



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 12:25 AM EST

PDB ID : 6XL5  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

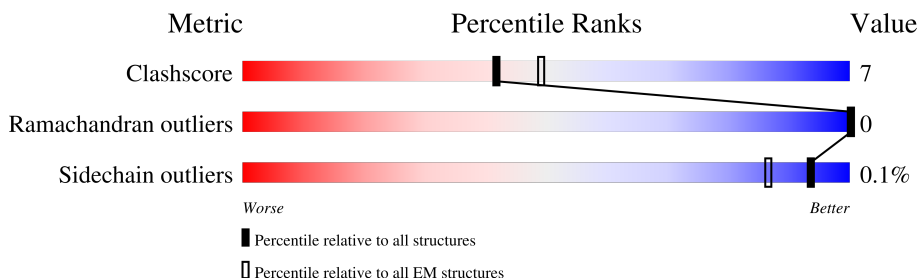
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
6	N	54	
7	T	54	

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Mol	Chain	Length	Quality of chain
8	G	268	<div><div>63%</div><div>75%</div><div>25%</div></div>
8	H	268	<div><div>55%</div><div>78%</div><div>22%</div></div>

## 2 Entry composition

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		

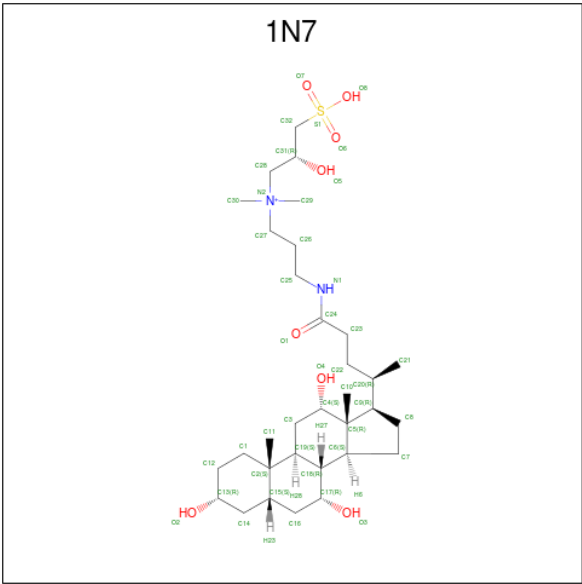
- Molecule 7 is a DNA chain called synthetic template strand DNA (54-MER).

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 (three-letter code: 1N7) (formula: C<sub>32</sub>H<sub>59</sub>N<sub>2</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			52	46	6	
9	C	1	Total	C	O	0
			52	46	6	
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	

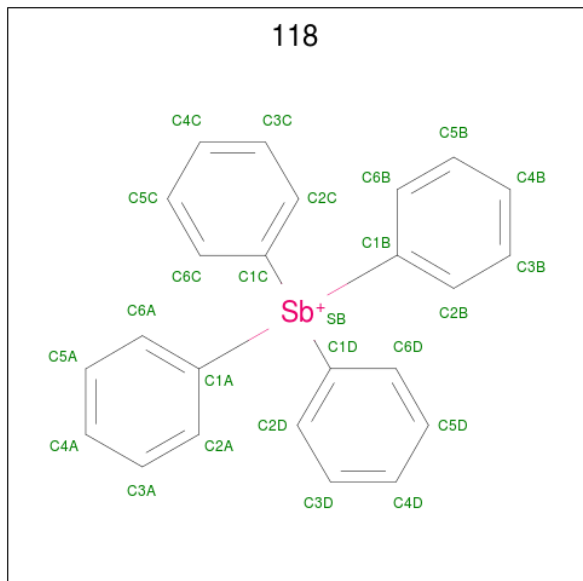
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is TETRAPHENYLANTIMONIUM ION (three-letter code: 118) (formula: C<sub>24</sub>H<sub>20</sub>Sb) (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	

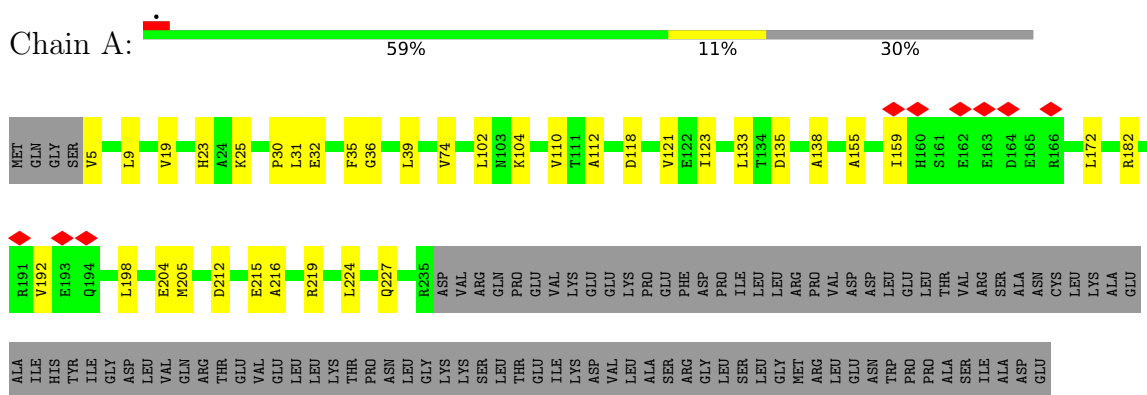
- Molecule 13 is water.

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

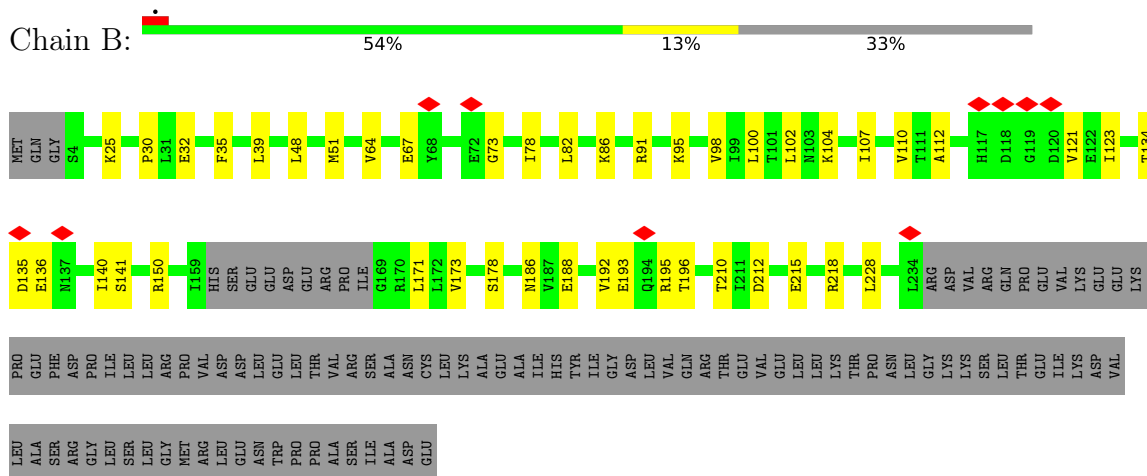
### 3 Residue-property plots

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.

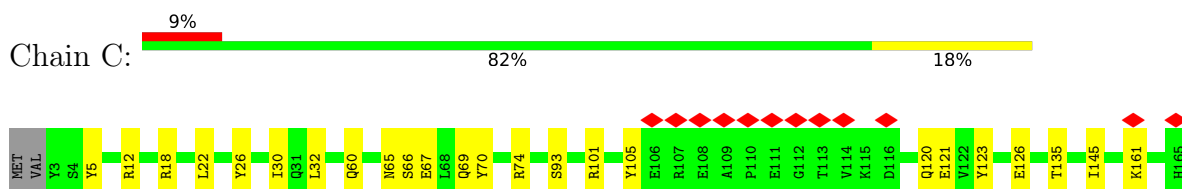
- Molecule 1: DNA-directed RNA polymerase subunit alpha



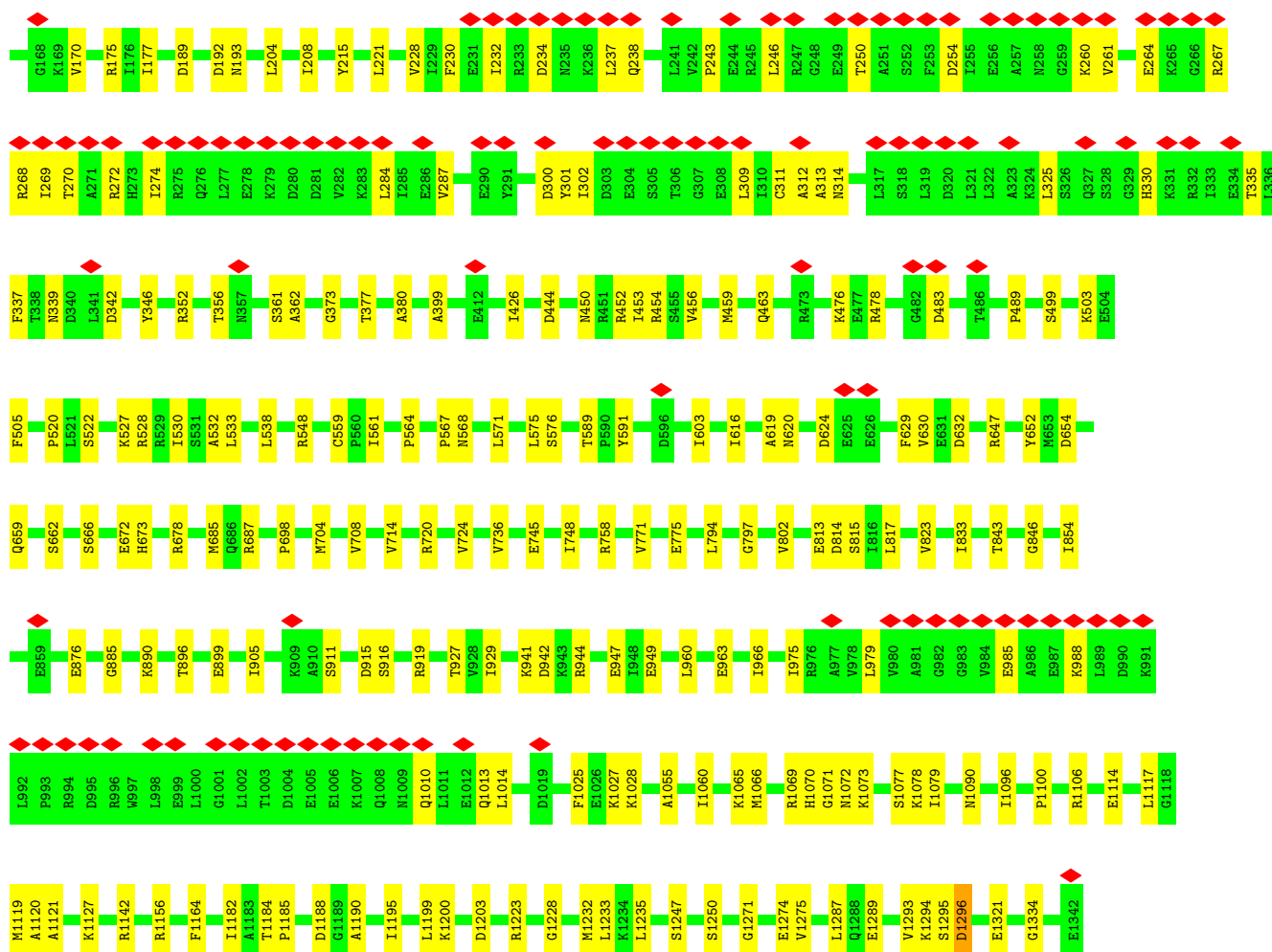
- Molecule 1: DNA-directed RNA polymerase subunit alpha



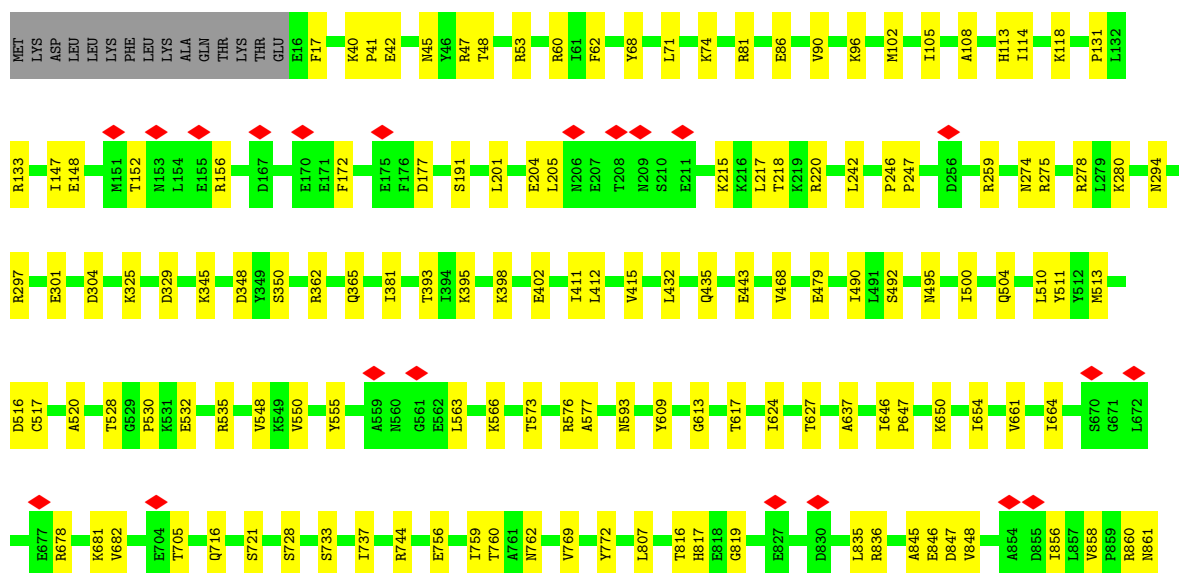
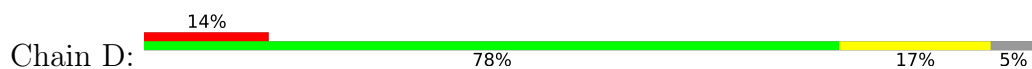
- Molecule 2: DNA-directed RNA polymerase subunit beta

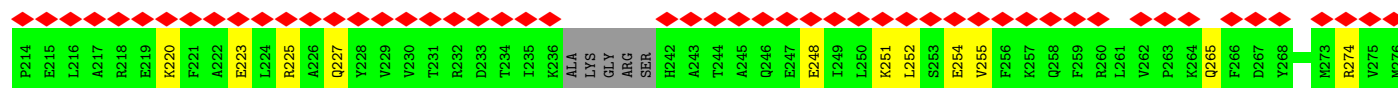


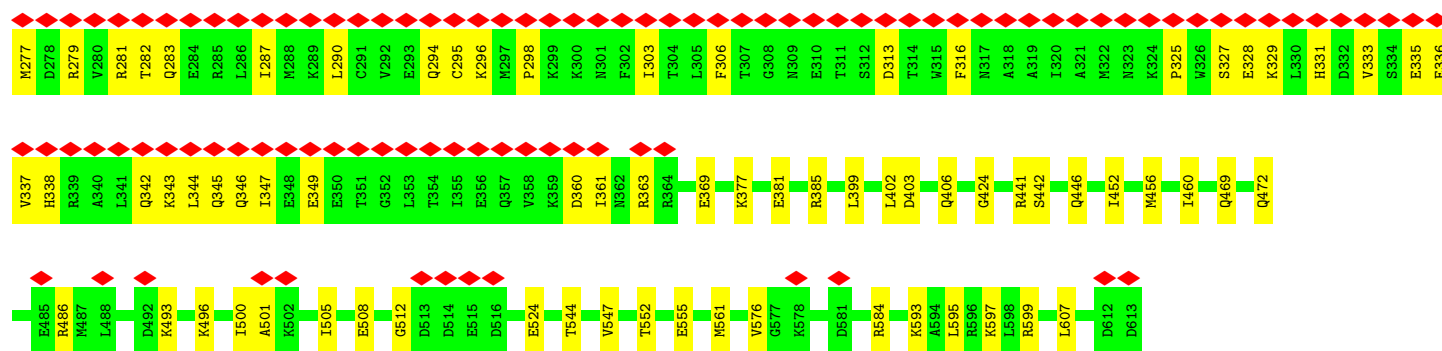




• Molecule 3: DNA-directed RNA polymerase subunit beta'



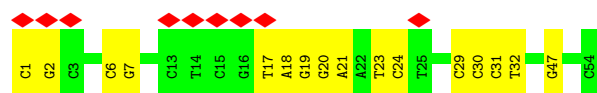




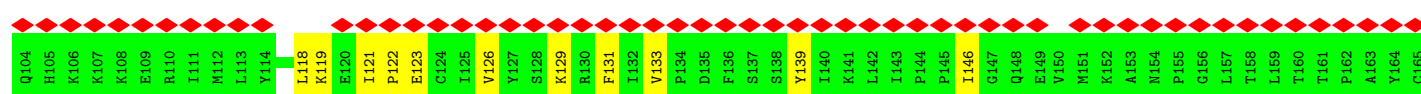
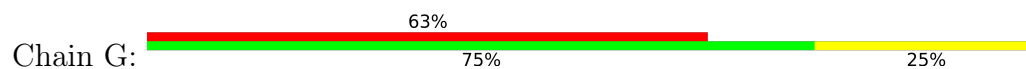
- Molecule 6: synthetic non-template strand DNA (54-MER)



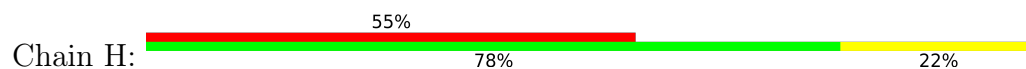
- Molecule 7: synthetic template strand DNA (54-MER)

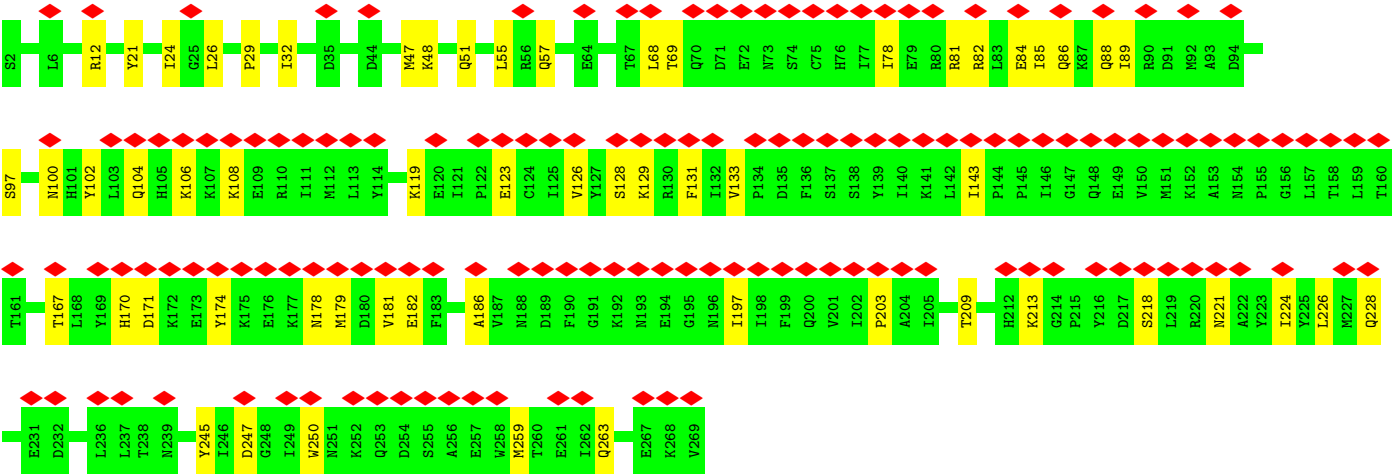


- Molecule 8: MerR family transcriptional regulator EcmrR



- 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 ( $\text{\AA}$ )	341.2481, 341.2481, 341.2481	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: ZN, 1N7, MG, 118

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	0.51	0/1815	0.55	0/2460
1	B	0.47	0/1730	0.57	0/2344
2	C	0.54	0/10739	0.55	0/14489
3	D	0.51	0/10551	0.55	0/14245
4	E	0.45	0/629	0.51	0/847
5	F	0.37	0/3930	0.53	0/5281
6	N	1.00	0/1243	0.96	0/1919
7	T	0.88	0/1239	0.91	0/1910
8	G	0.36	0/2260	0.65	0/3058
8	H	0.36	0/2260	0.62	0/3058
All	All	0.53	0/36396	0.60	0/49611

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1793	0	1822	24	0
1	B	1711	0	1748	28	0
2	C	10570	0	10582	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10394	0	10617	151	0
4	E	627	0	634	7	0
5	F	3878	0	3940	67	0
6	N	1109	0	609	13	0
7	T	1104	0	605	11	0
8	G	2208	0	2209	51	0
8	H	2208	0	2209	42	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	519	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 7.

All (519) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:813:GLU:CD	3:D:504:GLN:NE2	2.59	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
3:D:613:GLY:O	3:D:617:THR:OG1	2.20	0.55
2:C:941:LYS:NZ	2:C:949:GLU:OE1	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:564:PRO:HG2	2:C:568:ASN:O	2.09	0.53
5:F:227:GLN:HE22	5:F:251:LYS:HE2	1.74	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
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
8:G:223:TYR:OH	8:G:243:GLU:OE1	2.22	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
2:C:843:THR:OG1	2:C:846:GLY:O	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:C:890:LYS:NZ	2:C:911:SER:O	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
8:H:26:LEU:HD12	8:H:26:LEU:C	2.33	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
2:C:246:LEU:HD12	2:C:246:LEU:C	2.34	0.48
3:D:1199:PHE:HB2	3:D:1202:GLU:HG2	1.95	0.48
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: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
1:B:73:GLY:O	1:B:134:THR:OG1	2.29	0.47
2:C:802:VAL:HA	2:C:1096:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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
3:D:1058:SER:OG	3:D:1107:VAL:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:ASP:N	1:B:135:ASP:OD1	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.42
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: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: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
1:A:205:MET:HE1	1:A:216:ALA:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:678:ARG:HD3	3:D:678:ARG:C	2.40	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
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
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
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
3:D:513:MET:HE1	3:D:627:THR:HG22	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:916:SER:O	2:C:916:SER:OG	2.35	0.41
3:D:1284:ARG:HA	3:D:1284:ARG:HD3	1.83	0.41
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:H:167:THR:HG23	8:H:181:VAL:HG13	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/329 (70%)	226 (99%)	3 (1%)	0	100	100
1	B	218/329 (66%)	216 (99%)	2 (1%)	0	100	100
2	C	1338/1342 (100%)	1322 (99%)	16 (1%)	0	100	100
3	D	1330/1407 (94%)	1321 (99%)	9 (1%)	0	100	100
4	E	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
5	F	470/613 (77%)	466 (99%)	4 (1%)	0	100	100
8	G	266/268 (99%)	266 (100%)	0	0	100	100
8	H	266/268 (99%)	266 (100%)	0	0	100	100
All	All	4194/4647 (90%)	4159 (99%)	35 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/286 (70%)	199 (100%)	0	100	100
1	B	190/286 (66%)	190 (100%)	0	100	100
2	C	1155/1157 (100%)	1153 (100%)	2 (0%)	93	98
3	D	1120/1168 (96%)	1120 (100%)	0	100	100
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	424/540 (78%)	424 (100%)	0	100	100
8	G	245/245 (100%)	245 (100%)	0	100	100
8	H	245/245 (100%)	244 (100%)	1 (0%)	91	97
All	All	3645/4002 (91%)	3642 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	70	TYR
2	C	1296	ASP
8	H	213	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	B	66	HIS
1	B	93	GLN
1	B	186	ASN
2	C	31	GLN
2	C	69	GLN
2	C	120	GLN
2	C	330	HIS

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Mol	Chain	Res	Type
2	C	518	ASN
2	C	620	ASN
2	C	649	GLN
2	C	799	ASN
2	C	856	ASN
2	C	955	GLN
2	C	1013	GLN
2	C	1237	HIS
2	C	1268	GLN
3	D	45	ASN
3	D	274	ASN
3	D	294	ASN
3	D	364	HIS
3	D	424	ASN
3	D	504	GLN
3	D	951	GLN
3	D	962	ASN
3	D	979	ASN
3	D	1244	GLN
4	E	72	GLN
5	F	131	GLN
5	F	227	GLN
5	F	309	ASN
5	F	338	HIS
5	F	383	ASN
5	F	406	GLN
5	F	518	HIS
5	F	579	GLN
5	F	589	GLN
8	G	22	ASN
8	G	45	GLN
8	G	51	GLN
8	G	101	HIS
8	G	105	HIS
8	G	115	GLN
8	G	154	ASN
8	G	212	HIS
8	H	3	GLN
8	H	50	HIS
8	H	104	GLN
8	H	221	ASN
8	H	251	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 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	C	1401	-	29,29,46	0.75	1 (3%)	47,47,72	1.56	6 (12%)
9	1N7	H	301	-	30,30,46	0.75	1 (3%)	47,48,72	1.63	8 (17%)
12	118	G	302	-	28,28,28	0.69	0	24,38,38	0.31	0
9	1N7	T	101	-	29,29,46	0.75	1 (3%)	47,47,72	1.62	7 (14%)
9	1N7	C	1402	-	29,29,46	0.75	1 (3%)	47,47,72	1.60	7 (14%)
12	118	H	302	-	28,28,28	0.67	0	24,38,38	0.38	0
9	1N7	G	301	-	29,29,46	0.74	1 (3%)	47,47,72	1.73	9 (19%)

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	C	1401	-	-	5/6/71/92	0/4/4/4
9	1N7	H	301	-	-	6/7/72/92	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	118	G	302	-	-	-	0/4/4/4
9	1N7	T	101	-	-	6/6/71/92	0/4/4/4
9	1N7	C	1402	-	-	6/6/71/92	0/4/4/4
12	118	H	302	-	-	-	0/4/4/4
9	1N7	G	301	-	-	4/6/71/92	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	301	1N7	O4-C4	-2.07	1.40	1.43
9	C	1402	1N7	O4-C4	-2.07	1.40	1.43
9	T	101	1N7	O4-C4	-2.04	1.40	1.43
9	H	301	1N7	O4-C4	-2.03	1.40	1.43
9	C	1401	1N7	O4-C4	-2.01	1.40	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	301	1N7	C5-C9-C20	-5.85	112.52	119.50
9	C	1402	1N7	C5-C9-C20	-5.49	112.95	119.50
9	H	301	1N7	C5-C9-C20	-5.48	112.96	119.50
9	T	101	1N7	C5-C9-C20	-5.41	113.03	119.50
9	C	1401	1N7	C5-C9-C20	-5.13	113.37	119.50
9	G	301	1N7	C3-C19-C2	-4.85	108.72	113.73
9	G	301	1N7	C5-C6-C18	-4.01	109.61	114.74
9	T	101	1N7	C3-C19-C2	-4.00	109.60	113.73
9	C	1401	1N7	C3-C19-C2	-3.95	109.66	113.73
9	H	301	1N7	C3-C19-C2	-3.93	109.68	113.73
9	C	1402	1N7	C3-C19-C2	-3.82	109.79	113.73
9	C	1401	1N7	C3-C4-C5	-3.48	107.67	111.24
9	H	301	1N7	C3-C4-C5	-3.42	107.73	111.24
9	C	1402	1N7	C3-C4-C5	-3.27	107.89	111.24
9	T	101	1N7	C3-C4-C5	-3.20	107.96	111.24
9	T	101	1N7	C5-C6-C18	-2.97	110.94	114.74
9	C	1402	1N7	C5-C6-C18	-2.95	110.97	114.74
9	G	301	1N7	C2-C19-C18	-2.61	109.01	111.82
9	C	1401	1N7	C5-C6-C18	-2.56	111.47	114.74
9	H	301	1N7	C2-C19-C18	-2.55	109.08	111.82
9	G	301	1N7	C9-C5-C4	-2.53	115.36	117.67
9	G	301	1N7	C3-C4-C5	-2.47	108.71	111.24
9	H	301	1N7	C5-C6-C18	-2.44	111.62	114.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1402	1N7	O2-C13-C14	-2.43	105.01	109.85
9	C	1401	1N7	O2-C13-C14	-2.40	105.06	109.85
9	T	101	1N7	O2-C13-C14	-2.37	105.13	109.85
9	G	301	1N7	O2-C13-C14	-2.36	105.14	109.85
9	H	301	1N7	O2-C13-C14	-2.36	105.14	109.85
9	H	301	1N7	C9-C5-C4	-2.33	115.54	117.67
9	T	101	1N7	C9-C5-C4	-2.31	115.56	117.67
9	C	1401	1N7	C2-C19-C18	-2.22	109.44	111.82
9	C	1402	1N7	C9-C5-C4	-2.15	115.70	117.67
9	H	301	1N7	C6-C5-C4	2.14	109.39	107.40
9	G	301	1N7	C16-C17-C18	-2.08	109.26	111.48
9	C	1402	1N7	C2-C19-C18	-2.05	109.61	111.82
9	G	301	1N7	C14-C13-C12	-2.04	108.11	110.55
9	T	101	1N7	C2-C19-C18	-2.03	109.64	111.82

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	T	101	1N7	C21-C20-C22-C23
9	G	301	1N7	C21-C20-C9-C8
9	H	301	1N7	C22-C20-C9-C5
9	H	301	1N7	C22-C20-C9-C8
9	T	101	1N7	C9-C20-C22-C23
9	H	301	1N7	C9-C20-C22-C23
9	H	301	1N7	C21-C20-C22-C23
9	T	101	1N7	C21-C20-C9-C5
9	G	301	1N7	C22-C20-C9-C8
9	T	101	1N7	C22-C20-C9-C5
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	C9-C20-C22-C23
9	C	1402	1N7	C21-C20-C9-C8
9	C	1402	1N7	C21-C20-C22-C23

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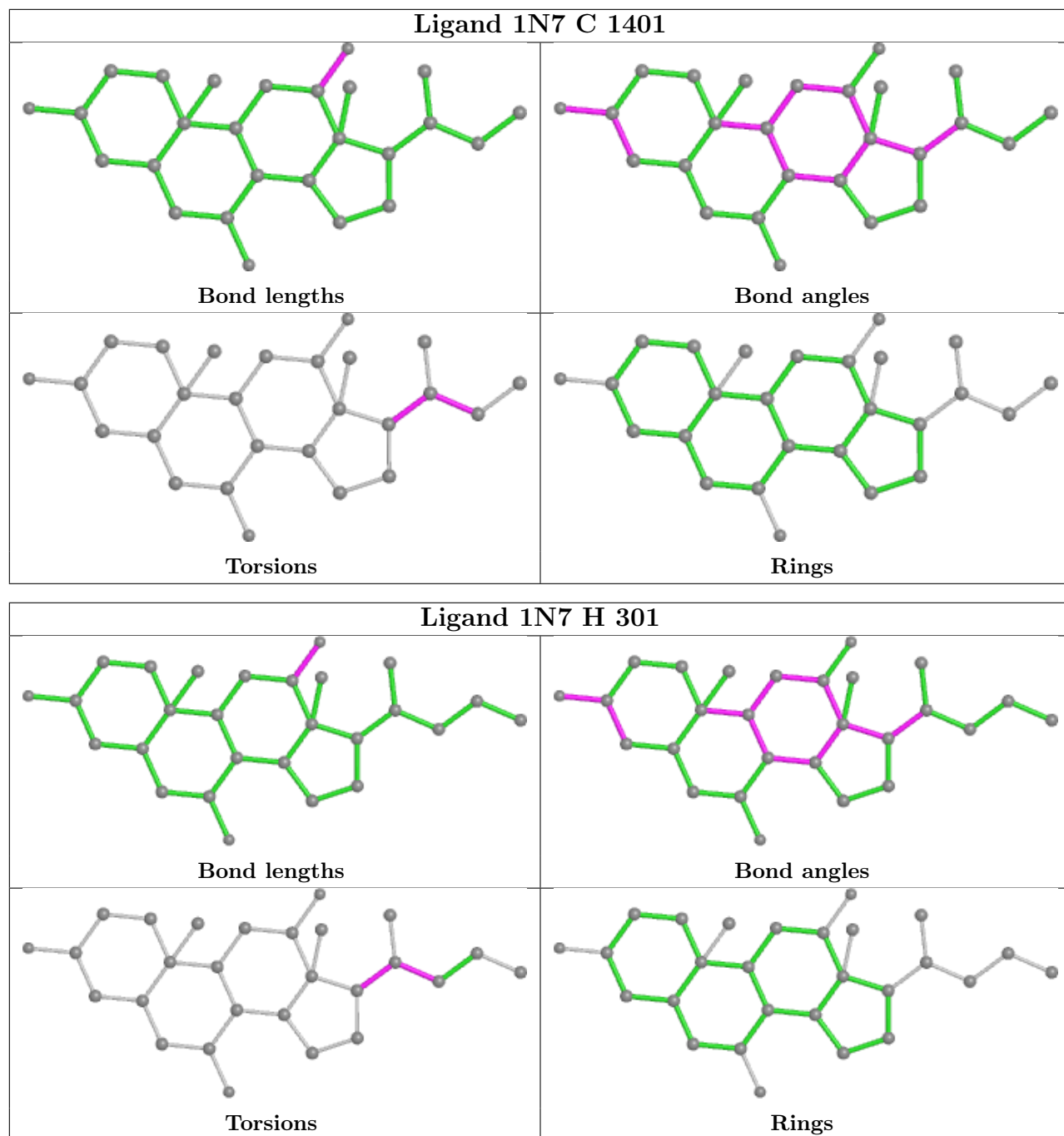
Mol	Chain	Res	Type	Atoms
9	T	101	1N7	C22-C20-C9-C8
9	C	1402	1N7	C22-C20-C9-C8
9	C	1401	1N7	C22-C20-C9-C8
9	C	1401	1N7	C21-C20-C22-C23

There are no ring outliers.

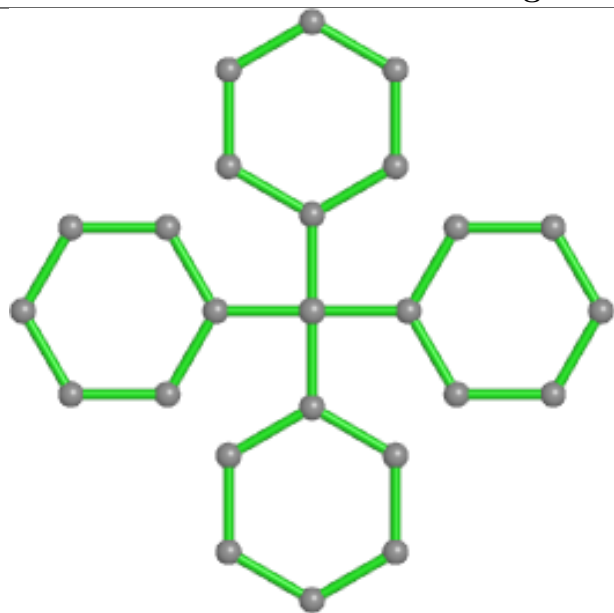
7 monomers are involved in 13 short contacts:

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

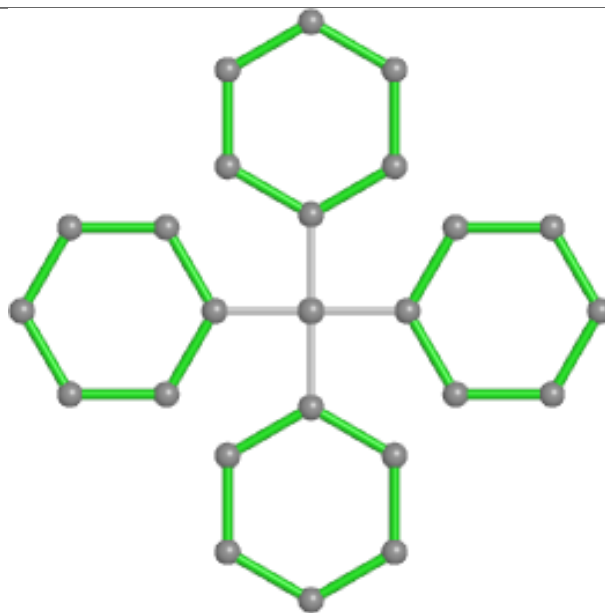
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



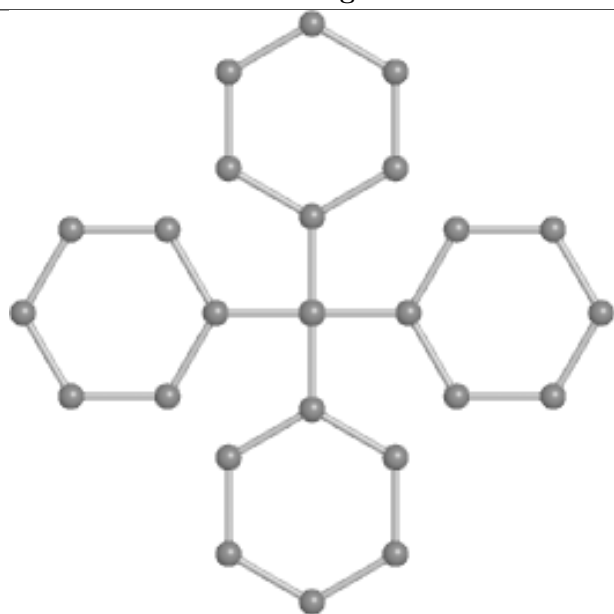
## Ligand 118 G 302



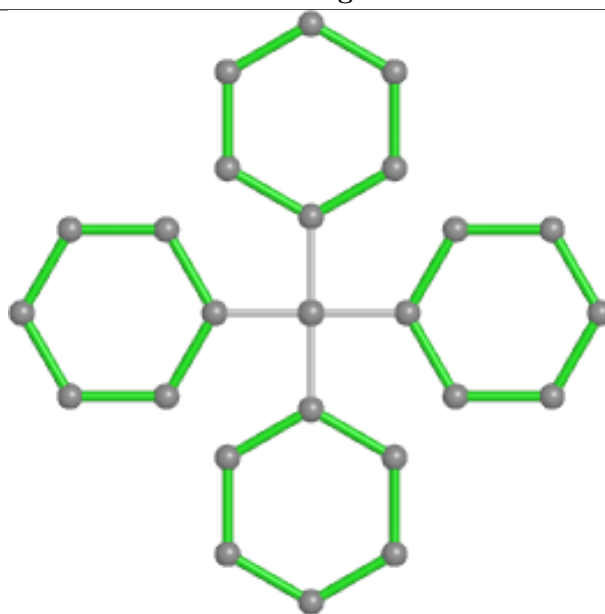
Bond lengths



Bond angles

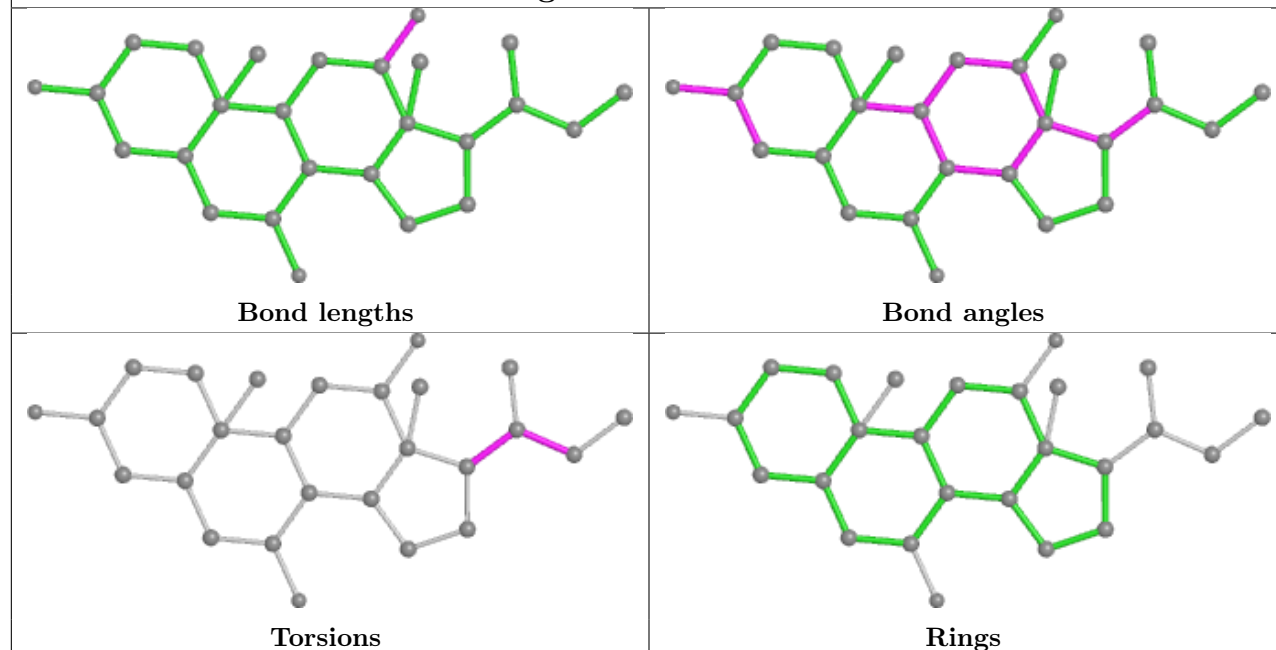


Torsions

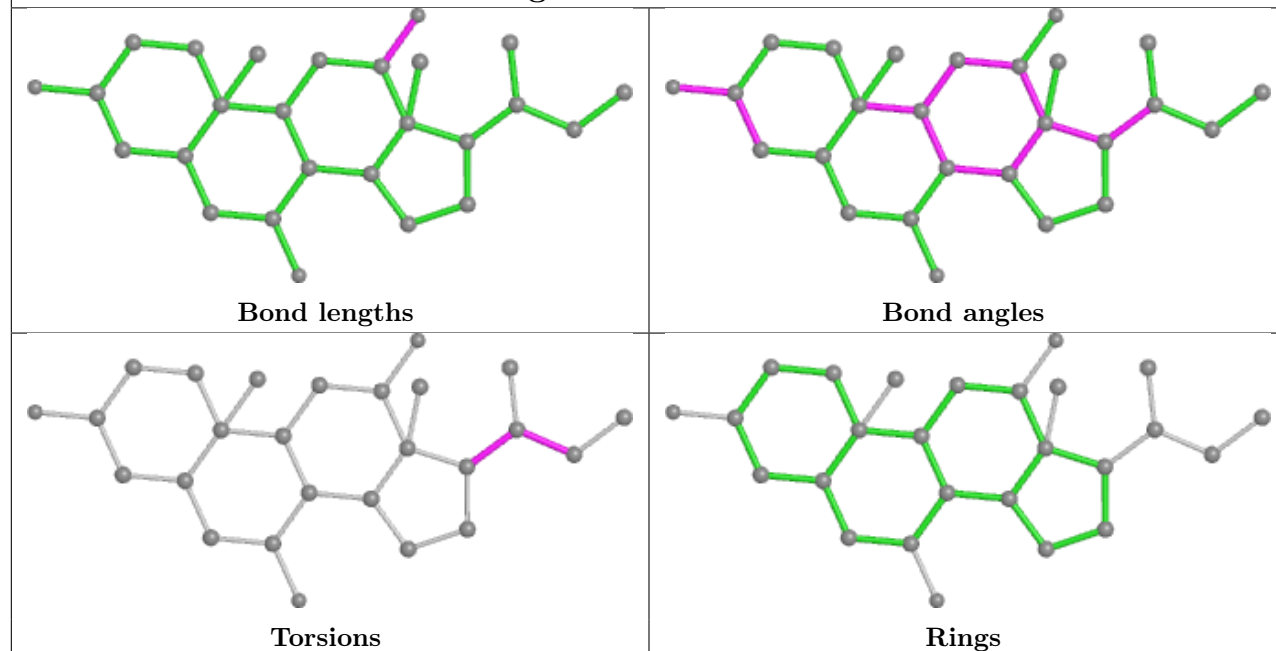


Rings

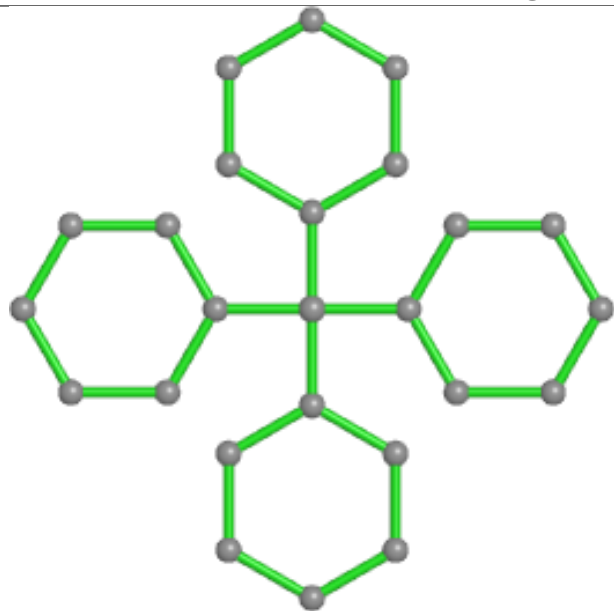
## Ligand 1N7 T 101



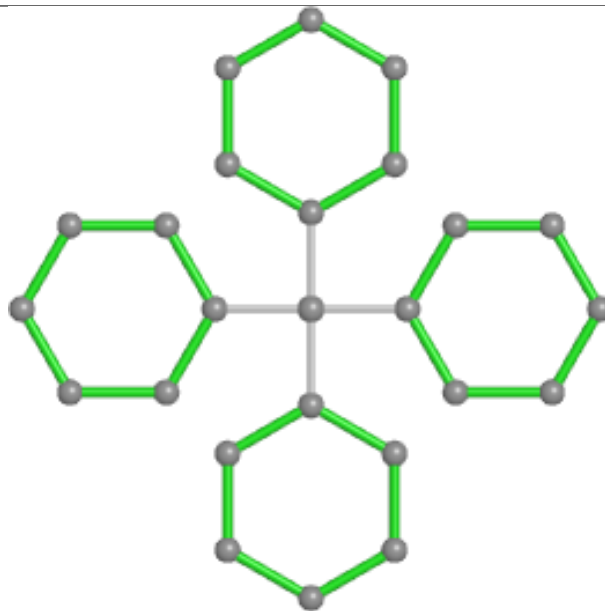
## Ligand 1N7 C 1402



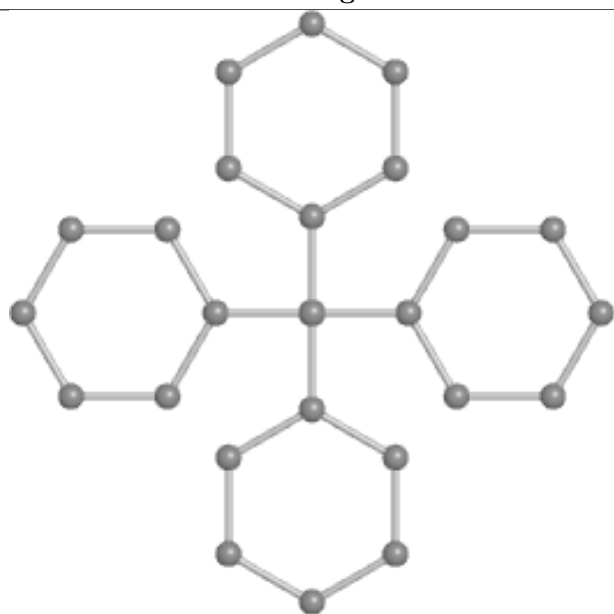
## Ligand 118 H 302



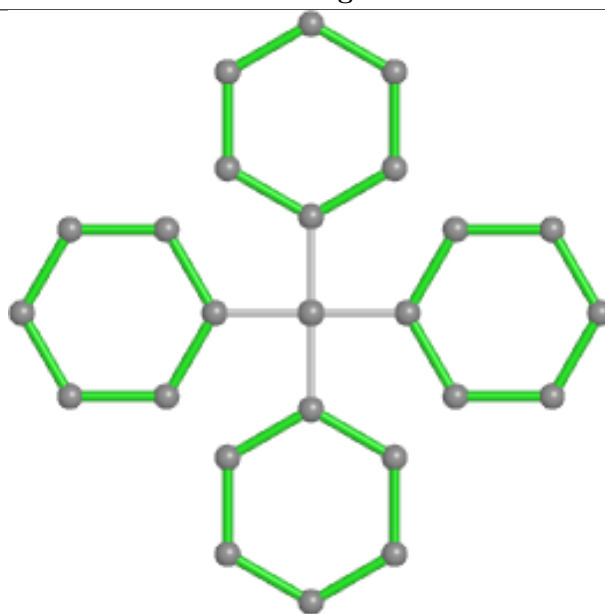
Bond lengths



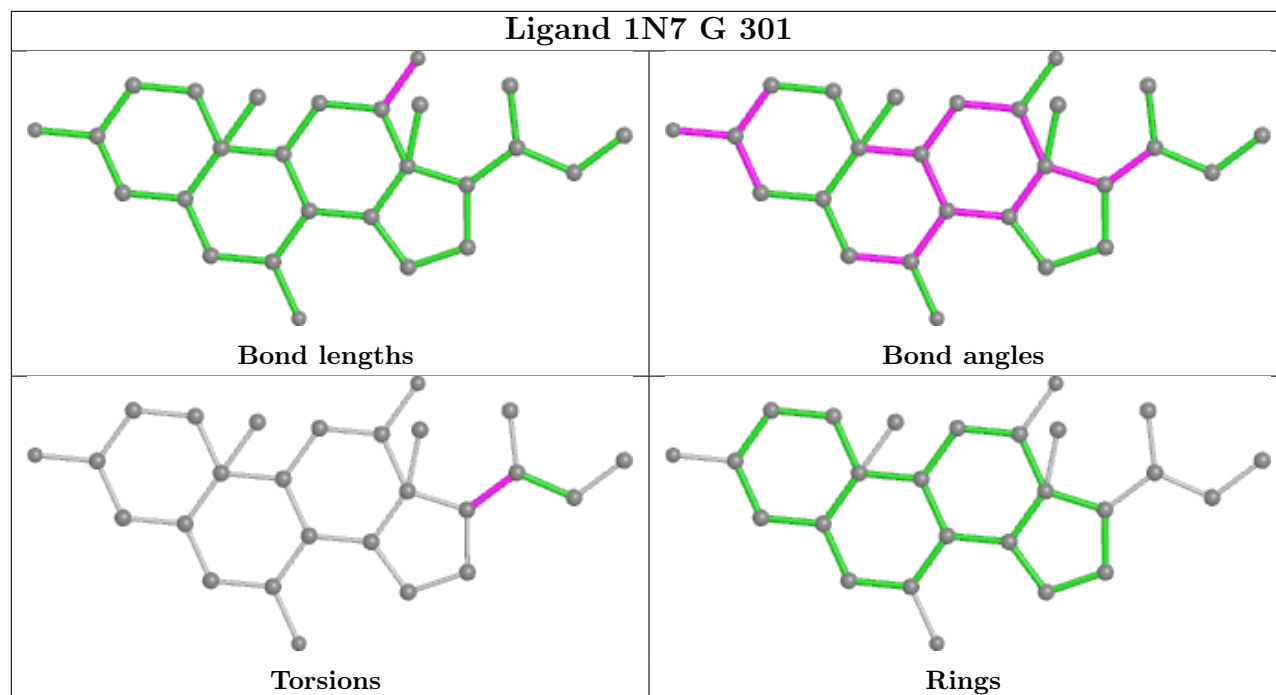
Bond angles



Torsions



Rings



## 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.

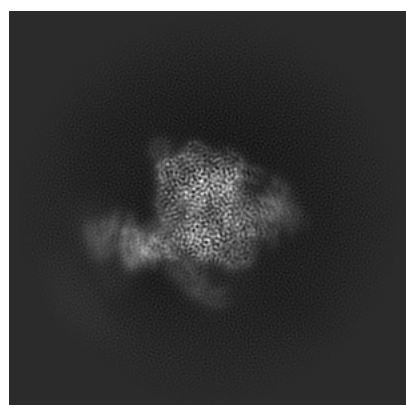
## 6 Map visualisation [i](#)

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.

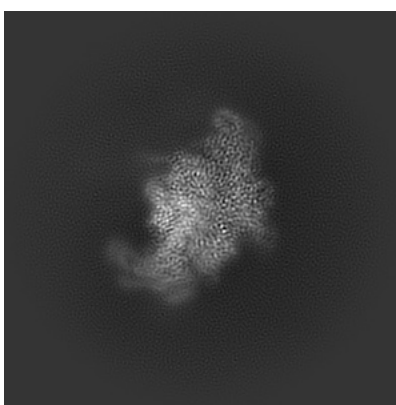
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

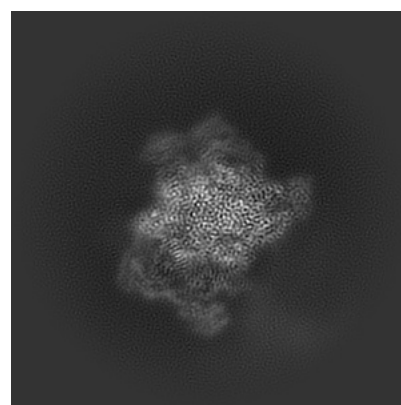
#### 6.1.1 Primary map



X



Y

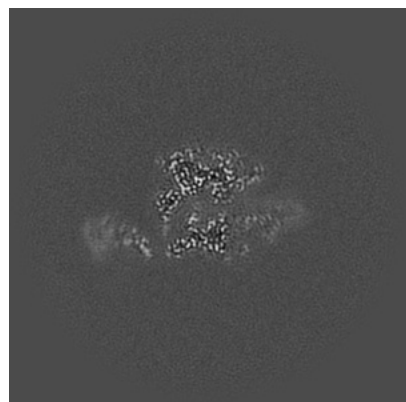


Z

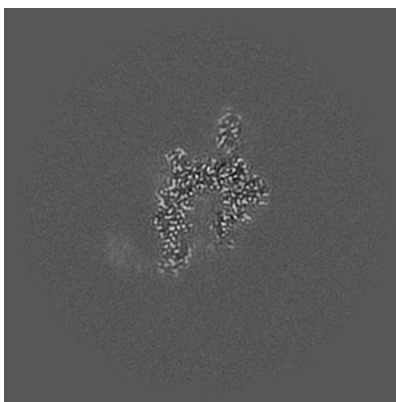
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

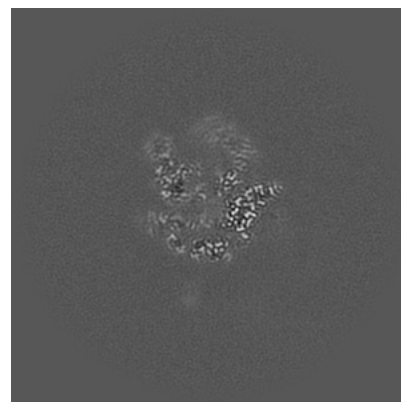
#### 6.2.1 Primary map



X Index: 192



Y Index: 192



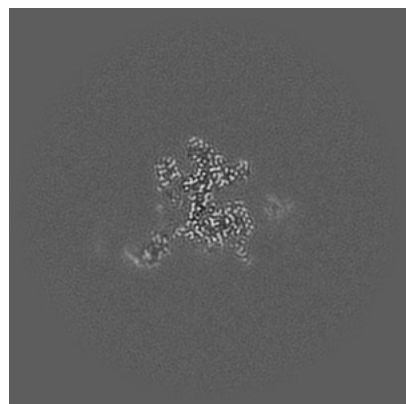
Z Index: 192



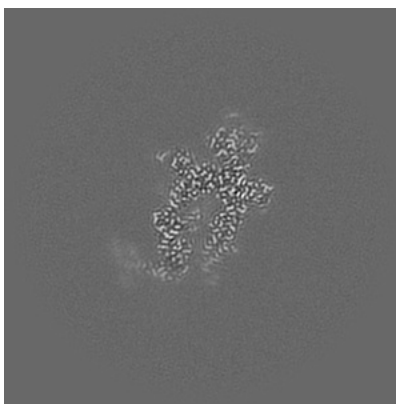
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

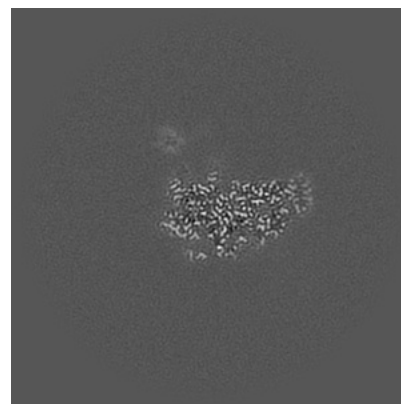
### 6.3.1 Primary map



X Index: 210



Y Index: 184

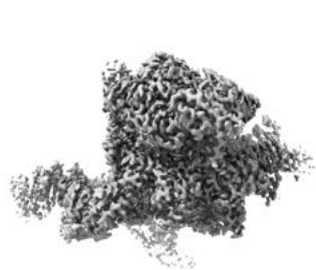


Z Index: 213

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

## 6.4 Orthogonal surface views [i](#)

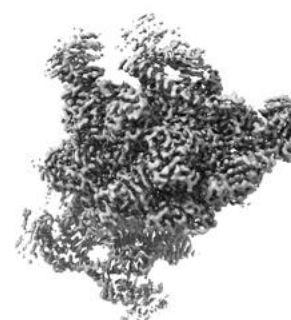
### 6.4.1 Primary map



X



Y



Z

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.

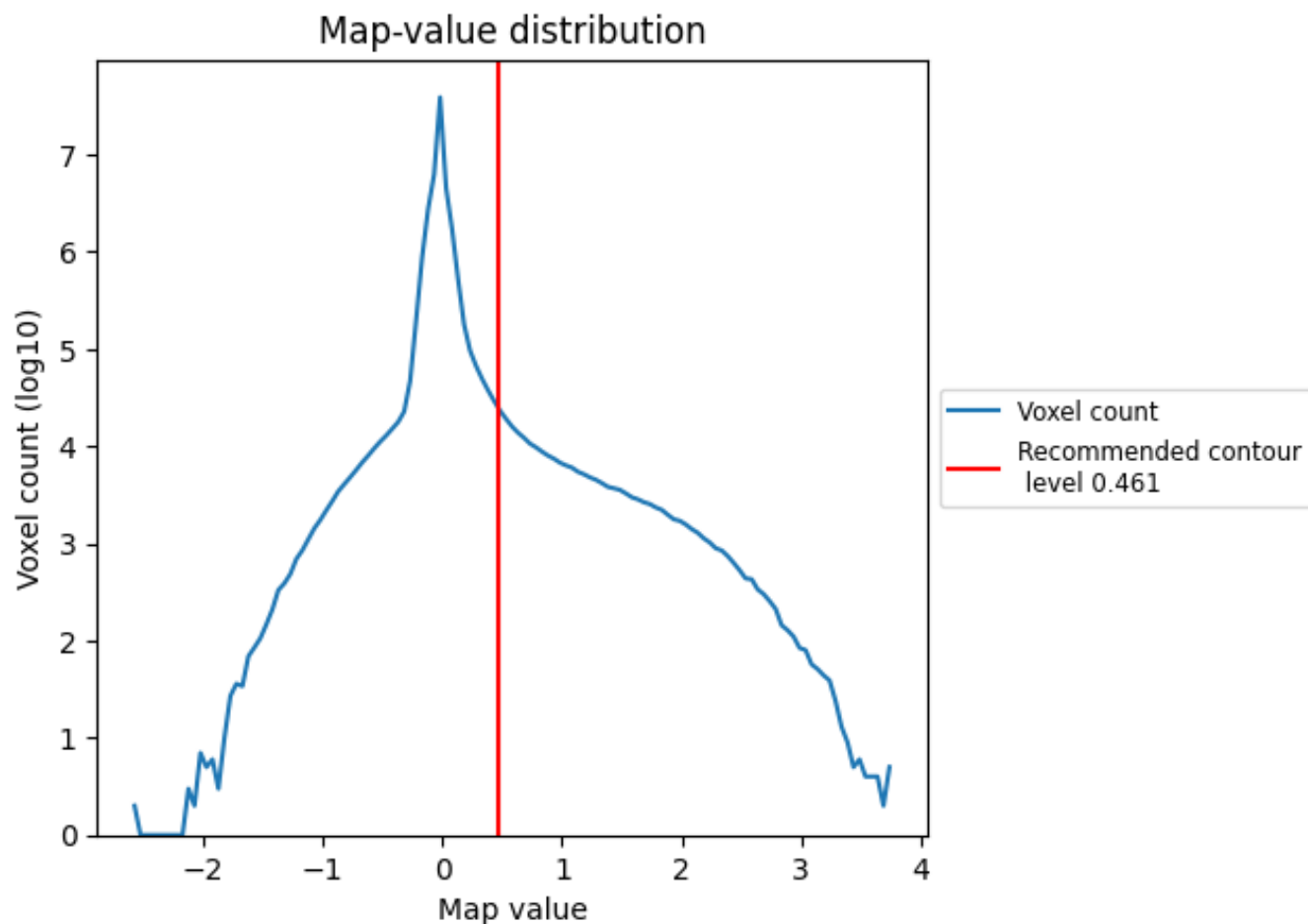
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

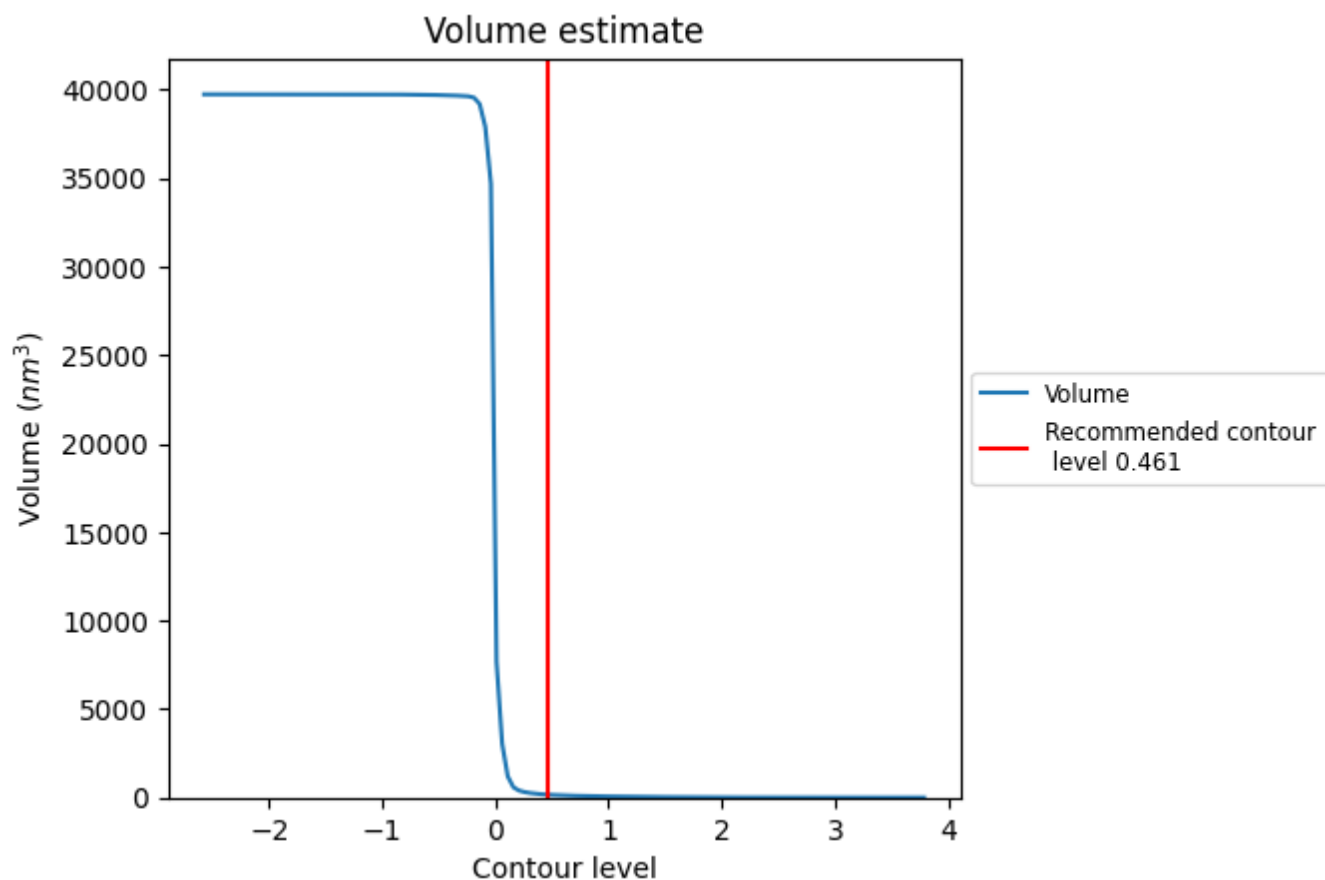
This section contains the results of statistical analysis of the map.

### 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.

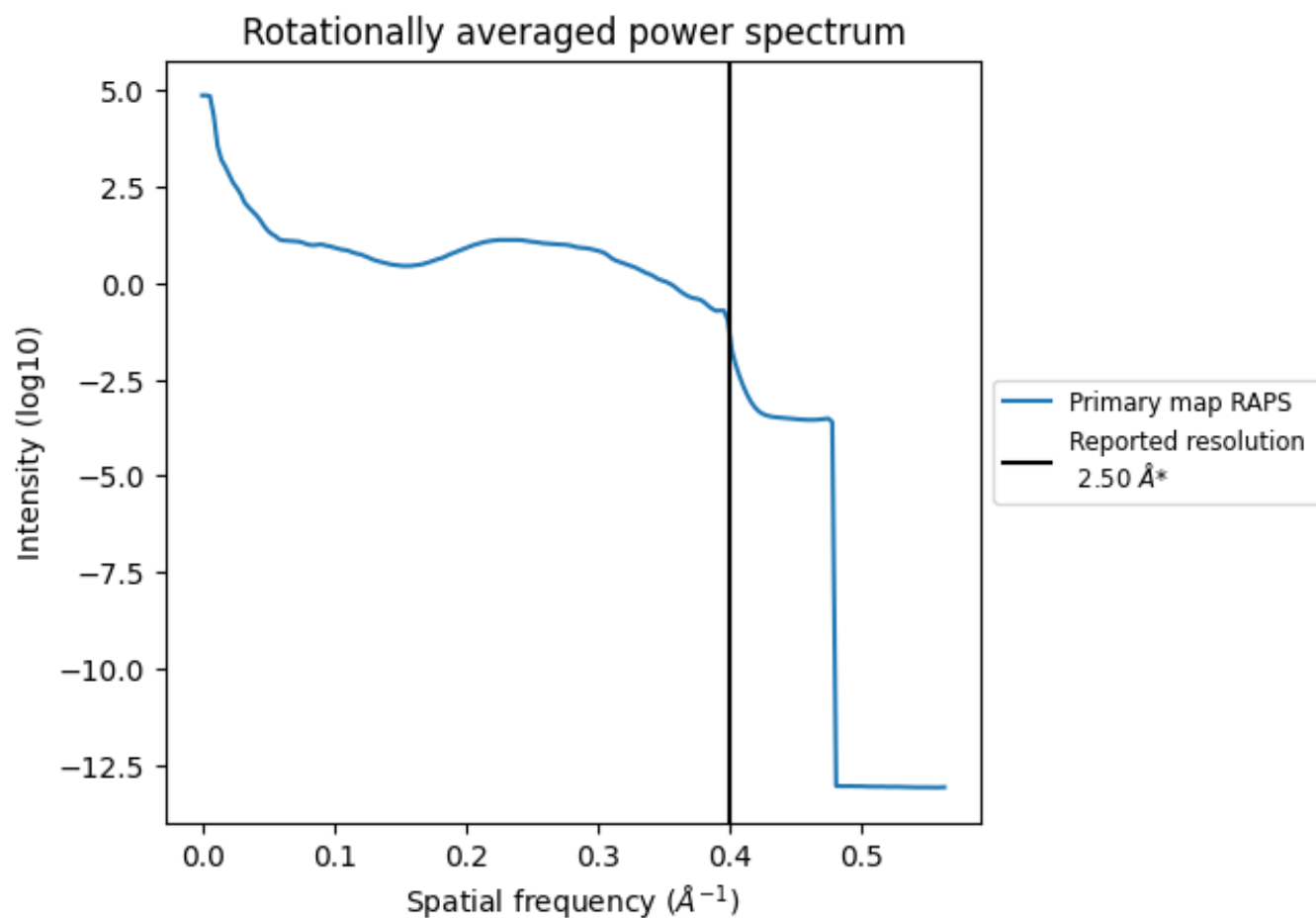
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm<sup>3</sup>; 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<sup>-1</sup>

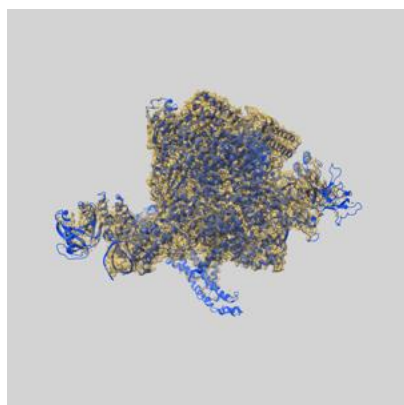
## 8 Fourier-Shell correlation

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

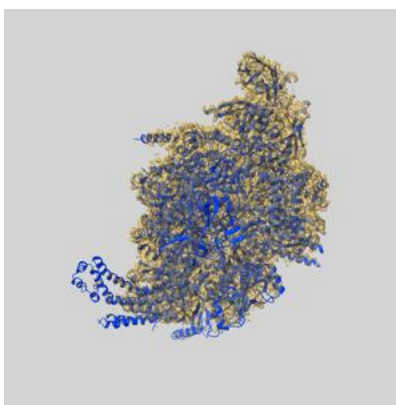
## 9 Map-model fit [i](#)

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](#).

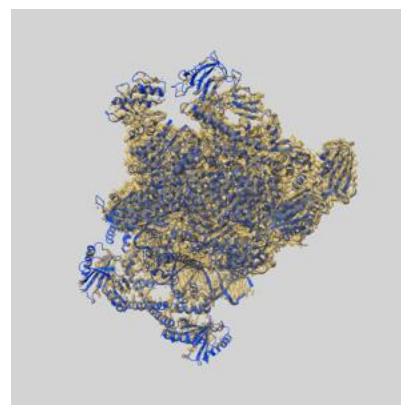
### 9.1 Map-model overlay [i](#)



X



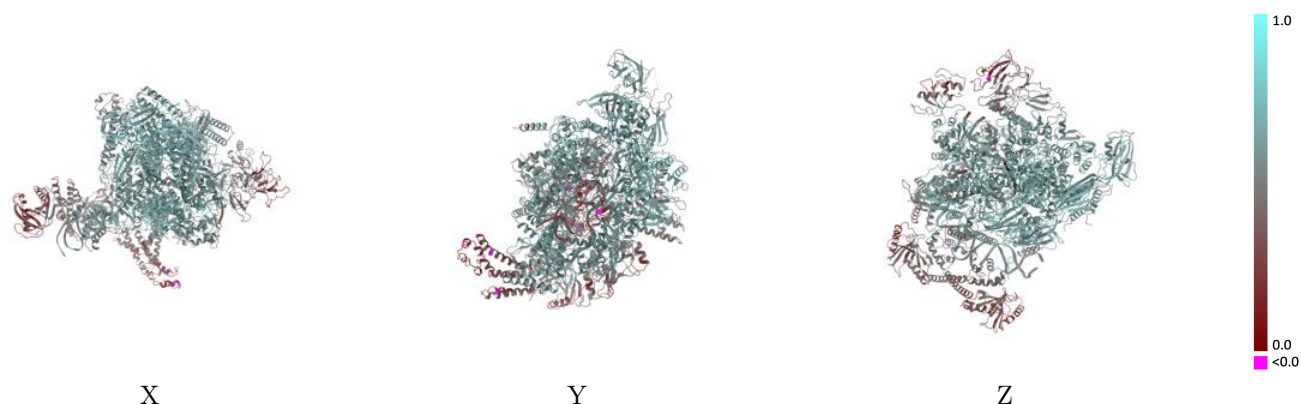
Y



Z

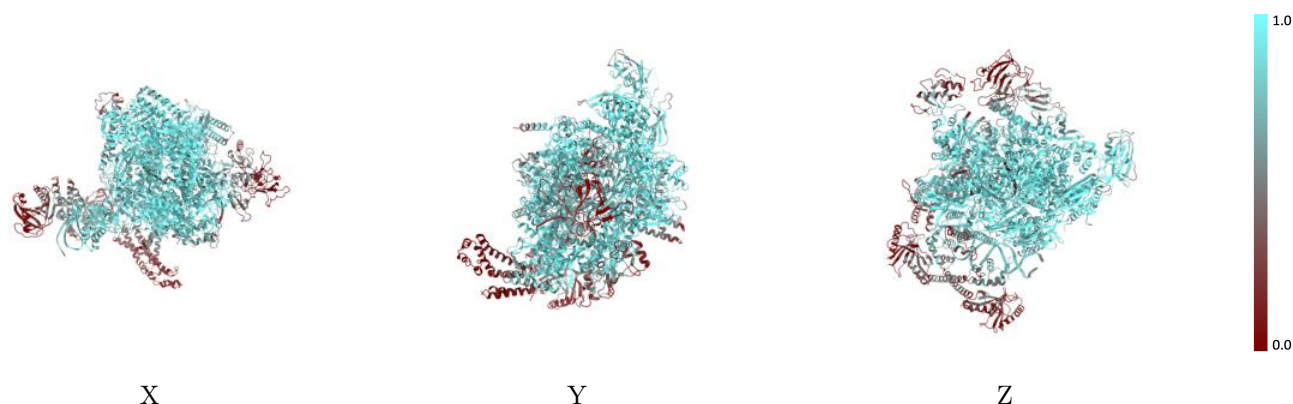
The images above show the 3D surface view of the map at the recommended contour level 0.461 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

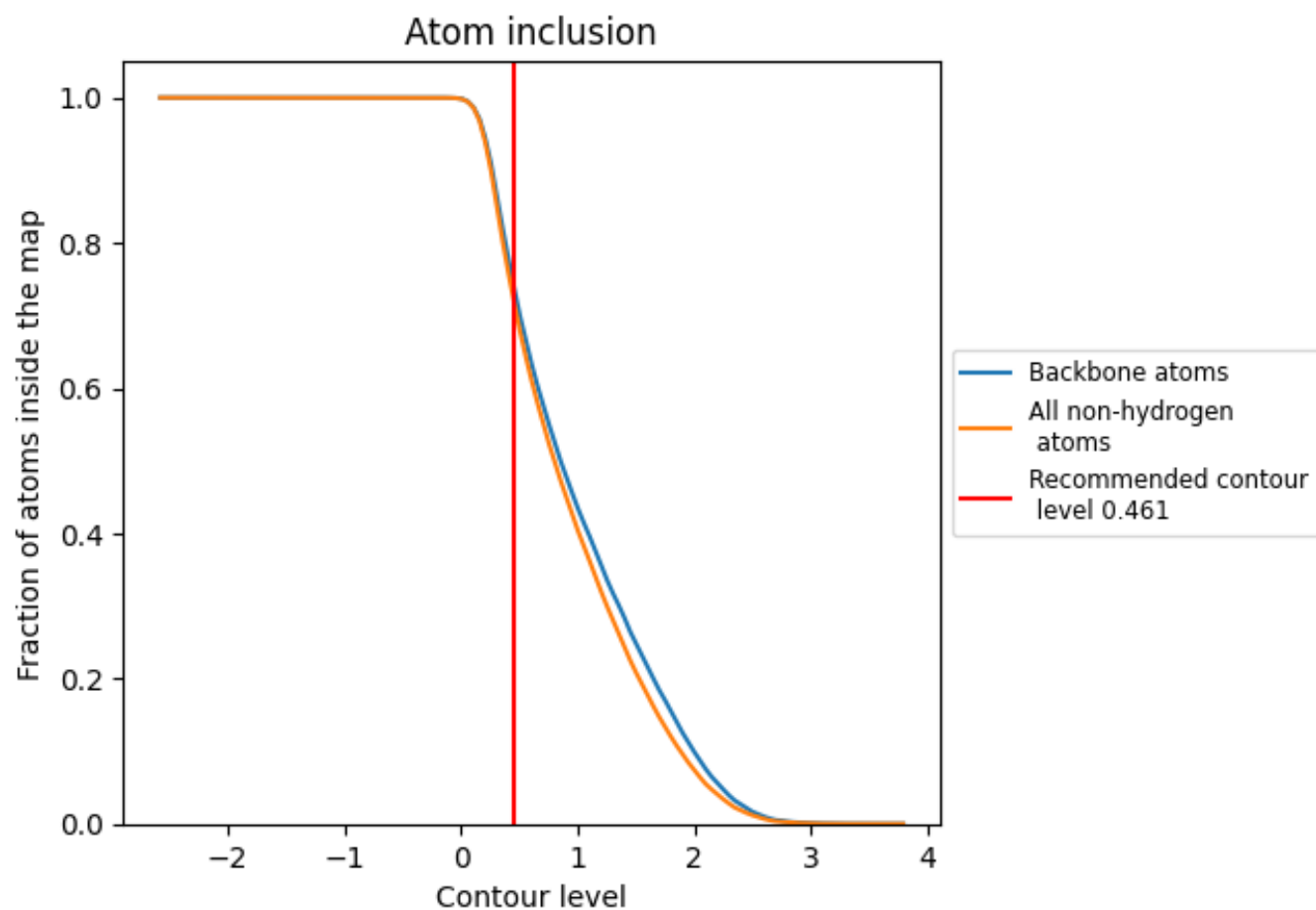
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.461).



## 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	<div></div> 0.7135	<div></div> 0.5410
A	<div></div> 0.8650	<div></div> 0.6150
B	<div></div> 0.8080	<div></div> 0.5920
C	<div></div> 0.8217	<div></div> 0.5910
D	<div></div> 0.7810	<div></div> 0.5730
E	<div></div> 0.8151	<div></div> 0.5930
F	<div></div> 0.5356	<div></div> 0.4640
G	<div></div> 0.3327	<div></div> 0.3560
H	<div></div> 0.3637	<div></div> 0.3710
N	<div></div> 0.7962	<div></div> 0.5410
T	<div></div> 0.7513	<div></div> 0.5220

1.0

0.0

<0.0