



Full wwPDB EM Validation Report ⓘ

Apr 30, 2026 – 04:47 pm BST

PDB ID : 9HNI / pdb_00009hni
EMDB ID : EMD-52310
Title : Drosophila melanogaster insulin receptor ectodomain in complex with two DILP2 molecules
Authors : Shafi, T.; Moroz, O.V.; Jenkins, H.T.; Chechik, M.; Isupov, M.N.; Brzozowski, A.M.
Deposited on : 2024-12-10
Resolution : 6.25 Å (reported)
Based on initial model : 8cls

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 : 1.8.4, CSD as541be (2020)
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

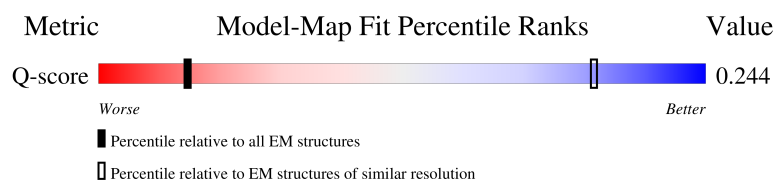
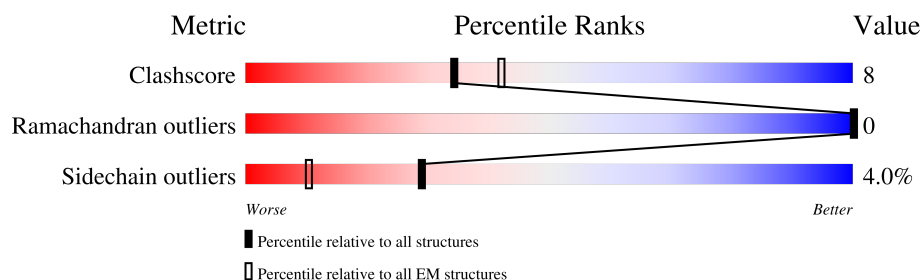
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.25 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	506 (5.75 - 6.75)

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	E	26	
1	G	26	
2	F	24	

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Mol	Chain	Length	Quality of chain
2	H	24	
3	A	1048	
3	B	1048	
4	C	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	1	-	-	X	-
5	NAG	B	1402	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14354 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 Probable insulin-like peptide 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	26	Total	C	N	O	S	0	0
			206	123	40	38	5		
1	G	26	Total	C	N	O	S	0	0
			206	123	40	38	5		

- Molecule 2 is a protein called Probable insulin-like peptide 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	24	Total	C	N	O	S	0	0
			190	119	29	39	3		
2	H	24	Total	C	N	O	S	0	0
			190	119	29	39	3		

- Molecule 3 is a protein called Insulin-like receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	821	Total	C	N	O	S	0	0
			6519	4106	1117	1249	47		
3	B	853	Total	C	N	O	S	0	0
			6777	4268	1160	1299	50		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	MET	-	initiating methionine	UNP P09208
B	263	MET	-	initiating methionine	UNP P09208

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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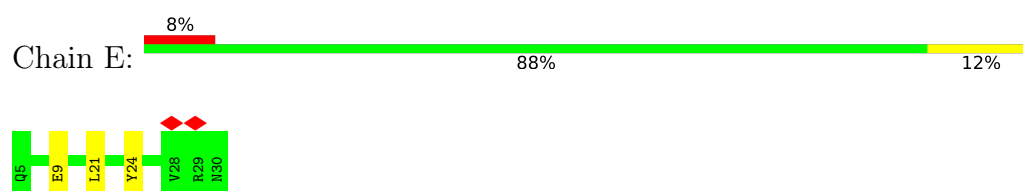
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

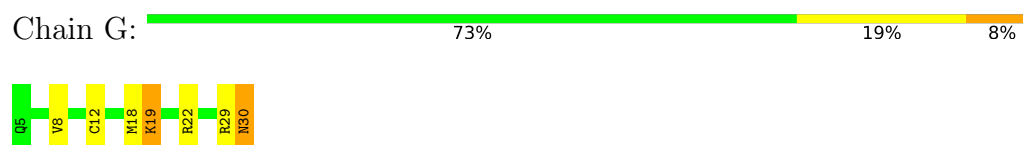
3 Residue-property plots [i](#)

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.

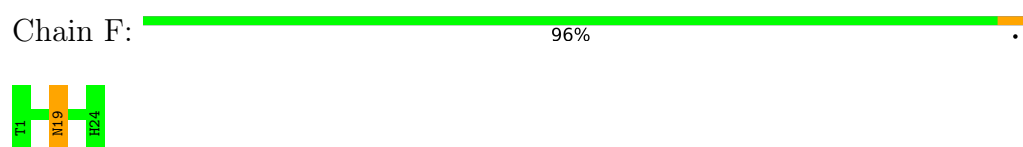
- Molecule 1: Probable insulin-like peptide 2



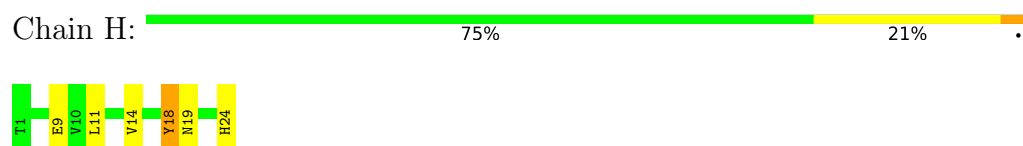
- Molecule 1: Probable insulin-like peptide 2



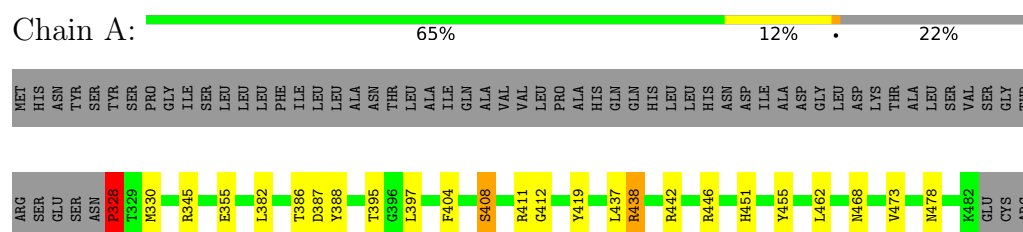
- Molecule 2: Probable insulin-like peptide 2

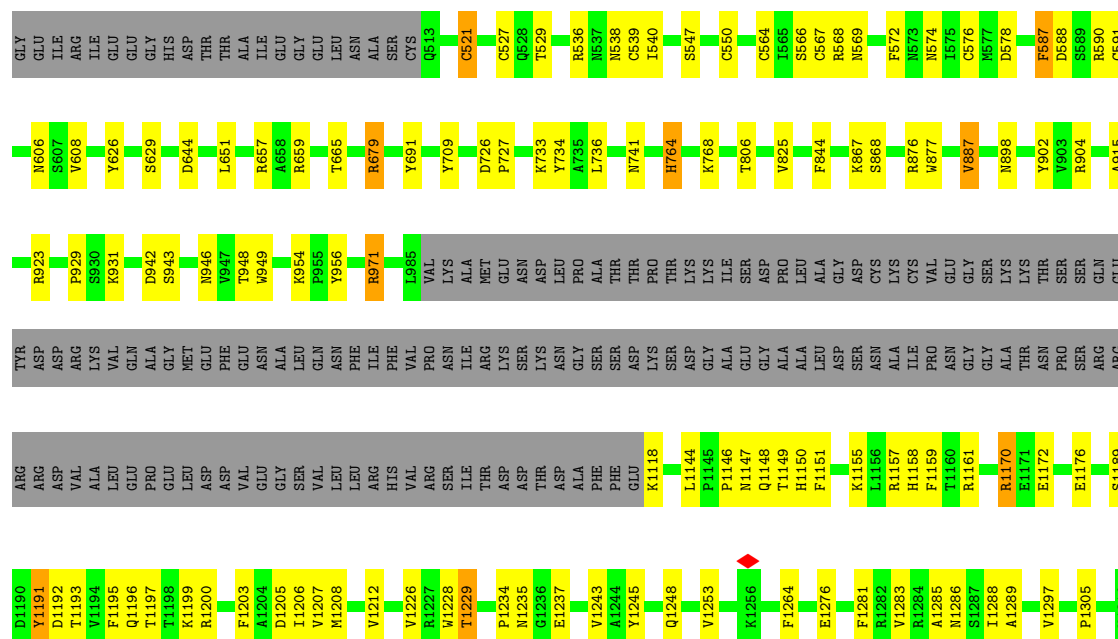


- Molecule 2: Probable insulin-like peptide 2



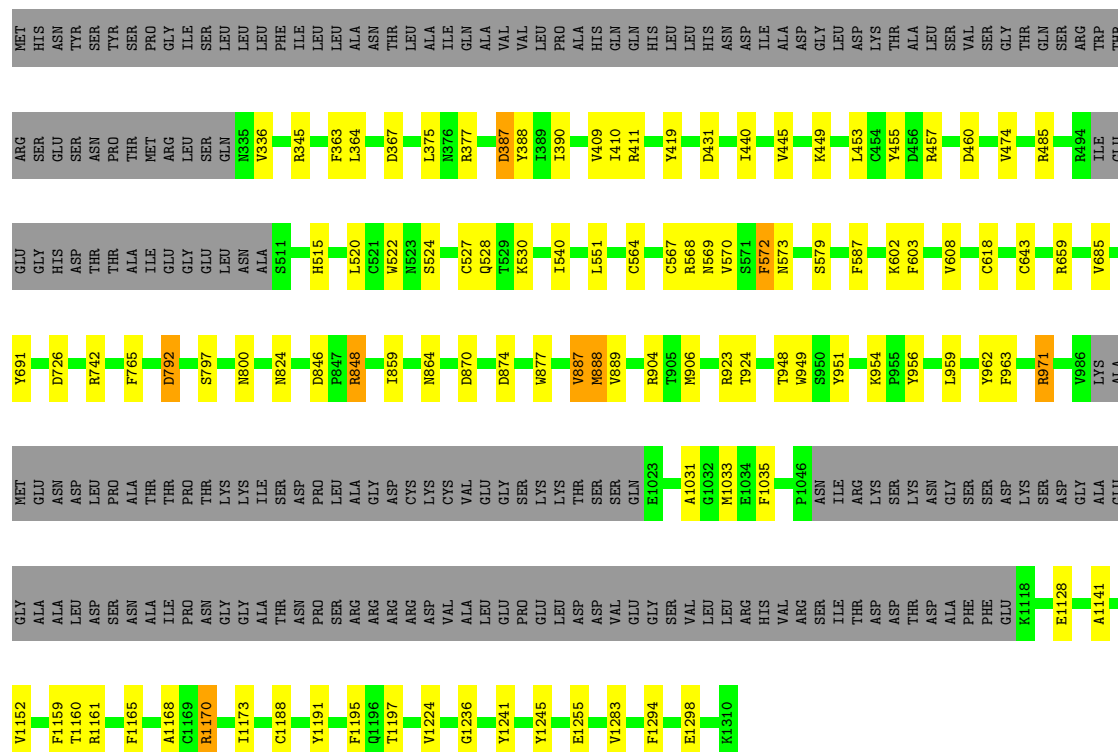
- Molecule 3: Insulin-like receptor





• Molecule 3: Insulin-like receptor

Chain B: 71% 9% 19%



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.003	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0006	Depositor
Map size (Å)	293.888, 293.888, 293.888	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	E	0.77	0/206	1.35	0/270
1	G	0.59	0/206	1.27	1/270 (0.4%)
2	F	0.84	0/193	1.49	1/261 (0.4%)
2	H	0.79	0/193	1.42	2/261 (0.8%)
3	A	0.73	0/6657	1.35	16/9007 (0.2%)
3	B	0.77	0/6919	1.40	18/9358 (0.2%)
All	All	0.75	0/14374	1.37	38/19427 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1158	HIS	N-CA-C	9.07	124.13	112.89
3	B	1165	PHE	CA-CB-CG	7.54	121.33	113.80
3	B	336	VAL	N-CA-C	7.47	117.59	110.42
3	B	643	CYS	N-CA-C	7.04	119.42	110.33
3	A	764	HIS	CA-CB-CG	-6.69	107.11	113.80
3	A	451	HIS	N-CA-C	6.46	119.14	111.33
3	A	1305	PRO	N-CA-CB	6.38	106.54	103.22
3	A	521	CYS	N-CA-C	6.32	118.68	109.07
2	H	24	HIS	CB-CG-CD2	-6.10	123.27	131.20
2	F	19	ASN	CA-CB-CG	6.06	118.66	112.60
3	B	870	ASP	CA-CB-CG	5.96	118.56	112.60
3	B	572	PHE	N-CA-C	5.72	117.76	109.07
3	A	455	TYR	CA-C-N	5.71	127.92	120.28
3	A	455	TYR	C-N-CA	5.71	127.92	120.28
3	B	527	CYS	N-CA-C	5.62	117.94	109.23
3	B	765	PHE	CA-CB-CG	-5.59	108.21	113.80
3	B	726	ASP	CA-CB-CG	5.58	118.18	112.60
3	B	1173	ILE	CA-C-N	5.55	125.01	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1173	ILE	C-N-CA	5.55	125.01	119.24
3	B	579	SER	N-CA-C	5.52	116.66	108.60
3	A	942	ASP	CA-CB-CG	5.49	118.09	112.60
3	B	608	VAL	N-CA-C	5.47	116.10	110.36
3	B	564	CYS	N-CA-C	5.46	118.16	109.96
3	A	1276	GLU	N-CA-C	5.45	117.11	110.41
3	B	431	ASP	CA-CB-CG	5.42	118.02	112.60
1	G	30	ASN	CA-CB-CG	5.36	117.96	112.60
2	H	18	TYR	N-CA-C	5.35	116.90	109.31
3	A	825	VAL	CA-C-N	5.32	127.72	120.54
3	A	825	VAL	C-N-CA	5.32	127.72	120.54
3	B	367	ASP	CA-CB-CG	5.31	117.91	112.60
3	A	1248	GLN	OE1-CD-NE2	-5.25	117.35	122.60
3	A	567	CYS	N-CA-C	5.22	119.40	112.30
3	B	874	ASP	CA-CB-CG	5.20	117.80	112.60
3	B	792	ASP	CA-CB-CG	5.17	117.77	112.60
3	B	864	ASN	CA-CB-CG	5.17	117.77	112.60
3	A	328	PRO	CA-N-CD	-5.11	104.85	112.00
3	A	1253	VAL	N-CA-C	5.05	117.24	111.88
3	A	727	PRO	N-CA-C	-5.03	104.57	110.70

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	E	206	0	208	2	0
1	G	206	0	208	7	0
2	F	190	0	186	0	0
2	H	190	0	186	7	0
3	A	6519	0	6395	130	0
3	B	6777	0	6635	92	0
4	C	28	0	25	8	0
5	A	126	0	117	5	0
5	B	112	0	104	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14354	0	14064	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1170:ARG:HH21	3:A:1172:GLU:HA	0.98	1.11
3:B:888:MET:HE3	3:B:888:MET:HA	1.34	1.09
3:A:578:ASP:O	5:A:1409:NAG:H82	1.54	1.08
3:A:1200:ARG:NH1	3:A:1200:ARG:HB3	1.70	1.05
3:B:1170:ARG:HG2	3:B:1170:ARG:HH11	1.21	1.05
3:A:1170:ARG:O	3:A:1170:ARG:HD3	1.56	1.01
3:B:848:ARG:HH11	3:B:848:ARG:HG2	1.20	1.00
3:A:1200:ARG:HH11	3:A:1200:ARG:CB	1.74	0.99
3:B:888:MET:HE2	3:B:889:VAL:H	1.22	0.98
3:A:887:VAL:HG11	4:C:1:NAG:H82	1.44	0.97
3:A:419:TYR:OH	3:A:446:ARG:HD2	1.65	0.96
3:B:923:ARG:HD3	5:B:1402:NAG:HN2	1.26	0.96
3:B:888:MET:CE	3:B:889:VAL:H	1.79	0.95
3:A:1170:ARG:NH2	3:A:1172:GLU:HA	1.81	0.94
3:B:419:TYR:OH	3:B:474:VAL:HB	1.68	0.92
3:B:1152:VAL:HB	5:B:1404:NAG:H82	1.54	0.90
3:A:1200:ARG:NH1	3:A:1200:ARG:CB	2.35	0.88
3:B:888:MET:HE2	3:B:889:VAL:N	1.91	0.86
3:A:572:PHE:HD1	3:A:590:ARG:HG3	1.40	0.86
3:A:1170:ARG:NH2	3:A:1176:GLU:HG2	1.92	0.85
3:B:846:ASP:HB3	3:B:848:ARG:HH12	1.41	0.85
3:B:1170:ARG:O	3:B:1170:ARG:HD3	1.79	0.83
3:B:846:ASP:HB3	3:B:848:ARG:NH1	1.93	0.82
3:A:355:GLU:HB2	5:A:1401:NAG:H82	1.59	0.82
3:B:971:ARG:HG3	3:B:971:ARG:HH11	1.43	0.82
3:B:1170:ARG:HH11	3:B:1170:ARG:CG	1.92	0.82
1:G:29:ARG:HD2	2:H:18:TYR:HD2	1.44	0.81
3:A:1170:ARG:HH12	3:A:1176:GLU:CD	1.91	0.79
1:G:29:ARG:HD2	2:H:18:TYR:CD2	2.17	0.79
3:A:1200:ARG:HH11	3:A:1200:ARG:HB2	1.47	0.78
3:A:572:PHE:HD1	3:A:590:ARG:CG	1.96	0.78
3:A:419:TYR:CE1	3:A:446:ARG:HB2	2.21	0.76
3:B:848:ARG:HG2	3:B:848:ARG:NH1	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:948:THR:OG1	5:A:1404:NAG:H62	1.86	0.75
3:B:951:TYR:CD2	3:B:959:LEU:HD13	2.21	0.75
3:B:923:ARG:HD3	5:B:1402:NAG:N2	2.02	0.75
3:A:1161:ARG:HG2	3:A:1197:THR:HG22	1.67	0.75
3:A:971:ARG:HA	3:A:1161:ARG:HD3	1.69	0.75
3:A:419:TYR:HH	3:A:679:ARG:HH21	1.33	0.74
3:B:1170:ARG:HD3	3:B:1170:ARG:C	2.13	0.73
3:A:419:TYR:CZ	3:A:446:ARG:HD2	2.23	0.73
3:B:848:ARG:HG3	3:B:1033:MET:SD	2.28	0.73
3:B:923:ARG:HG2	5:B:1402:NAG:H82	1.70	0.71
3:B:485:ARG:O	3:B:485:ARG:HG2	1.89	0.71
3:A:419:TYR:CZ	3:A:446:ARG:CD	2.74	0.70
3:B:888:MET:HE3	3:B:888:MET:CA	2.18	0.69
3:A:1118:LYS:HA	3:A:1191:TYR:CZ	2.28	0.69
3:A:1191:TYR:H	3:A:1191:TYR:HD2	1.39	0.68
3:B:888:MET:CE	3:B:889:VAL:N	2.52	0.68
3:B:971:ARG:HH11	3:B:971:ARG:CG	2.06	0.68
3:A:572:PHE:CD1	3:A:590:ARG:HG3	2.25	0.68
3:A:1118:LYS:N	3:A:1191:TYR:HH	1.91	0.68
3:A:1161:ARG:HG2	3:A:1197:THR:CG2	2.23	0.68
3:B:848:ARG:HH11	3:B:848:ARG:CG	1.99	0.67
3:B:824:ASN:OD1	3:B:887:VAL:HG12	1.95	0.66
3:B:888:MET:HA	3:B:888:MET:CE	2.21	0.66
3:A:419:TYR:OH	3:A:446:ARG:CD	2.43	0.66
3:B:411:ARG:NH2	3:B:569:ASN:HA	2.10	0.66
3:B:948:THR:HG21	5:B:1404:NAG:H62	1.77	0.66
3:A:568:ARG:HG2	3:A:569:ASN:OD1	1.95	0.66
3:A:971:ARG:CA	3:A:1161:ARG:HD3	2.26	0.65
1:G:18:MET:HE3	2:H:14:VAL:HG22	1.79	0.65
3:A:679:ARG:HH11	3:B:1031:ALA:HB1	1.62	0.64
3:A:971:ARG:NH1	3:A:1288:ILE:HB	2.11	0.64
3:A:1207:VAL:HG11	3:A:1228:TRP:CE3	2.33	0.64
3:A:1170:ARG:CZ	3:A:1176:GLU:HG2	2.27	0.63
3:A:679:ARG:NH1	3:B:1031:ALA:HB1	2.12	0.62
3:B:363:PHE:HB3	3:B:387:ASP:HB2	1.82	0.62
3:A:1161:ARG:CG	3:A:1197:THR:HG22	2.29	0.62
3:B:1170:ARG:HG2	3:B:1170:ARG:NH1	2.03	0.62
3:A:564:CYS:SG	3:A:566:SER:O	2.58	0.61
3:B:419:TYR:CD1	3:B:445:VAL:C	2.78	0.61
3:A:971:ARG:NH2	3:A:1235:ASN:C	2.58	0.61
3:A:1170:ARG:HH22	3:A:1176:GLU:HG2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1170:ARG:O	3:A:1170:ARG:CD	2.42	0.60
3:B:411:ARG:HH21	3:B:569:ASN:HA	1.65	0.60
3:B:848:ARG:NH1	3:B:848:ARG:CG	2.62	0.60
3:B:959:LEU:HD12	3:B:1168:ALA:HB1	1.82	0.60
3:A:1192:ASP:O	3:A:1193:THR:HG22	2.02	0.59
3:A:876:ARG:HG3	3:A:877:TRP:CD1	2.38	0.59
3:A:568:ARG:HG2	3:A:569:ASN:N	2.18	0.58
3:A:328:PRO:HD2	3:A:547:SER:HB3	1.85	0.58
4:C:1:NAG:H61	4:C:2:NAG:C7	2.33	0.57
3:A:887:VAL:HG21	4:C:1:NAG:H82	1.87	0.57
3:B:587:PHE:HA	3:B:618:CYS:HB2	1.87	0.57
3:A:657:ARG:HG2	3:A:657:ARG:HH11	1.70	0.57
3:B:1170:ARG:CG	3:B:1170:ARG:NH1	2.56	0.57
3:A:330:MET:CE	3:A:547:SER:OG	2.53	0.56
3:A:419:TYR:CZ	3:A:446:ARG:HD3	2.40	0.56
3:A:1118:LYS:HA	3:A:1191:TYR:CE2	2.40	0.56
3:A:868:SER:HG	3:A:877:TRP:CD1	2.24	0.56
3:A:330:MET:HE3	3:A:547:SER:OG	2.05	0.55
3:B:460:ASP:H	3:B:520:LEU:CD2	2.19	0.55
3:B:959:LEU:CD1	3:B:1168:ALA:HB1	2.37	0.55
3:A:1207:VAL:HG11	3:A:1228:TRP:CZ3	2.42	0.55
3:B:888:MET:HE3	3:B:889:VAL:H	1.71	0.54
3:B:846:ASP:CB	3:B:848:ARG:HH12	2.17	0.54
3:A:550:CYS:C	3:A:564:CYS:SG	2.89	0.54
3:A:1161:ARG:HH21	3:A:1195:PHE:HB3	1.73	0.54
3:B:1152:VAL:HB	5:B:1404:NAG:C8	2.31	0.54
3:A:1170:ARG:HD3	3:A:1170:ARG:C	2.29	0.54
3:B:419:TYR:OH	3:B:474:VAL:CB	2.49	0.54
3:B:1170:ARG:C	3:B:1170:ARG:CD	2.79	0.54
3:A:867:LYS:HE2	3:A:902:TYR:CG	2.43	0.54
3:A:1148:GLN:HE22	3:A:1150:HIS:CE1	2.26	0.53
3:B:363:PHE:CZ	3:B:603:PHE:HB3	2.43	0.53
3:B:1161:ARG:HE	3:B:1195:PHE:HB3	1.73	0.53
3:A:651:LEU:O	3:A:657:ARG:NH1	2.42	0.53
3:B:1170:ARG:HD2	3:B:1188:CYS:SG	2.49	0.53
3:B:923:ARG:CG	5:B:1402:NAG:H82	2.38	0.53
3:A:572:PHE:CD1	3:A:590:ARG:CG	2.87	0.52
3:A:330:MET:CE	3:A:547:SER:HG	2.22	0.52
3:A:1235:ASN:CG	3:A:1289:ALA:HB2	2.34	0.52
1:G:29:ARG:N	1:G:29:ARG:HD3	2.24	0.52
3:A:1200:ARG:HB3	3:A:1200:ARG:CZ	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:363:PHE:HB2	3:B:388:TYR:CD1	2.44	0.52
1:G:19:LYS:HA	1:G:22:ARG:HD3	1.92	0.52
3:A:1228:TRP:CE3	3:A:1264:PHE:CE1	2.98	0.52
3:A:887:VAL:HG11	4:C:1:NAG:C8	2.29	0.52
3:A:898:ASN:OD1	3:A:923:ARG:HB2	2.10	0.52
3:B:460:ASP:H	3:B:520:LEU:HD23	1.75	0.51
3:A:446:ARG:NH2	3:A:679:ARG:HH22	2.09	0.51
3:B:1170:ARG:HD2	3:B:1170:ARG:H	1.76	0.51
3:A:971:ARG:N	3:A:1161:ARG:HB2	2.26	0.51
3:B:419:TYR:HD1	3:B:445:VAL:C	2.18	0.50
3:A:971:ARG:NH2	3:A:1235:ASN:O	2.44	0.50
3:B:1152:VAL:HG13	3:B:1152:VAL:O	2.12	0.50
3:B:923:ARG:CD	5:B:1402:NAG:H82	2.41	0.50
3:B:971:ARG:CG	3:B:971:ARG:NH1	2.67	0.50
1:G:18:MET:O	1:G:22:ARG:HG3	2.12	0.49
1:G:29:ARG:CD	2:H:18:TYR:HD2	2.18	0.49
3:A:626:TYR:N	3:A:626:TYR:CD2	2.78	0.49
3:A:438:ARG:HG2	3:A:539:CYS:O	2.12	0.49
3:B:742:ARG:O	3:B:742:ARG:HG2	2.12	0.49
3:A:887:VAL:HG21	4:C:1:NAG:C8	2.42	0.49
3:A:1205:ASP:C	3:A:1285:ALA:HB3	2.37	0.49
3:A:590:ARG:HG2	3:A:591:CYS:N	2.28	0.49
3:A:1157:ARG:HH21	3:A:1234:PRO:HG2	1.77	0.49
3:A:442:ARG:NH1	3:A:442:ARG:HB3	2.28	0.49
3:B:457:ARG:HH11	3:B:485:ARG:HB2	1.76	0.49
3:A:412:GLY:O	3:A:442:ARG:NH1	2.45	0.49
3:B:419:TYR:HH	3:B:474:VAL:HB	1.77	0.49
3:B:904:ARG:HD2	3:B:906:MET:CE	2.42	0.49
3:B:904:ARG:HD2	3:B:906:MET:HE1	1.94	0.49
3:B:971:ARG:HH11	3:B:1236:GLY:HA2	1.78	0.49
3:A:946:ASN:OD1	3:A:1151:PHE:O	2.31	0.48
1:E:9:GLU:CD	3:B:345:ARG:HH22	2.20	0.48
3:A:929:PRO:HA	3:A:956:TYR:CD1	2.48	0.48
3:B:1161:ARG:HA	3:B:1197:THR:HG22	1.96	0.48
3:A:564:CYS:HB3	3:A:576:CYS:SG	2.54	0.47
3:A:419:TYR:CE2	3:A:446:ARG:HD3	2.49	0.47
3:A:386:THR:HG22	3:A:411:ARG:HD3	1.95	0.47
3:A:387:ASP:HB3	3:A:388:TYR:CD2	2.50	0.47
3:A:644:ASP:H	3:A:665:THR:HG21	1.79	0.47
3:A:659:ARG:HG2	3:A:691:TYR:CE2	2.49	0.46
3:B:659:ARG:NH1	3:B:691:TYR:CZ	2.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:923:ARG:CD	5:B:1402:NAG:C8	2.92	0.46
3:A:971:ARG:HB3	3:A:1161:ARG:CD	2.45	0.46
3:A:1228:TRP:CD2	3:A:1264:PHE:CE1	3.04	0.46
3:A:1243:VAL:HG22	3:A:1283:VAL:HG13	1.98	0.46
3:A:330:MET:HE3	3:A:547:SER:HG	1.79	0.46
3:A:578:ASP:C	5:A:1409:NAG:H82	2.36	0.46
3:A:887:VAL:CG1	4:C:1:NAG:H82	2.32	0.46
3:B:923:ARG:HD3	5:B:1402:NAG:C8	2.46	0.45
3:A:419:TYR:CE2	3:B:1035:PHE:CZ	3.04	0.45
3:B:363:PHE:HB2	3:B:388:TYR:O	2.17	0.45
3:A:733:LYS:HB3	3:A:734:TYR:CE2	2.51	0.45
3:A:948:THR:CG2	5:A:1404:NAG:H62	2.47	0.45
3:A:1205:ASP:O	3:A:1285:ALA:HB3	2.17	0.45
3:A:1159:PHE:CD2	3:A:1289:ALA:HA	2.51	0.45
3:A:1191:TYR:CD2	3:A:1191:TYR:N	2.79	0.45
3:A:902:TYR:HE2	3:A:904:ARG:HE	1.64	0.45
3:B:1245:TYR:CD2	3:B:1255:GLU:HB2	2.51	0.45
2:H:11:LEU:HD23	2:H:11:LEU:C	2.42	0.45
3:A:419:TYR:HE2	3:B:1035:PHE:CZ	2.35	0.45
3:B:411:ARG:NH2	3:B:568:ARG:O	2.50	0.45
3:B:971:ARG:NH2	3:B:1159:PHE:O	2.37	0.44
3:A:931:LYS:HA	3:A:1189:SER:HB2	1.99	0.44
4:C:1:NAG:H61	4:C:2:NAG:N2	2.33	0.44
3:A:949:TRP:CZ2	3:A:1149:THR:HA	2.53	0.44
3:B:411:ARG:HD3	3:B:551:LEU:HD12	1.98	0.44
3:A:438:ARG:NH2	3:A:540:ILE:O	2.51	0.44
3:A:442:ARG:NH1	3:A:442:ARG:CB	2.81	0.44
3:B:954:LYS:HB3	3:B:956:TYR:CE1	2.53	0.44
3:A:419:TYR:OH	3:A:679:ARG:NH2	2.26	0.44
3:A:462:LEU:O	3:A:536:ARG:HD2	2.17	0.44
3:A:1170:ARG:CD	3:A:1170:ARG:C	2.91	0.44
3:B:364:LEU:O	3:B:390:ILE:HB	2.19	0.43
3:A:806:THR:HG23	3:A:915:ALA:HA	2.00	0.43
3:B:453:LEU:HD13	3:B:455:TYR:CD2	2.53	0.43
3:B:410:ILE:HD12	3:B:440:ILE:HG23	2.00	0.43
3:A:568:ARG:HG2	3:A:569:ASN:H	1.84	0.43
3:B:659:ARG:NH1	3:B:691:TYR:CE2	2.87	0.43
4:C:1:NAG:H61	4:C:2:NAG:H82	2.00	0.43
3:B:363:PHE:CG	3:B:388:TYR:CE1	3.06	0.43
3:B:888:MET:CE	3:B:888:MET:CA	2.89	0.43
3:A:521:CYS:HA	3:A:527:CYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1208:MET:SD	3:A:1229:THR:HG23	2.59	0.43
3:A:943:SER:HB3	3:A:1155:LYS:HA	2.01	0.43
3:A:1203:PHE:H	3:A:1206:ILE:HD12	1.84	0.43
2:H:18:TYR:HA	3:A:345:ARG:CZ	2.49	0.42
3:B:949:TRP:CD1	3:B:962:TYR:CD1	3.07	0.42
3:B:587:PHE:O	3:B:602:LYS:HE2	2.19	0.42
3:A:1228:TRP:CD1	3:A:1228:TRP:C	2.97	0.42
3:A:954:LYS:HE2	3:A:956:TYR:CZ	2.55	0.42
3:A:1212:VAL:HG22	3:A:1226:VAL:HA	2.01	0.42
3:B:963:PHE:CZ	3:B:1141:ALA:HB1	2.54	0.42
3:A:572:PHE:HE1	3:A:590:ARG:CZ	2.33	0.42
3:A:408:SER:HA	3:A:437:LEU:HA	2.01	0.42
3:A:572:PHE:HA	3:A:590:ARG:HG3	2.02	0.42
3:A:587:PHE:CG	3:A:588:ASP:N	2.87	0.42
3:A:733:LYS:HB3	3:A:734:TYR:CD2	2.55	0.41
2:H:19:ASN:H	3:A:345:ARG:HG3	1.85	0.41
3:A:572:PHE:HE1	3:A:590:ARG:NH2	2.18	0.41
3:B:375:LEU:HD12	3:B:377:ARG:HG2	2.02	0.41
1:E:21:LEU:HA	1:E:24:TYR:CE2	2.56	0.41
3:A:949:TRP:CZ2	3:A:1144:LEU:HD13	2.55	0.41
3:A:1245:TYR:HB2	3:A:1281:PHE:CE2	2.56	0.41
3:A:764:HIS:CG	3:B:800:ASN:HD21	2.39	0.41
3:A:971:ARG:HH21	3:A:1237:GLU:N	2.19	0.41
3:A:1146:PRO:O	3:A:1147:ASN:OD1	2.38	0.41
3:A:1159:PHE:CD2	3:A:1199:LYS:HA	2.55	0.41
3:B:1159:PHE:CZ	3:B:1197:THR:HG21	2.56	0.41
3:B:515:HIS:NE2	3:B:530:LYS:HE3	2.36	0.41
3:B:522:TRP:CE2	3:B:528:GLN:HA	2.56	0.41
3:B:971:ARG:NH1	3:B:1236:GLY:HA2	2.36	0.41
3:A:709:TYR:N	3:A:709:TYR:CD2	2.88	0.40
3:B:1191:TYR:CD1	3:B:1191:TYR:C	2.99	0.40
3:A:971:ARG:NH1	3:A:1288:ILE:CB	2.84	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	E	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	G	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
2	F	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
2	H	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
3	A	815/1048 (78%)	695 (85%)	120 (15%)	0	100	100
3	B	845/1048 (81%)	714 (84%)	131 (16%)	0	100	100
All	All	1752/2196 (80%)	1486 (85%)	266 (15%)	0	100	100

There are no Ramachandran outliers to report.

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	E	24/24 (100%)	24 (100%)	0	100	100
1	G	24/24 (100%)	20 (83%)	4 (17%)	2	10
2	F	24/24 (100%)	23 (96%)	1 (4%)	26	48
2	H	24/24 (100%)	23 (96%)	1 (4%)	26	48
3	A	744/936 (80%)	713 (96%)	31 (4%)	26	48
3	B	772/936 (82%)	745 (96%)	27 (4%)	32	53
All	All	1612/1968 (82%)	1548 (96%)	64 (4%)	29	49

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	19	ASN
1	G	8	VAL
1	G	12	CYS

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Mol	Chain	Res	Type
1	G	19	LYS
1	G	30	ASN
2	H	9	GLU
3	A	328	PRO
3	A	382	LEU
3	A	395	THR
3	A	397	LEU
3	A	404	PHE
3	A	408	SER
3	A	438	ARG
3	A	468	ASN
3	A	473	VAL
3	A	478	ASN
3	A	529	THR
3	A	538	ASN
3	A	574	ASN
3	A	587	PHE
3	A	606	ASN
3	A	608	VAL
3	A	629	SER
3	A	679	ARG
3	A	726	ASP
3	A	736	LEU
3	A	741	ASN
3	A	768	LYS
3	A	844	PHE
3	A	887	VAL
3	A	971	ARG
3	A	1170	ARG
3	A	1191	TYR
3	A	1196	GLN
3	A	1229	THR
3	A	1286	ASN
3	A	1297	VAL
3	B	387	ASP
3	B	409	VAL
3	B	449	LYS
3	B	524	SER
3	B	540	ILE
3	B	567	CYS
3	B	570	VAL
3	B	572	PHE

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Mol	Chain	Res	Type
3	B	573	ASN
3	B	685	VAL
3	B	792	ASP
3	B	797	SER
3	B	848	ARG
3	B	859	ILE
3	B	877	TRP
3	B	887	VAL
3	B	888	MET
3	B	924	THR
3	B	971	ARG
3	B	1128	GLU
3	B	1160	THR
3	B	1170	ARG
3	B	1224	VAL
3	B	1241	TYR
3	B	1283	VAL
3	B	1294	PHE
3	B	1298	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	ASN
2	F	19	ASN
3	A	346	ASN
3	A	413	ASN
3	A	513	GLN
3	A	627	GLN
3	A	776	GLN
3	A	857	HIS
3	A	892	ASN
3	A	1148	GLN
3	A	1150	HIS
3	A	1252	GLN
3	A	1286	ASN
3	B	370	ASN
3	B	376	ASN
3	B	426	ASN
3	B	471	GLN
3	B	513	GLN
3	B	543	HIS

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Mol	Chain	Res	Type
3	B	606	ASN
3	B	766	ASN
3	B	798	ASN
3	B	1037	ASN
3	B	1265	ASN
3	B	1286	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1	4,3	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	C	2	4	14,14,15	0.40	0	17,19,21	2.38	4 (23%)

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	NAG	C	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	2	NAG	O5-C5-C6	8.38	120.35	107.20
4	C	2	NAG	C4-C3-C2	2.73	115.01	111.02
4	C	2	NAG	O3-C3-C4	2.51	116.15	110.35
4	C	2	NAG	O4-C4-C5	2.05	114.38	109.30

There are no chirality outliers.

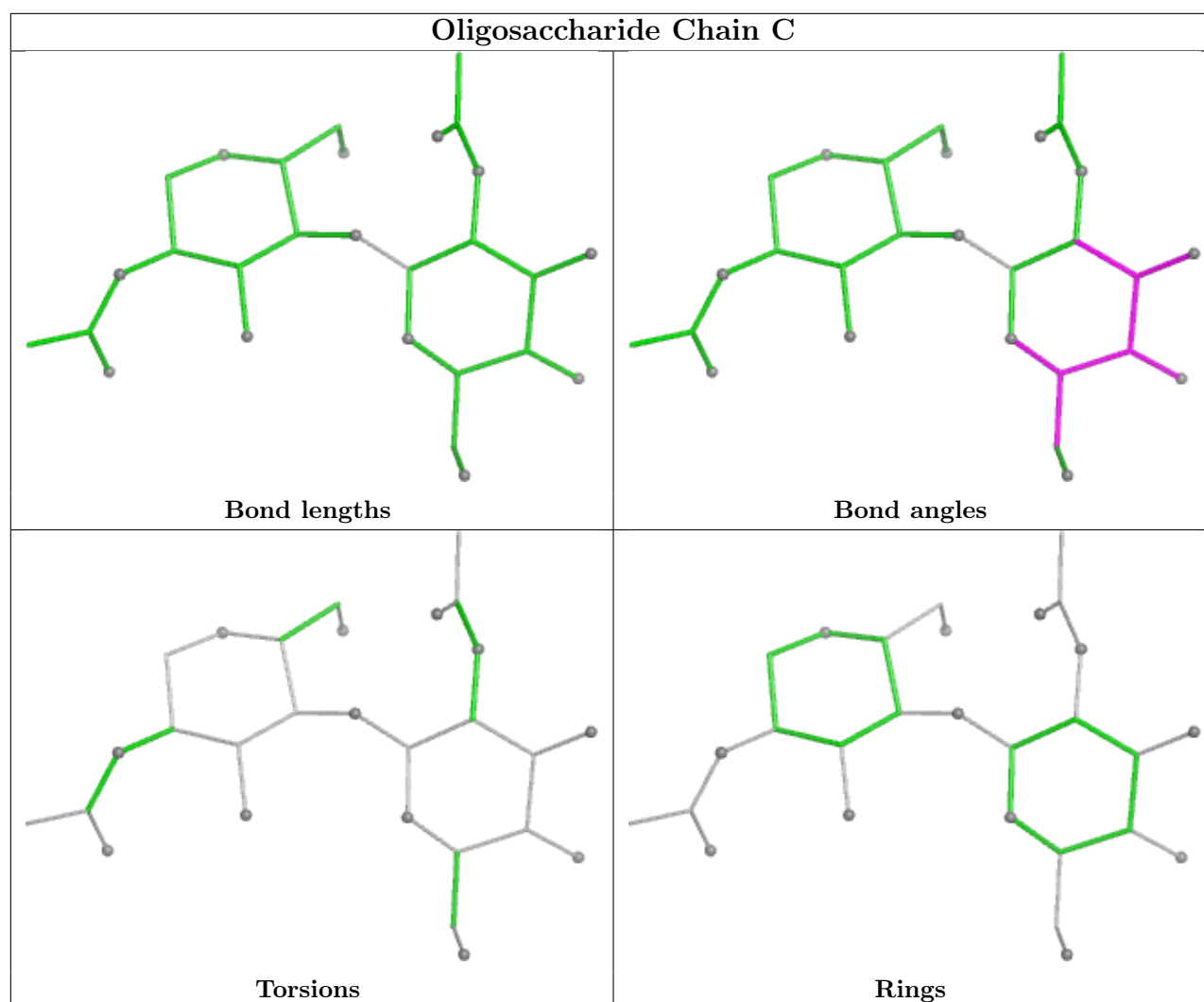
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	8	0
4	C	2	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
5	NAG	B	1406	3	14,14,15	0.40	0	17,19,21	0.81	0
5	NAG	A	1405	3	14,14,15	0.40	0	17,19,21	0.81	0
5	NAG	B	1408	3	14,14,15	0.40	0	17,19,21	0.82	0
5	NAG	B	1402	3	14,14,15	0.41	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1405	3	14,14,15	0.39	0	17,19,21	0.81	0
5	NAG	A	1401	3	14,14,15	0.26	0	17,19,21	0.79	1 (5%)
5	NAG	B	1403	3	14,14,15	0.41	0	17,19,21	0.82	0
5	NAG	A	1402	3	14,14,15	0.40	0	17,19,21	0.81	0
5	NAG	A	1404	3	14,14,15	0.40	0	17,19,21	0.81	0
5	NAG	A	1407	3	14,14,15	0.40	0	17,19,21	0.82	0
5	NAG	A	1409	3	14,14,15	0.40	0	17,19,21	0.82	0
5	NAG	B	1401	3	14,14,15	0.41	0	17,19,21	0.81	0
5	NAG	A	1403	3	14,14,15	0.41	0	17,19,21	0.81	0
5	NAG	A	1406	3	14,14,15	0.40	0	17,19,21	0.82	0
5	NAG	B	1404	3	14,14,15	0.40	0	17,19,21	0.81	0
5	NAG	B	1407	3	14,14,15	0.41	0	17,19,21	0.82	0
5	NAG	A	1408	3	14,14,15	0.41	0	17,19,21	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1406	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1401	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1408	3	-	0/6/23/26	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	A	1401	NAG	C4-C3-C2	-2.06	108.00	111.02

There are no chirality outliers.

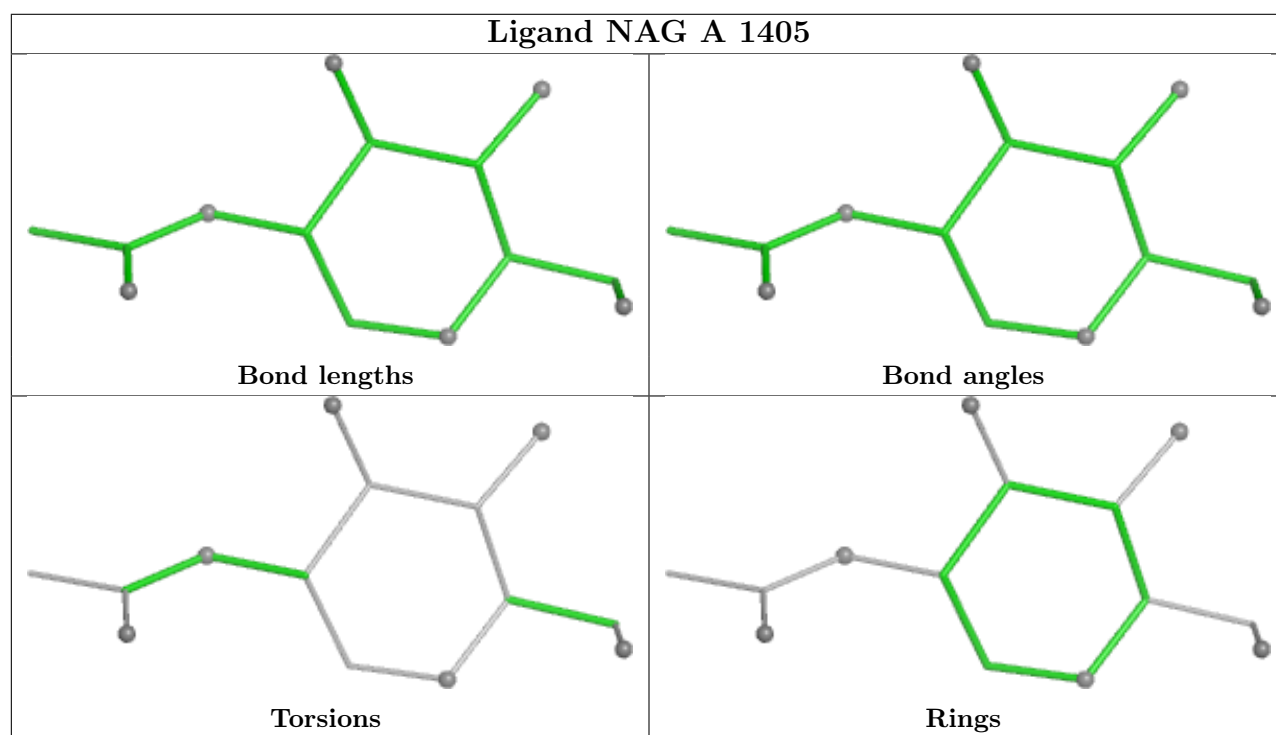
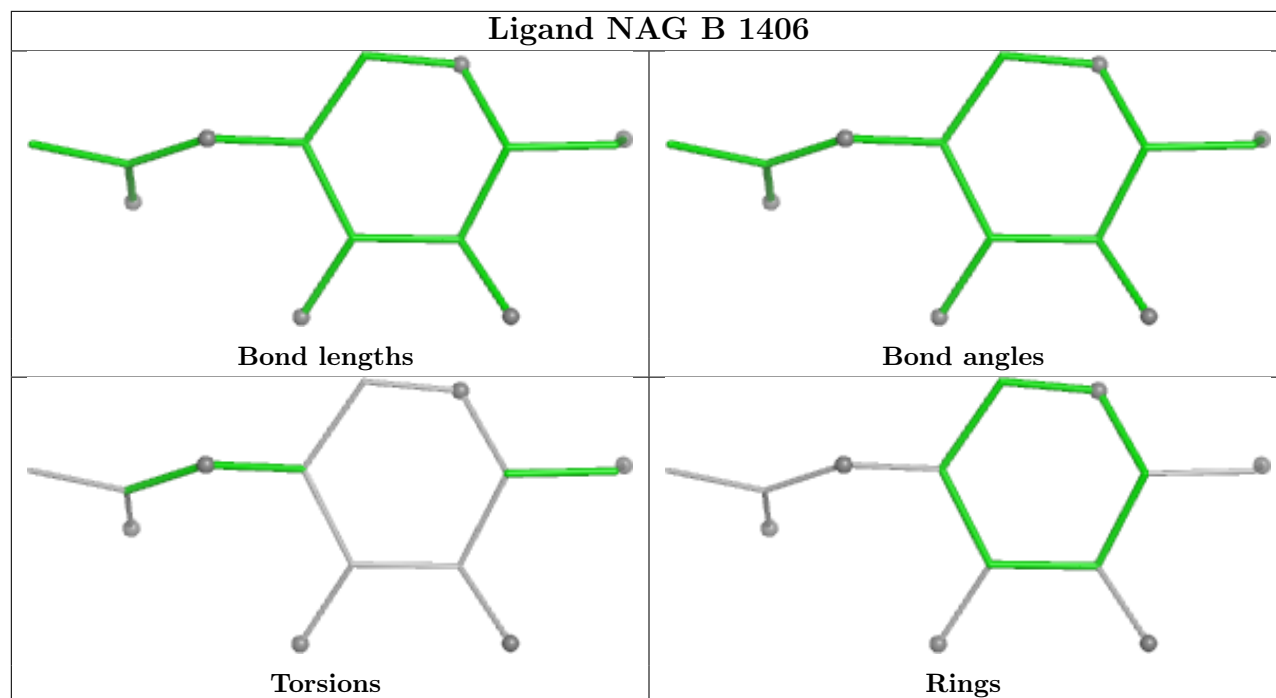
There are no torsion outliers.

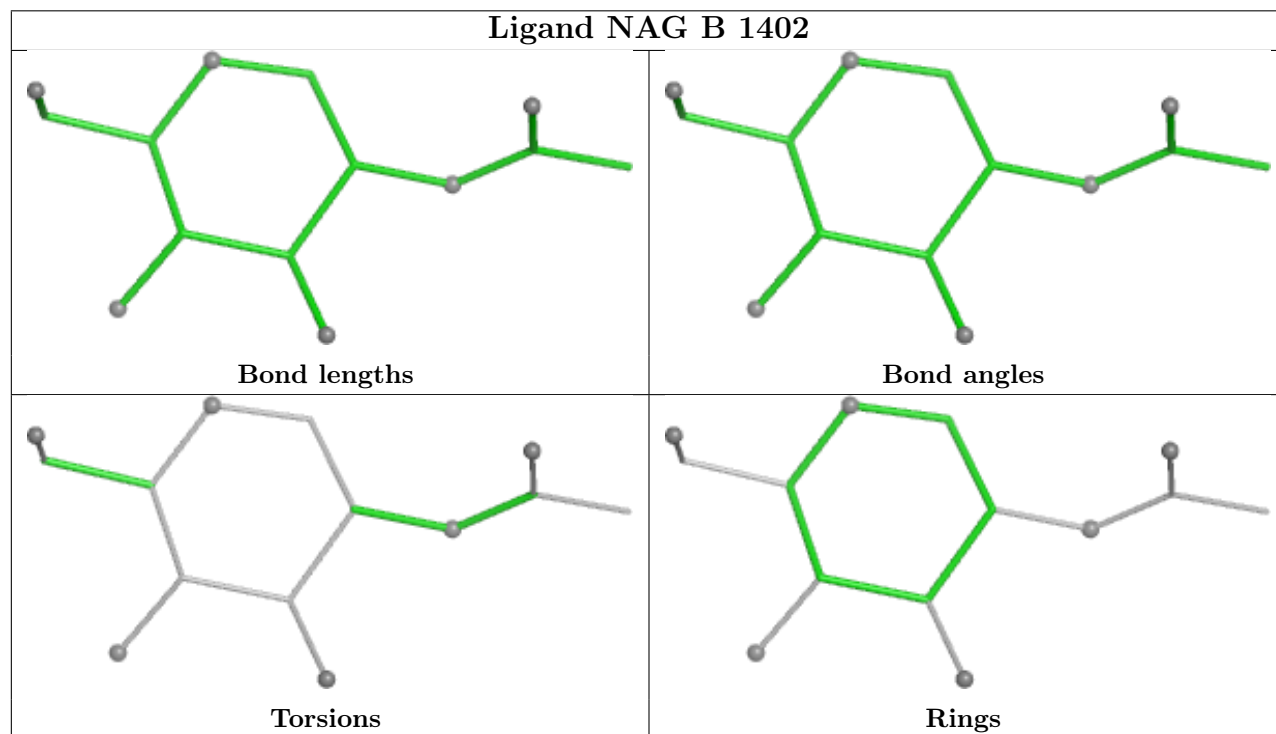
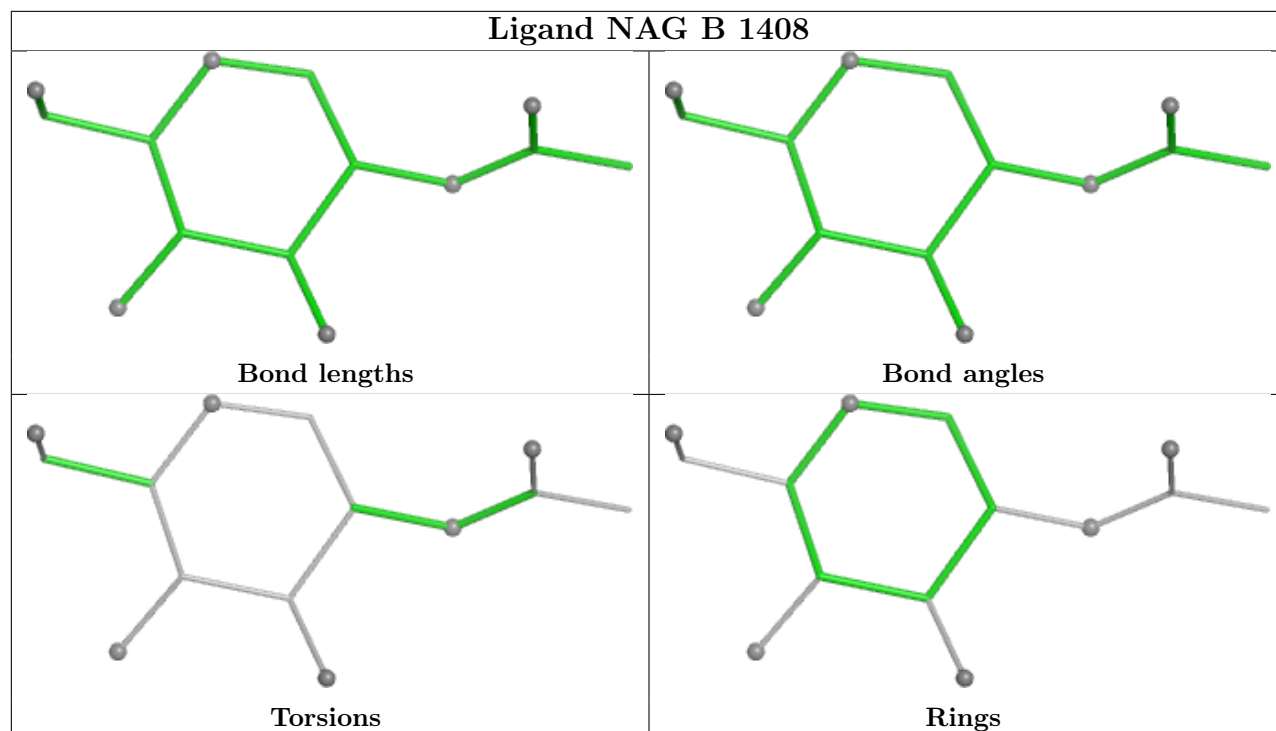
There are no ring outliers.

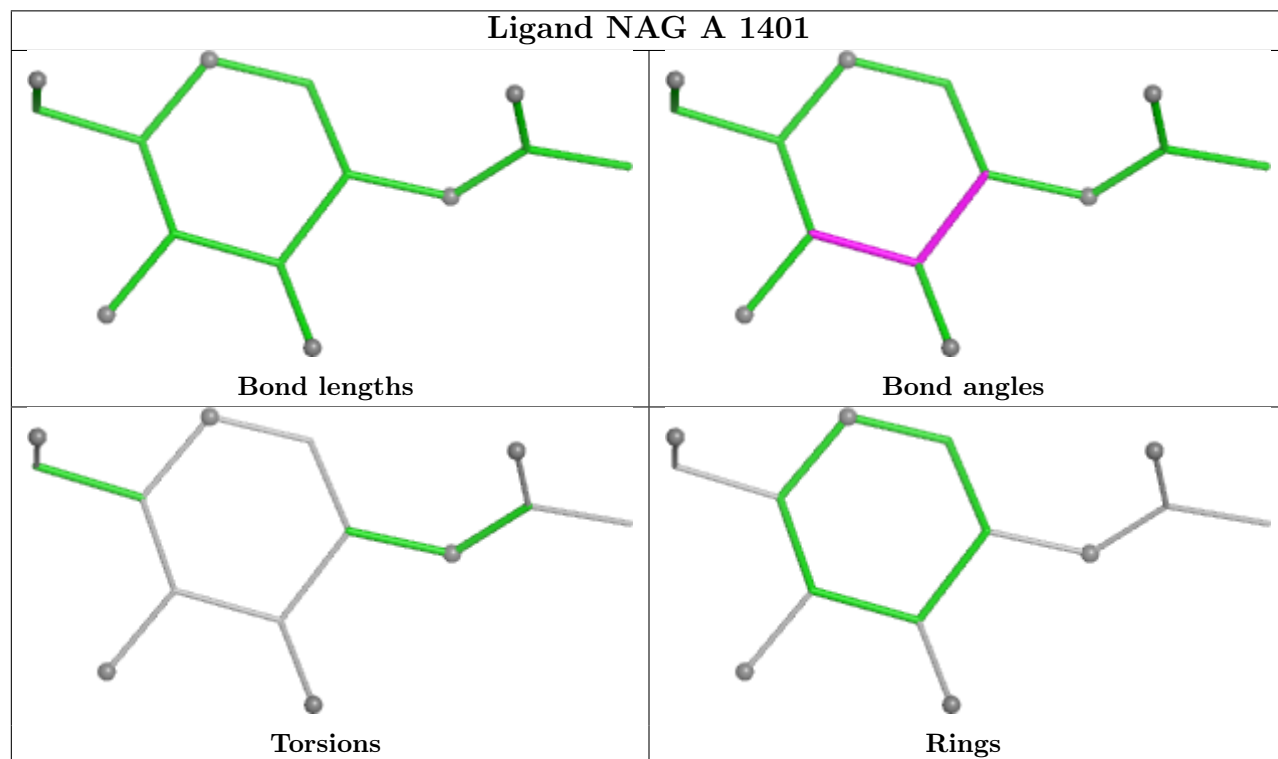
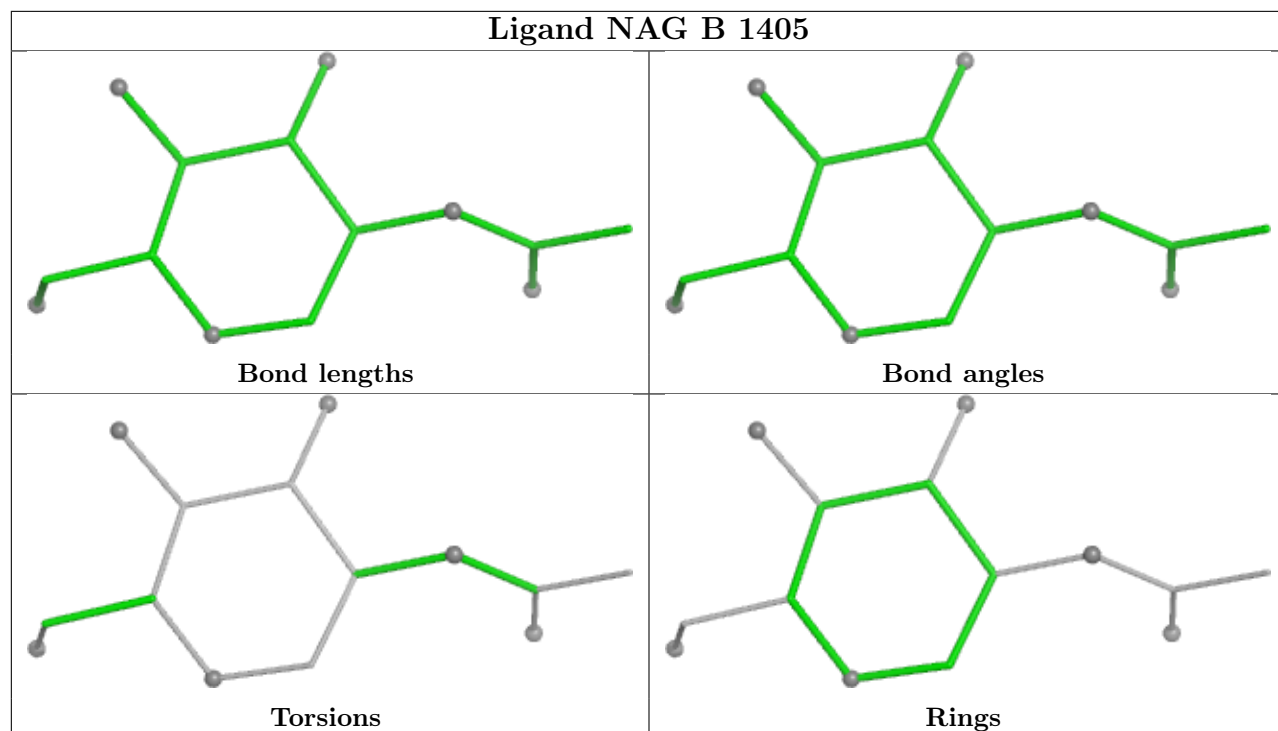
5 monomers are involved in 15 short contacts:

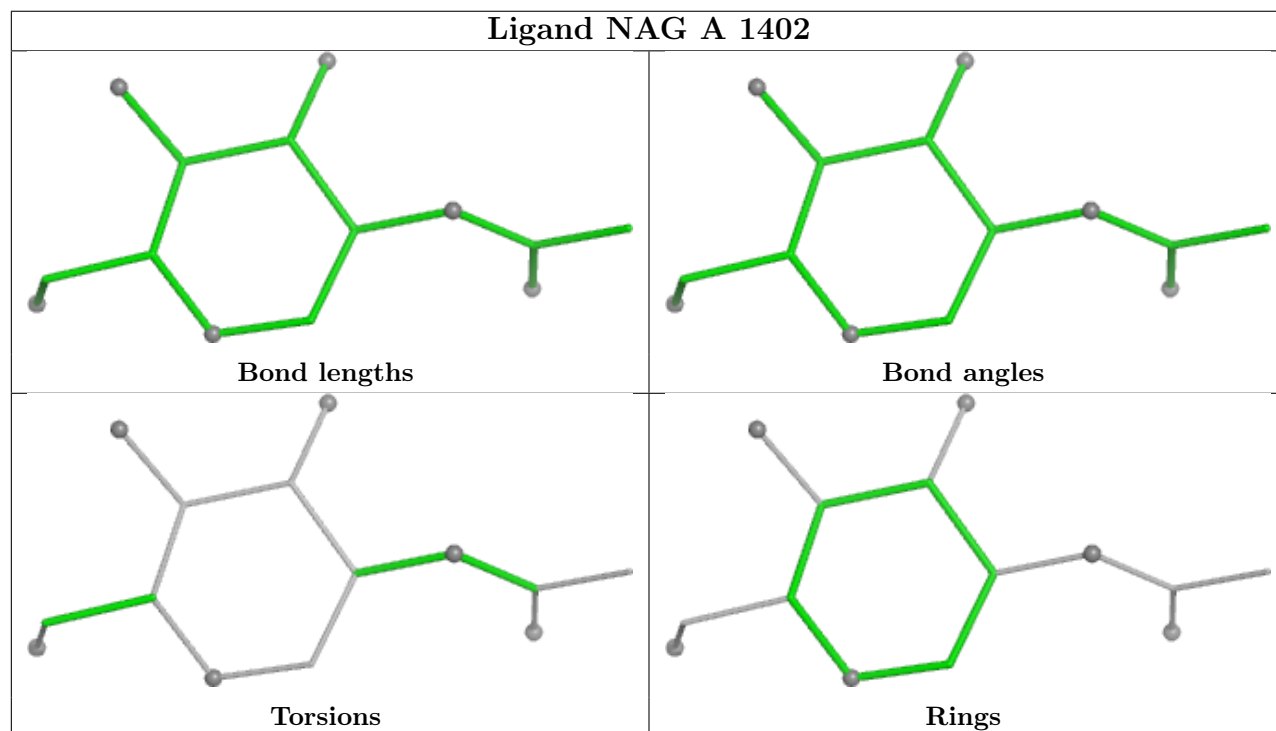
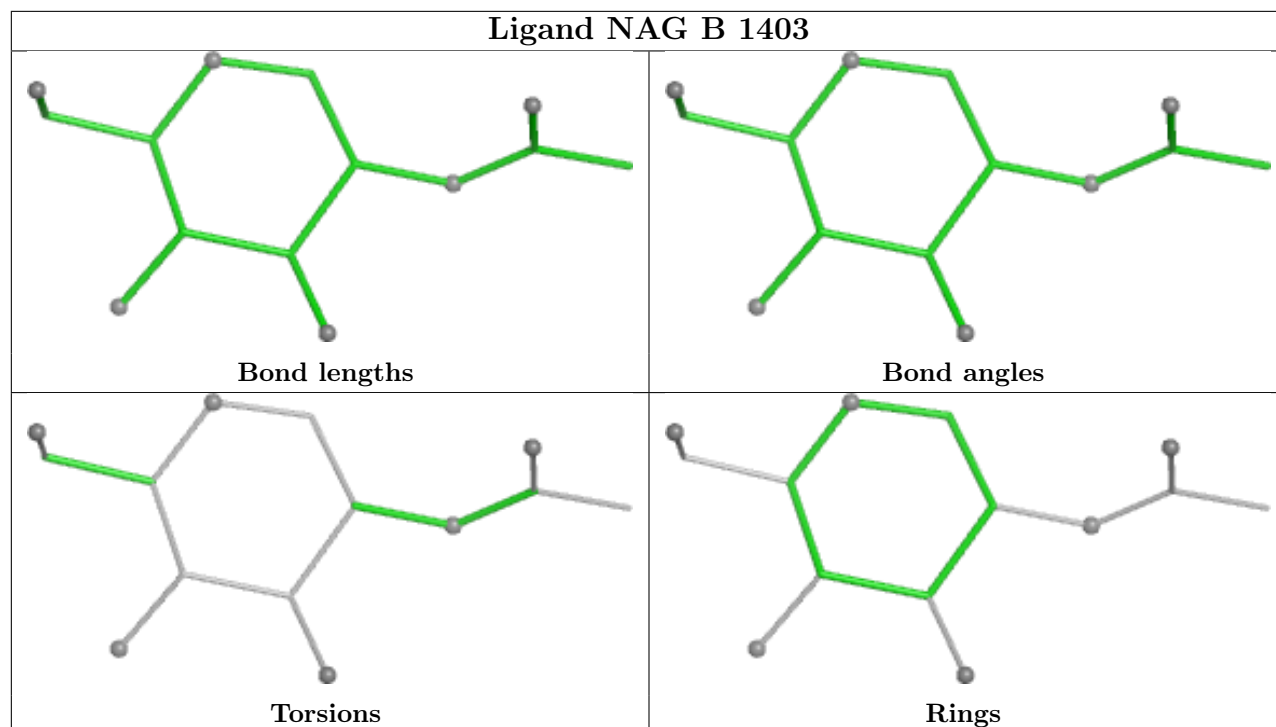
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1402	NAG	7	0
5	A	1401	NAG	1	0
5	A	1404	NAG	2	0
5	A	1409	NAG	2	0
5	B	1404	NAG	3	0

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.

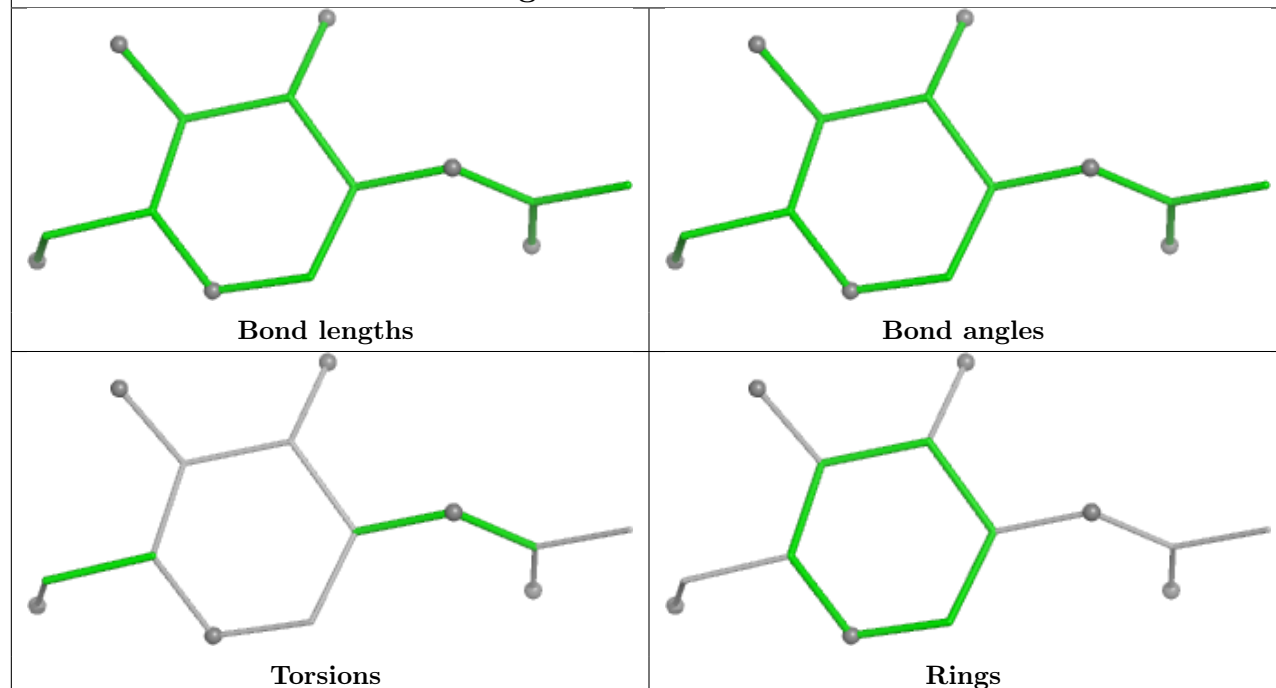




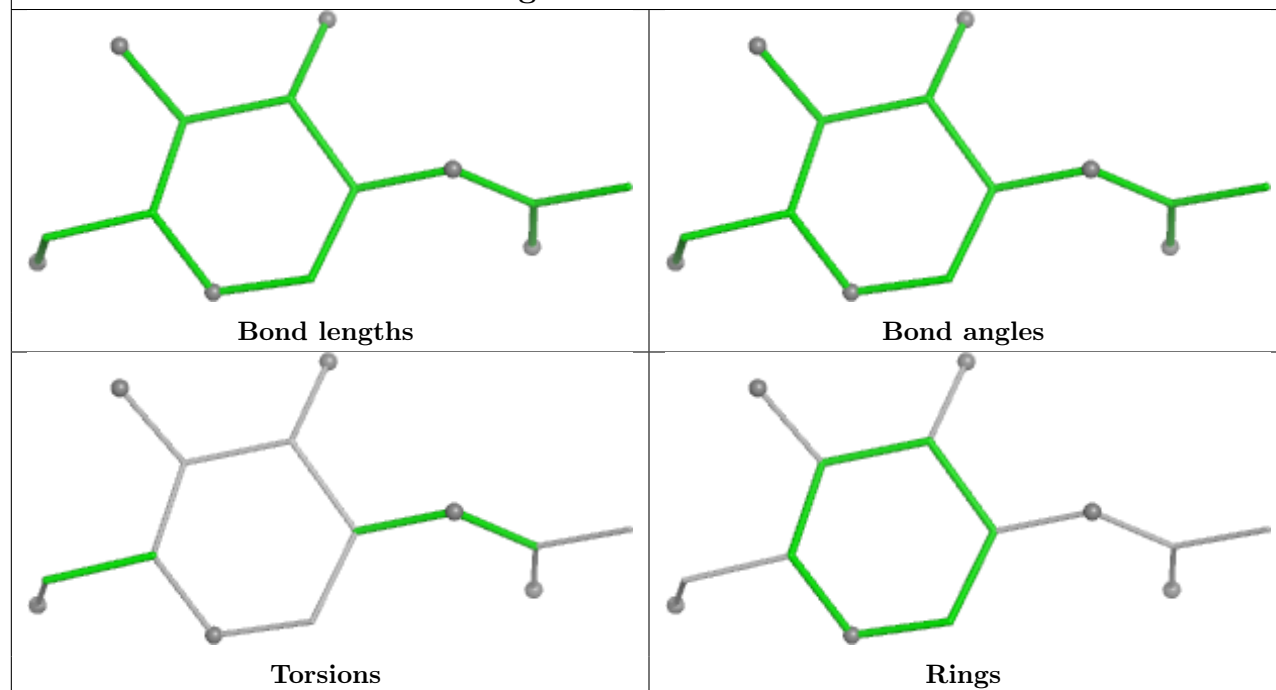


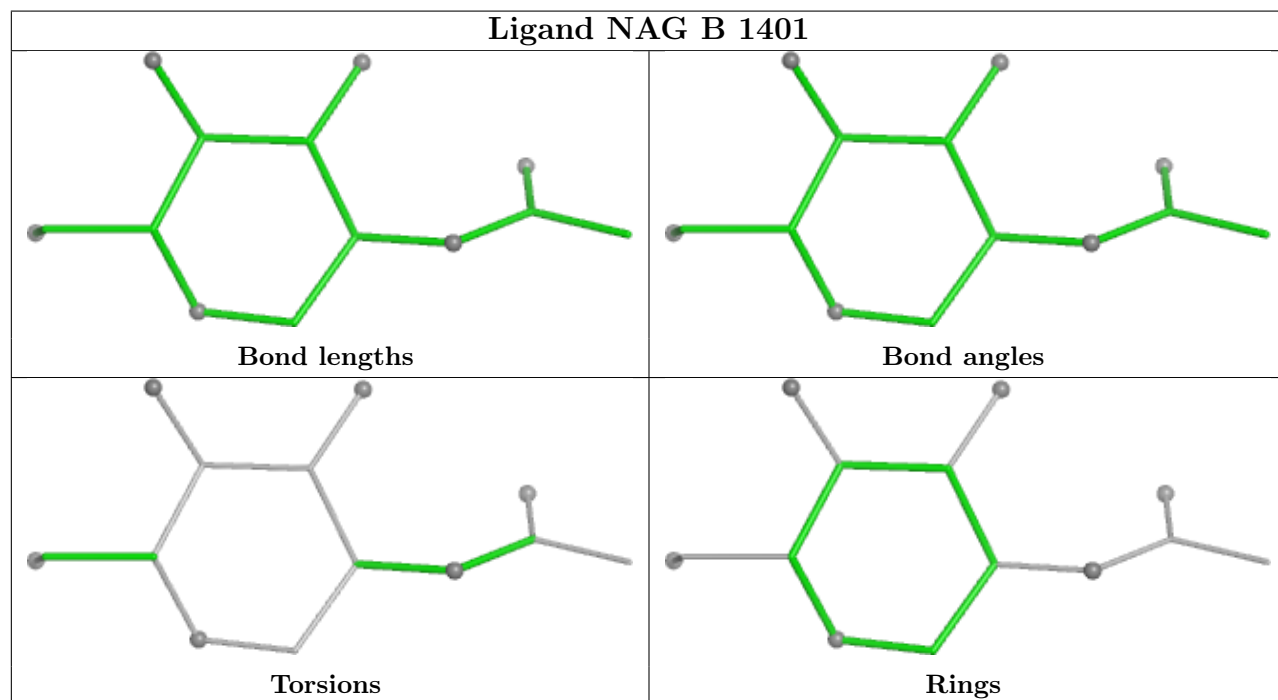
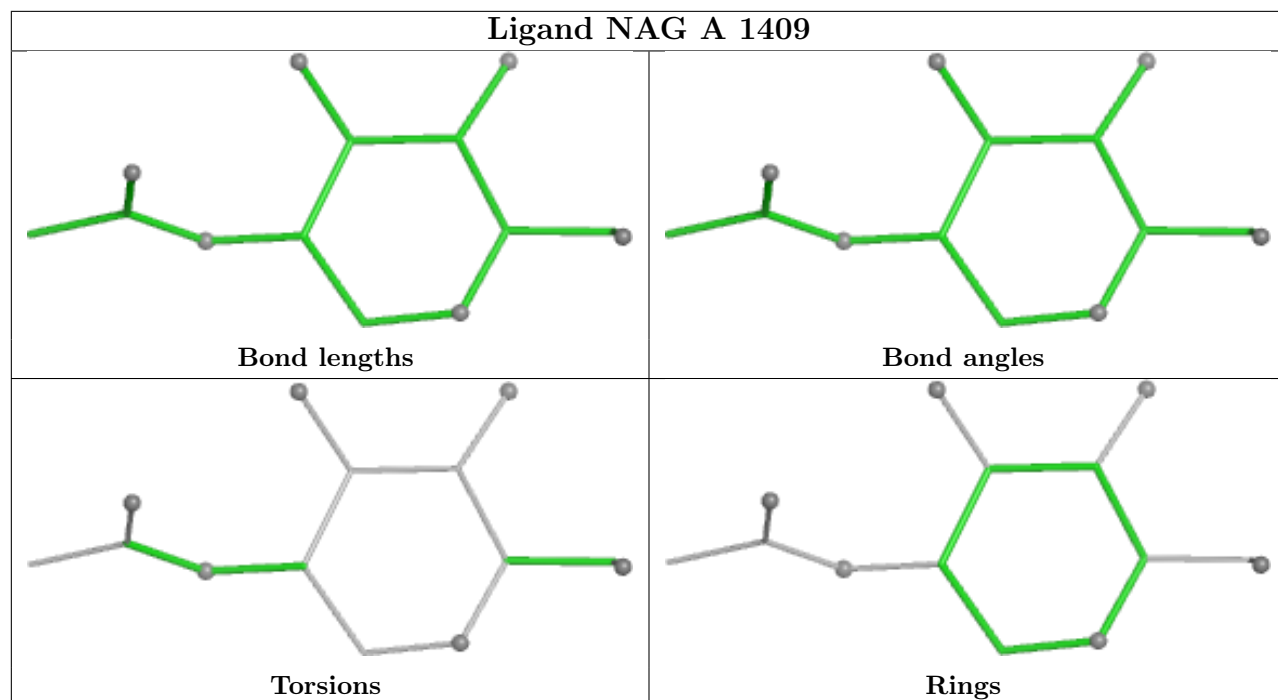


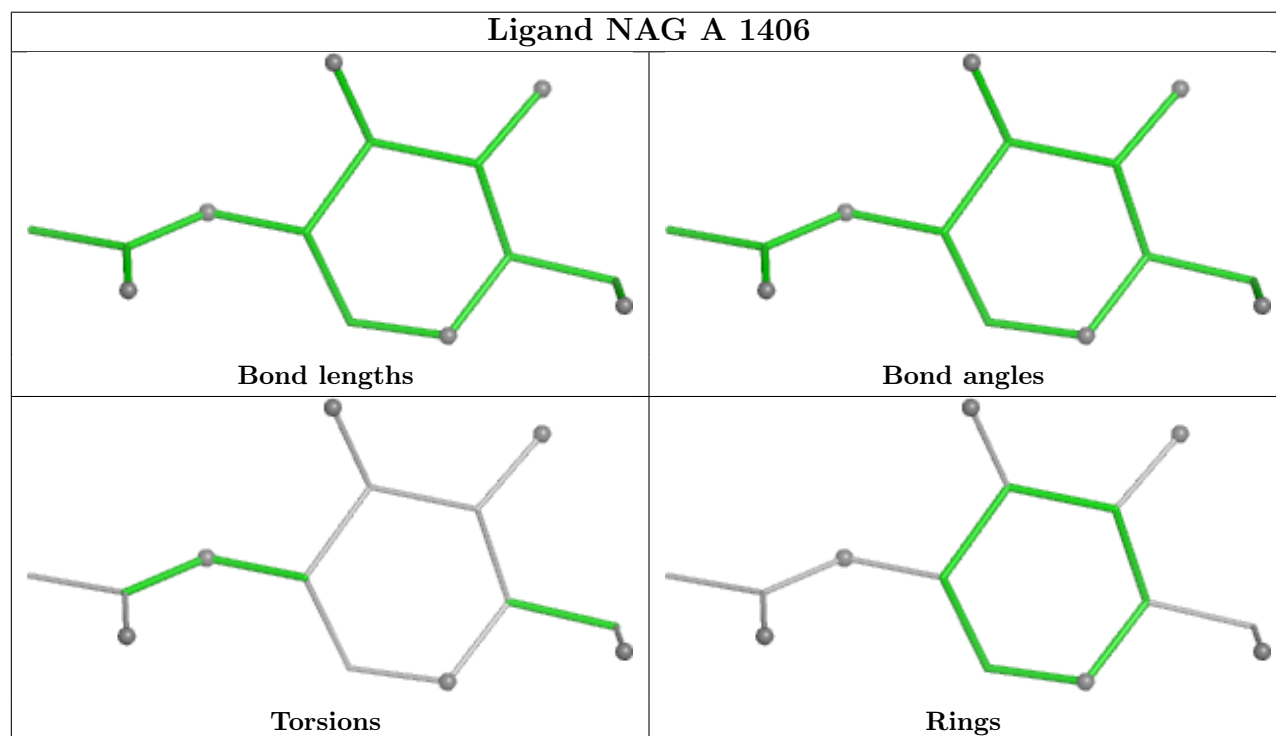
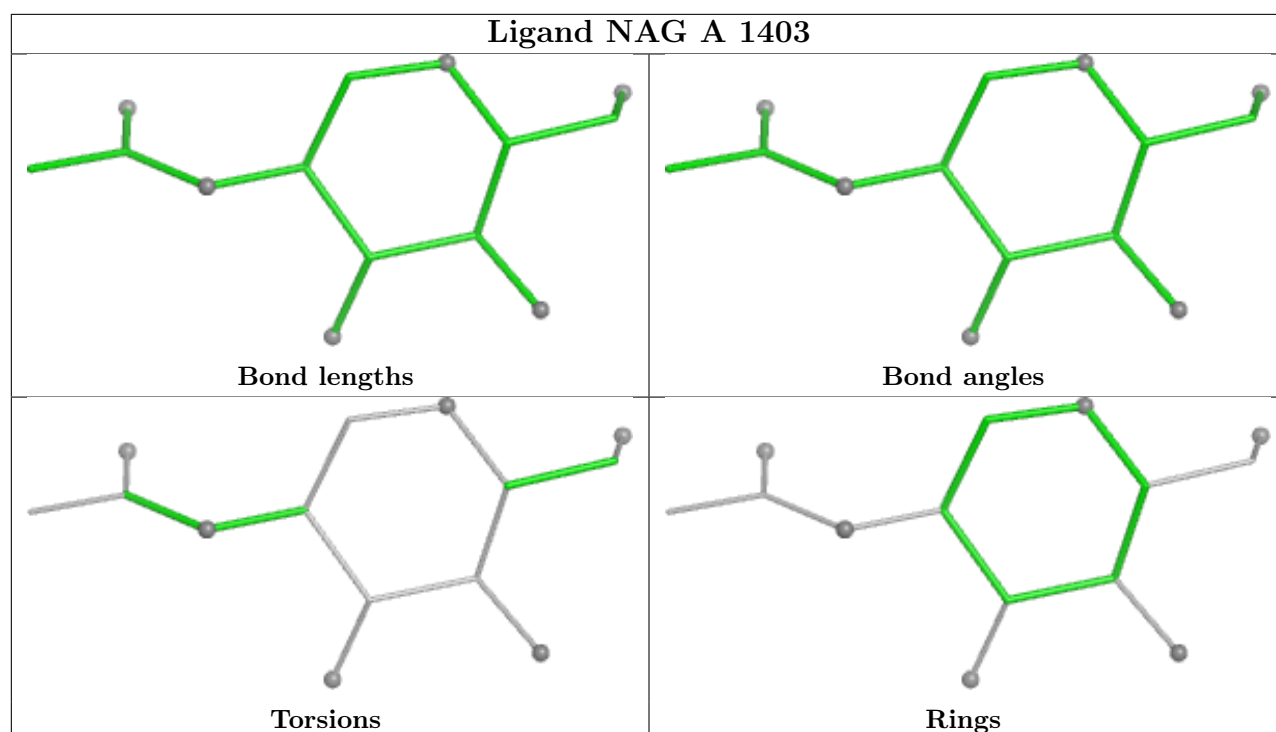
Ligand NAG A 1404

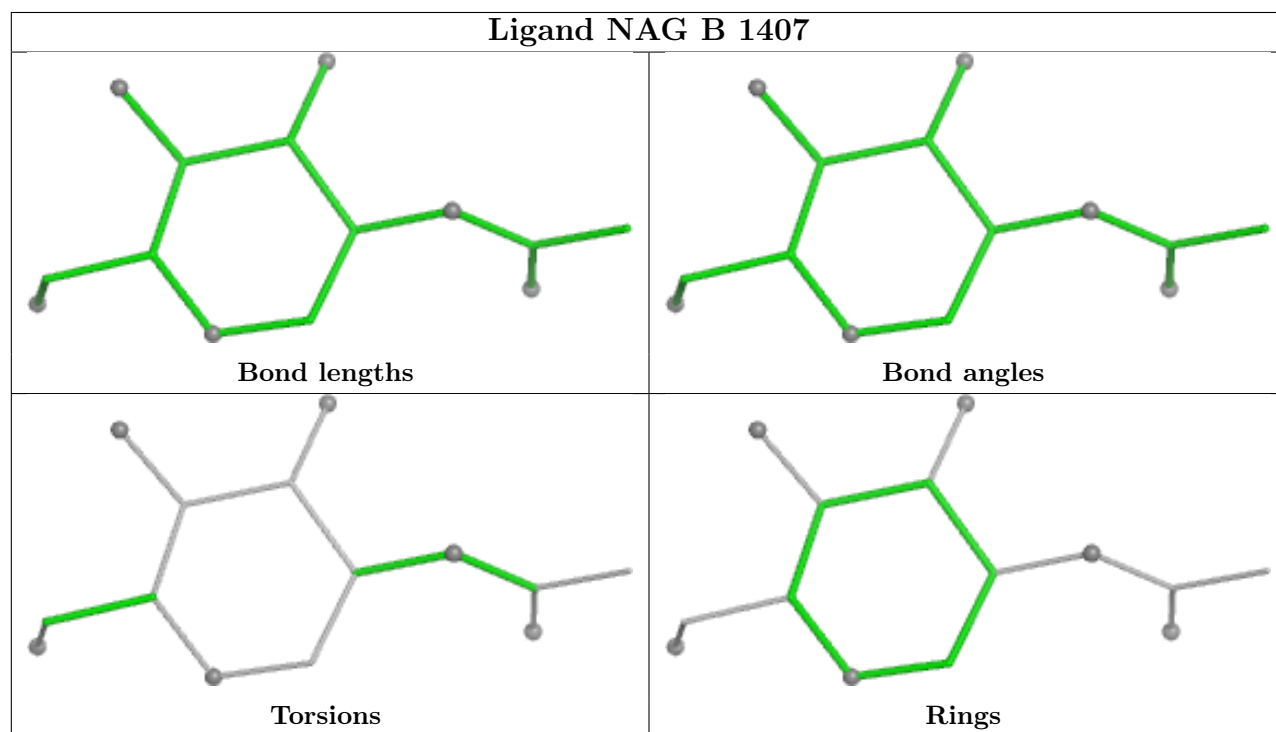
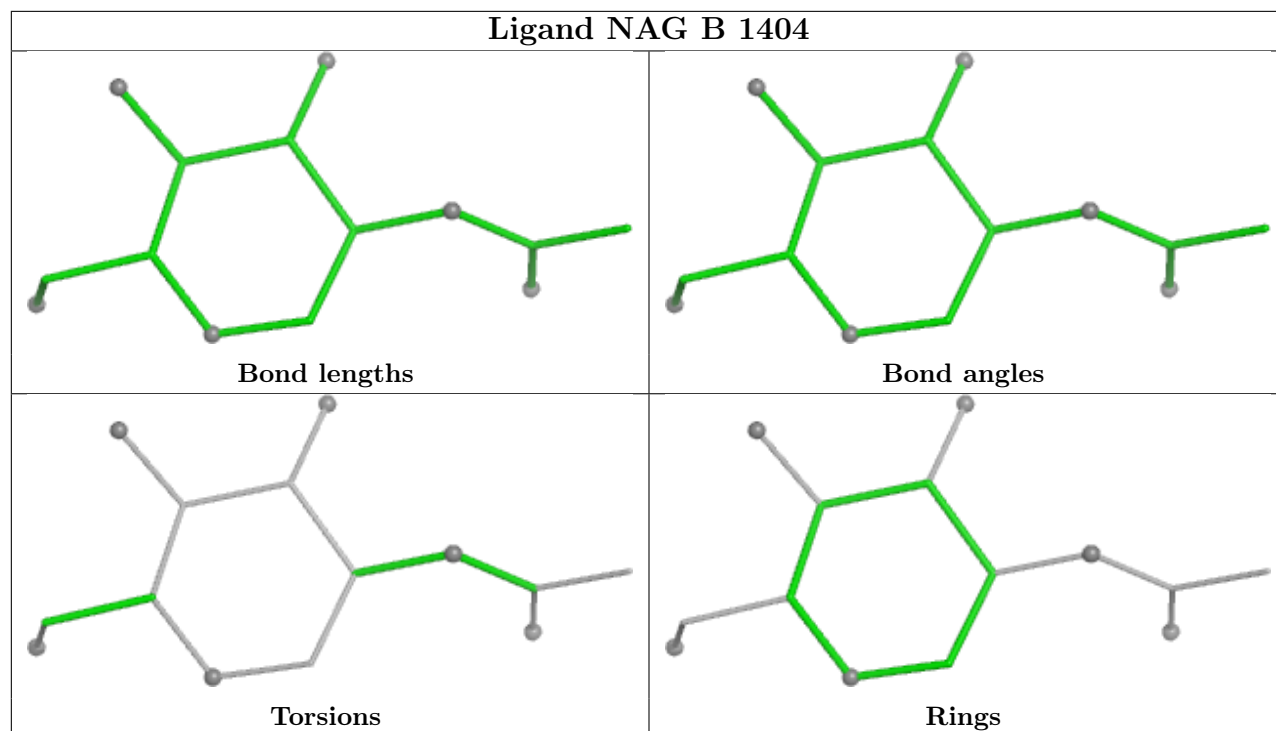


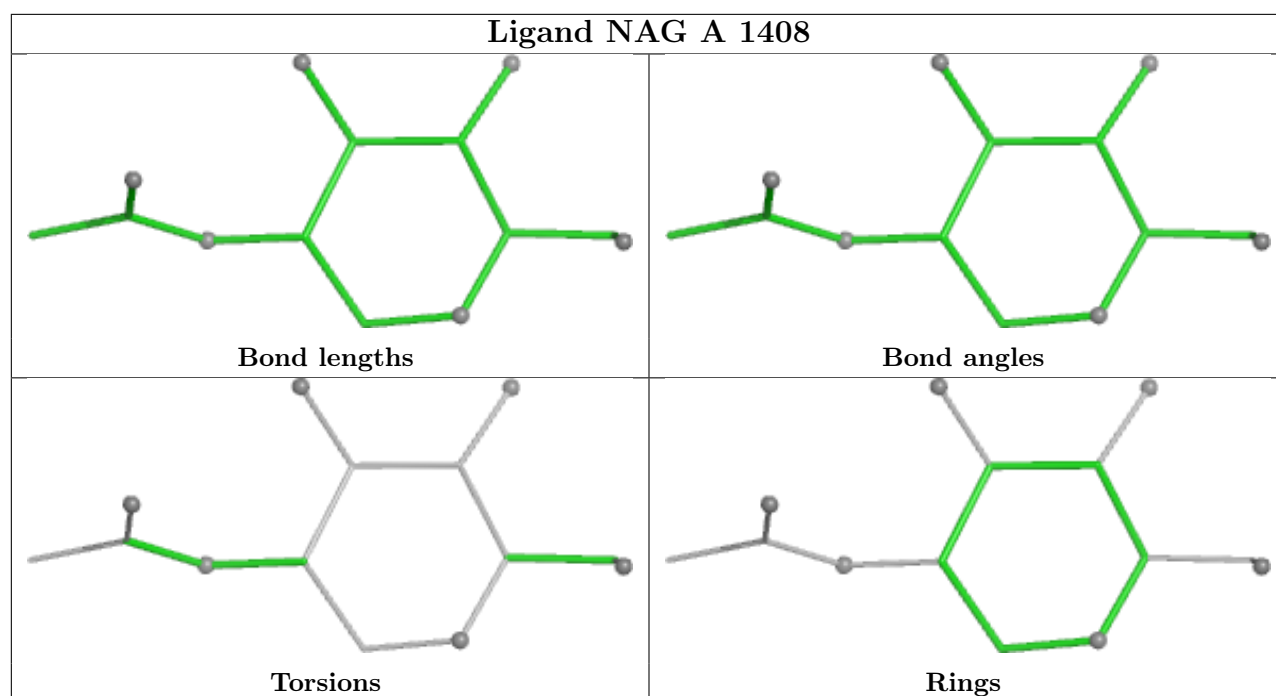
Ligand NAG A 1407











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-52310. These allow visual inspection of the internal detail of the map and identification of artifacts.

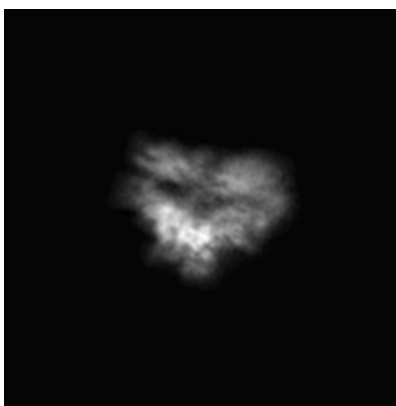
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

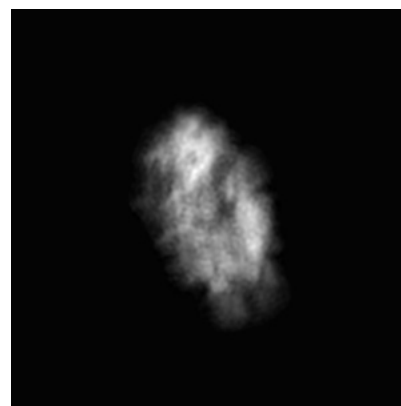
6.1.1 Primary map



X

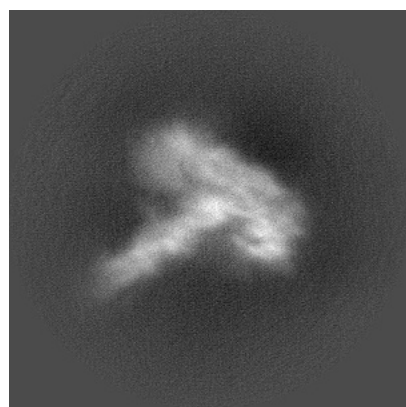


Y

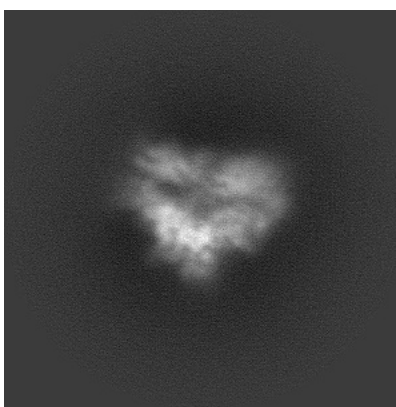


Z

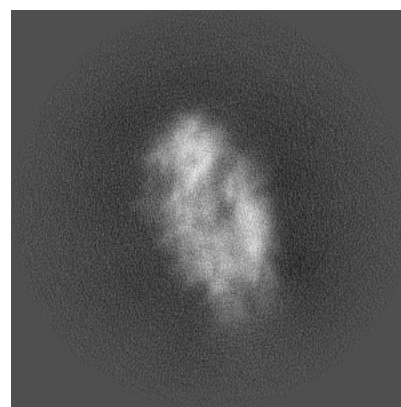
6.1.2 Raw map



X



Y

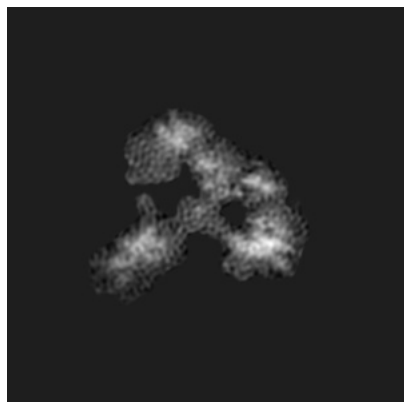


Z

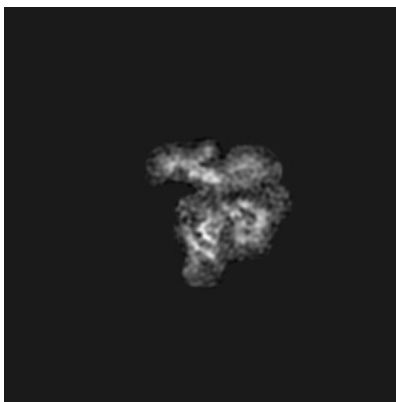
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

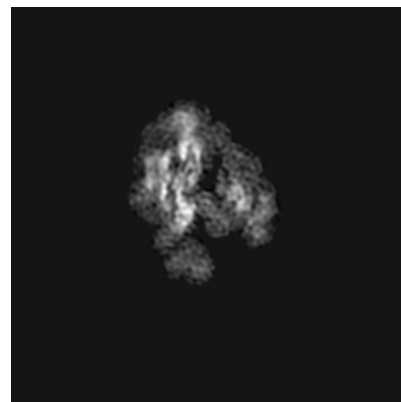
6.2.1 Primary map



X Index: 256

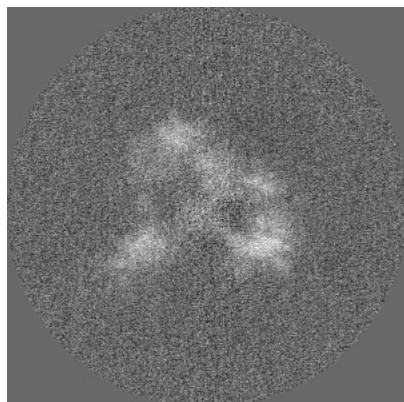


Y Index: 256

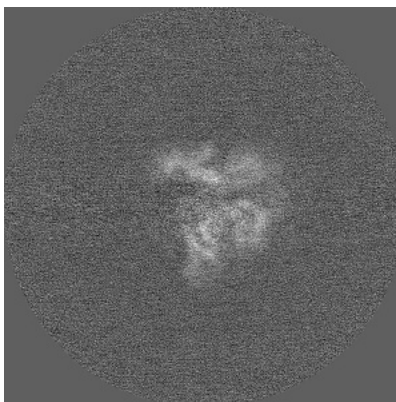


Z Index: 256

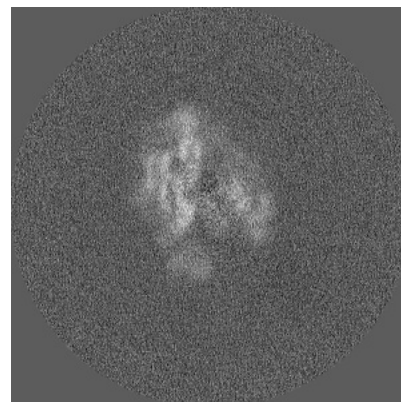
6.2.2 Raw map



X Index: 256



Y Index: 256

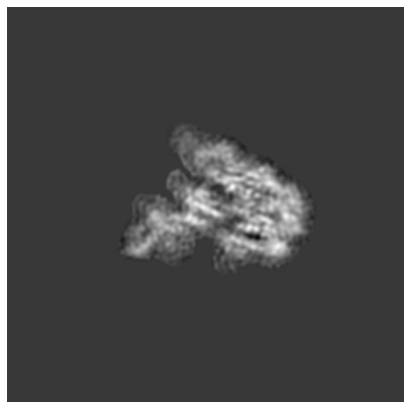


Z Index: 256

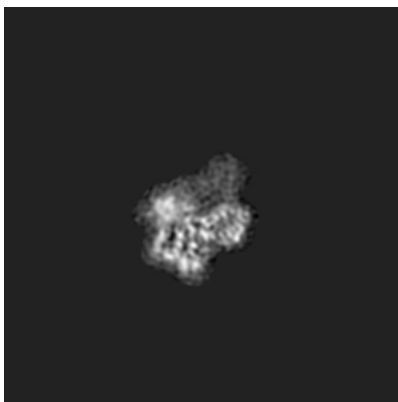
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

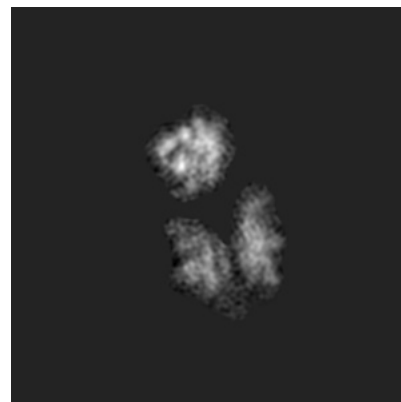
6.3.1 Primary map



X Index: 226

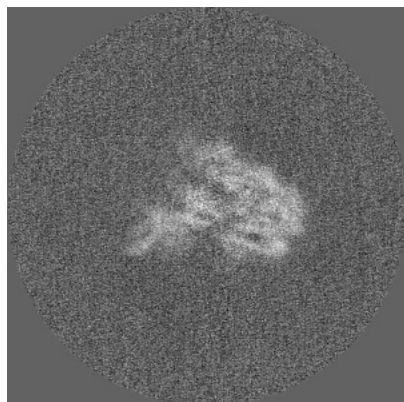


Y Index: 326

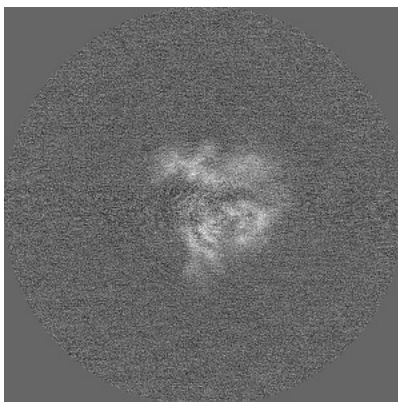


Z Index: 207

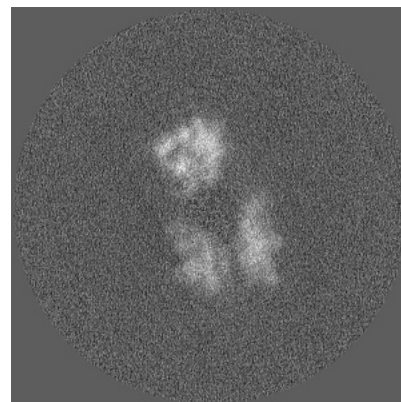
6.3.2 Raw map



X Index: 225



Y Index: 253

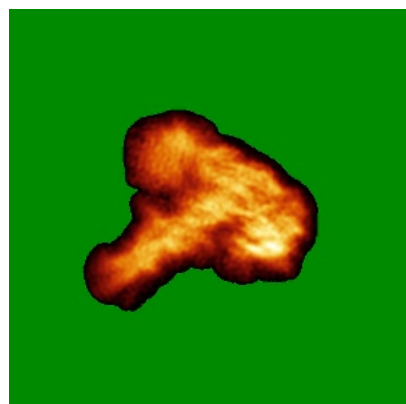


Z Index: 208

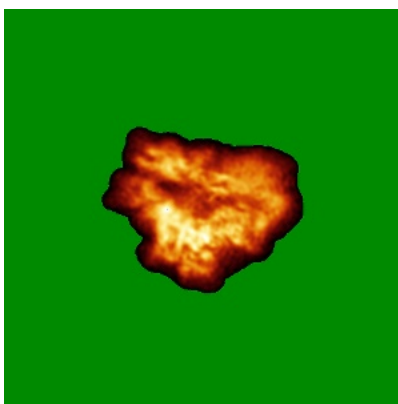
The images above show the largest variance slices of the map in three orthogonal directions.

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

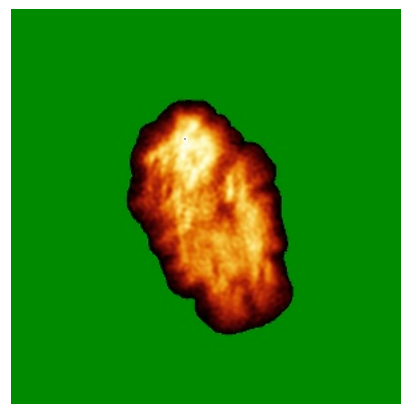
6.4.1 Primary map



X

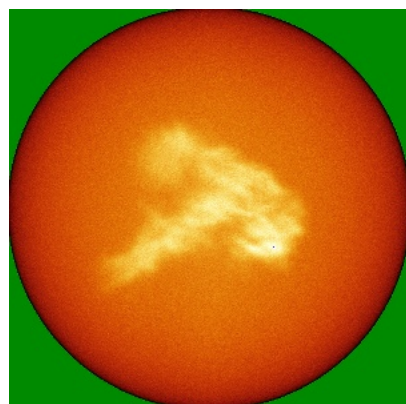


Y

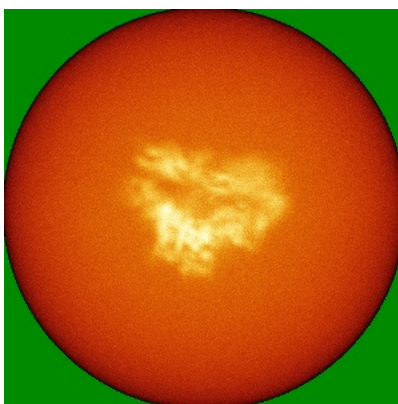


Z

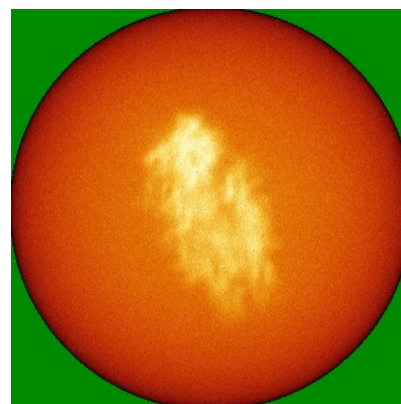
6.4.2 Raw map



X



Y

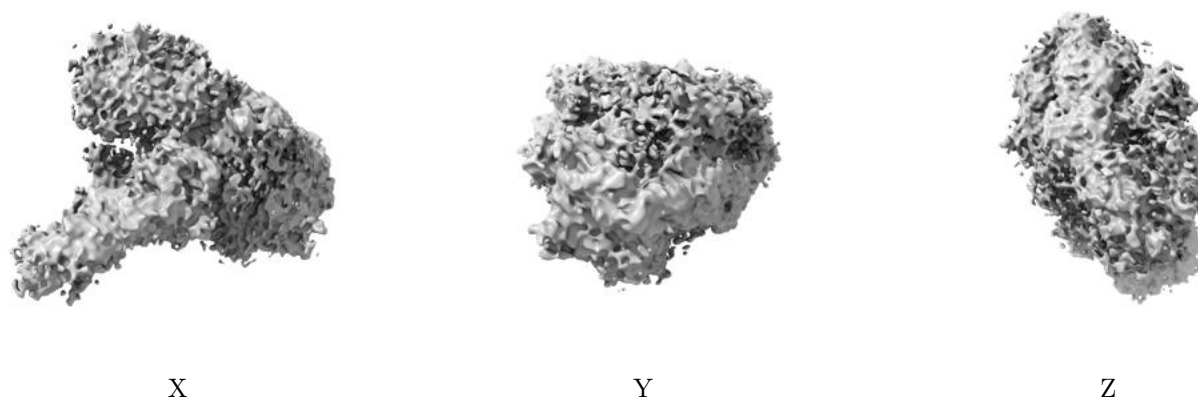


Z

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

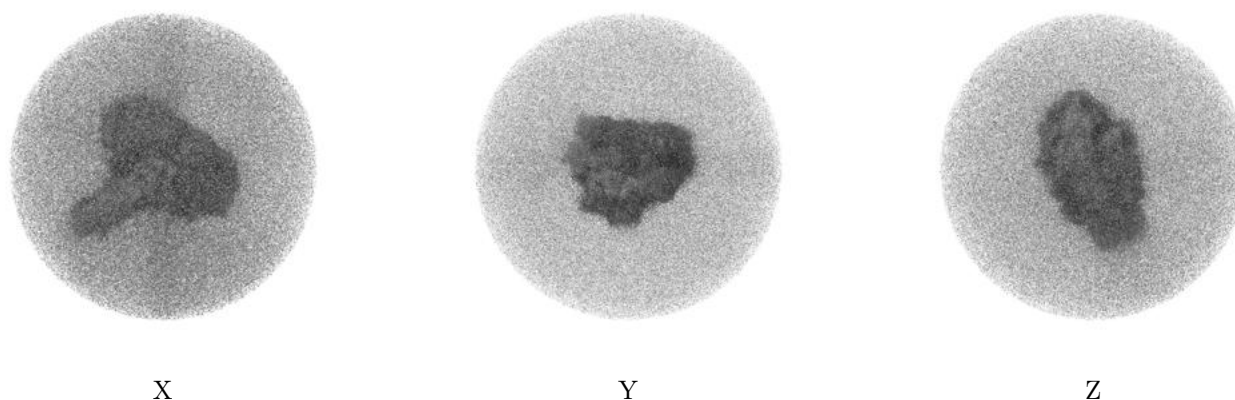
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

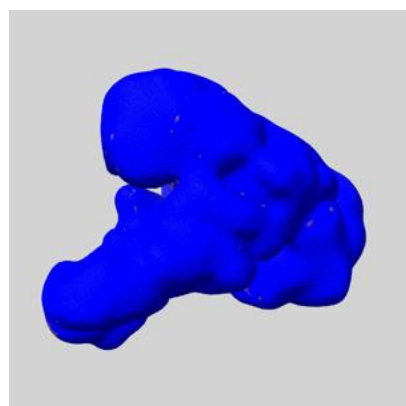
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

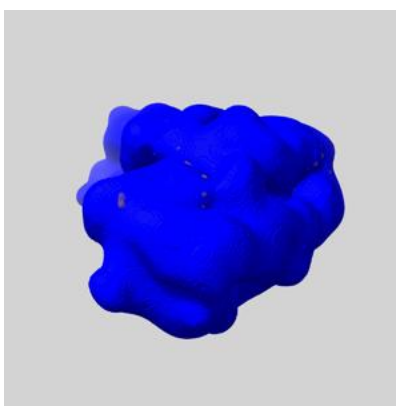
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

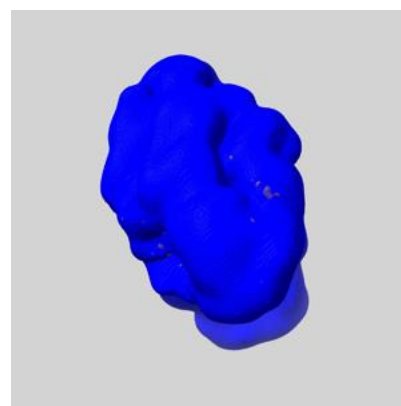
6.6.1 emd_52310_msk_1.map [i](#)



X



Y

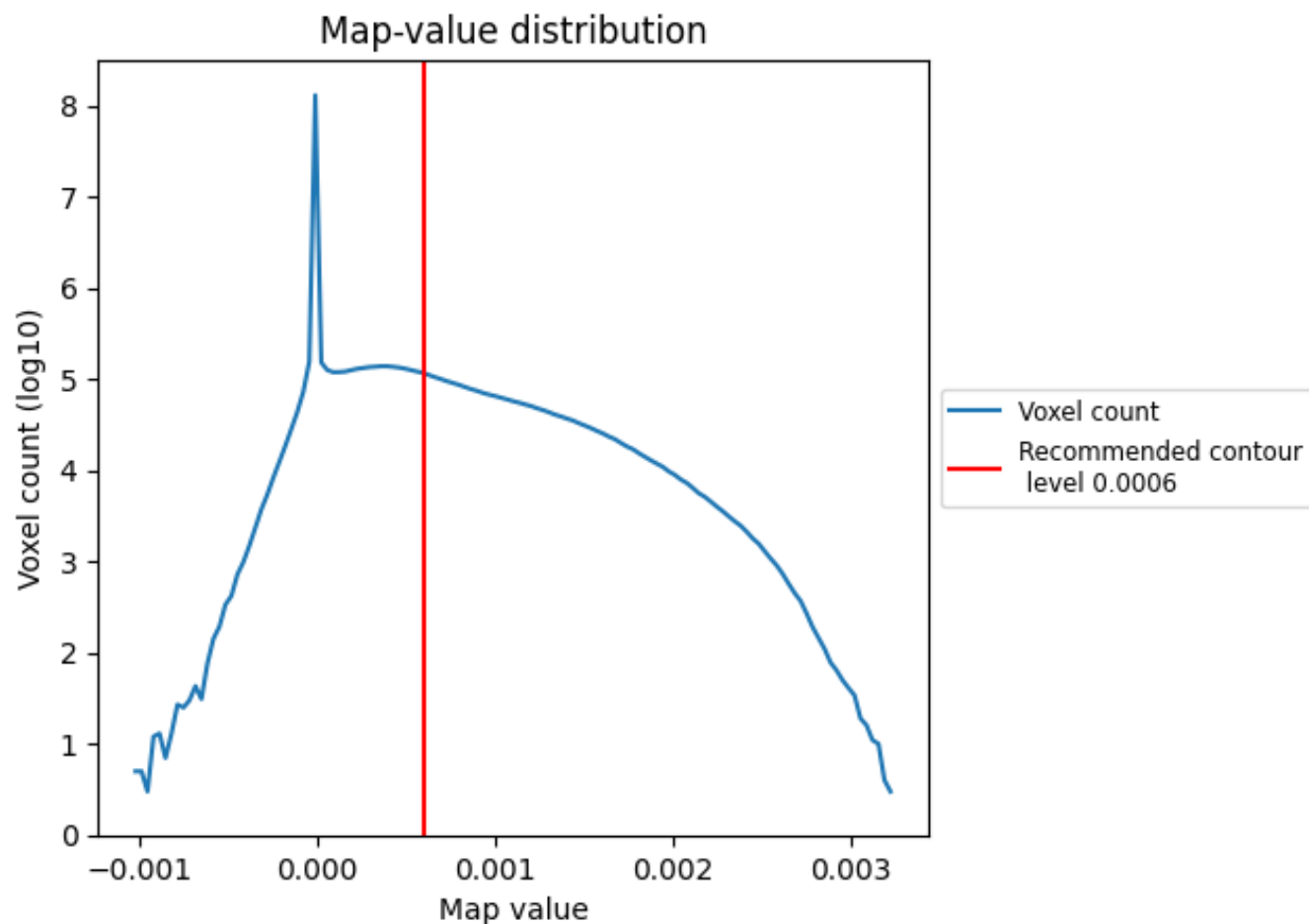


Z

7 Map analysis [i](#)

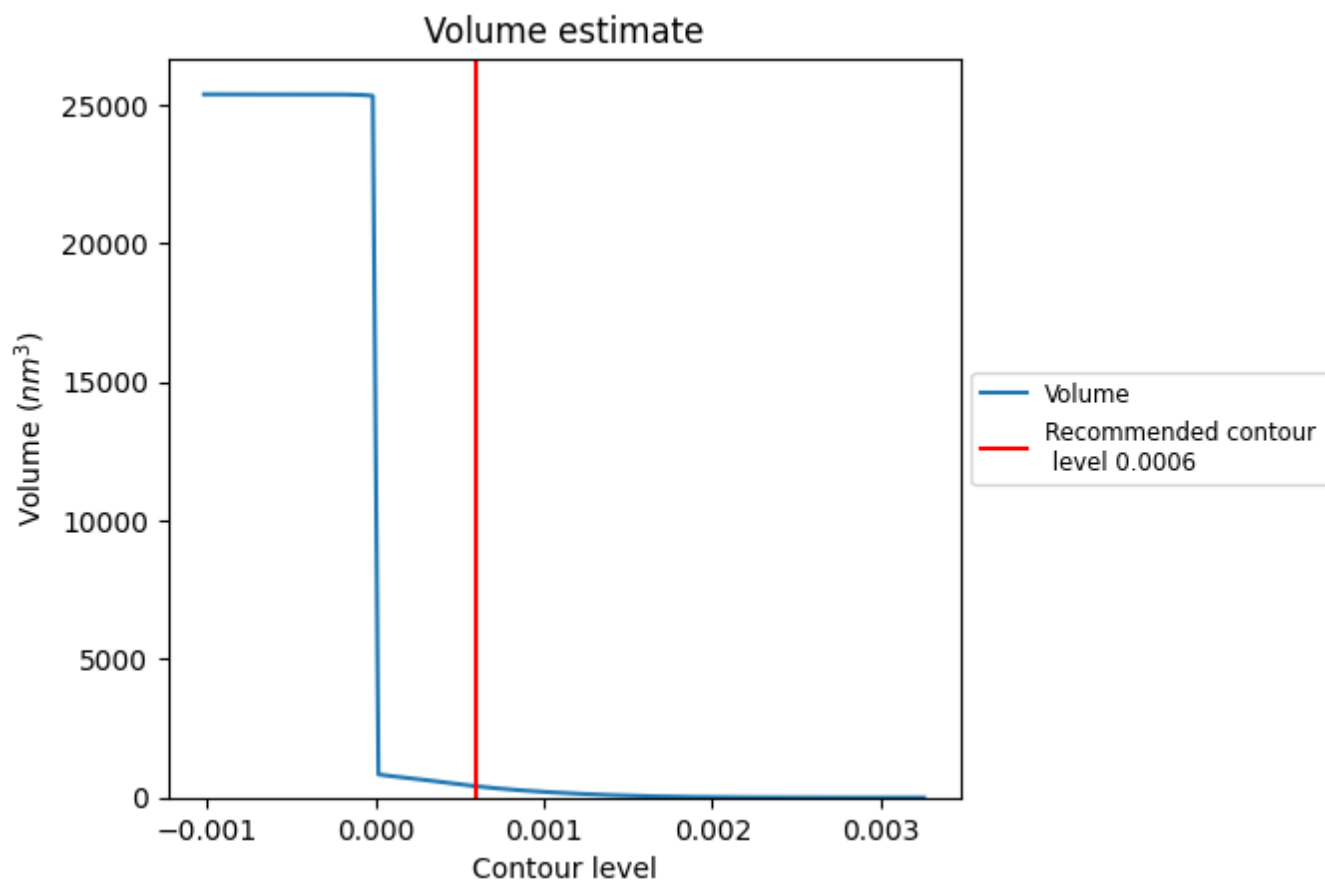
This section contains the results of statistical analysis of the map.

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.

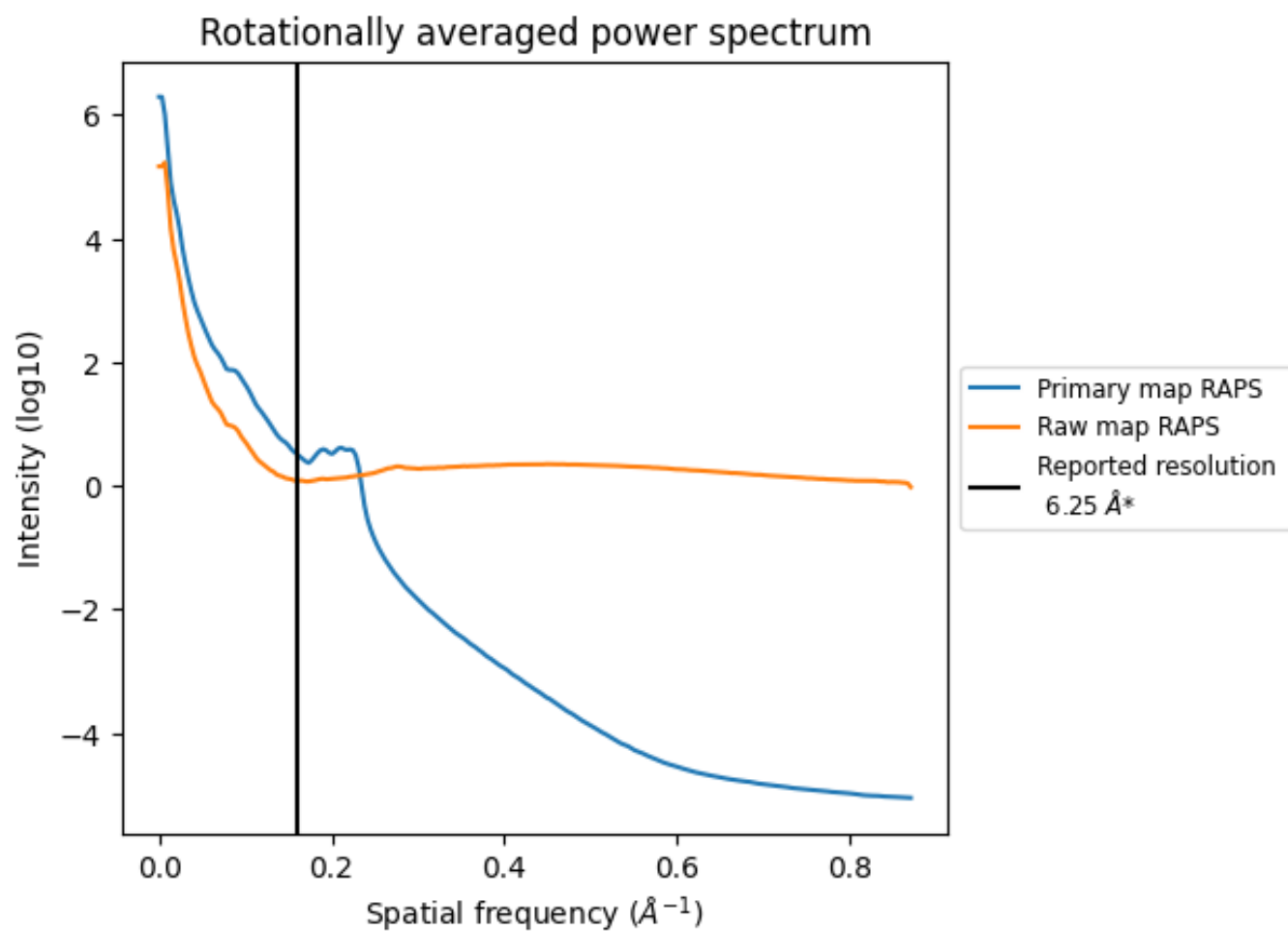
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 407 nm^3 ; this corresponds to an approximate mass of 368 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](#)

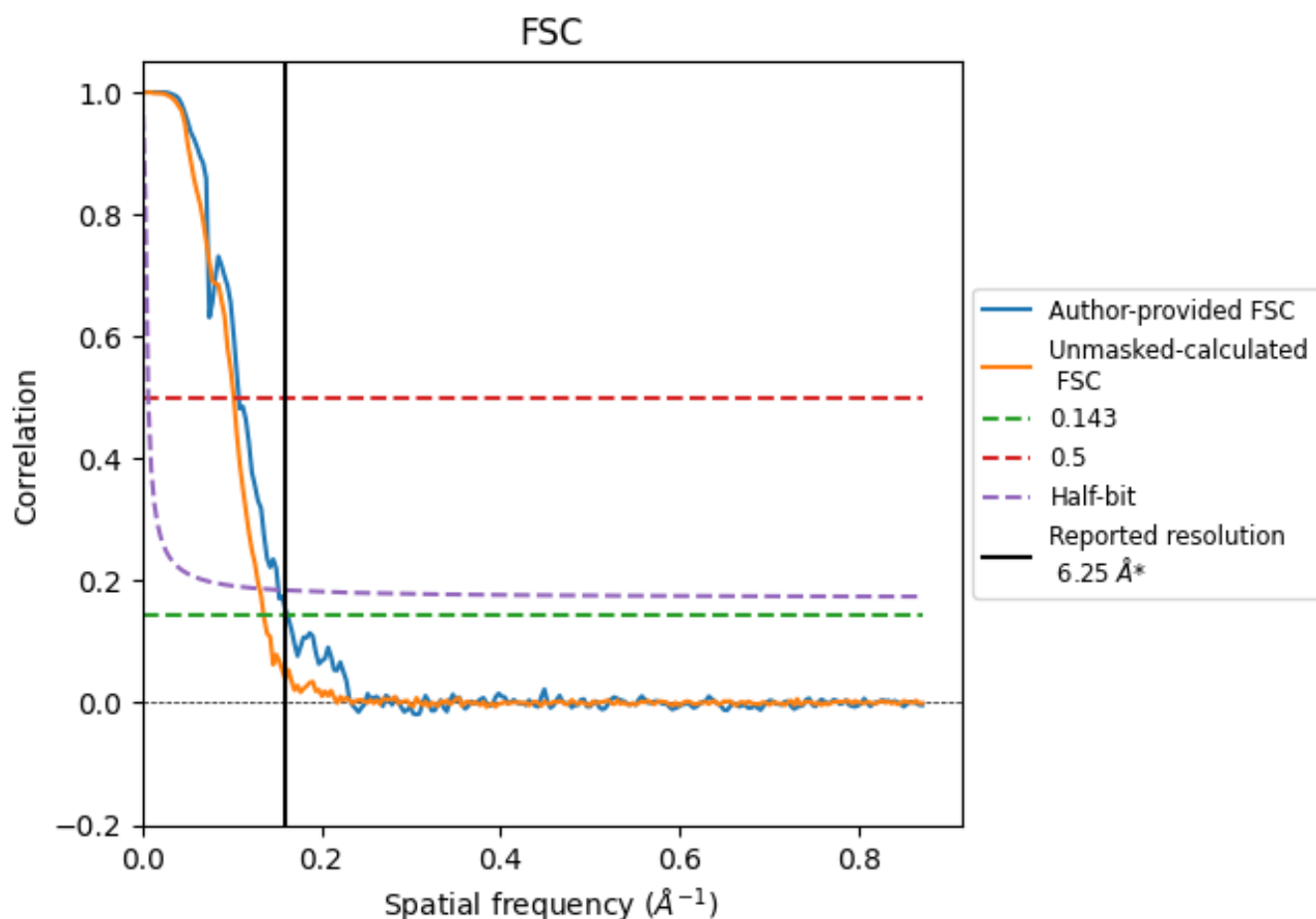


*Reported resolution corresponds to spatial frequency of 0.160 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.160 Å⁻¹

8.2 Resolution estimates [i](#)

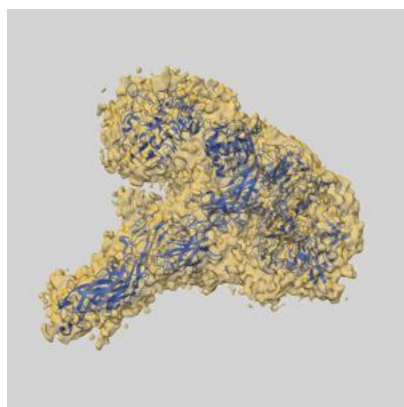
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.25	-	-
Author-provided FSC curve	6.17	9.28	6.57
Unmasked-calculated*	7.37	9.78	7.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.37 differs from the reported value 6.25 by more than 10 %

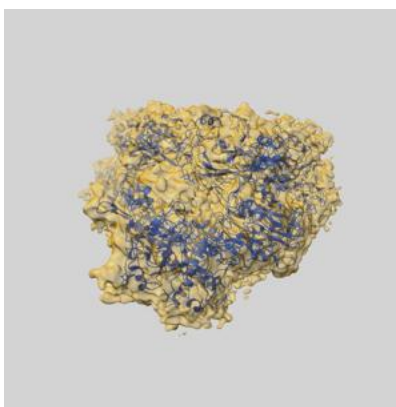
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52310 and PDB model 9HNI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

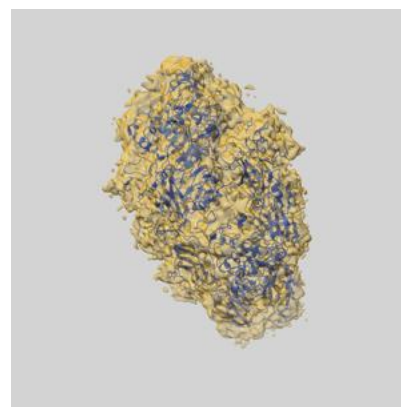
9.1 Map-model overlay [i](#)



X



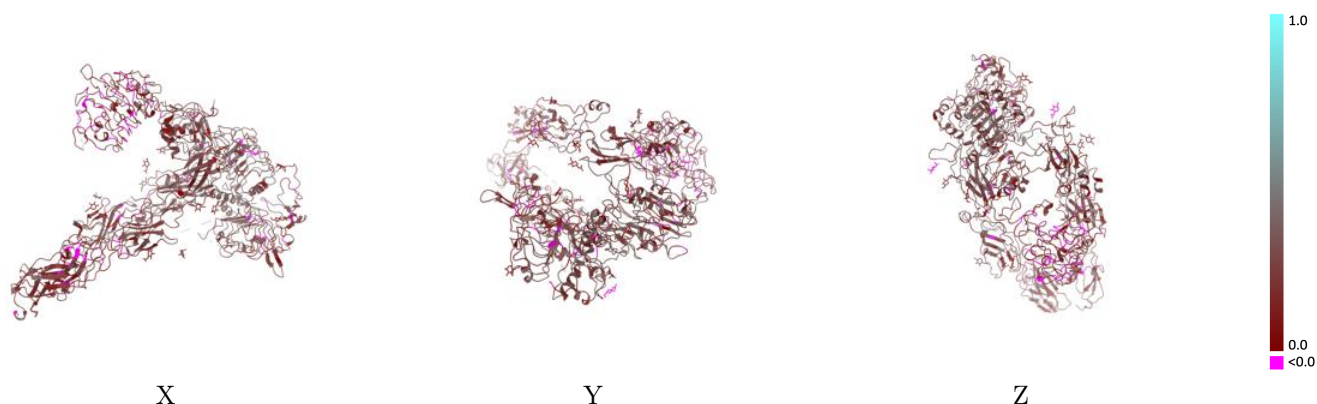
Y



Z

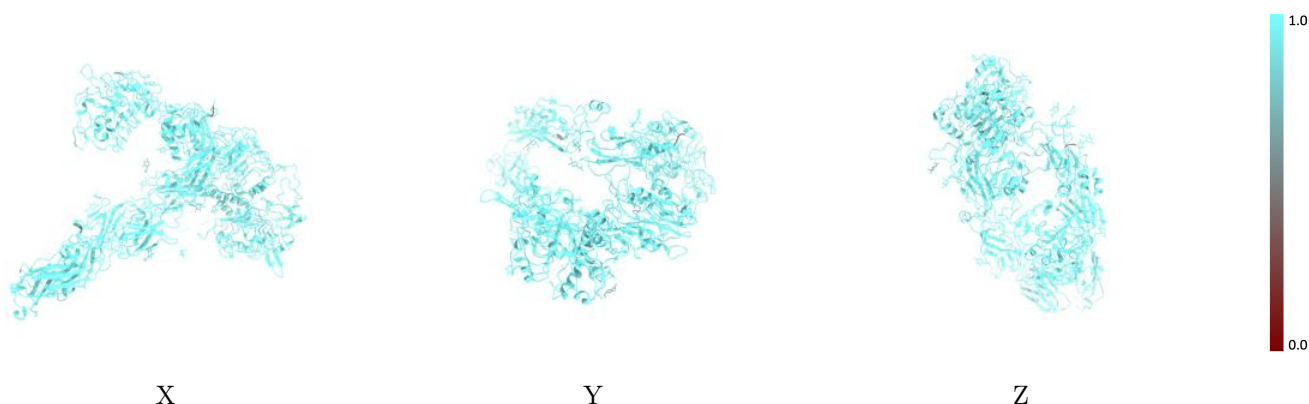
The images above show the 3D surface view of the map at the recommended contour level 0.0006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



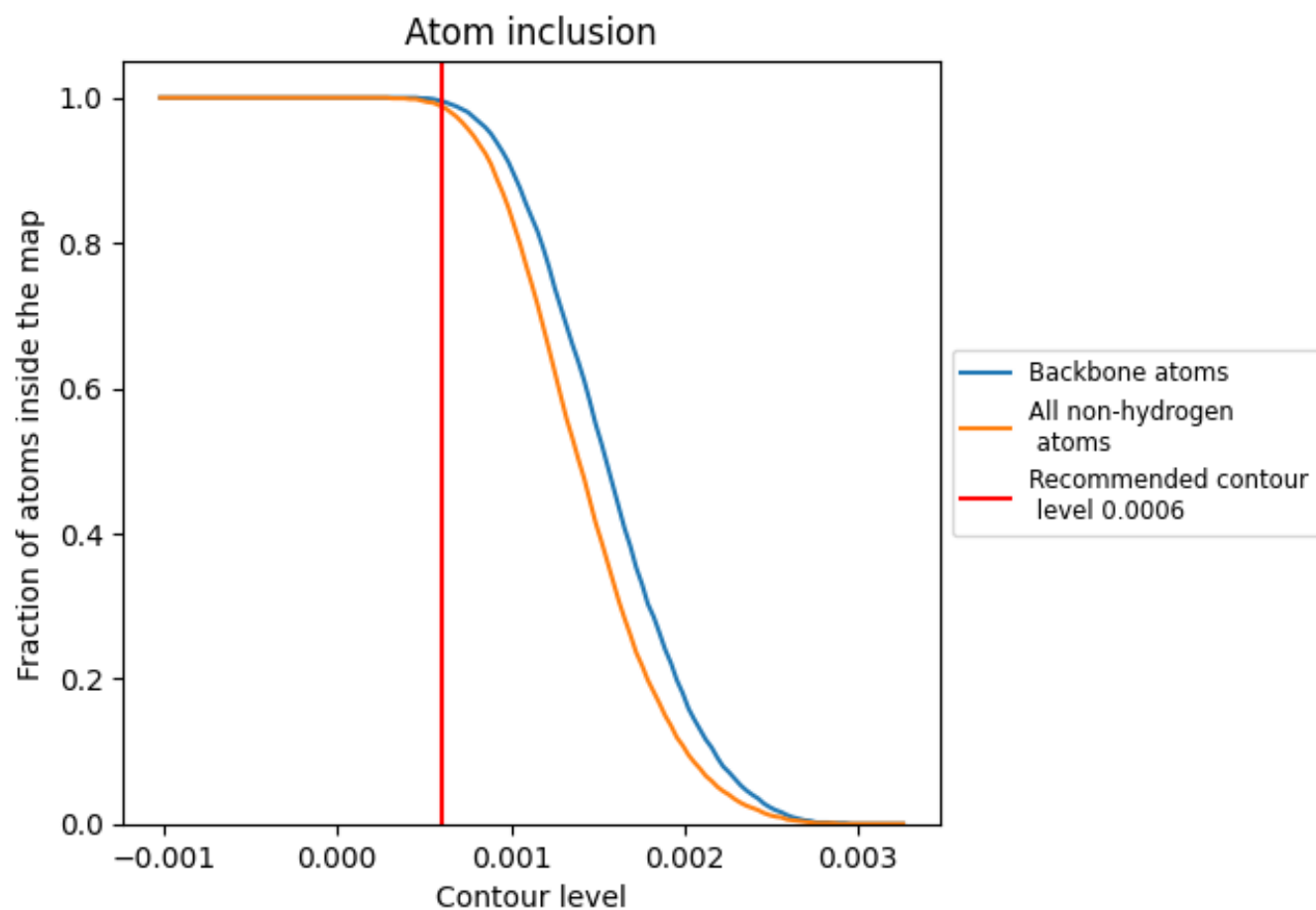
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9880</div>	<div><div></div>0.2440</div>
A	<div><div></div>0.9900</div>	<div><div></div>0.2580</div>
B	<div><div></div>0.9870</div>	<div><div></div>0.2310</div>
C	<div><div></div>1.0000</div>	<div><div></div>0.2350</div>
E	<div><div></div>0.9400</div>	<div><div></div>0.2420</div>
F	<div><div></div>0.9890</div>	<div><div></div>0.2270</div>
G	<div><div></div>0.9750</div>	<div><div></div>0.2020</div>
H	<div><div></div>0.9890</div>	<div><div></div>0.2810</div>

1.0

0.0

<0.0