Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 03:31 PM EST

PDB ID	:	5W3S
EMDB ID	:	EMD-8764
Title	:	Cryo-electron microscopy structure of a TRPML3 ion channel
Authors	:	Hirschi, M.; Herzik, M.A.; Wie, J.; Suo, Y.; Borschel, W.F.; Ren, D.; Lander, G.C.; Lee, S.Y.
Deposited on	:	2017-06-08
Resolution	:	2.94 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

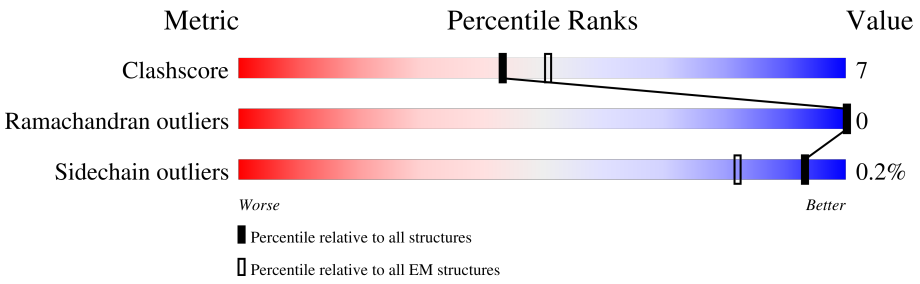
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 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	561	14% 75% 11% 14%
1	B	561	15% 75% 11% 14%
1	C	561	15% 75% 11% 14%
1	D	561	15% 75% 12% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31486 atoms, of which 15288 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 Mucolipin-3 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	485	7749	2574	3822	627	696	30	0	0
1	B	485	7749	2574	3822	627	696	30	0	0
1	C	485	7749	2574	3822	627	696	30	0	0
1	D	485	7749	2574	3822	627	696	30	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLN	ASN	engineered mutation	UNP F6RG56
A	554	SER	-	expression tag	UNP F6RG56
A	555	ASN	-	expression tag	UNP F6RG56
A	556	LEU	-	expression tag	UNP F6RG56
A	557	GLU	-	expression tag	UNP F6RG56
A	558	VAL	-	expression tag	UNP F6RG56
A	559	LEU	-	expression tag	UNP F6RG56
A	560	PHE	-	expression tag	UNP F6RG56
A	561	GLN	-	expression tag	UNP F6RG56
B	138	GLN	ASN	engineered mutation	UNP F6RG56
B	554	SER	-	expression tag	UNP F6RG56
B	555	ASN	-	expression tag	UNP F6RG56
B	556	LEU	-	expression tag	UNP F6RG56
B	557	GLU	-	expression tag	UNP F6RG56
B	558	VAL	-	expression tag	UNP F6RG56
B	559	LEU	-	expression tag	UNP F6RG56
B	560	PHE	-	expression tag	UNP F6RG56
B	561	GLN	-	expression tag	UNP F6RG56
C	138	GLN	ASN	engineered mutation	UNP F6RG56
C	554	SER	-	expression tag	UNP F6RG56
C	555	ASN	-	expression tag	UNP F6RG56
C	556	LEU	-	expression tag	UNP F6RG56

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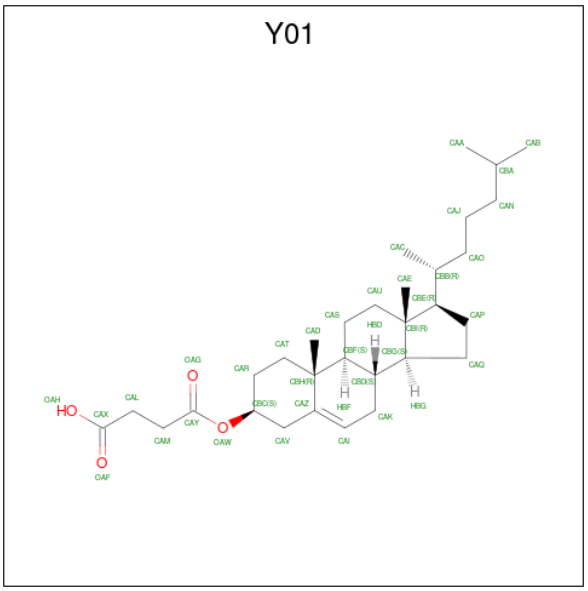
Chain	Residue	Modelled	Actual	Comment	Reference
C	557	GLU	-	expression tag	UNP F6RG56
C	558	VAL	-	expression tag	UNP F6RG56
C	559	LEU	-	expression tag	UNP F6RG56
C	560	PHE	-	expression tag	UNP F6RG56
C	561	GLN	-	expression tag	UNP F6RG56
D	138	GLN	ASN	engineered mutation	UNP F6RG56
D	554	SER	-	expression tag	UNP F6RG56
D	555	ASN	-	expression tag	UNP F6RG56
D	556	LEU	-	expression tag	UNP F6RG56
D	557	GLU	-	expression tag	UNP F6RG56
D	558	VAL	-	expression tag	UNP F6RG56
D	559	LEU	-	expression tag	UNP F6RG56
D	560	PHE	-	expression tag	UNP F6RG56
D	561	GLN	-	expression tag	UNP F6RG56

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	A	1	32	30	2	0
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	B	1	35	31	4	0

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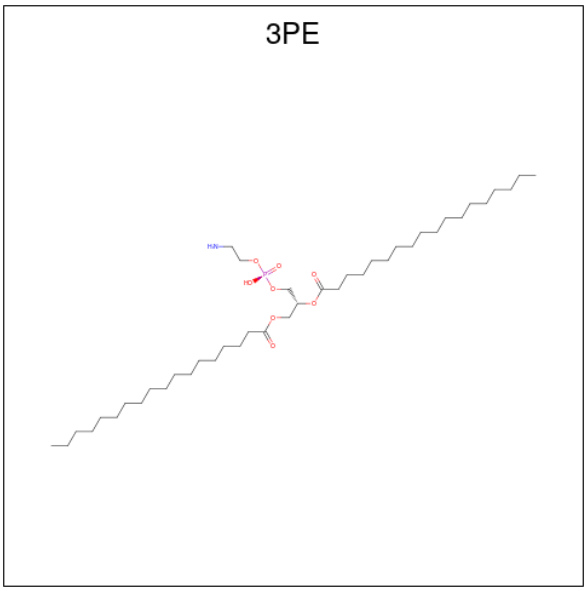
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	B	1	35	31	4	0
			Total	C	O	
2	B	1	32	30	2	0
			Total	C	O	
2	C	1	32	30	2	0
			Total	C	O	
2	C	1	35	31	4	0
			Total	C	O	
2	C	1	35	31	4	0
			Total	C	O	
2	D	1	35	31	4	0
			Total	C	O	
2	D	1	32	30	2	0
			Total	C	O	
2	D	1	35	31	4	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
3	A	2	2	2	0
			Total	Na	
3	C	3	3	3	0
			Total	Na	
3	D	1	1	1	0

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
4	A	1	18	18	0
4	B	1	18	18	0
4	C	1	18	18	0
4	D	1	18	18	0

- Molecule 5 is water.

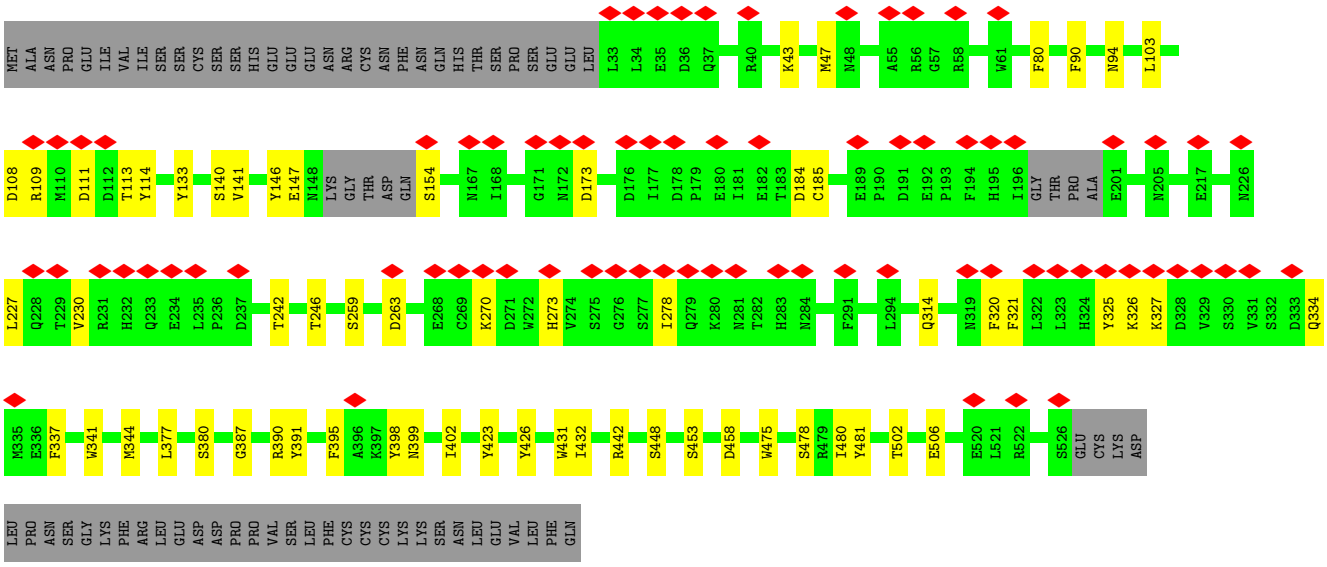
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	A	1	1	1	0
5	B	1	1	1	0
5	C	1	1	1	0
5	D	1	1	1	0

3 Residue-property plots (i)

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

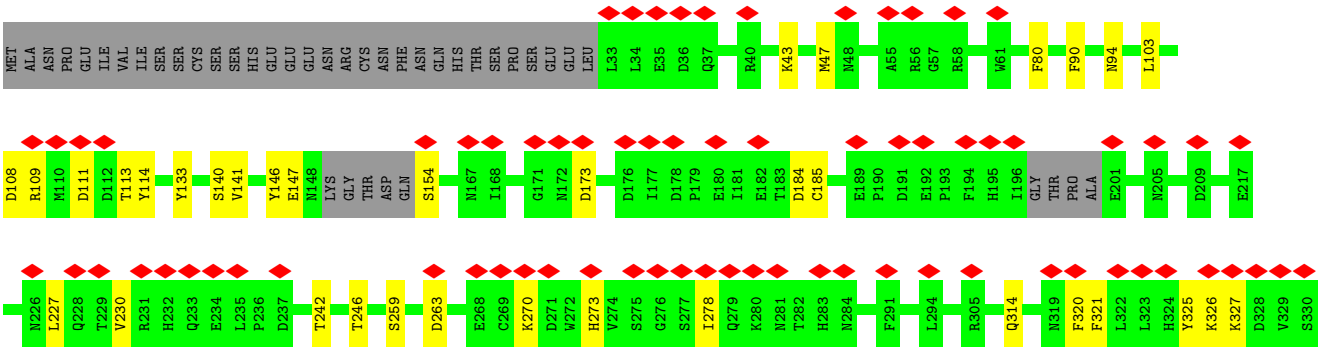
- Molecule 1: Mucolipin-3 isoform 1

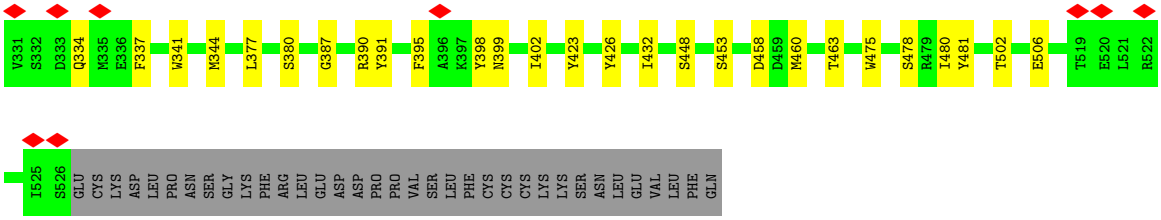
Chain A:



- Molecule 1: Mucolipin-3 isoform 1

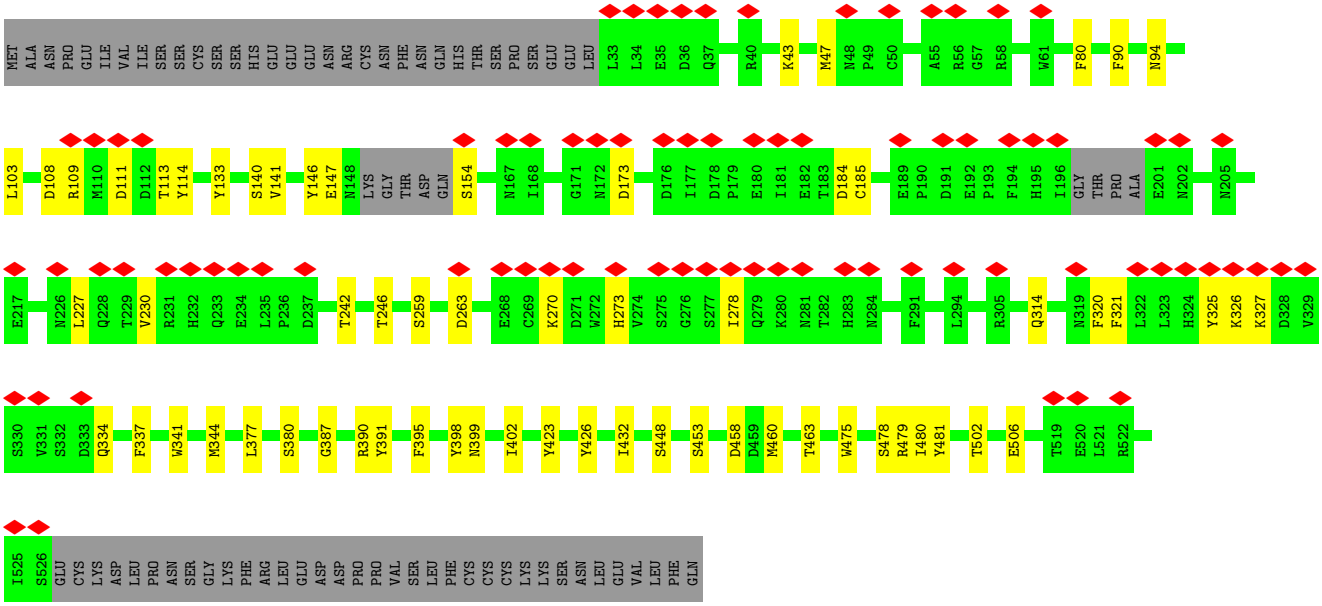
Chain B:





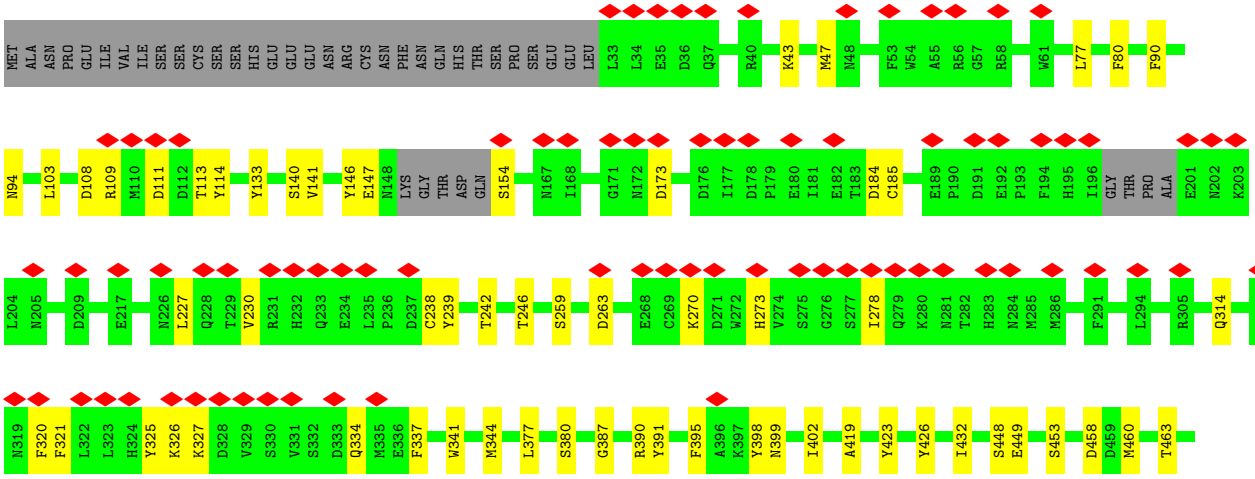
• Molecule 1: Mucolipin-3 isoform 1

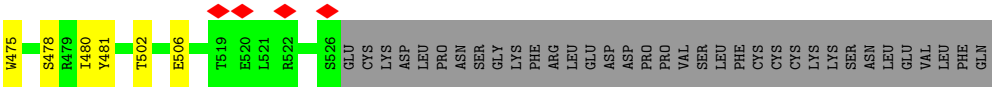
Chain C:



• Molecule 1: Mucolipin-3 isoform 1

Chain D:




W475
S478
R479
I480
Y481
T502
E506
T519
E520
L521
R522
S526
GLU
CYS
LYS
ASP
LEU
PRO
ASN
SER
GLY
LYS
PHE
ARG
LEU
GLU
ASP
ASP
PRO
PRO
VAL
SER
LEU
PHE
CYS
CYS
CYS
LYS
LYS
SER
SER
ASN
LEU
GLU
VAL
LEU
PHE
GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	104084	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 ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	167.68, 167.68, 167.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.655, 0.655, 0.655	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: 3PE, Y01, NA

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	0.35	0/4018	0.54	0/5441
1	B	0.35	0/4018	0.54	0/5441
1	C	0.35	0/4018	0.54	0/5441
1	D	0.35	0/4018	0.54	0/5441
All	All	0.35	0/16072	0.54	0/21764

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	3927	3822	3904	54	0
1	B	3927	3822	3904	55	0
1	C	3927	3822	3904	55	0
1	D	3927	3822	3904	58	0
2	A	102	0	145	16	0
2	B	102	0	145	15	0
2	C	102	0	145	18	0
2	D	102	0	145	18	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	35	0	0
4	B	18	0	35	0	0
4	C	18	0	35	0	0
4	D	18	0	35	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	16198	15288	16336	229	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 (229) 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:43:LYS:O	1:C:47:MET:HG3	1.77	0.85
1:C:341:TRP:CE3	1:C:344:MET:HE2	2.12	0.84
1:D:43:LYS:O	1:D:47:MET:HG3	1.77	0.84
1:A:43:LYS:O	1:A:47:MET:HG3	1.77	0.84
1:C:391:TYR:O	2:C:602:Y01:HAR1	1.77	0.83
1:B:43:LYS:O	1:B:47:MET:HG3	1.77	0.83
1:A:341:TRP:CE3	1:A:344:MET:HE2	2.15	0.81
1:A:80:PHE:CD2	1:B:432:ILE:HD11	2.17	0.80
1:B:314:GLN:HE21	1:B:337:PHE:HB2	1.48	0.79
1:D:341:TRP:CE3	1:D:344:MET:HE2	2.17	0.79
1:A:314:GLN:HE21	1:A:337:PHE:HB2	1.48	0.79
1:B:80:PHE:CD2	1:D:432:ILE:HD11	2.17	0.79
1:D:314:GLN:HE21	1:D:337:PHE:HB2	1.48	0.78
1:B:341:TRP:CE3	1:B:344:MET:HE2	2.20	0.77
1:C:314:GLN:HE21	1:C:337:PHE:HB2	1.48	0.77
1:D:242:THR:OG1	1:D:263:ASP:O	2.05	0.75
1:D:391:TYR:O	2:D:604:Y01:HAR1	1.87	0.74
1:A:432:ILE:HD11	1:C:80:PHE:CD2	2.23	0.74
1:C:242:THR:OG1	1:C:263:ASP:O	2.05	0.74
2:A:606:Y01:HBA	2:C:606:Y01:HAC2	1.70	0.73
2:B:602:Y01:HAC2	2:D:602:Y01:HBA	1.70	0.72
1:B:341:TRP:CE3	1:B:344:MET:CE	2.74	0.70
1:B:391:TYR:O	2:B:604:Y01:HAR1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:TRP:CE3	1:D:344:MET:CE	2.74	0.70
1:C:341:TRP:CE3	1:C:344:MET:CE	2.74	0.70
1:A:341:TRP:CE3	1:A:344:MET:CE	2.74	0.70
1:C:341:TRP:HE3	1:C:344:MET:HE2	1.57	0.69
1:A:242:THR:OG1	1:A:263:ASP:O	2.05	0.69
2:A:601:Y01:HAC2	2:B:601:Y01:HBA	1.75	0.69
2:C:607:Y01:HBA	2:D:605:Y01:HAC2	1.75	0.69
1:A:391:TYR:O	2:A:605:Y01:HAR1	1.93	0.68
1:A:80:PHE:HD2	1:B:432:ILE:HD11	1.59	0.68
1:B:242:THR:OG1	1:B:263:ASP:O	2.05	0.67
1:D:475:TRP:O	1:D:478:SER:OG	2.12	0.67
1:B:80:PHE:HD2	1:D:432:ILE:HD11	1.61	0.66
1:B:426:TYR:O	1:B:481:TYR:OH	2.12	0.66
1:C:387:GLY:O	1:C:390:ARG:HB3	1.96	0.65
1:B:387:GLY:O	1:B:390:ARG:HB3	1.96	0.65
1:C:432:ILE:HD11	1:D:80:PHE:CD2	2.31	0.65
1:B:475:TRP:O	1:B:478:SER:OG	2.12	0.65
1:A:387:GLY:O	1:A:390:ARG:HB3	1.96	0.65
1:A:426:TYR:O	1:A:481:TYR:OH	2.12	0.65
1:B:80:PHE:CE2	1:D:432:ILE:HD11	2.32	0.64
1:D:387:GLY:O	1:D:390:ARG:HB3	1.96	0.64
1:A:475:TRP:O	1:A:478:SER:OG	2.12	0.64
1:D:426:TYR:O	1:D:481:TYR:OH	2.12	0.64
1:C:133:TYR:O	1:C:146:TYR:OH	2.16	0.64
1:B:133:TYR:O	1:B:146:TYR:OH	2.16	0.64
1:B:341:TRP:HE3	1:B:344:MET:HE2	1.61	0.63
1:A:341:TRP:HE3	1:A:344:MET:CE	2.12	0.63
1:A:326:LYS:O	1:A:326:LYS:HG2	1.99	0.63
1:C:341:TRP:HE3	1:C:344:MET:CE	2.12	0.63
1:A:80:PHE:CE2	1:B:432:ILE:HD11	2.34	0.63
1:B:341:TRP:HE3	1:B:344:MET:CE	2.12	0.62
1:B:326:LYS:HG2	1:B:326:LYS:O	1.99	0.62
1:C:326:LYS:O	1:C:326:LYS:HG2	1.99	0.62
1:D:341:TRP:HE3	1:D:344:MET:HE2	1.60	0.62
1:A:133:TYR:O	1:A:146:TYR:OH	2.16	0.62
1:D:133:TYR:O	1:D:146:TYR:OH	2.16	0.62
1:D:341:TRP:HE3	1:D:344:MET:CE	2.12	0.62
1:D:326:LYS:O	1:D:326:LYS:HG2	1.99	0.62
1:A:432:ILE:HD11	1:C:80:PHE:HD2	1.64	0.61
1:A:341:TRP:HE3	1:A:344:MET:HE2	1.59	0.61
1:C:426:TYR:O	1:C:481:TYR:OH	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:TRP:O	1:C:478:SER:OG	2.12	0.60
1:C:453:SER:HB3	1:C:458:ASP:HB3	1.85	0.59
1:C:432:ILE:HD11	1:D:80:PHE:HD2	1.68	0.59
1:A:453:SER:HB3	1:A:458:ASP:HB3	1.85	0.59
1:C:480:ILE:HG23	2:C:607:Y01:HAC1	1.84	0.59
1:D:453:SER:HB3	1:D:458:ASP:HB3	1.85	0.59
1:B:453:SER:HB3	1:B:458:ASP:HB3	1.85	0.59
1:B:341:TRP:CZ3	1:B:344:MET:HE1	2.39	0.58
1:B:423:TYR:OH	1:B:448:SER:O	2.22	0.57
1:A:227:LEU:O	1:A:230:VAL:HG22	2.04	0.57
1:C:246:THR:OG1	1:C:259:SER:OG	2.22	0.57
1:A:246:THR:OG1	1:A:259:SER:OG	2.22	0.57
1:D:475:TRP:HZ3	2:D:602:Y01:HAL2	1.69	0.57
1:C:423:TYR:CE2	2:C:606:Y01:HAE2	2.39	0.57
1:A:432:ILE:HD11	1:C:80:PHE:CE2	2.39	0.57
1:D:227:LEU:O	1:D:230:VAL:HG22	2.04	0.57
1:A:423:TYR:OH	1:A:448:SER:O	2.22	0.57
1:D:246:THR:OG1	1:D:259:SER:OG	2.22	0.57
1:D:423:TYR:OH	1:D:448:SER:O	2.22	0.56
1:C:227:LEU:O	1:C:230:VAL:HG22	2.04	0.56
1:B:314:GLN:NE2	1:B:334:GLN:O	2.39	0.56
1:D:314:GLN:NE2	1:D:334:GLN:O	2.39	0.56
1:C:423:TYR:OH	1:C:448:SER:O	2.22	0.56
1:B:227:LEU:O	1:B:230:VAL:HG22	2.04	0.56
1:C:314:GLN:NE2	1:C:334:GLN:O	2.39	0.55
1:C:475:TRP:HZ3	2:C:607:Y01:HAL2	1.70	0.55
1:B:475:TRP:HZ3	2:B:601:Y01:HAL2	1.71	0.55
1:A:314:GLN:NE2	1:A:334:GLN:O	2.39	0.55
1:A:108:ASP:O	1:A:109:ARG:HB3	2.07	0.54
1:B:423:TYR:CE2	2:B:602:Y01:HAE2	2.42	0.54
1:A:423:TYR:CE2	2:A:601:Y01:HAE2	2.43	0.54
1:B:108:ASP:O	1:B:109:ARG:CB	2.55	0.54
1:B:108:ASP:O	1:B:109:ARG:HB3	2.07	0.54
1:C:113:THR:O	1:C:113:THR:HG22	2.08	0.54
1:A:108:ASP:O	1:A:109:ARG:CB	2.55	0.54
1:A:475:TRP:HZ3	2:A:606:Y01:HAL2	1.72	0.54
1:D:108:ASP:O	1:D:109:ARG:HB3	2.07	0.54
1:D:341:TRP:CZ3	1:D:344:MET:HE1	2.42	0.54
1:B:113:THR:HG22	1:B:113:THR:O	2.08	0.53
1:A:173:ASP:HB2	1:C:270:LYS:NZ	2.22	0.53
1:D:113:THR:HG22	1:D:113:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLU:OE2	1:C:154:SER:N	2.42	0.53
1:C:108:ASP:O	1:C:109:ARG:HB3	2.07	0.53
1:A:147:GLU:OE2	1:A:154:SER:N	2.42	0.53
1:A:113:THR:HG22	1:A:113:THR:O	2.08	0.53
1:D:108:ASP:O	1:D:109:ARG:CB	2.55	0.53
1:B:109:ARG:HG3	1:B:109:ARG:O	2.09	0.52
1:B:246:THR:OG1	1:B:259:SER:OG	2.22	0.52
1:C:109:ARG:O	1:C:109:ARG:HG3	2.09	0.52
1:B:147:GLU:OE2	1:B:154:SER:N	2.42	0.52
1:C:108:ASP:O	1:C:109:ARG:CB	2.55	0.52
1:D:109:ARG:HG3	1:D:109:ARG:O	2.09	0.52
1:D:502:THR:O	1:D:506:GLU:HG2	2.10	0.52
1:B:270:LYS:NZ	1:D:173:ASP:HB2	2.24	0.52
1:A:109:ARG:O	1:A:109:ARG:HG3	2.09	0.52
1:D:147:GLU:OE2	1:D:154:SER:N	2.42	0.52
1:C:502:THR:O	1:C:506:GLU:HG2	2.10	0.52
1:A:341:TRP:CZ3	1:A:344:MET:HE1	2.46	0.51
1:D:273:HIS:NE2	1:D:278:ILE:HG12	2.25	0.51
1:B:502:THR:O	1:B:506:GLU:HG2	2.10	0.51
1:A:502:THR:O	1:A:506:GLU:HG2	2.10	0.51
1:B:273:HIS:NE2	1:B:278:ILE:HG12	2.25	0.51
1:C:273:HIS:NE2	1:C:278:ILE:HG12	2.25	0.51
1:A:273:HIS:NE2	1:A:278:ILE:HG12	2.25	0.50
1:C:320:PHE:C	1:C:320:PHE:CD2	2.86	0.49
1:A:320:PHE:C	1:A:320:PHE:CD2	2.86	0.49
1:D:320:PHE:C	1:D:320:PHE:CD2	2.86	0.49
1:A:270:LYS:NZ	1:B:173:ASP:HB2	2.27	0.49
1:A:90:PHE:O	1:A:94:ASN:ND2	2.46	0.49
1:D:90:PHE:O	1:D:94:ASN:ND2	2.46	0.49
1:B:90:PHE:O	1:B:94:ASN:ND2	2.46	0.48
1:D:423:TYR:CE2	2:D:605:Y01:HAE2	2.48	0.48
2:D:604:Y01:CAL	2:D:604:Y01:HAV1	2.43	0.48
2:A:605:Y01:CAL	2:A:605:Y01:HAV1	2.44	0.48
1:B:320:PHE:C	1:B:320:PHE:CD2	2.86	0.48
2:B:604:Y01:CAL	2:B:604:Y01:HAV1	2.43	0.48
1:B:377:LEU:O	1:B:380:SER:OG	2.27	0.48
1:B:480:ILE:HG23	2:B:601:Y01:HAC1	1.95	0.48
1:C:90:PHE:O	1:C:94:ASN:ND2	2.46	0.48
1:C:475:TRP:CZ3	2:C:607:Y01:HAL2	2.47	0.48
2:C:602:Y01:HAV1	2:C:602:Y01:CAL	2.43	0.48
1:B:321:PHE:CD2	1:B:327:LYS:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:CD2	1:A:327:LYS:O	2.67	0.48
1:C:321:PHE:CD2	1:C:327:LYS:O	2.67	0.48
1:A:140:SER:OG	1:A:141:VAL:N	2.47	0.47
1:C:391:TYR:HB3	2:C:602:Y01:HAT1	1.97	0.47
1:B:140:SER:OG	1:B:141:VAL:N	2.47	0.47
1:D:475:TRP:CZ3	2:D:602:Y01:HAL2	2.50	0.47
1:D:480:ILE:HG23	2:D:602:Y01:HAC1	1.96	0.47
1:D:321:PHE:CD2	1:D:327:LYS:O	2.67	0.47
2:A:605:Y01:HAO2	2:A:605:Y01:HAP1	1.39	0.47
1:C:423:TYR:CD2	2:C:606:Y01:HAE2	2.49	0.47
1:B:395:PHE:O	1:B:399:ASN:HB2	2.15	0.47
1:B:460:MET:O	1:B:463:THR:OG1	2.20	0.46
2:C:602:Y01:HAO2	2:C:602:Y01:HAP1	1.37	0.46
2:B:604:Y01:HAP1	2:B:604:Y01:HAO2	1.37	0.46
1:D:377:LEU:O	1:D:380:SER:OG	2.27	0.46
1:B:341:TRP:CE3	1:B:344:MET:HE1	2.50	0.46
1:D:140:SER:OG	1:D:141:VAL:N	2.47	0.46
1:A:423:TYR:CD2	2:A:601:Y01:HAE2	2.50	0.46
1:C:140:SER:OG	1:C:141:VAL:N	2.47	0.46
1:A:480:ILE:HG23	2:A:606:Y01:HAC1	1.97	0.46
1:B:475:TRP:CZ3	2:B:601:Y01:HAL2	2.50	0.46
1:C:395:PHE:O	1:C:399:ASN:HB2	2.16	0.46
1:D:395:PHE:O	1:D:399:ASN:HB2	2.16	0.45
1:C:341:TRP:CZ3	1:C:344:MET:HE1	2.51	0.45
2:C:607:Y01:HAA3	2:D:605:Y01:HAN2	1.97	0.45
1:A:395:PHE:O	1:A:399:ASN:HB2	2.16	0.45
1:C:432:ILE:HD12	1:D:77:LEU:HG	1.99	0.45
1:D:460:MET:O	1:D:463:THR:OG1	2.20	0.45
2:A:606:Y01:HAM1	2:C:606:Y01:OAG	2.17	0.45
1:B:184:ASP:OD1	1:B:185:CYS:N	2.50	0.45
2:D:604:Y01:HAC3	2:D:604:Y01:HAJ1	1.79	0.44
2:A:601:Y01:HAN2	2:B:601:Y01:HAA3	1.99	0.44
1:B:423:TYR:CD2	2:B:602:Y01:HAE2	2.52	0.44
1:A:475:TRP:CZ3	2:A:606:Y01:HAL2	2.51	0.44
2:A:606:Y01:HAA3	2:C:606:Y01:HAN2	2.00	0.44
1:C:432:ILE:HD11	1:D:80:PHE:CE2	2.52	0.44
1:D:423:TYR:CD2	2:D:605:Y01:HAE2	2.53	0.43
2:B:602:Y01:OAG	2:D:602:Y01:HAM1	2.19	0.43
1:C:460:MET:O	1:C:463:THR:OG1	2.20	0.43
1:B:398:TYR:O	1:B:402:ILE:HD12	2.19	0.43
1:D:184:ASP:OD1	1:D:185:CYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:TYR:HB3	2:D:604:Y01:HAT1	2.01	0.43
2:A:601:Y01:HAO1	2:A:601:Y01:HAP1	1.62	0.43
2:A:605:Y01:HAJ1	2:A:605:Y01:HAC3	1.77	0.43
1:D:419:ALA:HB3	2:D:605:Y01:HAA2	2.00	0.43
2:B:602:Y01:HAN2	2:D:602:Y01:HAA3	2.01	0.42
2:D:605:Y01:HAP1	2:D:605:Y01:HAO1	1.63	0.42
2:C:606:Y01:HAO1	2:C:606:Y01:HAP1	1.66	0.42
2:C:607:Y01:HAB1	2:C:607:Y01:HAJ1	1.79	0.42
1:D:398:TYR:O	1:D:402:ILE:HD12	2.19	0.42
1:B:341:TRP:HZ3	1:B:344:MET:HE1	1.83	0.42
1:A:184:ASP:OD1	1:A:185:CYS:N	2.50	0.42
1:C:103:LEU:HD12	1:C:114:TYR:OH	2.19	0.42
1:C:184:ASP:OD1	1:C:185:CYS:N	2.50	0.42
1:A:398:TYR:O	1:A:402:ILE:HD12	2.19	0.42
1:B:109:ARG:C	1:B:111:ASP:H	2.23	0.42
2:B:602:Y01:HAP1	2:B:602:Y01:HAO1	1.66	0.42
1:C:398:TYR:O	1:C:402:ILE:HD12	2.19	0.42
1:A:80:PHE:HD2	1:B:432:ILE:CD1	2.30	0.42
1:A:103:LEU:HD12	1:A:114:TYR:OH	2.19	0.42
1:A:341:TRP:CZ3	1:A:344:MET:CE	3.03	0.42
1:A:109:ARG:C	1:A:111:ASP:H	2.23	0.42
1:A:431:TRP:NE1	1:A:442:ARG:O	2.48	0.42
1:C:173:ASP:HB2	1:D:270:LYS:NZ	2.35	0.42
2:C:602:Y01:HAJ1	2:C:602:Y01:HAC3	1.79	0.42
2:D:604:Y01:HAP1	2:D:604:Y01:HAO2	1.37	0.42
1:B:103:LEU:HD12	1:B:114:TYR:OH	2.19	0.41
1:D:103:LEU:HD12	1:D:114:TYR:OH	2.19	0.41
1:D:109:ARG:C	1:D:111:ASP:N	2.74	0.41
1:D:341:TRP:CZ3	1:D:344:MET:CE	3.03	0.41
1:C:479:ARG:NH2	1:D:449:GLU:OE2	2.53	0.41
2:A:601:Y01:OAG	2:B:601:Y01:HAM1	2.20	0.41
1:C:341:TRP:CZ3	1:C:344:MET:CE	3.03	0.41
1:A:109:ARG:C	1:A:111:ASP:N	2.74	0.41
1:B:109:ARG:C	1:B:111:ASP:N	2.74	0.41
1:C:377:LEU:O	1:C:380:SER:OG	2.27	0.41
1:D:109:ARG:C	1:D:111:ASP:H	2.23	0.41
1:D:238:CYS:SG	1:D:239:TYR:N	2.94	0.41
1:C:109:ARG:C	1:C:111:ASP:H	2.23	0.41
2:C:607:Y01:HAM1	2:D:605:Y01:OAG	2.20	0.41
1:A:173:ASP:HB2	1:C:270:LYS:HZ2	1.85	0.40
1:A:377:LEU:O	1:A:380:SER:OG	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:HD2	1:D:432:ILE:CD1	2.30	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	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
1	B	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
1	C	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
1	D	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
All	All	1916/2244 (85%)	1836 (96%)	80 (4%)	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	431/515 (84%)	430 (100%)	1 (0%)	93	98
1	B	431/515 (84%)	430 (100%)	1 (0%)	93	98
1	C	431/515 (84%)	430 (100%)	1 (0%)	93	98
1	D	431/515 (84%)	430 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1724/2060 (84%)	1720 (100%)	4 (0%)	93 98

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

Mol	Chain	Res	Type
1	A	325	TYR
1	B	325	TYR
1	C	325	TYR
1	D	325	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	314	GLN
1	B	314	GLN
1	C	314	GLN
1	D	314	GLN

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)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	Y01	D	602	-	38,38,38	0.69	0	57,57,57	0.86	0
2	Y01	C	607	-	38,38,38	0.69	0	57,57,57	0.87	1 (1%)
4	3PE	C	601	-	17,17,50	0.91	1 (5%)	16,16,55	0.91	0
4	3PE	D	603	-	17,17,50	0.91	1 (5%)	16,16,55	0.91	0
4	3PE	B	603	-	17,17,50	0.91	1 (5%)	16,16,55	0.91	0
2	Y01	A	601	-	38,38,38	0.67	0	57,57,57	0.79	0
2	Y01	B	601	-	38,38,38	0.70	0	57,57,57	0.87	0
2	Y01	D	605	-	38,38,38	0.66	0	57,57,57	0.80	0
2	Y01	B	602	-	38,38,38	0.67	0	57,57,57	0.80	1 (1%)
2	Y01	A	606	-	38,38,38	0.69	0	57,57,57	0.86	0
2	Y01	C	602	-	35,35,38	0.66	0	53,53,57	0.81	0
2	Y01	C	606	-	38,38,38	0.66	0	57,57,57	0.80	0
4	3PE	A	604	-	17,17,50	0.91	1 (5%)	16,16,55	0.91	0
2	Y01	D	604	-	35,35,38	0.66	0	53,53,57	0.81	0
2	Y01	A	605	-	35,35,38	0.65	0	53,53,57	0.81	0
2	Y01	B	604	-	35,35,38	0.66	0	53,53,57	0.81	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
2	Y01	D	602	-	-	10/19/77/77	0/4/4/4
2	Y01	C	607	-	-	11/19/77/77	0/4/4/4
4	3PE	C	601	-	-	6/15/15/54	-
4	3PE	D	603	-	-	6/15/15/54	-
4	3PE	B	603	-	-	6/15/15/54	-
2	Y01	A	601	-	-	13/19/77/77	0/4/4/4
2	Y01	B	601	-	-	11/19/77/77	0/4/4/4
2	Y01	D	605	-	-	13/19/77/77	0/4/4/4
2	Y01	B	602	-	-	13/19/77/77	0/4/4/4
2	Y01	A	606	-	-	10/19/77/77	0/4/4/4
2	Y01	C	602	-	-	12/16/74/77	0/4/4/4
2	Y01	C	606	-	-	13/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3PE	A	604	-	-	6/15/15/54	-
2	Y01	D	604	-	-	12/16/74/77	0/4/4/4
2	Y01	A	605	-	-	12/16/74/77	0/4/4/4
2	Y01	B	604	-	-	12/16/74/77	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	3PE	C3A-C39	-2.81	1.35	1.51
4	A	604	3PE	C3A-C39	-2.81	1.35	1.51
4	B	603	3PE	C3A-C39	-2.80	1.35	1.51
4	D	603	3PE	C3A-C39	-2.78	1.36	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	Y01	CAD-CBH-CBF	-2.02	109.27	111.68
2	C	607	Y01	CBH-CAZ-CAI	-2.01	119.83	122.90

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	Y01	CAO-CBB-CBE-CAP
2	A	601	Y01	CAO-CBB-CBE-CBI
2	A	601	Y01	CAC-CBB-CBE-CBI
2	A	601	Y01	CAR-CBC-OAW-CAY
2	A	601	Y01	CAM-CAY-OAW-CBC
2	A	605	Y01	CAV-CBC-OAW-CAY
2	A	605	Y01	CAM-CAY-OAW-CBC
2	A	606	Y01	CAM-CAY-OAW-CBC
2	B	601	Y01	CAM-CAY-OAW-CBC
2	B	602	Y01	CAO-CBB-CBE-CAP
2	B	602	Y01	CAO-CBB-CBE-CBI
2	B	602	Y01	CAC-CBB-CBE-CBI
2	B	602	Y01	CAM-CAY-OAW-CBC
2	B	604	Y01	CAV-CBC-OAW-CAY
2	B	604	Y01	CAM-CAY-OAW-CBC
2	C	602	Y01	CAV-CBC-OAW-CAY
2	C	602	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
2	C	606	Y01	CAO-CBB-CBE-CAP
2	C	606	Y01	CAO-CBB-CBE-CBI
2	C	606	Y01	CAC-CBB-CBE-CBI
2	C	606	Y01	CAM-CAY-OAW-CBC
2	C	607	Y01	CAM-CAY-OAW-CBC
2	D	602	Y01	CAM-CAY-OAW-CBC
2	D	604	Y01	CAV-CBC-OAW-CAY
2	D	604	Y01	CAM-CAY-OAW-CBC
2	D	605	Y01	CAO-CBB-CBE-CAP
2	D	605	Y01	CAO-CBB-CBE-CBI
2	D	605	Y01	CAC-CBB-CBE-CBI
2	D	605	Y01	CAM-CAY-OAW-CBC
2	B	602	Y01	CAR-CBC-OAW-CAY
2	A	601	Y01	CAC-CBB-CBE-CAP
2	B	602	Y01	CAC-CBB-CBE-CAP
2	C	606	Y01	CAC-CBB-CBE-CAP
2	D	605	Y01	CAC-CBB-CBE-CAP
2	A	601	Y01	OAG-CAY-OAW-CBC
2	A	605	Y01	OAG-CAY-OAW-CBC
2	B	602	Y01	OAG-CAY-OAW-CBC
2	B	604	Y01	OAG-CAY-OAW-CBC
2	C	602	Y01	OAG-CAY-OAW-CBC
2	C	606	Y01	OAG-CAY-OAW-CBC
2	D	604	Y01	OAG-CAY-OAW-CBC
2	D	605	Y01	OAG-CAY-OAW-CBC
2	D	605	Y01	CAR-CBC-OAW-CAY
2	A	606	Y01	CAC-CBB-CBE-CAP
2	B	601	Y01	CAC-CBB-CBE-CAP
2	C	607	Y01	CAC-CBB-CBE-CAP
2	D	602	Y01	CAC-CBB-CBE-CAP
2	A	606	Y01	CAC-CBB-CBE-CBI
2	B	601	Y01	CAC-CBB-CBE-CBI
2	C	607	Y01	CAC-CBB-CBE-CBI
2	D	602	Y01	CAC-CBB-CBE-CBI
2	A	606	Y01	CAO-CBB-CBE-CBI
2	B	601	Y01	CAO-CBB-CBE-CBI
2	C	607	Y01	CAO-CBB-CBE-CBI
2	D	602	Y01	CAO-CBB-CBE-CBI
2	A	606	Y01	OAG-CAY-OAW-CBC
2	B	601	Y01	OAG-CAY-OAW-CBC
2	C	607	Y01	OAG-CAY-OAW-CBC
2	D	602	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
2	A	606	Y01	CAO-CBB-CBE-CAP
2	B	601	Y01	CAO-CBB-CBE-CAP
2	C	607	Y01	CAO-CBB-CBE-CAP
2	D	602	Y01	CAO-CBB-CBE-CAP
2	C	606	Y01	CAR-CBC-OAW-CAY
2	A	605	Y01	CAJ-CAO-CBB-CAC
2	B	604	Y01	CAJ-CAO-CBB-CAC
2	C	602	Y01	CAJ-CAO-CBB-CAC
2	D	604	Y01	CAJ-CAO-CBB-CAC
2	A	605	Y01	CAO-CBB-CBE-CBI
2	C	606	Y01	CAV-CBC-OAW-CAY
2	B	604	Y01	CAO-CBB-CBE-CBI
2	C	602	Y01	CAO-CBB-CBE-CBI
2	D	604	Y01	CAO-CBB-CBE-CBI
2	A	605	Y01	CAC-CBB-CBE-CAP
2	B	604	Y01	CAC-CBB-CBE-CAP
2	C	602	Y01	CAC-CBB-CBE-CAP
2	D	604	Y01	CAC-CBB-CBE-CAP
2	A	605	Y01	CAO-CBB-CBE-CAP
2	A	605	Y01	CAC-CBB-CBE-CBI
2	D	605	Y01	CAV-CBC-OAW-CAY
2	C	602	Y01	CAC-CBB-CBE-CBI
2	D	604	Y01	CAC-CBB-CBE-CBI
2	B	604	Y01	CAO-CBB-CBE-CAP
2	C	602	Y01	CAO-CBB-CBE-CAP
2	D	604	Y01	CAO-CBB-CBE-CAP
2	B	604	Y01	CAC-CBB-CBE-CBI
2	B	602	Y01	CAV-CBC-OAW-CAY
2	B	601	Y01	CAN-CAJ-CAO-CBB
2	C	607	Y01	CAN-CAJ-CAO-CBB
2	A	606	Y01	CAN-CAJ-CAO-CBB
2	D	602	Y01	CAN-CAJ-CAO-CBB
4	D	603	3PE	C37-C38-C39-C3A
2	A	605	Y01	CAN-CAJ-CAO-CBB
2	A	601	Y01	CAV-CBC-OAW-CAY
4	A	604	3PE	C37-C38-C39-C3A
4	B	603	3PE	C37-C38-C39-C3A
4	C	601	3PE	C37-C38-C39-C3A
2	C	602	Y01	CAN-CAJ-CAO-CBB
2	D	604	Y01	CAN-CAJ-CAO-CBB
2	B	604	Y01	CAN-CAJ-CAO-CBB
4	D	603	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	B	603	3PE	C35-C36-C37-C38
4	A	604	3PE	C35-C36-C37-C38
4	C	601	3PE	C35-C36-C37-C38
4	A	604	3PE	C31-C32-C33-C34
4	D	603	3PE	C31-C32-C33-C34
4	B	603	3PE	C31-C32-C33-C34
4	C	601	3PE	C31-C32-C33-C34
2	D	605	Y01	CAN-CAJ-CAO-CBB
2	A	601	Y01	CAN-CAJ-CAO-CBB
2	C	606	Y01	CAN-CAJ-CAO-CBB
2	D	605	Y01	CAJ-CAN-CBA-CAB
4	A	604	3PE	C34-C35-C36-C37
4	B	603	3PE	C34-C35-C36-C37
4	C	601	3PE	C34-C35-C36-C37
4	D	603	3PE	C34-C35-C36-C37
2	A	601	Y01	CAJ-CAN-CBA-CAB
2	B	602	Y01	CAN-CAJ-CAO-CBB
2	A	605	Y01	CAO-CAJ-CAN-CBA
2	B	602	Y01	CAJ-CAN-CBA-CAB
2	C	606	Y01	CAJ-CAN-CBA-CAB
4	B	603	3PE	C32-C33-C34-C35
4	D	603	3PE	C32-C33-C34-C35
4	A	604	3PE	C32-C33-C34-C35
4	C	601	3PE	C32-C33-C34-C35
2	D	605	Y01	CAJ-CAN-CBA-CAA
4	C	601	3PE	C3A-C3B-C3C-C3D
4	A	604	3PE	C3A-C3B-C3C-C3D
4	B	603	3PE	C3A-C3B-C3C-C3D
2	A	601	Y01	CAJ-CAN-CBA-CAA
4	D	603	3PE	C3A-C3B-C3C-C3D
2	A	605	Y01	CAJ-CAN-CBA-CAA
2	B	602	Y01	CAJ-CAN-CBA-CAA
2	A	605	Y01	CAJ-CAN-CBA-CAB
2	C	606	Y01	CAJ-CAN-CBA-CAA
2	D	604	Y01	CAJ-CAN-CBA-CAA
2	D	604	Y01	CAJ-CAN-CBA-CAB
2	C	602	Y01	CAJ-CAN-CBA-CAA
2	C	602	Y01	CAJ-CAN-CBA-CAB
2	B	604	Y01	CAJ-CAN-CBA-CAB
2	C	607	Y01	CAM-CAL-CAX-OAH
2	C	607	Y01	CAM-CAL-CAX-OAF
2	B	604	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
2	B	601	Y01	CAM-CAL-CAX-OAH
2	B	601	Y01	CAM-CAL-CAX-OAF
2	D	602	Y01	CAM-CAL-CAX-OAF
2	D	602	Y01	CAM-CAL-CAX-OAH
2	A	606	Y01	CAM-CAL-CAX-OAH
2	A	606	Y01	CAM-CAL-CAX-OAF
2	A	606	Y01	CAX-CAL-CAM-CAY
2	D	602	Y01	CAX-CAL-CAM-CAY
2	C	606	Y01	CAM-CAL-CAX-OAH
2	D	605	Y01	CAM-CAL-CAX-OAH
2	A	601	Y01	CAM-CAL-CAX-OAH
2	B	602	Y01	CAM-CAL-CAX-OAH
2	B	602	Y01	CAM-CAL-CAX-OAF
2	C	606	Y01	CAM-CAL-CAX-OAF
2	A	601	Y01	CAM-CAL-CAX-OAF
2	D	605	Y01	CAM-CAL-CAX-OAF
2	D	604	Y01	CAO-CAJ-CAN-CBA
2	C	607	Y01	CAX-CAL-CAM-CAY
2	B	601	Y01	CAX-CAL-CAM-CAY
2	B	601	Y01	CAJ-CAN-CBA-CAB
2	C	607	Y01	CAJ-CAN-CBA-CAB
2	C	602	Y01	CAO-CAJ-CAN-CBA
2	B	604	Y01	CAO-CAJ-CAN-CBA

There are no ring outliers.

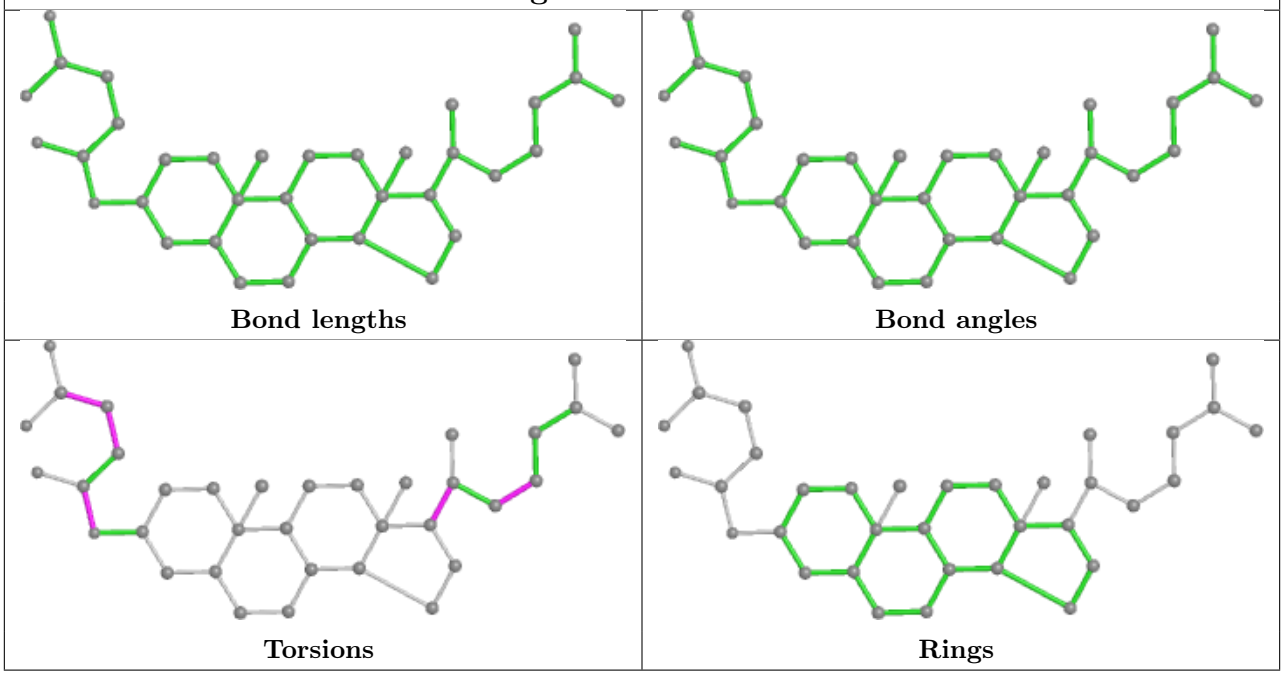
12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	Y01	6	0
2	C	607	Y01	7	0
2	A	601	Y01	6	0
2	B	601	Y01	6	0
2	D	605	Y01	7	0
2	B	602	Y01	6	0
2	A	606	Y01	6	0
2	C	602	Y01	5	0
2	C	606	Y01	6	0
2	D	604	Y01	5	0
2	A	605	Y01	4	0
2	B	604	Y01	3	0

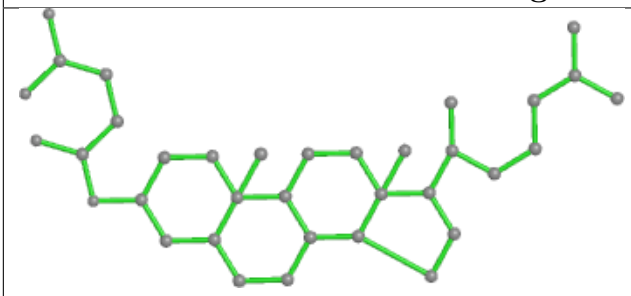
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

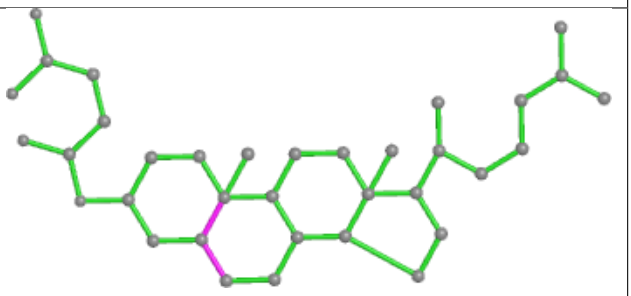
Ligand Y01 D 602



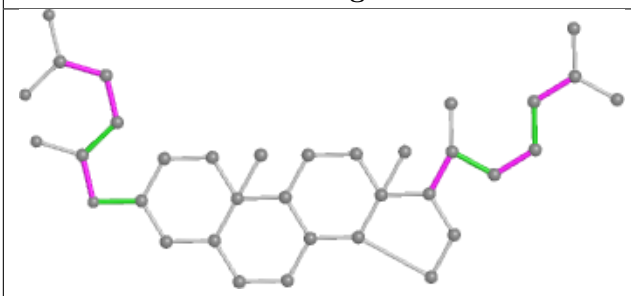
Ligand Y01 C 607



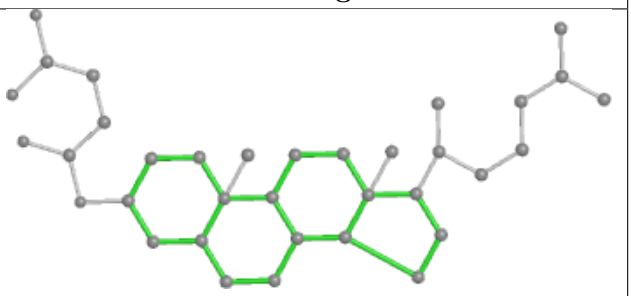
Bond lengths



Bond angles



Torsions



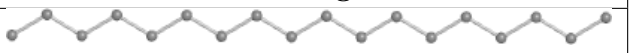
Rings

Ligand 3PE C 601

Bond lengths

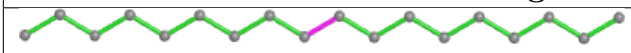
Bond angles

Torsions

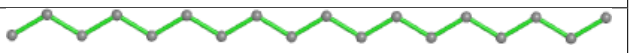


Rings

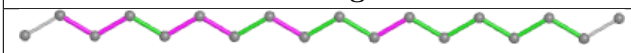
Ligand 3PE D 603



Bond lengths



Bond angles



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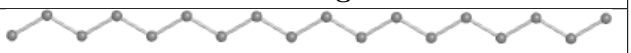
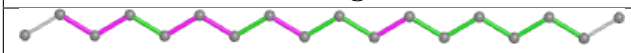


Rings

Ligand 3PE B 603

Bond lengths

Bond angles



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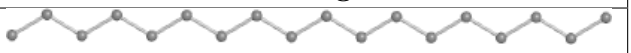
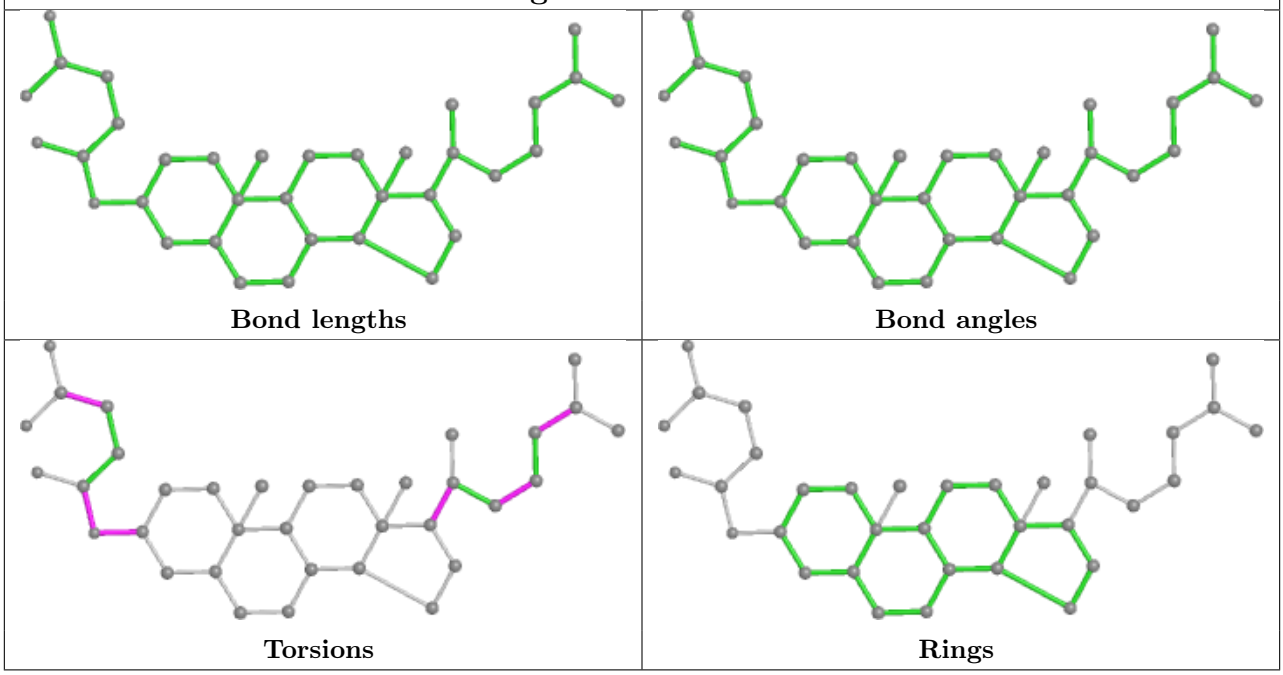
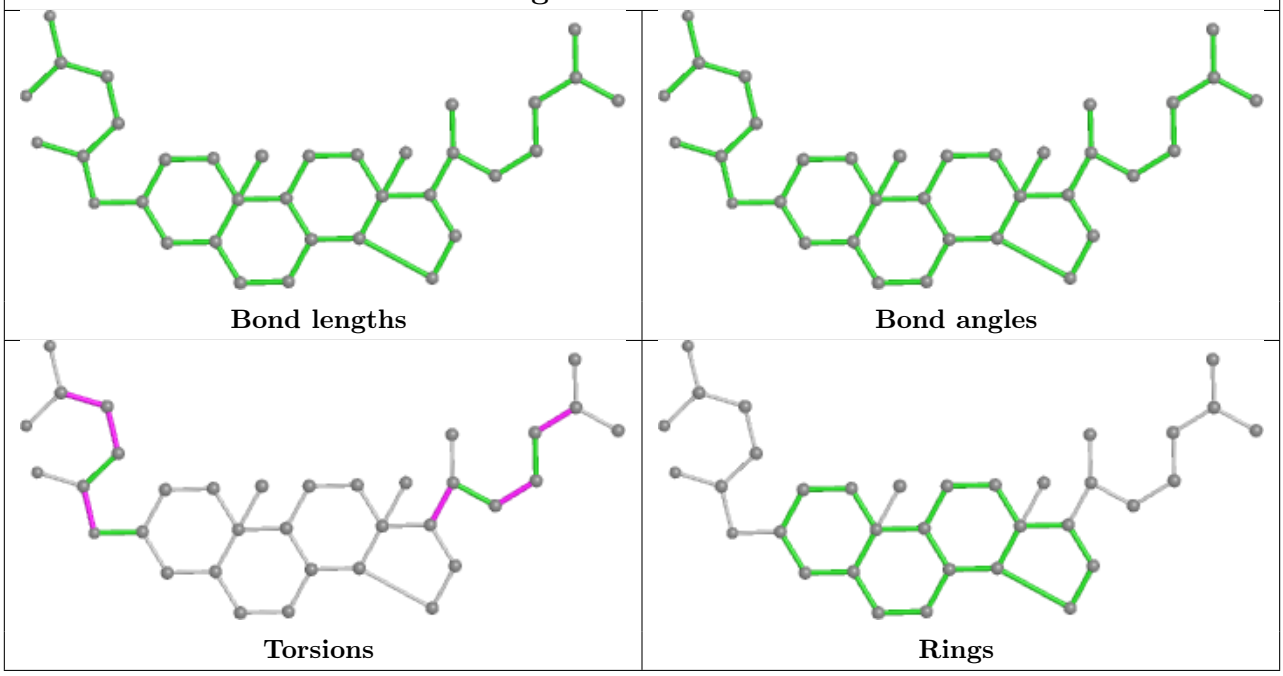


Rings

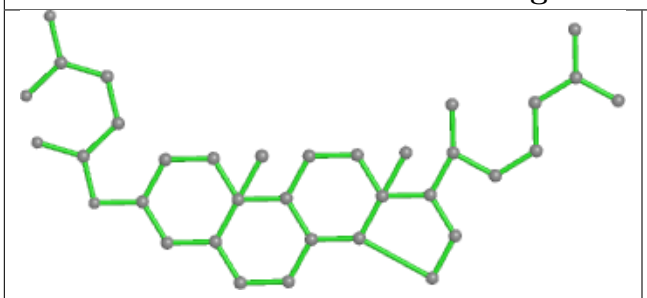
Ligand Y01 A 601



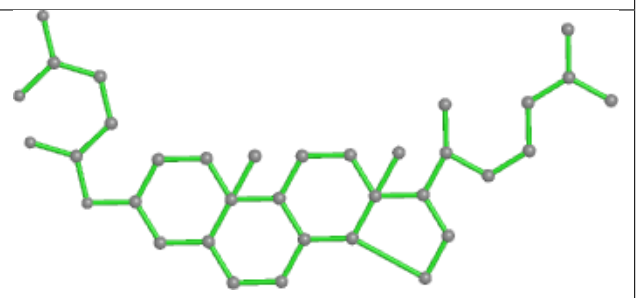
Ligand Y01 B 601



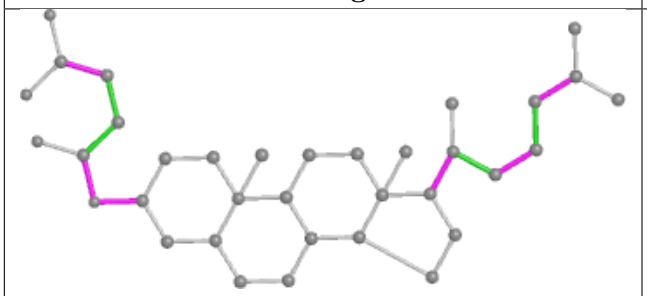
Ligand Y01 D 605



Bond lengths



Bond angles



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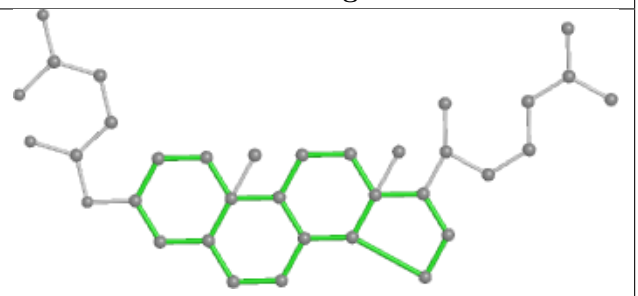
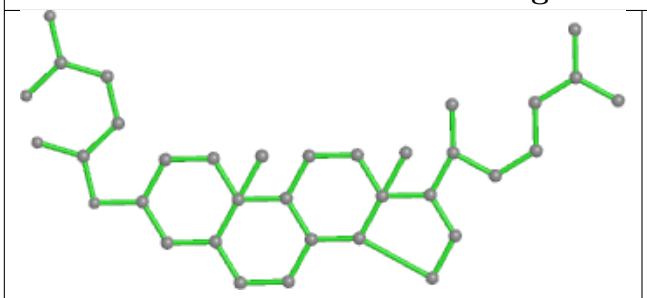
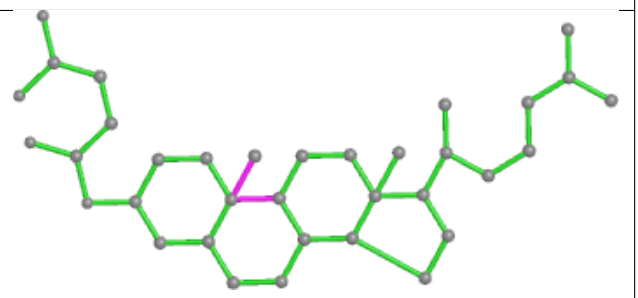


Rings

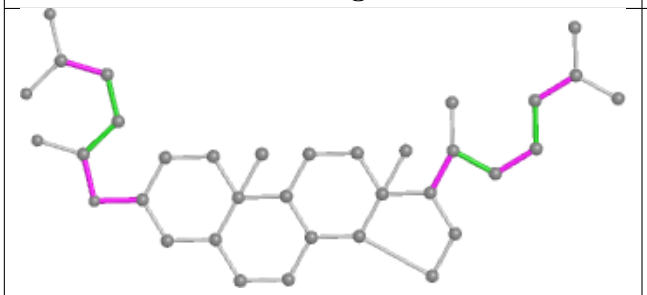
Ligand Y01 B 602



Bond lengths



Bond angles



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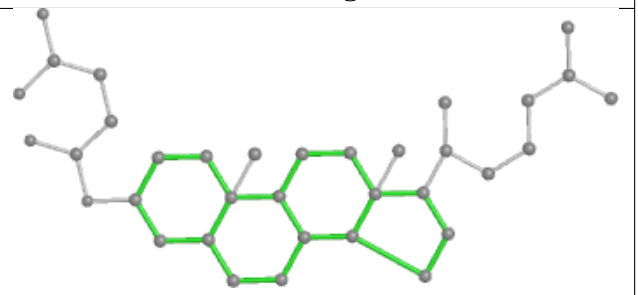
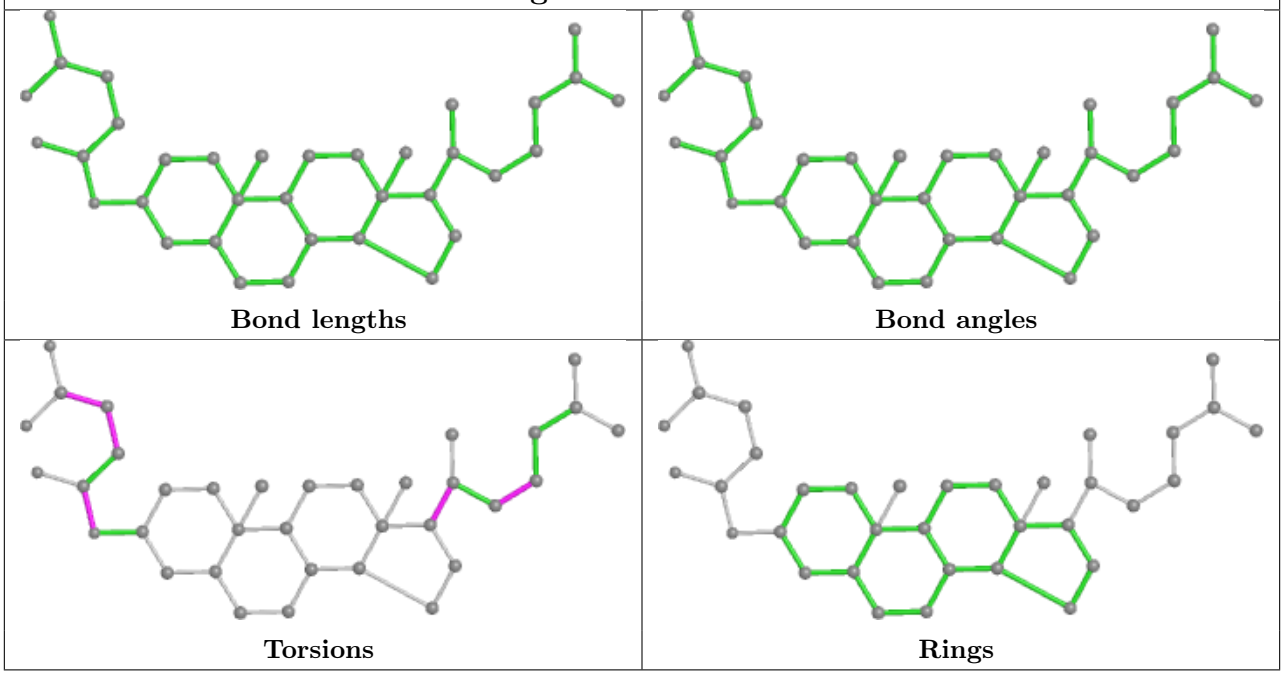
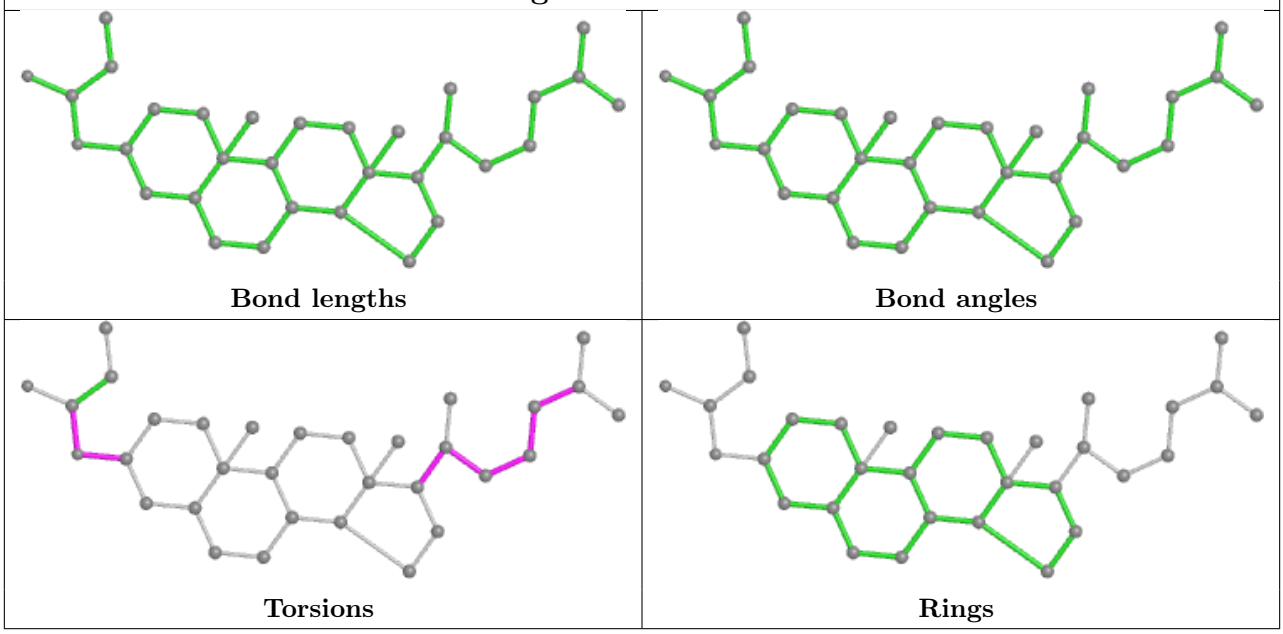


Rings

Ligand Y01 A 606



Ligand Y01 C 602



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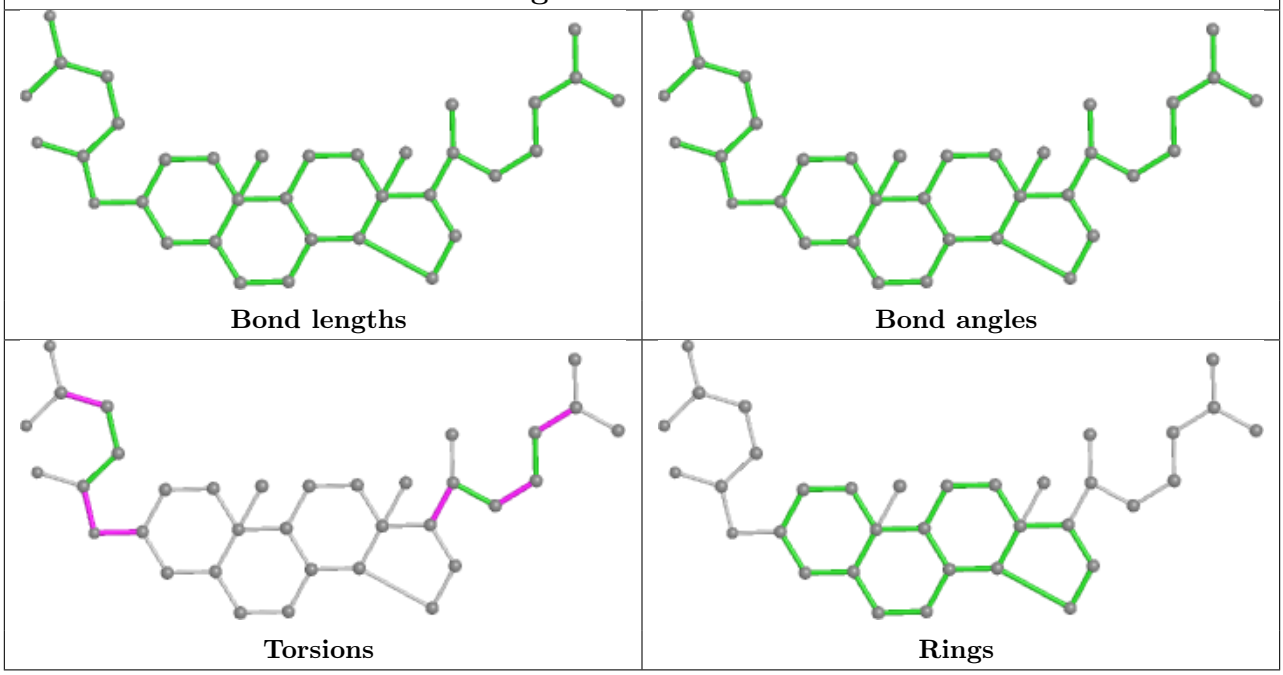

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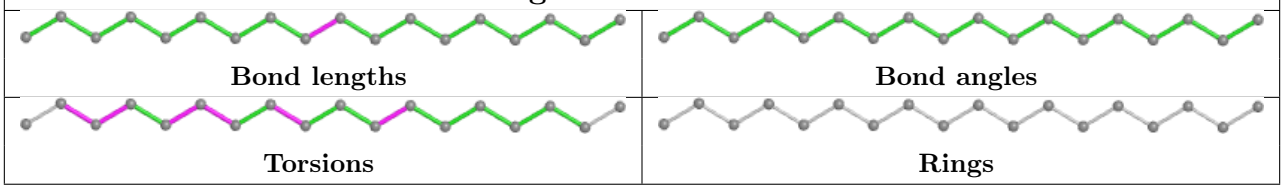
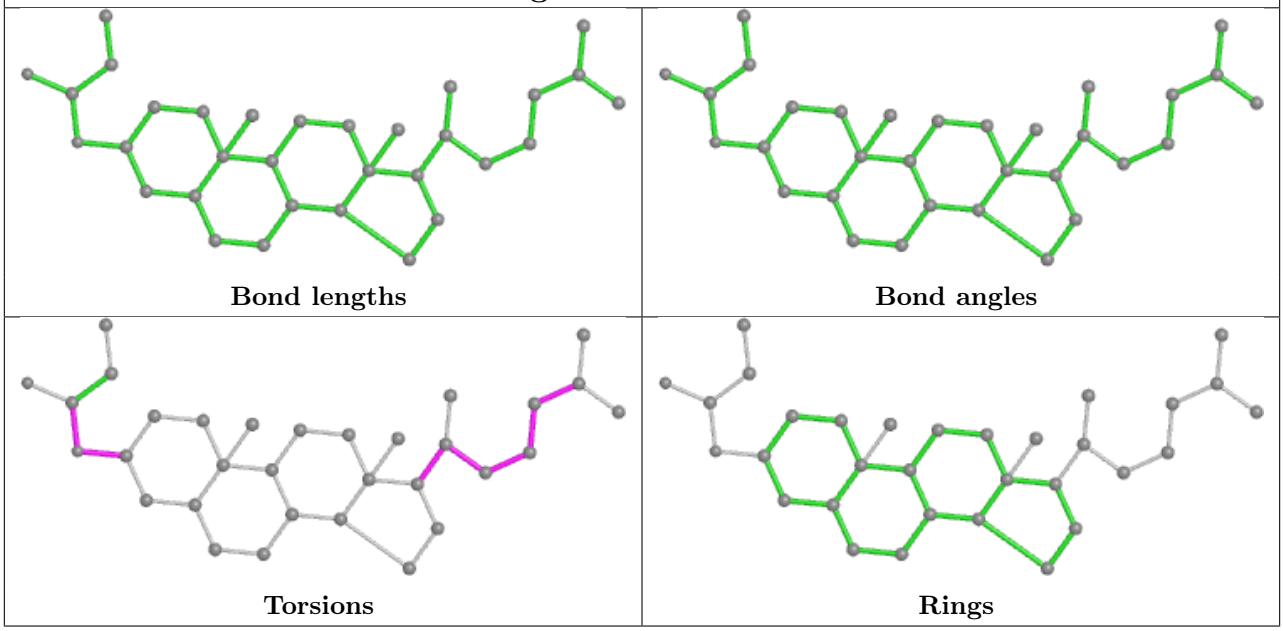
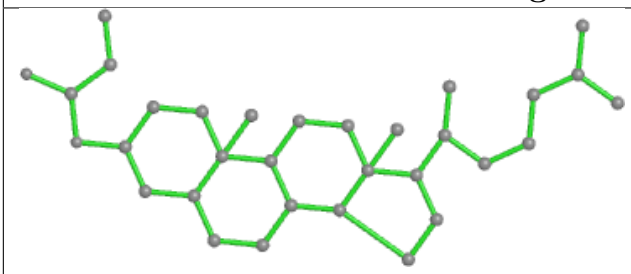
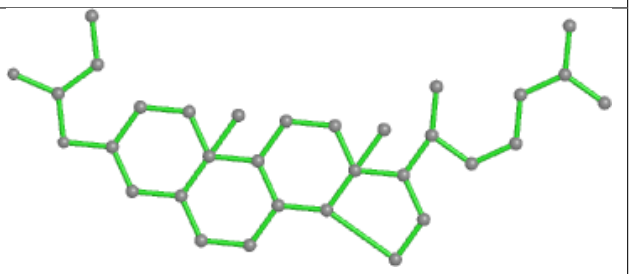
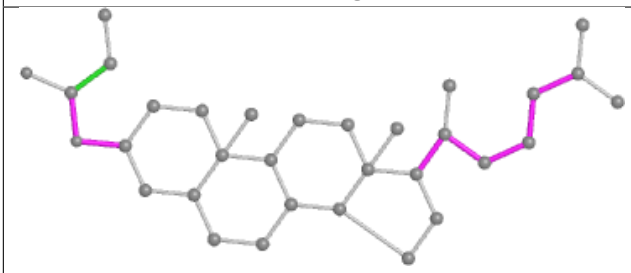
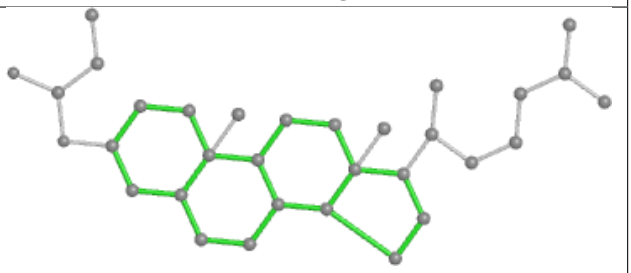
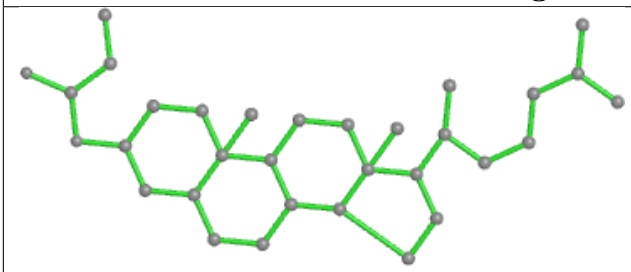
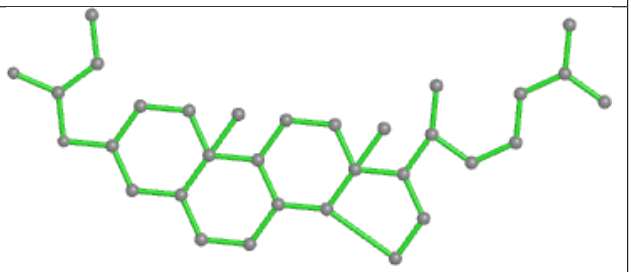
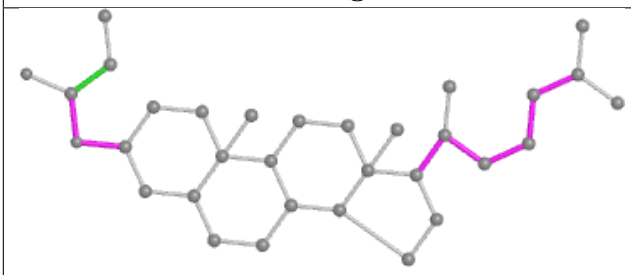
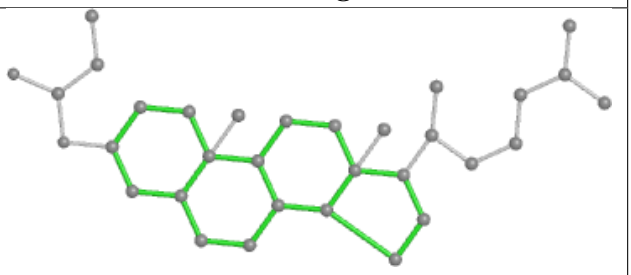


Ligand Y01 D 604



Ligand Y01 A 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 B 604	
 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.

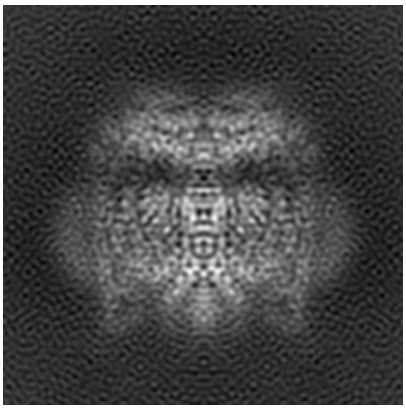
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8764. These allow visual inspection of the internal detail of the map and identification of artifacts.

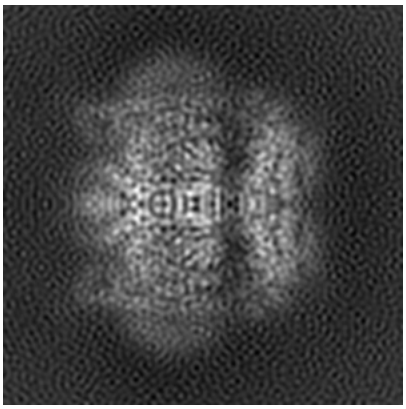
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

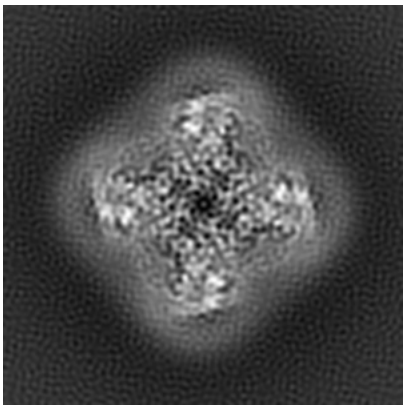
6.1.1 Primary map



X

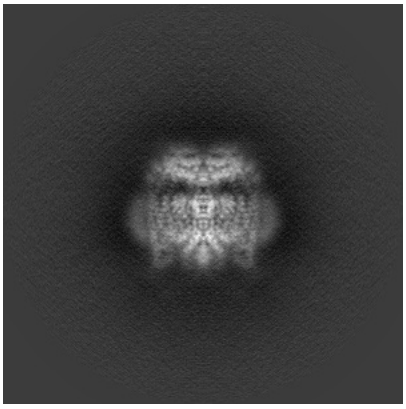


Y

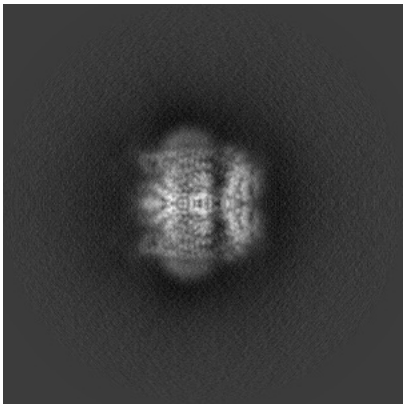


Z

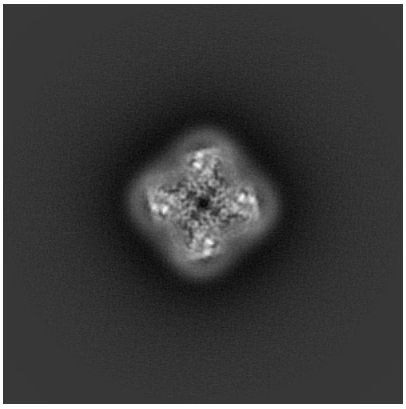
6.1.2 Raw map



X



Y

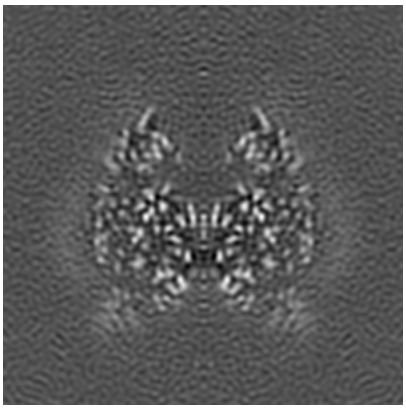


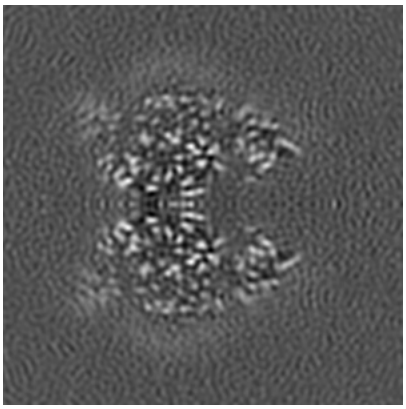
Z

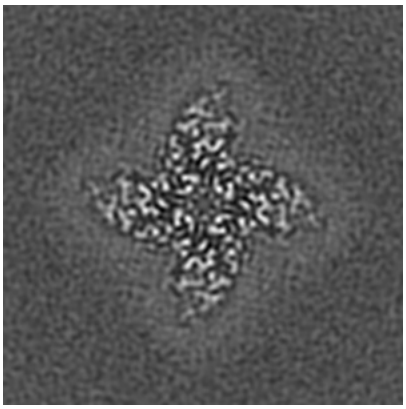
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

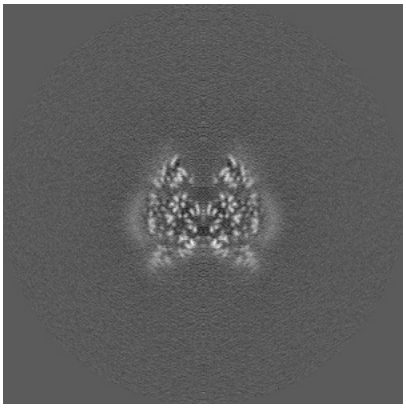
6.2.1 Primary map

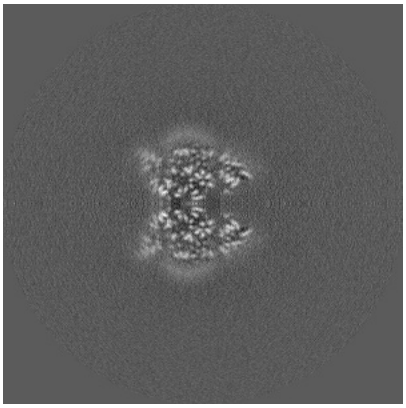

X Index: 128

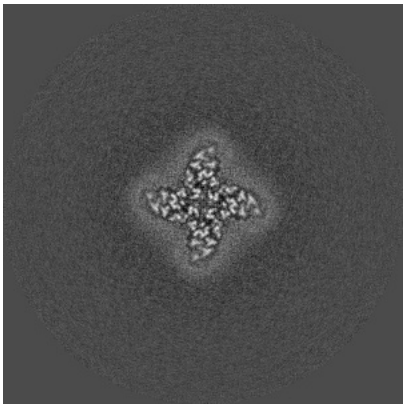

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 256

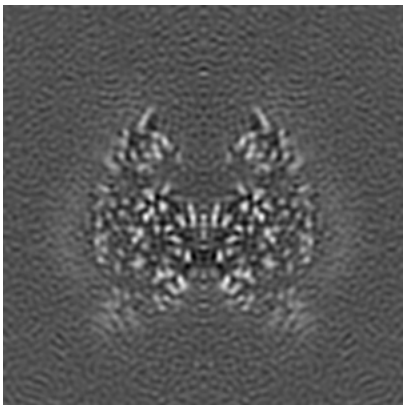

Y Index: 256

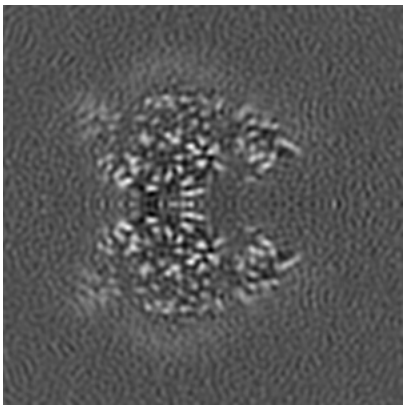

Z Index: 256

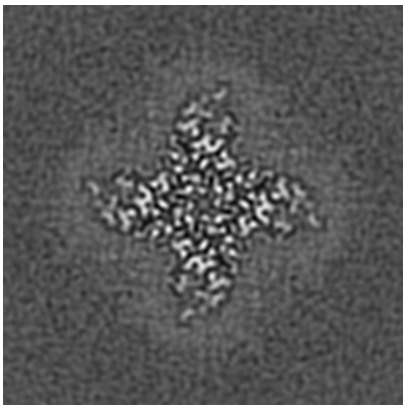
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

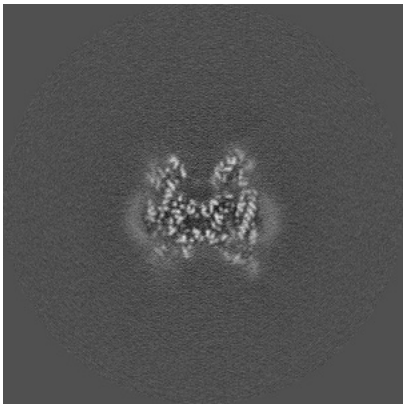
6.3.1 Primary map

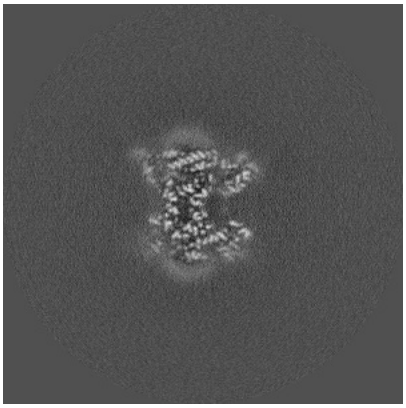

X Index: 128

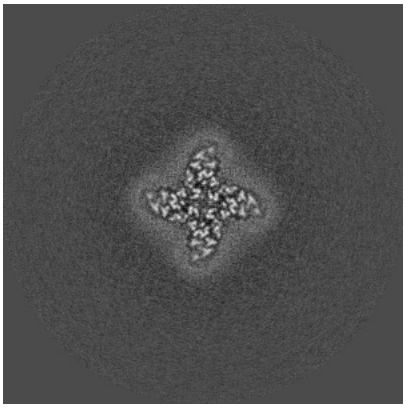

Y Index: 128


Z Index: 127

6.3.2 Raw map


X Index: 249

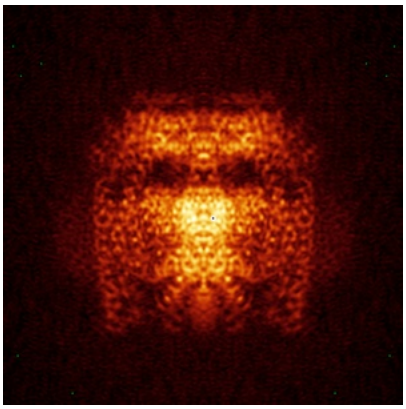

Y Index: 263

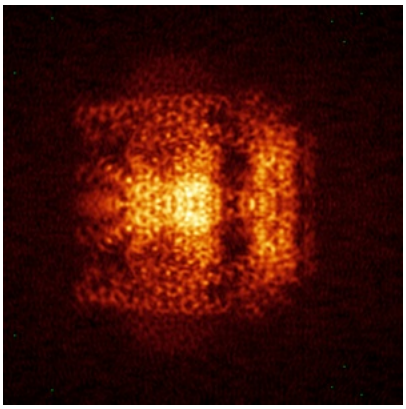

Z Index: 256

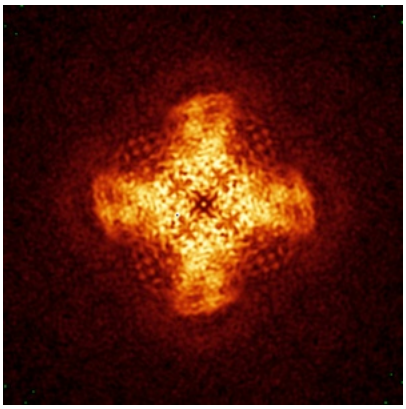
The images above show the largest variance slices of the map in three orthogonal directions.

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

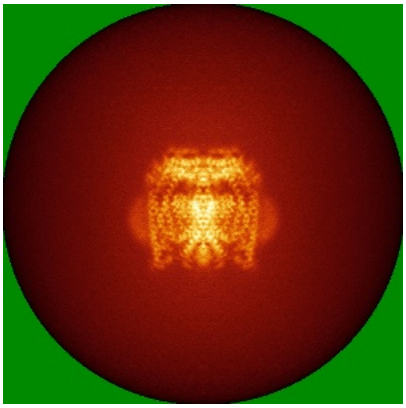
6.4.1 Primary map

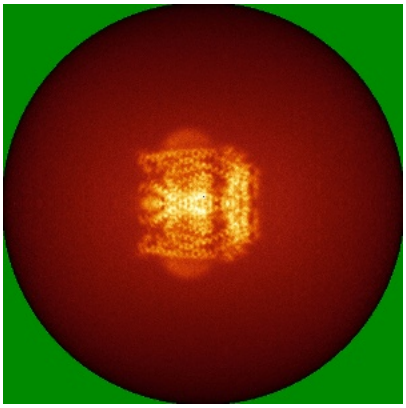

X

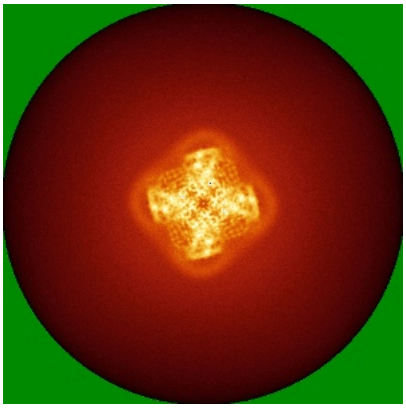

Y


Z

6.4.2 Raw map


X

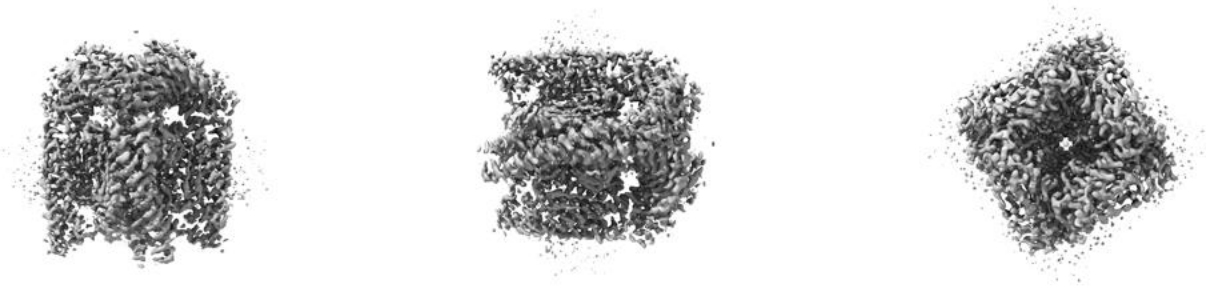

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

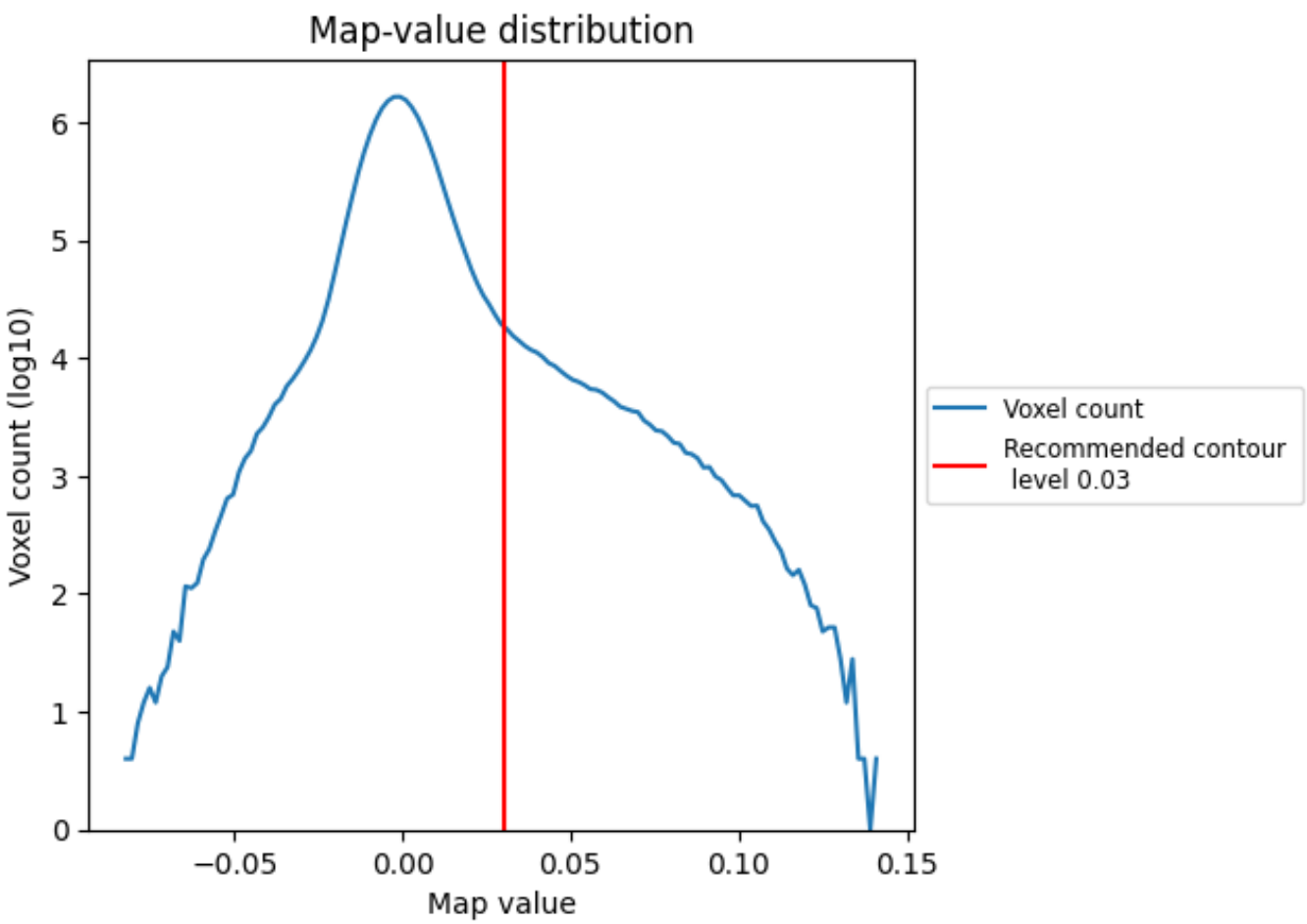
6.6 Mask visualisation (i)

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

7 Map analysis (i)

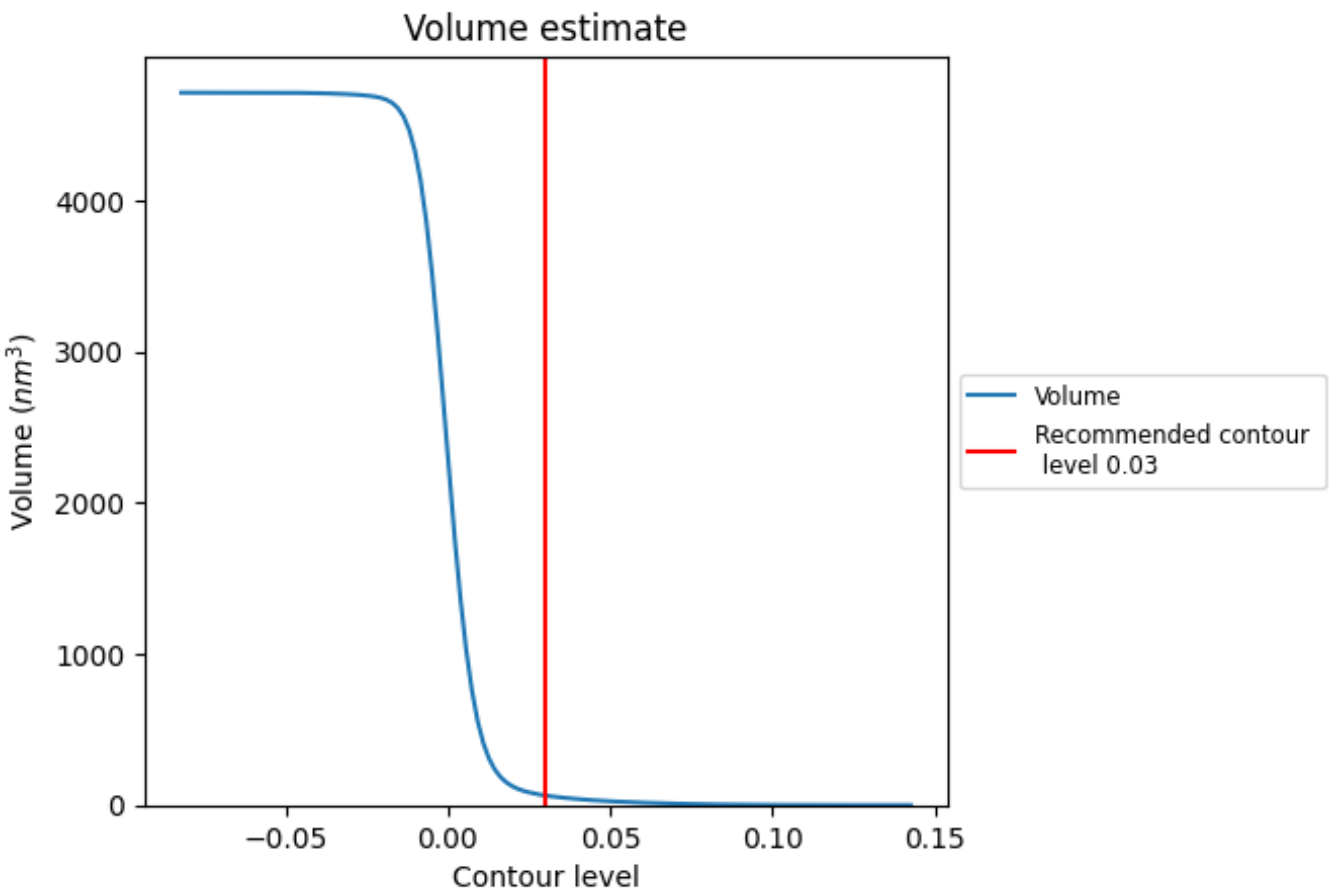
This section contains the results of statistical analysis of the map.

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.

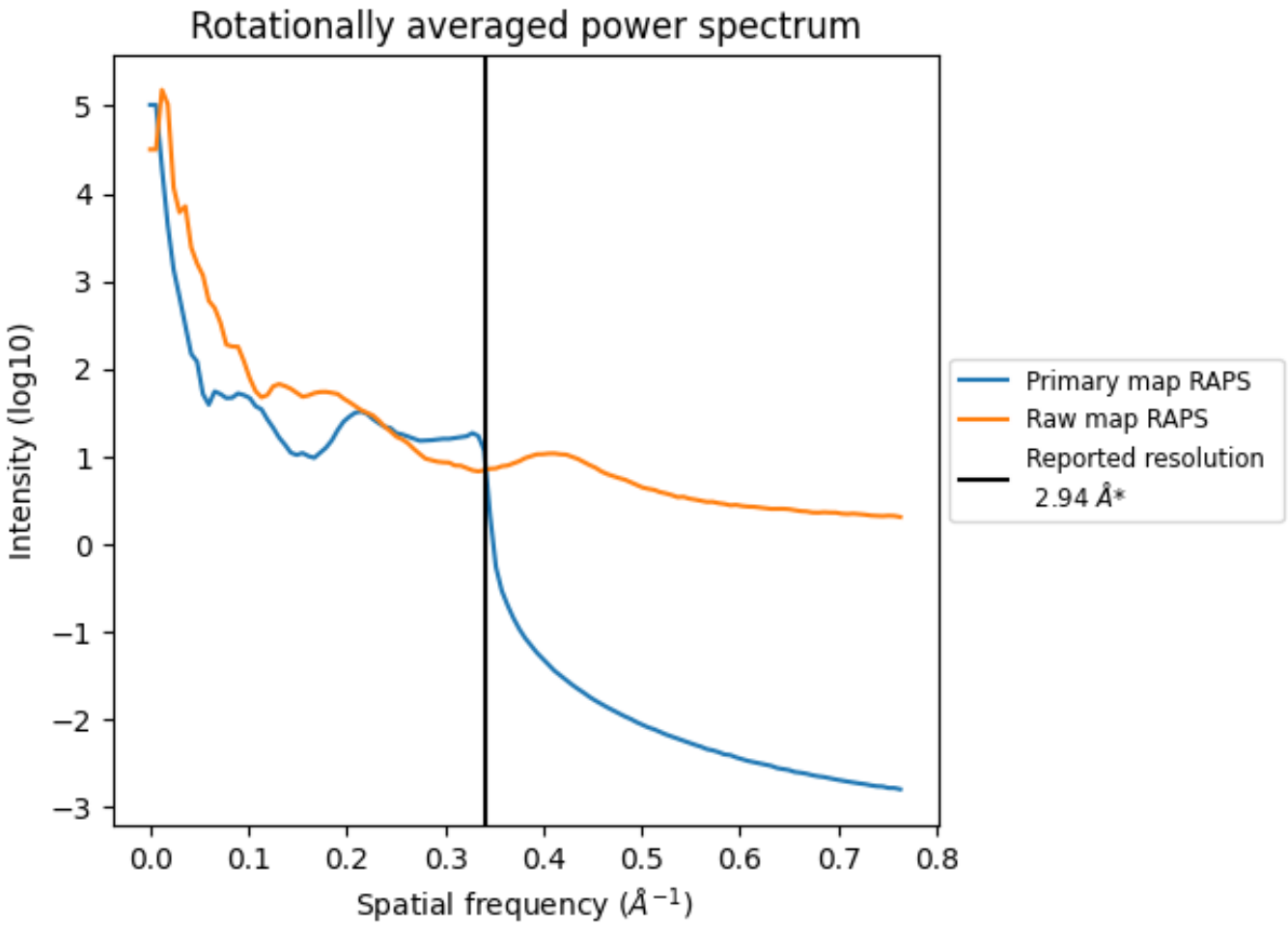
7.2 Volume estimate (i)



The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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)

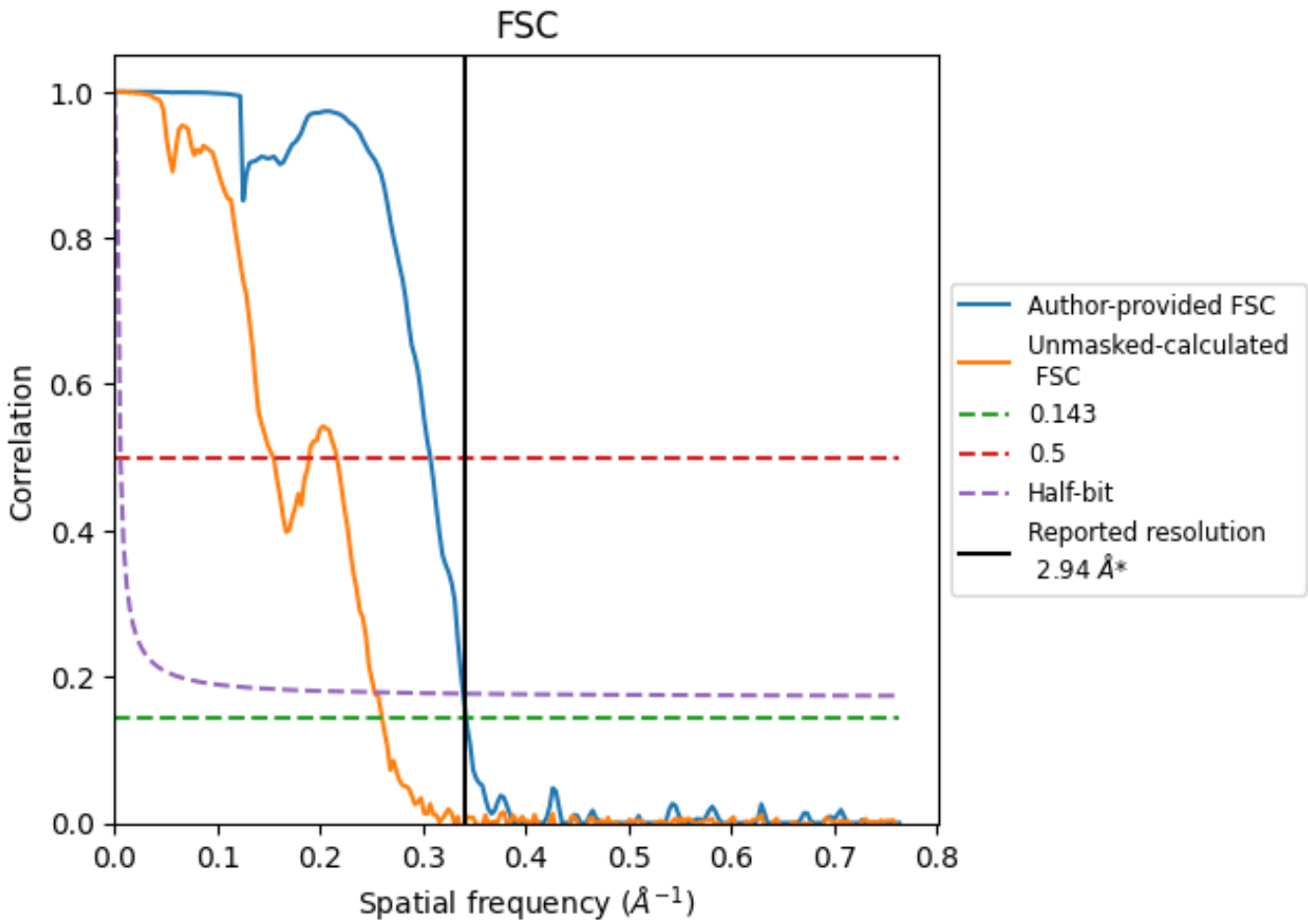


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8.2 Resolution estimates (i)

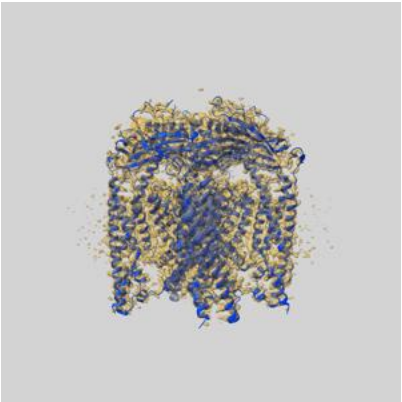
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.26	2.95
Unmasked-calculated*	3.84	6.48	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 2.94 by more than 10 %

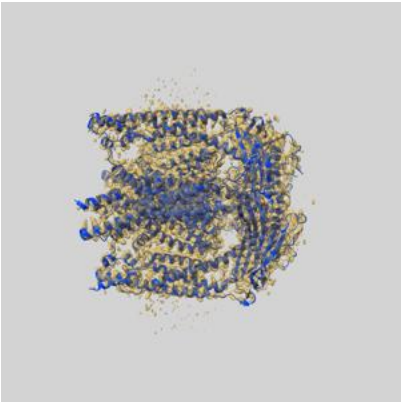
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8764 and PDB model 5W3S. Per-residue inclusion information can be found in section 3 on page 7.

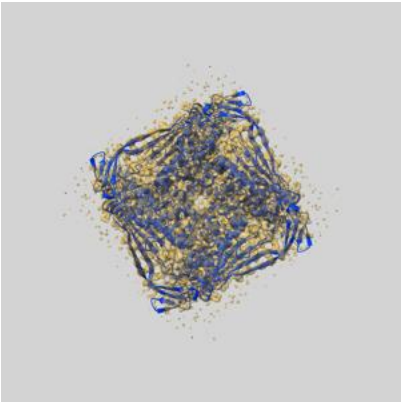
9.1 Map-model overlay (i)



X



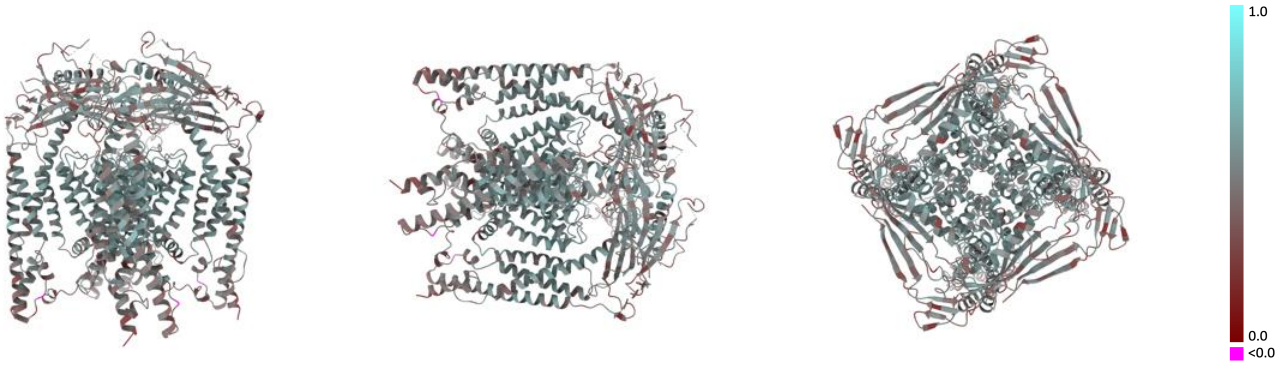
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

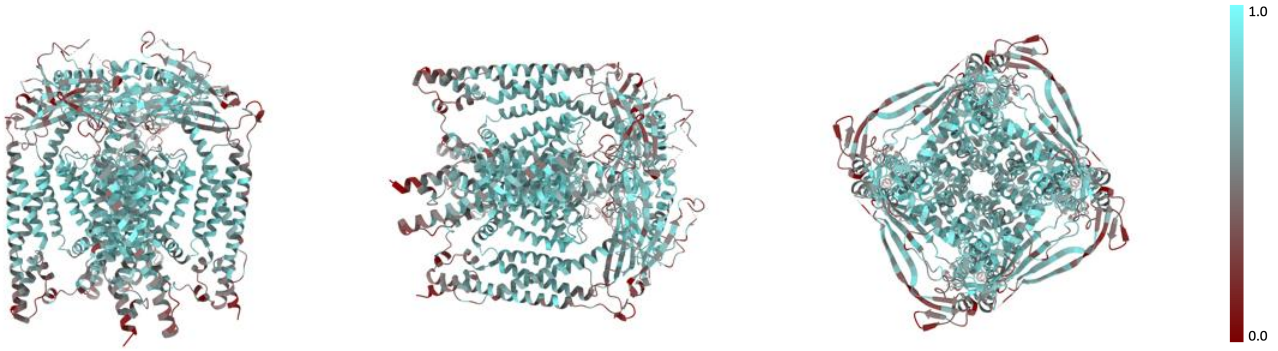
9.2 Q-score mapped to coordinate model (i)



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.

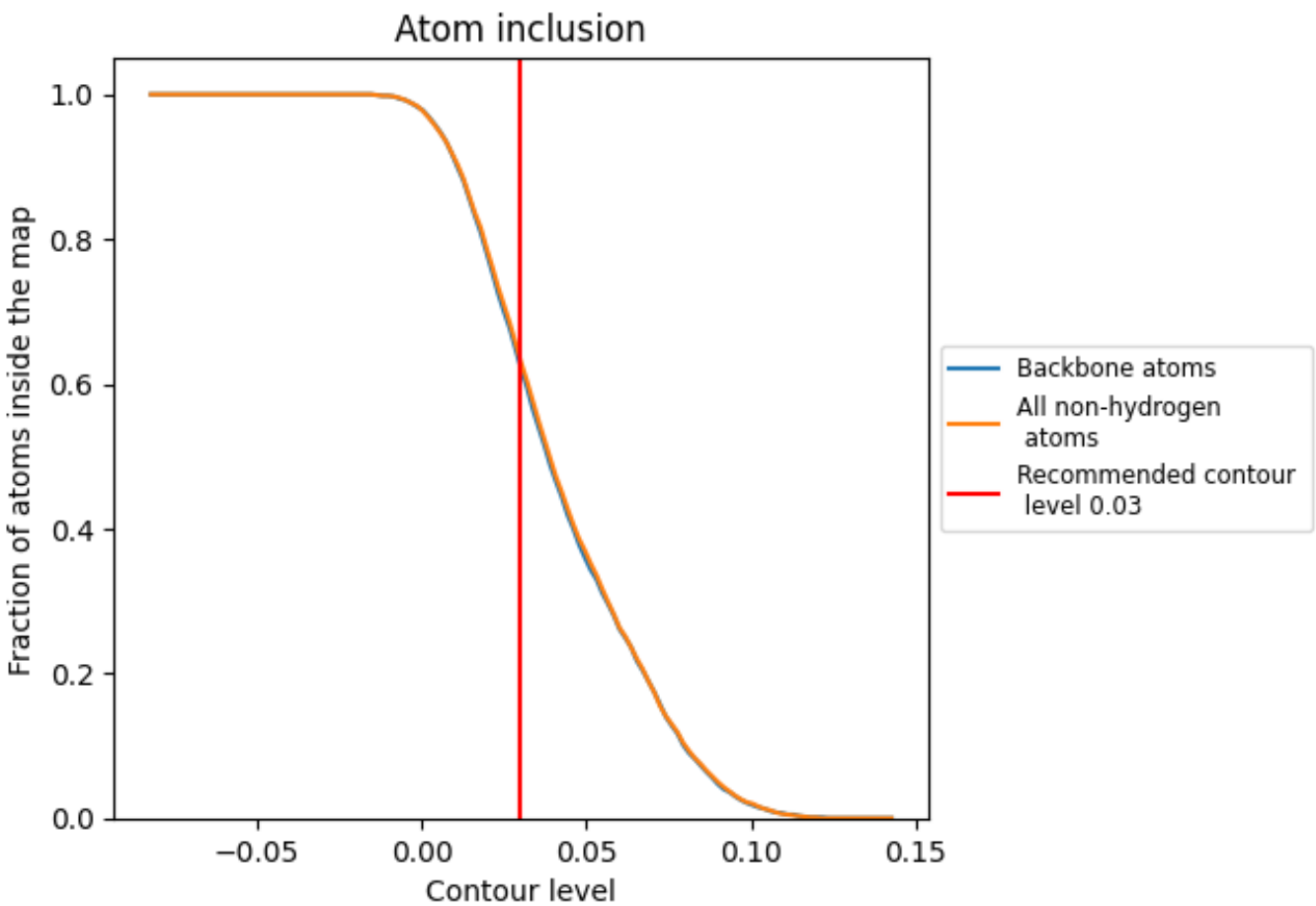
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6330	0.4910
A	0.6400	0.4940
B	0.6380	0.4900
C	0.6390	0.4910
D	0.6360	0.4900