



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:02 PM UTC

PDB ID : 7E2I / pdb_00007e2i
EMDB ID : EMD-30958
Title : Cryo-EM structure of hDisp1NNN-ShhN
Authors : Li, W.; Wang, L.; Gong, X.
Deposited on : 2021-02-05
Resolution : 4.07 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

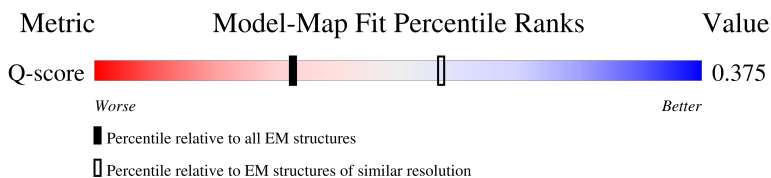
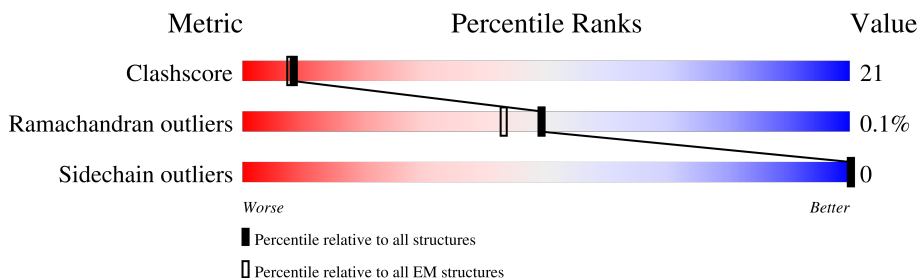
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

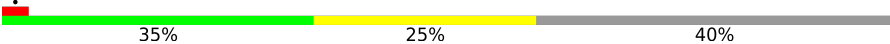
The reported resolution of this entry is 4.07 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6427 (3.58 - 4.57)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	462	
2	D	1524	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8569 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 Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	151	Total	C	N	O	S	0	0
			1209	754	215	235	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	907	Total	C	N	O	S	0	0
			7058	4592	1135	1269	62		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	572	ASN	ASP	engineered mutation	UNP Q96F81
D	573	ASN	ASP	engineered mutation	UNP Q96F81
D	1051	ASN	ASP	engineered mutation	UNP Q96F81

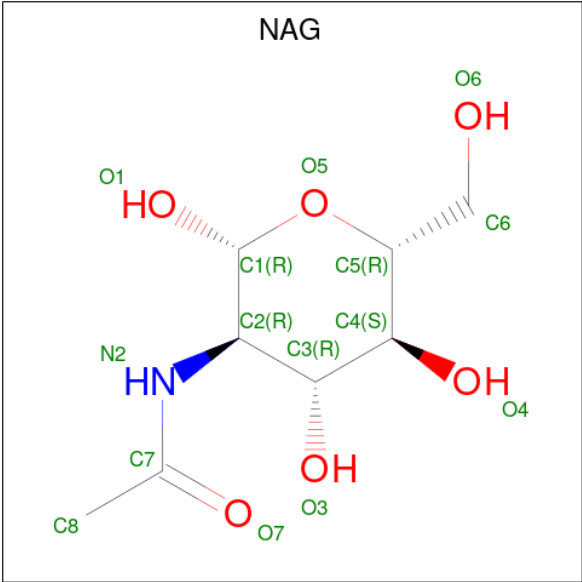
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	



SER	GLU	ASN
ILE	LEU	MET
GLU	SER	GLU
LEU	LEU	ALA
HIS	SER	ASN
LEU	GLN	VAL
PRO	THR	PRO
LYS	ASP	ALA
MET	ALA	VAL
ALA	SER	LEU
GLU	VAL	THR
PRO	ASN	HIS
SER	SER	SER
SER	GLU	GLU
PHE	HIS	LEU
VAL	PHE	SER
CYS	ASN	GLY
ARG	GLN	GLU
SER	ASN	SER
THR	GLU	LEU
GLY	PRO	LEU
SER	LYS	ILE
LEU	VAL	LYS
LEU	LEU	THR
LYS	PHE	THR
THR	ASN	ASN
CYS	HIS	LEU
CYS	LEU	CYS
ASP	MET	LEU
PRO	GLY	GLY
GLU	GLU	GLU
ASN	ALA	ALA
LYS	GLY	GLY
GLN	CYS	GLN
ARG	ARG	CYS
GLU	SER	THR
LEU	CYS	PRO
CYS	PRO	ASN
LYS	ASN	LYS
ASN	ASN	ASN
ARG	SER	SER
ASP	GLN	GLN
VAL	SER	SER
SER	CYS	CYS
ASN	GLY	GLY
LEU	ARG	ARG
GLU	ILE	ILE
SER	VAL	VAL
SER	ARG	ARG
GLY	VAL	VAL
GLY	LYS	LYS
THR	CYS	CYS
GLU	ASN	ASN
ASN	SER	SER
LYS	VAL	VAL
VAL	ASP	ASP
GLY	CYS	CYS
LYS	GLN	GLN
VAL	MET	MET
	PRO	PRO

ASN
MET
GLU
ALA
ASN
VAL
PRO
ALA
VAL
LEU
THR
HIS
SER
GLU
LEU
SER
GLY
GLU
SER
LEU
ILE
LYS
THR
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173169	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 ($e^-/\text{\AA}^2$)	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	0.124	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	187.152, 187.152, 187.152	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	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: ZN, 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	G	0.17	0/1235	0.39	0/1668
2	D	0.30	0/7244	0.49	1/9862 (0.0%)
All	All	0.28	0/8479	0.47	1/11530 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	255	PHE	N-CA-C	6.31	116.33	108.19

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	G	1209	0	1159	59	0
2	D	7058	0	6881	305	0
3	G	1	0	0	0	0
4	D	245	0	343	8	0
5	D	56	0	52	0	0
All	All	8569	0	8435	365	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 21.

All (365) 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:D:350:PRO:O	2:D:356:ASN:ND2	2.06	0.89
2:D:314:TRP:HE1	2:D:449:LEU:HD13	1.38	0.86
2:D:1024:VAL:HA	2:D:1027:LEU:HD12	1.63	0.80
2:D:501:LEU:HD12	4:D:1604:Y01:HAT2	1.67	0.74
2:D:313:LEU:H	2:D:448:ALA:HB1	1.53	0.74
2:D:340:CYS:N	2:D:348:CYS:SG	2.58	0.72
2:D:316:LEU:HG	2:D:317:PRO:HD3	1.71	0.72
1:G:56:LEU:HD11	2:D:338:ASP:HA	1.72	0.72
2:D:1048:LEU:HD12	2:D:1116:MET:HE1	1.72	0.71
1:G:45:LYS:NZ	1:G:176:GLU:O	2.23	0.70
2:D:514:VAL:HG22	2:D:518:MET:HE2	1.72	0.70
1:G:144:ARG:HH21	1:G:186:LYS:HA	1.58	0.69
1:G:158:TYR:HB3	1:G:181:ILE:HD11	1.74	0.69
2:D:432:VAL:HA	2:D:453:MET:H	1.57	0.69
1:G:44:TYR:HD1	1:G:45:LYS:HG2	1.58	0.68
2:D:611:THR:OG1	2:D:1051:ASN:ND2	2.27	0.68
2:D:915:ASP:OD1	2:D:916:ILE:N	2.26	0.67
2:D:294:ASP:OD1	2:D:295:VAL:N	2.24	0.67
2:D:476:ASN:OD1	2:D:477:SER:N	2.27	0.67
2:D:317:PRO:HA	2:D:320:LYS:HG2	1.77	0.67
2:D:547:ARG:HH21	2:D:553:GLU:HB2	1.60	0.67
2:D:1058:VAL:O	2:D:1061:ARG:NH2	2.27	0.66
2:D:913:ARG:O	2:D:921:ARG:N	2.23	0.66
2:D:1059:ALA:O	2:D:1075:SER:OG	2.10	0.66
2:D:296:PRO:HG3	2:D:352:TRP:HE1	1.60	0.66
2:D:995:ALA:HB1	2:D:1050:VAL:HG11	1.76	0.66
2:D:422:ASN:OD1	2:D:426:GLN:NE2	2.30	0.65
2:D:306:THR:O	2:D:482:THR:OG1	2.15	0.65
2:D:601:LEU:HD21	4:D:1607:Y01:HAU1	1.78	0.64
2:D:859:TRP:O	2:D:862:ASN:ND2	2.31	0.64
1:G:68:ARG:NH1	1:G:92:THR:OG1	2.31	0.64
2:D:478:SER:OG	2:D:482:THR:O	2.15	0.63
2:D:438:THR:O	2:D:440:LYS:NZ	2.25	0.63
2:D:951:ILE:HD12	2:D:967:PHE:HB2	1.79	0.63
2:D:464:MET:HA	2:D:467:ILE:HD13	1.80	0.63
2:D:256:LYS:NZ	2:D:898:GLU:OE2	2.29	0.63
2:D:691:CYS:O	2:D:695:LEU:HG	1.99	0.63
2:D:304:VAL:HA	2:D:453:MET:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:362:ASN:HD21	2:D:364:ARG:HH11	1.46	0.63
2:D:929:SER:OG	2:D:930:THR:N	2.27	0.62
2:D:739:ASN:CG	2:D:740:PRO:HD2	2.24	0.61
2:D:349:CYS:HB3	2:D:457:PRO:HB3	1.81	0.61
2:D:503:ASP:OD2	2:D:1101:THR:OG1	2.16	0.61
2:D:314:TRP:NE1	2:D:449:LEU:HD13	2.15	0.61
2:D:252:ASN:C	2:D:254:PRO:HD2	2.25	0.61
2:D:1143:ILE:HG22	2:D:1145:LEU:H	1.66	0.61
2:D:300:TYR:HA	2:D:459:GLU:HA	1.83	0.61
1:G:155:ARG:HH22	1:G:178:LYS:HB2	1.65	0.60
2:D:238:ASN:O	2:D:241:VAL:HG12	2.01	0.60
2:D:934:THR:HG21	2:D:939:LYS:HB2	1.81	0.60
2:D:287:HIS:ND1	2:D:289:ASP:O	2.34	0.60
2:D:890:ILE:HG13	2:D:891:LYS:H	1.67	0.60
2:D:865:CYS:SG	2:D:892:ARG:NH1	2.74	0.60
2:D:1064:PRO:HB2	2:D:1066:PRO:HD2	1.84	0.60
2:D:742:MET:HE1	2:D:1032:TRP:O	2.02	0.59
2:D:818:ILE:O	2:D:823:SER:OG	2.19	0.59
2:D:296:PRO:HG3	2:D:352:TRP:NE1	2.18	0.59
2:D:353:THR:H	2:D:356:ASN:ND2	2.00	0.58
2:D:1098:MET:SD	2:D:1110:THR:OG1	2.61	0.58
2:D:942:GLN:NE2	2:D:946:GLU:OE1	2.36	0.58
2:D:1112:MET:HA	2:D:1115:ILE:HG22	1.83	0.58
2:D:350:PRO:O	2:D:352:TRP:N	2.37	0.58
2:D:215:ASP:OD1	2:D:216:PHE:N	2.37	0.58
2:D:739:ASN:OD1	2:D:740:PRO:HD2	2.03	0.58
2:D:1056:TYR:HE2	2:D:1124:THR:HA	1.69	0.58
1:G:171:ASP:HB2	1:G:185:VAL:HA	1.86	0.57
2:D:1002:THR:HG23	2:D:1003:THR:HG23	1.86	0.57
1:G:53:GLU:HG3	1:G:54:LYS:HD2	1.87	0.57
2:D:497:GLN:NE2	2:D:498:ASP:OD1	2.37	0.57
2:D:560:LEU:HD11	4:D:1604:Y01:HAP1	1.85	0.57
1:G:55:THR:O	1:G:60:GLY:N	2.38	0.57
2:D:711:PRO:O	2:D:715:ILE:HG12	2.03	0.57
2:D:525:MET:O	2:D:528:THR:OG1	2.20	0.57
1:G:121:LYS:H	1:G:151:SER:HB3	1.69	0.57
2:D:464:MET:HG2	2:D:489:PHE:HD2	1.70	0.57
2:D:737:CYS:SG	2:D:738:ILE:N	2.78	0.57
2:D:515:LEU:HA	2:D:518:MET:HE3	1.86	0.56
2:D:742:MET:HE2	2:D:1034:LEU:HG	1.86	0.56
2:D:791:TRP:CD1	2:D:960:GLU:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1006:ILE:HD12	2:D:1006:ILE:H	1.70	0.56
2:D:338:ASP:OD1	2:D:338:ASP:N	2.36	0.56
2:D:453:MET:HB2	2:D:772:PHE:CZ	2.40	0.56
1:G:53:GLU:O	1:G:59:SER:OG	2.11	0.56
1:G:171:ASP:OD2	1:G:186:LYS:N	2.24	0.56
2:D:352:TRP:CD1	2:D:455:PHE:HB2	2.42	0.55
2:D:313:LEU:HB3	2:D:448:ALA:O	2.06	0.55
2:D:1131:CYS:HA	2:D:1134:LEU:HG	1.88	0.55
2:D:329:ARG:HE	2:D:472:PHE:HE1	1.54	0.55
2:D:496:PHE:HD1	2:D:755:PHE:HE1	1.55	0.55
2:D:820:SER:O	2:D:823:SER:OG	2.11	0.55
2:D:1003:THR:HB	2:D:1008:ILE:HD11	1.88	0.55
2:D:219:PRO:HG3	2:D:496:PHE:CE2	2.41	0.55
2:D:709:VAL:O	2:D:713:ILE:HG12	2.06	0.55
2:D:717:PHE:C	2:D:719:TYR:H	2.15	0.54
1:G:134:HIS:O	1:G:141:TYR:OH	2.26	0.54
2:D:358:ILE:HG12	2:D:375:VAL:HG22	1.89	0.54
1:G:122:LEU:HD11	1:G:161:LEU:HD11	1.90	0.54
2:D:479:ASP:OD1	2:D:480:GLY:N	2.41	0.54
2:D:519:CYS:SG	2:D:525:MET:HG2	2.48	0.54
1:G:49:PRO:HG2	1:G:172:TRP:CD1	2.43	0.54
2:D:326:ASP:OD1	2:D:330:ILE:HD12	2.08	0.54
1:G:55:THR:O	1:G:59:SER:OG	2.25	0.54
1:G:150:THR:H	1:G:158:TYR:HE1	1.54	0.54
2:D:315:ASN:OD1	2:D:317:PRO:HD2	2.08	0.54
2:D:1044:VAL:HG22	2:D:1048:LEU:HD23	1.90	0.54
2:D:644:ASN:O	2:D:648:MET:HG2	2.08	0.53
1:G:47:PHE:HB3	1:G:174:TYR:HD1	1.73	0.53
2:D:350:PRO:C	2:D:352:TRP:H	2.16	0.53
2:D:351:SER:O	2:D:454:LEU:HD11	2.09	0.53
2:D:1041:THR:HA	2:D:1044:VAL:HG12	1.91	0.53
2:D:559:ASN:HD21	2:D:633:PHE:HA	1.73	0.53
2:D:299:ARG:HG3	2:D:300:TYR:CD1	2.44	0.52
2:D:305:PHE:HE2	2:D:322:MET:HG3	1.73	0.52
2:D:584:THR:HG21	2:D:600:THR:HB	1.91	0.52
1:G:48:ILE:HG21	1:G:166:VAL:HG22	1.90	0.52
2:D:1011:TYR:HB3	2:D:1130:MET:HE3	1.91	0.52
2:D:791:TRP:HD1	2:D:960:GLU:HB2	1.74	0.52
2:D:481:VAL:HG23	2:D:482:THR:HG22	1.90	0.52
2:D:635:VAL:O	2:D:639:THR:HG23	2.09	0.52
1:G:53:GLU:O	1:G:55:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:THR:HG22	1:G:158:TYR:CE1	2.44	0.52
2:D:298:ASP:HA	2:D:302:ARG:NH1	2.25	0.52
2:D:691:CYS:O	2:D:694:VAL:HG12	2.09	0.52
2:D:1015:SER:O	2:D:1019:THR:HG23	2.10	0.52
2:D:310:GLY:O	2:D:311:GLU:HG3	2.10	0.51
2:D:496:PHE:HA	2:D:755:PHE:HZ	1.74	0.51
2:D:530:MET:HG3	2:D:651:TRP:HE1	1.75	0.51
2:D:553:GLU:N	2:D:553:GLU:OE1	2.44	0.51
1:G:61:ARG:NH1	1:G:63:GLU:OE2	2.42	0.51
2:D:296:PRO:HG3	2:D:352:TRP:CZ2	2.46	0.51
2:D:715:ILE:HG13	2:D:716:LYS:N	2.26	0.51
2:D:745:PRO:O	2:D:977:GLN:NE2	2.44	0.51
1:G:47:PHE:HD2	1:G:174:TYR:HE1	1.58	0.51
1:G:58:ALA:O	1:G:171:ASP:HB3	2.11	0.51
2:D:808:GLY:C	2:D:809:LYS:HD3	2.36	0.51
2:D:878:SER:OG	2:D:880:PRO:O	2.29	0.51
2:D:934:THR:O	2:D:935:LEU:HD23	2.11	0.51
2:D:1089:THR:HG23	2:D:1090:THR:H	1.75	0.51
2:D:821:PRO:HA	2:D:824:GLN:NE2	2.26	0.51
2:D:840:PHE:HD1	2:D:842:GLN:HE21	1.59	0.50
2:D:327:ASN:ND2	2:D:331:ARG:HG3	2.26	0.50
2:D:752:PHE:O	2:D:754:VAL:HG23	2.12	0.50
1:G:150:THR:HG22	1:G:158:TYR:HE1	1.76	0.50
2:D:941:HIS:NE2	2:D:945:LYS:HD3	2.26	0.50
2:D:890:ILE:O	2:D:894:ILE:HG22	2.11	0.50
2:D:1008:ILE:HA	2:D:1011:TYR:HD2	1.76	0.50
2:D:1004:TRP:HZ3	2:D:1142:GLN:H	1.59	0.50
1:G:106:LEU:HD11	1:G:124:VAL:HG11	1.93	0.50
1:G:149:THR:HG22	1:G:180:HIS:HA	1.93	0.50
2:D:384:THR:O	2:D:387:LYS:HB3	2.12	0.50
2:D:489:PHE:C	2:D:491:ILE:H	2.19	0.50
2:D:352:TRP:HD1	2:D:455:PHE:HB2	1.76	0.50
2:D:516:LEU:O	2:D:520:VAL:HG23	2.11	0.50
2:D:1128:GLN:O	2:D:1132:ARG:N	2.40	0.50
2:D:546:TYR:OH	2:D:554:PHE:O	2.24	0.49
1:G:105:LYS:NZ	1:G:169:GLY:O	2.43	0.49
2:D:362:ASN:ND2	2:D:364:ARG:HH11	2.08	0.49
2:D:1118:ILE:HD11	4:D:1601:Y01:HAP2	1.94	0.49
2:D:467:ILE:H	2:D:467:ILE:HD12	1.77	0.49
2:D:320:LYS:O	2:D:324:ASN:ND2	2.46	0.49
2:D:893:ALA:O	2:D:897:LEU:HG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ARG:HG2	2:D:366:SER:H	1.77	0.49
1:G:59:SER:O	1:G:144:ARG:NH2	2.45	0.49
2:D:291:PHE:HD1	2:D:291:PHE:H	1.60	0.49
2:D:468:TYR:CD1	2:D:472:PHE:HB3	2.48	0.49
2:D:478:SER:HG	2:D:483:THR:HA	1.77	0.49
1:G:44:TYR:CD1	1:G:45:LYS:HG2	2.44	0.49
1:G:57:GLY:HA2	2:D:339:LEU:HD22	1.94	0.49
1:G:87:LYS:HZ2	1:G:89:GLU:HB3	1.77	0.49
2:D:316:LEU:CG	2:D:317:PRO:HD3	2.42	0.49
2:D:824:GLN:HE21	2:D:881:TYR:H	1.59	0.49
2:D:435:ASP:C	2:D:437:MET:H	2.21	0.49
2:D:315:ASN:CG	2:D:317:PRO:HD2	2.38	0.48
2:D:1126:PHE:HE1	2:D:1130:MET:HE2	1.78	0.48
2:D:219:PRO:HG3	2:D:496:PHE:CZ	2.49	0.48
2:D:856:PHE:O	2:D:860:MET:HG2	2.12	0.48
2:D:954:GLU:HG2	2:D:955:LEU:N	2.28	0.48
1:G:109:LEU:HD13	1:G:165:ALA:HA	1.94	0.48
2:D:223:PHE:CD1	2:D:1036:VAL:HG11	2.49	0.48
2:D:353:THR:HG23	2:D:356:ASN:H	1.78	0.48
2:D:587:ASP:OD2	2:D:588:LYS:NZ	2.30	0.48
2:D:246:TYR:H	2:D:250:LEU:CB	2.27	0.48
2:D:909:THR:HB	2:D:910:PRO:HD2	1.95	0.48
2:D:595:GLU:N	2:D:595:GLU:OE1	2.47	0.48
2:D:622:ASN:ND2	2:D:1040:VAL:HG23	2.29	0.48
1:G:104:ASP:OD1	1:G:105:LYS:N	2.47	0.48
2:D:372:GLU:HA	2:D:375:VAL:HG23	1.95	0.48
2:D:475:TRP:H	2:D:475:TRP:HE3	1.62	0.48
2:D:627:ILE:HB	2:D:630:ILE:HG12	1.95	0.48
2:D:305:PHE:CE2	2:D:322:MET:HG3	2.49	0.47
1:G:123:ARG:HH21	1:G:153:ARG:HG2	1.78	0.47
2:D:519:CYS:HA	2:D:528:THR:HG21	1.95	0.47
1:G:101:ARG:NE	1:G:188:GLU:OE2	2.44	0.47
2:D:296:PRO:HG2	2:D:430:TYR:HD2	1.79	0.47
2:D:427:ILE:HA	2:D:431:LEU:CB	2.44	0.47
1:G:47:PHE:HB3	1:G:174:TYR:CD1	2.49	0.47
2:D:745:PRO:HA	2:D:1033:GLU:CD	2.40	0.47
2:D:1126:PHE:O	2:D:1129:CYS:N	2.47	0.47
1:G:42:LEU:N	1:G:159:GLY:O	2.48	0.47
2:D:246:TYR:CB	2:D:250:LEU:HA	2.45	0.47
2:D:327:ASN:HD21	2:D:331:ARG:NH1	2.12	0.47
2:D:223:PHE:CZ	2:D:1036:VAL:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:890:ILE:HG13	2:D:891:LYS:N	2.28	0.47
1:G:47:PHE:HD1	1:G:50:ASN:HA	1.79	0.47
2:D:437:MET:SD	2:D:449:LEU:HD11	2.54	0.47
2:D:478:SER:OG	2:D:483:THR:HA	2.15	0.47
2:D:643:VAL:HA	2:D:646:VAL:HG12	1.97	0.47
2:D:906:ASP:O	2:D:908:LYS:HG2	2.14	0.47
2:D:964:ASN:C	2:D:966:TRP:HD1	2.22	0.47
2:D:432:VAL:CA	2:D:453:MET:H	2.26	0.47
2:D:488:GLU:OE2	2:D:490:GLY:N	2.36	0.47
2:D:530:MET:SD	2:D:651:TRP:HZ2	2.38	0.47
2:D:554:PHE:HE1	2:D:556:PRO:HB3	1.80	0.47
2:D:464:MET:HG2	2:D:489:PHE:CD2	2.48	0.46
2:D:620:TYR:CE1	2:D:638:GLY:HA3	2.50	0.46
2:D:960:GLU:C	2:D:964:ASN:ND2	2.72	0.46
2:D:313:LEU:HD13	2:D:449:LEU:O	2.16	0.46
2:D:960:GLU:O	2:D:964:ASN:ND2	2.48	0.46
2:D:851:CYS:SG	2:D:853:ILE:HG12	2.55	0.46
1:G:123:ARG:NH2	1:G:153:ARG:HG2	2.30	0.46
2:D:254:PRO:O	2:D:913:ARG:HA	2.16	0.46
2:D:358:ILE:HD11	2:D:374:ASP:C	2.40	0.46
2:D:558:MET:O	2:D:561:THR:OG1	2.31	0.46
2:D:1005:ASN:OD1	2:D:1008:ILE:HG12	2.15	0.46
1:G:172:TRP:HB3	1:G:184:SER:OG	2.16	0.46
2:D:315:ASN:O	2:D:318:ALA:HB3	2.16	0.46
2:D:313:LEU:HD11	2:D:452:SER:HB3	1.97	0.45
2:D:293:CYS:SG	2:D:294:ASP:N	2.88	0.45
2:D:305:PHE:HB2	2:D:452:SER:OG	2.17	0.45
2:D:717:PHE:HB3	2:D:720:LEU:HB2	1.99	0.45
2:D:716:LYS:HD2	2:D:716:LYS:HA	1.77	0.45
2:D:876:HIS:O	2:D:876:HIS:CG	2.69	0.45
2:D:1008:ILE:HA	2:D:1011:TYR:CD2	2.52	0.45
2:D:1098:MET:HE2	2:D:1098:MET:HB2	1.72	0.45
2:D:292:PHE:HE2	2:D:357:TYR:CZ	2.35	0.45
2:D:416:ARG:HG3	2:D:418:CYS:H	1.81	0.45
2:D:458:THR:OG1	2:D:459:GLU:N	2.49	0.45
2:D:385:CYS:O	2:D:388:HIS:N	2.50	0.45
2:D:514:VAL:HA	2:D:517:VAL:HG22	1.98	0.45
2:D:556:PRO:HD2	2:D:559:ASN:OD1	2.16	0.45
2:D:774:PHE:CE2	2:D:775:GLU:HG2	2.52	0.45
2:D:198:MET:O	2:D:202:VAL:HG12	2.17	0.45
2:D:297:SER:OG	2:D:298:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1607:Y01:HAP1	4:D:1607:Y01:HAO1	1.65	0.45
2:D:329:ARG:NH1	2:D:475:TRP:CD1	2.85	0.45
2:D:411:CYS:SG	2:D:412:THR:N	2.89	0.45
2:D:614:THR:HG23	2:D:615:THR:H	1.82	0.45
2:D:937:TYR:HE2	2:D:978:ASP:HA	1.82	0.44
2:D:1124:THR:OG1	2:D:1125:PHE:N	2.51	0.44
2:D:186:ALA:HB2	2:D:594:SER:HB3	2.00	0.44
2:D:774:PHE:O	2:D:778:HIS:CB	2.65	0.44
2:D:947:VAL:O	2:D:951:ILE:HG13	2.17	0.44
2:D:546:TYR:HE1	2:D:552:PHE:CE2	2.35	0.44
2:D:759:HIS:CE1	2:D:761:PHE:H	2.35	0.44
2:D:546:TYR:HE2	2:D:555:PHE:HD1	1.66	0.44
2:D:1016:ILE:HG22	2:D:1049:SER:OG	2.18	0.44
2:D:783:LEU:HA	2:D:783:LEU:HD12	1.63	0.44
2:D:1005:ASN:HD22	2:D:1139:THR:HB	1.82	0.44
2:D:373:ARG:O	2:D:377:HIS:ND1	2.51	0.44
2:D:773:MET:O	2:D:777:VAL:HB	2.17	0.44
2:D:296:PRO:HG3	2:D:352:TRP:CE2	2.52	0.44
1:G:84:ILE:HD12	1:G:122:LEU:HB2	2.00	0.43
2:D:285:ASN:N	2:D:350:PRO:HG3	2.33	0.43
2:D:453:MET:HG2	2:D:454:LEU:N	2.33	0.43
2:D:518:MET:HG2	2:D:575:PHE:CE1	2.53	0.43
2:D:856:PHE:O	2:D:860:MET:N	2.50	0.43
2:D:947:VAL:HG11	2:D:967:PHE:CE1	2.53	0.43
2:D:324:ASN:OD1	2:D:325:VAL:N	2.51	0.43
2:D:518:MET:HG2	2:D:575:PHE:CZ	2.54	0.43
2:D:883:GLN:HA	2:D:886:PHE:HB3	1.98	0.43
2:D:1089:THR:HG23	2:D:1090:THR:N	2.33	0.43
2:D:468:TYR:HD1	2:D:472:PHE:HB3	1.82	0.43
2:D:232:GLN:HG3	2:D:795:PRO:HB2	2.01	0.43
2:D:232:GLN:HE22	2:D:797:ASP:N	2.15	0.43
2:D:291:PHE:CE1	2:D:360:ILE:HG12	2.53	0.43
2:D:711:PRO:HG3	2:D:1076:LEU:HD22	2.00	0.43
2:D:226:ARG:HG3	2:D:804:PRO:HG2	2.00	0.43
2:D:264:SER:OG	2:D:265:HIS:N	2.51	0.43
2:D:938:GLU:HG2	2:D:939:LYS:N	2.34	0.43
1:G:144:ARG:HB3	1:G:185:VAL:O	2.19	0.43
2:D:226:ARG:NE	2:D:797:ASP:OD2	2.41	0.43
2:D:253:TYR:N	2:D:254:PRO:HD2	2.34	0.43
2:D:545:LEU:HD23	2:D:545:LEU:HA	1.87	0.43
2:D:614:THR:HG23	2:D:615:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:717:PHE:O	2:D:719:TYR:N	2.52	0.43
2:D:840:PHE:CD1	2:D:841:TYR:N	2.87	0.43
1:G:90:GLU:OE1	1:G:90:GLU:N	2.47	0.42
2:D:560:LEU:HA	2:D:560:LEU:HD13	1.83	0.42
2:D:641:ILE:HD12	2:D:641:ILE:HA	1.87	0.42
2:D:996:PHE:HB2	2:D:1013:ILE:HD11	1.99	0.42
1:G:135:SER:O	1:G:138:SER:OG	2.32	0.42
2:D:478:SER:OG	2:D:479:ASP:N	2.52	0.42
2:D:943:PHE:O	2:D:946:GLU:HG2	2.19	0.42
1:G:48:ILE:HG22	1:G:173:VAL:O	2.20	0.42
2:D:511:ILE:HA	2:D:514:VAL:HG12	2.01	0.42
1:G:48:ILE:HG23	1:G:49:PRO:HD3	2.00	0.42
1:G:100:GLN:HA	1:G:103:LYS:HB3	2.01	0.42
2:D:230:ILE:HB	2:D:975:ASP:OD2	2.20	0.42
2:D:958:ALA:HB3	2:D:959:PRO:HD3	2.01	0.42
2:D:606:LEU:HD21	4:D:1607:Y01:HAQ2	2.01	0.42
2:D:1005:ASN:ND2	2:D:1138:GLY:O	2.53	0.42
2:D:745:PRO:HA	2:D:1033:GLU:OE1	2.19	0.42
2:D:1018:GLY:O	2:D:1022:VAL:HG12	2.20	0.42
4:D:1605:Y01:HAC2	4:D:1605:Y01:HAJ2	1.85	0.42
1:G:47:PHE:CD1	1:G:50:ASN:HA	2.54	0.42
2:D:192:VAL:O	2:D:195:MET:HG3	2.20	0.42
2:D:554:PHE:CE1	2:D:556:PRO:HB3	2.55	0.42
2:D:999:MET:HE1	2:D:1053:ALA:C	2.45	0.42
2:D:293:CYS:SG	2:D:339:LEU:HD12	2.59	0.42
2:D:531:THR:O	2:D:535:ILE:HG12	2.20	0.42
2:D:816:PHE:HE2	2:D:818:ILE:HB	1.84	0.42
2:D:357:TYR:O	2:D:360:ILE:HG22	2.20	0.41
2:D:557:PHE:O	2:D:557:PHE:CG	2.72	0.41
2:D:220:LEU:O	2:D:220:LEU:HD12	2.20	0.41
2:D:298:ASP:HA	2:D:302:ARG:HH12	1.84	0.41
2:D:535:ILE:HG21	2:D:567:VAL:HG23	2.01	0.41
2:D:626:ASN:HB2	2:D:979:SER:OG	2.19	0.41
2:D:946:GLU:O	2:D:949:SER:OG	2.22	0.41
2:D:1020:ILE:HA	2:D:1023:THR:HG22	2.01	0.41
1:G:155:ARG:NH2	1:G:178:LYS:HE2	2.34	0.41
2:D:646:VAL:HA	2:D:649:VAL:HG12	2.02	0.41
2:D:182:ALA:HA	2:D:185:ILE:HG22	2.01	0.41
2:D:304:VAL:HG22	2:D:486:GLY:HA3	2.02	0.41
2:D:331:ARG:NH2	2:D:349:CYS:O	2.48	0.41
2:D:823:SER:O	2:D:827:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1055:HIS:HA	2:D:1058:VAL:HG12	2.02	0.41
2:D:499:TYR:HD2	2:D:755:PHE:CE2	2.39	0.41
2:D:539:LEU:HD21	2:D:563:LEU:HB2	2.03	0.41
2:D:1049:SER:HA	2:D:1119:SER:OG	2.20	0.41
2:D:212:GLU:O	2:D:547:ARG:NH1	2.54	0.41
2:D:244:THR:C	2:D:254:PRO:HG3	2.46	0.41
2:D:949:SER:O	2:D:952:SER:OG	2.38	0.41
1:G:155:ARG:NH2	1:G:178:LYS:HB2	2.35	0.41
2:D:383:ARG:NH2	2:D:446:THR:HB	2.36	0.41
2:D:435:ASP:HB3	2:D:437:MET:HE3	2.02	0.41
2:D:484:ILE:HB	2:D:487:ILE:HD11	2.02	0.41
2:D:556:PRO:O	2:D:558:MET:N	2.54	0.41
2:D:826:TRP:NE1	2:D:956:SER:HA	2.36	0.41
2:D:862:ASN:O	2:D:875:SER:HB2	2.21	0.41
2:D:1020:ILE:O	2:D:1024:VAL:HG13	2.21	0.41
2:D:1088:LEU:HD12	2:D:1088:LEU:HA	1.94	0.41
1:G:136:GLU:C	1:G:137:GLU:HG3	2.46	0.41
2:D:236:THR:HG21	2:D:966:TRP:HH2	1.85	0.41
2:D:305:PHE:N	2:D:452:SER:O	2.44	0.41
2:D:1108:LEU:HD12	2:D:1108:LEU:HA	1.86	0.41
1:G:78:PRO:O	1:G:103:LYS:NZ	2.44	0.40
2:D:777:VAL:O	2:D:781:GLU:HG3	2.20	0.40
2:D:819:ALA:HB1	2:D:883:GLN:HG2	2.02	0.40
2:D:826:TRP:HZ2	2:D:954:GLU:O	2.04	0.40
4:D:1603:Y01:HBA	4:D:1603:Y01:HAO1	1.92	0.40
1:G:56:LEU:HA	1:G:60:GLY:HA2	2.03	0.40
2:D:472:PHE:HZ	2:D:484:ILE:HG21	1.86	0.40
2:D:1011:TYR:CE2	2:D:1134:LEU:HD22	2.56	0.40
1:G:56:LEU:HD23	1:G:56:LEU:H	1.87	0.40
2:D:479:ASP:OD1	2:D:481:VAL:HG22	2.21	0.40
2:D:704:ILE:HA	2:D:707:GLU:HB2	2.02	0.40
2:D:788:THR:O	2:D:967:PHE:HA	2.20	0.40
1:G:47:PHE:HD2	1:G:174:TYR:CE1	2.38	0.40
1:G:117:TRP:HH2	1:G:160:MET:HB3	1.86	0.40
1:G:136:GLU:O	1:G:137:GLU:HG3	2.21	0.40
2:D:321:SER:O	2:D:325:VAL:HG22	2.21	0.40
2:D:437:MET:HE1	2:D:447:PRO:HG3	2.02	0.40
2:D:580:VAL:O	2:D:584:THR:HG22	2.21	0.40
2:D:759:HIS:HE1	2:D:761:PHE:CD1	2.39	0.40
2:D:1015:SER:OG	2:D:1016:ILE:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	149/462 (32%)	132 (89%)	17 (11%)	0	100	100
2	D	897/1524 (59%)	791 (88%)	105 (12%)	1 (0%)	48	81
All	All	1046/1986 (53%)	923 (88%)	122 (12%)	1 (0%)	49	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	351	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	128/356 (36%)	128 (100%)	0	100	100
2	D	761/1350 (56%)	761 (100%)	0	100	100
All	All	889/1706 (52%)	889 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	239	ASN
2	D	252	ASN
2	D	327	ASN

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Mol	Chain	Res	Type
2	D	356	ASN
2	D	362	ASN
2	D	426	GLN
2	D	466	ASN
2	D	559	ASN
2	D	572	ASN
2	D	659	HIS
2	D	824	GLN
2	D	842	GLN
2	D	862	ASN
2	D	964	ASN
2	D	1051	ASN
2	D	1107	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
5	NAG	D	1610	2	14,14,15	0.29	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Y01	D	1605	-	38,38,38	0.46	0	57,57,57	0.62	0
4	Y01	D	1601	-	38,38,38	0.43	0	57,57,57	0.73	1 (1%)
4	Y01	D	1602	-	38,38,38	0.45	0	57,57,57	0.55	0
4	Y01	D	1604	-	38,38,38	0.46	0	57,57,57	0.56	0
5	NAG	D	1611	2	14,14,15	0.19	0	17,19,21	0.64	1 (5%)
4	Y01	D	1603	-	38,38,38	0.47	0	57,57,57	0.57	0
4	Y01	D	1607	-	38,38,38	0.46	0	57,57,57	0.54	0
5	NAG	D	1608	2	14,14,15	0.36	0	17,19,21	0.31	0
4	Y01	D	1606	-	38,38,38	0.46	0	57,57,57	0.57	0
5	NAG	D	1609	-	14,14,15	0.24	0	17,19,21	0.46	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
5	NAG	D	1610	2	-	2/6/23/26	0/1/1/1
4	Y01	D	1605	-	-	3/19/77/77	0/4/4/4
4	Y01	D	1601	-	-	6/19/77/77	0/4/4/4
4	Y01	D	1602	-	-	2/19/77/77	0/4/4/4
4	Y01	D	1604	-	-	5/19/77/77	0/4/4/4
5	NAG	D	1611	2	-	0/6/23/26	0/1/1/1
4	Y01	D	1603	-	-	8/19/77/77	0/4/4/4
4	Y01	D	1607	-	-	7/19/77/77	0/4/4/4
5	NAG	D	1608	2	-	0/6/23/26	0/1/1/1
4	Y01	D	1606	-	-	2/19/77/77	0/4/4/4
5	NAG	D	1609	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1611	NAG	C1-O5-C5	2.23	115.17	112.19
4	D	1601	Y01	CBG-CBI-CBE	-2.04	97.75	100.10

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1603	Y01	CAV-CBC-OAW-CAY
4	D	1601	Y01	CAO-CBB-CBE-CBI
4	D	1601	Y01	CAC-CBB-CBE-CBI
4	D	1603	Y01	CAR-CBC-OAW-CAY
4	D	1601	Y01	CAC-CBB-CBE-CAP
4	D	1605	Y01	CAJ-CAO-CBB-CBE
5	D	1609	NAG	C4-C5-C6-O6
5	D	1609	NAG	O5-C5-C6-O6
5	D	1610	NAG	C4-C5-C6-O6
4	D	1604	Y01	CAV-CBC-OAW-CAY
4	D	1603	Y01	CAN-CAJ-CAO-CBB
4	D	1607	Y01	CAO-CBB-CBE-CBI
4	D	1607	Y01	CAC-CBB-CBE-CAP
4	D	1603	Y01	CAM-CAY-OAW-CBC
4	D	1607	Y01	CAO-CBB-CBE-CAP
5	D	1610	NAG	O5-C5-C6-O6
4	D	1607	Y01	CAC-CBB-CBE-CBI
4	D	1601	Y01	CAO-CBB-CBE-CAP
4	D	1603	Y01	OAG-CAY-OAW-CBC
4	D	1601	Y01	CAM-CAL-CAX-OAF
4	D	1607	Y01	CAM-CAL-CAX-OAF
4	D	1605	Y01	CAM-CAL-CAX-OAF
4	D	1604	Y01	CAR-CBC-OAW-CAY
4	D	1606	Y01	CAM-CAL-CAX-OAF
4	D	1607	Y01	CAM-CAL-CAX-OAH
4	D	1603	Y01	CAM-CAL-CAX-OAH
4	D	1602	Y01	CAM-CAL-CAX-OAH
4	D	1601	Y01	CAM-CAL-CAX-OAH
4	D	1605	Y01	CAM-CAL-CAX-OAH
4	D	1606	Y01	CAM-CAL-CAX-OAH
4	D	1604	Y01	CAM-CAL-CAX-OAH
4	D	1603	Y01	CAM-CAL-CAX-OAF
4	D	1602	Y01	CAM-CAL-CAX-OAF
4	D	1604	Y01	CAM-CAL-CAX-OAF
4	D	1603	Y01	CAO-CAJ-CAN-CBA
4	D	1607	Y01	CAR-CBC-OAW-CAY
4	D	1604	Y01	CAL-CAM-CAY-OAW

There are no ring outliers.

5 monomers are involved in 8 short contacts:

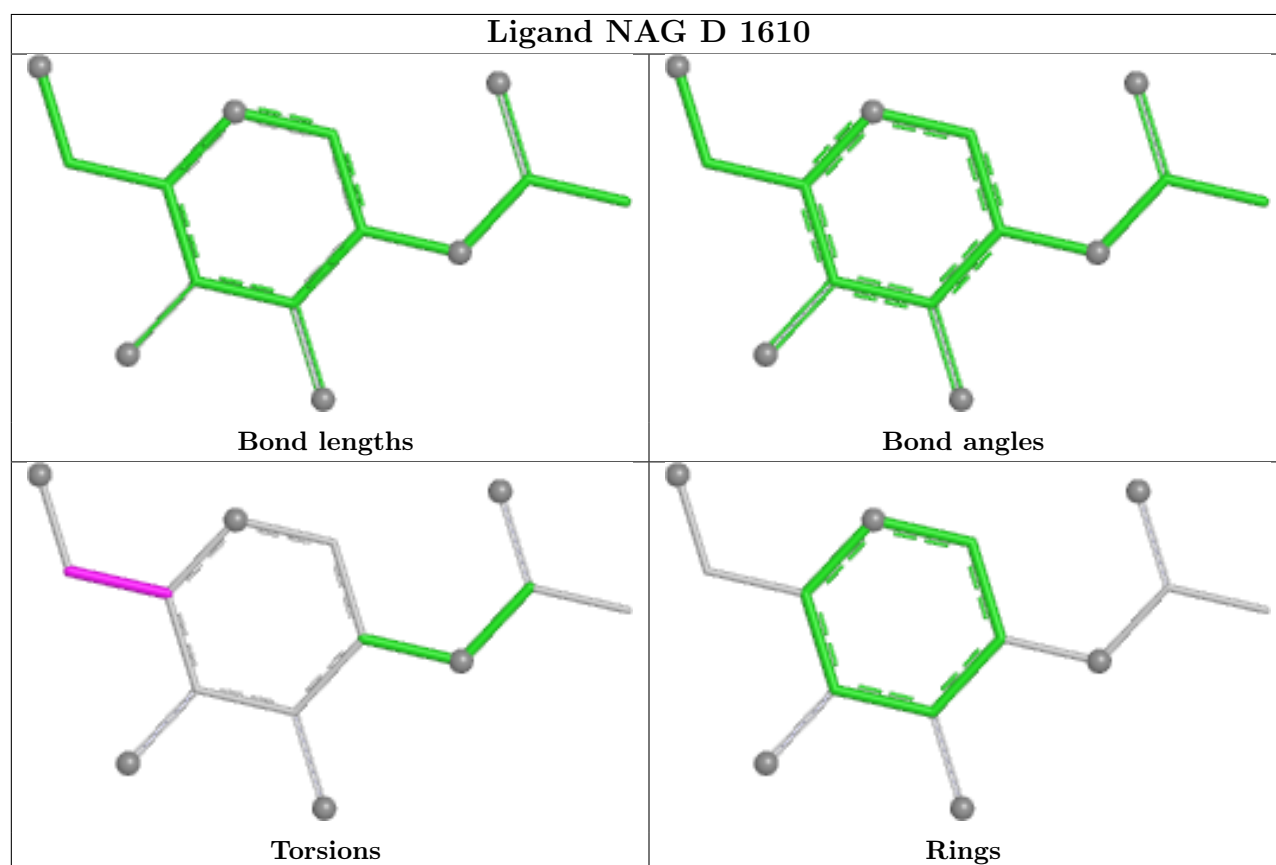
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1605	Y01	1	0

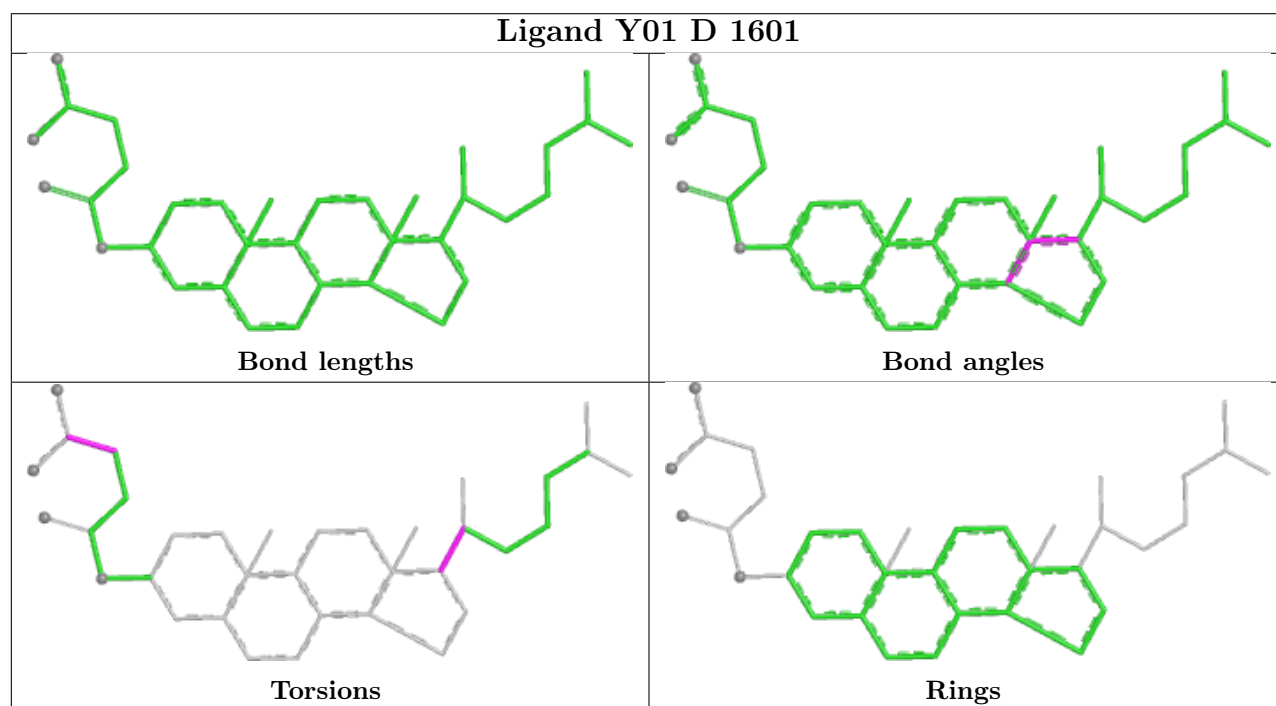
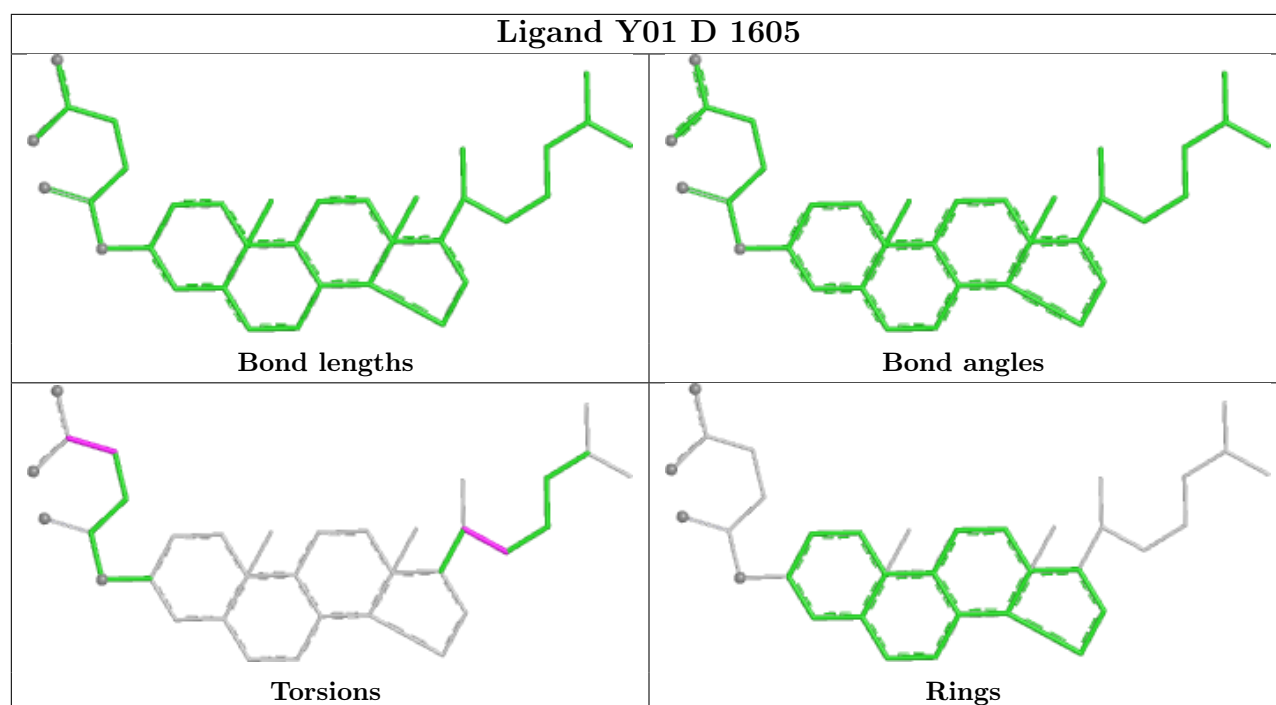
Continued on next page...

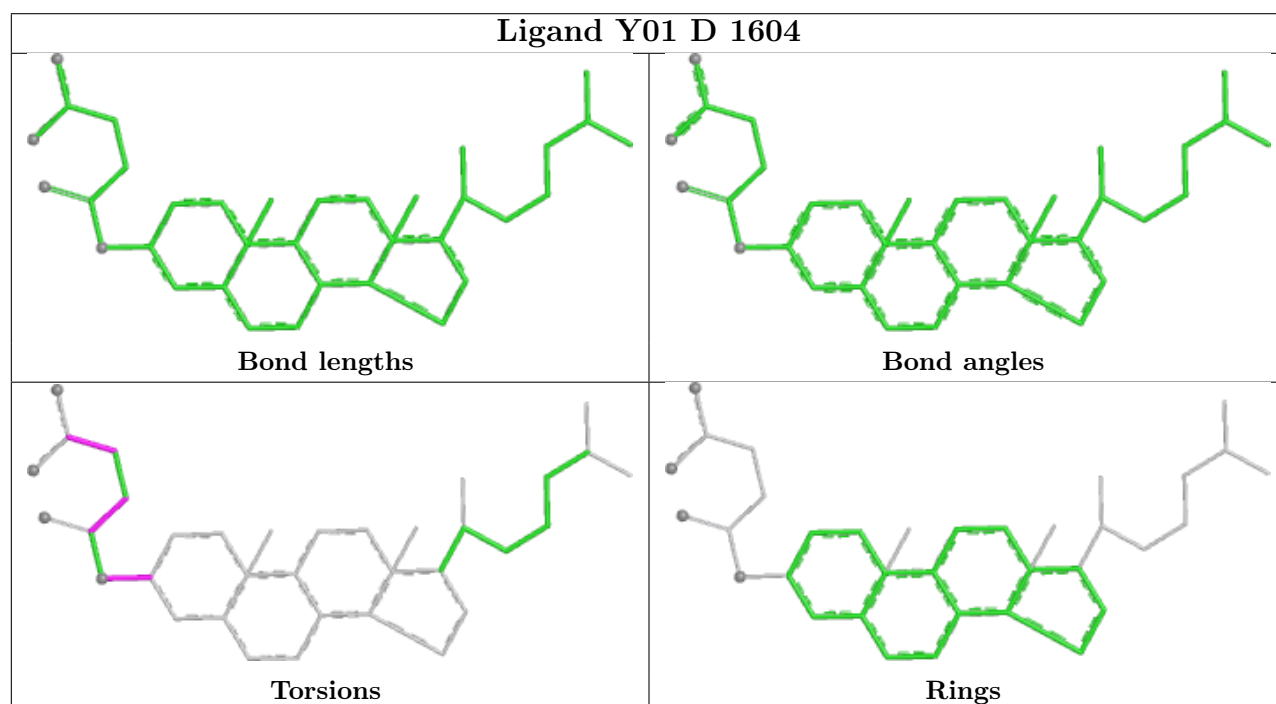
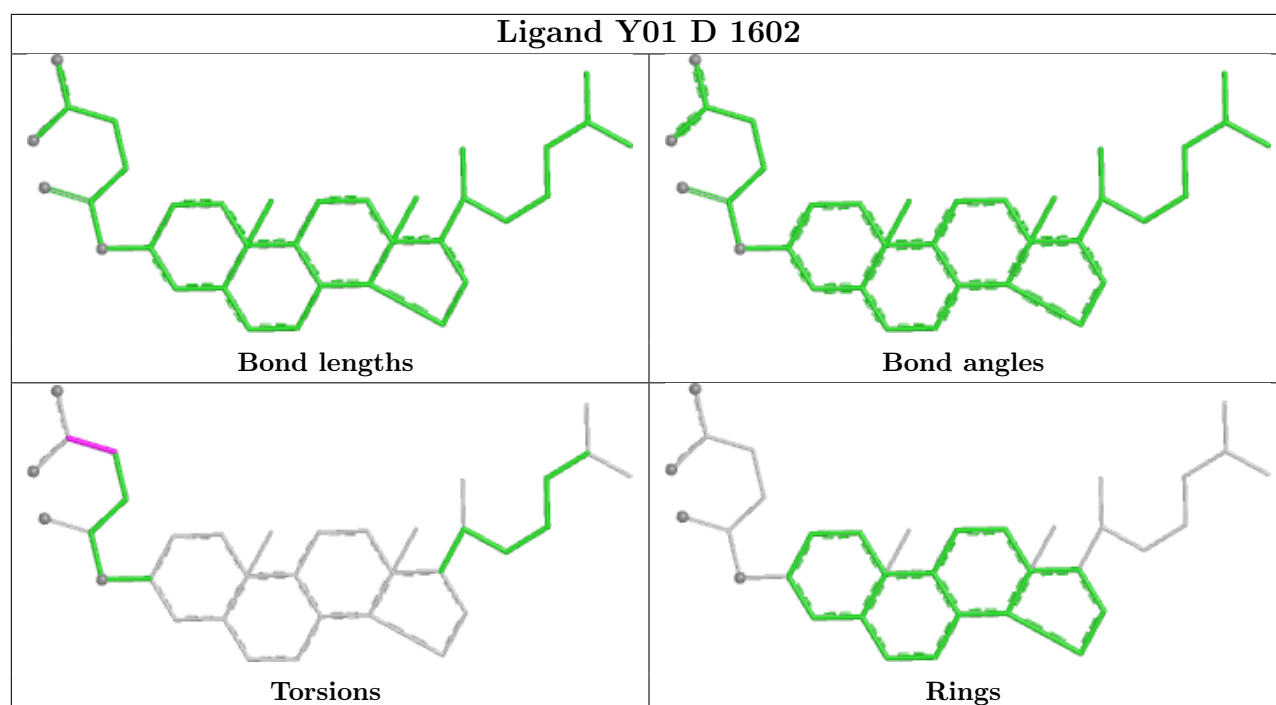
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1601	Y01	1	0
4	D	1604	Y01	2	0
4	D	1603	Y01	1	0
4	D	1607	Y01	3	0

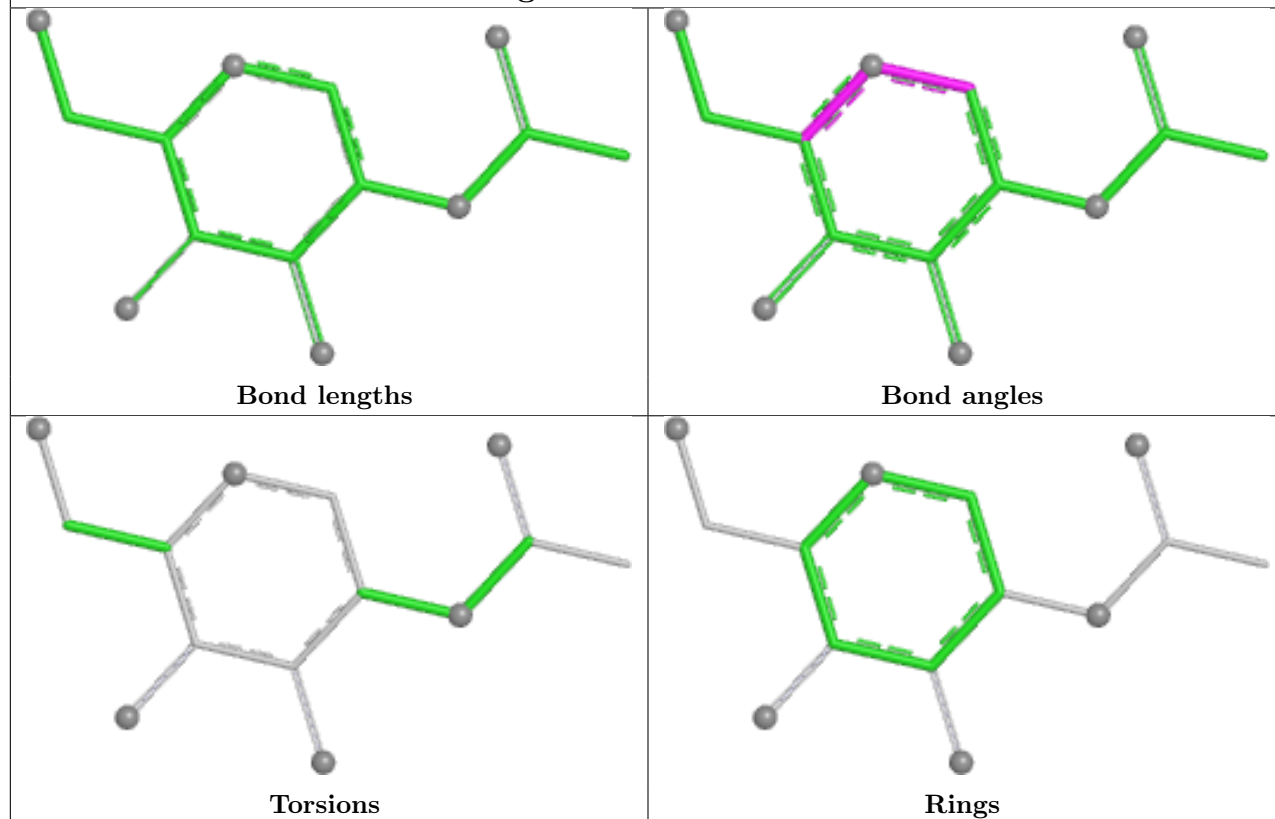
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



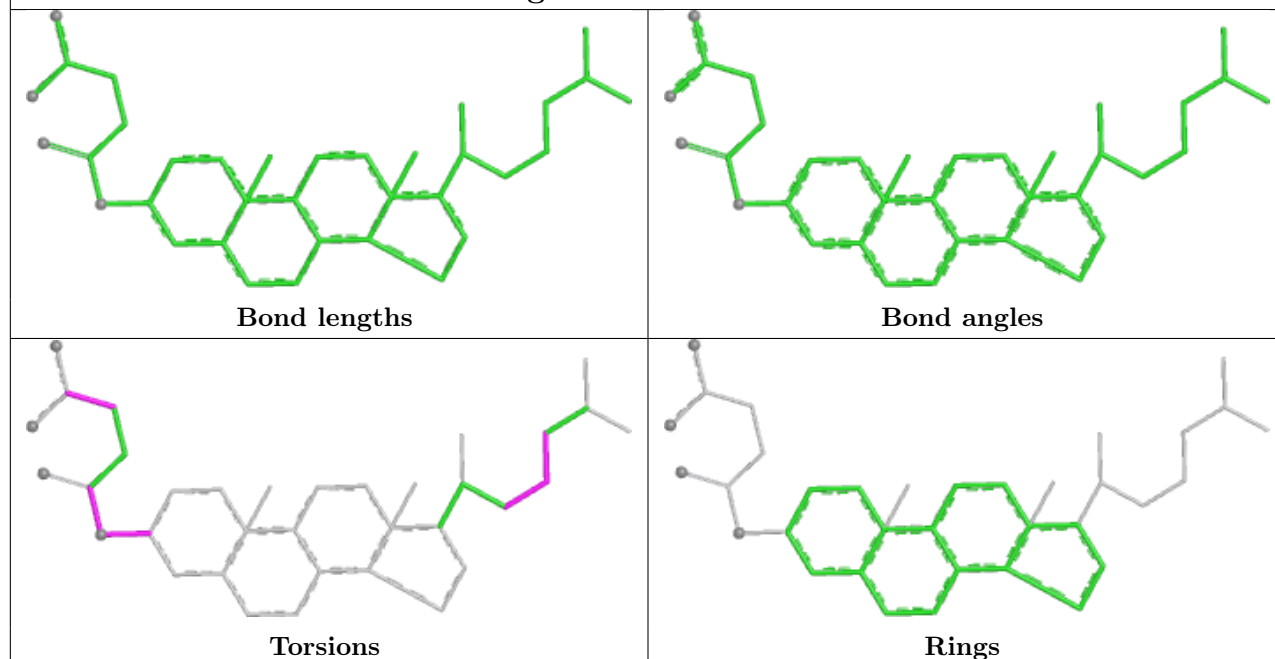


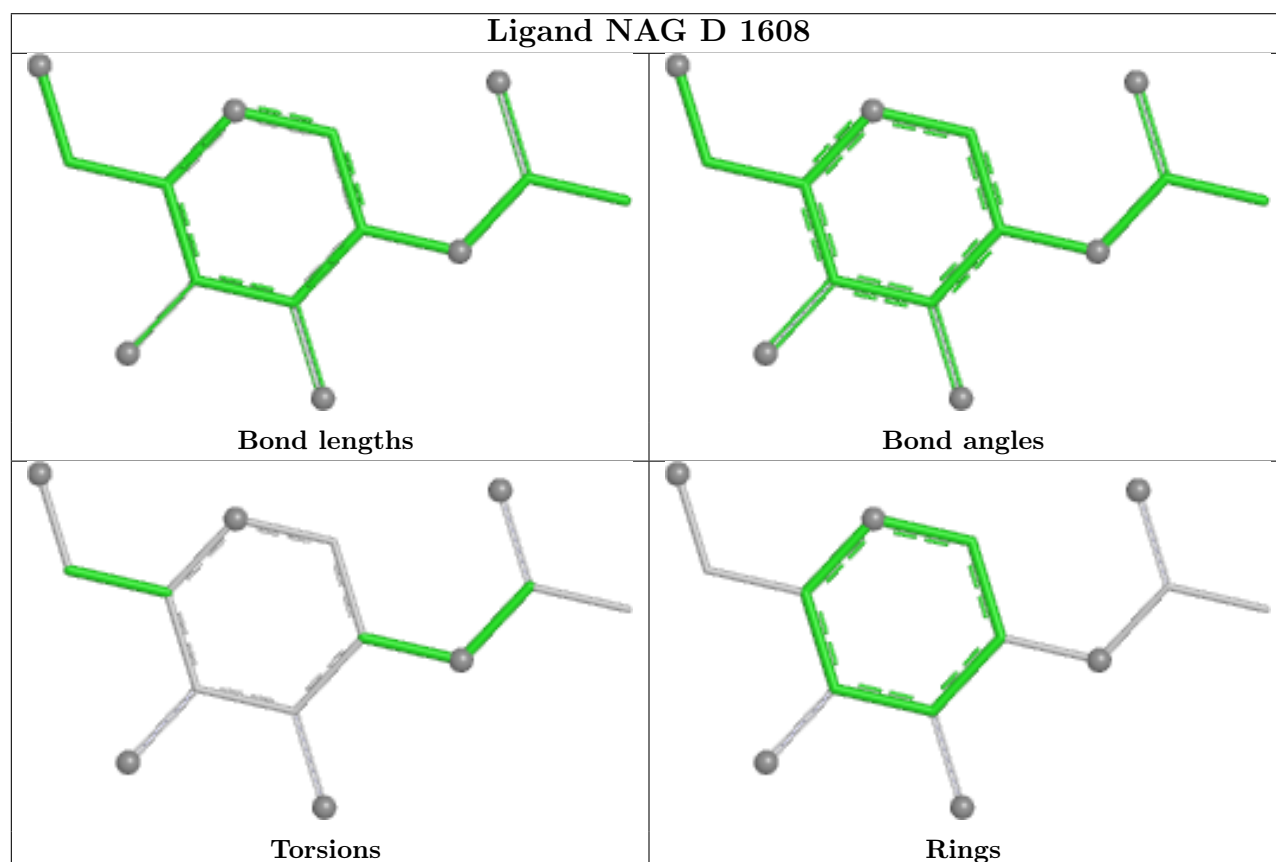
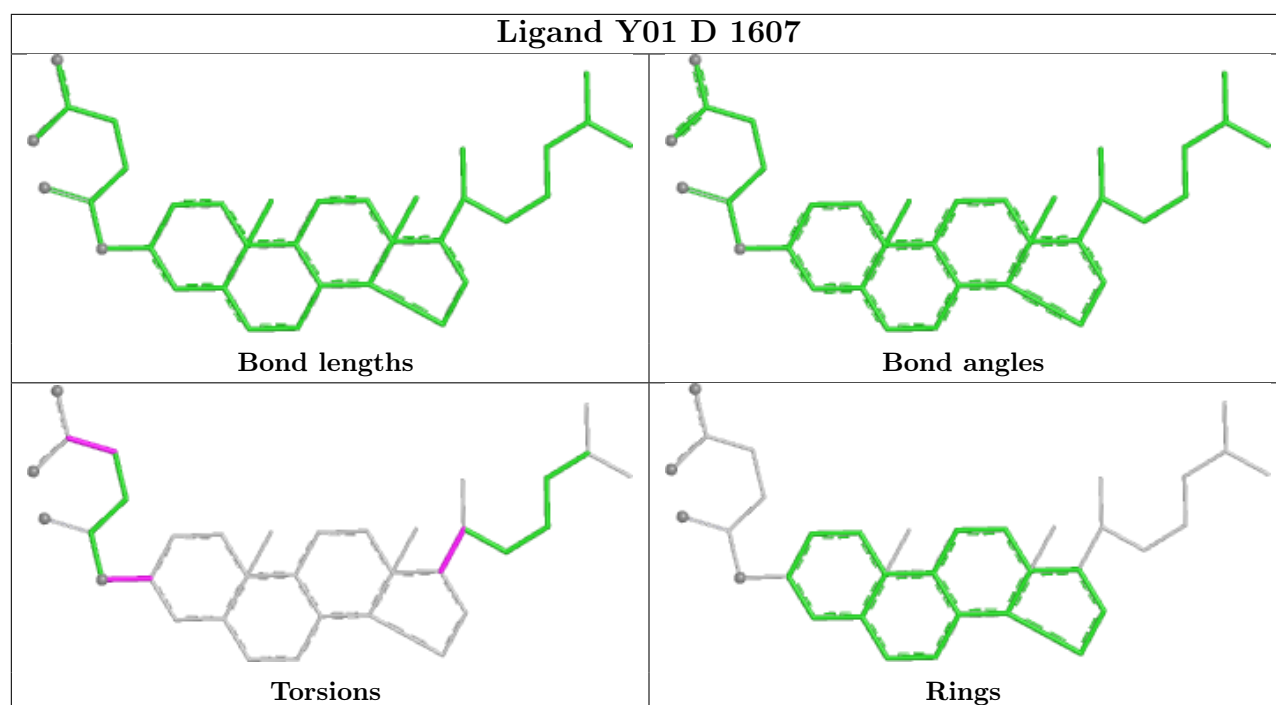


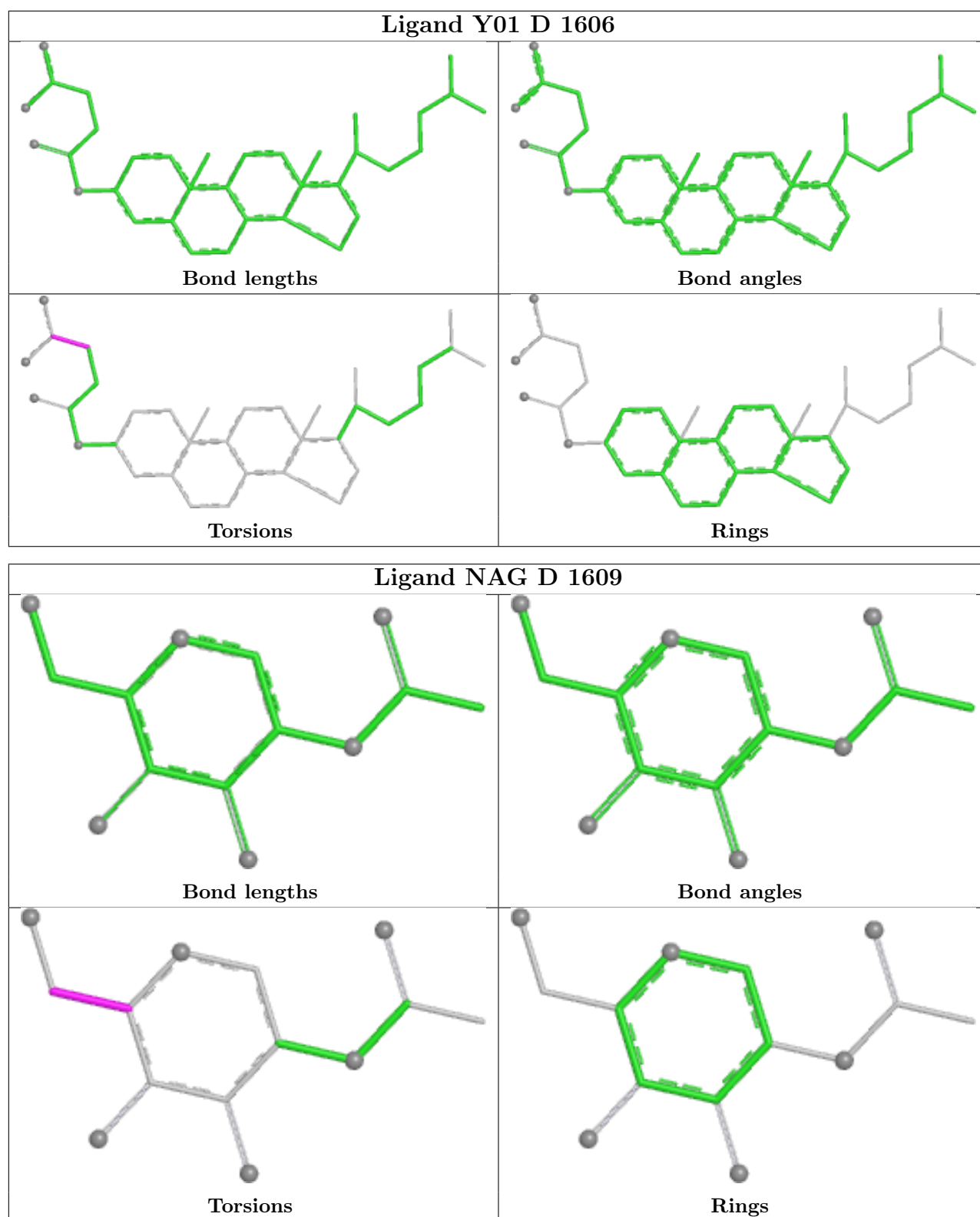
Ligand NAG D 1611



Ligand Y01 D 1603







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

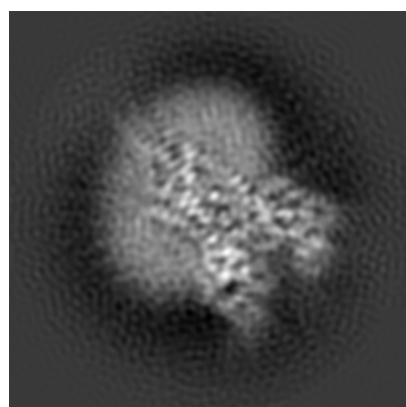
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30958. These allow visual inspection of the internal detail of the map and identification of artifacts.

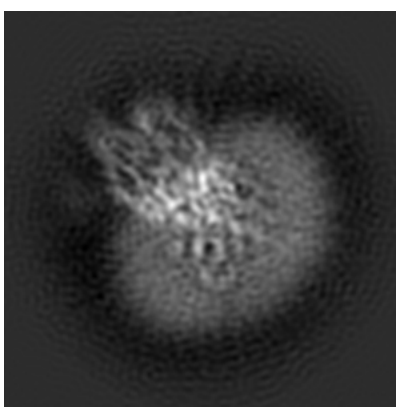
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

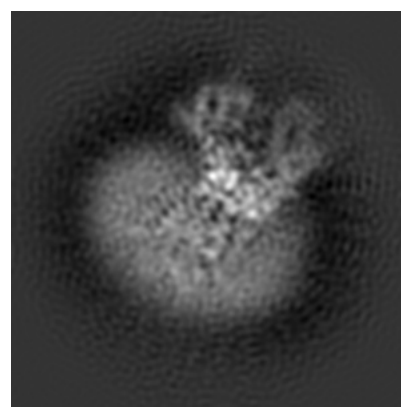
6.1.1 Primary map



X



Y

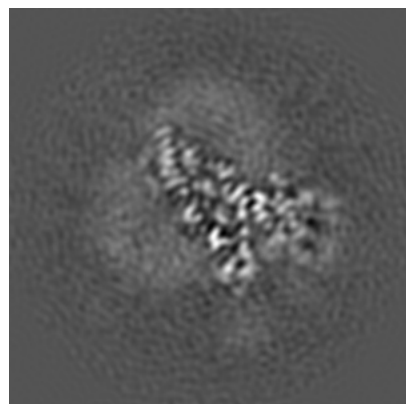


Z

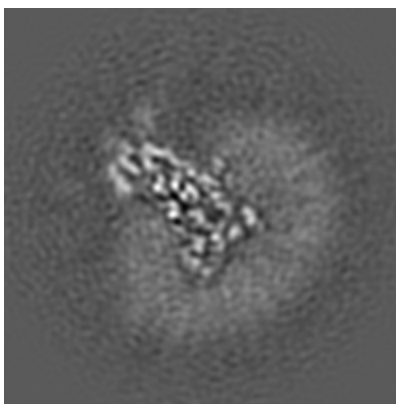
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

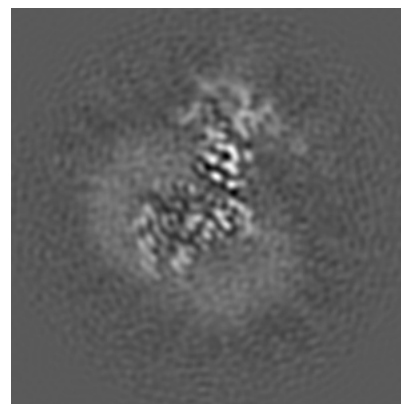
6.2.1 Primary map



X Index: 84



Y Index: 84

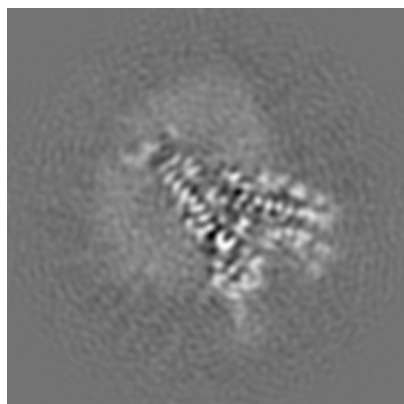


Z Index: 84

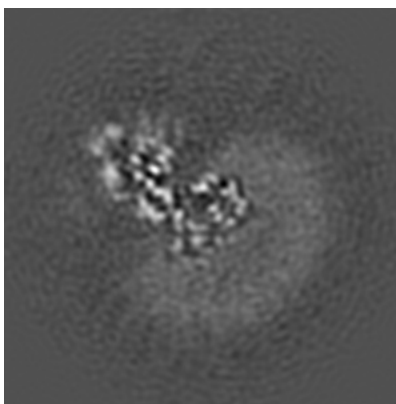
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

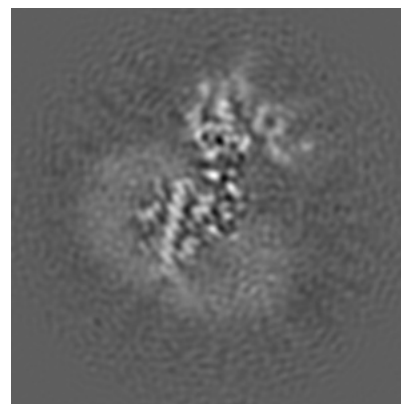
6.3.1 Primary map



X Index: 88



Y Index: 93

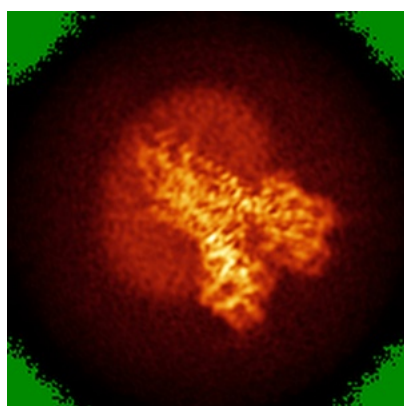


Z Index: 81

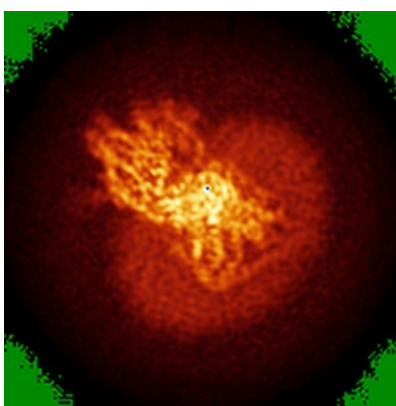
The images above show the largest variance slices of the map in three orthogonal directions.

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

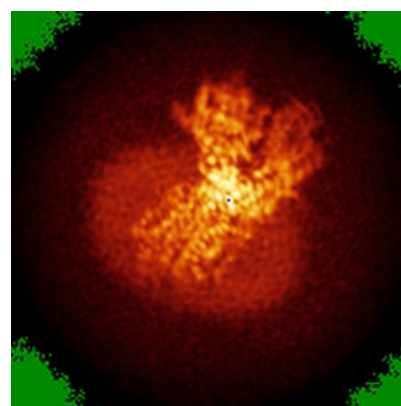
6.4.1 Primary map



X



Y

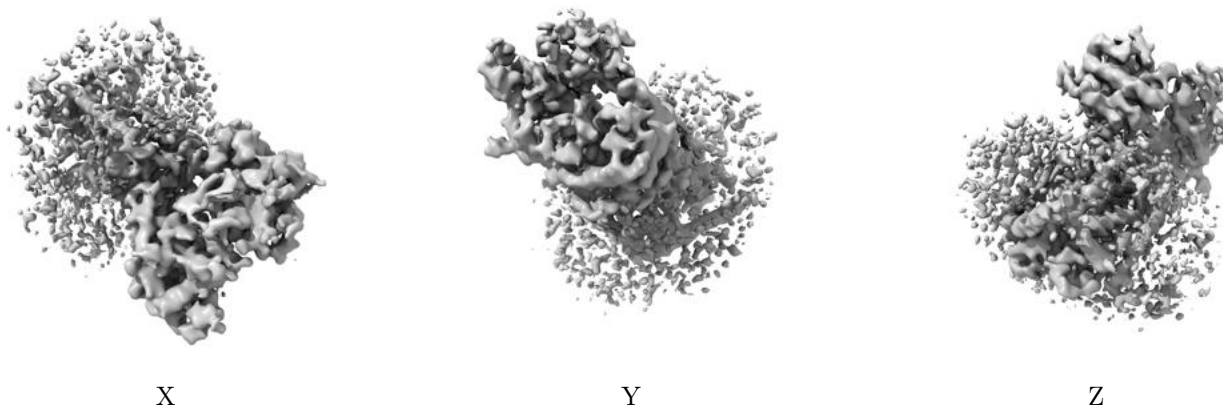


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

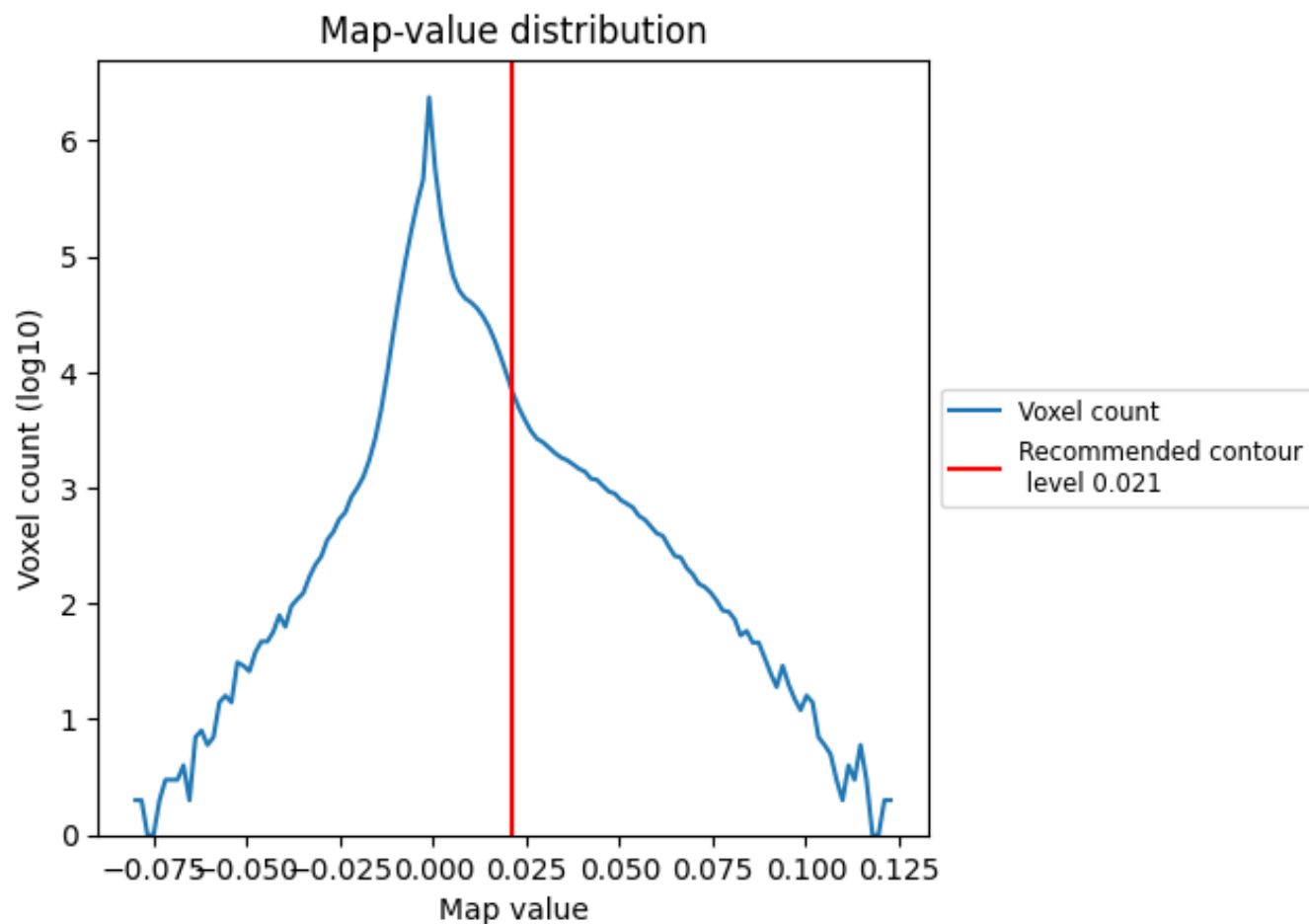
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

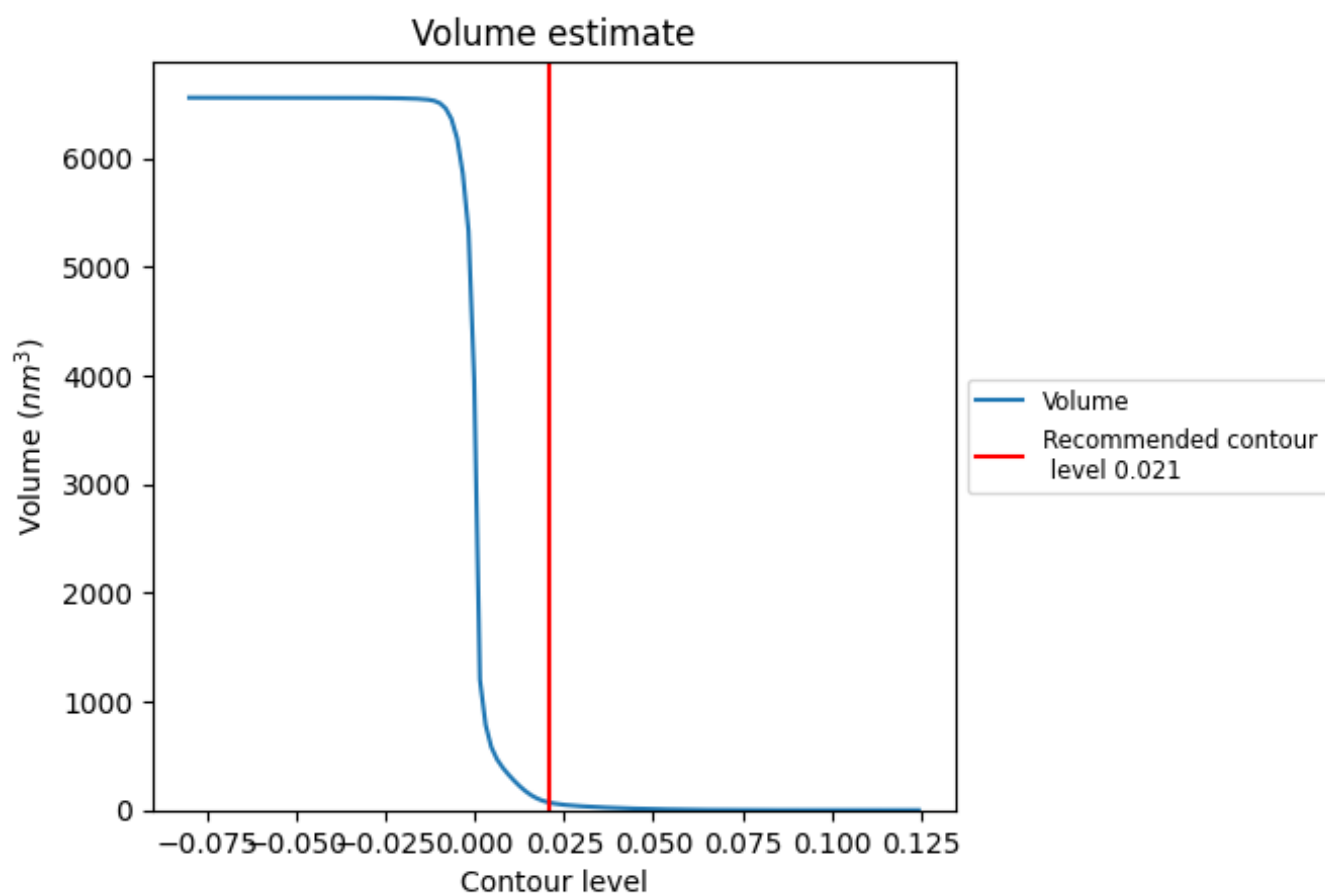
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

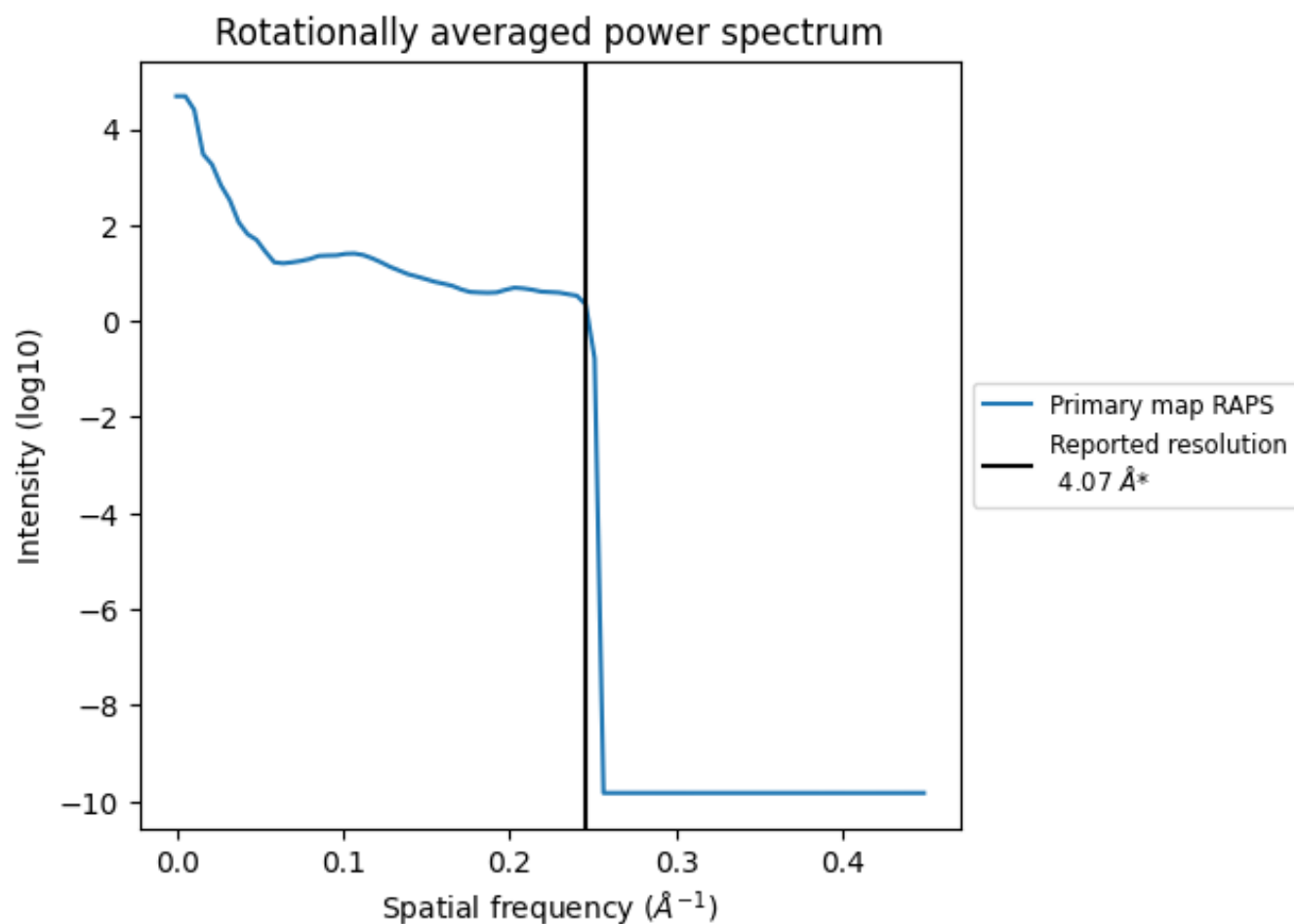
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm^3 ; this corresponds to an approximate mass of 63 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.246 $\text{\AA}^{-1}$

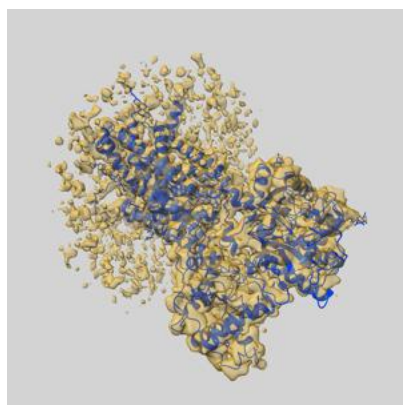
8 Fourier-Shell correlation

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

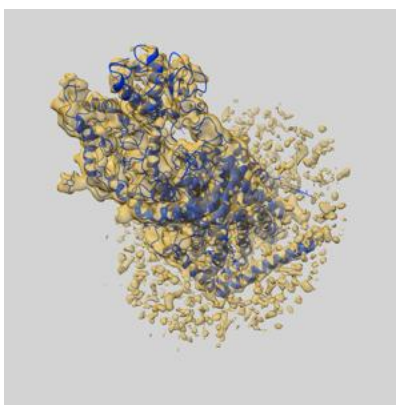
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30958 and PDB model 7E2I. Per-residue inclusion information can be found in section 3 on page 6.

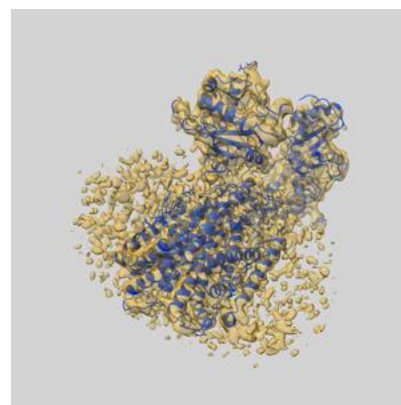
9.1 Map-model overlay [i](#)



X



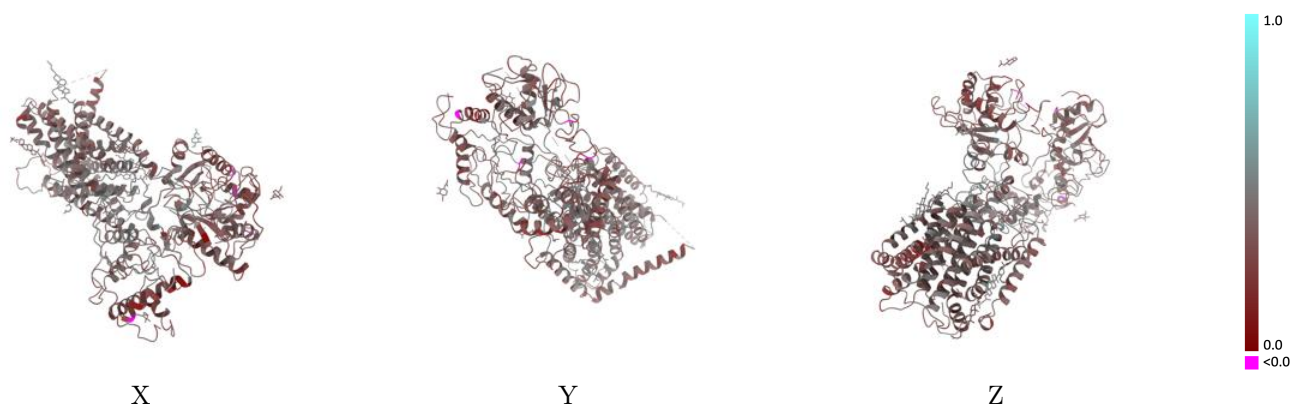
Y



Z

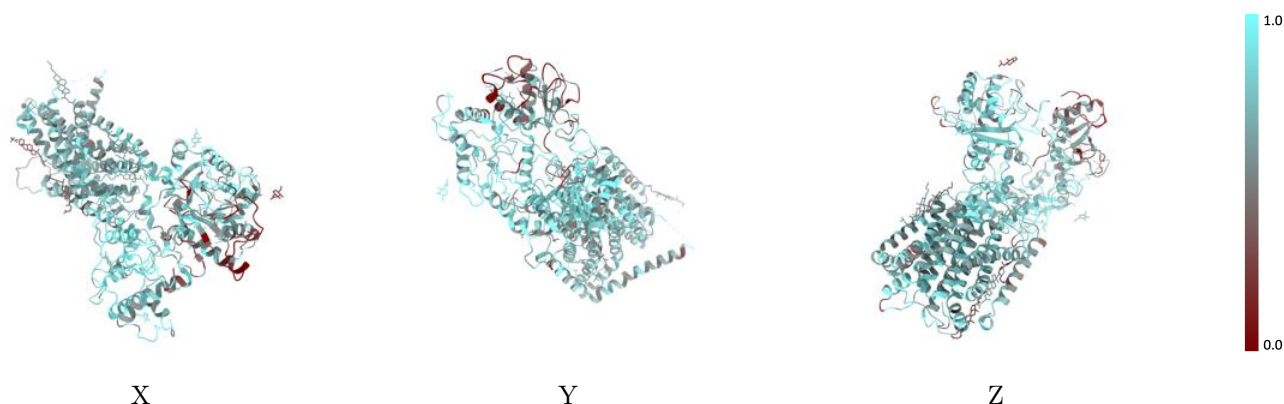
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



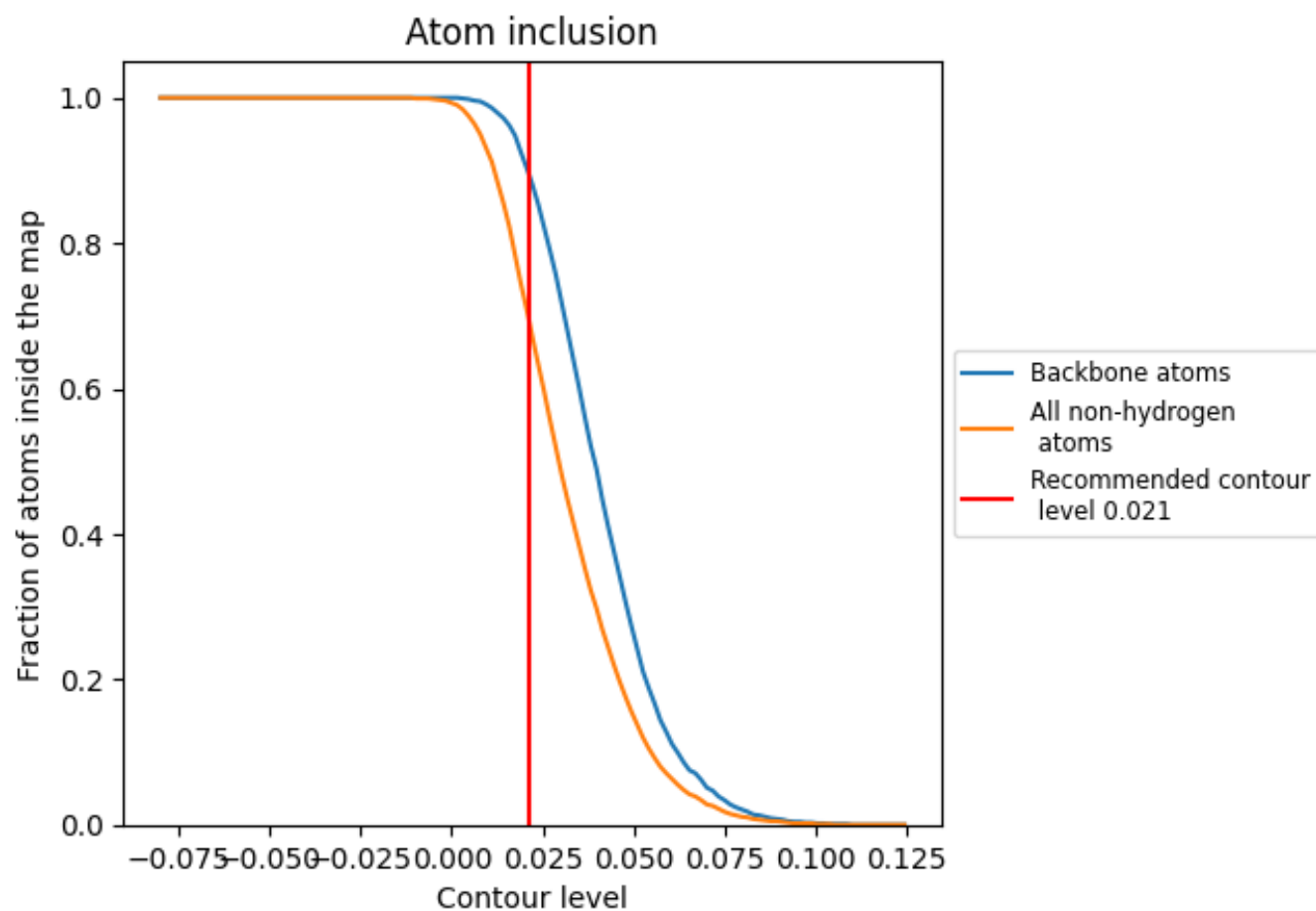
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7000	0.3750
D	0.7390	0.3780
G	0.4580	0.3570

