wwPDB EM Validation Summary Report

Jun 19, 2025 – 12:26 PM EDT

PDB ID	:	9CM7 / pdb_00009cm7
EMDB ID	:	EMD-45743
Title	:	Cryo-EM structure of Gi-coupled FFA2 in complex with TUG-1375 and AZ-1729
Authors	:	Zhang, X.; Tikhonova, I.; Milligan, G.; Zhang, C.
Deposited on	:	2024-07-12
Resolution	:	3.29 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:

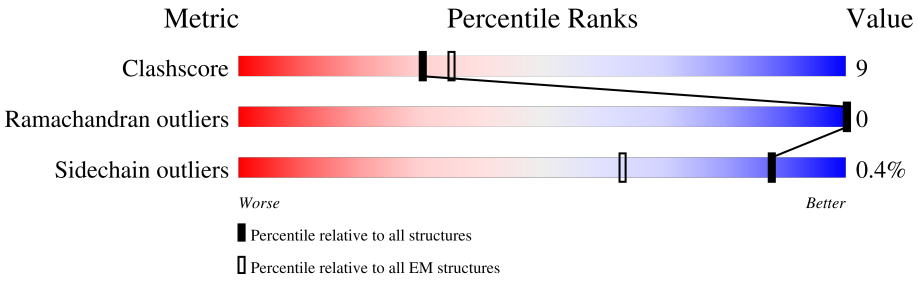
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 3.29 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	R	544	6% 38% 10% 51%
2	A	354	13% 53% 10% 37%
3	B	376	6% 72% 18% 10%
4	G	71	15% 73% • 23%
5	N	266	8% 63% 23% 14%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8408 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 Free fatty acid receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	266	Total	C	N	O	S	0	0
			2036	1368	333	325	10		

There are 214 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-44	ASP	-	expression tag	UNP O15552
R	-43	TYR	-	expression tag	UNP O15552
R	-42	LYS	-	expression tag	UNP O15552
R	-41	ASP	-	expression tag	UNP O15552
R	-40	ASP	-	expression tag	UNP O15552
R	-39	ASP	-	expression tag	UNP O15552
R	-38	ASP	-	expression tag	UNP O15552
R	-37	GLY	-	expression tag	UNP O15552
R	-36	GLN	-	expression tag	UNP O15552
R	-35	PRO	-	expression tag	UNP O15552
R	-34	GLY	-	expression tag	UNP O15552
R	-33	ASN	-	expression tag	UNP O15552
R	-32	GLY	-	expression tag	UNP O15552
R	-31	SER	-	expression tag	UNP O15552
R	-30	ALA	-	expression tag	UNP O15552
R	-29	PHE	-	expression tag	UNP O15552
R	-28	LEU	-	expression tag	UNP O15552
R	-27	LEU	-	expression tag	UNP O15552
R	-26	ALA	-	expression tag	UNP O15552
R	-25	PRO	-	expression tag	UNP O15552
R	-24	ASN	-	expression tag	UNP O15552
R	-23	GLY	-	expression tag	UNP O15552
R	-22	SER	-	expression tag	UNP O15552
R	-21	HIS	-	expression tag	UNP O15552
R	-20	ALA	-	expression tag	UNP O15552
R	-19	PRO	-	expression tag	UNP O15552
R	-18	ASP	-	expression tag	UNP O15552
R	-17	HIS	-	expression tag	UNP O15552

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-16	ASN	-	expression tag	UNP O15552
R	-15	VAL	-	expression tag	UNP O15552
R	-14	THR	-	expression tag	UNP O15552
R	-13	GLN	-	expression tag	UNP O15552
R	-12	GLN	-	expression tag	UNP O15552
R	-11	ARG	-	expression tag	UNP O15552
R	-10	ASP	-	expression tag	UNP O15552
R	-9	GLU	-	expression tag	UNP O15552
R	-8	GLU	-	expression tag	UNP O15552
R	-7	ASN	-	expression tag	UNP O15552
R	-6	LEU	-	expression tag	UNP O15552
R	-5	TYR	-	expression tag	UNP O15552
R	-4	PHE	-	expression tag	UNP O15552
R	-3	GLN	-	expression tag	UNP O15552
R	-2	GLY	-	expression tag	UNP O15552
R	-1	VAL	-	expression tag	UNP O15552
R	0	ASP	-	expression tag	UNP O15552
R	331	ALA	-	expression tag	UNP O15552
R	332	ALA	-	expression tag	UNP O15552
R	333	ALA	-	expression tag	UNP O15552
R	334	VAL	-	expression tag	UNP O15552
R	335	PHE	-	expression tag	UNP O15552
R	336	THR	-	expression tag	UNP O15552
R	337	LEU	-	expression tag	UNP O15552
R	338	GLU	-	expression tag	UNP O15552
R	339	ASP	-	expression tag	UNP O15552
R	340	PHE	-	expression tag	UNP O15552
R	341	VAL	-	expression tag	UNP O15552
R	342	GLY	-	expression tag	UNP O15552
R	343	ASP	-	expression tag	UNP O15552
R	344	TRP	-	expression tag	UNP O15552
R	345	GLU	-	expression tag	UNP O15552
R	346	GLN	-	expression tag	UNP O15552
R	347	THR	-	expression tag	UNP O15552
R	348	ALA	-	expression tag	UNP O15552
R	349	ALA	-	expression tag	UNP O15552
R	350	TYR	-	expression tag	UNP O15552
R	351	ASN	-	expression tag	UNP O15552
R	352	LEU	-	expression tag	UNP O15552
R	353	ASP	-	expression tag	UNP O15552
R	354	GLN	-	expression tag	UNP O15552
R	355	VAL	-	expression tag	UNP O15552

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Chain	Residue	Modelled	Actual	Comment	Reference
R	356	LEU	-	expression tag	UNP O15552
R	357	GLU	-	expression tag	UNP O15552
R	358	GLN	-	expression tag	UNP O15552
R	359	GLY	-	expression tag	UNP O15552
R	360	GLY	-	expression tag	UNP O15552
R	361	VAL	-	expression tag	UNP O15552
R	362	SER	-	expression tag	UNP O15552
R	363	SER	-	expression tag	UNP O15552
R	364	LEU	-	expression tag	UNP O15552
R	365	LEU	-	expression tag	UNP O15552
R	366	GLN	-	expression tag	UNP O15552
R	367	ASN	-	expression tag	UNP O15552
R	368	LEU	-	expression tag	UNP O15552
R	369	ALA	-	expression tag	UNP O15552
R	370	VAL	-	expression tag	UNP O15552
R	371	SER	-	expression tag	UNP O15552
R	372	VAL	-	expression tag	UNP O15552
R	373	THR	-	expression tag	UNP O15552
R	374	PRO	-	expression tag	UNP O15552
R	375	ILE	-	expression tag	UNP O15552
R	376	GLN	-	expression tag	UNP O15552
R	377	ARG	-	expression tag	UNP O15552
R	378	ILE	-	expression tag	UNP O15552
R	379	VAL	-	expression tag	UNP O15552
R	380	ARG	-	expression tag	UNP O15552
R	381	SER	-	expression tag	UNP O15552
R	382	GLY	-	expression tag	UNP O15552
R	383	GLU	-	expression tag	UNP O15552
R	384	ASN	-	expression tag	UNP O15552
R	385	ALA	-	expression tag	UNP O15552
R	386	LEU	-	expression tag	UNP O15552
R	387	LYS	-	expression tag	UNP O15552
R	388	ILE	-	expression tag	UNP O15552
R	389	ASP	-	expression tag	UNP O15552
R	390	ILE	-	expression tag	UNP O15552
R	391	HIS	-	expression tag	UNP O15552
R	392	VAL	-	expression tag	UNP O15552
R	393	ILE	-	expression tag	UNP O15552
R	394	ILE	-	expression tag	UNP O15552
R	395	PRO	-	expression tag	UNP O15552
R	396	TYR	-	expression tag	UNP O15552
R	397	GLU	-	expression tag	UNP O15552

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Chain	Residue	Modelled	Actual	Comment	Reference
R	398	GLY	-	expression tag	UNP O15552
R	399	LEU	-	expression tag	UNP O15552
R	400	SER	-	expression tag	UNP O15552
R	401	ALA	-	expression tag	UNP O15552
R	402	ASP	-	expression tag	UNP O15552
R	403	GLN	-	expression tag	UNP O15552
R	404	MET	-	expression tag	UNP O15552
R	405	ALA	-	expression tag	UNP O15552
R	406	GLN	-	expression tag	UNP O15552
R	407	ILE	-	expression tag	UNP O15552
R	408	GLU	-	expression tag	UNP O15552
R	409	GLU	-	expression tag	UNP O15552
R	410	VAL	-	expression tag	UNP O15552
R	411	PHE	-	expression tag	UNP O15552
R	412	LYS	-	expression tag	UNP O15552
R	413	VAL	-	expression tag	UNP O15552
R	414	VAL	-	expression tag	UNP O15552
R	415	TYR	-	expression tag	UNP O15552
R	416	PRO	-	expression tag	UNP O15552
R	417	VAL	-	expression tag	UNP O15552
R	418	ASP	-	expression tag	UNP O15552
R	419	ASP	-	expression tag	UNP O15552
R	420	HIS	-	expression tag	UNP O15552
R	421	HIS	-	expression tag	UNP O15552
R	422	PHE	-	expression tag	UNP O15552
R	423	LYS	-	expression tag	UNP O15552
R	424	VAL	-	expression tag	UNP O15552
R	425	ILE	-	expression tag	UNP O15552
R	426	LEU	-	expression tag	UNP O15552
R	427	PRO	-	expression tag	UNP O15552
R	428	TYR	-	expression tag	UNP O15552
R	429	GLY	-	expression tag	UNP O15552
R	430	THR	-	expression tag	UNP O15552
R	431	LEU	-	expression tag	UNP O15552
R	432	VAL	-	expression tag	UNP O15552
R	433	ILE	-	expression tag	UNP O15552
R	434	ASP	-	expression tag	UNP O15552
R	435	GLY	-	expression tag	UNP O15552
R	436	VAL	-	expression tag	UNP O15552
R	437	THR	-	expression tag	UNP O15552
R	438	PRO	-	expression tag	UNP O15552
R	439	ASN	-	expression tag	UNP O15552

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Chain	Residue	Modelled	Actual	Comment	Reference
R	440	MET	-	expression tag	UNP O15552
R	441	LEU	-	expression tag	UNP O15552
R	442	ASN	-	expression tag	UNP O15552
R	443	TYR	-	expression tag	UNP O15552
R	444	PHE	-	expression tag	UNP O15552
R	445	GLY	-	expression tag	UNP O15552
R	446	ARG	-	expression tag	UNP O15552
R	447	PRO	-	expression tag	UNP O15552
R	448	TYR	-	expression tag	UNP O15552
R	449	GLU	-	expression tag	UNP O15552
R	450	GLY	-	expression tag	UNP O15552
R	451	ILE	-	expression tag	UNP O15552
R	452	ALA	-	expression tag	UNP O15552
R	453	VAL	-	expression tag	UNP O15552
R	454	PHE	-	expression tag	UNP O15552
R	455	ASP	-	expression tag	UNP O15552
R	456	GLY	-	expression tag	UNP O15552
R	457	LYS	-	expression tag	UNP O15552
R	458	LYS	-	expression tag	UNP O15552
R	459	ILE	-	expression tag	UNP O15552
R	460	THR	-	expression tag	UNP O15552
R	461	VAL	-	expression tag	UNP O15552
R	462	THR	-	expression tag	UNP O15552
R	463	GLY	-	expression tag	UNP O15552
R	464	THR	-	expression tag	UNP O15552
R	465	LEU	-	expression tag	UNP O15552
R	466	TRP	-	expression tag	UNP O15552
R	467	ASN	-	expression tag	UNP O15552
R	468	GLY	-	expression tag	UNP O15552
R	469	ASN	-	expression tag	UNP O15552
R	470	LYS	-	expression tag	UNP O15552
R	471	ILE	-	expression tag	UNP O15552
R	472	ILE	-	expression tag	UNP O15552
R	473	ASP	-	expression tag	UNP O15552
R	474	GLU	-	expression tag	UNP O15552
R	475	ARG	-	expression tag	UNP O15552
R	476	LEU	-	expression tag	UNP O15552
R	477	ILE	-	expression tag	UNP O15552
R	478	THR	-	expression tag	UNP O15552
R	479	PRO	-	expression tag	UNP O15552
R	480	ASP	-	expression tag	UNP O15552
R	481	GLY	-	expression tag	UNP O15552

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Chain	Residue	Modelled	Actual	Comment	Reference
R	482	SER	-	expression tag	UNP O15552
R	483	MET	-	expression tag	UNP O15552
R	484	LEU	-	expression tag	UNP O15552
R	485	PHE	-	expression tag	UNP O15552
R	486	ARG	-	expression tag	UNP O15552
R	487	VAL	-	expression tag	UNP O15552
R	488	THR	-	expression tag	UNP O15552
R	489	ILE	-	expression tag	UNP O15552
R	490	ASN	-	expression tag	UNP O15552
R	491	SER	-	expression tag	UNP O15552
R	492	HIS	-	expression tag	UNP O15552
R	493	HIS	-	expression tag	UNP O15552
R	494	HIS	-	expression tag	UNP O15552
R	495	HIS	-	expression tag	UNP O15552
R	496	HIS	-	expression tag	UNP O15552
R	497	HIS	-	expression tag	UNP O15552
R	498	HIS	-	expression tag	UNP O15552
R	499	HIS	-	expression tag	UNP O15552

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	224	Total	C	N	O	S	0	0
			1696	1088	286	310	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	340	Total	C	N	O	S	0	0
			2555	1582	458	494	21		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

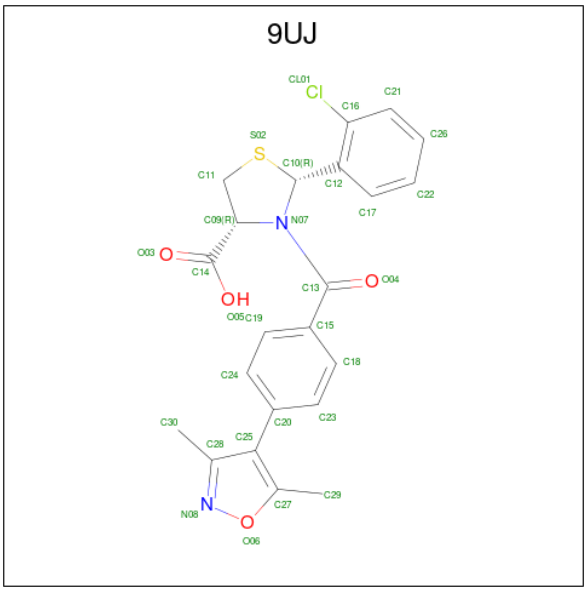
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	55	Total	C	N	O	S	0	0
			379	237	67	73	2		

- Molecule 5 is a protein called scFv16.

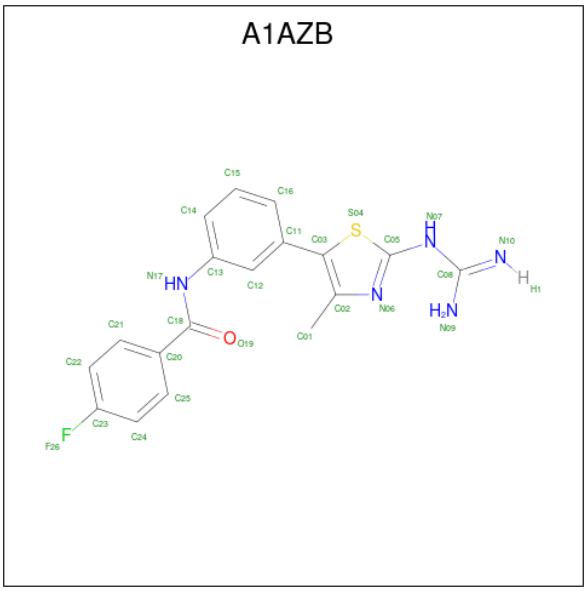
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	230	Total	C	N	O	S	0	0
			1686	1082	282	313	9		

- Molecule 6 is (2R,4R)-2-(2-chlorophenyl)-3-[4-(3,5-dimethyl-1,2-oxazol-4-yl)phenyl]carbonyl -1,3-thiazolidine-4-carboxylic acid (CCD ID: 9UJ) (formula: $C_{22}H_{19}ClN_2O_4S$).



Mol	Chain	Residues	Atoms						AltConf
6	R	1	Total	C	Cl	N	O	S	0
			30	22	1	2	4	1	

- Molecule 7 is N-[(3M)-3-(2-carbamimidamido-4-methyl-1,3-thiazol-5-yl)phenyl]-4-fluorobenz amide (CCD ID: A1AZB) (formula: $C_{18}H_{16}FN_5OS$).



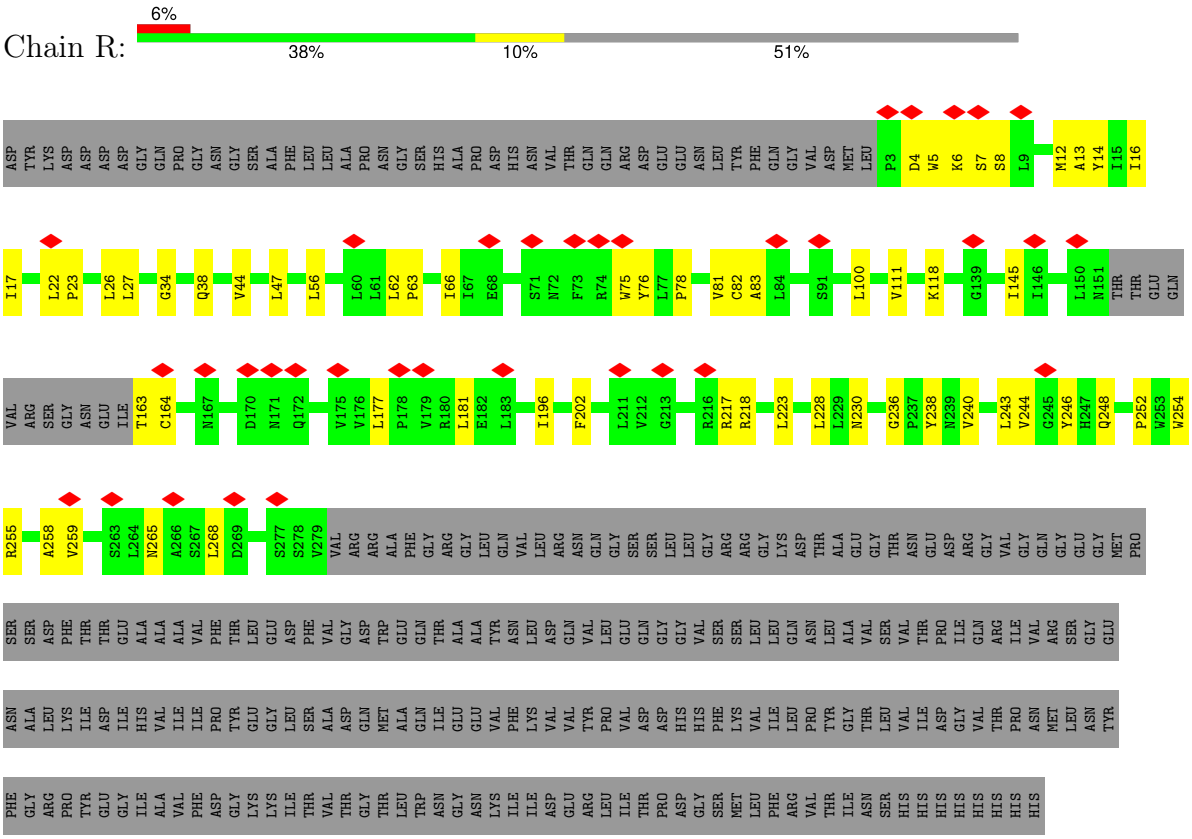
Mol	Chain	Residues	Atoms						AltConf
7	R	1	Total	C	F	N	O	S	0
			26	18	1	5	1	1	

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.

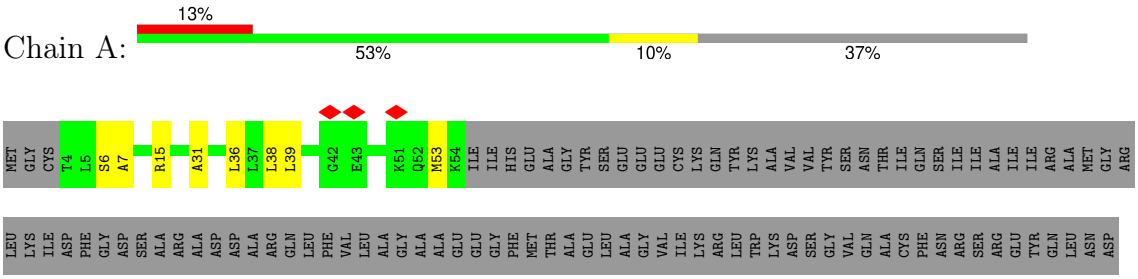
• Molecule 1: Free fatty acid receptor 2

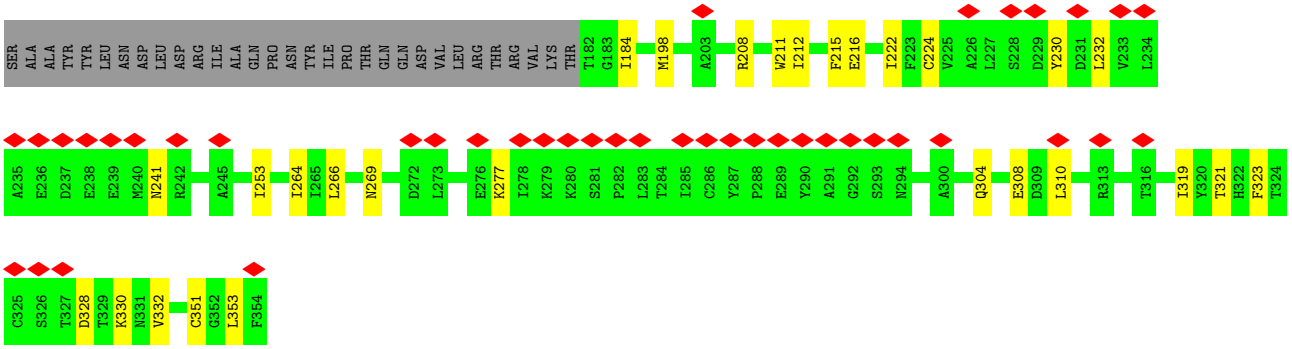
Chain R:



• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1

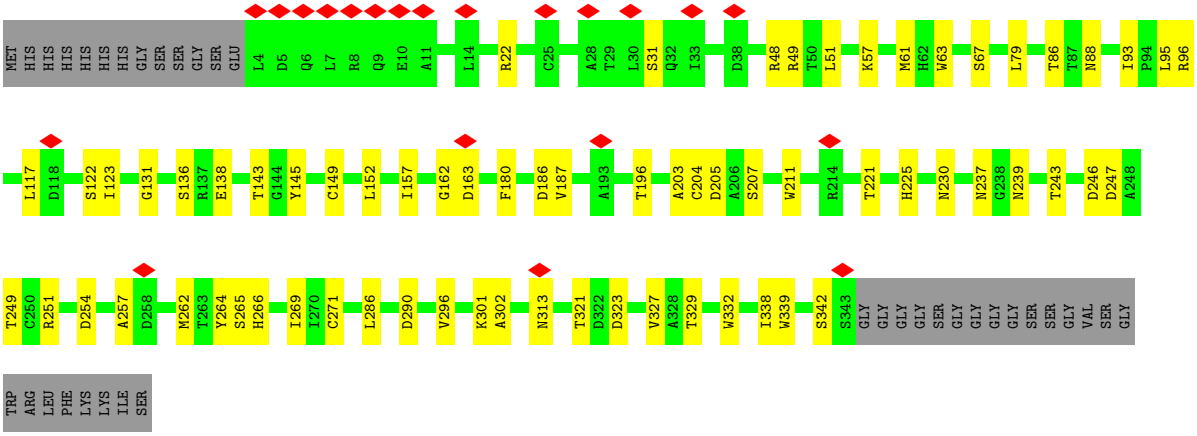
Chain A:





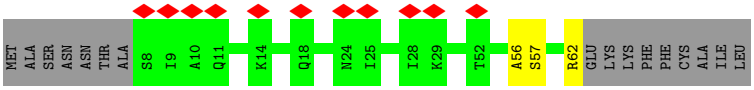
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



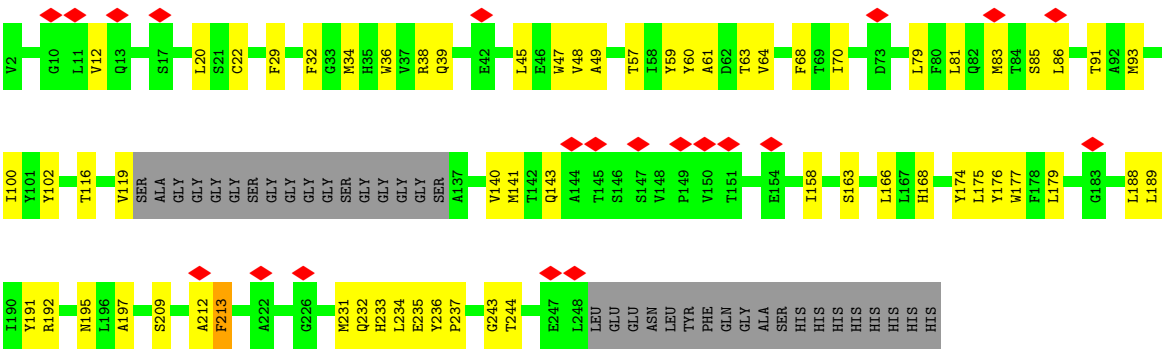
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



• Molecule 5: scFv16

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161839	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.763	Depositor
Minimum map value	-0.828	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	215.28, 215.28, 216.108	wwPDB
Map dimensions	260, 260, 261	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AZB, 9UJ

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	R	0.21	0/2096	0.38	0/2875
2	A	0.12	0/1725	0.27	0/2328
3	B	0.17	0/2602	0.32	0/3534
4	G	0.35	0/385	0.53	0/528
5	N	0.15	0/1730	0.36	0/2359
All	All	0.18	0/8538	0.35	0/11624

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	R	2036	0	2035	39	0
2	A	1696	0	1616	26	0
3	B	2555	0	2439	43	0
4	G	379	0	342	3	0
5	N	1686	0	1565	43	0
6	R	30	0	0	0	0
7	R	26	0	0	0	0
All	All	8408	0	7997	144	0

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

The worst 5 of 144 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:A:264:ILE:HB	2:A:319:ILE:HG22	1.67	0.77
5:N:175:LEU:HD13	5:N:213:PHE:HE2	1.53	0.72
5:N:22:CYS:HB3	5:N:79:LEU:HB3	1.76	0.67
2:A:224:CYS:SG	2:A:269:ASN:ND2	2.67	0.67
3:B:271:CYS:HB3	3:B:290:ASP:HB2	1.81	0.62

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	R	262/544 (48%)	252 (96%)	10 (4%)	0	100	100
2	A	220/354 (62%)	216 (98%)	4 (2%)	0	100	100
3	B	338/376 (90%)	327 (97%)	11 (3%)	0	100	100
4	G	53/71 (75%)	53 (100%)	0	0	100	100
5	N	226/266 (85%)	215 (95%)	11 (5%)	0	100	100
All	All	1099/1611 (68%)	1063 (97%)	36 (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	R	207/469 (44%)	205 (99%)	2 (1%)	73 84
2	A	167/305 (55%)	167 (100%)	0	100 100
3	B	269/306 (88%)	269 (100%)	0	100 100
4	G	33/58 (57%)	33 (100%)	0	100 100
5	N	168/215 (78%)	167 (99%)	1 (1%)	84 90
All	All	844/1353 (62%)	841 (100%)	3 (0%)	88 93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	217	ARG
1	R	218	ARG
5	N	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	17	GLN
3	B	266	HIS
3	B	32	GLN
4	G	18	GLN
3	B	220	GLN

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)

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	$\#\|Z\|>2$
6	9UJ	R	501	-	29,33,33	4.72	10 (34%)	40,48,48	2.21	6 (15%)
7	A1AZB	R	502	-	23,28,28	3.18	7 (30%)	26,39,39	1.26	2 (7%)

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	9UJ	R	501	-	-	1/20/33/33	0/4/4/4
7	A1AZB	R	502	-	-	4/14/16/16	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	9UJ	C10-S02	-12.52	1.69	1.84
6	R	501	9UJ	C11-S02	-12.17	1.47	1.81
6	R	501	9UJ	C11-C09	10.65	1.70	1.53
7	R	502	A1AZB	C08-N07	-10.53	1.24	1.38
6	R	501	9UJ	C10-N07	9.81	1.61	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	501	9UJ	C09-N07-C10	-9.84	107.88	116.58
6	R	501	9UJ	C11-S02-C10	7.09	103.89	90.88
7	R	502	A1AZB	C13-N17-C18	-3.30	117.92	126.61
6	R	501	9UJ	C30-C28-N08	2.44	126.69	119.19
6	R	501	9UJ	C17-C12-C16	2.43	119.26	116.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

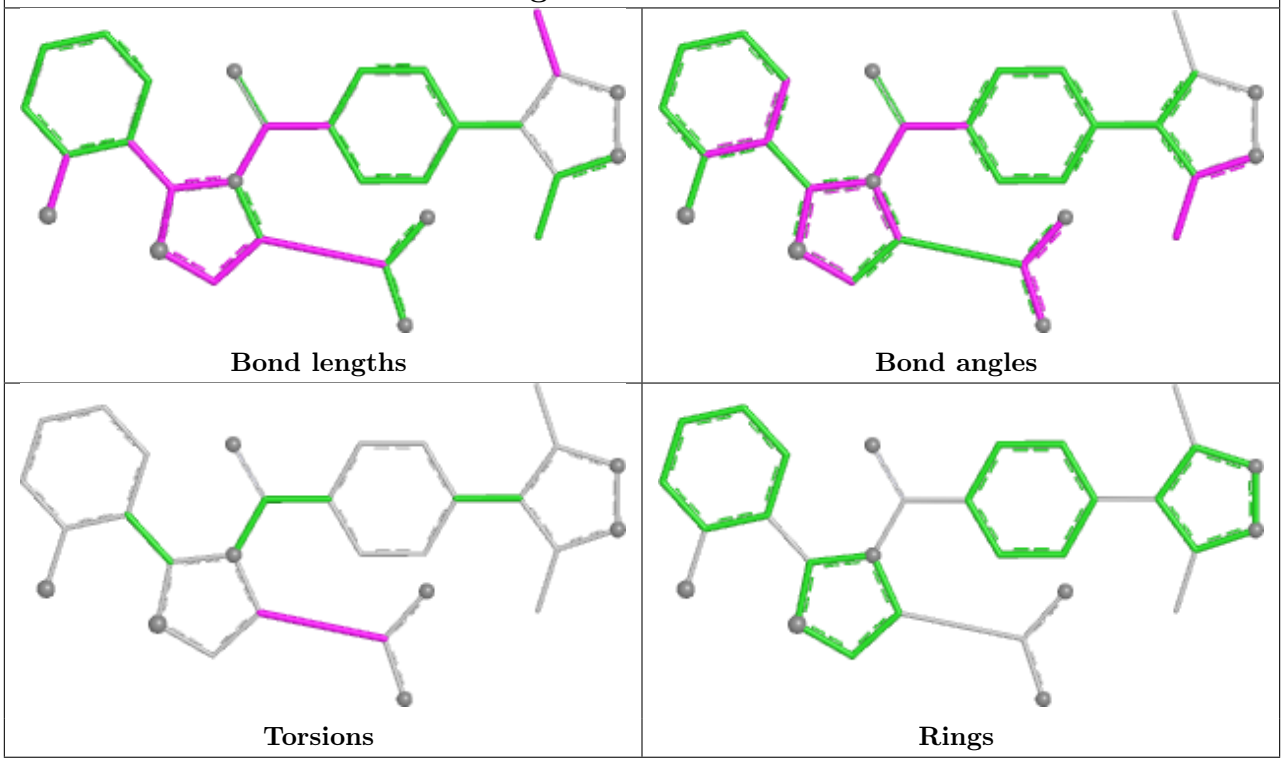
Mol	Chain	Res	Type	Atoms
7	R	502	A1AZB	C12-C13-N17-C18
7	R	502	A1AZB	C14-C13-N17-C18
6	R	501	9UJ	C11-C09-C14-O03
7	R	502	A1AZB	S04-C03-C11-C12
7	R	502	A1AZB	S04-C03-C11-C16

There are no ring outliers.

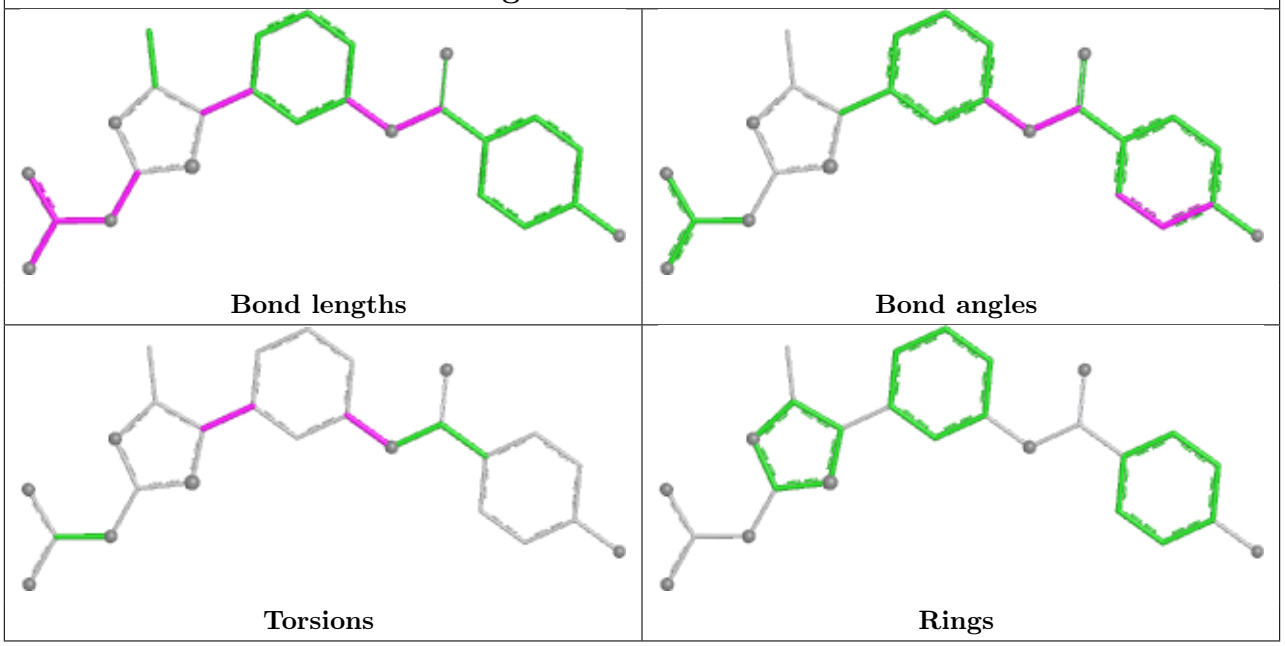
No monomer is involved in short contacts.

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 9UJ R 501



Ligand A1AZB R 502



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.

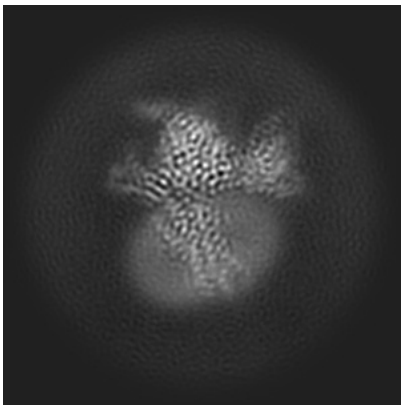
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45743. These allow visual inspection of the internal detail of the map and identification of artifacts.

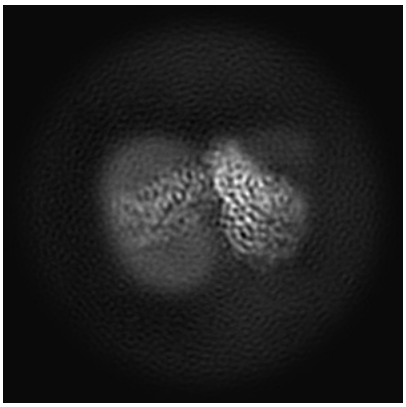
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

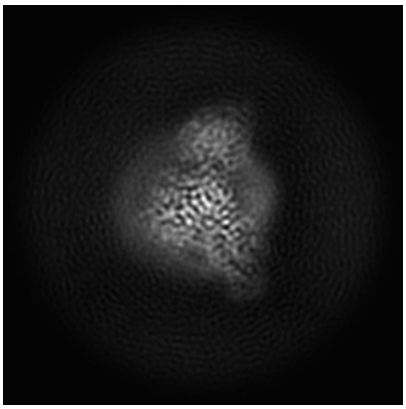
6.1.1 Primary map



X

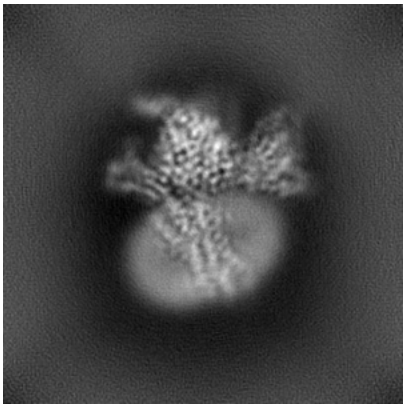


Y

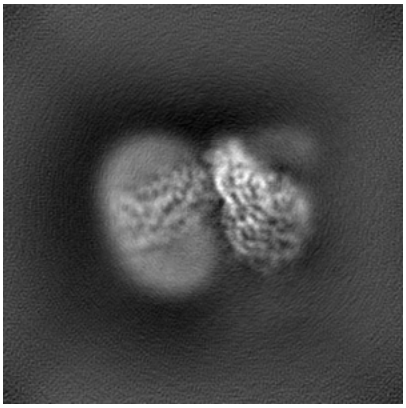


Z

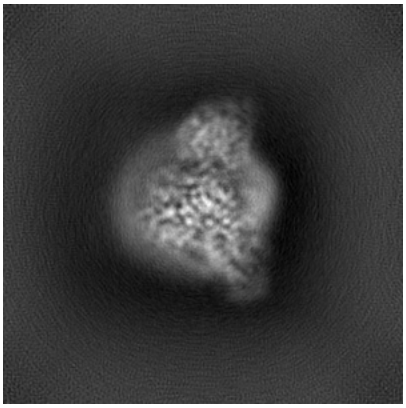
6.1.2 Raw map



X



Y

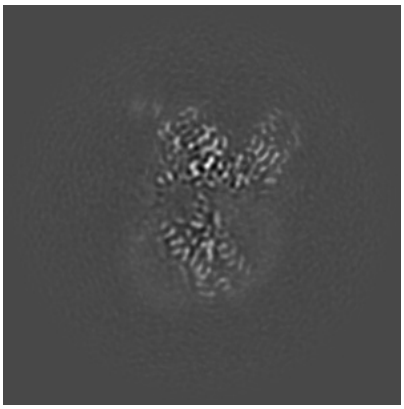


Z

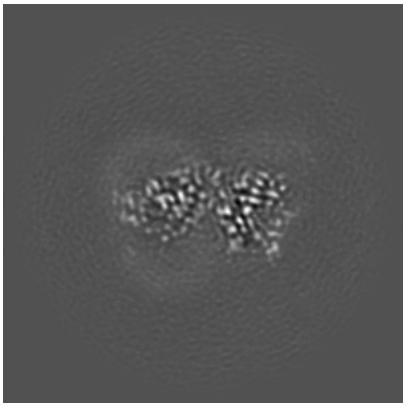
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

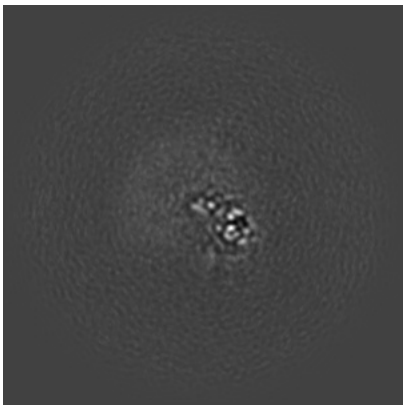
6.2.1 Primary map



X Index: 130

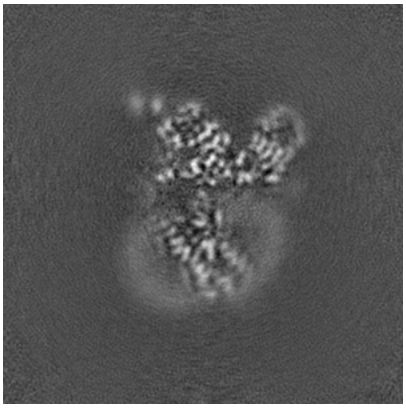


Y Index: 130

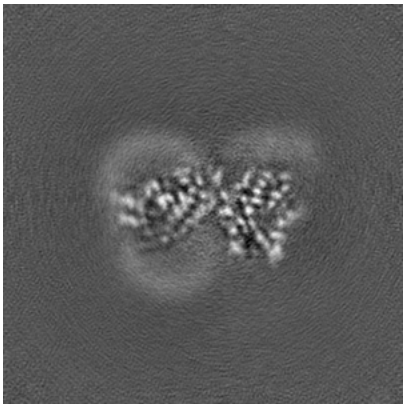


Z Index: 130

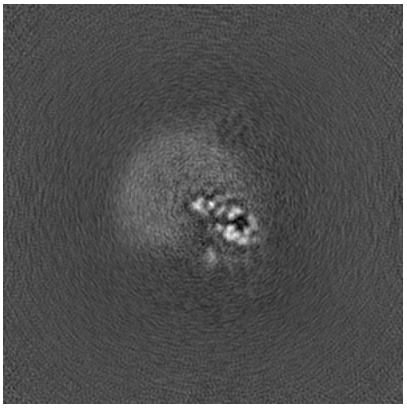
6.2.2 Raw map



X Index: 128



Y Index: 128

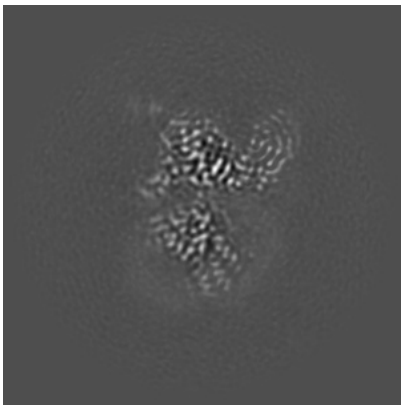


Z Index: 128

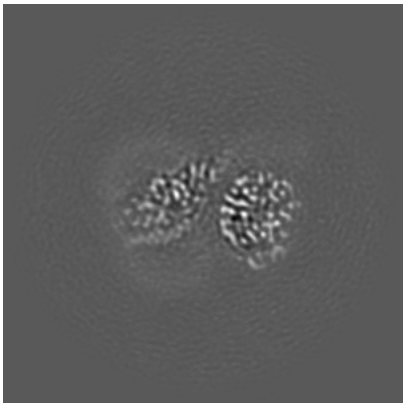
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

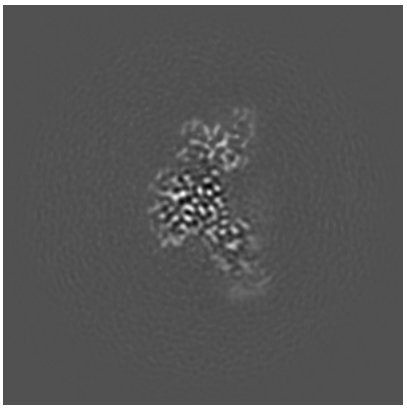
6.3.1 Primary map



X Index: 133

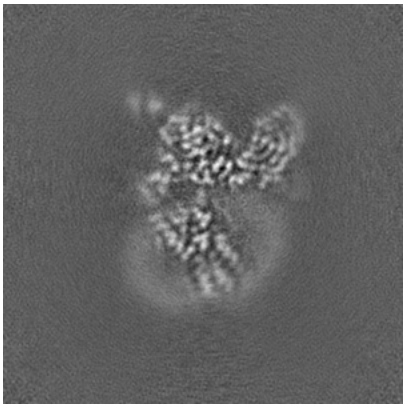


Y Index: 124

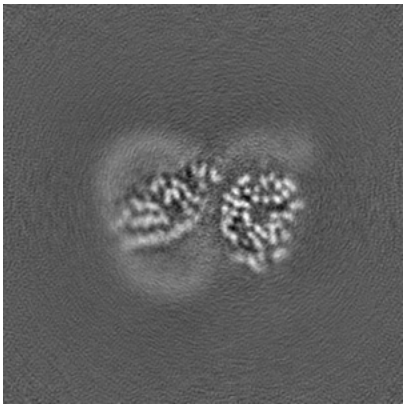


Z Index: 152

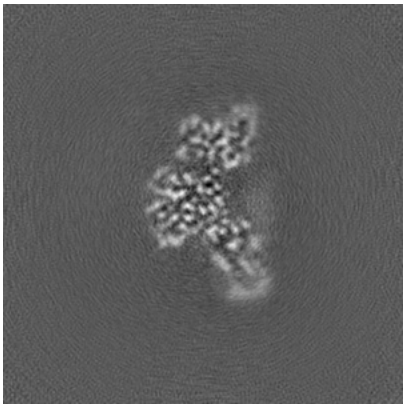
6.3.2 Raw map



X Index: 131



Y Index: 123

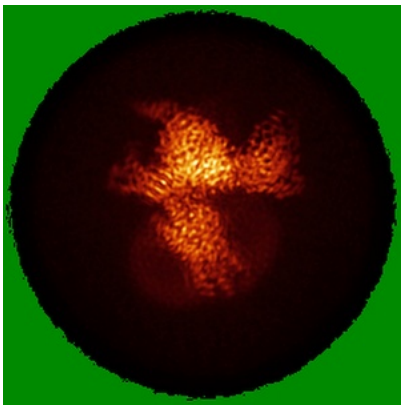


Z Index: 150

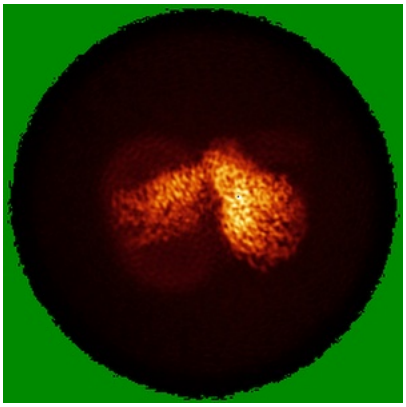
The images above show the largest variance slices of the map in three orthogonal directions.

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

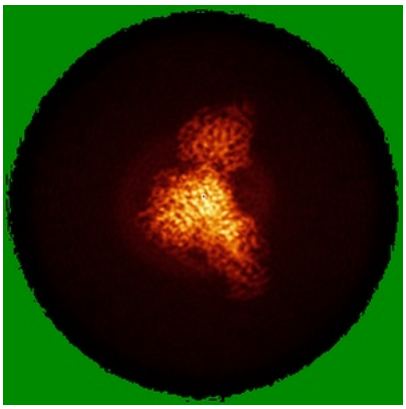
6.4.1 Primary map



X

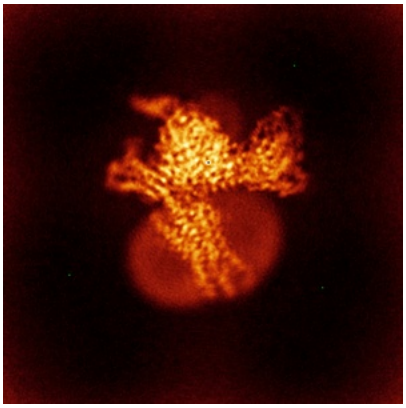


Y

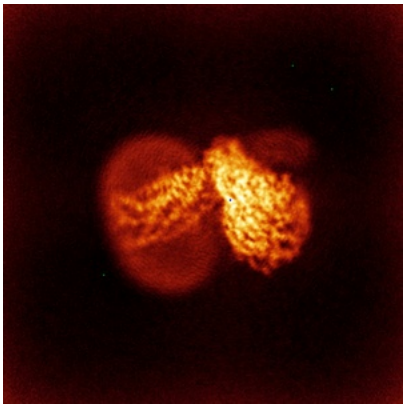


Z

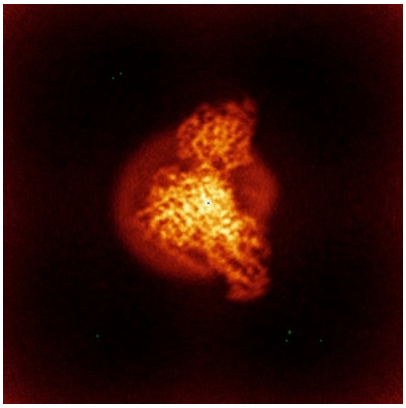
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

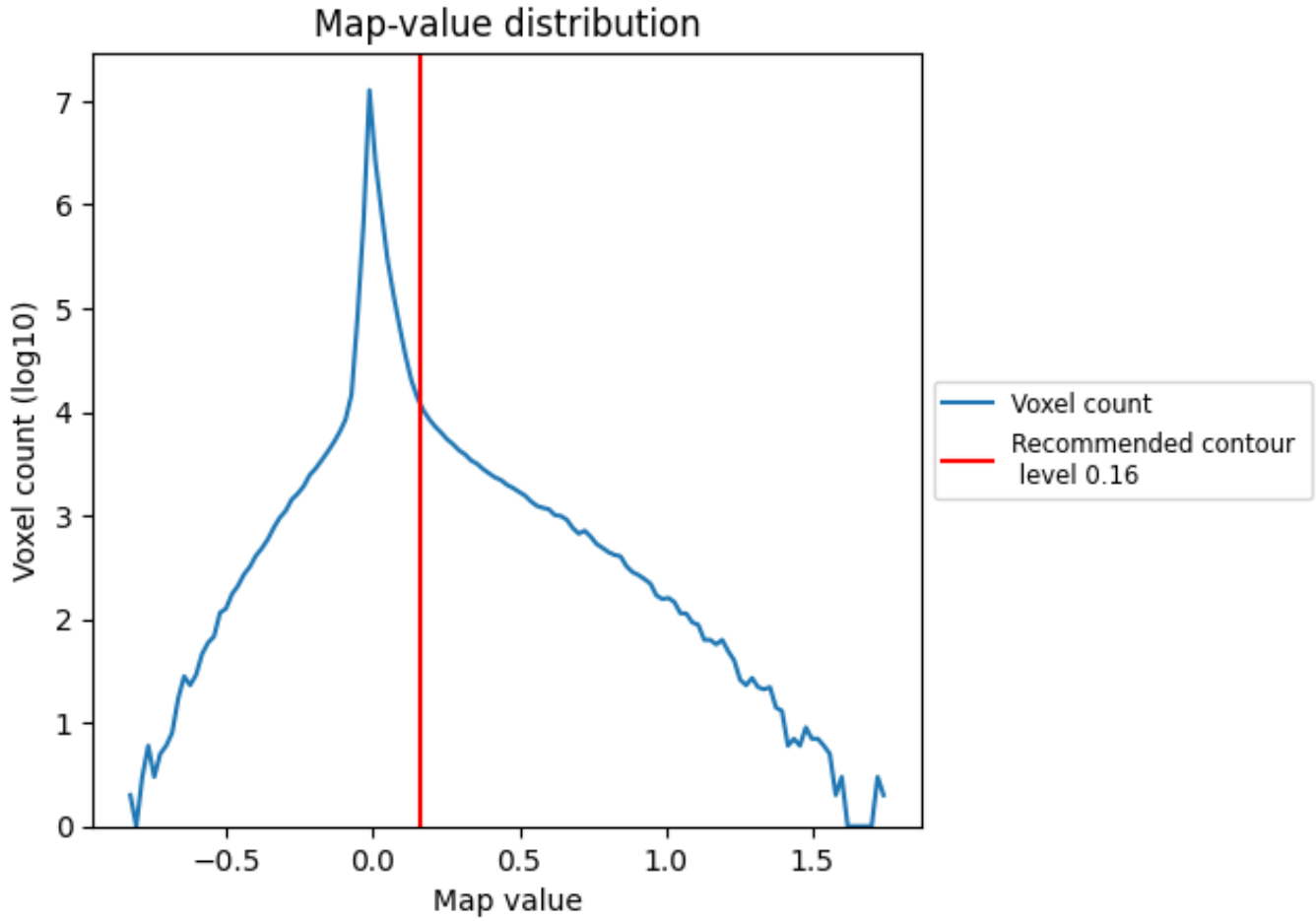
6.6 Mask visualisation (i)

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

7 Map analysis

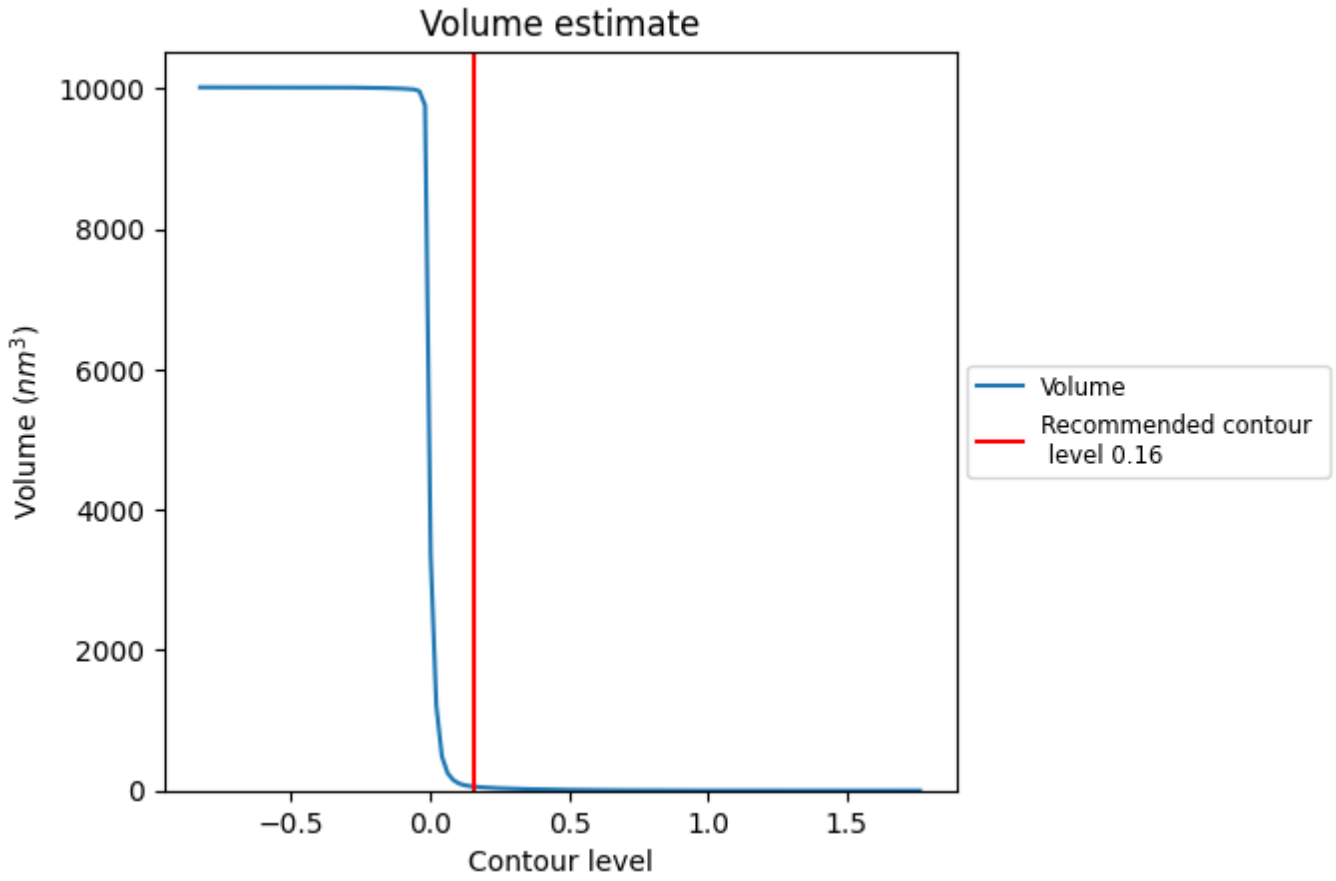
This section contains the results of statistical analysis of the map.

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 55 nm^3; this corresponds to an approximate mass of 50 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.

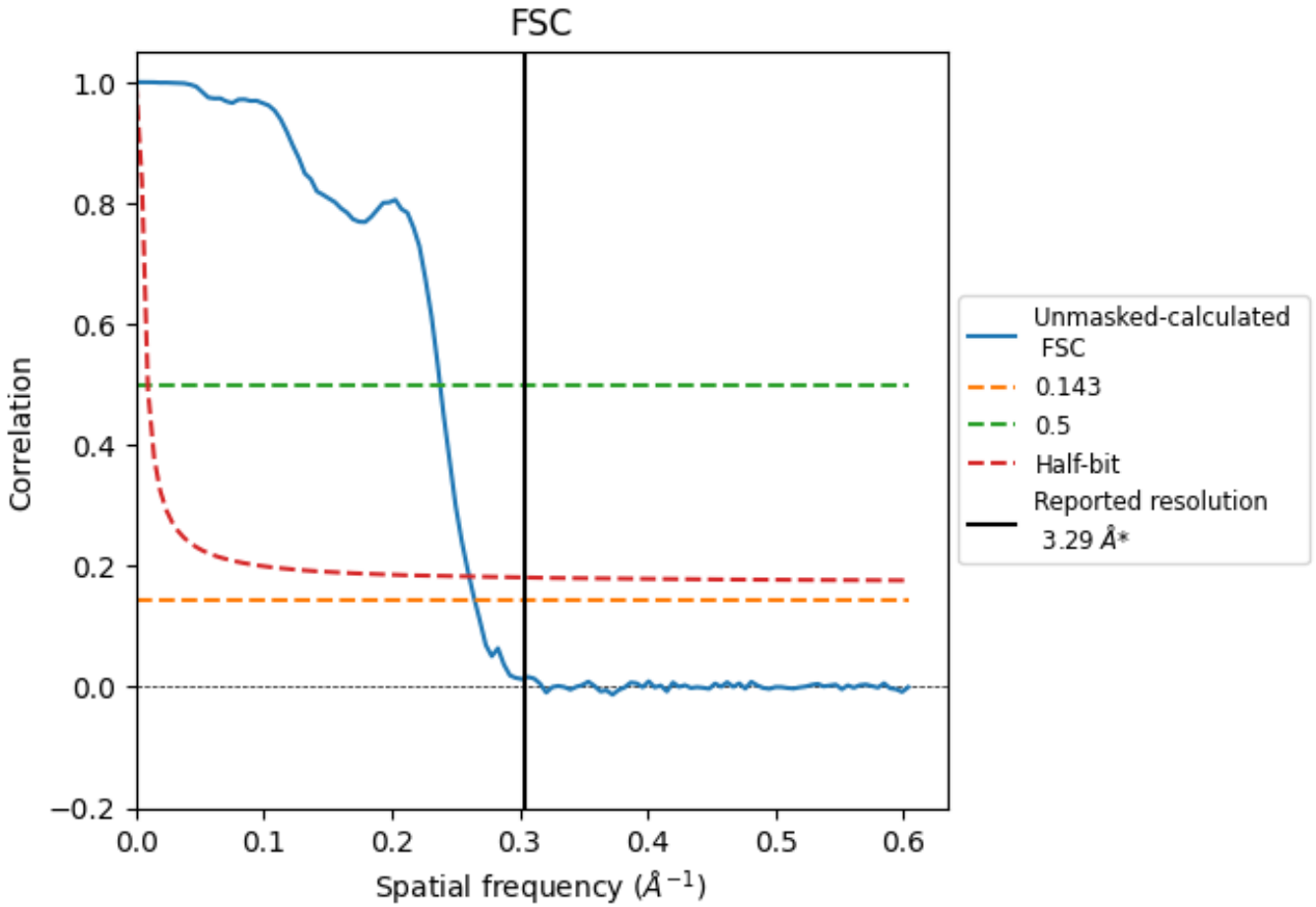
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.304 Å^{-1}

8.2 Resolution estimates (i)

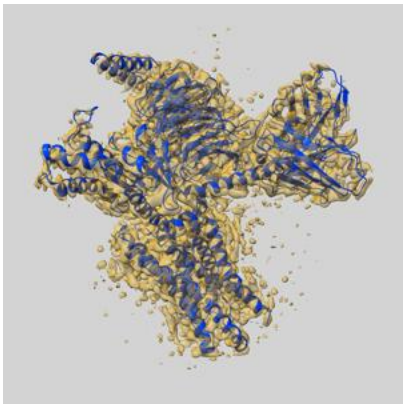
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	4.21	3.84

*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 3.78 differs from the reported value 3.29 by more than 10 %

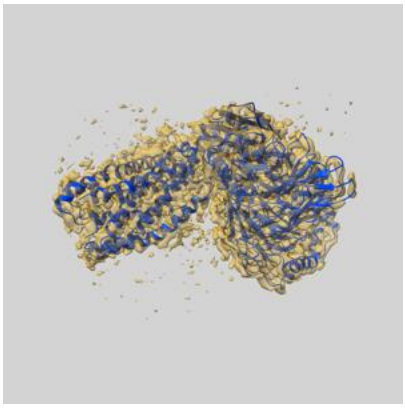
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45743 and PDB model 9CM7. Per-residue inclusion information can be found in section 3 on page 12.

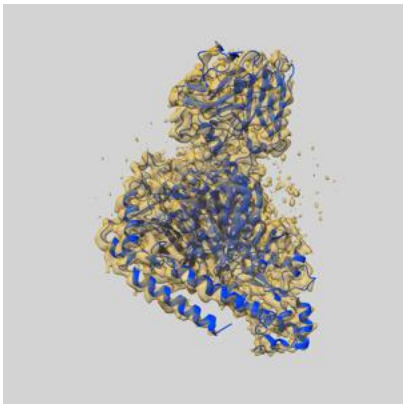
9.1 Map-model overlay



X



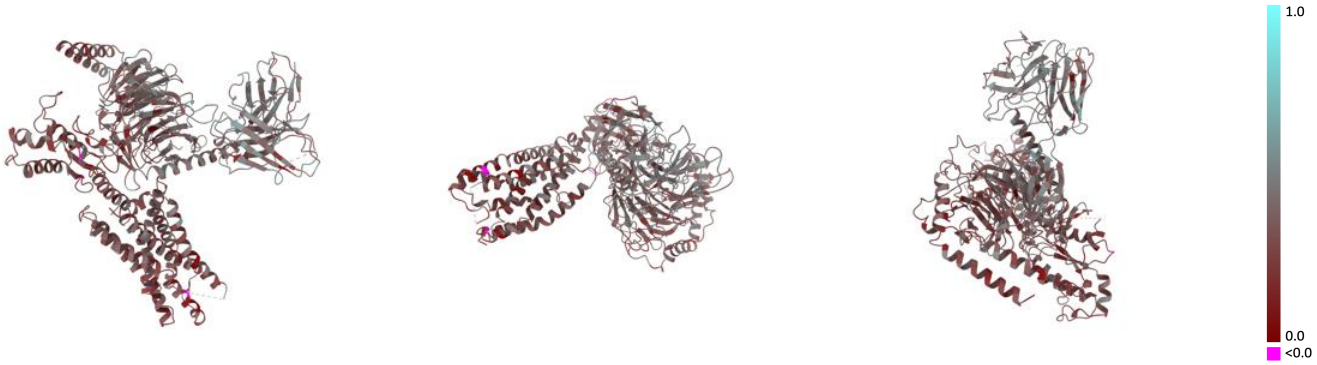
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

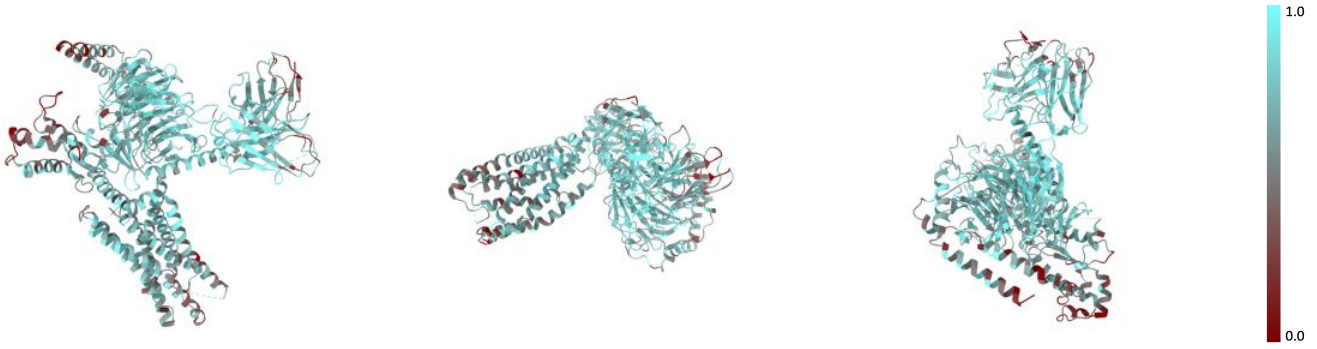
9.2 Q-score mapped to coordinate model (i)



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.

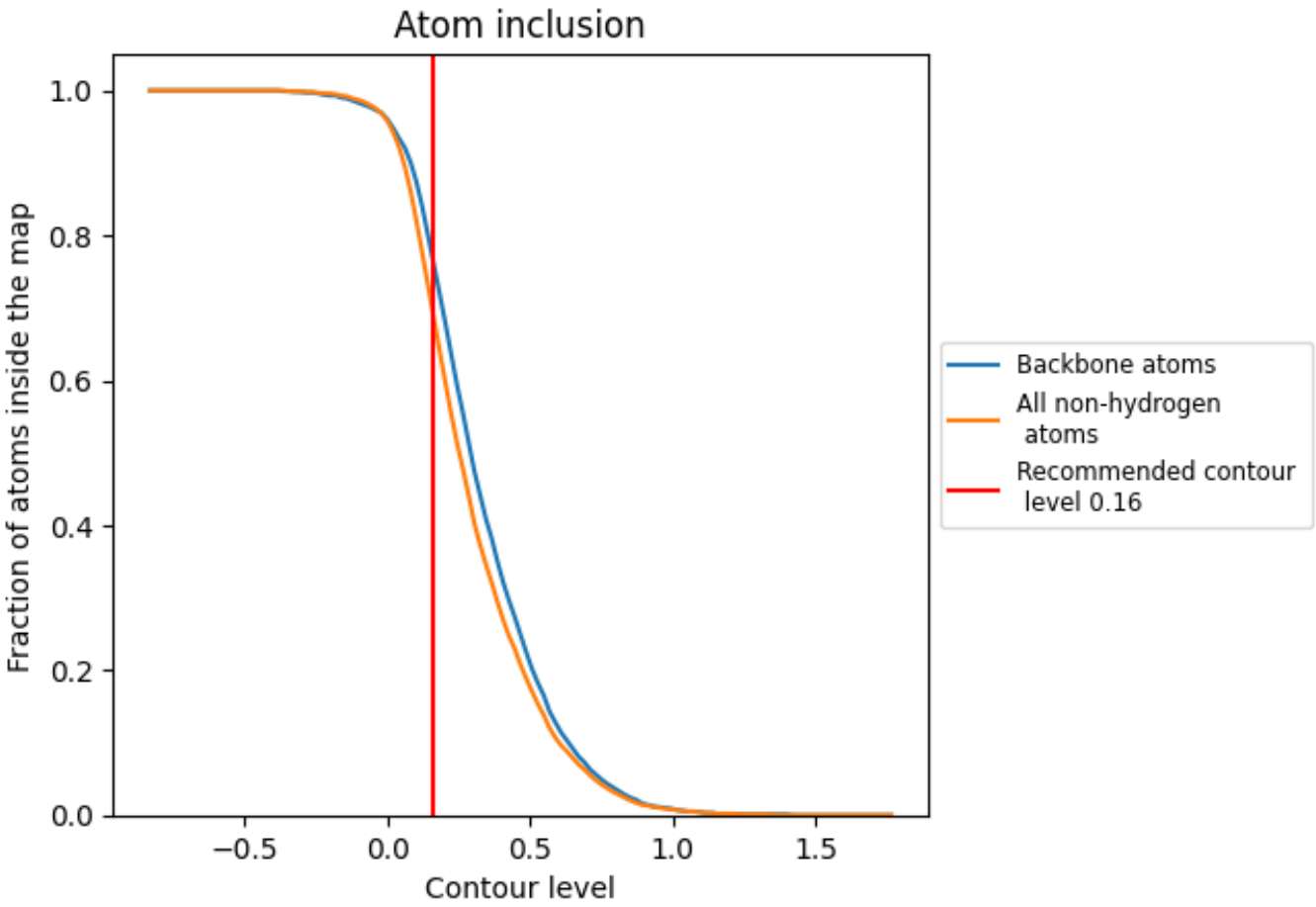
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 69% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.3470
A	0.6270	0.3230
B	0.7540	0.3540
G	0.6230	0.3180
N	0.7210	0.4310
R	0.6650	0.2970