Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 07:35 PM JST

PDB ID	:	7E2H
EMDB ID	:	EMD-30957
Title	:	Cryo-EM structure of hDisp1NNN-3C-Cleavage
Authors	:	Li, W.; Wang, L.; Gong, X.
Deposited on	:	2021-02-05
Resolution	:	3.68 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 ⓘ symbol.

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

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

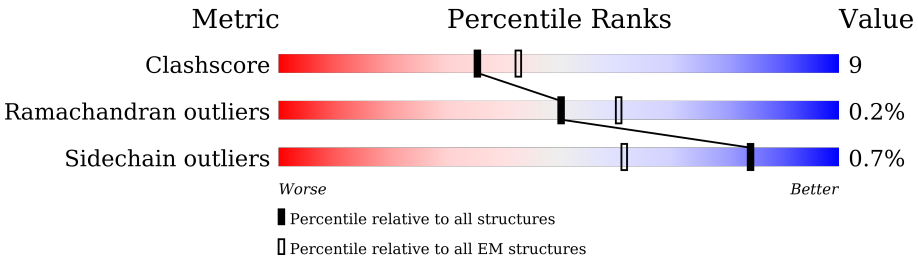
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.68 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	D	270	28% · 69%
2	E	1248	· 52% 14% 34%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7274 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 Protein dispatched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	83	Total	C	N	O	S	0	0
			615	403	98	109	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	263	SER	-	linker	UNP Q96F81
D	264	SER	-	linker	UNP Q96F81
D	271	LEU	-	linker	UNP Q96F81
D	272	GLU	-	linker	UNP Q96F81
D	273	VAL	-	linker	UNP Q96F81
D	274	LEU	-	linker	UNP Q96F81
D	275	PHE	-	linker	UNP Q96F81
D	276	GLN	-	linker	UNP Q96F81

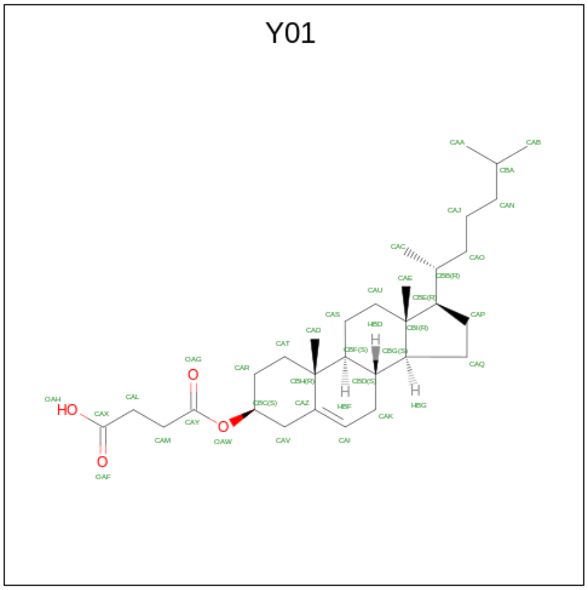
- Molecule 2 is a protein called Protein dispatched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	824	Total	C	N	O	S	0	0
			6323	4117	1018	1134	54		

There are 7 discrepancies between the modelled and reference sequences:

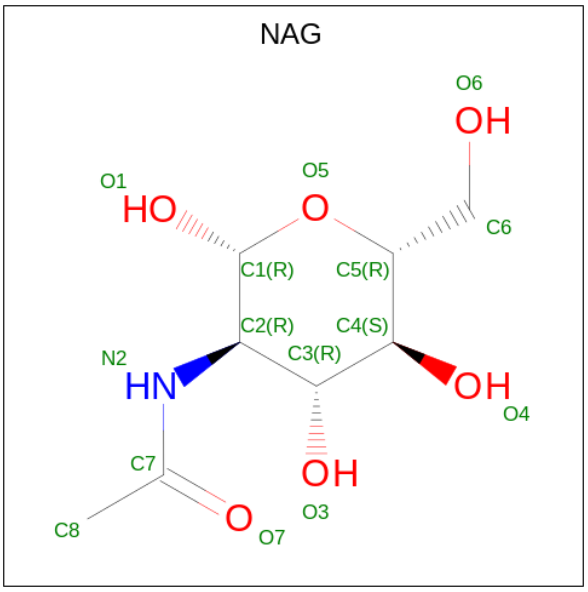
Chain	Residue	Modelled	Actual	Comment	Reference
E	277	GLY	-	linker	UNP Q96F81
E	278	PRO	-	linker	UNP Q96F81
E	279	GLY	-	linker	UNP Q96F81
E	280	SER	-	linker	UNP Q96F81
E	572	ASN	ASP	engineered mutation	UNP Q96F81
E	573	ASN	ASP	engineered mutation	UNP Q96F81
E	1051	ASN	ASP	engineered mutation	UNP Q96F81

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms	AltConf
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0
3	E	1	Total C O 280 248 32	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



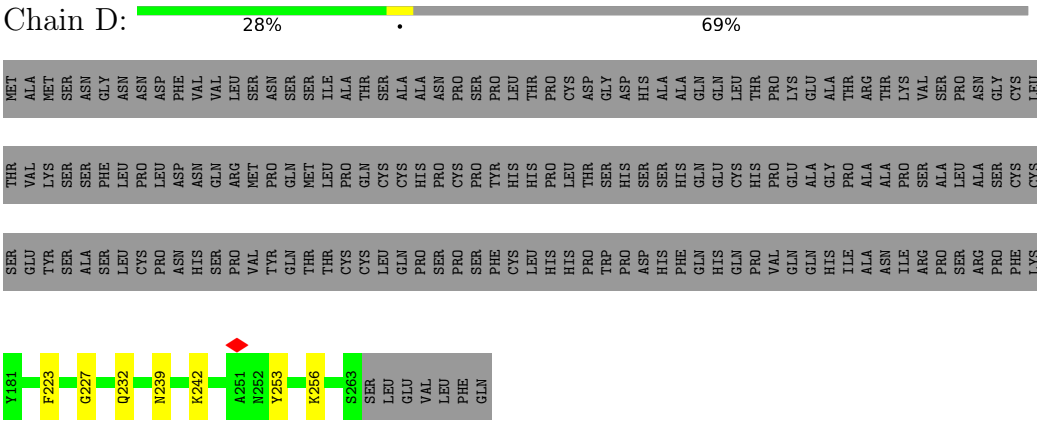
Mol	Chain	Residues	Atoms				AltConf
4	E	1	Total	C	N	O	0
			56	32	4	20	
4	E	1	Total	C	N	O	0
			56	32	4	20	
4	E	1	Total	C	N	O	0
			56	32	4	20	
4	E	1	Total	C	N	O	0
			56	32	4	20	

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.

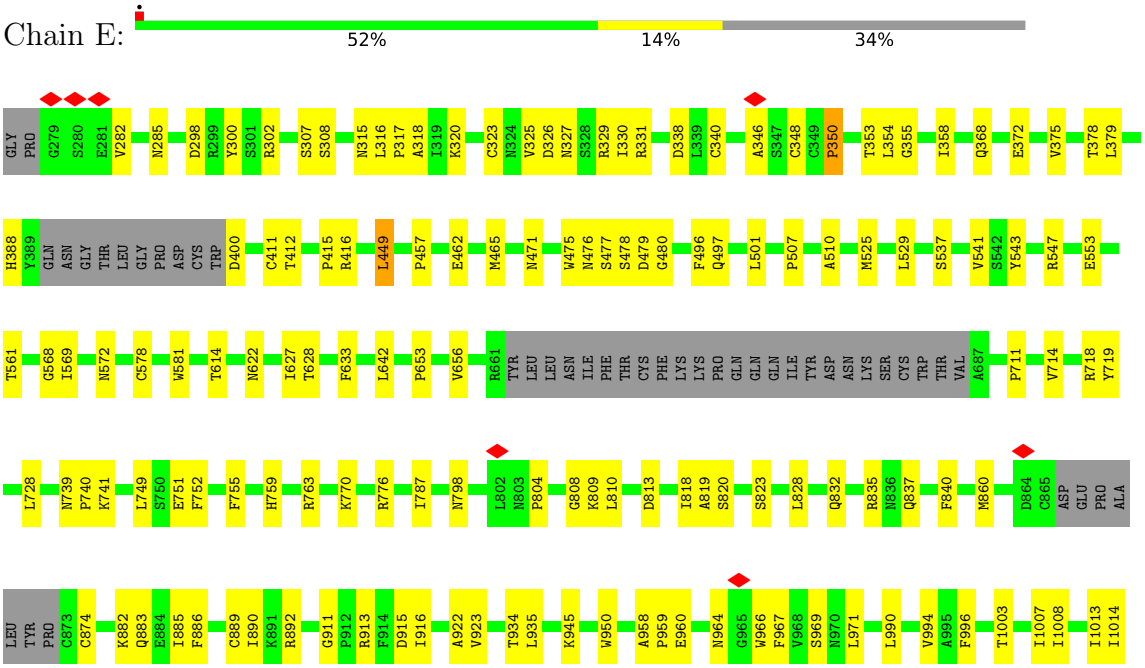
- Molecule 1: Protein dispatched homolog 1

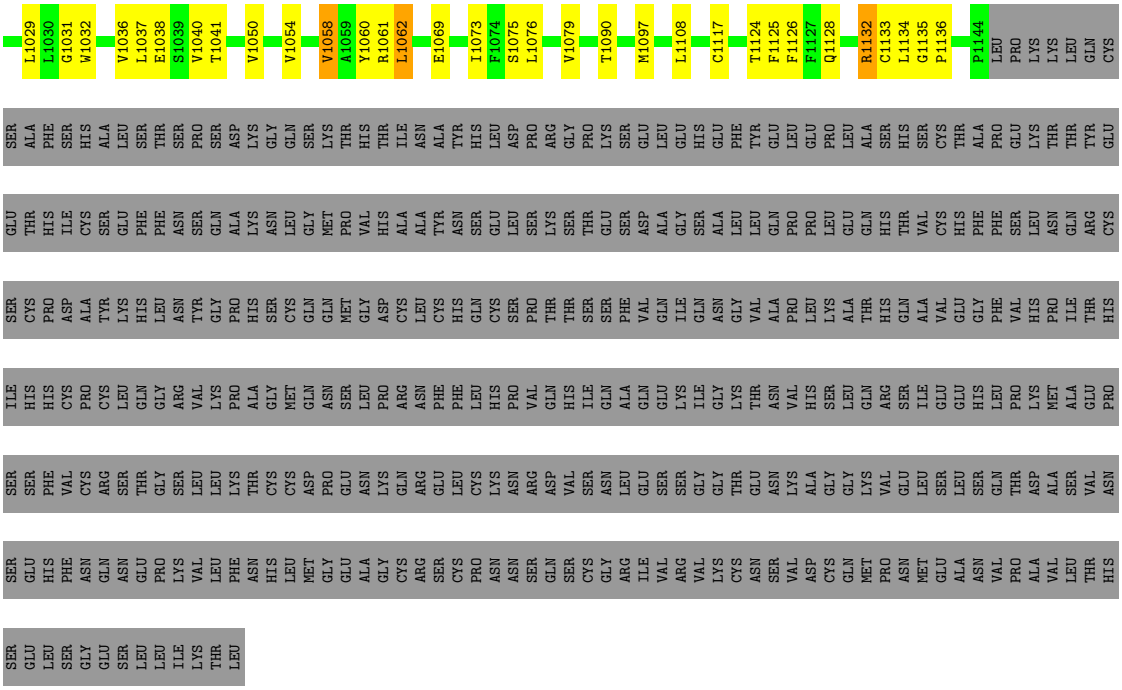
Chain D:



- Molecule 2: Protein dispatched homolog 1

Chain E:




L1029 L1030 G1031 W1032 V1036 L1037 E1038 S1039 V1040 T1041 V1050 V1054 V1058 A1059 Y1060 R1061 L1062 E1069 I1073 F1074 S1075 L1076 V1079 T1090 M1097 L1108 C1117 T1124 F1125 F1126 F1127 Q1128 R1132 C1133 L1134 G1135 P1136 P1144
SER ALA PHE SER HIS ALA LEU SER THR SER PRO SER ASP LYS GLY GLN SER LYS THR HIS THR ILE ASN ALA TYR HIS LEU ASP PRO ARG GLY PRO LYS SER GLU LEU GLU PHE TYR GLU LEU GLU PRO LEU ALA SER HIS SER CYS THR ALA PRO GLU LYS THR THR GLU
GLU THR HIS ILE CYS SER GLU PHE PHE ASN SER GLN ALA LYS ASN LEU GLY MET PRO VAL HIS ALA ALA TYR ASN SER GLU LEU SER LYS SER THR GLU SER ASP ALA GLY SER ALA LEU LEU GLN PRO PRO LEU GLU GLN HIS THR VAL CYS HIS PHE PHE SER LEU ASN GLN CYS ARG
SER CYS PRO ASP ALA TYR LYS HIS LEU ASN TYR GLY PRO HIS SER CYS GLN GLN MET GLY ASP CYS LEU CYS HIS GLN CYS SER PRO THR THR SER SER PHE VAL GLN ILE GLN ASN GLY VAL ALA PRO LEU LYS ALA THR HIS GLN GLN GLY PHE VAL HIS PRO ILE THR HIS
ILE HIS HIS CYS PRO CYS LEU GLN GLY ARG VAL LYS PRO ALA GLY MET GLN ASN SER LEU PRO ARG ASN PHE PHE LEU HIS PRO VAL GLN HIS ILE GLN ALA GLN GLU LYS ILE GLY LYS THR ASN VAL HIS SER LEU GLN ARG SER ILE GLU GLU HIS LEU PRO LYS MET ALA GLU PRO
SER SER PHE VAL CYS ARG SER THR GLY SER LEU LEU LYS THR CYS CYS ASP PRO GLU ASN LYS GLN ARG GLU LEU CYS LYS ASN ARG ASP VAL SER ASN LEU GLU SER SER GLY GLY THR GLU ASN LYS ALA GLY GLY LYS VAL LEU SER LEU SER GLN THR ASP ALA SER VAL ASN
SER GLU HIS PHE ASN GLN ASN GLU PRO LYS VAL LEU PHE ASN HIS LEU MET GLY GLU ALA GLY CYS ARG SER CYS PRO ASN ASN SER GLN SER CYS GLY ARG ILE VAL ARG VAL LYS CYS ASN SER VAL ASP CYS GLN MET PRO ASN MET GLU ALA ASN VAL PRO ALA VAL LEU THR HIS
SER GLU LEU SER GLY GLU SER LEU LEU ILE LYS THR LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	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	0.204	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	198.72, 198.72, 198.72	wwPDB
Map dimensions	184, 184, 184	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NAG

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	D	0.27	0/631	0.47	0/866
2	E	0.29	0/6487	0.45	0/8839
All	All	0.29	0/7118	0.45	0/9705

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	615	0	599	6	0
2	E	6323	0	6088	117	0
3	E	280	0	392	10	0
4	E	56	0	52	0	0
All	All	7274	0	7131	123	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 9.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1054:VAL:O	2:E:1058:VAL:HG12	1.76	0.85
2:E:1132:ARG:NH1	2:E:1133:CYS:SG	2.55	0.79
1:D:253:TYR:OH	2:E:813:ASP:OD1	2.05	0.74
2:E:329:ARG:HH22	2:E:475:TRP:HB2	1.57	0.69
2:E:543:TYR:OH	2:E:547:ARG:NH1	2.27	0.68
1:D:239:ASN:HD21	2:E:809:LYS:HB3	1.58	0.68
2:E:828:LEU:HG	2:E:832:GLN:HE22	1.59	0.68
2:E:1060:TYR:OH	2:E:1134:LEU:HD22	1.96	0.65
2:E:1038:GLU:OE1	2:E:1038:GLU:N	2.29	0.64
2:E:883:GLN:HA	2:E:886:PHE:HB3	1.80	0.63
2:E:739:ASN:HB3	2:E:740:PRO:HD3	1.82	0.62
2:E:718:ARG:NH1	2:E:1069:GLU:OE2	2.33	0.62
2:E:1076:LEU:HD12	2:E:1128:GLN:HG3	1.82	0.61
2:E:1050:VAL:HG22	2:E:1054:VAL:HG23	1.82	0.61
2:E:798:ASN:HD22	2:E:810:LEU:HD23	1.66	0.61
2:E:1029:LEU:HD22	3:E:1601:Y01:HAV2	1.81	0.61
2:E:996:PHE:HB2	2:E:1013:ILE:HD11	1.84	0.60
2:E:331:ARG:NH2	2:E:350:PRO:O	2.35	0.59
2:E:449:LEU:HD12	2:E:449:LEU:O	2.03	0.59
2:E:820:SER:O	2:E:823:SER:OG	2.20	0.59
2:E:282:VAL:HG21	2:E:346:ALA:H	1.68	0.58
2:E:882:LYS:O	2:E:883:GLN:HG3	2.04	0.56
2:E:298:ASP:O	2:E:302:ARG:NH2	2.38	0.56
2:E:751:GLU:N	2:E:751:GLU:OE2	2.38	0.56
2:E:1062:LEU:O	2:E:1062:LEU:HG	2.05	0.56
2:E:561:THR:HB	2:E:1108:LEU:HD22	1.89	0.54
2:E:886:PHE:O	2:E:890:ILE:HG12	2.06	0.54
3:E:1607:Y01:HAA1	3:E:1607:Y01:HAO1	1.88	0.54
2:E:326:ASP:O	2:E:330:ILE:HG22	2.07	0.54
2:E:578:CYS:O	2:E:581:TRP:HB3	2.06	0.54
2:E:1003:THR:HG21	2:E:1008:ILE:HB	1.89	0.54
2:E:653:PRO:HA	2:E:656:VAL:HG12	1.88	0.54
2:E:770:LYS:O	2:E:776:ARG:NH1	2.41	0.53
2:E:478:SER:OG	2:E:479:ASP:N	2.41	0.53
2:E:323:CYS:O	2:E:327:ASN:ND2	2.42	0.53
2:E:1031:GLY:O	2:E:1032:TRP:HD1	1.91	0.52
2:E:354:LEU:O	2:E:358:ILE:HG12	2.10	0.52
2:E:497:GLN:HE21	3:E:1604:Y01:HAD1	1.73	0.52
2:E:308:SER:OG	2:E:480:GLY:O	2.25	0.52
2:E:913:ARG:HB2	2:E:922:ALA:HB3	1.90	0.52
2:E:718:ARG:NH2	2:E:719:TYR:OH	2.43	0.51
2:E:496:PHE:HD1	2:E:755:PHE:HE1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:741:LYS:HE3	3:E:1607:Y01:HAL1	1.94	0.49
2:E:1036:VAL:HG23	2:E:1037:LEU:HD22	1.94	0.49
2:E:525:MET:HG3	2:E:529:LEU:HD13	1.94	0.49
2:E:749:LEU:HD12	2:E:752:PHE:HE2	1.76	0.49
2:E:960:GLU:O	2:E:964:ASN:ND2	2.46	0.49
2:E:415:PRO:HB2	2:E:416:ARG:HD2	1.94	0.49
2:E:614:THR:HG21	2:E:1050:VAL:HG11	1.94	0.48
2:E:476:ASN:OD1	2:E:477:SER:N	2.41	0.48
2:E:1038:GLU:HA	2:E:1041:THR:HB	1.95	0.48
2:E:711:PRO:HA	2:E:714:VAL:HG12	1.96	0.48
2:E:320:LYS:NZ	2:E:368:GLN:O	2.41	0.47
2:E:860:MET:HE1	2:E:889:CYS:HB3	1.94	0.47
2:E:388:HIS:O	2:E:400:ASP:N	2.47	0.47
2:E:969:SER:HB2	2:E:971:LEU:HD22	1.96	0.47
2:E:889:CYS:HA	2:E:892:ARG:HB3	1.96	0.47
2:E:990:LEU:O	2:E:994:VAL:HG23	2.15	0.47
2:E:338:ASP:HB3	2:E:348:CYS:SG	2.55	0.47
2:E:315:ASN:ND2	2:E:318:ALA:H	2.13	0.47
2:E:945:LYS:HD2	2:E:945:LYS:HA	1.73	0.46
1:D:239:ASN:ND2	2:E:809:LYS:HB3	2.29	0.46
2:E:307:SER:OG	2:E:308:SER:N	2.48	0.46
2:E:497:GLN:NE2	3:E:1604:Y01:HAV1	2.30	0.46
2:E:886:PHE:CE1	2:E:890:ILE:HD11	2.51	0.46
2:E:837:GLN:OE1	2:E:950:TRP:NE1	2.47	0.46
2:E:1124:THR:HG22	2:E:1125:PHE:HD1	1.80	0.46
1:D:223:PHE:CD1	2:E:1036:VAL:HG11	2.51	0.46
2:E:964:ASN:O	2:E:966:TRP:N	2.49	0.46
2:E:553:GLU:N	2:E:553:GLU:OE2	2.48	0.46
2:E:751:GLU:O	2:E:751:GLU:HG2	2.16	0.46
2:E:911:GLY:O	2:E:913:ARG:NH1	2.49	0.46
2:E:633:PHE:CE2	2:E:1040:VAL:HG11	2.50	0.45
2:E:835:ARG:HD3	2:E:840:PHE:CZ	2.51	0.45
2:E:787:ILE:HB	2:E:967:PHE:HE1	1.82	0.45
2:E:507:PRO:HA	2:E:1097:MET:HE1	1.98	0.45
2:E:934:THR:OG1	2:E:935:LEU:N	2.49	0.45
3:E:1607:Y01:HAO2	3:E:1607:Y01:HAP1	1.70	0.45
2:E:501:LEU:HD12	3:E:1604:Y01:HAS1	1.98	0.45
1:D:227:GLY:HA2	1:D:232:GLN:HG3	1.97	0.44
2:E:411:CYS:SG	2:E:412:THR:N	2.91	0.44
2:E:874:CYS:SG	2:E:885:ILE:HG12	2.58	0.44
2:E:325:VAL:HG21	2:E:478:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:358:ILE:HD12	2:E:378:THR:HG21	2.00	0.44
2:E:787:ILE:HB	2:E:967:PHE:CE1	2.53	0.43
2:E:1117:CYS:SG	3:E:1602:Y01:HAP2	2.58	0.43
2:E:553:GLU:O	2:E:553:GLU:HG2	2.18	0.43
2:E:642:LEU:HD23	2:E:642:LEU:HA	1.77	0.43
2:E:331:ARG:HH21	2:E:457:PRO:HG2	1.84	0.43
2:E:1075:SER:O	2:E:1079:VAL:HG22	2.17	0.43
2:E:828:LEU:HD12	2:E:828:LEU:HA	1.90	0.43
2:E:340:CYS:N	2:E:348:CYS:SG	2.67	0.43
2:E:353:THR:HG23	2:E:355:GLY:N	2.34	0.43
2:E:711:PRO:HB3	2:E:1073:ILE:HG22	2.00	0.43
3:E:1607:Y01:HAC1	3:E:1608:Y01:HAK2	2.01	0.42
2:E:375:VAL:O	2:E:379:LEU:HD23	2.18	0.42
2:E:628:THR:HG23	2:E:804:PRO:HG2	2.00	0.42
3:E:1607:Y01:HAU1	3:E:1608:Y01:HAI	2.01	0.42
2:E:818:ILE:HD12	2:E:923:VAL:HG21	2.00	0.42
2:E:1007:ILE:H	2:E:1007:ILE:HD12	1.84	0.42
2:E:300:TYR:O	2:E:302:ARG:NH2	2.53	0.42
2:E:471:ASN:HA	2:E:475:TRP:HZ3	1.85	0.42
2:E:958:ALA:HB3	2:E:959:PRO:HD3	2.01	0.42
1:D:242:LYS:HD3	1:D:242:LYS:HA	1.82	0.42
2:E:627:ILE:HG22	2:E:628:THR:H	1.84	0.41
2:E:537:SER:O	2:E:541:VAL:HG12	2.21	0.41
2:E:728:LEU:HD23	2:E:728:LEU:HA	1.92	0.41
2:E:568:GLY:O	2:E:1090:THR:OG1	2.35	0.41
2:E:759:HIS:O	2:E:763:ARG:HG2	2.20	0.41
2:E:462:GLU:O	2:E:465:MET:HG2	2.21	0.41
2:E:316:LEU:HD21	2:E:372:GLU:HA	2.03	0.41
2:E:547:ARG:HD2	2:E:547:ARG:HA	1.89	0.41
2:E:569:ILE:O	2:E:572:ASN:HB3	2.21	0.41
2:E:622:ASN:ND2	2:E:1040:VAL:HG13	2.36	0.41
2:E:819:ALA:HB1	2:E:883:GLN:HB2	2.02	0.41
2:E:915:ASP:OD1	2:E:916:ILE:N	2.42	0.41
2:E:1014:ILE:HG22	2:E:1126:PHE:HE2	1.85	0.41
2:E:507:PRO:O	2:E:510:ALA:HB3	2.20	0.40
2:E:885:ILE:HD12	2:E:885:ILE:H	1.86	0.40
2:E:808:GLY:C	2:E:809:LYS:HD3	2.41	0.40
2:E:315:ASN:HD22	2:E:317:PRO:HD2	1.86	0.40
2:E:285:ASN:HB3	2:E:350:PRO:HG3	2.03	0.40
2:E:1135:GLY:HA2	2:E:1136:PRO:HD3	1.99	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	D	81/270 (30%)	72 (89%)	8 (10%)	1 (1%)	13 49
2	E	816/1248 (65%)	747 (92%)	68 (8%)	1 (0%)	51 83
All	All	897/1518 (59%)	819 (91%)	76 (8%)	2 (0%)	50 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	LYS
2	E	350	PRO

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	D	62/236 (26%)	62 (100%)	0	100 100
2	E	666/1106 (60%)	661 (99%)	5 (1%)	81 89
All	All	728/1342 (54%)	723 (99%)	5 (1%)	84 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	449	LEU
2	E	1058	VAL
2	E	1061	ARG
2	E	1062	LEU

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Mol	Chain	Res	Type
2	E	1132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	239	ASN
2	E	315	ASN
2	E	497	GLN
2	E	622	ASN
2	E	832	GLN
2	E	862	ASN
2	E	964	ASN
2	E	977	GLN
2	E	1035	ASN

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)

12 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	$\#\|Z\|>2$
3	Y01	E	1604	-	38,38,38	0.43	0	57,57,57	0.59	0
3	Y01	E	1606	-	38,38,38	0.43	0	57,57,57	0.62	0
4	NAG	E	1611	2	14,14,15	0.25	0	17,19,21	0.44	0
3	Y01	E	1608	-	38,38,38	0.44	0	57,57,57	0.49	0
3	Y01	E	1602	-	38,38,38	0.42	0	57,57,57	0.60	0
3	Y01	E	1607	-	38,38,38	0.44	0	57,57,57	0.65	0
3	Y01	E	1601	-	38,38,38	0.45	0	57,57,57	0.63	0
3	Y01	E	1603	-	38,38,38	0.44	0	57,57,57	0.55	0
4	NAG	E	1610	2	14,14,15	0.25	0	17,19,21	0.32	0
4	NAG	E	1612	2	14,14,15	0.21	0	17,19,21	0.36	0
4	NAG	E	1609	2	14,14,15	1.15	1 (7%)	17,19,21	1.30	1 (5%)
3	Y01	E	1605	-	38,38,38	0.44	0	57,57,57	0.50	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
3	Y01	E	1604	-	-	3/19/77/77	0/4/4/4
3	Y01	E	1606	-	-	5/19/77/77	0/4/4/4
4	NAG	E	1611	2	-	2/6/23/26	0/1/1/1
3	Y01	E	1608	-	-	7/19/77/77	0/4/4/4
3	Y01	E	1602	-	-	6/19/77/77	0/4/4/4
3	Y01	E	1607	-	-	13/19/77/77	0/4/4/4
3	Y01	E	1601	-	-	10/19/77/77	0/4/4/4
3	Y01	E	1603	-	-	10/19/77/77	0/4/4/4
4	NAG	E	1610	2	-	0/6/23/26	0/1/1/1
4	NAG	E	1612	2	-	1/6/23/26	0/1/1/1
4	NAG	E	1609	2	-	0/6/23/26	0/1/1/1
3	Y01	E	1605	-	-	3/19/77/77	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1609	NAG	O5-C1	3.92	1.50	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1609	NAG	C1-O5-C5	5.17	119.20	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1607	Y01	OAG-CAY-OAW-CBC
3	E	1607	Y01	CAM-CAY-OAW-CBC
3	E	1608	Y01	CAR-CBC-OAW-CAY
3	E	1607	Y01	CAC-CBB-CBE-CAP
3	E	1607	Y01	CAC-CBB-CBE-CBI
3	E	1607	Y01	CAO-CBB-CBE-CBI
4	E	1611	NAG	O5-C5-C6-O6
3	E	1607	Y01	CAO-CBB-CBE-CAP
3	E	1601	Y01	CAJ-CAO-CBB-CBE
3	E	1607	Y01	CAJ-CAO-CBB-CBE
3	E	1607	Y01	CAJ-CAO-CBB-CAC
3	E	1601	Y01	CAC-CBB-CBE-CBI
3	E	1601	Y01	CAO-CBB-CBE-CBI
3	E	1603	Y01	CAO-CBB-CBE-CBI
4	E	1611	NAG	C4-C5-C6-O6
3	E	1601	Y01	CAJ-CAO-CBB-CAC
3	E	1601	Y01	CAC-CBB-CBE-CAP
3	E	1603	Y01	CAC-CBB-CBE-CAP
3	E	1603	Y01	CAC-CBB-CBE-CBI
3	E	1603	Y01	CAM-CAY-OAW-CBC
3	E	1605	Y01	CAN-CAJ-CAO-CBB
4	E	1612	NAG	O5-C5-C6-O6
3	E	1603	Y01	OAG-CAY-OAW-CBC
3	E	1602	Y01	CAJ-CAO-CBB-CBE
3	E	1603	Y01	CAO-CAJ-CAN-CBA
3	E	1601	Y01	CAO-CBB-CBE-CAP
3	E	1603	Y01	CAN-CAJ-CAO-CBB
3	E	1601	Y01	CAL-CAM-CAY-OAW
3	E	1603	Y01	CAO-CBB-CBE-CAP
3	E	1608	Y01	CAJ-CAO-CBB-CBE
3	E	1608	Y01	CAM-CAY-OAW-CBC
3	E	1607	Y01	CAJ-CAN-CBA-CAB
3	E	1606	Y01	CAO-CBB-CBE-CBI
3	E	1608	Y01	OAG-CAY-OAW-CBC
3	E	1606	Y01	CAC-CBB-CBE-CBI
3	E	1602	Y01	CAO-CBB-CBE-CBI
3	E	1604	Y01	CAM-CAL-CAX-OAF

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Mol	Chain	Res	Type	Atoms
3	E	1601	Y01	CAM-CAL-CAX-OAF
3	E	1604	Y01	CAM-CAL-CAX-OAH
3	E	1606	Y01	CAO-CBB-CBE-CAP
3	E	1602	Y01	CAM-CAL-CAX-OAH
3	E	1605	Y01	CAM-CAL-CAX-OAF
3	E	1607	Y01	CAM-CAL-CAX-OAF
3	E	1602	Y01	CAM-CAL-CAX-OAF
3	E	1601	Y01	CAM-CAL-CAX-OAH
3	E	1602	Y01	CAC-CBB-CBE-CBI
3	E	1607	Y01	CAM-CAL-CAX-OAH
3	E	1603	Y01	CAM-CAL-CAX-OAH
3	E	1605	Y01	CAM-CAL-CAX-OAH
3	E	1608	Y01	CAM-CAL-CAX-OAH
3	E	1606	Y01	CAM-CAL-CAX-OAH
3	E	1607	Y01	CAJ-CAN-CBA-CAA
3	E	1608	Y01	CAO-CBB-CBE-CAP
3	E	1608	Y01	CAM-CAL-CAX-OAF
3	E	1606	Y01	CAM-CAL-CAX-OAF
3	E	1603	Y01	CAM-CAL-CAX-OAF
3	E	1602	Y01	CAO-CBB-CBE-CAP
3	E	1607	Y01	CAO-CAJ-CAN-CBA
3	E	1604	Y01	CAV-CBC-OAW-CAY
3	E	1601	Y01	CAL-CAM-CAY-OAG

There are no ring outliers.

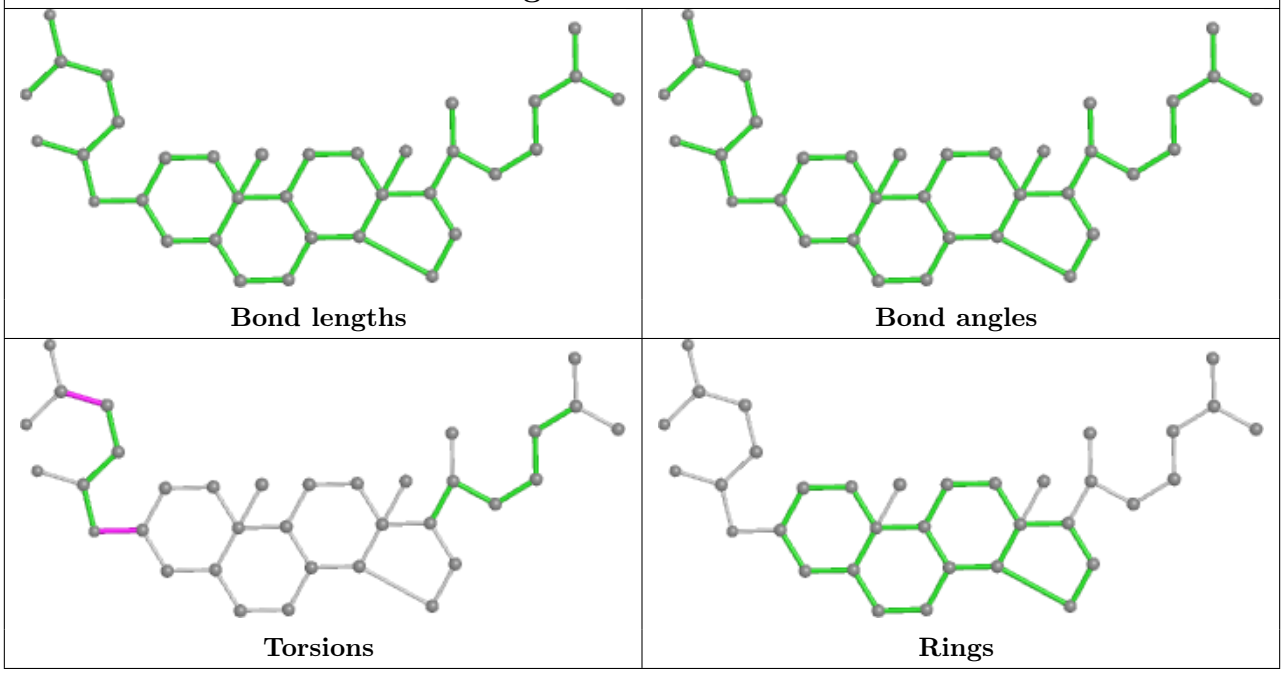
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1604	Y01	3	0
3	E	1608	Y01	2	0
3	E	1602	Y01	1	0
3	E	1607	Y01	5	0
3	E	1601	Y01	1	0

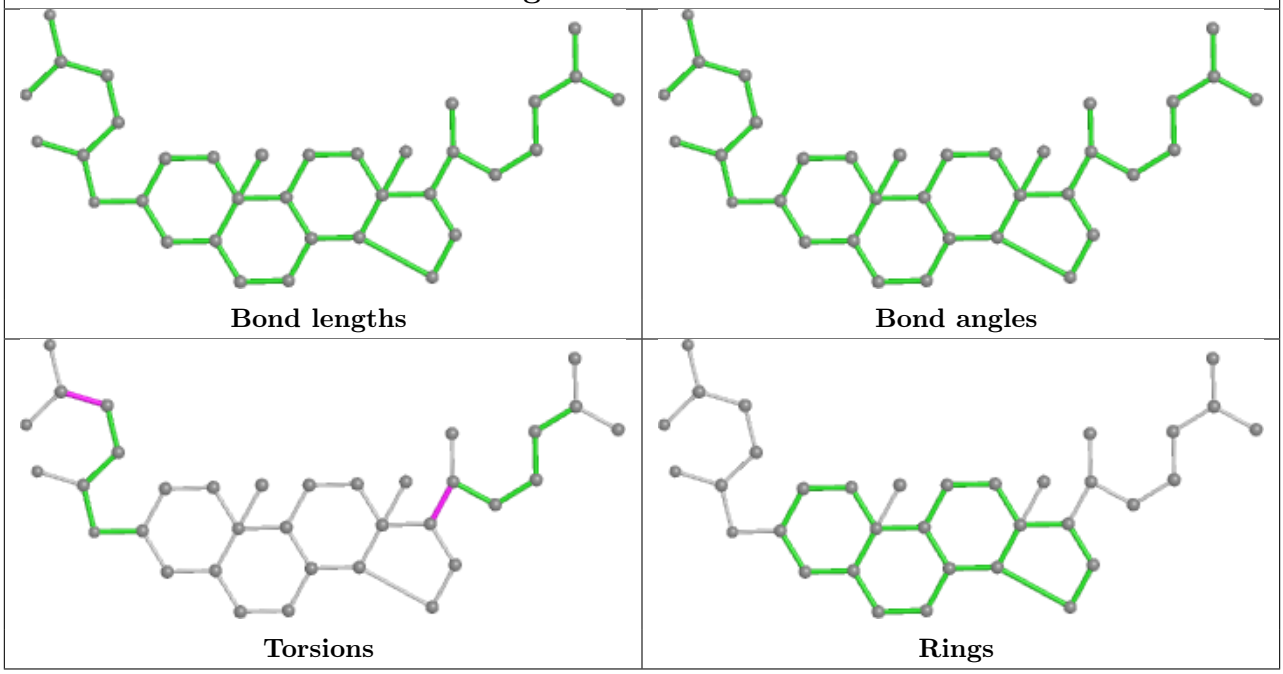
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

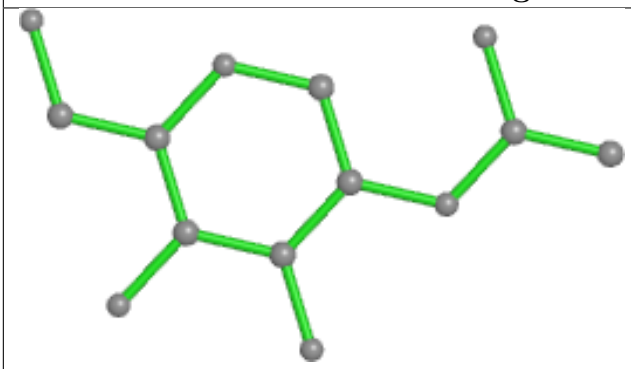
Ligand Y01 E 1604



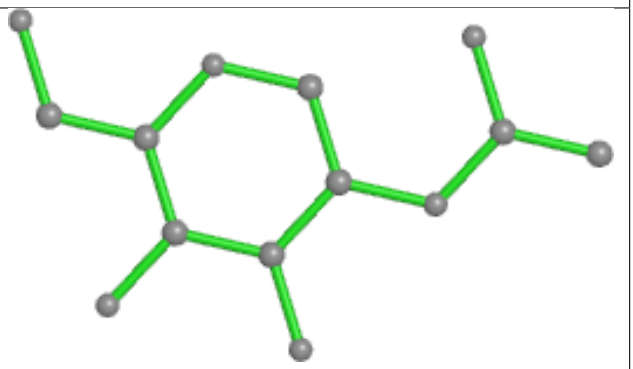
Ligand Y01 E 1606



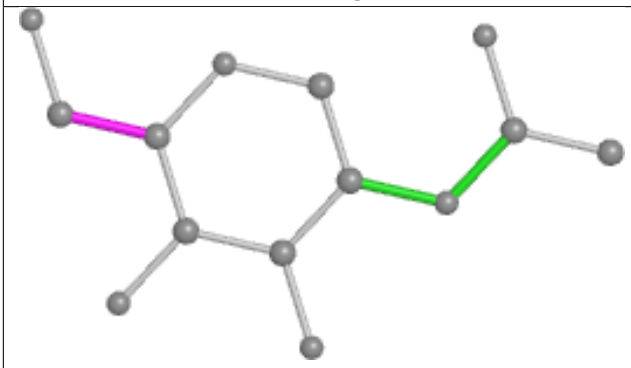
Ligand NAG E 1611



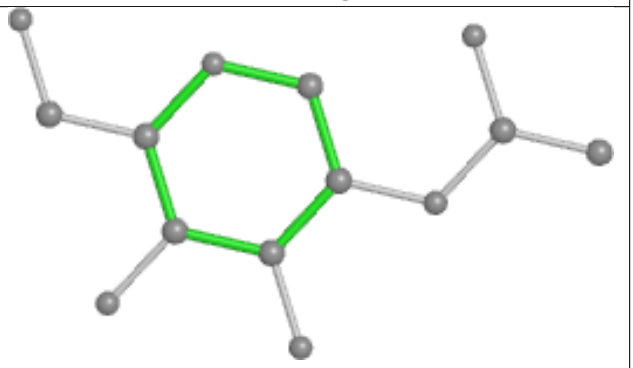
Bond lengths



Bond angles

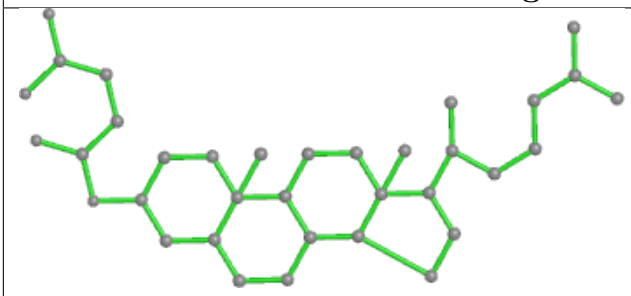


Torsions



Rings

Ligand Y01 E 1608



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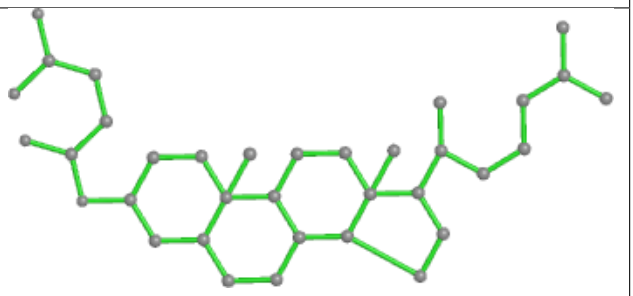
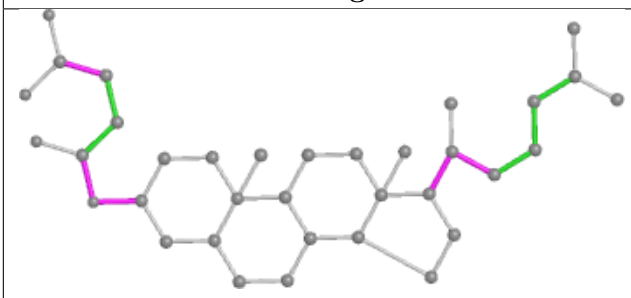
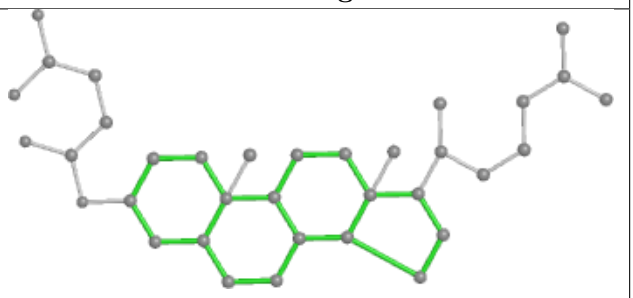


Bond angles

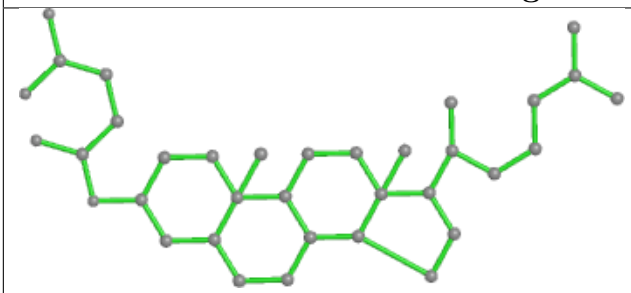


Torsions

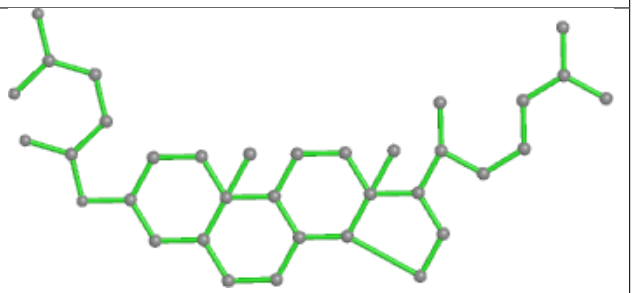


Rings

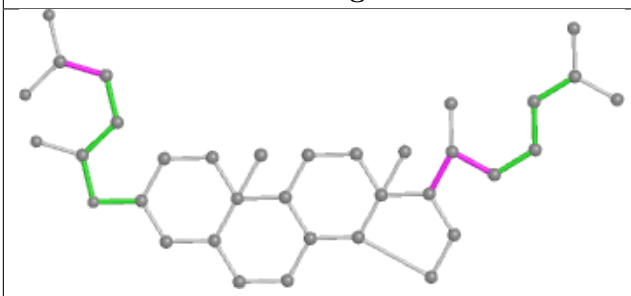
Ligand Y01 E 1602



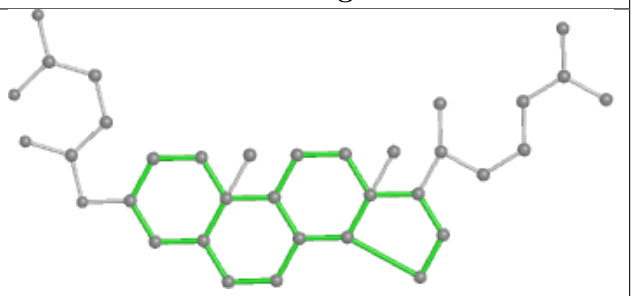
Bond lengths



Bond angles

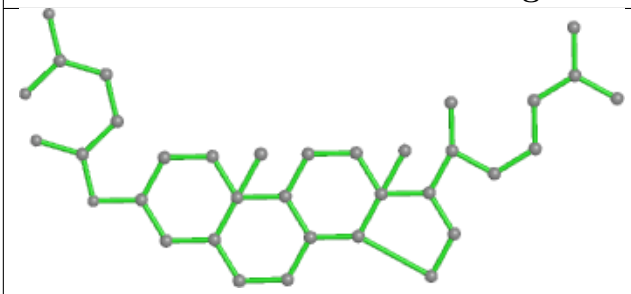


Torsions

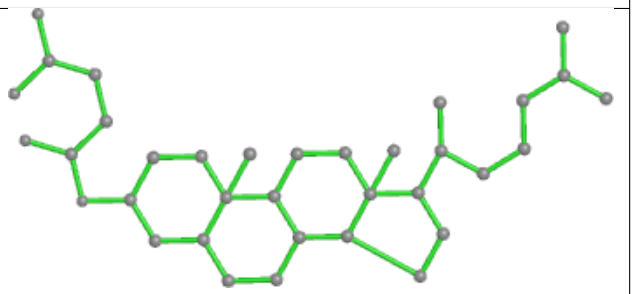


Rings

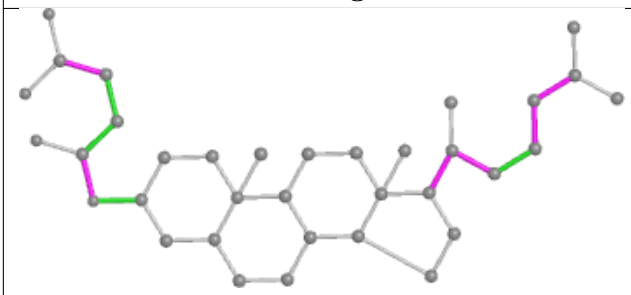
Ligand Y01 E 1607



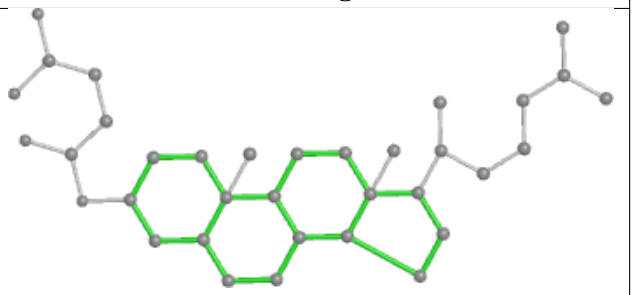
Bond lengths



Bond angles

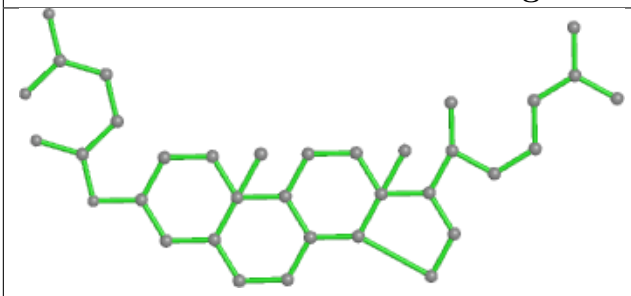


Torsions

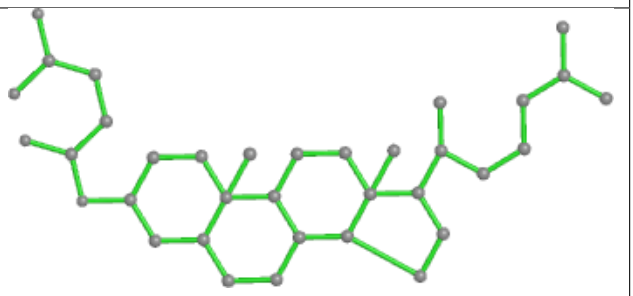


Rings

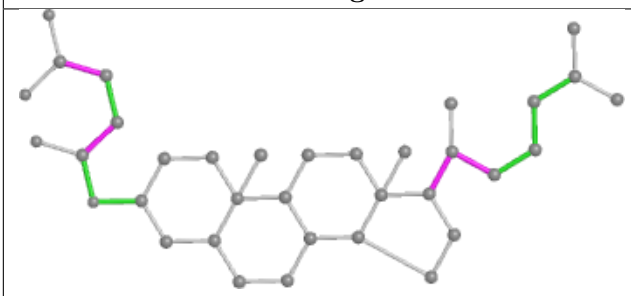
Ligand Y01 E 1601



Bond lengths



Bond angles



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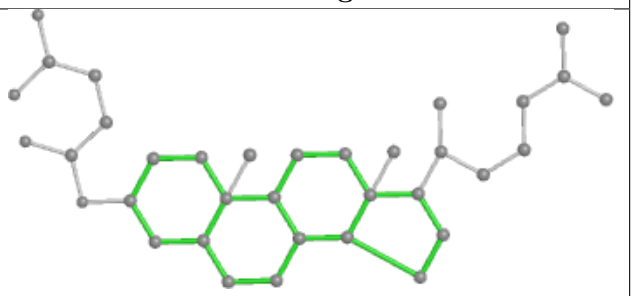
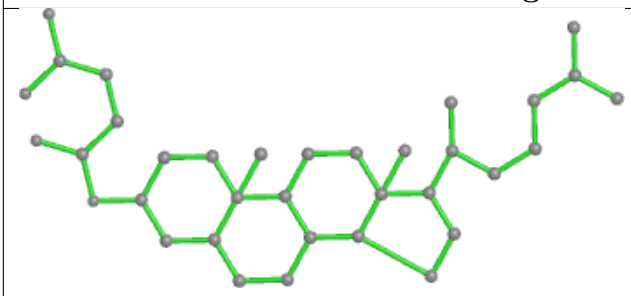
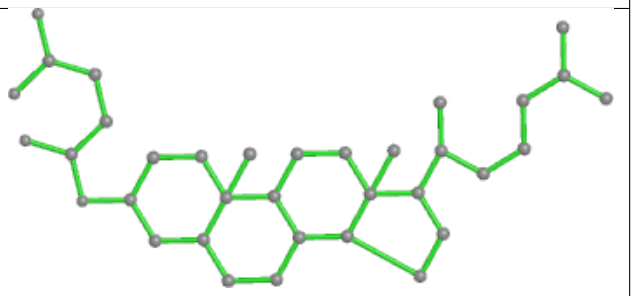


Rings

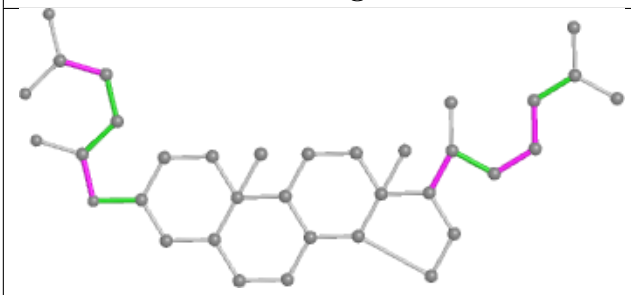
Ligand Y01 E 1603



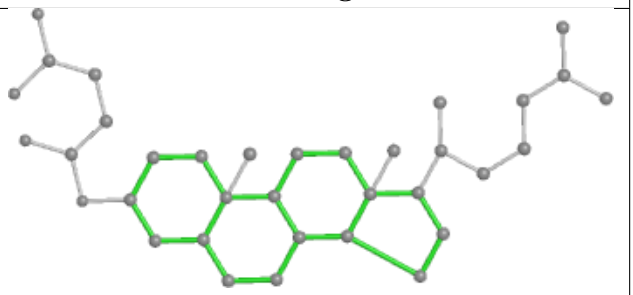
Bond lengths



Bond angles

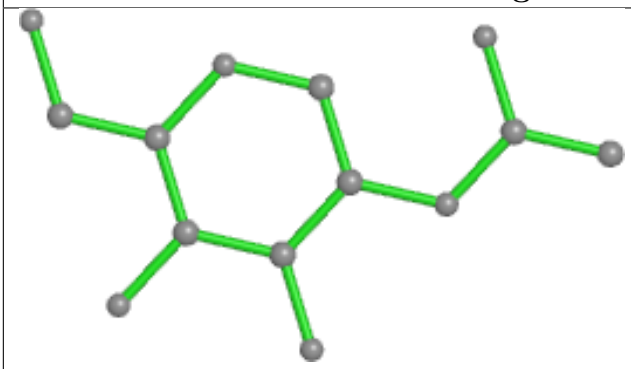


Torsions

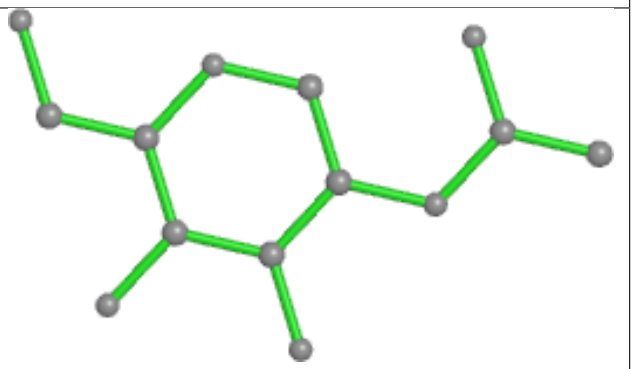


Rings

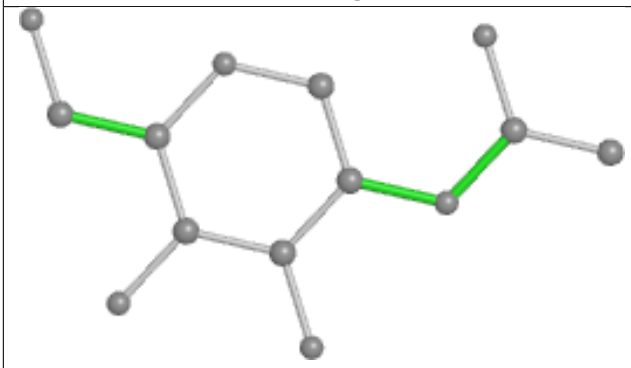
Ligand NAG E 1610



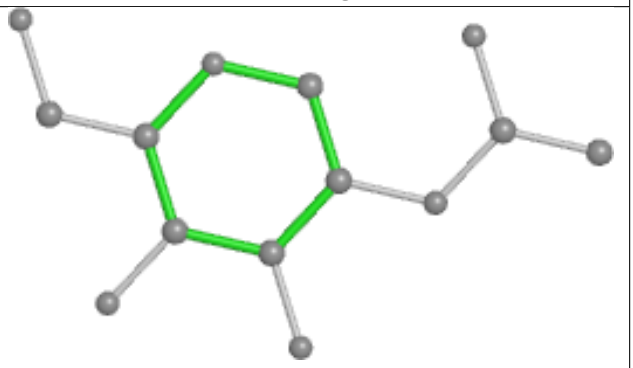
Bond lengths



Bond angles

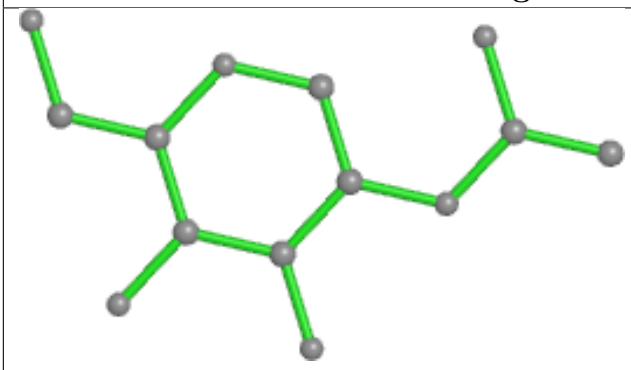


Torsions

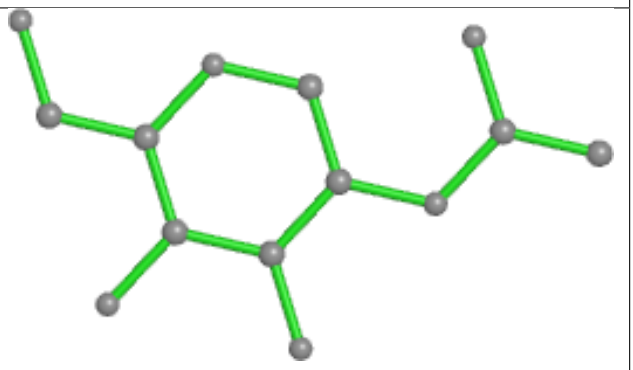


Rings

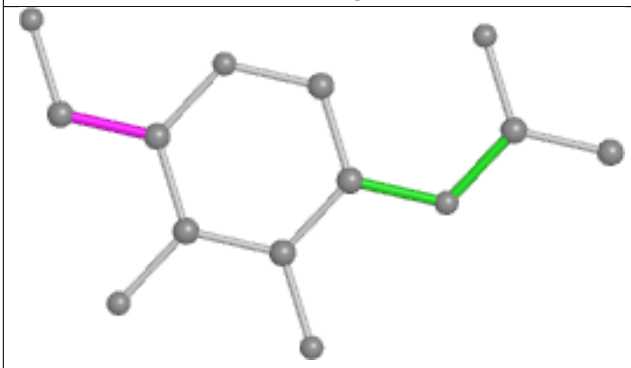
Ligand NAG E 1612



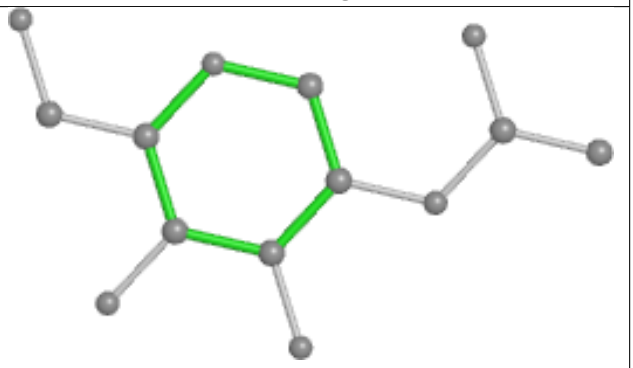
Bond lengths



Bond angles

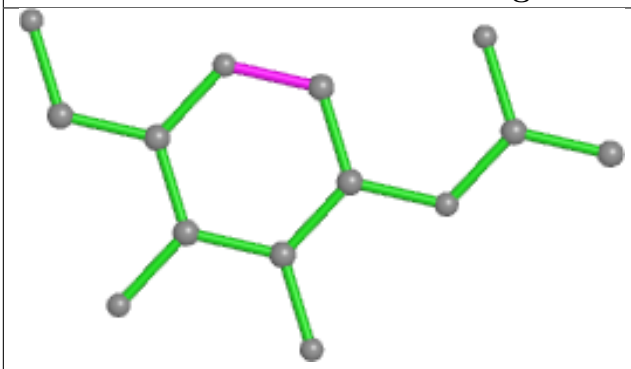


Torsions

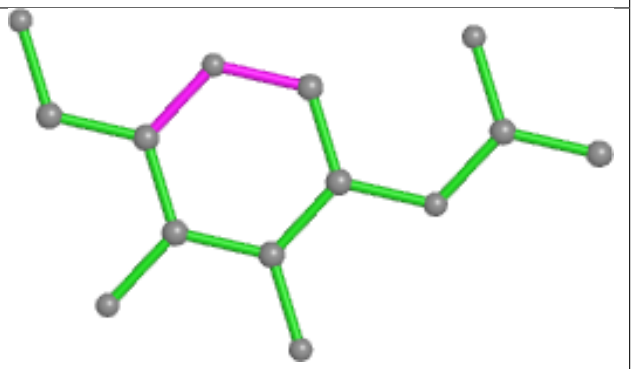


Rings

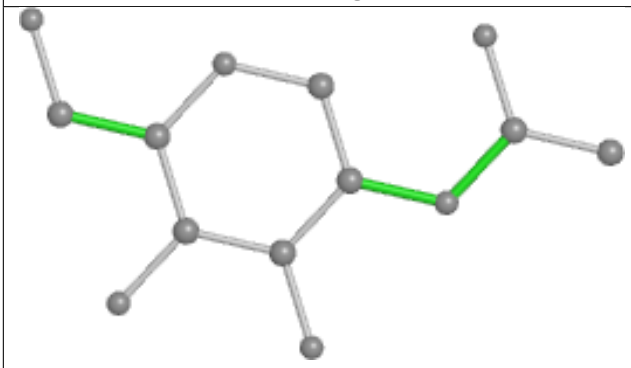
Ligand NAG E 1609



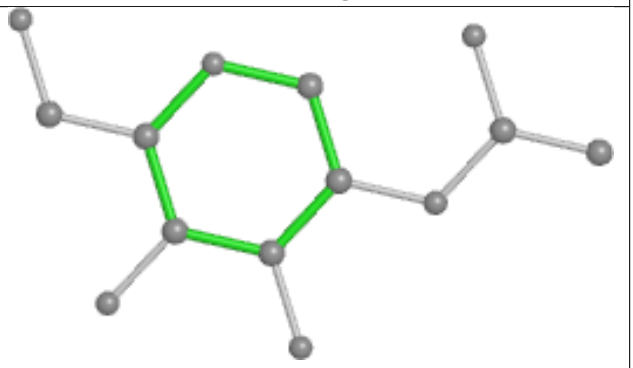
Bond lengths



Bond angles

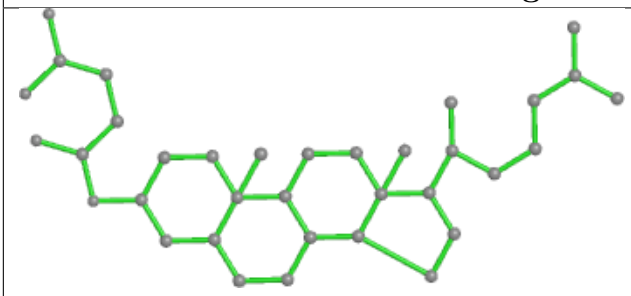


Torsions

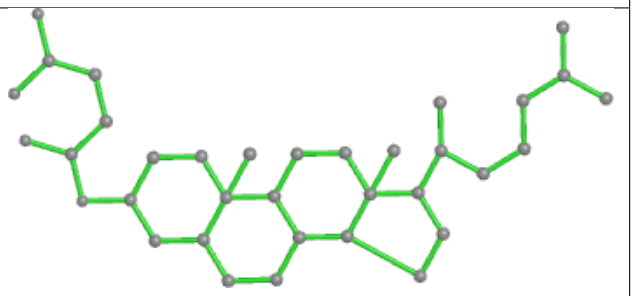


Rings

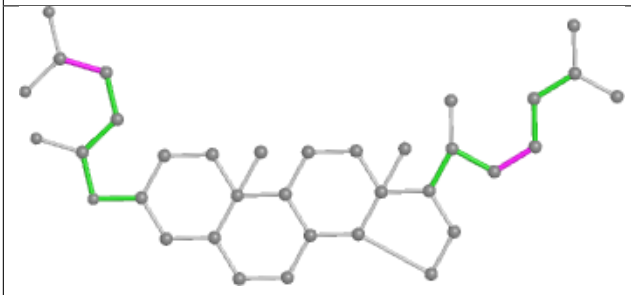
Ligand Y01 E 1605



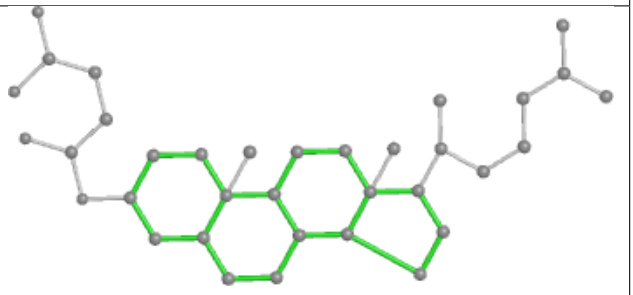
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

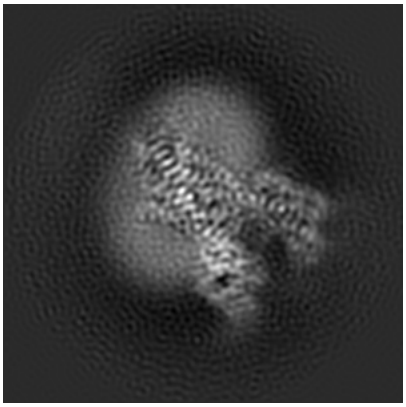
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30957. These allow visual inspection of the internal detail of the map and identification of artifacts.

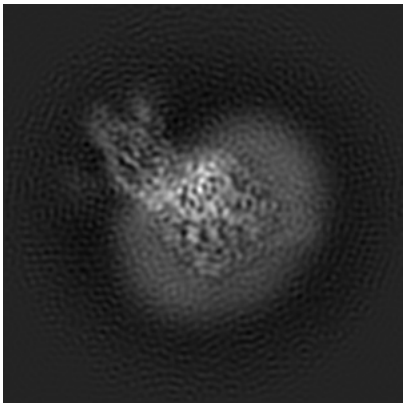
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

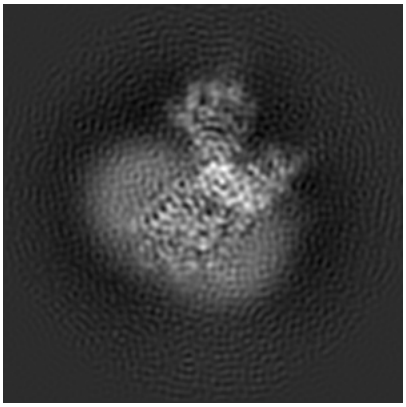
6.1.1 Primary map



X



Y

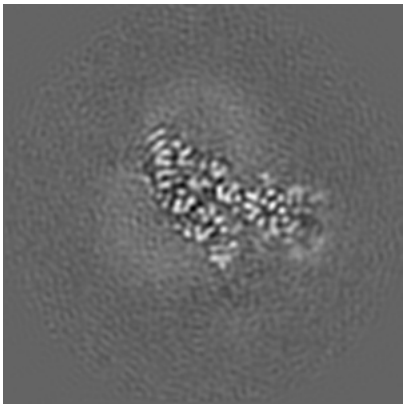


Z

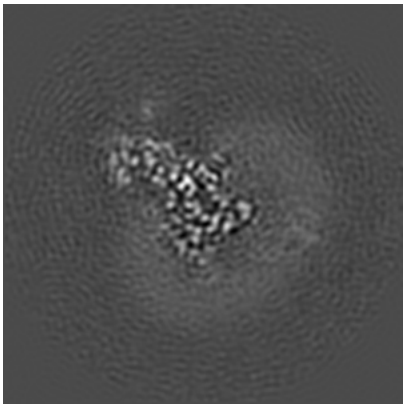
The images above show the map projected in three orthogonal directions.

6.2 Central slices

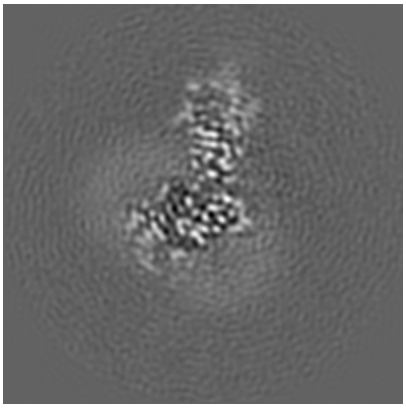
6.2.1 Primary map



X Index: 92



Y Index: 92

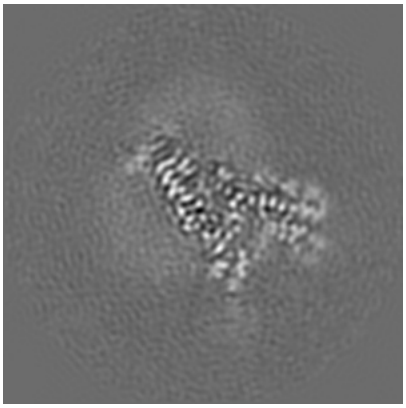


Z Index: 92

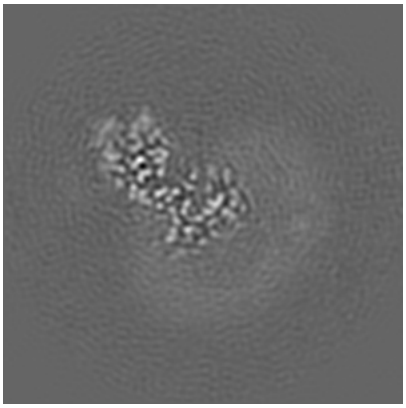
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

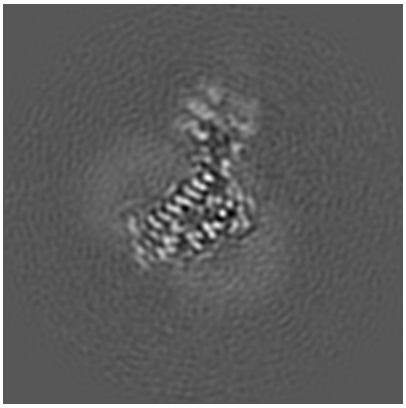
6.3.1 Primary map



X Index: 96



Y Index: 99

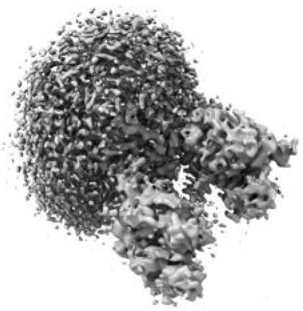


Z Index: 97

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

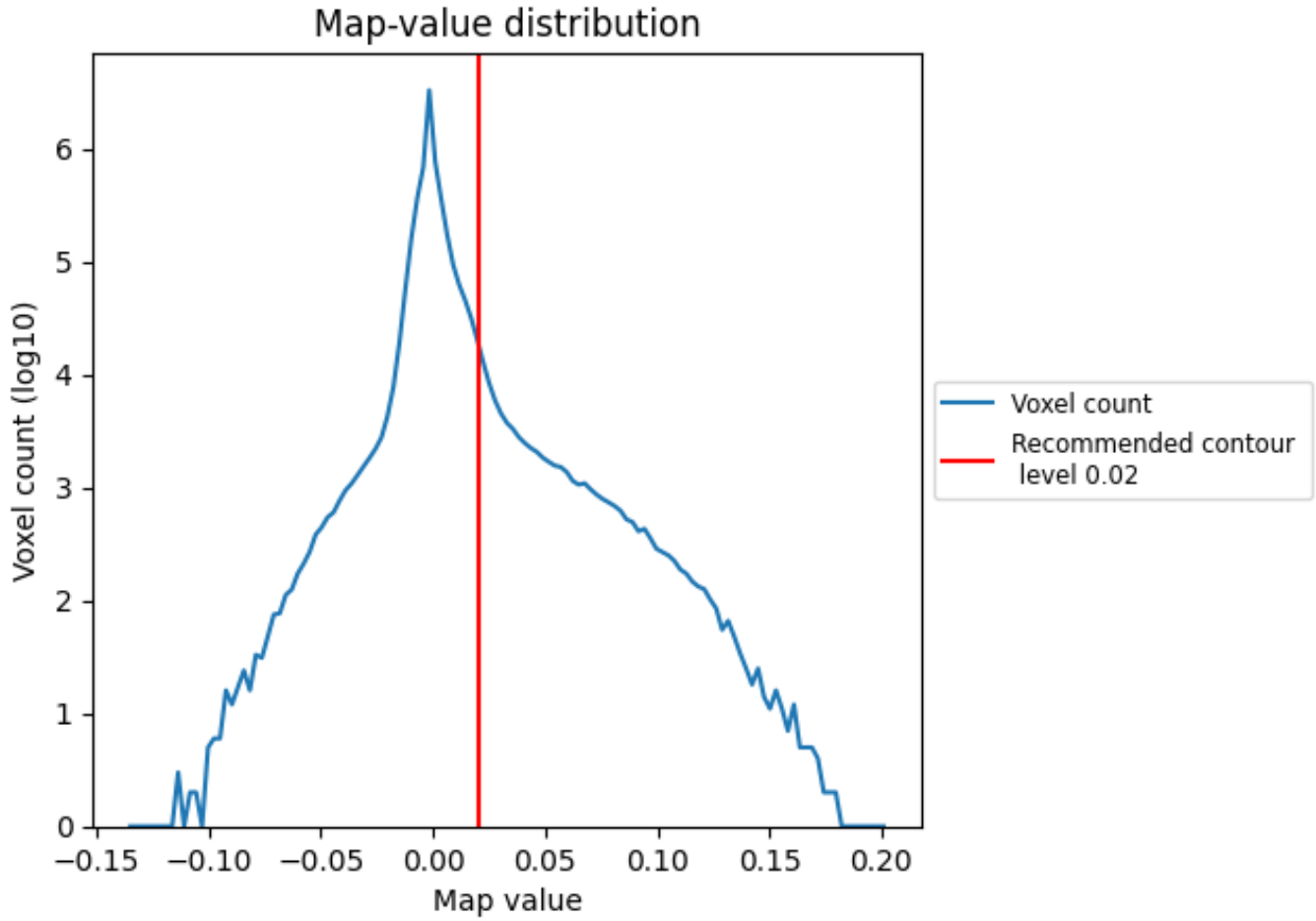
6.5 Mask visualisation (i)

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

7 Map analysis

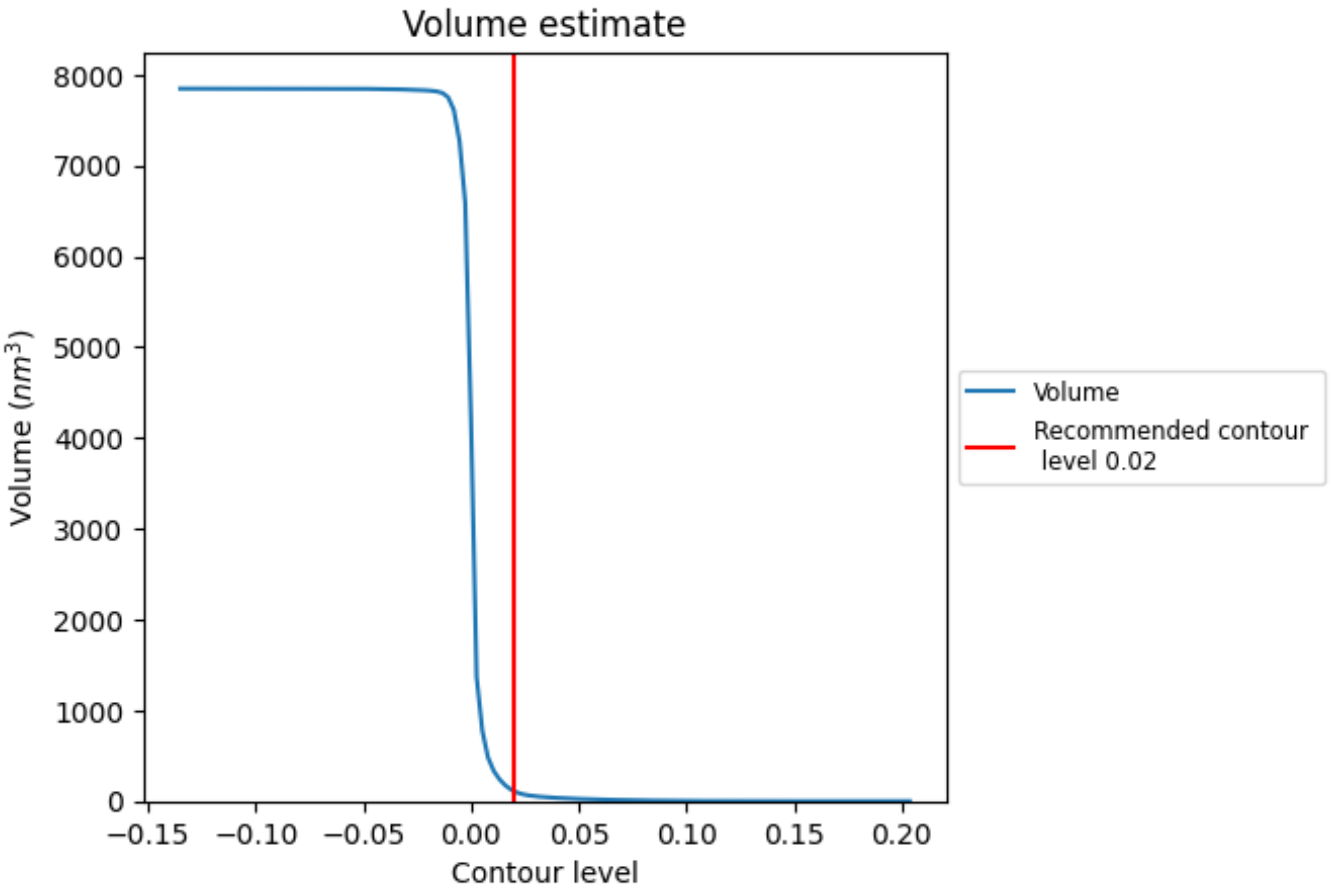
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

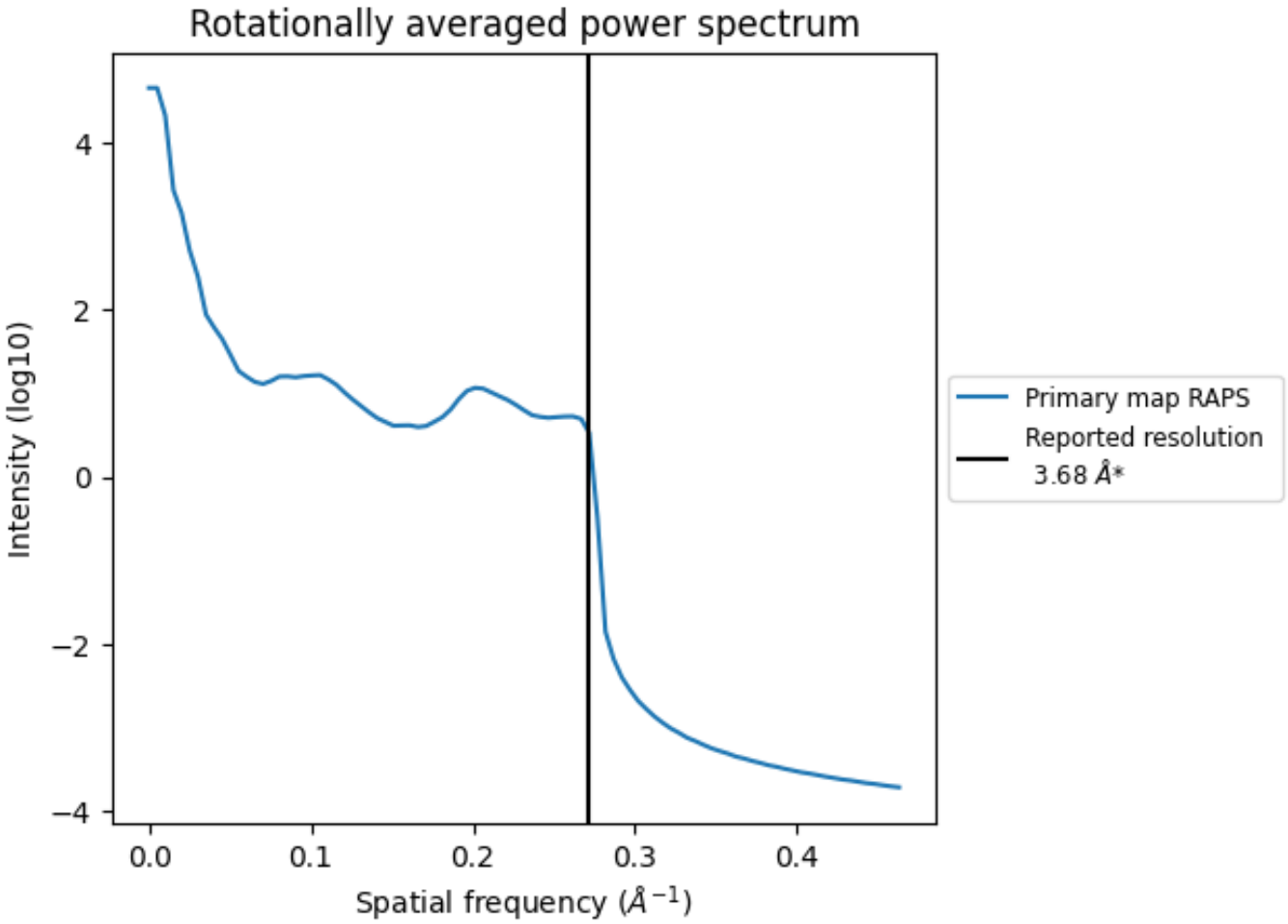
7.2 Volume estimate



The volume at the recommended contour level is 110 nm^3; this corresponds to an approximate mass of 100 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 0.272 Å^{-1}

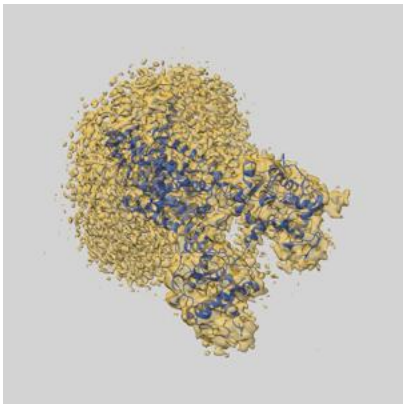
8 Fourier-Shell correlation (i)

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

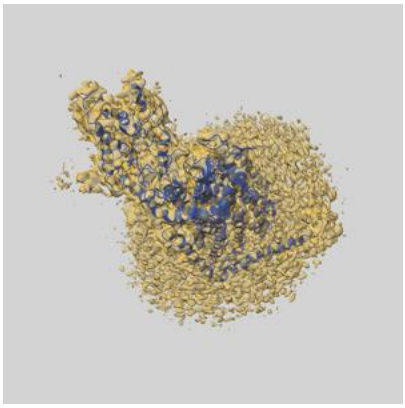
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30957 and PDB model 7E2H. Per-residue inclusion information can be found in section 3 on page 6.

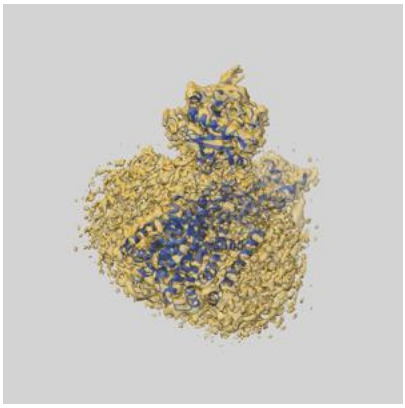
9.1 Map-model overlay



X



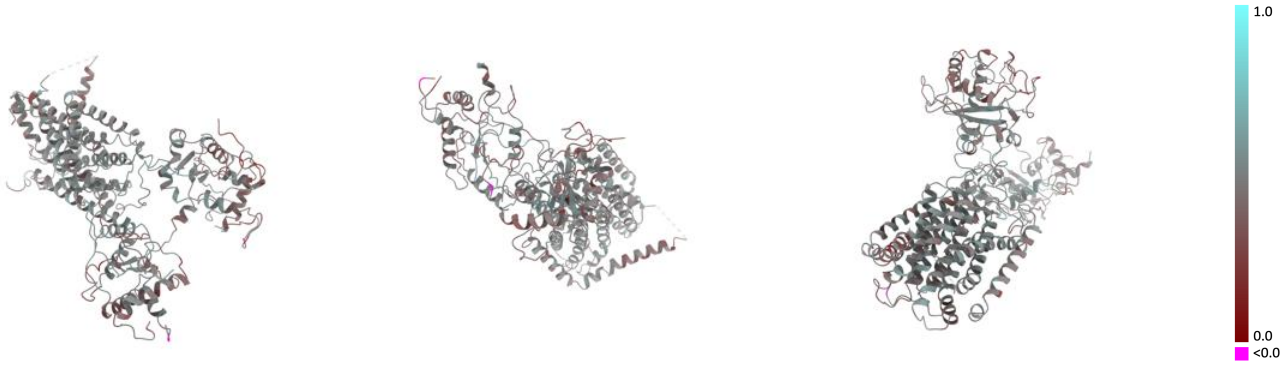
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

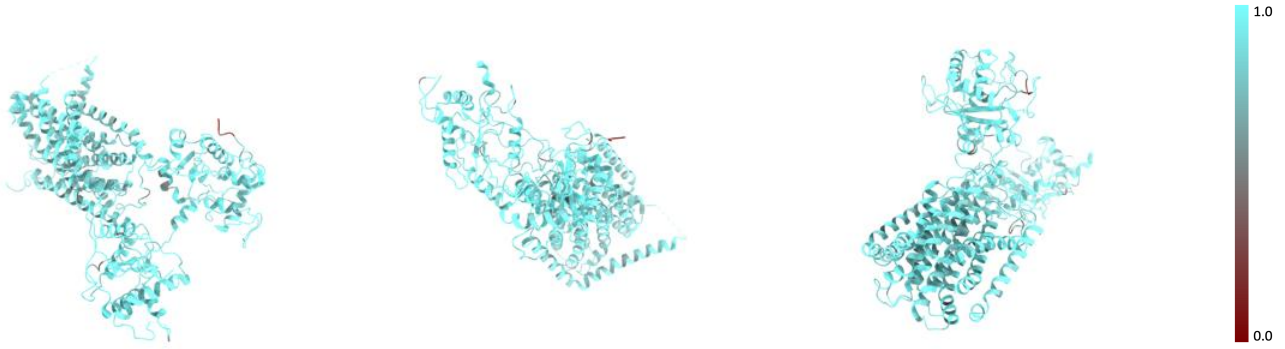
9.2 Q-score mapped to coordinate model (i)



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.

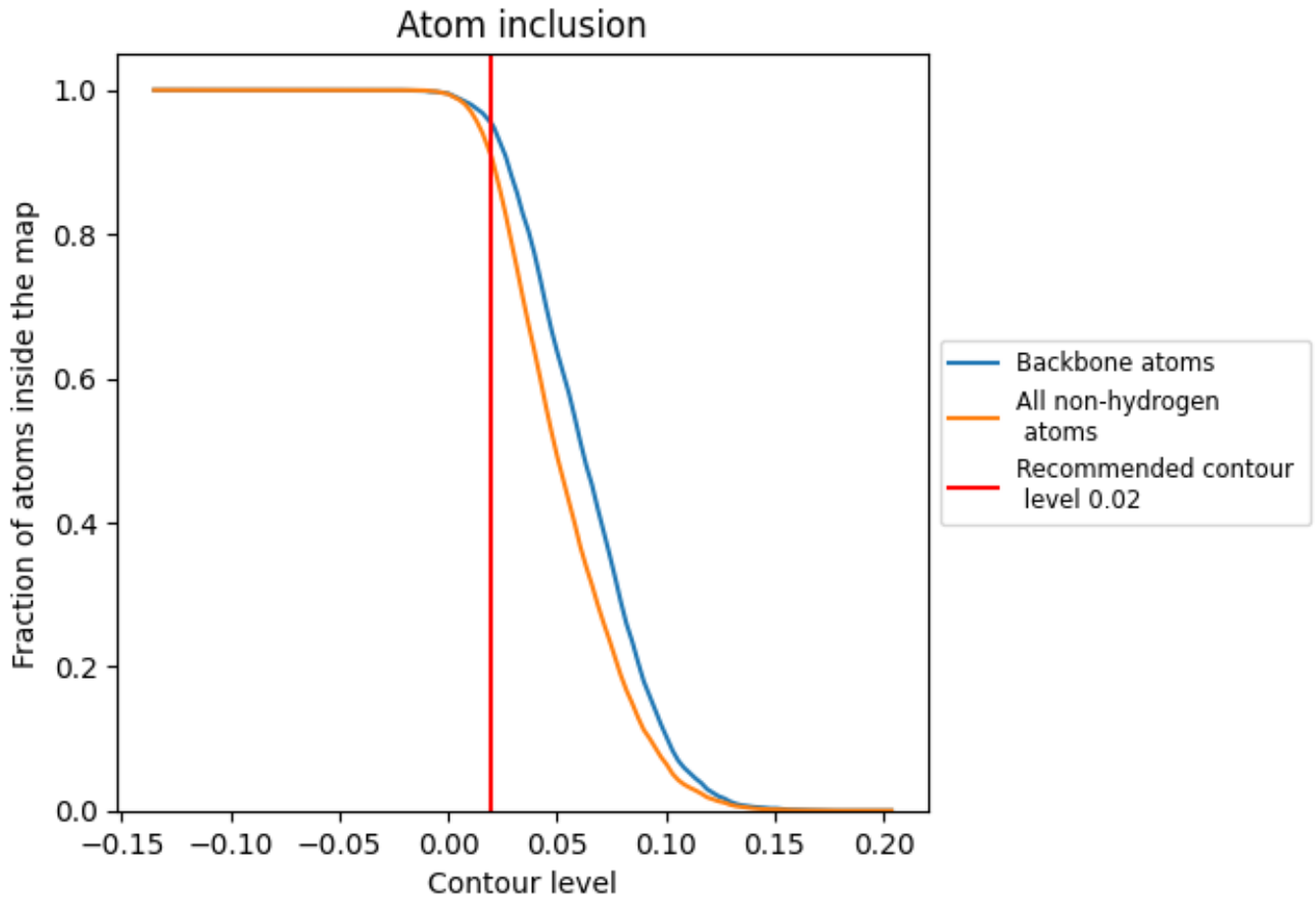
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9065	0.4640
D	0.9125	0.4700
E	0.9060	0.4630