



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 03:33 AM JST

PDB ID : 7E2I
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

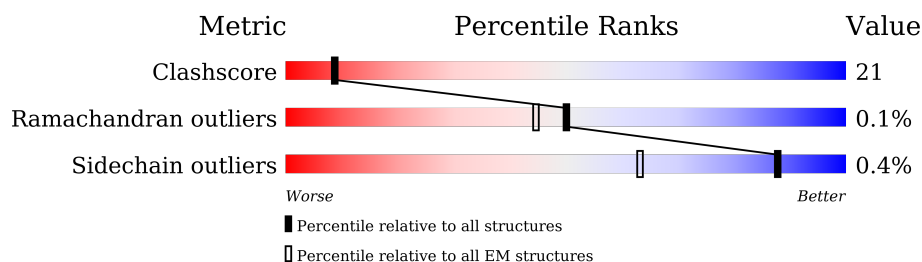
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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

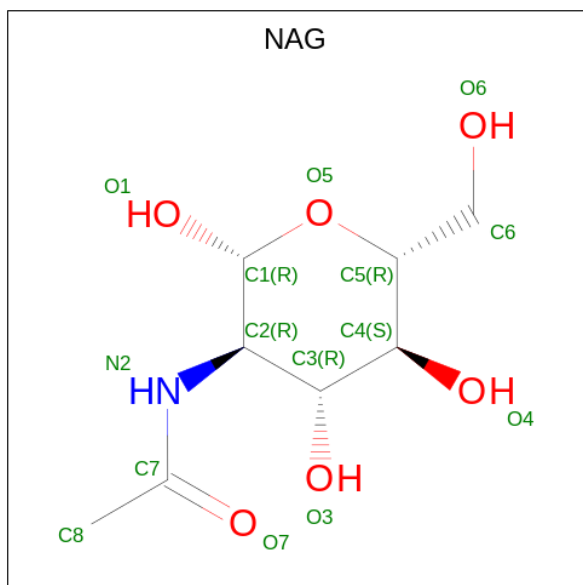
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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	

ASP	HIS	TYR	L339	C340	A346	S347	C348	C349	P350	S351	T353	N356	Y357	I358	A359	I360	L361	N362	N363	R364	S365	S366	Y444	A445	T446	P447	A448	L449	K450	Y451	S452	M453	L454	F455	S456	P457	T458	E459	M464	I467	Y468	F472	W475	N476	S477	S478	D479	G480	V481	T482	T483	I484	T485	G486	I487																																						
E488	F489	G490	I491	F496	Q497	D498	Y499	L500	L501	M502	D503	I511	V514	L515	L516	M517	M518	C519	V520	M525	T528	L529	P530	T531	I535	L539	L545	Y546	R547	F552	E553	F554	F555	P556	F557	M558	N559	L560	L563	V567	F575	V580	T584	D587	K588	S594	E595	T600	L601	Q602	L606	T611	T614	T615	Y620	A621	N622	N626	I627	T630	F633	G634	V635	G638	T639	A640	I641	L642	V643	N644	V646	L647	M648	V649	T650	W651	R661	TYR	LEU	LEU	ASN	ILE	PHE	THR	CYS	PHE	LYS	LYS	PRO	PRO	GLN	GLN	H778
ILE	TYR	ASP	ASN	LYS	SER	CYS	THR	VAL	A687	C688	Q689	K690	C691	V694	L695	F696	I704	E707	K708	V709	L710	P711	G712	I713	V714	I715	K716	F717	R718	Y719	L720	C737	I738	N739	P740	P745	F752	Q753	V754	F755	H759	F760	F761	F772	M773	F774	E775	R776	V777	H778																																											
H779	G780	E781	E782	L783	T788	W791	P795	E796	D797	L802	N803	P804	G808	K809	F816	N817	I818	A819	S820	P821	S823	V824	Q824	A825	W826	I827	F840	Y841	Q842	C851	F852	I853	F856	W859	N860	E861	N862	Q863	D864	C865	ASP	GLU	PRO	PRO	ALA	LEU	TYR	PRO	C873	C874																																											
S875	H876	W877	F879	P880	Y881	K882	Q883	F886	I890	K891	R892	A893	I894	L897	E898	R899	D906	S907	K908	T909	P910	R913	F914	D915	I916	N917	D918	R921	S929	T930	T934	A936	Y937	E938	K939	H941	Q942	F943	Y944	K945	E946	Y947	S949	W950	I951	S952	S953																																														
E954	L955	S956	Y1056	A958	P959	E960	N964	G965	F967	D975	Q976	D978	S979	A985	F996	T1002	T1003	W1004	N1005	I1006	I1007	I1008	S1009	F1010	Y1011	A1012	I1013	I1014	S1015	I1016	G1018	T1019	I1020	F1021	V1022	T1023	V1024	L1027	E1033	V1036	V1040	T1041	V1044	L1048	I951	S1049	V1050																																														
M1051	H1055	Y1056	G1057	V1058	A1059	Y1060	R1061	P1064	D1065	P1066	S1075	L1076	L1088	T1089	T1090	M1098	T1101	L1108	G1109	T1110	F1111	M1112	I1115	T1118	S1119	T1124	F1125	F1126	F1127	Q1128	C1129	M1130	C1131	R1132	G1133	L1134	T1139	G1138	Q1142	I1143	P1144	L1145	X1148	LEU	GLN	CYS																																															
SER	ALA	PHE	SER	HIS	ALA	LEU	SER	THR	PRO	ASP	GLY	SER	LYS	ASN	GLN	ILE	ALA	TYR	ASN	GLY	ASP	PRO	GLY	THR	GLY	THR	GLY	GLY	GLY	ALA	PHE	TYR	GLN	ALA	SER	HIS	THR	CYS	THR	PHE	ALA	PRO	GLU	LYS	THR	THR	TYR	GLU																																													
GLU	THR	HIS	ILE	CYS	SER	ALA	PHE	THR	ASN	GLN	LYS	ASN	GLY	GLY	MET	PRO	VAL	HIS	ALA	ALA	VAL	GLY	THR	GLY	THR	GLY	THR	GLY	ASP	GLY	ALA	GLY	GLN	VAL	GLY	THR	CYS	THR	PHE	ALA	VAL	SER	LEU	ASN	GLN	ARG	CYS																																														
SER	CYS	PRO	ASP	ALA	TYR	HIS	LEU	HIS	ASN	TYR	GLY	PRO	HIS	SER	GLN	MET	GLY	ASP	ARG	ASN	PHE	THR	GLY	THR	GLY	PHE	GLN	GLY	ILE	GLY	ASN	VAL	GLY	THR	VAL	GLY	THR	VAL	GLY	THR	GLY	PHE	VAL	VAL	HIS	PRO	ILE	THR	HIS																																												

[illegible]

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

5.1 Standard geometry

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	0.28	0/1235	0.46	0/1668
2	D	0.37	0/7244	0.50	0/9862
All	All	0.36	0/8479	0.49	0/11530

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	G	1209	0	1159	57	0
2	D	7058	0	6881	293	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	351	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 (351) 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
1:G:45:LYS:NZ	1:G:176:GLU:O	2.23	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:929:SER:OG	2:D:930:THR:N	2.27	0.65
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: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
2:D:362:ASN:HD21	2:D:364:ARG:HH11	1.46	0.63
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:739:ASN:CG	2:D:740:PRO:HD2	2.24	0.57
2:D:711:PRO:O	2:D:715:ILE:HG12	2.03	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:791:TRP:CD1	2:D:960:GLU:HB2	2.40	0.56
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:252:ASN:C	2:D:254:PRO:HD2	2.25	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:1003:THR:HB	2:D:1008:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:256:LYS:NZ	2:D:898:GLU:OE2	2.29	0.52
2:D:791:TRP:HD1	2:D:960:GLU:HB2	1.74	0.52
2:D:820:SER:O	2:D:823:SER:OG	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ALA:O	1:G:171:ASP:HB3	2.11	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: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:717:PHE:C	2:D:719:TYR:H	2.15	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
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:350:PRO:C	2:D:352:TRP:H	2.16	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:293:CYS:SG	2:D:294:ASP:N	2.88	0.46
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: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
2:D:489:PHE:C	2:D:491:ILE:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:808:GLY:C	2:D:809:LYS:HD3	2.36	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:525:MET:O	2:D:528:THR:OG1	2.20	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: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:CG	2:D:876:HIS:O	2.69	0.45
2:D:1008:ILE:HA	2:D:1011:TYR:CD2	2.52	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
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:315:ASN:CG	2:D:317:PRO:HD2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:ASP:C	2:D:437:MET:H	2.21	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
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
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:745:PRO:HA	2:D:1033:GLU:CD	2.40	0.42
2:D:511:ILE:HA	2:D:514:VAL:HG12	2.01	0.42
2:D:960:GLU:C	2:D:964:ASN:ND2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:964:ASN:C	2:D:966:TRP:HD1	2.22	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:293:CYS:SG	2:D:339:LEU:HD12	2.59	0.42
2:D:358:ILE:HD11	2:D:374:ASP:C	2.40	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
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: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: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
2:D:236:THR:HG21	2:D:966:TRP:HH2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1060:TYR:OH	2:D:1131:CYS:SG	2.79	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: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 [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	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%)	50	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	351	SER

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	G	128/356 (36%)	127 (99%)	1 (1%)	79	85
2	D	761/1350 (56%)	758 (100%)	3 (0%)	89	91
All	All	889/1706 (52%)	885 (100%)	4 (0%)	88	91

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

Mol	Chain	Res	Type
1	G	61	ARG
2	D	661	ARG
2	D	891	LYS
2	D	899	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	239	ASN
2	D	252	ASN
2	D	327	ASN
2	D	356	ASN
2	D	362	ASN
2	D	388	HIS
2	D	426	GLN
2	D	559	ASN
2	D	572	ASN
2	D	622	ASN
2	D	659	HIS
2	D	842	GLN

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Mol	Chain	Res	Type
2	D	862	ASN
2	D	964	ASN
2	D	1051	ASN
2	D	1055	HIS
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	$\# Z > 2$
4	Y01	D	1602	-	38,38,38	0.44	0	57,57,57	0.54	0
4	Y01	D	1605	-	38,38,38	0.45	0	57,57,57	0.61	0
5	NAG	D	1608	2	14,14,15	0.37	0	17,19,21	0.30	0
4	Y01	D	1603	-	38,38,38	0.46	0	57,57,57	0.57	0
4	Y01	D	1601	-	38,38,38	0.43	0	57,57,57	0.71	0
5	NAG	D	1609	-	14,14,15	0.23	0	17,19,21	0.44	0
4	Y01	D	1607	-	38,38,38	0.45	0	57,57,57	0.54	0
4	Y01	D	1606	-	38,38,38	0.45	0	57,57,57	0.56	0
4	Y01	D	1604	-	38,38,38	0.45	0	57,57,57	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	1611	2	14,14,15	0.20	0	17,19,21	0.63	1 (5%)
5	NAG	D	1610	2	14,14,15	0.28	0	17,19,21	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	D	1602	-	-	2/19/77/77	0/4/4/4
4	Y01	D	1605	-	-	3/19/77/77	0/4/4/4
5	NAG	D	1608	2	-	1/6/23/26	0/1/1/1
4	Y01	D	1603	-	-	9/19/77/77	0/4/4/4
4	Y01	D	1601	-	-	6/19/77/77	0/4/4/4
5	NAG	D	1609	-	-	2/6/23/26	0/1/1/1
4	Y01	D	1607	-	-	7/19/77/77	0/4/4/4
4	Y01	D	1606	-	-	2/19/77/77	0/4/4/4
4	Y01	D	1604	-	-	6/19/77/77	0/4/4/4
5	NAG	D	1611	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1610	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1611	NAG	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

All (40) 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-CAP
4	D	1601	Y01	CAC-CBB-CBE-CBI
4	D	1603	Y01	CAR-CBC-OAW-CAY
4	D	1605	Y01	CAJ-CAO-CBB-CBE
5	D	1609	NAG	C4-C5-C6-O6
5	D	1610	NAG	C4-C5-C6-O6

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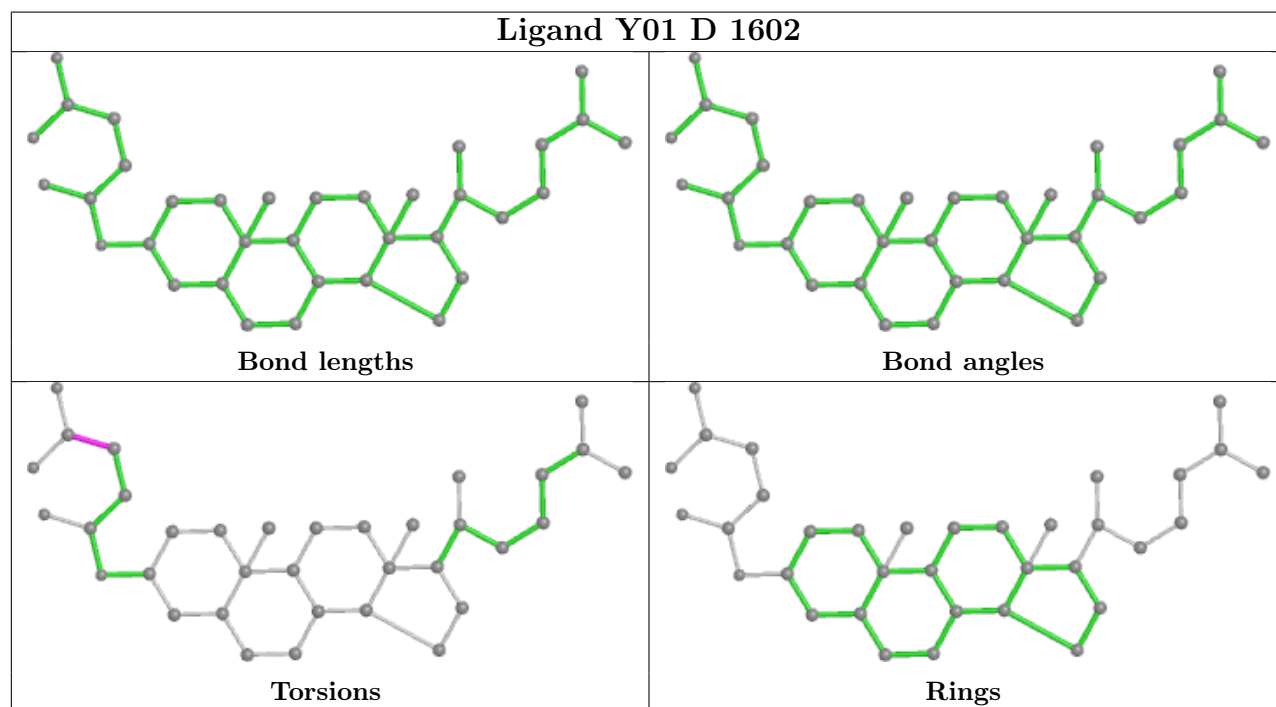
Mol	Chain	Res	Type	Atoms
5	D	1609	NAG	O5-C5-C6-O6
4	D	1604	Y01	CAV-CBC-OAW-CAY
4	D	1603	Y01	CAN-CAJ-CAO-CBB
4	D	1607	Y01	CAO-CBB-CBE-CAP
4	D	1607	Y01	CAO-CBB-CBE-CBI
4	D	1607	Y01	CAC-CBB-CBE-CAP
4	D	1603	Y01	CAM-CAY-OAW-CBC
4	D	1601	Y01	CAO-CBB-CBE-CAP
5	D	1610	NAG	O5-C5-C6-O6
4	D	1607	Y01	CAC-CBB-CBE-CBI
5	D	1608	NAG	C1-C2-N2-C7
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	1606	Y01	CAM-CAL-CAX-OAF
4	D	1607	Y01	CAM-CAL-CAX-OAH
4	D	1603	Y01	CAM-CAL-CAX-OAH
4	D	1604	Y01	CAR-CBC-OAW-CAY
4	D	1601	Y01	CAM-CAL-CAX-OAH
4	D	1605	Y01	CAM-CAL-CAX-OAH
4	D	1602	Y01	CAM-CAL-CAX-OAH
4	D	1606	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-OAH
4	D	1604	Y01	CAM-CAL-CAX-OAF
4	D	1603	Y01	CAO-CAJ-CAN-CBA
4	D	1604	Y01	CAL-CAM-CAY-OAW
4	D	1603	Y01	CAL-CAM-CAY-OAW
4	D	1604	Y01	CAL-CAM-CAY-OAG
4	D	1607	Y01	CAR-CBC-OAW-CAY

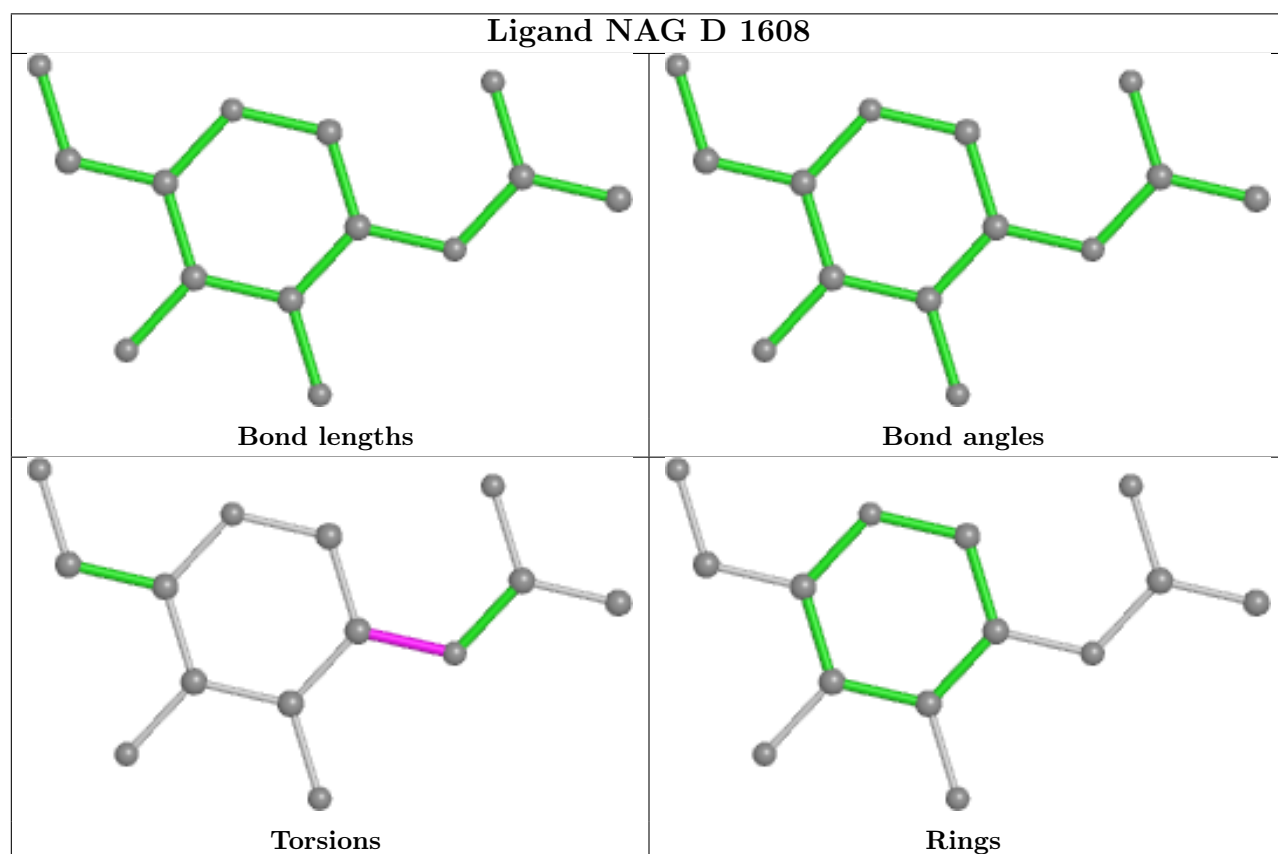
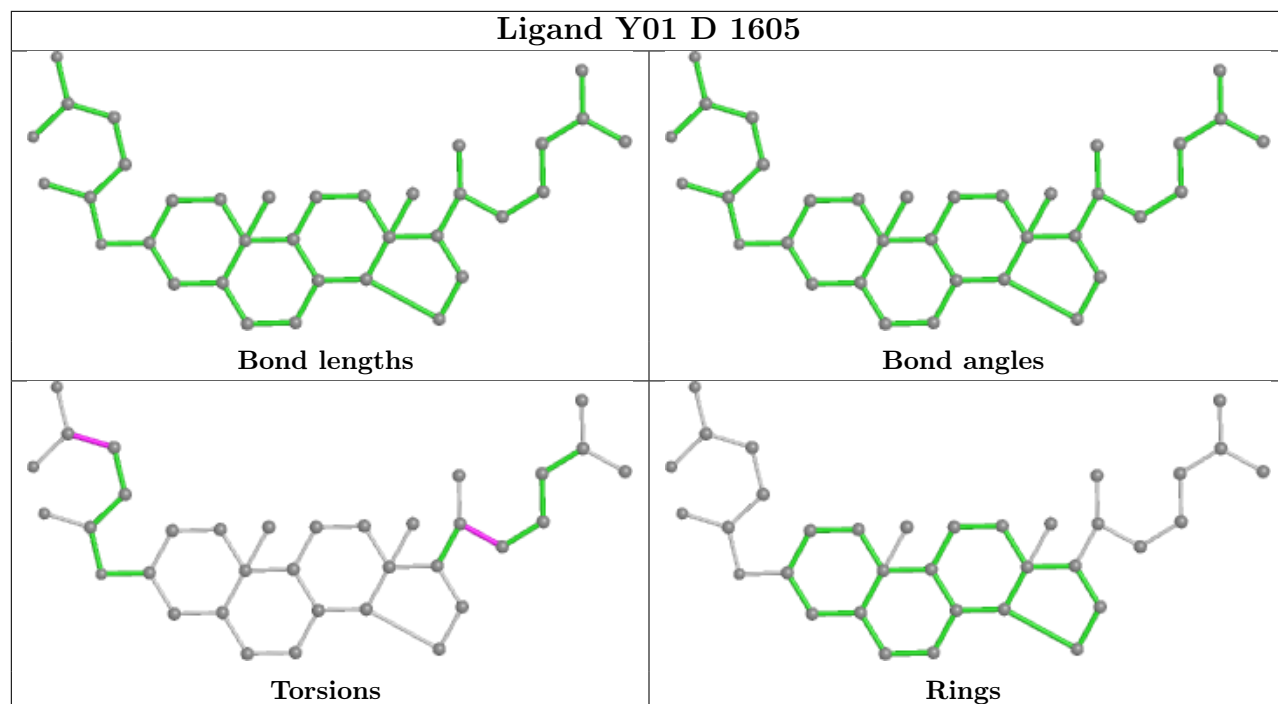
There are no ring outliers.

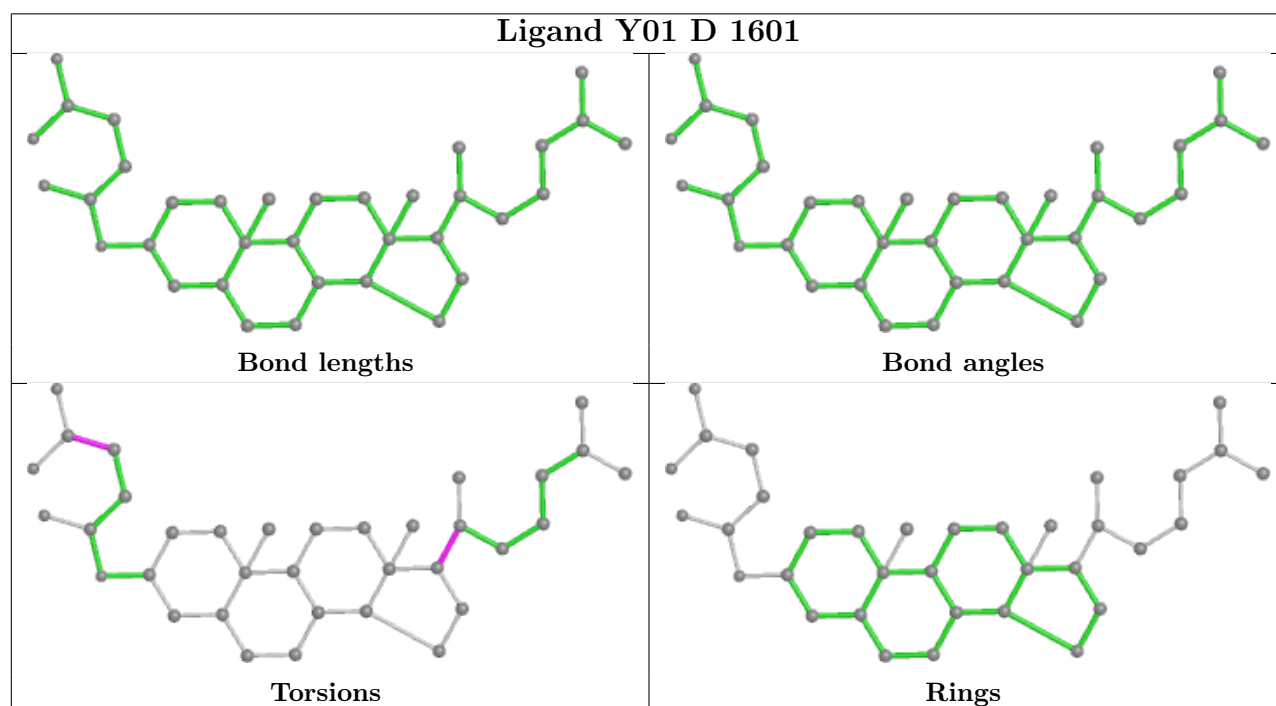
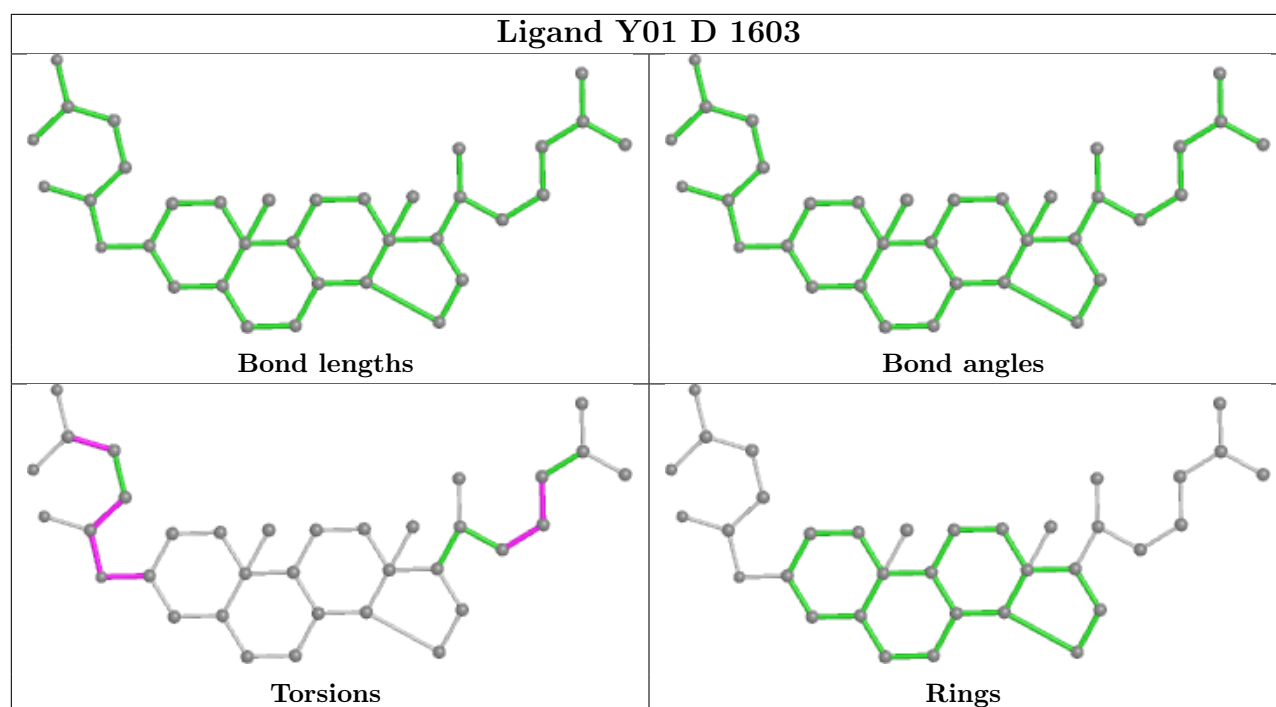
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1605	Y01	1	0
4	D	1603	Y01	1	0
4	D	1601	Y01	1	0
4	D	1607	Y01	3	0
4	D	1604	Y01	2	0

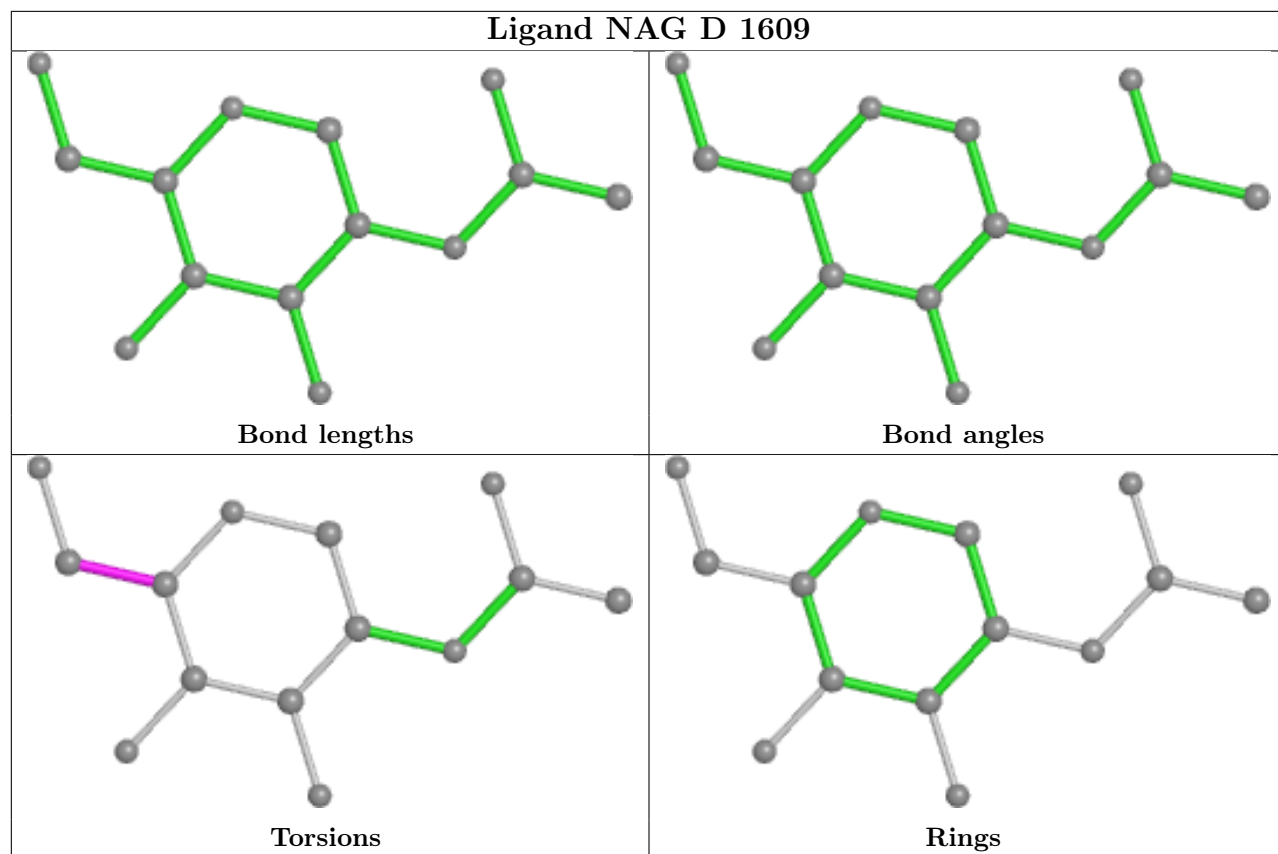
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



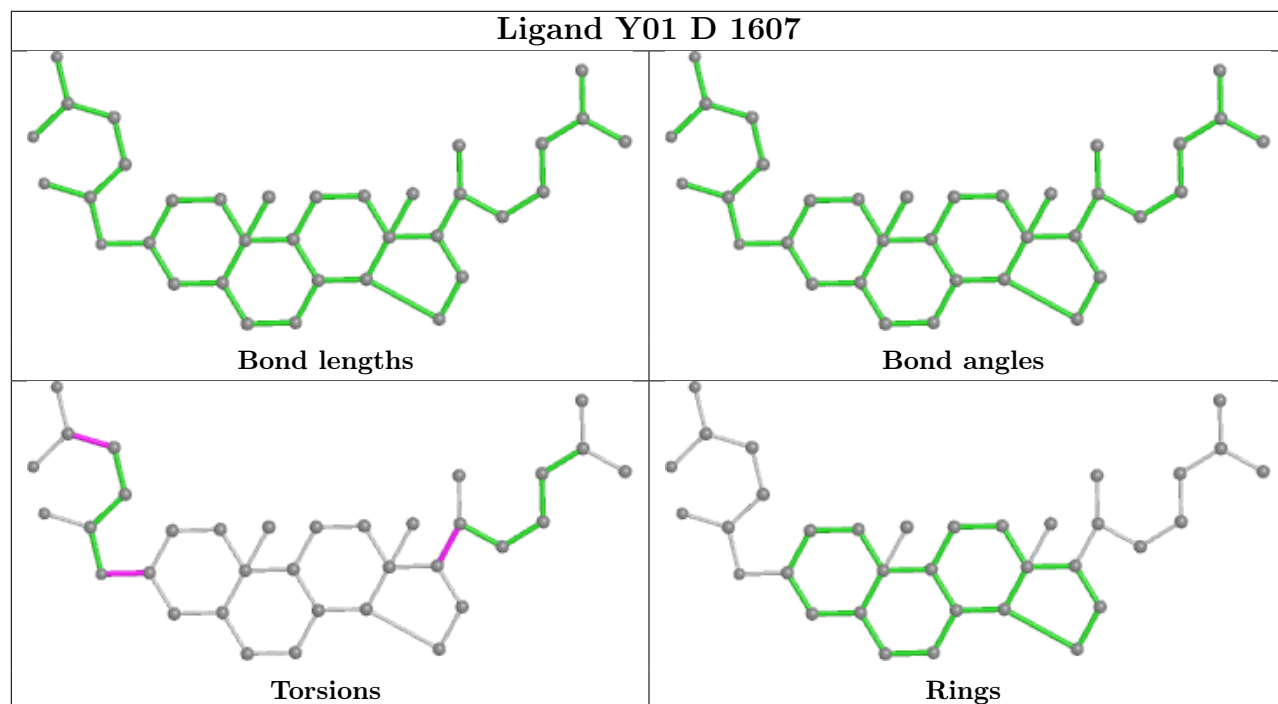


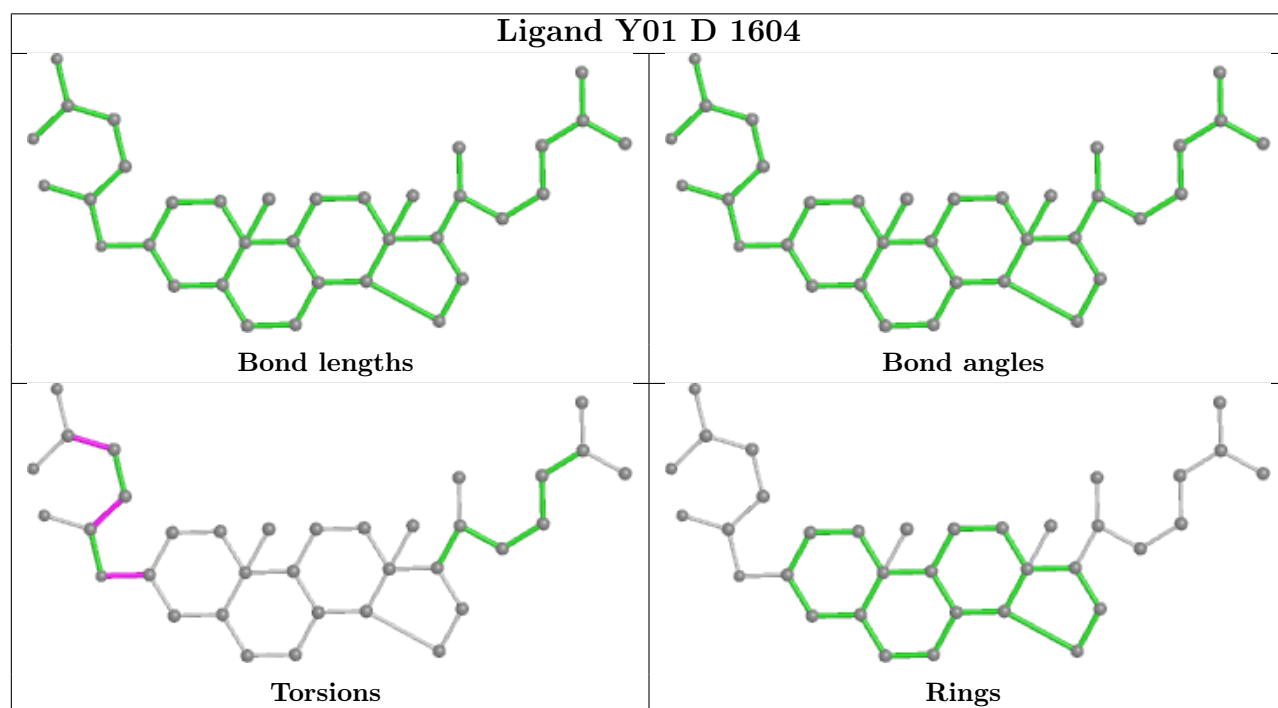
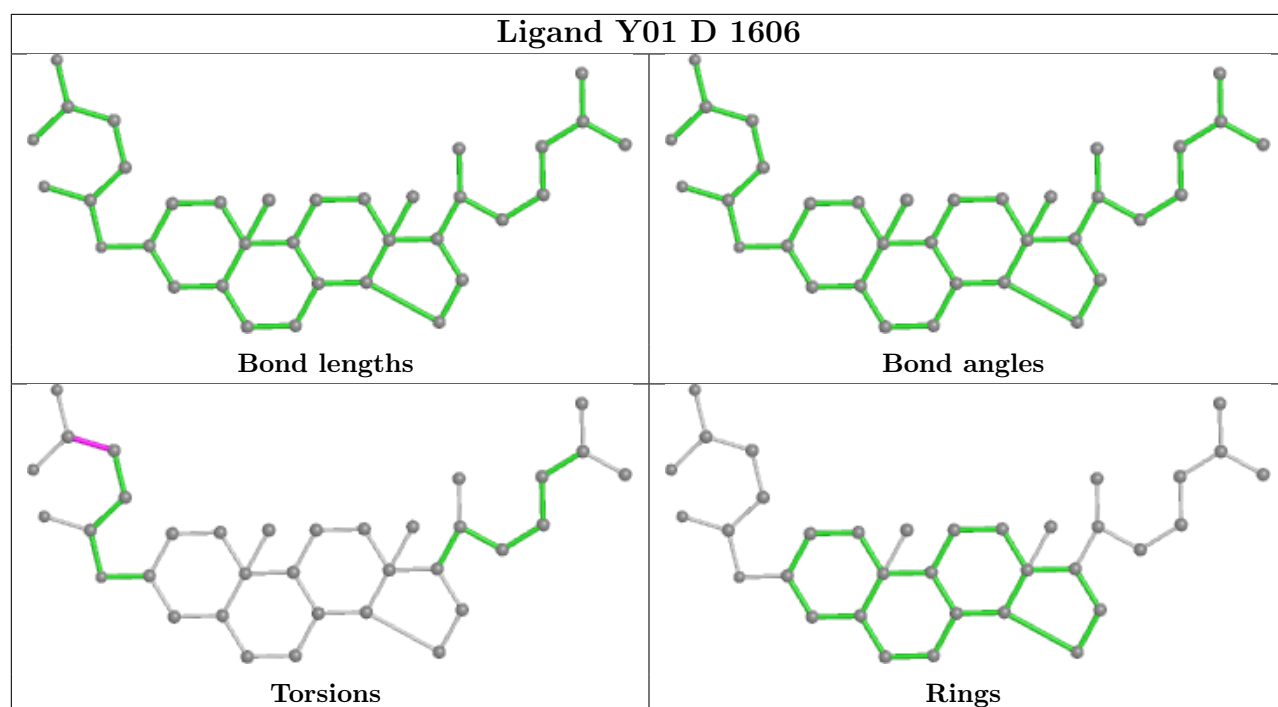


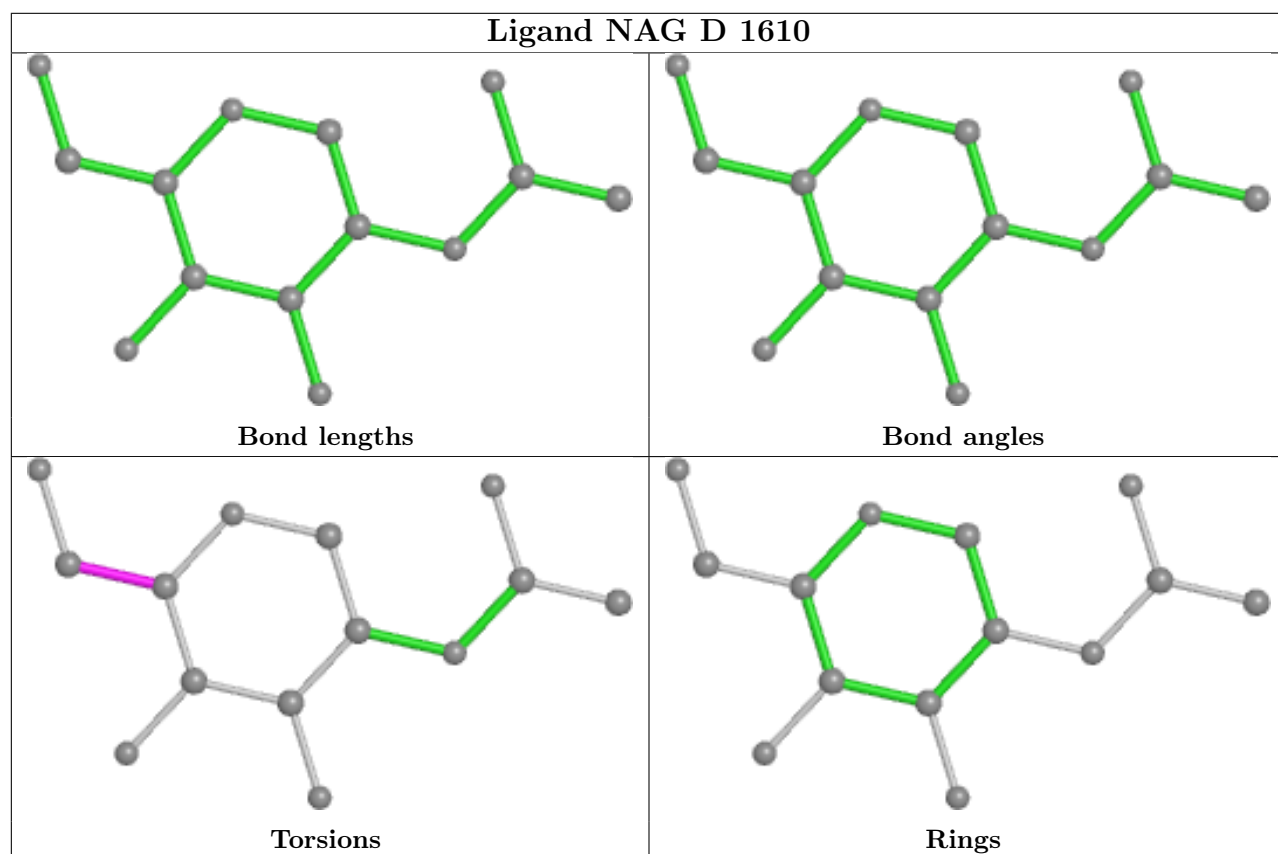
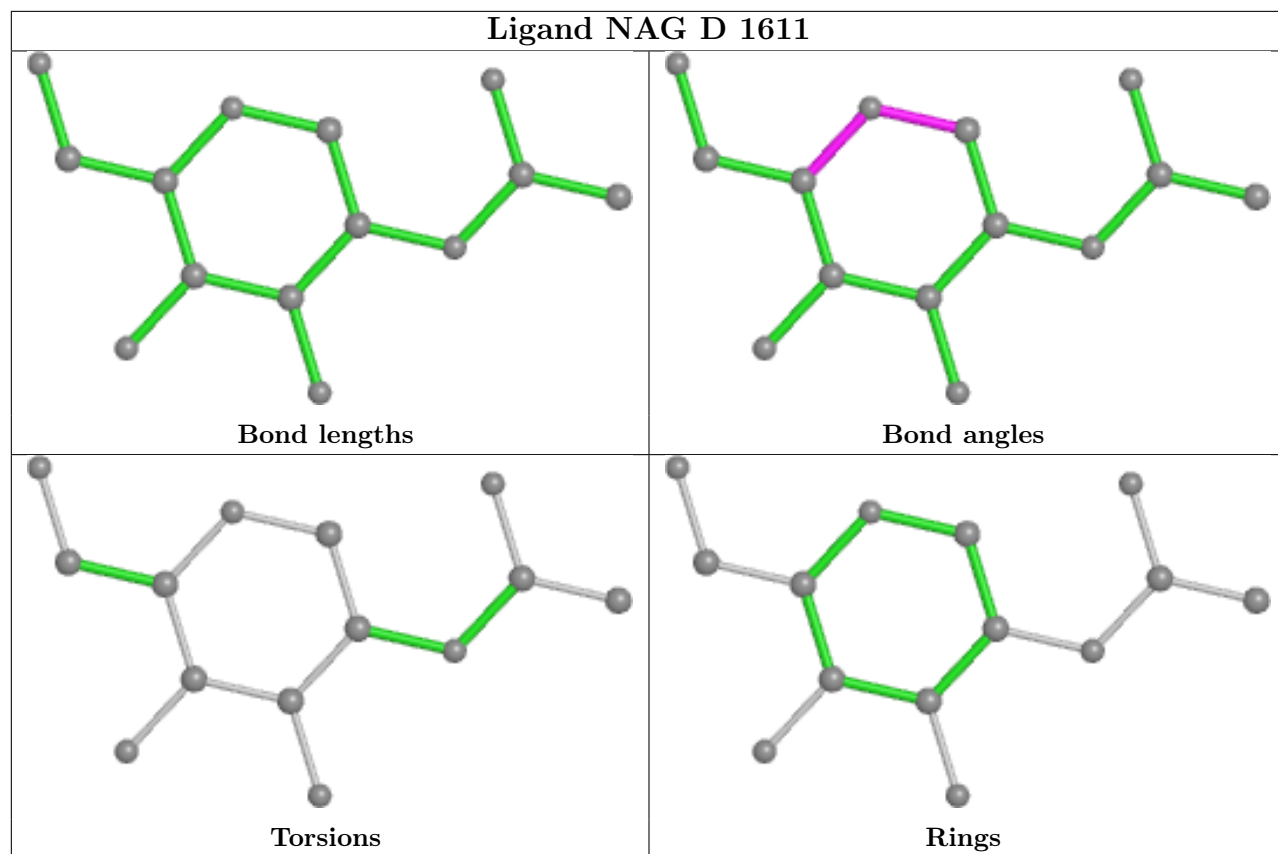
Ligand NAG D 1609



Ligand Y01 D 1607







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.

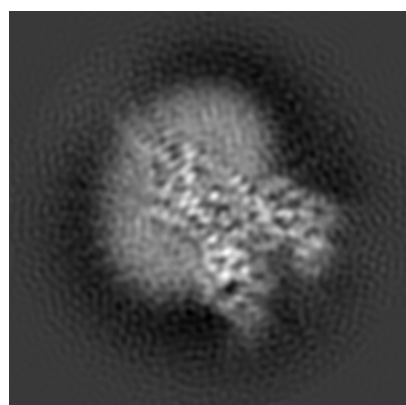
6 Map visualisation [i](#)

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

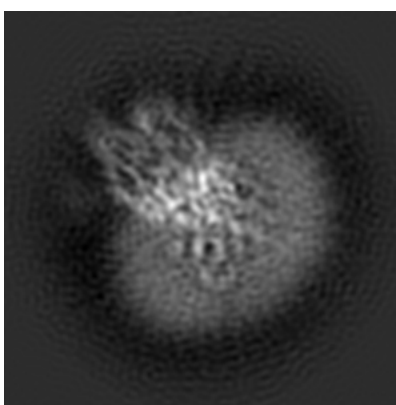
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

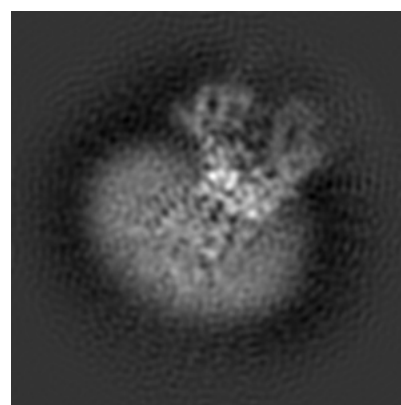
6.1.1 Primary map



X



Y

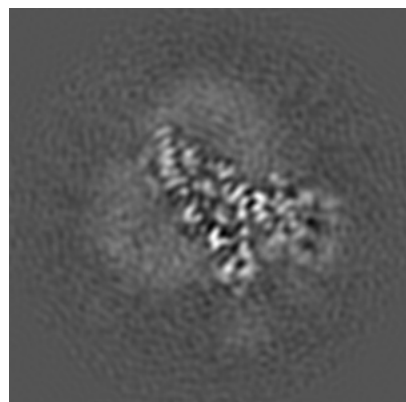


Z

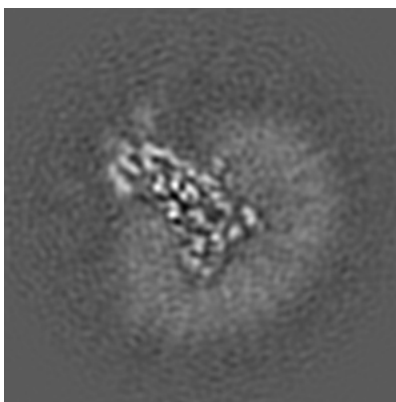
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

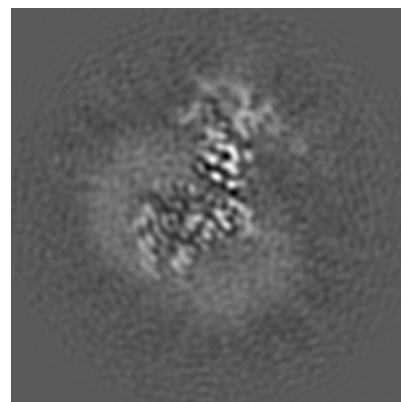
6.2.1 Primary map



X Index: 84



Y Index: 84

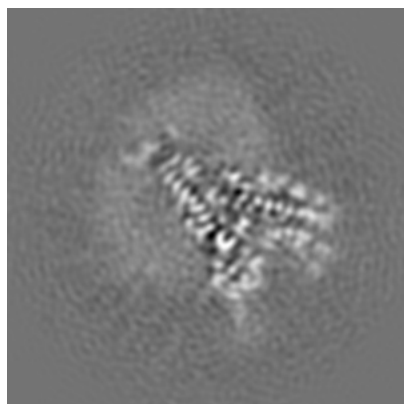


Z Index: 84

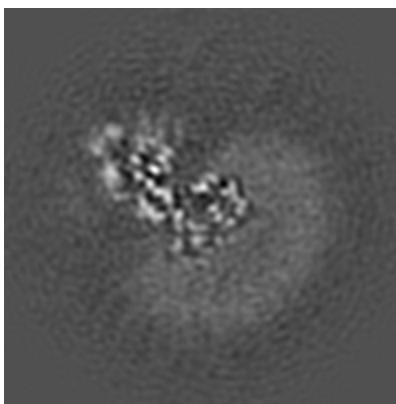
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

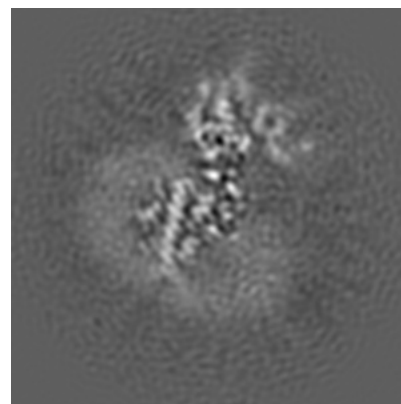
6.3.1 Primary map



X Index: 88



Y Index: 93

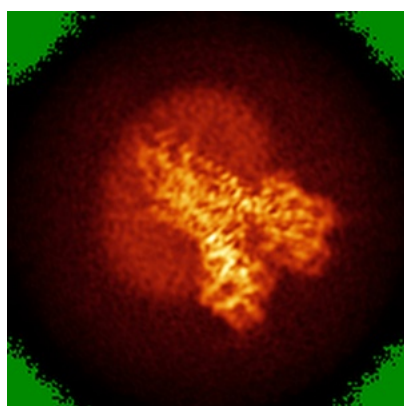


Z Index: 81

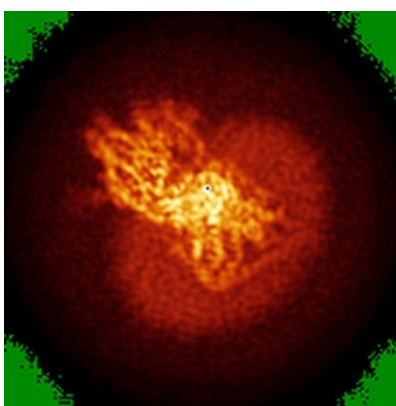
The images above show the largest variance slices of the map in three orthogonal directions.

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

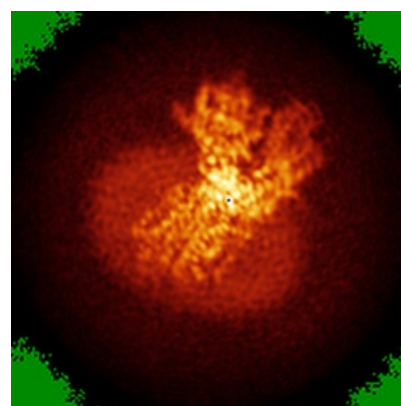
6.4.1 Primary map



X



Y

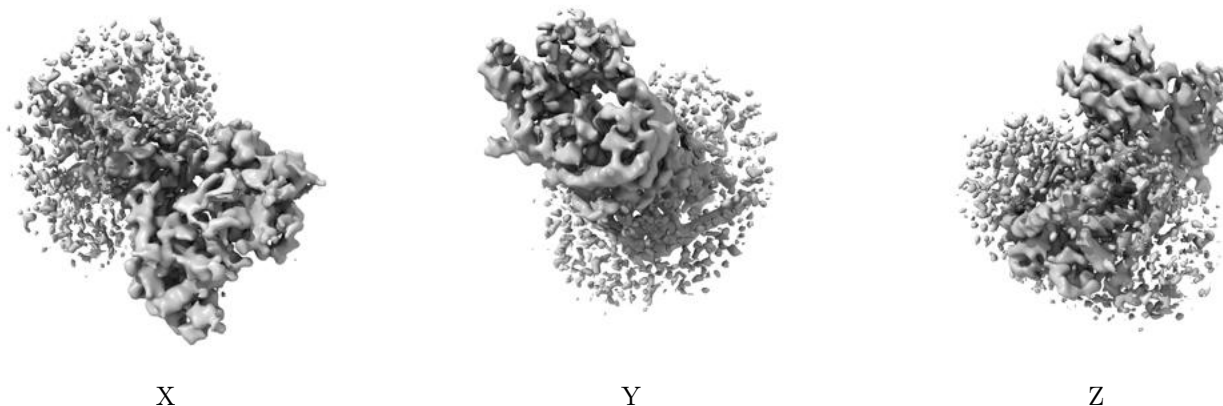


Z

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.

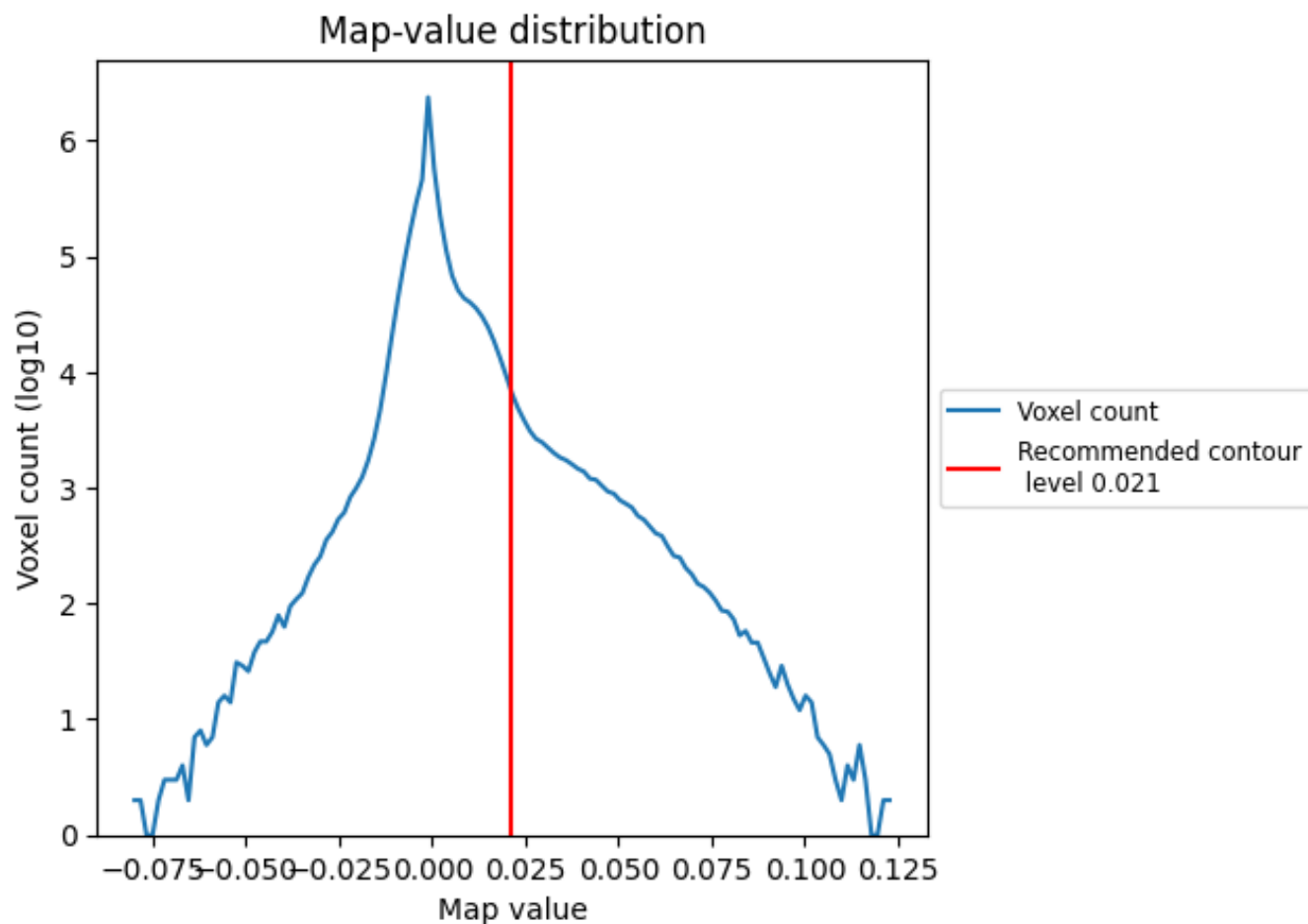
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

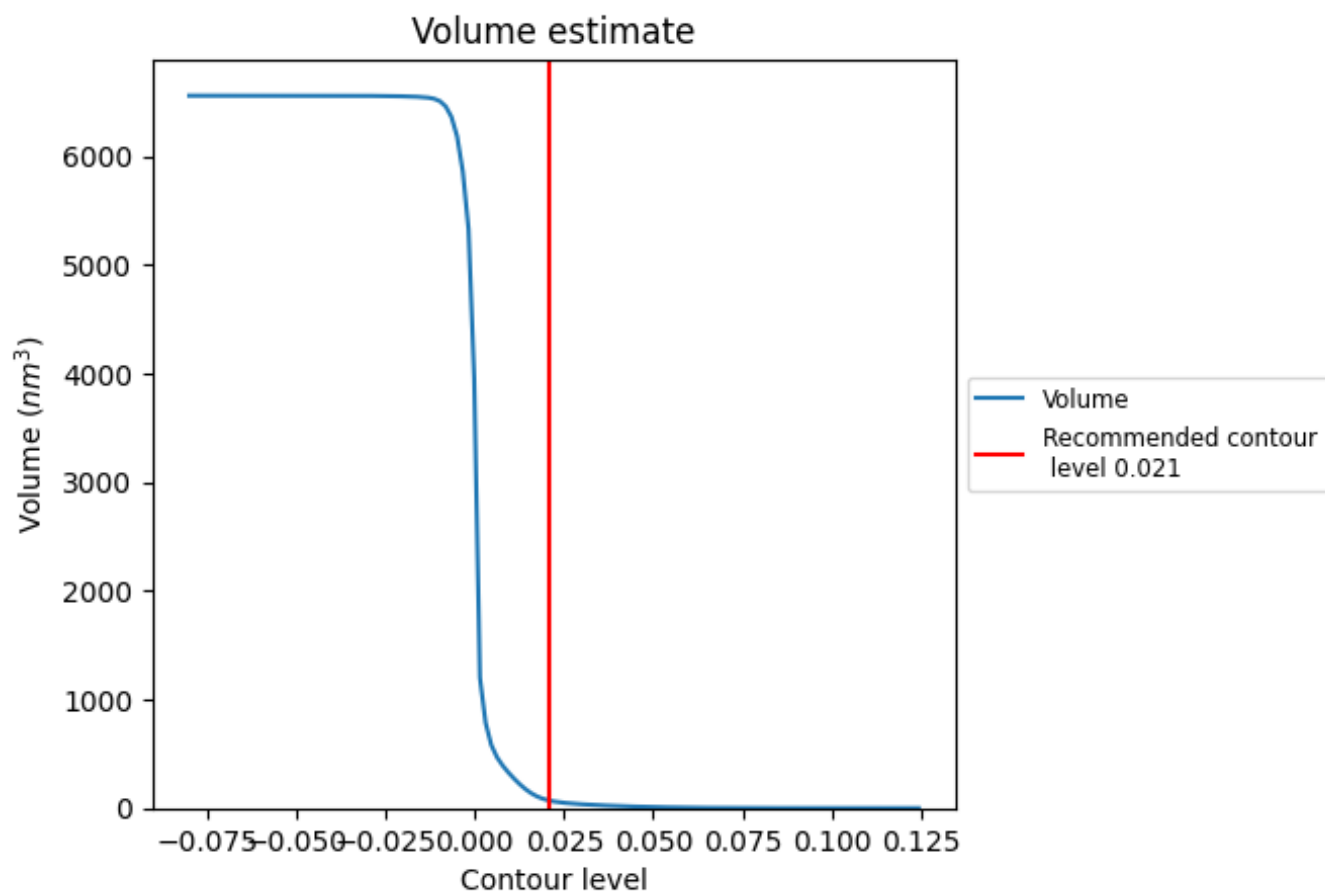
This section contains the results of statistical analysis of the map.

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.

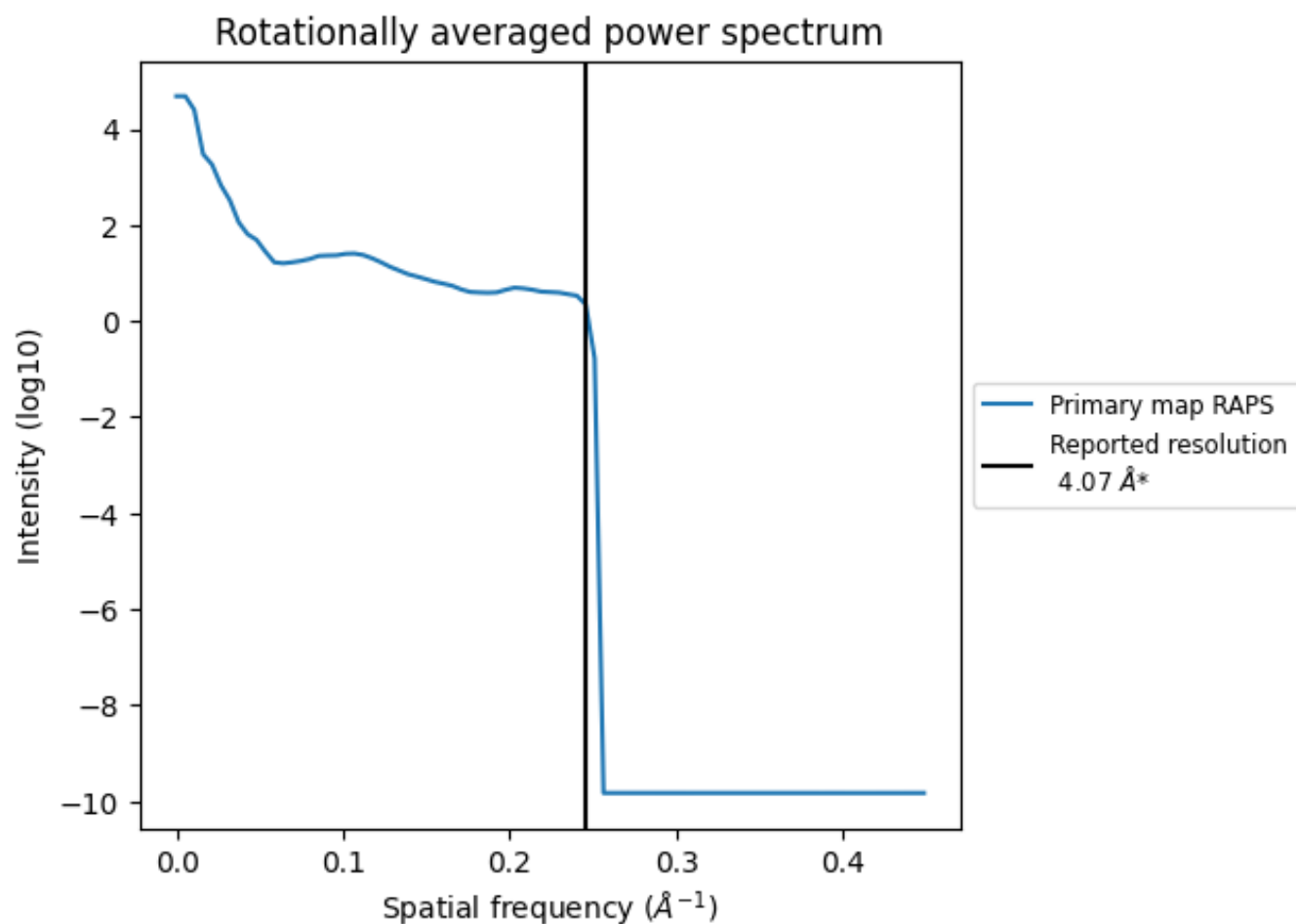
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm³; 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 Å⁻¹

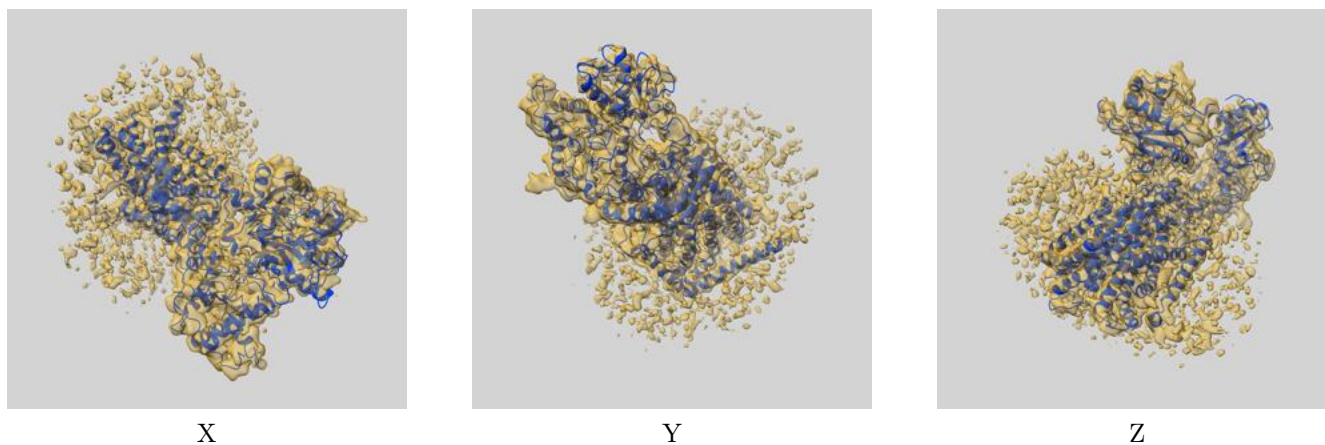
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

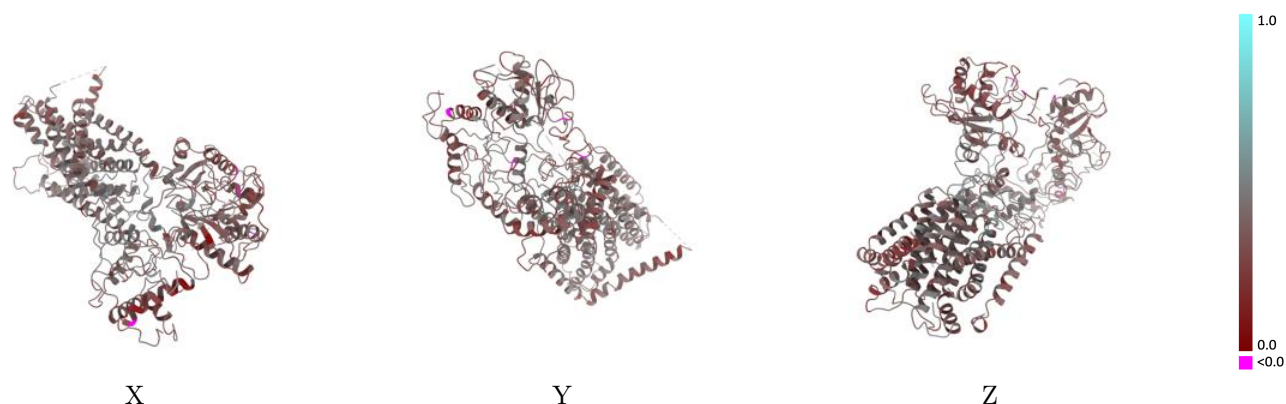
This section contains information regarding the fit between EMDB map EMD-30958 and PDB model 7E2I. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



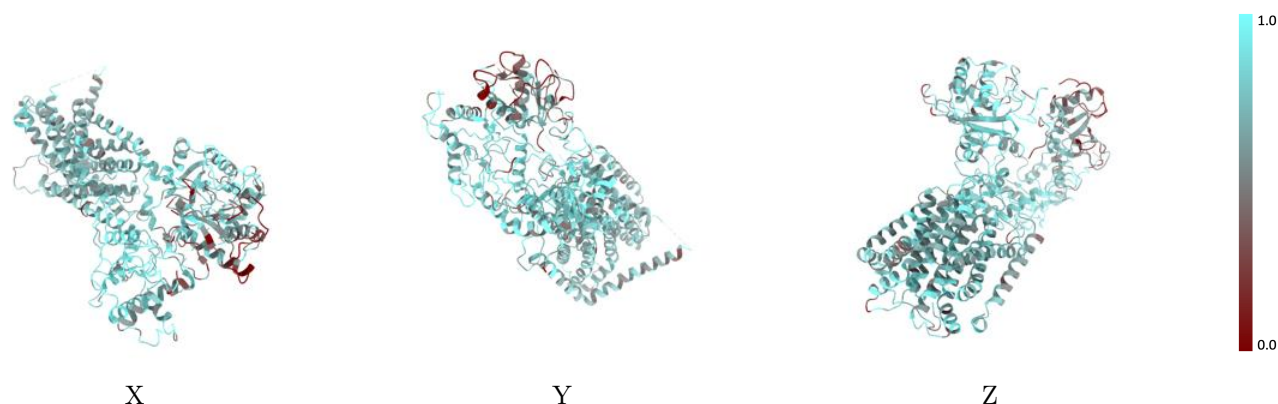
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



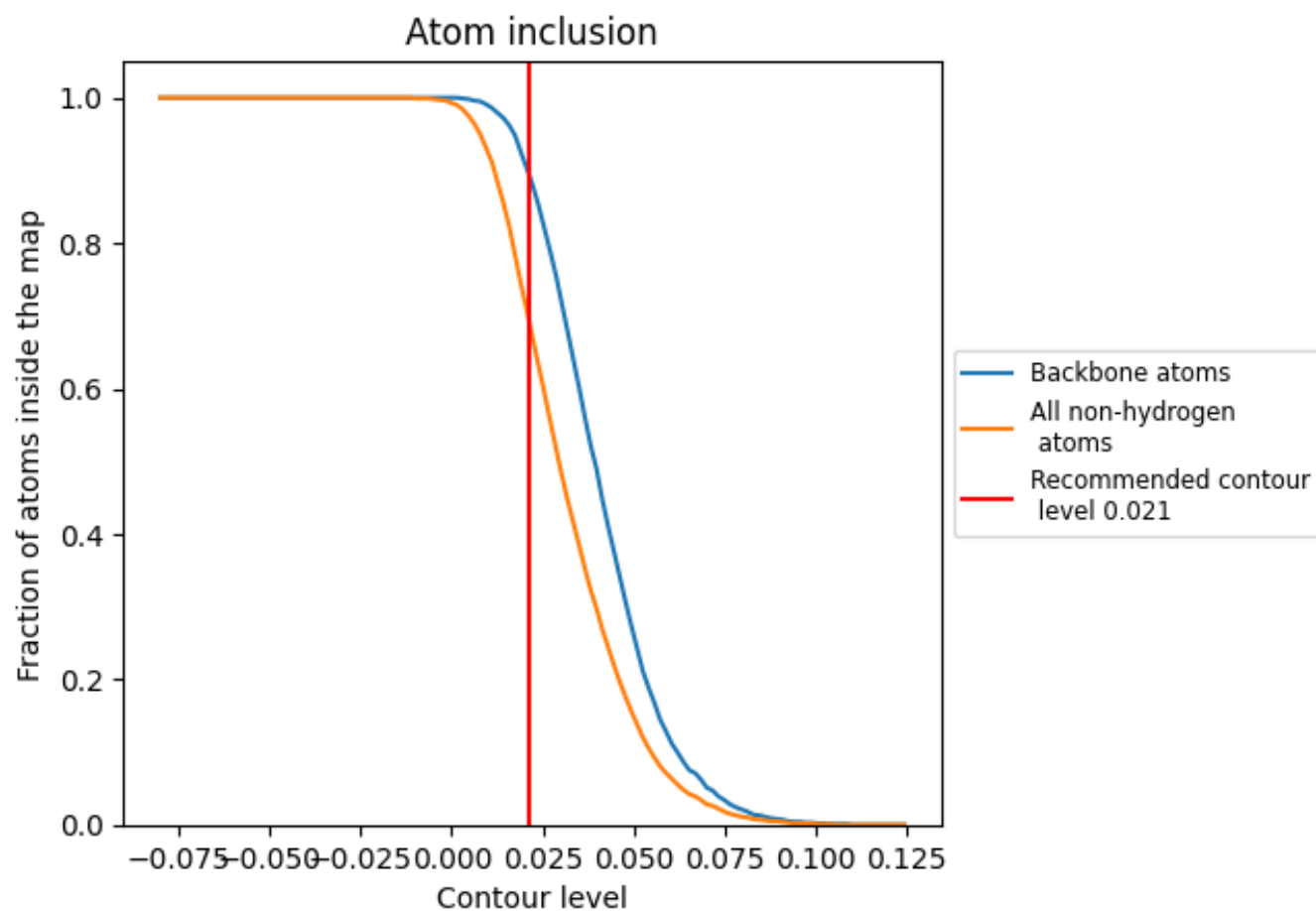
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.7000	<div></div> 0.3750
D	<div></div> 0.7390	<div></div> 0.3780
G	<div></div> 0.4580	<div></div> 0.3570

