



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2026 – 02:34 PM JST

PDB ID : 9WEU / pdb_00009weu
EMDB ID : EMD-65916
Title : D1R-Gs in complexed with SKF81297/LY3154207/BMSA1
Authors : Xu, Y.; Wang, K.; Zhuang, Y.; Xu, H.E.
Deposited on : 2025-08-20
Resolution : 2.65 Å(reported)

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

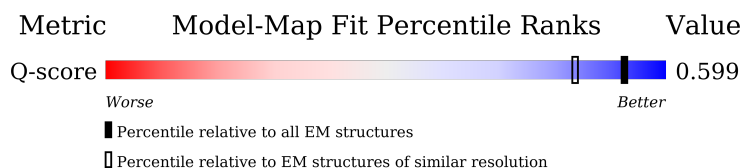
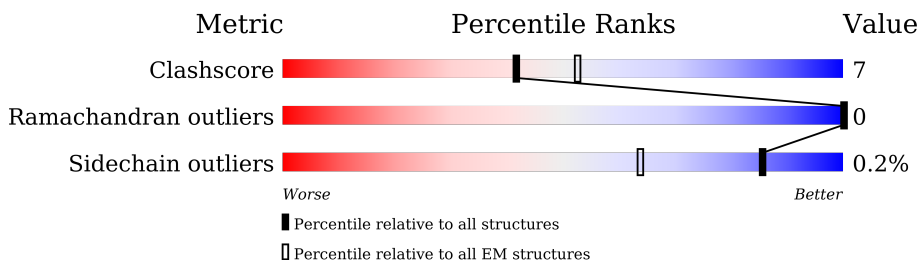
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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	246	
2	B	371	
3	G	68	
4	N	160	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	R	603	40% 6% 54%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8399 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	238	Total	C	N	O	S	0	0
			1989	1250	361	370	8		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	LYS	conflict	UNP P63092
A	49	ASP	GLY	conflict	UNP P63092
A	50	ASN	GLU	conflict	UNP P63092
A	63	TYR	LEU	conflict	UNP P63092
A	88	ALA	GLY	conflict	UNP P63092
A	111	ASP	ALA	conflict	UNP P63092
A	114	ASP	SER	conflict	UNP P63092
A	124	ASP	LEU	conflict	UNP P63092
A	218	SER	ALA	conflict	UNP P63092
A	224	ALA	ILE	conflict	UNP P63092
A	227	ILE	VAL	conflict	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	57	Total	C	N	O	S	0	0
			436	273	77	83	3		

- Molecule 4 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	127	Total	C	N	O	S	0	0
			967	602	169	190	6		

- Molecule 5 is a protein called Beta-2 adrenergic receptor,D(1A) dopamine receptor,Engineered oplophorus-luciferin 2-monooxygenase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	280	Total	C	N	O	S	0	0
			2226	1478	366	365	17		

There are 42 discrepancies between the modelled and reference sequences:

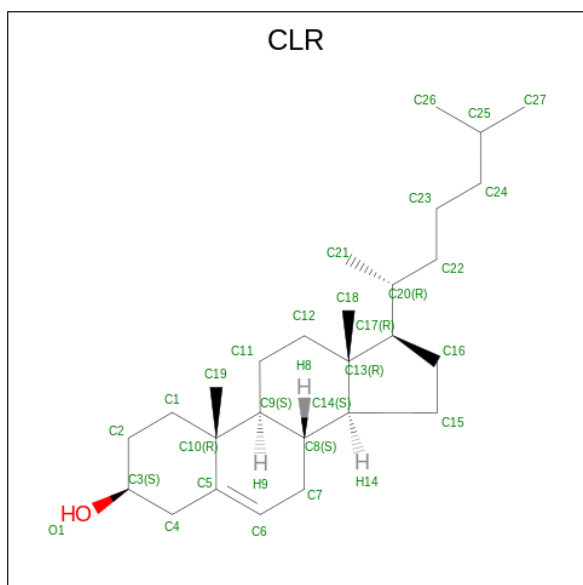
Chain	Residue	Modelled	Actual	Comment	Reference
R	-69	MET	-	initiating methionine	UNP P07550
R	-68	ASP	-	expression tag	UNP P07550
R	-67	SER	-	expression tag	UNP P07550
R	-66	LYS	-	expression tag	UNP P07550
R	-65	GLY	-	expression tag	UNP P07550
R	-64	SER	-	expression tag	UNP P07550
R	-63	SER	-	expression tag	UNP P07550
R	-62	GLN	-	expression tag	UNP P07550
R	-61	LYS	-	expression tag	UNP P07550
R	-60	GLY	-	expression tag	UNP P07550
R	-59	SER	-	expression tag	UNP P07550
R	-58	ARG	-	expression tag	UNP P07550
R	-57	LEU	-	expression tag	UNP P07550
R	-56	LEU	-	expression tag	UNP P07550
R	-55	LEU	-	expression tag	UNP P07550
R	-54	LEU	-	expression tag	UNP P07550
R	-53	LEU	-	expression tag	UNP P07550
R	-52	VAL	-	expression tag	UNP P07550
R	-51	VAL	-	expression tag	UNP P07550
R	-50	SER	-	expression tag	UNP P07550
R	-49	ASN	-	expression tag	UNP P07550
R	-48	LEU	-	expression tag	UNP P07550
R	-47	LEU	-	expression tag	UNP P07550
R	-46	LEU	-	expression tag	UNP P07550
R	-45	CYS	-	expression tag	UNP P07550
R	-44	GLN	-	expression tag	UNP P07550
R	-43	GLY	-	expression tag	UNP P07550
R	-42	VAL	-	expression tag	UNP P07550
R	-41	VAL	-	expression tag	UNP P07550
R	-40	SER	-	expression tag	UNP P07550
R	-39	ASP	-	expression tag	UNP P07550
R	-38	TYR	-	expression tag	UNP P07550
R	-37	LYS	-	expression tag	UNP P07550
R	-36	ASP	-	expression tag	UNP P07550
R	-35	ASP	-	expression tag	UNP P07550

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-34	ASP	-	expression tag	UNP P07550
R	-33	ASP	-	expression tag	UNP P07550
R	-32	VAL	-	expression tag	UNP P07550
R	-31	ASP	-	expression tag	UNP P07550
R	-4	GLN	GLU	conflict	UNP P07550
R	0	ALA	-	linker	UNP P07550
R	1	SER	-	linker	UNP P07550

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	O	0
			28	27	1	

- Molecule 7 is 1-[(1 {S},3 {R},6 {R})-6-(1,3-benzodioxol-5-yl)-3-bicyclo[4.1.0]heptan-yl]-4-[(2-bromanyl-5-chloranyl-phenyl)methyl]piperazine (CCD ID: A1EV3) (formula: $C_{25}H_{28}BrClN_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
7	R	1	Total	Br	C	Cl	N	O	0
			31	1	25	1	2	2	

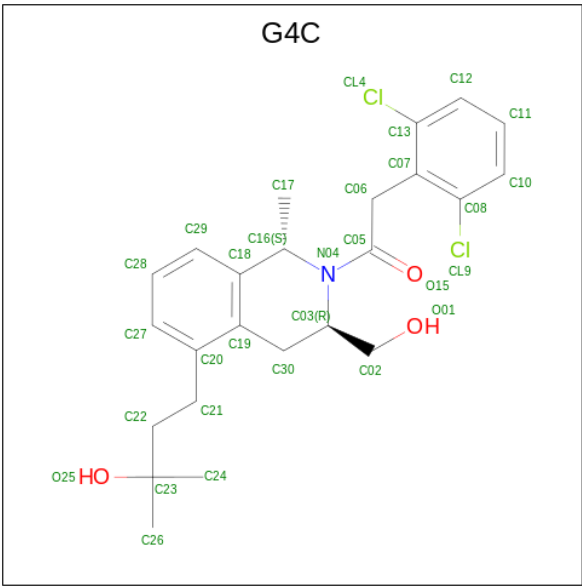
- Molecule 8 is (1R)-6-chloro-1-phenyl-2,3,4,5-tetrahydro-1H-3-benzazepine-7,8-diol (CCD ID: SK0) (formula: $\text{C}_{16}\text{H}_{16}\text{ClNO}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
8	R	1	Total 20	C 16	Cl 1	N 1	O 2	0

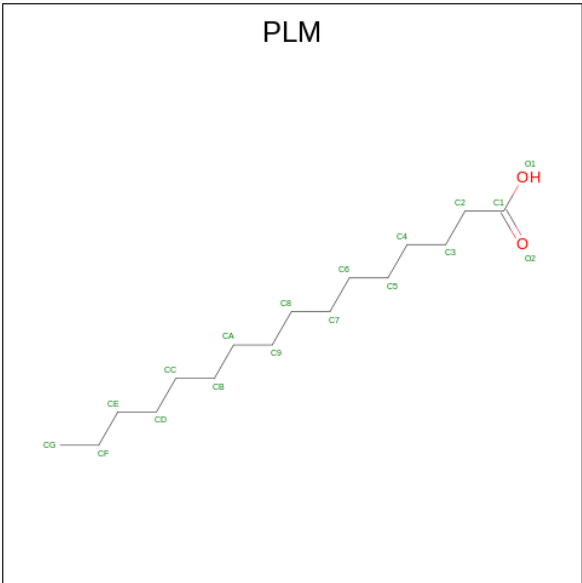
- Molecule 9 is 2-[2,6-bis(chloranyl)phenyl]-1-[(1S,3R)-3-(hydroxymethyl)-1-methyl-5-(3-methyl-3-oxidanyl-butyl)-3,4-dihydro-1H-isoquinolin-2-yl]ethanone (CCD ID: G4C) (formula:

C₂₄H₂₉Cl₂NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
9	R	1	30	24	2	1	3	0

- Molecule 10 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	R	1	18	16	2	0
10	R	1	Total 18	C 16	O 2	0

Continued on next page...

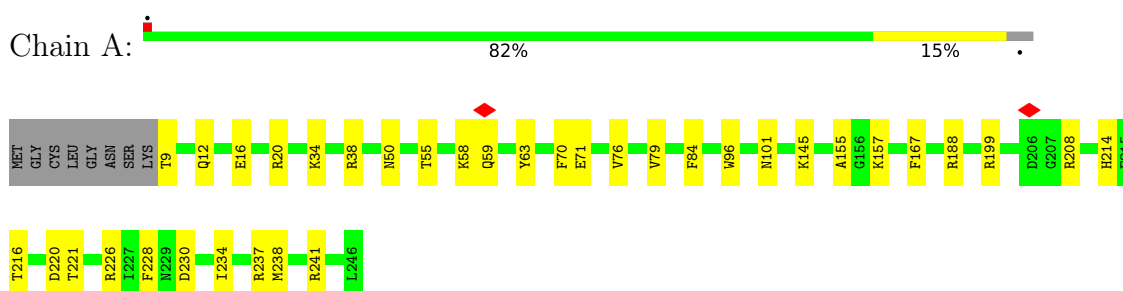
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
10	R	1	Total	C	O	0
			18	16	2	
10	R	1	Total	C	O	0
			18	16	2	

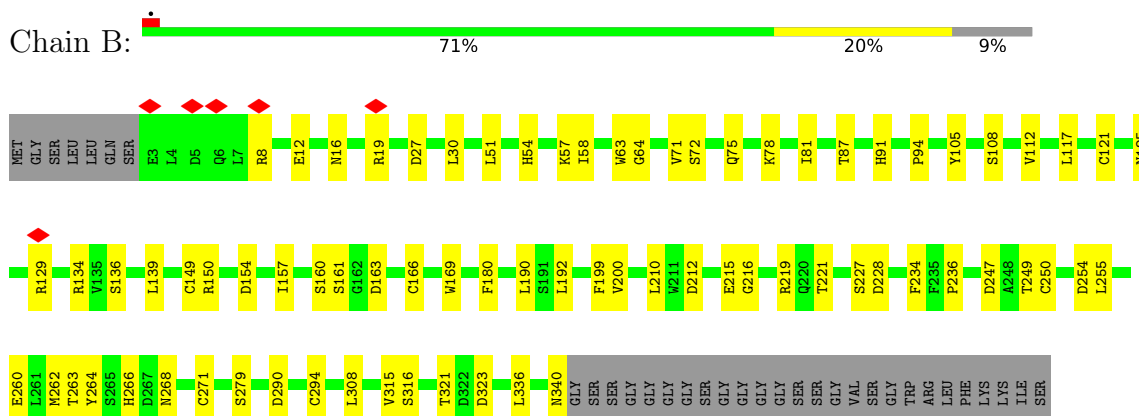
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

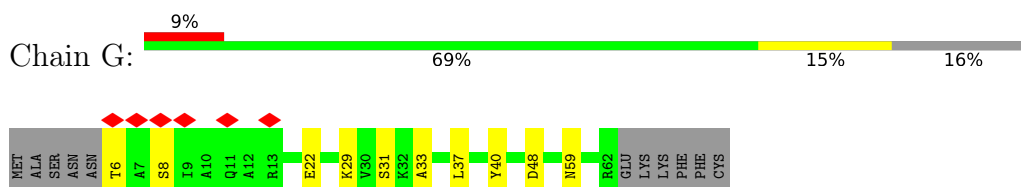
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

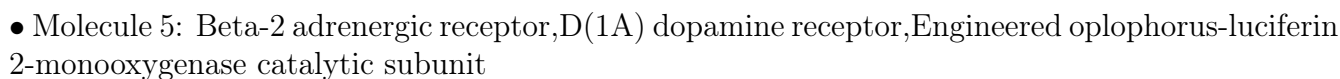


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: Nanobody35





ILE	THR	VAL	THR	GLY	THR	THR	LEU	THR	ASP	SER	R121	HIS	MET
THR	VAL	THR	ASP	GLN	ASP	THR	SER	PHE	PHE	SER	Y122	ASP	ASP
GLY	THR	GLN	THR	GLY	GLY	THR	THR	GLY	GLY	LYS	R133	THR	LYS
THR	THR	MET	THR	MET	SER	THR	SER	THR	THR	SER	M135	GLN	GLY
LEU	THR	ALA	GLU	GLU	THR	GLU	GLN	GLU	GLU	THR	K138	ARG	SER
THR	ASN	ILE	THR	THR	THR	THR	THR	THR	THR	THR	S145	ALA	GLN
ASN	GLY	GLU	GLU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	T149	SER	SER
LYS	ASN	GLU	VAL	VAL	THR	THR	THR	THR	THR	THR	T168	ARG	ARG
ILE	PHE	PHE	ASN	ASN	THR	THR	THR	THR	THR	THR	P168	THR	LEU
ILE	LYS	VAL	VAL	VAL	ASP	GLY	GLY	GLY	GLY	GLY	THR	ASN	LEU
ASP	ASP	VAL	VAL	VAL	GLN	GLY	GLY	GLY	GLY	GLY	SER	SER	LEU
GLU	GLU	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	PRO	THR	LEU
LEU	LEU	PRO	PRO	PRO	LEU	GLY	GLY	GLY	GLY	GLY	SER	ALA	VAL
ILE	ILE	VAL	VAL	VAL	GLU	GLY	GLY	GLY	GLY	GLY	ASP	MET	VAL
THR	THR	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	THR	ASP	SER
PRO	PRO	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	ASN
HIS	GLY	HIS	HIS	HIS	VAL	VAL	VAL	VAL	VAL	PHE	THR	GLY	LEU
GLY	PHE	PHE	PHE	PHE	THR	THR	THR	THR	THR	THR	THR	THR	LEU
VAL	VAL	VAL	VAL	VAL	ASN	ASN	ASN	ASN	ASN	ASN	ILE	VAL	VAL
THR	THR	THR	THR	THR	LEU	LEU	LEU	LEU	LEU	LEU	ASP	PHE	SER
ILE	ILE	GLY	GLY	GLY	ALA	ALA	ALA	ALA	ALA	ALA	N185	THR	THR
ASN	ASN	THR	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	I205	LYS	LYS
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	P206	ASP	ASP
HIS	HIS	ILE	ILE	ILE	THR	THR	THR	THR	THR	THR	V207	ASP	ASP
HIS	HIS	ASP	ASP	ASP	PRO	PRO	PRO	PRO	PRO	PRO	A208	ASP	ASP
HIS	HIS	GLY	GLY	GLY	ILE	ILE	ILE	ILE	ILE	ILE	I209	VAL	VAL
HIS	HIS	VAL	VAL	VAL	ARG	ARG	ARG	ARG	ARG	ARG	V212	ASP	ASP
HIS	HIS	THR	THR	THR	GLN	GLN	GLN	GLN	GLN	GLN	T213	MET	MET
HIS	HIS	PRO	PRO	PRO	ILE	ILE	ILE	ILE	ILE	ILE	K239	GLY	GLY
HIS	HIS	ASN	ASN	ASN	VAL	VAL	VAL	VAL	VAL	VAL	N240	GLN	GLN
HIS	HIS	MET	MET	MET	ARG	ARG	ARG	ARG	ARG	ARG	CYS	PRO	PRO
HIS	HIS	ASN	ASN	ASN	SER	SER	SER	SER	SER	SER	V58	GLY	GLY
HIS	HIS	ASN	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLN	ASN	ASN
HIS	HIS	THR	THR	THR	ALA	ALA	ALA	ALA	ALA	ALA	T59	GLY	GLY
HIS	HIS	PHE	PHE	PHE	ASN	ASN	ASN	ASN	ASN	ASN	THR	THR	SER
HIS	HIS	GLY	GLY	GLY	ALA	ALA	ALA	ALA	ALA	ALA	THR	THR	ALA
HIS	HIS	ARG	ARG	ARG	LEU	LEU	LEU	LEU	LEU	LEU	THR	THR	SER
HIS	HIS	PRO	PRO	PRO	LYS	LYS	LYS	LYS	LYS	LYS	GLY	GLY	ALA
HIS	HIS	TYR	TYR	TYR	ILE	ILE	ILE	ILE	ILE	ILE	THR	THR	PHE
HIS	HIS	GLU	GLU	GLU	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	LEU
HIS	HIS	GLY	GLY	GLY	ILE	ILE	ILE	ILE	ILE	ILE	LYS	LYS	ALA
HIS	HIS	ILE	ILE	ILE	HIS	HIS	HIS	HIS	HIS	HIS	PRO	PRO	PRO
HIS	HIS	ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	F102	ASN	ASN
HIS	HIS	PHE	PHE	PHE	ILE	ILE	ILE	ILE	ILE	ILE	CYS	GLY	SER
HIS	HIS	ASP	ASP	ASP									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	898739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	4.841	Depositor
Minimum map value	-3.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	263.68, 263.68, 263.68	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	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: SK0, G4C, PLM, A1EV3, CLR

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	0.14	0/2029	0.30	0/2731
2	B	0.13	0/2647	0.30	0/3589
3	G	0.14	0/442	0.31	0/597
4	N	0.12	0/987	0.34	0/1337
5	R	0.19	0/2283	0.41	0/3105
All	All	0.15	0/8388	0.34	0/11359

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	1989	0	1950	29	0
2	B	2600	0	2505	53	0
3	G	436	0	448	9	0
4	N	967	0	937	9	0
5	R	2226	0	2304	24	0
6	R	28	0	46	2	0
7	R	31	0	0	3	0
8	R	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	R	30	0	0	1	0
10	R	72	0	124	0	0
All	All	8399	0	8314	114	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.

The worst 5 of 114 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:208:ARG:NH2	1:A:241:ARG:HD2	1.39	1.36
1:A:208:ARG:HH21	1:A:241:ARG:CD	1.60	1.14
1:A:208:ARG:HH21	1:A:241:ARG:HD2	0.86	1.02
5:R:329:ILE:HG22	7:R:602:A1EV3:C30	2.11	0.81
1:A:208:ARG:NH2	1:A:241:ARG:CD	2.30	0.79

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	236/246 (96%)	229 (97%)	7 (3%)	0	100	100
2	B	336/371 (91%)	325 (97%)	11 (3%)	0	100	100
3	G	55/68 (81%)	55 (100%)	0	0	100	100
4	N	125/160 (78%)	123 (98%)	2 (2%)	0	100	100
5	R	272/603 (45%)	265 (97%)	7 (3%)	0	100	100
All	All	1024/1448 (71%)	997 (97%)	27 (3%)	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	216/222 (97%)	216 (100%)	0	100	100
2	B	281/302 (93%)	281 (100%)	0	100	100
3	G	46/56 (82%)	46 (100%)	0	100	100
4	N	105/129 (81%)	105 (100%)	0	100	100
5	R	247/526 (47%)	245 (99%)	2 (1%)	73	85
All	All	895/1235 (72%)	893 (100%)	2 (0%)	85	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	29	PHE
5	R	333	PHE

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

Mol	Chain	Res	Type
2	B	340	ASN
3	G	18	GLN
5	R	160	GLN
4	N	120	GLN
2	B	88	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
6	CLR	R	601	-	31,31,31	1.12	3 (9%)	48,48,48	1.49	11 (22%)
10	PLM	R	607	-	17,17,17	0.58	0	17,17,17	0.70	0
10	PLM	R	608	-	17,17,17	0.59	0	17,17,17	0.70	0
8	SK0	R	603	-	20,22,22	1.70	4 (20%)	23,31,31	0.73	1 (4%)
10	PLM	R	605	-	17,17,17	0.59	0	17,17,17	0.68	0
10	PLM	R	606	-	17,17,17	0.59	0	17,17,17	0.68	0
9	G4C	R	604	-	32,32,32	2.74	12 (37%)	41,47,47	1.19	4 (9%)
7	A1EV3	R	602	-	35,36,36	3.24	14 (40%)	45,54,54	3.00	17 (37%)

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	CLR	R	601	-	-	5/10/68/68	0/4/4/4
10	PLM	R	607	-	-	6/15/15/15	-
10	PLM	R	608	-	-	3/15/15/15	-
8	SK0	R	603	-	-	0/4/15/15	0/3/3/3
10	PLM	R	605	-	-	1/15/15/15	-
10	PLM	R	606	-	-	4/15/15/15	-
9	G4C	R	604	-	-	5/16/32/32	0/3/3/3
7	A1EV3	R	602	-	-	3/14/48/48	0/6/6/6

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	604	G4C	C05-N04	10.80	1.50	1.36
7	R	602	A1EV3	C12-N11	-9.50	1.29	1.47
7	R	602	A1EV3	C07-C01	-6.27	1.43	1.53
7	R	602	A1EV3	C22-N08	-6.18	1.35	1.47
7	R	602	A1EV3	C09-N08	-5.89	1.35	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	602	A1EV3	C02-C03-C23	-11.36	93.18	118.85
7	R	602	A1EV3	C04-C03-C02	-11.11	97.07	118.64
7	R	602	A1EV3	BR15-C14-C13	-4.43	114.26	120.34
7	R	602	A1EV3	C12-C13-C14	-4.26	113.53	122.47
7	R	602	A1EV3	C12-C13-C20	3.63	126.85	120.38

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	R	604	G4C	O01-C02-C03-C30
9	R	604	G4C	O01-C02-C03-N04
9	R	604	G4C	C21-C22-C23-C24
9	R	604	G4C	C21-C22-C23-O25
6	R	601	CLR	C21-C20-C22-C23

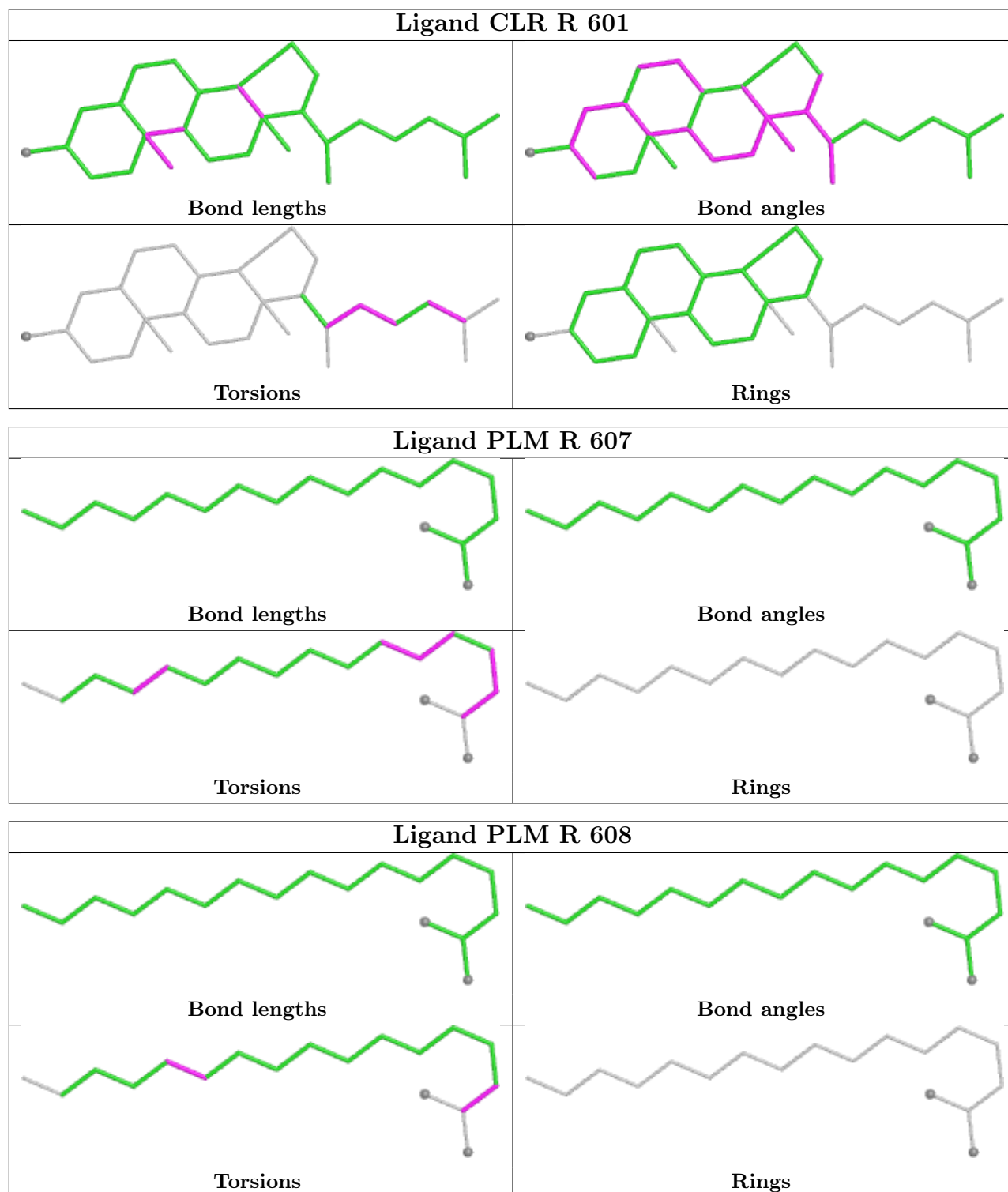
There are no ring outliers.

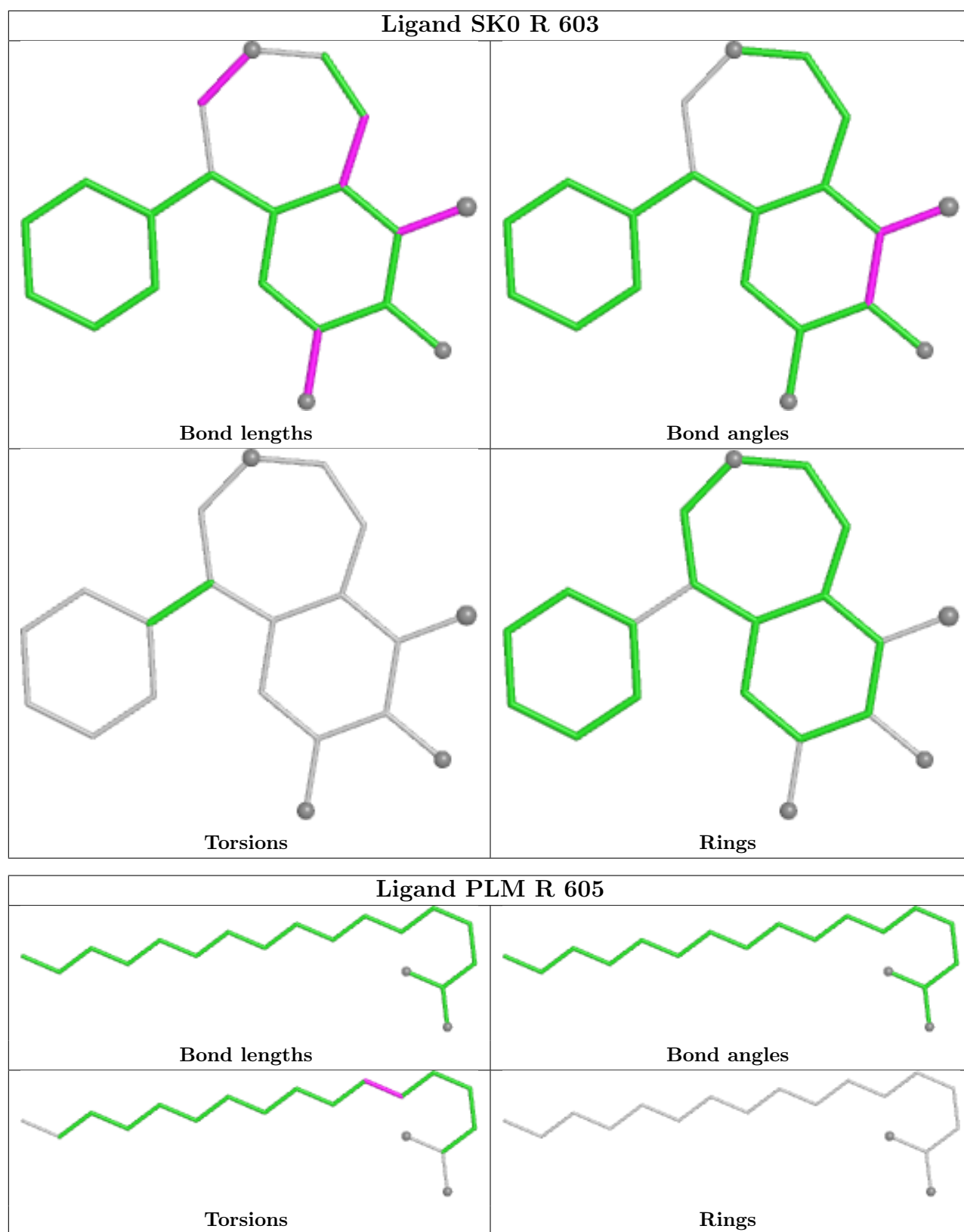
3 monomers are involved in 6 short contacts:

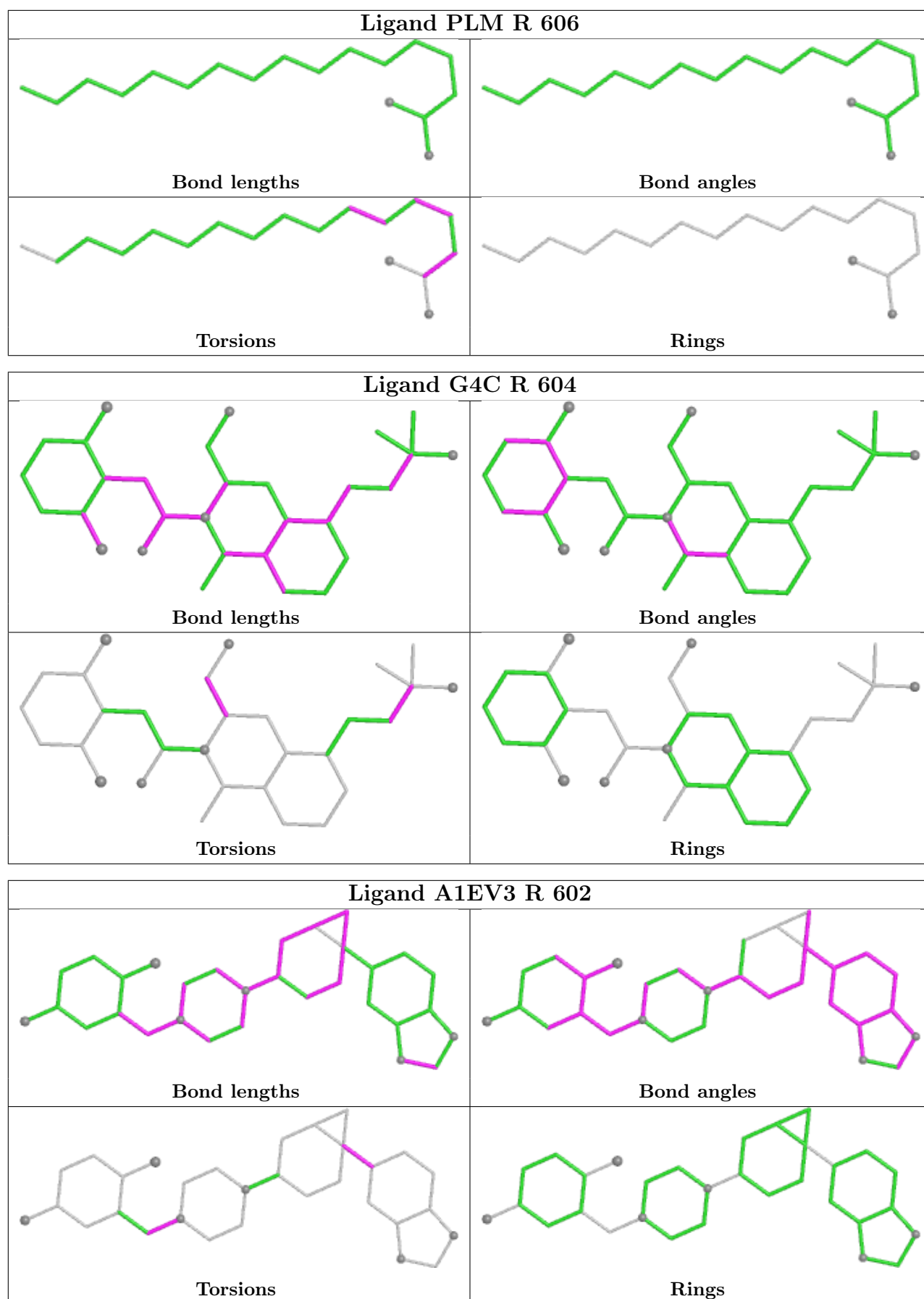
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	601	CLR	2	0
9	R	604	G4C	1	0
7	R	602	A1EV3	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

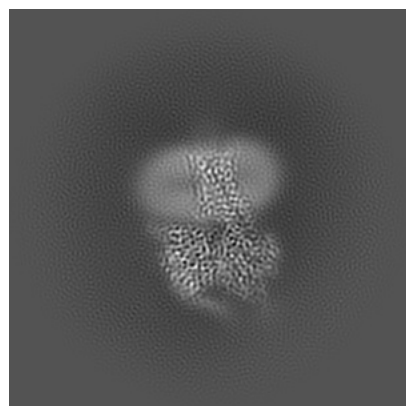
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65916. These allow visual inspection of the internal detail of the map and identification of artifacts.

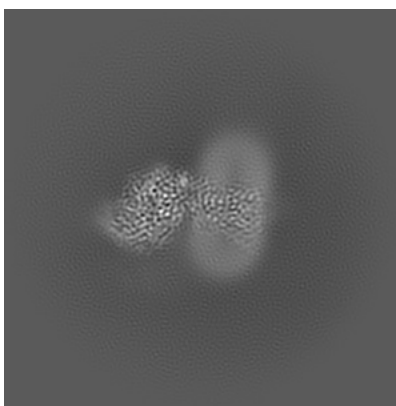
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

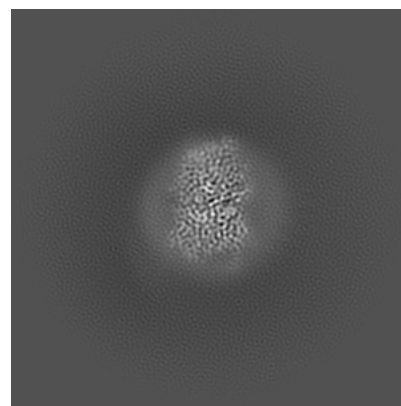
6.1.1 Primary map



X

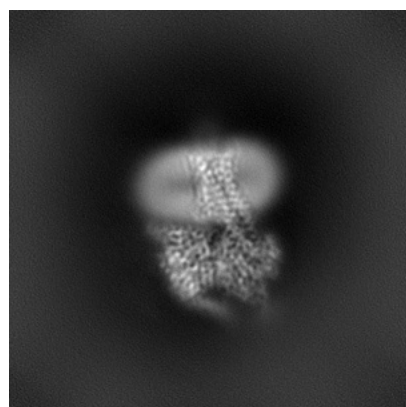


Y

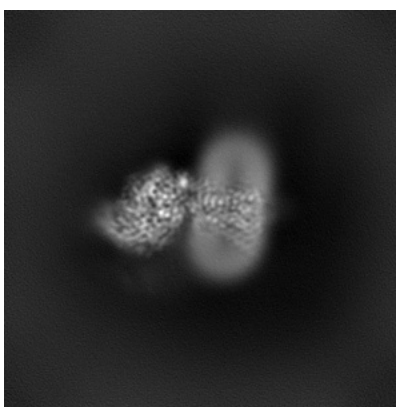


Z

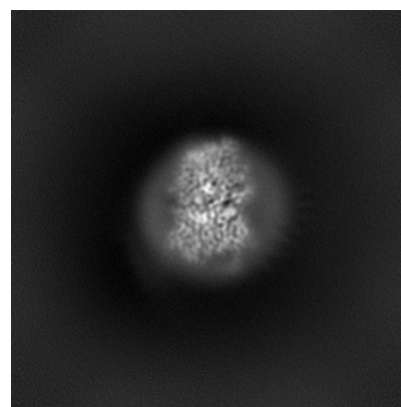
6.1.2 Raw map



X



Y

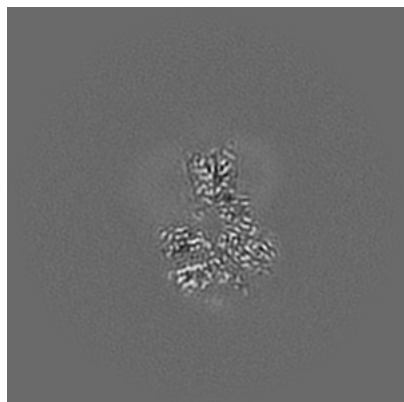


Z

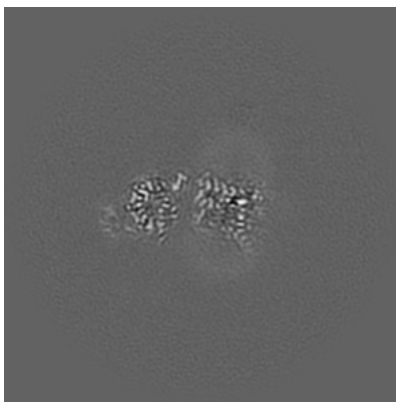
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

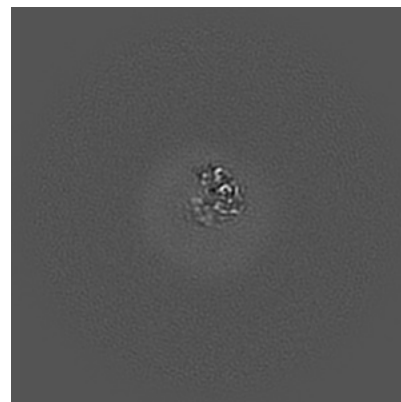
6.2.1 Primary map



X Index: 160

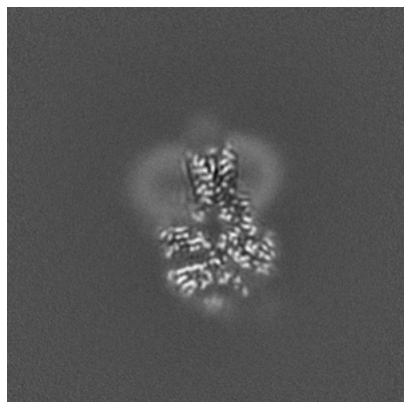


Y Index: 160

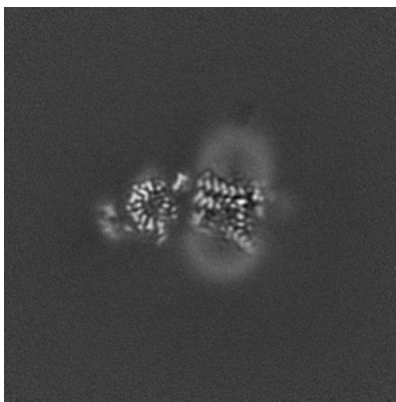


Z Index: 160

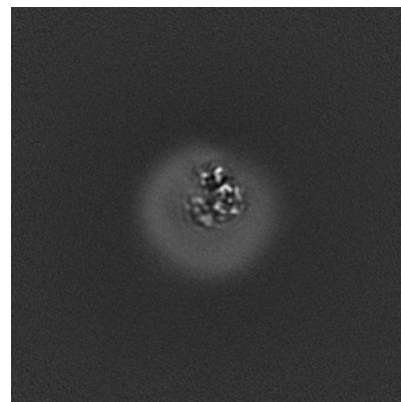
6.2.2 Raw map



X Index: 160



Y Index: 160

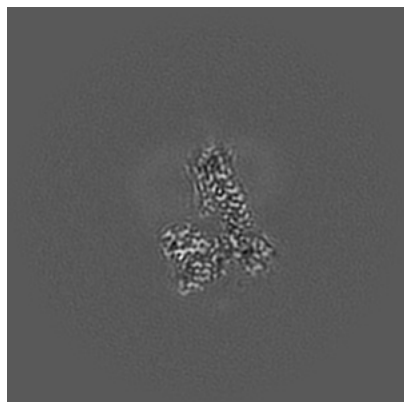


Z Index: 160

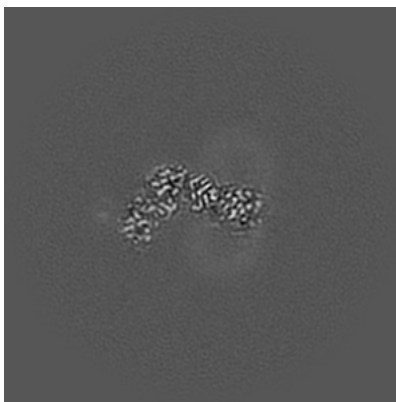
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

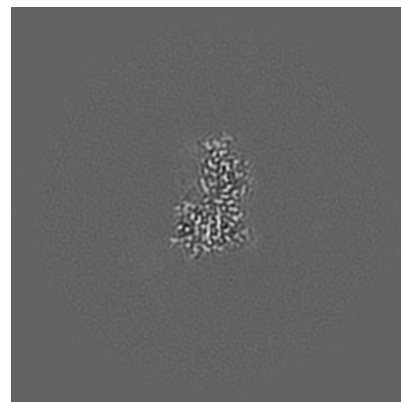
6.3.1 Primary map



X Index: 166

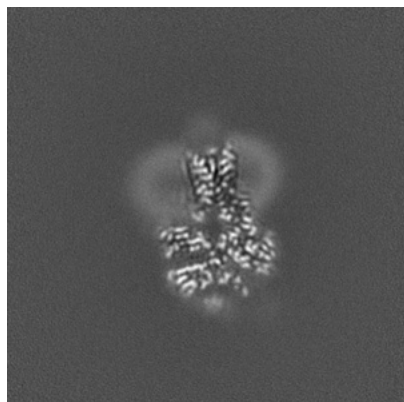


Y Index: 173

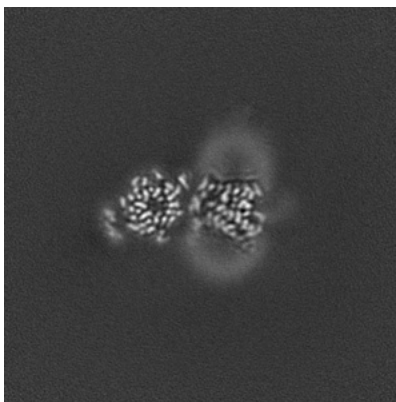


Z Index: 125

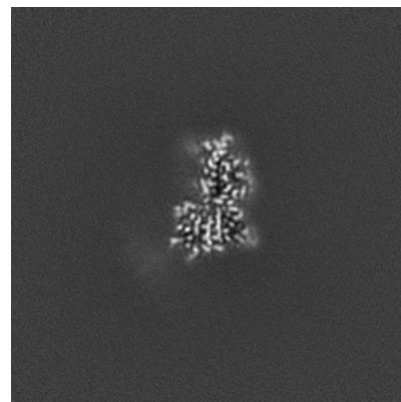
6.3.2 Raw map



X Index: 160



Y Index: 155

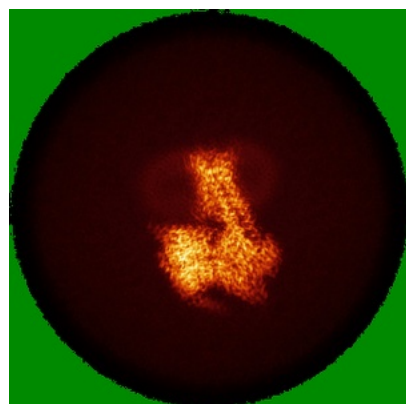


Z Index: 125

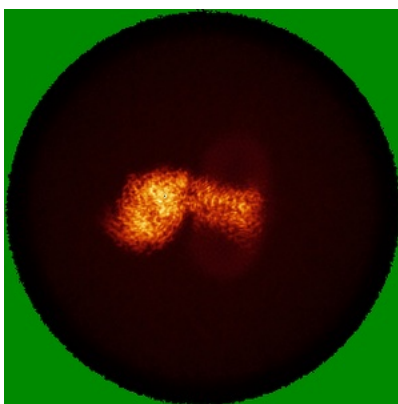
The images above show the largest variance slices of the map in three orthogonal directions.

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

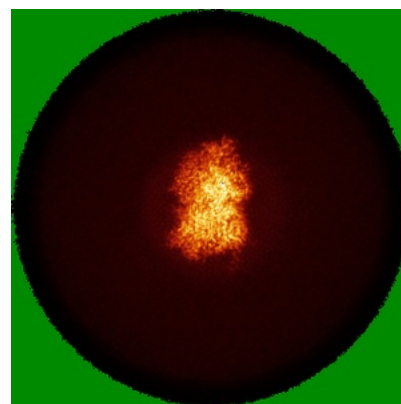
6.4.1 Primary map



X

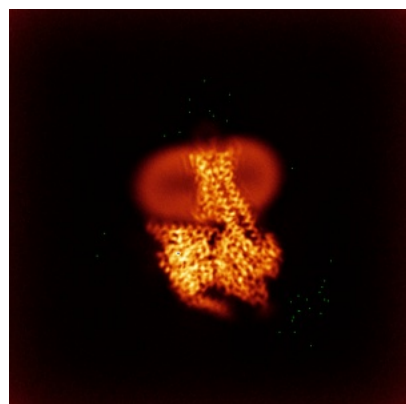


Y

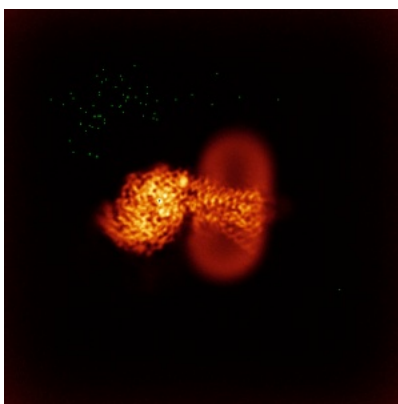


Z

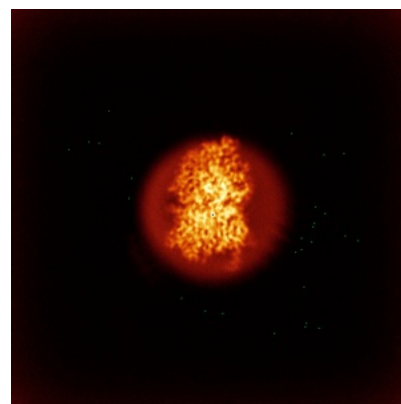
6.4.2 Raw map



X



Y

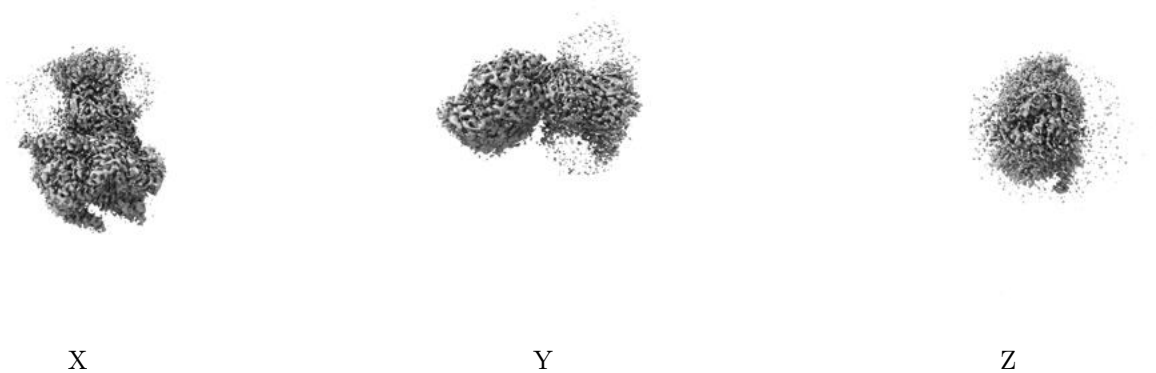


Z

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

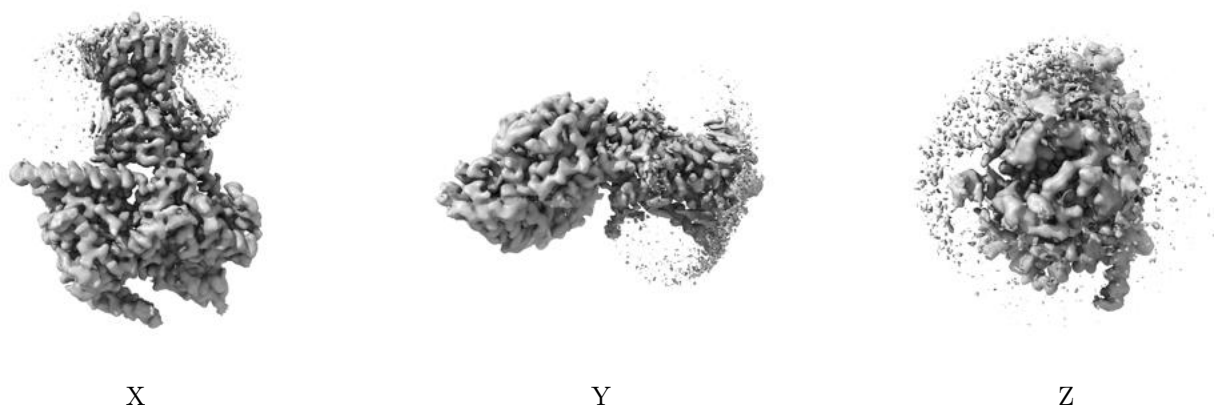
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

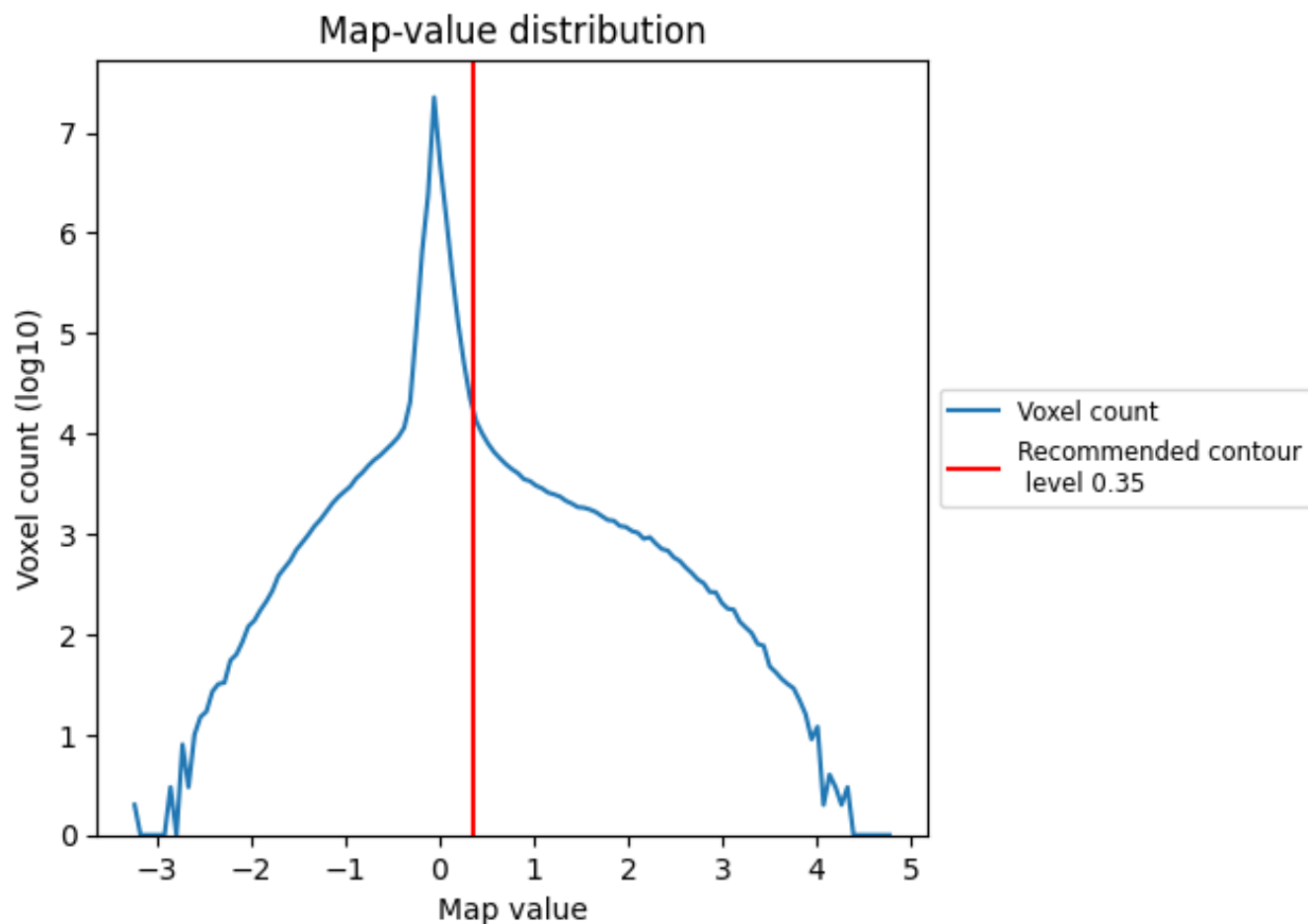
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

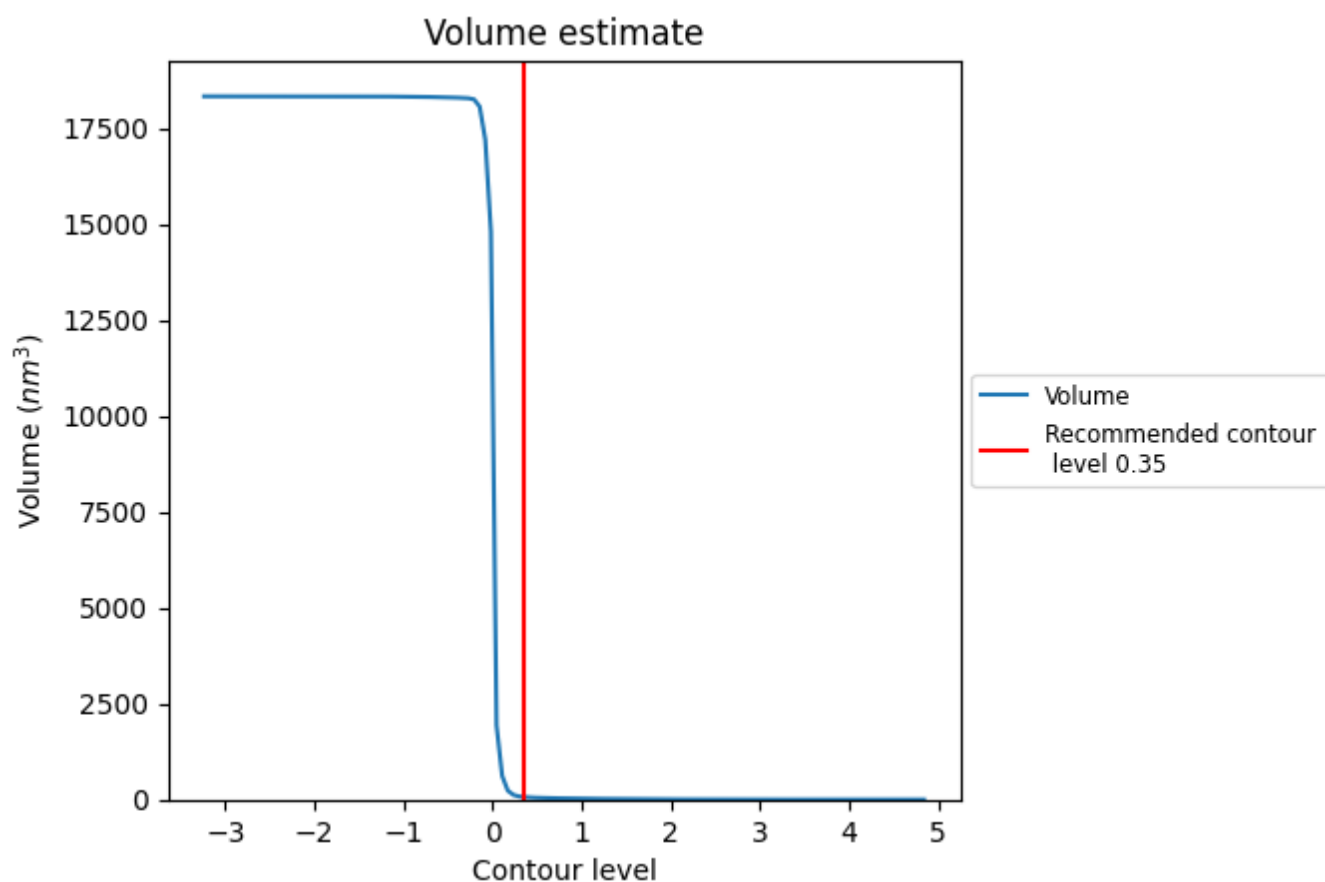
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

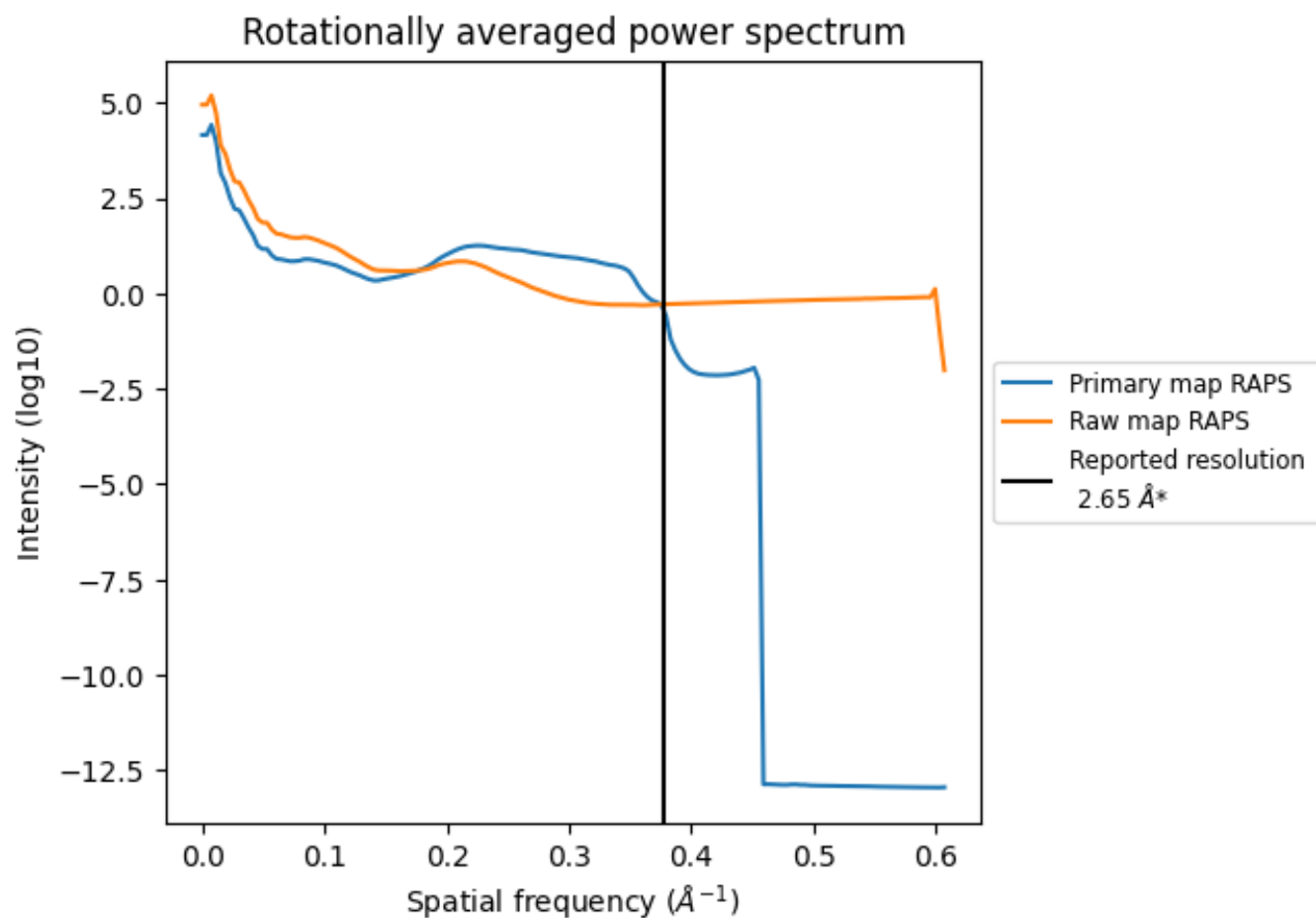
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm³; this corresponds to an approximate mass of 60 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 ⓘ

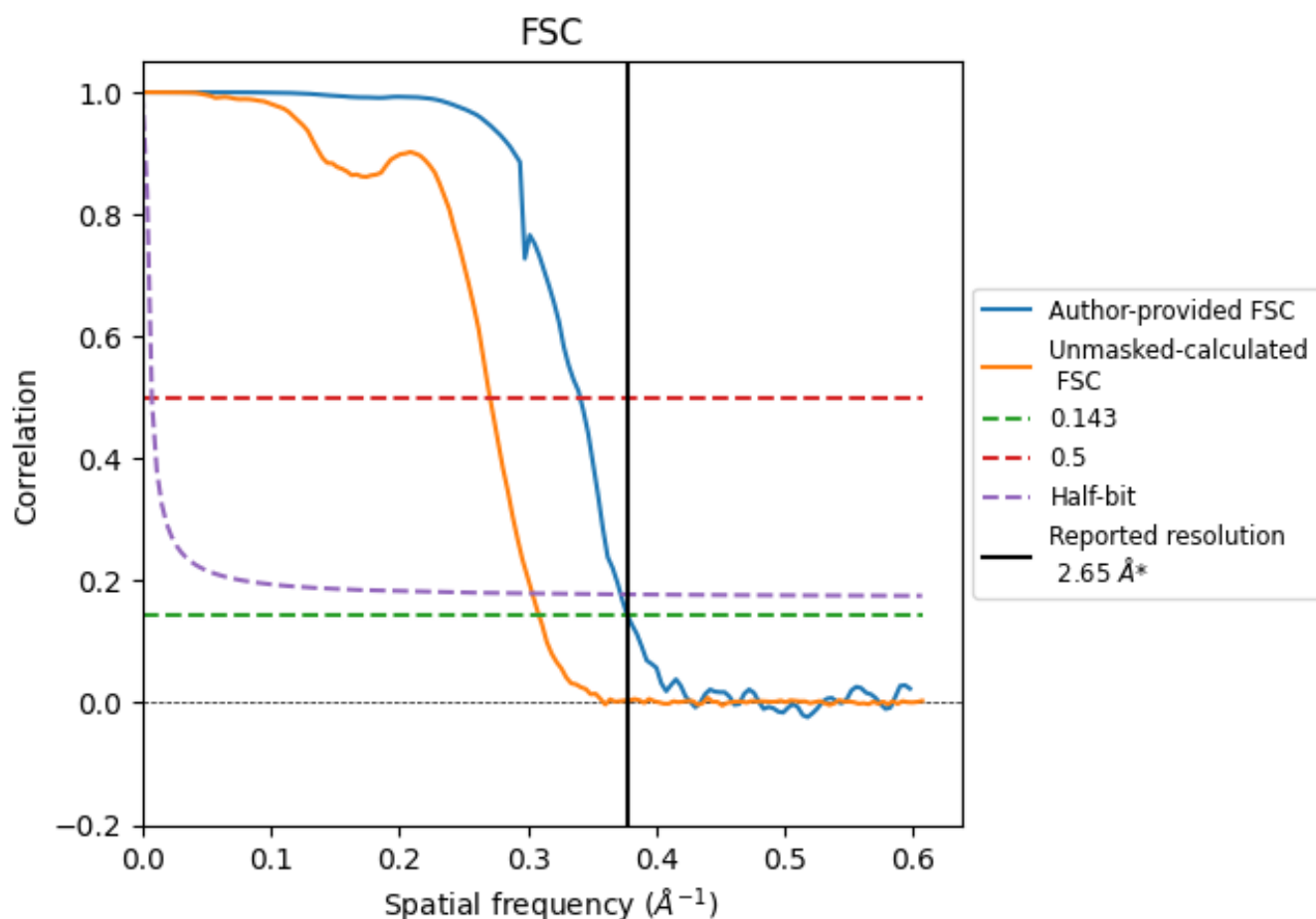


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8.2 Resolution estimates [i](#)

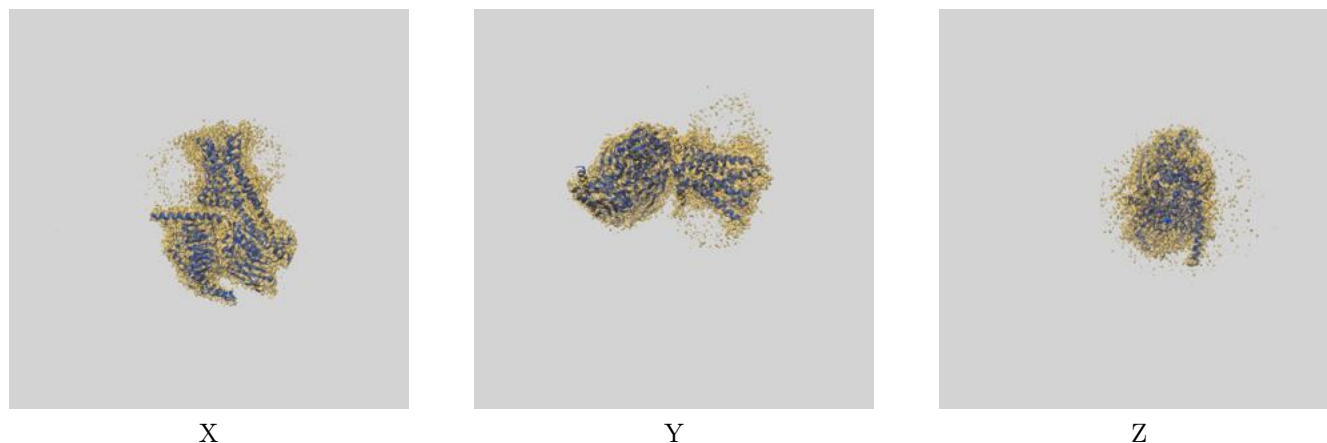
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	2.94	2.69
Unmasked-calculated*	3.24	3.70	3.29

*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 3.24 differs from the reported value 2.65 by more than 10 %

9 Map-model fit [i](#)

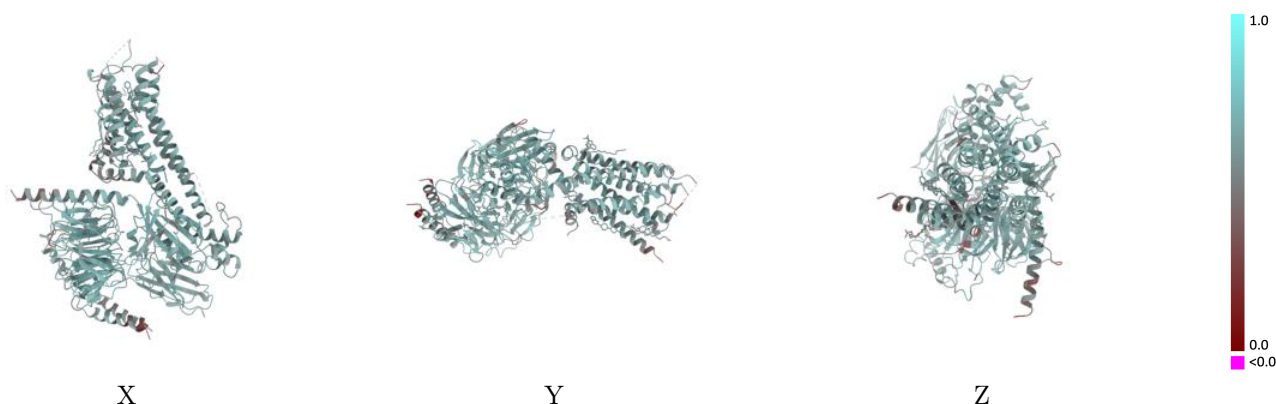
This section contains information regarding the fit between EMDB map EMD-65916 and PDB model 9WEU. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



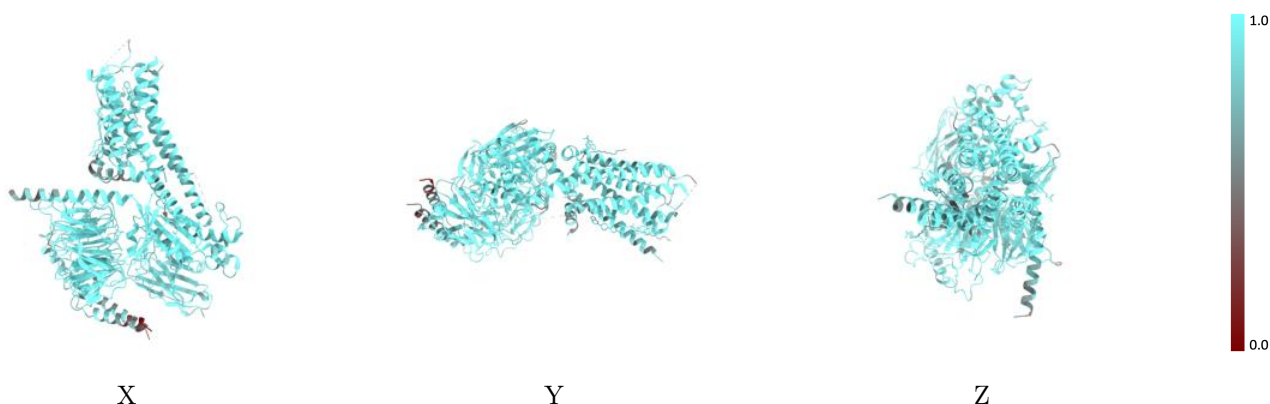
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



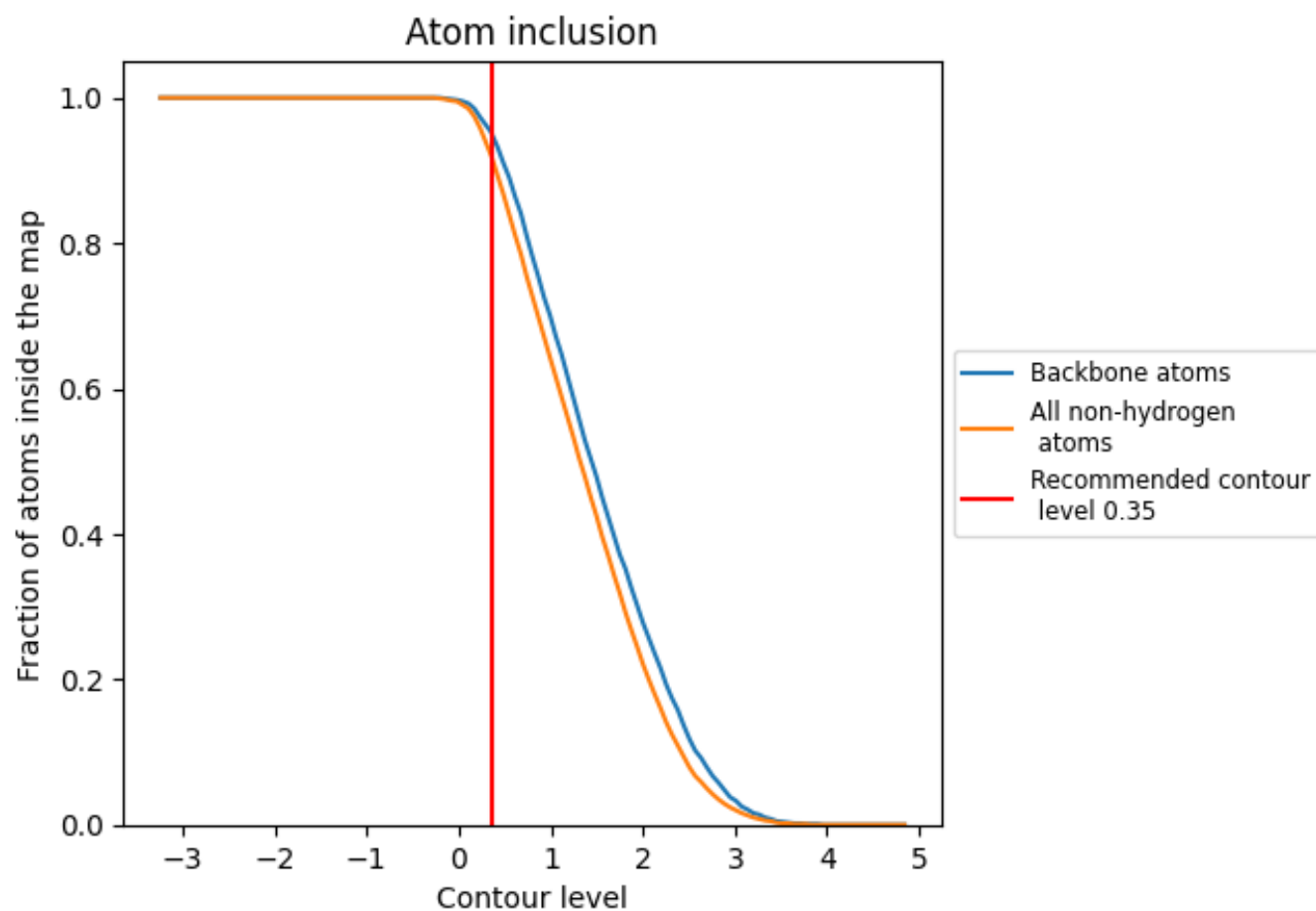
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.5990
A	0.9230	0.6010
B	0.9410	0.6170
G	0.7810	0.5370
N	0.9480	0.6170
R	0.9130	0.5840

