:GLU:HG3	2.20	0.42
6:7:149:ARG:HG3	6:7:238:GLU:OE2	2.20	0.42
6:7:205:CYS:HA	6:7:219:LEU:HD13	2.02	0.42
8:N:145:LEU:O	11:Q:201:GLN:HB2	2.19	0.42
10:P:60:THR:O	10:P:64:GLU:HG3	2.19	0.42
12:R:166:LYS:HB2	12:R:493:ILE:HB	2.02	0.42
10:J:192:TYR:HE1	10:J:522:PHE:HD2	1.67	0.42
12:L:14:LYS:HG3	12:L:15:PRO:HD2	2.01	0.42
6:F:98:LEU:HD23	6:F:98:LEU:HA	1.92	0.42
6:F:205:CYS:HA	6:F:219:LEU:HD13	2.02	0.42
1:A:184:PHE:HD2	1:A:247:ALA:HB3	1.85	0.41
1:A:374:ARG:HH11	1:A:377:ARG:HH21	1.68	0.41
3:C:154:GLY:HA2	6:F:104:HIS:HB2	2.01	0.41
5:E:217:LEU:HD21	5:E:223:PRO:HB3	2.01	0.41
8:N:74:ILE:HD13	8:N:88:PRO:HD3	2.01	0.41
12:R:229:HIS:HB3	12:R:230:PRO:HD3	2.01	0.41
11:K:32:TRP:HZ3	8:H:9:LEU:HD21	1.85	0.41
9:I:200:TYR:HA	9:I:203:ARG:HD3	2.01	0.41
3:4:251:ASP:OD1	3:4:251:ASP:N	2.52	0.41
4:5:107:VAL:O	4:5:111:VAL:HG23	2.20	0.41
5:6:66:ASN:O	5:6:70:ILE:HG13	2.19	0.41
4:D:176:CYS:HB3	4:D:208:CYS:SG	2.60	0.41
6:F:65:ILE:O	6:F:69:THR:HG22	2.20	0.41
7:M:168:LEU:HG	7:M:170:LYS:HG3	2.02	0.41
10:P:411:ASP:O	10:P:415:THR:HG23	2.19	0.41
1:2:239:GLU:O	1:2:243:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:10:HIS:NE2	12:L:256:GLN:OE1	2.49	0.41
10:P:11:PHE:O	10:P:15:VAL:HG23	2.20	0.41
7:G:136:ILE:O	11:K:92:ARG:NH1	2.52	0.41
8:H:71:LEU:HD23	8:H:71:LEU:HA	1.88	0.41
10:J:411:ASP:O	10:J:415:THR:HG23	2.19	0.41
2:B:90:THR:O	2:B:94:GLN:HG3	2.20	0.41
4:D:257:LYS:HE2	4:D:257:LYS:HB3	1.78	0.41
5:E:97:ARG:NH1	5:E:108:ALA:O	2.53	0.41
6:F:149:ARG:HG3	6:F:238:GLU:OE2	2.19	0.41
8:N:9:LEU:HD21	11:Q:32:TRP:HZ3	1.86	0.41
8:N:12:LYS:HB3	8:N:12:LYS:HE2	1.84	0.41
5:6:124:LYS:HE3	5:6:124:LYS:HB2	1.89	0.41
6:7:88:LYS:HE3	6:7:92:VAL:HG13	2.02	0.41
12:L:275:LEU:HD12	12:L:275:LEU:HA	1.92	0.41
7:G:140:MET:SD	7:G:187:ARG:NH1	2.93	0.41
2:3:162:LEU:HD11	2:3:169:PRO:HD3	2.03	0.41
4:5:61:LYS:HB2	4:5:111:VAL:HG11	2.02	0.41
5:6:217:LEU:HD21	5:6:223:PRO:HB3	2.01	0.41
12:R:14:LYS:HG3	12:R:15:PRO:HD2	2.02	0.41
12:R:321:ARG:O	12:R:325:LYS:HG3	2.21	0.41
11:K:104:HIS:NE2	11:K:162:LYS:HG2	2.36	0.41
8:H:26:VAL:HB	8:H:33:LEU:HB2	2.02	0.41
2:3:90:THR:O	2:3:94:GLN:HG3	2.20	0.41
2:3:162:LEU:HD21	2:3:169:PRO:HB3	2.03	0.41
4:D:61:LYS:HB2	4:D:111:VAL:HG11	2.02	0.41
7:G:43:ASN:OD1	7:G:62:ILE:HA	2.21	0.41
11:K:62:ASN:OD1	12:L:12:PHE:HA	2.20	0.41
2:3:25:ASP:O	2:3:30:GLY:HA2	2.20	0.41
6:7:65:ILE:O	6:7:69:THR:HG22	2.20	0.41
12:L:321:ARG:O	12:L:325:LYS:HG3	2.21	0.41
2:B:138:ARG:HB2	6:F:292:LEU:HD11	2.03	0.41
2:B:142:MET:HG2	2:B:194:LYS:HG2	2.02	0.41
9:O:35:ILE:HD12	9:O:39:PHE:CE2	2.56	0.41
9:O:40:PRO:HA	9:O:53:SER:HB3	2.03	0.41
7:G:84:LEU:HD11	11:K:138:LEU:HD22	2.03	0.41
1:2:392:LYS:HE2	1:2:392:LYS:HB3	1.84	0.41
2:3:146:HIS:CE1	2:3:186:THR:HG22	2.56	0.41
5:6:85:TYR:HD2	5:6:249:THR:HB	1.85	0.41
12:L:166:LYS:HB2	12:L:493:ILE:HB	2.03	0.41
1:A:229:LEU:HG	1:A:240:MET:HE1	2.02	0.41
2:B:61:ARG:HD3	2:B:61:ARG:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:43:ASN:OD1	7:M:62:ILE:HA	2.21	0.41
7:M:92:TRP:O	7:M:187:ARG:NH2	2.54	0.41
7:M:98:LEU:HD23	7:M:98:LEU:HA	1.85	0.41
7:M:140:MET:SD	7:M:187:ARG:NH1	2.94	0.41
8:N:26:VAL:HB	8:N:33:LEU:HB2	2.03	0.41
2:3:199:LEU:HD13	2:3:219:ILE:HD11	2.02	0.41
3:4:154:GLY:HA2	6:7:104:HIS:HB2	2.01	0.41
2:B:138:ARG:HD2	6:F:292:LEU:HD21	2.01	0.41
3:C:341:HIS:H	3:C:341:HIS:HD1	1.69	0.41
10:P:387:ASN:HD22	10:P:390:ARG:HE	1.67	0.41
11:Q:104:HIS:NE2	11:Q:162:LYS:HG2	2.36	0.41
8:H:48:LEU:HD12	8:H:48:LEU:HA	1.83	0.41
9:I:40:PRO:HA	9:I:53:SER:HB3	2.03	0.41
2:3:142:MET:HG2	2:3:194:LYS:HG2	2.03	0.41
5:E:93:CYS:O	5:E:96:VAL:HG12	2.21	0.40
5:E:147:HIS:ND1	5:E:207:LYS:O	2.54	0.40
10:P:71:TYR:CD1	10:P:94:ILE:HB	2.56	0.40
7:G:185:LEU:HD23	7:G:185:LEU:HA	1.91	0.40
10:J:393:LYS:HB3	10:J:396:ASP:HB2	2.04	0.40
1:2:229:LEU:HG	1:2:240:MET:HE1	2.03	0.40
3:C:302:ALA:N	3:C:315:VAL:O	2.54	0.40
6:F:102:ILE:HG12	6:F:105:ARG:HH22	1.86	0.40
11:Q:56:LEU:O	11:Q:60:GLU:HG3	2.22	0.40
11:Q:143:ALA:O	11:Q:147:MET:HG2	2.21	0.40
12:R:405:LYS:HD3	12:R:405:LYS:HA	1.69	0.40
1:2:215:LEU:HD12	1:2:216:PRO:HD2	2.03	0.40
4:5:173:CYS:SG	4:5:176:CYS:N	2.89	0.40
6:7:173:LYS:HB2	6:7:173:LYS:HE3	1.85	0.40
4:D:107:VAL:O	4:D:111:VAL:HG23	2.21	0.40
12:R:188:GLU:O	12:R:192:LEU:HG	2.22	0.40
10:J:71:TYR:CD1	10:J:94:ILE:HB	2.56	0.40
3:4:302:ALA:N	3:4:315:VAL:O	2.54	0.40
12:L:169:LEU:HD13	12:L:493:ILE:HG13	2.04	0.40
6:F:210:CYS:HB3	6:F:216:GLY:HA2	2.04	0.40
10:P:295:CYS:HB2	10:P:473:TYR:CE2	2.57	0.40
11:Q:19:LEU:HD23	11:Q:19:LEU:HA	1.92	0.40
7:G:4:GLU:H	7:G:4:GLU:HG2	1.71	0.40
10:J:277:LEU:HD21	10:J:342:ARG:HG2	2.03	0.40
1:A:215:LEU:HD12	1:A:216:PRO:HD2	2.03	0.40
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.90	0.40
5:E:84:GLU:HB3	5:E:87:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:88:LYS:HE2	6:F:91:GLU:HA	2.03	0.40
6:F:173:LYS:HE3	6:F:173:LYS:HB2	1.85	0.40
7:M:161:ILE:HG22	7:M:162:ASP:H	1.85	0.40
12:R:169:LEU:HD13	12:R:493:ILE:HG13	2.03	0.40
10:J:205:GLU:O	10:J:209:ILE:HG12	2.20	0.40
3:4:203:VAL:HG12	3:4:205:ASP:H	1.87	0.40
5:6:147:HIS:ND1	5:6:207:LYS:O	2.54	0.40
12:L:238:PHE:HB3	12:L:239:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	265/886 (30%)	256 (97%)	9 (3%)	0	100	100
1	A	265/886 (30%)	256 (97%)	9 (3%)	0	100	100
2	3	260/807 (32%)	252 (97%)	8 (3%)	0	100	100
2	B	260/807 (32%)	253 (97%)	7 (3%)	0	100	100
3	4	254/863 (29%)	253 (100%)	1 (0%)	0	100	100
3	C	254/863 (29%)	253 (100%)	1 (0%)	0	100	100
4	5	250/735 (34%)	244 (98%)	6 (2%)	0	100	100
4	D	250/735 (34%)	243 (97%)	7 (3%)	0	100	100
5	6	245/821 (30%)	240 (98%)	5 (2%)	0	100	100
5	E	245/821 (30%)	240 (98%)	5 (2%)	0	100	100
6	7	267/720 (37%)	260 (97%)	7 (3%)	0	100	100
6	F	267/720 (37%)	260 (97%)	7 (3%)	0	100	100
7	G	194/196 (99%)	192 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
8	H	173/185 (94%)	170 (98%)	3 (2%)	0	100	100
8	N	173/185 (94%)	170 (98%)	3 (2%)	0	100	100
9	I	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
9	O	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
10	J	519/567 (92%)	502 (97%)	17 (3%)	0	100	100
10	P	519/567 (92%)	504 (97%)	15 (3%)	0	100	100
11	K	201/221 (91%)	197 (98%)	4 (2%)	0	100	100
11	Q	201/221 (91%)	198 (98%)	3 (2%)	0	100	100
12	L	351/579 (61%)	338 (96%)	13 (4%)	0	100	100
12	R	351/579 (61%)	337 (96%)	14 (4%)	0	100	100
All	All	6358/13580 (47%)	6203 (98%)	155 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	238/767 (31%)	238 (100%)	0	100	100
1	A	238/767 (31%)	238 (100%)	0	100	100
2	3	231/701 (33%)	231 (100%)	0	100	100
2	B	231/701 (33%)	231 (100%)	0	100	100
3	4	240/761 (32%)	239 (100%)	1 (0%)	91	96
3	C	240/761 (32%)	239 (100%)	1 (0%)	91	96
4	5	225/627 (36%)	222 (99%)	3 (1%)	69	86
4	D	225/627 (36%)	222 (99%)	3 (1%)	69	86
5	6	219/712 (31%)	219 (100%)	0	100	100
5	E	219/712 (31%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	7	248/629 (39%)	248 (100%)	0	100 100
6	F	248/629 (39%)	248 (100%)	0	100 100
7	G	176/176 (100%)	176 (100%)	0	100 100
7	M	176/176 (100%)	176 (100%)	0	100 100
8	H	159/168 (95%)	158 (99%)	1 (1%)	86 94
8	N	159/168 (95%)	158 (99%)	1 (1%)	86 94
9	I	174/180 (97%)	174 (100%)	0	100 100
9	O	174/180 (97%)	174 (100%)	0	100 100
10	J	478/515 (93%)	476 (100%)	2 (0%)	91 96
10	P	478/515 (93%)	476 (100%)	2 (0%)	91 96
11	K	187/203 (92%)	187 (100%)	0	100 100
11	Q	187/203 (92%)	187 (100%)	0	100 100
12	L	317/499 (64%)	315 (99%)	2 (1%)	86 94
12	R	317/499 (64%)	315 (99%)	2 (1%)	86 94
All	All	5784/11876 (49%)	5766 (100%)	18 (0%)	92 97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	267	LYS
4	D	60	LEU
4	D	173	CYS
4	D	270	TYR
8	N	160	PHE
10	P	285	TRP
10	P	484	ASN
12	R	272	PHE
12	R	315	PRO
8	H	160	PHE
10	J	285	TRP
10	J	484	ASN
3	4	267	LYS
4	5	60	LEU
4	5	173	CYS
4	5	270	TYR
12	L	272	PHE
12	L	315	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
10	P	484	ASN
10	J	484	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

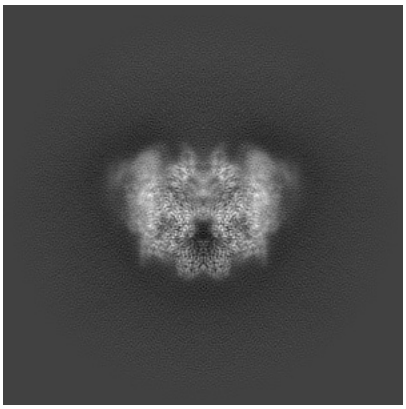
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18191. These allow visual inspection of the internal detail of the map and identification of artifacts.

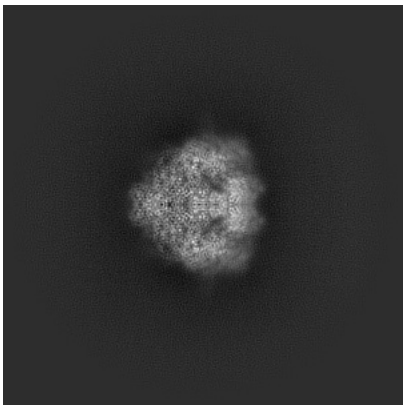
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

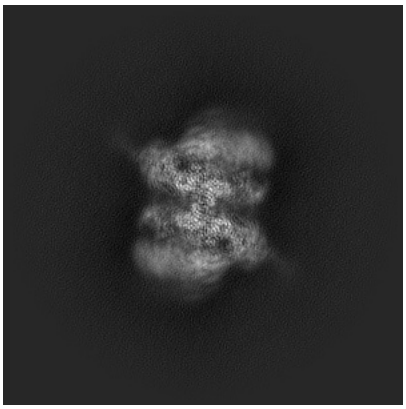
6.1.1 Primary map



X

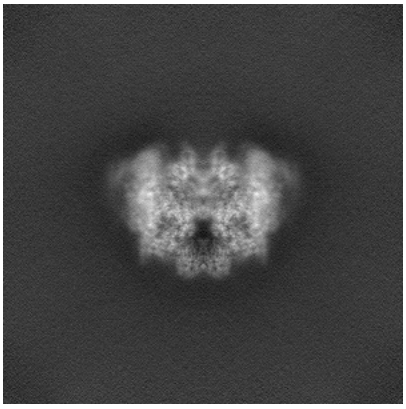


Y

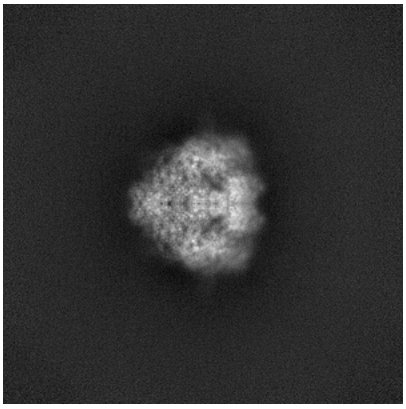


Z

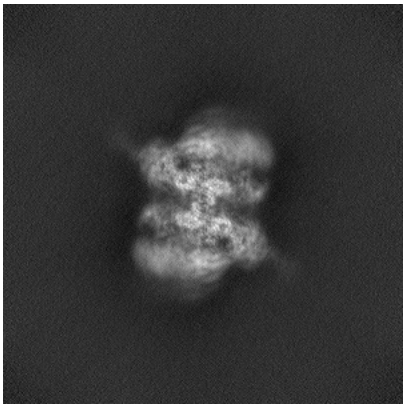
6.1.2 Raw map



X



Y

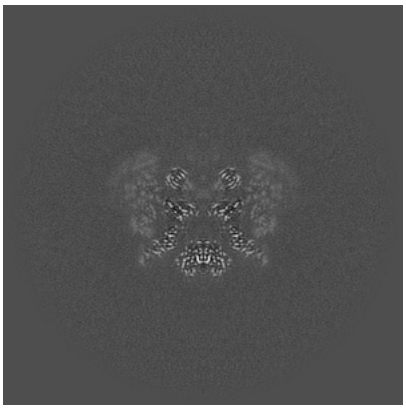


Z

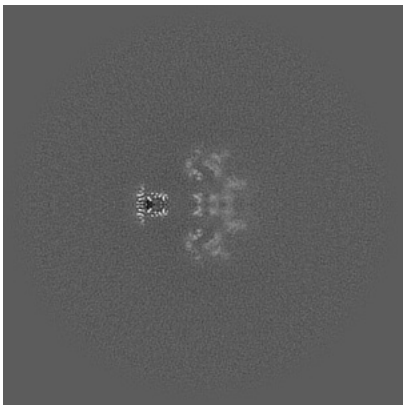
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

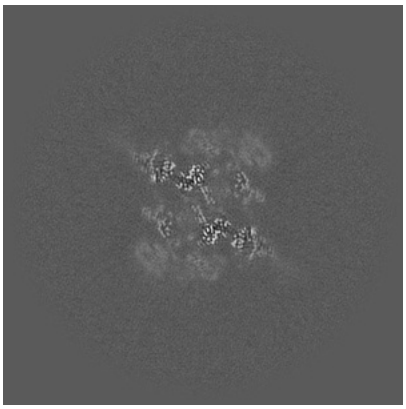
6.2.1 Primary map



X Index: 270

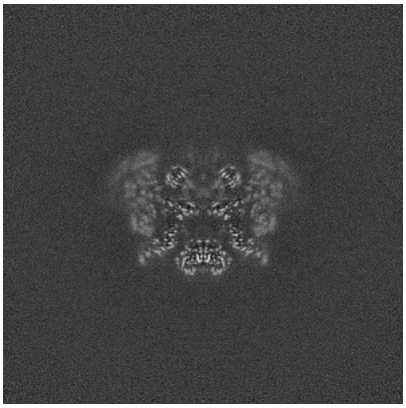


Y Index: 270

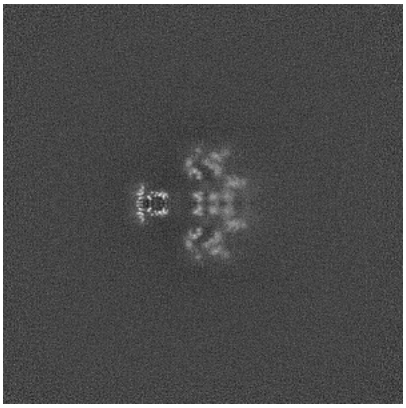


Z Index: 270

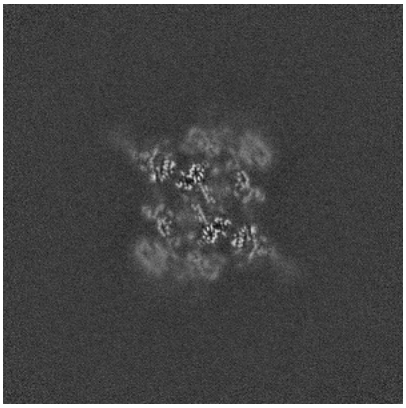
6.2.2 Raw map



X Index: 270



Y Index: 270

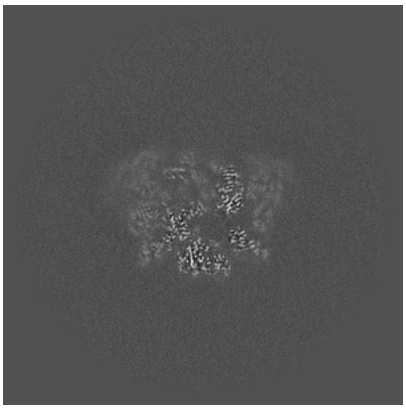


Z Index: 270

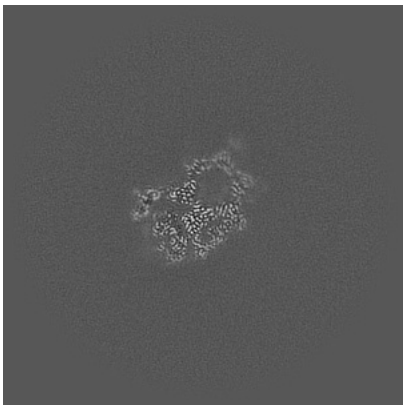
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

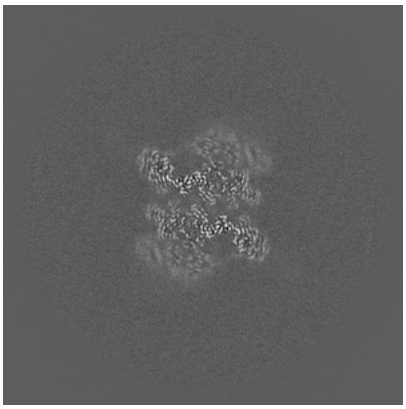
6.3.1 Primary map



X Index: 263

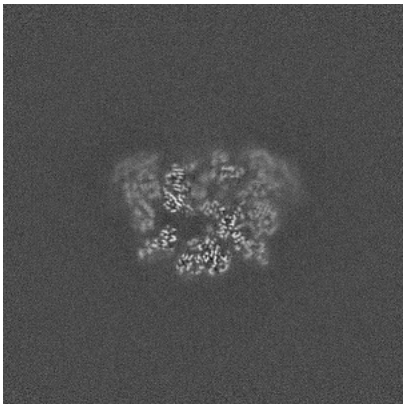


Y Index: 303

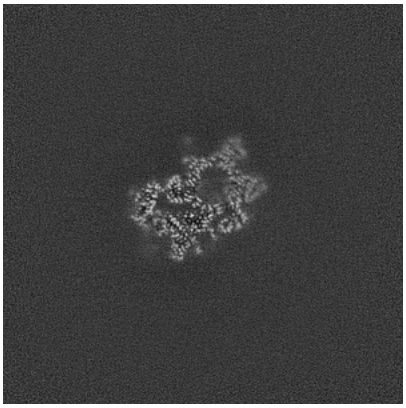


Z Index: 260

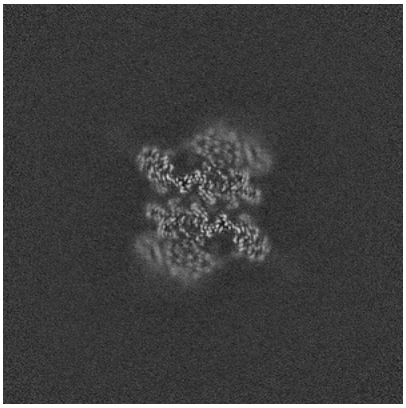
6.3.2 Raw map



X Index: 276



Y Index: 297

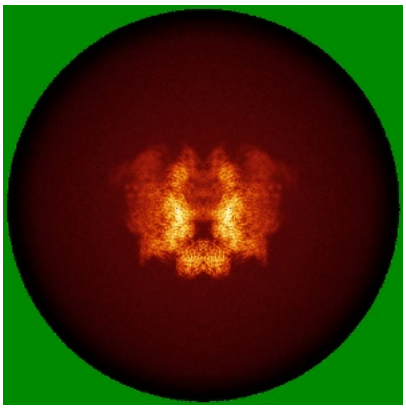


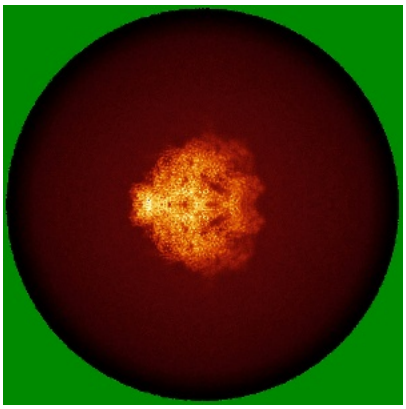
Z Index: 260

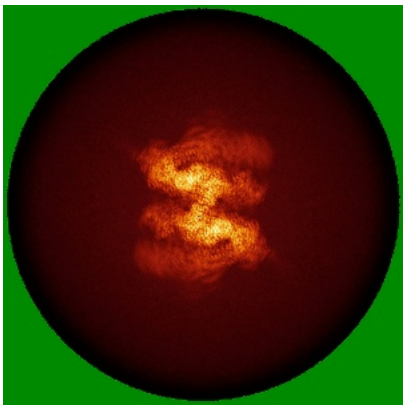
The images above show the largest variance slices of the map in three orthogonal directions.

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

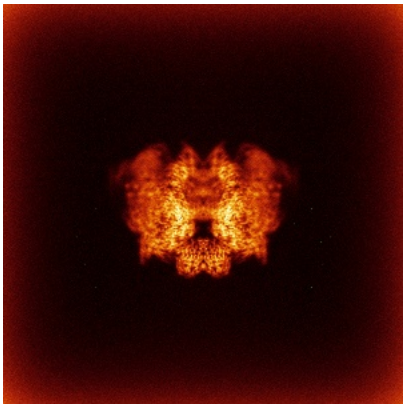
6.4.1 Primary map

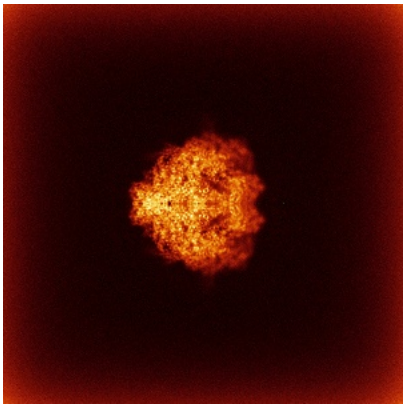

X

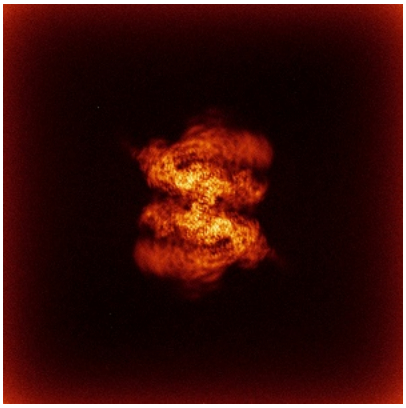

Y


Z

6.4.2 Raw 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 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

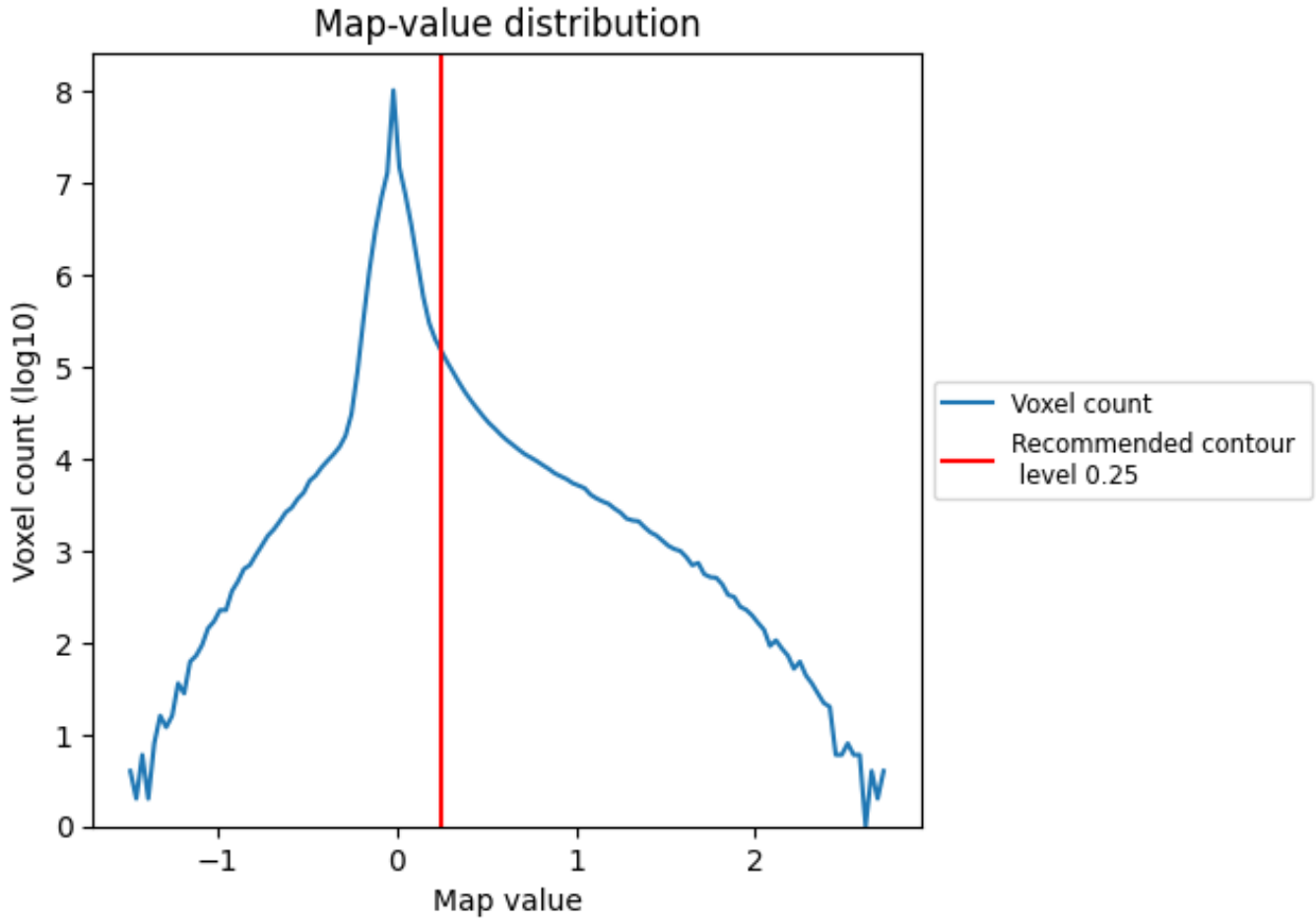
6.6 Mask visualisation (i)

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

7 Map analysis

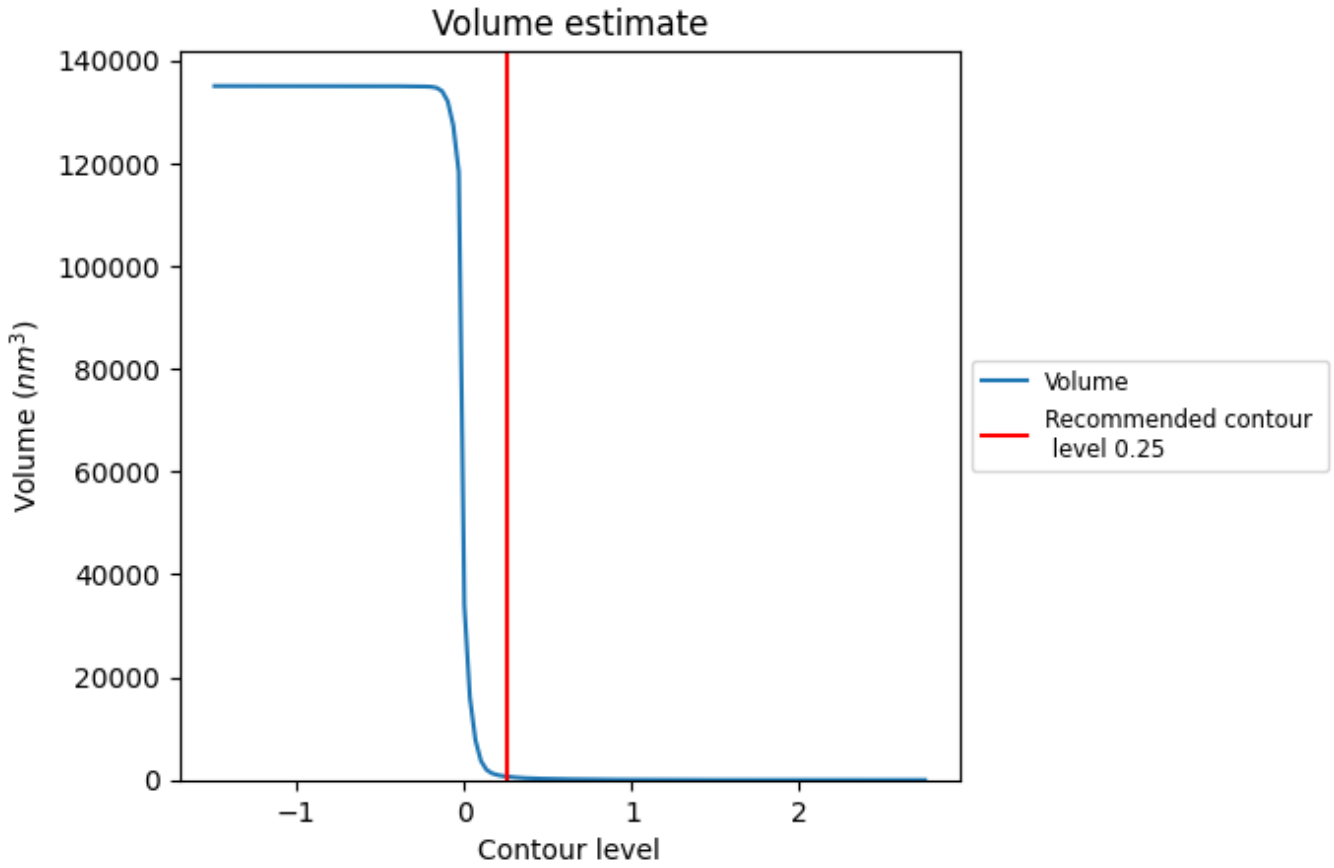
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

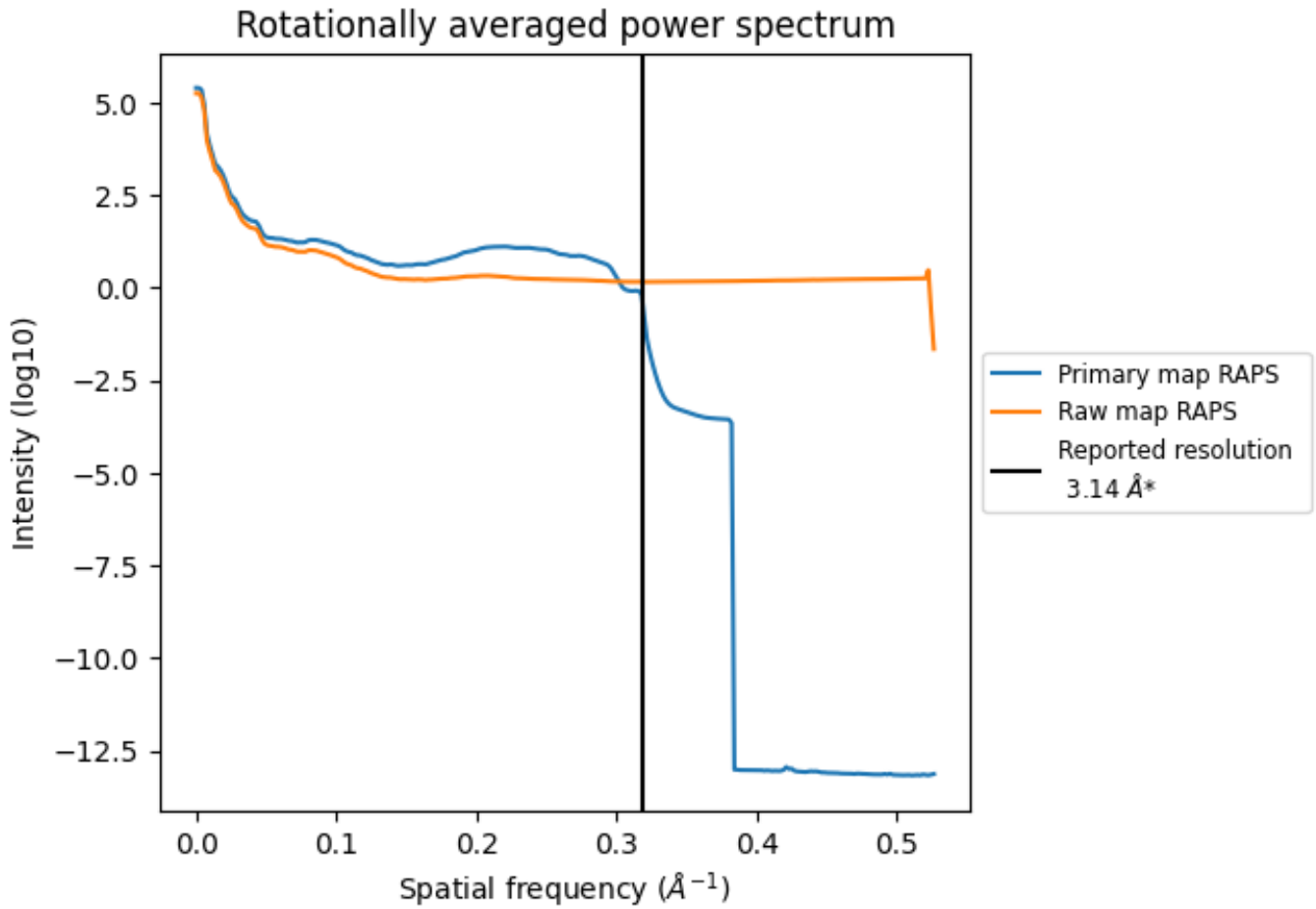
7.2 Volume estimate



The volume at the recommended contour level is 684 nm^3; this corresponds to an approximate mass of 618 kDa.

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

7.3 Rotationally averaged power spectrum (i)

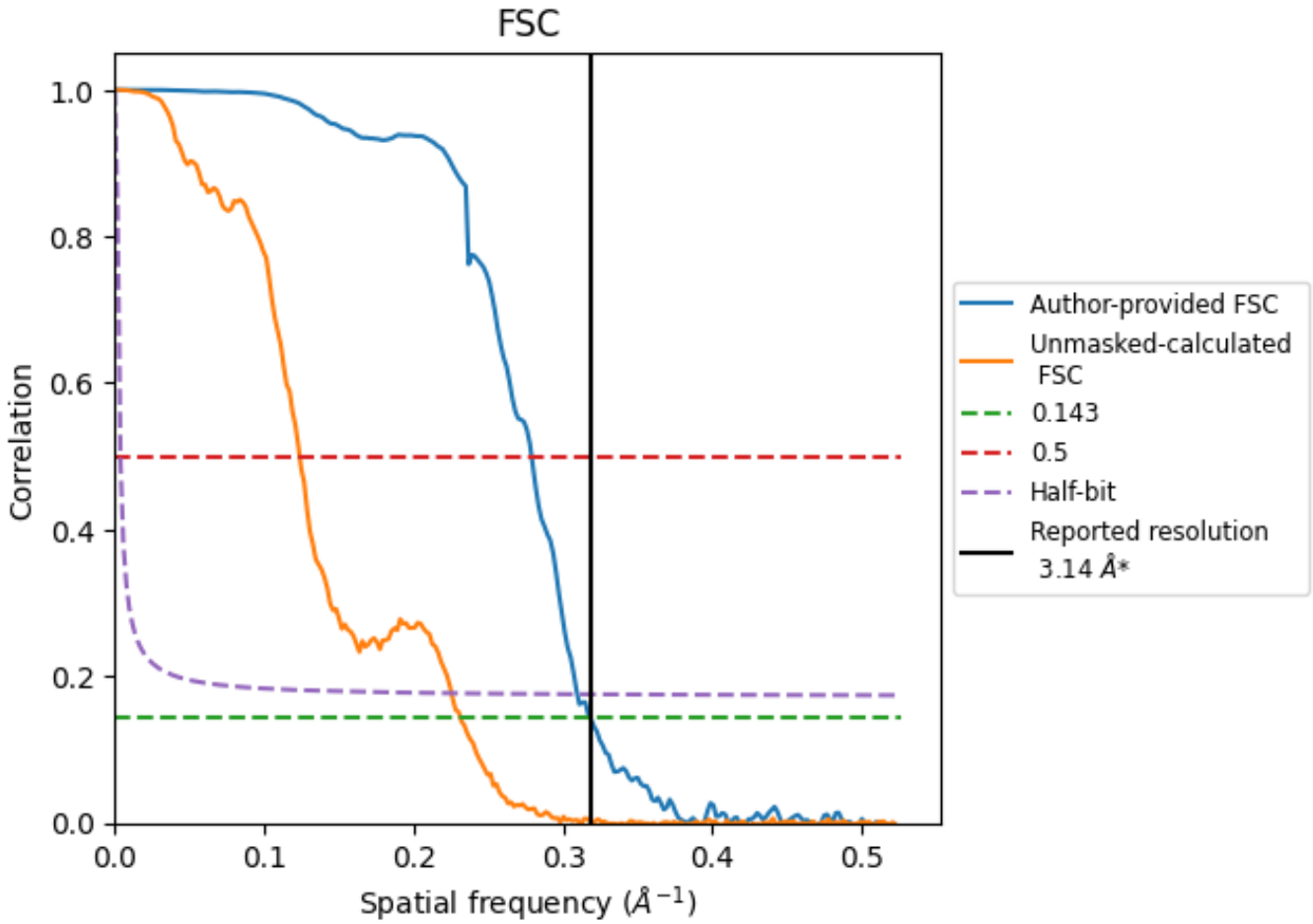


*Reported resolution corresponds to spatial frequency of 0.318 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.318 Å^{-1}

8.2 Resolution estimates (i)

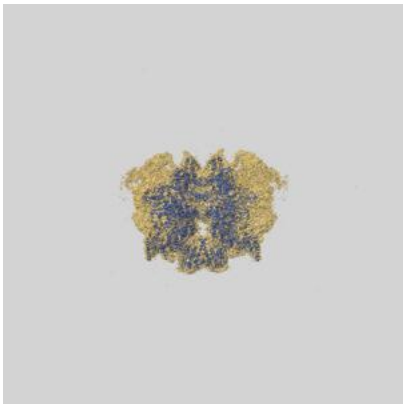
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.59	3.23
Unmasked-calculated*	4.32	8.08	4.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.14 by more than 10 %

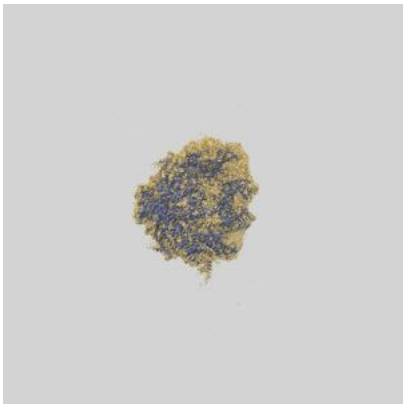
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18191 and PDB model 8Q6O. Per-residue inclusion information can be found in section 3 on page 7.

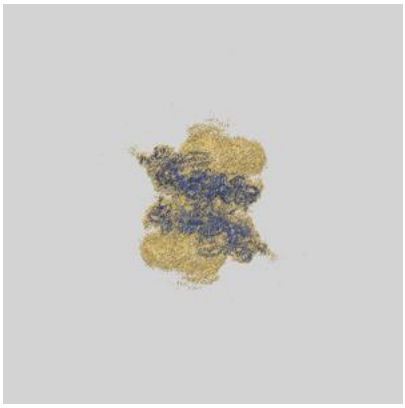
9.1 Map-model overlay



X



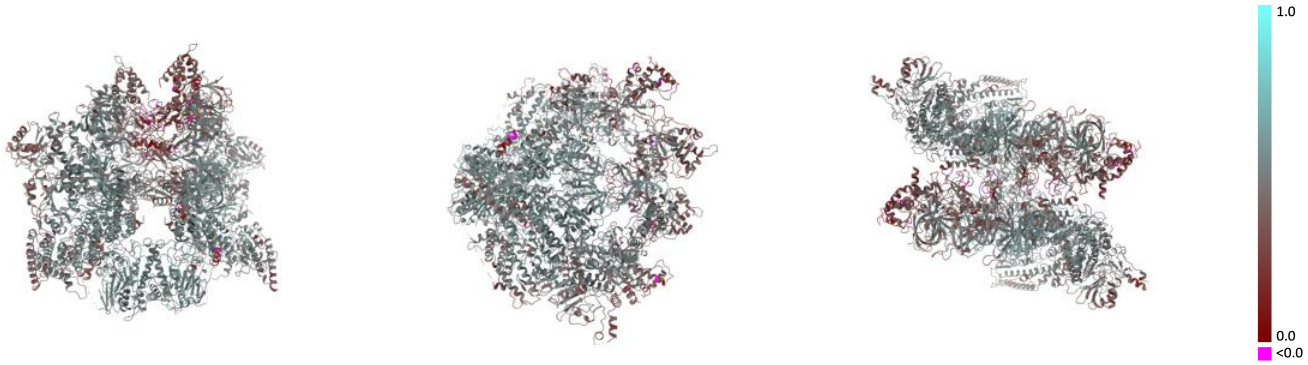
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

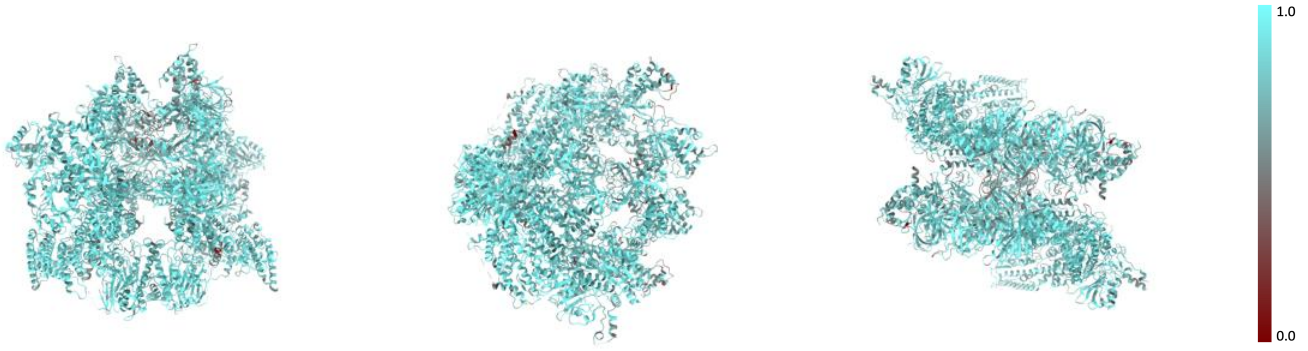
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

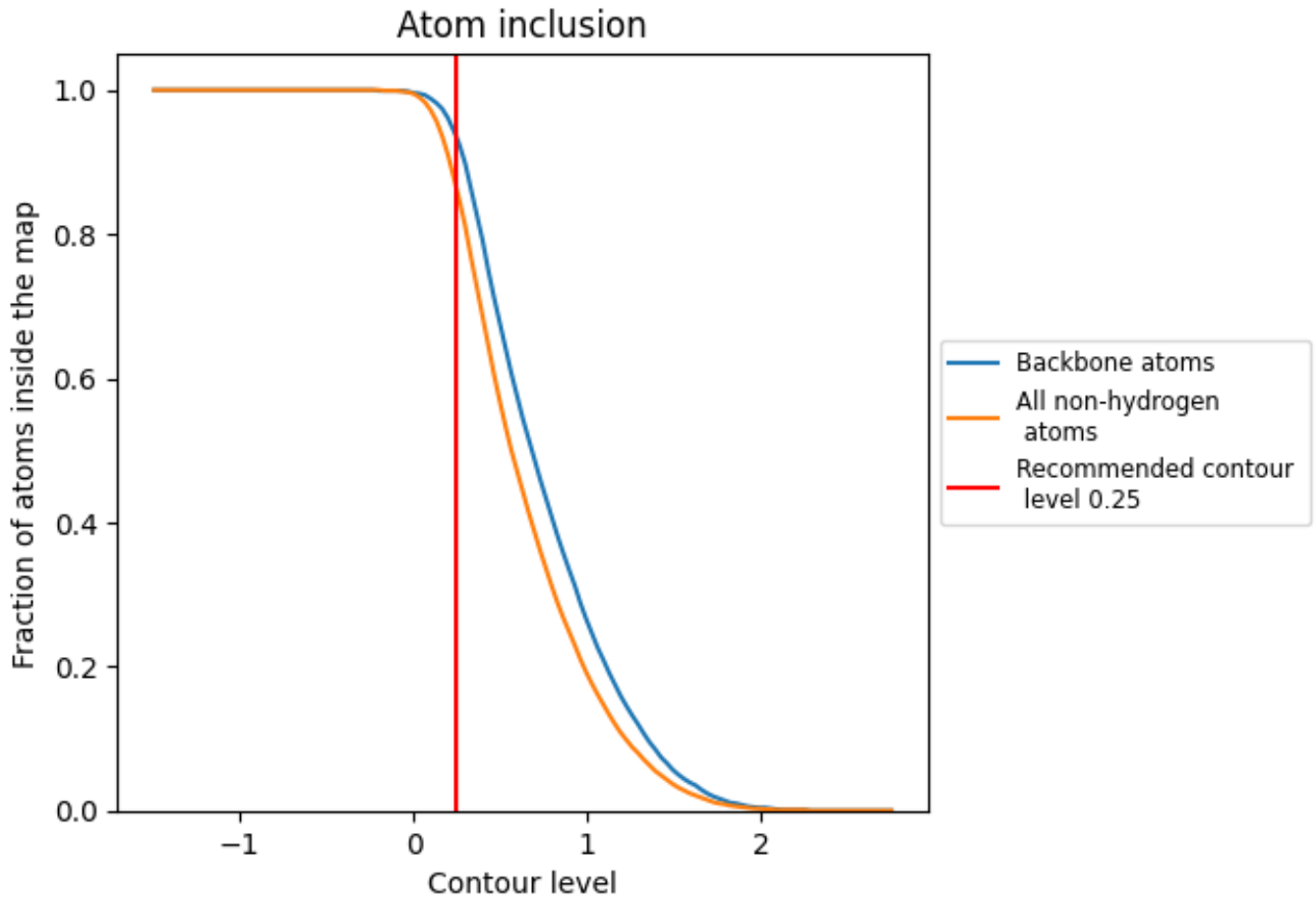
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 93% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.4710
2	0.8420	0.4600
3	0.9090	0.5270
4	0.7620	0.3370
5	0.9130	0.5390
6	0.7650	0.3590
7	0.8230	0.4030
A	0.8420	0.4610
B	0.9110	0.5300
C	0.7590	0.3410
D	0.9130	0.5380
E	0.7630	0.3620
F	0.8210	0.4040
G	0.8720	0.4660
H	0.9300	0.5350
I	0.9050	0.5290
J	0.8640	0.4770
K	0.8960	0.5050
L	0.8990	0.5220
M	0.8720	0.4690
N	0.9300	0.5390
O	0.9070	0.5290
P	0.8630	0.4780
Q	0.8960	0.5040
R	0.8980	0.5200