



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:08 PM UTC

PDB ID : 6XL5 / pdb_00006xl5
EMDB ID : EMD-22234
Title : Cryo-EM structure of EcmrR-RNAP-promoter open complex (EcmrR-RPo)
Authors : Yang, Y.; Liu, C.; Liu, B.
Deposited on : 2020-06-28
Resolution : 2.50 Å(reported)
Based on initial model : 6OUL

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

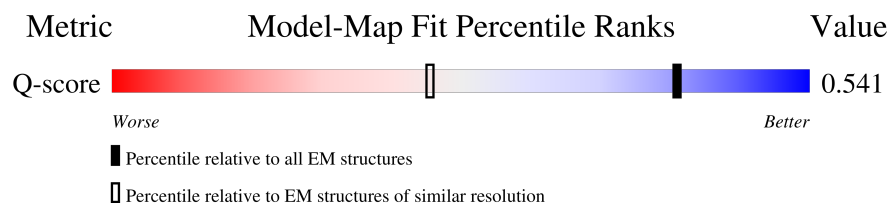
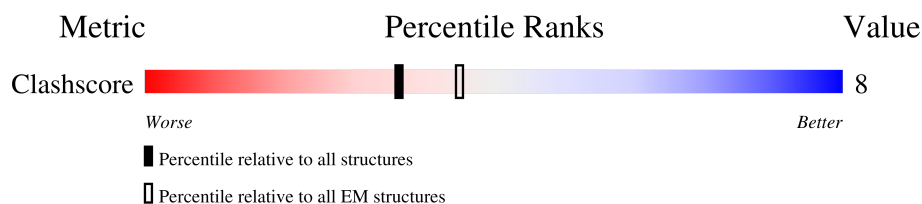
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

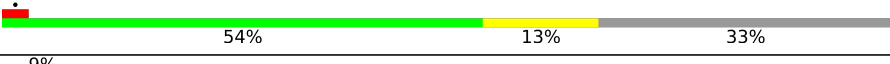
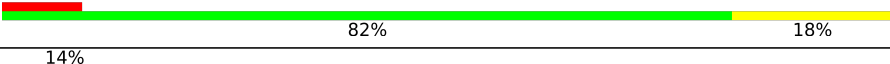
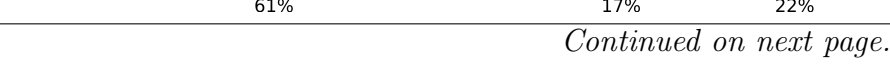
The reported resolution of this entry is 2.50 Å.

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



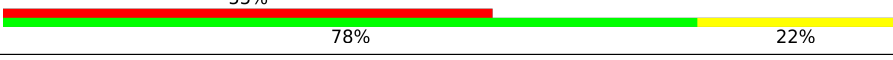
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	613	

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Mol	Chain	Length	Quality of chain
6	N	54	
7	T	54	
8	G	268	
8	H	268	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 35828 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1793	1117	318	352	6		
1	B	222	Total	C	N	O	S	0	0
			1711	1069	301	335	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1336	Total	C	N	O	S	0	0
			10394	6530	1855	1959	50		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	476	Total	C	N	O	S	0	0
			3878	2427	691	737	23		

- Molecule 6 is a DNA chain called synthetic non-template strand DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	54	Total	C	N	O	P	0	0
			1109	526	203	327	53		

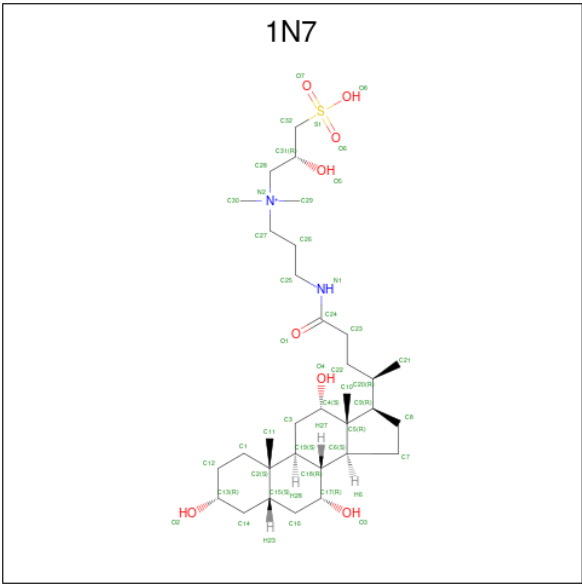
- Molecule 7 is a DNA chain called synthetic template strand DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	54	Total	C	N	O	P	0	0
			1104	523	209	319	53		

- Molecule 8 is a protein called MerR family transcriptional regulator EcmrR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	268	Total	C	N	O	S	0	0
			2208	1423	368	404	13		
8	H	268	Total	C	N	O	S	0	0
			2208	1423	368	404	13		

- Molecule 9 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			26	23	3	
9	C	1	Total	C	O	0
			26	23	3	
9	T	1	Total	C	O	0
			26	23	3	

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Mol	Chain	Residues	Atoms			AltConf
9	G	1	Total	C	O	0
			26	23	3	
9	H	1	Total	C	O	0
			27	24	3	

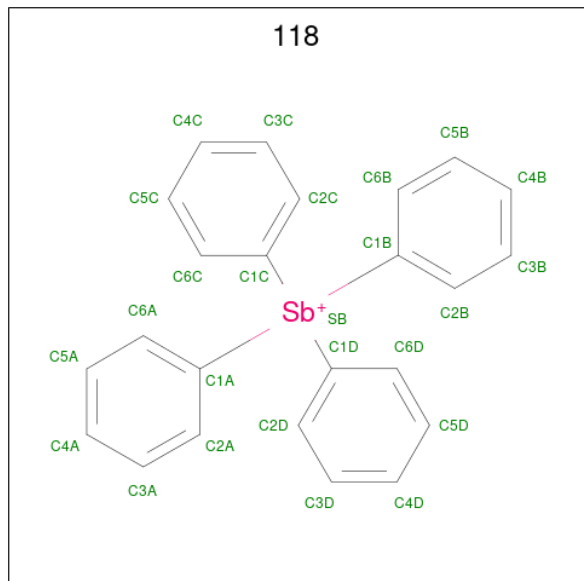
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is TETRAPHENYLANTIMONIUM ION (CCD ID: 118) (formula: C₂₄H₂₀Sb) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	G	1	Total	C	Sb	0
			25	24	1	
12	H	1	Total	C	Sb	0
			25	24	1	

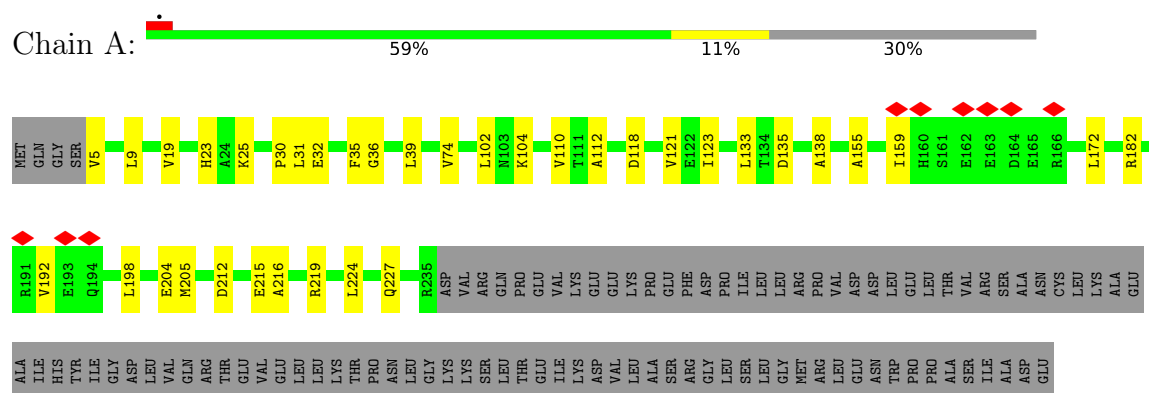
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 1	O 1	0
13	C	22	Total 22	O 22	0
13	D	15	Total 15	O 15	0
13	F	3	Total 3	O 3	0
13	N	1	Total 1	O 1	0

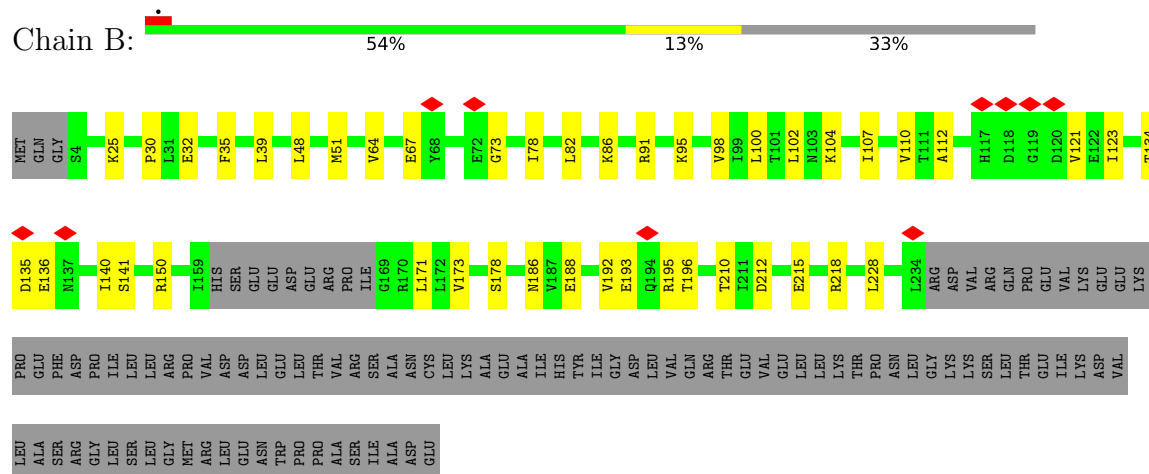
3 Residue-property plots [i](#)

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

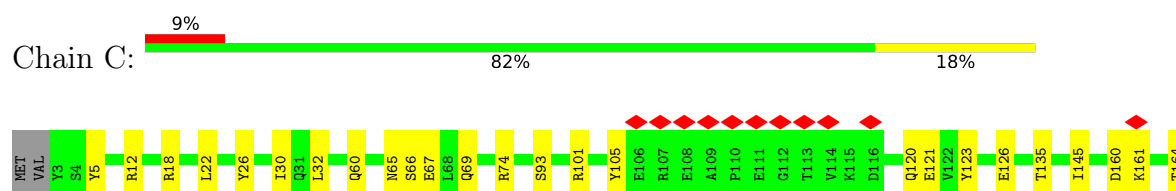
- Molecule 1: DNA-directed RNA polymerase subunit alpha

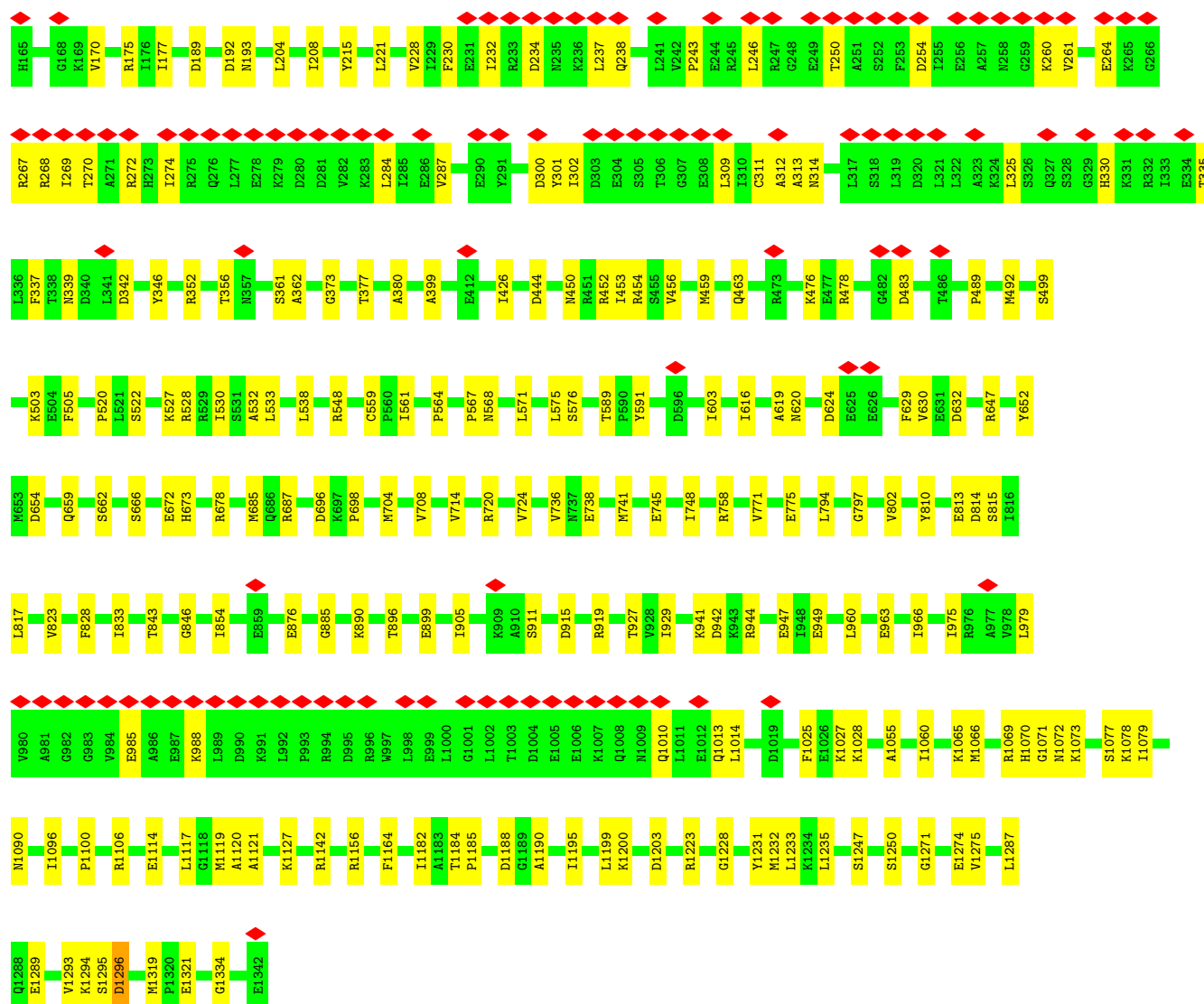


- Molecule 1: DNA-directed RNA polymerase subunit alpha

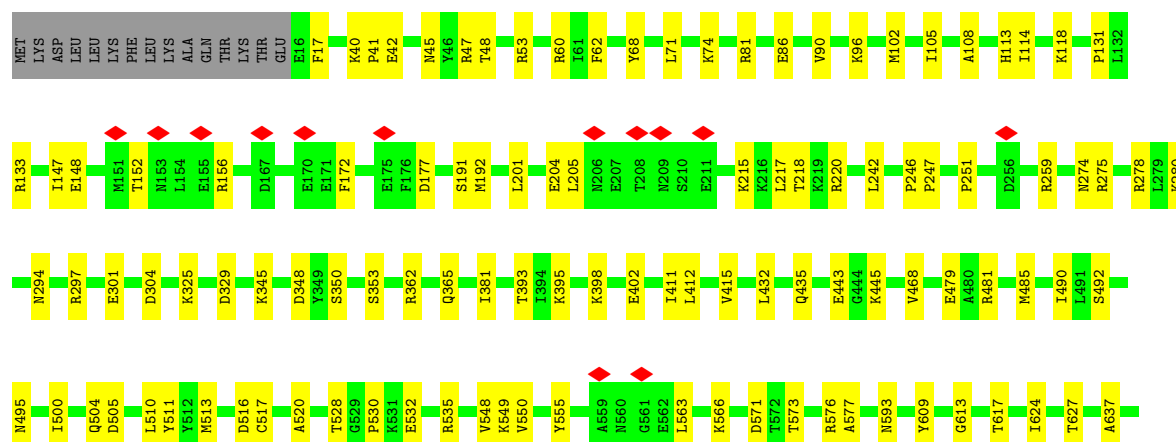
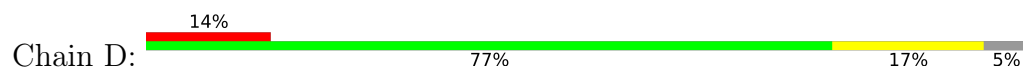


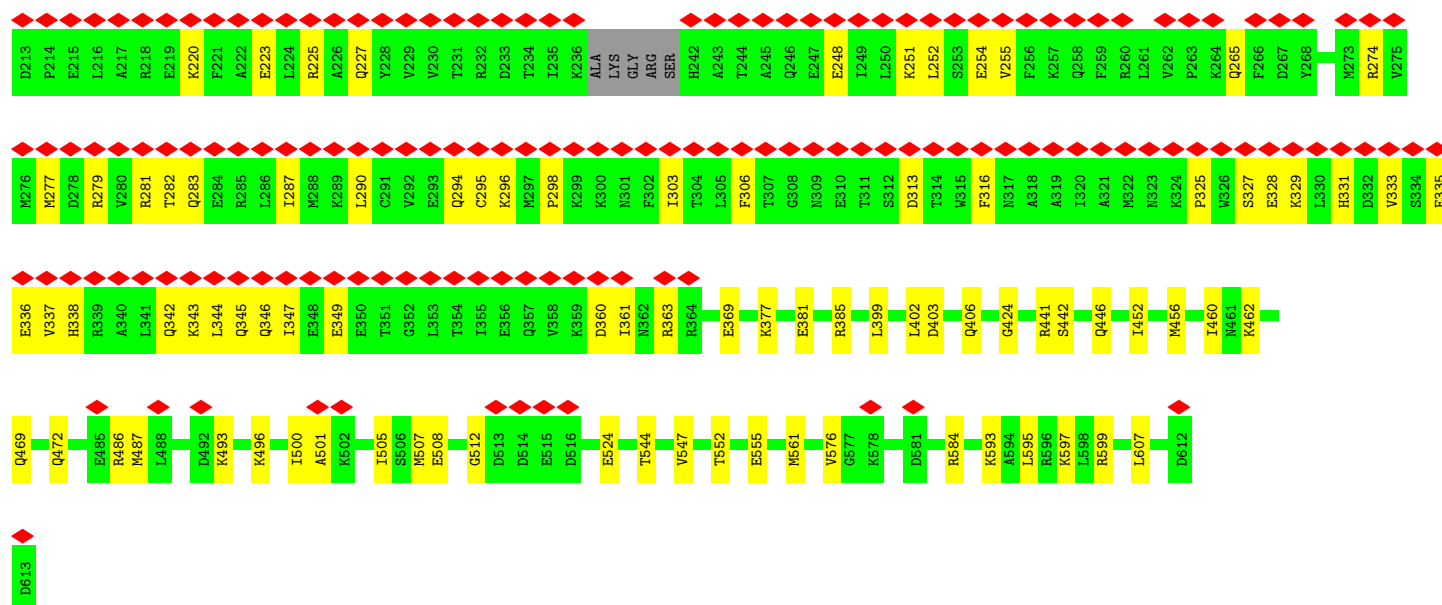
- Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'

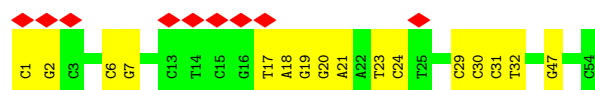




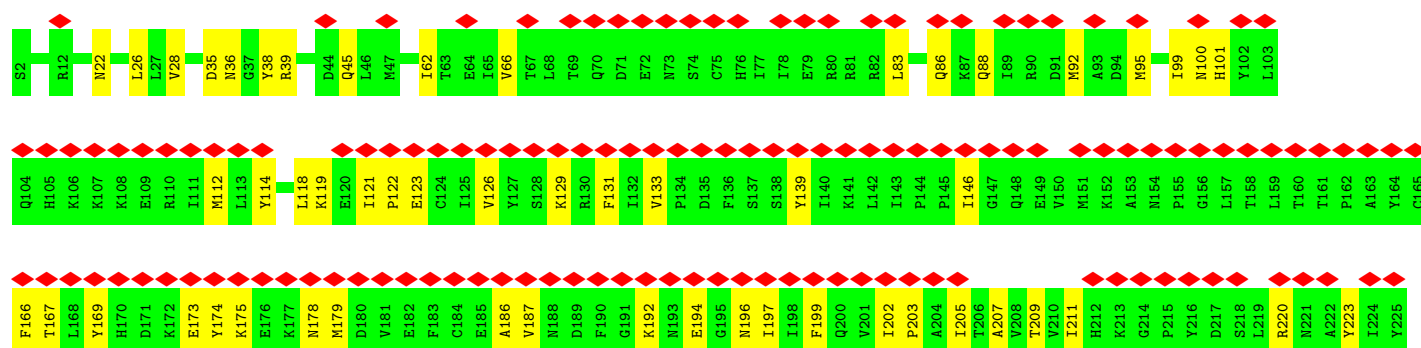
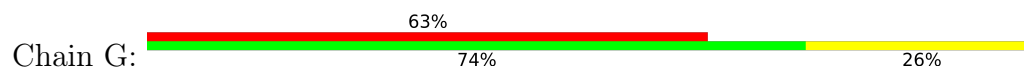
- Molecule 6: synthetic non-template strand DNA (54-MER)

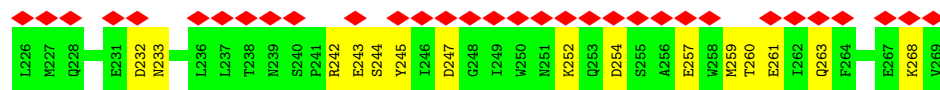


- Molecule 7: synthetic template strand DNA (54-MER)

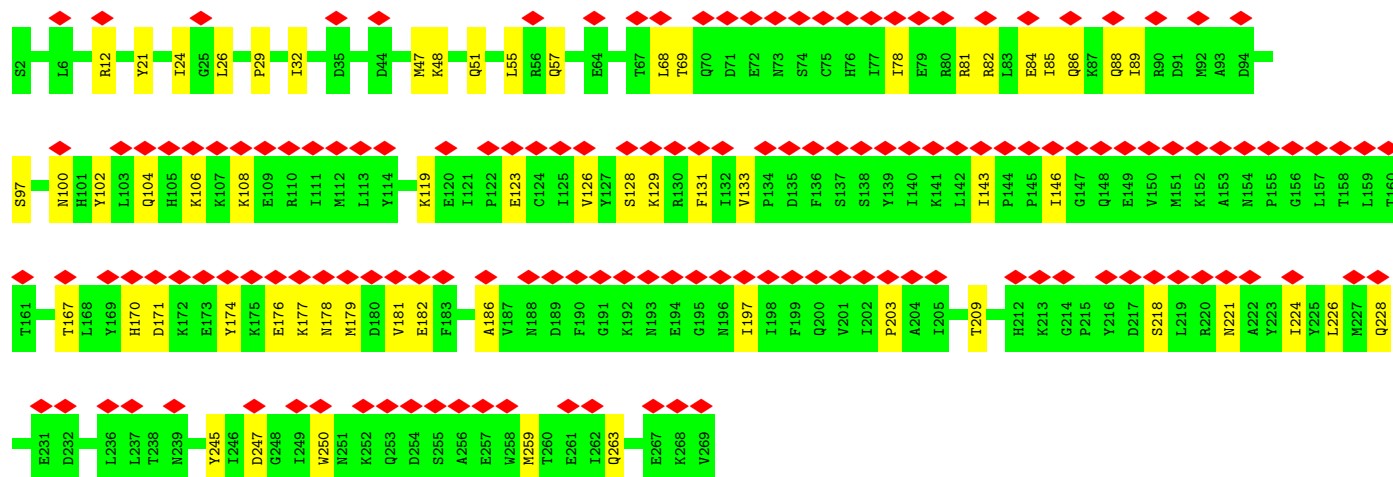
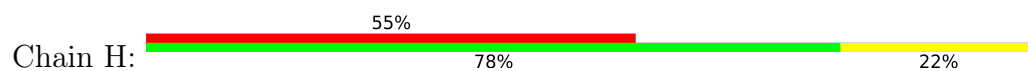


- Molecule 8: MerR family transcriptional regulator EcmrR





• Molecule 8: MerR family transcriptional regulator EcmrR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	214970	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.68	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.788	Depositor
Minimum map value	-2.575	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.461	Depositor
Map size (Å)	341.2481, 341.2481, 341.2481	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8886669, 0.8886669, 0.8886669	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 118, 1N7, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/1815	0.51	0/2460
1	B	0.43	0/1730	0.49	0/2344
2	C	0.48	0/10739	0.55	1/14489 (0.0%)
3	D	0.46	0/10551	0.53	1/14245 (0.0%)
4	E	0.43	0/629	0.50	0/847
5	F	0.34	0/3930	0.56	0/5281
6	N	0.45	0/1243	0.51	0/1919
7	T	0.39	0/1239	0.48	0/1910
8	G	0.30	0/2260	0.72	1/3058 (0.0%)
8	H	0.29	0/2260	0.68	0/3058
All	All	0.43	0/36396	0.56	3/49611 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1296	ASP	N-CA-C	8.17	123.55	113.50
8	G	114	TYR	N-CA-C	6.24	120.74	107.70
3	D	505	ASP	N-CA-C	5.31	117.76	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1793	0	1822	24	0
1	B	1711	0	1748	28	0
2	C	10570	0	10582	164	0
3	D	10394	0	10617	159	0
4	E	627	0	634	7	0
5	F	3878	0	3940	70	0
6	N	1109	0	609	13	0
7	T	1104	0	605	11	0
8	G	2208	0	2209	57	0
8	H	2208	0	2209	46	0
9	C	52	0	74	3	0
9	G	26	0	37	4	0
9	H	27	0	39	2	0
9	T	26	0	37	1	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
12	G	25	0	20	2	0
12	H	25	0	20	1	0
13	A	1	0	0	0	0
13	C	22	0	0	0	0
13	D	15	0	0	0	0
13	F	3	0	0	0	0
13	N	1	0	0	0	0
All	All	35828	0	35202	545	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 8.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:246:LEU:HD13	2:C:269:ILE:HG21	1.27	1.14
2:C:246:LEU:HD11	2:C:274:ILE:HG13	1.30	1.08
2:C:246:LEU:CD1	2:C:274:ILE:HG13	2.06	0.85
2:C:246:LEU:CD1	2:C:269:ILE:HG21	2.05	0.84
8:G:252:LYS:HD3	8:G:257:GLU:HG3	1.66	0.77
5:F:342:GLN:O	5:F:345:GLN:HB3	1.85	0.77
8:G:92:MET:HE3	8:H:85:ILE:HG13	1.67	0.75
3:D:816:THR:O	3:D:860:ARG:NH2	2.20	0.75
8:G:118:LEU:HB3	8:H:57:GLN:HE22	1.51	0.74
3:D:1368:ASP:HA	3:D:1371:ARG:HG2	1.70	0.73
8:G:119:LYS:NZ	8:G:209:THR:OG1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:179:MET:HG3	8:H:181:VAL:HG23	1.69	0.72
8:G:167:THR:O	8:G:242:ARG:HA	1.90	0.72
2:C:444:ASP:O	2:C:450:ASN:ND2	2.23	0.71
8:G:28:VAL:O	8:G:45:GLN:NE2	2.24	0.71
8:H:26:LEU:HD12	8:H:26:LEU:O	1.92	0.69
8:G:129:LYS:HB2	8:G:197:ILE:HD13	1.74	0.69
2:C:246:LEU:O	2:C:246:LEU:HD12	1.95	0.67
1:A:5:VAL:O	1:B:150:ARG:NH1	2.27	0.67
2:C:1184:THR:HG23	2:C:1190:ALA:H	1.59	0.67
8:H:21:TYR:CG	8:H:26:LEU:HD11	2.29	0.67
5:F:344:LEU:HA	5:F:347:ILE:HG22	1.76	0.67
12:H:302:118:H6A	12:H:302:118:H6C	1.77	0.67
2:C:1295:SER:OG	3:D:345:LYS:HD3	1.96	0.66
8:G:211:ILE:HD11	8:H:47:MET:HA	1.78	0.66
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.77	0.66
3:D:961:SER:O	3:D:980:THR:HA	1.96	0.66
2:C:915:ASP:OD2	2:C:919:ARG:NH2	2.29	0.65
2:C:478:ARG:NH1	2:C:483:ASP:OD2	2.29	0.65
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.77	0.65
3:D:1219:ASP:OD1	3:D:1222:ARG:NH2	2.29	0.65
8:G:244:SER:HB2	8:G:261:GLU:HG3	1.79	0.65
8:H:81:ARG:NH2	8:H:84:GLU:OE1	2.30	0.65
1:B:186:ASN:ND2	1:B:188:GLU:OE1	2.30	0.65
2:C:758:ARG:HB3	2:C:833:ILE:HB	1.79	0.64
2:C:1289:GLU:HA	2:C:1293:VAL:HG22	1.78	0.64
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.80	0.64
2:C:1127:LYS:NZ	2:C:1203:ASP:OD2	2.31	0.64
3:D:74:LYS:NZ	3:D:86:GLU:OE2	2.30	0.64
8:H:84:GLU:OE2	8:H:88:GLN:NE2	2.31	0.63
8:H:218:SER:OG	8:H:221:ASN:ND2	2.31	0.63
2:C:243:PRO:HB2	2:C:274:ILE:HG23	1.81	0.63
2:C:528:ARG:NH2	2:C:576:SER:O	2.32	0.63
3:D:47:ARG:NH1	6:N:58:DG:OP1	2.31	0.63
2:C:60:GLN:HG2	2:C:67:GLU:HG3	1.81	0.62
1:A:192:VAL:HG11	1:A:198:LEU:HD12	1.82	0.61
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.66	0.61
3:D:393:THR:HG22	3:D:395:LYS:H	1.65	0.61
2:C:720:ARG:NH2	2:C:745:GLU:OE2	2.34	0.61
1:B:102:LEU:O	1:B:141:SER:HA	1.99	0.61
3:D:1067:ARG:HE	3:D:1072:LYS:HA	1.66	0.61
3:D:53:ARG:HH11	3:D:60:ARG:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:131:PRO:HB2	3:D:133:ARG:HG2	1.83	0.61
5:F:496:LYS:O	5:F:500:ILE:HG13	2.00	0.61
2:C:161:LYS:HA	2:C:170:VAL:HG22	1.82	0.61
8:G:166:PHE:HA	8:G:243:GLU:O	2.00	0.61
5:F:113:ARG:NH2	5:F:424:GLY:O	2.34	0.61
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.82	0.60
2:C:813:GLU:CD	3:D:504:GLN:NE2	2.59	0.60
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.82	0.60
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.83	0.60
3:D:398:LYS:NZ	3:D:402:GLU:OE2	2.33	0.60
3:D:747:MET:HE2	3:D:775:SER:HA	1.82	0.60
3:D:1005:LYS:HE3	3:D:1011:VAL:HG12	1.84	0.60
2:C:314:ASN:O	2:C:352:ARG:NH1	2.35	0.60
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.84	0.60
3:D:1045:THR:HG23	3:D:1046:ILE:HG13	1.83	0.60
1:B:104:LYS:HG2	1:B:110:VAL:HG22	1.84	0.59
2:C:489:PRO:HA	2:C:492:MET:HE3	1.84	0.59
3:D:68:TYR:OH	3:D:81:ARG:NH2	2.35	0.59
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.84	0.59
3:D:156:ARG:HH21	3:D:191:SER:HB2	1.66	0.59
6:N:78:DC:OP2	6:N:78:DC:H6	1.84	0.59
2:C:60:GLN:NE2	2:C:67:GLU:OE2	2.33	0.59
2:C:678:ARG:NH1	2:C:1071:GLY:O	2.35	0.59
5:F:290:LEU:HD21	5:F:337:VAL:HG23	1.83	0.59
5:F:441:ARG:NH2	6:N:60:DG:OP2	2.36	0.59
8:G:22:ASN:HD22	8:G:39:ARG:HE	1.49	0.59
5:F:547:VAL:HG21	5:F:607:LEU:HD11	1.84	0.58
8:G:175:LYS:HD3	8:G:178:ASN:HB2	1.85	0.58
8:G:129:LYS:HD3	8:G:131:PHE:CD1	2.39	0.58
2:C:1250:SER:HB2	5:F:524:GLU:HG3	1.86	0.58
3:D:45:ASN:HD22	3:D:48:THR:H	1.52	0.58
8:G:169:TYR:HE2	8:G:243:GLU:HB2	1.69	0.58
8:H:170:HIS:NE2	8:H:182:GLU:OE1	2.37	0.57
8:H:245:TYR:HB3	8:H:250:TRP:HH2	1.69	0.57
3:D:362:ARG:H	3:D:365:GLN:HE21	1.52	0.57
1:B:67:GLU:HG3	1:B:171:LEU:HD23	1.85	0.57
8:G:223:TYR:OH	8:G:243:GLU:OE1	2.22	0.57
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.52	0.57
1:B:91:ARG:NH1	1:B:210:THR:O	2.38	0.57
5:F:162:ILE:HG22	5:F:164:GLY:H	1.69	0.56
2:C:246:LEU:CD1	2:C:274:ILE:CG1	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:516:ASP:OD1	3:D:516:ASP:N	2.37	0.56
3:D:863:LEU:HD21	3:D:901:ARG:HG3	1.88	0.56
4:E:29:GLN:HB3	4:E:35:LYS:HG3	1.87	0.56
6:N:44:DC:H2'	6:N:45:DT:C6	2.41	0.56
2:C:339:ASN:HD21	2:C:342:ASP:HB3	1.70	0.56
2:C:356:THR:HG23	2:C:361:SER:HB2	1.87	0.56
3:D:1148:ARG:NH1	6:N:80:DG:OP1	2.39	0.56
1:B:192:VAL:HG12	1:B:193:GLU:HG3	1.87	0.56
3:D:1167:LYS:H	3:D:1174:ARG:HD2	1.71	0.56
5:F:460:ILE:HD13	5:F:501:ALA:HB2	1.87	0.56
2:C:548:ARG:NH1	2:C:567:PRO:O	2.37	0.56
5:F:584:ARG:NH1	7:T:47:DG:N7	2.48	0.56
8:H:174:TYR:HD1	9:H:301:1N7:H6	1.70	0.56
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.87	0.56
3:D:1197:ASN:ND2	3:D:1212:ASP:OD2	2.39	0.56
3:D:41:PRO:HG3	3:D:274:ASN:HD21	1.71	0.55
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.88	0.55
2:C:942:ASP:N	2:C:942:ASP:OD1	2.39	0.55
2:C:941:LYS:NZ	2:C:949:GLU:OE1	2.38	0.55
3:D:513:MET:HE1	3:D:627:THR:HG22	1.89	0.55
5:F:110:LEU:HD21	5:F:385:ARG:HD2	1.88	0.55
8:H:21:TYR:CD1	8:H:26:LEU:HD11	2.41	0.55
2:C:1010:GLN:HA	2:C:1013:GLN:HE21	1.71	0.55
8:G:245:TYR:HA	8:G:260:THR:HG22	1.88	0.55
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.88	0.55
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.89	0.55
3:D:517:CYS:HB3	3:D:520:ALA:HB2	1.89	0.55
3:D:492:SER:HB3	3:D:495:ASN:O	2.07	0.55
8:G:26:LEU:HD13	8:G:66:VAL:HG22	1.89	0.55
8:H:209:THR:HG22	8:H:263:GLN:HG2	1.89	0.55
2:C:797:GLY:HA3	2:C:1233:LEU:HD23	1.88	0.55
8:H:55:LEU:HD13	8:H:68:LEU:HD23	1.89	0.55
8:H:179:MET:HG3	8:H:181:VAL:CG2	2.36	0.55
2:C:1142:ARG:NH2	2:C:1164:PHE:O	2.40	0.55
2:C:5:TYR:CE2	2:C:775:GLU:HG3	2.43	0.54
12:G:302:118:H6A	12:G:302:118:H6C	1.89	0.54
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.71	0.54
3:D:156:ARG:NH2	3:D:191:SER:HB2	2.21	0.54
3:D:807:LEU:HD23	3:D:1255:VAL:HG13	1.89	0.54
2:C:814:ASP:OD1	2:C:1106:ARG:NH2	2.35	0.54
2:C:843:THR:OG1	2:C:846:GLY:O	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:105:ILE:HD12	3:D:242:LEU:HD23	1.89	0.54
8:G:146:ILE:HD12	8:G:197:ILE:HD11	1.89	0.54
3:D:204:GLU:HG2	3:D:217:LEU:HD21	1.88	0.54
2:C:175:ARG:HG2	2:C:177:ILE:HG13	1.88	0.54
2:C:270:THR:OG1	2:C:272:ARG:NH1	2.40	0.54
3:D:817:HIS:HA	3:D:860:ARG:HH21	1.73	0.54
3:D:259:ARG:HG2	5:F:505:ILE:HD11	1.88	0.54
5:F:133:SER:OG	5:F:361:ILE:O	2.26	0.54
5:F:552:THR:HB	5:F:555:GLU:HG3	1.90	0.54
2:C:1296:ASP:OD1	2:C:1321:GLU:HB3	2.07	0.53
8:G:174:TYR:CE1	8:G:220:ARG:HD3	2.43	0.53
1:B:95:LYS:HE3	1:B:98:VAL:HG12	1.90	0.53
2:C:1121:ALA:HB2	2:C:1182:ILE:HD12	1.90	0.53
5:F:342:GLN:O	5:F:345:GLN:CB	2.55	0.53
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.91	0.53
2:C:960:LEU:HD21	2:C:1028:LYS:HB3	1.91	0.53
6:N:61:DT:H2'	6:N:62:DT:C6	2.43	0.53
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.74	0.53
2:C:135:THR:HG23	2:C:527:LYS:HE2	1.91	0.53
5:F:462:LYS:HG2	5:F:487:MET:HE3	1.91	0.53
1:A:182:ARG:NH1	2:C:1090:ASN:O	2.41	0.53
1:B:32:GLU:OE2	1:B:195:ARG:NH2	2.40	0.53
5:F:377:LYS:NZ	5:F:381:GLU:OE1	2.42	0.53
2:C:813:GLU:OE2	3:D:504:GLN:NE2	2.41	0.53
2:C:1223:ARG:NH2	3:D:721:SER:OG	2.40	0.53
3:D:549:LYS:NZ	3:D:571:ASP:OD1	2.36	0.53
8:H:26:LEU:HD12	8:H:26:LEU:C	2.33	0.53
2:C:564:PRO:HG2	2:C:568:ASN:O	2.09	0.53
2:C:828:PHE:CZ	2:C:1066:MET:HE1	2.43	0.53
5:F:227:GLN:HE22	5:F:251:LYS:HE2	1.74	0.52
2:C:246:LEU:HD12	2:C:246:LEU:C	2.34	0.52
3:D:835:LEU:HD21	3:D:880:VAL:HG23	1.90	0.52
5:F:248:GLU:HG3	5:F:251:LYS:HZ3	1.74	0.52
3:D:678:ARG:NH1	3:D:756:GLU:OE1	2.41	0.52
3:D:1215:GLU:HB3	3:D:1220:ILE:HD11	1.92	0.52
2:C:309:LEU:HD11	2:C:312:ALA:HB2	1.90	0.52
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	1.91	0.52
8:G:100:ASN:OD1	8:G:101:HIS:N	2.43	0.52
12:G:302:118:H2D	12:G:302:118:H2A	1.92	0.52
8:H:129:LYS:HG3	8:H:131:PHE:HE1	1.75	0.52
2:C:975:ILE:HG13	2:C:1014:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:890:LYS:NZ	2:C:911:SER:O	2.43	0.52
5:F:252:LEU:HA	5:F:255:VAL:HG12	1.91	0.52
7:T:29:DC:H2'	7:T:30:DC:C6	2.45	0.52
3:D:555:TYR:HB3	3:D:563:LEU:HG	1.90	0.52
5:F:360:ASP:HA	5:F:363:ARG:HG2	1.91	0.52
8:H:48:LYS:O	8:H:51:GLN:HG3	2.10	0.52
2:C:823:VAL:HG21	2:C:1079:ILE:HD13	1.92	0.51
2:C:499:SER:O	2:C:503:LYS:HB2	2.11	0.51
3:D:251:PRO:HG2	5:F:507:MET:HE1	1.92	0.51
3:D:965:SER:HB2	3:D:973:LEU:HD11	1.91	0.51
2:C:1060:ILE:HD11	2:C:1066:MET:SD	2.51	0.51
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.92	0.51
3:D:845:ALA:HB3	3:D:881:LYS:HG2	1.93	0.51
5:F:335:GLU:HA	5:F:338:HIS:CD2	2.46	0.51
3:D:511:TYR:CG	3:D:728:SER:HB3	2.46	0.51
3:D:846:GLU:HG2	3:D:881:LYS:HB3	1.93	0.51
8:H:133:VAL:O	8:H:178:ASN:HA	2.11	0.51
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.92	0.50
2:C:876:GLU:OE2	2:C:927:THR:OG1	2.28	0.50
3:D:490:ILE:HD11	3:D:609:TYR:CD1	2.46	0.50
1:A:9:LEU:HD12	1:A:198:LEU:HD11	1.93	0.50
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.93	0.50
2:C:620:ASN:HD21	3:D:769:VAL:HG23	1.75	0.50
5:F:274:ARG:NH2	5:F:369:GLU:OE1	2.40	0.50
5:F:295:CYS:HB2	5:F:329:LYS:HG3	1.91	0.50
2:C:532:ALA:HB1	2:C:538:LEU:HD13	1.92	0.50
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.93	0.50
8:G:133:VAL:HB	8:G:179:MET:HE3	1.92	0.50
3:D:275:ARG:NH1	3:D:301:GLU:OE2	2.33	0.50
8:G:261:GLU:OE2	8:G:263:GLN:NE2	2.44	0.50
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.29	0.50
8:G:35:ASP:OD1	8:G:35:ASP:N	2.42	0.50
2:C:748:ILE:HG21	2:C:966:ILE:HG22	1.93	0.50
3:D:1262:ARG:HH12	3:D:1316:THR:HG22	1.76	0.50
2:C:629:PHE:O	2:C:647:ARG:NH2	2.45	0.50
8:G:254:ASP:HB3	8:G:257:GLU:HG2	1.92	0.50
5:F:161:LEU:HD12	5:F:265:GLN:HG3	1.94	0.50
8:H:247:ASP:HB3	8:H:259:MET:HG3	1.94	0.50
1:B:212:ASP:N	1:B:212:ASP:OD1	2.40	0.49
5:F:493:LYS:HD2	5:F:496:LYS:HE2	1.92	0.49
7:T:31:DC:H2'	7:T:32:DT:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:664:ILE:HD12	3:D:681:LYS:HD3	1.92	0.49
4:E:44:ASP:OD2	4:E:52:ARG:NH1	2.46	0.49
5:F:399:LEU:HD21	5:F:446:GLN:HG3	1.94	0.49
2:C:813:GLU:OE1	3:D:504:GLN:NE2	2.45	0.49
3:D:964:LYS:O	3:D:976:THR:N	2.43	0.49
8:G:22:ASN:ND2	8:G:39:ARG:HE	2.10	0.49
6:N:79:DT:H2''	6:N:80:DG:H5''	1.94	0.49
8:G:88:GLN:NE2	8:G:92:MET:SD	2.73	0.49
3:D:528:THR:OG1	3:D:532:GLU:OE2	2.28	0.49
1:B:196:THR:HG21	3:D:443:GLU:HG3	1.94	0.49
5:F:512:GLY:N	7:T:20:DG:OP1	2.43	0.48
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.95	0.48
6:N:78:DC:OP2	6:N:78:DC:H2'	2.13	0.48
7:T:30:DC:H2'	7:T:31:DC:C6	2.47	0.48
2:C:228:VAL:N	2:C:335:THR:O	2.46	0.48
3:D:1109:LEU:HG	3:D:1121:LEU:HG	1.96	0.48
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.47	0.48
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.96	0.48
2:C:530:ILE:HD11	2:C:575:LEU:HD13	1.94	0.48
3:D:41:PRO:HG3	3:D:274:ASN:ND2	2.29	0.48
3:D:848:VAL:HB	3:D:858:VAL:HB	1.94	0.48
8:G:187:VAL:HG21	8:G:199:PHE:HE2	1.79	0.48
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.95	0.48
3:D:17:PHE:O	3:D:1369:ARG:NH2	2.46	0.48
3:D:17:PHE:HZ	3:D:1353:VAL:HG21	1.78	0.48
3:D:481:ARG:HA	3:D:485:MET:HE2	1.95	0.48
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.95	0.48
4:E:37:PRO:HB3	4:E:49:ILE:HG21	1.95	0.48
3:D:294:ASN:HD21	5:F:402:LEU:HD22	1.78	0.48
3:D:530:PRO:HB3	3:D:577:ALA:O	2.13	0.48
3:D:647:PRO:HG2	3:D:650:LYS:HB2	1.95	0.48
3:D:1107:VAL:HG12	3:D:1109:LEU:H	1.79	0.48
1:B:48:LEU:HD11	3:D:535:ARG:HG2	1.94	0.48
2:C:228:VAL:HG23	2:C:337:PHE:HB2	1.96	0.48
5:F:251:LYS:HA	5:F:254:GLU:HG2	1.96	0.48
2:C:243:PRO:O	2:C:246:LEU:HG	2.13	0.48
5:F:452:ILE:HG22	5:F:456:MET:HB3	1.96	0.48
6:N:37:DC:H2'	6:N:38:DT:H71	1.96	0.48
7:T:20:DG:H2''	7:T:21:DA:C8	2.49	0.48
8:G:167:THR:HB	8:G:243:GLU:HB3	1.96	0.48
3:D:1199:PHE:HB2	3:D:1202:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:151:VAL:HG11	5:F:158:LEU:HB3	1.96	0.48
5:F:279:ARG:HA	5:F:282:THR:HG22	1.96	0.48
1:B:215:GLU:OE1	1:B:218:ARG:NH2	2.41	0.47
3:D:1039:ASP:HB3	3:D:1074:LEU:HD21	1.95	0.47
3:D:1059:LEU:HG	3:D:1107:VAL:HB	1.95	0.47
8:H:86:GLN:HA	8:H:89:ILE:HG22	1.96	0.47
1:A:212:ASP:HB3	1:A:215:GLU:HB3	1.96	0.47
2:C:813:GLU:CD	3:D:504:GLN:HE22	2.22	0.47
2:C:616:ILE:HG12	2:C:652:TYR:HB2	1.96	0.47
8:G:133:VAL:HG11	8:G:139:TYR:HB2	1.96	0.47
2:C:802:VAL:HA	2:C:1096:ILE:O	2.14	0.47
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.49	0.47
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.96	0.47
1:B:30:PRO:HG3	1:B:192:VAL:HG21	1.96	0.47
2:C:234:ASP:OD1	2:C:234:ASP:N	2.48	0.47
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.26	0.47
2:C:738:GLU:HA	2:C:741:MET:HE3	1.97	0.47
3:D:1157:ALA:O	3:D:1207:GLY:N	2.45	0.47
5:F:248:GLU:HA	5:F:251:LYS:HG2	1.96	0.47
7:T:17:DT:H2"	7:T:18:DA:C8	2.50	0.47
2:C:905:ILE:O	5:F:599:ARG:NH1	2.47	0.47
8:H:104:GLN:HE22	8:H:228:GLN:HE21	1.62	0.47
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	1.96	0.47
4:E:5:THR:HG22	4:E:7:GLN:H	1.79	0.47
1:B:64:VAL:HG11	1:B:78:ILE:HG21	1.96	0.47
2:C:960:LEU:HB3	2:C:1025:PHE:CD1	2.50	0.47
3:D:678:ARG:HD3	3:D:678:ARG:C	2.40	0.47
3:D:912:GLY:O	3:D:1360:GLY:N	2.39	0.47
8:G:83:LEU:HA	8:G:86:GLN:NE2	2.30	0.47
2:C:624:ASP:HB3	2:C:630:VAL:HG12	1.96	0.46
6:N:74:DC:H2"	6:N:75:DA:N7	2.31	0.46
1:B:25:LYS:HB3	1:B:25:LYS:HE2	1.74	0.46
3:D:353:SER:OG	3:D:445:LYS:O	2.32	0.46
3:D:613:GLY:O	3:D:617:THR:OG1	2.20	0.46
3:D:705:THR:HG21	3:D:716:GLN:HE21	1.80	0.46
5:F:90:GLU:HA	5:F:93:ARG:HD2	1.97	0.46
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.97	0.46
3:D:45:ASN:HB3	3:D:48:THR:O	2.15	0.46
3:D:733:SER:O	3:D:737:ILE:HG12	2.16	0.46
9:H:301:1N7:H10	9:H:301:1N7:H34	1.43	0.46
2:C:1100:PRO:HG3	3:D:637:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:661:VAL:HG23	3:D:682:VAL:HG22	1.96	0.46
8:G:99:ILE:HD11	8:H:78:ILE:HG23	1.98	0.46
8:H:126:VAL:HG12	8:H:186:ALA:HA	1.97	0.46
1:A:227:GLN:HB3	1:B:39:LEU:HD11	1.97	0.46
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.51	0.46
8:H:123:GLU:HG3	8:H:203:PRO:HA	1.97	0.46
2:C:123:TYR:O	5:F:472:GLN:NE2	2.48	0.46
2:C:145:ILE:HB	2:C:456:VAL:HB	1.98	0.46
9:G:301:1N7:H14	9:G:301:1N7:H29	1.75	0.46
3:D:952:VAL:HG13	3:D:984:LEU:HD22	1.97	0.46
5:F:460:ILE:CD1	5:F:501:ALA:HB2	2.46	0.46
1:A:102:LEU:HD21	1:A:110:VAL:HG11	1.97	0.46
1:B:112:ALA:HB1	1:B:123:ILE:HG21	1.98	0.46
2:C:356:THR:HG21	2:C:362:ALA:HB2	1.97	0.46
5:F:544:THR:HA	5:F:547:VAL:HG22	1.97	0.46
2:C:561:ILE:HD11	3:D:772:TYR:HE2	1.80	0.45
3:D:654:ILE:HD13	3:D:760:THR:HB	1.97	0.45
8:H:51:GLN:HE22	8:H:69:THR:HB	1.80	0.45
2:C:192:ASP:HB3	2:C:346:TYR:HD1	1.81	0.45
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.97	0.45
3:D:1021:ASP:OD1	3:D:1024:THR:N	2.49	0.45
3:D:1174:ARG:HE	3:D:1189:MET:HE1	1.81	0.45
3:D:1200:GLU:OE1	3:D:1200:GLU:N	2.46	0.45
8:G:131:PHE:CE2	8:G:133:VAL:HG22	2.51	0.45
8:H:129:LYS:HZ3	8:H:146:ILE:HG13	1.81	0.45
2:C:93:SER:OG	2:C:126:GLU:OE1	2.34	0.45
5:F:343:LYS:O	5:F:346:GLN:HG3	2.15	0.45
3:D:148:GLU:HG2	3:D:177:ASP:HB3	1.98	0.45
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.45	0.45
5:F:290:LEU:O	5:F:294:GLN:HG2	2.16	0.45
1:B:32:GLU:HB3	1:B:35:PHE:CD1	2.52	0.45
3:D:1279:GLN:NE2	3:D:1305:ASP:OD2	2.41	0.45
5:F:595:LEU:O	5:F:599:ARG:HG3	2.15	0.45
2:C:896:THR:HB	2:C:899:GLU:HG2	1.98	0.45
3:D:951:GLN:NE2	3:D:1016:THR:OG1	2.41	0.45
8:H:128:SER:OG	8:H:182:GLU:OE2	2.32	0.45
8:H:171:ASP:OD1	8:H:171:ASP:N	2.48	0.45
2:C:399:ALA:HB3	9:C:1401:1N7:H6	1.99	0.45
8:G:211:ILE:HG22	8:G:261:GLU:HB3	1.98	0.45
3:D:108:ALA:HB2	3:D:280:LYS:HG3	1.99	0.45
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:HB2	1:A:198:LEU:HD13	1.98	0.45
1:B:86:LYS:NZ	3:D:532:GLU:OE1	2.39	0.45
2:C:817:LEU:HD12	2:C:1078:LYS:HB3	1.99	0.45
2:C:250:THR:HA	2:C:268:ARG:HG3	1.98	0.45
2:C:944:ARG:HA	2:C:947:GLU:HG2	1.99	0.45
8:G:101:HIS:HB2	8:G:232:ASP:OD2	2.17	0.45
2:C:377:THR:HG23	2:C:380:ALA:H	1.82	0.44
8:G:179:MET:HE3	8:G:179:MET:HB2	1.76	0.44
2:C:854:ILE:HD11	2:C:885:GLY:HA3	2.00	0.44
8:H:12:ARG:O	8:H:12:ARG:HG2	2.16	0.44
1:B:51:MET:HB2	1:B:178:SER:HB2	1.99	0.44
2:C:696:ASP:O	2:C:1231:TYR:OH	2.34	0.44
3:D:479:GLU:HG3	4:E:20:VAL:HG11	2.00	0.44
5:F:593:LYS:HG2	5:F:597:LYS:HE3	1.99	0.44
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.99	0.44
1:A:159:ILE:HD13	1:A:172:LEU:HD22	1.98	0.44
3:D:325:LYS:HG2	3:D:329:ASP:HB2	1.99	0.44
3:D:1221:LEU:HD22	3:D:1306:LEU:HB2	1.99	0.44
2:C:810:TYR:O	2:C:1077:SER:OG	2.29	0.44
8:G:220:ARG:HG2	9:G:301:1N7:H19	2.00	0.44
2:C:522:SER:OG	2:C:687:ARG:O	2.33	0.44
2:C:619:ALA:HB2	2:C:654:ASP:HB2	2.00	0.44
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.43	0.44
1:B:73:GLY:O	1:B:134:THR:OG1	2.29	0.44
2:C:1119:MET:HE2	2:C:1228:GLY:HA2	2.00	0.44
8:G:92:MET:HB3	8:H:89:ILE:HD13	2.00	0.44
1:A:31:LEU:HD21	1:A:39:LEU:HD12	2.00	0.44
3:D:978:ARG:HG2	3:D:999:TYR:HB2	1.99	0.44
8:H:97:SER:HA	8:H:100:ASN:ND2	2.33	0.44
1:A:155:ALA:O	1:A:159:ILE:HG12	2.17	0.44
2:C:985:GLU:HB3	2:C:988:LYS:HB3	2.00	0.44
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	2.00	0.44
3:D:48:THR:O	3:D:48:THR:OG1	2.26	0.44
2:C:65:ASN:OD1	2:C:66:SER:N	2.51	0.43
2:C:230:PHE:HE2	2:C:287:VAL:HG21	1.83	0.43
2:C:452:ARG:NH2	9:C:1401:1N7:H25	2.33	0.43
2:C:797:GLY:HA3	2:C:1232:MET:O	2.18	0.43
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.83	0.43
3:D:847:ASP:HB3	3:D:856:ILE:HD12	1.99	0.43
3:D:1194:ARG:NH1	3:D:1211:SER:OG	2.50	0.43
8:G:36:ASN:HB3	8:G:38:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASP:OD1	1:B:135:ASP:N	2.51	0.43
3:D:411:ILE:O	3:D:415:VAL:HG13	2.17	0.43
3:D:1273:ASP:OD1	3:D:1273:ASP:N	2.38	0.43
8:G:179:MET:SD	9:G:301:1N7:H24	2.59	0.43
9:G:301:1N7:H10	9:G:301:1N7:H34	1.60	0.43
1:A:32:GLU:HB2	1:A:35:PHE:HD2	1.83	0.43
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.00	0.43
8:G:205:ILE:HD12	8:G:207:ALA:HB2	2.00	0.43
2:C:30:ILE:HD12	2:C:30:ILE:H	1.83	0.43
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.49	0.43
3:D:1176:VAL:HG22	3:D:1187:GLU:HG3	2.00	0.43
8:G:187:VAL:HG21	8:G:199:PHE:CE2	2.53	0.43
1:A:224:LEU:HD13	1:B:228:LEU:HD11	2.00	0.43
2:C:724:VAL:HG21	2:C:771:VAL:HB	2.01	0.43
1:B:82:LEU:HD22	1:B:173:VAL:HG22	2.01	0.43
2:C:215:TYR:CE2	2:C:426:ILE:HD11	2.53	0.43
3:D:1158:GLU:OE1	3:D:1222:ARG:NH1	2.52	0.43
5:F:313:ASP:HB3	5:F:316:PHE:HB3	2.00	0.43
8:G:129:LYS:HE3	8:G:196:ASN:ND2	2.33	0.43
8:G:209:THR:HG22	8:G:263:GLN:HG2	2.01	0.43
2:C:685:MET:SD	2:C:1073:LYS:HB3	2.59	0.43
3:D:215:LYS:HA	3:D:218:THR:HG22	2.00	0.43
3:D:325:LYS:HD2	5:F:508:GLU:HG2	2.00	0.43
3:D:516:ASP:HB3	3:D:573:THR:HG21	2.00	0.43
5:F:303:ILE:HD12	5:F:306:PHE:HD2	1.84	0.43
5:F:442:SER:O	5:F:446:GLN:HG2	2.19	0.43
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.54	0.43
2:C:666:SER:HB3	2:C:704:MET:HG3	1.99	0.43
2:C:1271:GLY:N	2:C:1274:GLU:OE1	2.51	0.43
3:D:71:LEU:HB2	3:D:90:VAL:HG21	2.01	0.43
3:D:96:LYS:HB3	3:D:96:LYS:HE3	1.82	0.43
3:D:102:MET:HG2	3:D:246:PRO:HD3	2.01	0.43
3:D:819:GLY:HA3	3:D:882:VAL:O	2.18	0.43
2:C:160:ASP:OD2	2:C:164:THR:OG1	2.32	0.43
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	2.01	0.43
6:N:59:DG:H2'	6:N:60:DG:C8	2.54	0.43
8:G:211:ILE:HG21	8:G:211:ILE:HD13	1.81	0.43
1:A:118:ASP:HB3	1:A:121:VAL:HB	2.00	0.42
2:C:254:ASP:HB2	2:C:261:VAL:HG13	2.01	0.42
2:C:1066:MET:HE3	2:C:1066:MET:HB3	1.96	0.42
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:THR:HG23	3:D:172:PHE:CD2	2.53	0.42
3:D:984:LEU:HD23	3:D:993:GLU:HG3	2.01	0.42
4:E:3:ARG:HB2	4:E:48:VAL:HG13	1.99	0.42
5:F:349:GLU:OE1	5:F:349:GLU:N	2.52	0.42
1:A:112:ALA:HB1	1:A:123:ILE:HG21	2.00	0.42
5:F:296:LYS:HD2	5:F:298:PRO:HD3	2.00	0.42
8:G:95:MET:HE2	8:H:85:ILE:HD12	2.00	0.42
8:H:102:TYR:CE1	8:H:106:LYS:HE3	2.54	0.42
2:C:204:LEU:HB3	2:C:208:ILE:HD12	2.00	0.42
2:C:300:ASP:OD1	2:C:313:ALA:N	2.48	0.42
2:C:1289:GLU:HG3	2:C:1294:LYS:HE3	2.01	0.42
8:G:112:MET:HE2	8:G:112:MET:HB3	1.90	0.42
8:G:123:GLU:OE1	8:G:203:PRO:HA	2.18	0.42
2:C:18:ARG:O	2:C:1156:ARG:NE	2.48	0.42
3:D:1036:ARG:HB2	3:D:1081:VAL:HG22	2.01	0.42
5:F:105:MET:HE3	5:F:105:MET:HB3	1.96	0.42
2:C:1127:LYS:HE2	2:C:1127:LYS:HB2	1.77	0.42
3:D:147:ILE:N	3:D:147:ILE:HD12	2.35	0.42
3:D:1173:ARG:NE	3:D:1192:LYS:HE2	2.34	0.42
5:F:333:VAL:HG12	5:F:336:GLU:HB3	2.02	0.42
8:H:224:ILE:HD13	8:H:224:ILE:HA	1.90	0.42
2:C:189:ASP:OD1	2:C:193:ASN:N	2.33	0.42
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.60	0.42
3:D:1155:ILE:HB	3:D:1211:SER:HB3	2.01	0.42
5:F:145:LEU:HD12	5:F:225:ARG:NH2	2.34	0.42
5:F:279:ARG:HH12	5:F:346:GLN:HE22	1.67	0.42
8:H:143:ILE:HD13	8:H:143:ILE:HA	1.94	0.42
2:C:65:ASN:O	2:C:105:TYR:N	2.47	0.42
2:C:325:LEU:HB2	2:C:330:HIS:HD2	1.84	0.42
2:C:708:VAL:HG11	2:C:794:LEU:HD22	2.02	0.42
3:D:566:LYS:HB2	3:D:566:LYS:HE2	1.76	0.42
3:D:1029:THR:OG1	3:D:1117:SER:HA	2.20	0.42
3:D:1081:VAL:HG12	3:D:1087:ASP:HA	2.02	0.42
5:F:277:MET:O	5:F:281:ARG:HB2	2.19	0.42
2:C:1027:LYS:HD3	2:C:1027:LYS:HA	1.86	0.42
3:D:1140:ARG:NH2	3:D:1236:GLU:OE1	2.41	0.42
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.20	0.42
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.53	0.42
2:C:1200:LYS:HE3	2:C:1200:LYS:HB2	1.61	0.42
3:D:297:ARG:NH2	5:F:104:GLU:OE2	2.45	0.42
3:D:350:SER:HA	3:D:468:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1191:PRO:HB2	3:D:1193:TRP:CE2	2.54	0.42
7:T:1:DC:H2''	7:T:2:DG:C8	2.55	0.42
9:T:101:1N7:H14	9:T:101:1N7:H29	1.84	0.42
8:G:173:GLU:HG3	8:G:174:TYR:N	2.35	0.42
2:C:232:ILE:HG12	2:C:237:LEU:HA	2.02	0.41
2:C:1289:GLU:HB2	2:C:1293:VAL:CG2	2.50	0.41
6:N:74:DC:H2''	6:N:75:DA:C8	2.55	0.41
8:G:62:ILE:O	8:G:66:VAL:HG23	2.20	0.41
8:G:166:PHE:CZ	8:G:202:ILE:HD12	2.55	0.41
2:C:22:LEU:HD13	2:C:603:ILE:HD13	2.02	0.41
2:C:1289:GLU:CA	2:C:1293:VAL:HG22	2.47	0.41
2:C:1319:MET:HE2	2:C:1319:MET:HB2	1.94	0.41
5:F:469:GLN:OE1	5:F:486:ARG:NH2	2.53	0.41
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.88	0.41
2:C:12:ARG:NH2	2:C:698:PRO:O	2.45	0.41
2:C:260:LYS:HA	2:C:260:LYS:HD3	1.88	0.41
2:C:672:GLU:HG2	2:C:673:HIS:CD2	2.56	0.41
3:D:646:ILE:HD13	3:D:762:ASN:HD21	1.85	0.41
1:A:205:MET:HE1	1:A:216:ALA:HB3	2.01	0.41
2:C:246:LEU:CD1	2:C:246:LEU:O	2.63	0.41
2:C:264:GLU:H	2:C:267:ARG:HH12	1.67	0.41
3:D:432:LEU:O	3:D:435:GLN:NE2	2.44	0.41
1:A:19:VAL:HB	1:A:23:HIS:HD2	1.85	0.41
2:C:1247:SER:O	3:D:348:ASP:HB3	2.20	0.41
8:G:233:ASN:O	8:G:268:LYS:NZ	2.51	0.41
8:H:226:LEU:HD23	8:H:226:LEU:HA	1.74	0.41
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.54	0.41
3:D:205:LEU:HD23	3:D:205:LEU:HA	1.92	0.41
3:D:1158:GLU:HB3	3:D:1186:TYR:CE2	2.56	0.41
8:H:129:LYS:HB3	8:H:197:ILE:HG22	2.02	0.41
2:C:815:SER:HB3	2:C:1077:SER:HB3	2.02	0.41
3:D:1102:PRO:HG2	3:D:1124:ILE:HG12	2.02	0.41
3:D:1188:GLU:O	3:D:1189:MET:HE2	2.21	0.41
6:N:85:DG:H1'	6:N:86:DG:H5'	2.03	0.41
3:D:490:ILE:HA	3:D:500:ILE:HG12	2.03	0.41
3:D:576:ARG:HD3	3:D:593:ASN:HA	2.02	0.41
8:H:24:ILE:HD11	8:H:26:LEU:HD21	2.02	0.41
8:H:119:LYS:HD2	8:H:209:THR:HG21	2.02	0.41
2:C:373:GLY:O	5:F:103:ARG:NH1	2.41	0.41
2:C:632:ASP:HA	2:C:647:ARG:HD2	2.03	0.41
3:D:1284:ARG:HA	3:D:1284:ARG:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:220:LYS:O	5:F:223:GLU:HG3	2.21	0.41
5:F:327:SER:O	5:F:331:HIS:ND1	2.53	0.41
7:T:6:DC:H2"	7:T:7:DG:C8	2.55	0.41
7:T:23:DT:H2"	7:T:24:DC:C6	2.56	0.41
8:G:123:GLU:CD	8:G:203:PRO:HA	2.46	0.41
8:H:167:THR:HG23	8:H:181:VAL:HG13	2.03	0.41
8:H:176:GLU:C	8:H:177:LYS:HD3	2.45	0.41
2:C:591:TYR:HB3	2:C:652:TYR:HB3	2.02	0.41
5:F:248:GLU:HG3	5:F:251:LYS:NZ	2.36	0.41
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.89	0.40
2:C:960:LEU:O	2:C:963:GLU:HG3	2.21	0.40
2:C:966:ILE:HD11	9:C:1402:1N7:H15	2.03	0.40
3:D:192:MET:HE3	3:D:192:MET:HB2	1.98	0.40
3:D:860:ARG:NH1	3:D:861:ASN:OD1	2.54	0.40
5:F:138:PRO:O	5:F:142:THR:HG23	2.20	0.40
5:F:347:ILE:HD12	5:F:347:ILE:HA	1.90	0.40
8:H:82:ARG:HA	8:H:85:ILE:HG22	2.03	0.40
1:B:110:VAL:HG21	1:B:140:ILE:HG21	2.03	0.40
2:C:453:ILE:HD12	2:C:530:ILE:HD12	2.03	0.40
2:C:979:LEU:HA	2:C:979:LEU:HD23	1.77	0.40
3:D:118:LYS:HE3	3:D:118:LYS:HB3	1.82	0.40
3:D:1024:THR:HA	3:D:1125:PRO:HA	2.03	0.40
3:D:1046:ILE:HG23	3:D:1059:LEU:HB2	2.03	0.40
7:T:19:DG:H4'	7:T:20:DG:OP1	2.20	0.40
8:G:192:LYS:HG3	8:G:194:GLU:OE1	2.22	0.40
8:G:247:ASP:OD1	8:G:259:MET:N	2.53	0.40
1:B:107:ILE:HD12	1:B:136:GLU:HG2	2.02	0.40
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	2.04	0.40
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.19	0.40
3:D:548:VAL:HG13	3:D:550:VAL:HG23	2.03	0.40
4:E:75:GLN:NE2	4:E:76:GLU:OE2	2.55	0.40
8:H:29:PRO:HG2	8:H:32:ILE:HD11	2.02	0.40
8:H:108:LYS:HB2	8:H:108:LYS:HE3	1.87	0.40
5:F:283:GLN:O	5:F:287:ILE:HG12	2.22	0.40
8:G:121:ILE:HA	8:G:122:PRO:HD3	1.97	0.40
8:G:126:VAL:HG12	8:G:186:ALA:HA	2.04	0.40
1:A:74:VAL:HG22	1:A:133:LEU:HD23	2.03	0.40
2:C:120:GLN:HG2	2:C:489:PRO:HG2	2.04	0.40
2:C:476:LYS:HB2	2:C:476:LYS:HE3	1.84	0.40
3:D:278:ARG:NH2	5:F:403:ASP:OD1	2.46	0.40
5:F:325:PRO:O	5:F:328:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:126:VAL:HG21	8:G:202:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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
9	1N7	T	101	-	29,29,46	0.76	1 (3%)	47,47,72	1.62	6 (12%)
9	1N7	C	1401	-	29,29,46	0.75	1 (3%)	47,47,72	1.56	7 (14%)
12	118	G	302	-	28,28,28	0.56	0	24,38,38	0.34	0
9	1N7	H	301	-	30,30,46	0.75	1 (3%)	47,48,72	1.63	8 (17%)
12	118	H	302	-	28,28,28	0.54	0	24,38,38	0.43	0
9	1N7	G	301	-	29,29,46	0.75	1 (3%)	47,47,72	1.73	9 (19%)
9	1N7	C	1402	-	29,29,46	0.76	1 (3%)	47,47,72	1.60	6 (12%)

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
9	1N7	T	101	-	-	6/6/71/92	0/4/4/4
9	1N7	C	1401	-	-	5/6/71/92	0/4/4/4
12	118	G	302	-	-	-	0/4/4/4
9	1N7	H	301	-	-	6/7/72/92	0/4/4/4
12	118	H	302	-	-	-	0/4/4/4
9	1N7	G	301	-	-	4/6/71/92	0/4/4/4
9	1N7	C	1402	-	-	6/6/71/92	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	301	1N7	O4-C4	-2.09	1.40	1.43
9	C	1402	1N7	O4-C4	-2.08	1.40	1.43
9	T	101	1N7	O4-C4	-2.05	1.40	1.43
9	H	301	1N7	O4-C4	-2.04	1.40	1.43
9	C	1401	1N7	O4-C4	-2.02	1.40	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	301	1N7	C5-C9-C20	-5.75	112.52	119.48
9	C	1402	1N7	C5-C9-C20	-5.40	112.95	119.48
9	H	301	1N7	C5-C9-C20	-5.39	112.96	119.48
9	T	101	1N7	C5-C9-C20	-5.33	113.03	119.48
9	C	1401	1N7	C5-C9-C20	-5.05	113.37	119.48
9	G	301	1N7	C3-C19-C2	-4.91	108.72	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	101	1N7	C3-C19-C2	-4.04	109.60	113.70
9	G	301	1N7	C5-C6-C18	-4.03	109.61	114.72
9	C	1401	1N7	C3-C19-C2	-3.99	109.66	113.70
9	H	301	1N7	C3-C19-C2	-3.97	109.68	113.70
9	C	1402	1N7	C3-C19-C2	-3.85	109.79	113.70
9	C	1401	1N7	C3-C4-C5	-3.54	107.67	111.26
9	H	301	1N7	C3-C4-C5	-3.47	107.73	111.26
9	C	1402	1N7	C3-C4-C5	-3.32	107.89	111.26
9	T	101	1N7	C3-C4-C5	-3.25	107.96	111.26
9	T	101	1N7	C5-C6-C18	-2.98	110.94	114.72
9	C	1402	1N7	C5-C6-C18	-2.95	110.97	114.72
9	G	301	1N7	C9-C5-C4	-2.56	115.36	117.67
9	C	1401	1N7	C5-C6-C18	-2.56	111.47	114.72
9	G	301	1N7	C2-C19-C18	-2.53	109.01	111.84
9	G	301	1N7	C3-C4-C5	-2.51	108.71	111.26
9	H	301	1N7	C2-C19-C18	-2.47	109.08	111.84
9	H	301	1N7	C5-C6-C18	-2.44	111.62	114.72
9	C	1402	1N7	O2-C13-C14	-2.43	105.01	109.84
9	C	1401	1N7	O2-C13-C14	-2.40	105.06	109.84
9	H	301	1N7	C9-C5-C4	-2.37	115.54	117.67
9	T	101	1N7	O2-C13-C14	-2.37	105.13	109.84
9	G	301	1N7	O2-C13-C14	-2.36	105.14	109.84
9	H	301	1N7	O2-C13-C14	-2.36	105.14	109.84
9	T	101	1N7	C9-C5-C4	-2.34	115.56	117.67
9	C	1402	1N7	C9-C5-C4	-2.19	115.70	117.67
9	H	301	1N7	C6-C5-C4	2.16	109.39	107.42
9	C	1401	1N7	C2-C19-C18	-2.16	109.44	111.84
9	G	301	1N7	C16-C17-C18	-2.05	109.26	111.50
9	G	301	1N7	C14-C13-C12	-2.05	108.11	110.62
9	C	1401	1N7	C14-C13-C12	-2.01	108.17	110.62

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	H	301	1N7	C21-C20-C9-C8
9	G	301	1N7	C21-C20-C9-C5
9	H	301	1N7	C21-C20-C9-C5
9	G	301	1N7	C22-C20-C9-C5
9	G	301	1N7	C21-C20-C9-C8
9	H	301	1N7	C22-C20-C9-C5
9	T	101	1N7	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
9	H	301	1N7	C9-C20-C22-C23
9	H	301	1N7	C21-C20-C22-C23
9	T	101	1N7	C9-C20-C22-C23
9	H	301	1N7	C22-C20-C9-C8
9	T	101	1N7	C21-C20-C9-C5
9	T	101	1N7	C22-C20-C9-C5
9	G	301	1N7	C22-C20-C9-C8
9	C	1401	1N7	C21-C20-C9-C5
9	C	1401	1N7	C22-C20-C9-C5
9	C	1402	1N7	C22-C20-C9-C5
9	C	1402	1N7	C21-C20-C9-C5
9	T	101	1N7	C21-C20-C9-C8
9	C	1401	1N7	C21-C20-C9-C8
9	C	1402	1N7	C21-C20-C9-C8
9	C	1402	1N7	C9-C20-C22-C23
9	C	1402	1N7	C21-C20-C22-C23
9	T	101	1N7	C22-C20-C9-C8
9	C	1402	1N7	C22-C20-C9-C8
9	C	1401	1N7	C22-C20-C9-C8
9	C	1401	1N7	C21-C20-C22-C23

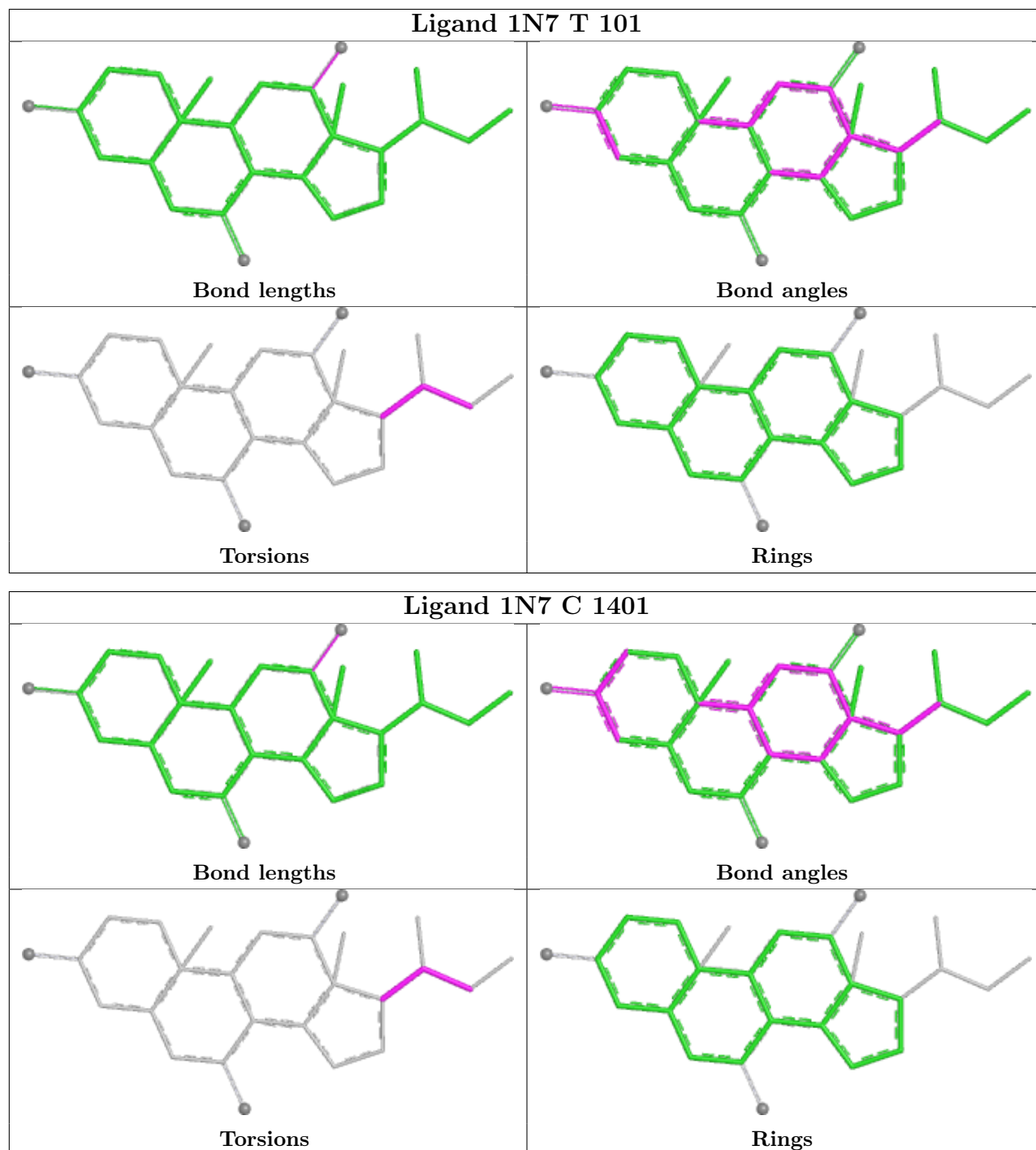
There are no ring outliers.

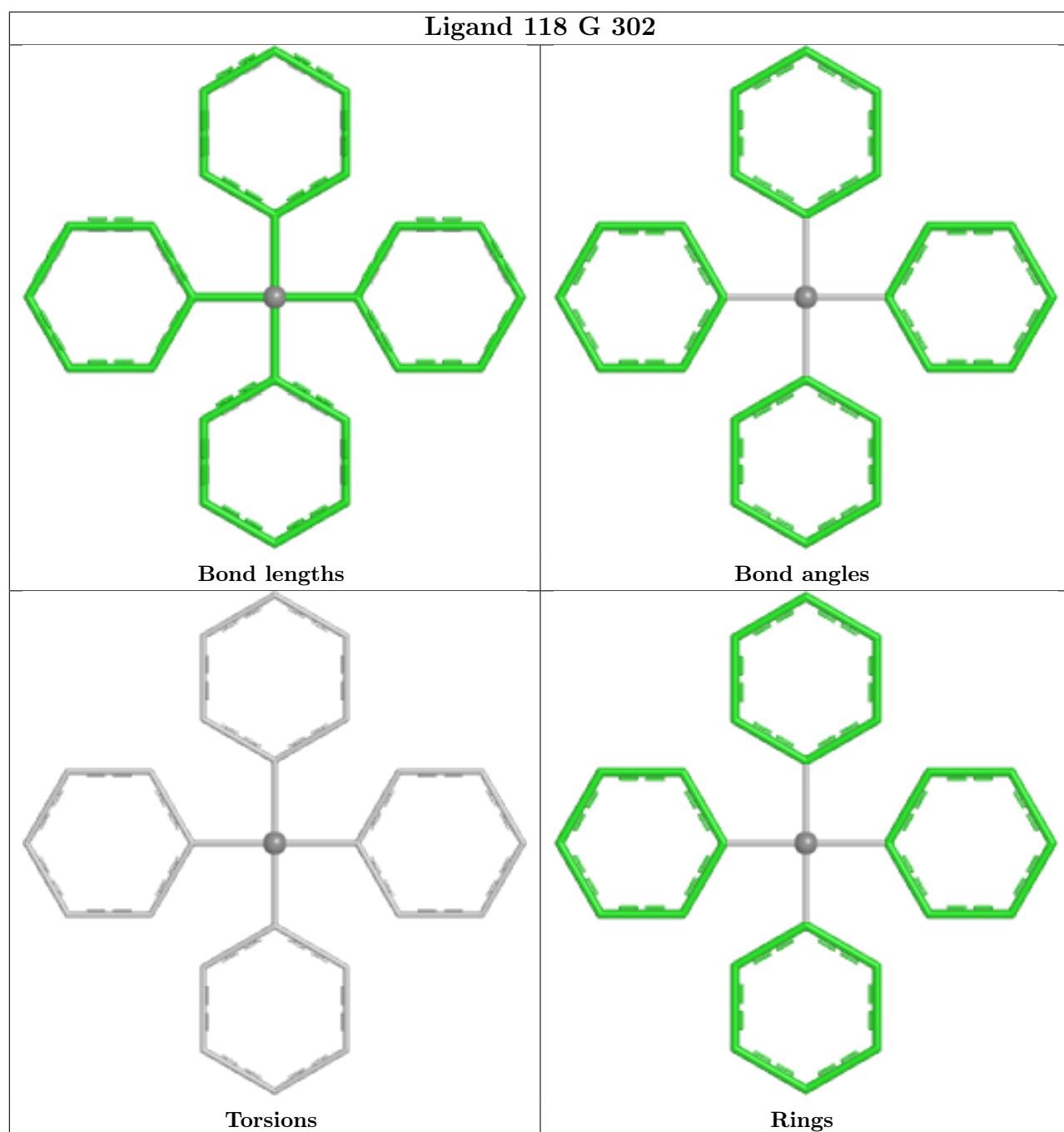
7 monomers are involved in 13 short contacts:

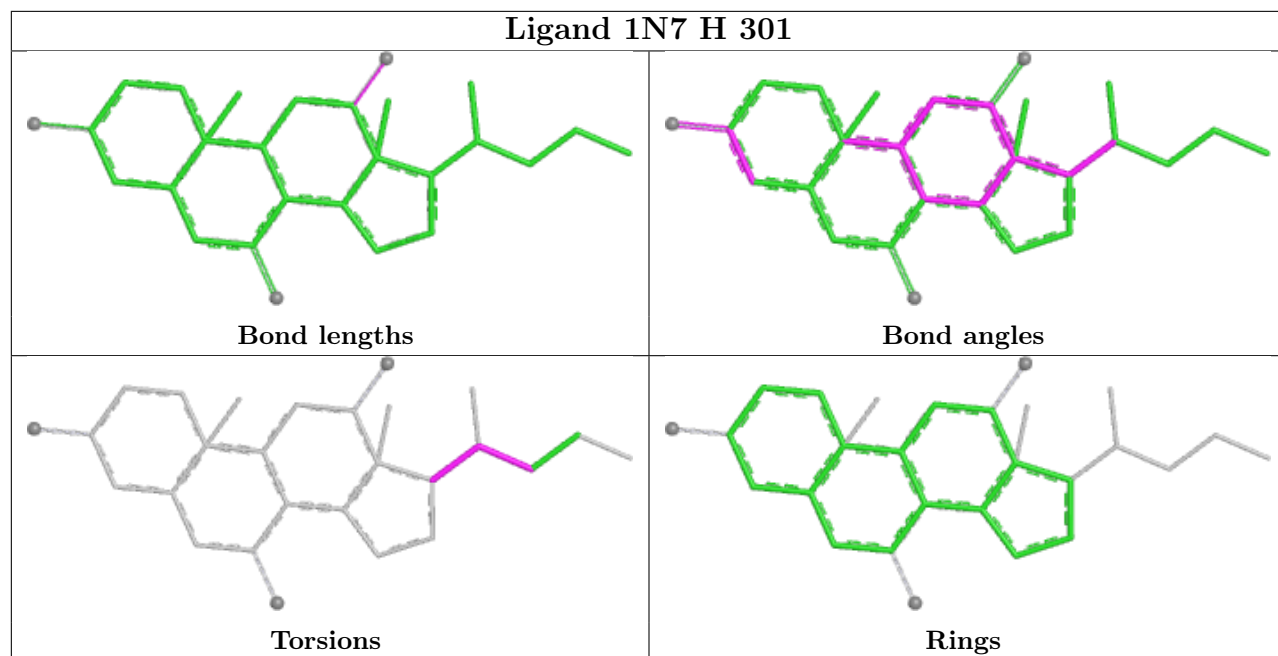
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	T	101	1N7	1	0
9	C	1401	1N7	2	0
12	G	302	118	2	0
9	H	301	1N7	2	0
12	H	302	118	1	0
9	G	301	1N7	4	0
9	C	1402	1N7	1	0

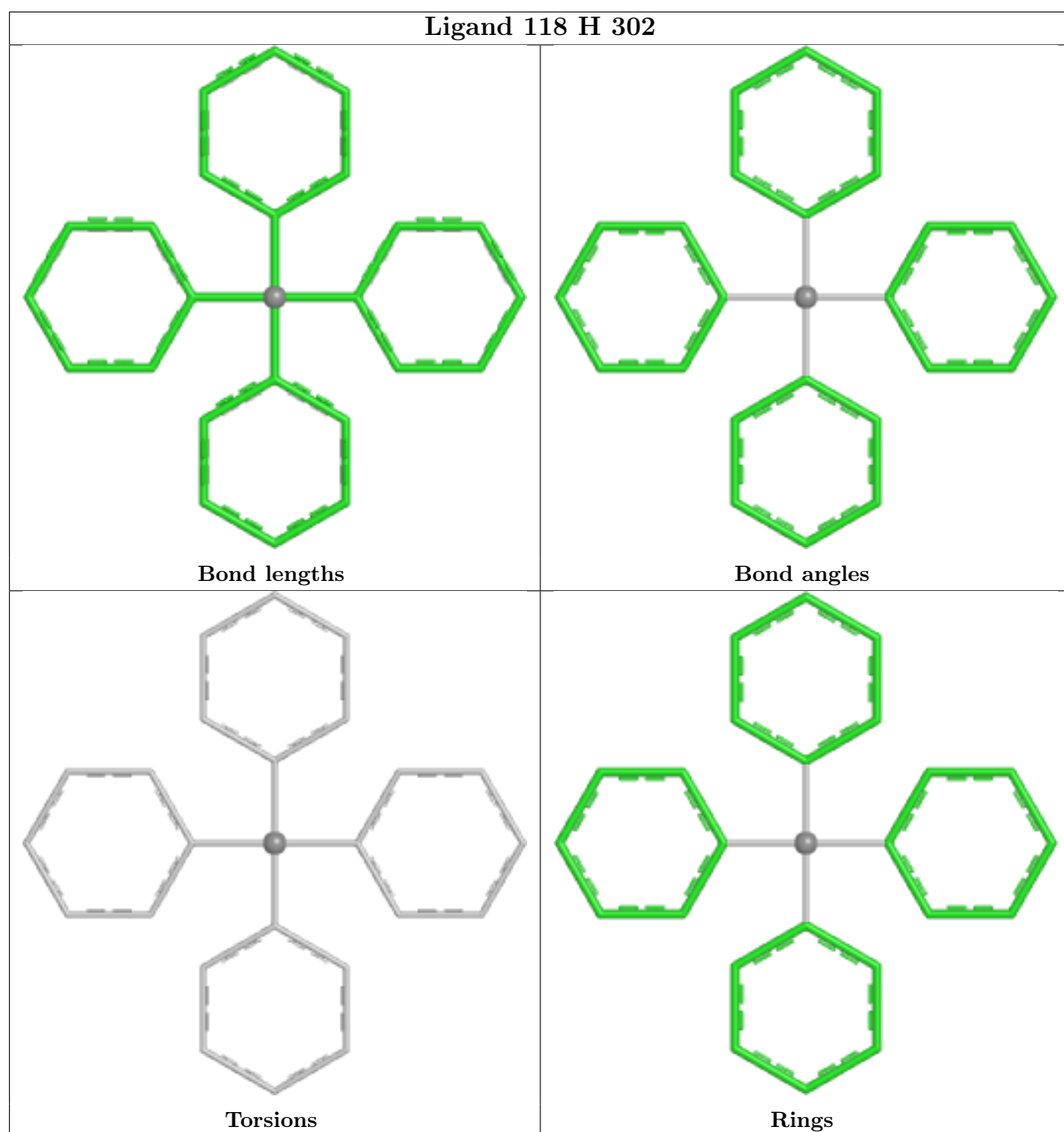
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

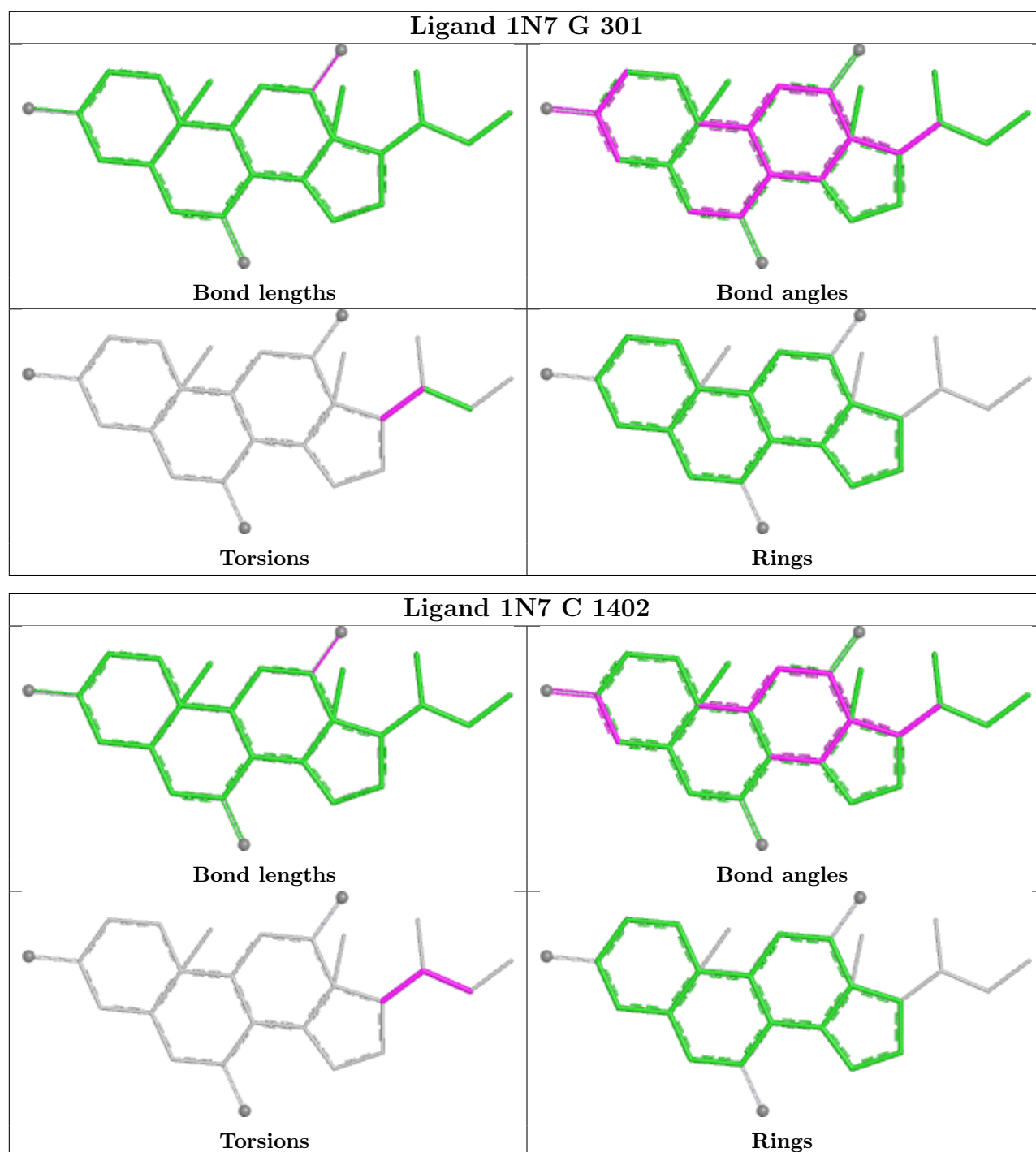
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

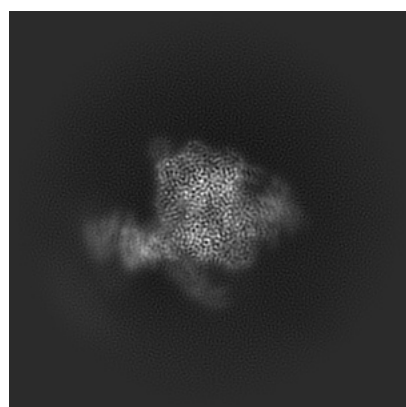
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22234. These allow visual inspection of the internal detail of the map and identification of artifacts.

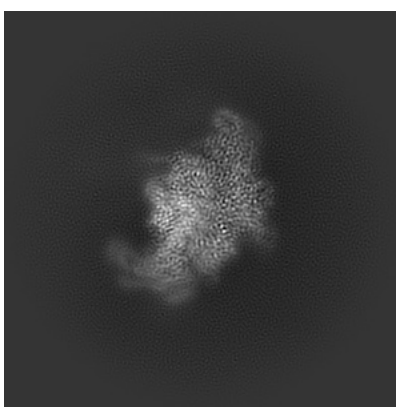
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

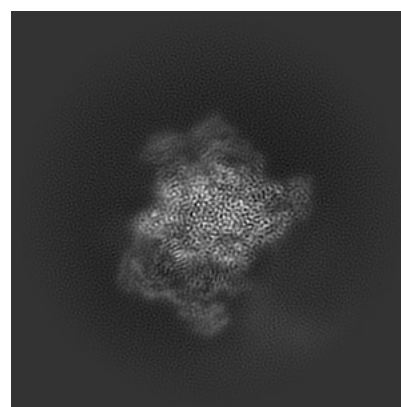
6.1.1 Primary map



X



Y

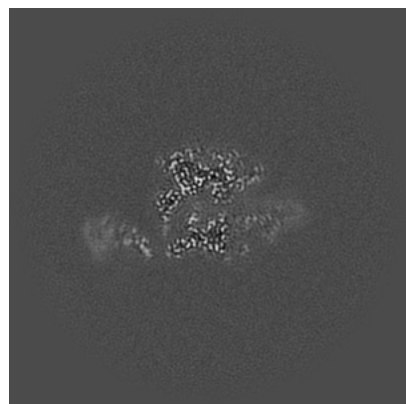


Z

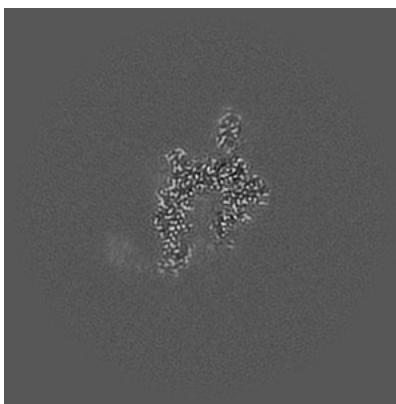
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

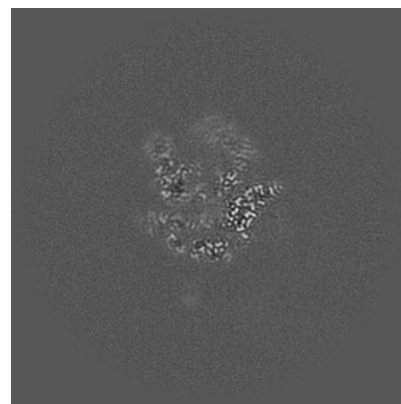
6.2.1 Primary map



X Index: 192



Y Index: 192

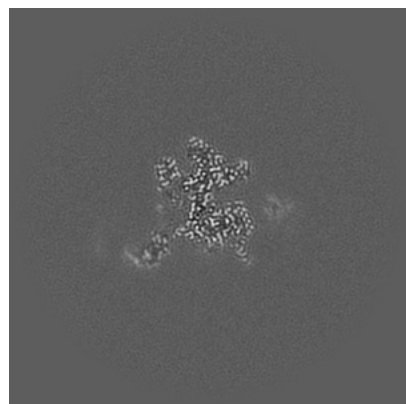


Z Index: 192

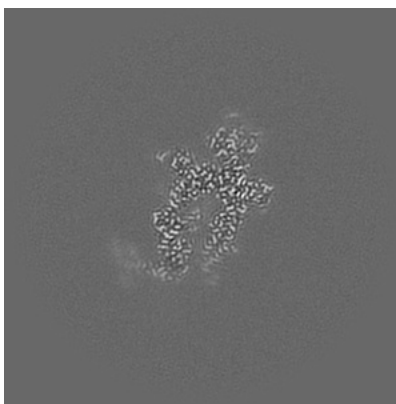
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

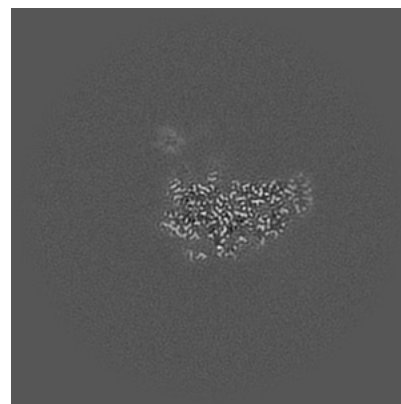
6.3.1 Primary map



X Index: 210



Y Index: 184

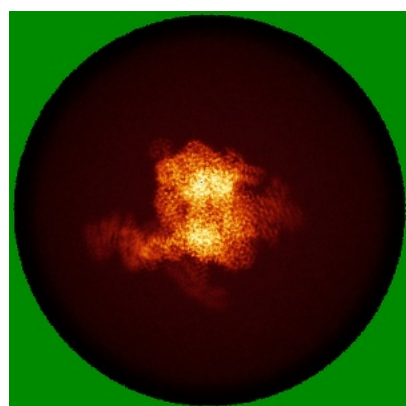


Z Index: 213

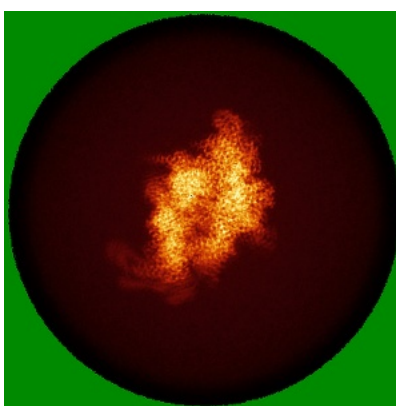
The images above show the largest variance slices of the map in three orthogonal directions.

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

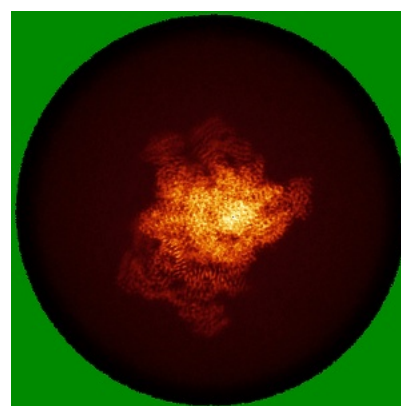
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.461. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

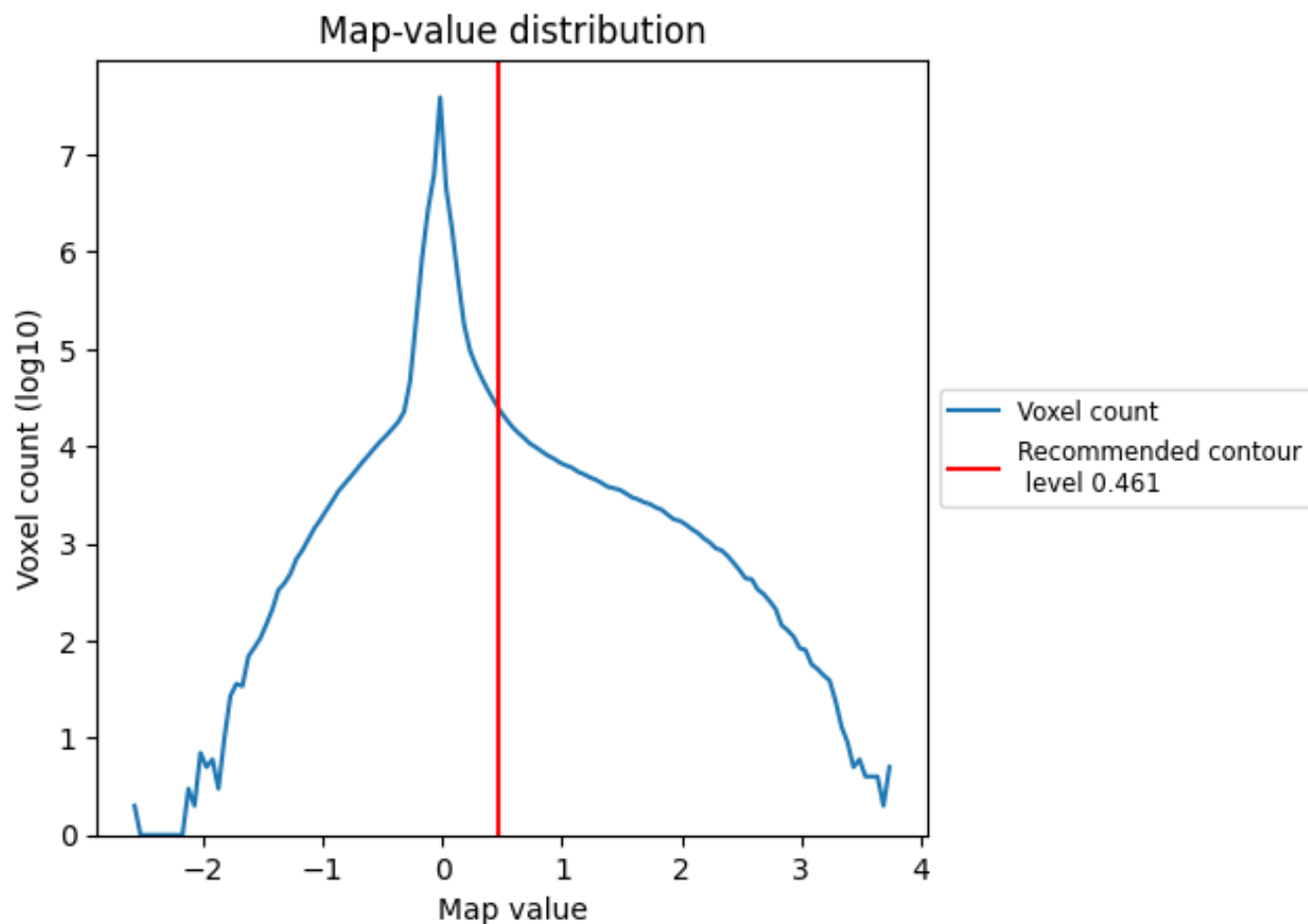
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

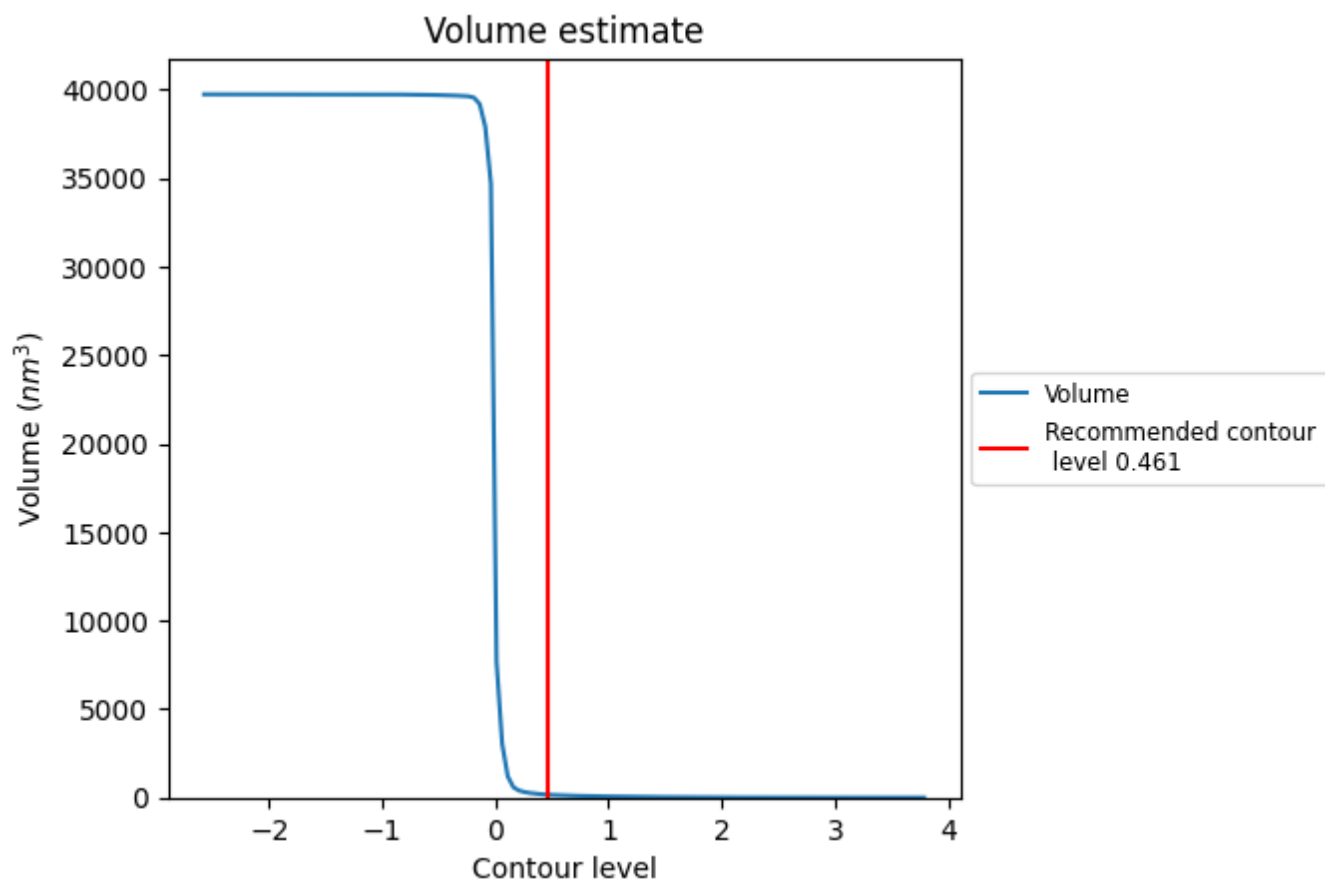
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

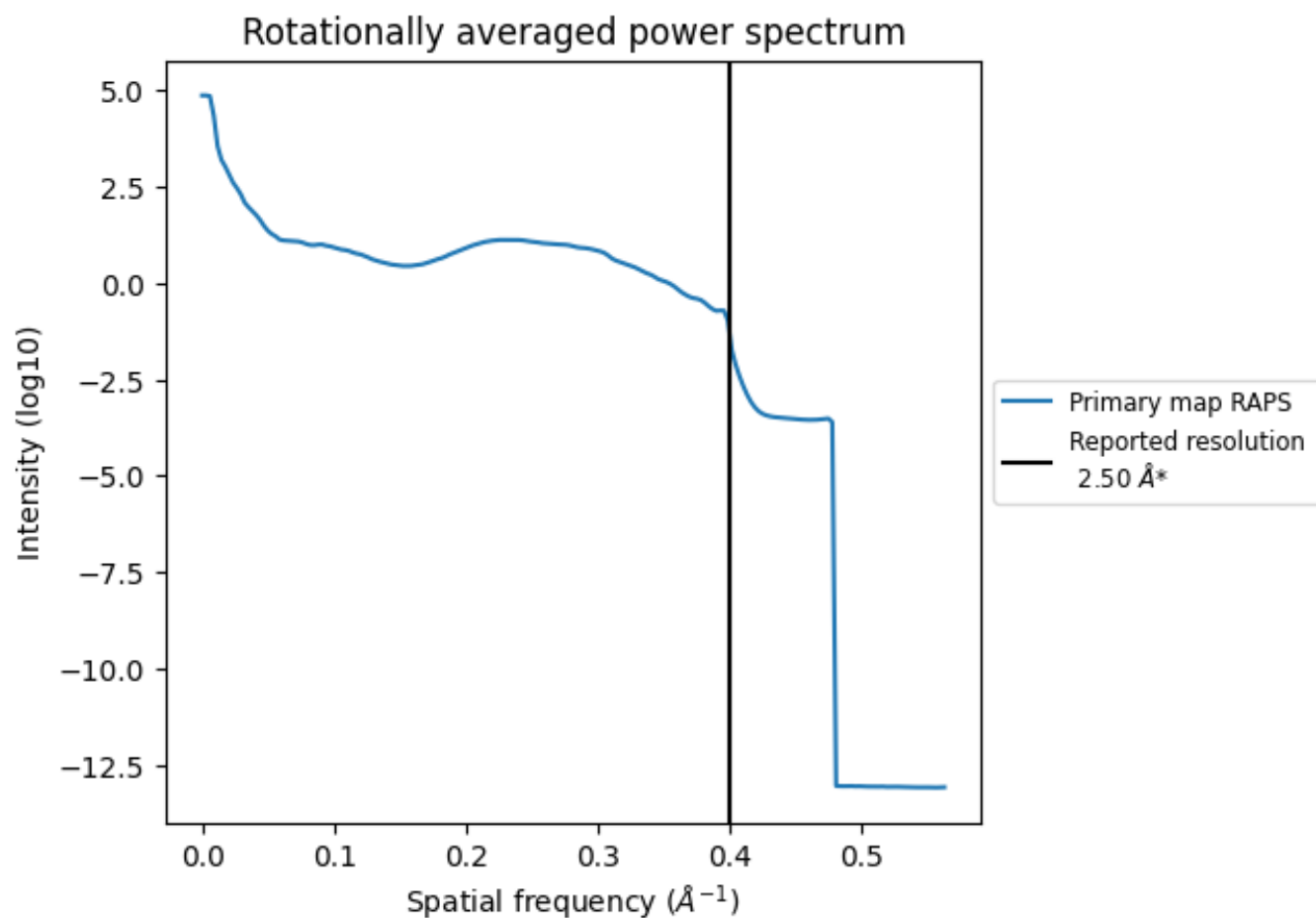
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

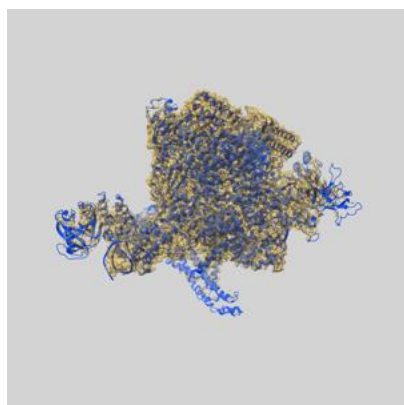
8 Fourier-Shell correlation ⓘ

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

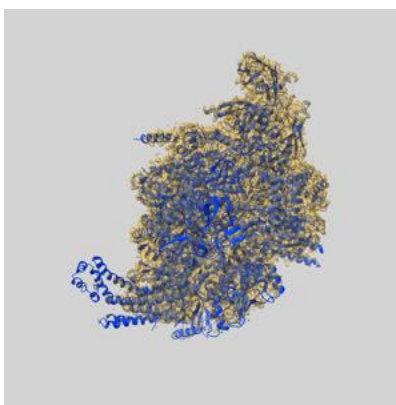
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22234 and PDB model 6XL5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

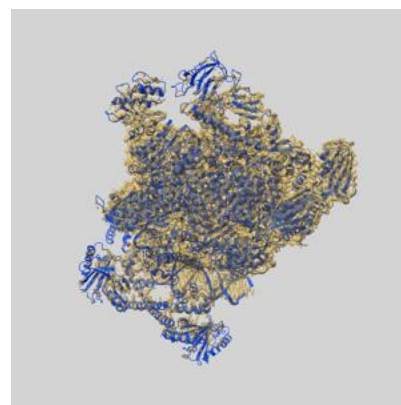
9.1 Map-model overlay [i](#)



X



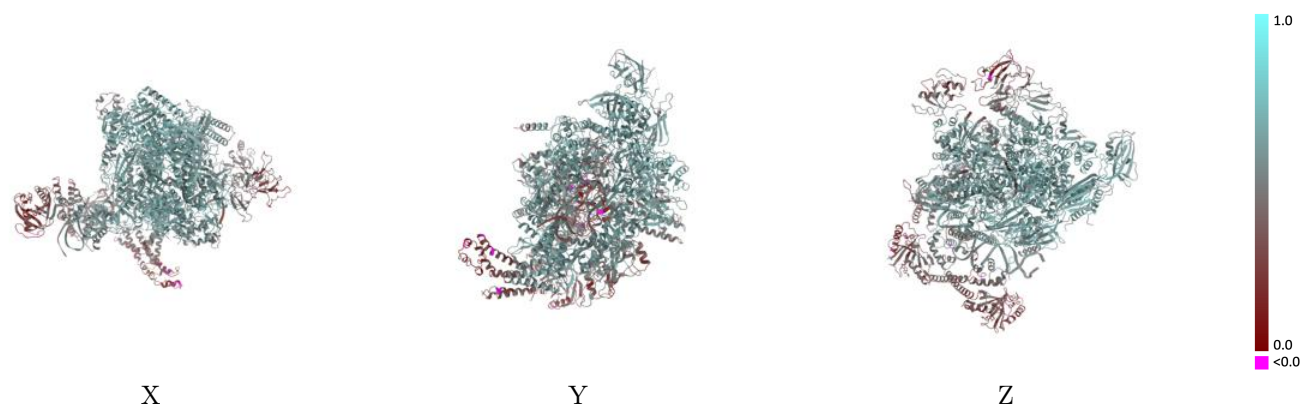
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.461 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

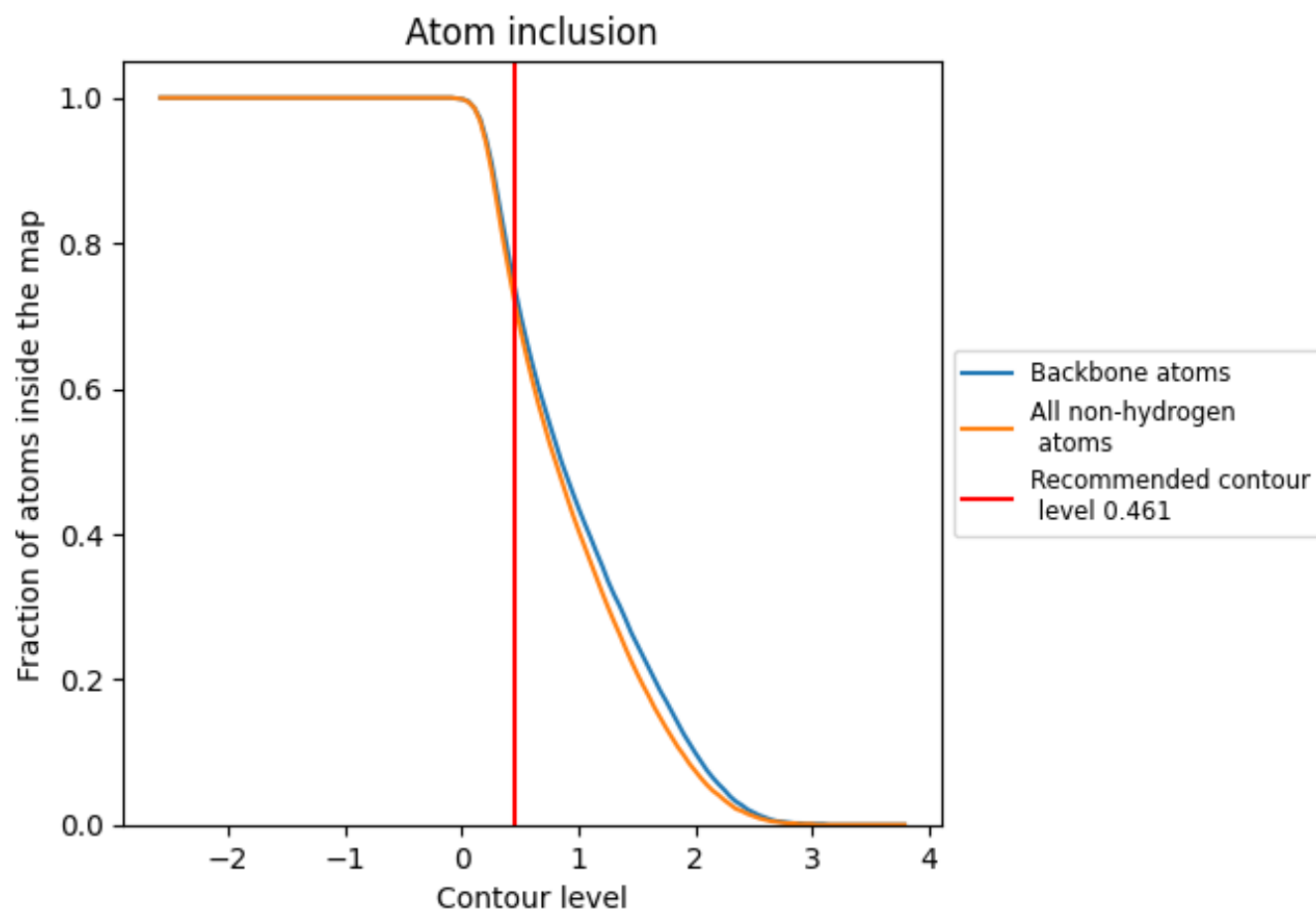


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 71% 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 (0.461) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.5410
A	0.8650	0.6150
B	0.8080	0.5920
C	0.8220	0.5910
D	0.7810	0.5730
E	0.8150	0.5930
F	0.5360	0.4640
G	0.3330	0.3560
H	0.3640	0.3710
N	0.7960	0.5410
T	0.7510	0.5220

1.0

0.0

<0.0