wwPDB EM Validation Summary Report (i)

Feb 24, 2024 – 06:52 PM EST

PDB ID	:	6XLJ
EMDB ID	:	EMD-22245
Title	:	Cryo-EM structure of EcmrR-RNAP-promoter initial transcribing complex with 4-nt RNA transcript (EcmrR-RPitc-4nt)
Authors	:	Yang, Y.; Liu, C.; Liu, B.
Deposited on	:	2020-06-28
Resolution	:	2.70 Å(reported)
Based on initial model	:	6OUL

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

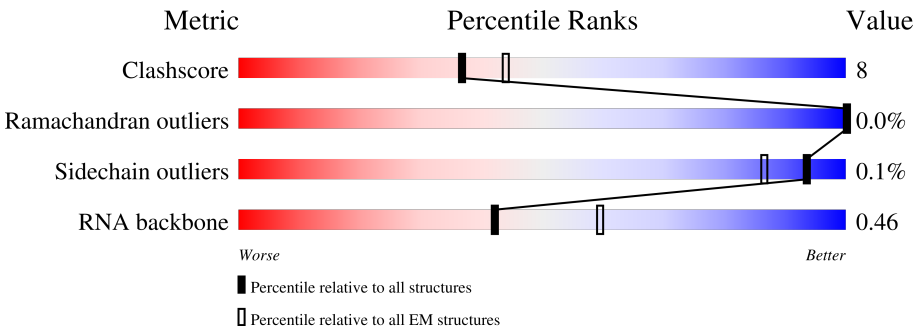
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	329	• 56% 15% 30%
1	B	329	• 57% 11% 32%
2	C	1342	8% 78% 21%
3	D	1407	13% 78% 17% 5%
4	E	91	9% 75% 12% 13%
5	F	613	27% 61% 17% 22%
6	G	268	52% 69% 31%

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Mol	Chain	Length	Quality of chain
6	H	268	50% 75% 25%
7	N	54	6% 57% 43%
8	R	4	100%
9	T	54	69% 31%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 35902 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
			Total	C	N	O	S		
1	A	231	1793	1117	318	352	6	0	0
1	B	224	1726	1080	303	337	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1339	10560	6626	1840	2051	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1336	10387	6526	1852	1959	50	0	0

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

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

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

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

- Molecule 6 is a protein called MerR family transcriptional regulator EcmrR.

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

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

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

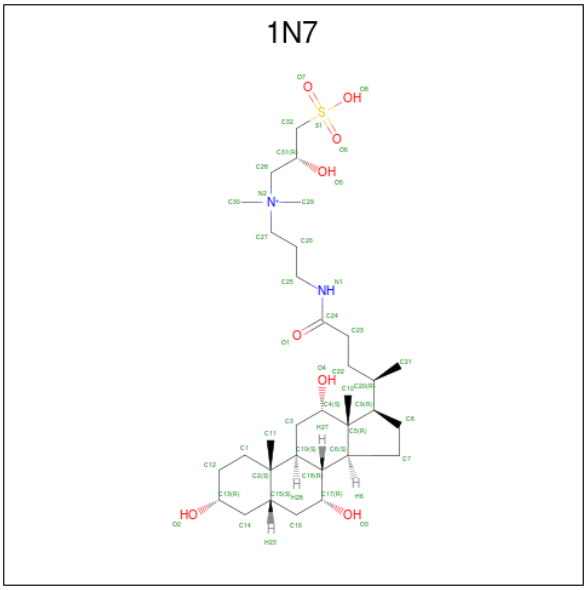
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	R	4	97	39	18	34	6	0	0

- Molecule 9 is a DNA chain called synthetic template strand DNA (54-MER).

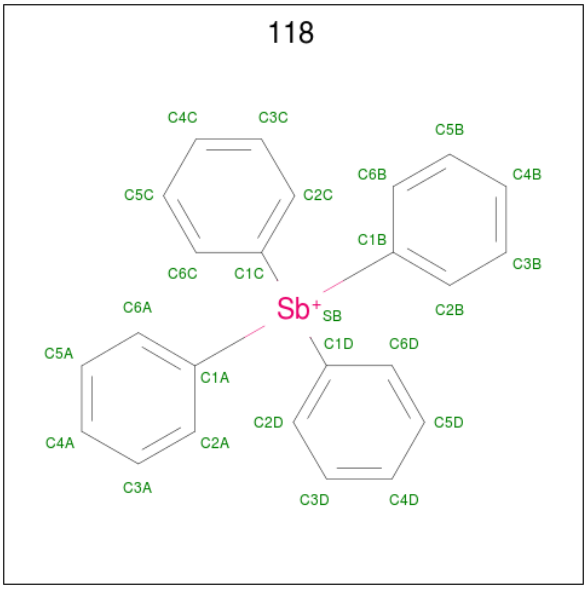
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	T	54	1099	521	208	317	53	0	0

- Molecule 10 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



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

- Molecule 11 is TETRAPHENYLANTIMONIUM ION (three-letter code: 118) (formula: $C_{24}H_{20}Sb$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
12	R	1	1	1	0

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

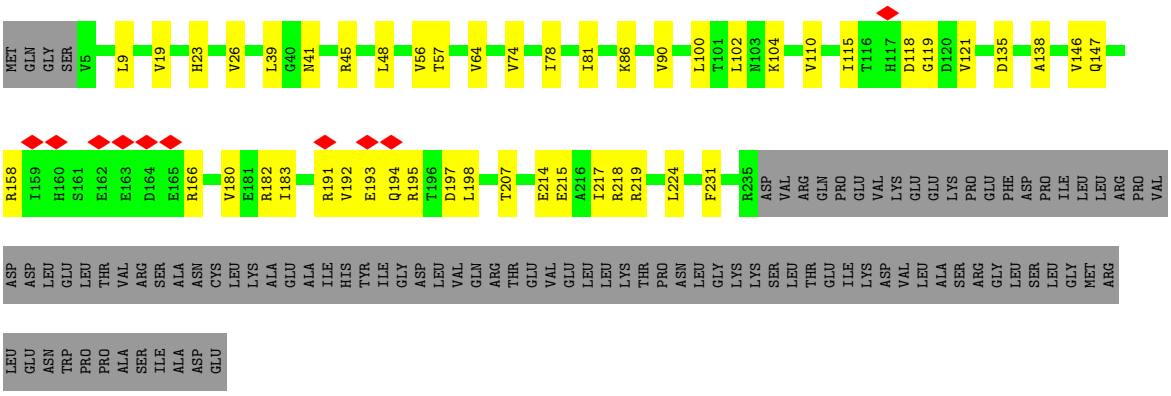
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
13	D	2	2	2	0

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.

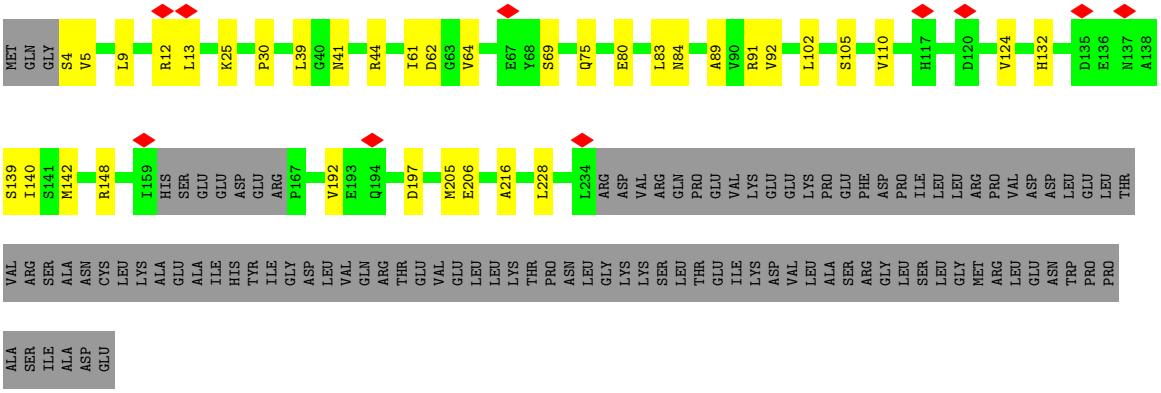
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

MET VAL Y3 S4 E7 R12 K13 D14 D23 Y26 L27 L28 L32 D33 S34 Q60 N65 S66 E67 L68 Q69 S93 R101 L102 V103 I104 Y105 E106 R107 E108 A109 P110 E111 G112 K115 D116 I117 Q120 G125 E126 L129 D132 E142 Q148

S159 D160 H165 S166 V170 L171 R175 I176 I177 P178 Y179 R180 D185 L194 I198 D199 R200 R201 P205 D222 L223 F224 F225 V228 E231 I232 R233 D234 N235 K236 L237 Q238 L241 E244 R245 L246 R247 G248 E249 T250 A251 S252 F253 D254 I255 E256 A257

N258 G259 K260 V263 E264 K265 G266 R267 R268 I269 T270 A271 R272 H273 I274 R275 Q276 L277 E278 K279 D280 D281 V282 K283 L284 I285 E286 V289 E290 G294 I302 D303 E304 S305 T306 G307 E308 L309 A312 A313 N314 M315 L319 D320 L321 K324 L325 S326 Q327 S328 G329 H330 K331

R332 F337 T338 N339 D340 L341 D342 H343 G344 P345 Y346 I347 S348 E349 R352 V353 D354 P355 T356 A362 R368 G373 F389 L397 V400 G401 R402 M403 K404 F405 N406 R411 L420 D424 I425 V428 M429 K439 D444 N450 I453 R454 S455 V456

G457 E458 M459 Q463 L468 E472 R473 A474 V475 R478 L479 G482 D483 L484 D485 T486 L487 M488 P489 Q490 K496 S499 A500 K503 E504 F505 M515 D516 Q517 N518 N519 P520 L521 S522 E523 I524 T525 R528 R529 I530 L533 L538 R542 A543 V547 R548

C559 P567 L571 L575 S576 Y591 V594 V599 I603 E611 I616 A617 N620 E626 G627 H628 D632 R637 Y652 M653 V660 V661 S662 S666 E672 H673 D674 D675 A676 N677 R678 M681 M685 Q686 R687 V690 P691 T692

M704 V710 V714 T715 A716 V717 R720 G721 I732 V736 E740 G744 E745 I748 R758 S759 N762 I763 C764 I765 N766 Q767 L783 A784 P787 L796 V802 N808 E813 D826 T830 E835 S840 R841 I854 L862 I870

E876 G885 K890 G891 E892 T893 Q894 S911 D912 F934 T935 R936 K941 D942 K943 R944 A945 K954 L960 E963 I966 R974 I975 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005

E1006 K1007 Q1008 N1009 E1012 Q1013 L1014 A1015 Y1018 K1022 R1033 R1034 A1043 V1046 L1047 K1048 K1051 V1052 Y1053 R1058 G1071 N1072 K1073 S1077 P1086 N1090 I1096 P1100 L1101 S1105 Q1111 L1117 G1118 M1119 A1120 R1142 V1159 F1164 A1183

T1184 A1190 I1195 L1199 K1200 L1204 R1216 F1221 E1222 R1223 K1234 D1241 H1244 S1247 Q1256 G1266 G1271 E1272 M1273 E1274 K1294 S1295 D1296 D1297 R1301 G1318 E1321 L1333 L1339 E1340 D1341 GLU

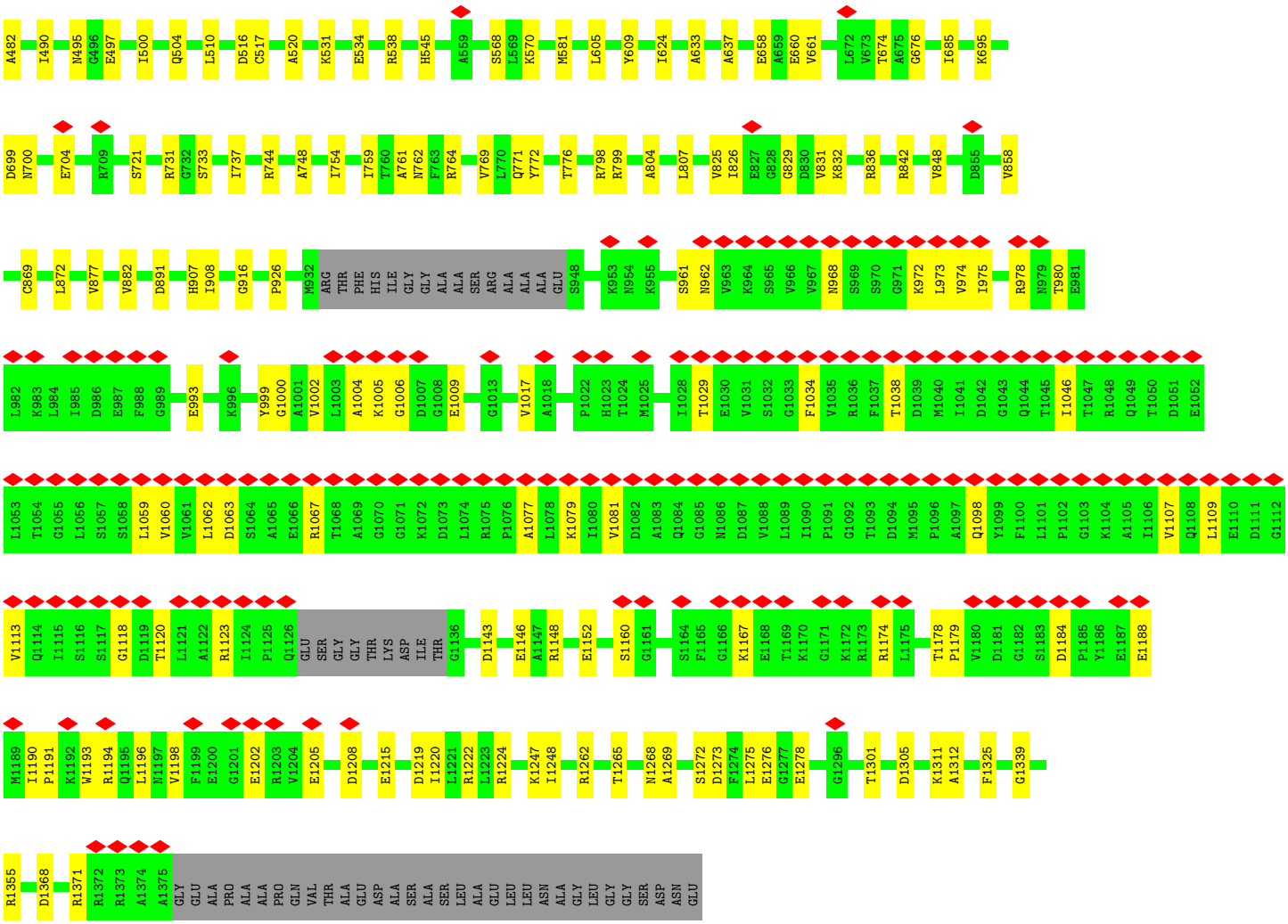
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

MET LYS ASP LEU LEU LYS PHE LEU LYS ALA GLN THR LYS THR GLU E16 F17 I20 K21 L24 K40 P41 E42 N45 Y46 R47 T48 C58 F62 L71 R77 L78 K79 V90 H113 I114 W115 L126 L127 R133 D134 I135 L139 V146 M151

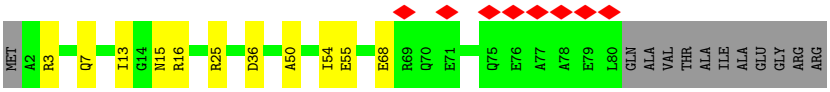
T152 N153 Q157 D167 A168 L169 E170 G173 D174 E175 A178 L188 R202 E203 E204 E207 T208 N209 S210 E211 T212 K213 R214 K215 K216 L217 L223 L224 E225 A226 Q229 S230 G231 N232 K233 P234 P247 D256 R259 T262 S263 D264 L265 N266 R270

N274 D289 V292 R293 N294 M298 N309 N320 K321 R322 S326 K334 S353 T356 V357 E375 I381 K384 R388 T393 I394 K395 K398 E402 L412 D413 E414 V415 V421 L422 L423 A436 I447 F461 M466 V470



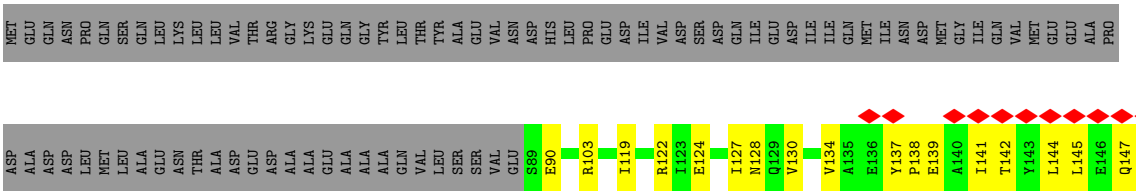
- Molecule 4: DNA-directed RNA polymerase subunit omega

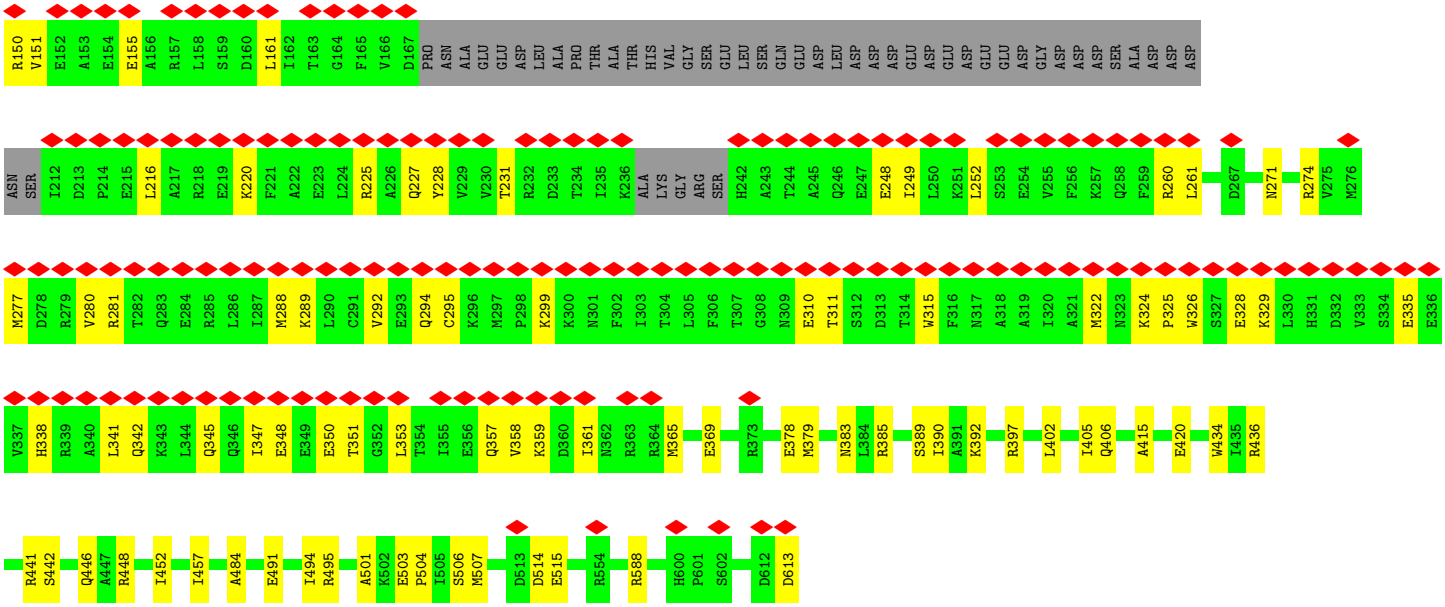
Chain E:



- Molecule 5: RNA polymerase sigma factor RpoD

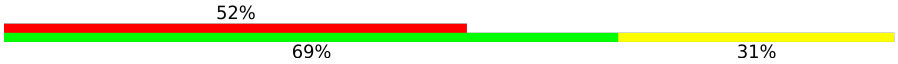
Chain F:

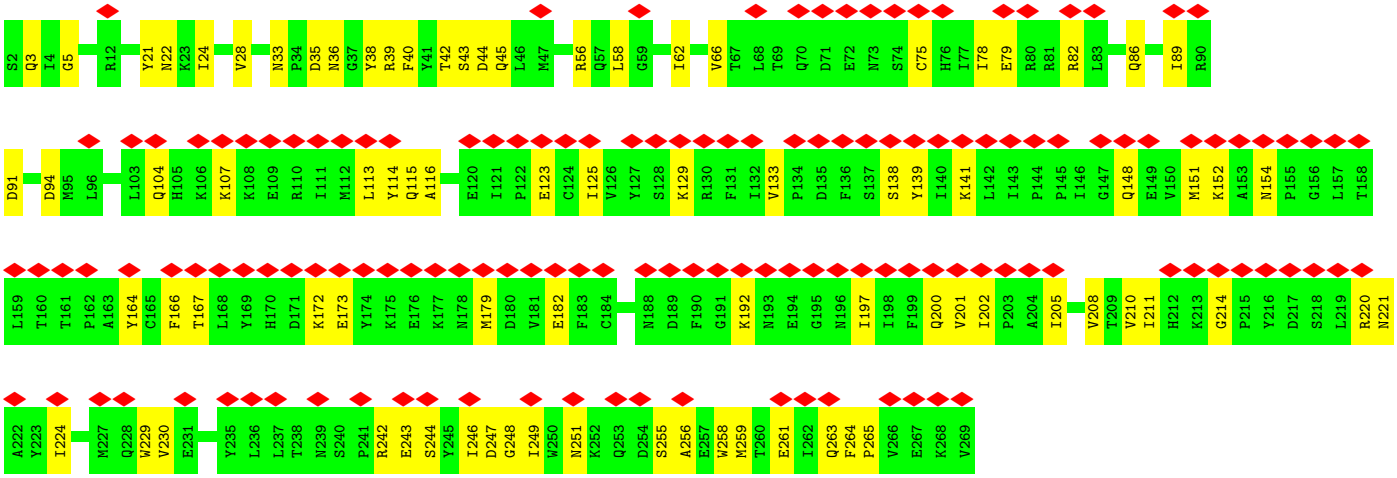




- Molecule 6: MerR family transcriptional regulator EcmrR

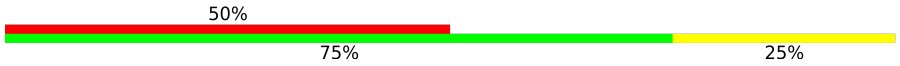
Chain G:

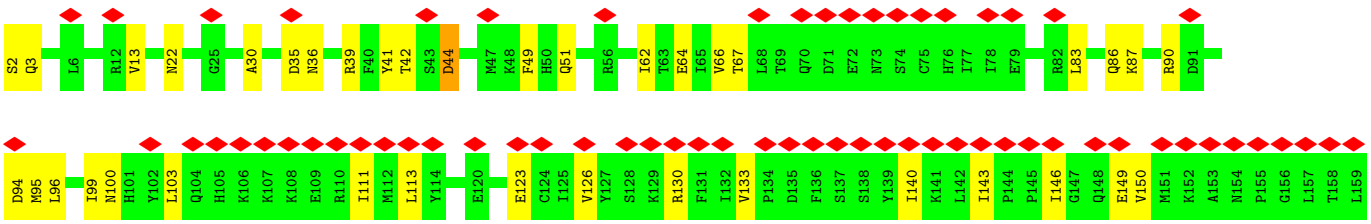


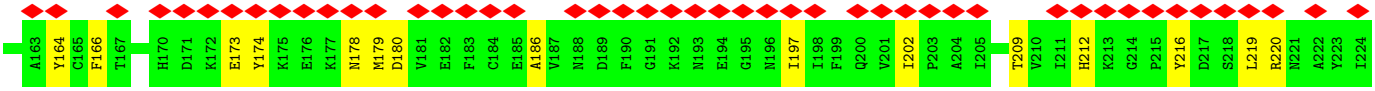


- Molecule 6: MerR family transcriptional regulator EcmrR

Chain H:

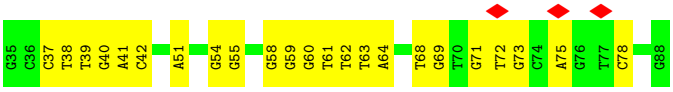






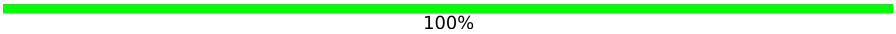
- Molecule 7: synthetic non-template strand DNA (54-MER)

Chain N:



- Molecule 8: RNA (5'-D(*(GTP))-R(P*CP*AP*G)-3')

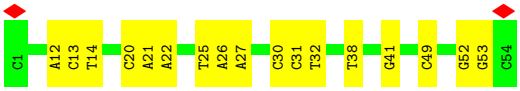
Chain R:



There are no outlier residues recorded for this chain.

- Molecule 9: synthetic template strand DNA (54-MER)

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.46	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	5.317	Depositor
Minimum map value	-2.787	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.76	Depositor
Map size (Å)	341.248, 341.248, 341.248	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 1N7, ZN, 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	0.66	0/1815	0.62	0/2460
1	B	0.59	0/1746	0.60	0/2366
2	C	0.73	0/10729	0.59	0/14477
3	D	0.69	0/10544	0.61	0/14236
4	E	0.63	0/629	0.58	0/847
5	F	0.47	0/3930	0.56	0/5281
6	G	0.42	0/2260	0.68	0/3058
6	H	0.41	0/2260	0.66	0/3058
7	N	1.24	0/1243	0.98	0/1919
8	R	1.36	0/72	1.19	0/110
9	T	1.20	0/1233	0.91	0/1899
All	All	0.70	0/36461	0.64	0/49711

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1793	0	1822	33	0
1	B	1726	0	1767	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10560	0	10576	185	0
3	D	10387	0	10607	153	0
4	E	627	0	634	7	0
5	F	3878	0	3940	75	0
6	G	2208	0	2209	60	0
6	H	2208	0	2209	51	0
7	N	1109	0	609	24	0
8	R	97	0	44	0	0
9	T	1099	0	604	21	0
10	A	26	0	37	2	0
10	C	26	0	37	2	0
10	D	26	0	37	0	0
10	G	26	0	37	3	0
10	H	27	0	39	4	0
11	C	25	0	20	1	0
11	G	25	0	20	0	0
11	H	25	0	20	1	0
12	D	1	0	0	0	0
12	R	1	0	0	0	0
13	D	2	0	0	0	0
All	All	35902	0	35268	589	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.

The worst 5 of 589 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)
3:D:1034:PHE:HB2	3:D:1081:VAL:O	1.62	0.99
5:F:342:GLN:O	5:F:345:GLN:HB2	1.67	0.95
9:T:14:DT:H6	9:T:14:DT:H5"	1.37	0.90
5:F:503:GLU:OE1	5:F:504:PRO:HD2	1.78	0.84
3:D:357:VAL:HG22	3:D:461:PHE:CE2	2.17	0.80

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%)	223 (97%)	5 (2%)	1 (0%)	34	60
1	B	220/329 (67%)	217 (99%)	3 (1%)	0	100	100
2	C	1337/1342 (100%)	1307 (98%)	30 (2%)	0	100	100
3	D	1330/1407 (94%)	1306 (98%)	24 (2%)	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
6	G	266/268 (99%)	263 (99%)	3 (1%)	0	100	100
6	H	266/268 (99%)	265 (100%)	1 (0%)	0	100	100
All	All	4195/4647 (90%)	4123 (98%)	71 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/286 (70%)	199 (100%)	0	100	100
1	B	192/286 (67%)	192 (100%)	0	100	100
2	C	1154/1157 (100%)	1153 (100%)	1 (0%)	93	98
3	D	1119/1168 (96%)	1118 (100%)	1 (0%)	93	98

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	424/540 (78%)	424 (100%)	0	100	100
6	G	245/245 (100%)	245 (100%)	0	100	100
6	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	764	CYS
3	D	139	LEU
6	H	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	51	GLN
6	H	3	GLN
6	G	86	GLN
6	G	193	ASN
6	H	154	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	1N7	C	1401	-	29,29,46	0.77	1 (3%)	47,47,72	1.69	8 (17%)
11	118	C	1402	-	28,28,28	0.55	0	24,38,38	0.40	0
11	118	G	302	-	28,28,28	0.63	0	24,38,38	0.36	0
10	1N7	A	1501	-	29,29,46	0.78	1 (3%)	47,47,72	1.66	9 (19%)
10	1N7	D	1504	-	29,29,46	0.78	1 (3%)	47,47,72	1.64	7 (14%)
11	118	H	302	-	28,28,28	0.64	0	24,38,38	0.43	0
10	1N7	H	301	-	30,30,46	0.76	1 (3%)	47,48,72	1.64	8 (17%)
10	1N7	G	301	-	29,29,46	0.75	1 (3%)	47,47,72	1.72	8 (17%)

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
10	1N7	C	1401	-	-	6/6/71/92	0/4/4/4
11	118	C	1402	-	-	-	0/4/4/4
11	118	G	302	-	-	-	0/4/4/4
10	1N7	A	1501	-	-	6/6/71/92	0/4/4/4
10	1N7	D	1504	-	-	6/6/71/92	0/4/4/4
11	118	H	302	-	-	-	0/4/4/4
10	1N7	H	301	-	-	6/7/72/92	0/4/4/4
10	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)
10	A	1501	1N7	O4-C4	-2.15	1.40	1.43
10	C	1401	1N7	O4-C4	-2.09	1.40	1.43
10	D	1504	1N7	O4-C4	-2.09	1.40	1.43
10	H	301	1N7	O4-C4	-2.07	1.40	1.43
10	G	301	1N7	O4-C4	-2.06	1.40	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1401	1N7	C5-C9-C20	-5.96	112.38	119.50
10	G	301	1N7	C5-C9-C20	-5.83	112.53	119.50
10	D	1504	1N7	C5-C9-C20	-5.54	112.88	119.50
10	A	1501	1N7	C5-C9-C20	-5.41	113.04	119.50
10	H	301	1N7	C5-C9-C20	-5.40	113.05	119.50

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	G	301	1N7	C21-C20-C9-C5
10	D	1504	1N7	C21-C20-C22-C23
10	C	1401	1N7	C22-C20-C9-C5
10	G	301	1N7	C22-C20-C9-C5
10	C	1401	1N7	C21-C20-C9-C5

There are no ring outliers.

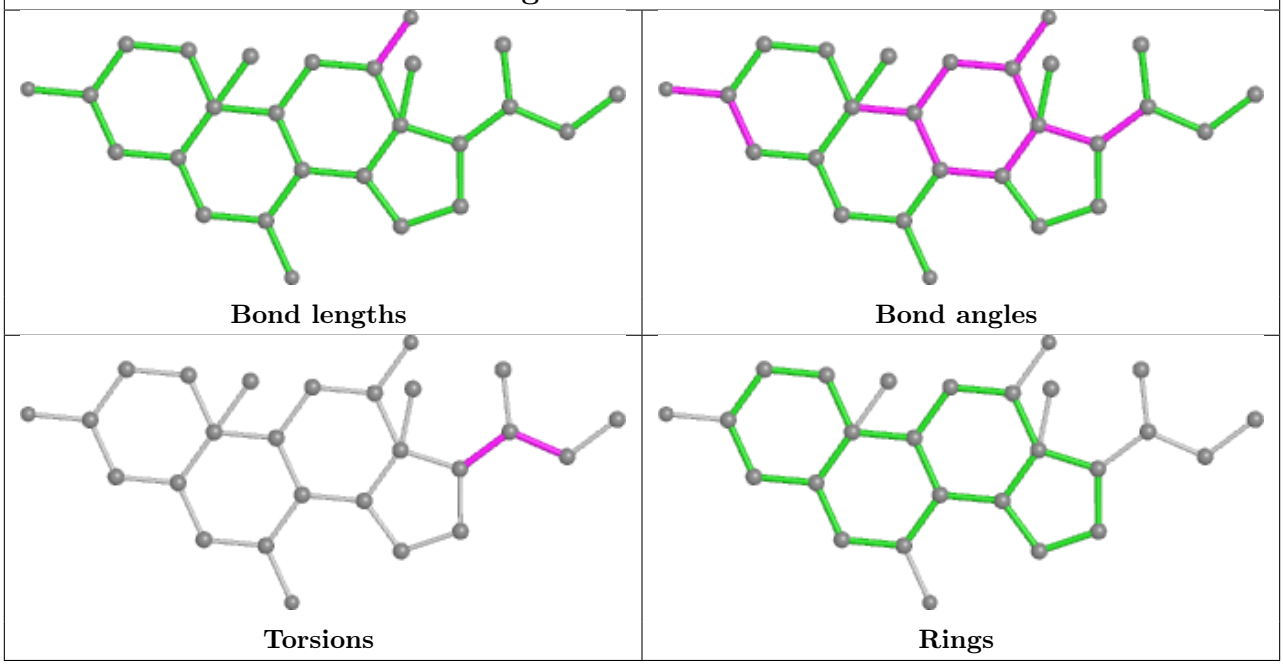
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1401	1N7	2	0
11	C	1402	118	1	0
10	A	1501	1N7	2	0
11	H	302	118	1	0
10	H	301	1N7	4	0
10	G	301	1N7	3	0

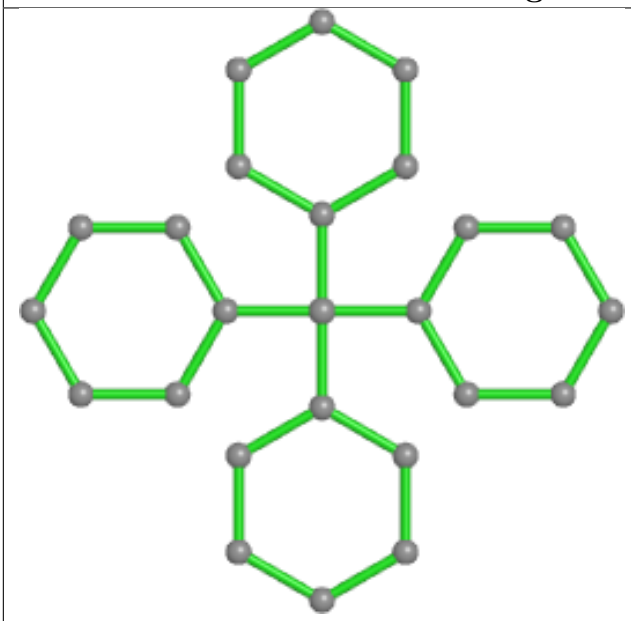
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

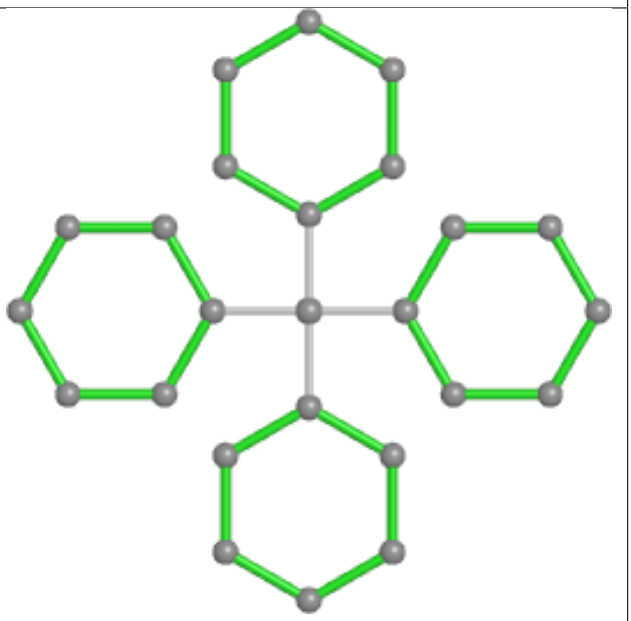
Ligand 1N7 C 1401



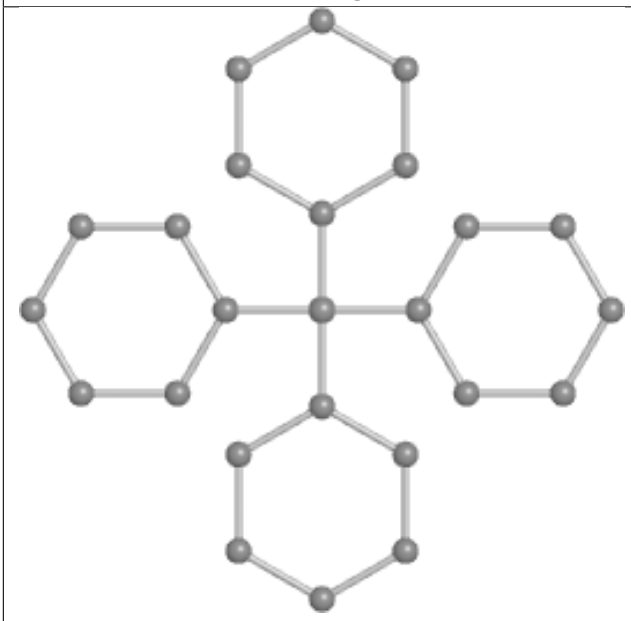
Ligand 118 C 1402



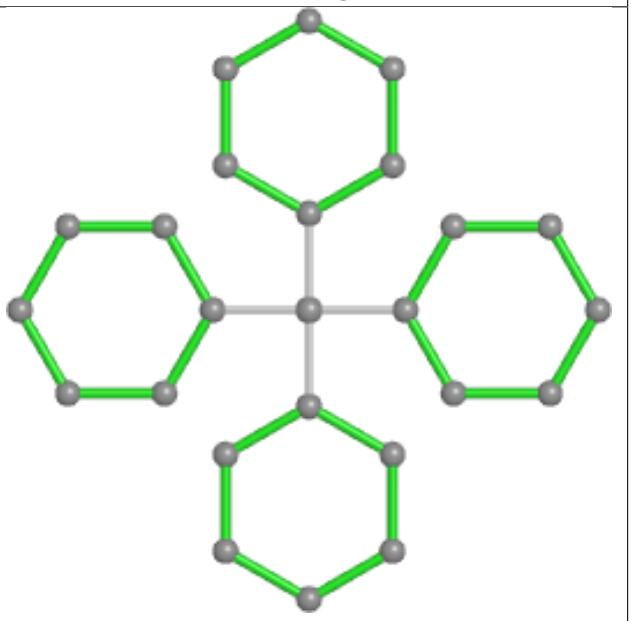
Bond lengths



Bond angles

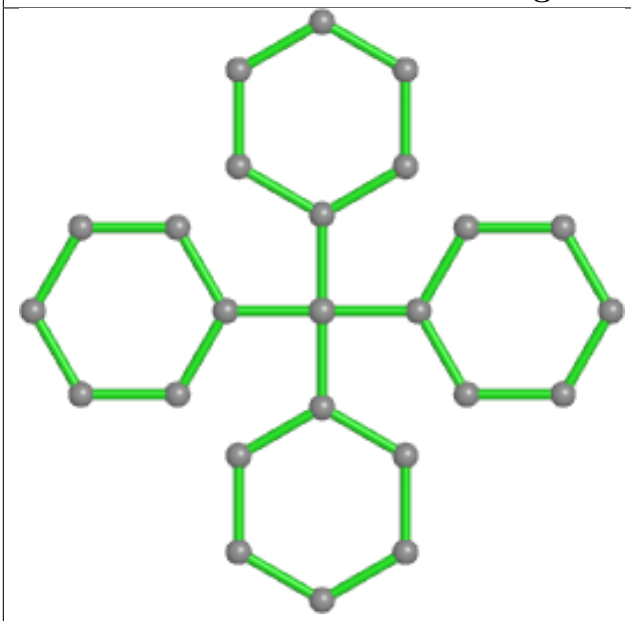


Torsions

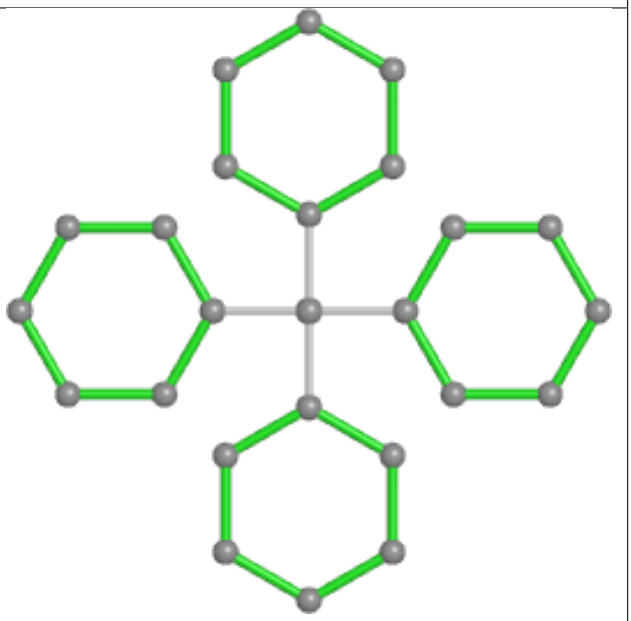


Rings

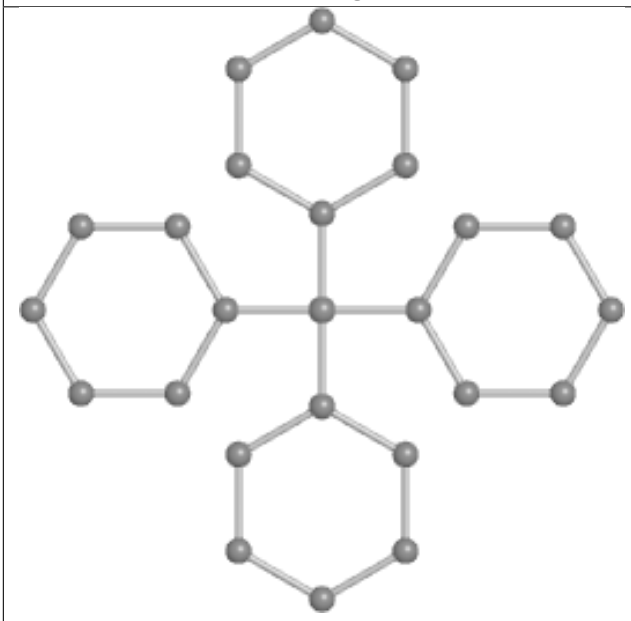
Ligand 118 G 302



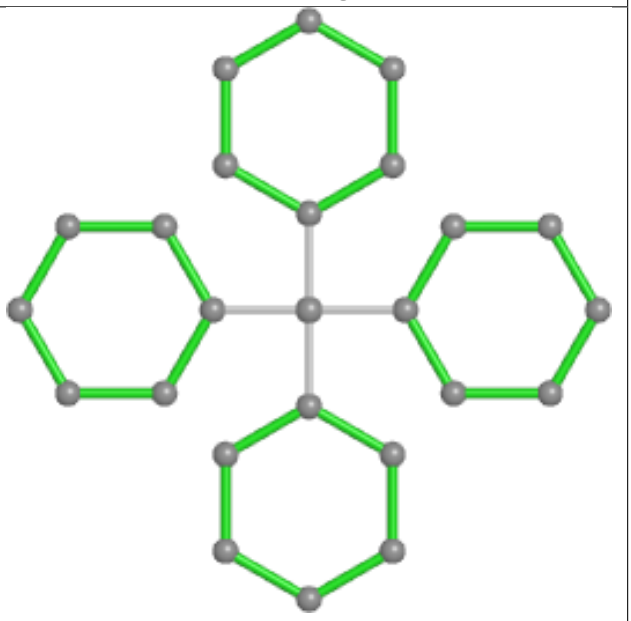
Bond lengths



Bond angles

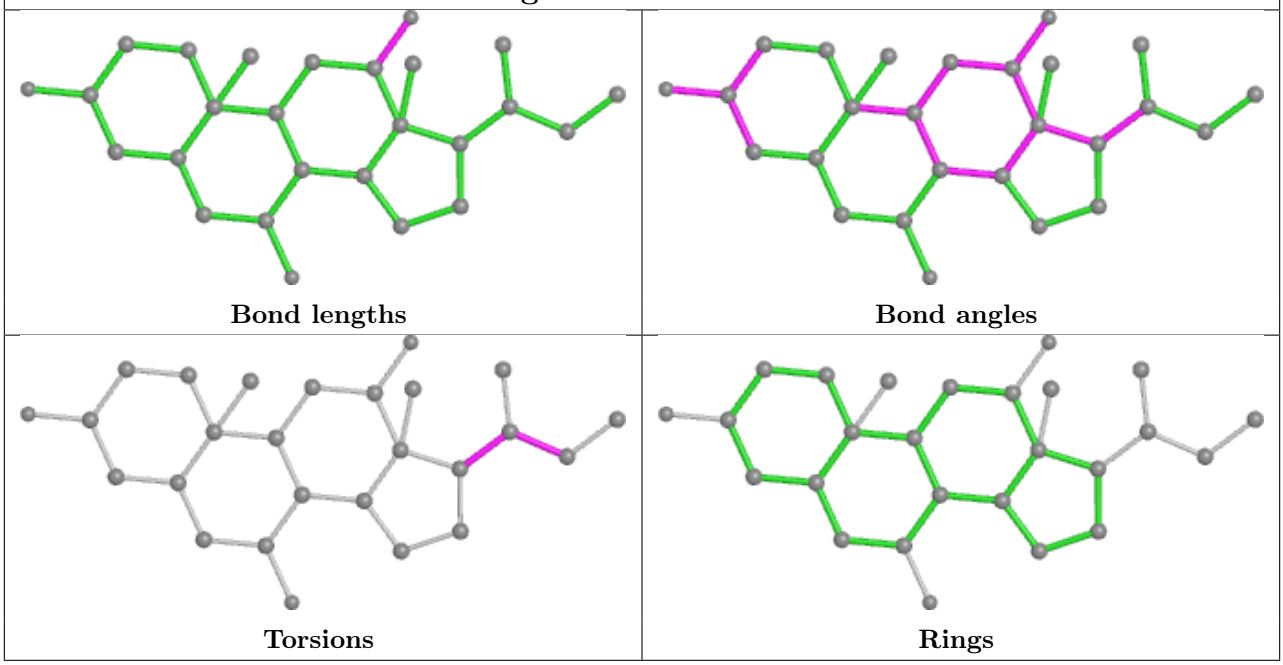


Torsions

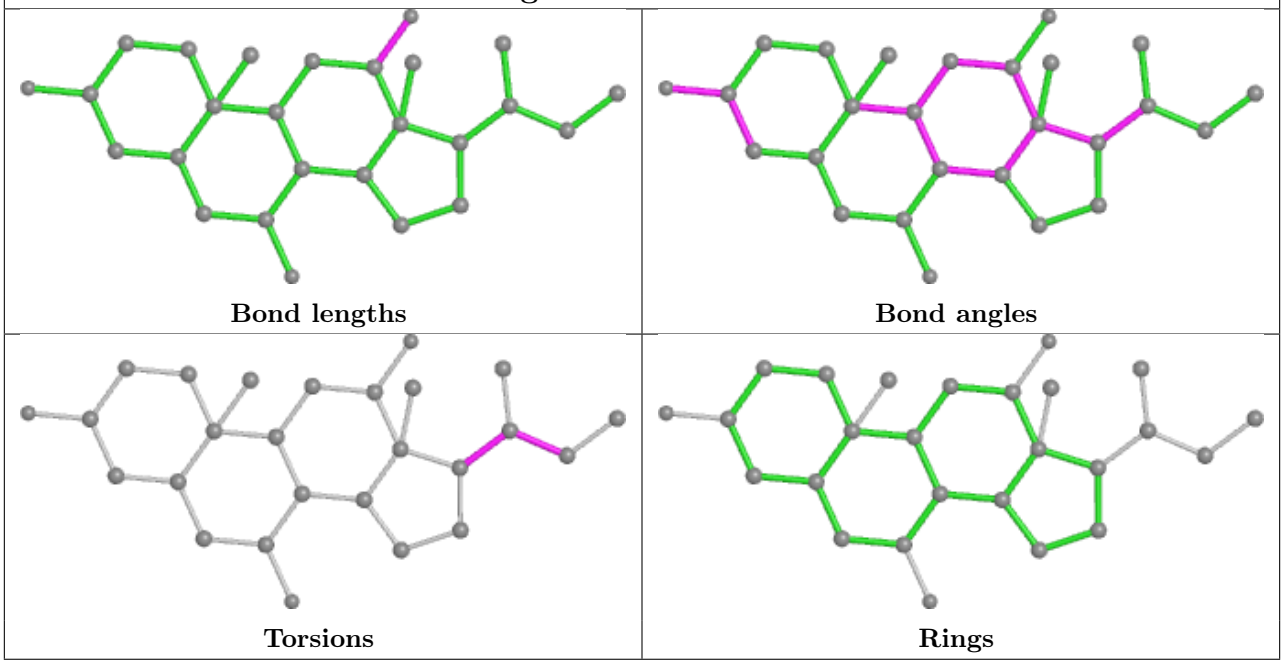


Rings

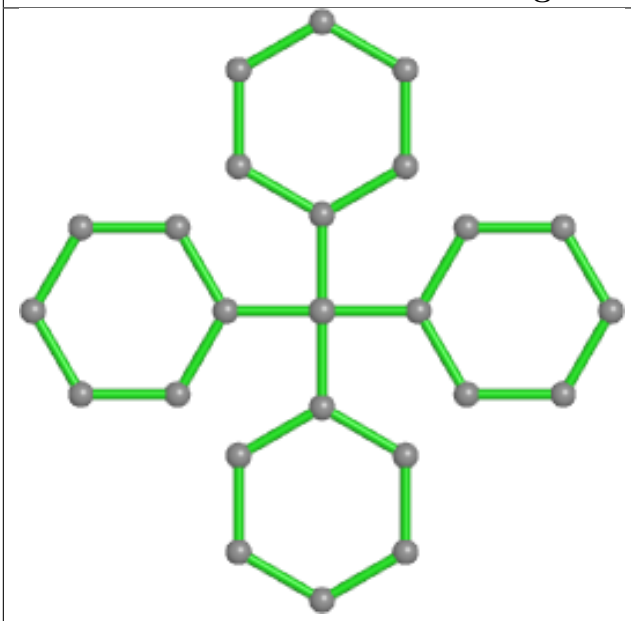
Ligand 1N7 A 1501



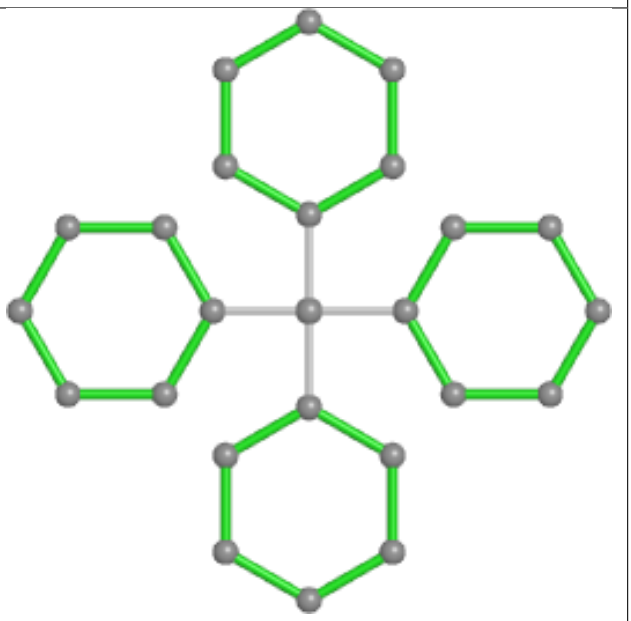
Ligand 1N7 D 1504



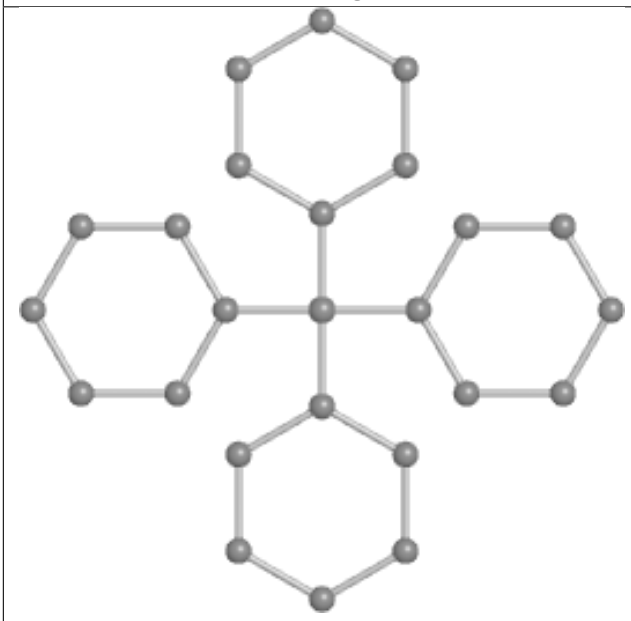
Ligand 118 H 302



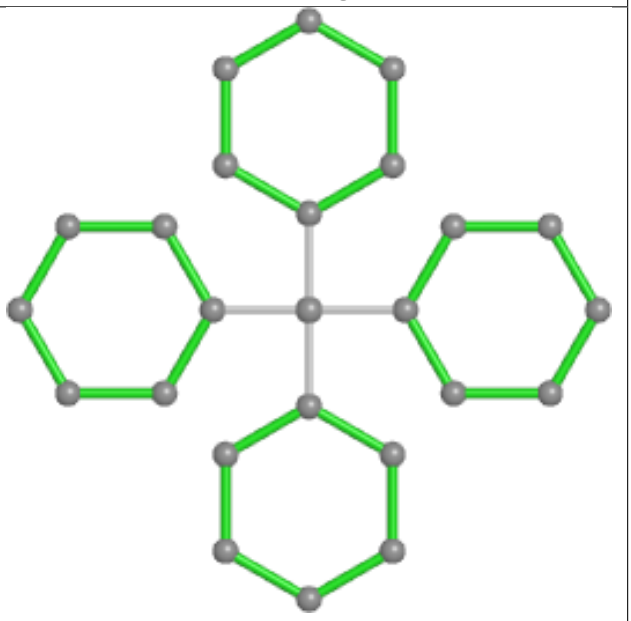
Bond lengths



Bond angles

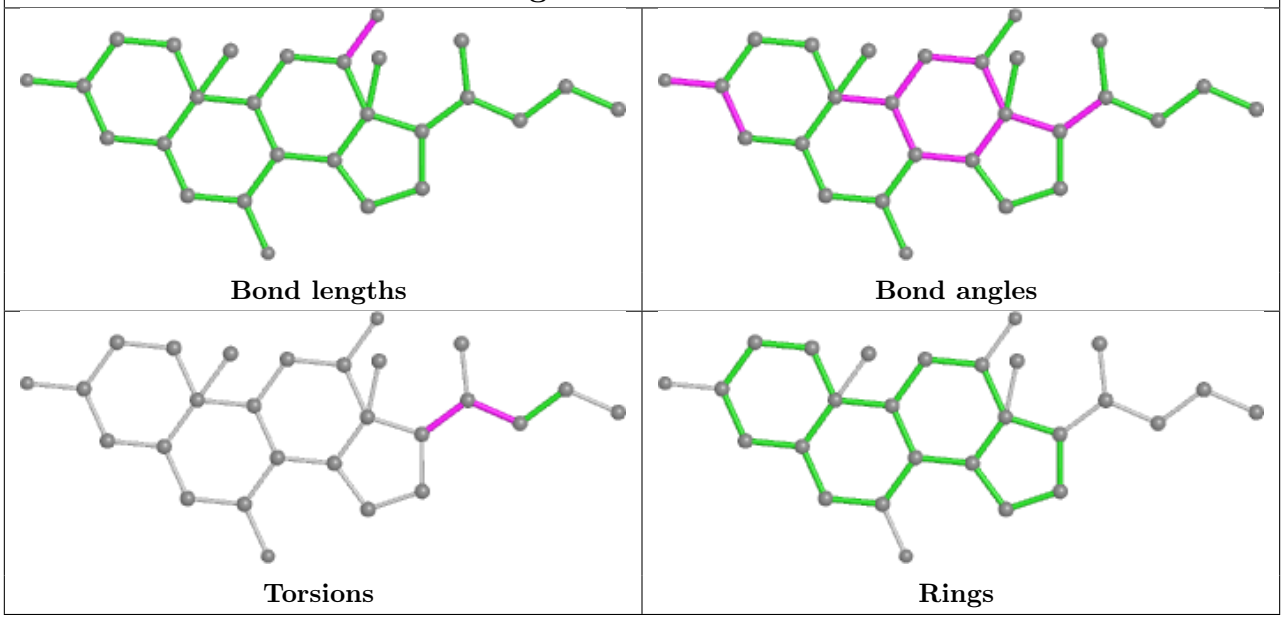


Torsions

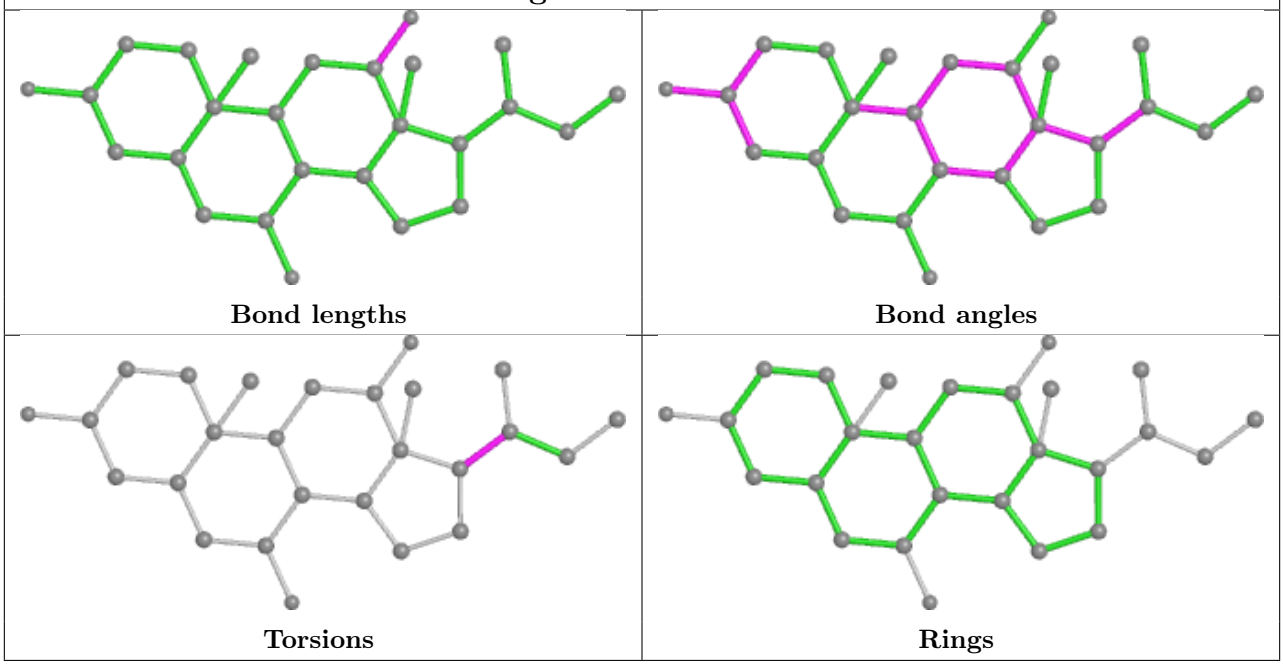


Rings

Ligand 1N7 H 301



Ligand 1N7 G 301



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.

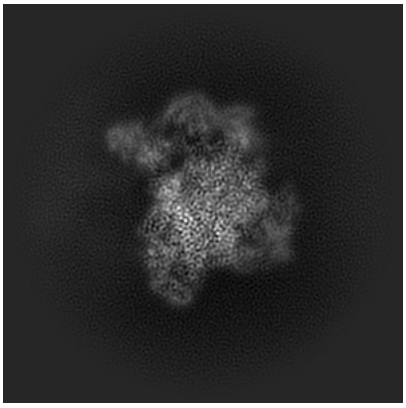
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22245. These allow visual inspection of the internal detail of the map and identification of artifacts.

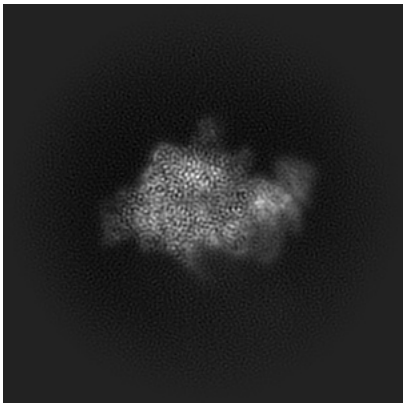
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

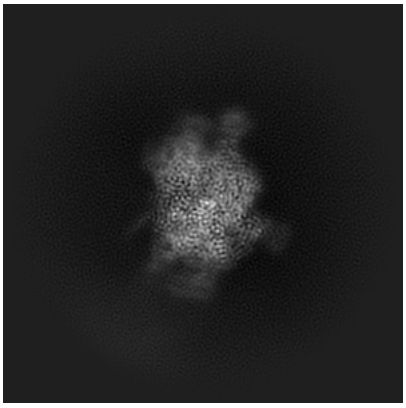
6.1.1 Primary map



X



Y

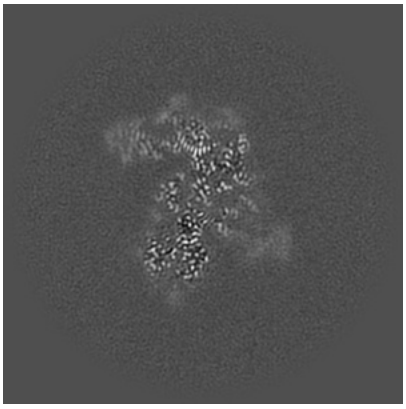


Z

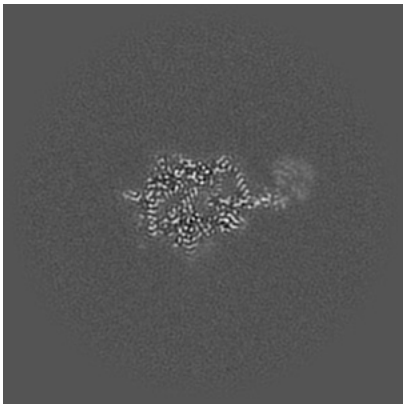
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

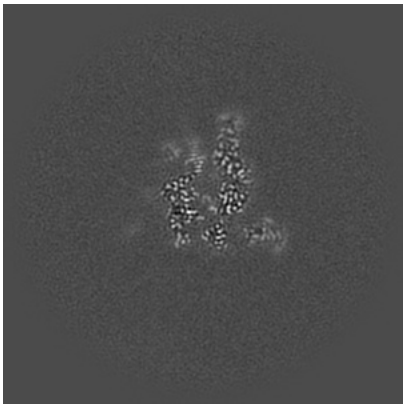
6.2.1 Primary map



X Index: 128



Y Index: 128

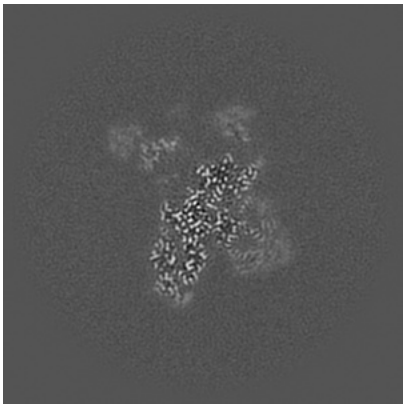


Z Index: 128

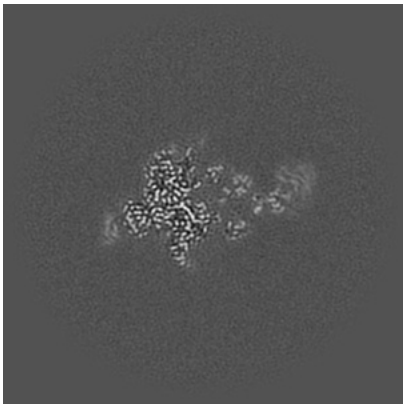
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

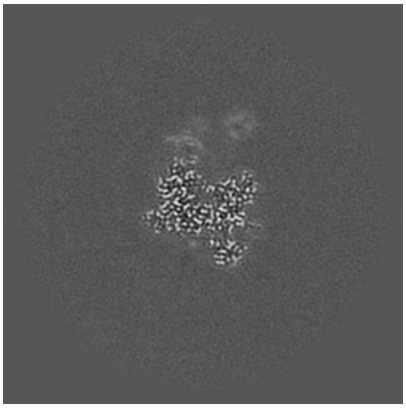
6.3.1 Primary map



X Index: 119



Y Index: 119

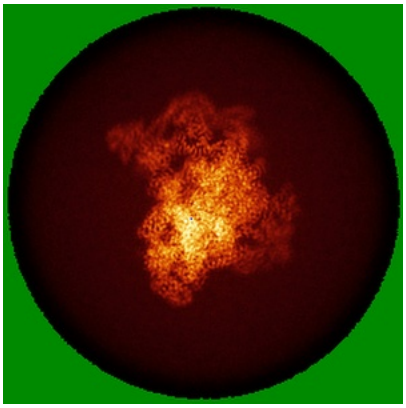


Z Index: 113

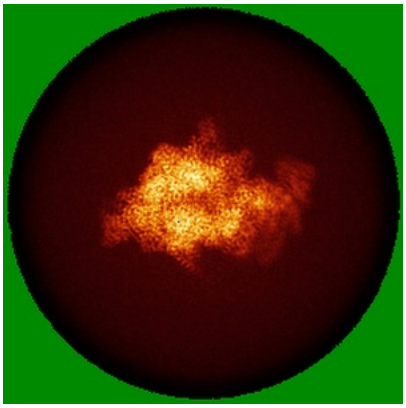
The images above show the largest variance slices of the map in three orthogonal directions.

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

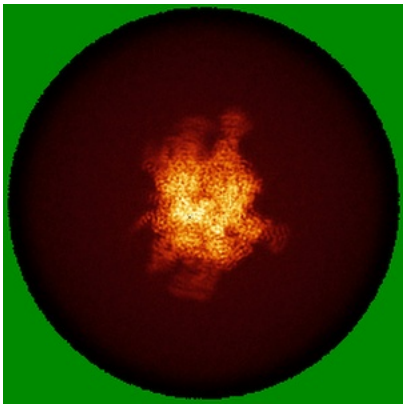
6.4.1 Primary map



X



Y

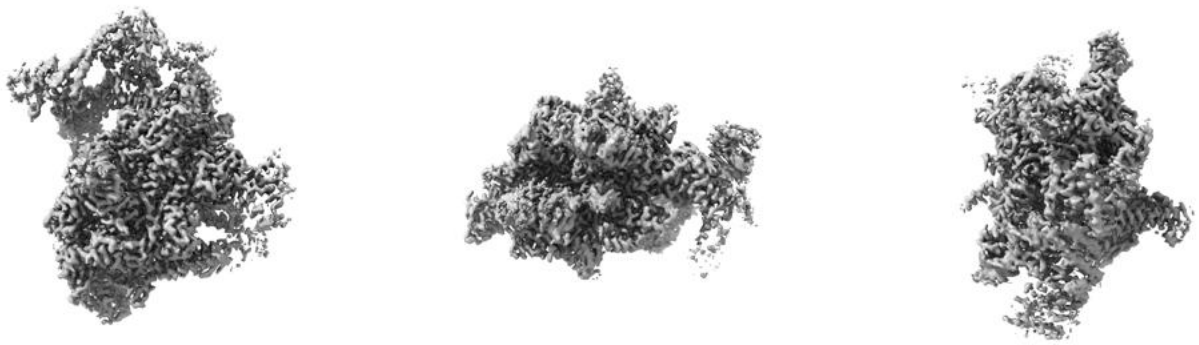


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.76. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

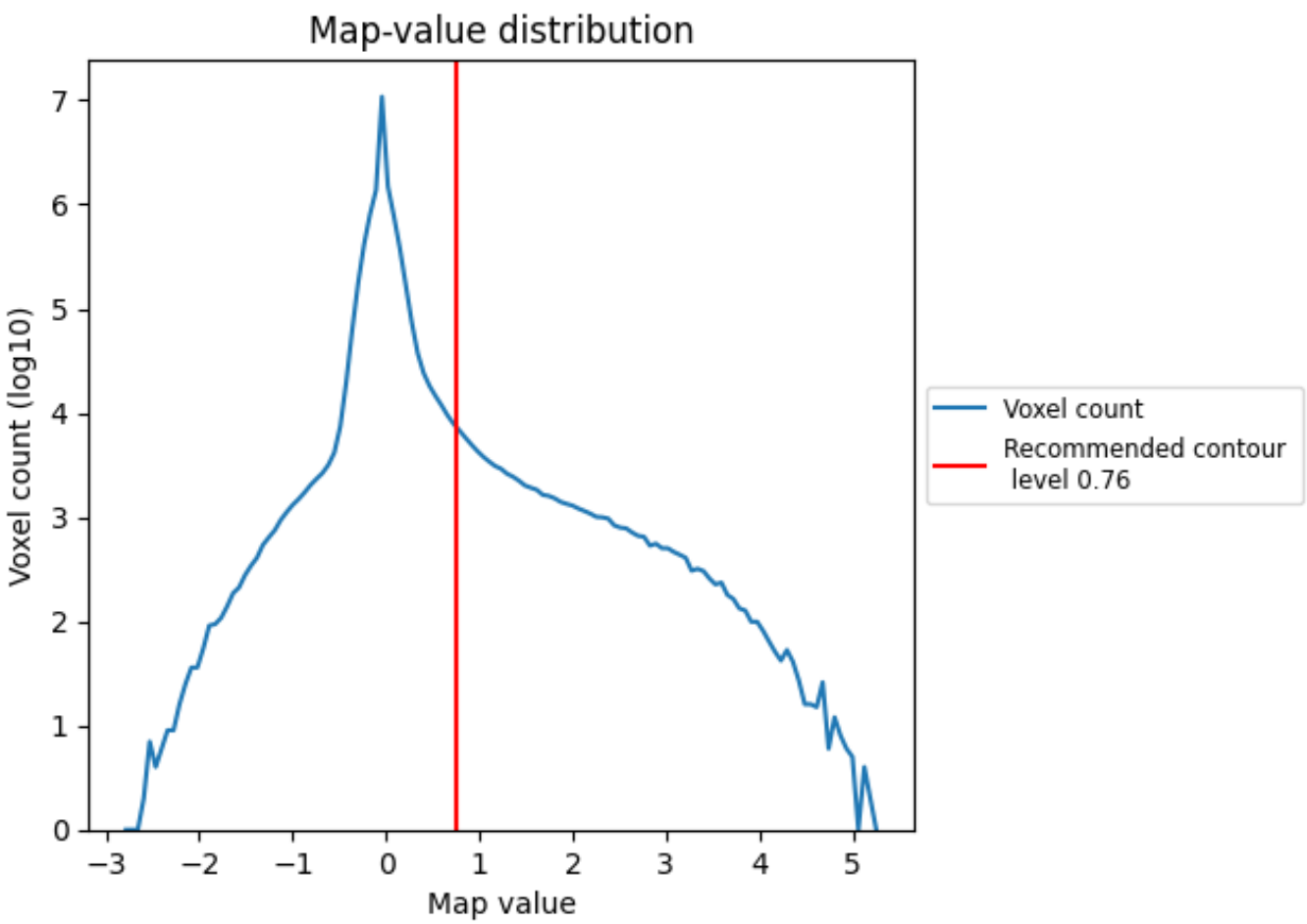
6.6 Mask visualisation (i)

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

7 Map analysis (i)

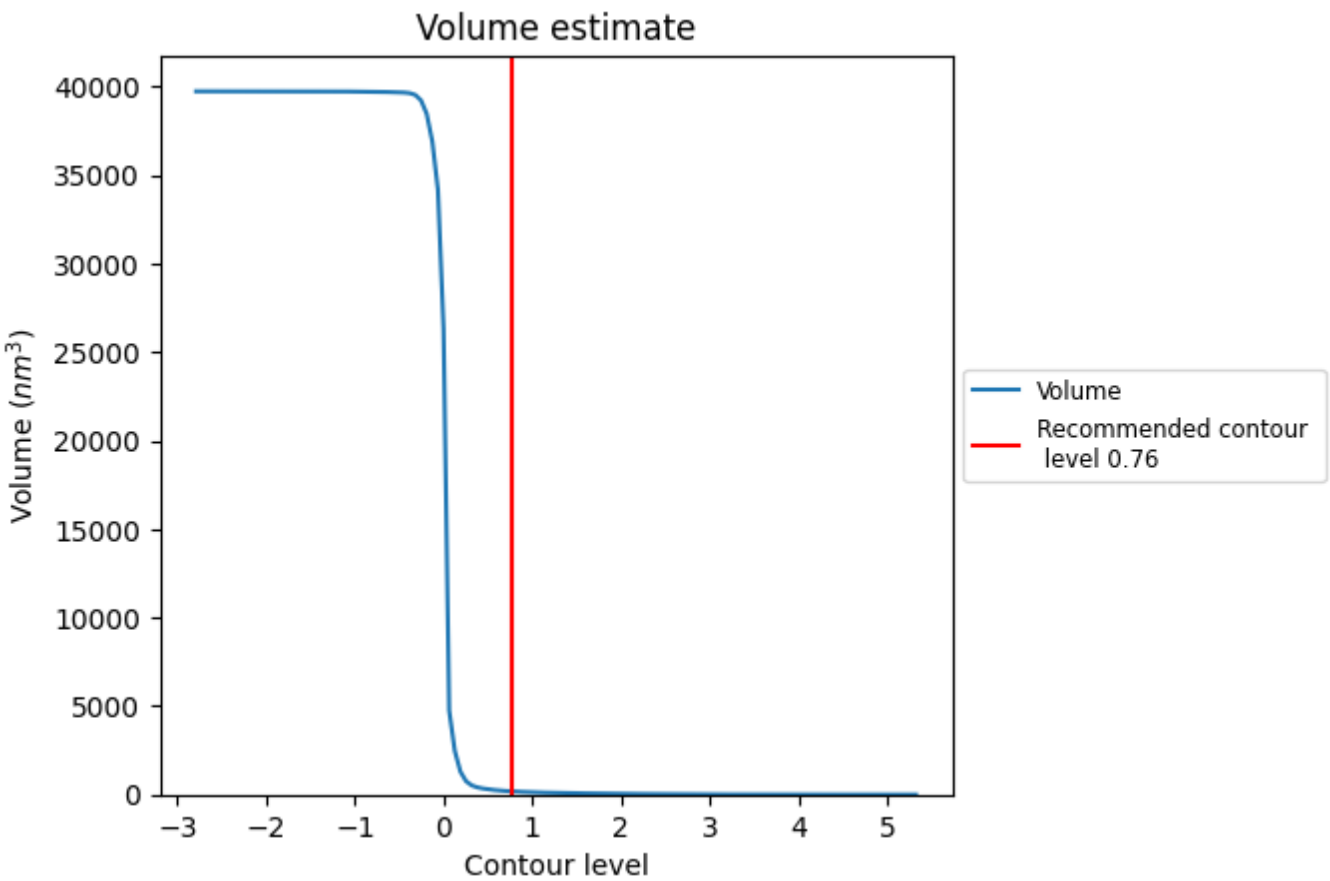
This section contains the results of statistical analysis of the map.

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.

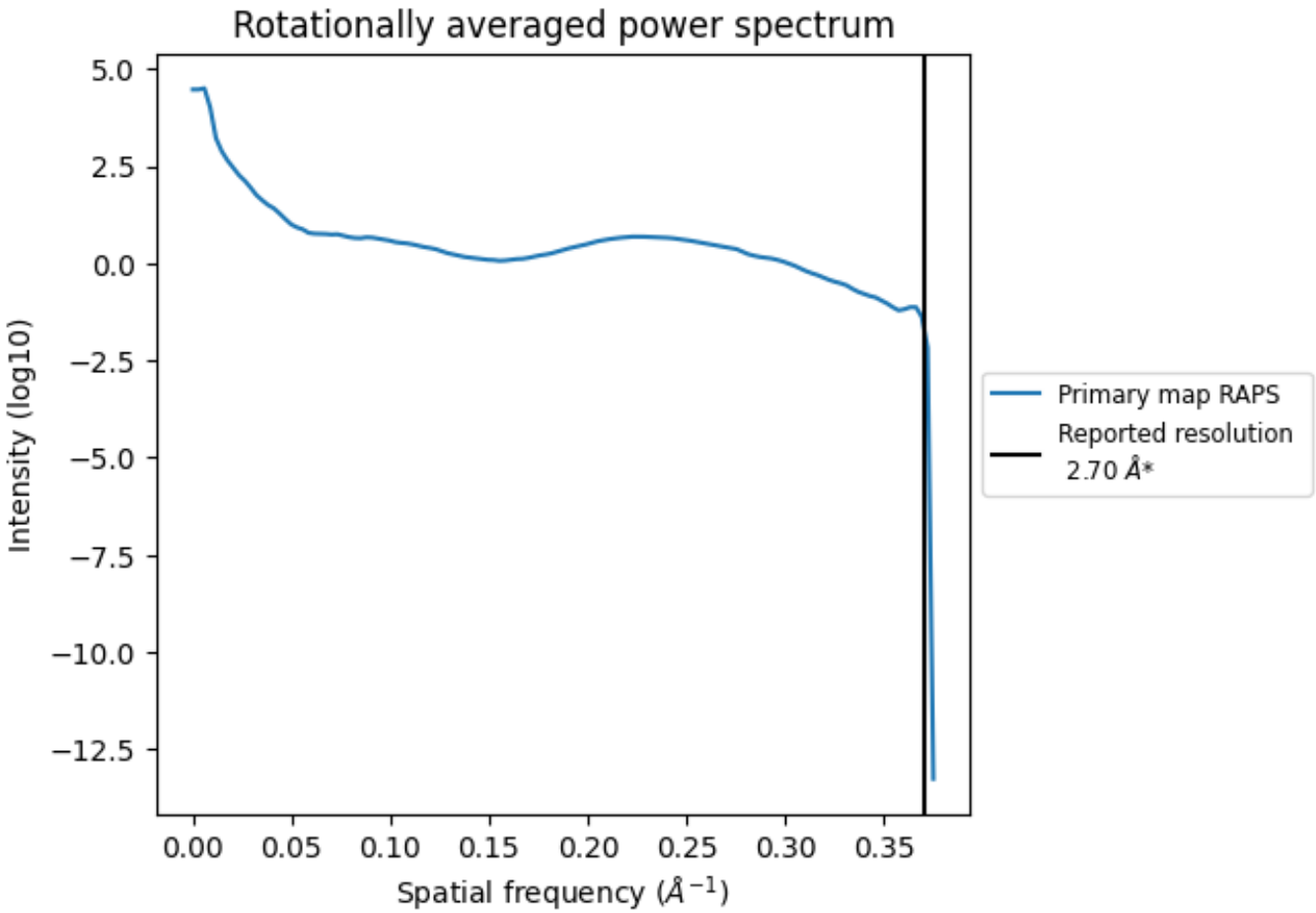
7.2 Volume estimate (i)



The volume at the recommended contour level is 183 nm^3; this corresponds to an approximate mass of 165 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

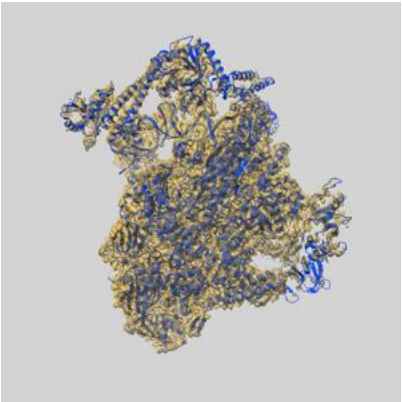
8 Fourier-Shell correlation (i)

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

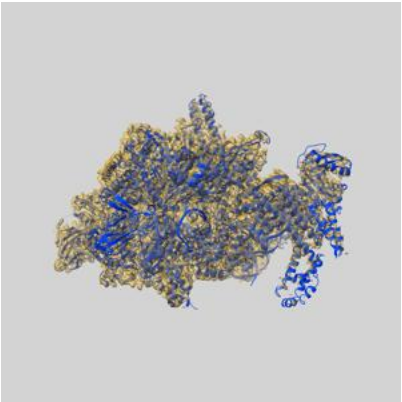
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22245 and PDB model 6XLJ. Per-residue inclusion information can be found in section 3 on page 8.

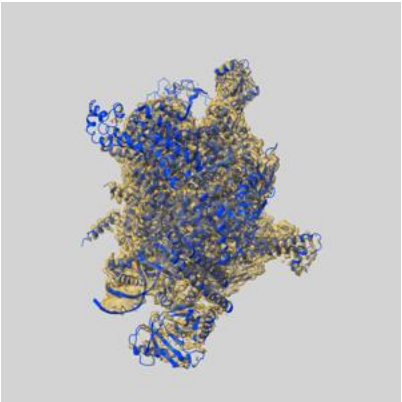
9.1 Map-model overlay (i)



X



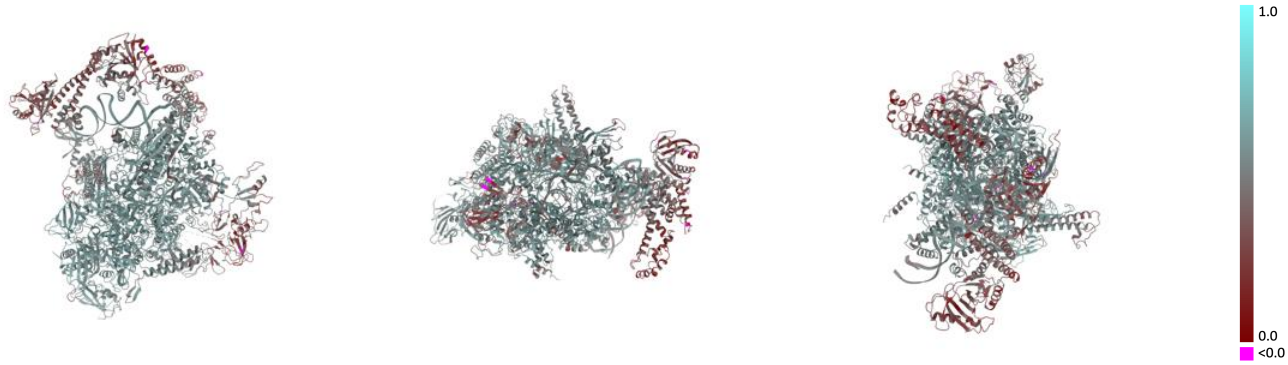
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.76 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

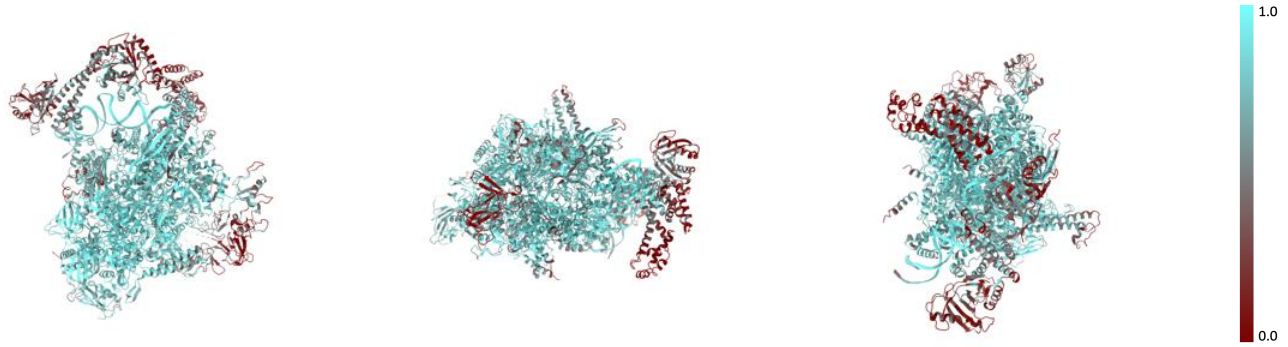
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

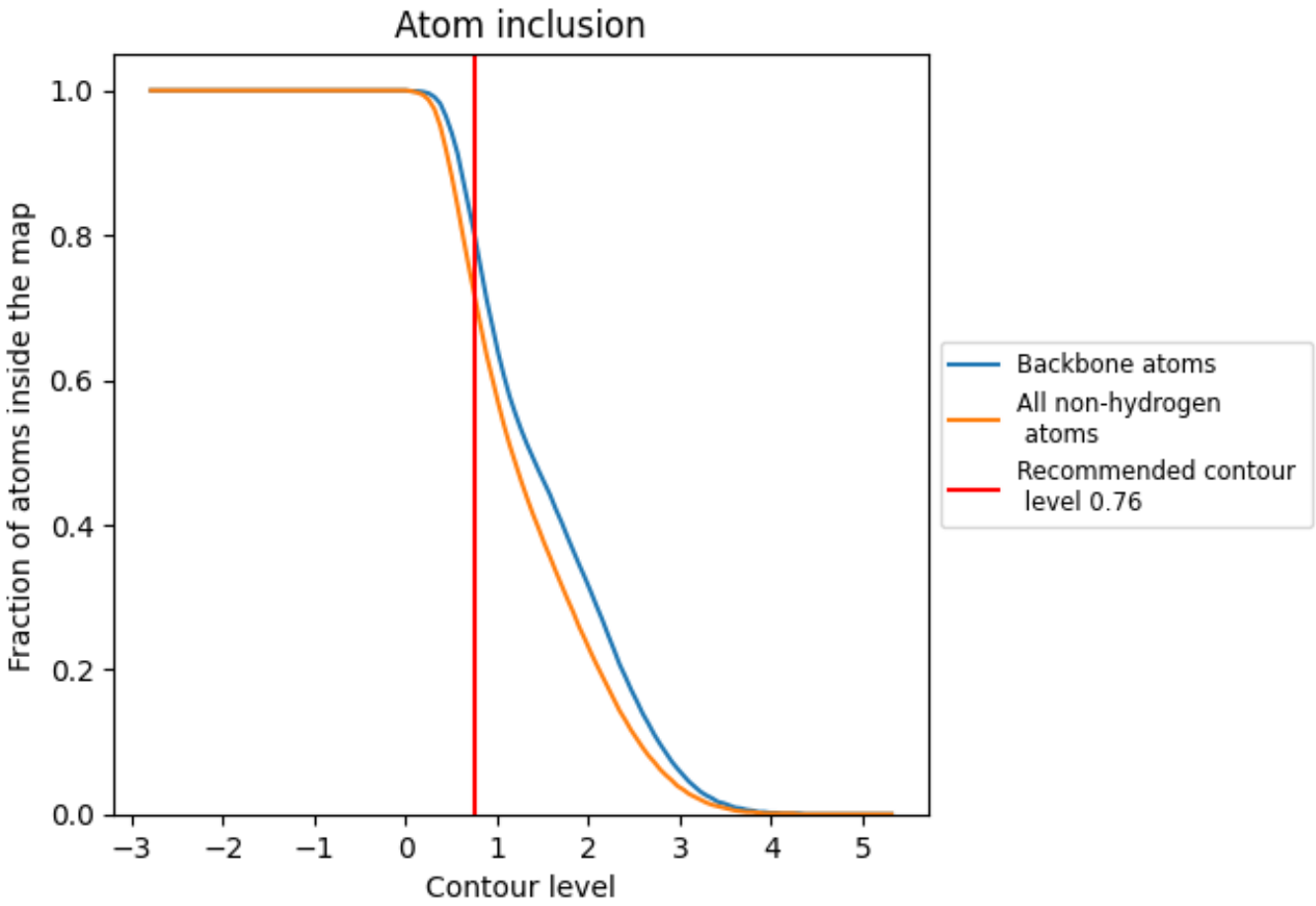
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.76).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.76) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.5120
A	0.8360	0.5710
B	0.7710	0.5540
C	0.8030	0.5550
D	0.7570	0.5390
E	0.7660	0.5580
F	0.5430	0.4420
G	0.3910	0.3420
H	0.3970	0.3530
N	0.8350	0.5350
R	0.9900	0.6120
T	0.8620	0.5430