



## Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 01:38 AM EDT

PDB ID : 8SRH / pdb\_00008srh  
EMDB ID : EMD-40731  
Title : Cryo-EM structure of TRPM2 chanzyme (E1114A) in the presence of Magnesium and ADP-ribose, open state  
Authors : Huang, Y.; Kumar, S.; Lu, W.; Du, J.  
Deposited on : 2023-05-05  
Resolution : 3.79 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

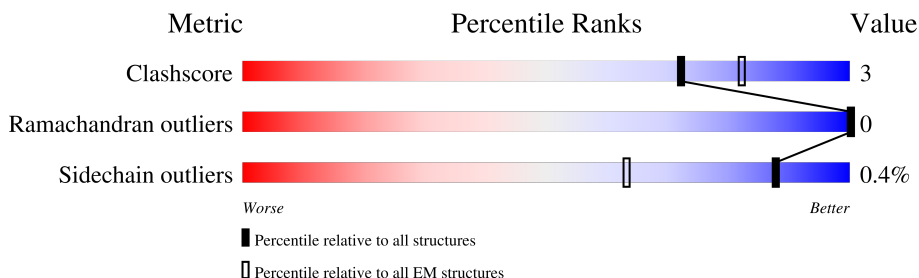
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.79 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1494	<div> <div>12%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	B	1494	<div> <div>12%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	C	1494	<div> <div>12%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	D	1494	<div> <div>12%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39468 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.

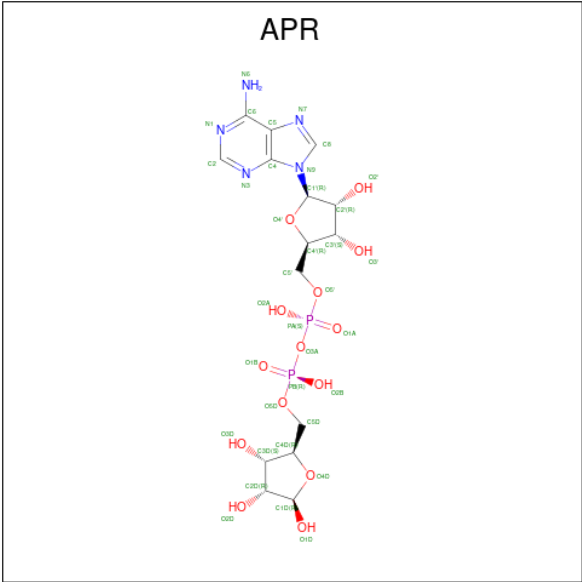
- Molecule 1 is a protein called TRPM2 chanzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1366	Total	C	N	O	S	0	0
			9707	6279	1713	1669	46		
1	B	1366	Total	C	N	O	S	0	0
			9707	6279	1713	1669	46		
1	C	1366	Total	C	N	O	S	0	0
			9707	6279	1713	1669	46		
1	D	1366	Total	C	N	O	S	0	0
			9707	6279	1713	1669	46		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1114	ALA	GLU	engineered mutation	UNP F2UB89
B	1114	ALA	GLU	engineered mutation	UNP F2UB89
C	1114	ALA	GLU	engineered mutation	UNP F2UB89
D	1114	ALA	GLU	engineered mutation	UNP F2UB89

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	A	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	B	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	B	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	C	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	C	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	D	1	Total	C	N	O	P	0
			36	15	5	14	2	
2	D	1	Total	C	N	O	P	0
			36	15	5	14	2	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

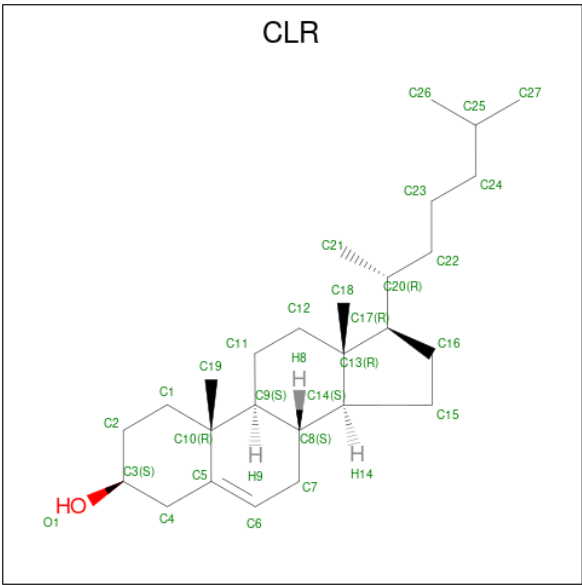
Mol	Chain	Residues	Atoms		AltConf
3	A	4	Total	Mg	0
			4	4	
3	B	4	Total	Mg	0
			4	4	
3	C	4	Total	Mg	0
			4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	D	4	Total	Mg	0
			4	4	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	C	1	Total	C	O	0
			28	27	1	
4	C	1	Total	C	O	0
			28	27	1	
4	C	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	

Continued on next page...

*Continued from previous page...*

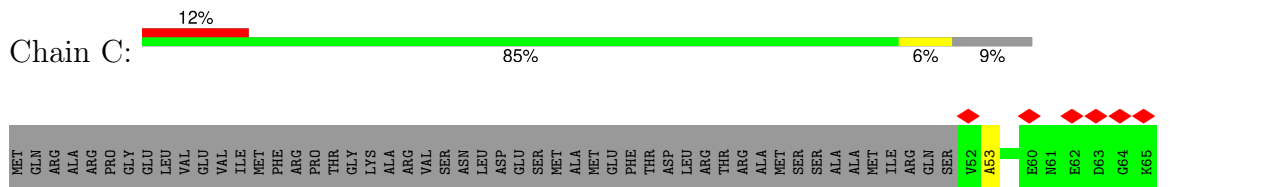
Mol	Chain	Residues	Atoms			AltConf
4	D	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	



Chain B:

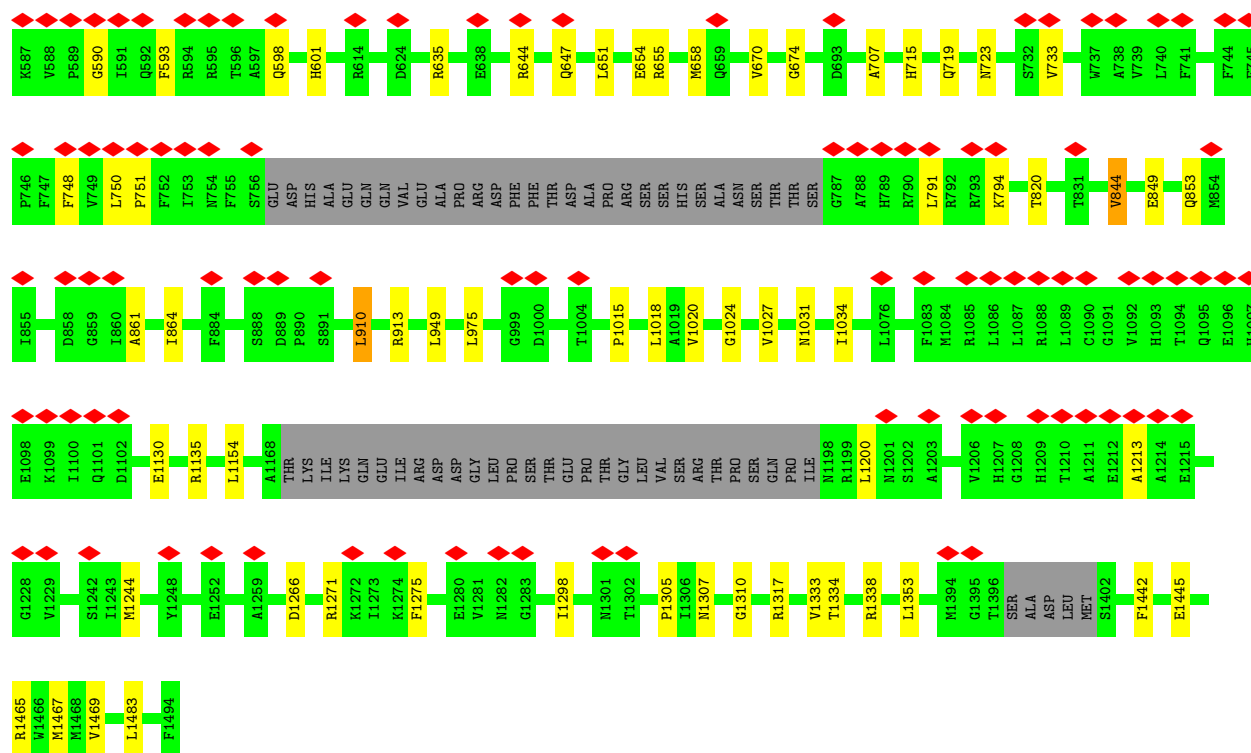


Chain C:









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	8279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	16.288	Depositor
Minimum map value	-6.751	Depositor
Average map value	0.060	Depositor
Map value standard deviation	0.431	Depositor
Recommended contour level	3	Depositor
Map size ( $\text{\AA}$ )	363.44, 363.44, 363.44	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82600003, 0.82600003, 0.82600003	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APR, MG, CLR

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	0.47	0/9940	0.83	14/13588 (0.1%)
1	B	0.47	0/9940	0.83	14/13588 (0.1%)
1	C	0.47	0/9940	0.83	14/13588 (0.1%)
1	D	0.47	0/9940	0.83	14/13588 (0.1%)
All	All	0.47	0/39760	0.83	56/54352 (0.1%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	PRO	N-CA-C	9.40	122.17	110.70
1	A	244	PRO	N-CA-C	9.39	122.16	110.70
1	C	244	PRO	N-CA-C	9.39	122.16	110.70
1	D	244	PRO	N-CA-C	9.39	122.16	110.70
1	B	844	VAL	N-CA-C	-7.62	103.37	110.53
1	A	844	VAL	N-CA-C	-7.58	103.40	110.53
1	C	844	VAL	N-CA-C	-7.58	103.40	110.53
1	D	844	VAL	N-CA-C	-7.58	103.40	110.53
1	C	1244	MET	CA-C-N	7.14	130.54	122.83
1	C	1244	MET	C-N-CA	7.14	130.54	122.83
1	A	1244	MET	CA-C-N	7.10	130.50	122.83
1	A	1244	MET	C-N-CA	7.10	130.50	122.83
1	B	1244	MET	CA-C-N	7.10	130.50	122.83
1	B	1244	MET	C-N-CA	7.10	130.50	122.83
1	D	1244	MET	CA-C-N	7.10	130.50	122.83
1	D	1244	MET	C-N-CA	7.10	130.50	122.83
1	B	913	ARG	N-CA-C	-6.07	104.95	112.90
1	A	913	ARG	N-CA-C	-6.05	104.98	112.90
1	C	913	ARG	N-CA-C	-6.05	104.98	112.90
1	D	913	ARG	N-CA-C	-6.05	104.98	112.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	SER	CA-C-N	5.71	130.47	122.08
1	D	93	SER	C-N-CA	5.71	130.47	122.08
1	A	93	SER	CA-C-N	5.69	130.44	122.08
1	A	93	SER	C-N-CA	5.69	130.44	122.08
1	B	93	SER	CA-C-N	5.69	130.44	122.08
1	B	93	SER	C-N-CA	5.69	130.44	122.08
1	C	93	SER	CA-C-N	5.68	130.43	122.08
1	C	93	SER	C-N-CA	5.68	130.43	122.08
1	A	1213	ALA	CA-C-N	5.66	130.17	122.19
1	A	1213	ALA	C-N-CA	5.66	130.17	122.19
1	B	1213	ALA	CA-C-N	5.66	130.17	122.19
1	B	1213	ALA	C-N-CA	5.66	130.17	122.19
1	C	1213	ALA	CA-C-N	5.66	130.17	122.19
1	C	1213	ALA	C-N-CA	5.66	130.17	122.19
1	D	1213	ALA	CA-C-N	5.66	130.17	122.19
1	D	1213	ALA	C-N-CA	5.66	130.17	122.19
1	A	1271	ARG	CA-C-N	5.50	129.95	122.19
1	A	1271	ARG	C-N-CA	5.50	129.95	122.19
1	B	1271	ARG	CA-C-N	5.50	129.95	122.19
1	B	1271	ARG	C-N-CA	5.50	129.95	122.19
1	C	1271	ARG	CA-C-N	5.50	129.95	122.19
1	C	1271	ARG	C-N-CA	5.50	129.95	122.19
1	D	1271	ARG	CA-C-N	5.50	129.95	122.19
1	D	1271	ARG	C-N-CA	5.50	129.95	122.19
1	A	733	VAL	N-CA-C	5.42	112.01	106.21
1	B	733	VAL	N-CA-C	5.42	112.01	106.21
1	C	733	VAL	N-CA-C	5.42	112.01	106.21
1	D	733	VAL	N-CA-C	5.42	112.01	106.21
1	A	1275	PHE	CA-C-N	5.38	130.20	122.40
1	A	1275	PHE	C-N-CA	5.38	130.20	122.40
1	B	1275	PHE	CA-C-N	5.38	130.20	122.40
1	B	1275	PHE	C-N-CA	5.38	130.20	122.40
1	C	1275	PHE	CA-C-N	5.38	130.20	122.40
1	C	1275	PHE	C-N-CA	5.38	130.20	122.40
1	D	1275	PHE	CA-C-N	5.38	130.20	122.40
1	D	1275	PHE	C-N-CA	5.38	130.20	122.40

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	9707	0	8825	55	0
1	B	9707	0	8825	59	0
1	C	9707	0	8825	51	0
1	D	9707	0	8825	57	0
2	A	72	0	42	2	0
2	B	72	0	42	2	0
2	C	72	0	42	2	0
2	D	72	0	42	2	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	84	0	138	5	0
4	B	84	0	138	5	0
4	C	84	0	138	4	0
4	D	84	0	138	4	0
All	All	39468	0	36020	244	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 3.

All (244) 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)
1:C:651:LEU:O	1:C:654:GLU:HB2	1.90	0.72
1:A:651:LEU:O	1:A:654:GLU:HB2	1.90	0.71
1:B:651:LEU:O	1:B:654:GLU:HB2	1.90	0.71
1:D:651:LEU:O	1:D:654:GLU:HB2	1.90	0.71
4:B:1707:CLR:H122	1:C:975:LEU:HD13	1.75	0.69
4:A:1707:CLR:H122	1:B:975:LEU:HD13	1.75	0.69
4:C:1707:CLR:H122	1:D:975:LEU:HD13	1.75	0.68
1:A:975:LEU:HD13	4:D:6001:CLR:H122	1.75	0.68
1:B:750:LEU:HD13	1:B:791:LEU:HD22	1.74	0.68
1:C:750:LEU:HD13	1:C:791:LEU:HD22	1.74	0.68
1:D:750:LEU:HD13	1:D:791:LEU:HD22	1.74	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:LEU:HD23	1:C:794:LYS:HD2	1.76	0.67
1:A:750:LEU:HD22	1:A:791:LEU:HD22	1.77	0.67
1:A:750:LEU:HD13	1:A:791:LEU:HD22	1.74	0.67
1:A:750:LEU:HD23	1:A:794:LYS:HD2	1.76	0.67
1:D:750:LEU:HD22	1:D:791:LEU:HD22	1.77	0.67
1:B:750:LEU:HD23	1:B:794:LYS:HD2	1.76	0.66
1:B:750:LEU:HD22	1:B:791:LEU:HD22	1.77	0.66
1:D:750:LEU:HD23	1:D:794:LYS:HD2	1.76	0.66
1:C:750:LEU:HD22	1:C:791:LEU:HD22	1.77	0.65
1:B:1200:LEU:C	1:B:1200:LEU:HD12	2.28	0.58
1:C:1200:LEU:HD12	1:C:1200:LEU:C	2.28	0.58
1:A:1200:LEU:HD12	1:A:1200:LEU:C	2.28	0.58
1:B:820:THR:HG21	1:B:910:LEU:HD13	1.87	0.57
1:D:820:THR:HG21	1:D:910:LEU:HD13	1.86	0.57
1:D:1200:LEU:HD12	1:D:1200:LEU:C	2.28	0.57
1:A:820:THR:HG21	1:A:910:LEU:HD13	1.87	0.57
1:C:820:THR:HG21	1:C:910:LEU:HD13	1.87	0.57
1:A:145:LEU:O	1:A:179:VAL:HA	2.05	0.57
1:A:750:LEU:HD22	1:A:791:LEU:CD2	2.35	0.57
1:B:145:LEU:O	1:B:179:VAL:HA	2.05	0.56
1:B:1015:PRO:O	1:B:1018:LEU:HB3	2.06	0.56
1:D:750:LEU:HD22	1:D:791:LEU:CD2	2.35	0.56
1:C:145:LEU:O	1:C:179:VAL:HA	2.05	0.56
1:C:53:ALA:HB2	1:C:233:ILE:HD13	1.88	0.56
1:D:145:LEU:O	1:D:179:VAL:HA	2.05	0.56
1:B:53:ALA:HB2	1:B:233:ILE:HD13	1.88	0.56
1:C:750:LEU:HD22	1:C:791:LEU:CD2	2.35	0.56
1:A:1015:PRO:O	1:A:1018:LEU:HB3	2.06	0.56
1:C:1015:PRO:O	1:C:1018:LEU:HB3	2.06	0.56
1:D:1015:PRO:O	1:D:1018:LEU:HB3	2.06	0.56
1:B:750:LEU:HD22	1:B:791:LEU:CD2	2.35	0.55
1:B:485:THR:HG22	1:B:549:LEU:HG	1.89	0.54
1:A:53:ALA:HB2	1:A:233:ILE:HD13	1.88	0.54
1:C:485:THR:HG22	1:C:549:LEU:HG	1.89	0.54
1:D:485:THR:HG22	1:D:549:LEU:HG	1.89	0.54
1:A:485:THR:HG22	1:A:549:LEU:HG	1.89	0.54
1:B:280:ASN:HD22	1:B:311:GLN:HB3	1.73	0.54
1:D:53:ALA:HB2	1:D:233:ILE:HD13	1.88	0.54
1:C:280:ASN:HD22	1:C:311:GLN:HB3	1.73	0.53
1:A:146:SER:O	1:A:292:THR:HA	2.09	0.53
1:A:280:ASN:HD22	1:A:311:GLN:HB3	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:SER:O	1:C:292:THR:HA	2.09	0.52
1:D:280:ASN:HD22	1:D:311:GLN:HB3	1.73	0.52
1:A:1298:ILE:HA	1:A:1305:PRO:HA	1.92	0.52
1:B:1298:ILE:HA	1:B:1305:PRO:HA	1.92	0.52
1:B:146:SER:O	1:B:292:THR:HA	2.09	0.52
1:C:1298:ILE:HA	1:C:1305:PRO:HA	1.92	0.51
1:D:146:SER:O	1:D:292:THR:HA	2.09	0.51
1:D:1298:ILE:HA	1:D:1305:PRO:HA	1.92	0.51
2:B:1706:APR:N3	2:B:1706:APR:H'2	2.27	0.50
1:B:750:LEU:CD2	1:B:794:LYS:HD2	2.40	0.50
1:A:750:LEU:CD2	1:A:794:LYS:HD2	2.40	0.50
1:D:750:LEU:CD2	1:D:794:LYS:HD2	2.40	0.50
1:A:1031:ASN:HA	1:A:1034:ILE:HG12	1.94	0.50
2:C:1706:APR:H'2	2:C:1706:APR:N3	2.27	0.50
1:D:1031:ASN:HA	1:D:1034:ILE:HG12	1.94	0.50
2:D:6009:APR:H'2	2:D:6009:APR:N3	2.27	0.50
2:A:1706:APR:H'2	2:A:1706:APR:N3	2.27	0.49
1:D:1027:VAL:O	1:D:1031:ASN:ND2	2.45	0.49
1:C:1027:VAL:O	1:C:1031:ASN:ND2	2.45	0.49
1:A:655:ARG:O	1:A:658:MET:HB2	2.12	0.49
1:B:415:LEU:HD11	1:B:431:LEU:HD21	1.95	0.49
1:A:1027:VAL:O	1:A:1031:ASN:ND2	2.45	0.49
1:D:415:LEU:HD11	1:D:431:LEU:HD21	1.95	0.49
1:B:655:ARG:O	1:B:658:MET:HB2	2.12	0.49
1:B:1031:ASN:HA	1:B:1034:ILE:HG12	1.93	0.49
1:A:415:LEU:HD11	1:A:431:LEU:HD21	1.95	0.49
1:B:1027:VAL:O	1:B:1031:ASN:ND2	2.45	0.49
1:C:1031:ASN:HA	1:C:1034:ILE:HG12	1.94	0.49
1:C:655:ARG:O	1:C:658:MET:HB2	2.13	0.49
1:C:750:LEU:CD2	1:C:794:LYS:HD2	2.40	0.49
1:C:415:LEU:HD11	1:C:431:LEU:HD21	1.95	0.49
1:A:1307:ASN:ND2	1:A:1310:GLY:O	2.46	0.48
1:D:655:ARG:O	1:D:658:MET:HB2	2.12	0.48
1:D:1307:ASN:ND2	1:D:1310:GLY:O	2.46	0.48
1:C:1307:ASN:ND2	1:C:1310:GLY:O	2.46	0.48
1:B:447:ILE:HA	1:B:450:ASN:HB2	1.97	0.47
1:C:447:ILE:HA	1:C:450:ASN:HB2	1.96	0.47
1:A:97:GLY:HA3	1:A:231:PRO:O	2.15	0.47
1:A:210:THR:H	1:A:255:ASN:HB2	1.79	0.47
1:B:97:GLY:HA3	1:B:231:PRO:O	2.15	0.47
1:B:1307:ASN:ND2	1:B:1310:GLY:O	2.46	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLY:HA3	1:C:231:PRO:O	2.15	0.47
1:B:210:THR:H	1:B:255:ASN:HB2	1.79	0.47
1:B:296:GLN:HG2	1:B:322:GLY:HA3	1.97	0.47
4:D:6002:CLR:H162	4:D:6002:CLR:H222	1.69	0.47
1:D:447:ILE:HA	1:D:450:ASN:HB2	1.96	0.47
1:D:97:GLY:HA3	1:D:231:PRO:O	2.15	0.47
1:D:1338:ARG:NH2	1:D:1445:GLU:O	2.48	0.47
1:A:644:ARG:HA	1:A:647:GLN:HE21	1.80	0.47
1:A:1338:ARG:NH2	1:A:1445:GLU:O	2.48	0.47
1:A:447:ILE:HA	1:A:450:ASN:HB2	1.96	0.47
1:A:296:GLN:HG2	1:A:322:GLY:HA3	1.97	0.46
2:D:6004:APR:H8	2:D:6004:APR:H'2	1.64	0.46
1:B:644:ARG:HA	1:B:647:GLN:HE21	1.80	0.46
1:D:210:THR:H	1:D:255:ASN:HB2	1.79	0.46
1:D:644:ARG:HA	1:D:647:GLN:HE21	1.80	0.46
1:D:750:LEU:CD1	1:D:791:LEU:HD22	2.45	0.46
1:B:748:PHE:O	1:B:751:PRO:HD2	2.16	0.46
1:C:210:THR:H	1:C:255:ASN:HB2	1.79	0.46
1:B:861:ALA:HA	1:B:864:ILE:HG22	1.98	0.46
1:B:1338:ARG:NH2	1:B:1445:GLU:O	2.48	0.46
1:B:231:PRO:O	1:B:232:LYS:C	2.59	0.46
1:C:748:PHE:O	1:C:751:PRO:HD2	2.16	0.46
1:D:296:GLN:HG2	1:D:322:GLY:HA3	1.97	0.46
1:C:644:ARG:HA	1:C:647:GLN:HE21	1.80	0.46
4:C:1709:CLR:H162	4:C:1709:CLR:H221	1.49	0.46
1:B:670:VAL:O	1:B:674:GLY:N	2.50	0.45
1:B:750:LEU:CD1	1:B:791:LEU:HD22	2.45	0.45
1:C:1338:ARG:NH2	1:C:1445:GLU:O	2.48	0.45
2:C:1701:APR:H8	2:C:1701:APR:H'2	1.64	0.45
1:D:748:PHE:O	1:D:751:PRO:HD2	2.16	0.45
1:A:748:PHE:O	1:A:751:PRO:HD2	2.16	0.45
1:A:861:ALA:HA	1:A:864:ILE:HG22	1.98	0.45
1:C:296:GLN:HG2	1:C:322:GLY:HA3	1.97	0.45
1:A:670:VAL:O	1:A:674:GLY:N	2.50	0.45
1:A:750:LEU:CD1	1:A:791:LEU:HD22	2.45	0.45
4:A:1708:CLR:H162	4:A:1708:CLR:H222	1.69	0.45
1:D:670:VAL:O	1:D:674:GLY:N	2.50	0.45
1:C:861:ALA:HA	1:C:864:ILE:HG22	1.98	0.45
1:D:861:ALA:HA	1:D:864:ILE:HG22	1.98	0.45
1:C:231:PRO:O	1:C:232:LYS:C	2.59	0.45
2:B:1701:APR:H'2	2:B:1701:APR:H8	1.65	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1707:CLR:H211	4:B:1707:CLR:H232	1.67	0.45
1:C:280:ASN:ND2	1:C:311:GLN:O	2.50	0.45
1:A:748:PHE:C	1:A:751:PRO:HD2	2.42	0.45
2:A:1701:APR:H8	2:A:1701:APR:H'2	1.64	0.44
1:A:280:ASN:ND2	1:A:311:GLN:O	2.50	0.44
1:C:748:PHE:C	1:C:751:PRO:HD2	2.42	0.44
1:C:1465:ARG:HH21	1:C:1467:MET:HE3	1.83	0.44
4:A:1707:CLR:H232	4:A:1707:CLR:H211	1.67	0.44
1:A:1465:ARG:HH21	1:A:1467:MET:HE3	1.83	0.44
1:D:1465:ARG:HH21	1:D:1467:MET:HE3	1.83	0.44
1:B:280:ASN:ND2	1:B:311:GLN:O	2.50	0.44
1:B:748:PHE:C	1:B:751:PRO:HD2	2.42	0.44
1:B:1465:ARG:HH21	1:B:1467:MET:HE3	1.83	0.44
1:A:635:ARG:HD3	1:A:707:ALA:HA	2.00	0.44
4:B:1708:CLR:H222	4:B:1708:CLR:H162	1.69	0.44
4:B:1709:CLR:H162	4:B:1709:CLR:H221	1.49	0.44
1:D:563:ILE:O	1:D:567:LEU:HB2	2.17	0.44
1:D:748:PHE:C	1:D:751:PRO:HD2	2.42	0.44
1:B:635:ARG:HD3	1:B:707:ALA:HA	2.00	0.43
4:B:1709:CLR:H272	4:B:1709:CLR:H231	1.76	0.43
1:D:280:ASN:ND2	1:D:311:GLN:O	2.50	0.43
1:A:230:PRO:HB2	1:A:231:PRO:HD3	2.00	0.43
1:A:563:ILE:O	1:A:567:LEU:HB2	2.17	0.43
1:B:230:PRO:HB2	1:B:231:PRO:HD3	2.00	0.43
1:B:563:ILE:O	1:B:567:LEU:HB2	2.17	0.43
1:C:563:ILE:O	1:C:567:LEU:HB2	2.17	0.43
1:A:750:LEU:CD2	1:A:791:LEU:HD22	2.47	0.43
1:A:231:PRO:O	1:A:232:LYS:C	2.59	0.43
1:D:231:PRO:O	1:D:232:LYS:C	2.59	0.43
1:D:635:ARG:HD3	1:D:707:ALA:HA	2.00	0.43
1:C:230:PRO:HB2	1:C:231:PRO:HD3	2.00	0.42
1:C:635:ARG:HD3	1:C:707:ALA:HA	2.00	0.42
1:A:670:VAL:HG13	1:A:715:HIS:HD2	1.85	0.42
1:B:467:LEU:HD11	1:B:473:ILE:HD11	2.01	0.42
1:C:719:GLN:O	1:C:723:ASN:HB2	2.20	0.42
1:D:230:PRO:HB2	1:D:231:PRO:HD3	2.00	0.42
1:C:670:VAL:O	1:C:674:GLY:N	2.50	0.42
1:D:719:GLN:O	1:D:723:ASN:HB2	2.20	0.42
1:D:750:LEU:CD2	1:D:791:LEU:HD22	2.47	0.42
1:A:467:LEU:HD11	1:A:473:ILE:HD11	2.01	0.42
1:A:213:ILE:HD12	1:A:275:ARG:HG3	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:GLY:O	1:B:593:PHE:HB3	2.20	0.42
1:B:670:VAL:HG13	1:B:715:HIS:HD2	1.85	0.42
1:C:670:VAL:HG13	1:C:715:HIS:HD2	1.85	0.42
1:D:670:VAL:HG13	1:D:715:HIS:HD2	1.85	0.42
1:C:590:GLY:O	1:C:593:PHE:HB3	2.20	0.42
1:B:719:GLN:O	1:B:723:ASN:HB2	2.20	0.42
1:A:590:GLY:O	1:A:593:PHE:HB3	2.20	0.42
1:C:750:LEU:CD1	1:C:791:LEU:HD22	2.45	0.42
1:B:702:ASN:OD1	1:B:1057:TYR:OH	2.38	0.41
1:C:467:LEU:HD11	1:C:473:ILE:HD11	2.01	0.41
1:B:807:ILE:HD12	1:B:807:ILE:HA	1.95	0.41
1:C:213:ILE:HD12	1:C:275:ARG:HG3	2.02	0.41
1:A:316:VAL:HG21	1:A:400:ILE:HD13	2.03	0.41
1:A:719:GLN:O	1:A:723:ASN:HB2	2.20	0.41
1:D:467:LEU:HD11	1:D:473:ILE:HD11	2.01	0.41
1:D:590:GLY:O	1:D:593:PHE:HB3	2.20	0.41
1:A:53:ALA:HB2	1:A:233:ILE:CD1	2.51	0.41
4:A:1708:CLR:H272	4:A:1708:CLR:H231	1.77	0.41
1:B:316:VAL:HG21	1:B:400:ILE:HD13	2.03	0.41
1:B:750:LEU:CD2	1:B:791:LEU:HD22	2.47	0.41
1:B:1154:LEU:HD12	1:B:1154:LEU:HA	1.87	0.41
4:C:1708:CLR:H162	4:C:1708:CLR:H222	1.69	0.41
4:C:1708:CLR:H272	4:C:1708:CLR:H231	1.77	0.41
1:D:1200:LEU:HD12	1:D:1200:LEU:O	2.21	0.41
4:D:6002:CLR:H272	4:D:6002:CLR:H231	1.77	0.41
1:A:1200:LEU:HD12	1:A:1200:LEU:O	2.21	0.41
1:B:598:GLN:O	1:B:601:HIS:HB3	2.21	0.41
1:C:316:VAL:HG21	1:C:400:ILE:HD13	2.03	0.41
1:D:316:VAL:HG21	1:D:400:ILE:HD13	2.03	0.41
1:B:213:ILE:HD12	1:B:275:ARG:HG3	2.02	0.41
1:D:53:ALA:HB2	1:D:233:ILE:CD1	2.51	0.41
1:D:598:GLN:O	1:D:601:HIS:HB3	2.21	0.41
1:D:1333:VAL:HG22	1:D:1442:PHE:HB2	2.02	0.41
1:A:927:LYS:HA	1:A:927:LYS:HD3	1.91	0.41
1:C:1333:VAL:HG22	1:C:1442:PHE:HB2	2.02	0.41
1:B:849:GLU:OE2	1:B:853:GLN:NE2	2.53	0.41
1:B:1266:ASP:O	1:B:1317:ARG:NH1	2.54	0.41
1:C:598:GLN:O	1:C:601:HIS:HB3	2.21	0.41
1:C:1130:GLU:O	1:C:1135:ARG:NH1	2.54	0.41
1:D:1020:VAL:O	1:D:1024:GLY:N	2.54	0.41
4:A:1709:CLR:H221	4:A:1709:CLR:H162	1.49	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ALA:HB2	1:B:233:ILE:CD1	2.51	0.41
1:B:697:LYS:HD3	1:B:697:LYS:HA	1.93	0.41
1:B:1130:GLU:O	1:B:1135:ARG:NH1	2.54	0.41
1:C:53:ALA:HB2	1:C:233:ILE:CD1	2.51	0.41
1:D:1130:GLU:O	1:D:1135:ARG:NH1	2.54	0.41
1:A:145:LEU:HD23	1:A:179:VAL:HG22	2.04	0.40
1:A:598:GLN:O	1:A:601:HIS:HB3	2.21	0.40
1:A:1041:TYR:O	1:A:1045:GLN:HB2	2.22	0.40
1:A:1130:GLU:O	1:A:1135:ARG:NH1	2.54	0.40
1:D:849:GLU:OE2	1:D:853:GLN:NE2	2.53	0.40
1:D:1307:ASN:OD1	1:D:1307:ASN:N	2.55	0.40
1:B:97:GLY:O	1:B:109:PRO:HA	2.21	0.40
1:C:1020:VAL:O	1:C:1024:GLY:N	2.54	0.40
1:D:213:ILE:HD12	1:D:275:ARG:HG3	2.02	0.40
1:A:1266:ASP:O	1:A:1317:ARG:NH1	2.54	0.40
1:A:1307:ASN:OD1	1:A:1307:ASN:N	2.55	0.40
1:B:145:LEU:HD23	1:B:179:VAL:HG22	2.04	0.40
1:B:1333:VAL:HG22	1:B:1442:PHE:HB2	2.02	0.40
1:C:1469:VAL:HG23	1:C:1483:LEU:HD13	2.03	0.40
1:D:1154:LEU:HD12	1:D:1154:LEU:HA	1.87	0.40
1:D:1469:VAL:HG23	1:D:1483:LEU:HD13	2.03	0.40
1:D:1266:ASP:O	1:D:1317:ARG:NH1	2.54	0.40
1:D:1334:THR:HB	1:D:1353:LEU:HD22	2.04	0.40
4:D:6001:CLR:H211	4:D:6001:CLR:H232	1.67	0.40
1:A:97:GLY:O	1:A:109:PRO:HA	2.21	0.40
1:B:927:LYS:HD3	1:B:927:LYS:HA	1.91	0.40
1:B:1020:VAL:O	1:B:1024:GLY:N	2.54	0.40
1:C:750:LEU:CD2	1:C:791:LEU:HD22	2.47	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	1356/1494 (91%)	1296 (96%)	60 (4%)	0	100	100
1	B	1356/1494 (91%)	1297 (96%)	59 (4%)	0	100	100
1	C	1356/1494 (91%)	1296 (96%)	60 (4%)	0	100	100
1	D	1356/1494 (91%)	1297 (96%)	59 (4%)	0	100	100
All	All	5424/5976 (91%)	5186 (96%)	238 (4%)	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	830/1275 (65%)	827 (100%)	3 (0%)	89	91
1	B	830/1275 (65%)	827 (100%)	3 (0%)	89	91
1	C	830/1275 (65%)	827 (100%)	3 (0%)	89	91
1	D	830/1275 (65%)	827 (100%)	3 (0%)	89	91
All	All	3320/5100 (65%)	3308 (100%)	12 (0%)	88	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	844	VAL
1	A	910	LEU
1	A	949	LEU
1	B	844	VAL
1	B	910	LEU
1	B	949	LEU
1	C	844	VAL
1	C	910	LEU
1	C	949	LEU
1	D	844	VAL
1	D	910	LEU
1	D	949	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	253	ASN
1	A	255	ASN
1	A	280	ASN
1	A	337	ASN
1	A	417	GLN
1	A	440	HIS
1	A	530	HIS
1	A	562	GLN
1	A	598	GLN
1	A	677	HIS
1	A	696	ASN
1	A	715	HIS
1	A	892	ASN
1	A	992	ASN
1	A	1078	HIS
1	A	1485	HIS
1	B	205	HIS
1	B	253	ASN
1	B	255	ASN
1	B	280	ASN
1	B	337	ASN
1	B	359	ASN
1	B	417	GLN
1	B	440	HIS
1	B	530	HIS
1	B	562	GLN
1	B	598	GLN
1	B	647	GLN
1	B	677	HIS
1	B	696	ASN
1	B	715	HIS
1	B	892	ASN
1	B	992	ASN
1	B	1078	HIS
1	B	1485	HIS
1	C	205	HIS
1	C	253	ASN
1	C	255	ASN
1	C	280	ASN
1	C	307	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	337	ASN
1	C	359	ASN
1	C	417	GLN
1	C	440	HIS
1	C	530	HIS
1	C	562	GLN
1	C	598	GLN
1	C	677	HIS
1	C	696	ASN
1	C	715	HIS
1	C	892	ASN
1	C	992	ASN
1	C	1031	ASN
1	C	1078	HIS
1	C	1485	HIS
1	D	205	HIS
1	D	253	ASN
1	D	255	ASN
1	D	280	ASN
1	D	307	GLN
1	D	337	ASN
1	D	359	ASN
1	D	417	GLN
1	D	440	HIS
1	D	530	HIS
1	D	562	GLN
1	D	598	GLN
1	D	677	HIS
1	D	696	ASN
1	D	715	HIS
1	D	892	ASN
1	D	992	ASN
1	D	1078	HIS
1	D	1485	HIS

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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	$\# Z  > 2$
4	CLR	B	1709	-	31,31,31	0.31	0	48,48,48	0.44	0
4	CLR	D	6001	-	31,31,31	0.30	0	48,48,48	0.43	0
4	CLR	B	1708	-	31,31,31	0.29	0	48,48,48	0.43	0
4	CLR	D	6002	-	31,31,31	0.29	0	48,48,48	0.43	0
2	APR	D	6004	-	35,39,39	0.74	0	42,60,60	1.30	4 (9%)
4	CLR	A	1707	-	31,31,31	0.30	0	48,48,48	0.43	0
2	APR	C	1706	3	35,39,39	0.80	0	42,60,60	1.21	5 (11%)
2	APR	C	1701	-	35,39,39	0.74	0	42,60,60	1.30	4 (9%)
4	CLR	C	1708	-	31,31,31	0.29	0	48,48,48	0.43	0
2	APR	A	1701	-	35,39,39	0.74	0	42,60,60	1.30	4 (9%)
2	APR	D	6009	3	35,39,39	0.80	0	42,60,60	1.21	5 (11%)
4	CLR	B	1707	-	31,31,31	0.30	0	48,48,48	0.43	0
4	CLR	D	6003	-	31,31,31	0.31	0	48,48,48	0.44	0
2	APR	B	1706	3	35,39,39	0.80	0	42,60,60	1.21	5 (11%)
2	APR	A	1706	3	35,39,39	0.80	0	42,60,60	1.21	5 (11%)
4	CLR	C	1707	-	31,31,31	0.30	0	48,48,48	0.43	0
2	APR	B	1701	-	35,39,39	0.74	0	42,60,60	1.30	4 (9%)
4	CLR	A	1709	-	31,31,31	0.31	0	48,48,48	0.44	0
4	CLR	A	1708	-	31,31,31	0.29	0	48,48,48	0.43	0
4	CLR	C	1709	-	31,31,31	0.31	0	48,48,48	0.44	0

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
4	CLR	B	1709	-	-	9/10/68/68	0/4/4/4
4	CLR	D	6001	-	-	9/10/68/68	0/4/4/4
4	CLR	B	1708	-	-	8/10/68/68	0/4/4/4
4	CLR	D	6002	-	-	8/10/68/68	0/4/4/4
2	APR	D	6004	-	-	10/18/54/54	0/4/4/4
4	CLR	A	1707	-	-	9/10/68/68	0/4/4/4
2	APR	C	1706	3	-	6/18/54/54	0/4/4/4
2	APR	C	1701	-	-	10/18/54/54	0/4/4/4
4	CLR	C	1708	-	-	8/10/68/68	0/4/4/4
2	APR	A	1701	-	-	10/18/54/54	0/4/4/4
2	APR	D	6009	3	-	6/18/54/54	0/4/4/4
4	CLR	B	1707	-	-	9/10/68/68	0/4/4/4
4	CLR	D	6003	-	-	9/10/68/68	0/4/4/4
2	APR	B	1706	3	-	6/18/54/54	0/4/4/4
2	APR	A	1706	3	-	6/18/54/54	0/4/4/4
4	CLR	C	1707	-	-	9/10/68/68	0/4/4/4
2	APR	B	1701	-	-	10/18/54/54	0/4/4/4
4	CLR	A	1709	-	-	9/10/68/68	0/4/4/4
4	CLR	A	1708	-	-	8/10/68/68	0/4/4/4
4	CLR	C	1709	-	-	9/10/68/68	0/4/4/4

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	APR	N3-C2-N1	-3.70	123.65	128.67
2	B	1701	APR	N3-C2-N1	-3.70	123.65	128.67
2	C	1701	APR	N3-C2-N1	-3.70	123.65	128.67
2	D	6004	APR	N3-C2-N1	-3.70	123.65	128.67
2	A	1706	APR	N3-C2-N1	-3.62	123.75	128.67
2	B	1706	APR	N3-C2-N1	-3.62	123.75	128.67
2	C	1706	APR	N3-C2-N1	-3.62	123.75	128.67
2	D	6009	APR	N3-C2-N1	-3.62	123.75	128.67
2	B	1701	APR	C1D-C2D-C3D	3.19	106.21	102.29
2	A	1701	APR	C1D-C2D-C3D	3.17	106.18	102.29
2	C	1701	APR	C1D-C2D-C3D	3.17	106.18	102.29
2	D	6004	APR	C1D-C2D-C3D	3.17	106.18	102.29
2	A	1706	APR	C1D-C2D-C3D	3.04	106.03	102.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1706	APR	C1D-C2D-C3D	3.04	106.03	102.29
2	C	1706	APR	C1D-C2D-C3D	3.04	106.03	102.29
2	D	6009	APR	C1D-C2D-C3D	3.02	106.00	102.29
2	A	1701	APR	C4-C5-N7	-2.32	106.88	109.34
2	B	1701	APR	C4-C5-N7	-2.32	106.88	109.34
2	C	1701	APR	C4-C5-N7	-2.32	106.88	109.34
2	D	6004	APR	C4-C5-N7	-2.32	106.88	109.34
2	A	1701	APR	O4D-C1D-C2D	2.26	107.80	104.67
2	C	1701	APR	O4D-C1D-C2D	2.26	107.80	104.67
2	D	6004	APR	O4D-C1D-C2D	2.26	107.80	104.67
2	B	1701	APR	O4D-C1D-C2D	2.24	107.78	104.67
2	D	6009	APR	O4D-C1D-C2D	2.23	107.77	104.67
2	A	1706	APR	O4D-C1D-C2D	2.21	107.74	104.67
2	B	1706	APR	O4D-C1D-C2D	2.21	107.74	104.67
2	C	1706	APR	O4D-C1D-C2D	2.21	107.74	104.67
2	A	1706	APR	C2D-C3D-C4D	2.09	106.65	102.61
2	B	1706	APR	C2D-C3D-C4D	2.09	106.65	102.61
2	C	1706	APR	C2D-C3D-C4D	2.09	106.65	102.61
2	D	6009	APR	C2D-C3D-C4D	2.09	106.65	102.61
2	B	1706	APR	C4-C5-N7	-2.02	107.20	109.34
2	D	6009	APR	C4-C5-N7	-2.02	107.20	109.34
2	A	1706	APR	C4-C5-N7	-2.01	107.22	109.34
2	C	1706	APR	C4-C5-N7	-2.01	107.22	109.34

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1701	APR	C5'-O5'-PA-O1A
2	A	1701	APR	C5'-O5'-PA-O3A
2	A	1701	APR	C5D-O5D-PB-O3A
2	A	1701	APR	C5D-O5D-PB-O1B
2	A	1701	APR	C5D-O5D-PB-O2B
2	A	1706	APR	C3'-C4'-C5'-O5'
2	A	1706	APR	C3D-C4D-C5D-O5D
2	B	1701	APR	C5'-O5'-PA-O1A
2	B	1701	APR	C5'-O5'-PA-O3A
2	B	1701	APR	C5D-O5D-PB-O3A
2	B	1701	APR	C5D-O5D-PB-O1B
2	B	1701	APR	C5D-O5D-PB-O2B
2	B	1706	APR	C3'-C4'-C5'-O5'
2	B	1706	APR	C3D-C4D-C5D-O5D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1701	APR	C5'-O5'-PA-O1A
2	C	1701	APR	C5'-O5'-PA-O3A
2	C	1701	APR	C5D-O5D-PB-O3A
2	C	1701	APR	C5D-O5D-PB-O1B
2	C	1701	APR	C5D-O5D-PB-O2B
2	C	1706	APR	C3'-C4'-C5'-O5'
2	C	1706	APR	C3D-C4D-C5D-O5D
2	D	6004	APR	C5'-O5'-PA-O1A
2	D	6004	APR	C5'-O5'-PA-O3A
2	D	6004	APR	C5D-O5D-PB-O3A
2	D	6004	APR	C5D-O5D-PB-O1B
2	D	6004	APR	C5D-O5D-PB-O2B
2	D	6009	APR	C3'-C4'-C5'-O5'
2	D	6009	APR	C3D-C4D-C5D-O5D
4	A	1707	CLR	C13-C17-C20-C21
4	A	1709	CLR	C13-C17-C20-C21
4	A	1709	CLR	C16-C17-C20-C22
4	B	1707	CLR	C13-C17-C20-C21
4	B	1709	CLR	C13-C17-C20-C21
4	B	1709	CLR	C16-C17-C20-C22
4	C	1707	CLR	C13-C17-C20-C21
4	C	1709	CLR	C13-C17-C20-C21
4	C	1709	CLR	C16-C17-C20-C22
4	D	6001	CLR	C13-C17-C20-C21
4	D	6003	CLR	C13-C17-C20-C21
4	D	6003	CLR	C16-C17-C20-C22
4	A	1709	CLR	C16-C17-C20-C21
4	B	1709	CLR	C16-C17-C20-C21
4	C	1709	CLR	C16-C17-C20-C21
4	D	6003	CLR	C16-C17-C20-C21
4	A	1709	CLR	C13-C17-C20-C22
4	B	1709	CLR	C13-C17-C20-C22
4	C	1709	CLR	C13-C17-C20-C22
4	D	6003	CLR	C13-C17-C20-C22
4	A	1707	CLR	C16-C17-C20-C21
4	B	1707	CLR	C16-C17-C20-C21
4	C	1707	CLR	C16-C17-C20-C21
4	D	6001	CLR	C16-C17-C20-C21
4	A	1707	CLR	C16-C17-C20-C22
4	B	1707	CLR	C16-C17-C20-C22
4	C	1707	CLR	C16-C17-C20-C22
4	D	6001	CLR	C16-C17-C20-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	1707	CLR	C13-C17-C20-C22
4	A	1708	CLR	C13-C17-C20-C22
4	B	1707	CLR	C13-C17-C20-C22
4	B	1708	CLR	C13-C17-C20-C22
4	C	1707	CLR	C13-C17-C20-C22
4	C	1708	CLR	C13-C17-C20-C22
4	D	6001	CLR	C13-C17-C20-C22
4	D	6002	CLR	C13-C17-C20-C22
4	A	1709	CLR	C21-C20-C22-C23
4	B	1709	CLR	C21-C20-C22-C23
4	C	1709	CLR	C21-C20-C22-C23
4	D	6003	CLR	C21-C20-C22-C23
4	A	1708	CLR	C13-C17-C20-C21
4	B	1708	CLR	C13-C17-C20-C21
4	C	1708	CLR	C13-C17-C20-C21
4	D	6002	CLR	C13-C17-C20-C21
2	A	1701	APR	C3D-C4D-C5D-O5D
2	B	1701	APR	C3D-C4D-C5D-O5D
2	C	1701	APR	C3D-C4D-C5D-O5D
2	D	6004	APR	C3D-C4D-C5D-O5D
4	A	1707	CLR	C21-C20-C22-C23
4	B	1707	CLR	C21-C20-C22-C23
4	C	1707	CLR	C21-C20-C22-C23
4	D	6001	CLR	C21-C20-C22-C23
4	A	1708	CLR	C16-C17-C20-C21
4	B	1708	CLR	C16-C17-C20-C21
4	C	1708	CLR	C16-C17-C20-C21
4	D	6002	CLR	C16-C17-C20-C21
2	A	1701	APR	C3'-C4'-C5'-O5'
2	A	1706	APR	O4'-C4'-C5'-O5'
2	A	1706	APR	O4D-C4D-C5D-O5D
2	B	1701	APR	C3'-C4'-C5'-O5'
2	B	1706	APR	O4'-C4'-C5'-O5'
2	B	1706	APR	O4D-C4D-C5D-O5D
2	C	1701	APR	C3'-C4'-C5'-O5'
2	C	1706	APR	O4'-C4'-C5'-O5'
2	C	1706	APR	O4D-C4D-C5D-O5D
2	D	6004	APR	C3'-C4'-C5'-O5'
2	D	6009	APR	O4'-C4'-C5'-O5'
2	D	6009	APR	O4D-C4D-C5D-O5D
4	A	1707	CLR	C20-C22-C23-C24
4	B	1707	CLR	C20-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	C	1707	CLR	C20-C22-C23-C24
4	D	6001	CLR	C20-C22-C23-C24
4	A	1707	CLR	C22-C23-C24-C25
4	B	1707	CLR	C22-C23-C24-C25
4	C	1707	CLR	C22-C23-C24-C25
4	D	6001	CLR	C22-C23-C24-C25
4	A	1709	CLR	C17-C20-C22-C23
4	B	1709	CLR	C17-C20-C22-C23
4	C	1709	CLR	C17-C20-C22-C23
4	D	6003	CLR	C17-C20-C22-C23
4	A	1709	CLR	C22-C23-C24-C25
4	B	1709	CLR	C22-C23-C24-C25
4	C	1709	CLR	C22-C23-C24-C25
4	D	6003	CLR	C22-C23-C24-C25
4	A	1708	CLR	C23-C24-C25-C26
4	B	1708	CLR	C23-C24-C25-C26
4	C	1708	CLR	C23-C24-C25-C26
4	D	6002	CLR	C23-C24-C25-C26
4	A	1707	CLR	C23-C24-C25-C26
4	B	1707	CLR	C23-C24-C25-C26
4	C	1707	CLR	C23-C24-C25-C26
4	D	6001	CLR	C23-C24-C25-C26
4	A	1708	CLR	C16-C17-C20-C22
4	B	1708	CLR	C16-C17-C20-C22
4	C	1708	CLR	C16-C17-C20-C22
4	D	6002	CLR	C16-C17-C20-C22
2	A	1701	APR	O4'-C4'-C5'-O5'
2	B	1701	APR	O4'-C4'-C5'-O5'
2	C	1701	APR	O4'-C4'-C5'-O5'
2	D	6004	APR	O4'-C4'-C5'-O5'
2	A	1701	APR	O4D-C4D-C5D-O5D
2	B	1701	APR	O4D-C4D-C5D-O5D
2	C	1701	APR	O4D-C4D-C5D-O5D
2	D	6004	APR	O4D-C4D-C5D-O5D
4	A	1709	CLR	C20-C22-C23-C24
4	B	1709	CLR	C20-C22-C23-C24
4	C	1709	CLR	C20-C22-C23-C24
4	D	6003	CLR	C20-C22-C23-C24
4	A	1708	CLR	C22-C23-C24-C25
4	B	1708	CLR	C22-C23-C24-C25
4	C	1708	CLR	C22-C23-C24-C25
4	D	6002	CLR	C22-C23-C24-C25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	1707	CLR	C23-C24-C25-C27
4	B	1707	CLR	C23-C24-C25-C27
4	C	1707	CLR	C23-C24-C25-C27
4	D	6001	CLR	C23-C24-C25-C27
4	A	1708	CLR	C23-C24-C25-C27
4	B	1708	CLR	C23-C24-C25-C27
4	C	1708	CLR	C23-C24-C25-C27
4	D	6002	CLR	C23-C24-C25-C27
4	A	1709	CLR	C23-C24-C25-C27
4	B	1709	CLR	C23-C24-C25-C27
4	C	1709	CLR	C23-C24-C25-C27
4	D	6003	CLR	C23-C24-C25-C27
2	A	1701	APR	C5'-O5'-PA-O2A
2	B	1701	APR	C5'-O5'-PA-O2A
2	C	1701	APR	C5'-O5'-PA-O2A
2	D	6004	APR	C5'-O5'-PA-O2A
4	A	1708	CLR	C20-C22-C23-C24
4	B	1708	CLR	C20-C22-C23-C24
4	C	1708	CLR	C20-C22-C23-C24
4	D	6002	CLR	C20-C22-C23-C24
2	A	1706	APR	PA-O3A-PB-O2B
2	B	1706	APR	PA-O3A-PB-O2B
2	C	1706	APR	PA-O3A-PB-O2B
2	D	6009	APR	PA-O3A-PB-O2B
2	A	1706	APR	PA-O3A-PB-O1B
2	B	1706	APR	PA-O3A-PB-O1B
2	C	1706	APR	PA-O3A-PB-O1B
2	D	6009	APR	PA-O3A-PB-O1B

There are no ring outliers.

19 monomers are involved in 26 short contacts:

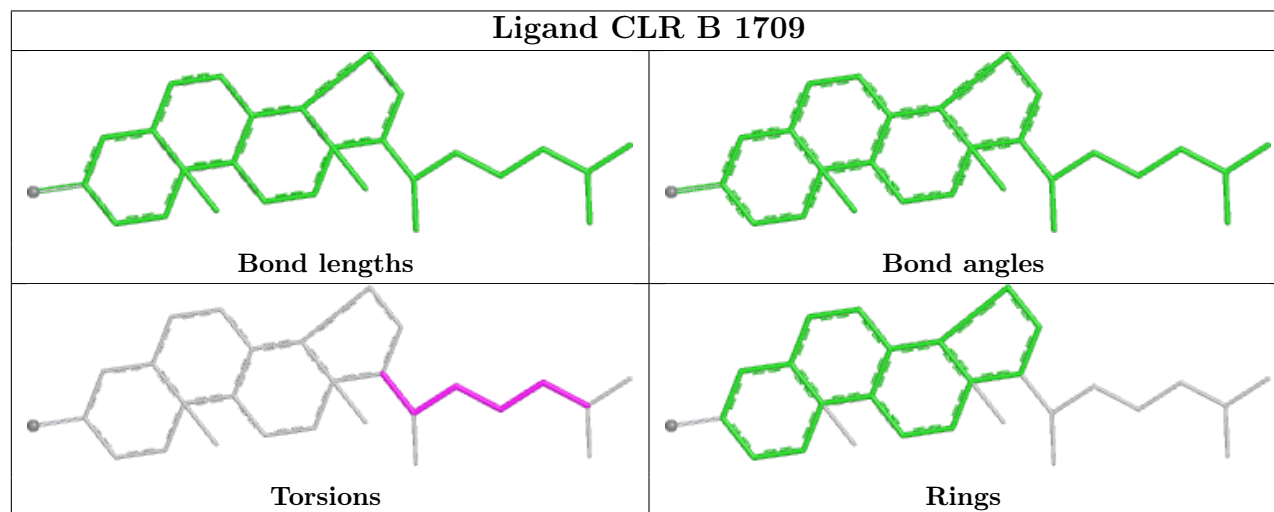
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1709	CLR	2	0
4	D	6001	CLR	2	0
4	B	1708	CLR	1	0
4	D	6002	CLR	2	0
2	D	6004	APR	1	0
4	A	1707	CLR	2	0
2	C	1706	APR	1	0
2	C	1701	APR	1	0
4	C	1708	CLR	2	0

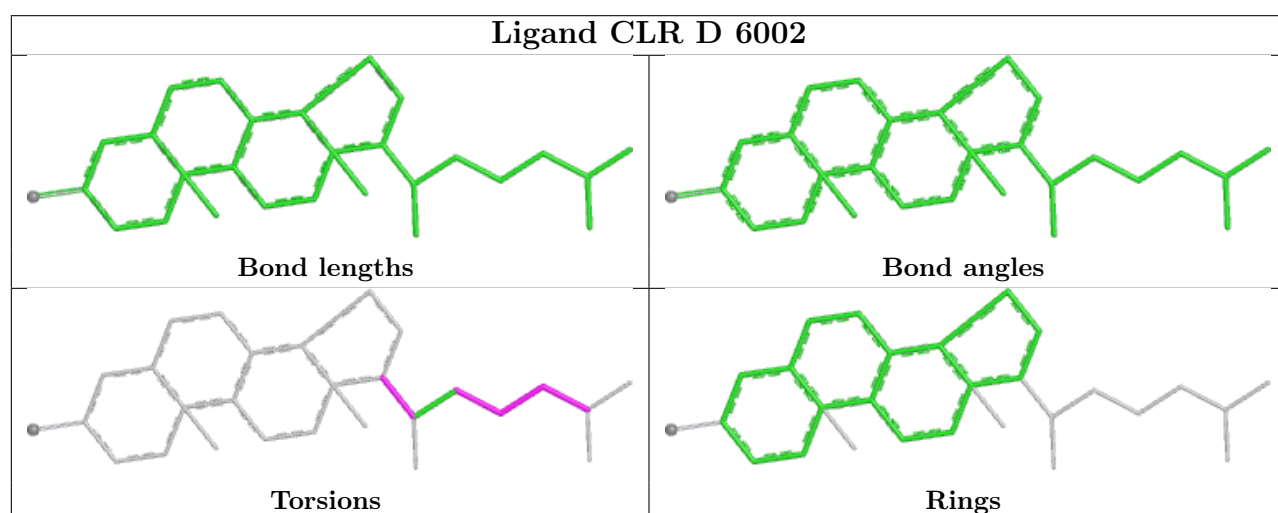
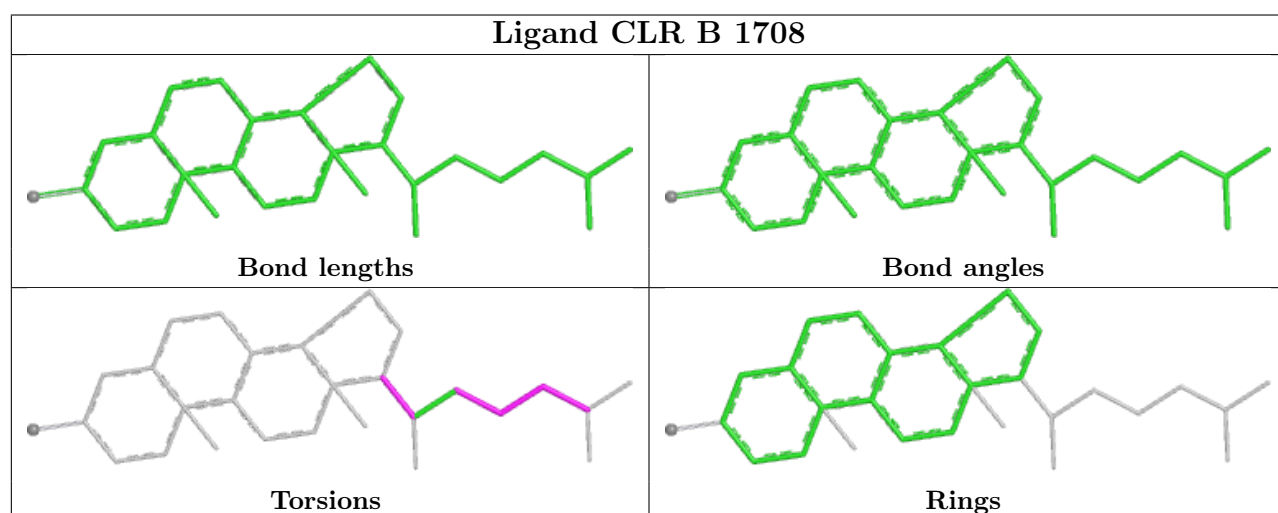
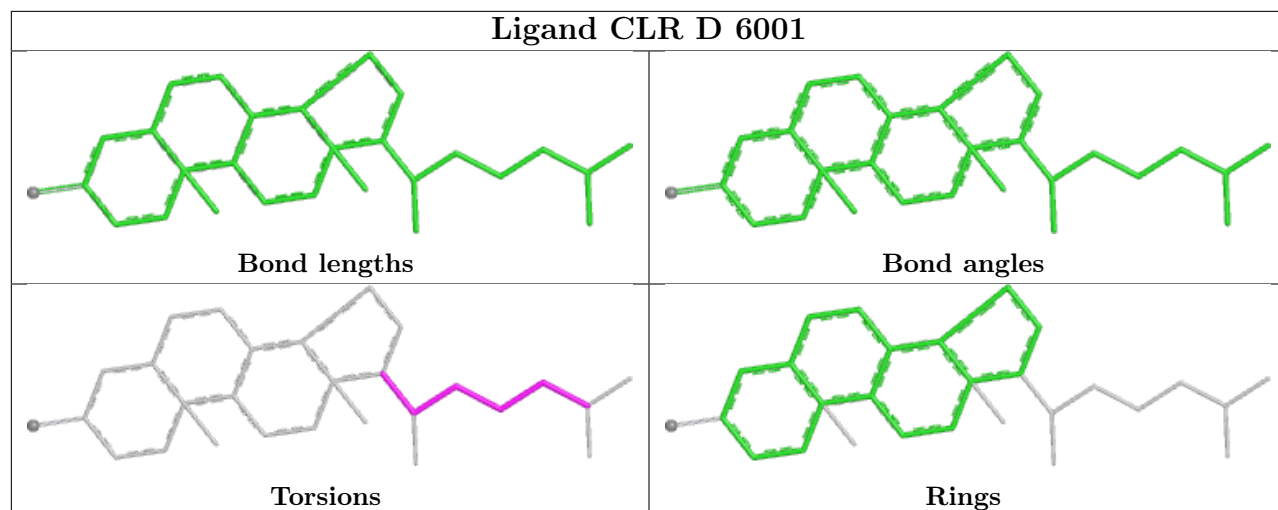
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1701	APR	1	0
2	D	6009	APR	1	0
4	B	1707	CLR	2	0
2	B	1706	APR	1	0
2	A	1706	APR	1	0
4	C	1707	CLR	1	0
2	B	1701	APR	1	0
4	A	1709	CLR	1	0
4	A	1708	CLR	2	0
4	C	1709	CLR	1	0

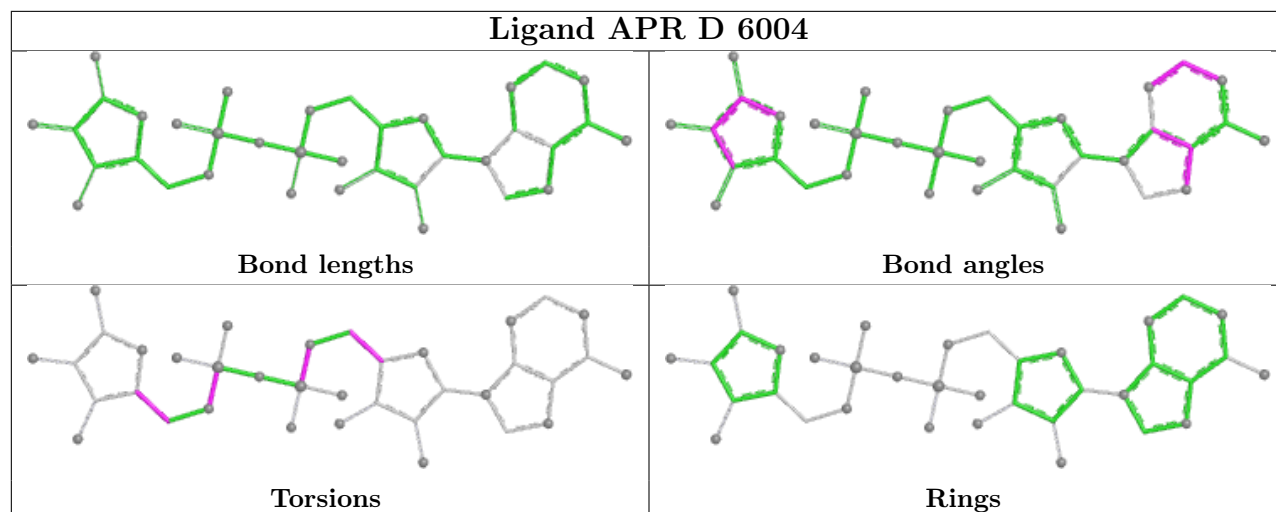
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



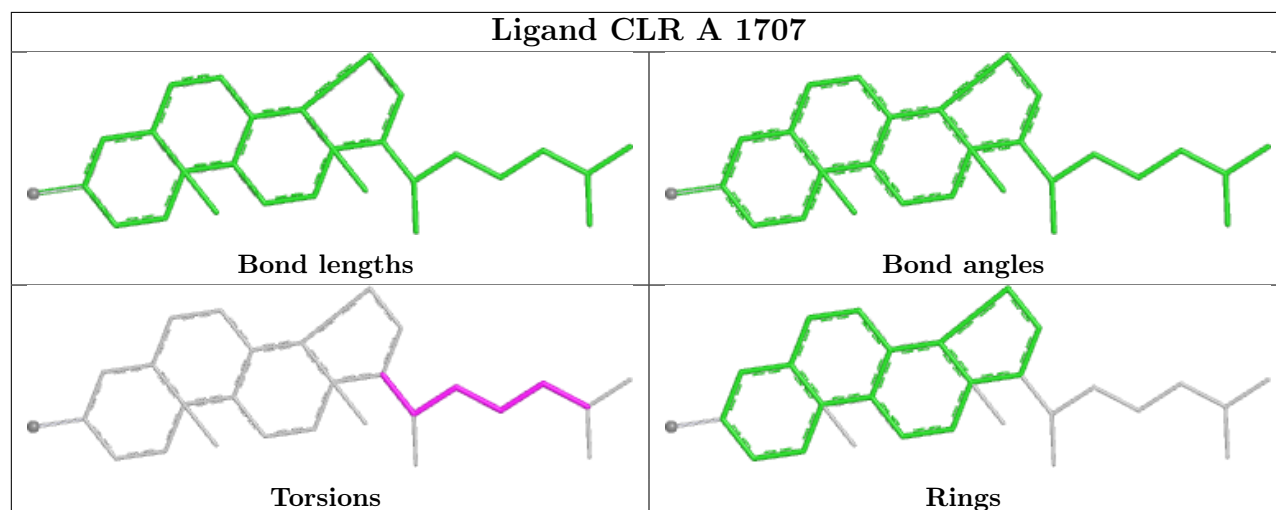




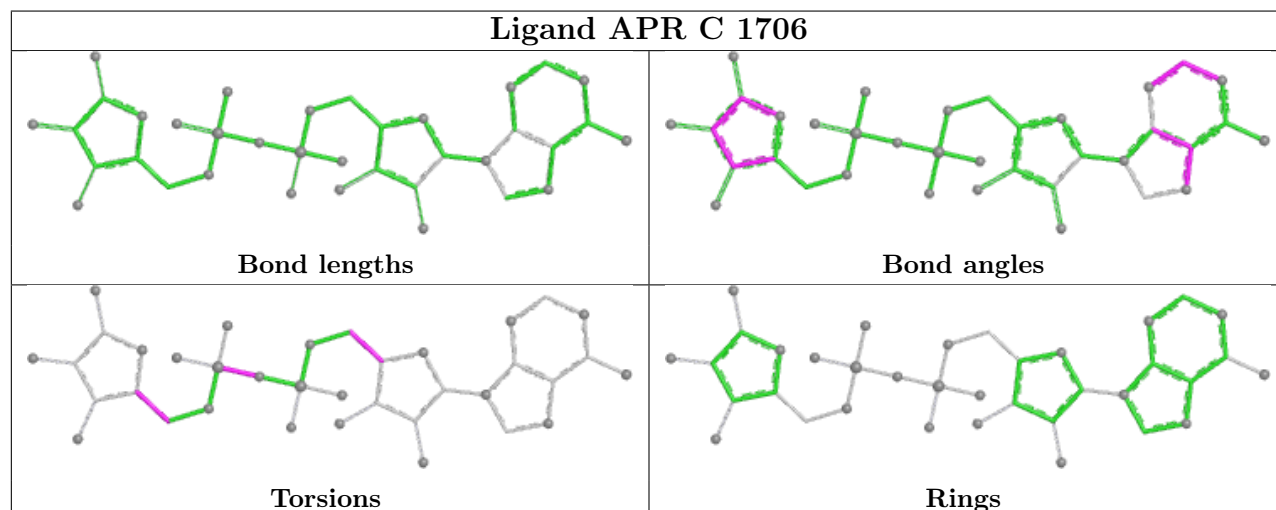
## Ligand APR D 6004



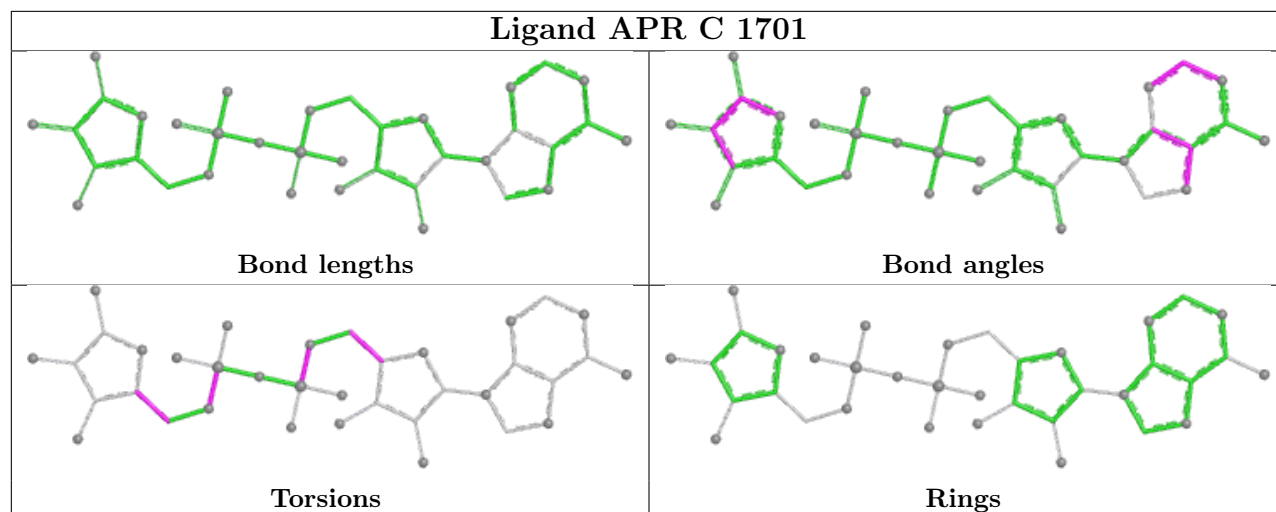
## Ligand CLR A 1707



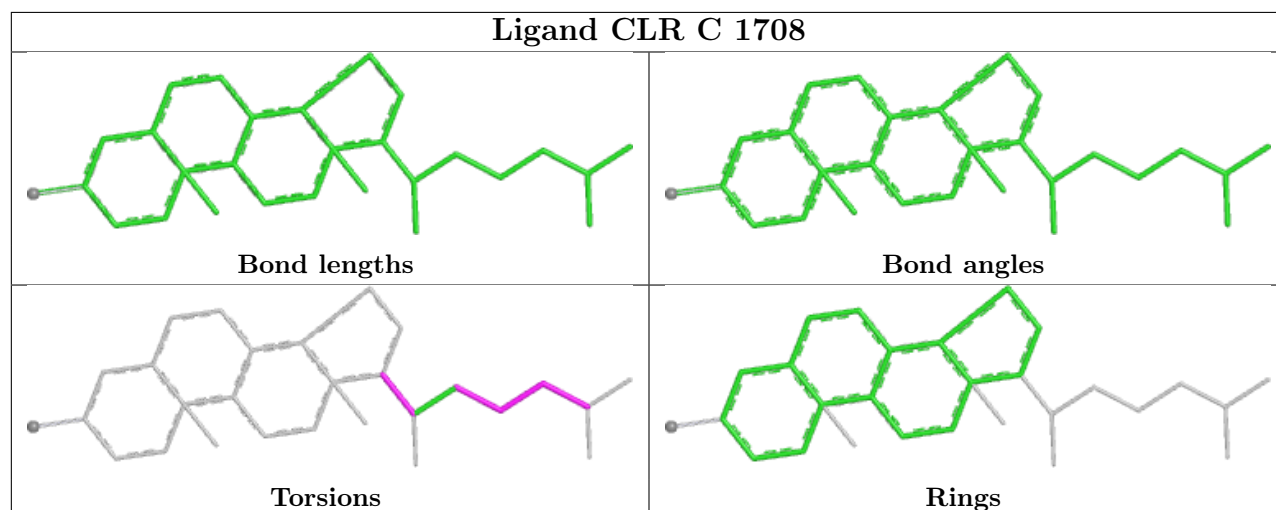
## Ligand APR C 1706



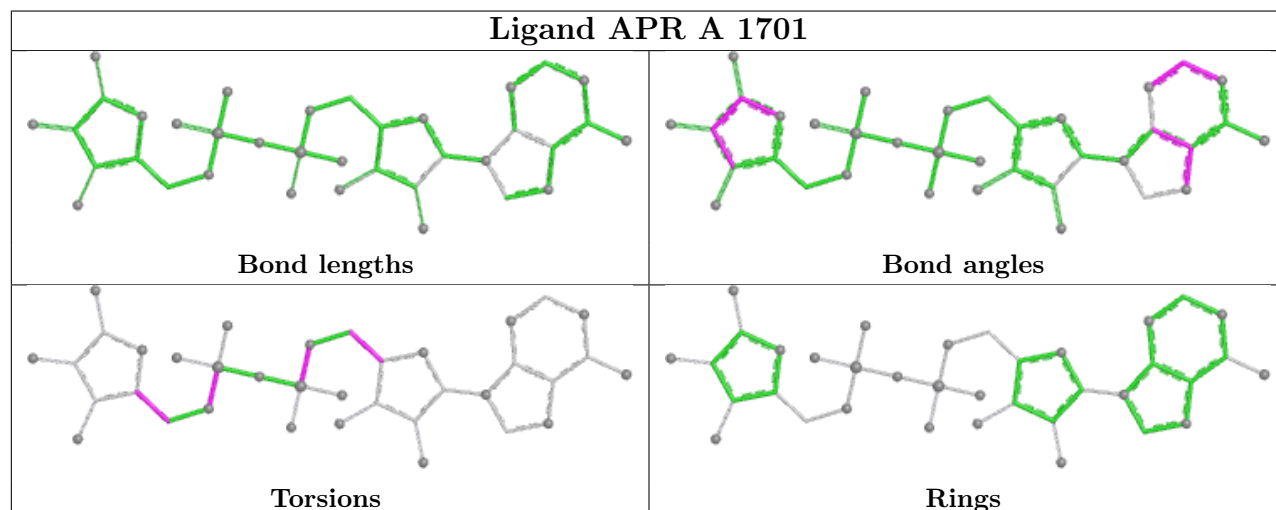
## Ligand APR C 1701



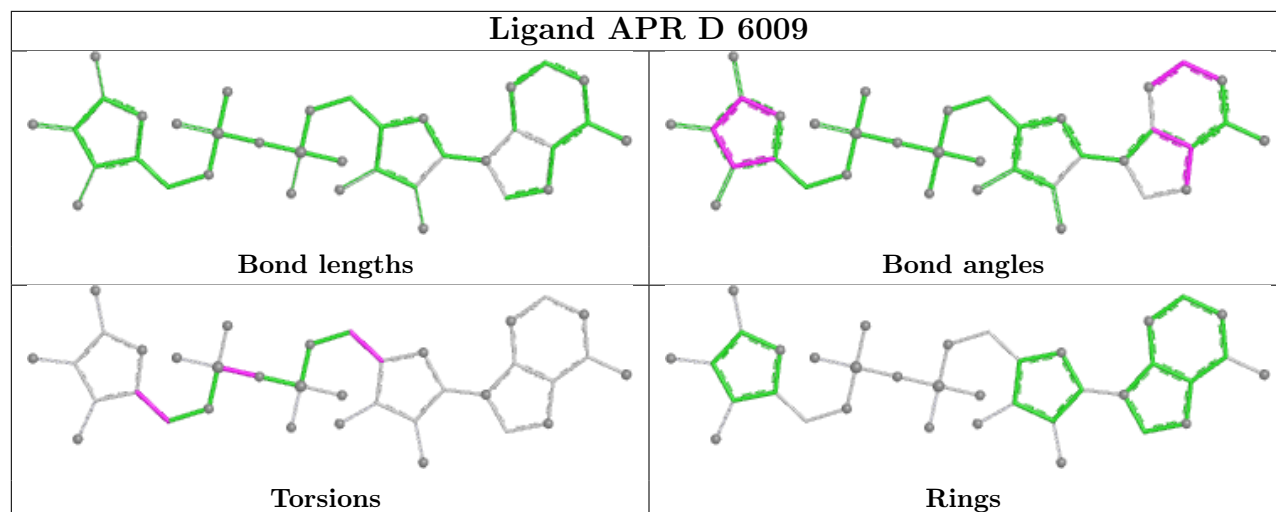
## Ligand CLR C 1708



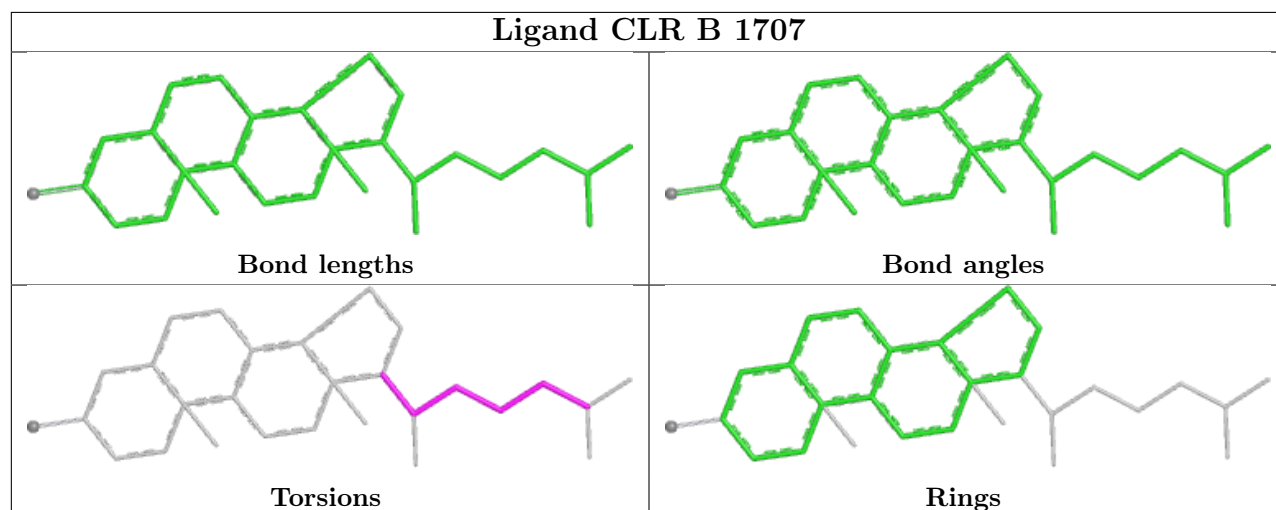
## Ligand APR A 1701



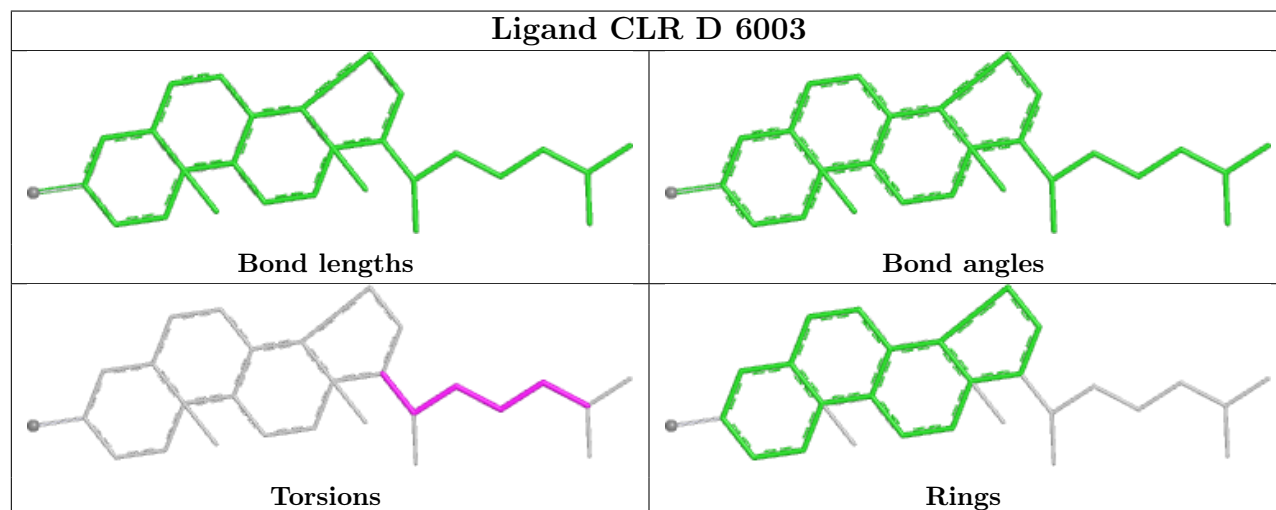
## Ligand APR D 6009



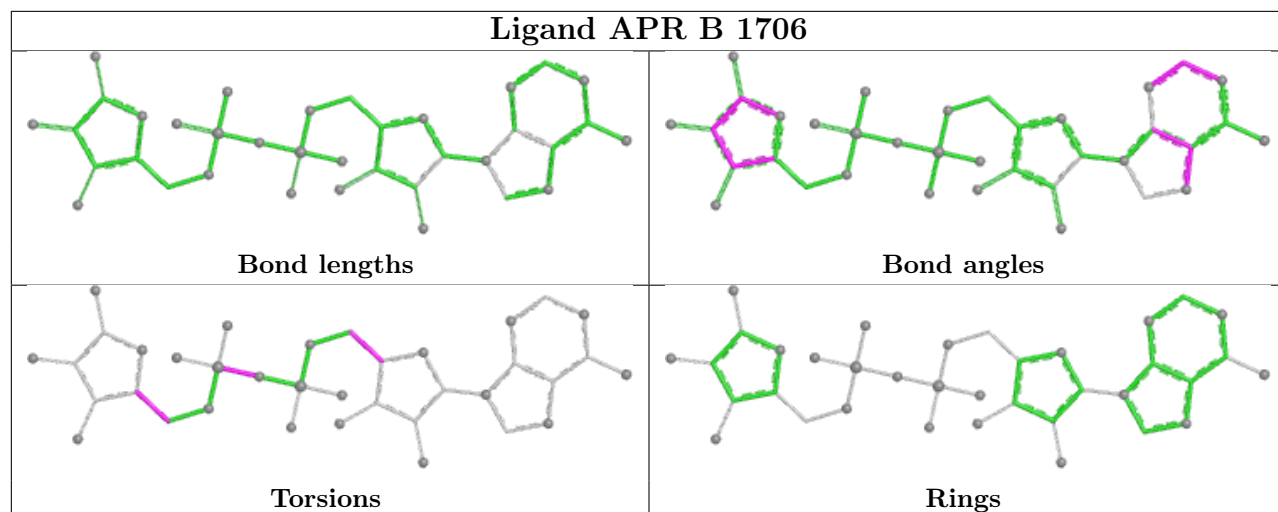
## Ligand CLR B 1707



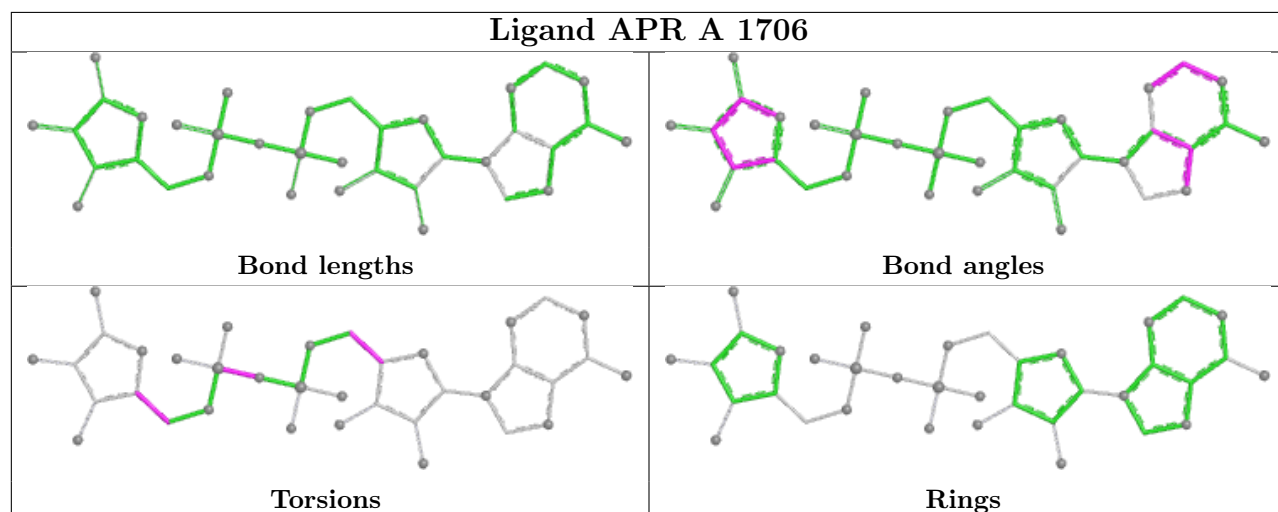
## Ligand CLR D 6003



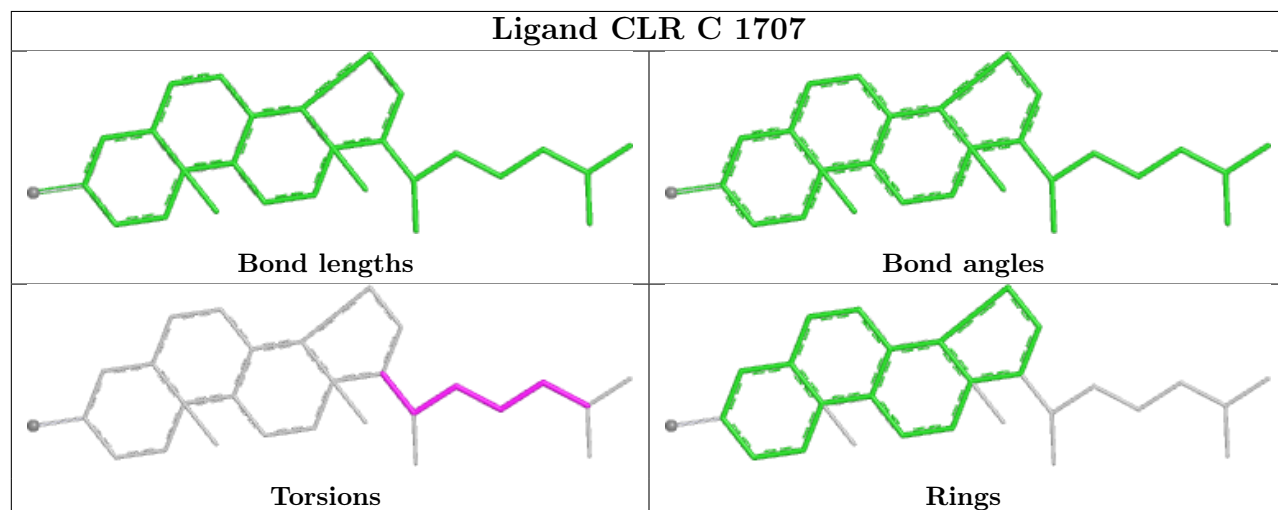
## Ligand APR B 1706



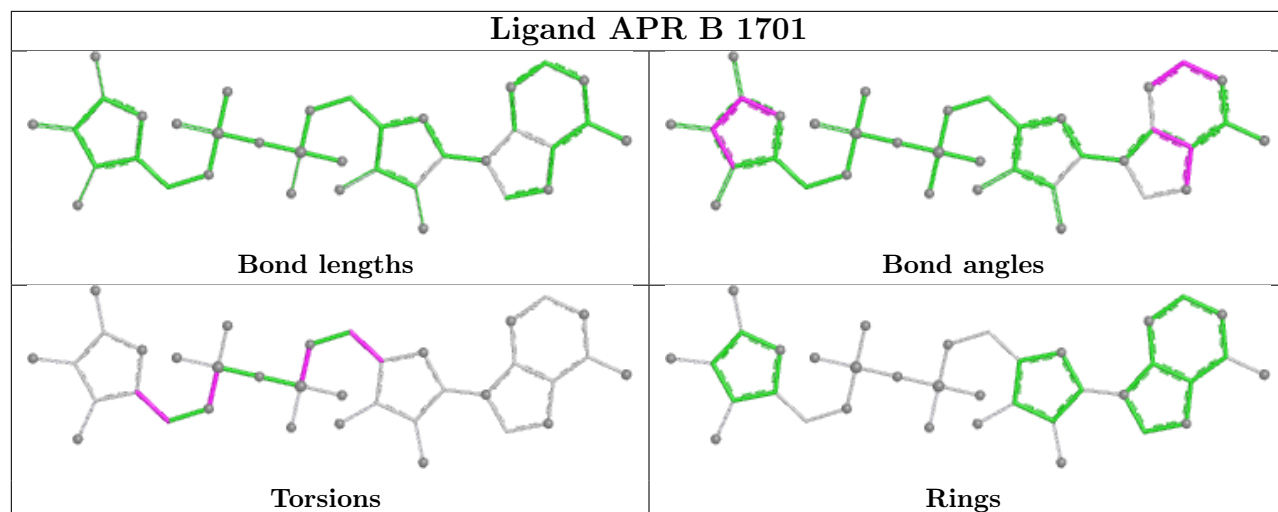
## Ligand APR A 1706



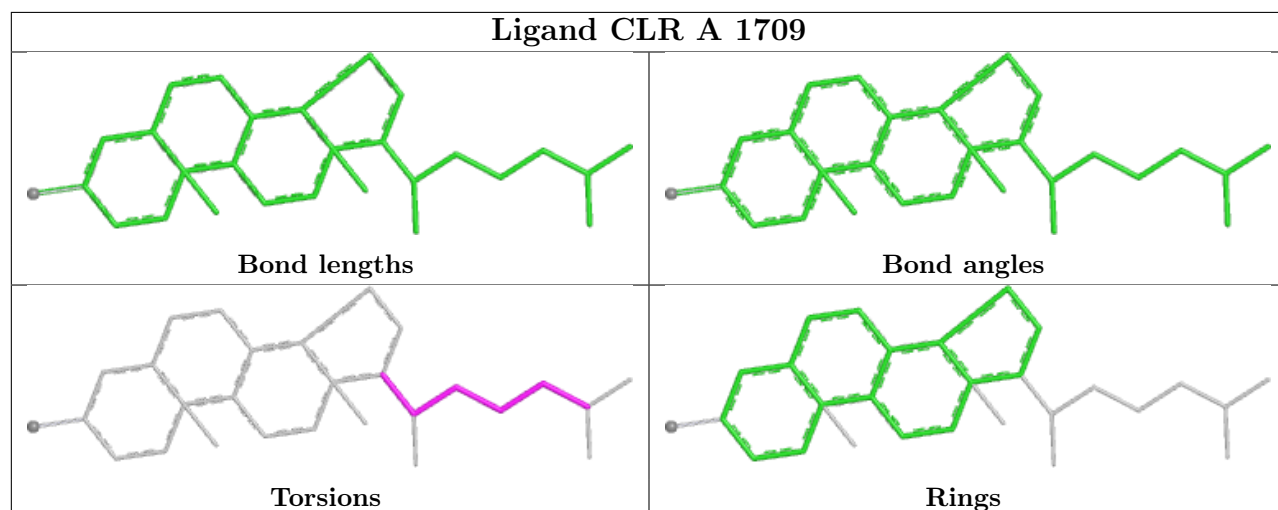
## Ligand CLR C 1707



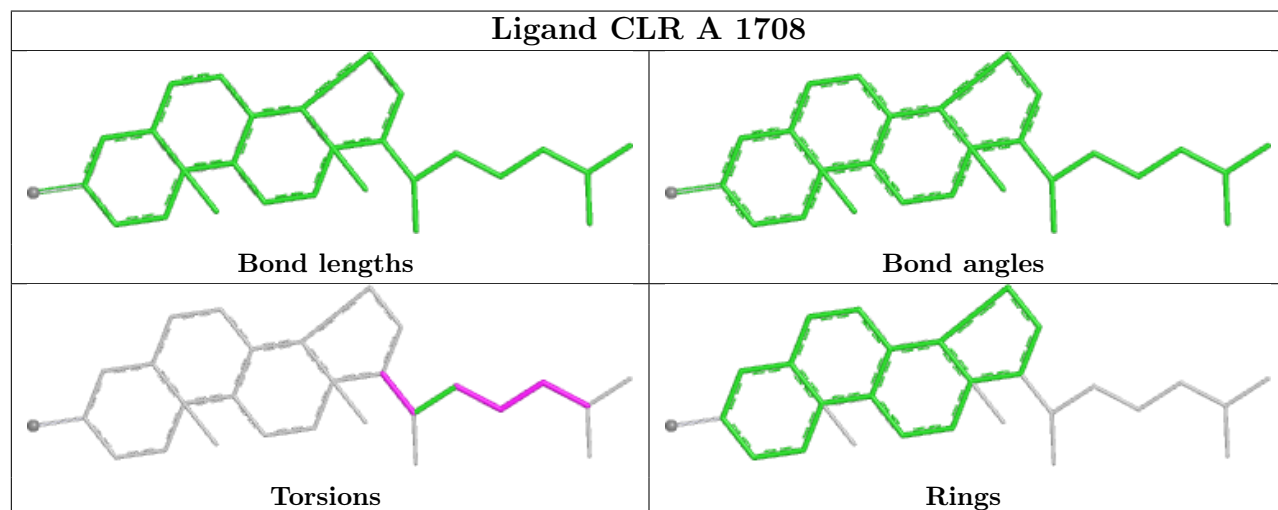
## Ligand APR B 1701

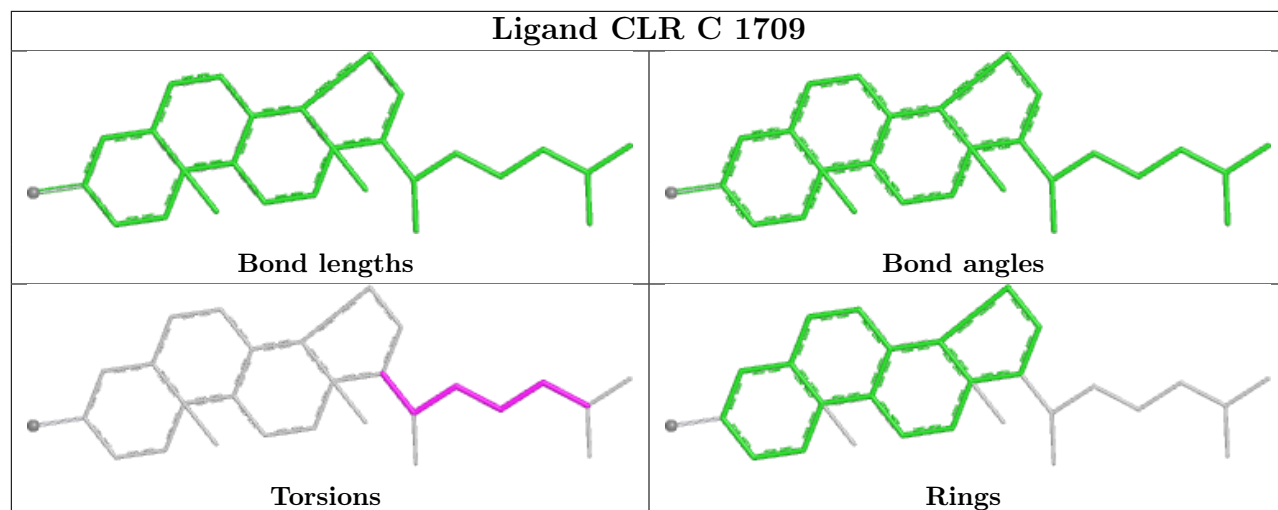


## Ligand CLR A 1709



## Ligand CLR A 1708





## 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.

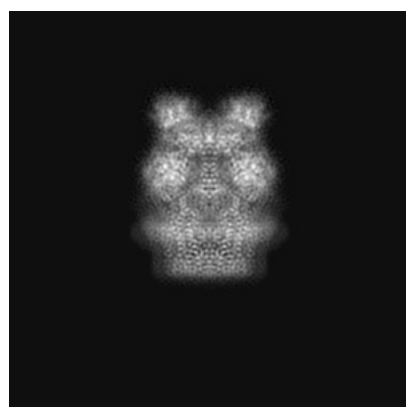
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40731. These allow visual inspection of the internal detail of the map and identification of artifacts.

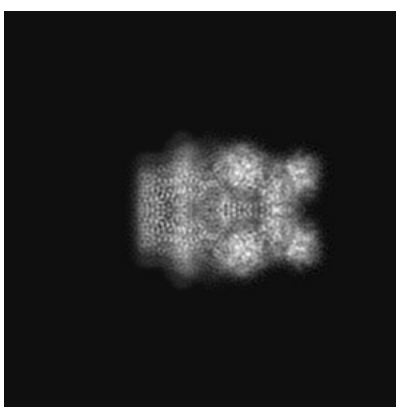
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

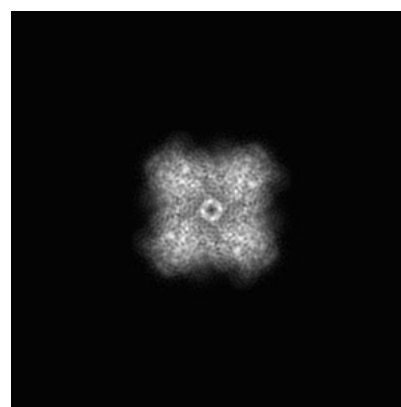
#### 6.1.1 Primary map



X



Y



Z

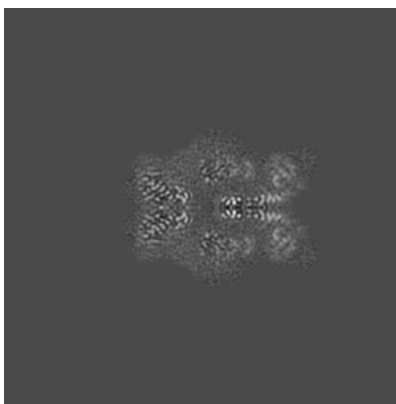
The images above show the map projected in three orthogonal directions.

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

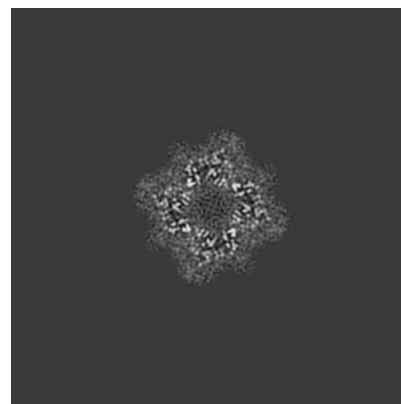
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

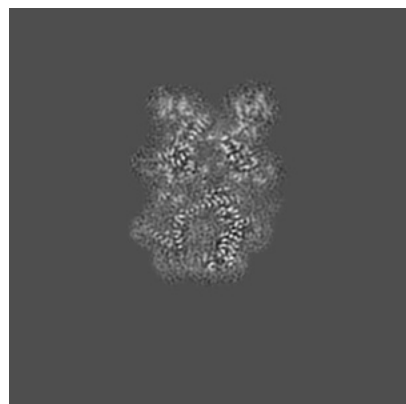


Z Index: 220

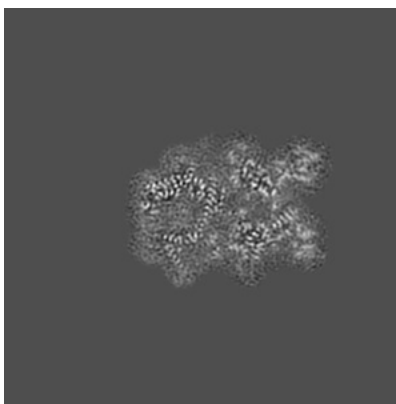
The images above show central slices of the map in three orthogonal directions.

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

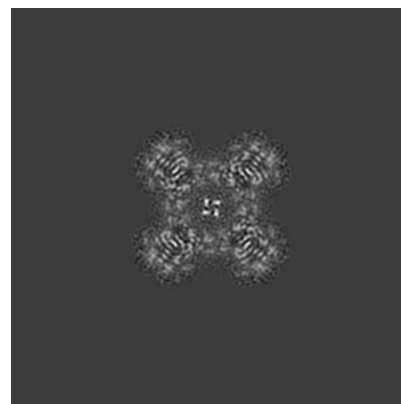
### 6.3.1 Primary map



X Index: 251



Y Index: 189

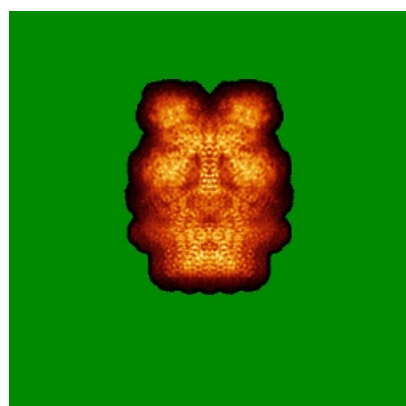


Z Index: 266

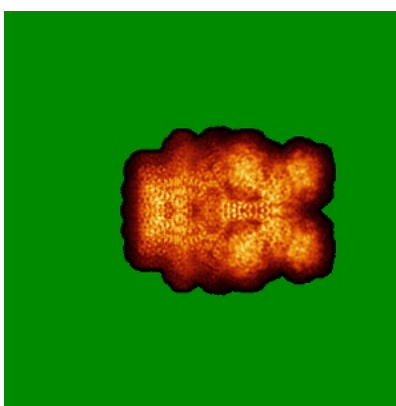
The images above show the largest variance slices of the map in three orthogonal directions.

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

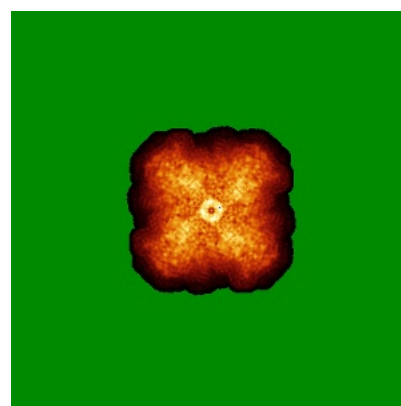
### 6.4.1 Primary map



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.

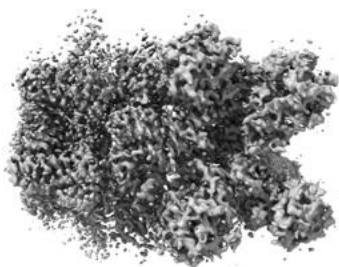


## 6.5 Orthogonal surface views [i](#)

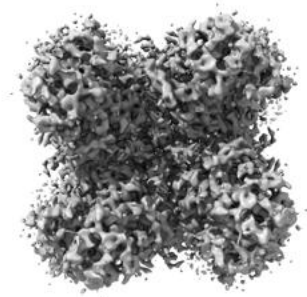
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

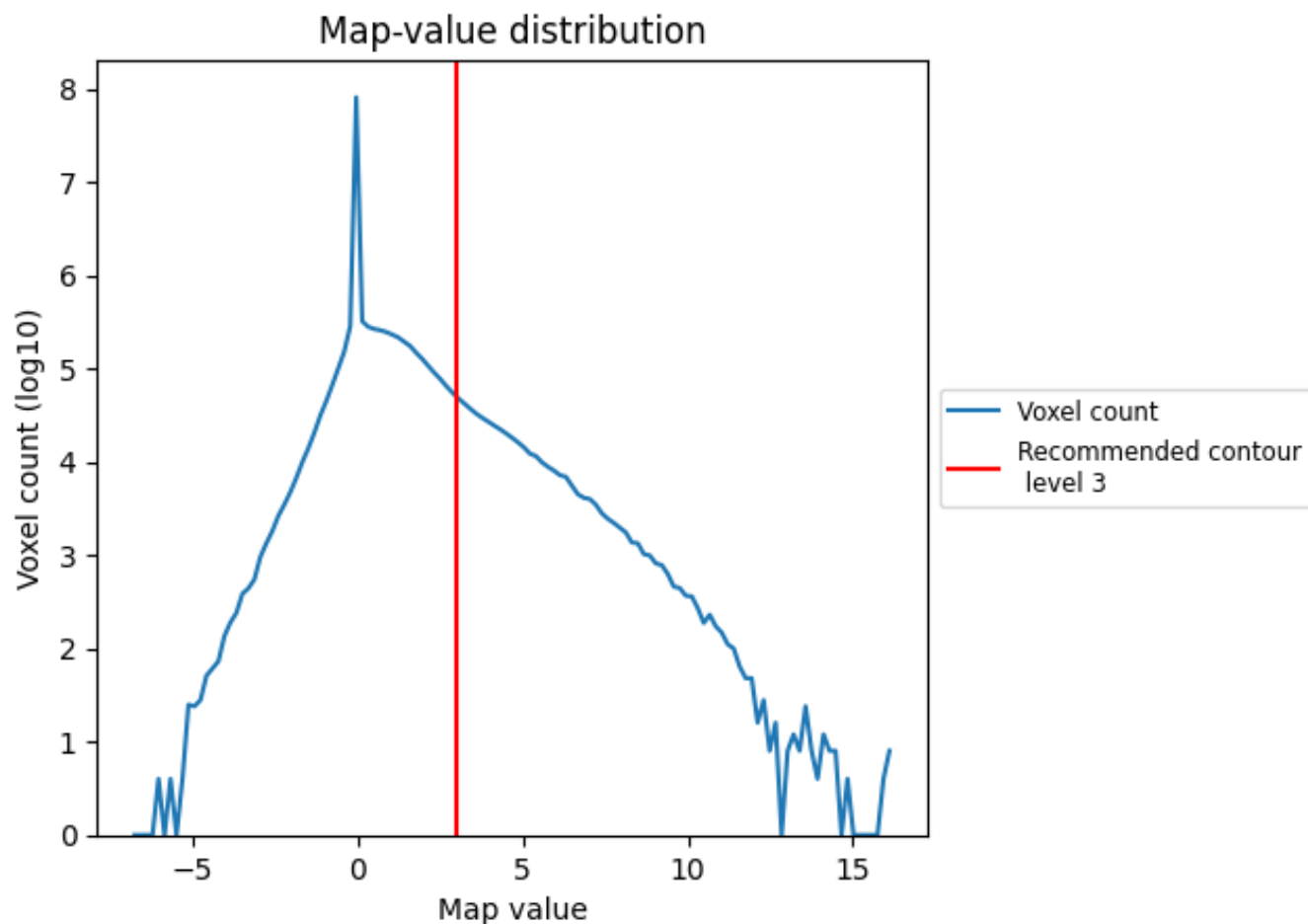
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

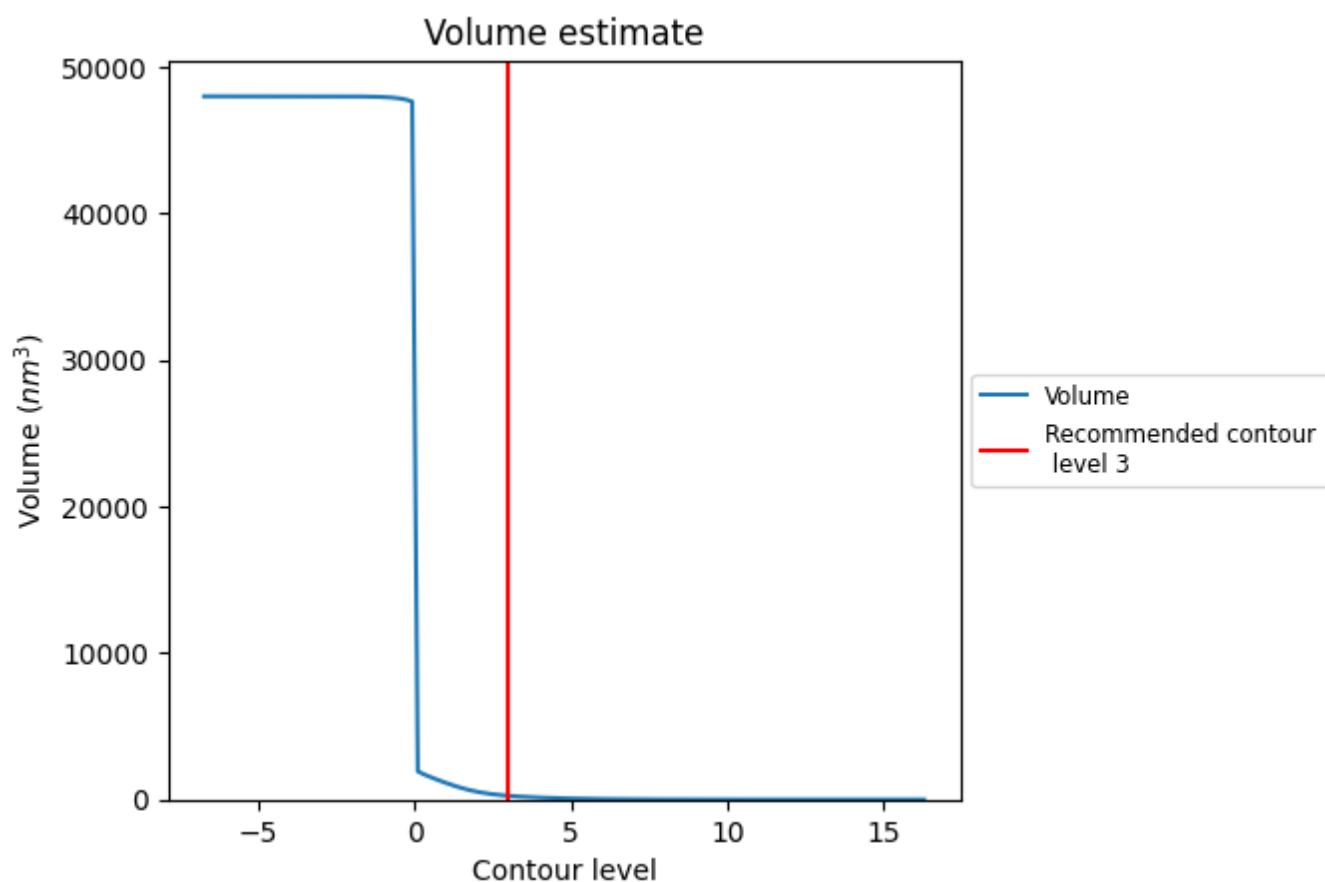
This section contains the results of statistical analysis of the map.

### 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.

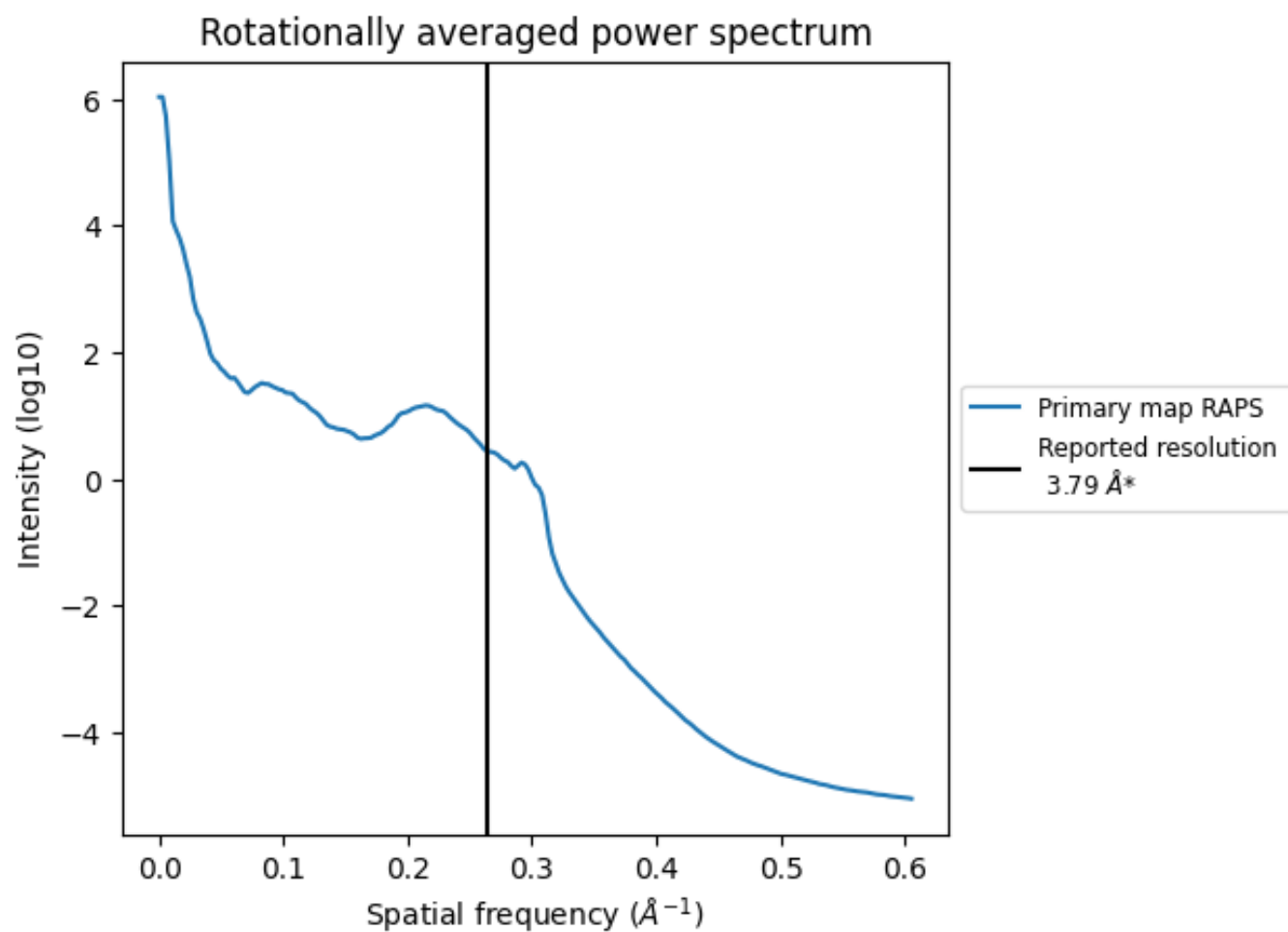
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm<sup>3</sup>; this corresponds to an approximate mass of 232 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 0.264 Å<sup>-1</sup>

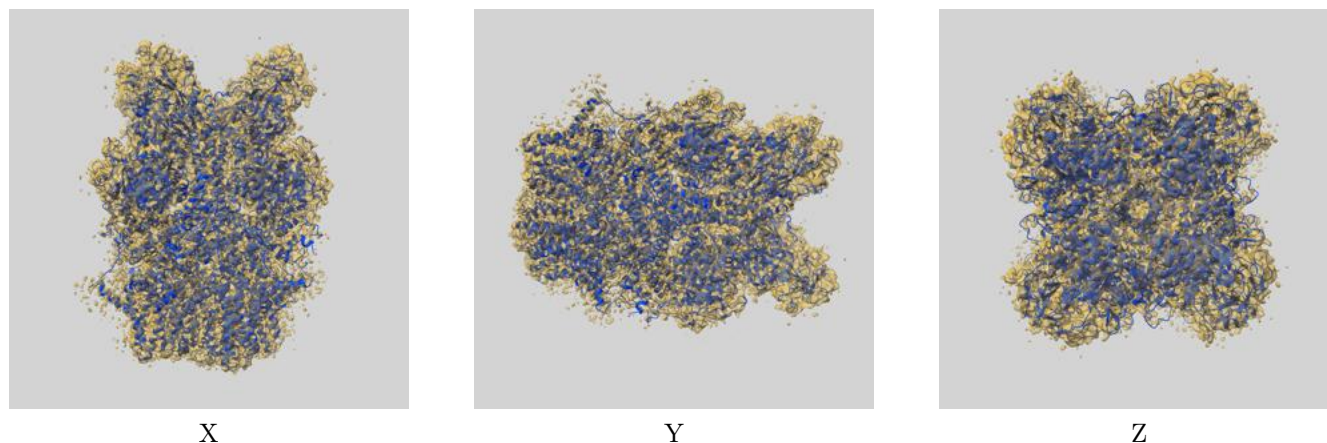
## 8 Fourier-Shell correlation ⓘ

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

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

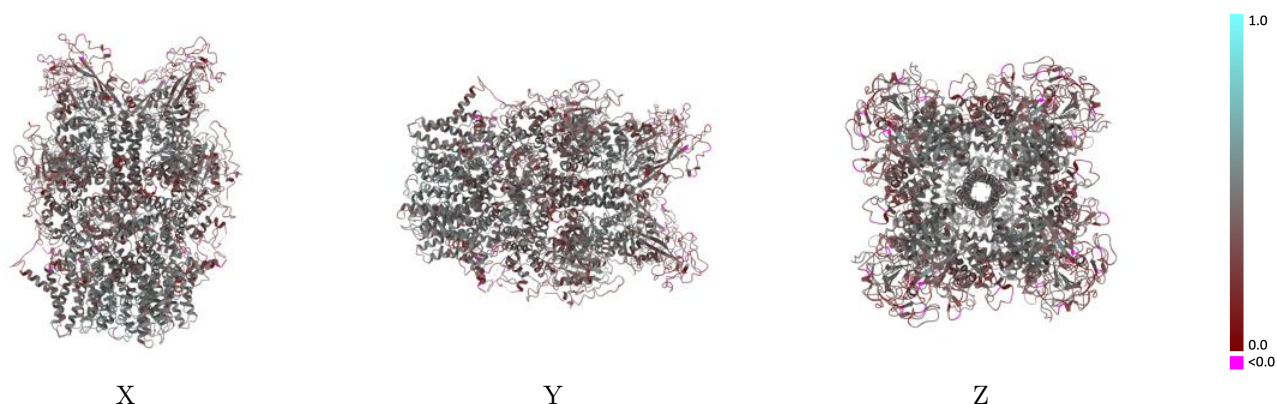
This section contains information regarding the fit between EMDB map EMD-40731 and PDB model 8SRH. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



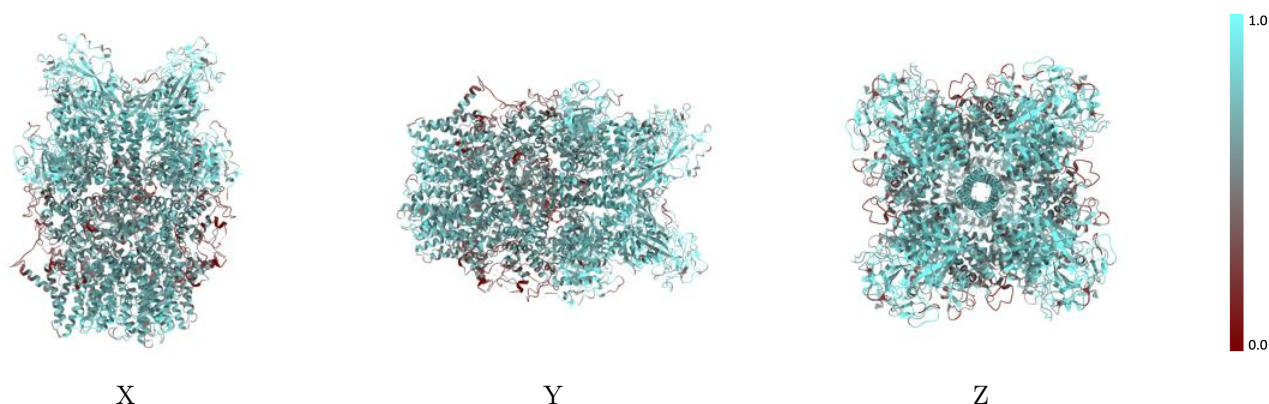
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



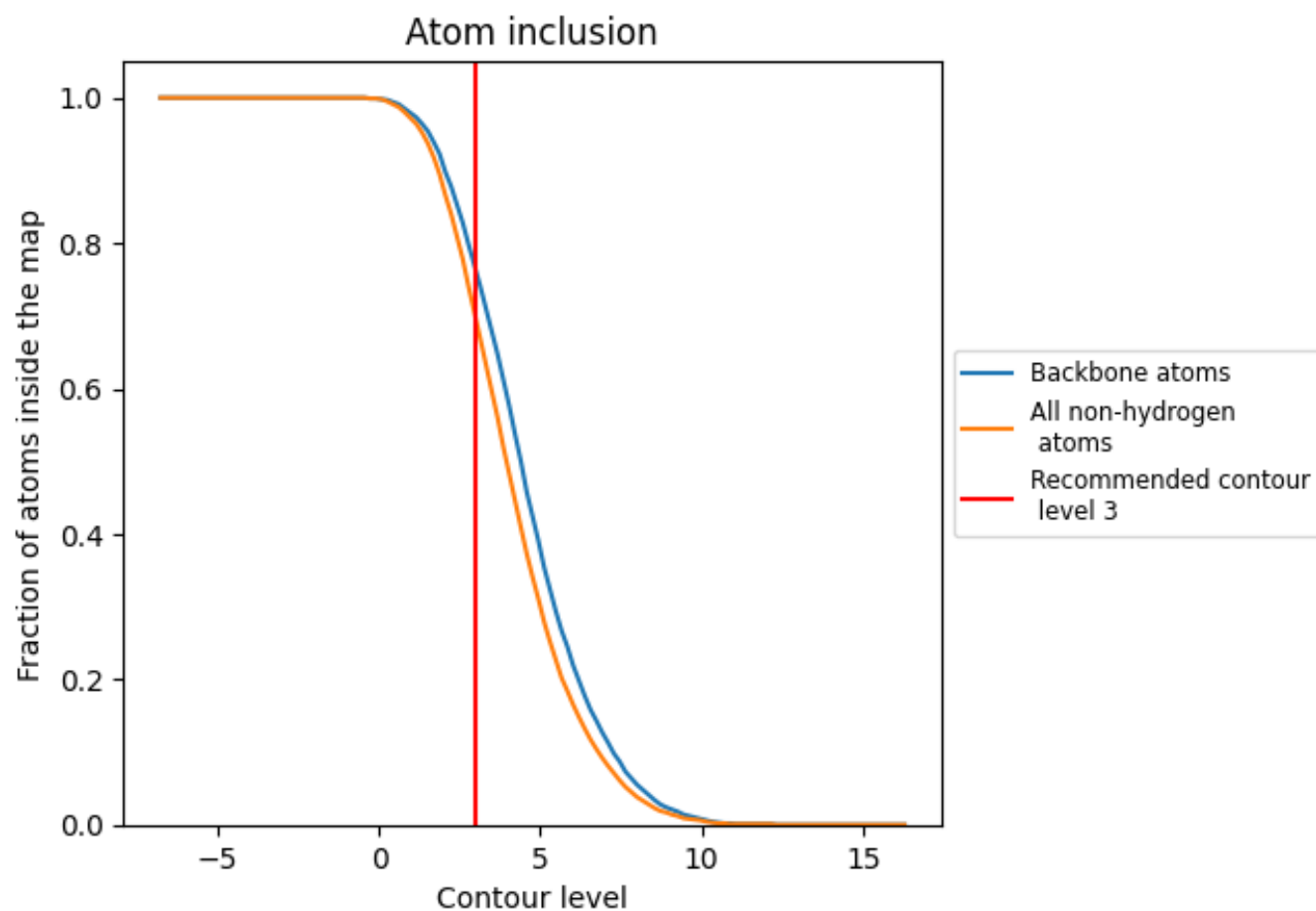
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6990	<div></div> 0.4100
A	<div></div> 0.7000	<div></div> 0.4100
B	<div></div> 0.6990	<div></div> 0.4100
C	<div></div> 0.7000	<div></div> 0.4100
D	<div></div> 0.7000	<div></div> 0.4110

