



## Full wwPDB EM Validation Report ⓘ

Sep 22, 2025 – 01:03 PM EDT

PDB ID : 9EF1 / pdb\_00009ef1  
EMDB ID : EMD-47967  
Title : Cryo-EM structure of Drosophila melanogaster insulin receptor (dmIR) bound with one DILP1, asymmetric conformation  
Authors : Bai, X.C.  
Deposited on : 2024-11-19  
Resolution : 4.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

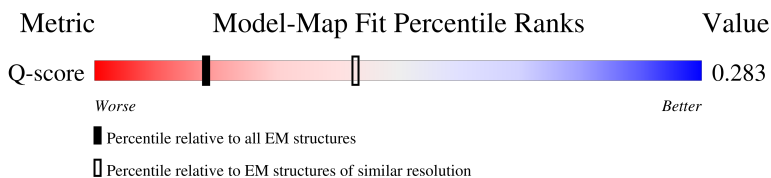
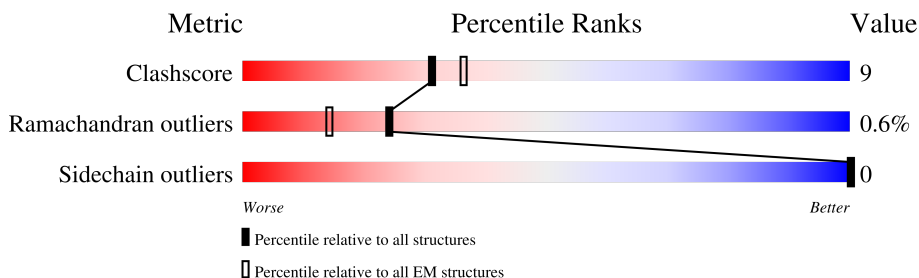
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	3132 ( 3.91 - 4.90 )

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  $\geq 3$ , 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	C	41	
2	D	27	
3	A	2144	
3	B	2144	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22546 atoms, of which 11155 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 DILP1 B-chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	27	Total	C	H	N	O	S	0	0
			377	121	184	34	35	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	LYS	ARG	conflict	UNP Q9VT50

- Molecule 2 is a protein called DILP1 A-chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	23	Total	C	H	N	O	S	0	0
			295	102	136	23	30	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	816	Total	C	H	N	O	S	0	0
			12834	4077	6361	1110	1236	50		
3	B	552	Total	C	H	N	O	S	0	0
			8704	2793	4306	736	850	19		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	





SER	PRO	THR	ASN	PRO	ASN	SER	GLY	ILE	GLY	ALA	THR	GLY	ALA	GLY	ASN	ARG	SER	ASN	LEU	LEU	LYS	GLU	ASN	TRP	LEU	ARG	PRO	ALA	SER	THR	PRO	ARG	PRO	PRO	PRO	ASN	GLY	PHE	ILE	GLY	ARG	GLU	ALA
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- Molecule 3: Insulin-like receptor

Chain B:  21% 1% 74%

ASP	SER	PRO	ALA	SER	SER	GLU	GLU	ALA	ALA	TYR	SER	SER	SER	SER	CYS	GLN	ALA	GLU	SER	SER	SER	ILE	SER	GLU	ALA	GLU	GLU	VAL	TRP	PHE	LEU	SER	SER	HIS	ASP	ASP	ILE	LEU	VAL	VAL	CYS	CYS	ARG	ARG	PRO	LYS	PHE	ASP	ASP	GLU	VAL	VAL	GLU	THR	THR	GLY	GLY	LYS	LYS	ARG	ASP	VAL	VAL	LYS	CYS	SER
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[illegible]

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

[illegible]

Residue	Score
THR	
LYS	
PHE	
GLU	
THR	
ASN	
SER	
VAL	
TYR	
SER	
GLY	
ILE	
PRO	
TYR	
ASN	
GLY	
GLN	
CYS	
ILE	
THR	
HIS	
CYS	
PRO	
THR	
GLY	
TYR	
GLN	
LYS	
SER	
GLU	
ASN	
LYS	
ARG	
MET	
CYS	
GLU	
PRO	
CYS	
PRO	
GLY	
GLY	
LYS	
CYS	
DG44	
K645	
E646	
S649	
T668	
E680	
L693	
V696	
T708	

PRO	MEI	D7 30	V7 38	N7 41	R7 42	D7 43	E7 46	L7 47	F7 63	N7 66	Q7 76	N7 98	T9 06	L8 13	V8 16	A9 21	V9 25	I8 31	G8 32	E8 33	P8 34	Q8 35	S8 38	F8 53	P8 61	D8 74	D8 75	R8 76	S8 80	E8 83	K8 84	S8 85	G8 86	V8 87	M8 88	T8 96	N8 98
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[illegible]

E1034
L1039
Q1040
F1044
V1045
P1046
ASN
ILE
ARG
LYS
SER
LYS
ASN
GLY
SER
SER
ASP
LYS
LYS
SER
ASP
GLY
ALA
GLU
GLY
ALA
ALA
LEU
ASP
SER
ASN
ILE
PRO
ASN
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ALA
ALA
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ARG
ARG
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VAL
ALA
LEU
GLU
PRO
GLU
LEU
ASP
ASP
VAL
GLY





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size ( $\text{\AA}$ )	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C	0.16	0/199	0.46	0/271
2	D	0.25	0/162	0.43	0/222
3	A	0.13	0/6603	0.40	1/8926 (0.0%)
3	B	0.14	0/4493	0.38	0/6080
All	All	0.14	0/11457	0.39	1/15499 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	639	PRO	N-CA-CB	6.95	110.64	103.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	193	184	183	6	0
2	D	159	136	135	5	0
3	A	6473	6361	6352	124	0
3	B	4398	4306	4301	66	0
4	A	98	98	91	3	0
4	B	70	70	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11391	11155	11127	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (194) 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:413:ASN:ND2	3:A:588:ASP:OD1	2.04	0.91
3:A:1124:TYR:OH	3:A:1143:GLU:OE1	1.92	0.85
3:A:1201:LYS:NZ	3:A:1233:ASP:O	2.13	0.81
3:A:702:SER:OG	3:A:735:ALA:O	2.01	0.79
3:B:1250:PRO:O	3:B:1252:GLN:NE2	2.17	0.77
2:D:4:GLY:O	2:D:23:TYR:OH	2.04	0.76
3:A:580:CYS:SG	3:A:586:GLN:NE2	2.61	0.74
3:A:1200:ARG:O	3:A:1235:ASN:ND2	2.23	0.72
3:B:816:VAL:O	3:B:925:ASN:ND2	2.23	0.71
3:A:535:CYS:SG	3:A:536:ARG:N	2.63	0.70
3:A:978:ARG:NH2	3:A:983:GLU:OE2	2.24	0.70
3:A:867:LYS:NZ	3:A:916:GLU:OE2	2.24	0.67
3:A:1227:ARG:NE	3:A:1268:ALA:O	2.28	0.66
3:A:707:LEU:O	3:A:707:LEU:HD12	1.95	0.66
3:A:586:GLN:OE1	3:A:590:ARG:N	2.30	0.65
3:A:887:VAL:HG21	4:A:2204:NAG:H82	1.79	0.64
3:B:1244:ALA:HB1	3:B:1254:GLU:OE2	1.99	0.63
3:A:745:ASP:OD2	3:A:746:GLU:N	2.32	0.62
3:A:355:GLU:OE1	3:A:356:ASN:ND2	2.32	0.62
1:C:27:ALA:O	1:C:31:VAL:HG23	2.00	0.61
3:A:595:ASN:OD1	3:A:596:GLU:N	2.33	0.61
3:A:724:SER:O	3:A:758:LYS:NZ	2.34	0.60
3:A:361:GLU:OE2	3:A:590:ARG:NH1	2.35	0.60
3:A:805:GLY:O	3:A:806:THR:OG1	2.11	0.60
3:A:927:GLY:O	3:A:1170:ARG:NE	2.35	0.59
3:A:1272:ILE:CG2	3:A:1274:LEU:HD23	2.33	0.58
3:A:555:VAL:O	3:A:563:SER:N	2.37	0.58
3:A:865:SER:OG	3:A:876:ARG:NH2	2.32	0.57
3:B:1148:GLN:N	3:B:1148:GLN:OE1	2.38	0.57
3:B:978:ARG:HH22	3:B:985:LEU:HD21	1.69	0.57
3:A:386:THR:O	3:A:412:GLY:N	2.37	0.57
3:A:455:TYR:OH	3:A:486:LEU:O	2.21	0.57
3:B:896:TYR:N	3:B:924:THR:OG1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:693:LEU:O	3:A:696:VAL:HG12	2.04	0.57
3:A:577:MET:SD	3:A:577:MET:N	2.78	0.56
3:B:980:TYR:O	3:B:982:THR:N	2.37	0.56
3:A:1239:VAL:N	3:A:1286:ASN:O	2.35	0.56
3:B:874:ASP:OD2	3:B:876:ARG:NH1	2.39	0.56
2:D:6:VAL:O	2:D:10:CYS:N	2.37	0.55
3:B:1126:ASP:N	3:B:1143:GLU:OE2	2.39	0.55
3:B:968:LEU:HD13	3:B:1160:THR:HG21	1.88	0.55
1:C:37:ASN:O	1:C:38:THR:OG1	2.13	0.54
3:B:1277:GLY:O	3:B:1302:VAL:N	2.40	0.54
3:A:964:ILE:HG13	3:A:1144:LEU:HD12	1.89	0.54
3:A:355:GLU:CB	4:A:2201:NAG:H82	2.37	0.54
3:A:821:ALA:O	3:A:890:LEU:N	2.35	0.54
3:A:1159:PHE:N	3:A:1198:THR:OG1	2.41	0.53
3:B:1215:GLU:O	3:B:1222:SER:OG	2.13	0.53
3:A:678:LYS:CD	3:B:1030:GLN:HB3	2.38	0.53
3:B:968:LEU:CD1	3:B:1160:THR:HG21	2.39	0.53
3:B:883:GLU:OE1	3:B:885:SER:N	2.39	0.53
3:A:908:ILE:HG23	3:A:909:SER:N	2.24	0.53
3:A:339:CYS:SG	3:A:360:ILE:HD13	2.48	0.52
3:A:417:ASP:OD1	3:A:679:ARG:NH2	2.39	0.52
3:B:1183:PHE:O	3:B:1185:LYS:N	2.42	0.52
3:A:888:MET:SD	3:A:889:VAL:N	2.82	0.52
3:A:1184:LYS:O	3:A:1185:LYS:C	2.52	0.52
3:B:746:GLU:OE1	3:B:747:LEU:N	2.42	0.51
3:A:585:TYR:O	3:A:592:VAL:HG22	2.10	0.51
3:A:745:ASP:OD2	3:A:745:ASP:C	2.52	0.51
1:C:21:GLY:O	1:C:24:LEU:HG	2.11	0.51
3:B:825:VAL:HG13	3:B:825:VAL:O	2.10	0.51
3:A:722:GLU:OE2	3:A:757:ARG:NE	2.34	0.50
3:A:706:HIS:O	3:A:708:THR:HG23	2.10	0.50
3:A:738:VAL:HG12	3:A:766:ASN:OD1	2.10	0.50
3:A:945:ILE:HD12	3:A:1156:LEU:CD2	2.41	0.50
3:A:678:LYS:NZ	3:B:1034:GLU:OE2	2.45	0.49
3:A:1239:VAL:HG12	3:A:1240:THR:HG23	1.92	0.49
3:A:1273:LYS:O	3:A:1274:LEU:HD22	2.12	0.49
3:A:1171:GLU:OE1	3:A:1171:GLU:N	2.37	0.49
3:A:830:GLU:OE1	3:A:835:GLN:N	2.45	0.49
3:B:1202:LYS:HD2	3:B:1203:PHE:N	2.27	0.49
3:B:1250:PRO:O	3:B:1251:ASP:OD1	2.31	0.49
3:B:708:THR:HG22	3:B:741:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1206:ILE:HG13	3:A:1207:VAL:H	1.77	0.49
3:A:896:TYR:N	3:A:924:THR:OG1	2.46	0.48
3:A:1126:ASP:CG	3:A:1127:GLU:H	2.21	0.48
3:B:853:PHE:N	3:B:883:GLU:O	2.44	0.48
3:B:1242:GLU:N	3:B:1284:ARG:O	2.34	0.48
2:D:23:TYR:CD2	3:B:1046:PRO:HD2	2.48	0.48
3:A:601:THR:OG1	3:A:608:VAL:O	2.32	0.48
3:A:596:GLU:O	3:A:600:LEU:HD23	2.13	0.47
3:A:856:TYR:CZ	3:A:879:VAL:HG23	2.50	0.47
3:A:614:TYR:O	3:A:615:ASN:OD1	2.32	0.47
3:A:1224:VAL:O	3:A:1272:ILE:N	2.43	0.47
3:B:874:ASP:OD1	3:B:875:ASP:N	2.48	0.47
3:A:435:HIS:O	3:A:438:ARG:NH1	2.44	0.47
3:B:1247:LEU:HD23	3:B:1248:GLN:N	2.29	0.47
3:A:891:SER:O	3:A:892:ASN:OD1	2.33	0.47
3:B:1039:LEU:C	3:B:1039:LEU:HD23	2.39	0.47
3:A:678:LYS:HZ2	3:B:1034:GLU:CD	2.22	0.47
3:B:880:SER:OG	3:B:888:MET:HE1	2.15	0.47
3:A:778:LEU:HD12	3:A:785:PRO:O	2.15	0.47
3:A:627:GLN:O	3:A:636:GLU:N	2.45	0.47
3:B:813:LEU:HD12	3:B:816:VAL:HG13	1.96	0.47
3:A:706:HIS:HA	3:A:739:LEU:O	2.15	0.46
3:A:355:GLU:HB3	4:A:2201:NAG:H82	1.98	0.46
3:B:693:LEU:O	3:B:696:VAL:HG12	2.15	0.46
3:B:1023:GLU:OE1	3:B:1023:GLU:N	2.48	0.46
3:A:1221:GLU:OE1	3:A:1221:GLU:N	2.49	0.46
3:B:816:VAL:HG12	3:B:821:ALA:CB	2.46	0.46
3:B:1251:ASP:OD1	3:B:1251:ASP:C	2.59	0.46
3:B:649:SER:N	3:B:668:THR:O	2.50	0.45
3:B:861:PRO:O	3:B:898:ASN:ND2	2.50	0.45
3:B:766:ASN:N	3:B:798:ASN:OD1	2.42	0.45
3:A:1166:VAL:O	3:A:1166:VAL:HG13	2.15	0.45
3:A:766:ASN:O	3:A:799:GLY:N	2.49	0.45
3:B:680:GLU:OE1	3:B:680:GLU:N	2.46	0.45
3:A:336:VAL:HG23	3:A:336:VAL:O	2.17	0.45
3:A:476:THR:HG21	3:B:1028:LYS:HE3	1.99	0.45
3:A:343:ASP:OD1	3:A:343:ASP:N	2.48	0.45
3:A:531:CYS:HB2	3:A:532:PRO:HD2	1.98	0.45
3:B:1045:VAL:HB	3:B:1046:PRO:HD3	1.99	0.45
3:A:960:THR:O	3:A:960:THR:HG22	2.17	0.44
3:A:464:ILE:HG23	3:A:465:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1216:HIS:O	3:B:1216:HIS:ND1	2.51	0.44
3:A:386:THR:OG1	3:A:588:ASP:OD1	2.35	0.44
3:A:454:CYS:SG	3:A:455:TYR:N	2.91	0.44
3:B:1202:LYS:HD2	3:B:1203:PHE:CD2	2.52	0.44
1:C:18:LYS:O	1:C:18:LYS:HG3	2.17	0.44
3:A:676:SER:HA	3:A:708:THR:HG22	1.98	0.44
3:B:1212:VAL:HG11	3:B:1300:ILE:CG1	2.48	0.44
3:A:612:ILE:O	3:A:619:ILE:N	2.51	0.44
3:A:655:LEU:HD13	3:A:688:GLU:HG2	1.99	0.44
3:A:898:ASN:OD1	3:A:923:ARG:NE	2.47	0.44
3:A:1213:ASP:OD2	3:A:1227:ARG:NH1	2.50	0.44
3:A:674:THR:HA	3:A:704:MET:O	2.18	0.44
3:B:1226:VAL:O	3:B:1270:TYR:N	2.50	0.44
3:A:362:GLY:N	3:A:386:THR:HG22	2.33	0.44
3:A:608:VAL:O	3:A:609:TYR:C	2.61	0.44
3:A:1235:ASN:O	3:A:1287:SER:OG	2.33	0.44
3:A:770:CYS:SG	3:A:804:CYS:C	3.01	0.43
1:C:17:HIS:HB3	1:C:19:LEU:HD23	2.00	0.43
2:D:23:TYR:CD2	3:B:1044:PHE:HB3	2.53	0.43
3:B:825:VAL:HG12	3:B:886:GLY:O	2.18	0.43
3:A:969:ILE:N	3:A:1161:ARG:O	2.46	0.43
3:A:1282:ARG:CG	3:A:1297:VAL:HG12	2.47	0.43
3:B:813:LEU:H	3:B:813:LEU:HD23	1.84	0.43
3:B:1172:GLU:O	3:B:1177:LYS:NZ	2.49	0.43
3:B:1216:HIS:O	3:B:1217:ALA:C	2.61	0.43
2:D:7:TYR:HB2	3:B:1040:GLN:HE21	1.84	0.43
3:A:677:ILE:HG23	3:A:711:LEU:HD21	2.00	0.43
3:A:587:PHE:HB2	3:A:592:VAL:HG21	2.00	0.43
3:A:756:ILE:HG13	3:A:781:LEU:HA	2.01	0.43
3:B:776:GLN:N	3:B:776:GLN:OE1	2.52	0.42
3:B:934:GLU:OE2	3:B:950:SER:OG	2.36	0.42
3:A:360:ILE:HB	3:A:385:VAL:HG23	2.02	0.42
3:A:414:LYS:C	3:A:415:LEU:HD22	2.45	0.42
3:A:1251:ASP:O	3:A:1251:ASP:OD1	2.38	0.42
3:A:386:THR:HG23	3:A:387:ASP:N	2.34	0.42
3:A:685:VAL:O	3:A:689:LEU:HD13	2.19	0.42
3:A:974:ARG:N	3:A:1237:GLU:OE2	2.41	0.42
3:B:1284:ARG:HB3	3:B:1294:PHE:HA	2.00	0.42
3:A:776:GLN:O	3:A:779:PRO:HD2	2.19	0.42
3:A:964:ILE:HD13	3:A:1166:VAL:HG23	2.00	0.42
3:A:856:TYR:CE2	3:A:879:VAL:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:990:GLU:O	3:B:991:ASN:C	2.62	0.42
3:A:539:CYS:SG	3:A:544:THR:C	3.03	0.41
3:A:913:THR:HG22	3:A:913:THR:O	2.20	0.41
3:B:1126:ASP:OD1	3:B:1127:GLU:N	2.53	0.41
3:B:1120:ASP:OD1	3:B:1191:TYR:OH	2.30	0.41
3:A:488:LYS:O	3:A:489:CYS:HB2	2.21	0.41
3:A:1206:ILE:HG13	3:A:1207:VAL:N	2.35	0.41
3:B:1278:LEU:HD12	3:B:1300:ILE:O	2.20	0.41
3:A:756:ILE:HG13	3:A:756:ILE:O	2.20	0.41
3:A:854:VAL:HG13	3:A:880:SER:O	2.20	0.41
3:A:908:ILE:O	3:A:911:GLU:N	2.42	0.41
3:A:690:LYS:O	3:A:694:ALA:HB2	2.21	0.41
3:A:989:MET:C	3:A:990:GLU:O	2.64	0.41
3:A:789:GLU:OE1	3:A:791:SER:N	2.47	0.41
3:B:1212:VAL:HG11	3:B:1300:ILE:HG13	2.01	0.41
3:A:1261:ALA:O	3:A:1262:ALA:C	2.63	0.41
3:A:1275:ASN:O	3:A:1279:TYR:OH	2.29	0.41
3:B:738:VAL:HG21	3:B:763:PHE:CE2	2.55	0.41
3:A:744:LEU:CD2	3:A:769:LEU:HD12	2.51	0.41
3:A:1210:LEU:C	3:A:1210:LEU:HD23	2.45	0.41
3:B:834:PRO:O	3:B:835:GLN:CG	2.69	0.41
3:B:1281:PHE:N	3:B:1298:GLU:O	2.49	0.41
3:A:692:GLY:C	3:A:693:LEU:HD22	2.46	0.41
3:A:714:LEU:HD21	3:A:744:LEU:HD11	2.03	0.41
3:A:855:PHE:CD1	3:A:903:VAL:HG22	2.56	0.41
3:A:989:MET:O	3:A:990:GLU:O	2.39	0.41
3:B:742:ARG:O	3:B:743:ASP:HB2	2.20	0.41
3:B:937:ALA:O	3:B:1196:GLN:NE2	2.43	0.41
3:A:394:VAL:HG22	3:A:426:ASN:OD1	2.21	0.40
3:B:831:ILE:HG13	3:B:832:GLY:N	2.37	0.40
1:C:39:LEU:HD23	1:C:40:PRO:HD3	2.02	0.40
3:A:417:ASP:HA	3:A:655:LEU:HD11	2.03	0.40
3:A:928:ARG:NH2	3:A:1190:ASP:OD1	2.52	0.40
3:A:372:ALA:C	3:A:374:PRO:HD2	2.46	0.40
3:A:1235:ASN:HB3	3:A:1289:ALA:HB3	2.04	0.40
3:A:1282:ARG:HG3	3:A:1297:VAL:HG12	2.04	0.40
3:A:604:GLU:O	3:A:605:THR:C	2.65	0.40
3:B:806:THR:HA	3:B:914:ASN:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	25/41 (61%)	22 (88%)	2 (8%)	1 (4%)	2	19
2	D	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
3	A	804/2144 (38%)	713 (89%)	85 (11%)	6 (1%)	19	56
3	B	542/2144 (25%)	497 (92%)	43 (8%)	2 (0%)	30	67
All	All	1392/4356 (32%)	1251 (90%)	132 (10%)	9 (1%)	24	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	990	GLU
3	A	1185	LYS
3	A	1262	ALA
3	A	726	ASP
3	A	840	ALA
3	A	1201	LYS
3	B	1184	LYS
3	B	925	ASN
1	C	38	THR

### 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	C	22/34 (65%)	22 (100%)	0	100	100
2	D	16/24 (67%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	739/1888 (39%)	739 (100%)	0	100	100
3	B	492/1888 (26%)	492 (100%)	0	100	100
All	All	1269/3834 (33%)	1269 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	HIS
3	A	346	ASN
3	A	606	ASN
3	A	1150	HIS
3	A	1265	ASN
3	B	741	ASN
3	B	1040	GLN
3	B	1158	HIS

### 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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	2202	3	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	B	2205	3	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	A	2206	3	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	A	2207	3	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
4	NAG	B	2202	3	14,14,15	0.21	0	17,19,21	0.37	0
4	NAG	A	2203	3	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	A	2205	3	14,14,15	0.21	0	17,19,21	0.37	0
4	NAG	B	2204	3	14,14,15	0.16	0	17,19,21	0.45	0
4	NAG	B	2203	3	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	A	2201	3	14,14,15	0.36	0	17,19,21	0.61	1 (5%)
4	NAG	B	2201	3	14,14,15	0.39	0	17,19,21	0.50	0
4	NAG	A	2204	3	14,14,15	0.23	0	17,19,21	0.54	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	NAG	A	2202	3	-	0/6/23/26	0/1/1/1
4	NAG	B	2205	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2206	3	-	1/6/23/26	0/1/1/1
4	NAG	A	2207	3	-	2/6/23/26	0/1/1/1
4	NAG	B	2202	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2203	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2205	3	-	0/6/23/26	0/1/1/1
4	NAG	B	2204	3	-	0/6/23/26	0/1/1/1
4	NAG	B	2203	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2201	3	-	0/6/23/26	0/1/1/1
4	NAG	B	2201	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2204	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2207	NAG	C1-O5-C5	2.22	115.16	112.19
4	A	2201	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2206	NAG	O5-C5-C6-O6
4	A	2207	NAG	O5-C5-C6-O6
4	A	2207	NAG	C4-C5-C6-O6

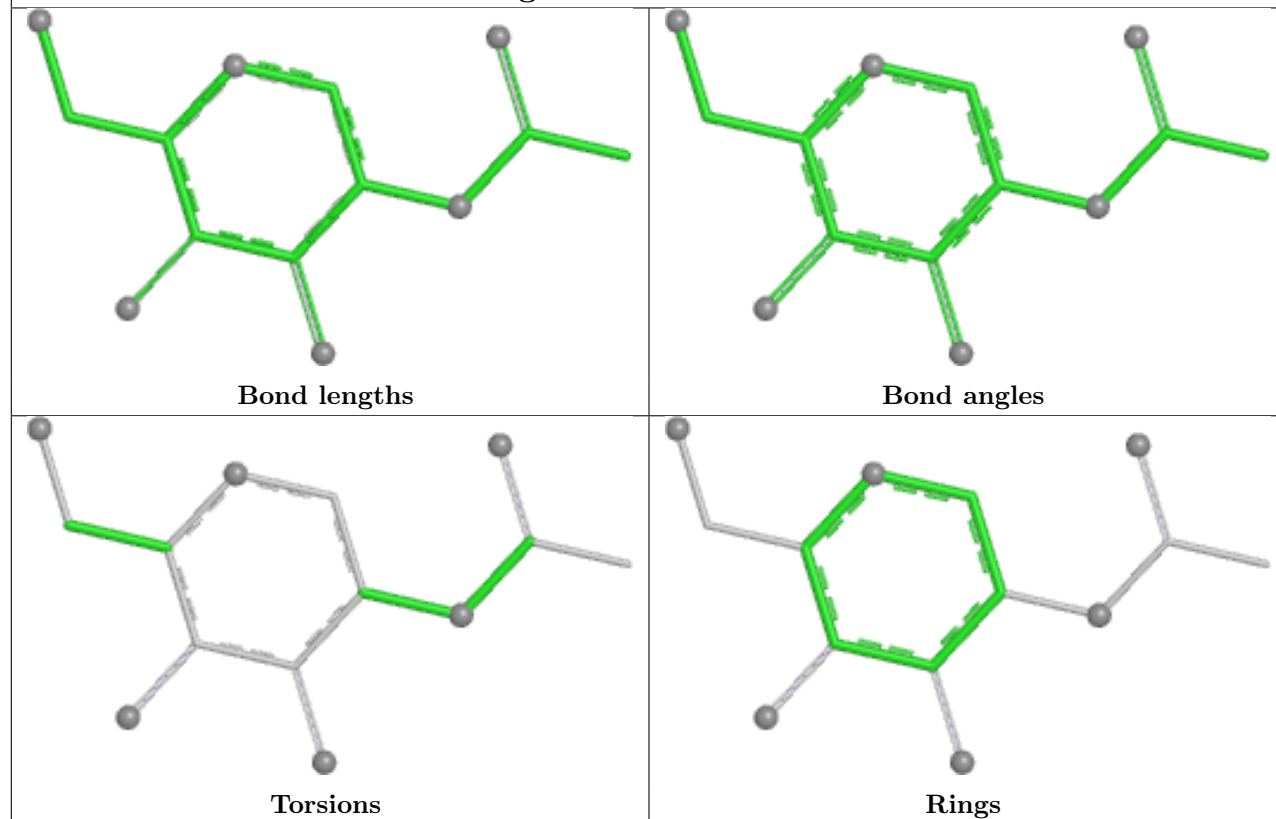
There are no ring outliers.

2 monomers are involved in 3 short contacts:

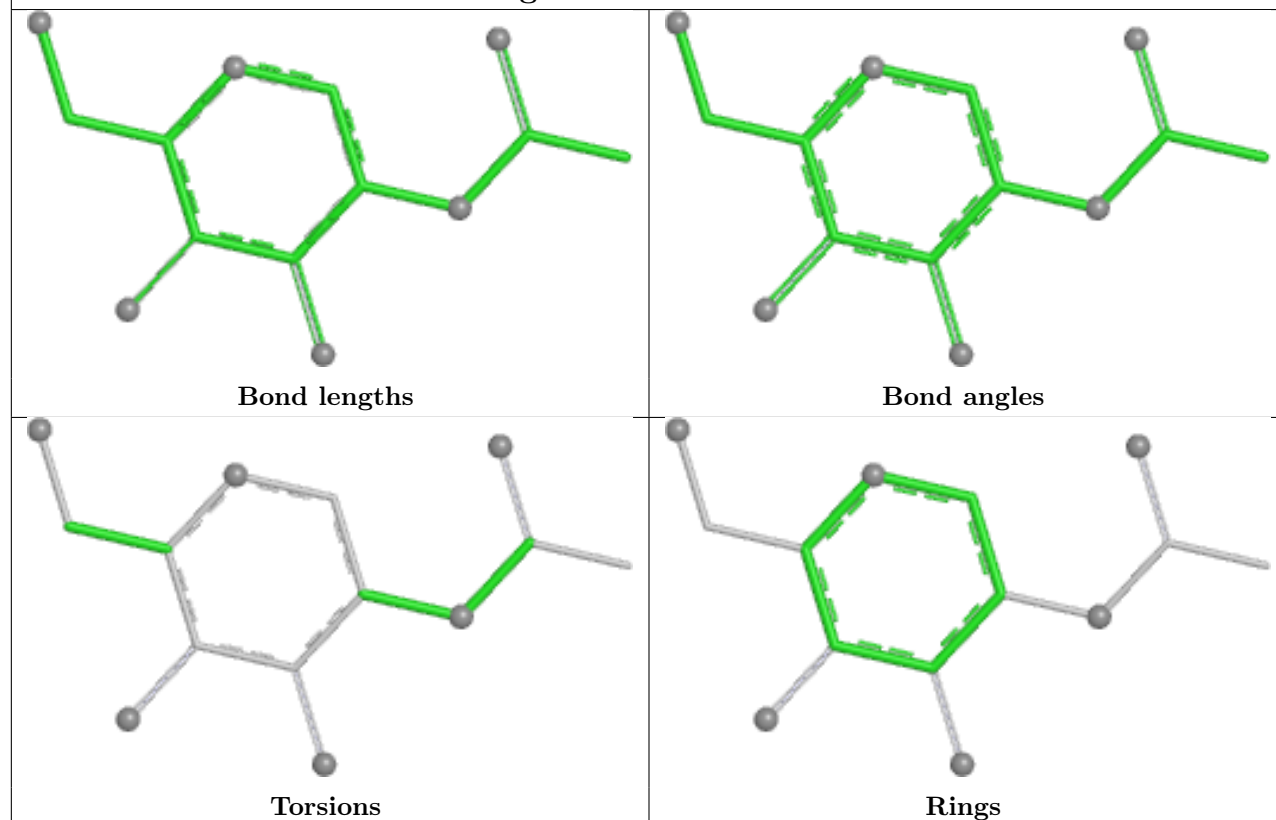
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2201	NAG	2	0
4	A	2204	NAG	1	0

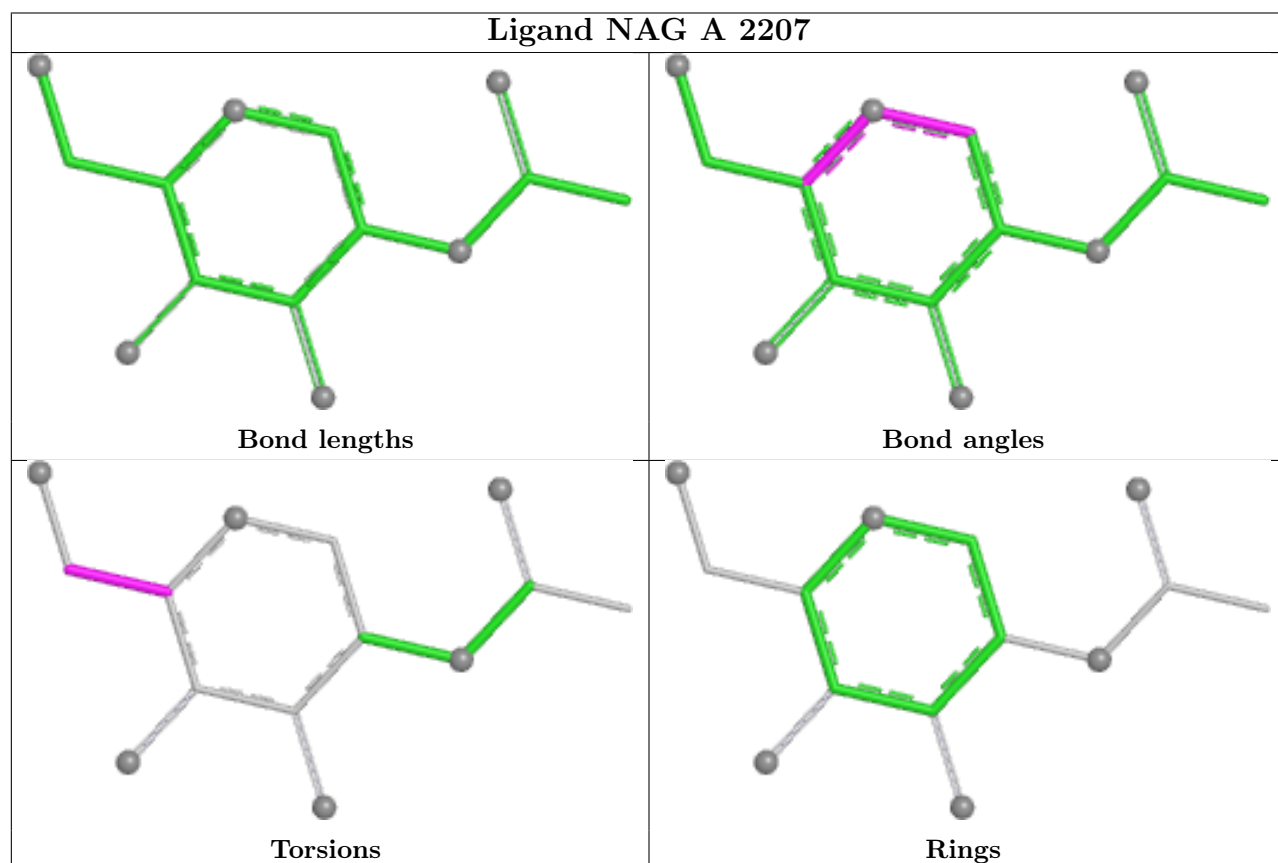
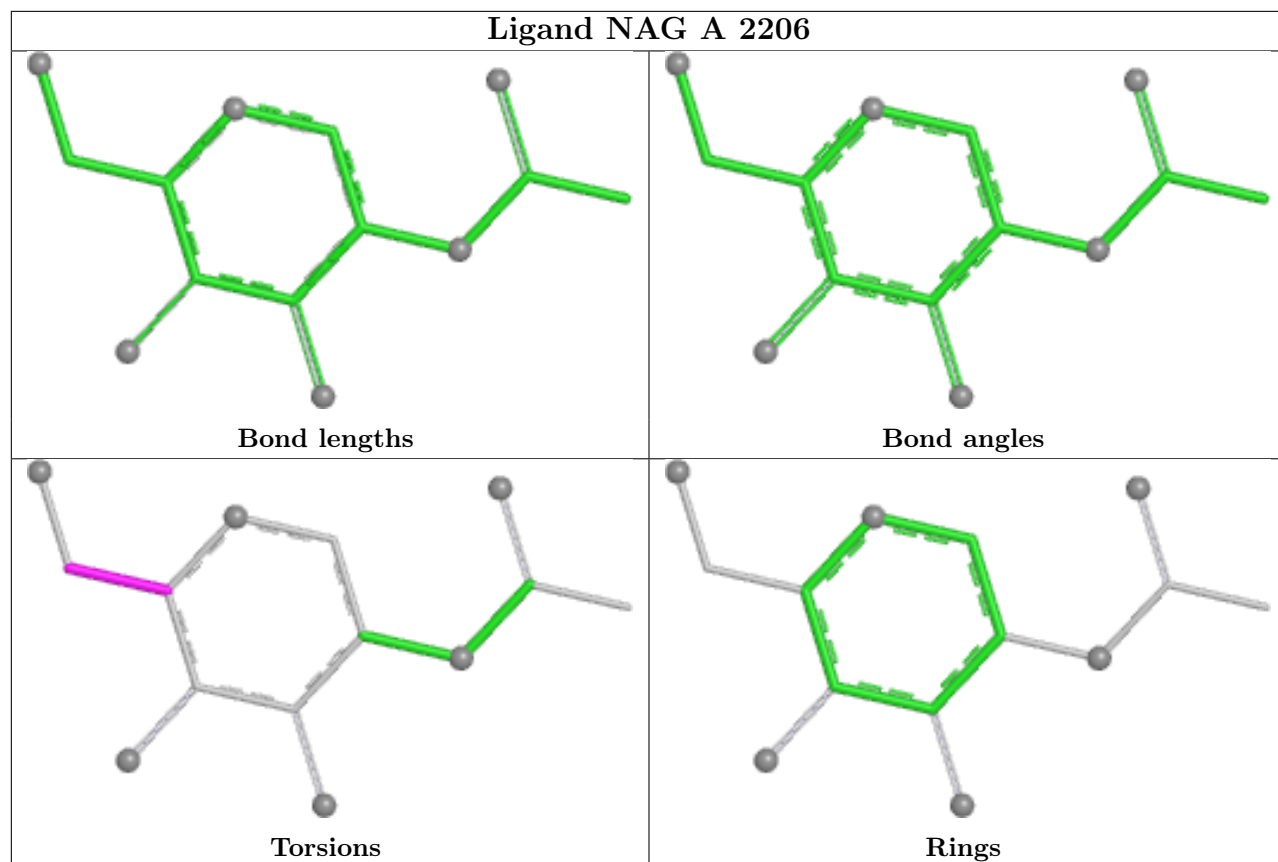
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 2202

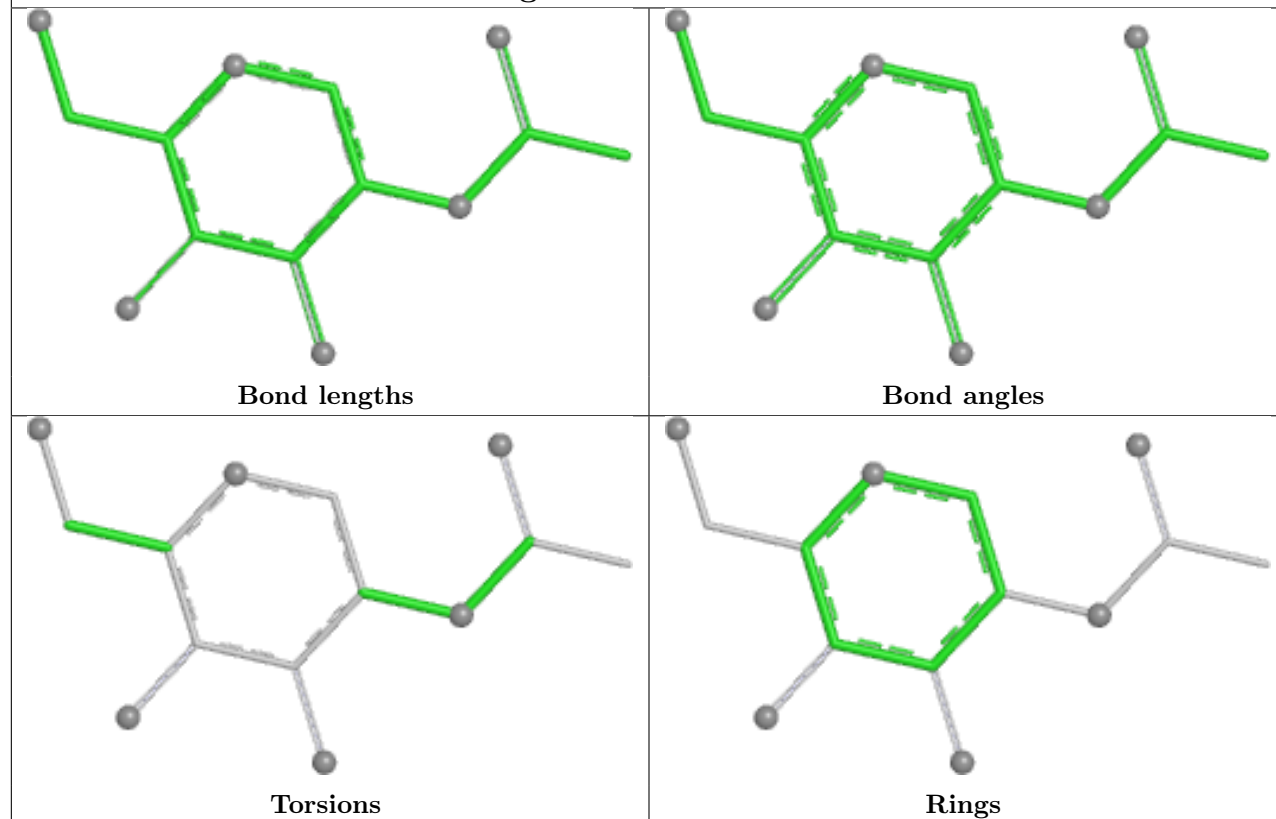


## Ligand NAG B 2205

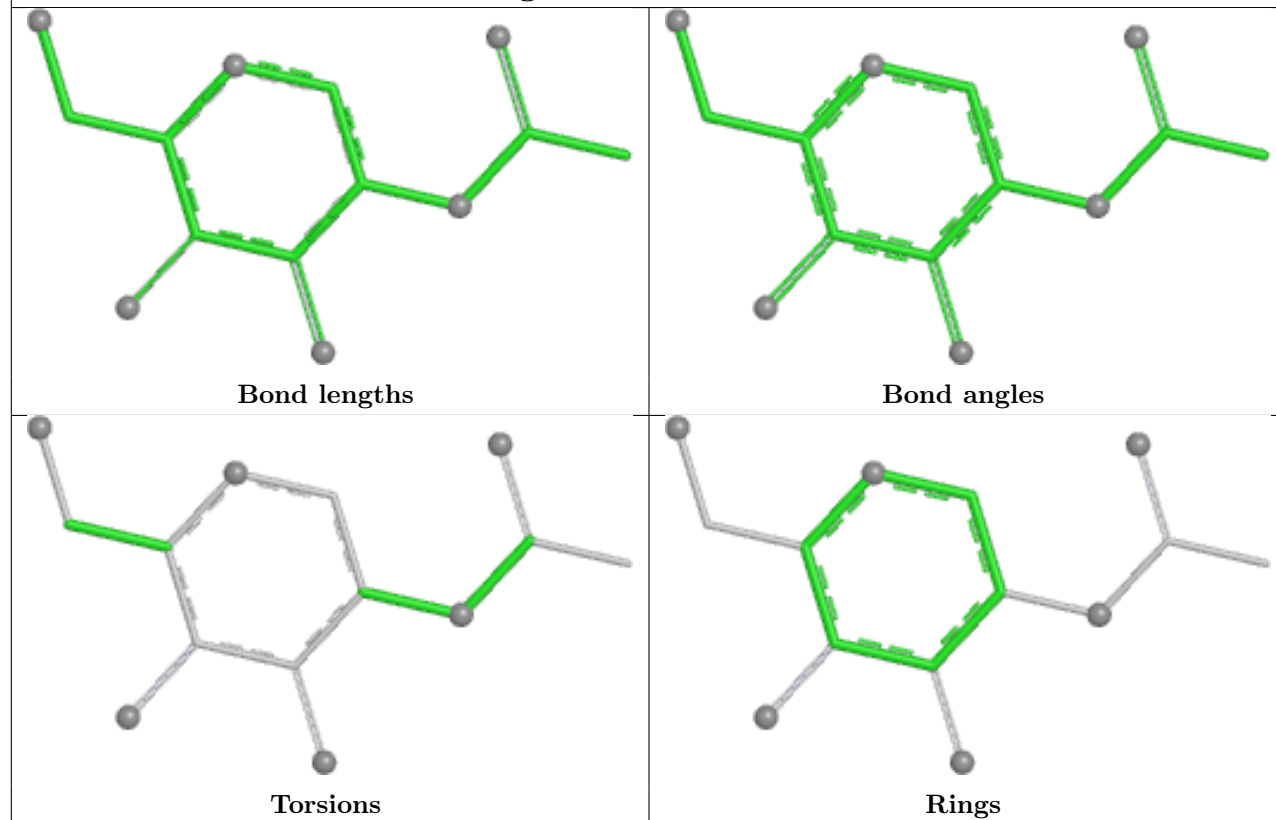




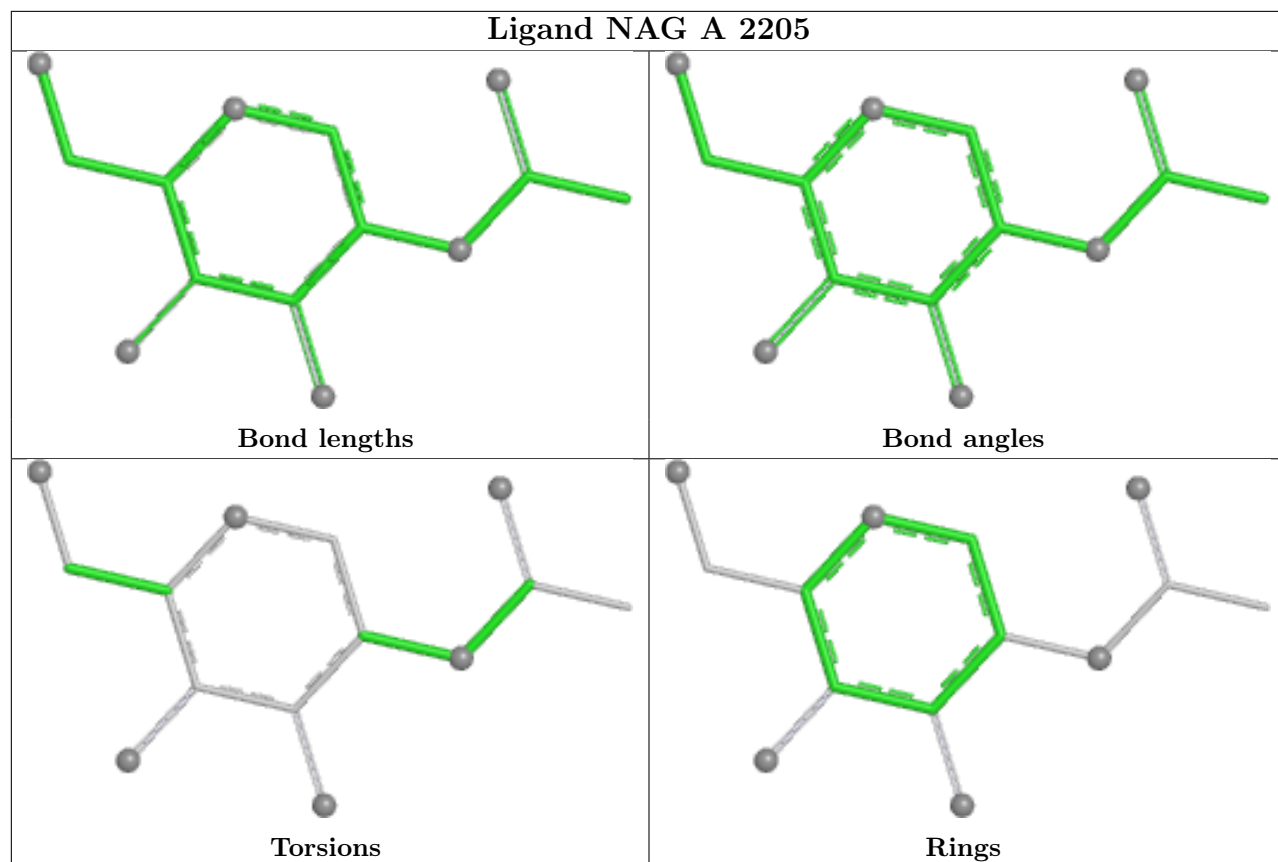
## Ligand NAG B 2202



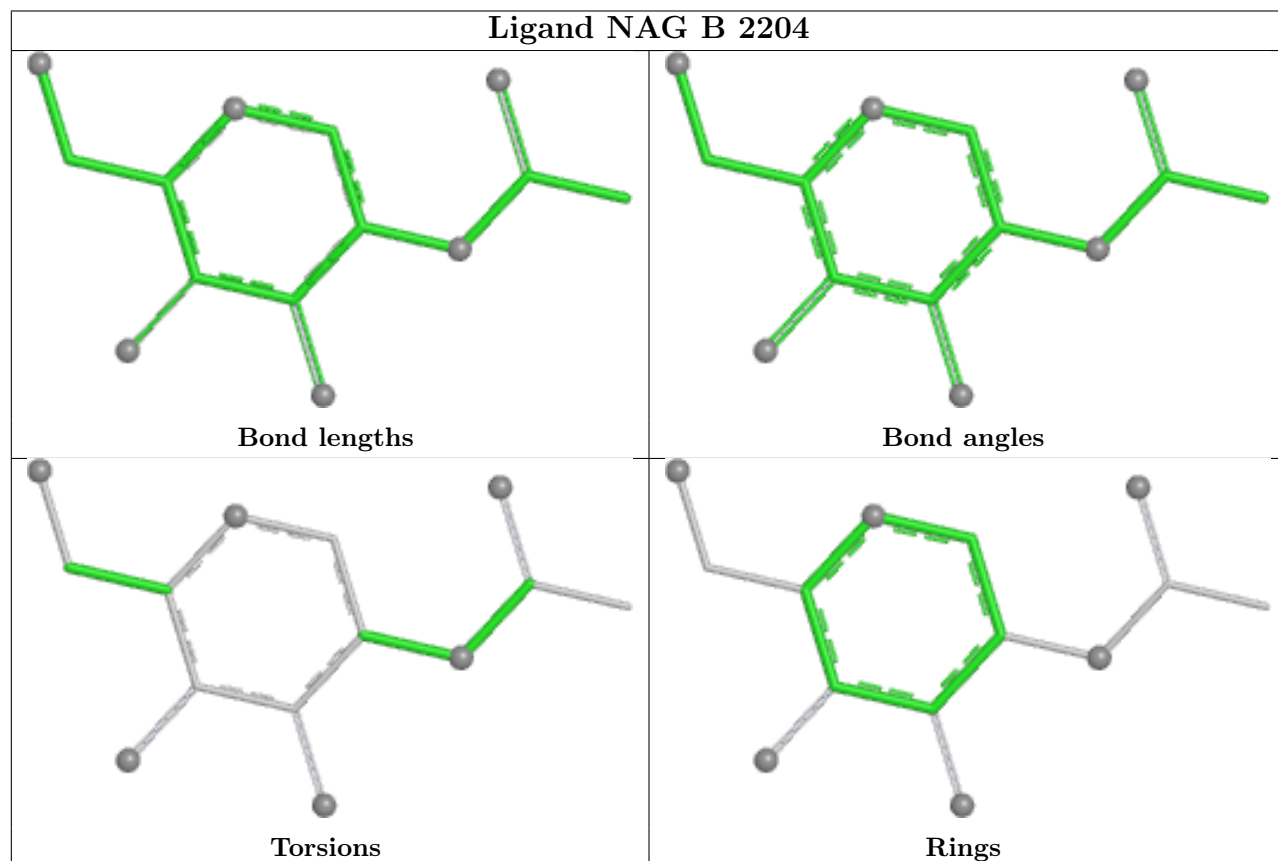
## Ligand NAG A 2203

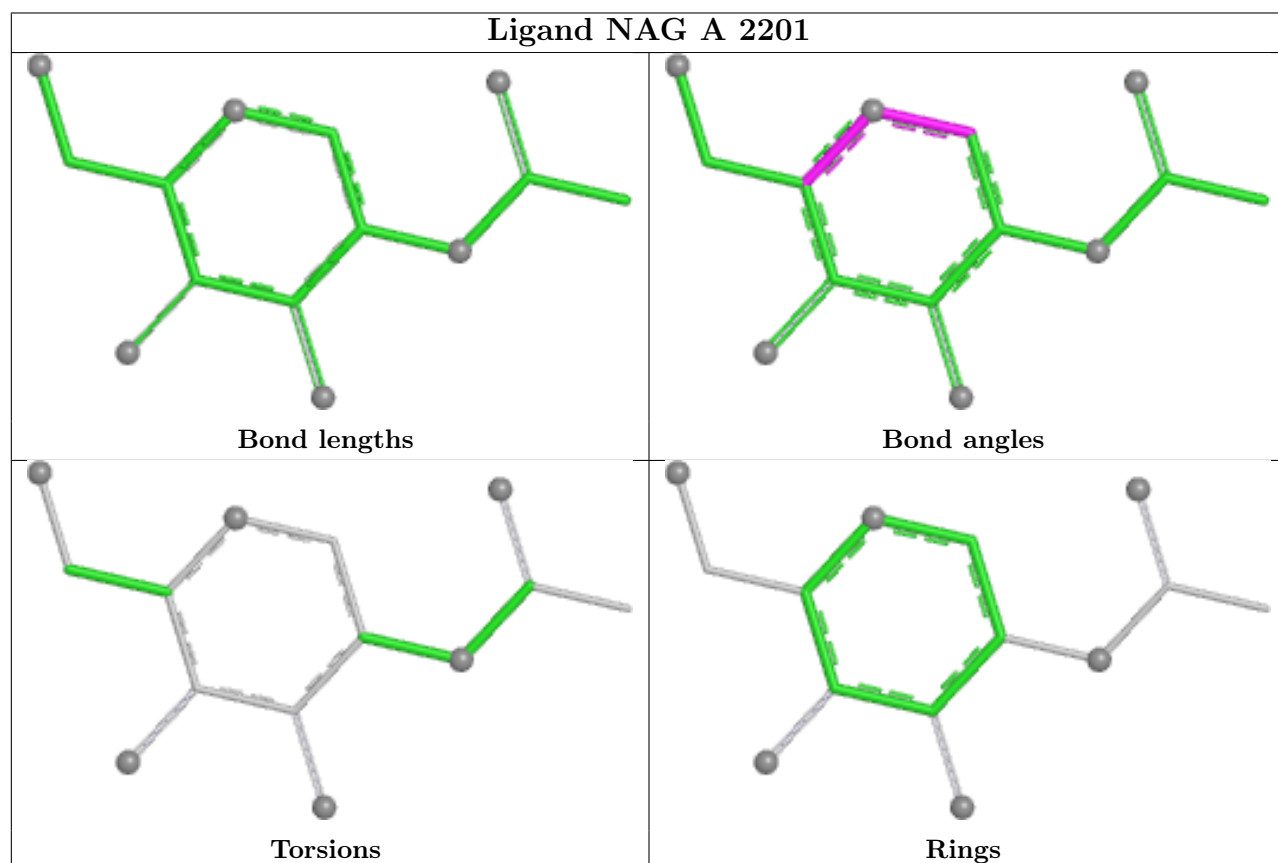
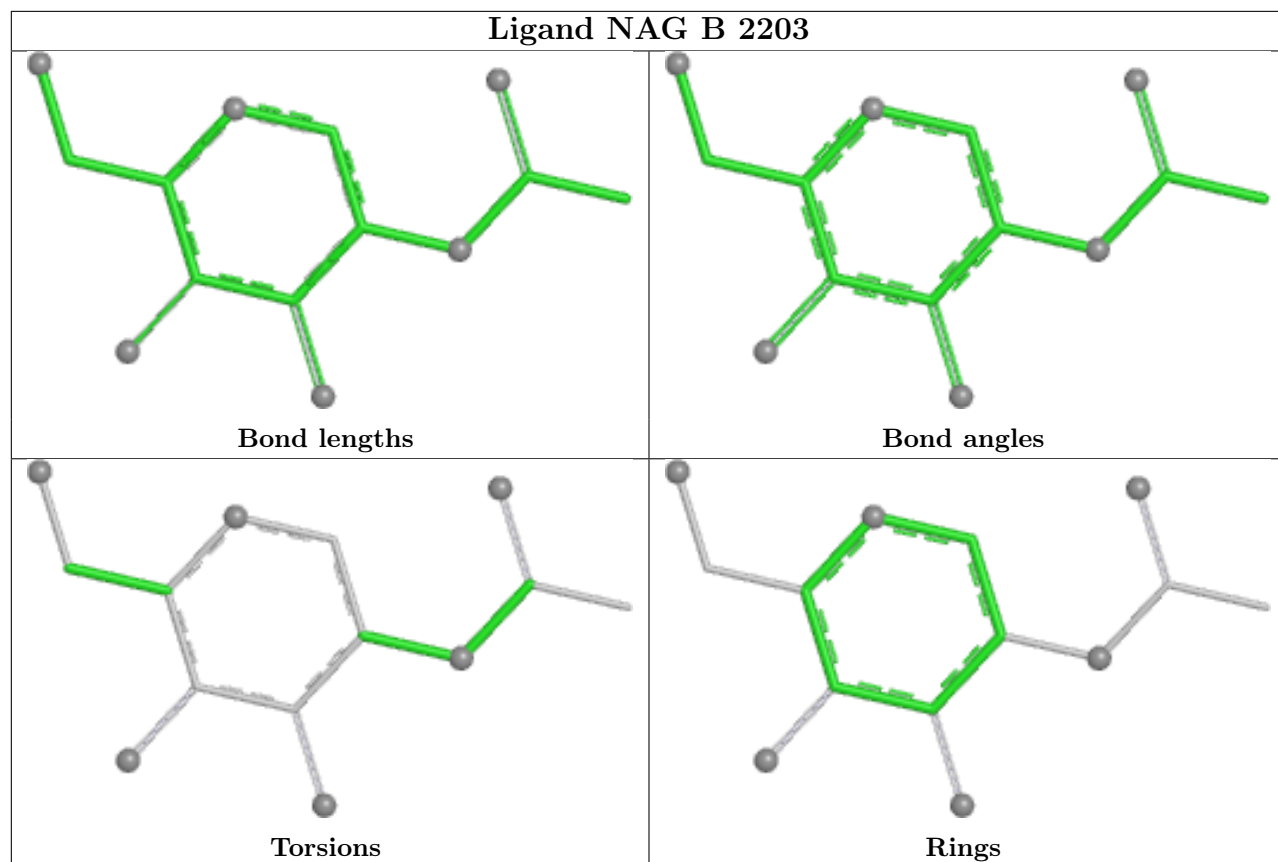


## Ligand NAG A 2205



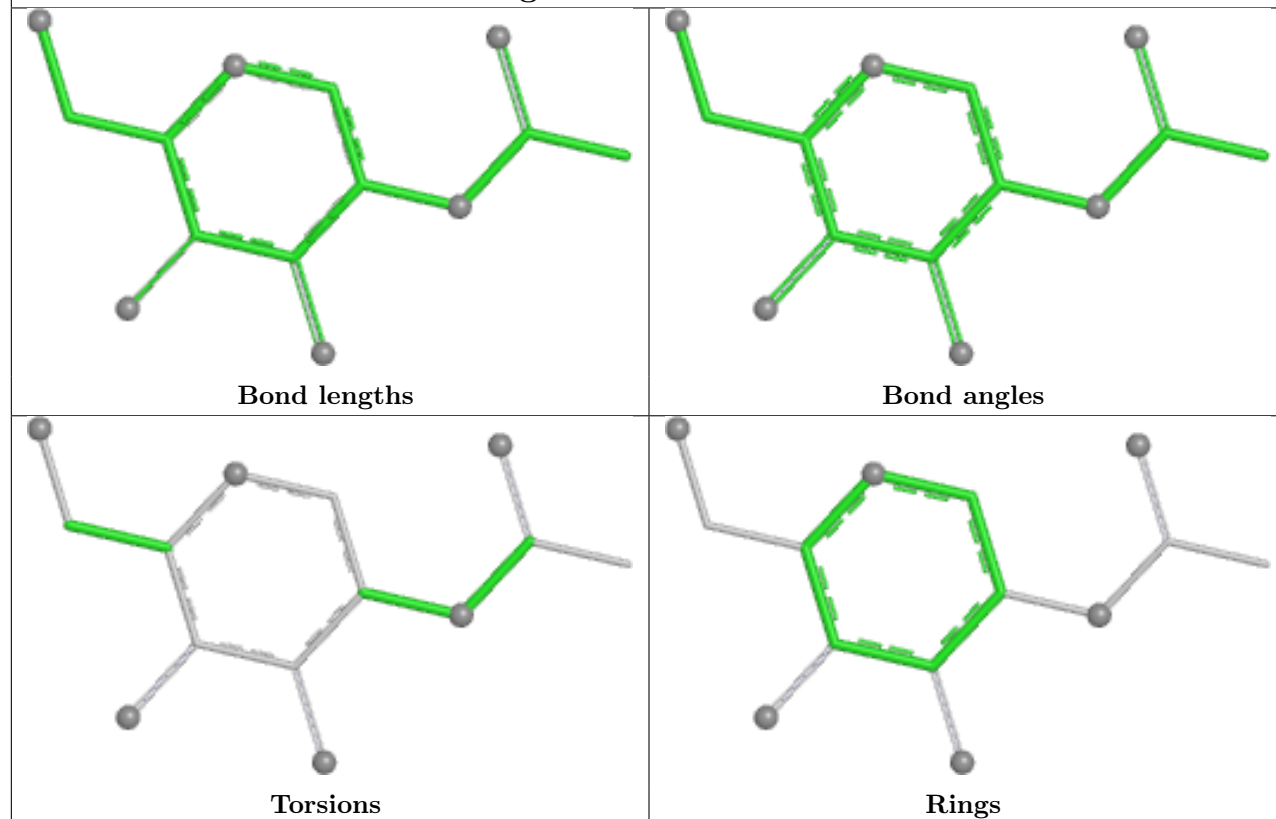
## Ligand NAG B 2204



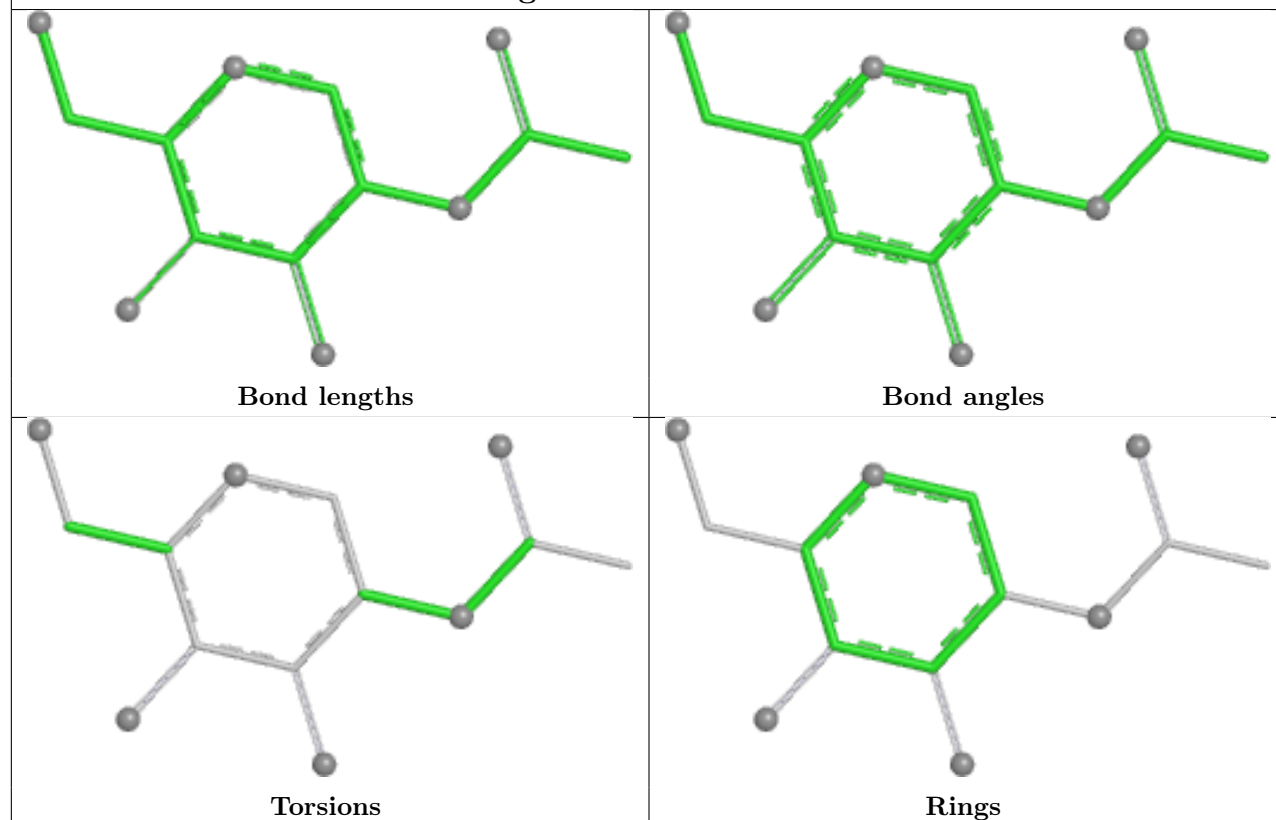




## Ligand NAG B 2201



## Ligand NAG A 2204



## 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.

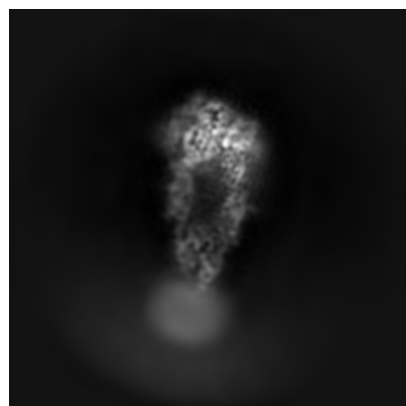
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47967. These allow visual inspection of the internal detail of the map and identification of artifacts.

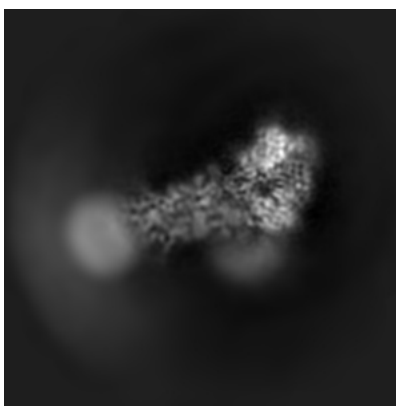
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

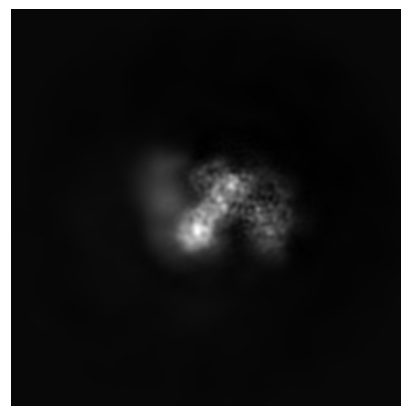
#### 6.1.1 Primary map



X

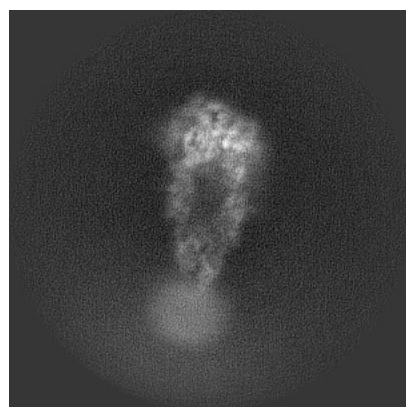


Y

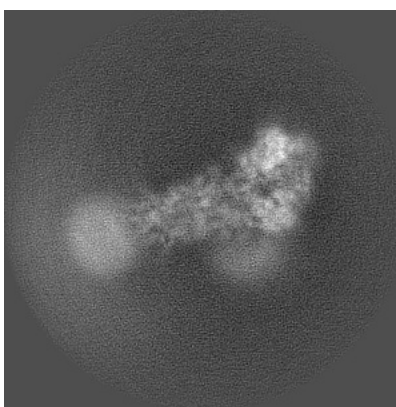


Z

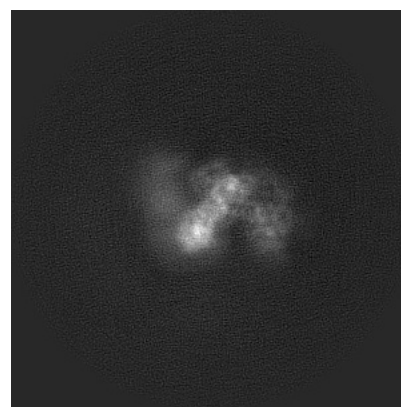
#### 6.1.2 Raw map



X



Y

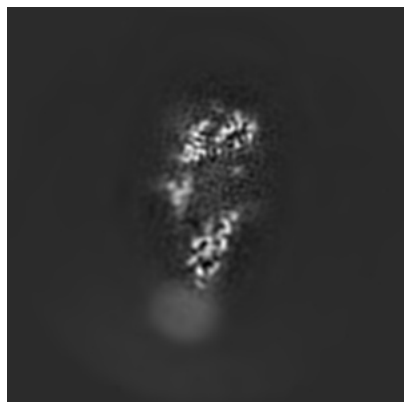


Z

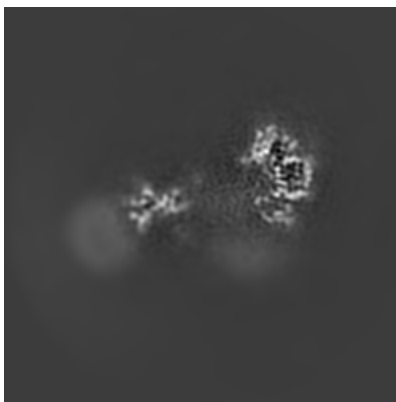
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

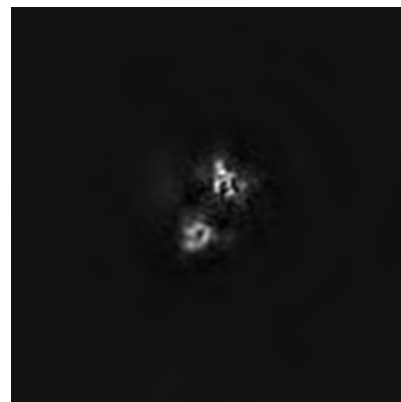
### 6.2.1 Primary map



X Index: 150

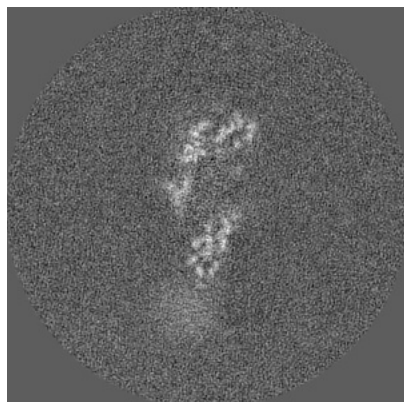


Y Index: 150

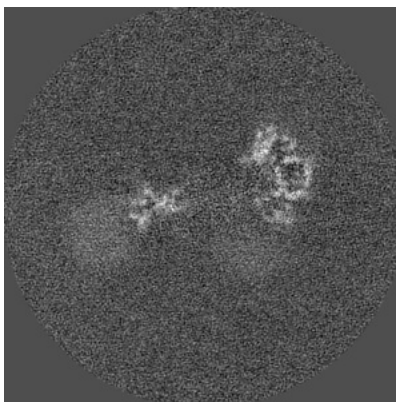


Z Index: 150

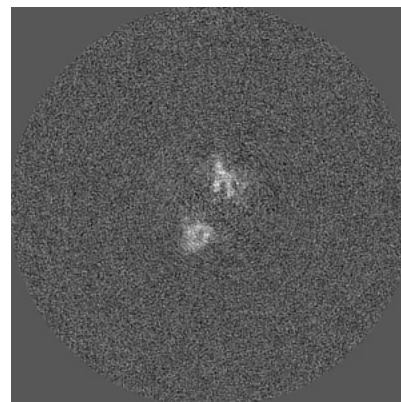
### 6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

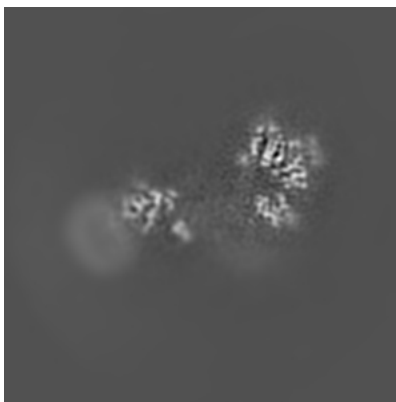
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

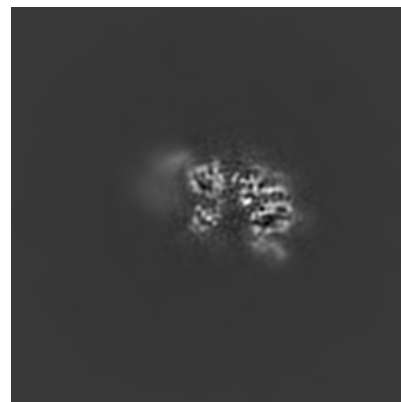
### 6.3.1 Primary map



X Index: 154

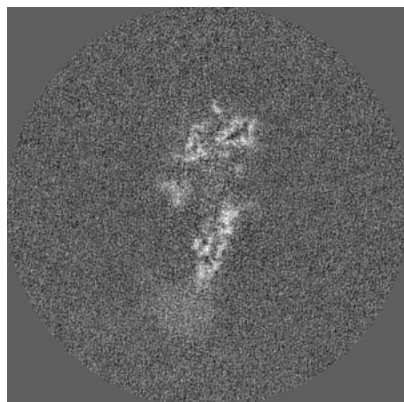


Y Index: 145

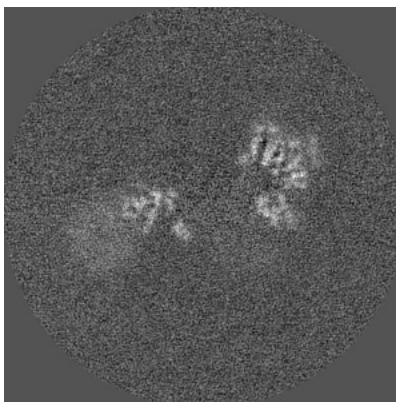


Z Index: 198

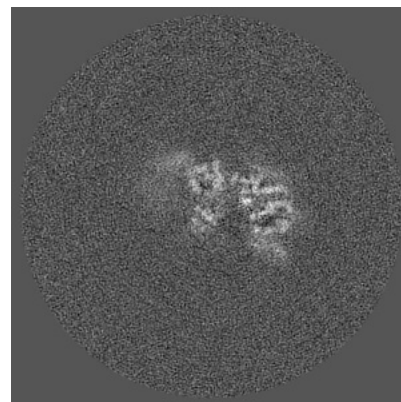
### 6.3.2 Raw map



X Index: 152



Y Index: 145



Z Index: 198

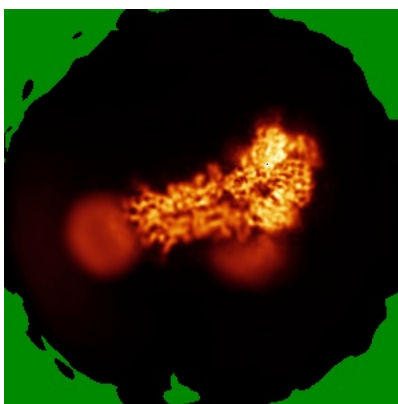
The images above show the largest variance slices of the map in three orthogonal directions.

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

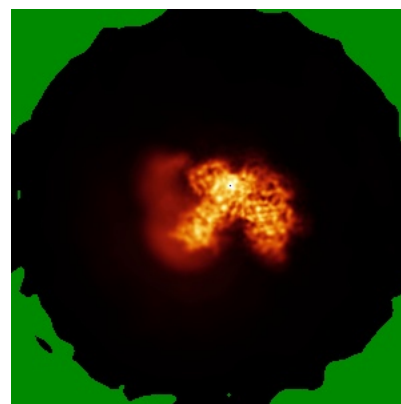
### 6.4.1 Primary map



X

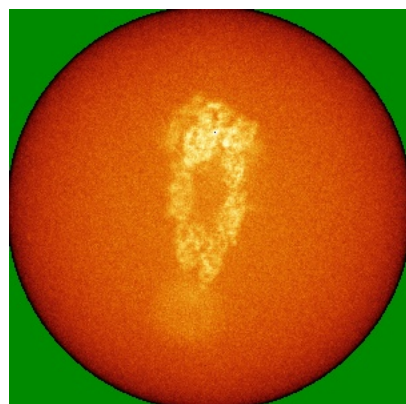


Y

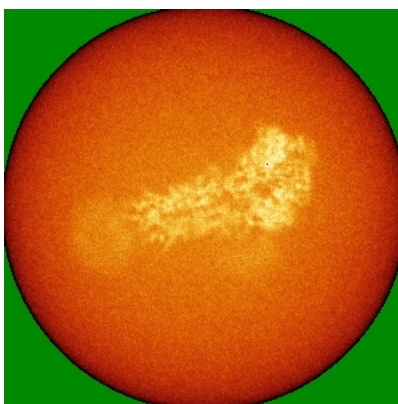


Z

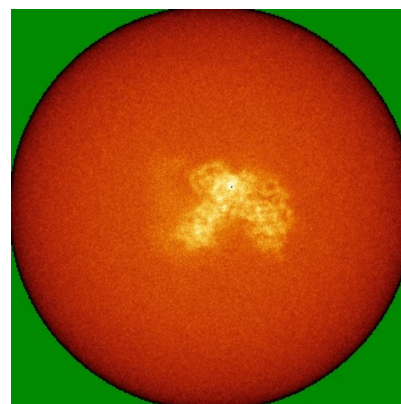
### 6.4.2 Raw map



X



Y



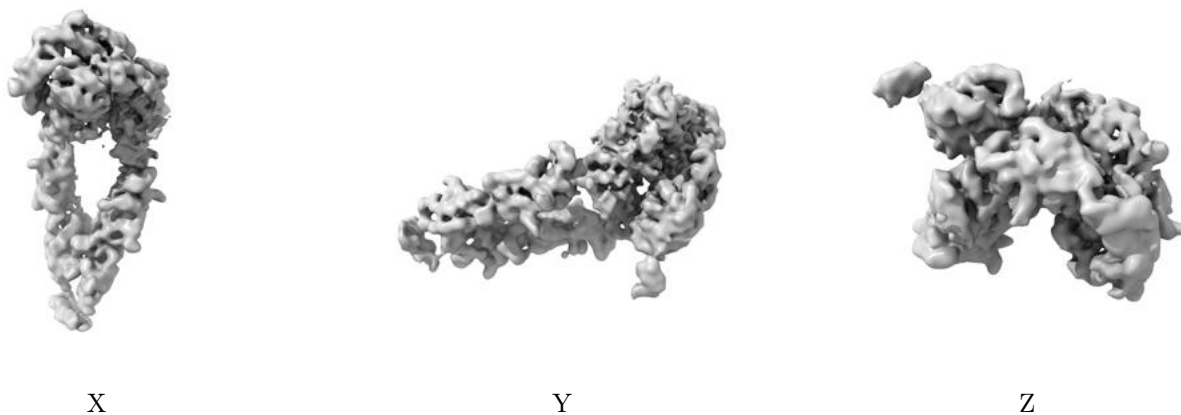
Z

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.



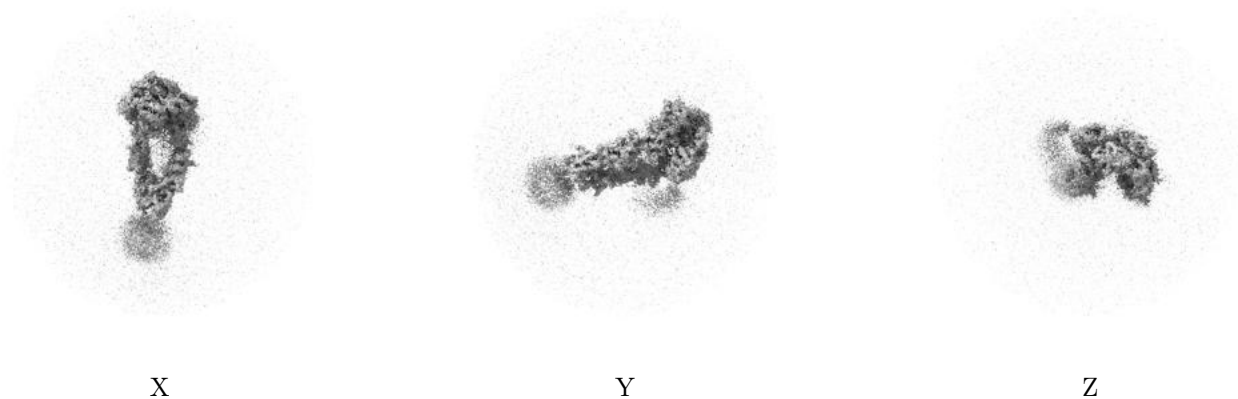
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

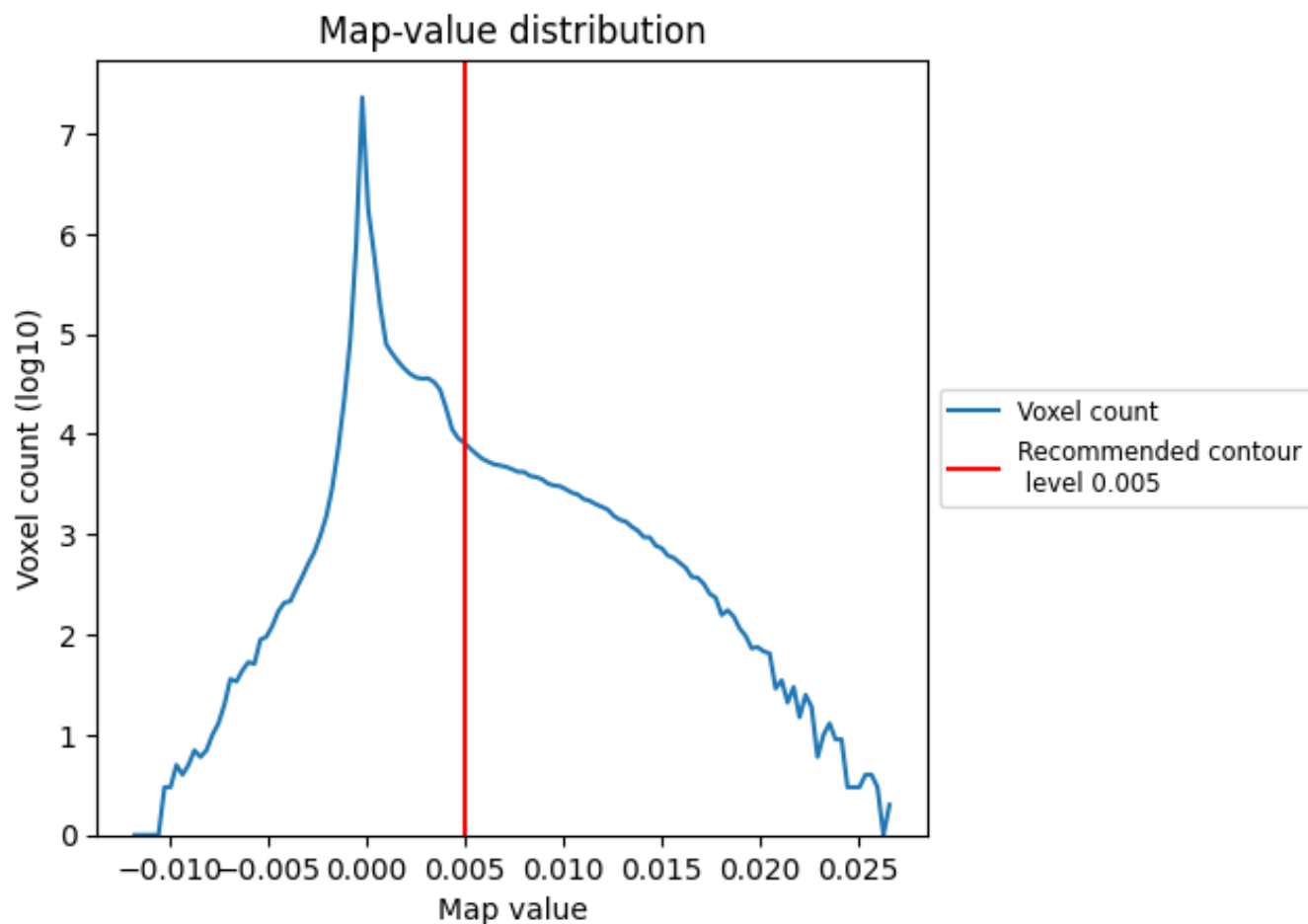
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

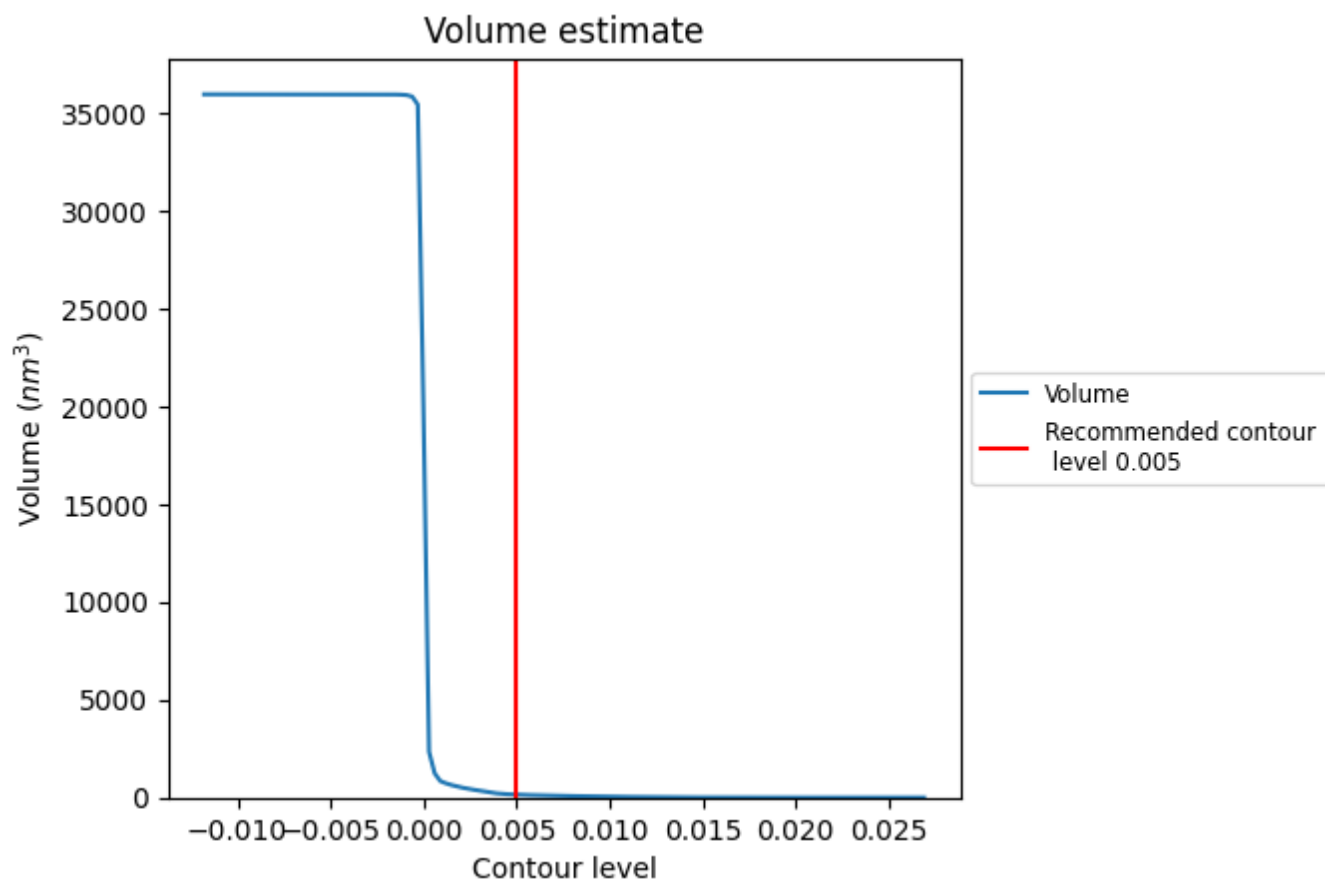
### 7.1 Map-value distribution [i](#)



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.



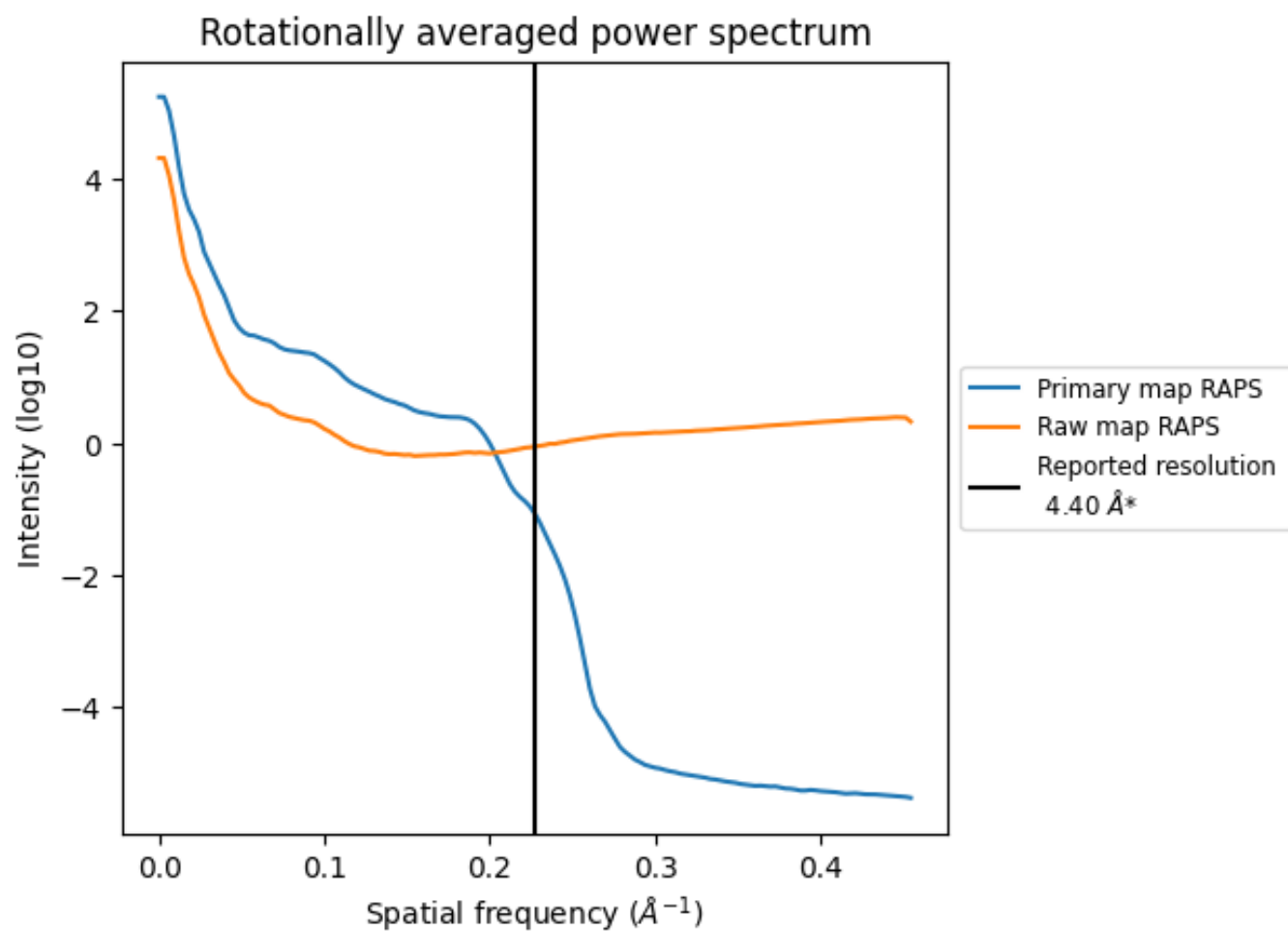
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150  $\text{nm}^3$ ; this corresponds to an approximate mass of 135 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 ⓘ

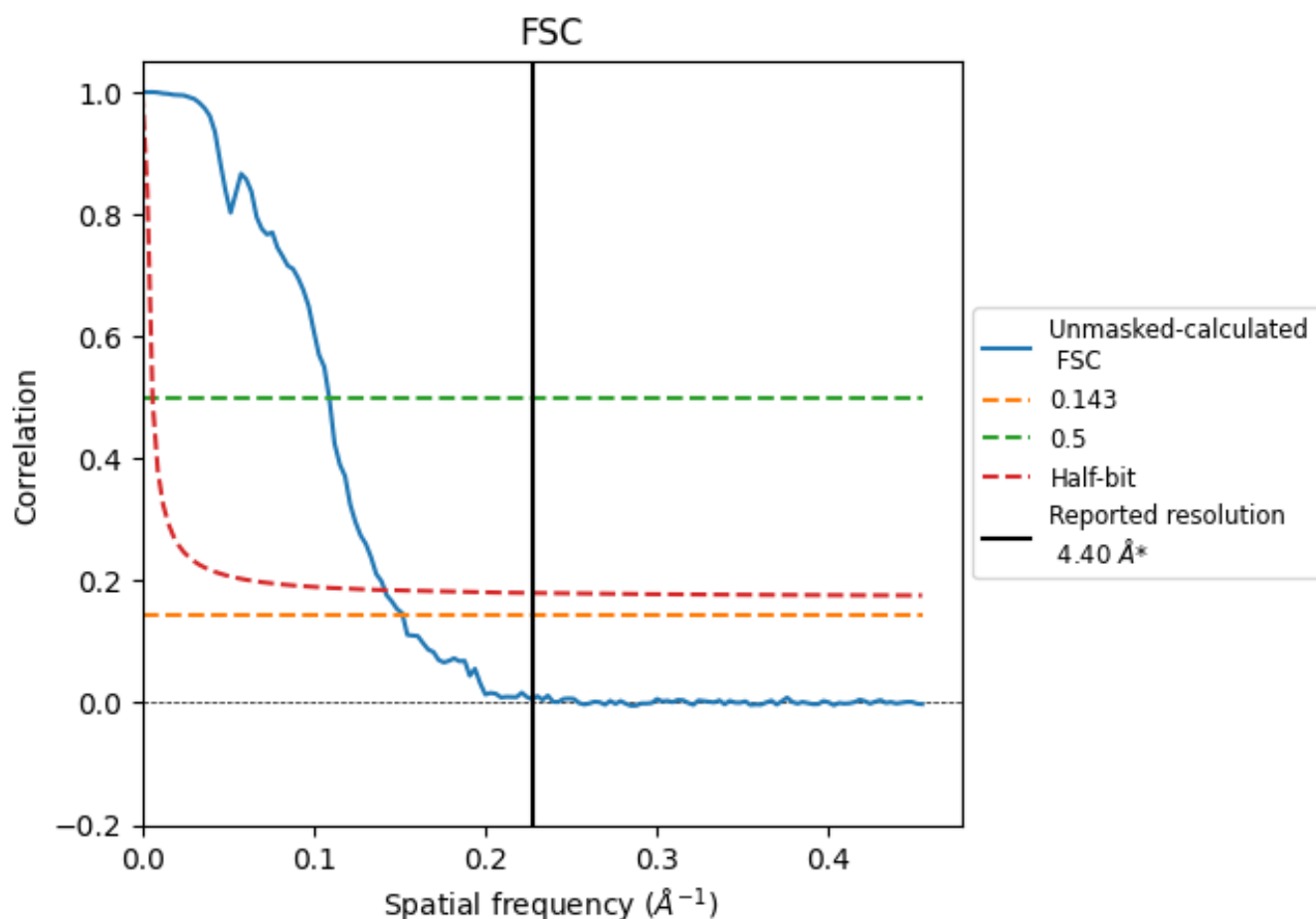


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 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 0.227  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

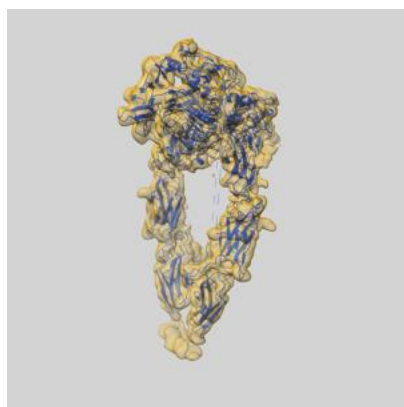
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.59	9.18	7.08

\*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 6.59 differs from the reported value 4.4 by more than 10 %

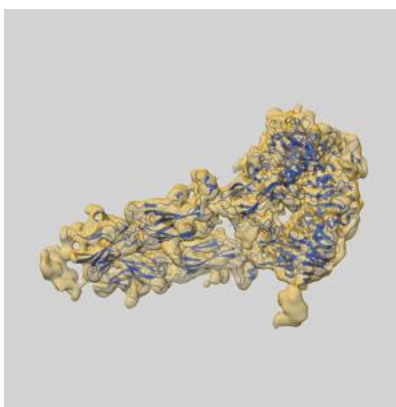
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47967 and PDB model 9EF1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

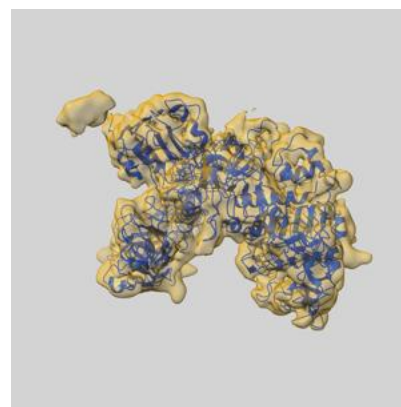
### 9.1 Map-model overlay [i](#)



X



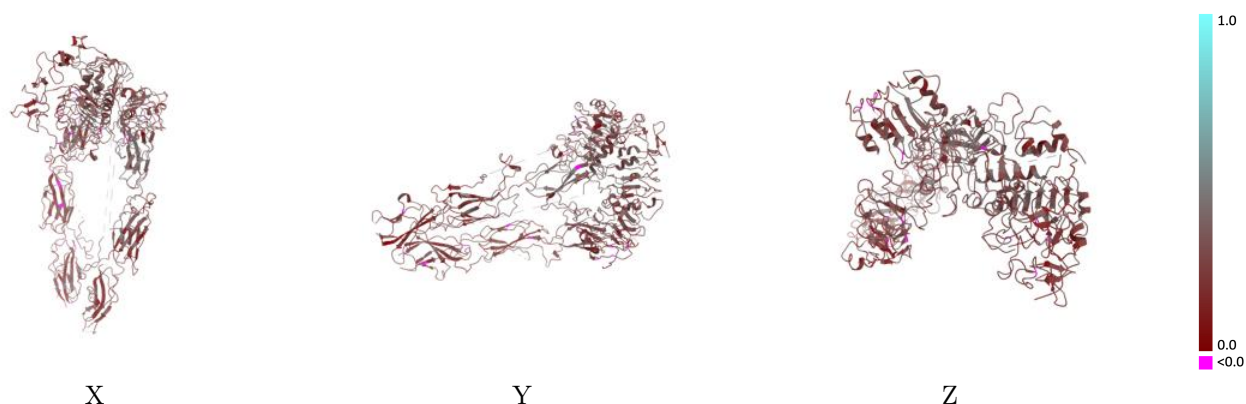
Y



Z

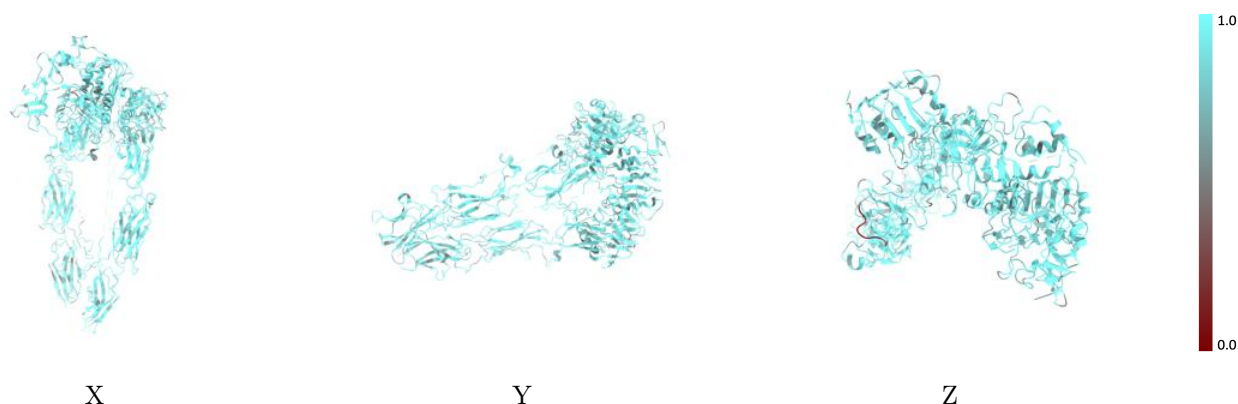
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



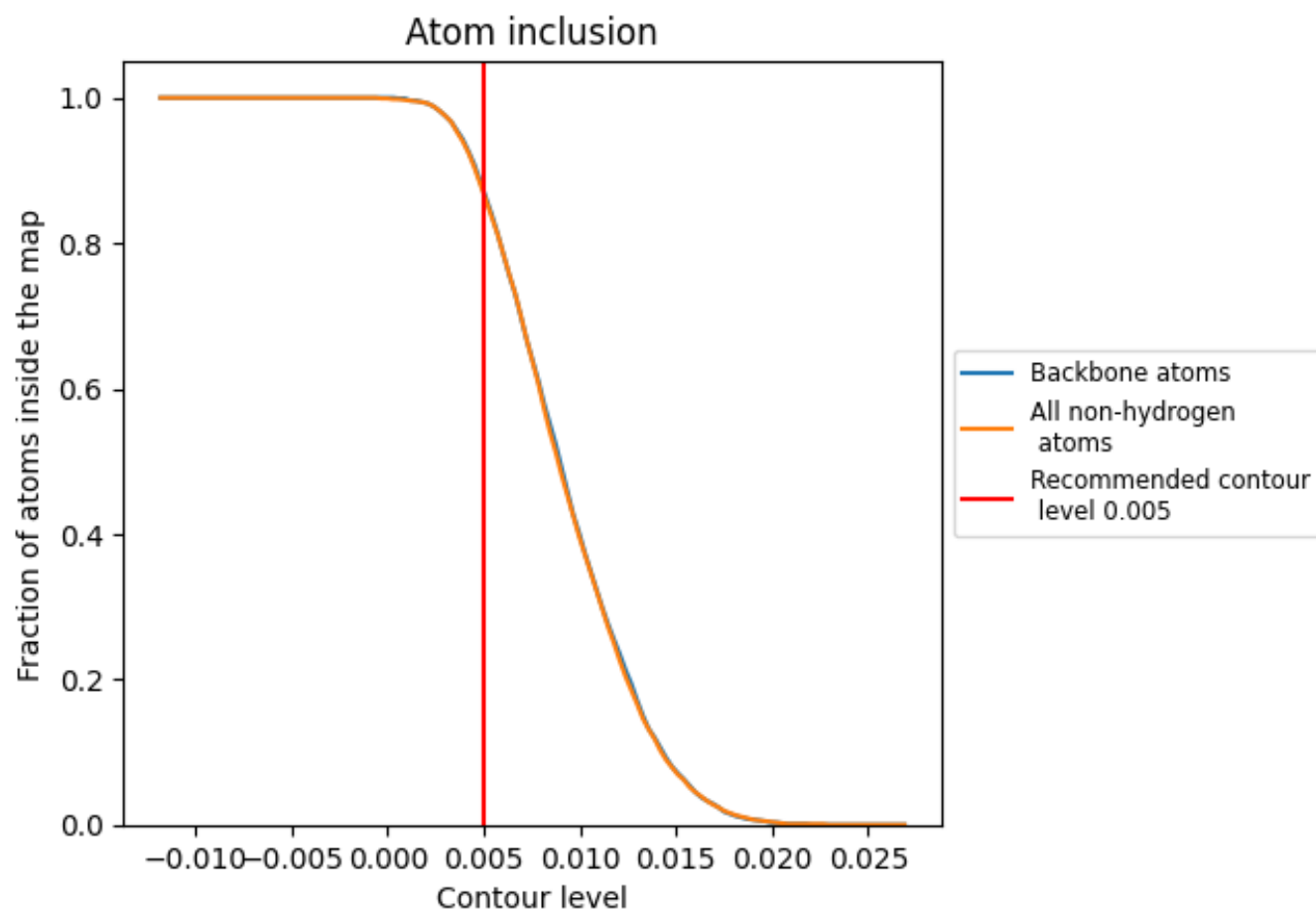
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8690	<div></div> 0.2830
A	<div></div> 0.8680	<div></div> 0.2720
B	<div></div> 0.8840	<div></div> 0.2990
C	<div></div> 0.9170	<div></div> 0.3100
D	<div></div> 0.9100	<div></div> 0.2970

