



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:25 PM UTC

PDB ID : 7L31 / pdb_00007l31
EMDB ID : EMD-23148
Title : Cyro-EM structure of human Glycine Receptor alpha2-beta heteromer, strychnine bound state, 3.8 Angstrom
Authors : Yu, H.; Wang, W.
Deposited on : 2020-12-17
Resolution : 3.80 Å(reported)
Based on initial model : 3JAD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

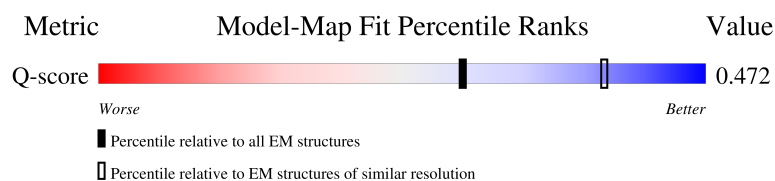
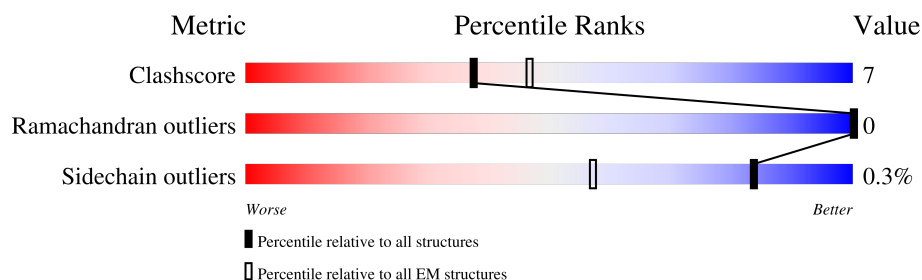
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	A	364	7% 81%12%7%
1	B	364	5% 77%16%7%
1	C	364	8% 81%12%7%
1	D	364	6% 73%20%7%

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Mol	Chain	Length	Quality of chain
2	E	702	37% 10% 53%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13596 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 Glycine receptor subunit alpha-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	339	Total	C	N	O	S	0	0
			2698	1754	437	490	17		
1	B	339	Total	C	N	O	S	0	0
			2697	1762	435	483	17		
1	C	339	Total	C	N	O	S	0	0
			2674	1741	432	484	17		
1	D	339	Total	C	N	O	S	0	0
			2663	1738	428	479	18		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLY	-	linker	UNP P23416
A	379	SER	-	linker	UNP P23416
A	380	SER	-	linker	UNP P23416
A	381	GLY	-	linker	UNP P23416
B	378	GLY	-	linker	UNP P23416
B	379	SER	-	linker	UNP P23416
B	380	SER	-	linker	UNP P23416
B	381	GLY	-	linker	UNP P23416
C	378	GLY	-	linker	UNP P23416
C	379	SER	-	linker	UNP P23416
C	380	SER	-	linker	UNP P23416
C	381	GLY	-	linker	UNP P23416
D	378	GLY	-	linker	UNP P23416
D	379	SER	-	linker	UNP P23416
D	380	SER	-	linker	UNP P23416
D	381	GLY	-	linker	UNP P23416

- Molecule 2 is a protein called Glycine receptor subunit beta, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	330	Total	C	N	O	S	0	0
			2613	1711	419	469	14		

There are 42 discrepancies between the modelled and reference sequences:

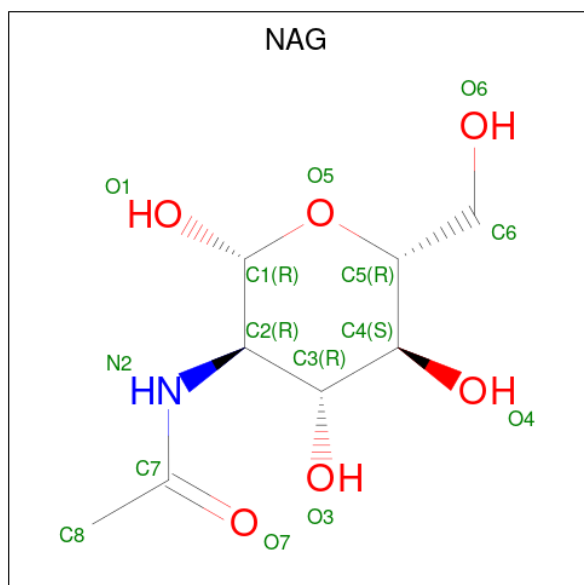
Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	GLY	-	expression tag	UNP P48167
E	-18	VAL	-	expression tag	UNP P48167
E	-17	ALA	-	expression tag	UNP P48167
E	-16	MET	-	expression tag	UNP P48167
E	-15	PRO	-	expression tag	UNP P48167
E	-14	GLY	-	expression tag	UNP P48167
E	-13	ALA	-	expression tag	UNP P48167
E	-12	GLU	-	expression tag	UNP P48167
E	-11	ASP	-	expression tag	UNP P48167
E	-10	ASP	-	expression tag	UNP P48167
E	-9	VAL	-	expression tag	UNP P48167
E	-8	VAL	-	expression tag	UNP P48167
E	-7	ALA	-	expression tag	UNP P48167
E	-6	ALA	-	expression tag	UNP P48167
E	-5	LEU	-	expression tag	UNP P48167
E	-4	GLU	-	expression tag	UNP P48167
E	-3	VAL	-	expression tag	UNP P48167
E	-2	LEU	-	expression tag	UNP P48167
E	-1	PHE	-	expression tag	UNP P48167
E	0	GLN	-	expression tag	UNP P48167
E	1	GLY	-	expression tag	UNP P48167
E	2	PRO	-	expression tag	UNP P48167
E	331A	LEU	-	linker	UNP P48167
E	331B	ASN	-	linker	UNP P48167
E	331C	GLY	-	linker	UNP P48167
E	331D	GLY	-	linker	UNP P48167
E	331E	SER	-	linker	UNP P48167
E	331F	SER	-	linker	UNP P48167
E	331G	ALA	-	linker	UNP P48167
E	331H	ALA	-	linker	UNP P48167
E	331I	ALA	-	linker	UNP P48167
E	331J	VAL	-	linker	UNP P48167
E	333U	LEU	PHE	engineered mutation	UNP P42212
E	333V	THR	SER	engineered mutation	UNP P42212
E	339G	LYS	ALA	engineered mutation	UNP P42212
E	340F	LEU	HIS	engineered mutation	UNP P42212
E	340N	SER	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	340O	GLY	-	linker	UNP P42212
E	340P	SER	-	linker	UNP P42212
E	340Q	GLY	-	linker	UNP P42212
E	340R	SER	-	linker	UNP P42212
E	340S	GLY	-	linker	UNP P42212

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



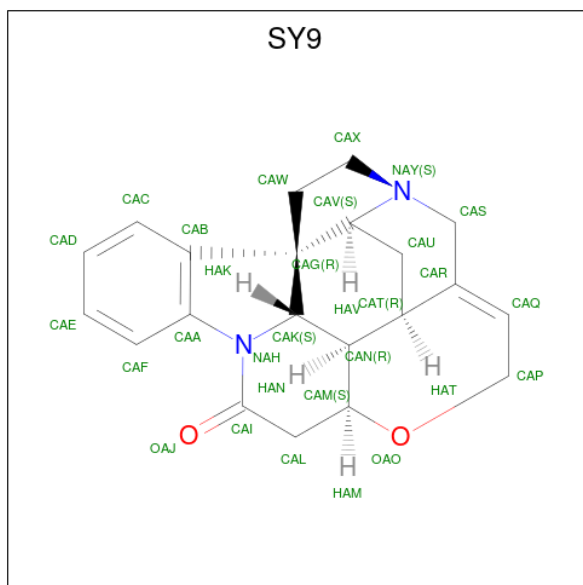
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 4 is STRYCHNINE (CCD ID: SY9) (formula: $C_{21}H_{22}N_2O_2$) (labeled as "Ligand of Interest" by depositor).

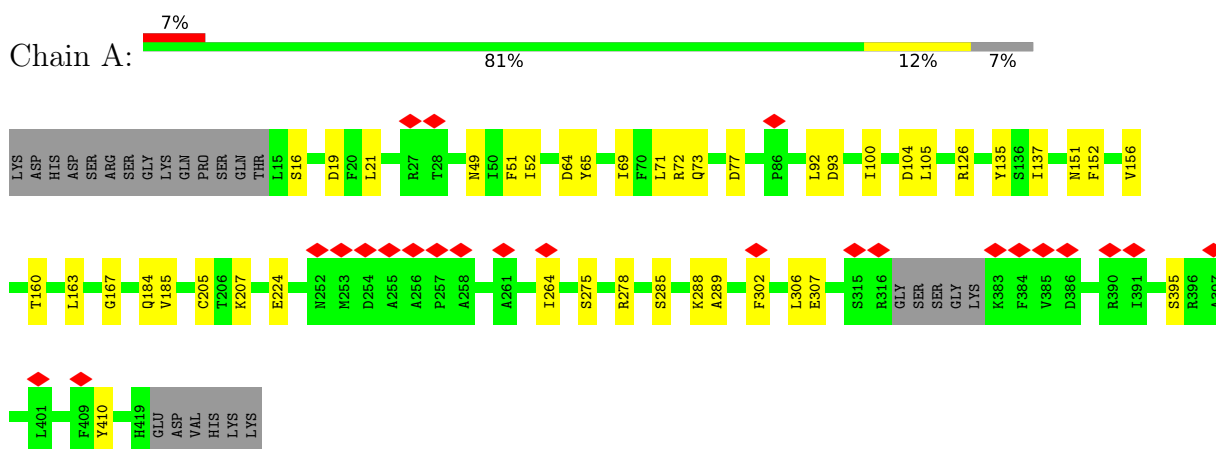


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			25	21	2	2	
4	B	1	Total	C	N	O	0
			25	21	2	2	
4	C	1	Total	C	N	O	0
			25	21	2	2	
4	D	1	Total	C	N	O	0
			25	21	2	2	
4	D	1	Total	C	N	O	0
			25	21	2	2	

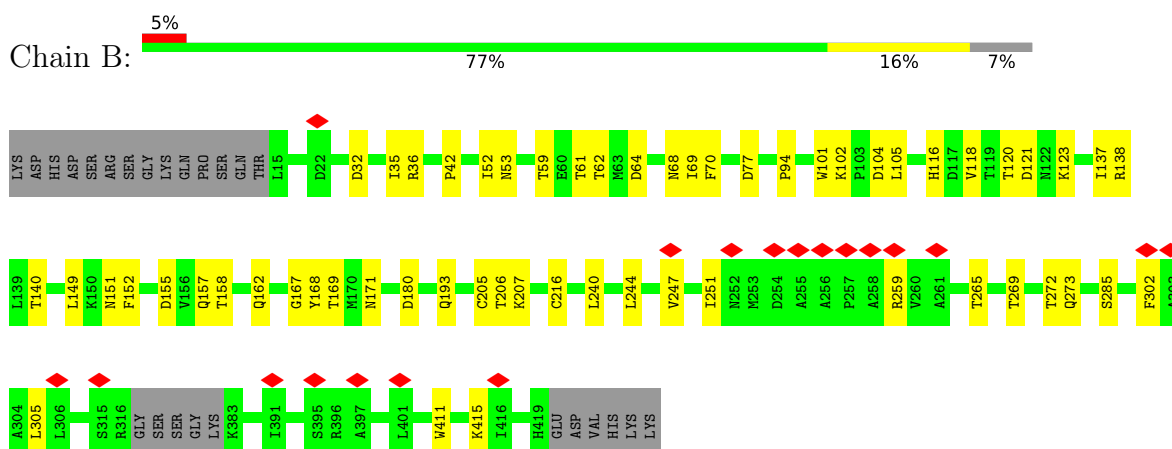
3 Residue-property plots

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.

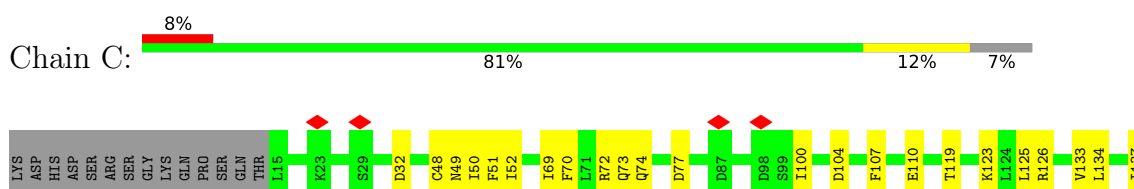
- Molecule 1: Glycine receptor subunit alpha-2

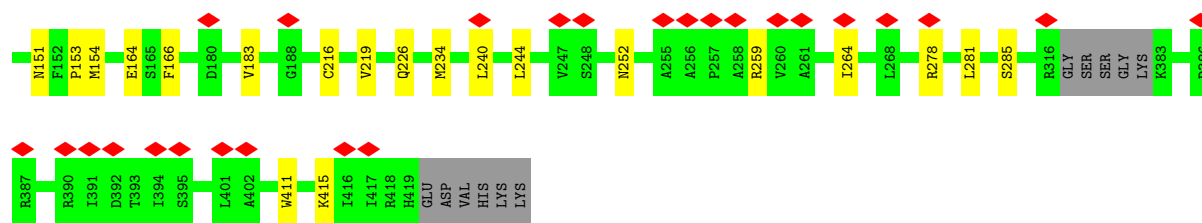


- Molecule 1: Glycine receptor subunit alpha-2

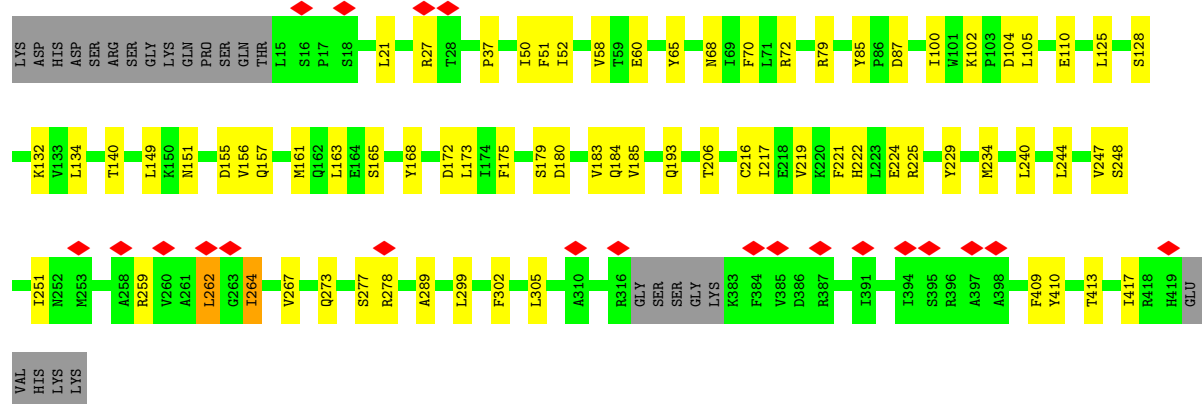


- Molecule 1: Glycine receptor subunit alpha-2

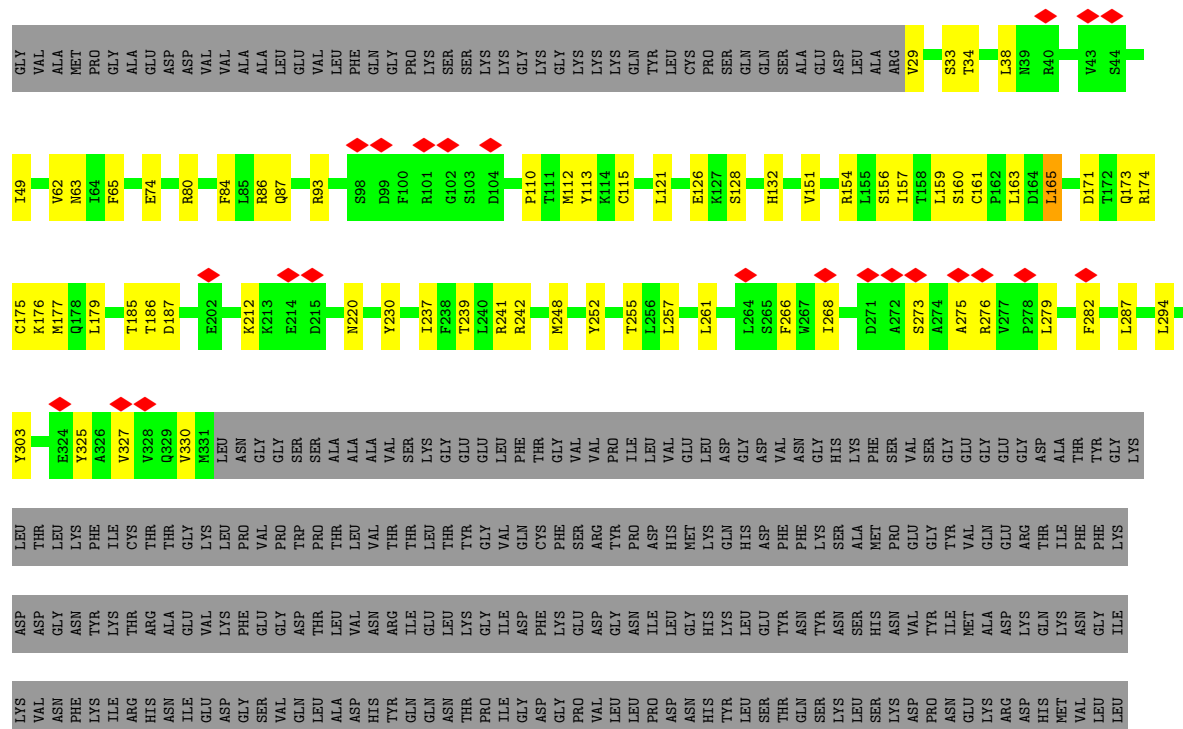
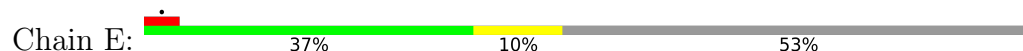




• Molecule 1: Glycine receptor subunit alpha-2



• Molecule 2: Glycine receptor subunit beta, Green fluorescent protein



GLU
PHE
VAL
THR
ALA
GLY
ILE
THR
LEU
GLY
MET
ASP
GLU
LEU
TYR
LYS
SER
GLY
SER
GLY
GLY
VAL
GLY
GLU
THR
ARG
CYS
LYS
LYS
VAL
CYS
THR
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LYS
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PRO
PRO
ALA
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VAL
ILE
PRO
THR
ALA
ALA
K449
L453
L458
V468
S472
L475

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38541	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0185	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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, SY9

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	A	0.21	0/2766	0.48	0/3761
1	B	0.26	0/2766	0.49	0/3761
1	C	0.22	0/2741	0.45	0/3729
1	D	0.24	0/2731	0.48	0/3717
2	E	0.23	0/2681	0.51	0/3655
All	All	0.23	0/13685	0.48	0/18623

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	A	2698	0	2648	29	0
1	B	2697	0	2662	41	0
1	C	2674	0	2623	39	0
1	D	2663	0	2600	69	0
2	E	2613	0	2559	57	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	26	0	0
3	E	14	0	13	1	0
4	A	25	0	22	1	0
4	B	25	0	22	2	0
4	C	25	0	22	1	0
4	D	50	0	44	4	0
All	All	13596	0	13319	201	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 7.

All (201) 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)
1:C:264:ILE:HG13	1:D:262:LEU:CD1	1.60	1.30
1:C:264:ILE:CG1	1:D:262:LEU:CD1	2.27	1.11
1:C:264:ILE:CG1	1:D:262:LEU:HD12	1.80	1.10
1:C:264:ILE:HG13	1:D:262:LEU:HD12	1.14	1.09
1:C:264:ILE:CD1	1:D:262:LEU:CD1	2.42	0.97
1:C:264:ILE:HG13	1:D:262:LEU:HD13	1.49	0.92
1:D:58:VAL:HG12	1:D:65:TYR:CB	2.01	0.91
1:D:58:VAL:HG12	1:D:65:TYR:HB2	1.53	0.87
1:C:264:ILE:CG1	1:D:262:LEU:HD13	2.00	0.87
1:C:264:ILE:CD1	1:D:262:LEU:HD12	2.04	0.86
1:D:264:ILE:HG21	2:E:282:PHE:HB2	1.61	0.82
1:C:264:ILE:HD11	1:D:262:LEU:CD1	2.10	0.80
1:D:58:VAL:HG12	1:D:65:TYR:HB3	1.72	0.69
2:E:165:LEU:HD23	2:E:303:TYR:OH	1.93	0.69
2:E:29:VAL:N	2:E:33:SER:HG	1.92	0.68
2:E:165:LEU:H	2:E:165:LEU:CD2	2.07	0.68
1:D:305:LEU:HD13	2:E:261:LEU:HD11	1.75	0.67
1:B:94:PRO:HB2	1:B:121:ASP:OD2	1.95	0.66
1:B:305:LEU:HD23	1:C:244:LEU:HD11	1.78	0.65
1:C:264:ILE:HD11	1:D:262:LEU:HD11	1.78	0.64
1:A:126:ARG:HH11	4:A:503:SY9:HAE	1.64	0.63
1:D:168:TYR:HB3	1:D:172:ASP:HB2	1.83	0.61
1:D:251:ILE:O	1:D:259:ARG:NH2	2.34	0.61
1:A:156:VAL:HG12	1:A:224:GLU:HG2	1.81	0.61
1:A:167:GLY:HA2	4:B:503:SY9:HAC	1.82	0.61
1:D:264:ILE:CG2	2:E:282:PHE:HB2	2.30	0.61
1:D:58:VAL:HG23	1:D:58:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:268:ILE:HG21	2:E:275:ALA:HB3	1.82	0.60
1:B:206:THR:HG22	1:B:206:THR:O	2.02	0.59
2:E:255:THR:HG23	2:E:287:LEU:HD11	1.84	0.59
1:D:264:ILE:CD1	2:E:279:LEU:HA	2.32	0.59
2:E:171:ASP:OD2	2:E:173:GLN:NE2	2.35	0.58
2:E:74:GLU:OE2	2:E:242:ARG:NH2	2.37	0.57
1:C:100:ILE:HD13	1:C:125:LEU:HD21	1.86	0.57
2:E:174:ARG:NH2	2:E:239:THR:OG1	2.38	0.56
1:A:93:ASP:OD1	1:A:93:ASP:N	2.38	0.56
1:D:278:ARG:HG3	2:E:294:LEU:HD21	1.87	0.56
1:C:285:SER:O	1:D:229:TYR:N	2.37	0.56
1:B:53:ASN:HD22	1:B:138:ARG:HH21	1.55	0.55
1:D:155:ASP:OD2	1:D:157:GLN:NE2	2.38	0.55
1:C:183:VAL:HG21	1:C:219:VAL:HG21	1.88	0.55
1:B:285:SER:OG	1:C:226:GLN:O	2.23	0.55
1:A:285:SER:HB3	1:B:193:GLN:HG2	1.89	0.55
1:D:299:LEU:HD12	2:E:257:LEU:HD21	1.89	0.55
1:B:121:ASP:O	1:B:121:ASP:OD1	2.24	0.54
1:C:49:ASN:HD21	1:C:72:ARG:HH11	1.55	0.54
1:B:180:ASP:OD1	1:B:180:ASP:N	2.40	0.54
1:D:165:SER:HB2	1:D:173:LEU:HD23	1.89	0.54
2:E:165:LEU:HD23	2:E:165:LEU:H	1.73	0.54
1:C:153:PRO:HG2	1:C:154:MET:HE2	1.90	0.54
2:E:65:PHE:HB3	2:E:84:PHE:HB2	1.89	0.54
1:D:264:ILE:CG2	2:E:282:PHE:CB	2.87	0.53
1:A:52:ILE:HG22	1:A:69:ILE:HG22	1.91	0.53
2:E:132:HIS:HD2	2:E:154:ARG:HG2	1.74	0.53
2:E:80:ARG:NH1	2:E:156:SER:OG	2.41	0.53
2:E:220:ASN:HB3	3:E:501:NAG:H82	1.90	0.53
1:D:72:ARG:NH2	4:D:503:SY9:OAJ	2.42	0.53
1:A:52:ILE:HD11	1:A:185:VAL:HG22	1.90	0.52
1:B:36:ARG:NH1	1:B:42:PRO:O	2.37	0.52
1:D:193:GLN:OE1	1:D:225:ARG:NH1	2.42	0.52
1:D:37:PRO:HA	1:D:79:ARG:HH22	1.74	0.52
2:E:266:PHE:O	2:E:276:ARG:NH1	2.43	0.52
2:E:63:ASN:OD1	2:E:86:ARG:NH2	2.42	0.52
1:A:104:ASP:OD1	1:A:104:ASP:N	2.39	0.52
1:B:104:ASP:N	1:B:104:ASP:OD1	2.41	0.52
1:D:183:VAL:HG21	1:D:219:VAL:HG21	1.92	0.51
2:E:165:LEU:CD2	2:E:303:TYR:OH	2.57	0.51
1:B:116:HIS:NE2	1:B:140:THR:OG1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ILE:HD13	1:D:161:MET:HE1	1.93	0.51
1:D:100:ILE:HD13	1:D:125:LEU:HD21	1.92	0.51
2:E:165:LEU:HD23	2:E:165:LEU:N	2.25	0.51
1:D:264:ILE:HD11	2:E:279:LEU:HA	1.93	0.51
1:D:264:ILE:HG21	2:E:282:PHE:CB	2.36	0.51
2:E:273:SER:OG	2:E:325:TYR:OH	2.26	0.51
1:A:49:ASN:HD21	1:A:72:ARG:HH21	1.58	0.51
1:B:251:ILE:O	1:B:259:ARG:NH2	2.45	0.50
2:E:185:THR:OG1	2:E:187:ASP:OD1	2.25	0.50
1:A:77:ASP:N	1:A:77:ASP:OD1	2.44	0.50
1:C:164:GLU:HG3	1:C:216:CYS:HB2	1.93	0.50
1:A:152:PHE:HB2	1:A:288:LYS:HD2	1.93	0.50
1:D:105:LEU:HD21	1:D:163:LEU:HD23	1.93	0.50
2:E:159:LEU:HD13	2:E:177:MET:HB2	1.93	0.50
1:D:267:VAL:HG21	1:D:305:LEU:HD12	1.94	0.50
1:C:77:ASP:N	1:C:77:ASP:OD1	2.43	0.50
1:D:413:THR:HA	1:D:417:ILE:HD12	1.93	0.50
1:A:16:SER:OG	1:A:19:ASP:OD1	2.30	0.50
1:A:289:ALA:O	1:A:410:TYR:OH	2.23	0.50
1:D:244:LEU:O	1:D:248:SER:OG	2.29	0.49
2:E:49:ILE:O	2:E:93:ARG:NH2	2.40	0.49
1:B:105:LEU:O	1:C:119:THR:OG1	2.30	0.49
1:B:169:THR:OG1	1:B:171:ASN:OD1	2.28	0.49
2:E:165:LEU:CD2	2:E:165:LEU:N	2.73	0.49
4:D:504:SY9:HAQ	2:E:84:PHE:CG	2.48	0.48
1:B:62:THR:OG1	1:B:64:ASP:OD2	2.29	0.48
1:B:70:PHE:CG	4:B:503:SY9:HAQ	2.48	0.48
1:D:206:THR:H	1:D:216:CYS:HB3	1.78	0.48
1:B:149:LEU:HD22	1:B:152:PHE:HD1	1.77	0.48
1:A:92:LEU:HD22	1:A:100:ILE:HD12	1.96	0.48
1:D:72:ARG:HH21	1:D:134:LEU:HD11	1.78	0.48
1:D:289:ALA:O	1:D:410:TYR:OH	2.27	0.48
1:B:118:VAL:C	1:B:120:THR:H	2.22	0.48
1:D:302:PHE:HD1	2:E:261:LEU:HD12	1.78	0.48
1:B:302:PHE:HD1	1:C:240:LEU:HD23	1.78	0.47
1:A:205:CYS:SG	1:A:207:LYS:NZ	2.81	0.47
1:B:162:GLN:OE1	1:B:207:LYS:NZ	2.47	0.47
1:D:70:PHE:CG	4:D:503:SY9:HAQ	2.50	0.47
1:D:104:ASP:OD1	1:D:104:ASP:N	2.40	0.47
1:D:102:LYS:HE3	1:D:102:LYS:HB2	1.71	0.47
2:E:212:LYS:HG3	2:E:241:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:OH	1:A:160:THR:O	2.30	0.47
1:B:155:ASP:OD2	1:B:157:GLN:NE2	2.46	0.47
1:D:234:MET:SD	1:D:277:SER:OG	2.66	0.46
1:C:72:ARG:HH21	1:C:134:LEU:HD11	1.80	0.46
1:D:151:ASN:OD1	1:D:151:ASN:N	2.48	0.46
1:A:275:SER:HA	1:A:278:ARG:HE	1.80	0.46
1:C:48:CYS:HB3	1:C:73:GLN:HB3	1.97	0.46
1:C:234:MET:HE1	1:C:281:LEU:HD21	1.97	0.46
1:D:50:ILE:HG21	1:D:161:MET:HE1	1.97	0.46
2:E:165:LEU:H	2:E:165:LEU:HD22	1.81	0.46
1:B:68:ASN:HD21	1:B:116:HIS:HE1	1.64	0.46
1:D:175:PHE:HB3	1:D:217:ILE:HD13	1.98	0.46
1:A:307:GLU:OE2	1:A:395:SER:OG	2.32	0.46
2:E:110:PRO:HA	2:E:113:TYR:HB2	1.97	0.46
2:E:165:LEU:O	2:E:165:LEU:HG	2.16	0.46
1:B:158:THR:O	1:B:158:THR:OG1	2.34	0.45
1:D:244:LEU:HA	1:D:247:VAL:HG12	1.97	0.45
1:D:85:TYR:HD2	1:D:87:ASP:H	1.64	0.45
1:D:156:VAL:HG12	1:D:224:GLU:HG2	1.97	0.45
1:D:110:GLU:HG2	2:E:154:ARG:HH21	1.79	0.45
2:E:157:ILE:HD12	2:E:159:LEU:HD21	1.98	0.45
1:A:151:ASN:OD1	1:A:151:ASN:O	2.34	0.45
2:E:186:THR:OG1	2:E:230:TYR:O	2.29	0.45
1:C:52:ILE:HG12	1:C:69:ILE:HG22	1.98	0.45
1:B:59:THR:HG22	1:B:61:THR:H	1.82	0.45
1:C:123:LYS:HG2	1:C:137:ILE:HG23	1.99	0.45
2:E:62:VAL:HG12	2:E:87:GLN:HB3	1.98	0.45
1:C:51:PHE:HB3	1:C:70:PHE:HB2	1.98	0.45
2:E:248:MET:HA	2:E:252:TYR:HB2	1.98	0.45
1:C:411:TRP:O	1:C:415:LYS:HB2	2.17	0.44
2:E:160:SER:O	2:E:160:SER:OG	2.35	0.44
1:C:74:GLN:HA	1:C:133:VAL:O	2.17	0.44
2:E:86:ARG:HA	2:E:151:VAL:O	2.17	0.44
1:A:21:LEU:HD13	1:A:92:LEU:HD12	1.99	0.44
2:E:112:MET:O	2:E:115:CYS:HB2	2.18	0.44
1:C:32:ASP:OD1	1:C:32:ASP:N	2.45	0.44
2:E:266:PHE:HE1	2:E:325:TYR:HB2	1.83	0.44
1:B:167:GLY:O	1:C:126:ARG:NH2	2.51	0.44
1:A:64:ASP:OD2	1:A:64:ASP:N	2.50	0.43
1:B:151:ASN:OD1	1:B:151:ASN:N	2.49	0.43
1:C:278:ARG:HH22	1:D:273:GLN:HE22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASN:HA	1:D:289:ALA:HB2	2.00	0.43
2:E:128:SER:O	2:E:128:SER:OG	2.35	0.43
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.92	0.43
1:C:151:ASN:OD1	1:C:151:ASN:N	2.51	0.43
1:A:302:PHE:HB2	1:B:240:LEU:HD21	2.01	0.43
1:B:32:ASP:HB3	1:B:35:ILE:HG12	2.00	0.43
1:B:123:LYS:HG2	1:B:137:ILE:HG22	2.01	0.43
2:E:273:SER:HB2	2:E:276:ARG:HB2	1.99	0.43
1:A:105:LEU:HD11	1:A:163:LEU:HB3	2.01	0.43
1:C:104:ASP:OD1	1:C:104:ASP:N	2.41	0.43
1:B:94:PRO:HB2	1:B:121:ASP:CG	2.43	0.42
1:A:278:ARG:NH1	1:B:273:GLN:OE1	2.52	0.42
1:A:73:GLN:HE21	1:A:135:TYR:HD2	1.66	0.42
1:D:60:GLU:HG2	1:D:149:LEU:HD11	2.01	0.42
2:E:126:GLU:HA	2:E:159:LEU:HA	2.02	0.42
1:D:52:ILE:HD11	1:D:185:VAL:HG13	2.02	0.42
1:C:252:ASN:O	1:C:259:ARG:NH2	2.52	0.42
1:D:128:SER:HB2	1:D:132:LYS:HB3	2.02	0.42
1:D:58:VAL:CG1	1:D:65:TYR:HB2	2.36	0.42
2:E:74:GLU:HA	2:E:163:LEU:HD12	2.01	0.42
1:B:269:THR:HA	1:B:272:THR:HG22	2.02	0.41
1:D:27:ARG:HA	1:D:27:ARG:HD3	1.91	0.41
1:D:68:ASN:ND2	1:D:140:THR:OG1	2.51	0.41
2:E:121:LEU:HD13	2:E:179:LEU:HD23	2.01	0.41
1:B:77:ASP:OD1	1:B:77:ASP:N	2.41	0.41
1:B:411:TRP:O	1:B:415:LYS:HB2	2.20	0.41
1:D:221:PHE:O	1:D:222:HIS:ND1	2.53	0.41
2:E:468:VAL:O	2:E:472:SER:HB3	2.20	0.41
1:D:409:PHE:O	1:D:413:THR:OG1	2.35	0.41
1:A:306:LEU:HD11	1:B:247:VAL:HG21	2.03	0.41
1:B:52:ILE:HG12	1:B:69:ILE:HG22	2.02	0.41
1:C:107:PHE:HB2	1:C:110:GLU:HG2	2.03	0.41
1:D:70:PHE:CD2	4:D:503:SY9:HAQ	2.54	0.41
2:E:34:THR:O	2:E:38:LEU:HB2	2.21	0.41
1:A:71:LEU:HB3	1:A:137:ILE:HG13	2.02	0.41
1:C:50:ILE:HD11	1:C:183:VAL:HG13	2.03	0.41
2:E:161:CYS:HB2	2:E:175:CYS:HB2	1.37	0.41
2:E:176:LYS:HB3	2:E:237:ILE:HG23	2.03	0.41
2:E:220:ASN:OD1	2:E:220:ASN:N	2.52	0.41
2:E:327:VAL:HA	2:E:330:VAL:HG12	2.03	0.41
1:C:166:PHE:HE1	1:D:70:PHE:HE2	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:SER:OG	1:D:180:ASP:N	2.54	0.40
1:A:51:PHE:HD2	1:A:184:GLN:HB2	1.85	0.40
1:D:51:PHE:HD2	1:D:184:GLN:HB2	1.86	0.40
1:B:101:TRP:HE1	1:B:168:TYR:HE2	1.70	0.40
1:B:102:LYS:HE2	1:B:102:LYS:HB2	1.92	0.40
1:C:72:ARG:NH2	4:C:503:SY9:OAJ	2.54	0.40
1:D:240:LEU:HD12	1:D:240:LEU:HA	1.93	0.40
1:B:206:THR:H	1:B:216:CYS:HB3	1.85	0.40
1:A:264:ILE:HG12	1:B:265:THR:HG21	2.03	0.40
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.91	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	A	335/364 (92%)	315 (94%)	20 (6%)	0	100	100
1	B	335/364 (92%)	314 (94%)	21 (6%)	0	100	100
1	C	335/364 (92%)	316 (94%)	19 (6%)	0	100	100
1	D	335/364 (92%)	319 (95%)	16 (5%)	0	100	100
2	E	326/702 (46%)	303 (93%)	23 (7%)	0	100	100
All	All	1666/2158 (77%)	1567 (94%)	99 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/327 (90%)	294 (100%)	0	100	100
1	B	293/327 (90%)	292 (100%)	1 (0%)	86	84
1	C	288/327 (88%)	288 (100%)	0	100	100
1	D	285/327 (87%)	283 (99%)	2 (1%)	76	77
2	E	282/614 (46%)	281 (100%)	1 (0%)	84	83
All	All	1442/1922 (75%)	1438 (100%)	4 (0%)	84	84

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

Mol	Chain	Res	Type
1	B	205	CYS
1	D	262	LEU
1	D	264	ILE
2	E	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	157	GLN
1	A	273	GLN
1	A	312	ASN
1	B	53	ASN
1	B	68	ASN
1	B	74	GLN
1	B	222	HIS
1	B	226	GLN
1	B	252	ASN
1	C	53	ASN
1	C	193	GLN
1	C	208	HIS
1	C	222	HIS
1	D	53	ASN
1	D	68	ASN
1	D	252	ASN
1	D	273	GLN
2	E	132	HIS

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Mol	Chain	Res	Type
2	E	194	GLN
2	E	269	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
3	NAG	D	501	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
3	NAG	C	501	1	14,14,15	0.97	1 (7%)	17,19,21	2.20	3 (17%)
4	SY9	C	503	-	31,31,31	1.16	3 (9%)	51,51,51	2.38	17 (33%)
3	NAG	A	502	1	14,14,15	0.34	0	17,19,21	0.52	0
3	NAG	C	502	1	14,14,15	0.28	0	17,19,21	0.48	0
4	SY9	B	503	-	31,31,31	1.16	4 (12%)	51,51,51	2.34	16 (31%)
3	NAG	B	501	1	14,14,15	0.31	0	17,19,21	0.38	0
3	NAG	E	501	2	14,14,15	0.73	1 (7%)	17,19,21	2.11	2 (11%)
3	NAG	B	502	1	14,14,15	0.62	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SY9	A	503	-	31,31,31	1.17	4 (12%)	51,51,51	2.32	19 (37%)
4	SY9	D	503	-	31,31,31	1.12	2 (6%)	51,51,51	2.29	17 (33%)
3	NAG	D	502	1	14,14,15	0.39	0	17,19,21	0.85	1 (5%)
4	SY9	D	504	-	31,31,31	1.17	5 (16%)	51,51,51	2.31	16 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1	-	4/6/23/26	0/1/1/1
3	NAG	D	501	1	-	4/6/23/26	0/1/1/1
3	NAG	C	501	1	-	4/6/23/26	0/1/1/1
3	NAG	A	502	1	-	1/6/23/26	0/1/1/1
3	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	NAG	E	501	2	-	6/6/23/26	0/1/1/1
3	NAG	B	502	1	-	3/6/23/26	0/1/1/1
3	NAG	D	502	1	-	4/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	SY9	CAA-CAB	3.06	1.43	1.39
4	B	503	SY9	CAA-CAB	2.90	1.42	1.39
3	C	501	NAG	C1-C2	2.84	1.56	1.52
4	D	504	SY9	CAA-CAB	2.75	1.42	1.39
4	C	503	SY9	CAA-CAB	2.75	1.42	1.39
4	D	504	SY9	CAL-CAI	2.67	1.55	1.51
4	A	503	SY9	CAL-CAI	2.66	1.55	1.51
4	C	503	SY9	CAL-CAI	2.61	1.55	1.51
4	B	503	SY9	CAL-CAI	2.57	1.55	1.51
4	A	503	SY9	CAA-CAB	2.52	1.42	1.39
4	D	503	SY9	CAL-CAI	2.35	1.54	1.51
4	D	504	SY9	CAI-NAH	2.28	1.41	1.36
3	E	501	NAG	C1-C2	2.23	1.55	1.52
4	C	503	SY9	CAG-CAK	-2.22	1.52	1.56
4	B	503	SY9	CAI-NAH	2.21	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	SY9	CAG-CAB	-2.21	1.48	1.51
4	A	503	SY9	CAT-CAN	-2.11	1.50	1.54
4	B	503	SY9	CAG-CAK	-2.06	1.52	1.56
4	D	504	SY9	CAG-CAK	-2.05	1.52	1.56
4	D	504	SY9	CAN-CAK	2.01	1.56	1.53

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	SY9	CAN-CAK-NAH	-7.67	99.37	106.08
4	C	503	SY9	CAN-CAK-NAH	-7.61	99.43	106.08
3	E	501	NAG	C2-N2-C7	7.29	132.67	122.90
3	C	501	NAG	C2-N2-C7	7.24	132.61	122.90
4	D	503	SY9	CAN-CAK-NAH	-6.64	100.27	106.08
4	B	503	SY9	CAN-CAK-NAH	-6.64	100.28	106.08
4	D	504	SY9	CAN-CAK-NAH	-6.43	100.46	106.08
4	D	504	SY9	CAS-CAR-CAQ	-6.14	117.42	123.07
4	B	503	SY9	CAS-CAR-CAQ	-5.87	117.66	123.07
4	D	503	SY9	CAS-CAR-CAQ	-5.71	117.81	123.07
4	C	503	SY9	CAS-CAR-CAQ	-5.49	118.01	123.07
4	A	503	SY9	CAS-CAR-CAQ	-5.35	118.14	123.07
4	C	503	SY9	CAS-NAY-CAV	4.68	117.36	113.05
4	B	503	SY9	CAS-NAY-CAV	4.54	117.23	113.05
4	D	503	SY9	CAS-NAY-CAV	4.48	117.18	113.05
4	B	503	SY9	CAK-CAG-CAV	4.44	118.13	113.82
4	D	504	SY9	CAS-NAY-CAV	4.35	117.06	113.05
4	A	503	SY9	CAS-NAY-CAV	4.29	117.00	113.05
4	D	504	SY9	CAK-CAG-CAV	4.20	117.90	113.82
4	D	503	SY9	CAK-CAG-CAV	4.20	117.89	113.82
4	C	503	SY9	CAK-CAG-CAV	4.19	117.89	113.82
4	B	503	SY9	CAS-NAY-CAX	-4.13	105.78	112.58
4	A	503	SY9	CAK-CAG-CAV	4.06	117.77	113.82
4	D	503	SY9	CAS-NAY-CAX	-4.03	105.95	112.58
4	C	503	SY9	CAA-NAH-CAI	4.02	130.72	125.45
4	A	503	SY9	CAS-CAR-CAT	4.01	122.49	114.01
4	D	504	SY9	CAA-NAH-CAI	3.99	130.68	125.45
4	A	503	SY9	CAA-NAH-CAI	3.97	130.66	125.45
4	C	503	SY9	CAS-CAR-CAT	3.95	122.36	114.01
4	D	503	SY9	CAA-NAH-CAI	3.92	130.59	125.45
4	B	503	SY9	CAA-NAH-CAI	3.91	130.58	125.45
4	D	504	SY9	CAS-NAY-CAX	-3.90	106.17	112.58
4	C	503	SY9	CAS-NAY-CAX	-3.87	106.21	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	SY9	CAS-CAR-CAT	3.84	122.13	114.01
4	D	504	SY9	CAS-CAR-CAT	3.67	121.77	114.01
4	B	503	SY9	CAS-CAR-CAT	3.67	121.76	114.01
4	A	503	SY9	CAS-NAY-CAX	-3.64	106.58	112.58
4	A	503	SY9	CAT-CAR-CAQ	-3.62	118.11	122.67
3	C	501	NAG	C1-C2-N2	3.62	116.13	110.43
3	E	501	NAG	C1-C2-N2	3.56	116.04	110.43
4	D	503	SY9	CAT-CAR-CAQ	-3.37	118.43	122.67
4	C	503	SY9	CAW-CAG-CAV	3.30	104.81	101.25
4	D	504	SY9	CAT-CAR-CAQ	-3.27	118.55	122.67
4	C	503	SY9	CAT-CAR-CAQ	-3.25	118.58	122.67
4	B	503	SY9	CAT-CAR-CAQ	-3.23	118.60	122.67
4	C	503	SY9	OAO-CAM-CAL	3.22	108.19	104.49
4	D	504	SY9	CAW-CAG-CAV	3.21	104.71	101.25
4	B	503	SY9	OAO-CAM-CAL	3.14	108.10	104.49
4	D	504	SY9	CAP-OAO-CAM	-3.11	111.66	114.86
4	D	503	SY9	CAW-CAG-CAV	3.08	104.57	101.25
4	B	503	SY9	CAW-CAG-CAV	3.05	104.53	101.25
4	D	504	SY9	CAW-CAG-CAB	-3.03	106.85	112.36
4	D	503	SY9	CAW-CAG-CAB	-2.99	106.93	112.36
4	B	503	SY9	CAW-CAG-CAB	-2.98	106.94	112.36
4	A	503	SY9	OAO-CAM-CAL	2.95	107.88	104.49
3	C	501	NAG	C1-O5-C5	2.95	116.13	112.19
4	A	503	SY9	CAW-CAG-CAV	2.94	104.42	101.25
4	D	504	SY9	OAO-CAM-CAL	2.93	107.86	104.49
4	B	503	SY9	CAT-CAN-CAK	2.92	115.46	112.60
4	D	504	SY9	CAT-CAN-CAK	2.90	115.44	112.60
4	B	503	SY9	CAP-OAO-CAM	-2.90	111.88	114.86
4	C	503	SY9	CAT-CAN-CAK	2.86	115.40	112.60
4	B	503	SY9	CAW-CAG-CAK	-2.81	107.63	111.27
4	C	503	SY9	CAW-CAG-CAB	-2.79	107.29	112.36
4	A	503	SY9	CAW-CAG-CAB	-2.77	107.32	112.36
4	D	504	SY9	CAW-CAG-CAK	-2.75	107.70	111.27
4	D	503	SY9	CAP-OAO-CAM	-2.74	112.04	114.86
4	C	503	SY9	CAP-OAO-CAM	-2.70	112.08	114.86
4	D	503	SY9	OAO-CAP-CAQ	-2.68	106.13	111.51
4	D	503	SY9	CAT-CAN-CAK	2.65	115.20	112.60
4	D	503	SY9	CAW-CAG-CAK	-2.65	107.84	111.27
4	A	503	SY9	CAT-CAN-CAK	2.64	115.18	112.60
4	C	503	SY9	OAO-CAP-CAQ	-2.60	106.30	111.51
4	C	503	SY9	CAM-CAL-CAI	-2.57	113.55	117.12
3	D	502	NAG	C2-N2-C7	2.57	126.34	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	SY9	OAQ-CAP-CAQ	-2.57	106.36	111.51
4	D	503	SY9	OAQ-CAM-CAL	2.57	107.44	104.49
3	A	501	NAG	C2-N2-C7	2.56	126.34	122.90
4	C	503	SY9	CAW-CAG-CAK	-2.55	107.96	111.27
3	D	501	NAG	C2-N2-C7	2.53	126.29	122.90
4	A	503	SY9	OAQ-CAP-CAQ	-2.52	106.46	111.51
4	A	503	SY9	CAM-CAL-CAI	-2.40	113.79	117.12
4	B	503	SY9	CAG-CAV-NAY	2.40	108.19	105.66
4	D	504	SY9	OAQ-CAP-CAQ	-2.38	106.73	111.51
4	C	503	SY9	CAG-CAV-NAY	2.27	108.06	105.66
4	A	503	SY9	CAP-OAQ-CAM	-2.27	112.52	114.86
4	D	504	SY9	CAG-CAV-NAY	2.19	107.97	105.66
4	A	503	SY9	CAW-CAG-CAK	-2.09	108.56	111.27
4	A	503	SY9	CAG-CAV-NAY	2.09	107.86	105.66
4	A	503	SY9	CAM-CAN-CAK	2.05	109.37	107.46
4	D	503	SY9	CAR-CAS-NAY	2.04	116.78	112.86
4	D	503	SY9	CAG-CAV-NAY	2.04	107.81	105.66
4	A	503	SY9	CAR-CAS-NAY	2.01	116.71	112.86

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	NAG	C4-C5-C6-O6
3	E	501	NAG	O5-C5-C6-O6
3	C	502	NAG	O5-C5-C6-O6
3	D	501	NAG	O5-C5-C6-O6
3	D	502	NAG	O5-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	E	501	NAG	C4-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	D	502	NAG	C4-C5-C6-O6
3	D	501	NAG	C4-C5-C6-O6
3	B	502	NAG	C8-C7-N2-C2
3	B	502	NAG	O7-C7-N2-C2
3	C	501	NAG	C8-C7-N2-C2
3	C	501	NAG	O7-C7-N2-C2
3	E	501	NAG	C8-C7-N2-C2
3	E	501	NAG	O7-C7-N2-C2
3	C	501	NAG	O5-C5-C6-O6
3	B	501	NAG	C4-C5-C6-O6

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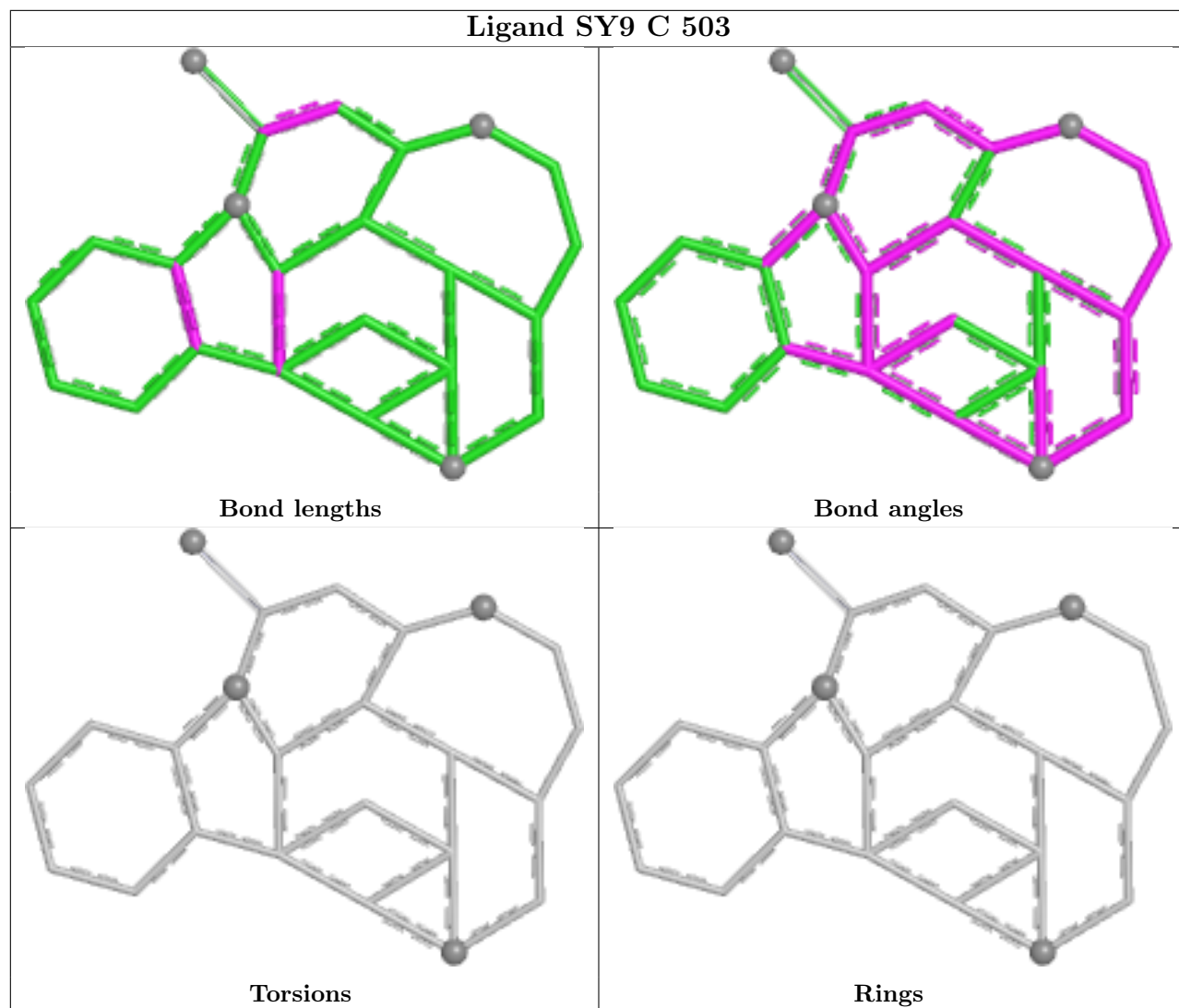
Mol	Chain	Res	Type	Atoms
3	B	502	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	D	501	NAG	C1-C2-N2-C7
3	D	502	NAG	C1-C2-N2-C7
3	A	501	NAG	C1-C2-N2-C7
3	E	501	NAG	C1-C2-N2-C7
3	A	501	NAG	C3-C2-N2-C7
3	C	501	NAG	C3-C2-N2-C7
3	D	501	NAG	C3-C2-N2-C7
3	D	502	NAG	C3-C2-N2-C7
3	E	501	NAG	C3-C2-N2-C7

There are no ring outliers.

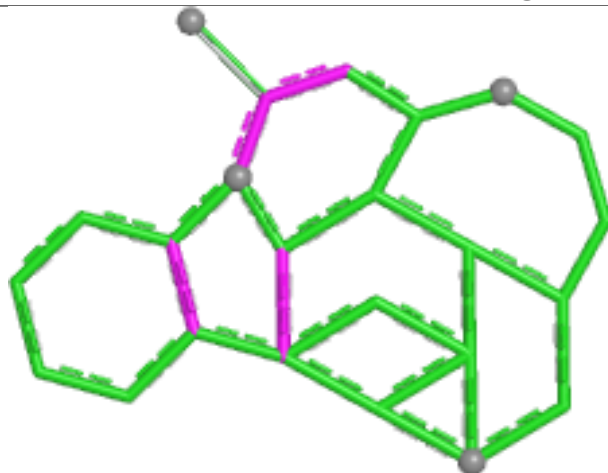
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	SY9	1	0
4	B	503	SY9	2	0
3	E	501	NAG	1	0
4	A	503	SY9	1	0
4	D	503	SY9	3	0
4	D	504	SY9	1	0

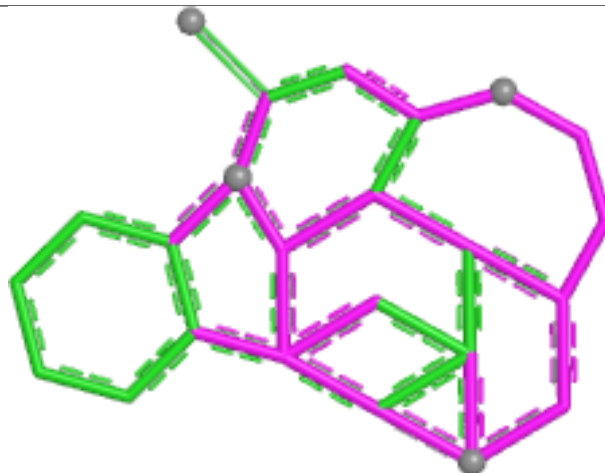
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



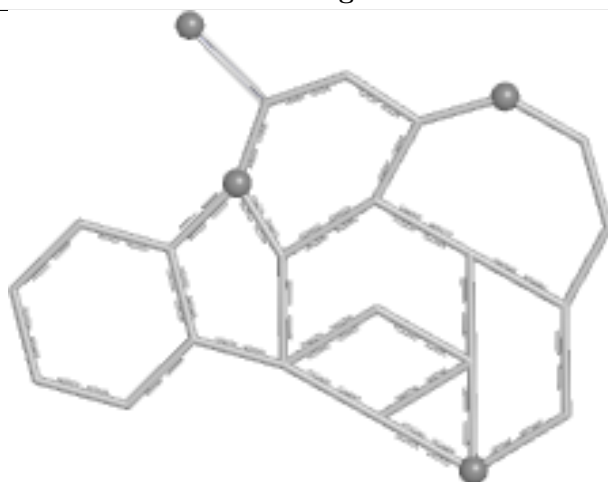
Ligand SY9 B 503



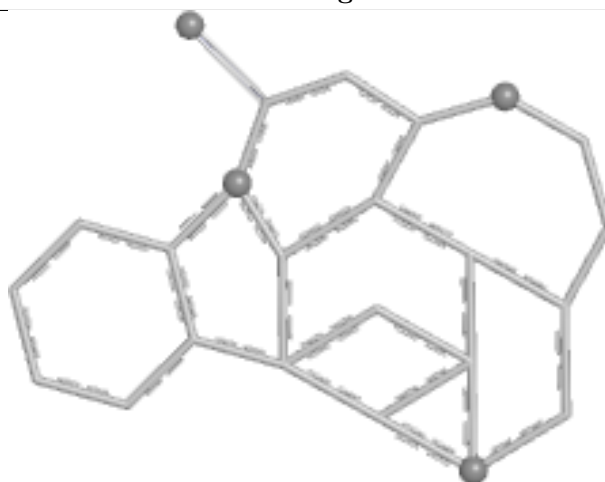
Bond lengths



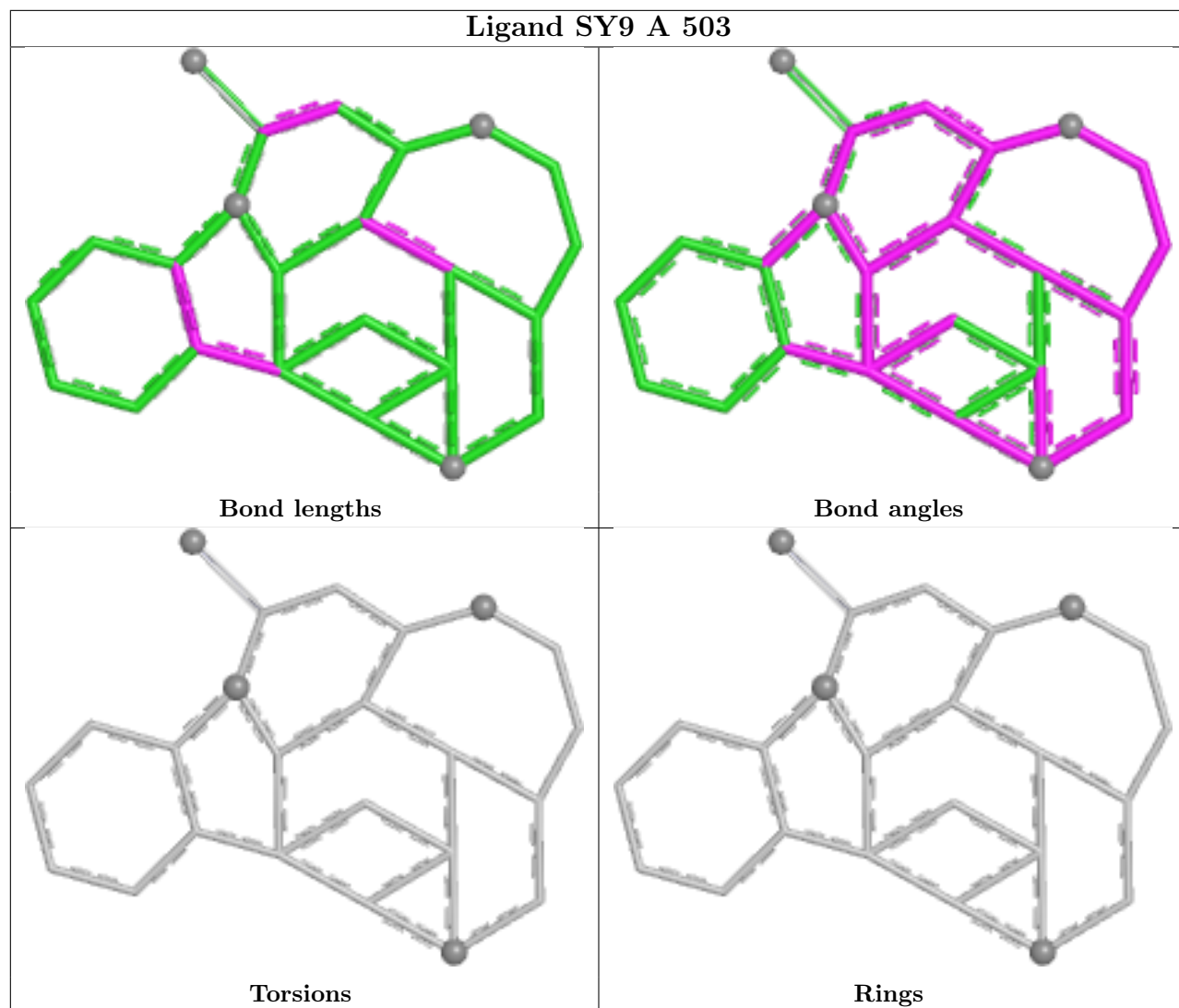
Bond angles

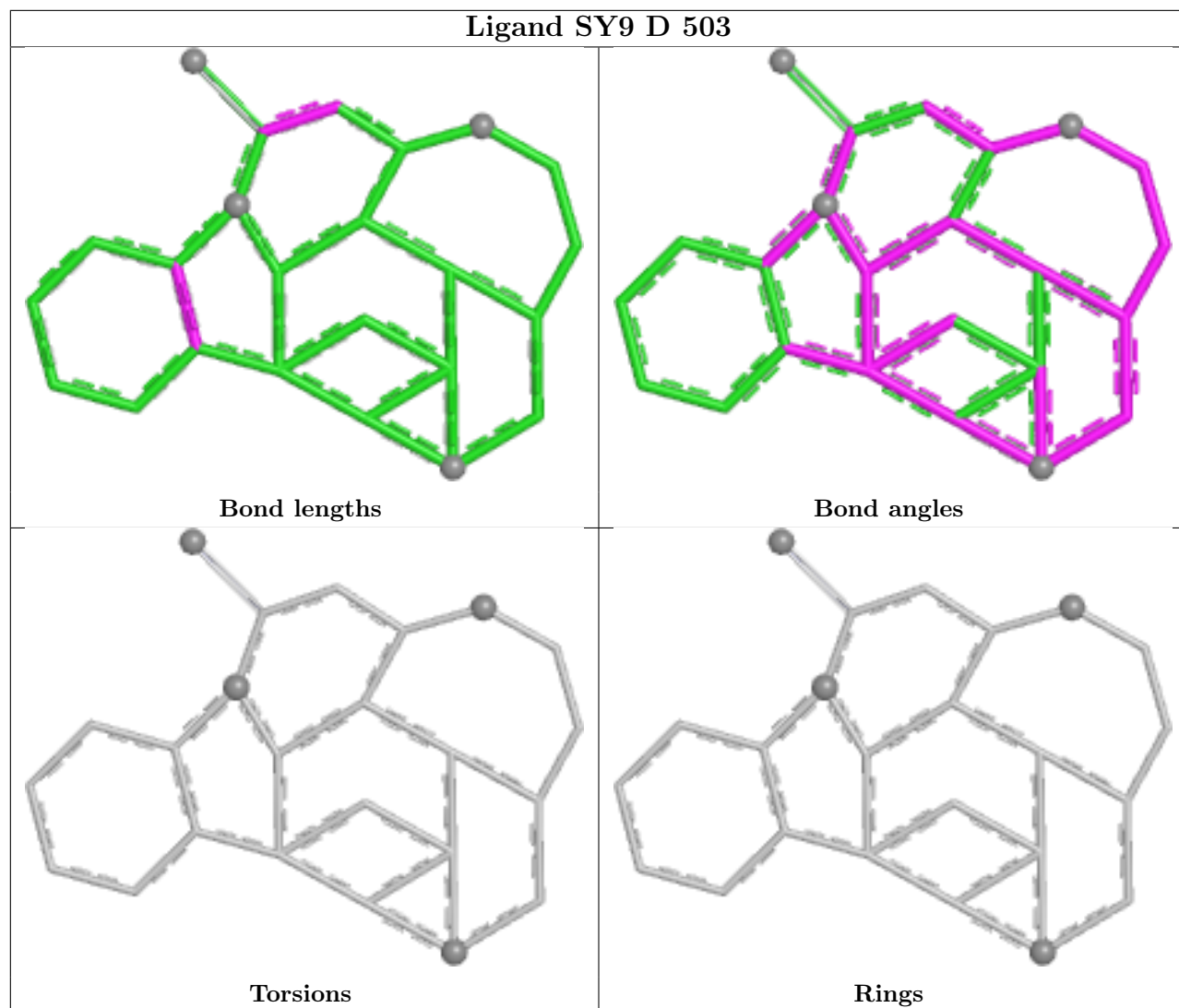


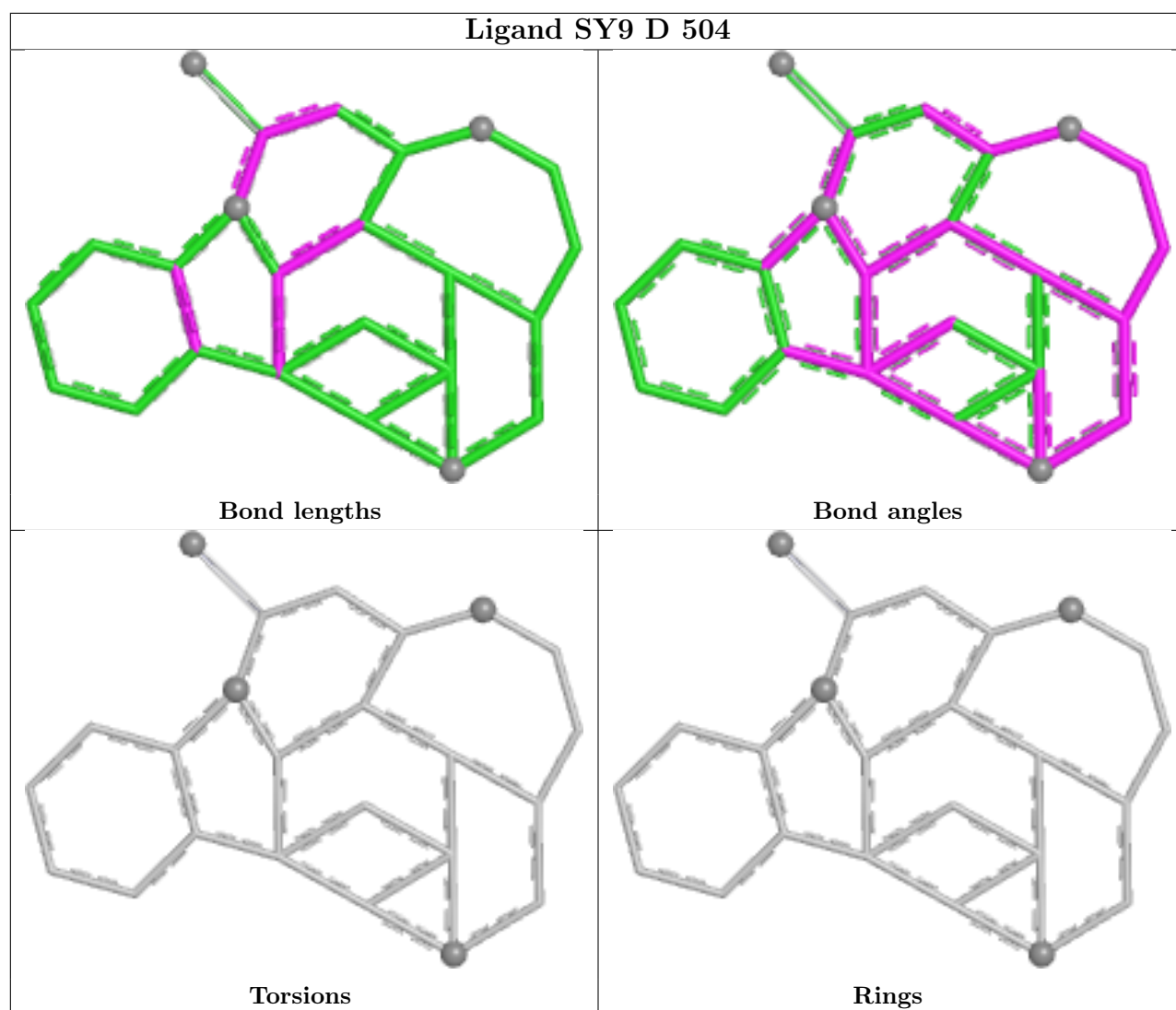
Torsions



Rings







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.

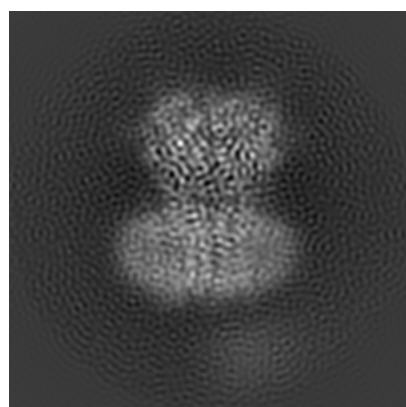
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23148. These allow visual inspection of the internal detail of the map and identification of artifacts.

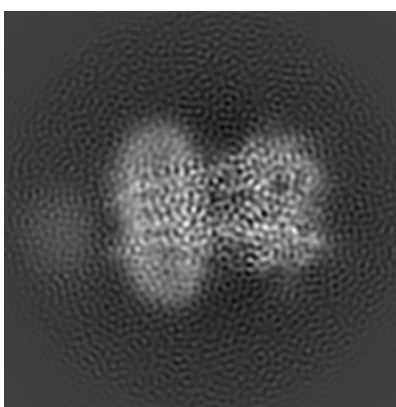
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

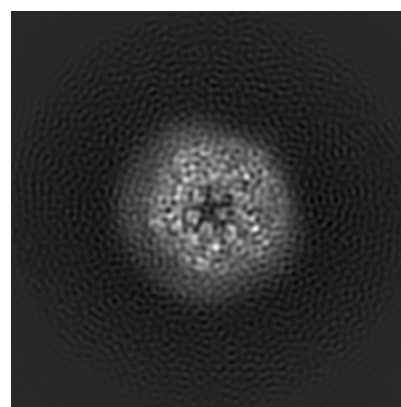
6.1.1 Primary map



X



Y

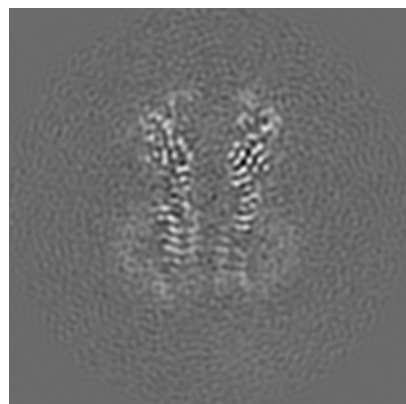


Z

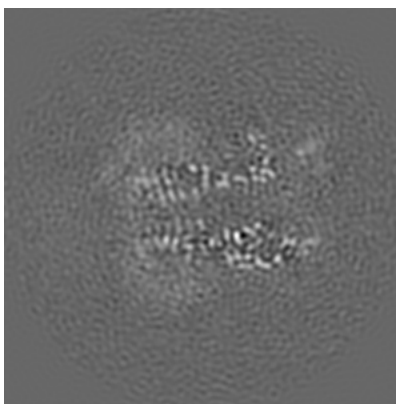
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

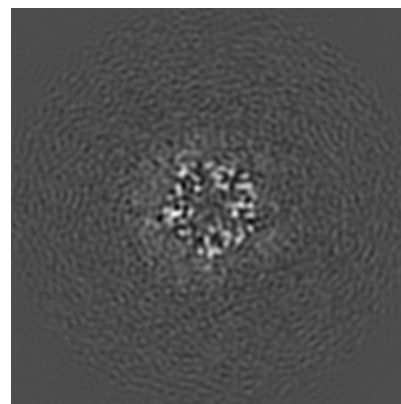
6.2.1 Primary map



X Index: 128



Y Index: 128

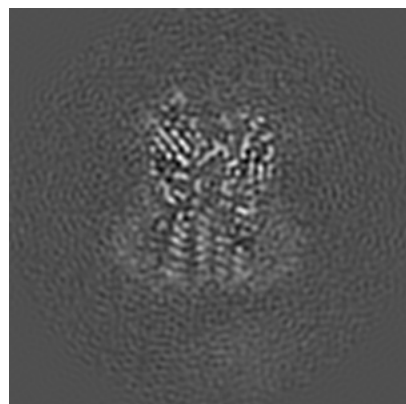


Z Index: 128

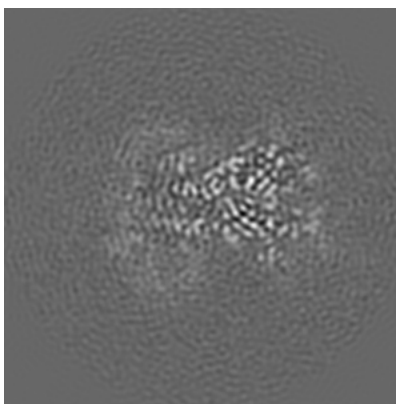
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

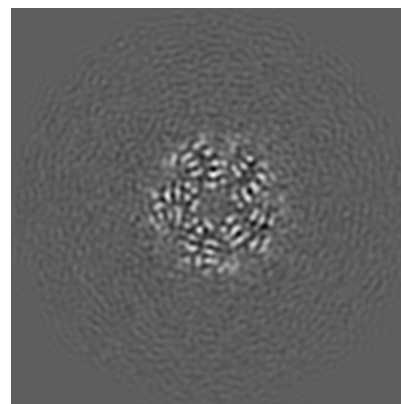
6.3.1 Primary map



X Index: 117



Y Index: 110

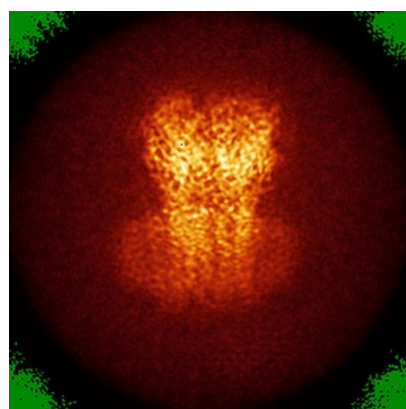


Z Index: 162

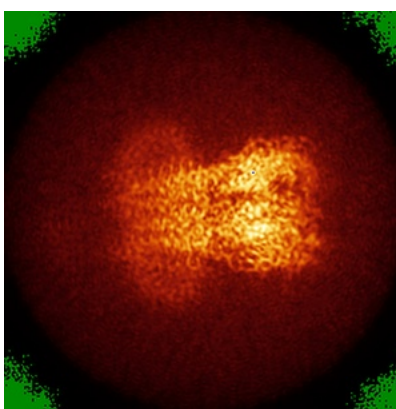
The images above show the largest variance slices of the map in three orthogonal directions.

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

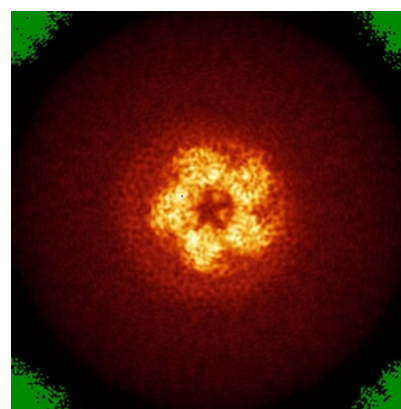
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0185. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

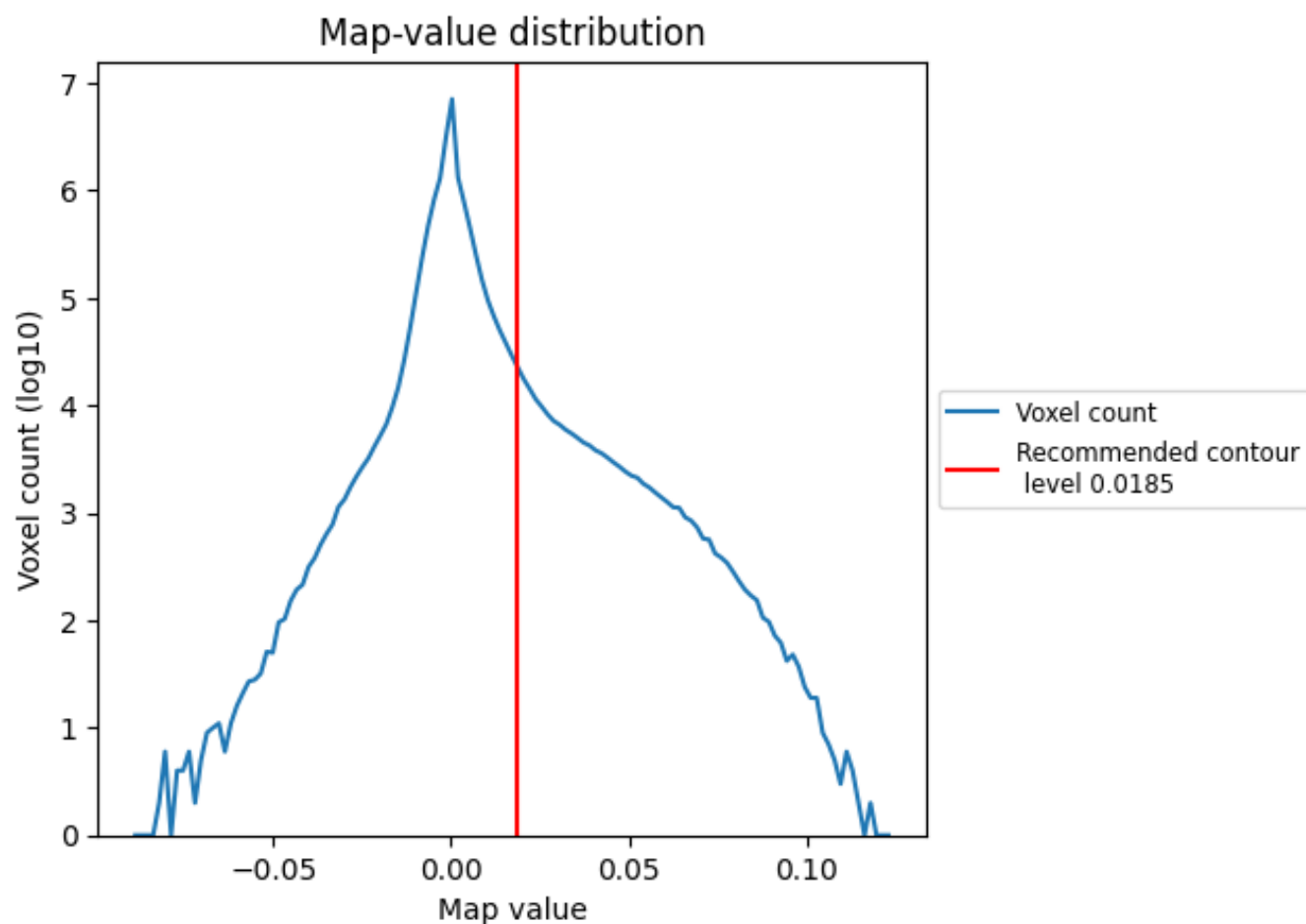
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

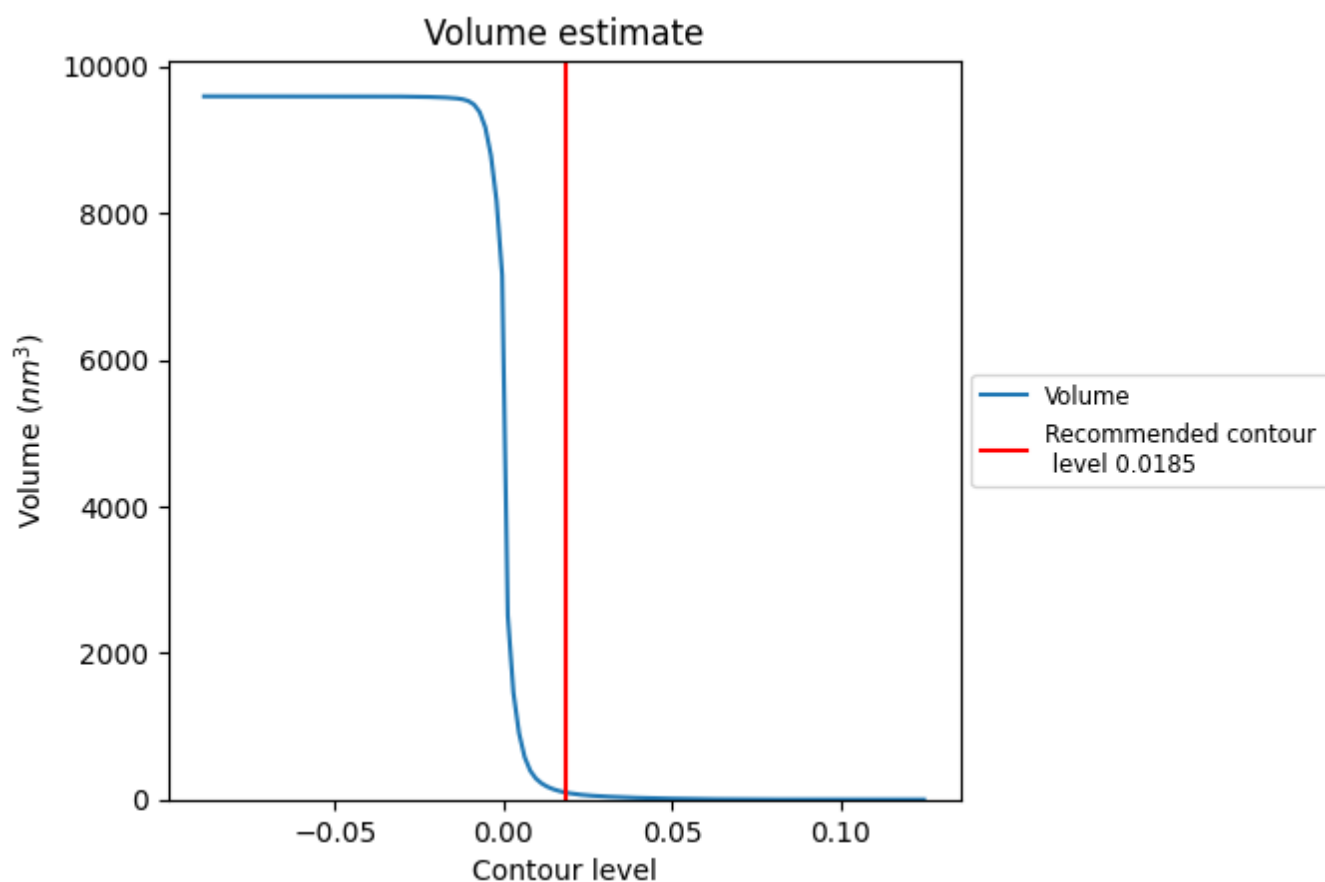
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

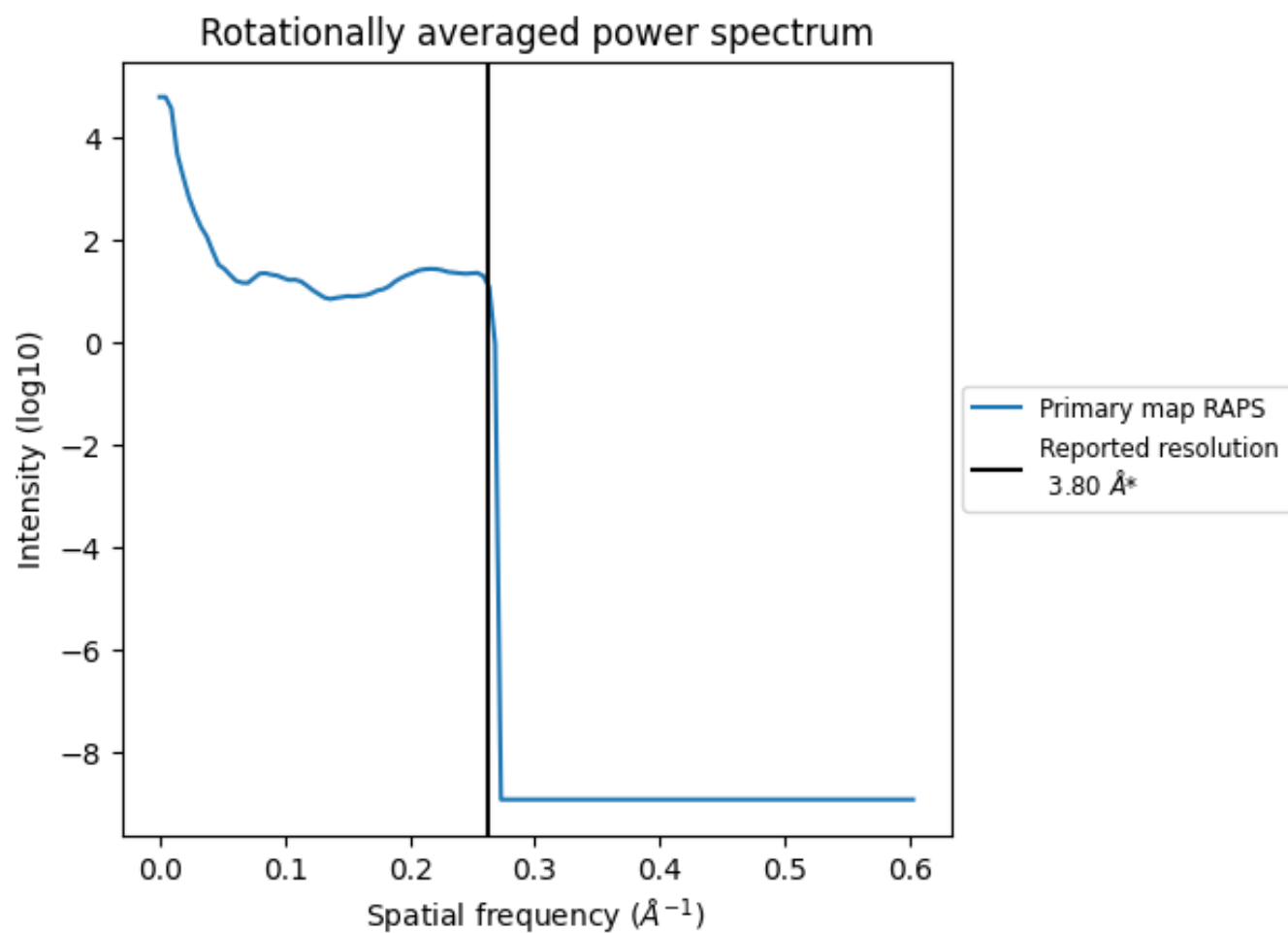
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 86 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 0.263 Å⁻¹

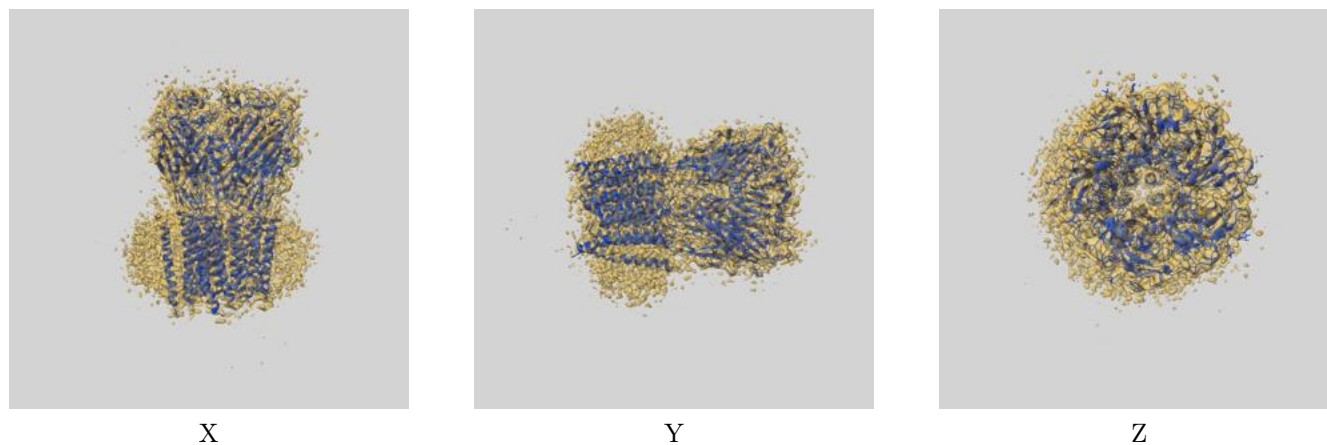
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

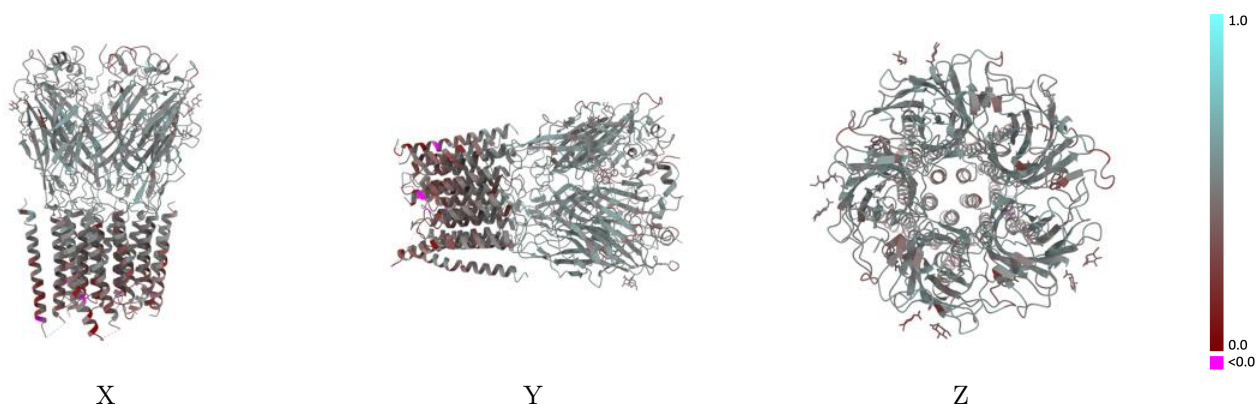
This section contains information regarding the fit between EMDB map EMD-23148 and PDB model 7L31. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



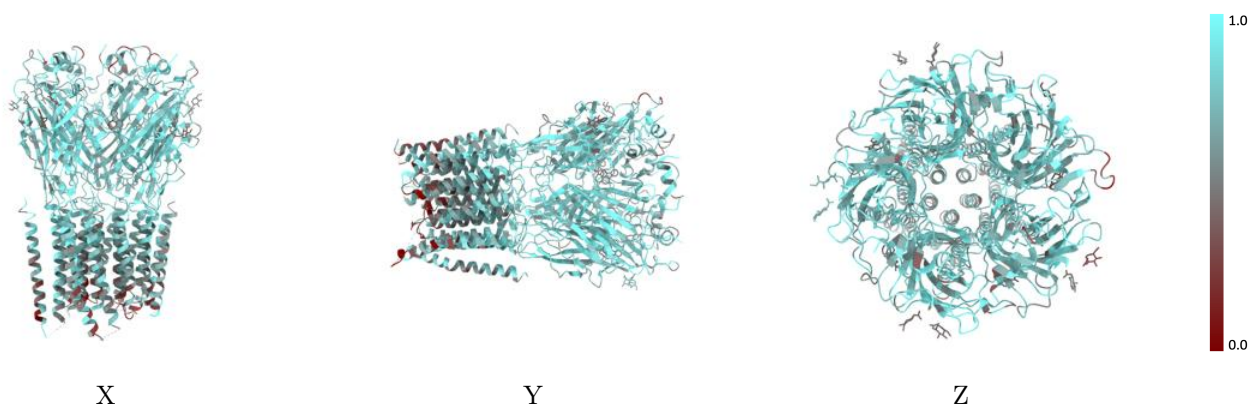
The images above show the 3D surface view of the map at the recommended contour level 0.0185 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



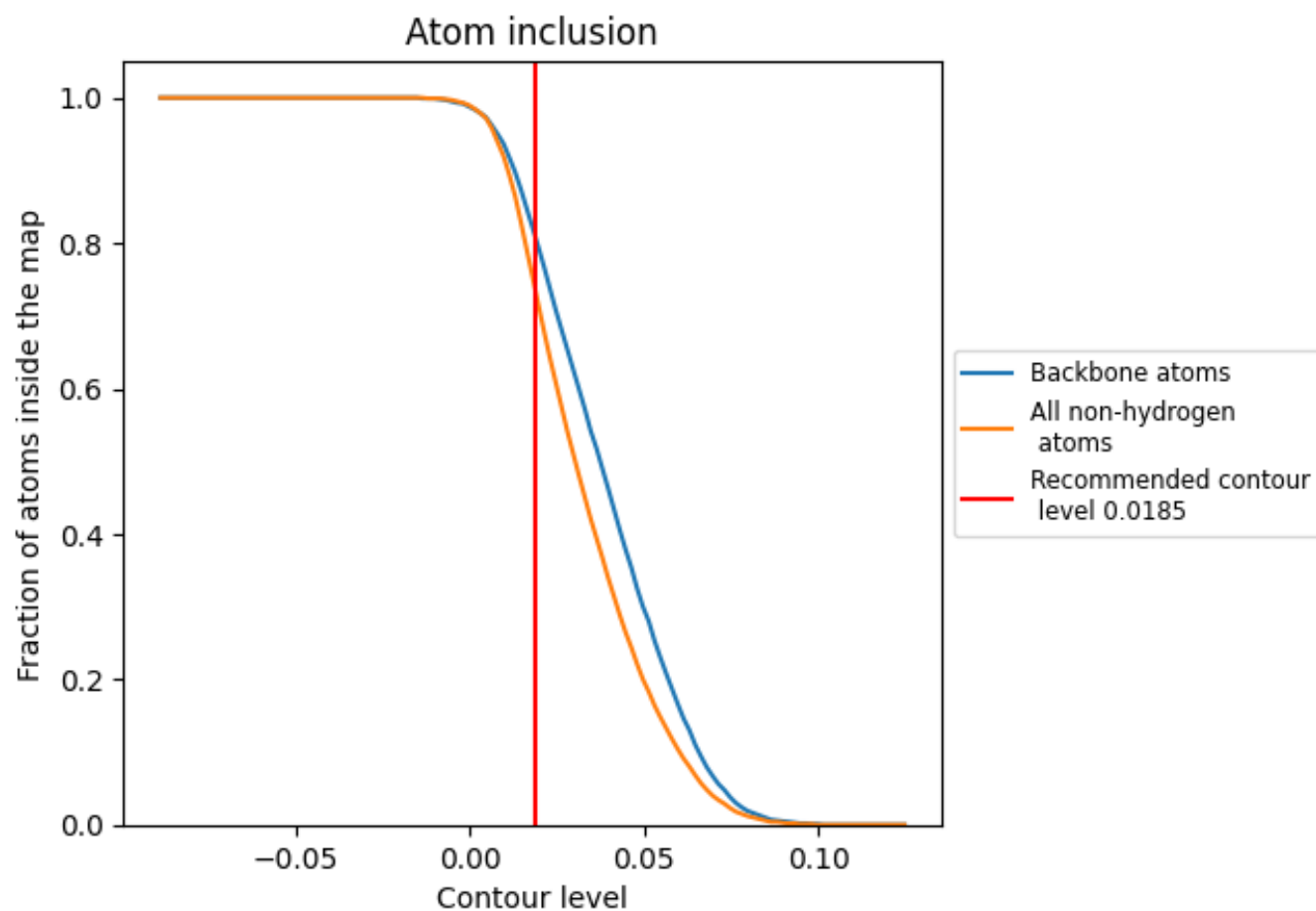
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0185).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.0185) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.4720
A	0.7430	0.4770
B	0.7450	0.4740
C	0.7430	0.4690
D	0.7410	0.4690
E	0.7330	0.4720

