WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

May 24, 2025 – 04:15 pm BST

PDB ID	:	9FG9 / pdb_00009fg9
EMDB ID	:	EMD-50389
Title	:	Cryo-EM structure of the full-length alpha1beta3gamma2 GABA(A) receptor in complex with GABA and Etomidate in the long-lived symmetric desensitised state
Authors	:	Mihaylov, D.B.; Malinauskas, T.; Aricescu, A.R.
Deposited on	:	2024-05-23
Resolution	:	2.70 Å(reported)
Based on initial model	:	6HUK

This is a wwPDB EM Validation Summary 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:
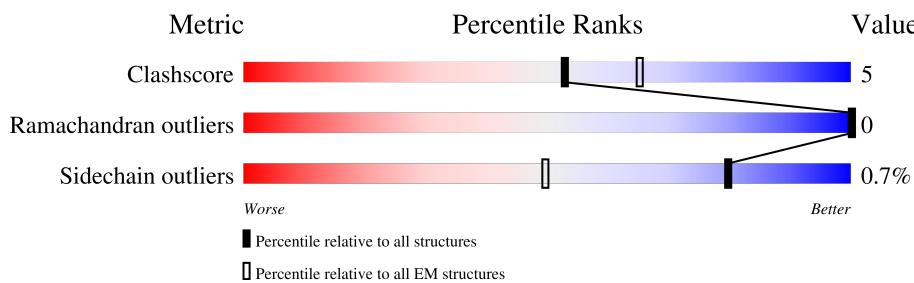
|		
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
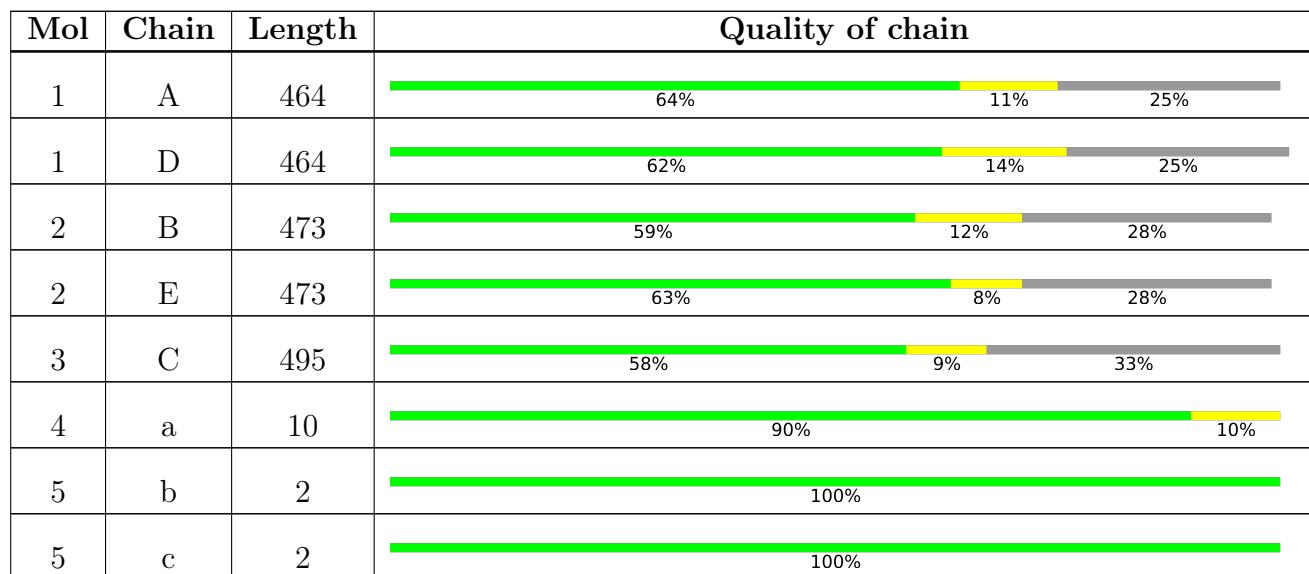
The reported resolution of this entry is 2.70 Å.

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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.7%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
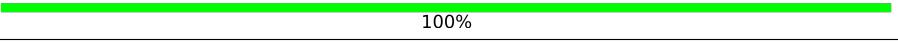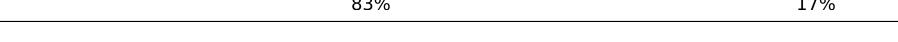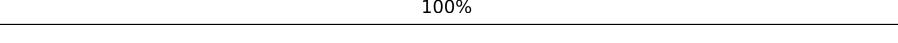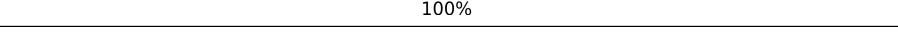
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	464	64% 11% 25%
1	D	464	62% 14% 25%
2	B	473	59% 12% 28%
2	E	473	63% 8% 28%
3	C	495	58% 9% 33%
4	a	10	90% 10%
5	b	2	100%
5	c	2	100%

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Mol	Chain	Length	Quality of chain
5	e	2	100%
6	F	6	83% 17%
6	G	6	100%
7	d	5	100%

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	MAN	a	5	X	-	-	-
4	MAN	a	6	X	-	-	-

2   Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 15031 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	349	Total 2864	C 1859	N 479	O 509	S 17	6	0
1	D	349	Total 2864	C 1860	N 479	O 509	S 16	6	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P14867
A	-33	LYS	-	expression tag	UNP P14867
A	-32	LYS	-	expression tag	UNP P14867
A	-31	SER	-	expression tag	UNP P14867
A	-30	PRO	-	expression tag	UNP P14867
A	-29	GLY	-	expression tag	UNP P14867
A	-28	LEU	-	expression tag	UNP P14867
A	-27	SER	-	expression tag	UNP P14867
A	-26	ASP	-	expression tag	UNP P14867
A	-25	TYR	-	expression tag	UNP P14867
A	-24	LEU	-	expression tag	UNP P14867
A	-23	TRP	-	expression tag	UNP P14867
A	-22	ALA	-	expression tag	UNP P14867
A	-21	TRP	-	expression tag	UNP P14867
A	-20	THR	-	expression tag	UNP P14867
A	-19	LEU	-	expression tag	UNP P14867
A	-18	PHE	-	expression tag	UNP P14867
A	-17	LEU	-	expression tag	UNP P14867
A	-16	SER	-	expression tag	UNP P14867
A	-15	THR	-	expression tag	UNP P14867
A	-14	LEU	-	expression tag	UNP P14867
A	-13	THR	-	expression tag	UNP P14867
A	-12	GLY	-	expression tag	UNP P14867
A	-11	ARG	-	expression tag	UNP P14867
A	-10	SER	-	expression tag	UNP P14867
A	-9	TYR	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P14867
A	-7	ASP	-	expression tag	UNP P14867
A	-6	TYR	-	expression tag	UNP P14867
A	-5	LYS	-	expression tag	UNP P14867
A	-4	ASP	-	expression tag	UNP P14867
A	-3	ASP	-	expression tag	UNP P14867
A	-2	ASP	-	expression tag	UNP P14867
A	-1	ASP	-	expression tag	UNP P14867
A	0	LYS	-	expression tag	UNP P14867
D	-34	MET	-	initiating methionine	UNP P14867
D	-33	LYS	-	expression tag	UNP P14867
D	-32	LYS	-	expression tag	UNP P14867
D	-31	SER	-	expression tag	UNP P14867
D	-30	PRO	-	expression tag	UNP P14867
D	-29	GLY	-	expression tag	UNP P14867
D	-28	LEU	-	expression tag	UNP P14867
D	-27	SER	-	expression tag	UNP P14867
D	-26	ASP	-	expression tag	UNP P14867
D	-25	TYR	-	expression tag	UNP P14867
D	-24	LEU	-	expression tag	UNP P14867
D	-23	TRP	-	expression tag	UNP P14867
D	-22	ALA	-	expression tag	UNP P14867
D	-21	TRP	-	expression tag	UNP P14867
D	-20	THR	-	expression tag	UNP P14867
D	-19	LEU	-	expression tag	UNP P14867
D	-18	PHE	-	expression tag	UNP P14867
D	-17	LEU	-	expression tag	UNP P14867
D	-16	SER	-	expression tag	UNP P14867
D	-15	THR	-	expression tag	UNP P14867
D	-14	LEU	-	expression tag	UNP P14867
D	-13	THR	-	expression tag	UNP P14867
D	-12	GLY	-	expression tag	UNP P14867
D	-11	ARG	-	expression tag	UNP P14867
D	-10	SER	-	expression tag	UNP P14867
D	-9	TYR	-	expression tag	UNP P14867
D	-8	GLY	-	expression tag	UNP P14867
D	-7	ASP	-	expression tag	UNP P14867
D	-6	TYR	-	expression tag	UNP P14867
D	-5	LYS	-	expression tag	UNP P14867
D	-4	ASP	-	expression tag	UNP P14867
D	-3	ASP	-	expression tag	UNP P14867
D	-2	ASP	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	expression tag	UNP P14867
D	0	LYS	-	expression tag	UNP P14867

• Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	340	Total 2846	C 1867	N 466	O 496	S 17	9	0
2	E	340	Total 2811	C 1842	N 460	O 493	S 16	3	0

• Molecule 3 is a protein called Gamma-aminobutyric acid receptor subunit gamma-2.
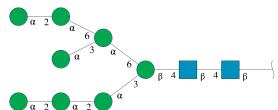
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	332	Total 2736	C 1785	N 453	O 483	S 15	1	0

There are 20 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
C	437	GLY	-	expression tag	UNP P18507
C	438	GLY	-	expression tag	UNP P18507
C	439	SER	-	expression tag	UNP P18507
C	440	GLY	-	expression tag	UNP P18507
C	441	GLY	-	expression tag	UNP P18507
C	442	SER	-	expression tag	UNP P18507
C	443	GLY	-	expression tag	UNP P18507
C	444	GLY	-	expression tag	UNP P18507
C	445	SER	-	expression tag	UNP P18507
C	446	GLY	-	expression tag	UNP P18507
C	447	LYS	-	expression tag	UNP P18507
C	448	THR	-	expression tag	UNP P18507
C	449	GLU	-	expression tag	UNP P18507
C	450	THR	-	expression tag	UNP P18507
C	451	SER	-	expression tag	UNP P18507
C	452	GLN	-	expression tag	UNP P18507
C	453	VAL	-	expression tag	UNP P18507
C	454	ALA	-	expression tag	UNP P18507
C	455	PRO	-	expression tag	UNP P18507
C	456	ALA	-	expression tag	UNP P18507
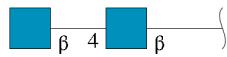
• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra
nose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyra
nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl
ucopyranose.
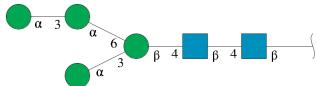
Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	10	Total 116	C 64	N 2	O 50	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a
  cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	2	Total 28	C 16	N 2	O 10	0	0
5	c	2	Total 28	C 16	N 2	O 10	0	0
5	e	2	Total 28	C 16	N 2	O 10	0	0
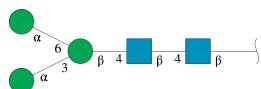
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran
  ose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-
  beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	6	Total 72	C 40	N 2	O 30	0	0
6	G	6	Total 72	C 40	N 2	O 30	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran
  ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.
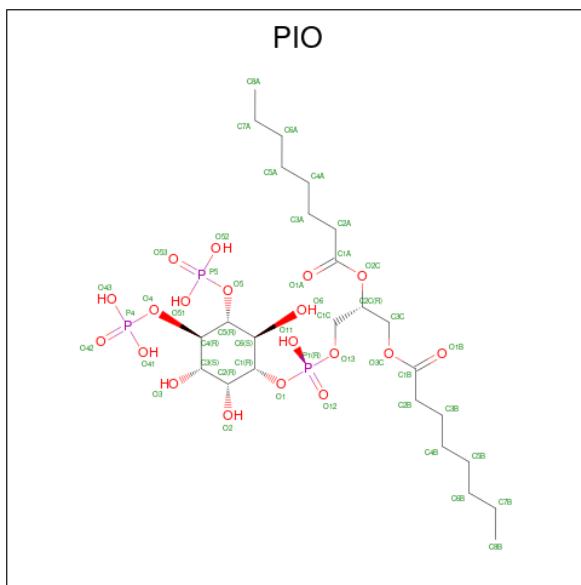
Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Cl	0
			1	1	
8	C	1	Total	Cl	0
			1	1	
8	D	1	Total	Cl	0
			1	1	

- Molecule 9 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: $C_{25}H_{49}O_{19}P_3$).
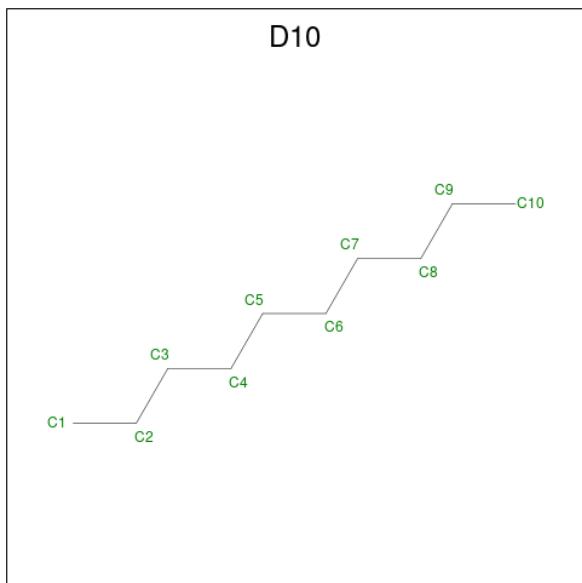
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			47	25	19	3	

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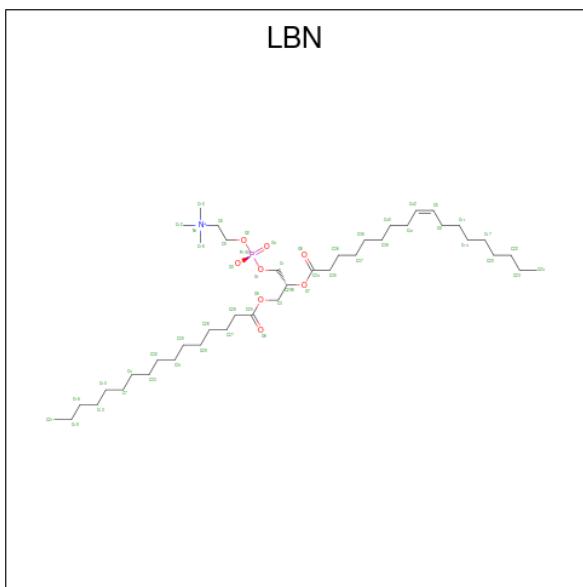
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	D	1	47	25	19	3	0

- Molecule 10 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).
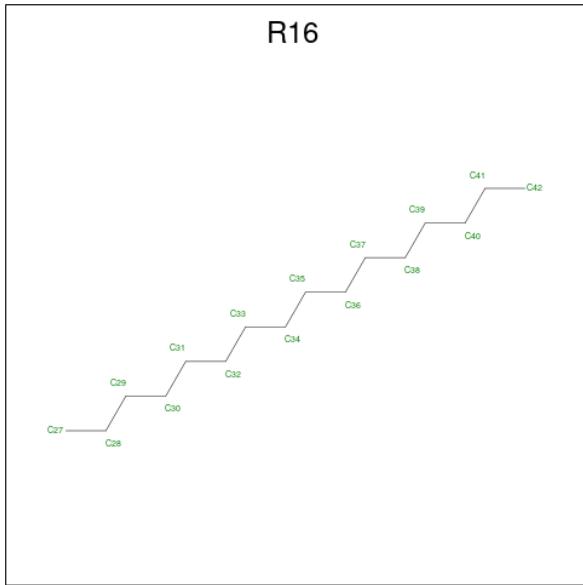
D10

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
10	A	1	10	10	0
10	B	1	10	10	0
10	C	1	10	10	0
10	D	1	10	10	0
10	E	1	10	10	0

- Molecule 11 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$).
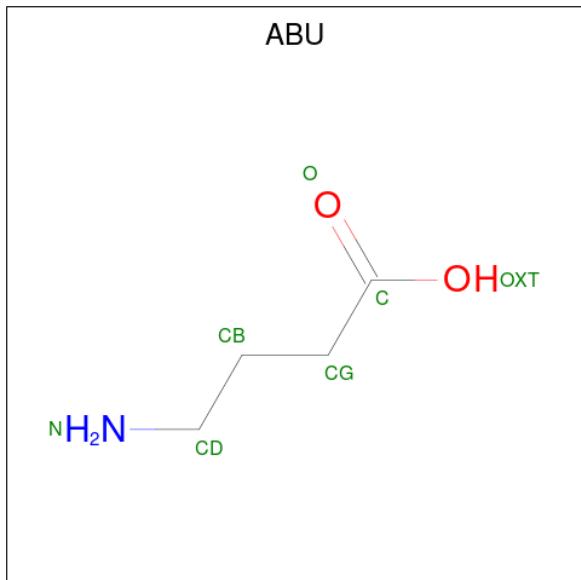
Mol	Chain	Residues	Atoms						AltConf
11	A	1	Total	C	N	O	P		0
			52	42	1	8	1		
11	D	1	Total	C	N	O	P		0
			52	42	1	8	1		

- Molecule 12 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).
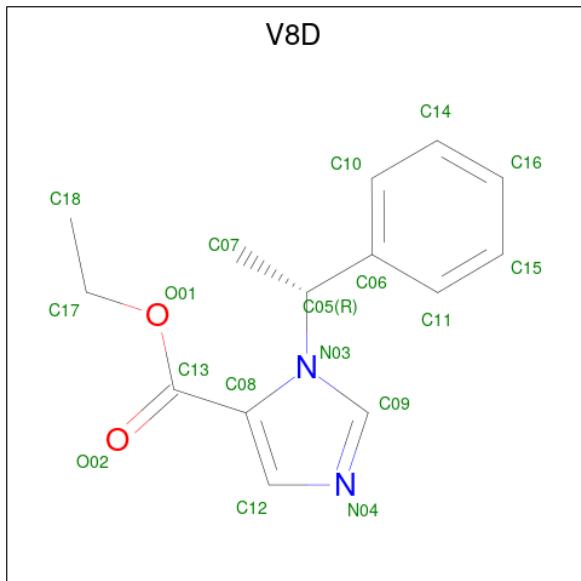
Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	C	0
			16	16	
12	E	1	Total	C	0
			16	16	

- Molecule 13 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total 7	C 4	N 1	O 2	0
13	E	1	Total 7	C 4	N 1	O 2	0

- Molecule 14 is Etomidate (CCD ID: V8D) (formula: $C_{14}H_{16}N_2O_2$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
14	B	1	Total 18	C 14	N 2	O 2	0
14	E	1	Total 18	C 14	N 2	O 2	0
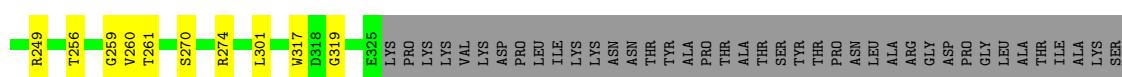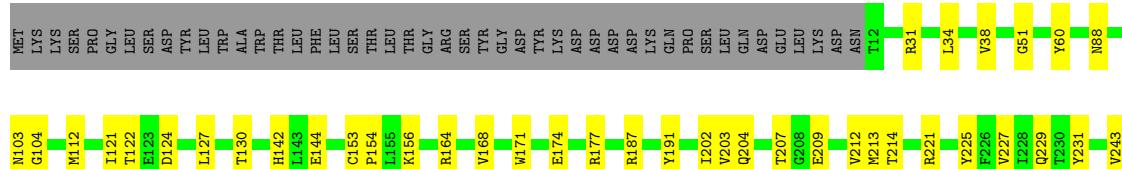
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	30	Total 30	O 30	0
15	B	39	Total 39	O 39	0
15	C	36	Total 36	O 36	0
15	D	33	Total 33	O 33	0
15	E	34	Total 34	O 34	0
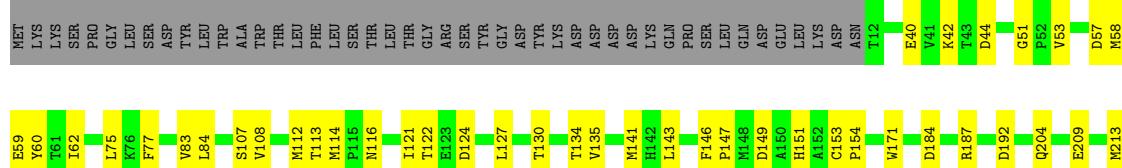
3   Residue-property plots ⓘ

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: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A:

• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain D:

• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain B:

MET CYS SER GLY LEU LEU GLU LEU LEU LEU PRO ILE TRP LEU SER TRP THR LEU GLY THR ARG GLY SER GLU PRO ARG SER VAL ASN ASP PRO **GLY** N8 N41 I42 D43 I44 D48 Y57 Q64 Q65 Y66 Y97 F98 L99 N100 D101 K102 V106 T123 V124 L125

R129 A135 D139 L140 R141 P144 L145 D146 E147 Q148 T151 L152 E153 I154 E155 R169 V175 V178 I181 R192 L193 V194 R207 L208 L210 S209 S211 I222 L223 Q224 T225 Y226 I230 L235 S239 V251 A252 L253 G254 I255 L259 L272

I275 K279 A280 I281 L296 V302 F306 R313 GLN LYS LYS LEU ALA GLU LYS THR ALA LYS ALA ASN ASP SER LYS SER GLU SER ASN ARG VAL ASP ALA HIS GLY ASN ILE LEU LEU THR SER LEU GLU VAL HIS ASN GLU MET ASN GLU VAL SER GLY ILE

GLY ASP THR ARG ASN SER ALA ILE SER PHE ASP ASN SER GLY ILE GLN TYR ARG LYS GLN SER MET PRO ARG GLU GLY HIS GLY ARG PHE LEU GLY ASP ARG SER LEU PRO HIS LYS LYS THR HIS LEU ARG ARG ARG SER SER GLN LEU LYS ILE LYS I414 V420 D424 R425 W426

S427 R428 I429 V430 Y446 V447 ASN

• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain E:63%8%28%

MET CYS SER GLY LEU LEU GLU LEU LEU LEU PRO ILE TRP LEU SER TRP THR LEU GLY THR ARG GLY SER GLU PRO ARG SER VAL ASN ASP PRO **GLY** N8 I42 D43 I44 Y66 F98 D101 M115 T123 V124 L125 R129 P144 T151 I164 V175

V178 I181 V198 T202 P206 R207 S211 Y220 Q224 T225 T233 I234 L235 S236 G254 I255 L259 T262 T266 L272 K279 A280 I281 L296 L297 F301 I305 R313 GLN LYS LYS LEU ALA GLU LYS THR ALA LYS ALA LYS ASN ASP

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

GLY ARG PHE LEU GLY ASP ARG SER LEU PRO HIS LYS LYS THR HIS LEU ARG ARG ARG SER SER GLN LEU LYS LYS ILE LYS I414 W426 V430 V447 ASN

• Molecule 3: Gamma-aminobutyric acid receptor subunit gamma-2

Chain C:58%9%33%

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

VAL PRO GLU G25 L34 D56 G63 N66 N69 M70 E71 Y72 T73 A79 R85 R86 L87 K88 N101 M102 P109 D110 S116 K117 I124 T125 L155 C165 S171 W183 S187 Q200 L206 R207 N208 Y226 R232 T237

Y241 I282 A283 R284 L287 P288 K289 V290 V293 D297 L311 H318 S322 N323 R324 LYS PRO SER LYS ASP LYS ASP LYS LYS ASN PRO LEU LEU ARG MET PHE SER PHE LYS ALA PRO THR ILE ASP ILE ARG PRO ARG SER ALA THR ILE GLN MET ASN ASN

ALA THR HIS LEU GLN GLU ARG ASP GLU GLU TYR GLY TYR GLU CYS LEU ASP GLY LYS ASP CYS ALA SER PHE PHE CYS PHE GLU ASP ARG THR GLY ALA TRP ARG HIS GLY ARG ILE LEU HIS ILE I406 L424 S432 L436 G437 GLY SER GLY SER GLY SER GLY

LYS THR GLU THR SER GLN VAL ALA PRO ALA

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran
ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-
(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl
ucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

90%　　　10%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8 MAN9 MAN10

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain b:

100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain c:

100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain e:

100%

NAG1 NAG2

• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam
ido-2-deoxy-beta-D-glucopyranose

Chain F:

83%　　　17%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam
ido-2-deoxy-beta-D-glucopyranose

Chain G:

100%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain d: 100%

NAG1 NAG2 BMA3 MAN4 MAN5

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110000	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.799	Depositor
Minimum map value	-0.612	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	260.28, 260.28, 260.28	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0845, 1.0845, 1.0845	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LBN, ABU, BMA, R16, D10, CL, V8D, NAG, PIO, MAN

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	0.28	0/2956	0.29	0/4015
1	D	0.28	0/2956	0.29	0/4017
2	B	0.28	0/2948	0.32	0/4009
2	E	0.28	0/2895	0.31	0/3939
3	C	0.28	0/2813	0.31	0/3828
All	All	0.28	0/14568	0.31	0/19808

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2864	0	2872	31	0
1	D	2864	0	2874	40	0
2	B	2846	0	2870	40	0
2	E	2811	0	2815	26	0
3	C	2736	0	2729	28	0
4	a	116	0	97	1	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	28	0	25	0	0
6	F	72	0	61	1	0
6	G	72	0	61	0	0
7	d	61	0	52	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	47	0	44	2	0
9	D	47	0	44	2	0
10	A	10	0	22	1	0
10	B	10	0	22	0	0
10	C	10	0	22	1	0
10	D	10	0	22	1	0
10	E	10	0	22	0	0
11	A	52	0	0	0	0
11	D	52	0	0	0	0
12	B	16	0	34	1	0
12	E	16	0	34	0	0
13	B	7	0	0	0	0
13	E	7	0	0	1	0
14	B	18	0	0	0	0
14	E	18	0	0	0	0
15	A	30	0	0	0	0
15	B	39	0	0	1	0
15	C	36	0	0	1	0
15	D	33	0	0	0	0
15	E	34	0	0	0	0
All	All	15031	0	14772	152	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 5.

The worst 5 of 152 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:A:301:LEU:HD23	2:E:235:LEU:HD11	1.68	0.75
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.20	0.74
1:A:395[A]:LEU:HD23	9:A:502:PIO:H6AA	1.72	0.71
2:B:254:GLY:HA3	2:B:296:LEU:HD13	1.74	0.67
1:A:51:GLY:HA2	1:A:187:ARG:HB2	1.77	0.66

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	351/464 (76%)	347 (99%)	4 (1%)	0	100	100
1	D	351/464 (76%)	342 (97%)	9 (3%)	0	100	100
2	B	345/473 (73%)	339 (98%)	6 (2%)	0	100	100
2	E	339/473 (72%)	335 (99%)	4 (1%)	0	100	100
3	C	329/495 (66%)	314 (95%)	15 (5%)	0	100	100
All	All	1715/2369 (72%)	1677 (98%)	38 (2%)	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	317/413 (77%)	315 (99%)	2 (1%)	84	94
1	D	317/413 (77%)	313 (99%)	4 (1%)	65	85
2	B	315/422 (75%)	312 (99%)	3 (1%)	73	89
2	E	309/422 (73%)	308 (100%)	1 (0%)	91	97
3	C	306/448 (68%)	304 (99%)	2 (1%)	81	93
All	All	1564/2118 (74%)	1552 (99%)	12 (1%)	80	91

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	130	THR
1	D	395[A]	LEU
2	E	297	LEU
1	D	395[B]	LEU
2	B	275	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	152	GLN
3	C	156	HIS
2	E	185	GLN
1	D	242	GLN
2	B	54	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 ⓘ

33 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	$\#|Z| > 2$
6	NAG	F	1	2,6	14,14,15	0.26	0	17,19,21	0.53	0
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.43	0
6	BMA	F	3	6	11,11,12	0.22	0	15,15,17	0.45	0
6	MAN	F	4	6	11,11,12	0.19	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	MAN	F	5	6	11,11,12	0.23	0	15,15,17	0.35	0
6	MAN	F	6	6	11,11,12	0.18	0	15,15,17	0.35	0
6	NAG	G	1	2,6	14,14,15	0.27	0	17,19,21	0.47	0
6	NAG	G	2	6	14,14,15	0.25	0	17,19,21	0.41	0
6	BMA	G	3	6	11,11,12	0.20	0	15,15,17	0.55	0
6	MAN	G	4	6	11,11,12	0.19	0	15,15,17	0.43	0
6	MAN	G	5	6	11,11,12	0.20	0	15,15,17	0.45	0
6	MAN	G	6	6	11,11,12	0.18	0	15,15,17	0.33	0
4	NAG	a	1	1,4	14,14,15	0.23	0	17,19,21	0.51	0
4	MAN	a	10	4	11,11,12	0.18	0	15,15,17	0.51	0
4	NAG	a	2	4	14,14,15	0.22	0	17,19,21	0.50	0
4	BMA	a	3	4	11,11,12	0.21	0	15,15,17	0.55	0
4	MAN	a	4	4	11,11,12	0.20	0	15,15,17	0.48	0
4	MAN	a	5	4	11,11,12	0.23	0	15,15,17	0.80	0
4	MAN	a	6	4	11,11,12	0.20	0	15,15,17	0.33	0
4	MAN	a	7	4	11,11,12	0.26	0	15,15,17	0.71	0
4	MAN	a	8	4	11,11,12	0.22	0	15,15,17	0.59	0
4	MAN	a	9	4	11,11,12	0.19	0	15,15,17	0.42	0
5	NAG	b	1	2,5	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	b	2	5	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	c	1	3,5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	c	2	5	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	d	1	7,1	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	d	2	7	14,14,15	0.22	0	17,19,21	0.63	0
7	BMA	d	3	7	11,11,12	0.17	0	15,15,17	0.36	0
7	MAN	d	4	7	11,11,12	0.24	0	15,15,17	0.30	0
7	MAN	d	5	7	11,11,12	0.22	0	15,15,17	0.48	0
5	NAG	e	1	2,5	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	e	2	5	14,14,15	0.21	0	17,19,21	0.50	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
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	1/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	1/2/19/22	0/1/1/1
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	1/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	a	10	4	-	0/2/19/22	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	BMA	a	3	4	-	2/2/19/22	0/1/1/1
4	MAN	a	4	4	-	1/2/19/22	0/1/1/1
4	MAN	a	5	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	a	6	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	a	7	4	-	0/2/19/22	0/1/1/1
4	MAN	a	8	4	-	1/2/19/22	0/1/1/1
4	MAN	a	9	4	-	0/2/19/22	0/1/1/1
5	NAG	b	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	3/6/23/26	0/1/1/1
7	NAG	d	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	BMA	d	3	7	-	0/2/19/22	0/1/1/1
7	MAN	d	4	7	-	0/2/19/22	0/1/1/1
7	MAN	d	5	7	-	0/2/19/22	0/1/1/1
5	NAG	e	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	a	5	MAN	C1
4	a	6	MAN	C1

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	c	2	NAG	C8-C7-N2-C2

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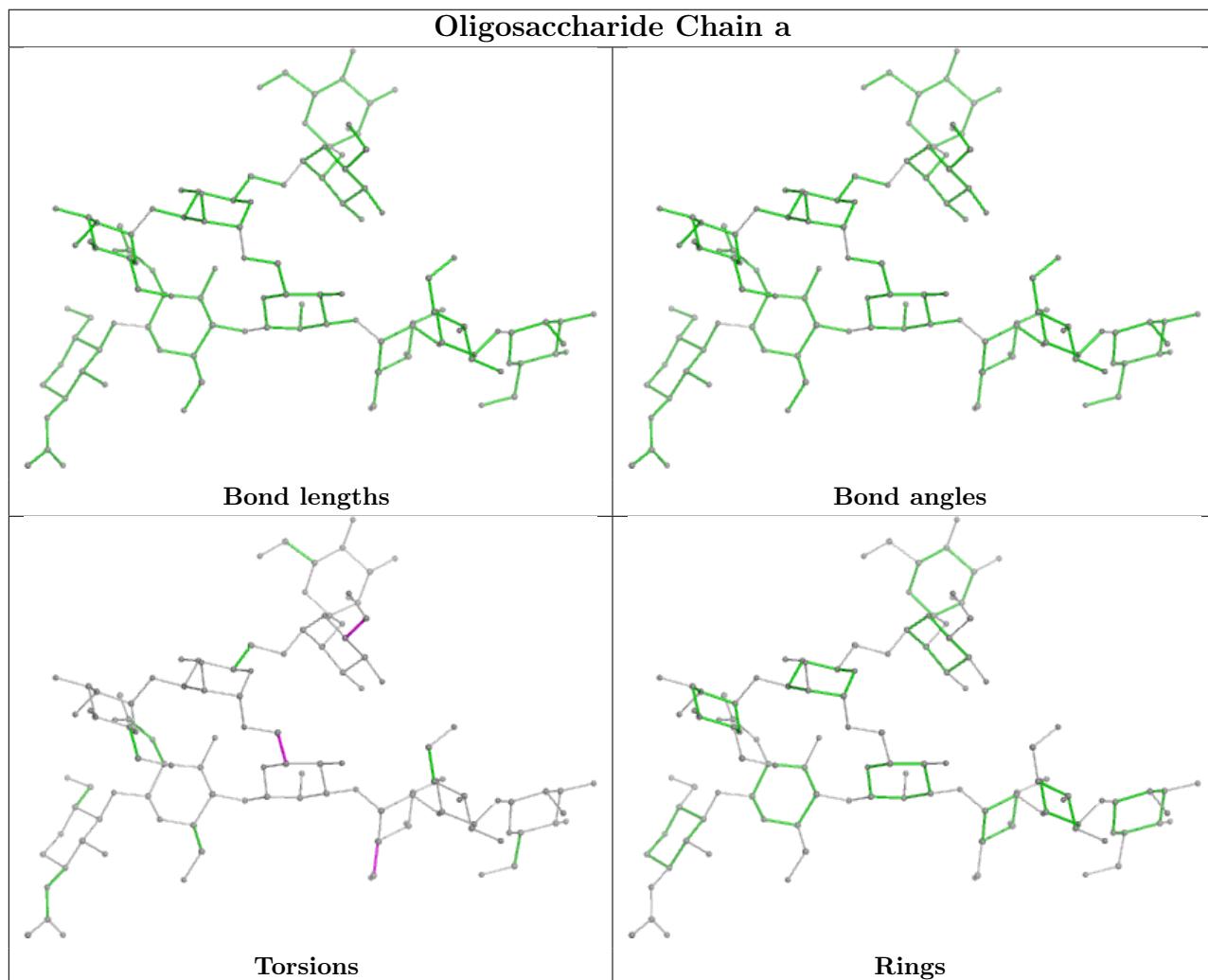
Mol	Chain	Res	Type	Atoms
5	c	2	NAG	O7-C7-N2-C2
4	a	3	BMA	O5-C5-C6-O6
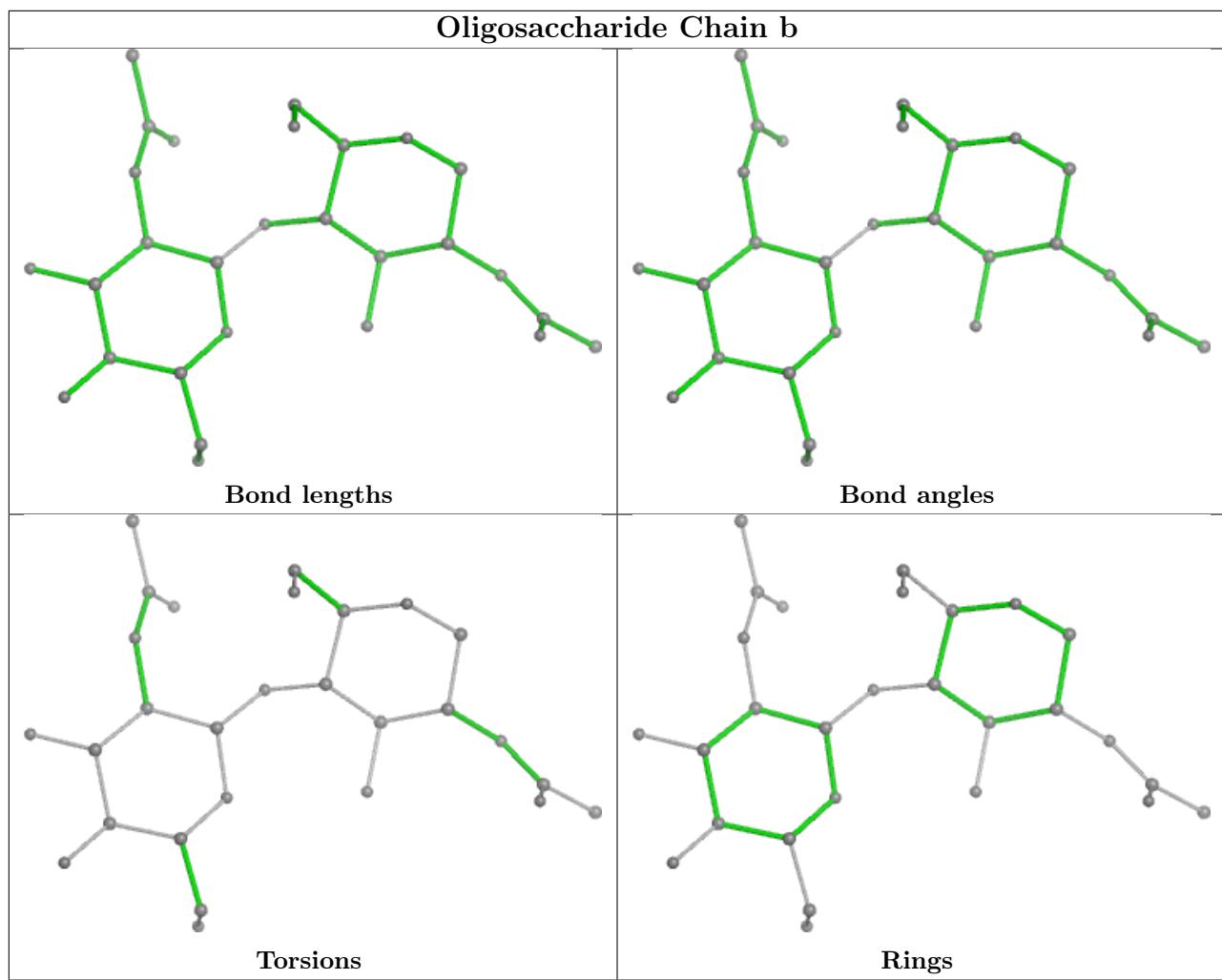
There are no ring outliers.
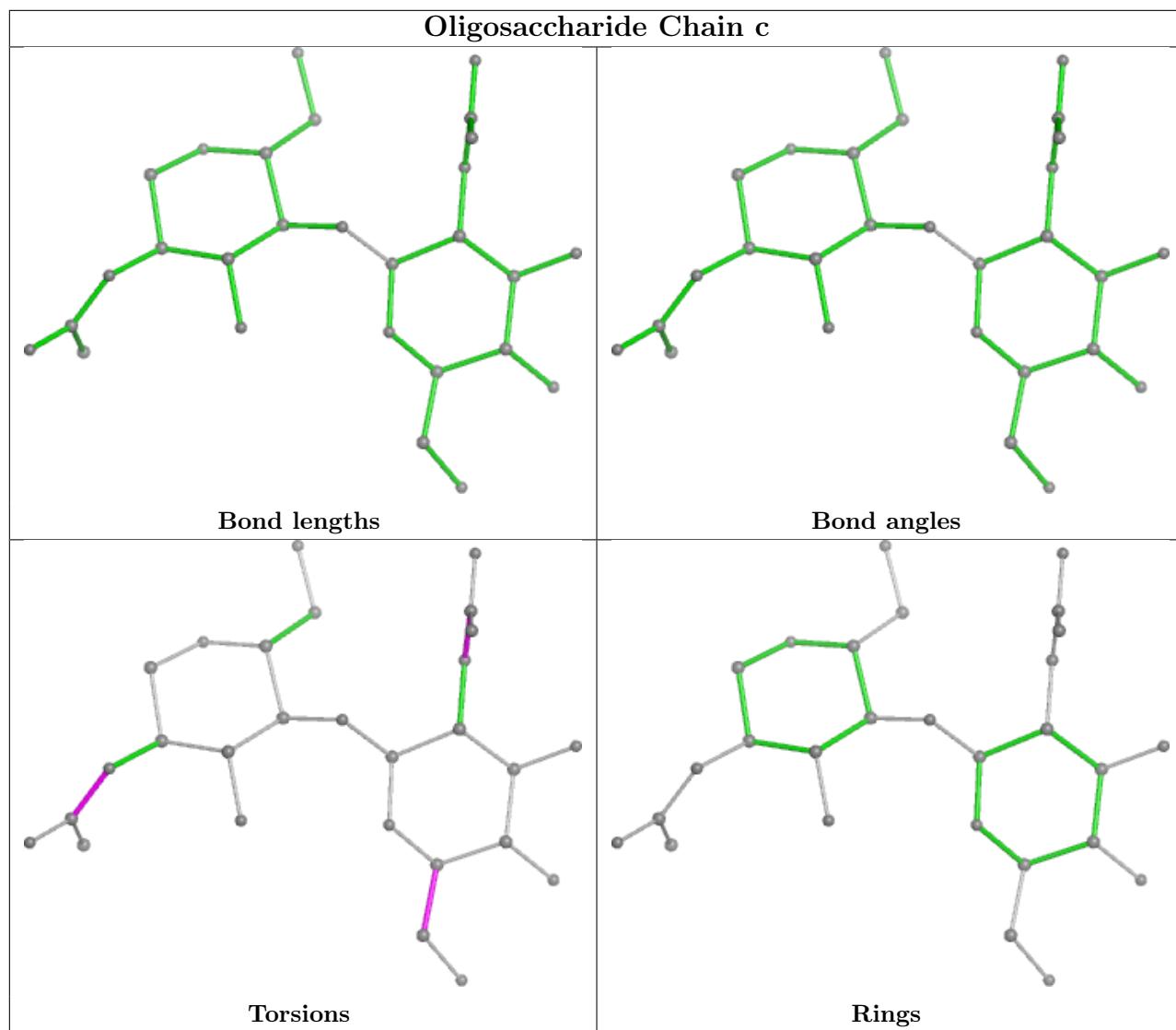
2 monomers are involved in 2 short contacts:
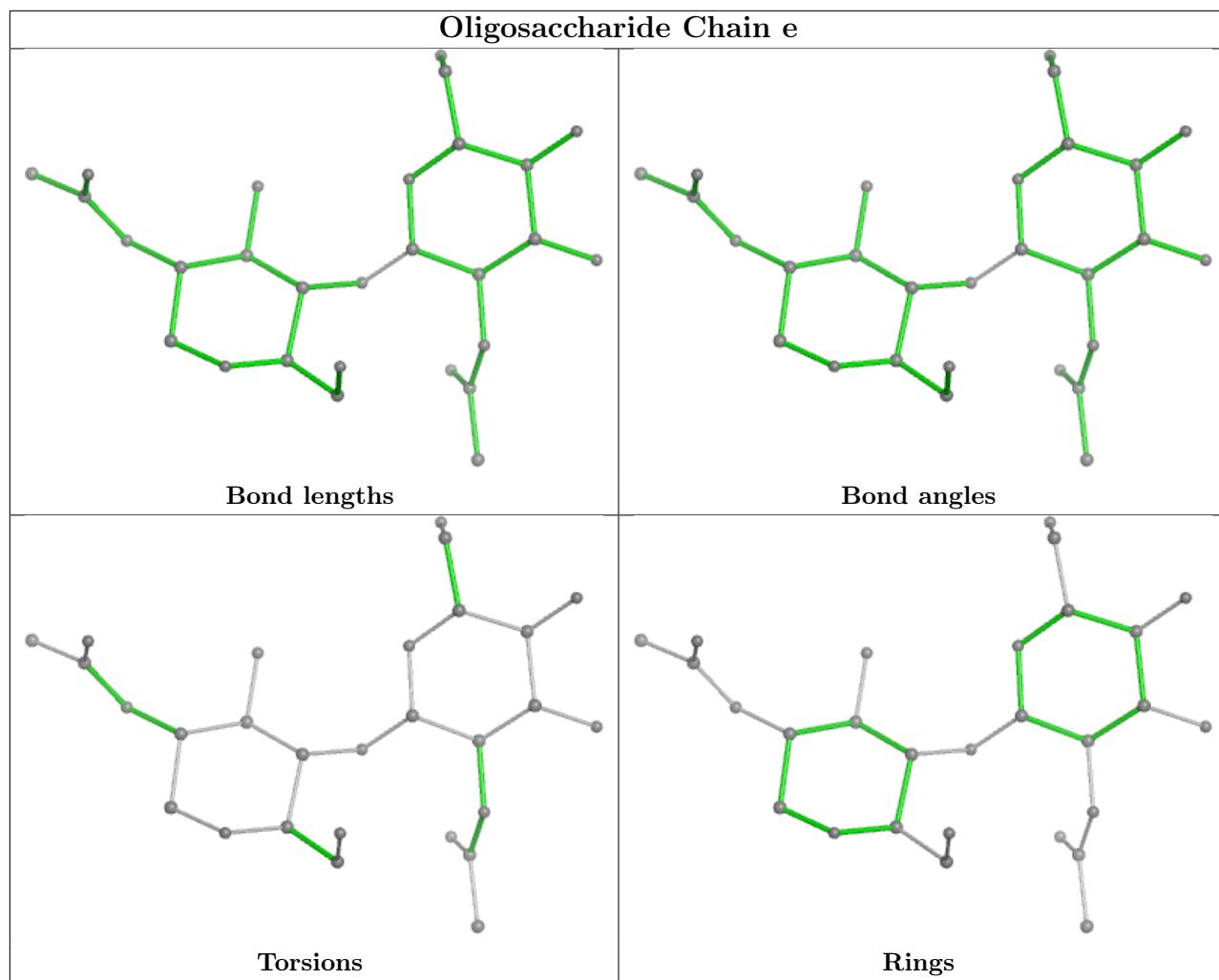
| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	a	5	MAN	1	0
6	F	1	NAG	1	0
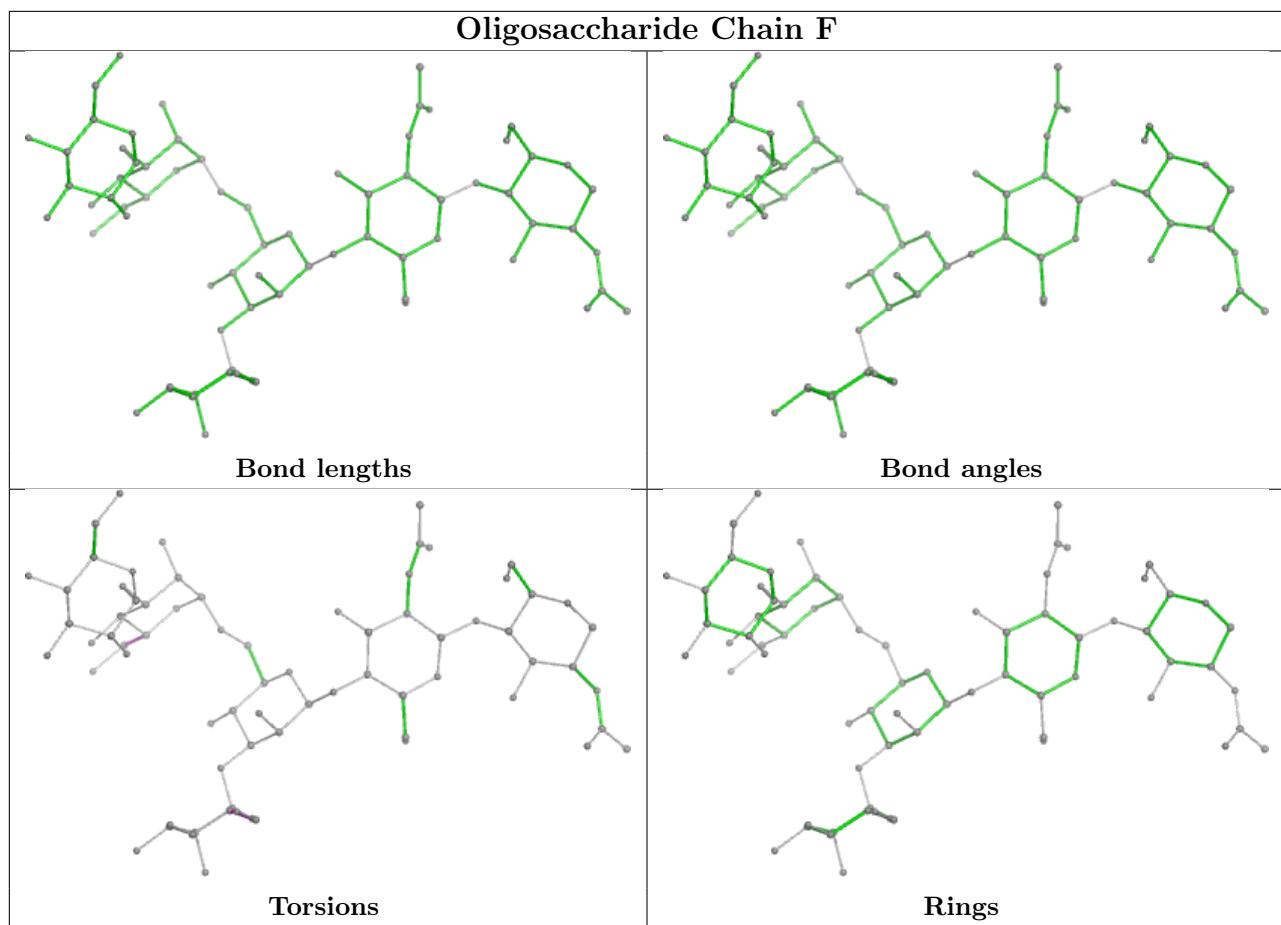
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain a

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain b

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain c

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain e

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain d

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
12	R16	E	504	-	15,15,15	0.14	0	14,14,14	0.23	0
10	D10	C	502	-	9,9,9	0.14	0	8,8,8	0.12	0
10	D10	B	502	-	9,9,9	0.11	0	8,8,8	0.12	0
11	LBN	D	504	-	51,51,51	0.29	0	57,59,59	0.28	0
10	D10	A	503	-	9,9,9	0.12	0	8,8,8	0.16	0
10	D10	E	501	-	9,9,9	0.12	0	8,8,8	0.11	0
14	V8D	B	504	-	17,19,19	0.47	0	22,25,25	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
13	ABU	E	502	-	6,6,6	0.89	0	6,6,6	0.91	0
13	ABU	B	503	-	6,6,6	0.77	0	6,6,6	0.77	0
9	PIO	A	502	-	47,47,47	0.56	0	61,65,65	0.45	0
12	R16	B	501	-	15,15,15	0.10	0	14,14,14	0.19	0
9	PIO	D	502	-	47,47,47	0.54	0	61,65,65	0.46	0
10	D10	D	503	-	9,9,9	0.13	0	8,8,8	0.14	0
11	LBN	A	504	-	51,51,51	0.29	0	57,59,59	0.28	0
14	V8D	E	503	-	17,19,19	0.46	0	22,25,25	0.59	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
12	R16	E	504	-	-	0/13/13/13	-
10	D10	C	502	-	-	0/7/7/7	-
10	D10	B	502	-	-	0/7/7/7	-
11	LBN	D	504	-	-	14/55/55/55	-
10	D10	A	503	-	-	0/7/7/7	-
10	D10	E	501	-	-	0/7/7/7	-
14	V8D	B	504	-	-	0/14/15/15	0/2/2/2
13	ABU	E	502	-	-	0/4/4/4	-
13	ABU	B	503	-	-	0/4/4/4	-
9	PIO	A	502	-	-	8/44/68/68	0/1/1/1
12	R16	B	501	-	-	0/13/13/13	-
9	PIO	D	502	-	-	7/44/68/68	0/1/1/1
10	D10	D	503	-	-	1/7/7/7	-
11	LBN	A	504	-	-	16/55/55/55	-
14	V8D	E	503	-	-	3/14/15/15	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	502	PIO	C4-O4-P4-O42
11	A	504	LBN	C1-O1-P1-O2
11	A	504	LBN	C1-O1-P1-O3

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...
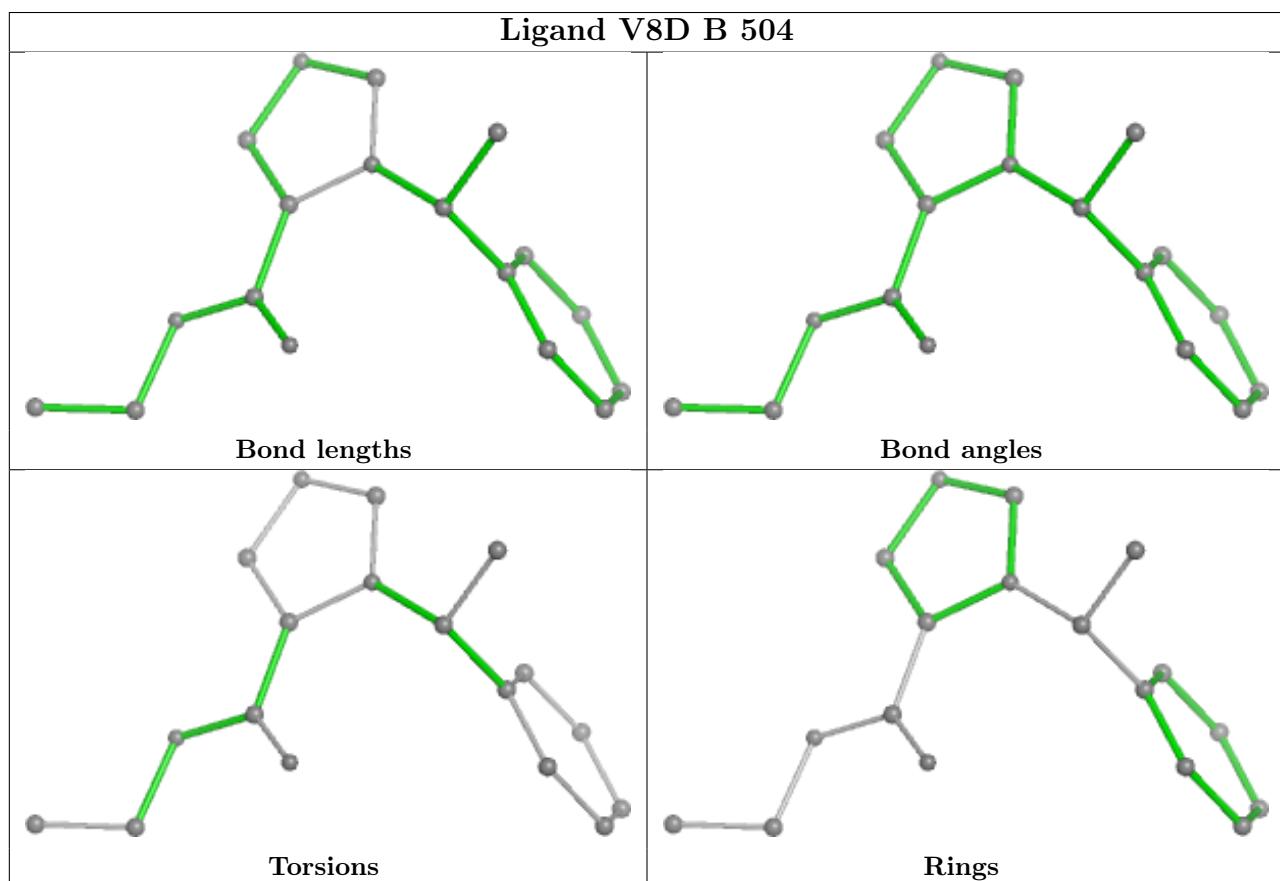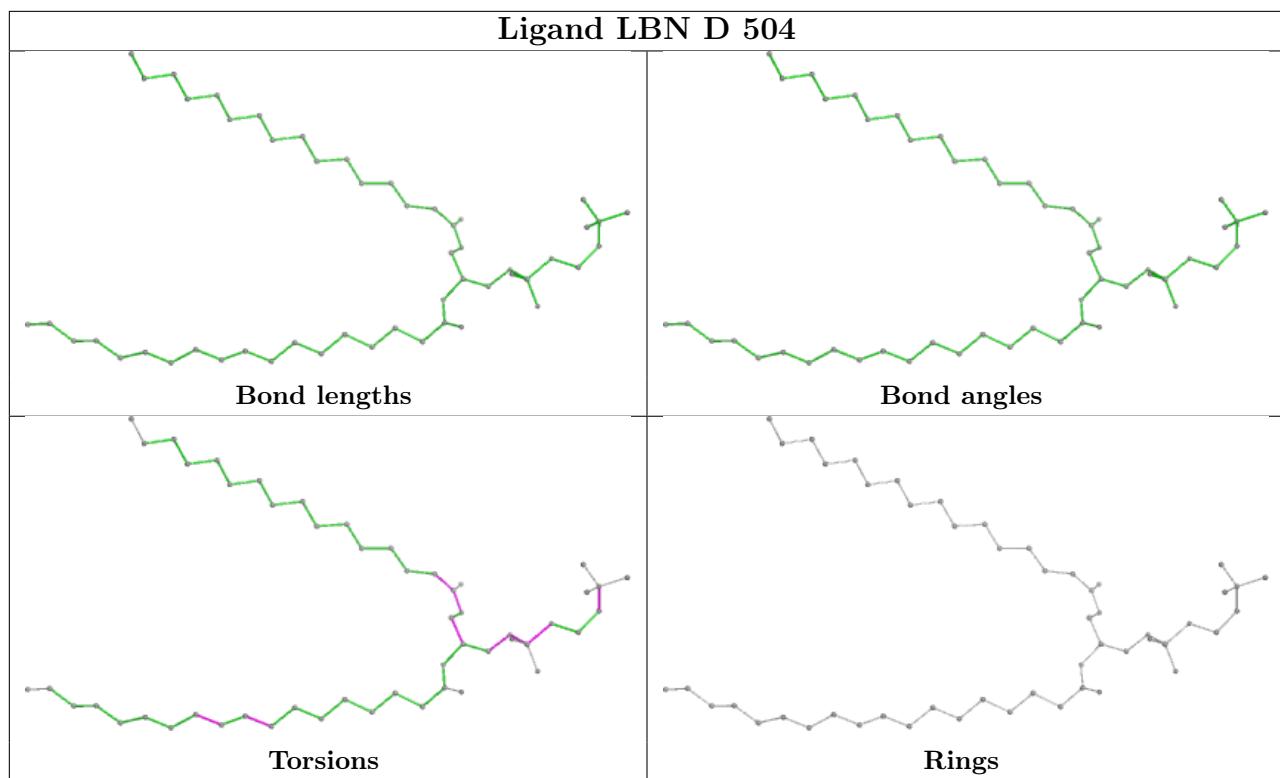
Mol	Chain	Res	Type	Atoms
11	A	504	LBN	C1-O1-P1-O4
11	A	504	LBN	C9-O2-P1-O1
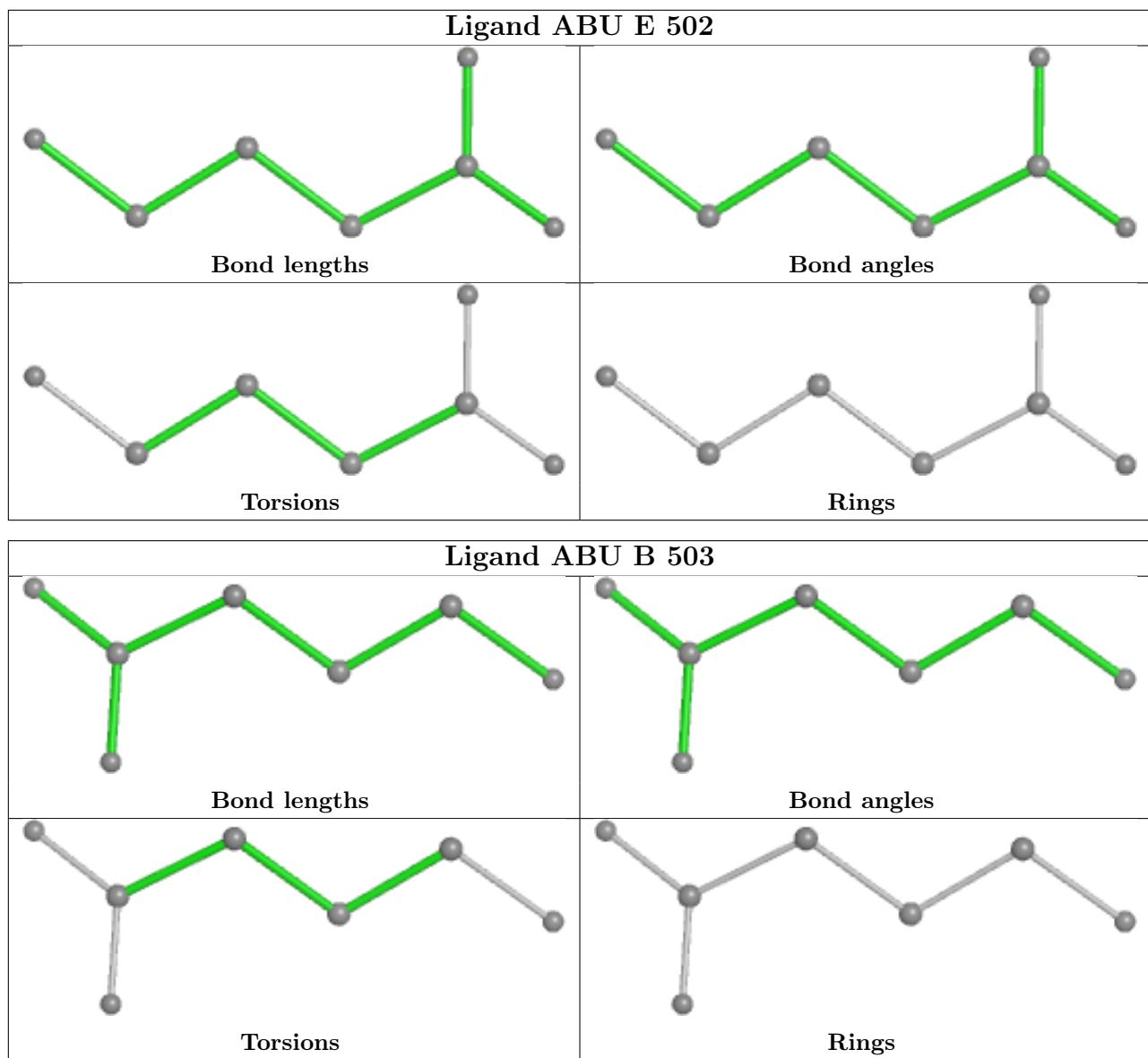
There are no ring outliers.
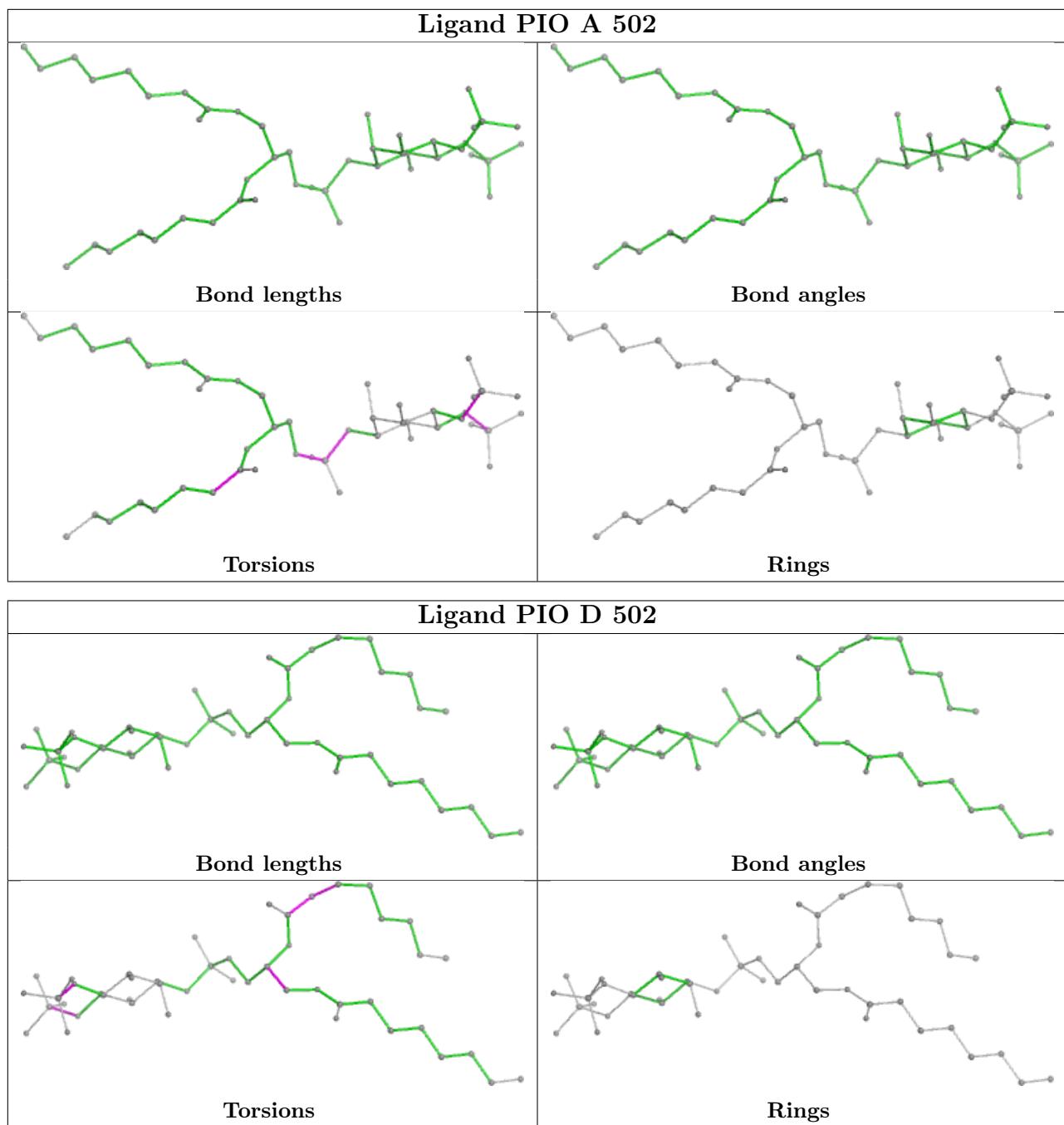
7 monomers are involved in 9 short contacts:
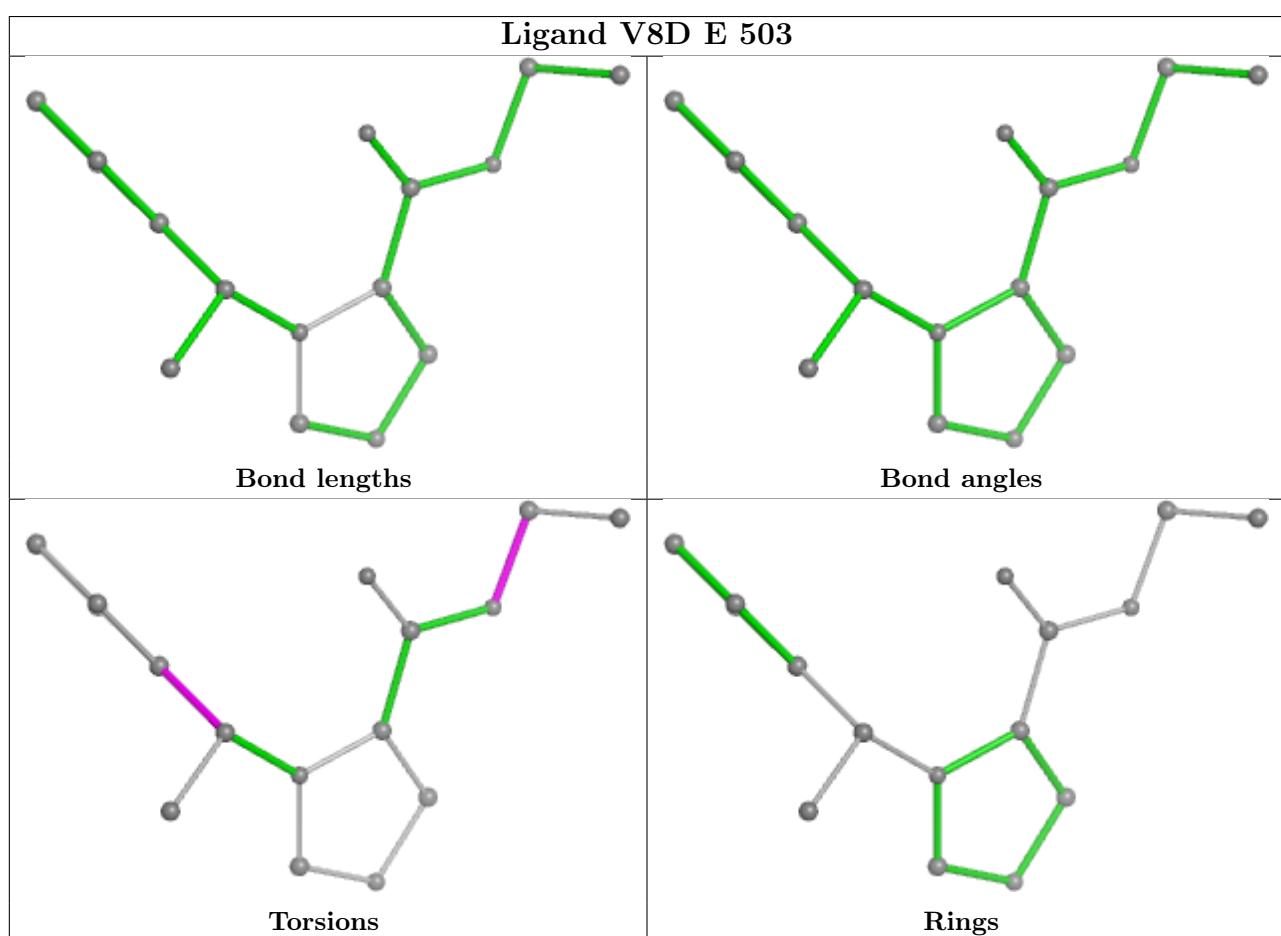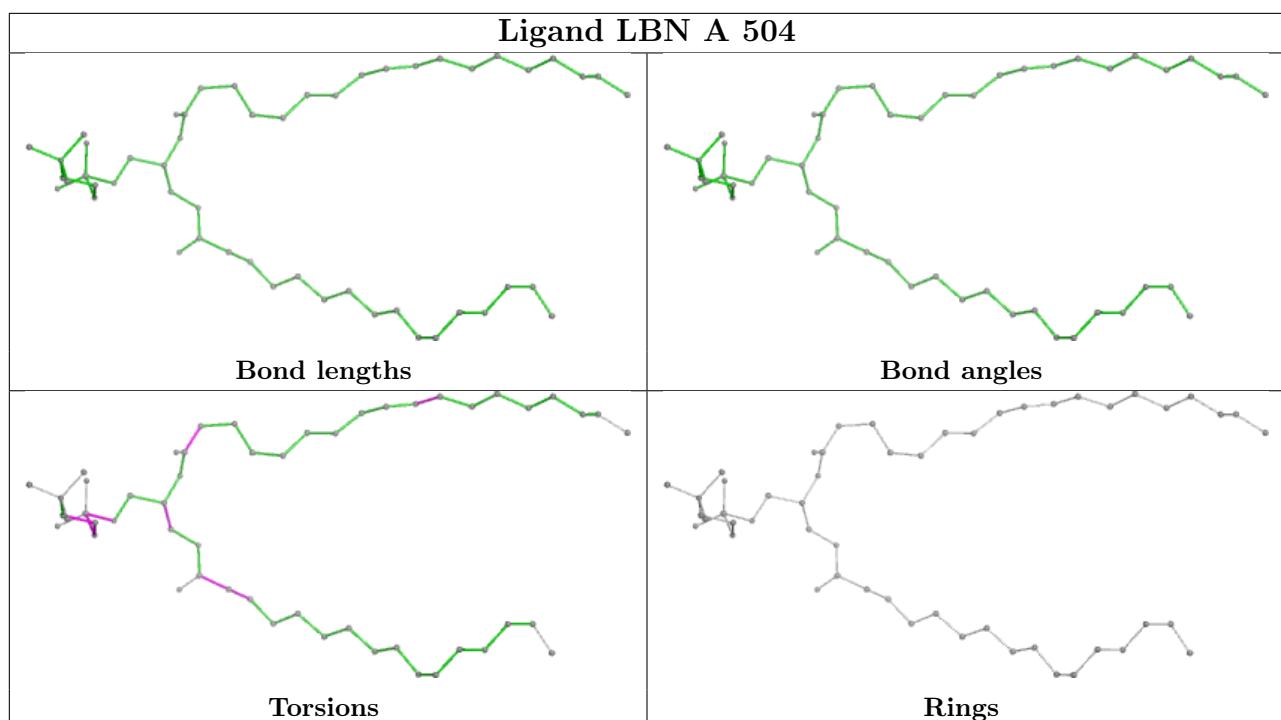
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	502	D10	1	0
10	A	503	D10	1	0
13	E	502	ABU	1	0
9	A	502	PIO	2	0
12	B	501	R16	1	0
9	D	502	PIO	2	0
10	D	503	D10	1	0

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 then 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 LBN D 504

Bond lengths

Bond angles

Torsions

Rings

Ligand V8D B 504

Bond lengths

Bond angles

Torsions

Rings

Ligand ABU E 502	

Bond lengths |

Bond angles |
|

Torsions |

Rings |

Ligand ABU B 503	

Bond lengths |

Bond angles |
|

Torsions |

Rings |

Ligand PIO A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand PIO D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN A 504

Bond lengths

Bond angles

Torsions

Rings

Ligand V8D E 503

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
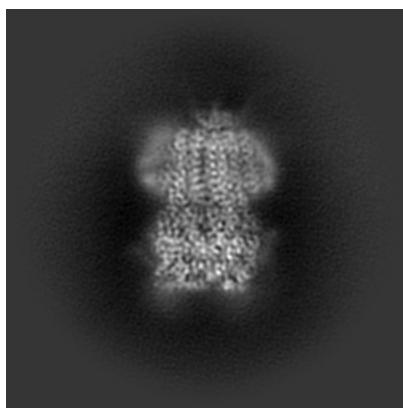
6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-50389. These allow visual inspection of the internal detail of the map and identification of artifacts.
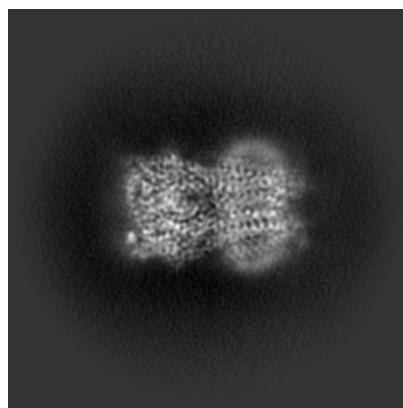
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1   Orthogonal projections ⓘ
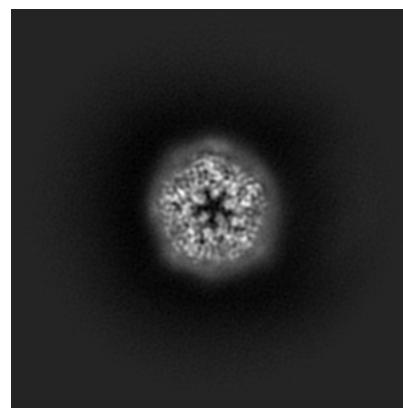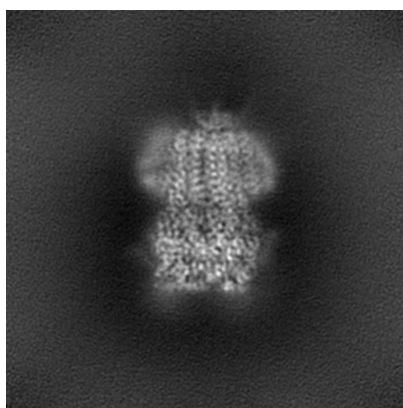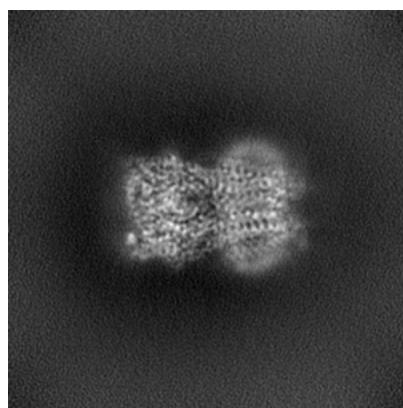
6.1.1   Primary map

X   Y   Z
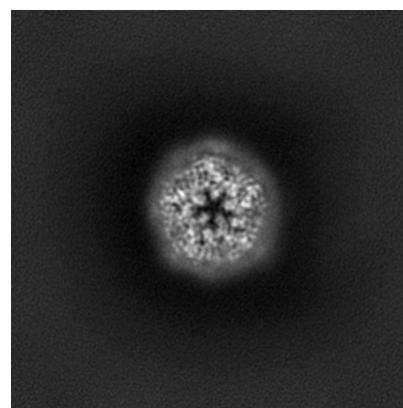
6.1.2   Raw map

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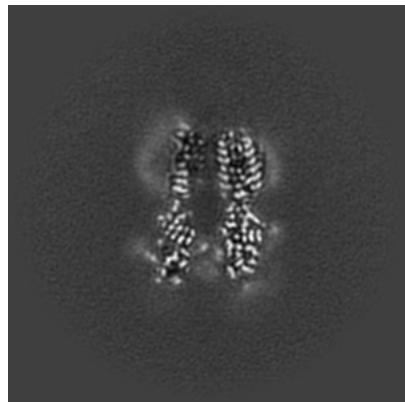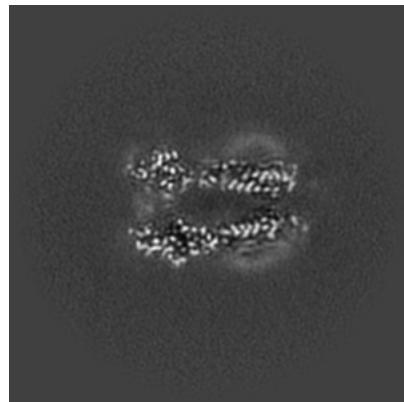
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)
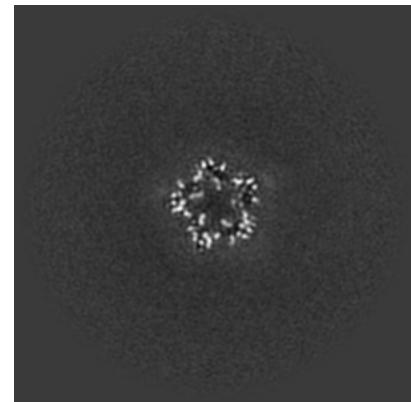
6.2.1 Primary map
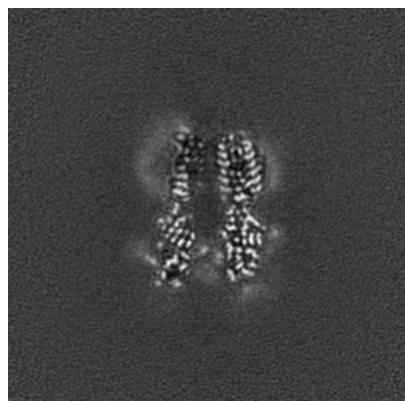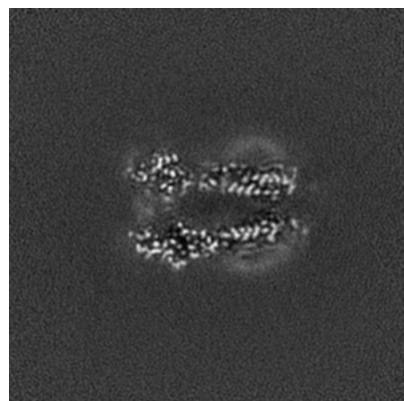
| X Index: 120 | Y Index: 120 | Z Index: 120 |
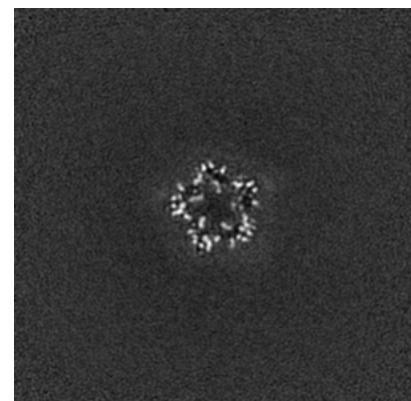
6.2.2 Raw map
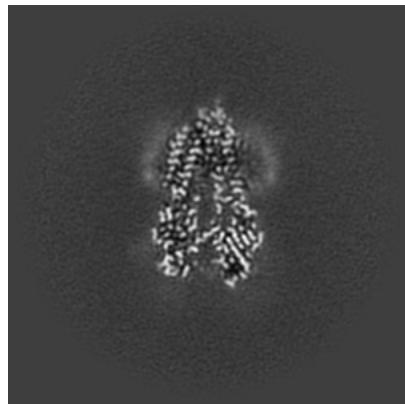
| X Index: 120 | Y Index: 120 | Z Index: 120 |
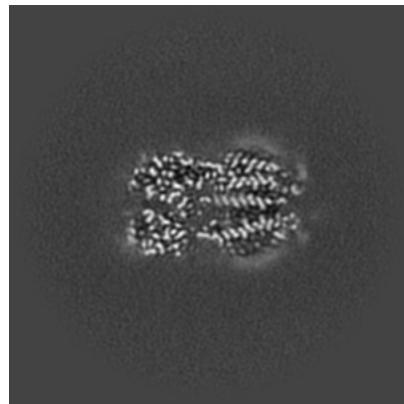
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)
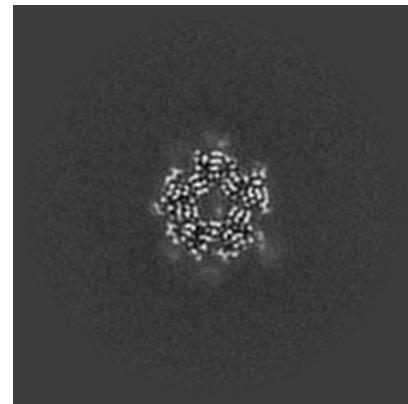
6.3.1 Primary map
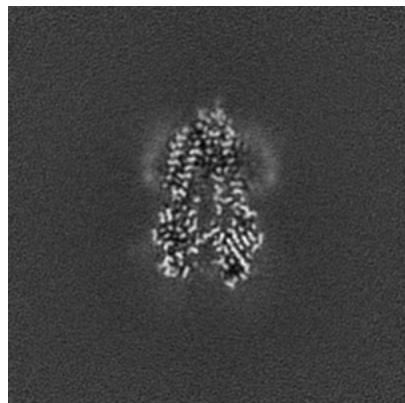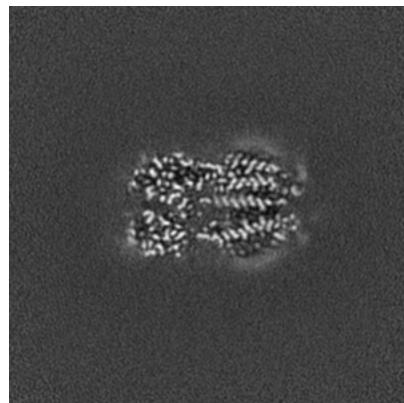
| X Index: 110 | Y Index: 130 | Z Index: 99 |
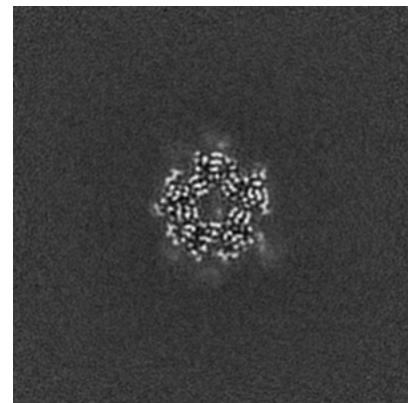
6.3.2 Raw map
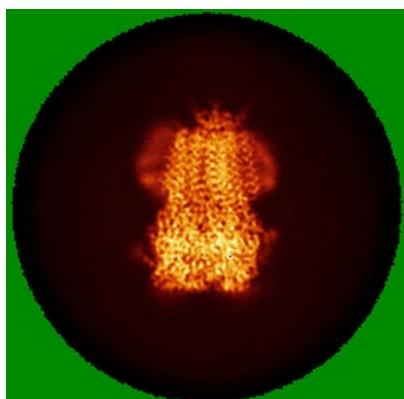
| X Index: 110 | Y Index: 130 | Z Index: 99 |
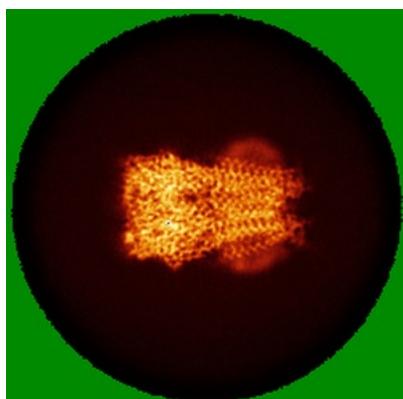
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)
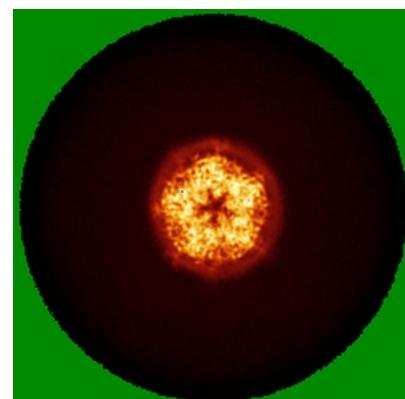
6.4.1 Primary map
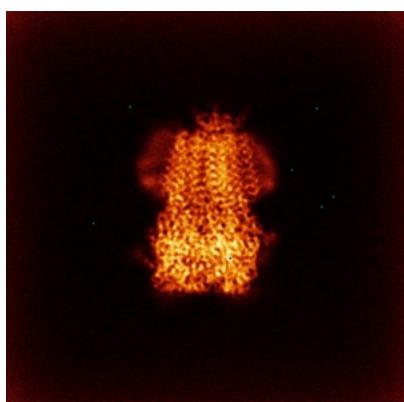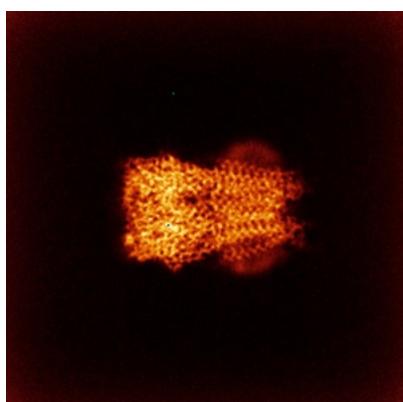
<center>X   Y   Z</center>
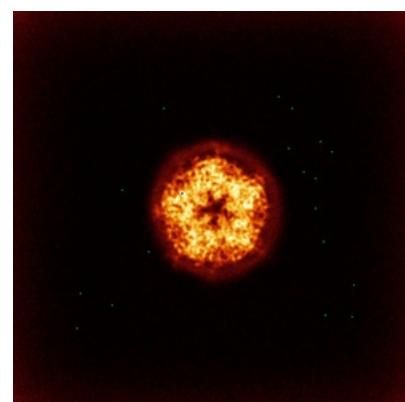
6.4.2 Raw map

<center>X   Y   Z</center>
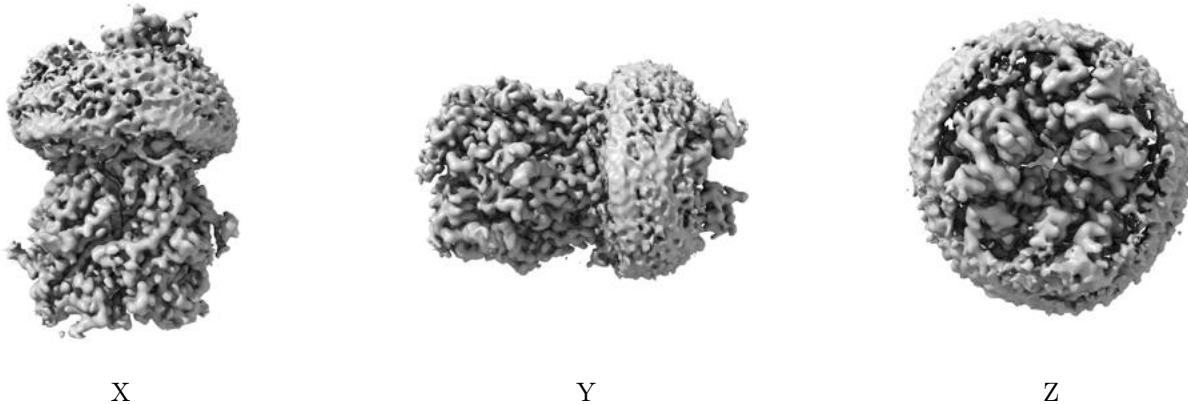
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.
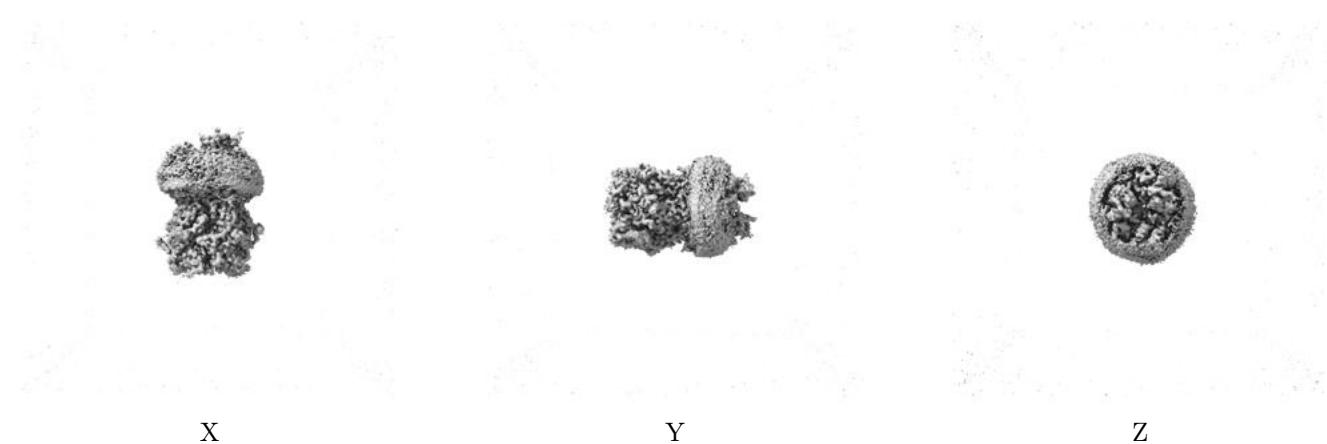
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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

X   Y   Z

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.
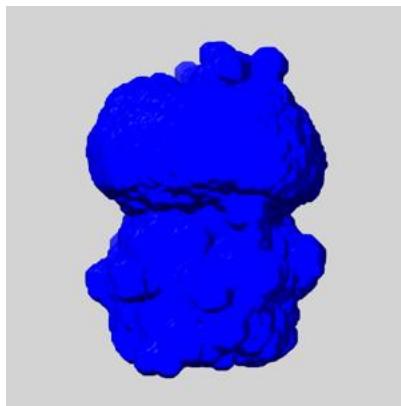
6.6　Mask visualisation ⓘ

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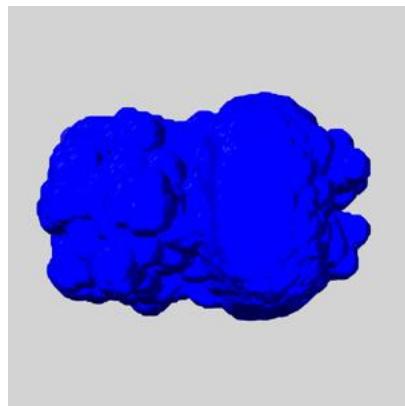
A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure
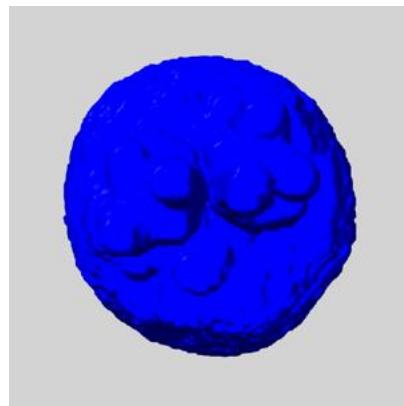
6.6.1　emd_50389_msk_1.map ⓘ
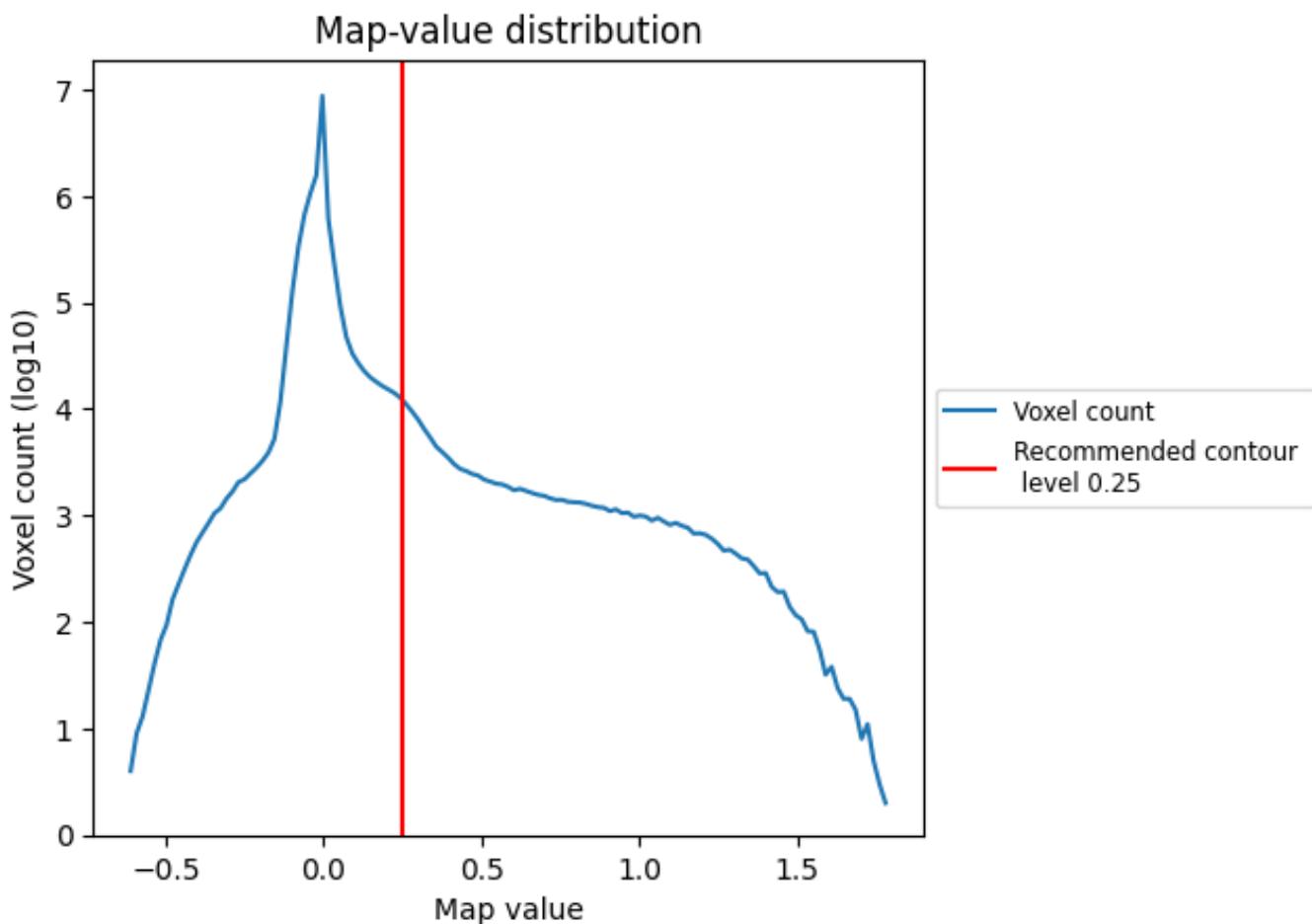
X　　　　　　　　　　　Y　　　　　　　　　　　Z

7   Map analysis (i)
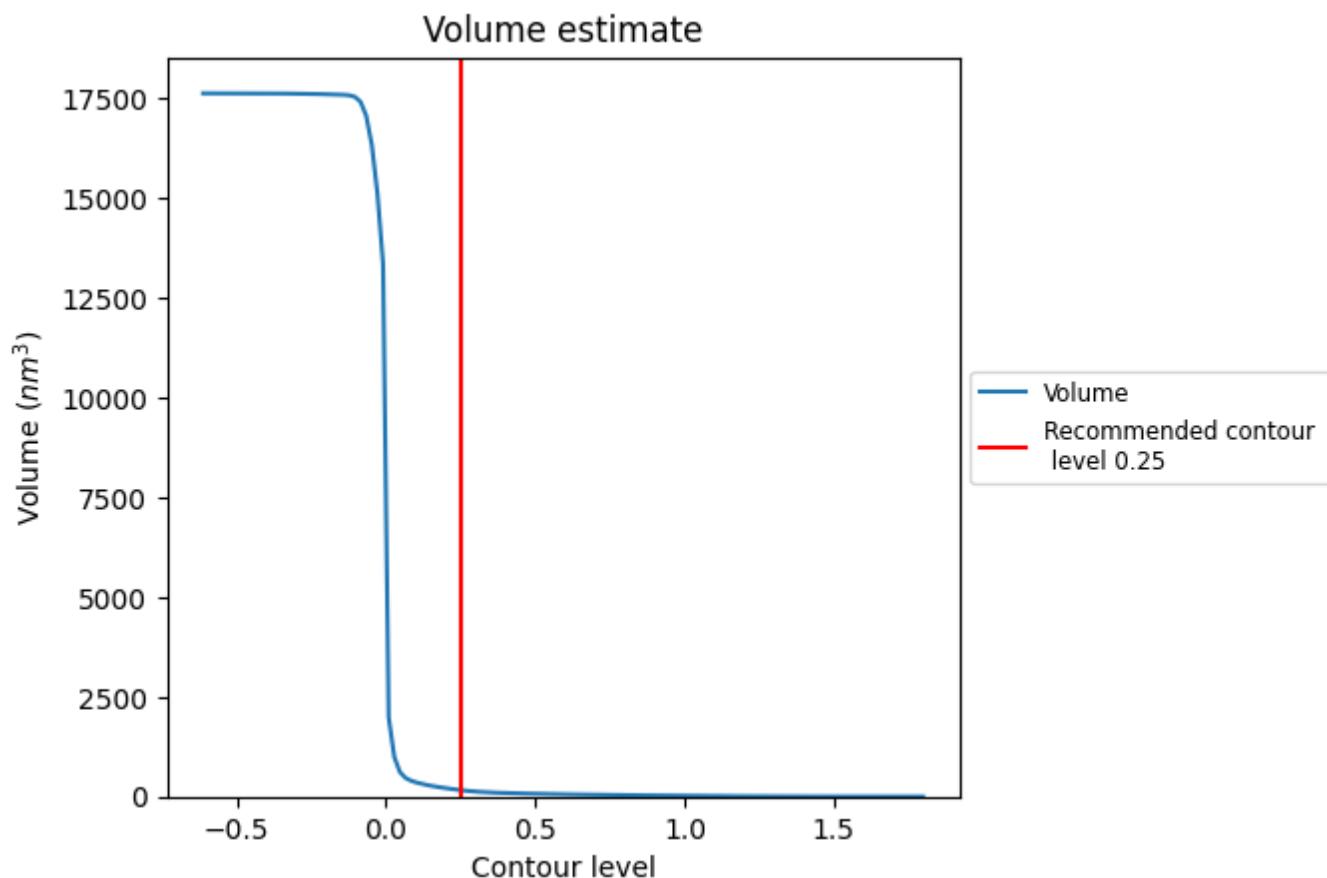
This section contains the results of statistical analysis of the map.

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.
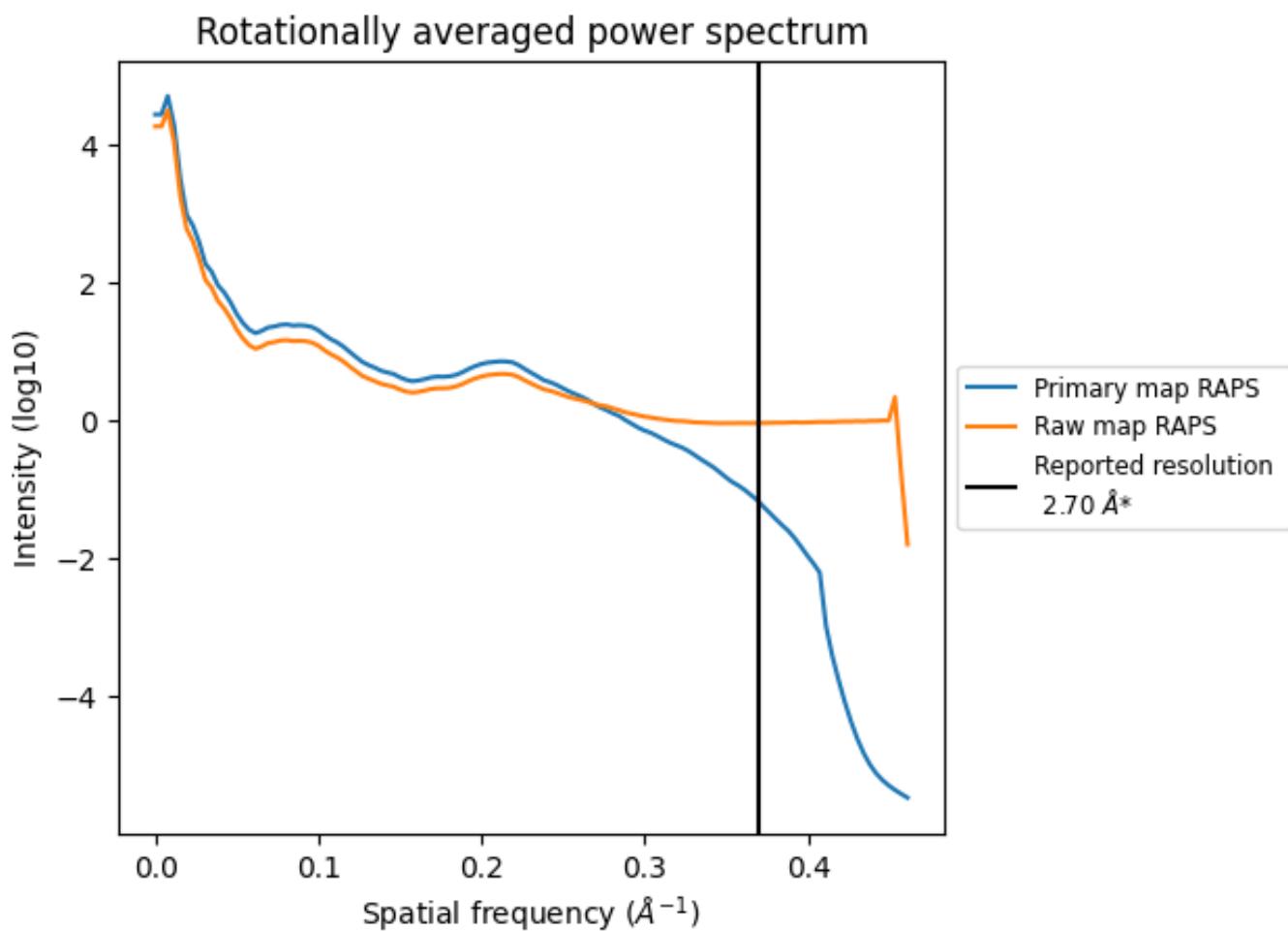
7.2 Volume estimate ⓘ

The volume at the recommended contour level is 162 nm^3; this corresponds to an approximate mass of 146 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 ⓘ
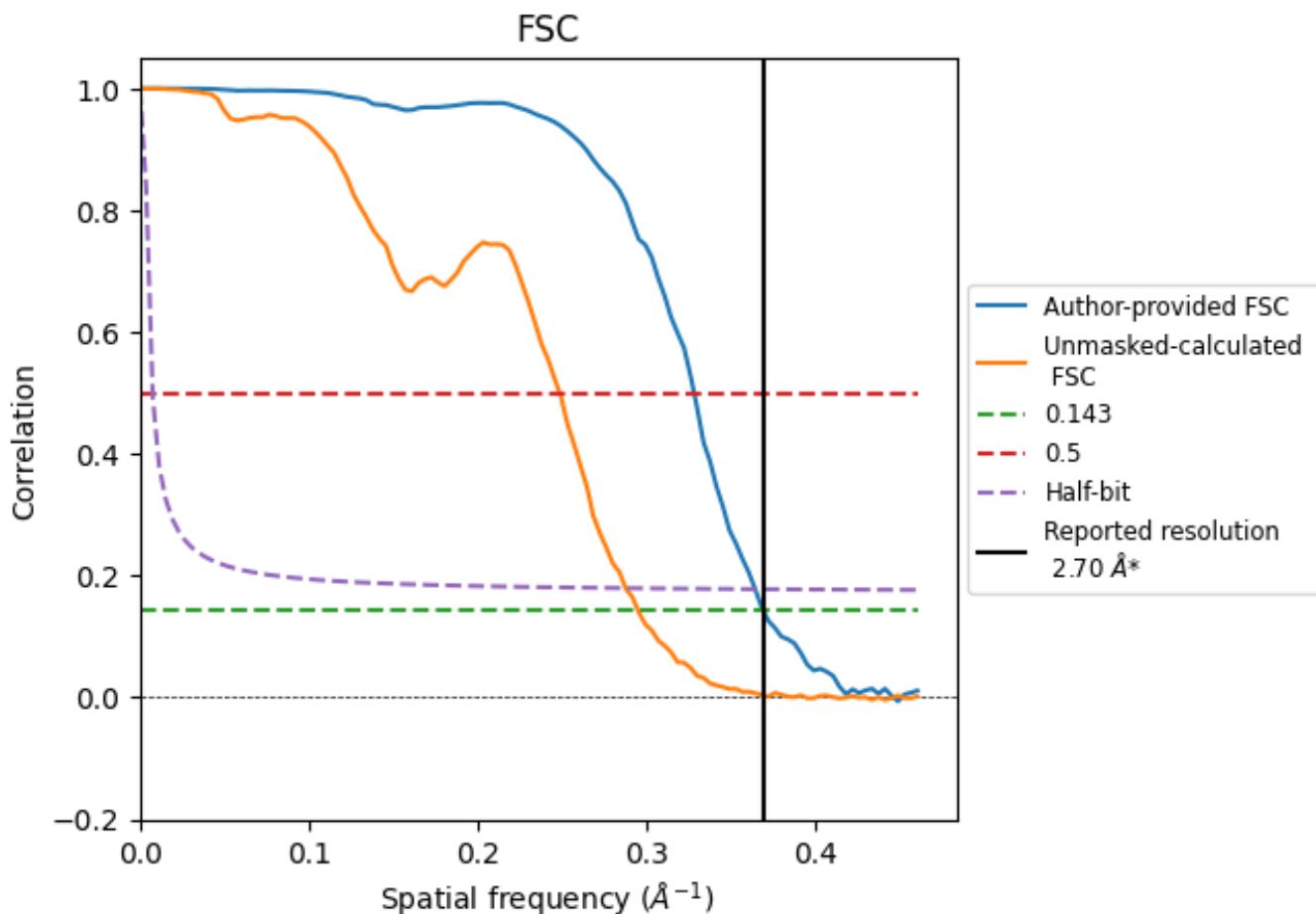
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ

*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2   Resolution estimates ⓘ
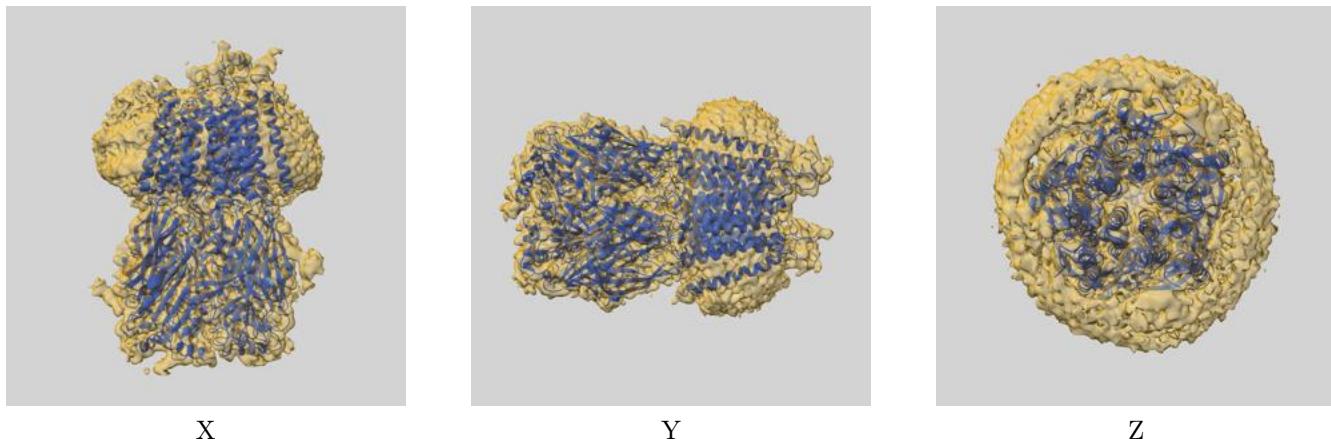
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.04	2.74
Unmasked-calculated*	3.39	4.02	3.47

*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 3.39 differs from the reported value 2.7 by more than 10 %

9 Map-model fit ⓘ
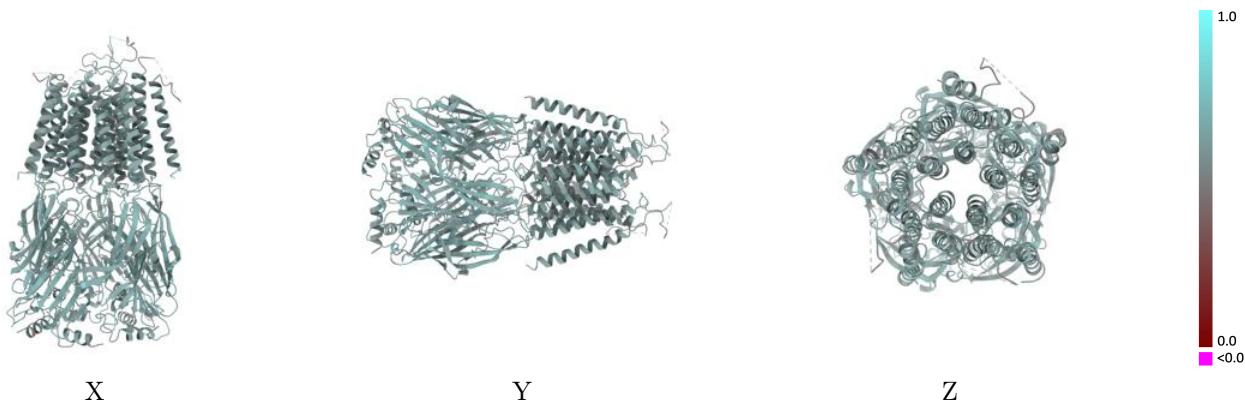
This section contains information regarding the fit between EMDB map EMD-50389 and PDB model 9FG9. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay ⓘ

| X | Y | Z |
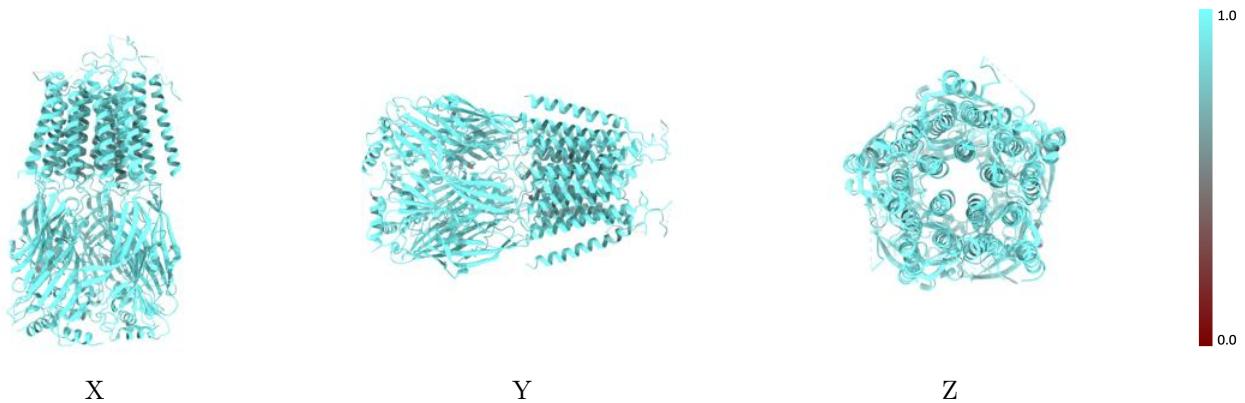
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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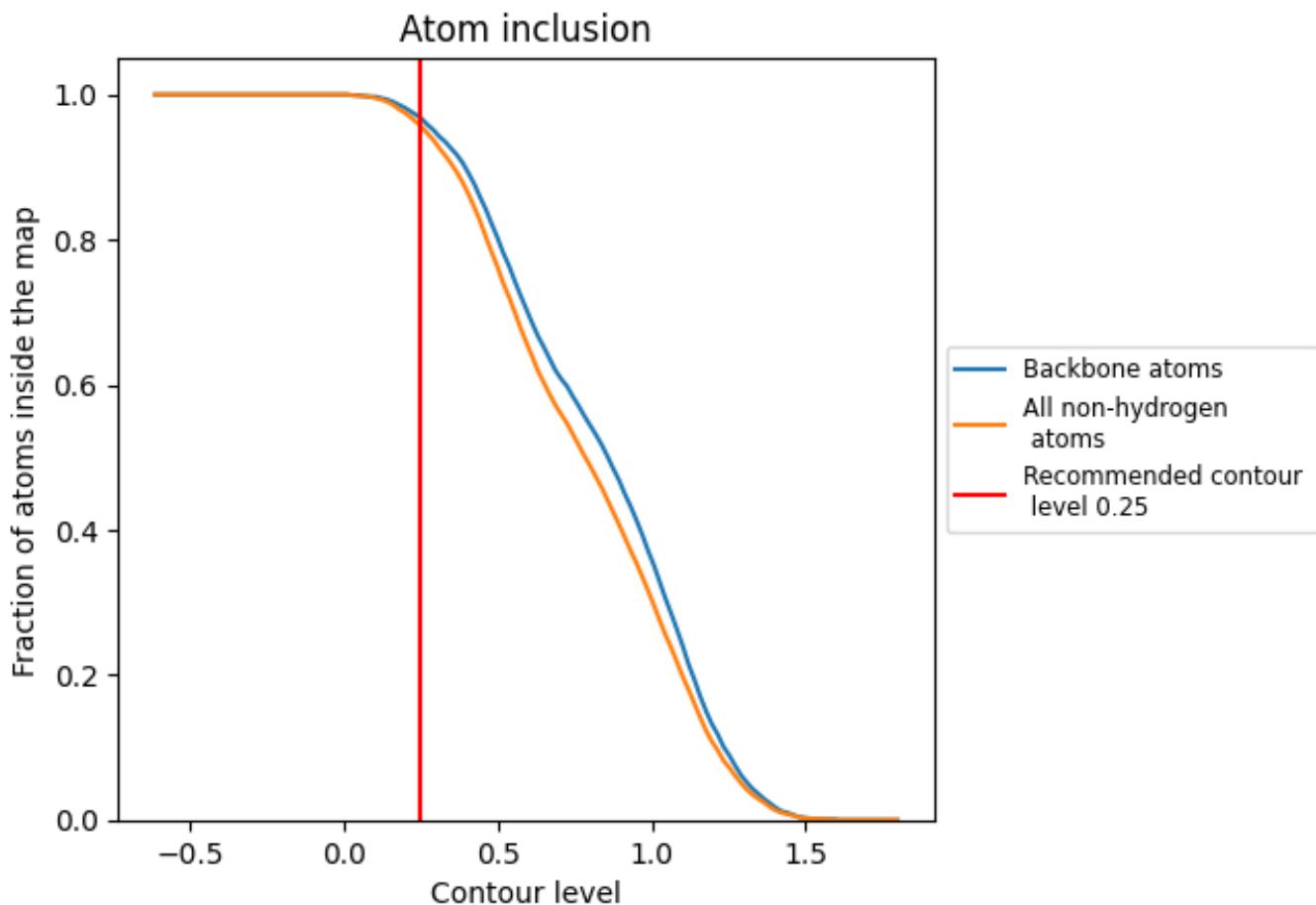
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z

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 (0.25).
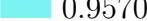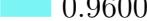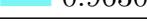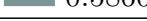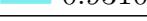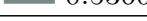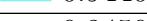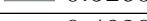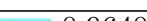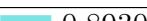
9.4 Atom inclusion ⓘ

At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.5840
A	0.9600	0.5850
B	0.9570	0.5870
C	0.9650	0.5850
D	0.9580	0.5860
E	0.9630	0.5860
F	0.9310	0.5360
G	0.9440	0.5260
a	0.8450	0.4920
b	0.9640	0.5140
c	0.8930	0.4540
d	0.8850	0.5120
e	0.9290	0.5180

1.0

0.0
<0.0