Full wwPDB EM Validation Report (i)

Dec 12, 2022 – 08:45 am GMT

PDB ID	:	6Y90
EMDB ID	:	EMD-10731
Title	:	Structure of full-length CD20 in complex with Rituximab Fab
Authors	:	Kumar, A.; Reyes, N.
Deposited on	:	2020-03-06
Resolution	:	3.69 Å(reported)
Based on initial model	:	2OSL

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

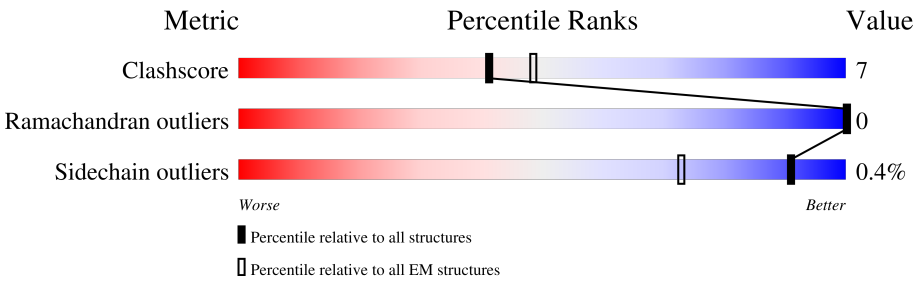
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.69 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	172	11% 80% 20%
1	B	172	15% 72% 28%
2	C	224	39% 88% 12%
2	H	224	39% 87% 13%
3	D	213	43% 86% 14%
3	L	213	42% 85% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9778 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 B-lymphocyte antigen CD20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	172	1341	883	212	232	14	0	0
1	B	172	1341	883	212	232	14	0	0

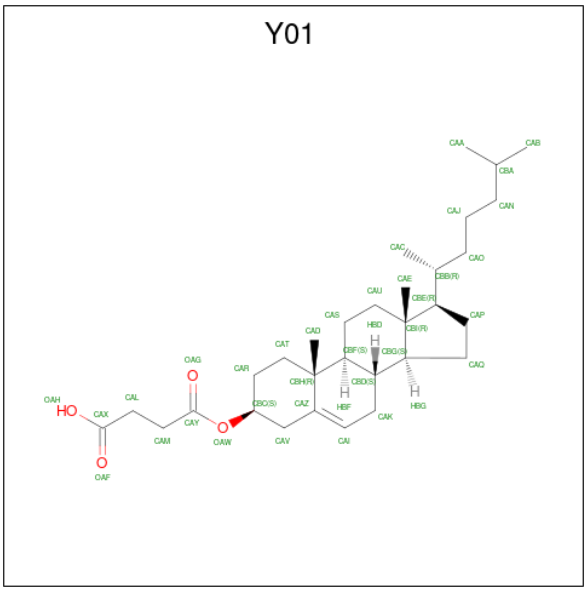
- Molecule 2 is a protein called Rituximab Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	224	1669	1055	274	332	8	0	0
2	H	224	1669	1055	274	332	8	0	0

- Molecule 3 is a protein called Rituximab Fab Light Chain.

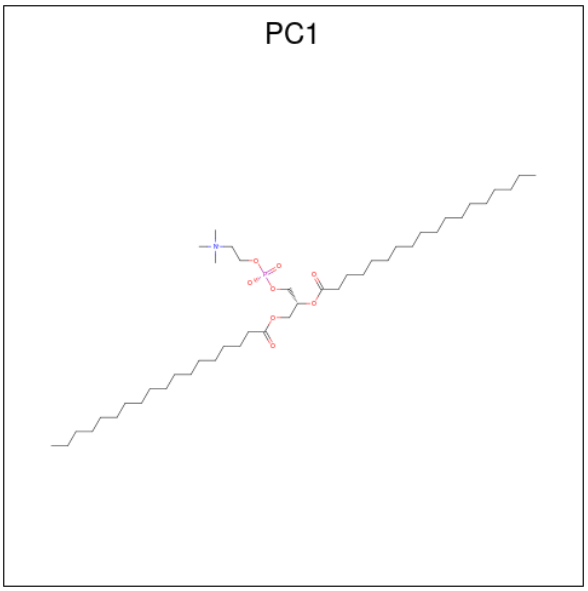
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	213	1623	1016	273	328	6	0	0
3	L	213	1623	1016	273	328	6	0	0

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



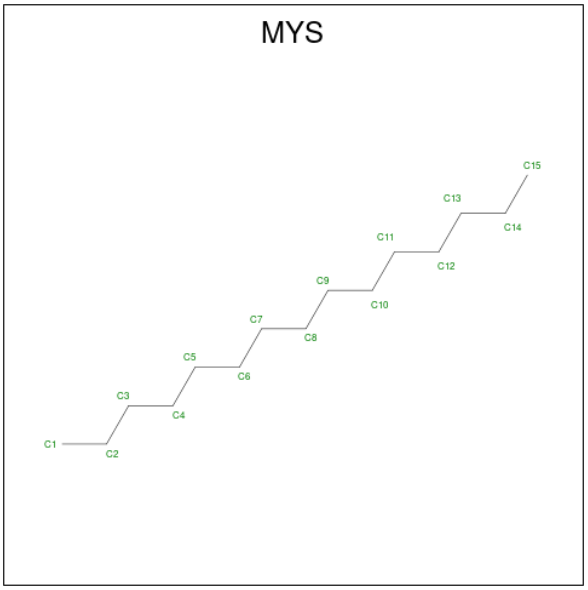
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 139	C 123	O 16	0
4	A	1	Total 139	C 123	O 16	0
4	A	1	Total 139	C 123	O 16	0
4	A	1	Total 139	C 123	O 16	0
4	B	1	Total 139	C 123	O 16	0
4	B	1	Total 139	C 123	O 16	0
4	B	1	Total 139	C 123	O 16	0
4	B	1	Total 139	C 123	O 16	0

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	42	32	1	8	1	0
			Total	C	N	O	P	
5	B	1	42	32	1	8	1	0

- Molecule 6 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
6	A	1	75	75	0
			Total	C	
6	A	1	75	75	0

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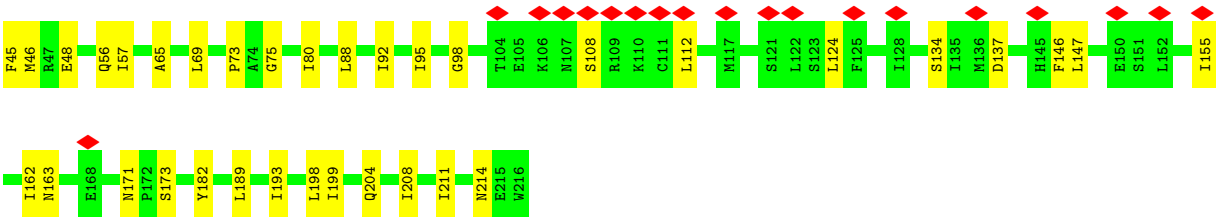
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
6	A	1	75	75	0
			Total	C	
6	A	1	75	75	0
			Total	C	
6	A	1	75	75	0
			Total	C	
6	B	1	75	75	0
			Total	C	
6	B	1	75	75	0
			Total	C	
6	B	1	75	75	0
			Total	C	
6	B	1	75	75	0
			Total	C	
6	B	1	75	75	0

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.

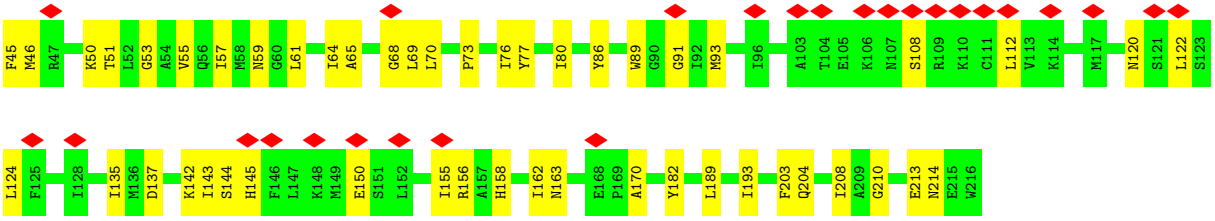
• Molecule 1: B-lymphocyte antigen CD20

Chain A:



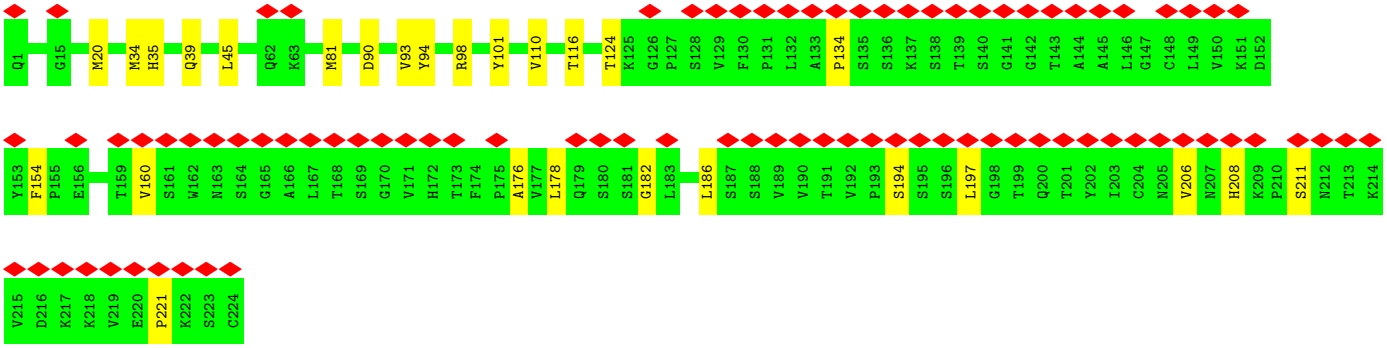
• Molecule 1: B-lymphocyte antigen CD20

Chain B:



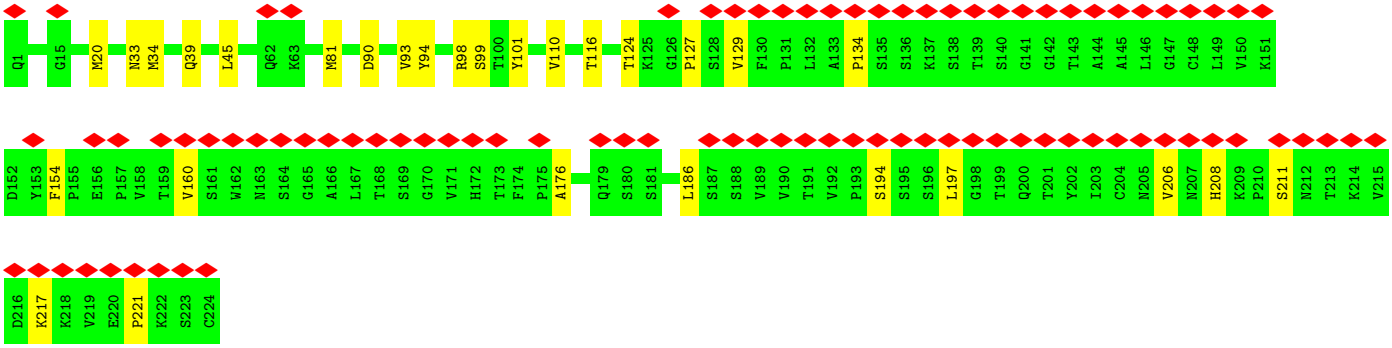
• Molecule 2: Rituximab Fab Heavy Chain

Chain C:



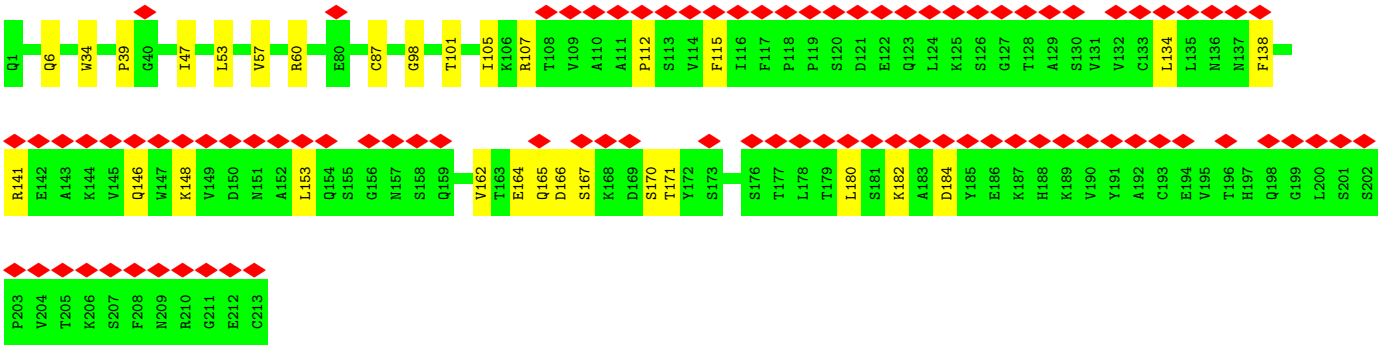
- Molecule 2: Rituximab Fab Heavy Chain

Chain H:



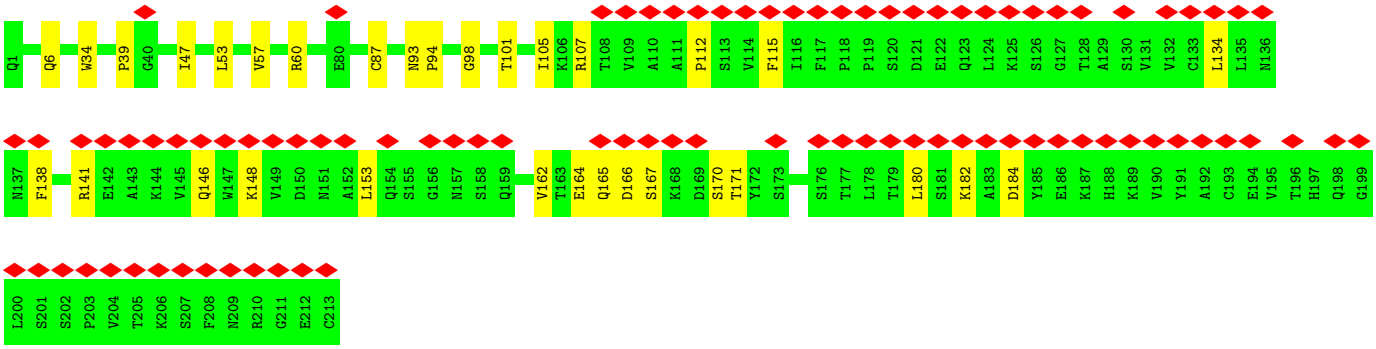
- Molecule 3: Rituximab Fab Light Chain

Chain D:



- Molecule 3: Rituximab Fab Light Chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	65203	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 ($e^-/Å^2$)	41.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.836	Depositor
Minimum map value	-1.357	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	244.2, 244.2, 244.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.814, 0.814, 0.814	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: Y01, MYS, PC1

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	0.25	0/1372	0.43	0/1857
1	B	0.26	0/1372	0.43	0/1857
2	C	0.25	0/1713	0.45	0/2334
2	H	0.25	0/1713	0.45	0/2334
3	D	0.24	0/1662	0.42	0/2260
3	L	0.24	0/1662	0.42	0/2260
All	All	0.25	0/9494	0.43	0/12902

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	1341	0	1385	30	0
1	B	1341	0	1385	38	0
2	C	1669	0	1624	15	0
2	H	1669	0	1624	17	0
3	D	1623	0	1574	19	0
3	L	1623	0	1574	20	0
4	A	139	0	192	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	139	0	191	11	0
5	A	42	0	58	2	0
5	B	42	0	56	5	0
6	A	75	0	160	3	0
6	B	75	0	160	1	0
All	All	9778	0	9983	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (147) 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:B:59:ASN:HD22	1:B:204:GLN:HB2	1.48	0.79
3:L:53:LEU:HB3	3:L:57:VAL:HG11	1.73	0.71
1:A:69:LEU:HD21	1:B:193:ILE:HD13	1.73	0.70
1:A:189:LEU:HD22	1:B:189:LEU:HD21	1.73	0.70
3:L:112:PRO:HB3	3:L:138:PHE:HB3	1.74	0.69
3:D:53:LEU:HB3	3:D:57:VAL:HG11	1.73	0.69
3:D:112:PRO:HB3	3:D:138:PHE:HB3	1.74	0.68
1:B:142:LYS:HG2	5:B:305:PC1:H12	1.80	0.64
4:A:301:Y01:HAC3	1:B:65:ALA:HA	1.81	0.63
1:B:150:GLU:OE2	1:B:156:ARG:NH2	2.32	0.62
3:D:105:ILE:H	3:D:165:GLN:HE22	1.50	0.60
3:L:105:ILE:H	3:L:165:GLN:HE22	1.50	0.59
1:A:193:ILE:HG12	1:B:69:LEU:HD21	1.84	0.58
1:A:108:SER:HB2	1:A:112:LEU:HB2	1.84	0.58
3:L:39:PRO:HG3	3:L:164:GLU:HG3	1.85	0.58
3:D:39:PRO:HG3	3:D:164:GLU:HG3	1.85	0.57
2:H:208:HIS:HD2	2:H:211:SER:HB3	1.70	0.57
2:C:208:HIS:HD2	2:C:211:SER:HB3	1.70	0.56
1:A:65:ALA:HA	4:B:302:Y01:HAC3	1.87	0.56
1:B:108:SER:HB2	1:B:112:LEU:HB2	1.87	0.56
3:D:6:GLN:NE2	3:D:87:CYS:HB2	2.21	0.55
3:L:6:GLN:NE2	3:L:87:CYS:HB2	2.21	0.55
1:A:57:ILE:HG22	1:A:95:ILE:HA	1.88	0.55
1:A:46:MET:HB3	1:A:214:ASN:HD21	1.73	0.54
1:A:199:ILE:HD13	5:A:304:PC1:H3A1	1.90	0.54
1:A:80:ILE:HG22	1:A:137:ASP:HB2	1.90	0.54
1:A:92:ILE:HA	1:A:95:ILE:HD12	1.90	0.54
1:B:46:MET:HB3	1:B:214:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD22	1:B:208:ILE:HD12	1.90	0.53
2:C:134:PRO:HD2	2:C:221:PRO:HA	1.89	0.53
2:H:98:ARG:HG2	2:H:110:VAL:HG12	1.91	0.52
2:H:134:PRO:HD2	2:H:221:PRO:HA	1.89	0.52
1:A:73:PRO:HD3	1:A:155:ILE:HD11	1.92	0.52
2:C:39:GLN:HB2	2:C:45:LEU:HD12	1.92	0.52
2:C:160:VAL:HG22	2:C:206:VAL:HG12	1.92	0.52
2:H:20:MET:HB2	2:H:81:MET:HB3	1.92	0.52
2:C:98:ARG:HG2	2:C:110:VAL:HG12	1.91	0.52
3:D:6:GLN:OE1	3:D:101:THR:HG23	2.10	0.52
3:L:6:GLN:OE1	3:L:101:THR:HG23	2.10	0.51
2:H:39:GLN:HB2	2:H:45:LEU:HD12	1.92	0.51
3:D:180:LEU:HD12	3:D:184:ASP:HB3	1.92	0.51
1:A:182:TYR:HB3	1:B:182:TYR:HB3	1.91	0.51
3:L:180:LEU:HD12	3:L:184:ASP:HB3	1.93	0.51
1:A:163:ASN:O	1:B:182:TYR:OH	2.27	0.51
1:B:53:GLY:O	1:B:57:ILE:HG12	2.09	0.51
2:H:160:VAL:HG22	2:H:206:VAL:HG12	1.92	0.50
1:B:204:GLN:O	1:B:208:ILE:HG12	2.11	0.50
2:H:39:GLN:HA	2:H:45:LEU:HA	1.93	0.50
2:C:20:MET:HB2	2:C:81:MET:HB3	1.92	0.50
2:C:39:GLN:HA	2:C:45:LEU:HA	1.93	0.49
2:H:124:THR:HA	2:H:154:PHE:HD2	1.78	0.49
1:A:57:ILE:HG23	1:A:98:GLY:HA3	1.95	0.49
1:A:204:GLN:O	1:A:208:ILE:HG12	2.13	0.49
2:C:124:THR:HA	2:C:154:PHE:HD2	1.78	0.49
1:B:170:ALA:HB1	2:C:35:HIS:HE1	1.78	0.48
2:C:93:VAL:HG22	2:C:116:THR:HG22	1.94	0.48
2:H:93:VAL:HG22	2:H:116:THR:HG22	1.94	0.48
2:H:90:ASP:OD1	2:H:94:TYR:OH	2.28	0.48
1:A:124:LEU:HD22	1:A:208:ILE:HD12	1.95	0.48
1:B:210:GLY:HA2	1:B:213:GLU:HG2	1.96	0.48
1:B:80:ILE:HG22	1:B:137:ASP:HB2	1.94	0.48
1:B:93:MET:HE2	1:B:122:LEU:HB3	1.96	0.47
3:L:141:ARG:HE	3:L:162:VAL:HG21	1.79	0.47
1:A:199:ILE:HG13	4:B:301:Y01:HAB2	1.96	0.47
1:B:143:ILE:HG22	1:B:144:SER:H	1.79	0.47
3:L:115:PHE:HB2	3:L:134:LEU:HB3	1.95	0.47
3:D:141:ARG:HE	3:D:162:VAL:HG21	1.79	0.47
3:D:6:GLN:HE21	3:D:87:CYS:HB2	1.81	0.46
3:D:115:PHE:HB2	3:D:134:LEU:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:309:MYS:H51	6:B:309:MYS:H82	1.75	0.46
1:B:135:ILE:HG13	5:B:305:PC1:H281	1.64	0.46
3:D:107:ARG:NH2	3:D:171:THR:HG23	2.31	0.46
3:L:107:ARG:NH2	3:L:171:THR:HG23	2.31	0.46
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.98	0.46
6:A:305:MYS:H72	6:A:305:MYS:H42	1.71	0.45
1:A:48:GLU:OE2	1:B:50:LYS:HD3	2.16	0.45
4:A:310:Y01:HAE2	4:A:310:Y01:HBB	1.82	0.45
1:A:45:PHE:N	1:A:214:ASN:HD22	2.15	0.45
3:L:87:CYS:O	3:L:98:GLY:N	2.50	0.45
4:A:310:Y01:HAP1	4:A:310:Y01:HAO2	1.77	0.45
3:L:34:TRP:HB2	3:L:47:ILE:HB	1.97	0.45
1:B:73:PRO:HD3	1:B:155:ILE:HD11	1.99	0.45
3:L:6:GLN:HE21	3:L:87:CYS:HB2	1.80	0.45
3:D:170:SER:OG	3:D:171:THR:N	2.49	0.45
1:B:70:LEU:HD23	1:B:70:LEU:HA	1.83	0.44
3:L:170:SER:OG	3:L:171:THR:N	2.50	0.44
2:H:176:ALA:HB2	2:H:186:LEU:HB3	1.99	0.44
5:A:304:PC1:H222	5:A:304:PC1:H251	1.78	0.44
1:B:145:HIS:H	1:B:145:HIS:CD2	2.35	0.44
3:D:87:CYS:O	3:D:98:GLY:N	2.50	0.44
1:A:134:SER:HB3	1:A:198:LEU:HD12	2.00	0.44
1:B:57:ILE:O	1:B:61:LEU:HD13	2.18	0.44
2:C:176:ALA:HB2	2:C:186:LEU:HB3	1.99	0.44
1:A:208:ILE:HA	1:A:211:ILE:HD12	1.99	0.44
1:B:76:ILE:HG13	1:B:77:TYR:CD1	2.54	0.43
6:A:308:MYS:H82	6:A:308:MYS:H51	1.75	0.43
2:C:90:ASP:OD1	2:C:94:TYR:OH	2.28	0.43
1:A:162:ILE:HD11	1:B:182:TYR:CD1	2.54	0.43
3:L:146:GLN:HG3	3:L:153:LEU:HD22	2.01	0.43
1:A:88:LEU:HD21	4:A:302:Y01:HAB2	2.01	0.43
1:A:182:TYR:OH	1:B:163:ASN:O	2.32	0.43
3:D:148:LYS:HE2	3:D:148:LYS:HB3	1.85	0.43
4:B:301:Y01:HAD3	4:B:301:Y01:HBD	1.83	0.43
5:B:305:PC1:H242	5:B:305:PC1:H271	1.87	0.43
3:D:146:GLN:HG3	3:D:153:LEU:HD22	2.01	0.43
1:A:56:GLN:HB3	1:A:204:GLN:HE22	1.83	0.42
1:B:45:PHE:N	1:B:214:ASN:HD22	2.16	0.42
5:B:305:PC1:H282	5:B:305:PC1:H2B2	1.86	0.42
4:A:301:Y01:HAD2	4:A:301:Y01:HAS2	1.84	0.42
1:B:59:ASN:ND2	1:B:204:GLN:HB2	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:SER:HA	2:H:197:LEU:HG	2.01	0.42
3:L:148:LYS:HE2	3:L:148:LYS:HB3	1.85	0.42
4:A:301:Y01:HAC1	1:B:68:GLY:HA3	2.01	0.42
3:D:107:ARG:HH21	3:D:171:THR:HG23	1.85	0.42
1:A:146:PHE:CD2	1:A:147:LEU:HD23	2.55	0.42
4:B:304:Y01:HAD2	4:B:304:Y01:HAS2	1.86	0.42
2:C:194:SER:HA	2:C:197:LEU:HG	2.01	0.42
3:D:60:ARG:HE	3:D:60:ARG:HB2	1.69	0.42
3:L:166:ASP:OD2	3:L:167:SER:N	2.53	0.42
4:A:302:Y01:HAE2	4:A:302:Y01:HBB	1.95	0.42
3:D:166:ASP:OD2	3:D:167:SER:N	2.53	0.42
3:L:107:ARG:HH21	3:L:171:THR:HG23	1.85	0.42
4:B:302:Y01:HAD3	4:B:302:Y01:HBD	1.88	0.41
4:A:310:Y01:HBE	1:B:203:PHE:CZ	2.55	0.41
4:B:301:Y01:HAS2	4:B:301:Y01:HAD2	1.71	0.41
5:B:305:PC1:H251	5:B:305:PC1:H222	1.78	0.41
4:B:301:Y01:HAE2	4:B:301:Y01:HBB	1.82	0.41
4:B:301:Y01:HAP1	4:B:301:Y01:HAO2	1.77	0.41
1:A:171:ASN:ND2	2:H:99:SER:OG	2.49	0.41
1:A:182:TYR:CD1	1:B:162:ILE:HD11	2.56	0.41
4:B:302:Y01:HAE2	4:B:302:Y01:HBB	1.92	0.41
2:C:178:LEU:HD11	2:C:182:GLY:HA2	2.03	0.41
6:A:307:MYS:H31	6:A:307:MYS:H62	1.78	0.41
4:B:304:Y01:HAD3	4:B:304:Y01:HBD	1.80	0.41
4:A:310:Y01:HAD3	4:A:310:Y01:HBD	1.83	0.41
1:B:158:HIS:CE1	4:B:303:Y01:HAV1	2.56	0.41
3:L:93:ASN:HA	3:L:94:PRO:HA	1.91	0.41
1:B:64:ILE:HG23	1:B:91:GLY:HA3	2.03	0.41
1:B:51:THR:O	1:B:55:VAL:HG23	2.21	0.41
1:A:173:SER:HB3	2:H:33:ASN:HD21	1.86	0.40
2:C:101:TYR:HB3	2:H:101:TYR:HB3	2.02	0.40
1:B:86:TYR:HA	1:B:89:TRP:NE1	2.36	0.40
3:L:60:ARG:HE	3:L:60:ARG:HB2	1.69	0.40
1:B:120:ASN:O	1:B:124:LEU:HD23	2.22	0.40
1:A:75:GLY:H	1:A:162:ILE:HG23	1.87	0.40
2:H:127:PRO:HG3	2:H:208:HIS:HB2	2.04	0.40
2:H:129:VAL:HG22	2:H:217:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
1	B	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
2	C	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
2	H	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
3	D	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
3	L	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
All	All	1206/1218 (99%)	1172 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/148 (100%)	148 (100%)	0	100	100
1	B	148/148 (100%)	148 (100%)	0	100	100
2	C	186/186 (100%)	185 (100%)	1 (0%)	88	94
2	H	186/186 (100%)	185 (100%)	1 (0%)	88	94
3	D	185/185 (100%)	184 (100%)	1 (0%)	88	94
3	L	185/185 (100%)	184 (100%)	1 (0%)	88	94
All	All	1038/1038 (100%)	1034 (100%)	4 (0%)	91	95

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

Mol	Chain	Res	Type
2	C	34	MET
3	D	182	LYS
2	H	34	MET
3	L	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	181	GLN
1	A	214	ASN
1	B	59	ASN
1	B	171	ASN
1	B	181	GLN
1	B	214	ASN
2	C	207	ASN
2	C	208	HIS
2	H	33	ASN
2	H	207	ASN
2	H	208	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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	Y01	A	301	-	38,38,38	1.78	6 (15%)	57,57,57	1.74	12 (21%)
4	Y01	B	303	-	38,38,38	1.78	6 (15%)	57,57,57	1.71	13 (22%)
5	PC1	A	304	-	41,41,53	1.06	4 (9%)	47,49,61	1.06	2 (4%)
6	MYS	B	309	-	14,14,14	0.30	0	13,13,13	0.85	0
6	MYS	A	305	-	14,14,14	0.29	0	13,13,13	0.87	0
4	Y01	B	304	-	37,37,38	1.80	7 (18%)	52,55,57	1.81	13 (25%)
6	MYS	A	309	-	14,14,14	0.30	0	13,13,13	0.86	0
4	Y01	B	301	1	38,38,38	1.79	5 (13%)	57,57,57	1.77	10 (17%)
5	PC1	B	305	1	41,41,53	1.06	4 (9%)	47,49,61	1.06	2 (4%)
4	Y01	B	302	-	38,38,38	1.78	6 (15%)	57,57,57	1.74	12 (21%)
4	Y01	A	310	-	38,38,38	1.78	5 (13%)	57,57,57	1.76	10 (17%)
6	MYS	B	310	-	14,14,14	0.30	0	13,13,13	0.86	0
4	Y01	A	302	-	38,38,38	1.78	6 (15%)	57,57,57	1.72	13 (22%)
6	MYS	B	307	-	14,14,14	0.29	0	13,13,13	0.87	0
6	MYS	A	308	-	14,14,14	0.30	0	13,13,13	0.84	0
6	MYS	A	307	-	14,14,14	0.29	0	13,13,13	0.87	0
6	MYS	B	308	-	14,14,14	0.30	0	13,13,13	0.87	0
4	Y01	A	303	-	37,37,38	1.80	7 (18%)	52,55,57	1.82	13 (25%)
6	MYS	A	306	-	14,14,14	0.29	0	13,13,13	0.87	0
6	MYS	B	306	-	14,14,14	0.29	0	13,13,13	0.87	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	Y01	A	301	-	-	11/19/77/77	0/4/4/4
4	Y01	B	303	-	-	8/19/77/77	0/4/4/4
5	PC1	A	304	-	-	12/45/45/57	-
6	MYS	B	309	-	-	4/12/12/12	-
6	MYS	A	305	-	-	2/12/12/12	-
4	Y01	B	304	-	-	4/16/74/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MYS	A	309	-	-	0/12/12/12	-
4	Y01	B	301	1	-	12/19/77/77	0/4/4/4
5	PC1	B	305	1	-	12/45/45/57	-
4	Y01	B	302	-	-	11/19/77/77	0/4/4/4
4	Y01	A	310	-	-	12/19/77/77	0/4/4/4
6	MYS	B	310	-	-	0/12/12/12	-
4	Y01	A	302	-	-	8/19/77/77	0/4/4/4
6	MYS	B	307	-	-	2/12/12/12	-
6	MYS	A	308	-	-	4/12/12/12	-
6	MYS	A	307	-	-	1/12/12/12	-
6	MYS	B	308	-	-	1/12/12/12	-
4	Y01	A	303	-	-	4/16/74/77	0/4/4/4
6	MYS	A	306	-	-	2/12/12/12	-
6	MYS	B	306	-	-	2/12/12/12	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	Y01	CBH-CAZ	-6.02	1.40	1.52
4	B	304	Y01	CBH-CAZ	-6.01	1.41	1.52
4	A	302	Y01	CBH-CAZ	-5.95	1.41	1.52
4	B	301	Y01	CBH-CAZ	-5.94	1.41	1.52
4	B	302	Y01	CBH-CAZ	-5.94	1.41	1.52
4	A	310	Y01	CBH-CAZ	-5.93	1.41	1.52
4	A	301	Y01	CBH-CAZ	-5.93	1.41	1.52
4	B	303	Y01	CBH-CAZ	-5.93	1.41	1.52
4	A	301	Y01	CAV-CAZ	-5.13	1.40	1.51
4	B	302	Y01	CAV-CAZ	-5.10	1.40	1.51
4	B	303	Y01	CAV-CAZ	-5.10	1.40	1.51
4	A	302	Y01	CAV-CAZ	-5.08	1.40	1.51
4	B	301	Y01	CAV-CAZ	-5.08	1.40	1.51
4	A	310	Y01	CAV-CAZ	-5.07	1.40	1.51
4	A	310	Y01	CAK-CAI	-4.84	1.39	1.50
4	B	304	Y01	CAV-CAZ	-4.84	1.41	1.51
4	B	301	Y01	CAK-CAI	-4.83	1.39	1.50
4	A	303	Y01	CAV-CAZ	-4.83	1.41	1.51
4	A	301	Y01	CAK-CAI	-4.79	1.39	1.50
4	A	302	Y01	CAK-CAI	-4.77	1.39	1.50
4	B	302	Y01	CAK-CAI	-4.77	1.39	1.50
4	B	303	Y01	CAK-CAI	-4.76	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	Y01	CAK-CAI	-4.62	1.40	1.50
4	A	303	Y01	CAK-CAI	-4.62	1.40	1.50
4	A	302	Y01	CAI-CAZ	3.23	1.40	1.33
4	B	301	Y01	CAI-CAZ	3.22	1.40	1.33
4	A	301	Y01	CAI-CAZ	3.21	1.40	1.33
4	A	303	Y01	CAI-CAZ	3.20	1.40	1.33
4	A	310	Y01	CAI-CAZ	3.19	1.40	1.33
4	B	303	Y01	CAI-CAZ	3.19	1.40	1.33
4	B	304	Y01	CAI-CAZ	3.18	1.40	1.33
4	B	302	Y01	CAI-CAZ	3.18	1.40	1.33
5	B	305	PC1	O21-C2	-2.49	1.40	1.46
5	A	304	PC1	O21-C2	-2.48	1.40	1.46
4	A	301	Y01	CBI-CBG	-2.45	1.50	1.55
4	B	302	Y01	CBI-CBG	-2.42	1.50	1.55
5	B	305	PC1	O31-C31	2.41	1.40	1.33
5	A	304	PC1	O31-C31	2.41	1.40	1.33
4	A	303	Y01	CBI-CBG	-2.41	1.50	1.55
4	A	310	Y01	CBI-CBG	-2.39	1.50	1.55
4	B	304	Y01	CBI-CBG	-2.38	1.50	1.55
4	A	303	Y01	CBH-CBF	-2.37	1.52	1.56
4	B	304	Y01	CBH-CBF	-2.36	1.52	1.56
4	B	301	Y01	CBI-CBG	-2.35	1.50	1.55
4	B	303	Y01	CBI-CBG	-2.34	1.50	1.55
4	A	302	Y01	CBI-CBG	-2.33	1.50	1.55
4	B	303	Y01	CBH-CBF	-2.28	1.52	1.56
4	A	302	Y01	CBH-CBF	-2.27	1.52	1.56
5	A	304	PC1	O21-C21	2.17	1.40	1.34
5	B	305	PC1	O21-C21	2.15	1.40	1.34
4	B	302	Y01	CBH-CBF	-2.13	1.52	1.56
5	A	304	PC1	O31-C3	-2.13	1.40	1.45
5	B	305	PC1	O31-C3	-2.10	1.40	1.45
4	A	303	Y01	CBI-CBE	-2.08	1.50	1.54
4	A	301	Y01	CBH-CBF	-2.08	1.52	1.56
4	B	304	Y01	CBI-CBE	-2.06	1.51	1.54

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	302	Y01	CBI-CBE-CBB	-4.56	112.35	119.49
4	A	301	Y01	CBI-CBE-CBB	-4.55	112.36	119.49
4	A	303	Y01	CAP-CBE-CBI	-4.50	100.32	104.29
4	A	310	Y01	CAQ-CBG-CBD	-4.48	111.70	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	304	Y01	CAP-CBE-CBI	-4.47	100.34	104.29
4	B	301	Y01	CAQ-CBG-CBD	-4.46	111.74	119.08
4	B	301	Y01	CBI-CBE-CBB	-4.22	112.88	119.49
4	A	310	Y01	CBI-CBE-CBB	-4.20	112.90	119.49
4	A	303	Y01	CAV-CAZ-CBH	4.20	121.99	116.42
4	B	304	Y01	CAV-CAZ-CBH	4.15	121.94	116.42
4	A	310	Y01	CBH-CBF-CBD	-4.14	106.52	112.73
4	B	301	Y01	CAP-CBE-CBI	-4.11	98.89	103.84
4	B	301	Y01	CBH-CBF-CBD	-4.11	106.58	112.73
4	A	310	Y01	CAP-CBE-CBI	-4.07	98.94	103.84
4	B	302	Y01	CAV-CAZ-CBH	3.94	121.66	116.42
4	A	301	Y01	CAV-CAZ-CBH	3.92	121.63	116.42
5	B	305	PC1	O21-C21-C22	3.89	119.88	111.50
5	A	304	PC1	O21-C21-C22	3.88	119.85	111.50
4	A	302	Y01	CAV-CAZ-CBH	3.86	121.55	116.42
4	A	302	Y01	CBI-CBE-CBB	-3.85	113.45	119.49
4	B	303	Y01	CAV-CAZ-CBH	3.84	121.52	116.42
4	B	303	Y01	CBI-CBE-CBB	-3.83	113.48	119.49
4	A	301	Y01	CAP-CBE-CBI	-3.80	99.27	103.84
4	B	302	Y01	CAP-CBE-CBI	-3.77	99.30	103.84
4	B	304	Y01	CAD-CBH-CBF	-3.75	107.21	111.68
4	A	303	Y01	CAD-CBH-CBF	-3.74	107.22	111.68
4	B	304	Y01	CBH-CBF-CBD	-3.57	107.38	112.73
4	A	303	Y01	CBH-CBF-CBD	-3.57	107.38	112.73
4	B	302	Y01	CAQ-CBG-CBD	-3.55	113.24	119.08
4	A	301	Y01	CAQ-CBG-CBD	-3.54	113.25	119.08
4	B	301	Y01	CAV-CAZ-CBH	3.48	121.04	116.42
4	A	302	Y01	CAQ-CBG-CBD	-3.48	113.35	119.08
4	A	310	Y01	CAV-CAZ-CBH	3.47	121.03	116.42
4	B	303	Y01	CAQ-CBG-CBD	-3.46	113.38	119.08
4	A	302	Y01	CAP-CBE-CBI	-3.44	99.70	103.84
4	B	303	Y01	CAP-CBE-CBI	-3.42	99.72	103.84
4	A	310	Y01	CAS-CBF-CBH	-3.40	108.61	113.08
4	B	301	Y01	CAS-CBF-CBH	-3.39	108.61	113.08
4	B	301	Y01	CBI-CBG-CBD	-3.35	109.42	114.38
4	A	310	Y01	CBI-CBG-CBD	-3.34	109.44	114.38
4	A	303	Y01	CBC-OAW-CAY	-3.33	109.59	117.79
4	B	302	Y01	CBH-CBF-CBD	-3.32	107.75	112.73
4	B	304	Y01	CBC-OAW-CAY	-3.31	109.65	117.79
4	A	301	Y01	CBH-CBF-CBD	-3.30	107.78	112.73
4	A	310	Y01	CAD-CBH-CBF	-3.26	107.79	111.68
4	B	301	Y01	CAD-CBH-CBF	-3.25	107.80	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	303	Y01	CAQ-CBG-CBD	-3.23	113.76	119.08
4	B	304	Y01	CAQ-CBG-CBD	-3.19	113.83	119.08
4	B	303	Y01	CAS-CBF-CBH	-3.06	109.05	113.08
4	A	302	Y01	CAS-CBF-CBH	-3.03	109.09	113.08
4	A	301	Y01	CAS-CBF-CBH	-3.00	109.13	113.08
4	B	302	Y01	CAS-CBF-CBH	-2.96	109.17	113.08
4	A	302	Y01	CBH-CBF-CBD	-2.92	108.36	112.73
4	B	303	Y01	CBH-CBF-CBD	-2.91	108.37	112.73
4	A	302	Y01	CBG-CBI-CBE	-2.88	96.66	100.07
4	A	302	Y01	CBC-OAW-CAY	-2.85	110.78	117.79
4	B	303	Y01	CBG-CBI-CBE	-2.84	96.70	100.07
4	B	303	Y01	CBC-OAW-CAY	-2.84	110.81	117.79
4	A	303	Y01	CAS-CAU-CBI	-2.74	108.08	112.78
4	B	304	Y01	CAS-CAU-CBI	-2.74	108.08	112.78
4	A	301	Y01	CAD-CBH-CBF	-2.67	108.49	111.68
4	A	301	Y01	CAS-CAU-CBI	-2.66	108.22	112.78
4	B	302	Y01	CAD-CBH-CBF	-2.64	108.53	111.68
4	B	302	Y01	CAS-CAU-CBI	-2.64	108.25	112.78
4	A	303	Y01	CBI-CBG-CBD	-2.64	110.47	114.38
4	B	302	Y01	CBG-CBI-CBE	-2.63	96.95	100.07
4	A	301	Y01	CBG-CBI-CBE	-2.63	96.95	100.07
4	A	301	Y01	CAV-CAZ-CAI	-2.62	116.83	120.61
4	B	304	Y01	CBI-CBG-CBD	-2.62	110.50	114.38
4	B	302	Y01	CAV-CAZ-CAI	-2.62	116.84	120.61
4	B	304	Y01	CAD-CBH-CAZ	2.57	112.50	108.34
4	A	303	Y01	CAO-CBB-CBE	-2.57	108.75	113.63
4	B	304	Y01	CAO-CBB-CBE	-2.57	108.75	113.63
4	A	303	Y01	CAD-CBH-CAZ	2.55	112.47	108.34
5	A	304	PC1	O31-C31-C32	2.54	119.88	111.91
5	B	305	PC1	O31-C31-C32	2.54	119.88	111.91
4	B	301	Y01	CAS-CAU-CBI	-2.53	108.44	112.78
4	A	303	Y01	CAS-CBF-CBH	-2.53	109.75	113.08
4	B	304	Y01	CAS-CBF-CBH	-2.52	109.75	113.08
4	B	301	Y01	CAV-CAZ-CAI	-2.52	116.97	120.61
4	A	301	Y01	CBI-CBG-CBD	-2.52	110.65	114.38
4	A	310	Y01	CAS-CAU-CBI	-2.51	108.47	112.78
4	A	303	Y01	CAV-CAZ-CAI	-2.51	116.99	120.61
4	A	310	Y01	CAV-CAZ-CAI	-2.50	117.00	120.61
4	B	302	Y01	CBI-CBG-CBD	-2.48	110.71	114.38
4	A	302	Y01	CAT-CAR-CBC	-2.48	106.10	110.33
4	B	304	Y01	CAV-CAZ-CAI	-2.48	117.04	120.61
4	B	303	Y01	CAT-CAR-CBC	-2.47	106.11	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	302	Y01	CAS-CAU-CBI	-2.46	108.56	112.78
4	B	303	Y01	CAS-CAU-CBI	-2.45	108.57	112.78
4	A	302	Y01	CBI-CBG-CBD	-2.44	110.77	114.38
4	B	303	Y01	CAV-CAZ-CAI	-2.43	117.11	120.61
4	A	302	Y01	CAV-CAZ-CAI	-2.42	117.12	120.61
4	A	302	Y01	CAD-CBH-CBF	-2.42	108.80	111.68
4	B	303	Y01	CBI-CBG-CBD	-2.41	110.81	114.38
4	A	301	Y01	CAT-CAR-CBC	-2.40	106.23	110.33
4	B	302	Y01	CAT-CAR-CBC	-2.39	106.25	110.33
4	B	303	Y01	CAD-CBH-CBF	-2.38	108.84	111.68
4	B	304	Y01	CAQ-CBG-CBI	-2.24	101.14	103.84
4	A	303	Y01	CAQ-CBG-CBI	-2.24	101.15	103.84

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	Y01	CAR-CBC-OAW-CAY
4	A	302	Y01	CAM-CAY-OAW-CBC
4	A	310	Y01	CAX-CAL-CAM-CAY
4	B	301	Y01	CAX-CAL-CAM-CAY
4	B	302	Y01	CAR-CBC-OAW-CAY
4	B	303	Y01	CAM-CAY-OAW-CBC
5	A	304	PC1	C11-O13-P-O11
5	B	305	PC1	C11-O13-P-O11
4	A	301	Y01	CAC-CBB-CBE-CBI
4	A	310	Y01	CAC-CBB-CBE-CBI
4	B	301	Y01	CAC-CBB-CBE-CBI
4	B	302	Y01	CAC-CBB-CBE-CBI
4	A	302	Y01	OAG-CAY-OAW-CBC
4	B	303	Y01	OAG-CAY-OAW-CBC
4	A	310	Y01	CAV-CBC-OAW-CAY
4	B	301	Y01	CAV-CBC-OAW-CAY
4	A	302	Y01	CAC-CBB-CBE-CBI
4	B	303	Y01	CAC-CBB-CBE-CBI
4	A	301	Y01	CAO-CBB-CBE-CBI
4	A	310	Y01	CAO-CBB-CBE-CBI
4	B	301	Y01	CAO-CBB-CBE-CBI
4	B	302	Y01	CAO-CBB-CBE-CBI
4	A	302	Y01	CAO-CBB-CBE-CBI
4	B	303	Y01	CAO-CBB-CBE-CBI
4	A	301	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
4	B	302	Y01	CAJ-CAO-CBB-CBE
4	A	302	Y01	CAO-CAJ-CAN-CBA
4	B	303	Y01	CAO-CAJ-CAN-CBA
4	B	302	Y01	CAC-CBB-CBE-CAP
4	A	302	Y01	CAN-CAJ-CAO-CBB
4	B	303	Y01	CAN-CAJ-CAO-CBB
4	A	301	Y01	CAC-CBB-CBE-CAP
4	A	303	Y01	CAO-CAJ-CAN-CBA
4	B	304	Y01	CAO-CAJ-CAN-CBA
6	A	308	MYS	C2-C3-C4-C5
6	B	309	MYS	C2-C3-C4-C5
4	A	310	Y01	CAR-CBC-OAW-CAY
6	A	308	MYS	C11-C10-C9-C8
6	B	309	MYS	C11-C10-C9-C8
4	B	301	Y01	CAR-CBC-OAW-CAY
4	A	301	Y01	OAG-CAY-OAW-CBC
4	B	302	Y01	OAG-CAY-OAW-CBC
4	A	301	Y01	CAM-CAY-OAW-CBC
4	B	302	Y01	CAM-CAY-OAW-CBC
4	A	303	Y01	CAN-CAJ-CAO-CBB
4	B	304	Y01	CAN-CAJ-CAO-CBB
4	A	301	Y01	CAJ-CAO-CBB-CAC
4	B	302	Y01	CAJ-CAO-CBB-CAC
4	A	310	Y01	CAC-CBB-CBE-CAP
4	B	301	Y01	CAC-CBB-CBE-CAP
4	A	301	Y01	CAO-CBB-CBE-CAP
4	B	302	Y01	CAO-CBB-CBE-CAP
5	A	304	PC1	C1-C2-C3-O31
5	B	305	PC1	C1-C2-C3-O31
4	A	310	Y01	CAO-CBB-CBE-CAP
4	B	301	Y01	CAO-CBB-CBE-CAP
4	A	302	Y01	CAC-CBB-CBE-CAP
4	B	303	Y01	CAC-CBB-CBE-CAP
6	A	306	MYS	C4-C5-C6-C7
6	B	307	MYS	C4-C5-C6-C7
4	A	310	Y01	CAJ-CAO-CBB-CBE
4	B	301	Y01	CAJ-CAO-CBB-CBE
4	A	310	Y01	OAG-CAY-OAW-CBC
4	B	301	Y01	OAG-CAY-OAW-CBC
6	A	305	MYS	C6-C7-C8-C9
6	B	306	MYS	C6-C7-C8-C9
5	A	304	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
5	B	305	PC1	C26-C27-C28-C29
4	A	310	Y01	CAM-CAY-OAW-CBC
4	B	301	Y01	CAM-CAY-OAW-CBC
6	B	309	MYS	C3-C4-C5-C6
6	A	308	MYS	C3-C4-C5-C6
5	A	304	PC1	O21-C2-C3-O31
5	B	305	PC1	O21-C2-C3-O31
4	A	302	Y01	CAO-CBB-CBE-CAP
4	B	303	Y01	CAO-CBB-CBE-CAP
5	A	304	PC1	O13-C11-C12-N
5	B	305	PC1	O13-C11-C12-N
6	A	307	MYS	C4-C5-C6-C7
6	B	308	MYS	C4-C5-C6-C7
4	A	303	Y01	CAJ-CAO-CBB-CBE
4	B	304	Y01	CAJ-CAO-CBB-CBE
6	A	305	MYS	C3-C4-C5-C6
6	B	306	MYS	C3-C4-C5-C6
5	A	304	PC1	C31-C32-C33-C34
5	B	305	PC1	C31-C32-C33-C34
6	B	307	MYS	C2-C3-C4-C5
6	A	306	MYS	C2-C3-C4-C5
5	A	304	PC1	O31-C31-C32-C33
5	B	305	PC1	O31-C31-C32-C33
5	A	304	PC1	O21-C21-C22-C23
5	B	305	PC1	O21-C21-C22-C23
4	A	301	Y01	CAL-CAM-CAY-OAW
4	B	302	Y01	CAL-CAM-CAY-OAW
4	A	310	Y01	CAM-CAL-CAX-OAF
4	B	301	Y01	CAM-CAL-CAX-OAF
5	B	305	PC1	C32-C33-C34-C35
5	A	304	PC1	C32-C33-C34-C35
5	B	305	PC1	O32-C31-C32-C33
5	A	304	PC1	O32-C31-C32-C33
5	A	304	PC1	O22-C21-C22-C23
5	B	305	PC1	O22-C21-C22-C23
6	B	309	MYS	C7-C8-C9-C10
6	A	308	MYS	C7-C8-C9-C10
5	A	304	PC1	C11-O13-P-O12
5	B	305	PC1	C11-O13-P-O12
4	A	310	Y01	CAM-CAL-CAX-OAH
4	B	301	Y01	CAM-CAL-CAX-OAH
4	A	301	Y01	CAM-CAL-CAX-OAH

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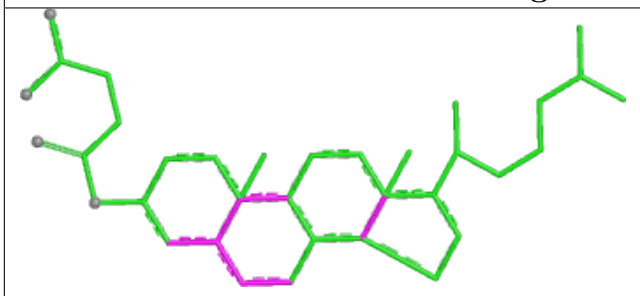
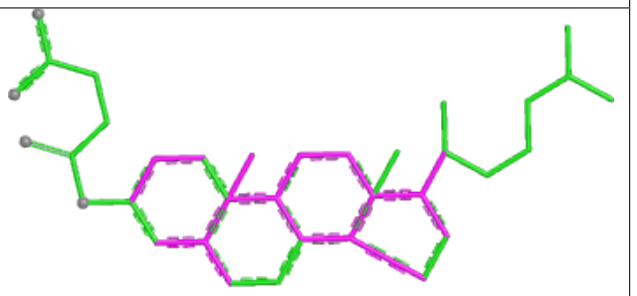
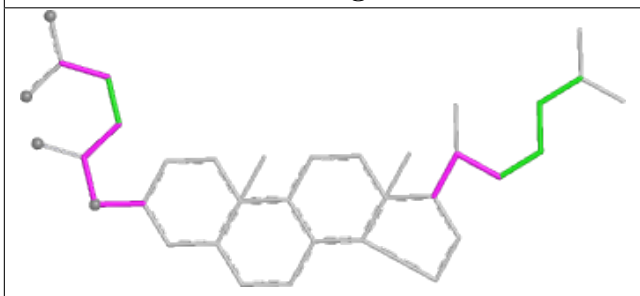
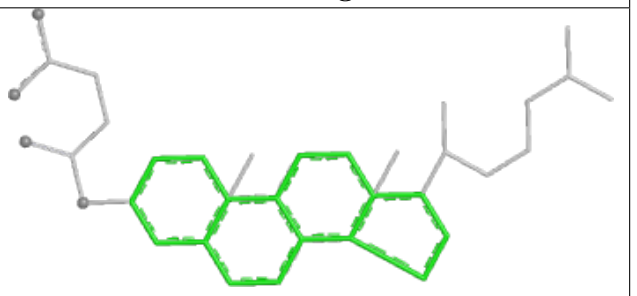
Mol	Chain	Res	Type	Atoms
4	A	303	Y01	CAM-CAL-CAX-OAF
4	B	302	Y01	CAM-CAL-CAX-OAH
4	B	304	Y01	CAM-CAL-CAX-OAF

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	Y01	3	0
4	B	303	Y01	1	0
5	A	304	PC1	2	0
6	B	309	MYS	1	0
6	A	305	MYS	1	0
4	B	304	Y01	2	0
4	B	301	Y01	5	0
5	B	305	PC1	5	0
4	B	302	Y01	3	0
4	A	310	Y01	4	0
4	A	302	Y01	2	0
6	A	308	MYS	1	0
6	A	307	MYS	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 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 Y01 A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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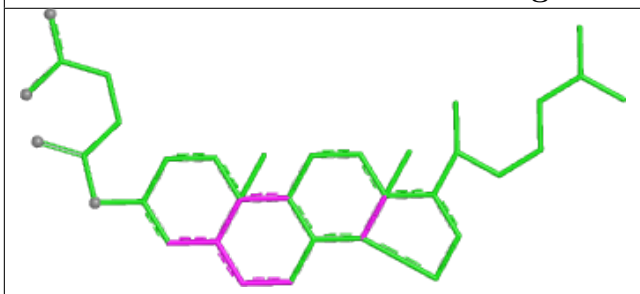
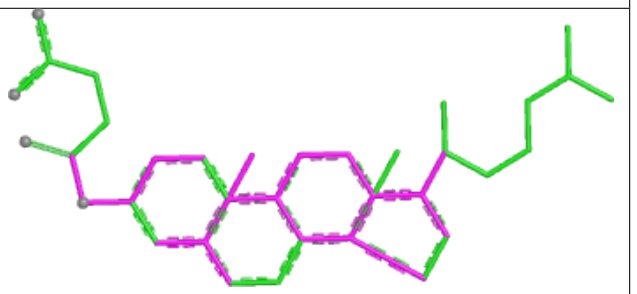
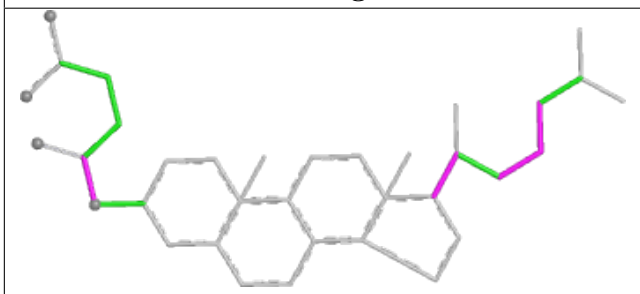
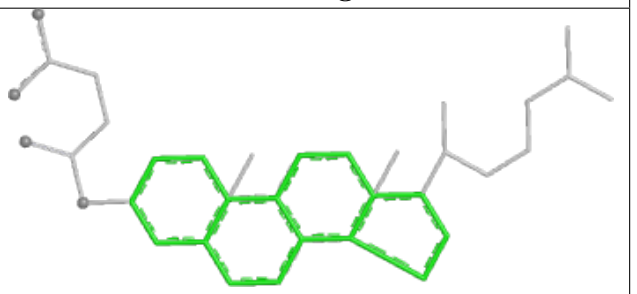
 Bond lengths	 Bond angles
 Torsions	 Rings

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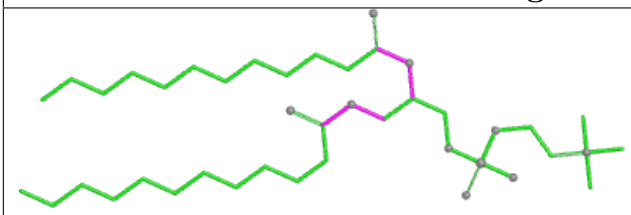
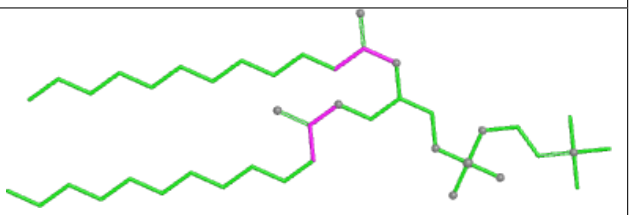
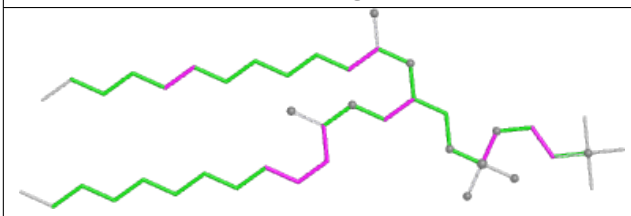
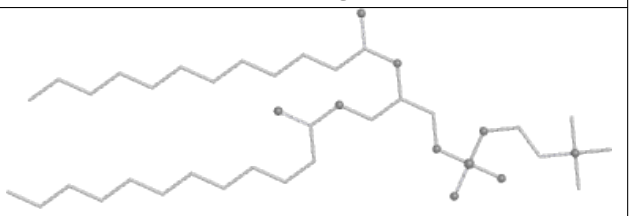
 Bond lengths	 Bond angles
 Torsions	 Rings

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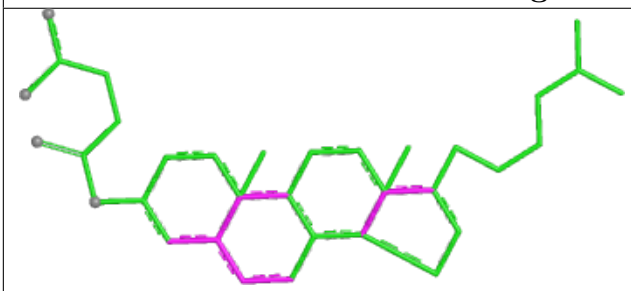
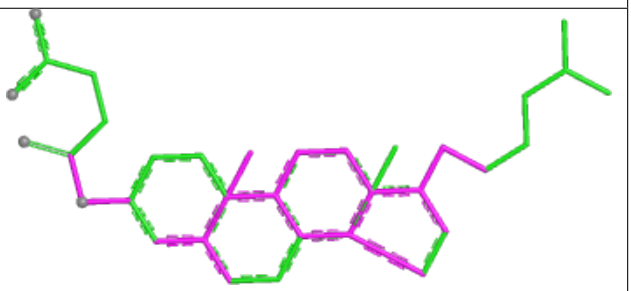
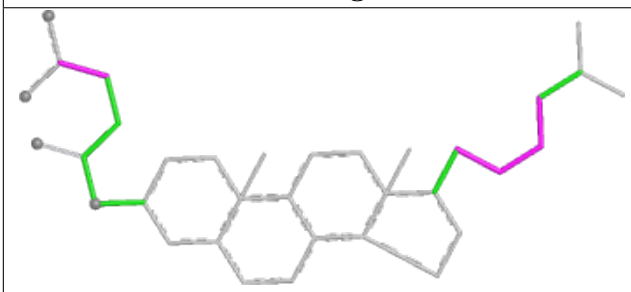
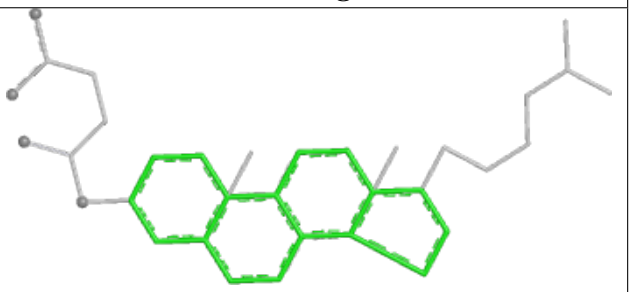
 Bond lengths	 Bond angles
 Torsions	 Rings

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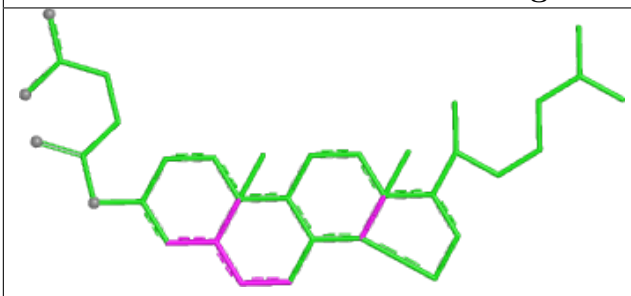
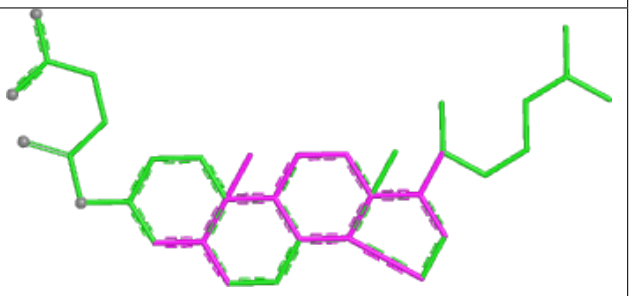
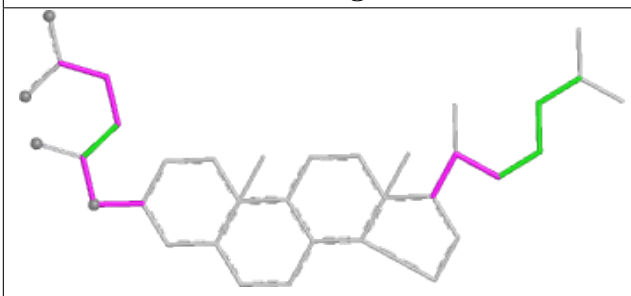
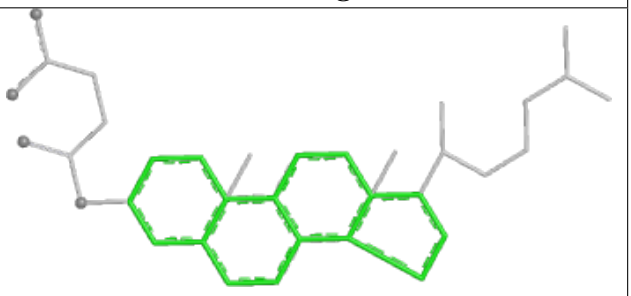
 Bond lengths	 Bond angles
 Torsions	 Rings

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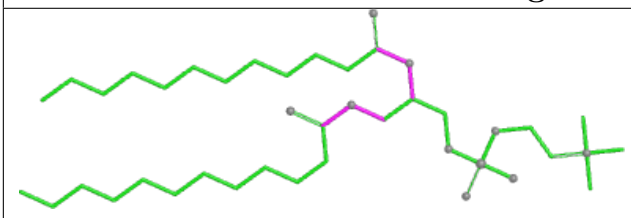
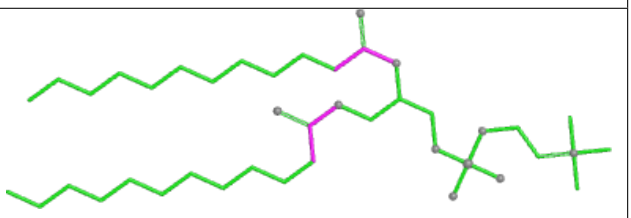
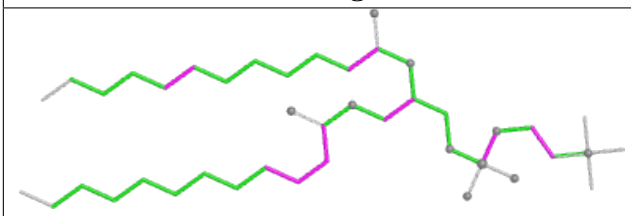
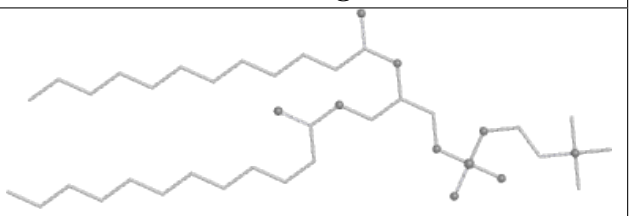
 Bond lengths	 Bond angles
 Torsions	 Rings

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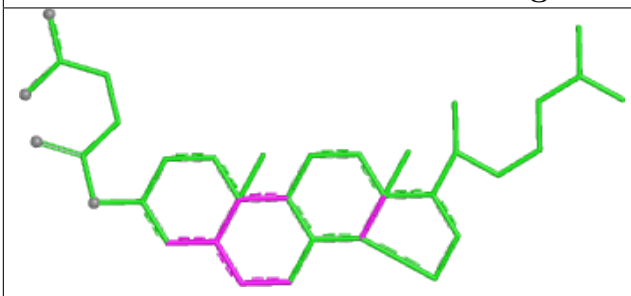
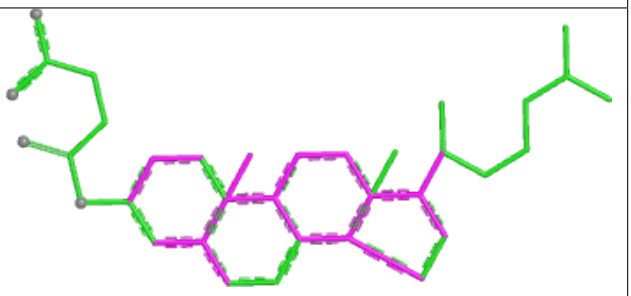
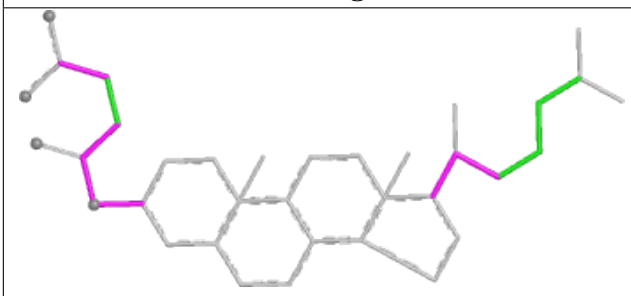
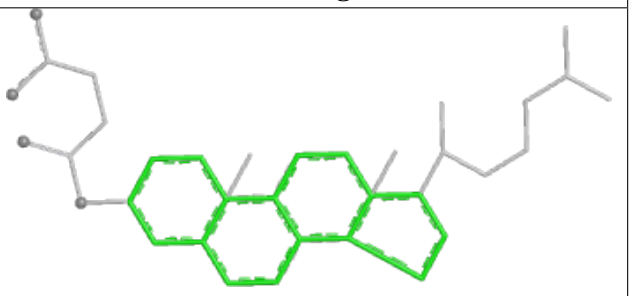
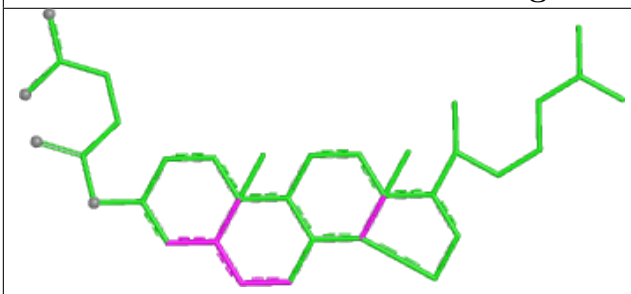
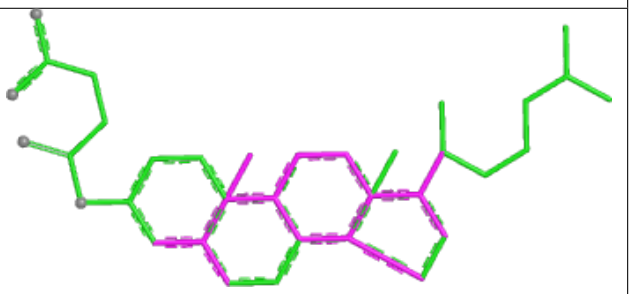
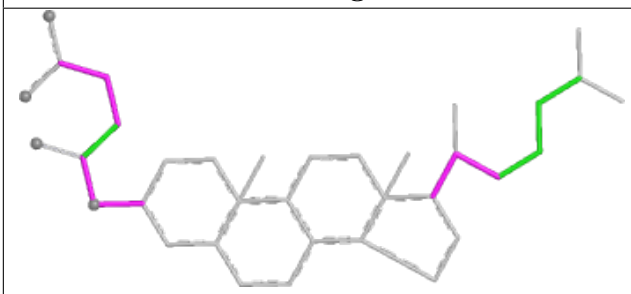
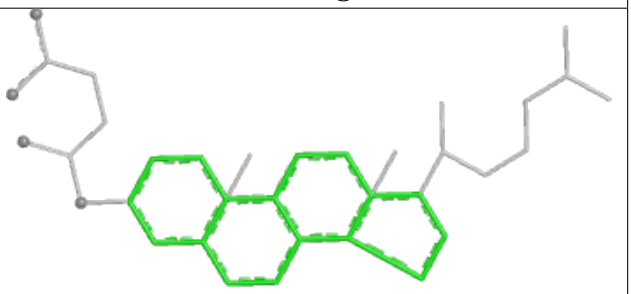
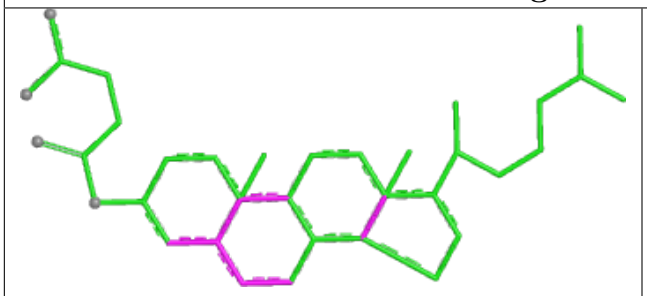
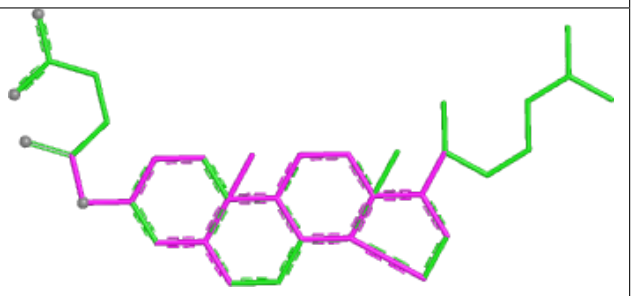
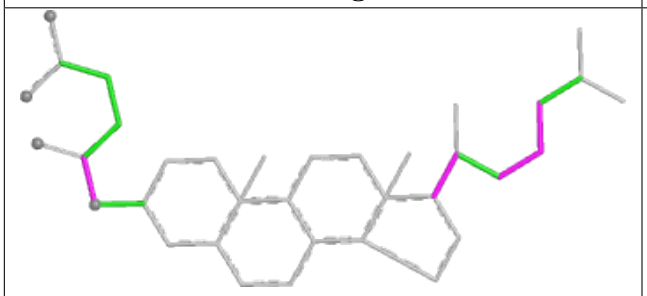
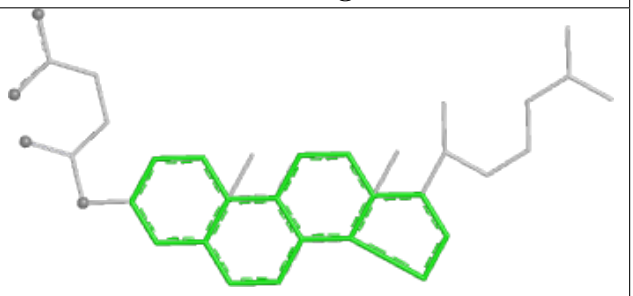
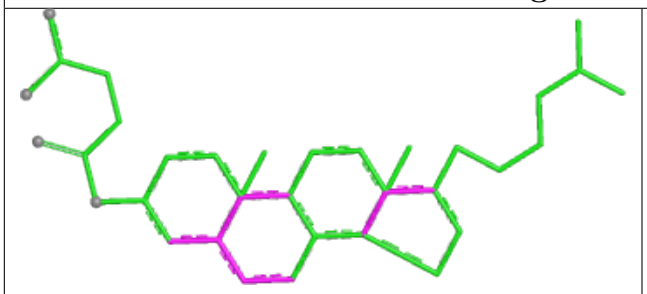
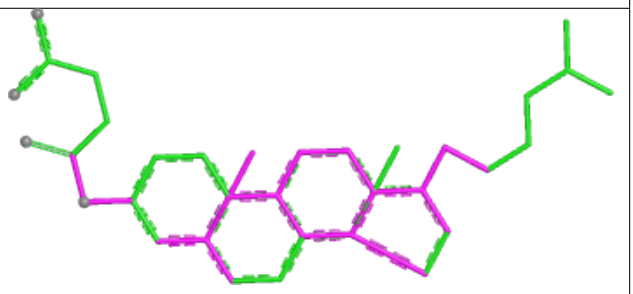
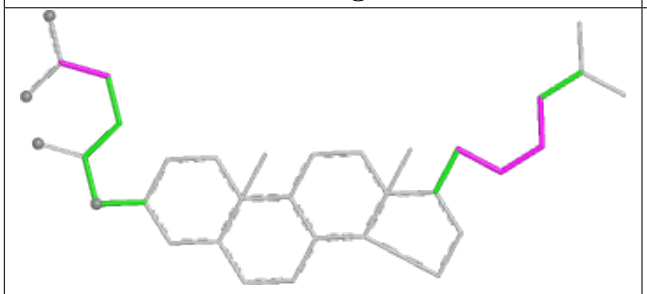
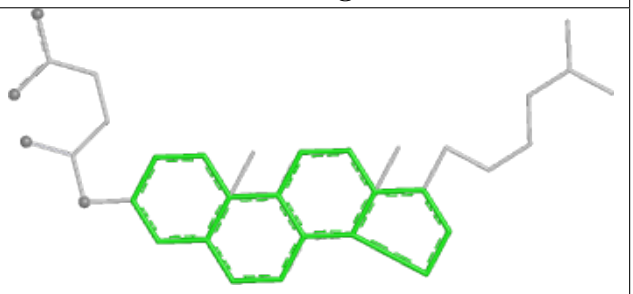
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 A 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 A 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 A 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

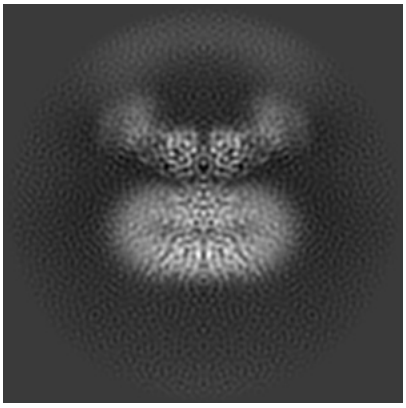
6 Map visualisation (i)

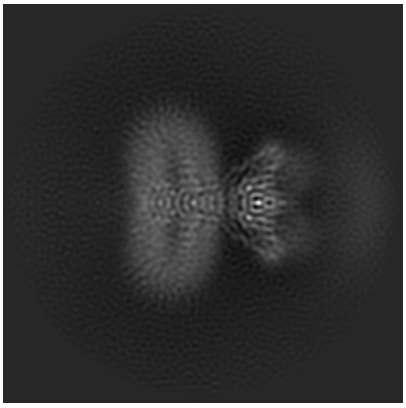
This section contains visualisations of the EMDB entry EMD-10731. These allow visual inspection of the internal detail of the map and identification of artifacts.

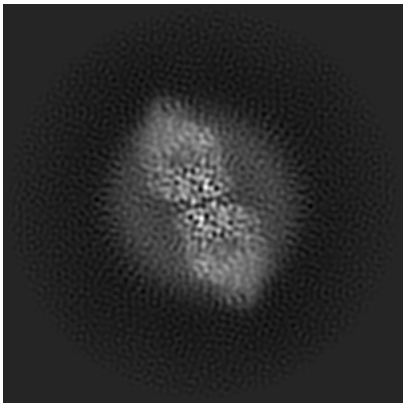
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

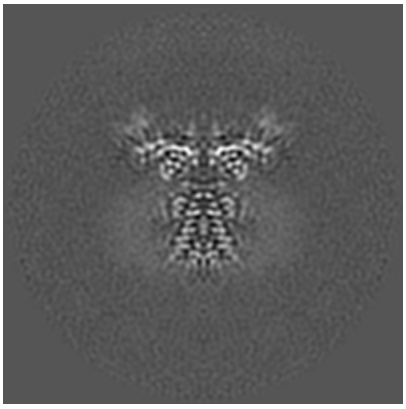

Y

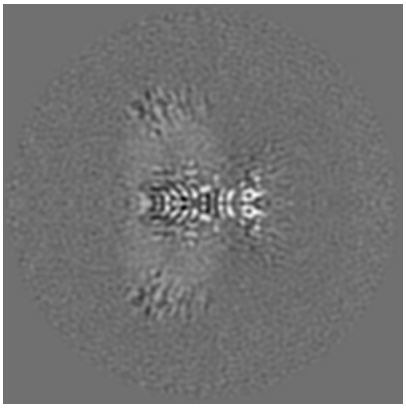

Z

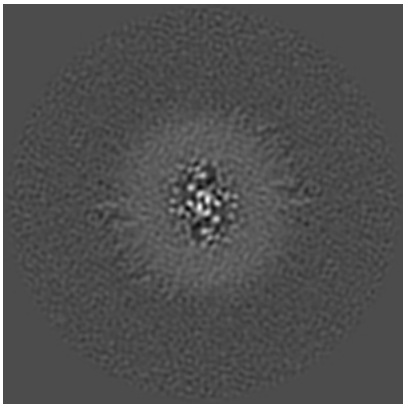
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 150

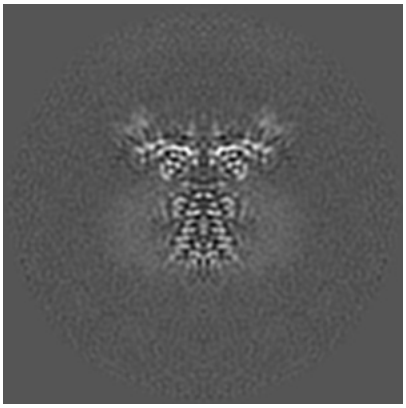

Y Index: 150


Z Index: 150

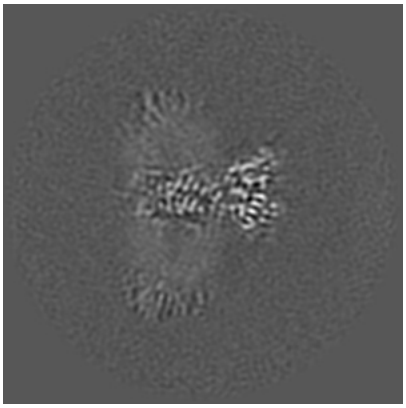
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

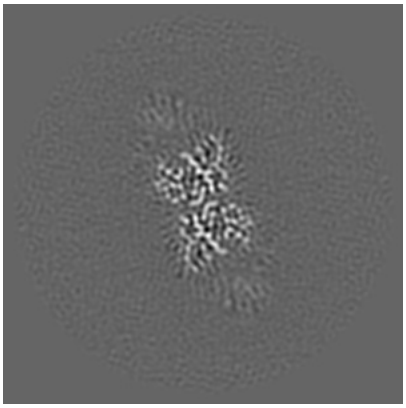
6.3.1 Primary map



X Index: 150



Y Index: 139



Z Index: 187

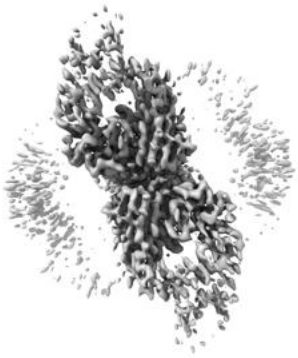
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

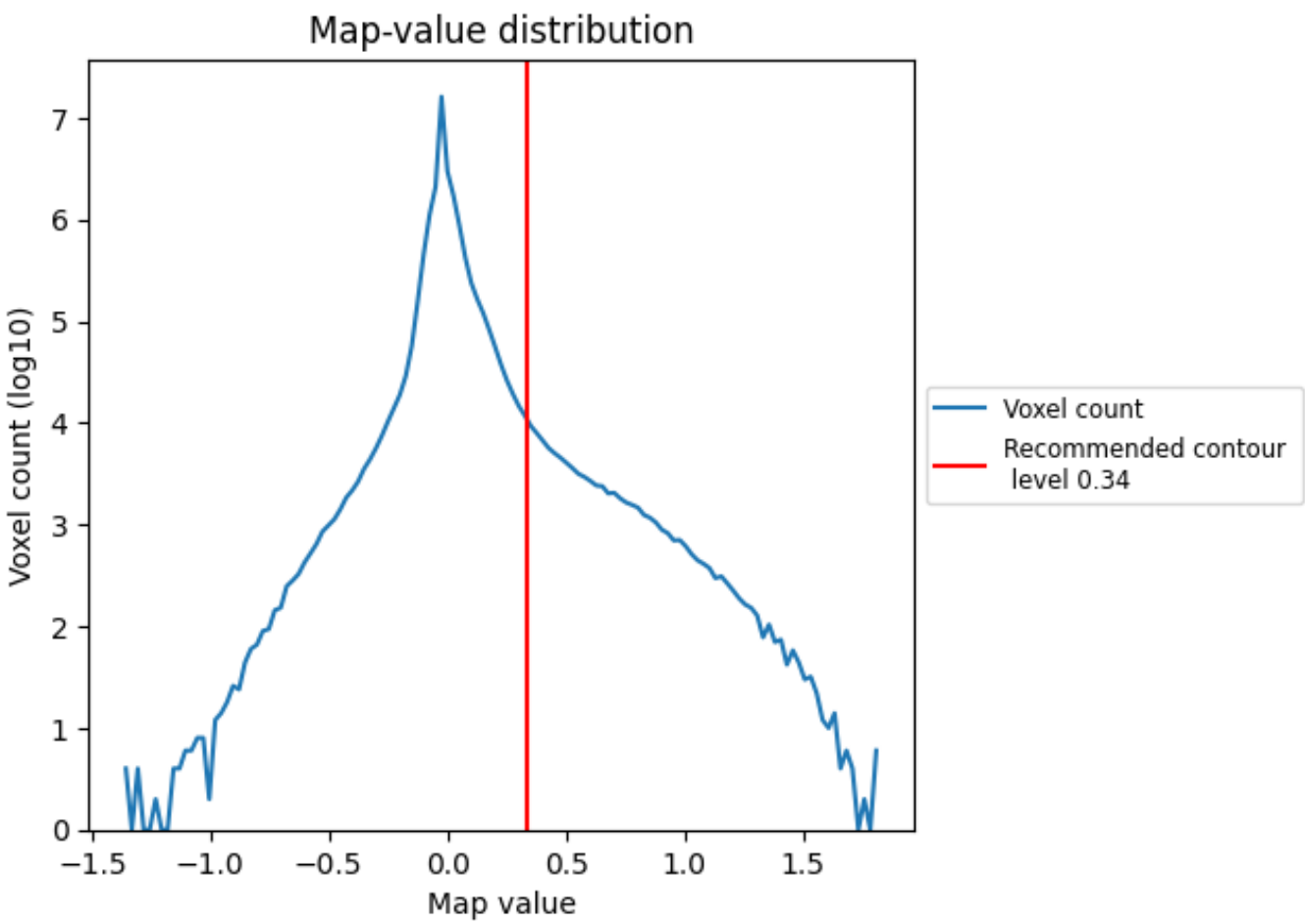
6.5 Mask visualisation (i)

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

7 Map analysis (i)

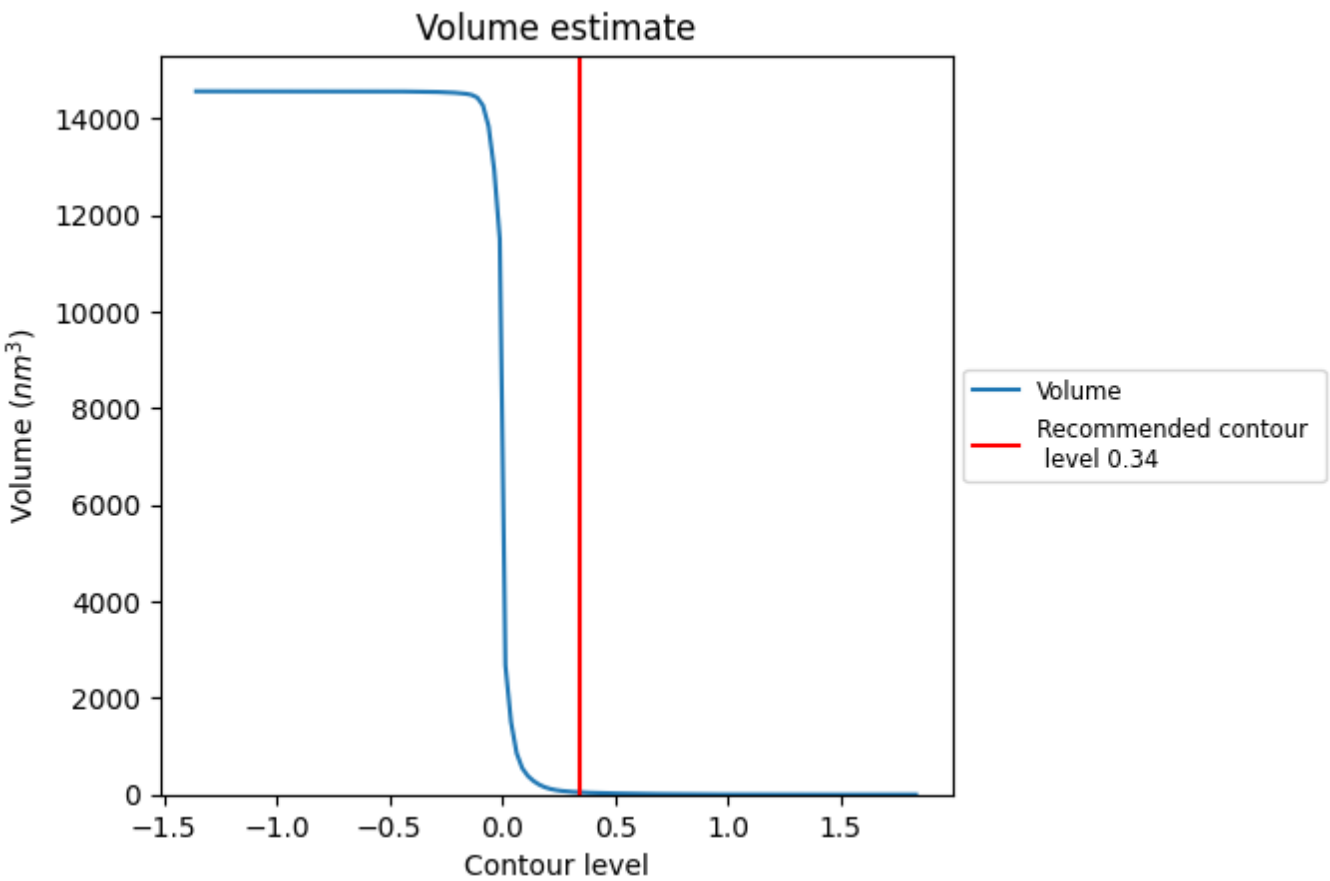
This section contains the results of statistical analysis of the map.

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.

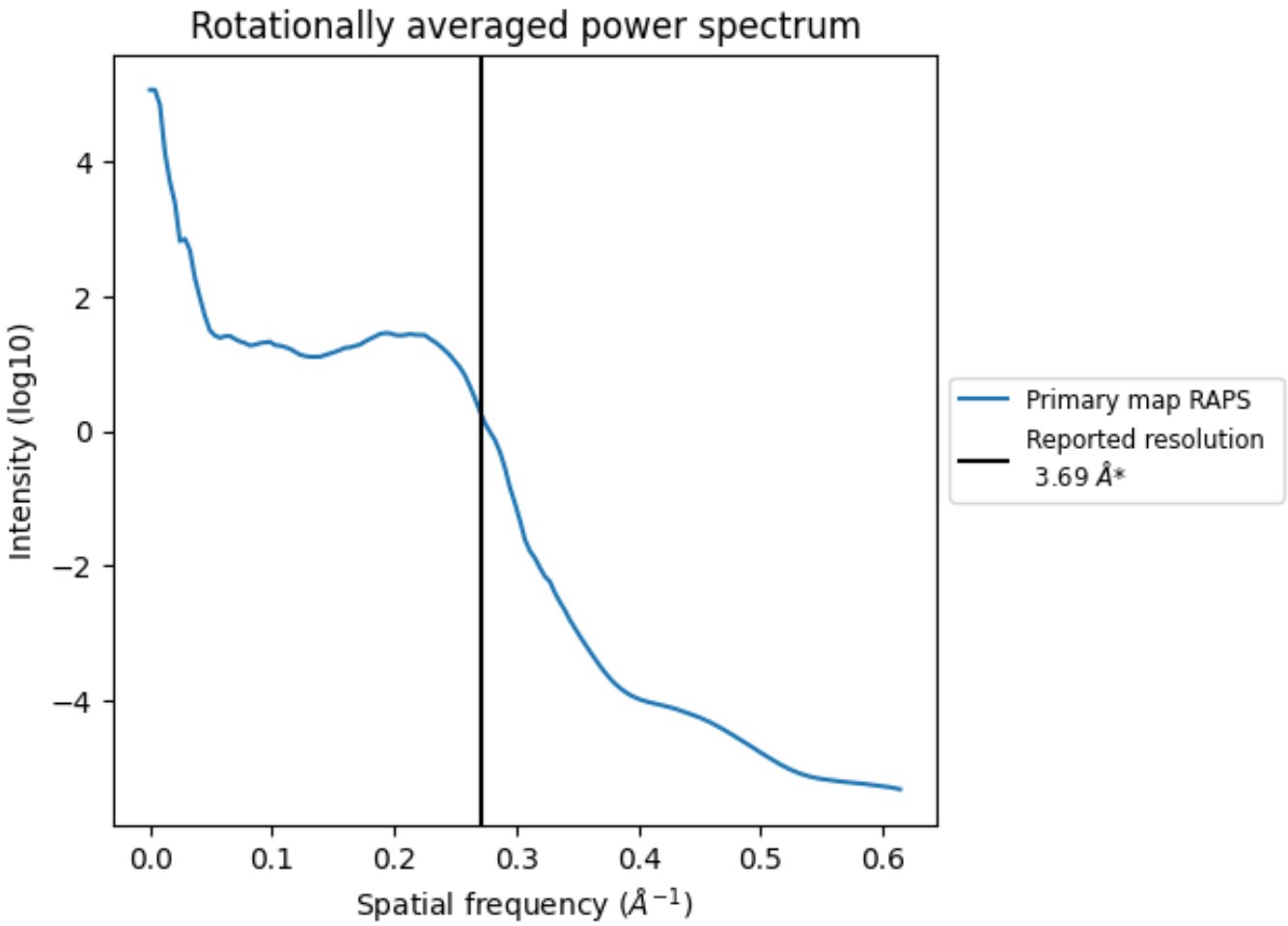
7.2 Volume estimate (i)



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 43 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 0.271 Å^{-1}

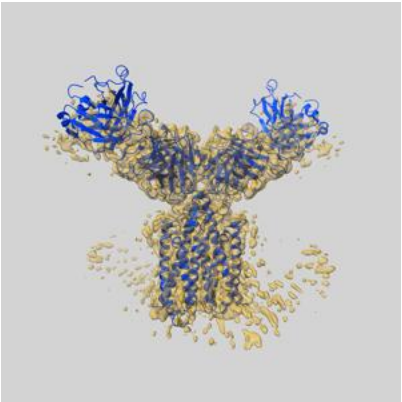
8 Fourier-Shell correlation (i)

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

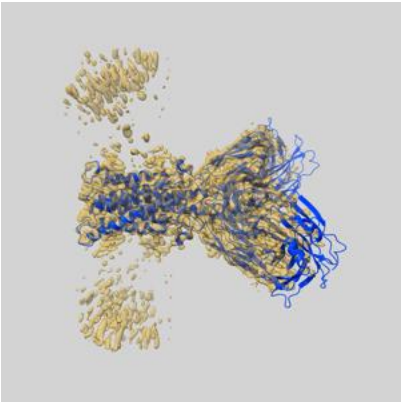
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10731 and PDB model 6Y90. Per-residue inclusion information can be found in section 3 on page 7.

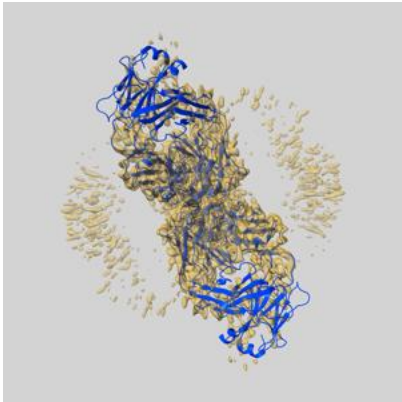
9.1 Map-model overlay (i)



X



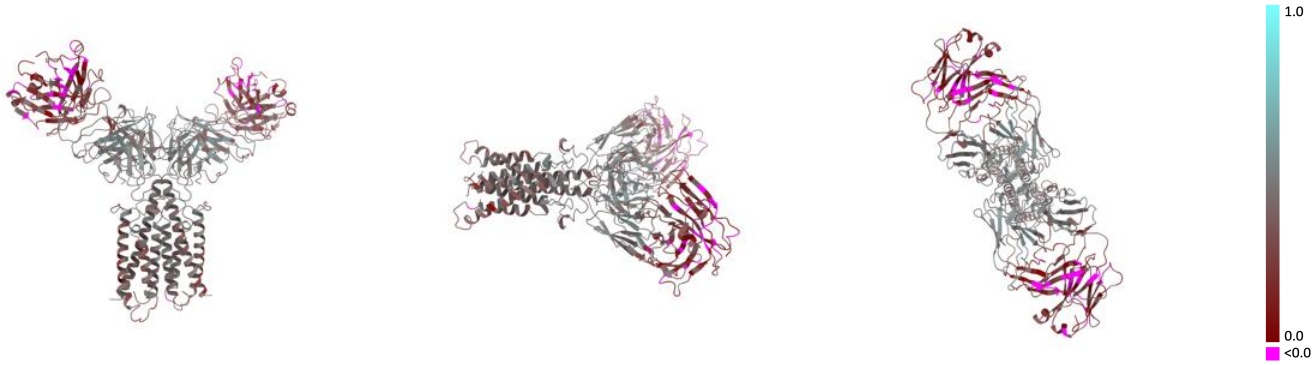
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.34 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.

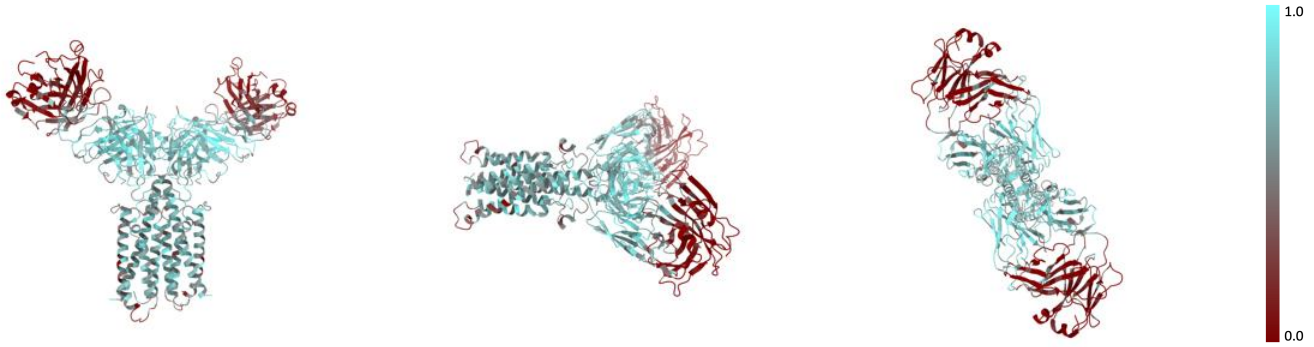
9.2 Q-score mapped to coordinate model (i)



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.

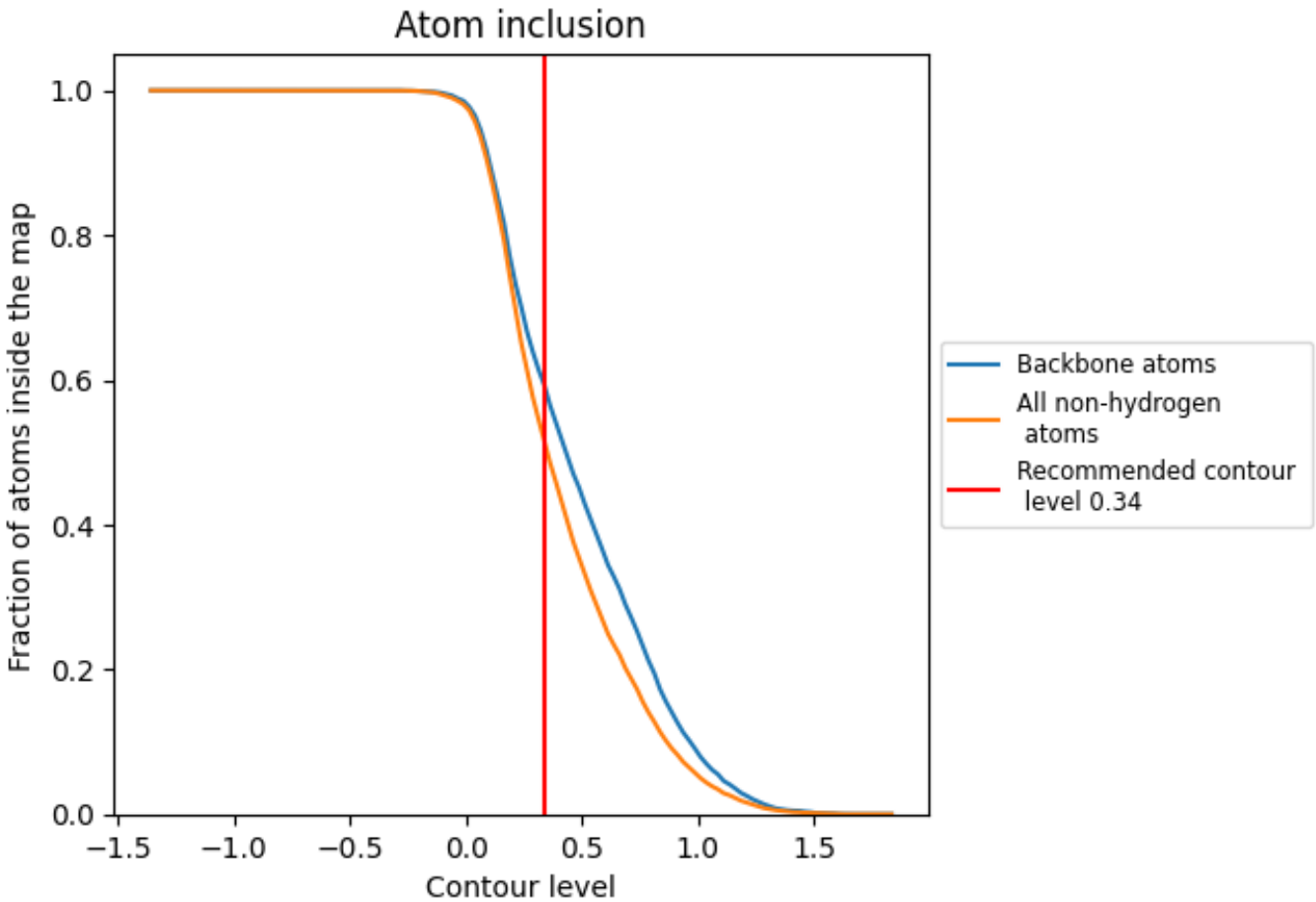
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.34).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 51% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5147	0.3650
A	0.5868	0.4070
B	0.5963	0.4130
C	0.4954	0.3460
D	0.4606	0.3370
H	0.4942	0.3490
L	0.4587	0.3370