wwPDB EM Validation Summary Report (i)

Feb 26, 2025 – 06:11 pm GMT

PDB ID	:	9GE2
EMDB ID	:	EMD-51284
Title	:	Structure of GPR55 in complex with G13 and synthetic agonist ML184
Authors	:	Claff, T.; Ebenhoch, R.; Weichert, D.
Deposited on	:	2024-08-06
Resolution	:	2.51 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 (i) 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 (i)) were used in the production of this report:

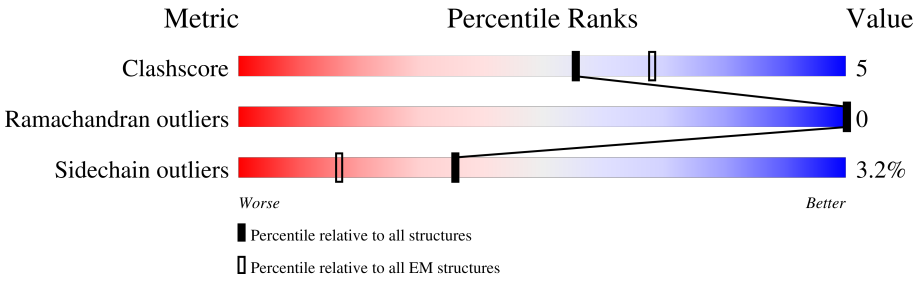
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 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)
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	230	23% 80% 14% 6%
2	B	358	8% 78% 15% • 6%
3	F	253	10% 79% 14% 7%
4	G	80	31% 65% 5% 30%
5	R	650	• 39% 6% 55%
6	X	2	50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9081 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 subunit alpha-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	217	1794	1139	315	333	7	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q14344
A	2	GLY	-	expression tag	UNP Q14344
A	3	SER	-	expression tag	UNP Q14344
A	4	THR	-	expression tag	UNP Q14344
A	5	VAL	-	expression tag	UNP Q14344
A	6	SER	-	expression tag	UNP Q14344
A	7	ALA	-	expression tag	UNP Q14344
A	8	GLU	-	expression tag	UNP Q14344
A	9	ASP	-	expression tag	UNP Q14344
A	10	LYS	-	expression tag	UNP Q14344
A	11	ALA	-	expression tag	UNP Q14344
A	12	ALA	-	expression tag	UNP Q14344
A	13	ALA	-	expression tag	UNP Q14344
A	14	GLU	-	expression tag	UNP Q14344
A	15	ARG	-	expression tag	UNP Q14344
A	42	ASP	GLY	engineered mutation	UNP Q14344
A	43	ASN	GLU	engineered mutation	UNP Q14344
A	59	GLY	-	linker	UNP Q14344
A	60	SER	-	linker	UNP Q14344
A	61	GLY	-	linker	UNP Q14344
A	62	GLY	-	linker	UNP Q14344
A	63	SER	-	linker	UNP Q14344
A	64	GLY	-	linker	UNP Q14344
A	65	GLY	-	linker	UNP Q14344
A	111	ASP	SER	engineered mutation	UNP Q14344
A	114	ASP	GLU	engineered mutation	UNP Q14344
A	?	-	ASP	deletion	UNP Q14344
A	?	-	GLN	deletion	UNP Q14344

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q14344
A	?	-	LEU	deletion	UNP Q14344
A	?	-	MET	deletion	UNP Q14344
A	?	-	GLU	deletion	UNP Q14344
A	?	-	ASP	deletion	UNP Q14344
A	?	-	ARG	deletion	UNP Q14344
A	?	-	LEU	deletion	UNP Q14344
A	?	-	THR	deletion	UNP Q14344
A	124	ASP	ILE	engineered mutation	UNP Q14344
A	208	ALA	ILE	engineered mutation	UNP Q14344
A	211	ILE	VAL	engineered mutation	UNP Q14344

- 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 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	HIS	-	expression tag	UNP P62873
B	3	HIS	-	expression tag	UNP P62873
B	4	HIS	-	expression tag	UNP P62873
B	5	HIS	-	expression tag	UNP P62873
B	6	HIS	-	expression tag	UNP P62873
B	7	HIS	-	expression tag	UNP P62873
B	8	LEU	-	expression tag	UNP P62873
B	9	GLU	-	expression tag	UNP P62873
B	10	VAL	-	expression tag	UNP P62873
B	11	LEU	-	expression tag	UNP P62873
B	12	PHE	-	expression tag	UNP P62873
B	13	GLN	-	expression tag	UNP P62873
B	14	GLY	-	expression tag	UNP P62873
B	15	PRO	-	expression tag	UNP P62873
B	16	GLY	-	expression tag	UNP P62873
B	17	SER	-	expression tag	UNP P62873
B	18	SER	-	expression tag	UNP P62873
B	19	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Single-chain variable fragment ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	235	Total	C	N	O	S	0	0
			1794	1136	297	351	10		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	56	Total	C	N	O	S	0	0
			433	271	76	83	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	72	GLY	-	expression tag	UNP P59768
G	73	SER	-	expression tag	UNP P59768
G	74	ALA	-	expression tag	UNP P59768
G	75	GLY	-	expression tag	UNP P59768
G	76	SER	-	expression tag	UNP P59768
G	77	ALA	-	expression tag	UNP P59768
G	78	GLY	-	expression tag	UNP P59768
G	79	SER	-	expression tag	UNP P59768
G	80	ALA	-	expression tag	UNP P59768

- Molecule 5 is a protein called Green fluorescent protein,G-protein coupled receptor 55.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	291	Total	C	N	O	S	0	0
			2357	1572	373	386	26		

There are 101 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-280	MET	-	initiating methionine	UNP P42212
R	-279	LYS	-	expression tag	UNP P42212
R	-278	THR	-	expression tag	UNP P42212
R	-277	ILE	-	expression tag	UNP P42212
R	-276	ILE	-	expression tag	UNP P42212
R	-275	ALA	-	expression tag	UNP P42212
R	-274	LEU	-	expression tag	UNP P42212
R	-273	SER	-	expression tag	UNP P42212
R	-272	TYR	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-271	ILE	-	expression tag	UNP P42212
R	-270	PHE	-	expression tag	UNP P42212
R	-269	CYS	-	expression tag	UNP P42212
R	-268	LEU	-	expression tag	UNP P42212
R	-267	VAL	-	expression tag	UNP P42212
R	-266	PHE	-	expression tag	UNP P42212
R	-265	ALA	-	expression tag	UNP P42212
R	-264	ASP	-	expression tag	UNP P42212
R	-263	TYR	-	expression tag	UNP P42212
R	-262	LYS	-	expression tag	UNP P42212
R	-261	ASP	-	expression tag	UNP P42212
R	-260	ASP	-	expression tag	UNP P42212
R	-259	ASP	-	expression tag	UNP P42212
R	-258	ASP	-	expression tag	UNP P42212
R	-257	LYS	-	expression tag	UNP P42212
R	-195	LEU	PHE	engineered mutation	UNP P42212
R	-194	THR	SER	engineered mutation	UNP P42212
R	-179	ARG	GLN	engineered mutation	UNP P42212
R	-160	SER	PHE	engineered mutation	UNP P42212
R	-106	THR	MET	engineered mutation	UNP P42212
R	-96	ALA	VAL	engineered mutation	UNP P42212
R	-20	ALA	-	linker	UNP P42212
R	-19	ALA	-	linker	UNP P42212
R	-18	GLY	-	linker	UNP P42212
R	-17	SER	-	linker	UNP P42212
R	-16	GLY	-	linker	UNP P42212
R	-15	GLU	-	linker	UNP P42212
R	-14	PHE	-	linker	UNP P42212
R	-13	LEU	-	linker	UNP P42212
R	-12	GLU	-	linker	UNP P42212
R	-11	VAL	-	linker	UNP P42212
R	-10	LEU	-	linker	UNP P42212
R	-9	PHE	-	linker	UNP P42212
R	-8	GLN	-	linker	UNP P42212
R	-7	GLY	-	linker	UNP P42212
R	-6	PRO	-	linker	UNP P42212
R	-5	GLY	-	linker	UNP P42212
R	-4	ALA	-	linker	UNP P42212
R	-3	GLY	-	linker	UNP P42212
R	-2	SER	-	linker	UNP P42212
R	-1	ASP	-	linker	UNP P42212
R	0	SER	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
R	320	ALA	-	expression tag	UNP Q9Y2T6
R	321	GLY	-	expression tag	UNP Q9Y2T6
R	322	SER	-	expression tag	UNP Q9Y2T6
R	323	GLY	-	expression tag	UNP Q9Y2T6
R	324	ALA	-	expression tag	UNP Q9Y2T6
R	325	GLY	-	expression tag	UNP Q9Y2T6
R	326	SER	-	expression tag	UNP Q9Y2T6
R	327	ALA	-	expression tag	UNP Q9Y2T6
R	328	TRP	-	expression tag	UNP Q9Y2T6
R	329	SER	-	expression tag	UNP Q9Y2T6
R	330	HIS	-	expression tag	UNP Q9Y2T6
R	331	PRO	-	expression tag	UNP Q9Y2T6
R	332	GLN	-	expression tag	UNP Q9Y2T6
R	333	PHE	-	expression tag	UNP Q9Y2T6
R	334	GLU	-	expression tag	UNP Q9Y2T6
R	335	LYS	-	expression tag	UNP Q9Y2T6
R	336	GLY	-	expression tag	UNP Q9Y2T6
R	337	GLY	-	expression tag	UNP Q9Y2T6
R	338	GLY	-	expression tag	UNP Q9Y2T6
R	339	SER	-	expression tag	UNP Q9Y2T6
R	340	GLY	-	expression tag	UNP Q9Y2T6
R	341	GLY	-	expression tag	UNP Q9Y2T6
R	342	GLY	-	expression tag	UNP Q9Y2T6
R	343	SER	-	expression tag	UNP Q9Y2T6
R	344	GLY	-	expression tag	UNP Q9Y2T6
R	345	GLY	-	expression tag	UNP Q9Y2T6
R	346	SER	-	expression tag	UNP Q9Y2T6
R	347	ALA	-	expression tag	UNP Q9Y2T6
R	348	TRP	-	expression tag	UNP Q9Y2T6
R	349	SER	-	expression tag	UNP Q9Y2T6
R	350	HIS	-	expression tag	UNP Q9Y2T6
R	351	PRO	-	expression tag	UNP Q9Y2T6
R	352	GLN	-	expression tag	UNP Q9Y2T6
R	353	PHE	-	expression tag	UNP Q9Y2T6
R	354	GLU	-	expression tag	UNP Q9Y2T6
R	355	LYS	-	expression tag	UNP Q9Y2T6
R	356	GLY	-	expression tag	UNP Q9Y2T6
R	357	ALA	-	expression tag	UNP Q9Y2T6
R	358	GLY	-	expression tag	UNP Q9Y2T6
R	359	SER	-	expression tag	UNP Q9Y2T6
R	360	HIS	-	expression tag	UNP Q9Y2T6
R	361	HIS	-	expression tag	UNP Q9Y2T6

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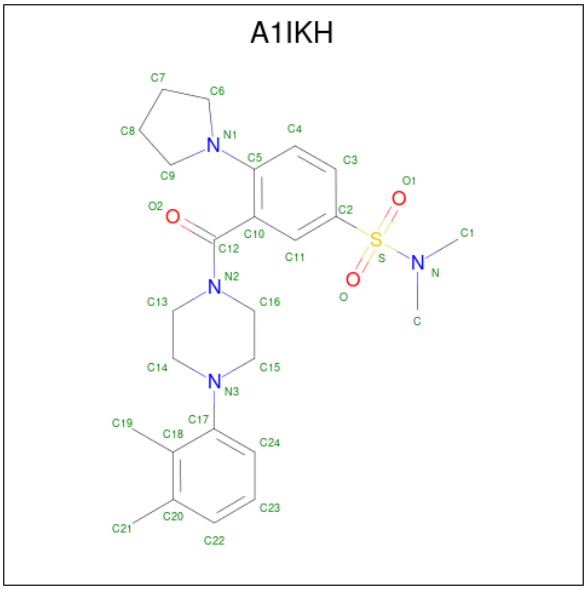
Chain	Residue	Modelled	Actual	Comment	Reference
R	362	HIS	-	expression tag	UNP Q9Y2T6
R	363	HIS	-	expression tag	UNP Q9Y2T6
R	364	HIS	-	expression tag	UNP Q9Y2T6
R	365	HIS	-	expression tag	UNP Q9Y2T6
R	366	HIS	-	expression tag	UNP Q9Y2T6
R	367	HIS	-	expression tag	UNP Q9Y2T6
R	368	HIS	-	expression tag	UNP Q9Y2T6
R	369	HIS	-	expression tag	UNP Q9Y2T6

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

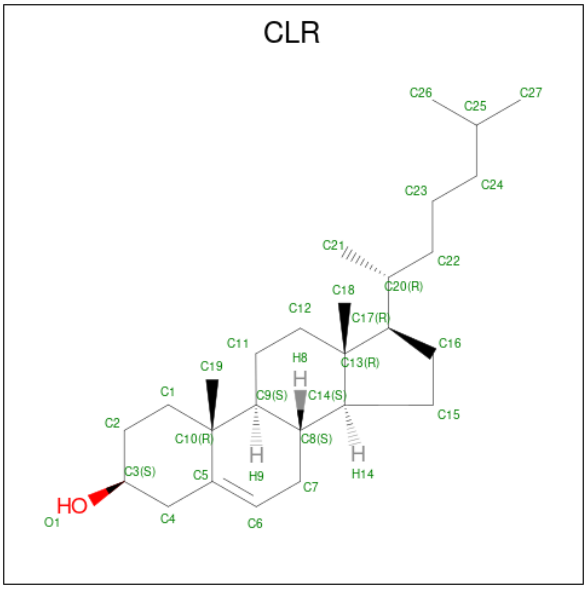
Mol	Chain	Residues	Atoms				AltConf	Trace
6	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 3-[4-(2,3-dimethylphenyl)piperazin-1-yl]carbonyl-N,N-dimethyl-4-pyrrolidin-1-yl-benzenesulfonamide (three-letter code: A1IKH) (formula: $C_{25}H_{34}N_4O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	R	1	Total	C	N	O	S	0
			33	25	4	3	1	

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

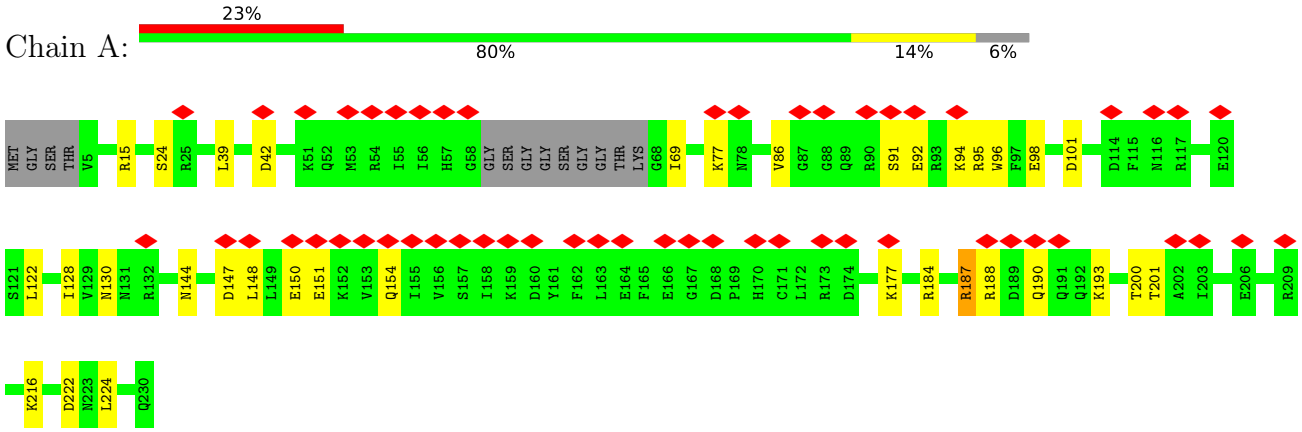
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	3	Total	O	0
			3	3	
9	B	6	Total	O	0
			6	6	
9	R	5	Total	O	0
			5	5	

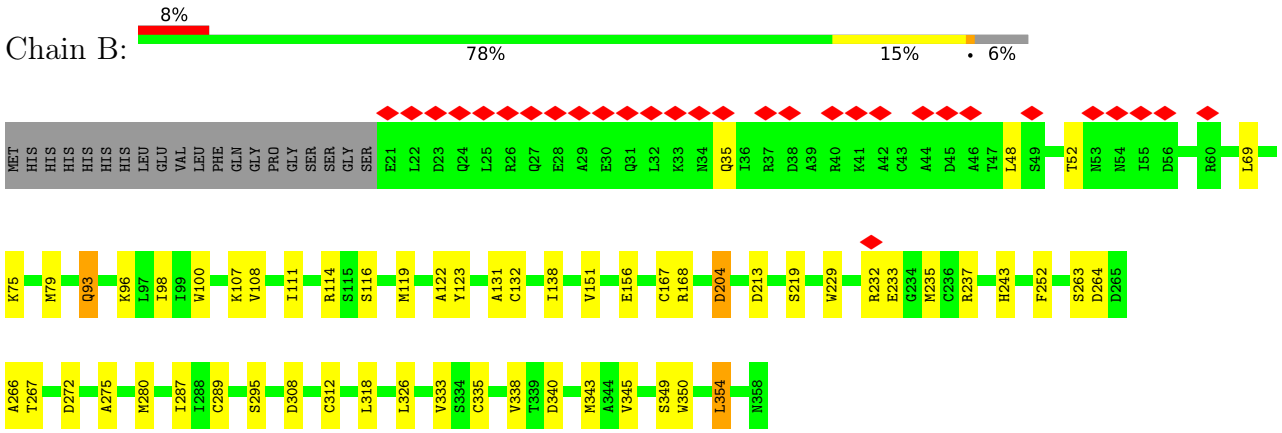
3 Residue-property plots (i)

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

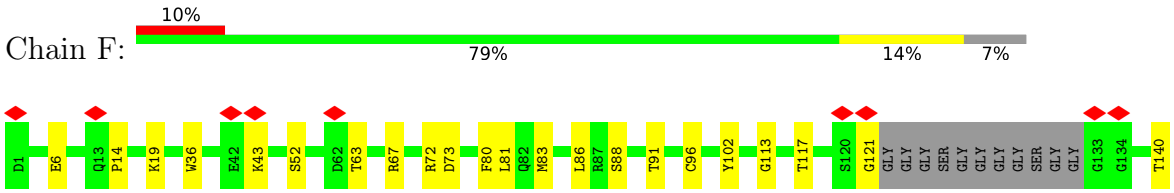
• Molecule 1: Guanine nucleotide-binding protein subunit alpha-13

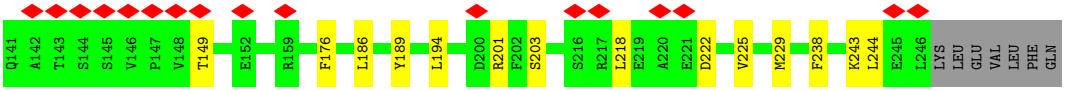


• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

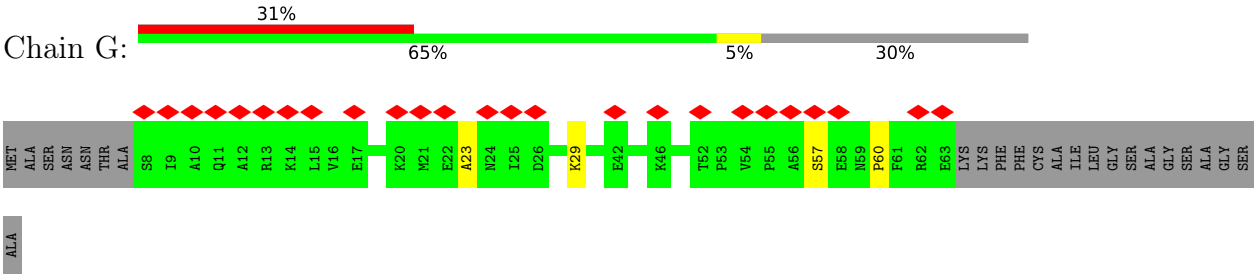


• Molecule 3: Single-chain variable fragment ScFv16

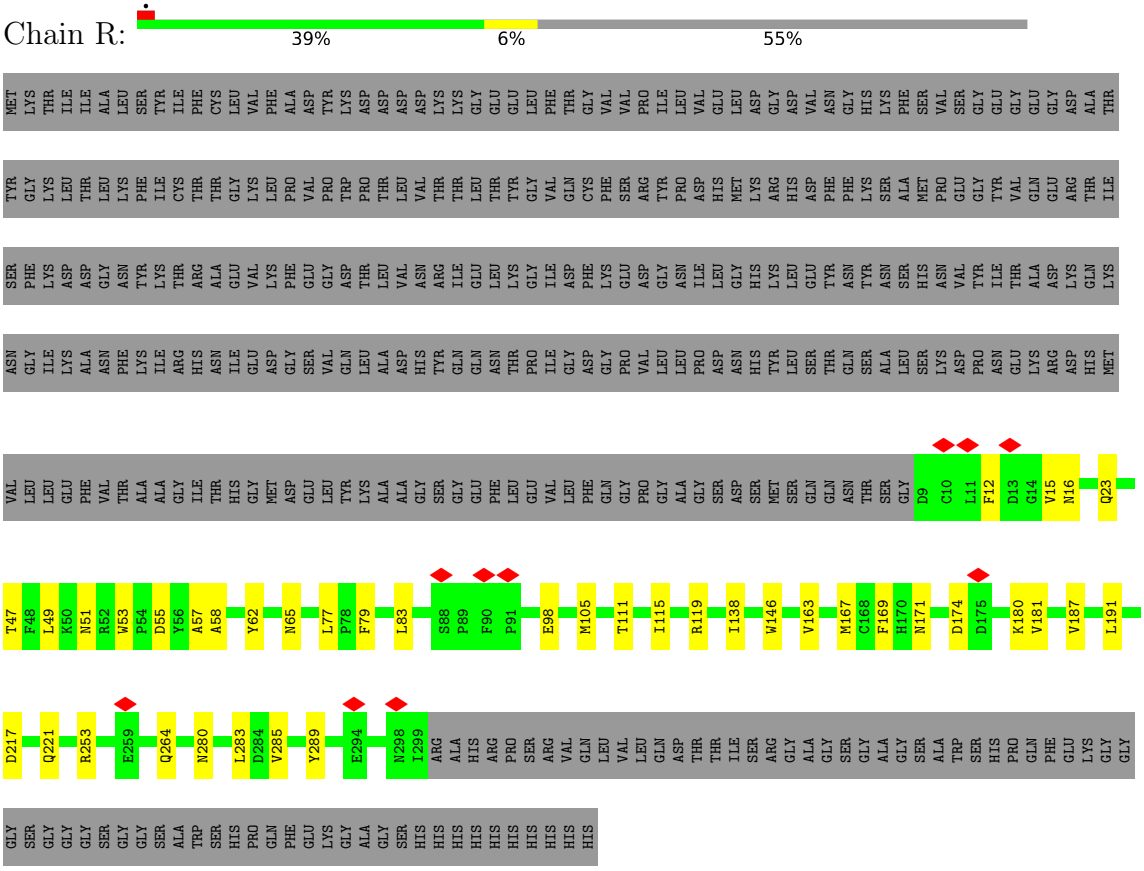




• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



• Molecule 5: Green fluorescent protein,G-protein coupled receptor 55



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	829193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	77.674	Depositor
Minimum map value	-56.282	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.104	Depositor
Recommended contour level	8	Depositor
Map size (Å)	265.28, 265.28, 265.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, NAG, A1IKH

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	0.26	0/1823	0.47	0/2445
2	B	0.26	0/2647	0.52	0/3589
3	F	0.28	0/1838	0.50	0/2491
4	G	0.24	0/439	0.44	0/592
5	R	0.28	0/2427	0.46	0/3292
All	All	0.27	0/9174	0.49	0/12409

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	1794	0	1806	20	0
2	B	2600	0	2505	31	0
3	F	1794	0	1727	18	0
4	G	433	0	442	2	0
5	R	2357	0	2380	24	0
6	X	28	0	25	1	0
7	R	33	0	0	0	0
8	R	28	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	3	0	0	0	0
9	B	6	0	0	0	0
9	R	5	0	0	1	0
All	All	9081	0	8931	87	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 87 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)
2:B:52:THR:HG21	2:B:318:LEU:HB3	1.66	0.76
1:A:92:GLU:N	1:A:92:GLU:OE2	2.21	0.73
2:B:114:ARG:NH1	2:B:156:GLU:OE1	2.23	0.72
3:F:218:LEU:HD11	3:F:244:LEU:HD21	1.79	0.65
2:B:69:LEU:HB2	2:B:354:LEU:HB2	1.80	0.64

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	213/230 (93%)	212 (100%)	1 (0%)	0	100	100
2	B	336/358 (94%)	324 (96%)	12 (4%)	0	100	100
3	F	231/253 (91%)	226 (98%)	5 (2%)	0	100	100
4	G	54/80 (68%)	53 (98%)	1 (2%)	0	100	100
5	R	289/650 (44%)	281 (97%)	8 (3%)	0	100	100
All	All	1123/1571 (72%)	1096 (98%)	27 (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	203/210 (97%)	196 (97%)	7 (3%)	32 58
2	B	281/298 (94%)	265 (94%)	16 (6%)	17 35
3	F	197/206 (96%)	192 (98%)	5 (2%)	42 69
4	G	46/61 (75%)	44 (96%)	2 (4%)	25 48
5	R	267/564 (47%)	265 (99%)	2 (1%)	81 93
All	All	994/1339 (74%)	962 (97%)	32 (3%)	36 60

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	29	LYS
4	G	57	SER
2	B	132	CYS
2	B	123	TYR
5	R	23	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
2	B	358	ASN
4	G	59	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)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	X	1	6,5	14,14,15	0.77	0	17,19,21	0.89	0
6	NAG	X	2	6	14,14,15	0.72	0	17,19,21	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

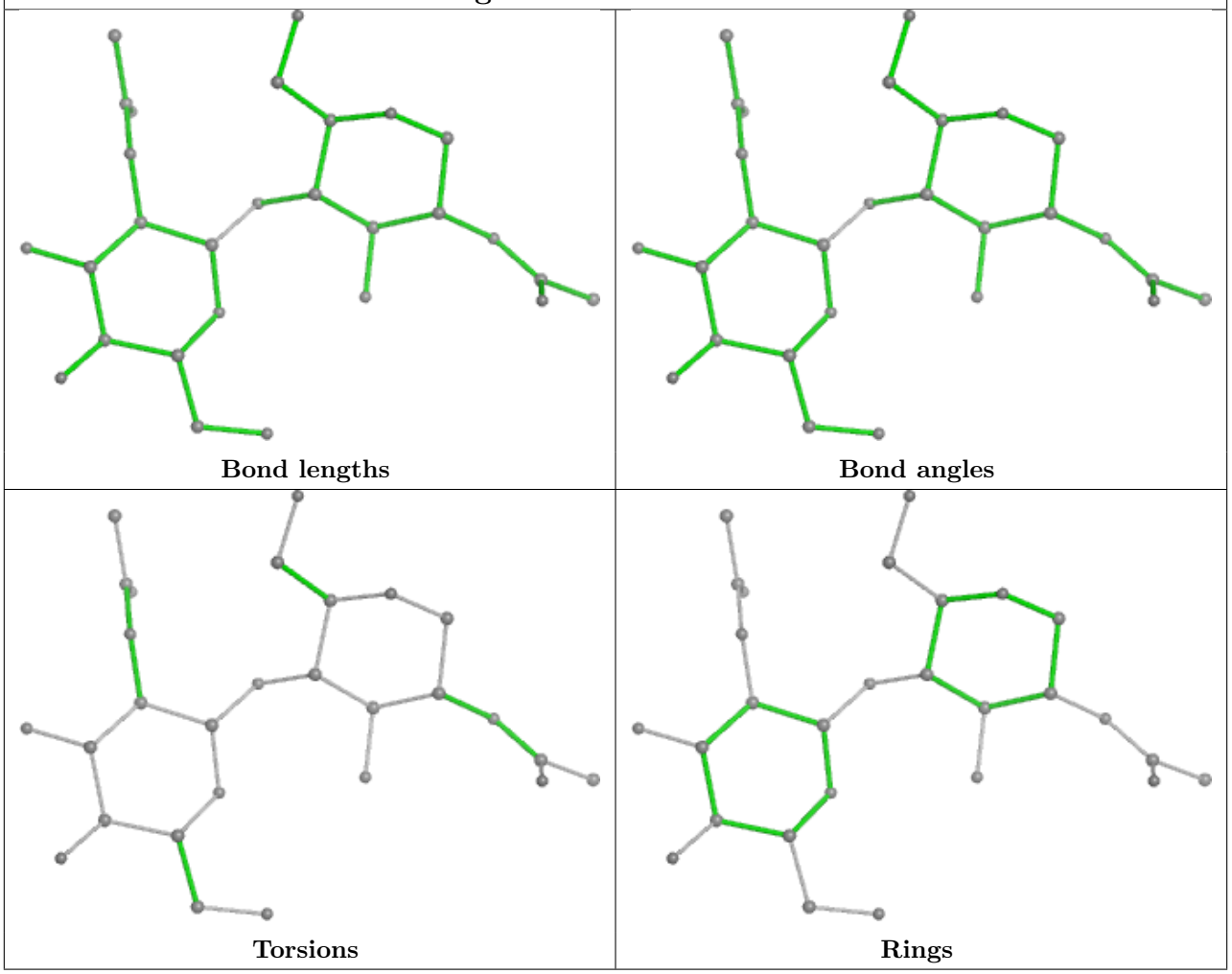
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	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 X



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
8	CLR	R	402	-	31,31,31	0.40	0	48,48,48	0.90	3 (6%)
7	A1IKH	R	401	-	36,36,36	0.14	0	52,53,53	0.88	1 (1%)

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
8	CLR	R	402	-	-	9/10/68/68	0/4/4/4
7	A1IKH	R	401	-	-	9/28/45/45	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	401	A1IKH	C18-C17-N3	-5.69	115.37	118.55
8	R	402	CLR	C10-C9-C8	-2.47	109.03	112.73
8	R	402	CLR	C16-C17-C20	2.41	115.87	112.15
8	R	402	CLR	C14-C8-C9	2.09	111.89	109.09

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	401	A1IKH	C10-C5-N1-C9
8	R	402	CLR	C13-C17-C20-C21
8	R	402	CLR	C16-C17-C20-C21
8	R	402	CLR	C13-C17-C20-C22
8	R	402	CLR	C16-C17-C20-C22

There are no ring outliers.

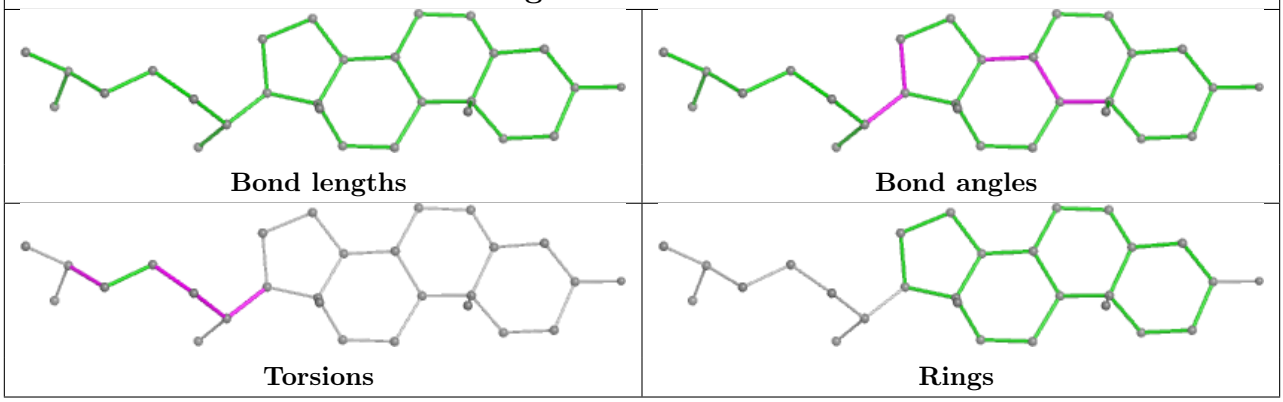
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	402	CLR	1	0

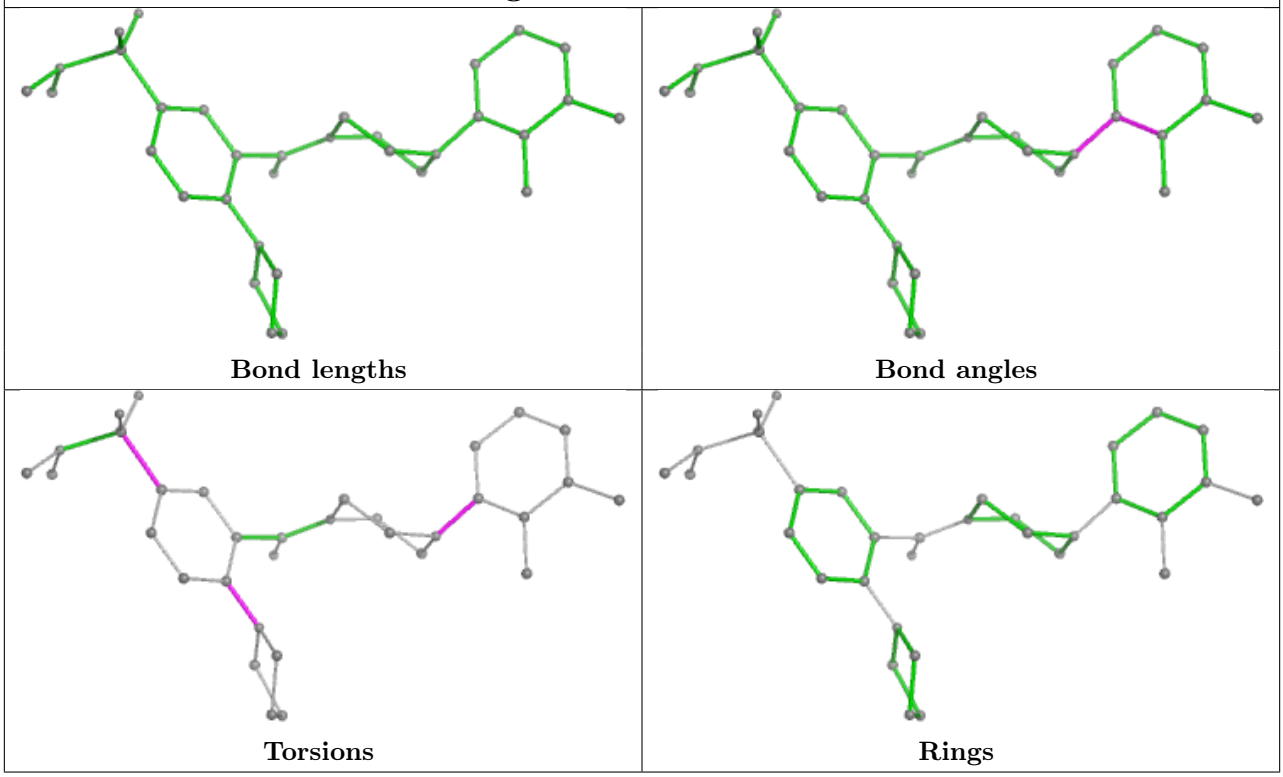
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CLR R 402



Ligand A1IKH R 401



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.

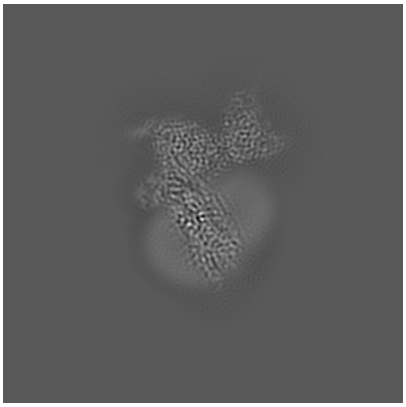
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51284. These allow visual inspection of the internal detail of the map and identification of artifacts.

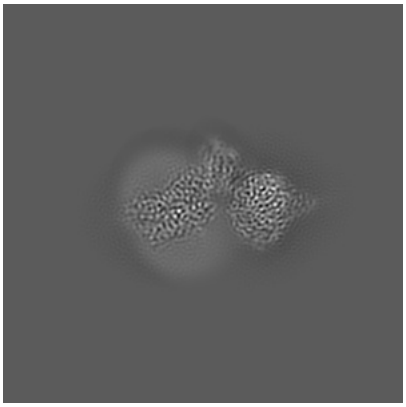
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

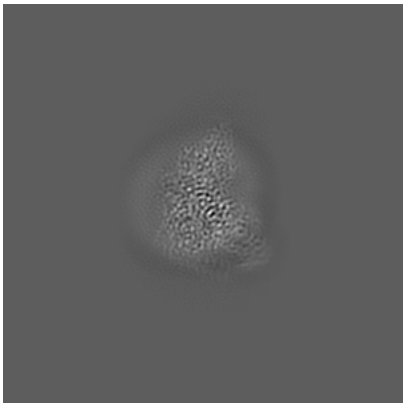
6.1.1 Primary map



X



Y

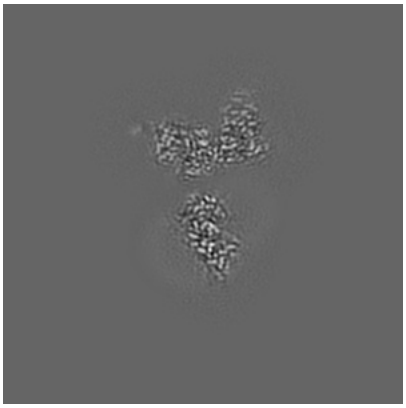


Z

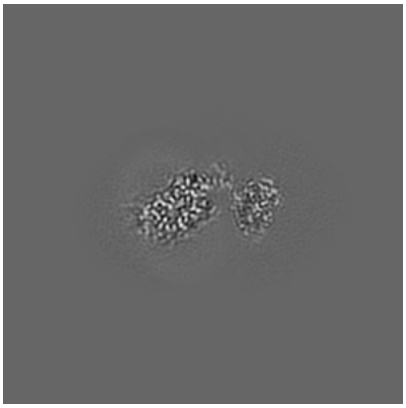
The images above show the map projected in three orthogonal directions.

6.2 Central slices

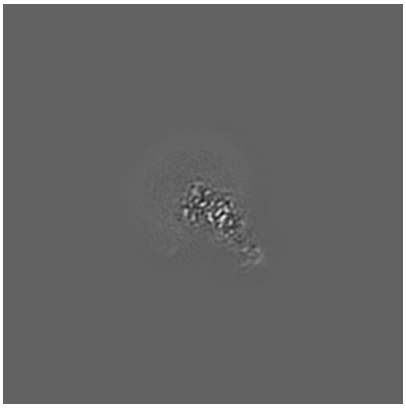
6.2.1 Primary map



X Index: 160



Y Index: 160

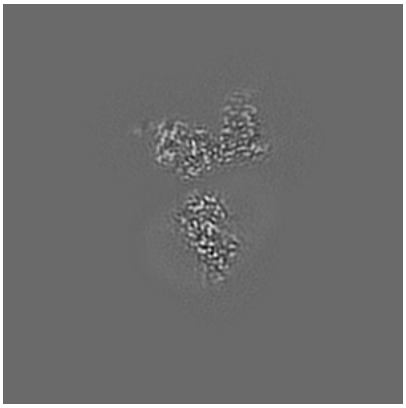


Z Index: 160

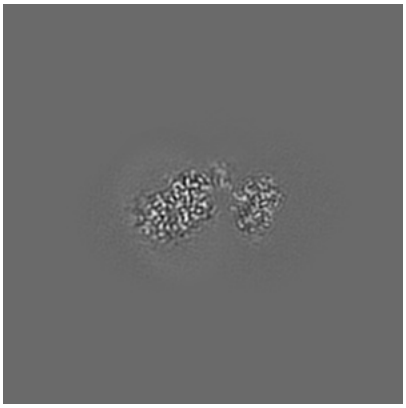
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

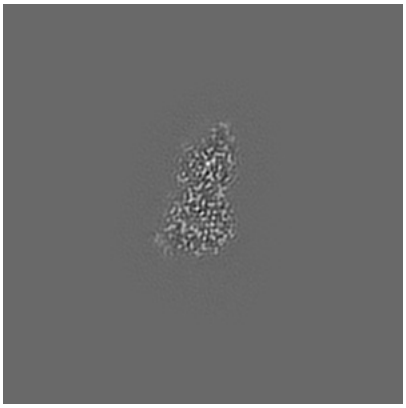
6.3.1 Primary map



X Index: 159



Y Index: 159

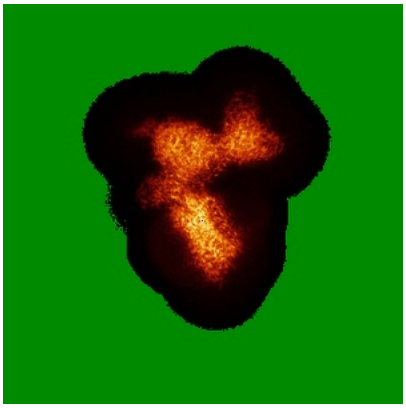


Z Index: 207

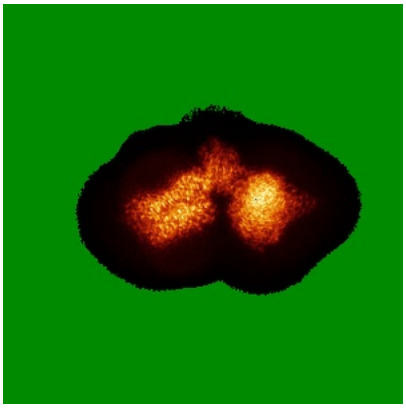
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

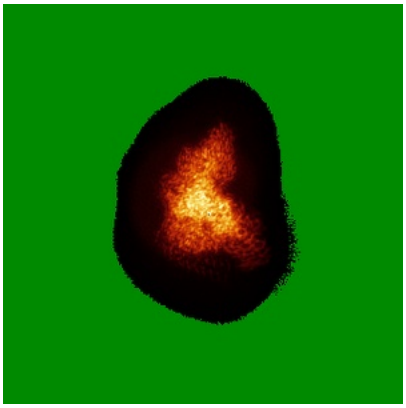
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

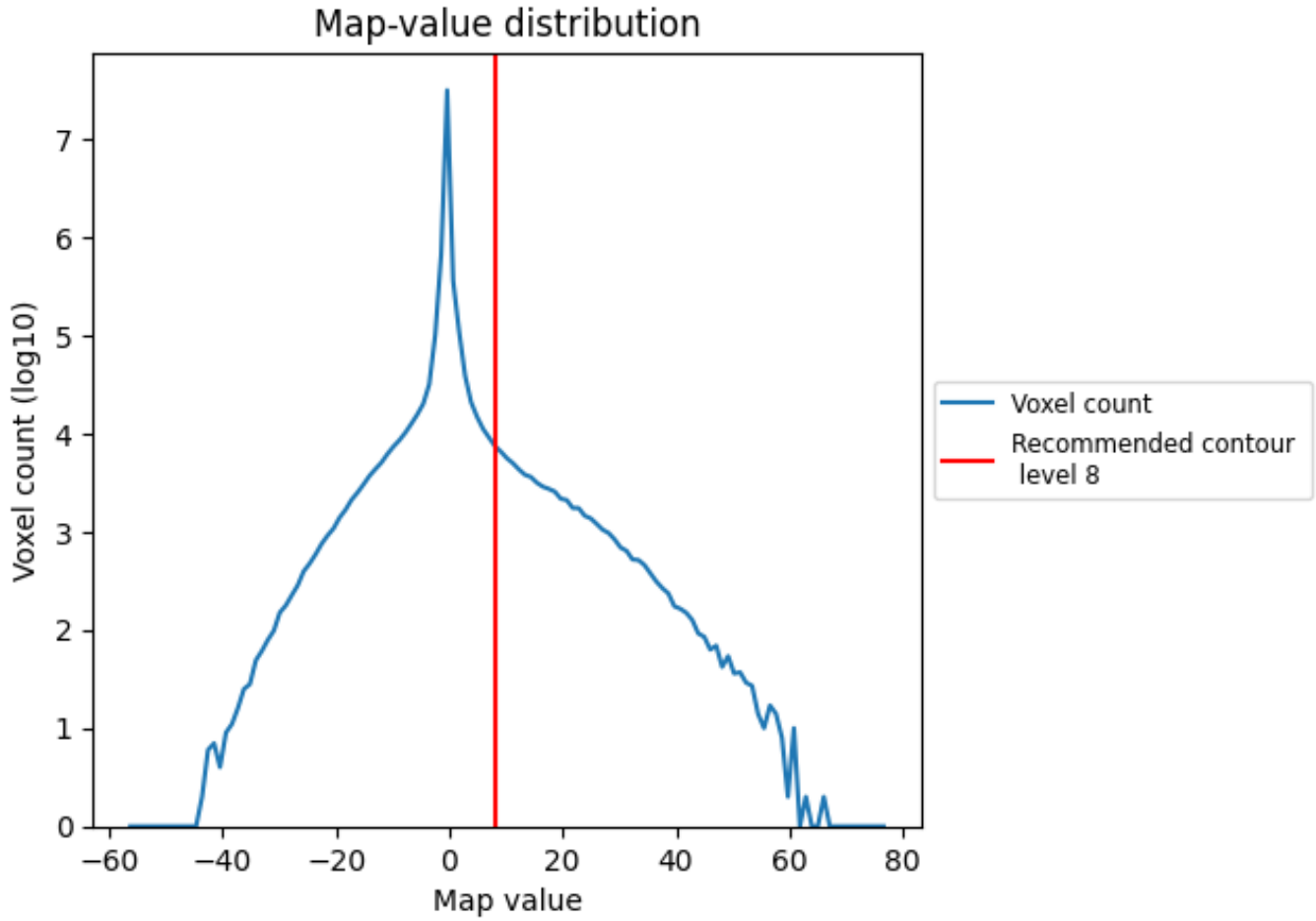
6.6 Mask visualisation (i)

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

7 Map analysis

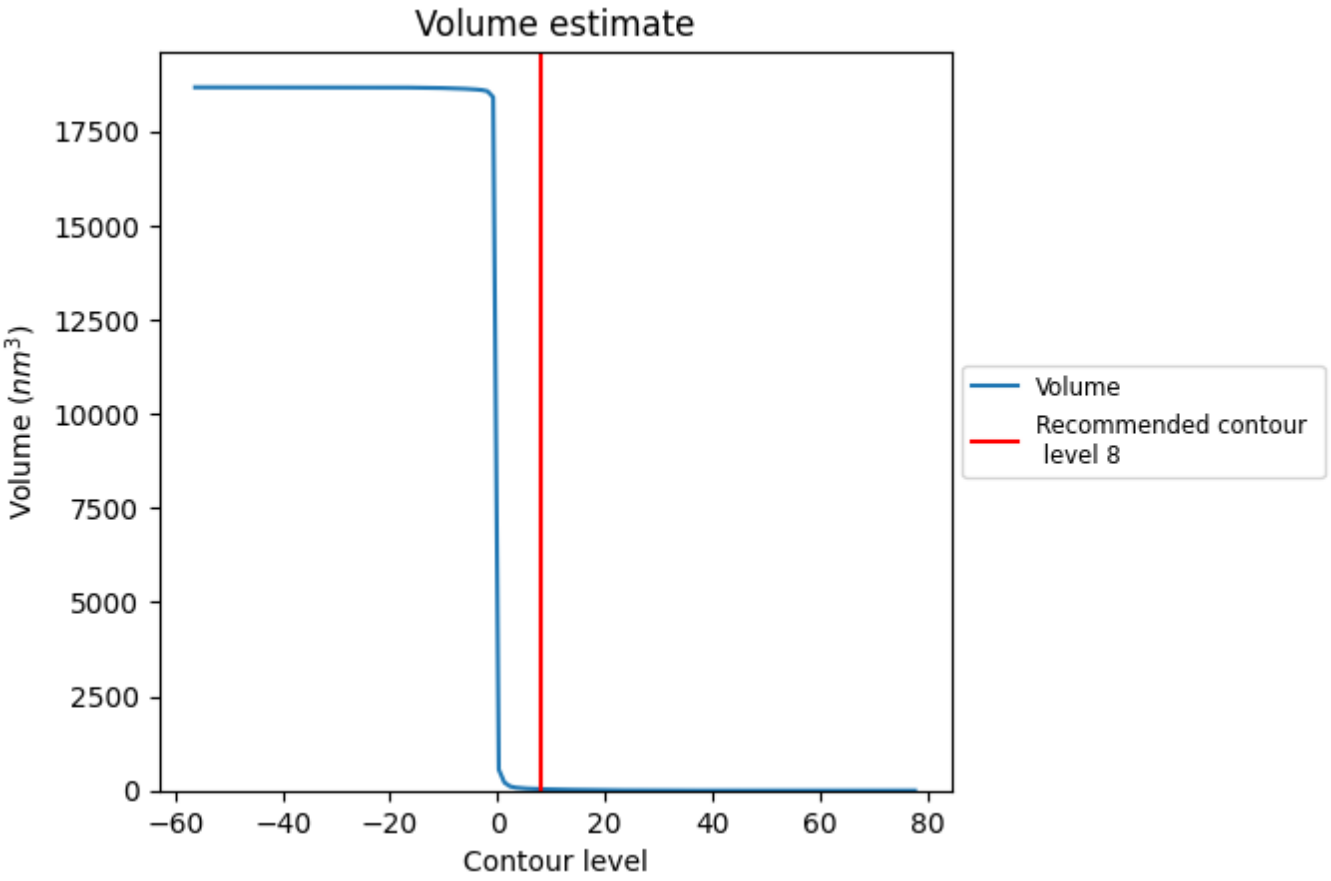
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

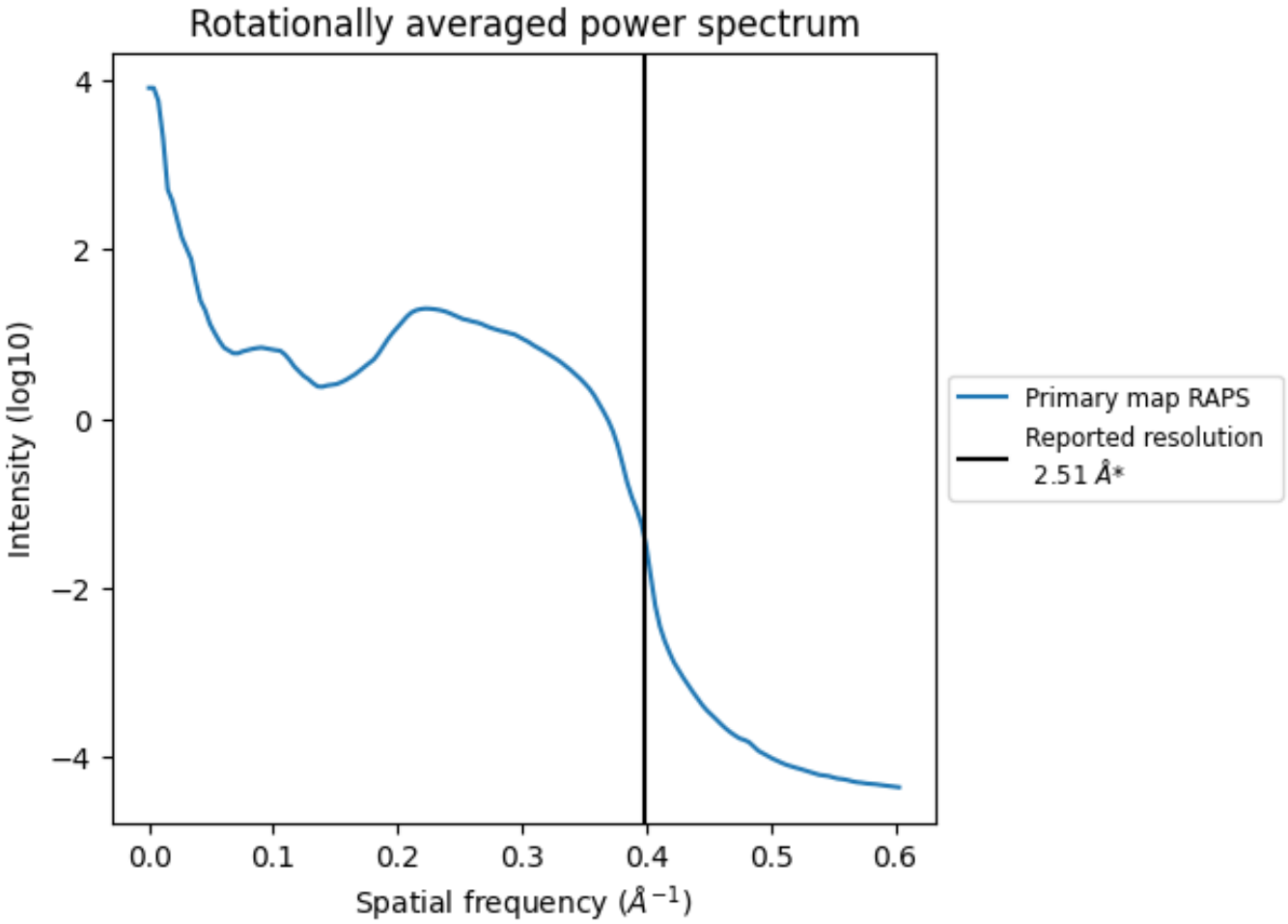
7.2 Volume estimate (i)



The volume at the recommended contour level is 39 nm^3; this corresponds to an approximate mass of 35 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.398 Å^{-1}

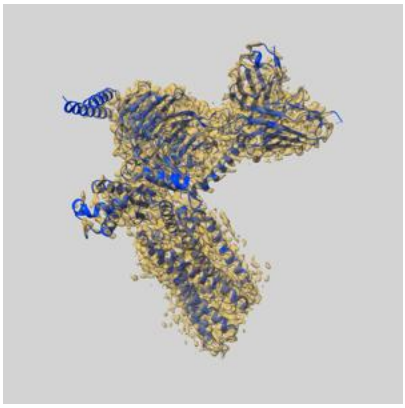
8 Fourier-Shell correlation (i)

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

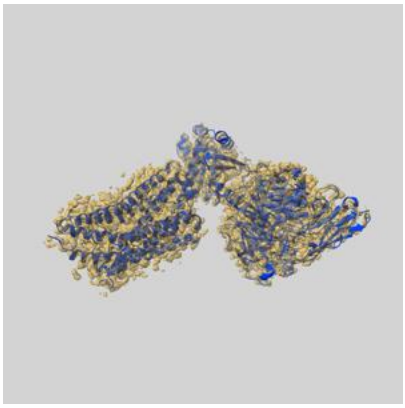
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51284 and PDB model 9GE2. Per-residue inclusion information can be found in section 3 on page 10.

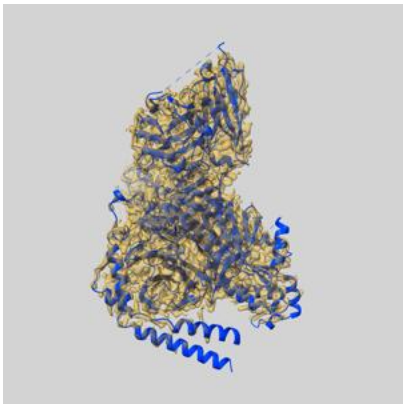
9.1 Map-model overlay



X



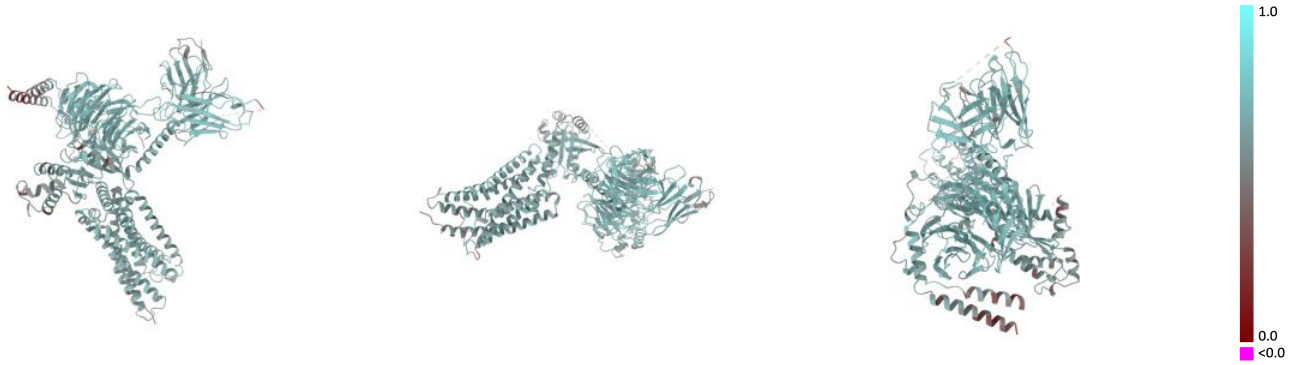
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

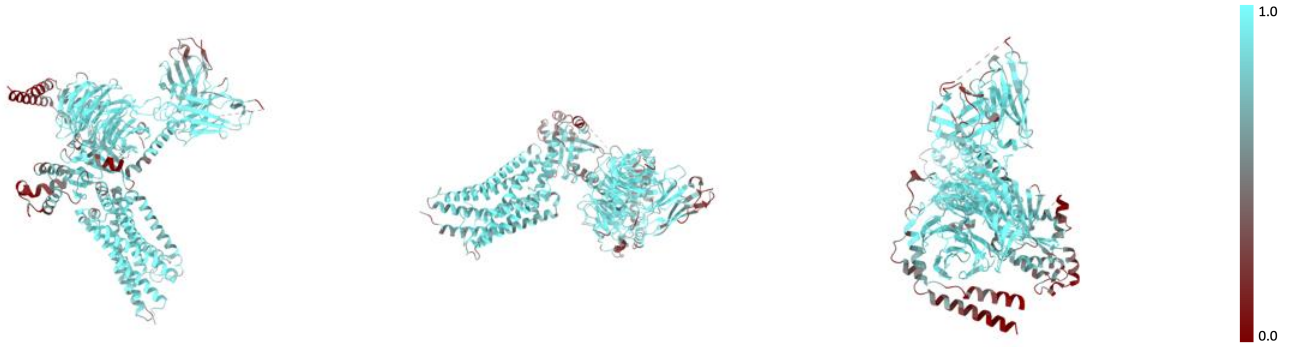
9.2 Q-score mapped to coordinate model (i)



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.

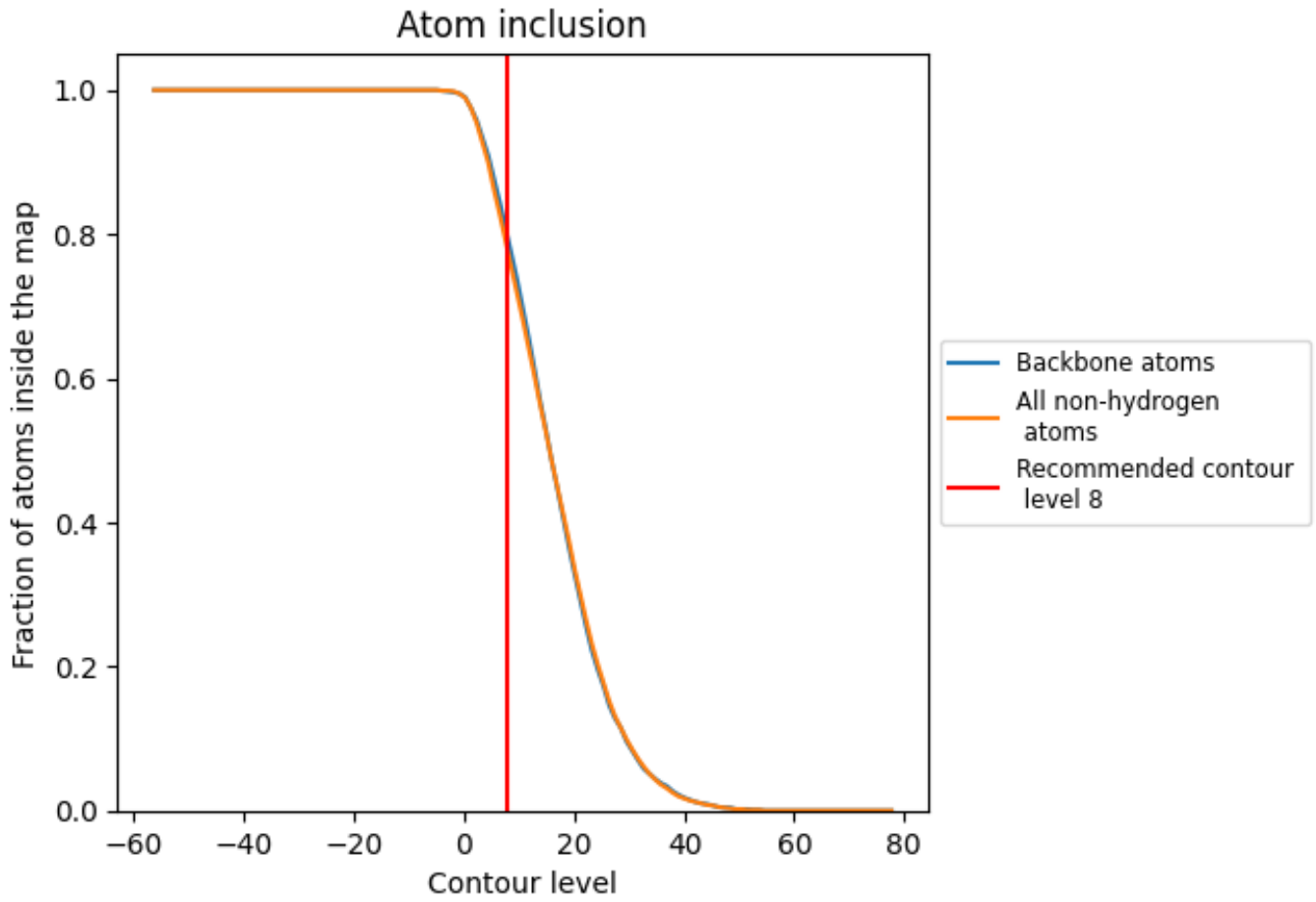
9.3 Atom inclusion mapped to coordinate model (i)



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 (8).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.6140
A	0.6430	0.5830
B	0.8480	0.6480
F	0.8110	0.6390
G	0.4600	0.5440
R	0.8510	0.5960
X	0.5360	0.5870