Full wwPDB EM Validation Report

Sep 26, 2024 – 01:38 pm BST

PDB ID	:	8S0D
EMDB ID	:	EMD-19622
Title	:	H. sapiens MCM bound to double stranded DNA and ORC1-6
Authors	:	Greiwe, J.F.; Weissmann, F.; Diffley, J.F.X.; Costa, A.
Deposited on	:	2024-02-13
Resolution	:	3.60 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:

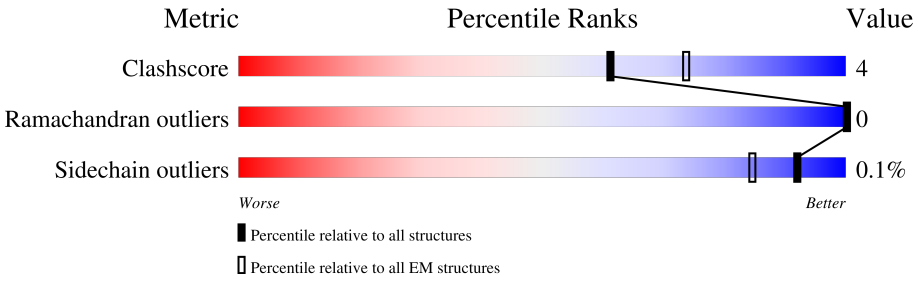
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.60 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

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	F	251	16% 63% 7% 30%
2	2	902	6% 64% 7% 29%
3	3	810	7% 66% 8% 26%
4	4	863	5% 67% 5% 28%
5	5	734	5% 75% 6% 19%
6	6	821	6% 74% 6% 21%
7	7	719	6% 69% 7% 24%
8	X	58	40% 48% 52%

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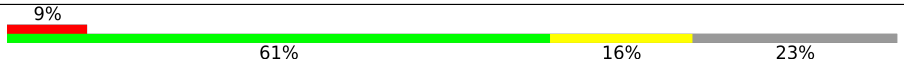
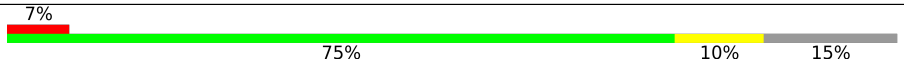
Mol	Chain	Length	Quality of chain
9	Y	58	
10	A	861	
11	B	577	
12	C	712	
13	D	436	
14	E	435	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 46024 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 Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	175	1341	846	232	250	13	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	643	5093	3206	909	948	30	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	598	4715	2954	837	898	26	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-1	GLY	-	expression tag	UNP P25205
3	0	GLU	-	expression tag	UNP P25205

- Molecule 4 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	623	4969	3130	880	932	27	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	650	MET	LEU	variant	UNP P33991

- Molecule 5 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	595	Total	C	N	O	S	0	0
			4679	2936	834	874	35		

- Molecule 6 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	652	Total	C	N	O	S	0	0
			5259	3322	930	980	27		

- Molecule 7 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	548	Total	C	N	O	S	0	0
			4338	2737	760	811	30		

- Molecule 8 is a DNA chain called DNA (58-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	58	Total	C	N	O	P	0	0
			1182	565	206	353	58		

- Molecule 9 is a DNA chain called DNA (58-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	58	Total	C	N	O	P	0	0
			1196	568	227	343	58		

- Molecule 10 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	113	Total	C	N	O	S	0	0
			890	558	153	171	8		

- Molecule 11 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	186	Total	C	N	O	S	0	0
			1538	996	254	283	5		

- Molecule 12 is a protein called Isoform 2 of Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	546	Total	C	N	O	S	0	0
			4481	2904	749	801	27		

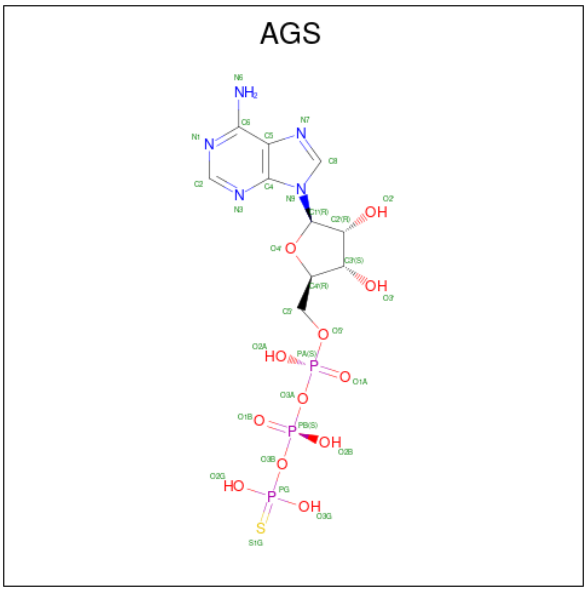
- Molecule 13 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	370	Total	C	N	O	S	0	0
			3029	1944	529	538	18		

- Molecule 14 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	375	Total	C	N	O	S	0	0
			3065	1997	503	555	10		

- Molecule 15 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
15	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
15	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
15	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
15	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
15	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

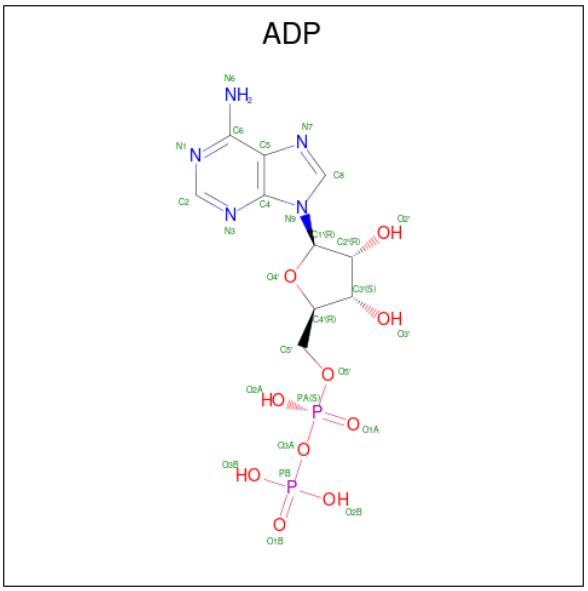
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	2	1	Total	Mg	0
			1	1	
16	3	1	Total	Mg	0
			1	1	
16	5	1	Total	Mg	0
			1	1	
16	6	1	Total	Mg	0
			1	1	
16	7	2	Total	Mg	0
			2	2	
16	D	1	Total	Mg	0
			1	1	
16	E	1	Total	Mg	0
			1	1	

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	
17	5	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



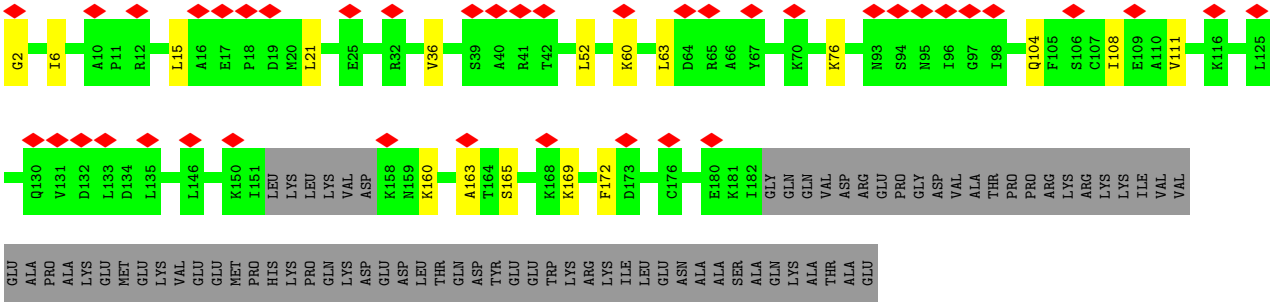
Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	5	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

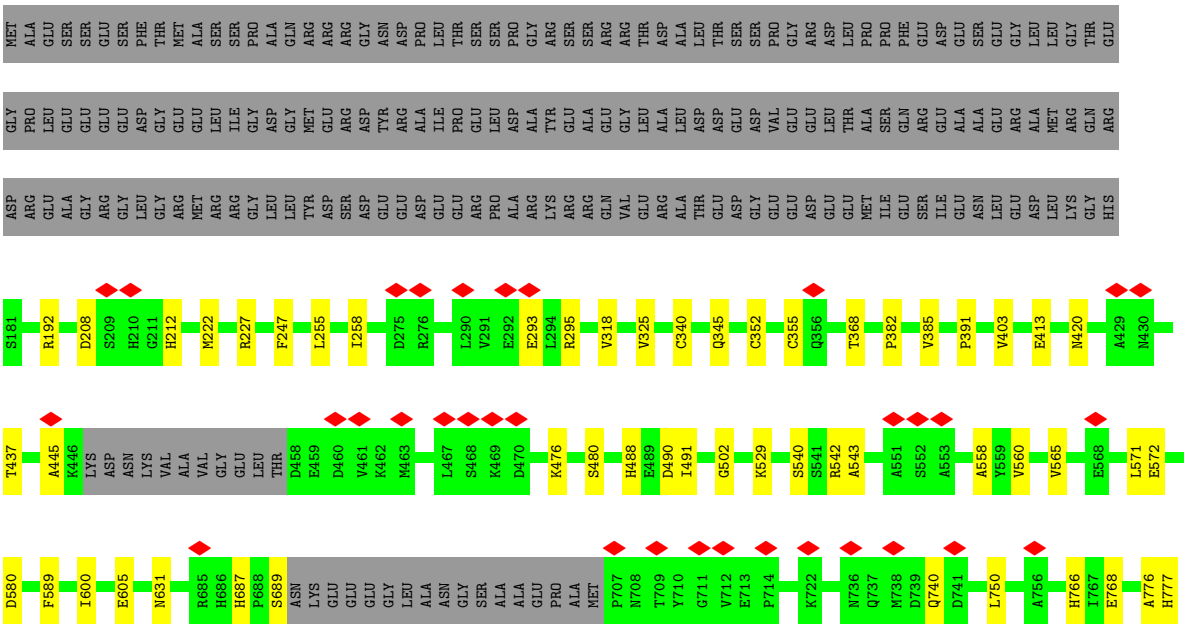
• Molecule 1: Origin recognition complex subunit 6

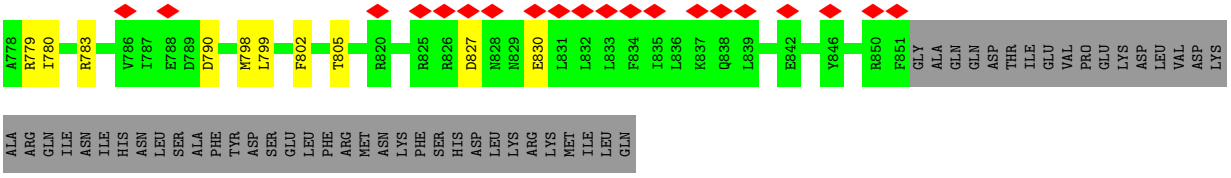
Chain F:



• Molecule 2: DNA replication licensing factor MCM2

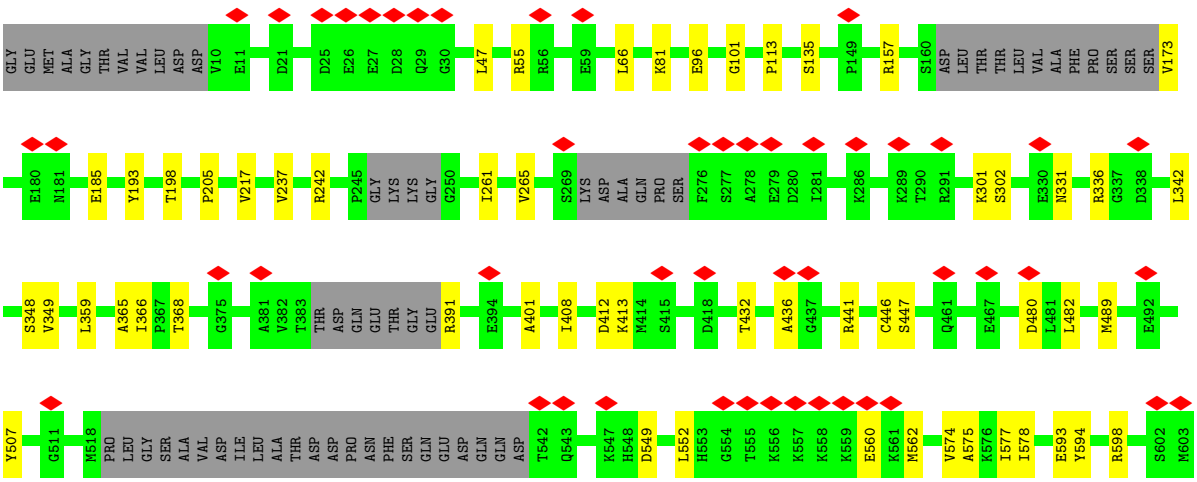
Chain 2:





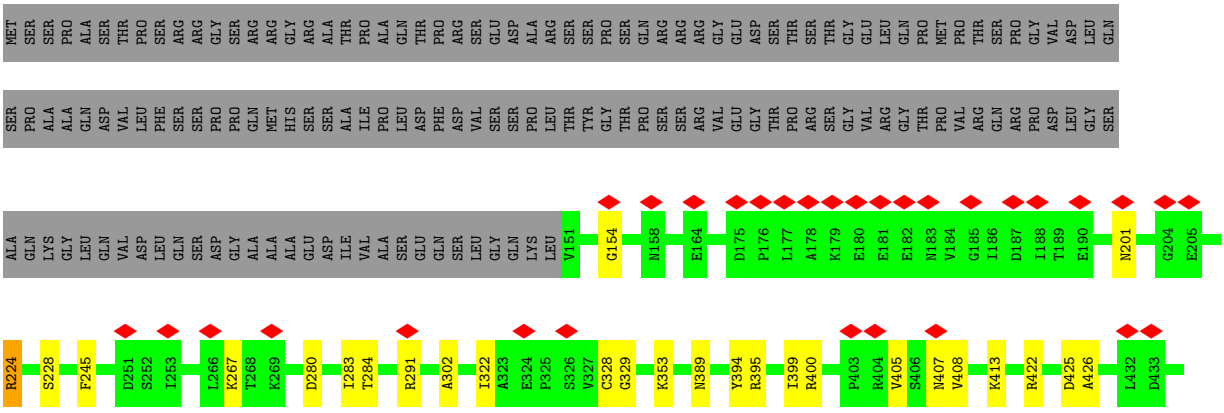
• Molecule 3: DNA replication licensing factor MCM3

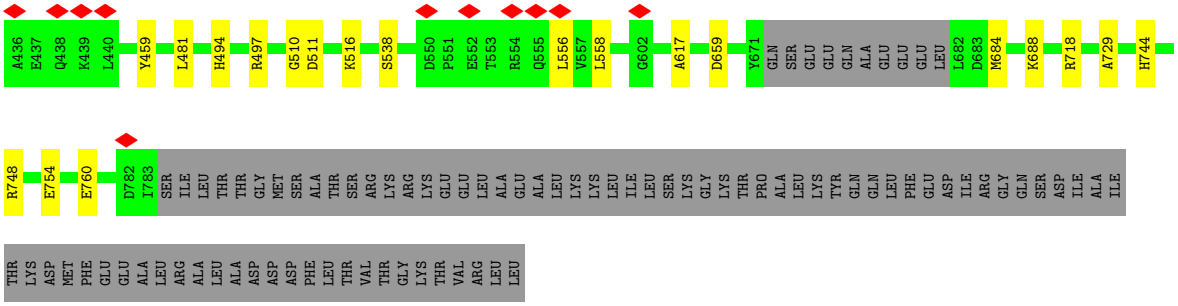
Chain 3:



• Molecule 4: DNA replication licensing factor MCM4

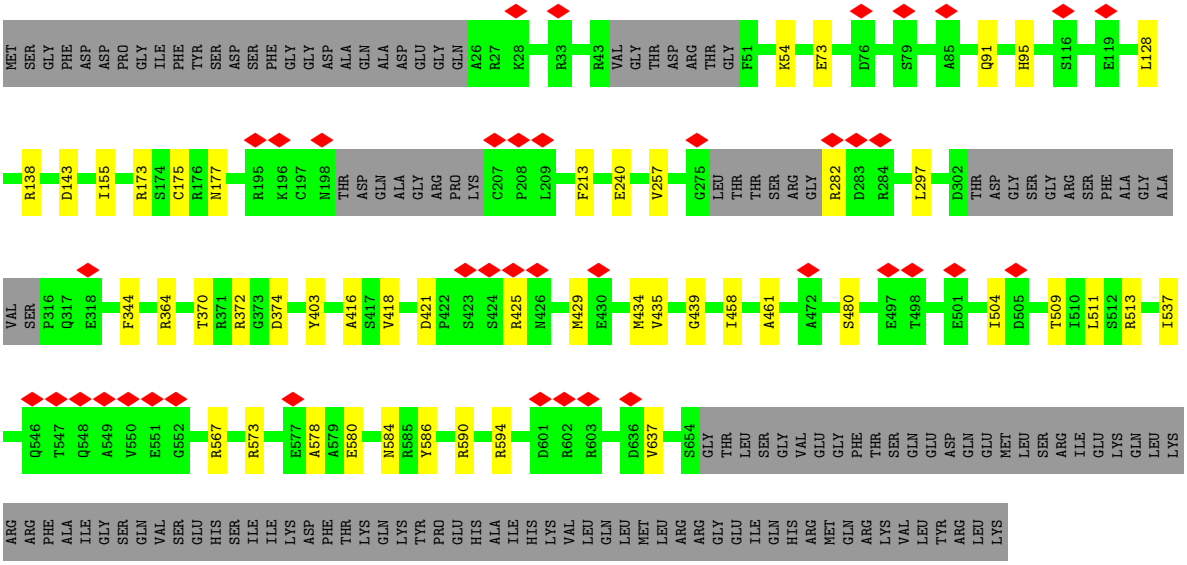
Chain 4:





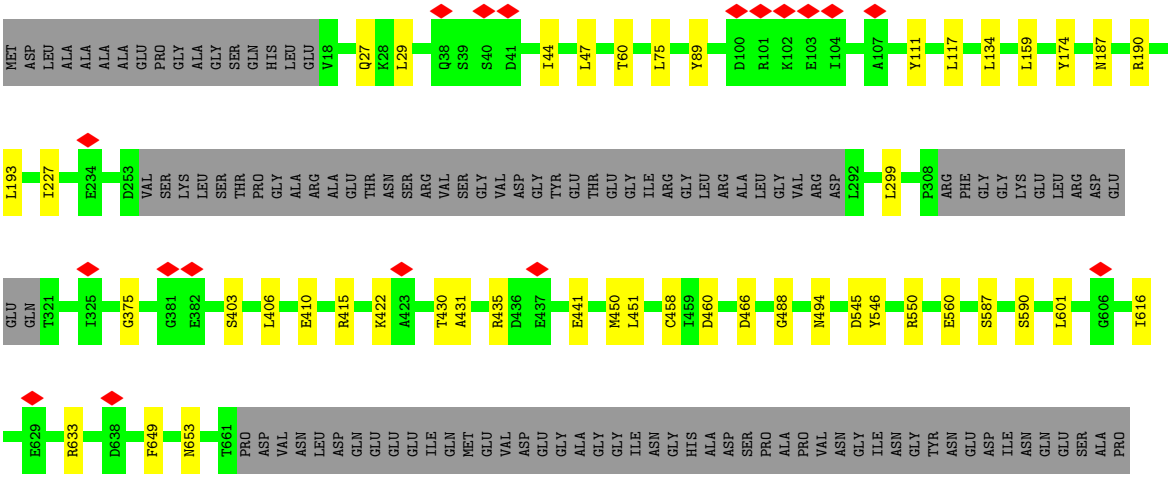
• Molecule 5: DNA replication licensing factor MCM5

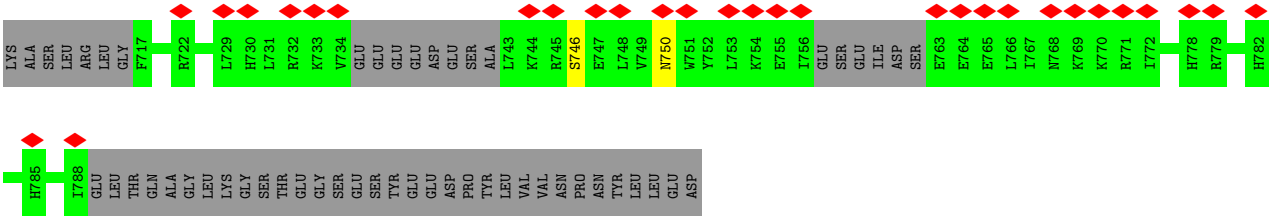
Chain 5:



• Molecule 6: DNA replication licensing factor MCM6

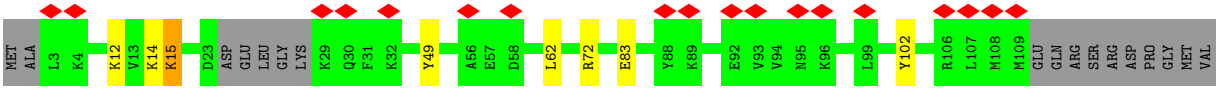
Chain 6:

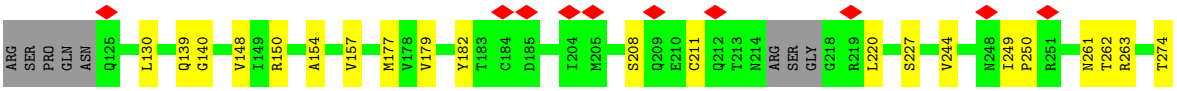


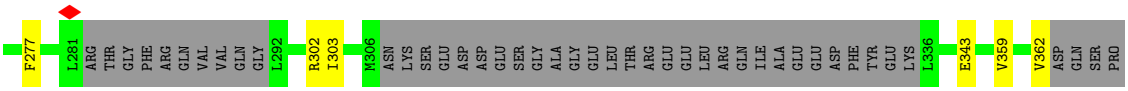


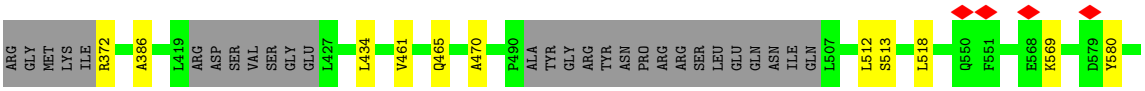
• Molecule 7: DNA replication licensing factor MCM7

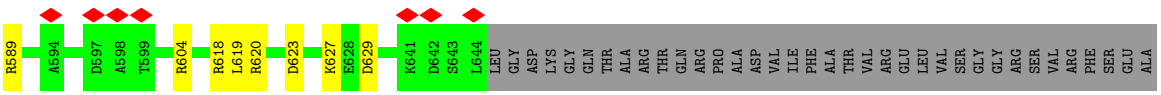
Chain 7:





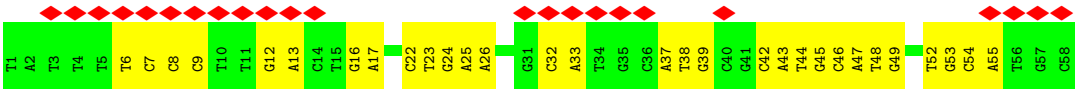






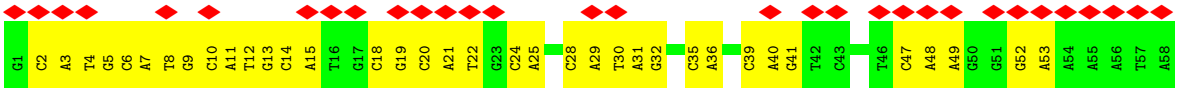
• Molecule 8: DNA (58-mer)

Chain X:



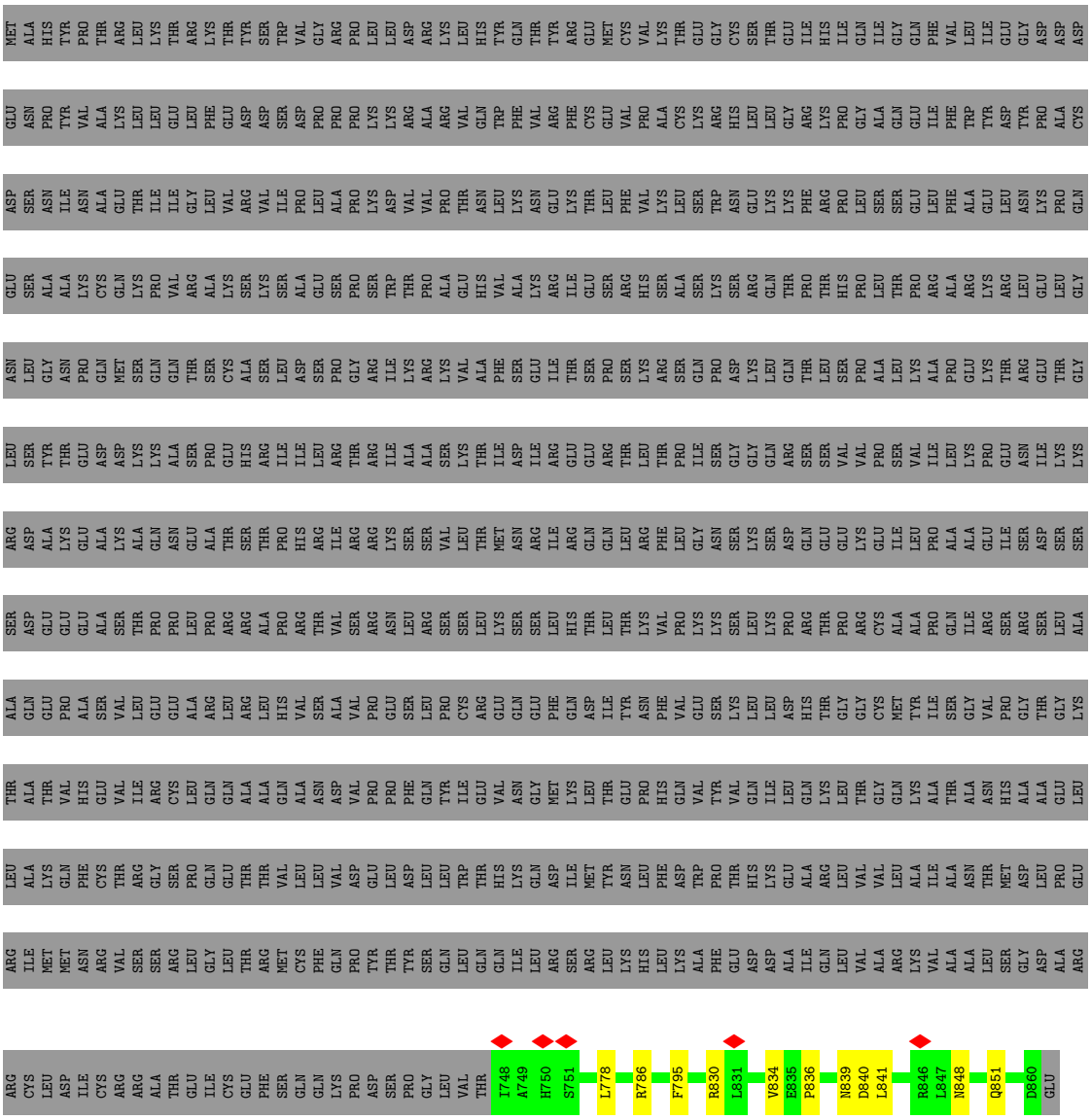
• Molecule 9: DNA (58-mer)

Chain Y:



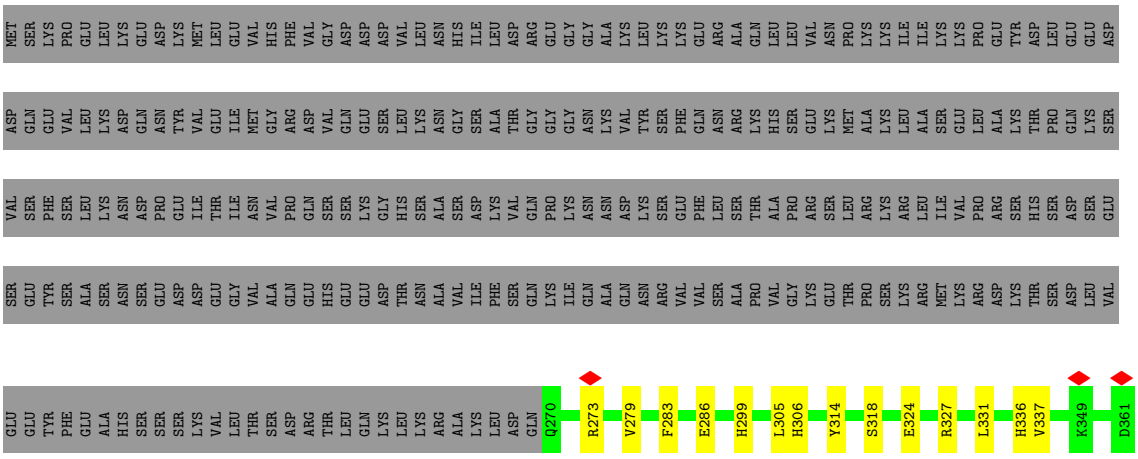
• Molecule 10: Origin recognition complex subunit 1

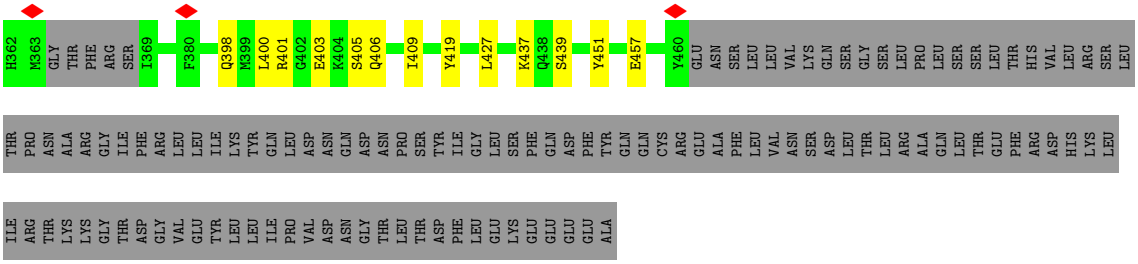
Chain A:



• Molecule 11: Origin recognition complex subunit 2

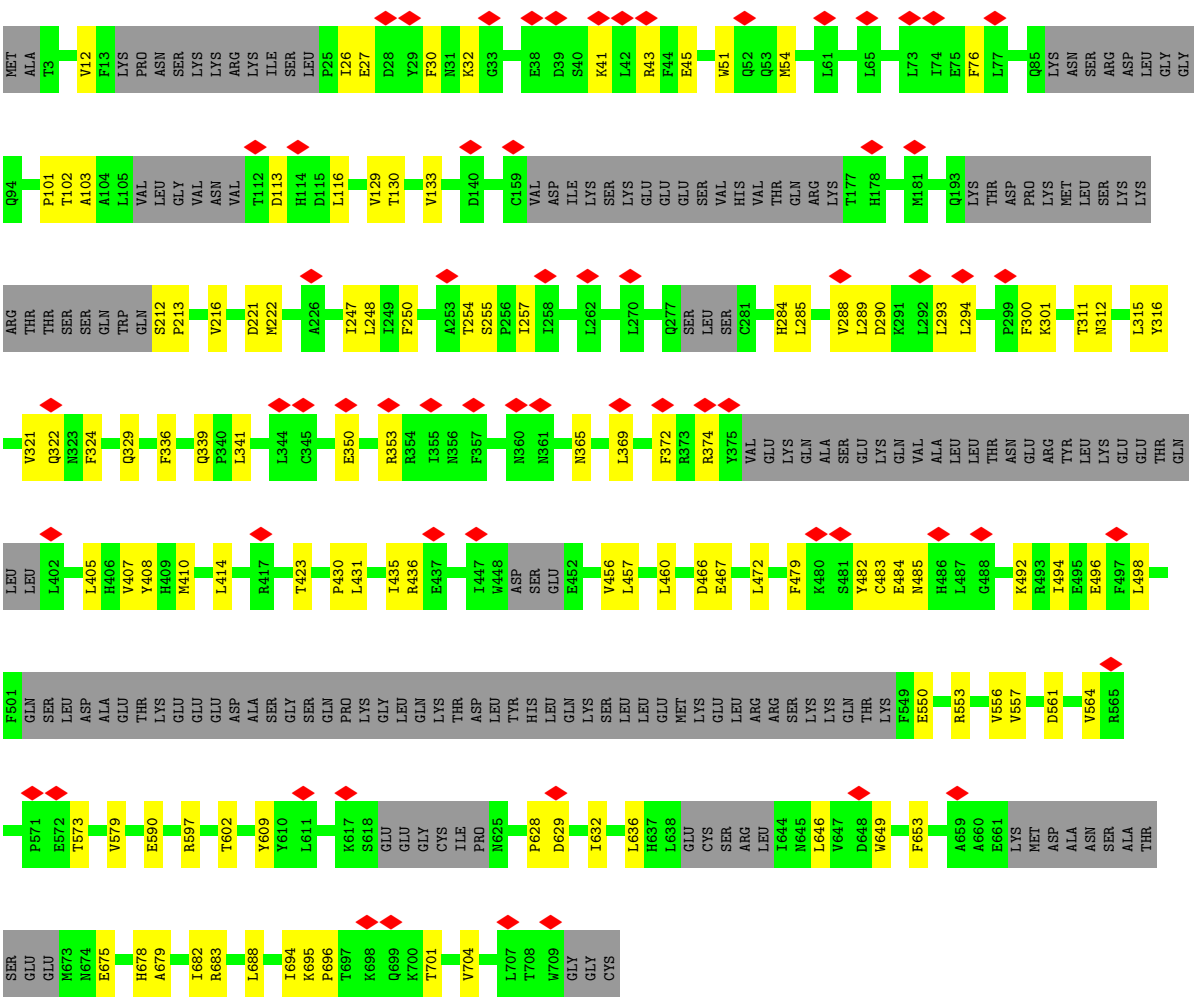
Chain B:





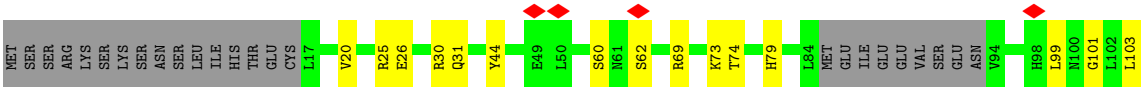
• Molecule 12: Isoform 2 of Origin recognition complex subunit 3

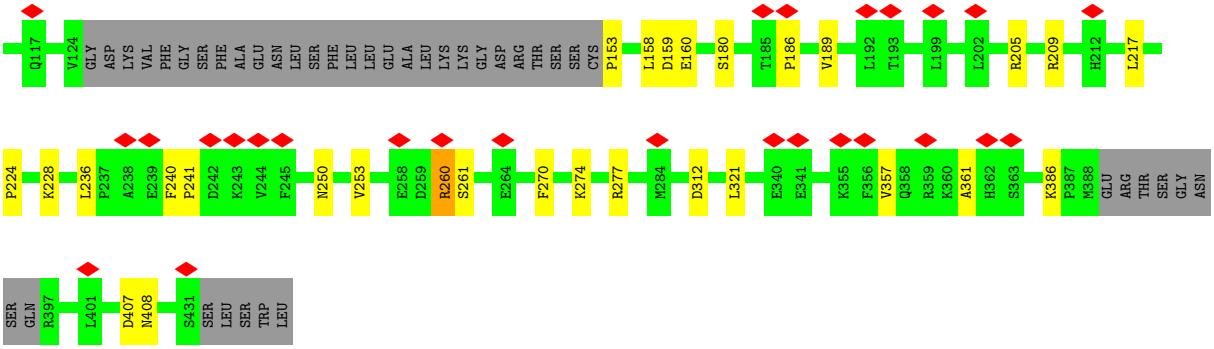
Chain C:



• Molecule 13: Origin recognition complex subunit 4

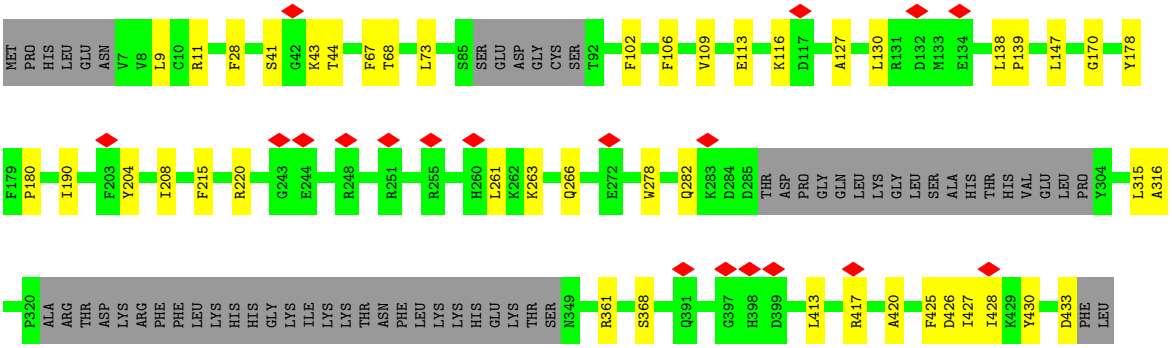
Chain D:





• Molecule 14: Origin recognition complex subunit 5

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182341	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 ($e^-/Å^2$)	49.28	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	48.610	Depositor
Minimum map value	-33.405	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.106	Depositor
Recommended contour level	7	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, MG, ADP, 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	F	0.23	0/1354	0.45	0/1817
2	2	0.23	0/5190	0.46	0/7015
3	3	0.23	0/4784	0.48	0/6447
4	4	0.23	0/5059	0.47	0/6841
5	5	0.24	0/4750	0.48	0/6386
6	6	0.24	0/5345	0.47	0/7207
7	7	0.23	0/4402	0.47	0/5942
8	X	0.51	0/1322	0.98	0/2037
9	Y	0.50	0/1344	0.89	0/2073
10	A	0.23	0/903	0.45	0/1219
11	B	0.23	0/1574	0.42	0/2131
12	C	0.24	0/4577	0.43	0/6184
13	D	0.24	0/3087	0.42	0/4161
14	E	0.24	0/3137	0.45	0/4260
All	All	0.26	0/46828	0.51	0/63720

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	F	1341	0	1418	20	0
2	2	5093	0	5097	40	0
3	3	4715	0	4760	36	0
4	4	4969	0	5002	29	0
5	5	4679	0	4755	28	0
6	6	5259	0	5313	29	0
7	7	4338	0	4402	34	0
8	X	1182	0	657	23	0
9	Y	1196	0	652	30	0
10	A	890	0	890	7	0
11	B	1538	0	1529	21	0
12	C	4481	0	4510	72	0
13	D	3029	0	3091	30	0
14	E	3065	0	3082	36	0
15	2	31	0	12	0	0
15	6	31	0	12	1	0
15	7	31	0	12	1	0
15	D	31	0	12	4	0
15	E	31	0	12	3	0
16	2	1	0	0	0	0
16	3	1	0	0	0	0
16	5	1	0	0	0	0
16	6	1	0	0	0	0
16	7	2	0	0	0	0
16	D	1	0	0	0	0
16	E	1	0	0	0	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
18	3	27	0	12	1	0
18	4	27	0	12	0	0
18	5	27	0	12	2	0
All	All	46024	0	45254	383	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 4.

All (383) 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)
7:7:208:SER:HB2	7:7:211:CYS:SG	1.99	1.01
1:F:60:LYS:HZ3	14:E:427:ILE:H	1.27	0.82
7:7:208:SER:CB	7:7:211:CYS:SG	2.66	0.79
1:F:2:GLY:N	2:2:340:CYS:HG	1.85	0.73
8:X:24:DG:N1	9:Y:36:DA:C6	2.59	0.70
13:D:26:GLU:HG2	13:D:30:ARG:HH12	1.55	0.70
12:C:339:GLN:HE22	12:C:579:VAL:HA	1.56	0.69
1:F:6:ILE:HG23	1:F:52:LEU:HD21	1.75	0.69
4:4:659:ASP:OD1	7:7:589:ARG:NH1	2.25	0.68
9:Y:21:DA:H2"	9:Y:22:DT:H5"	1.74	0.68
2:2:777:HIS:ND1	2:2:790:ASP:OD1	2.26	0.67
6:6:60:THR:HG22	6:6:111:TYR:HB2	1.75	0.67
3:3:507:TYR:O	5:5:573:ARG:NH1	2.27	0.67
13:D:31:GLN:HG2	15:D:901:AGS:H5'2	1.76	0.67
11:B:400:LEU:O	11:B:406:GLN:NE2	2.28	0.67
2:2:565:VAL:HA	6:6:488:GLY:HA2	1.77	0.67
4:4:224:ARG:NH1	4:4:228:SER:OG	2.28	0.66
1:F:60:LYS:NZ	14:E:428:ILE:HG12	2.10	0.66
2:2:325:VAL:HA	2:2:368:THR:HG23	1.79	0.64
4:4:302:ALA:HB2	4:4:322:ILE:HD13	1.80	0.64
4:4:328:CYS:SG	4:4:329:GLY:N	2.71	0.64
7:7:262:THR:HG22	7:7:263:ARG:HG3	1.80	0.63
5:5:586:TYR:OH	5:5:590:ARG:NH2	2.27	0.63
6:6:406:LEU:HG	6:6:458:CYS:HB3	1.81	0.63
11:B:327:ARG:HA	11:B:331:LEU:HB2	1.82	0.62
2:2:502:GLY:O	2:2:779:ARG:NH1	2.31	0.62
12:C:293:LEU:O	12:C:301:LYS:NZ	2.30	0.62
3:3:366:ILE:HD12	3:3:401:ALA:HB2	1.82	0.61
12:C:350:GLU:HA	12:C:353:ARG:HG2	1.82	0.61
13:D:357:VAL:HA	13:D:361:ALA:HB3	1.82	0.61
2:2:420:ASN:HD21	2:2:437:THR:HG22	1.64	0.61
2:2:488:HIS:HB3	2:2:491:ILE:HD12	1.81	0.60
9:Y:47:DC:H2"	9:Y:48:DA:H5"	1.82	0.60
4:4:201:ASN:HB2	4:4:245:PHE:HE1	1.66	0.60
12:C:76:PHE:CE2	12:C:103:ALA:HB2	2.36	0.60
4:4:494:HIS:ND1	6:6:560:GLU:OE1	2.33	0.60
5:5:509:THR:O	5:5:513:ARG:NH1	2.33	0.60
7:7:620:ARG:NH2	7:7:629:ASP:OD1	2.33	0.59
4:4:405:VAL:HG12	4:4:407:ASN:H	1.67	0.59
4:4:497:ARG:NH2	15:6:901:AGS:O3'	2.35	0.59
3:3:574:VAL:HA	3:3:577:ILE:HD12	1.83	0.59
5:5:578:ALA:HB1	5:5:637:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:38:DT:H2"	8:X:39:DG:C8	2.38	0.59
11:B:403:GLU:O	11:B:437:LYS:NZ	2.36	0.59
2:2:558:ALA:HA	2:2:572:GLU:O	2.03	0.59
8:X:42:DC:H2"	8:X:43:DA:C8	2.38	0.59
12:C:483:CYS:SG	12:C:484:GLU:N	2.76	0.59
4:4:400:ARG:HA	4:4:408:VAL:HG12	1.85	0.58
12:C:129:VAL:HG12	12:C:130:THR:HG23	1.85	0.58
6:6:649:PHE:O	6:6:653:ASN:ND2	2.36	0.58
8:X:12:DG:H2"	8:X:13:DA:C8	2.37	0.58
13:D:44:TYR:HH	13:D:79:HIS:HD1	1.52	0.58
4:4:283:ILE:HD12	4:4:394:TYR:HB2	1.86	0.58
5:5:138:ARG:NH1	5:5:240:GLU:OE2	2.37	0.57
12:C:646:LEU:HD12	12:C:701:THR:HG22	1.86	0.57
14:E:215:PHE:HE2	14:E:261:LEU:HD12	1.68	0.57
5:5:175:CYS:SG	5:5:177:ASN:ND2	2.64	0.57
8:X:22:DC:H2'	8:X:23:DT:H71	1.86	0.57
12:C:133:VAL:HG22	12:C:216:VAL:HB	1.86	0.57
5:5:54:LYS:NZ	5:5:73:GLU:OE1	2.38	0.57
3:3:359:LEU:HD23	3:3:365:ALA:HB1	1.87	0.57
3:3:237:VAL:HG22	3:3:265:VAL:HG12	1.86	0.57
11:B:398:GLN:OE1	11:B:401:ARG:NH1	2.38	0.57
4:4:291:ARG:HD2	4:4:353:LYS:HD2	1.87	0.56
12:C:374:ARG:NH1	12:C:573:THR:O	2.38	0.56
12:C:695:LYS:H	12:C:704:VAL:HG11	1.70	0.56
3:3:336:ARG:NH2	3:3:480:ASP:OD2	2.38	0.56
5:5:91:GLN:O	5:5:95:HIS:ND1	2.39	0.56
9:Y:10:DC:H2"	9:Y:11:DA:C8	2.41	0.56
6:6:27:GLN:HG3	6:6:89:TYR:HB3	1.86	0.56
1:F:104:GLN:HG2	14:E:430:TYR:HA	1.88	0.56
8:X:54:DC:H2"	8:X:55:DA:C8	2.41	0.56
9:Y:40:DA:H2"	9:Y:41:DG:C8	2.40	0.56
11:B:314:TYR:OH	12:C:590:GLU:OE2	2.24	0.56
4:4:399:ILE:HD11	4:4:413:LYS:HB2	1.88	0.56
6:6:415:ARG:NH1	6:6:451:LEU:O	2.39	0.56
11:B:273:ARG:NH2	12:C:679:ALA:O	2.39	0.55
6:6:29:LEU:HB3	6:6:75:LEU:HD22	1.88	0.55
8:X:24:DG:C2	9:Y:36:DA:N1	2.74	0.55
9:Y:30:DT:H2"	9:Y:31:DA:C8	2.42	0.55
6:6:601:LEU:HG	6:6:616:ILE:HD13	1.87	0.55
10:A:834:VAL:HG13	10:A:836:PRO:HD3	1.87	0.55
1:F:60:LYS:HZ1	14:E:428:ILE:HG12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:277:ARG:NH2	15:D:901:AGS:S1G	2.78	0.55
14:E:44:THR:HB	15:E:501:AGS:O1B	2.06	0.55
1:F:160:LYS:HE2	14:E:433:ASP:HA	1.88	0.55
2:2:529:LYS:NZ	2:2:631:ASN:OD1	2.38	0.55
7:7:130:LEU:HB2	7:7:179:VAL:HG11	1.89	0.55
12:C:294:LEU:HD21	12:C:435:ILE:HG12	1.89	0.55
12:C:407:VAL:HA	12:C:410:MET:HG2	1.89	0.55
1:F:165:SER:HB3	1:F:172:PHE:HZ	1.73	0.54
11:B:337:VAL:HG23	12:C:12:VAL:HG22	1.89	0.54
9:Y:39:DC:H2"	9:Y:40:DA:C8	2.42	0.54
7:7:244:VAL:HG21	7:7:250:PRO:HG3	1.88	0.54
10:A:786:ARG:NH2	10:A:851:GLN:OE1	2.40	0.54
5:5:416:ALA:HB2	5:5:435:VAL:HG21	1.89	0.54
6:6:375:GLY:O	6:6:633:ARG:NH1	2.41	0.54
3:3:489:MET:O	5:5:594:ARG:NH1	2.41	0.54
7:7:14:LYS:NZ	7:7:83:GLU:OE1	2.38	0.54
2:2:687:HIS:CD2	2:2:689:SER:H	2.26	0.53
6:6:159:LEU:HD12	6:6:190:ARG:HB3	1.89	0.53
3:3:391:ARG:NH1	3:3:436:ALA:O	2.41	0.53
3:3:628:HIS:HB3	3:3:641:ASP:OD1	2.09	0.53
8:X:6:DT:H2"	8:X:7:DC:C6	2.44	0.53
9:Y:28:DC:H2"	9:Y:29:DA:C8	2.44	0.53
12:C:254:THR:HG22	12:C:255:SER:H	1.74	0.53
2:2:768:GLU:OE2	18:5:801:ADP:O2'	2.26	0.53
6:6:430:THR:OG1	6:6:431:ALA:N	2.41	0.53
12:C:695:LYS:HD3	12:C:696:PRO:HD2	1.90	0.52
12:C:102:THR:HG22	12:C:248:LEU:HB2	1.91	0.52
12:C:423:THR:HG21	12:C:431:LEU:HB2	1.91	0.52
7:7:182:TYR:HB3	7:7:220:LEU:HB3	1.92	0.52
12:C:311:THR:HG22	12:C:436:ARG:HH21	1.74	0.52
13:D:20:VAL:HG23	13:D:236:LEU:HD21	1.91	0.52
7:7:261:ASN:HB3	7:7:303:ILE:HD12	1.90	0.52
7:7:359:VAL:HG21	7:7:619:LEU:HD21	1.91	0.52
13:D:25:ARG:NH1	14:E:28:PHE:O	2.43	0.52
5:5:143:ASP:OD1	5:5:143:ASP:N	2.42	0.52
5:5:364:ARG:HG2	5:5:370:THR:HG22	1.92	0.52
8:X:25:DA:H2"	8:X:26:DA:C8	2.44	0.52
9:Y:52:DG:H2"	9:Y:53:DA:C8	2.44	0.52
3:3:482:LEU:HD12	3:3:611:SER:HB2	1.91	0.52
6:6:422:LYS:NZ	6:6:466:ASP:OD1	2.42	0.52
4:4:718:ARG:NH1	6:6:545:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:7:DC:H2”	8:X:8:DC:C5	2.45	0.52
14:E:263:LYS:NZ	14:E:266:GLN:OE1	2.38	0.52
6:6:187:ASN:ND2	6:6:190:ARG:O	2.43	0.51
7:7:148:VAL:HG12	7:7:150:ARG:H	1.76	0.51
2:2:382:PRO:O	6:6:494:ASN:ND2	2.43	0.51
1:F:60:LYS:NZ	14:E:427:ILE:H	2.05	0.51
2:2:385:VAL:HG21	2:2:391:PRO:HG3	1.92	0.51
3:3:242:ARG:HD3	3:3:261:ILE:HD12	1.92	0.51
13:D:312:ASP:OD1	13:D:312:ASP:N	2.42	0.51
14:E:420:ALA:HB1	14:E:425:PHE:O	2.09	0.51
1:F:60:LYS:HZ3	14:E:427:ILE:N	2.03	0.51
1:F:76:LYS:HE2	1:F:163:ALA:HB1	1.93	0.51
2:2:352:CYS:HB3	2:2:355:CYS:SG	2.50	0.51
2:2:605:GLU:OE2	5:5:403:TYR:OH	2.29	0.51
3:3:47:LEU:O	3:3:101:GLY:N	2.43	0.51
3:3:593:GLU:OE1	3:3:646:VAL:HG21	2.11	0.51
9:Y:6:DC:H2”	9:Y:7:DA:C8	2.46	0.50
9:Y:24:DC:H2”	9:Y:25:DA:C8	2.46	0.50
10:A:795:PHE:HD2	10:A:841:LEU:HD12	1.76	0.50
9:Y:18:DC:H2”	9:Y:19:DG:C8	2.45	0.50
3:3:157:ARG:NH1	3:3:173:VAL:O	2.42	0.50
8:X:24:DG:C2	9:Y:36:DA:C2	3.00	0.50
11:B:427:LEU:HD11	12:C:597:ARG:HG3	1.93	0.50
3:3:55:ARG:HH21	3:3:66:LEU:HD11	1.76	0.50
6:6:746:SER:O	6:6:750:ASN:ND2	2.45	0.49
9:Y:14:DC:H2”	9:Y:15:DA:C8	2.47	0.49
3:3:301:LYS:NZ	3:3:560:GLU:OE1	2.45	0.49
9:Y:48:DA:H2”	9:Y:49:DA:H5”	1.95	0.49
12:C:101:PRO:HG2	12:C:247:ILE:HG12	1.92	0.49
13:D:321:LEU:O	14:E:220:ARG:NH1	2.44	0.49
14:E:316:ALA:O	14:E:361:ARG:NH2	2.34	0.49
2:2:222:MET:HG2	2:2:227:ARG:HB2	1.93	0.49
6:6:187:ASN:HD21	6:6:190:ARG:HB2	1.76	0.49
11:B:279:VAL:HG21	12:C:683:ARG:HH22	1.78	0.49
14:E:215:PHE:CE2	14:E:261:LEU:HD12	2.46	0.49
12:C:43:ARG:NE	12:C:336:PHE:O	2.46	0.49
12:C:636:LEU:HD22	12:C:649:TRP:CD1	2.48	0.49
1:F:108:ILE:HD13	14:E:368:SER:HB2	1.95	0.49
14:E:41:SER:OG	14:E:43:LYS:NZ	2.42	0.49
5:5:418:VAL:HG22	5:5:429:MET:HG2	1.94	0.48
7:7:12:LYS:HE2	7:7:62:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:459:TYR:HE1	4:4:481:LEU:HD23	1.79	0.48
4:4:511:ASP:N	4:4:511:ASP:OD1	2.42	0.48
9:Y:18:DC:H2"	9:Y:19:DG:H8	1.79	0.48
12:C:254:THR:HG22	12:C:255:SER:N	2.28	0.48
1:F:169:LYS:HA	1:F:172:PHE:HD2	1.77	0.48
6:6:406:LEU:O	6:6:410:GLU:HG3	2.13	0.48
8:X:52:DT:H2"	8:X:53:DG:C8	2.48	0.48
1:F:108:ILE:O	1:F:111:VAL:HB	2.13	0.48
3:3:81:LYS:NZ	3:3:96:GLU:O	2.35	0.48
2:2:542:ARG:NH1	2:2:580:ASP:O	2.46	0.48
12:C:472:LEU:HB3	12:C:498:LEU:HD13	1.95	0.48
1:F:60:LYS:HG3	14:E:417:ARG:NH2	2.29	0.48
11:B:405:SER:O	11:B:409:ILE:HG12	2.14	0.48
14:E:44:THR:CB	15:E:501:AGS:O1B	2.60	0.48
7:7:513:SER:O	7:7:604:ARG:NH1	2.46	0.48
9:Y:39:DC:H2"	9:Y:40:DA:N7	2.28	0.48
10:A:840:ASP:OD1	10:A:840:ASP:N	2.43	0.48
3:3:302:SER:OG	3:3:562:MET:SD	2.59	0.48
11:B:331:LEU:HD12	11:B:336:HIS:HB3	1.96	0.48
3:3:193:TYR:HB2	7:7:154:ALA:HB1	1.95	0.47
7:7:150:ARG:NH2	7:7:249:ILE:O	2.47	0.47
8:X:24:DG:N1	9:Y:36:DA:N1	2.62	0.47
12:C:460:LEU:HD21	12:C:557:VAL:HG13	1.95	0.47
13:D:260:ARG:NH1	13:D:261:SER:HB3	2.29	0.47
14:E:113:GLU:HA	14:E:116:LYS:HE2	1.95	0.47
14:E:11:ARG:HG3	15:E:501:AGS:HN62	1.79	0.47
8:X:24:DG:C2	9:Y:36:DA:C6	3.01	0.47
5:5:421:ASP:O	5:5:425:ARG:N	2.43	0.47
9:Y:31:DA:H2"	9:Y:32:DG:C8	2.48	0.47
1:F:60:LYS:NZ	14:E:426:ASP:OD1	2.44	0.47
2:2:247:PHE:HB3	2:2:255:LEU:HD11	1.96	0.47
2:2:318:VAL:HG13	2:2:403:VAL:HG11	1.95	0.47
6:6:117:LEU:HD21	6:6:134:LEU:HG	1.97	0.47
3:3:594:TYR:CZ	3:3:598:ARG:HD2	2.50	0.47
4:4:280:ASP:OD1	4:4:395:ARG:NH1	2.42	0.47
12:C:430:PRO:HB2	12:C:456:VAL:HG22	1.97	0.47
5:5:173:ARG:HD2	5:5:213:PHE:HE1	1.79	0.47
14:E:178:TYR:CE2	14:E:180:PRO:HA	2.49	0.47
11:B:283:PHE:HB3	11:B:286:GLU:HB3	1.97	0.47
12:C:629:ASP:HB2	12:C:653:PHE:HZ	1.79	0.47
3:3:342:LEU:HB3	3:3:482:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:575:ALA:HA	3:3:578:ILE:HD12	1.98	0.46
12:C:550:GLU:HA	12:C:553:ARG:HE	1.80	0.46
2:2:776:ALA:O	2:2:780:ILE:HG13	2.16	0.46
7:7:49:TYR:HB3	7:7:139:GLN:HE21	1.80	0.46
12:C:113:ASP:O	12:C:116:LEU:HG	2.16	0.46
13:D:103:LEU:HD11	14:E:147:LEU:HD13	1.98	0.46
9:Y:8:DT:H2"	9:Y:9:DG:C8	2.50	0.46
9:Y:12:DT:H2"	9:Y:13:DG:C8	2.50	0.46
13:D:224:PRO:O	13:D:228:LYS:HG2	2.16	0.46
5:5:155:ILE:HG13	5:5:257:VAL:HG11	1.97	0.46
12:C:27:GLU:HA	12:C:30:PHE:HB2	1.98	0.46
12:C:54:MET:HE3	12:C:300:PHE:HE1	1.81	0.45
12:C:339:GLN:HE21	12:C:341:LEU:HB3	1.81	0.45
3:3:205:PRO:HB3	5:5:429:MET:SD	2.56	0.45
8:X:46:DC:H2"	8:X:47:DA:C8	2.51	0.45
11:B:318:SER:OG	11:B:457:GLU:OE2	2.27	0.45
14:E:106:PHE:HA	14:E:109:VAL:HG12	1.99	0.45
3:3:446:CYS:SG	3:3:447:SER:N	2.90	0.45
12:C:289:LEU:HD11	12:C:324:PHE:CE1	2.52	0.45
12:C:482:TYR:O	12:C:485:ASN:ND2	2.41	0.45
4:4:718:ARG:HD2	4:4:729:ALA:HB3	1.97	0.45
3:3:607:THR:HG22	3:3:656:LYS:HG2	1.99	0.45
8:X:48:DT:H2"	8:X:49:DG:C8	2.52	0.45
2:2:589:PHE:HE1	2:2:600:ILE:HD13	1.82	0.45
6:6:403:SER:OG	6:6:460:ASP:OD2	2.35	0.45
13:D:99:LEU:O	13:D:159:ASP:N	2.48	0.45
8:X:24:DG:N1	9:Y:36:DA:N6	2.65	0.44
2:2:293:GLU:OE1	2:2:295:ARG:NH2	2.51	0.44
11:B:439:SER:OG	12:C:322:GLN:OE1	2.35	0.44
2:2:208:ASP:OD1	2:2:212:HIS:N	2.50	0.44
12:C:257:ILE:HD12	12:C:257:ILE:H	1.82	0.44
12:C:457:LEU:HA	12:C:460:LEU:HB3	2.00	0.44
13:D:270:PHE:CE1	13:D:274:LYS:HE3	2.52	0.44
13:D:60:SER:OG	13:D:180:SER:O	2.23	0.44
7:7:434:LEU:HD13	7:7:461:VAL:HG21	1.99	0.44
1:F:15:LEU:HD21	1:F:63:LEU:HD21	1.99	0.44
2:2:490:ASP:OD1	2:2:490:ASP:N	2.51	0.44
5:5:580:GLU:O	5:5:584:ASN:ND2	2.51	0.44
13:D:73:LYS:N	15:D:901:AGS:O2B	2.50	0.44
2:2:827:ASP:HB3	2:2:830:GLU:HG3	1.99	0.44
3:3:135:SER:HG	3:3:198:THR:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:44:DT:H2"	8:X:45:DG:C8	2.53	0.44
3:3:549:ASP:HB3	3:3:552:LEU:HB2	1.99	0.44
5:5:439:GLY:O	5:5:567:ARG:NH1	2.46	0.44
7:7:512:LEU:HA	7:7:518:LEU:HD11	1.99	0.44
12:C:41:LYS:O	12:C:45:GLU:HG2	2.16	0.44
12:C:51:TRP:CH2	12:C:329:GLN:HB3	2.53	0.44
14:E:73:LEU:HD13	14:E:102:PHE:HB2	1.99	0.44
12:C:629:ASP:HA	12:C:632:ILE:HD12	1.98	0.43
14:E:127:ALA:HB1	14:E:130:LEU:HD12	2.00	0.43
1:F:60:LYS:HZ2	14:E:428:ILE:HG12	1.83	0.43
12:C:285:LEU:HA	12:C:288:VAL:HG12	1.98	0.43
12:C:479:PHE:HE2	12:C:494:ILE:HG21	1.83	0.43
14:E:204:TYR:O	14:E:208:ILE:HG12	2.18	0.43
4:4:389:ASN:HB2	4:4:422:ARG:HB3	2.00	0.43
8:X:7:DC:H2"	8:X:8:DC:H5	1.83	0.43
5:5:504:ILE:HG21	5:5:511:LEU:HD11	2.00	0.43
6:6:227:ILE:HB	6:6:299:LEU:HD23	2.01	0.43
6:6:587:SER:HG	6:6:590:SER:HG	1.65	0.43
12:C:311:THR:O	12:C:315:LEU:HG	2.18	0.43
2:2:420:ASN:ND2	2:2:437:THR:HG22	2.33	0.43
3:3:633:MET:H	3:3:633:MET:HG2	1.65	0.43
5:5:372:ARG:HG2	5:5:374:ASP:H	1.83	0.43
11:B:305:LEU:HD21	11:B:419:TYR:HB3	1.99	0.43
12:C:688:LEU:HD23	12:C:694:ILE:HD13	2.01	0.43
2:2:687:HIS:HD2	2:2:689:SER:H	1.65	0.43
7:7:12:LYS:O	7:7:15:LYS:HG3	2.18	0.43
8:X:37:DA:H1'	8:X:38:DT:H5'	2.01	0.43
12:C:561:ASP:HA	12:C:564:VAL:HG12	2.01	0.43
7:7:177:MET:SD	7:7:227:SER:HB3	2.59	0.43
9:Y:4:DT:H2"	9:Y:5:DG:C8	2.53	0.43
10:A:830:ARG:O	10:A:848:ASN:ND2	2.36	0.43
14:E:9:LEU:HD12	14:E:190:ILE:HA	2.00	0.43
5:5:458:ILE:HA	5:5:461:ALA:HB3	2.01	0.43
13:D:69:ARG:NE	14:E:170:GLY:O	2.51	0.43
4:4:556:LEU:HD21	9:Y:20:DC:H5"	2.01	0.43
8:X:16:DG:H2"	8:X:17:DA:C8	2.53	0.43
11:B:299:HIS:HB2	12:C:32:LYS:HD2	2.00	0.43
11:B:451:TYR:HE2	12:C:628:PRO:HG2	1.84	0.43
7:7:157:VAL:HA	7:7:277:PHE:HD2	1.84	0.42
3:3:349:VAL:HG12	3:3:349:VAL:O	2.18	0.42
4:4:684:MET:HG2	4:4:688:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:748:ARG:NH2	4:4:754:GLU:OE2	2.50	0.42
12:C:602:THR:HG23	12:C:609:TYR:HD2	1.84	0.42
3:3:348:SER:HA	18:3:901:ADP:H5'2	2.00	0.42
12:C:492:LYS:O	12:C:496:GLU:HG3	2.20	0.42
13:D:205:ARG:HB3	13:D:209:ARG:NH1	2.34	0.42
5:5:128:LEU:HD12	5:5:297:LEU:HD13	2.01	0.42
6:6:174:TYR:HE1	6:6:193:LEU:HD11	1.84	0.42
7:7:140:GLY:H	7:7:274:THR:HG21	1.84	0.42
12:C:221:ASP:OD1	12:C:221:ASP:N	2.52	0.42
12:C:466:ASP:OD1	12:C:467:GLU:N	2.53	0.42
12:C:675:GLU:OE1	12:C:675:GLU:N	2.44	0.42
2:2:560:VAL:HG22	2:2:571:LEU:HD13	2.02	0.42
5:5:344:PHE:H	18:5:801:ADP:HN62	1.67	0.42
6:6:431:ALA:HB2	6:6:450:MET:SD	2.59	0.42
9:Y:52:DG:H2"	9:Y:53:DA:N7	2.35	0.42
13:D:62:SER:HA	13:D:189:VAL:O	2.19	0.42
13:D:224:PRO:O	13:D:228:LYS:NZ	2.50	0.42
14:E:315:LEU:HD13	14:E:430:TYR:HD2	1.85	0.42
6:6:44:ILE:HG22	6:6:47:LEU:H	1.84	0.42
7:7:362:VAL:HA	7:7:618:ARG:HH22	1.85	0.42
7:7:386:ALA:HB2	15:7:802:AGS:C8	2.50	0.42
12:C:431:LEU:HG	12:C:456:VAL:HG21	2.02	0.42
4:4:267:LYS:HA	4:4:284:THR:OG1	2.20	0.42
12:C:629:ASP:OD1	12:C:629:ASP:N	2.53	0.42
13:D:205:ARG:HB3	13:D:209:ARG:HH12	1.85	0.42
2:2:192:ARG:HG2	2:2:258:ILE:HD11	2.02	0.42
2:2:476:LYS:O	2:2:480:SER:OG	2.30	0.42
2:2:777:HIS:HA	2:2:780:ILE:HD12	2.02	0.42
2:2:783:ARG:NH1	2:2:790:ASP:OD1	2.53	0.42
3:3:432:THR:HG22	3:3:441:ARG:HG2	2.02	0.42
4:4:425:ASP:OD1	4:4:426:ALA:N	2.53	0.42
4:4:510:GLY:O	4:4:516:LYS:NZ	2.51	0.42
5:5:434:MET:O	5:5:480:SER:OG	2.30	0.42
12:C:284:HIS:CE1	12:C:321:VAL:HG21	2.55	0.42
12:C:405:LEU:HD12	12:C:408:TYR:HD2	1.85	0.42
3:3:412:ASP:OD2	3:3:413:LYS:NZ	2.45	0.41
8:X:32:DC:H2"	8:X:33:DA:C8	2.54	0.41
12:C:369:LEU:HB2	12:C:372:PHE:HB3	2.02	0.41
13:D:217:LEU:HD23	13:D:217:LEU:HA	1.95	0.41
2:2:540:SER:HB3	2:2:543:ALA:HB2	2.02	0.41
2:2:740:GLN:HG2	5:5:537:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:113:PRO:HB3	3:3:217:VAL:HG23	2.03	0.41
3:3:185:GLU:OE1	7:7:72:ARG:NH1	2.45	0.41
7:7:372:ARG:HD2	7:7:465:GLN:HG3	2.02	0.41
11:B:451:TYR:CE2	12:C:628:PRO:HG2	2.56	0.41
12:C:341:LEU:HB2	12:C:365:ASN:ND2	2.35	0.41
7:7:274:THR:HB	7:7:302:ARG:HB2	2.02	0.41
9:Y:2:DC:H2"	9:Y:3:DA:C8	2.56	0.41
13:D:74:THR:N	15:D:901:AGS:O2B	2.33	0.41
14:E:138:LEU:HB3	14:E:139:PRO:HD3	2.03	0.41
2:2:766:HIS:HB3	2:2:798:MET:SD	2.60	0.41
12:C:212:SER:HB3	12:C:213:PRO:HD3	2.02	0.41
14:E:413:LEU:O	14:E:417:ARG:HG3	2.20	0.41
2:2:802:PHE:O	2:2:805:THR:OG1	2.37	0.41
3:3:331:ASN:ND2	7:7:343:GLU:OE2	2.53	0.41
13:D:26:GLU:HG2	13:D:30:ARG:NH1	2.31	0.41
13:D:240:PHE:CD1	13:D:241:PRO:HD2	2.55	0.41
13:D:407:ASP:OD1	13:D:408:ASN:N	2.53	0.41
2:2:750:LEU:HD11	2:2:799:LEU:HD21	2.03	0.41
2:2:799:LEU:HD23	2:2:799:LEU:HA	1.86	0.41
4:4:744:HIS:CD2	4:4:760:GLU:HG2	2.56	0.41
6:6:435:ARG:HE	9:Y:22:DT:P	2.44	0.41
10:A:778:LEU:HD23	10:A:778:LEU:HA	1.92	0.41
4:4:154:GLY:HA3	7:7:102:TYR:CE1	2.56	0.41
4:4:516:LYS:NZ	4:4:617:ALA:O	2.54	0.41
5:5:282:ARG:NH2	6:6:441:GLU:O	2.51	0.41
8:X:8:DC:H2"	8:X:9:DC:C6	2.55	0.41
7:7:569:LYS:NZ	7:7:623:ASP:OD1	2.44	0.41
7:7:580:TYR:CE2	7:7:627:LYS:HE3	2.55	0.41
11:B:324:GLU:HA	11:B:327:ARG:HG2	2.02	0.41
13:D:101:GLY:H	13:D:160:GLU:HB2	1.84	0.41
13:D:250:ASN:HA	13:D:253:VAL:HG12	2.03	0.41
1:F:6:ILE:HG22	1:F:21:LEU:HD22	2.03	0.41
1:F:36:VAL:O	2:2:345:GLN:NE2	2.54	0.41
9:Y:35:DC:H2"	9:Y:36:DA:C8	2.56	0.41
10:A:839:ASN:OD1	10:A:839:ASN:N	2.54	0.41
13:D:158:LEU:HD13	13:D:189:VAL:HG13	2.02	0.41
3:3:368:THR:O	3:3:408:ILE:HA	2.21	0.40
4:4:558:LEU:HD23	4:4:558:LEU:HA	1.96	0.40
7:7:140:GLY:N	7:7:274:THR:HG21	2.36	0.40
2:2:413:GLU:HB2	2:2:445:ALA:HB3	2.03	0.40
11:B:306:HIS:CE1	12:C:26:ILE:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:67:PHE:CD1	14:E:68:THR:HG23	2.56	0.40
14:E:278:TRP:O	14:E:282:GLN:HG2	2.21	0.40
11:B:273:ARG:NH2	12:C:683:ARG:HB2	2.36	0.40
12:C:472:LEU:HD11	12:C:556:VAL:HG21	2.02	0.40
4:4:538:SER:HA	7:7:470:ALA:O	2.22	0.40
6:6:546:TYR:O	6:6:550:ARG:HG2	2.22	0.40
12:C:222:MET:HG3	12:C:250:PHE:CD2	2.55	0.40
12:C:290:ASP:HA	12:C:294:LEU:HB2	2.02	0.40
12:C:312:ASN:O	12:C:316:TYR:HB2	2.22	0.40
12:C:460:LEU:HD11	12:C:557:VAL:HG22	2.03	0.40
12:C:678:HIS:O	12:C:682:ILE:HG12	2.21	0.40
12:C:410:MET:O	12:C:414:LEU:HD13	2.21	0.40
13:D:153:PRO:HB3	13:D:186:PRO:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	171/251 (68%)	169 (99%)	2 (1%)	0	100	100
2	2	637/902 (71%)	614 (96%)	23 (4%)	0	100	100
3	3	586/810 (72%)	573 (98%)	13 (2%)	0	100	100
4	4	619/863 (72%)	603 (97%)	16 (3%)	0	100	100
5	5	585/734 (80%)	565 (97%)	20 (3%)	0	100	100
6	6	640/821 (78%)	625 (98%)	15 (2%)	0	100	100
7	7	530/719 (74%)	516 (97%)	14 (3%)	0	100	100
10	A	111/861 (13%)	110 (99%)	1 (1%)	0	100	100
11	B	182/577 (32%)	177 (97%)	5 (3%)	0	100	100
12	C	520/712 (73%)	504 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	D	362/436 (83%)	354 (98%)	8 (2%)	0	100	100
14	E	367/435 (84%)	357 (97%)	10 (3%)	0	100	100
All	All	5310/8121 (65%)	5167 (97%)	143 (3%)	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	F	151/217 (70%)	151 (100%)	0	100	100
2	2	563/779 (72%)	563 (100%)	0	100	100
3	3	516/708 (73%)	516 (100%)	0	100	100
4	4	551/753 (73%)	550 (100%)	1 (0%)	92	96
5	5	510/625 (82%)	510 (100%)	0	100	100
6	6	590/724 (82%)	590 (100%)	0	100	100
7	7	475/619 (77%)	474 (100%)	1 (0%)	92	96
10	A	101/766 (13%)	101 (100%)	0	100	100
11	B	175/529 (33%)	175 (100%)	0	100	100
12	C	508/659 (77%)	508 (100%)	0	100	100
13	D	343/403 (85%)	341 (99%)	2 (1%)	84	92
14	E	344/399 (86%)	344 (100%)	0	100	100
All	All	4827/7181 (67%)	4823 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	224	ARG
7	7	15	LYS
13	D	260	ARG
13	D	386	LYS

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

Mol	Chain	Res	Type
2	2	687	HIS
3	3	236	GLN
3	3	310	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	AGS	D	901	16	26,33,33	0.70	1 (3%)	26,52,52	1.13	3 (11%)
18	ADP	3	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
15	AGS	E	501	16	26,33,33	0.72	1 (3%)	26,52,52	1.05	2 (7%)
15	AGS	7	802	16	26,33,33	0.71	1 (3%)	26,52,52	1.04	2 (7%)
15	AGS	6	901	16	26,33,33	0.71	1 (3%)	26,52,52	1.08	2 (7%)
18	ADP	5	801	16	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
15	AGS	2	1001	16	26,33,33	0.71	1 (3%)	26,52,52	1.04	2 (7%)
18	ADP	4	902	16	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	AGS	D	901	16	-	3/17/38/38	0/3/3/3
18	ADP	3	901	-	-	1/12/32/32	0/3/3/3
15	AGS	E	501	16	-	3/17/38/38	0/3/3/3
15	AGS	7	802	16	-	5/17/38/38	0/3/3/3
15	AGS	6	901	16	-	0/17/38/38	0/3/3/3
18	ADP	5	801	16	-	6/12/32/32	0/3/3/3
15	AGS	2	1001	16	-	5/17/38/38	0/3/3/3
18	ADP	4	902	16	-	5/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	901	ADP	C5-C4	2.52	1.47	1.40
18	4	902	ADP	C5-C4	2.51	1.47	1.40
18	5	801	ADP	C5-C4	2.50	1.47	1.40
15	2	1001	AGS	PG-S1G	2.17	1.95	1.90
15	E	501	AGS	PG-S1G	2.14	1.95	1.90
15	D	901	AGS	PG-S1G	2.13	1.95	1.90
15	7	802	AGS	PG-S1G	2.12	1.95	1.90
15	6	901	AGS	PG-S1G	2.12	1.95	1.90

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	E	501	AGS	PA-O3A-PB	-3.81	119.74	132.83
15	6	901	AGS	PA-O3A-PB	-3.81	119.75	132.83
15	D	901	AGS	PA-O3A-PB	-3.80	119.78	132.83
18	4	902	ADP	C3'-C2'-C1'	3.65	106.47	100.98
18	5	801	ADP	C3'-C2'-C1'	3.57	106.36	100.98
18	3	901	ADP	PA-O3A-PB	-3.52	120.76	132.83
18	5	801	ADP	PA-O3A-PB	-3.49	120.83	132.83
18	4	902	ADP	PA-O3A-PB	-3.48	120.90	132.83
18	3	901	ADP	C3'-C2'-C1'	3.47	106.20	100.98
15	2	1001	AGS	PA-O3A-PB	-3.47	120.93	132.83
15	7	802	AGS	PA-O3A-PB	-3.22	121.79	132.83
18	4	902	ADP	N3-C2-N1	-3.20	123.67	128.68
18	5	801	ADP	N3-C2-N1	-3.18	123.71	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	901	ADP	N3-C2-N1	-3.17	123.72	128.68
18	3	901	ADP	C4-C5-N7	-2.68	106.60	109.40
18	4	902	ADP	C4-C5-N7	-2.64	106.64	109.40
18	5	801	ADP	C4-C5-N7	-2.61	106.68	109.40
15	2	1001	AGS	C5-C6-N6	2.30	123.84	120.35
15	6	901	AGS	C5-C6-N6	2.29	123.83	120.35
15	D	901	AGS	C5-C6-N6	2.29	123.83	120.35
15	E	501	AGS	C5-C6-N6	2.26	123.79	120.35
15	7	802	AGS	C5-C6-N6	2.26	123.79	120.35
15	D	901	AGS	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	2	1001	AGS	C5'-O5'-PA-O1A
15	2	1001	AGS	C5'-O5'-PA-O2A
15	7	802	AGS	C5'-O5'-PA-O1A
15	7	802	AGS	C5'-O5'-PA-O2A
15	D	901	AGS	C5'-O5'-PA-O1A
15	D	901	AGS	C5'-O5'-PA-O2A
15	E	501	AGS	C5'-O5'-PA-O3A
18	4	902	ADP	C5'-O5'-PA-O1A
18	5	801	ADP	C5'-O5'-PA-O1A
18	4	902	ADP	O4'-C4'-C5'-O5'
18	4	902	ADP	C3'-C4'-C5'-O5'
18	5	801	ADP	O4'-C4'-C5'-O5'
18	5	801	ADP	C3'-C4'-C5'-O5'
18	4	902	ADP	C5'-O5'-PA-O3A
15	2	1001	AGS	PA-O3A-PB-O1B
15	E	501	AGS	C5'-O5'-PA-O1A
18	4	902	ADP	C5'-O5'-PA-O2A
18	5	801	ADP	C5'-O5'-PA-O2A
15	E	501	AGS	C4'-C5'-O5'-PA
15	2	1001	AGS	PG-O3B-PB-O2B
18	5	801	ADP	PA-O3A-PB-O2B
15	7	802	AGS	PG-O3B-PB-O2B
15	2	1001	AGS	C5'-O5'-PA-O3A
15	7	802	AGS	C5'-O5'-PA-O3A
15	D	901	AGS	C5'-O5'-PA-O3A
18	5	801	ADP	C5'-O5'-PA-O3A
18	3	901	ADP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	7	802	AGS	PA-O3A-PB-O1B

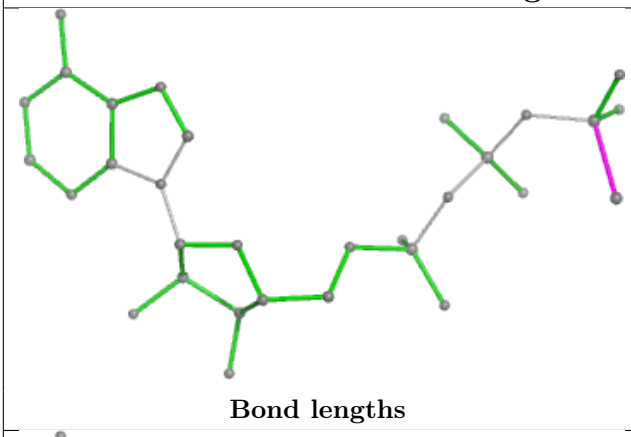
There are no ring outliers.

6 monomers are involved in 12 short contacts:

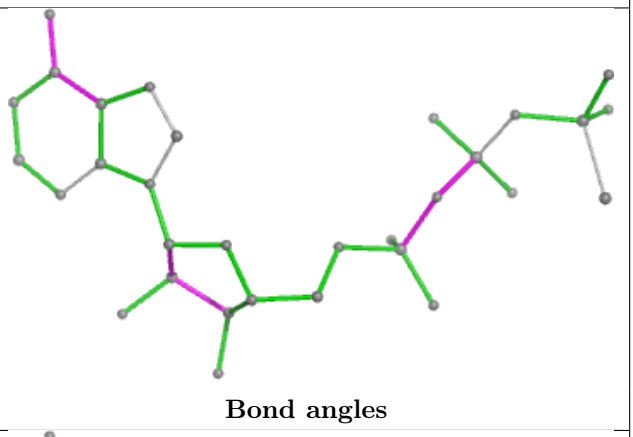
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	901	AGS	4	0
18	3	901	ADP	1	0
15	E	501	AGS	3	0
15	7	802	AGS	1	0
15	6	901	AGS	1	0
18	5	801	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

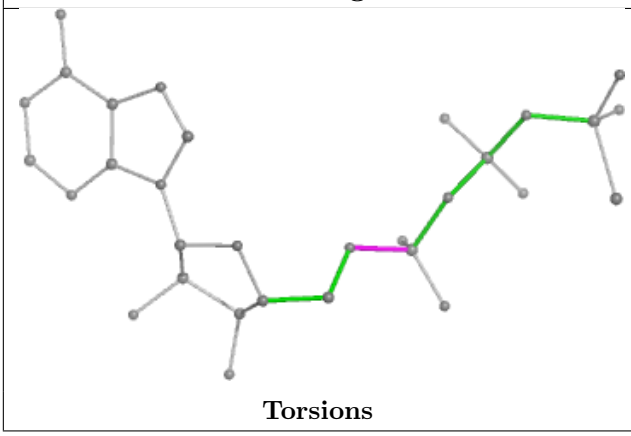
Ligand AGS D 901



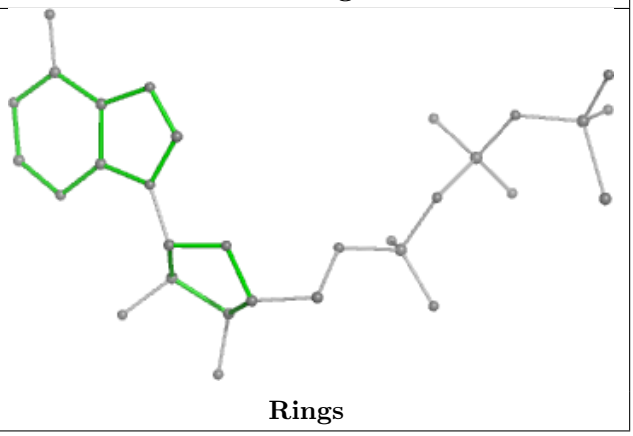
Bond lengths



Bond angles

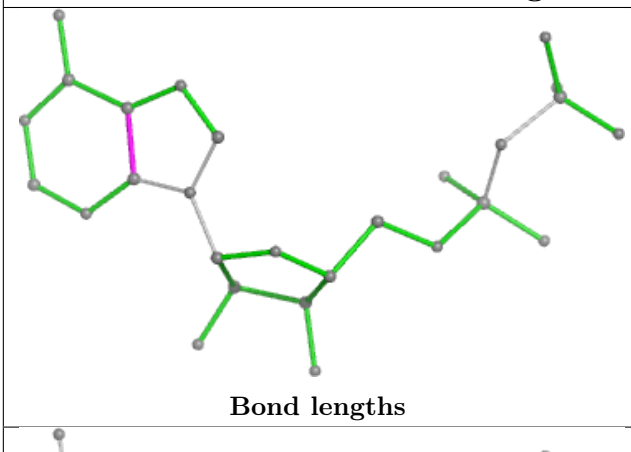


Torsions

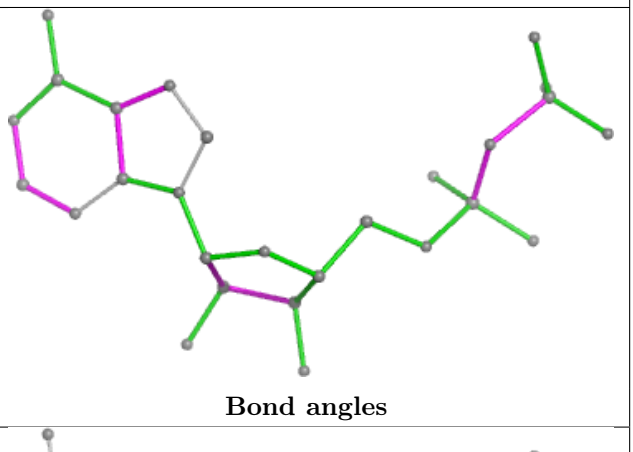


Rings

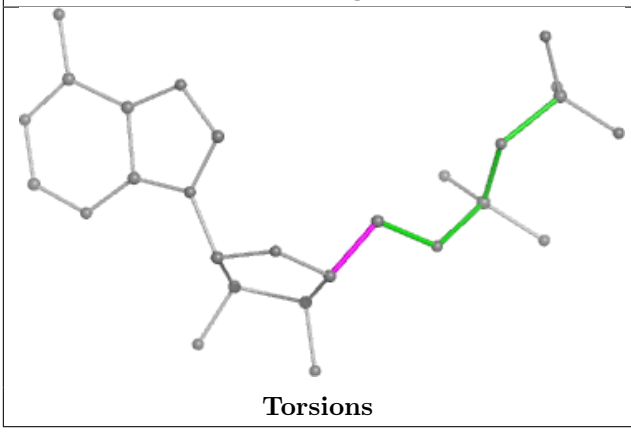
Ligand ADP 3 901



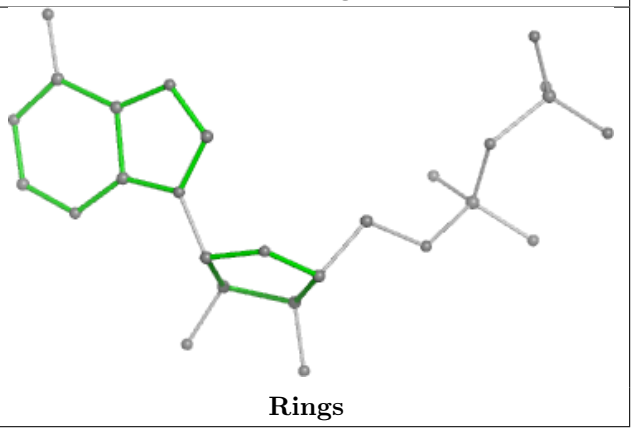
Bond lengths



Bond angles

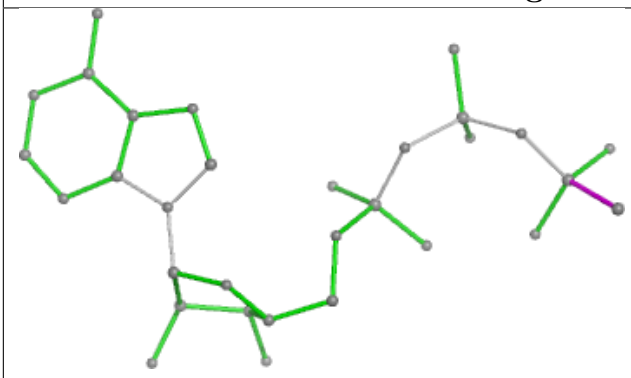


Torsions

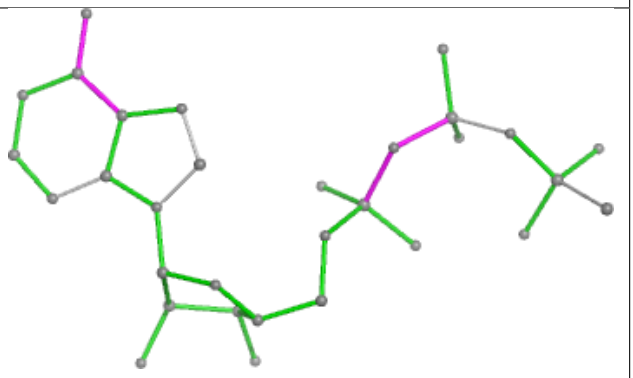


Rings

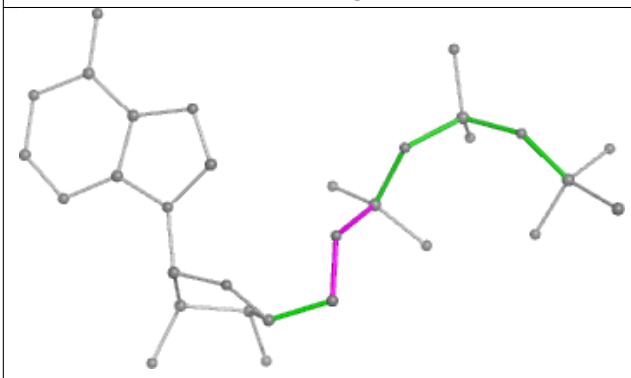
Ligand AGS E 501



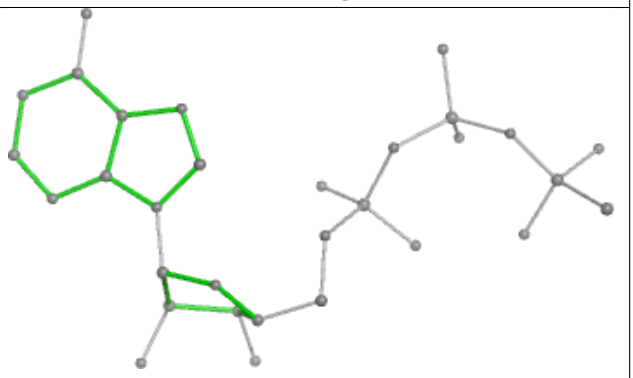
Bond lengths



Bond angles

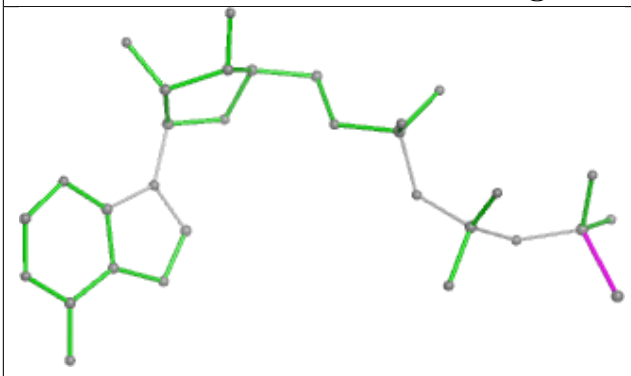


Torsions

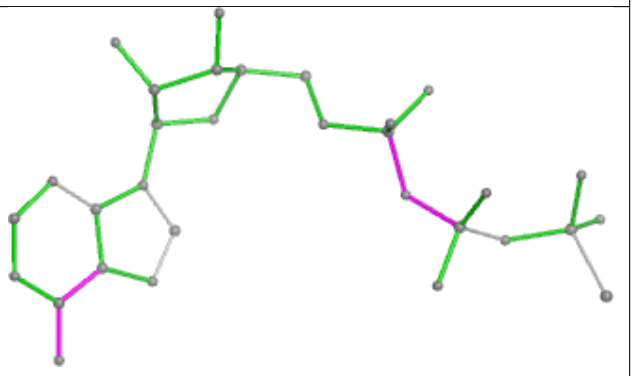


Rings

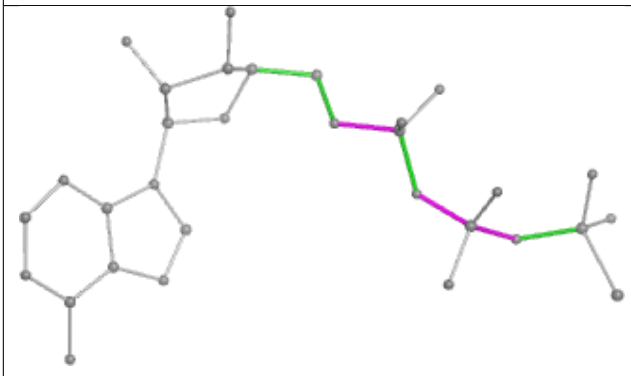
Ligand AGS 7 802



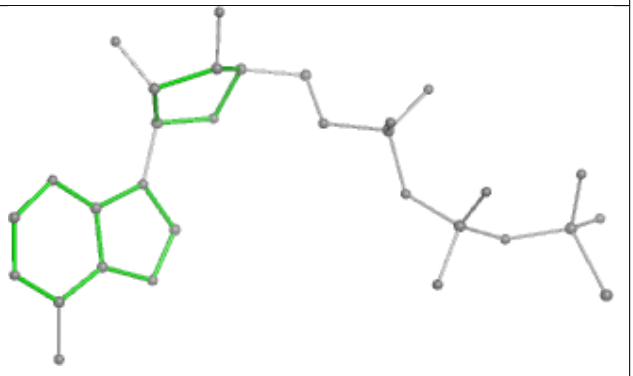
Bond lengths



Bond angles

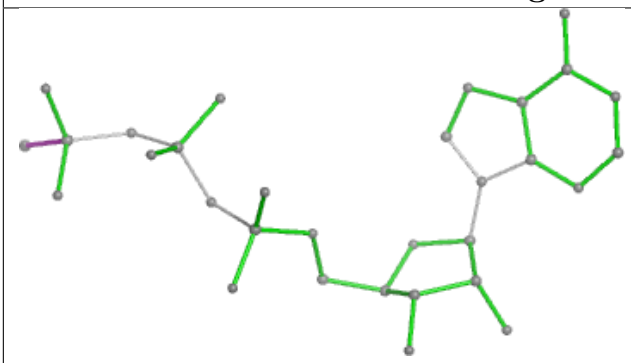


Torsions

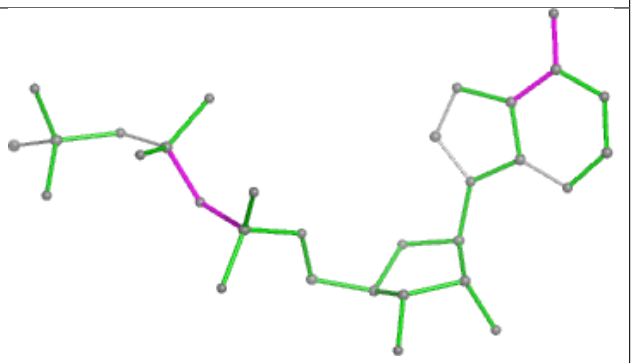


Rings

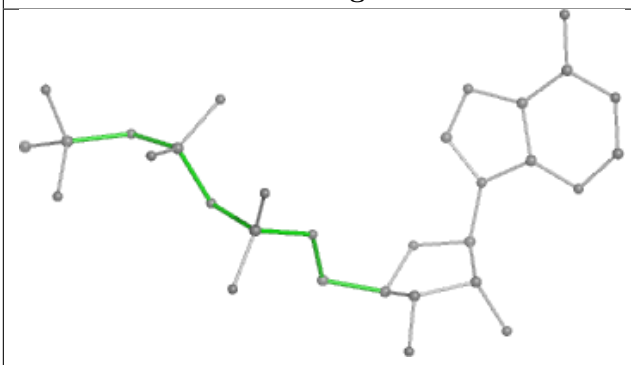
Ligand AGS 6 901



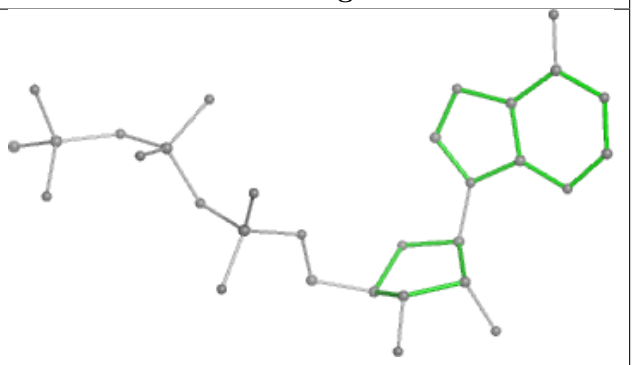
Bond lengths



Bond angles

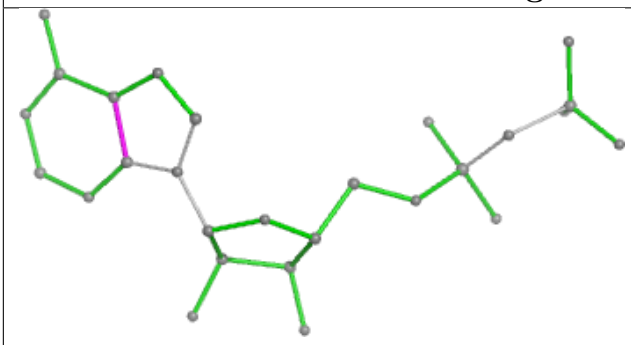


Torsions

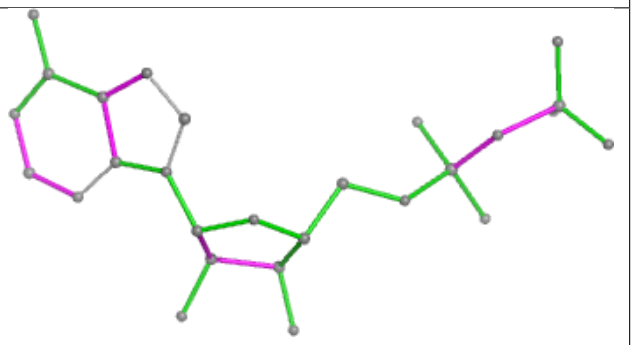


Rings

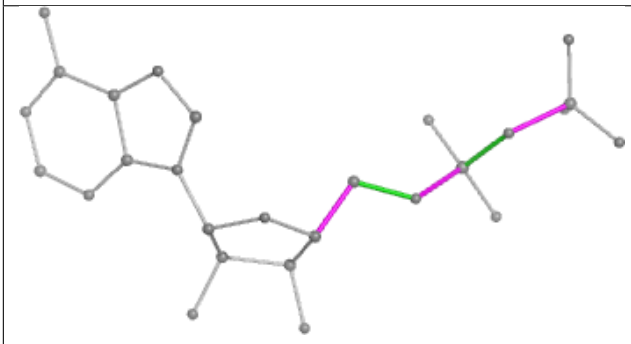
Ligand ADP 5 801



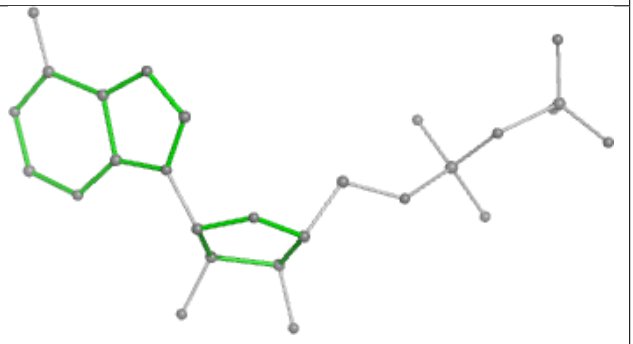
Bond lengths



Bond angles

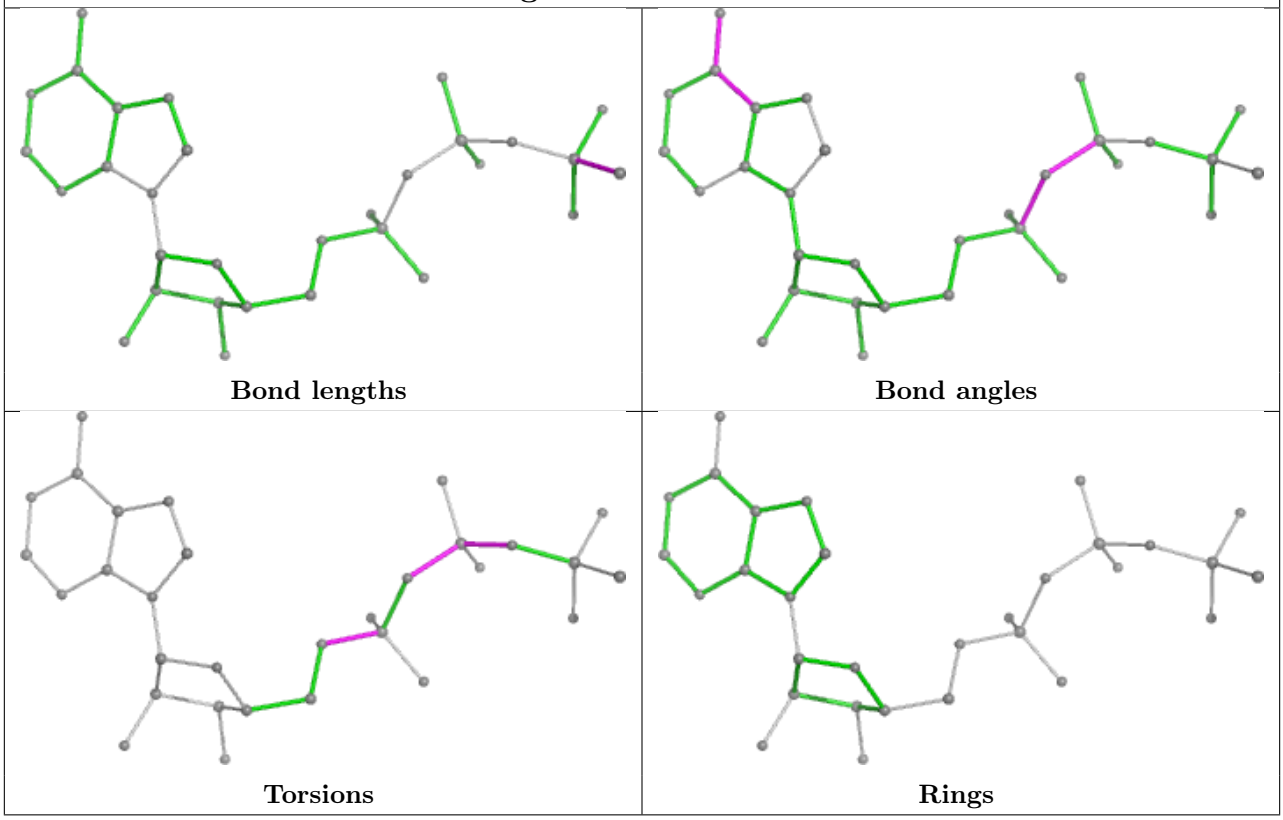


Torsions

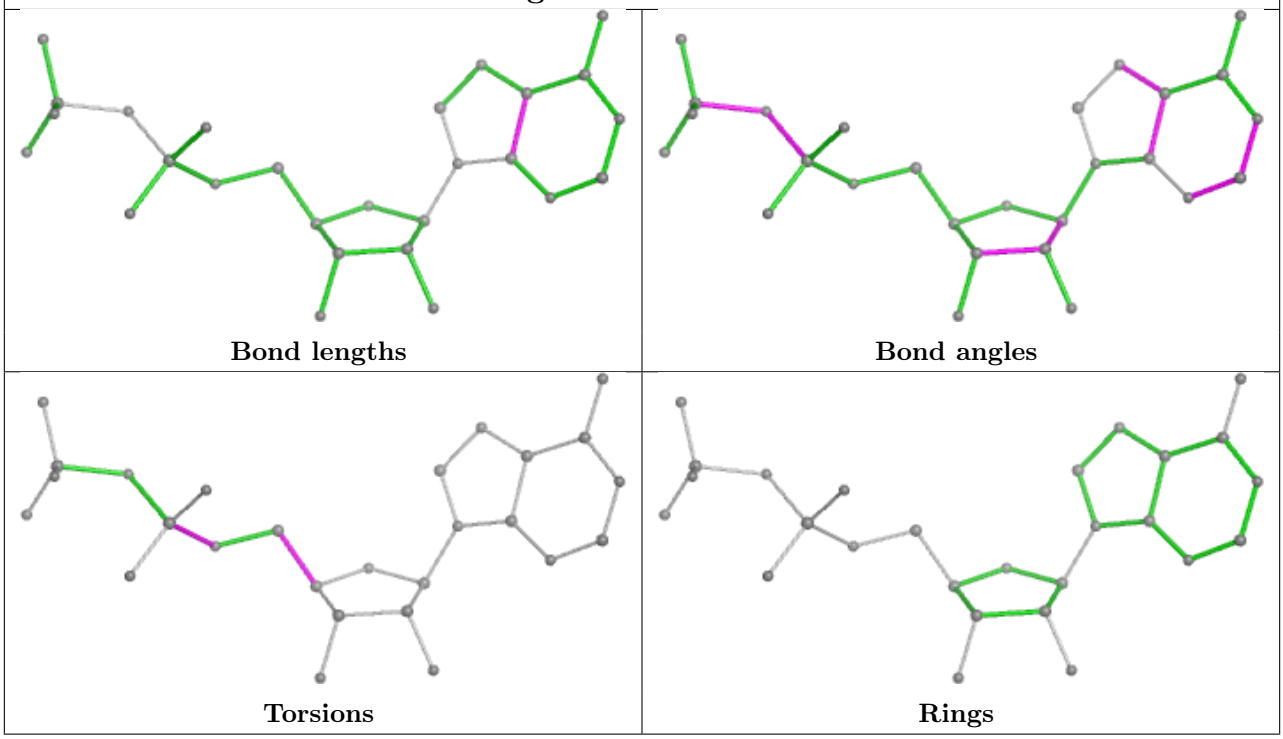


Rings

Ligand AGS 2 1001



Ligand ADP 4 902



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.

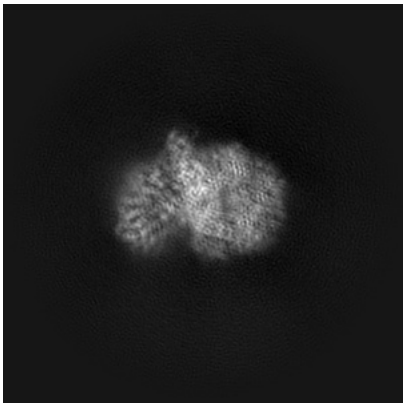
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19622. These allow visual inspection of the internal detail of the map and identification of artifacts.

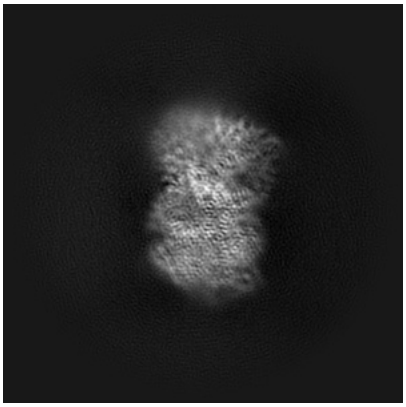
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

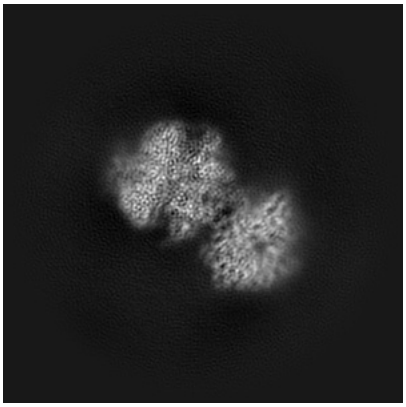
6.1.1 Primary map



X



Y

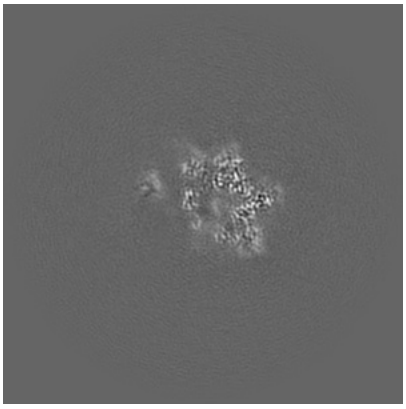


Z

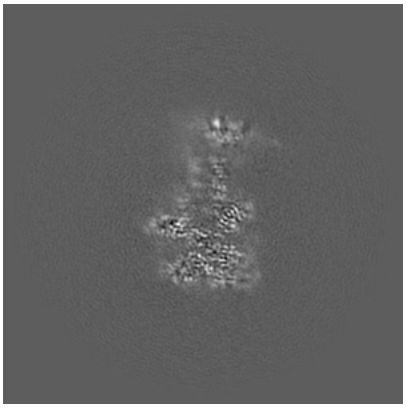
The images above show the map projected in three orthogonal directions.

6.2 Central slices

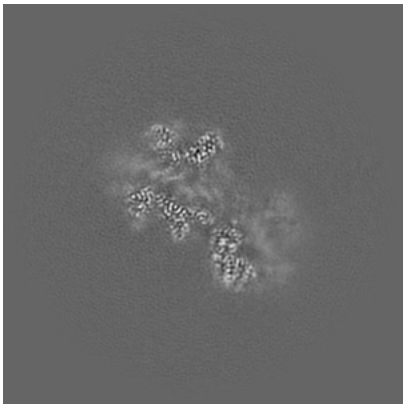
6.2.1 Primary map



X Index: 200



Y Index: 200

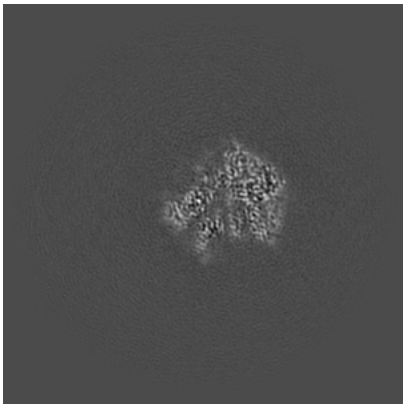


Z Index: 200

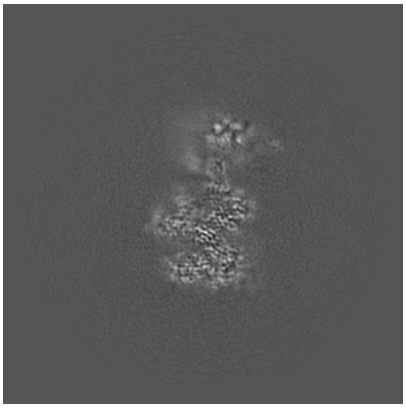
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

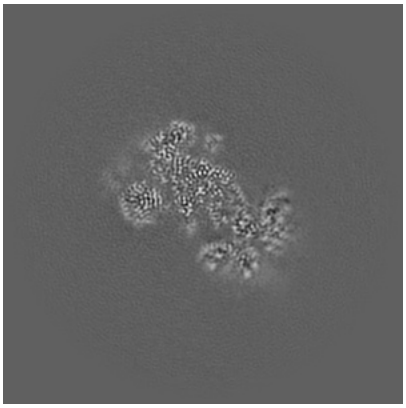
6.3.1 Primary map



X Index: 171



Y Index: 196

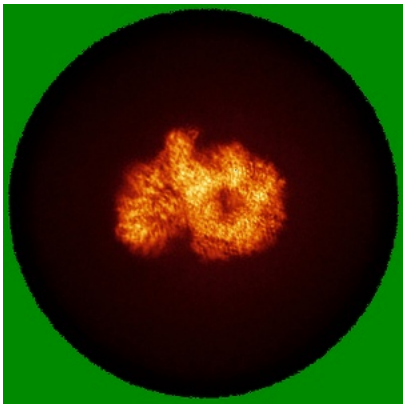


Z Index: 221

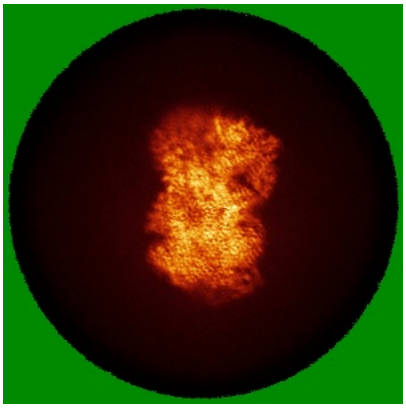
The images above show the largest variance slices of the map in three orthogonal directions.

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

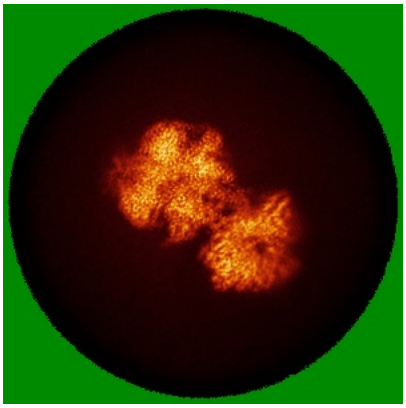
6.4.1 Primary map



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

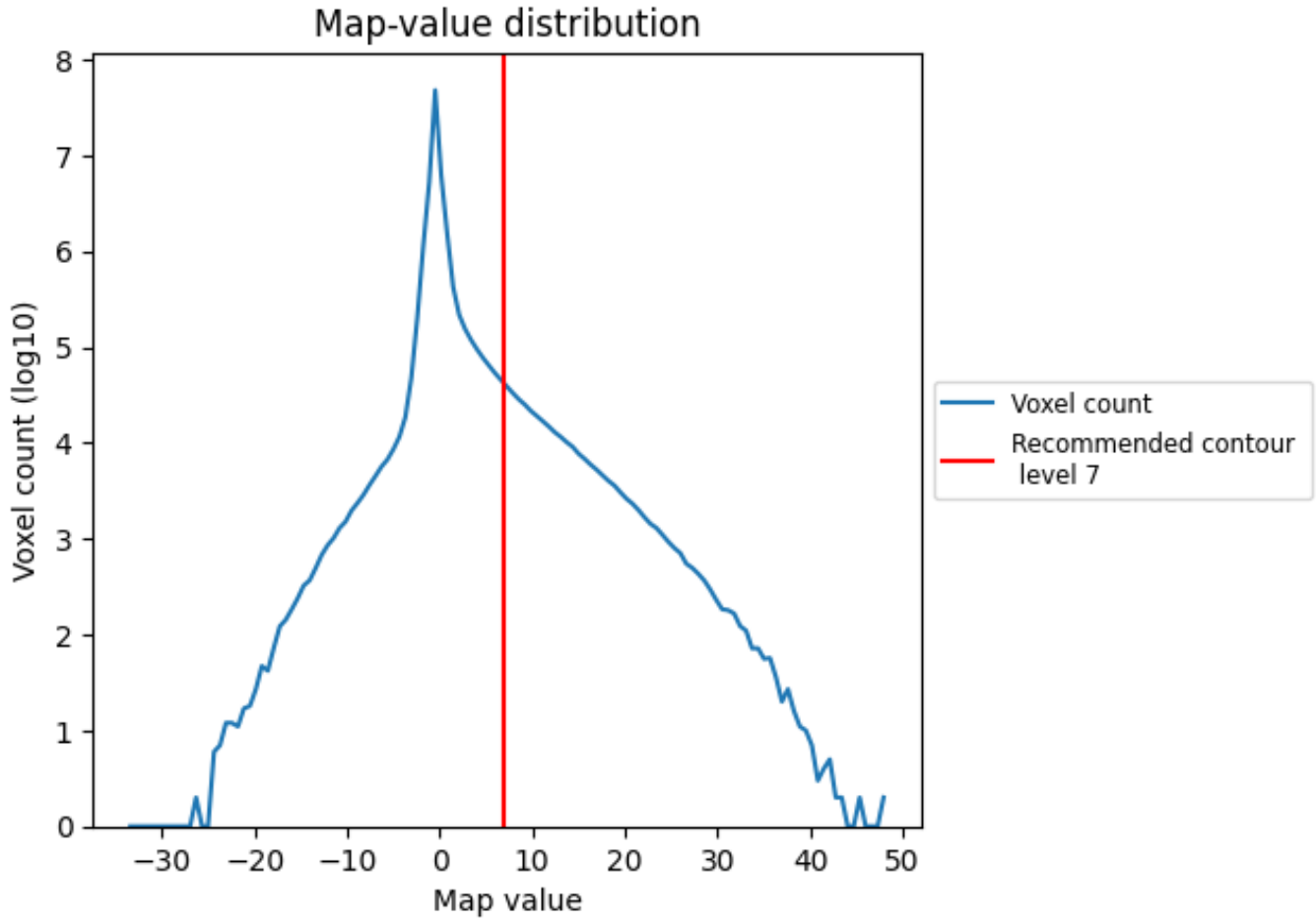
6.6 Mask visualisation (i)

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

7 Map analysis

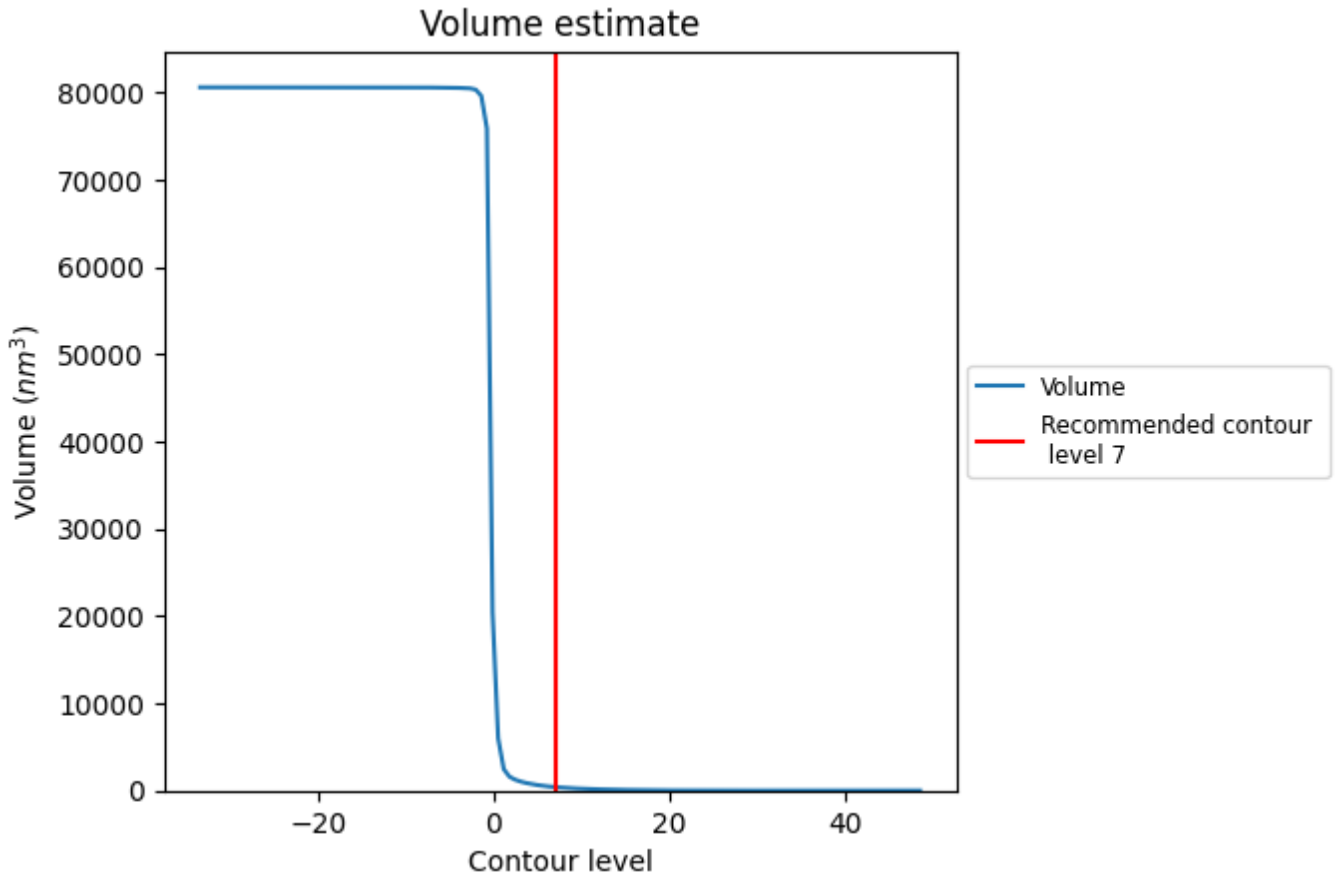
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

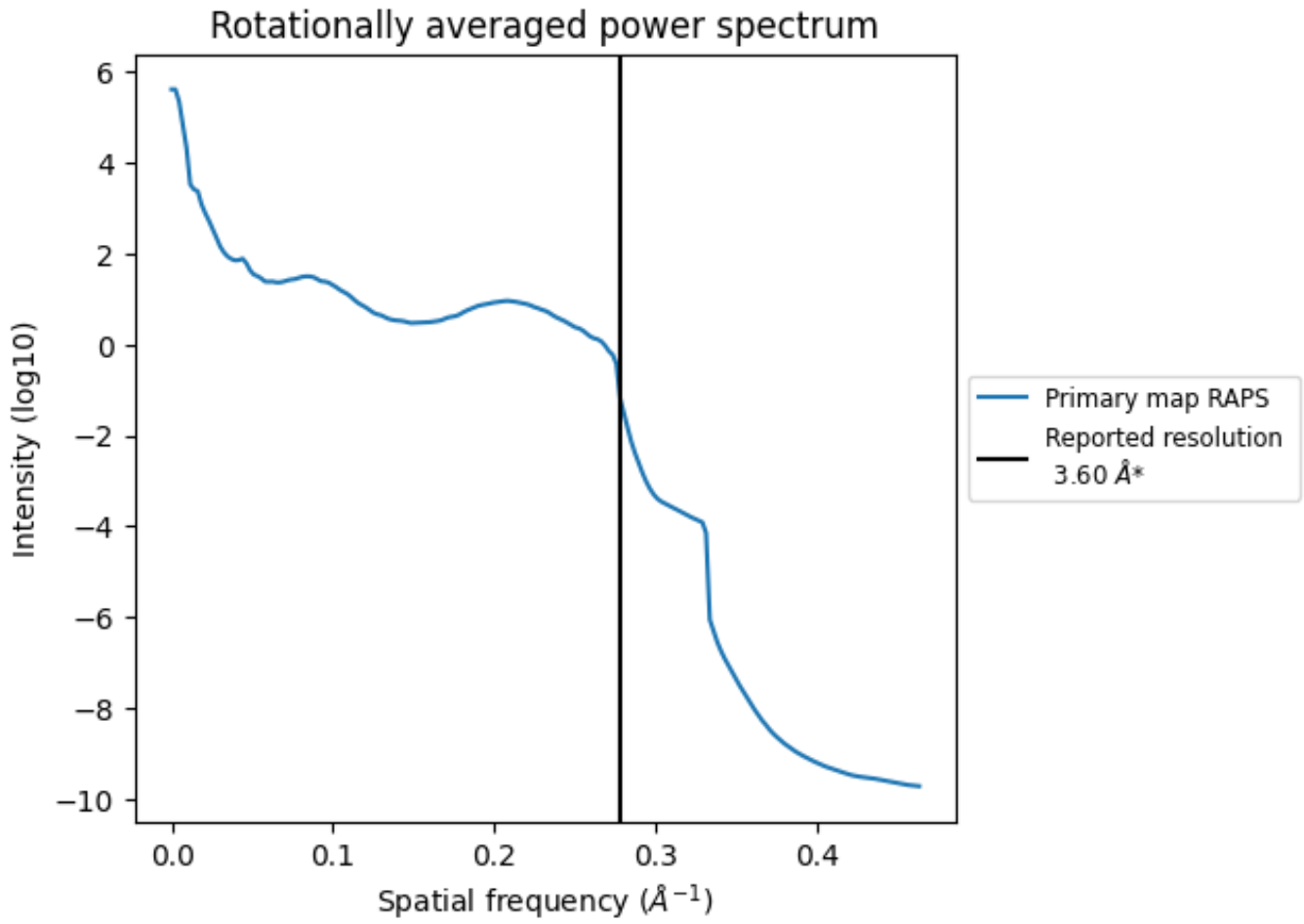
7.2 Volume estimate



The volume at the recommended contour level is 403 nm^3; this corresponds to an approximate mass of 364 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 0.278 $Å^{-1}$

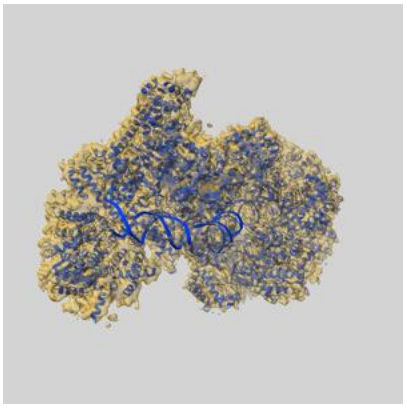
8 Fourier-Shell correlation

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

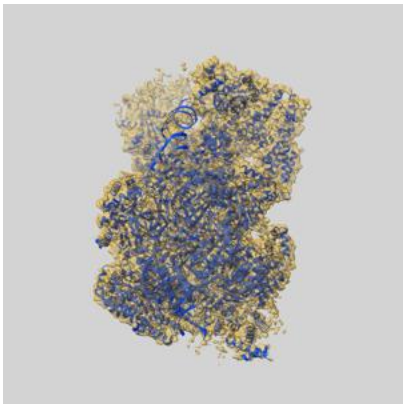
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19622 and PDB model 8S0D. Per-residue inclusion information can be found in section 3 on page 9.

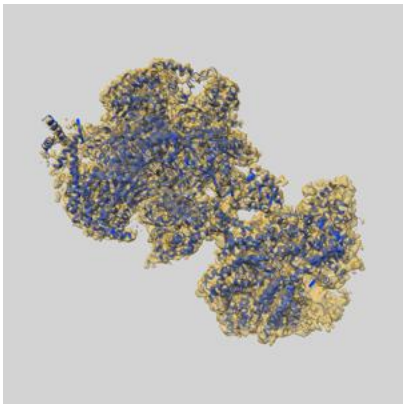
9.1 Map-model overlay



X



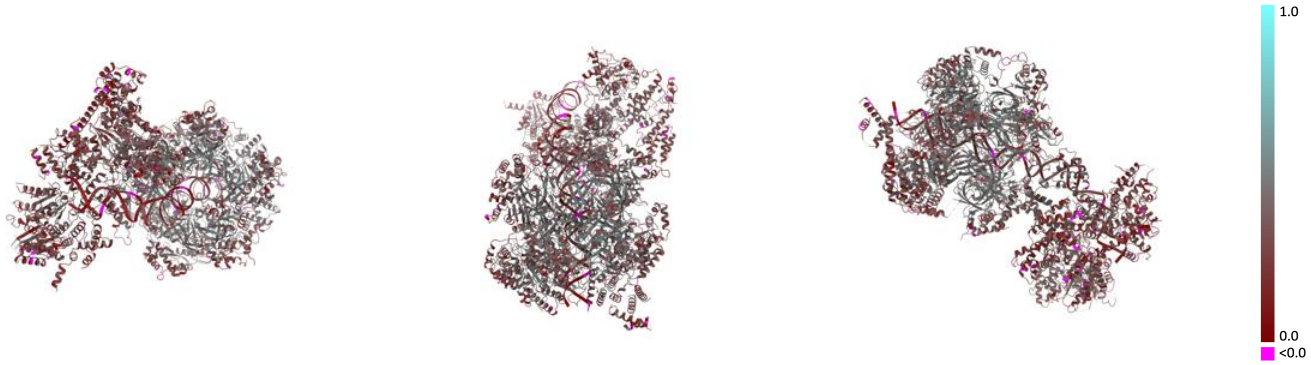
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

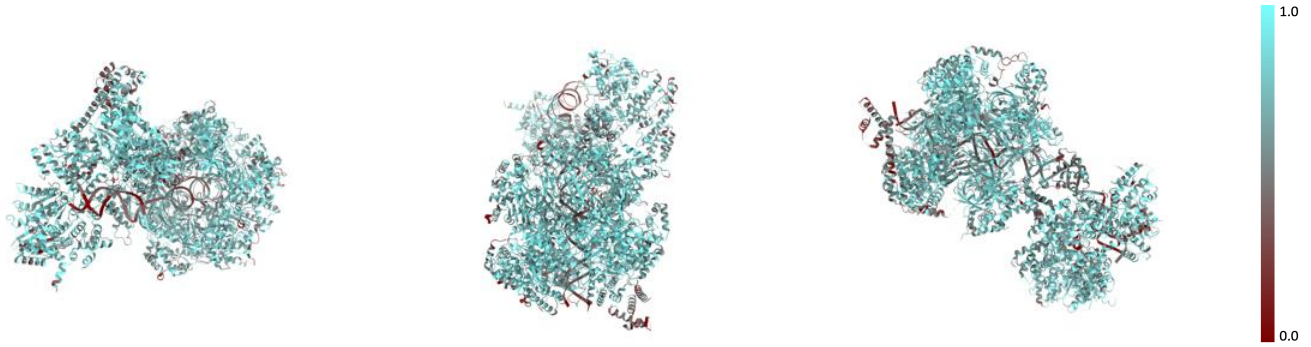
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

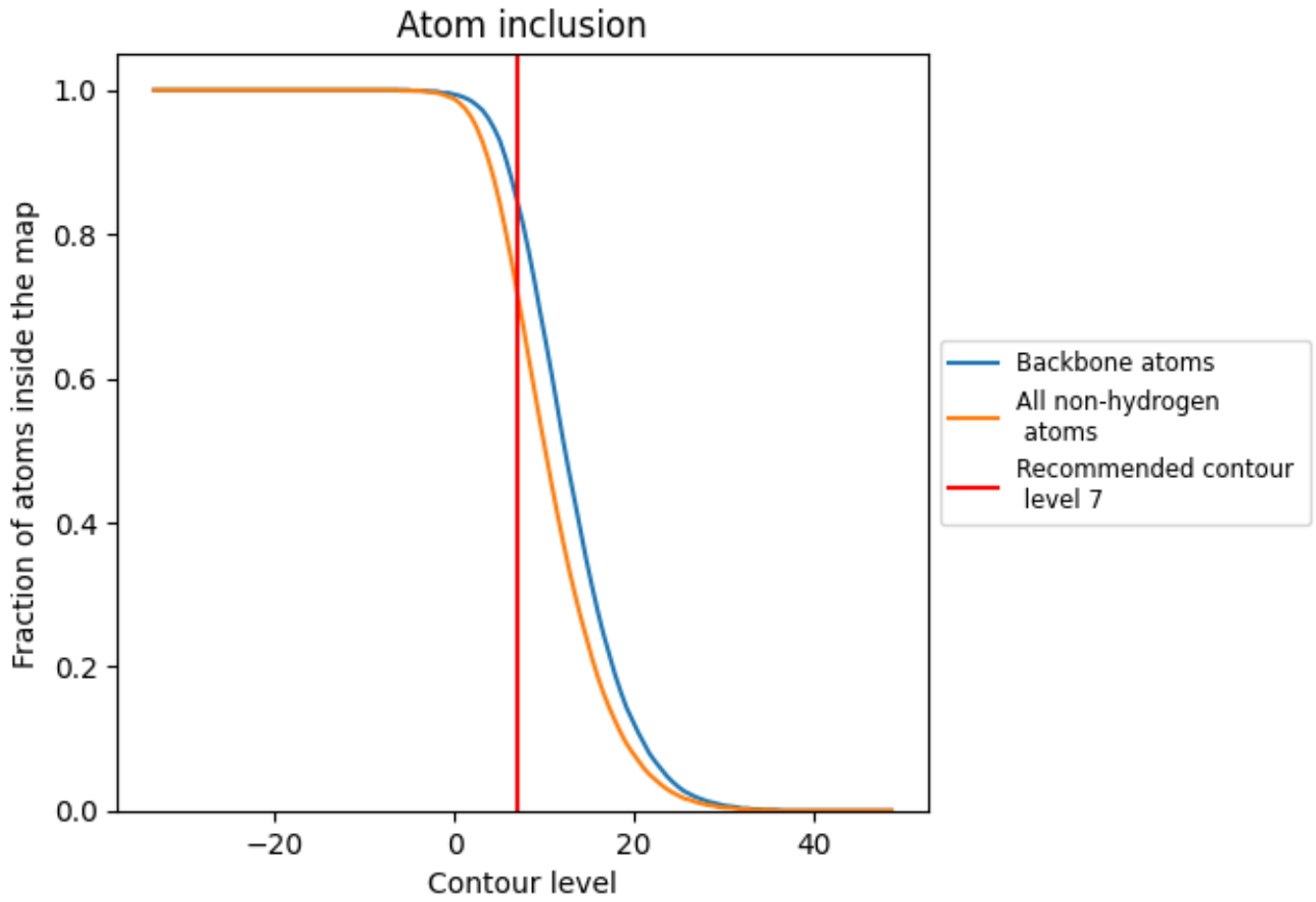
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 72% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.3460
2	0.7300	0.3780
3	0.7200	0.3710
4	0.7720	0.4110
5	0.7500	0.3870
6	0.7470	0.3900
7	0.7390	0.3690
A	0.7300	0.2740
B	0.7840	0.3010
C	0.6930	0.2600
D	0.7300	0.3050
E	0.7500	0.3310
F	0.5540	0.3750
X	0.4390	0.1520
Y	0.4160	0.1450