Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 06:53 PM JST

PDB ID	:	8XOS / pdb_00008xos
EMDB ID	:	EMD-38539
Title	:	Cryo-EM structure of the tethered agonist-bound human PAR1-Gi complex
Authors	:	Guo, J.; Zhang, Y.
Deposited on	:	2024-01-02
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

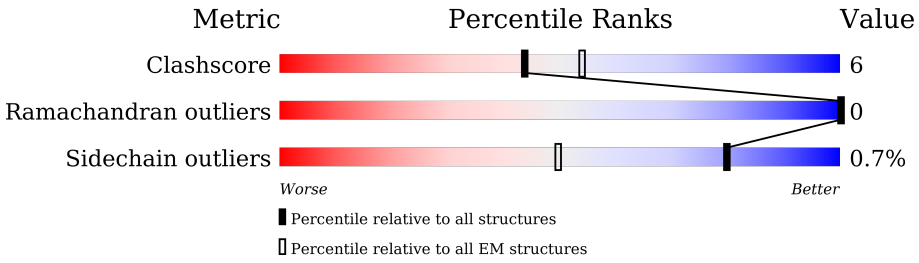
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	353	5% 53% 8% 39%
2	B	379	7% 77% 12% 11%
3	C	67	28% 75% 6% 19%
4	E	375	55% 7% 38%
5	R	532	49% 7% 44%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8919 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(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	217	1752	1117	292	331	12	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- 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
			Total	C	N	O	S		
2	B	336	2577	1590	462	504	21	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	initiating methionine	UNP P54311
B	-29	VAL	-	expression tag	UNP P54311
B	-28	SER	-	expression tag	UNP P54311
B	-27	GLY	-	expression tag	UNP P54311
B	-26	TRP	-	expression tag	UNP P54311
B	-25	ARG	-	expression tag	UNP P54311
B	-24	LEU	-	expression tag	UNP P54311
B	-23	PHE	-	expression tag	UNP P54311
B	-22	LYS	-	expression tag	UNP P54311
B	-21	LYS	-	expression tag	UNP P54311
B	-20	ILE	-	expression tag	UNP P54311
B	-19	SER	-	expression tag	UNP P54311
B	-18	GLY	-	expression tag	UNP P54311
B	-17	SER	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P54311
B	-15	GLY	-	expression tag	UNP P54311
B	-14	GLY	-	expression tag	UNP P54311
B	-13	GLY	-	expression tag	UNP P54311
B	-12	GLY	-	expression tag	UNP P54311
B	-11	SER	-	expression tag	UNP P54311
B	-10	GLY	-	expression tag	UNP P54311
B	-9	GLY	-	expression tag	UNP P54311
B	-8	GLY	-	expression tag	UNP P54311
B	-7	GLY	-	expression tag	UNP P54311
B	-6	SER	-	expression tag	UNP P54311
B	-5	SER	-	expression tag	UNP P54311
B	-4	GLY	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	HIS	-	expression tag	UNP P54311
B	342	HIS	-	expression tag	UNP P54311
B	343	HIS	-	expression tag	UNP P54311
B	344	HIS	-	expression tag	UNP P54311
B	345	HIS	-	expression tag	UNP P54311
B	346	HIS	-	expression tag	UNP P54311
B	347	HIS	-	expression tag	UNP P54311
B	348	HIS	-	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	C	54	Total	C	N	O	S	0	0
			418	263	74	78	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	232	Total	C	N	O	S	0	0
			1781	1131	295	345	10		

- Molecule 5 is a protein called Proteinase-activated receptor 1 LgBiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	297	Total	C	N	O	S	0	0
			2335	1558	353	405	19		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	398	GLY	-	expression tag	UNP P25116
R	399	SER	-	expression tag	UNP P25116
R	400	SER	-	expression tag	UNP P25116
R	401	GLY	-	expression tag	UNP P25116
R	402	GLY	-	expression tag	UNP P25116
R	403	GLY	-	expression tag	UNP P25116
R	404	GLY	-	expression tag	UNP P25116
R	405	SER	-	expression tag	UNP P25116
R	406	GLY	-	expression tag	UNP P25116
R	407	GLY	-	expression tag	UNP P25116
R	408	GLY	-	expression tag	UNP P25116
R	409	GLY	-	expression tag	UNP P25116
R	410	SER	-	expression tag	UNP P25116
R	411	SER	-	expression tag	UNP P25116
R	412	GLY	-	expression tag	UNP P25116
R	413	VAL	-	expression tag	UNP P25116
R	414	PHE	-	expression tag	UNP P25116
R	415	THR	-	expression tag	UNP P25116
R	416	LEU	-	expression tag	UNP P25116
R	417	GLU	-	expression tag	UNP P25116
R	418	ASP	-	expression tag	UNP P25116
R	419	PHE	-	expression tag	UNP P25116
R	420	VAL	-	expression tag	UNP P25116
R	421	GLY	-	expression tag	UNP P25116
R	422	ASP	-	expression tag	UNP P25116
R	423	TRP	-	expression tag	UNP P25116
R	424	GLU	-	expression tag	UNP P25116
R	425	GLN	-	expression tag	UNP P25116
R	426	THR	-	expression tag	UNP P25116
R	427	ALA	-	expression tag	UNP P25116
R	428	ALA	-	expression tag	UNP P25116
R	429	TYR	-	expression tag	UNP P25116
R	430	ASN	-	expression tag	UNP P25116
R	431	LEU	-	expression tag	UNP P25116
R	432	ASP	-	expression tag	UNP P25116
R	433	GLN	-	expression tag	UNP P25116
R	434	VAL	-	expression tag	UNP P25116

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Chain	Residue	Modelled	Actual	Comment	Reference
R	435	LEU	-	expression tag	UNP P25116
R	436	GLU	-	expression tag	UNP P25116
R	437	GLN	-	expression tag	UNP P25116
R	438	GLY	-	expression tag	UNP P25116
R	439	GLY	-	expression tag	UNP P25116
R	440	VAL	-	expression tag	UNP P25116
R	441	SER	-	expression tag	UNP P25116
R	442	SER	-	expression tag	UNP P25116
R	443	LEU	-	expression tag	UNP P25116
R	444	LEU	-	expression tag	UNP P25116
R	445	GLN	-	expression tag	UNP P25116
R	446	ASN	-	expression tag	UNP P25116
R	447	LEU	-	expression tag	UNP P25116
R	448	ALA	-	expression tag	UNP P25116
R	449	VAL	-	expression tag	UNP P25116
R	450	SER	-	expression tag	UNP P25116
R	451	VAL	-	expression tag	UNP P25116
R	452	THR	-	expression tag	UNP P25116
R	453	PRO	-	expression tag	UNP P25116
R	454	ILE	-	expression tag	UNP P25116
R	455	GLN	-	expression tag	UNP P25116
R	456	ARG	-	expression tag	UNP P25116
R	457	ILE	-	expression tag	UNP P25116
R	458	VAL	-	expression tag	UNP P25116
R	459	ARG	-	expression tag	UNP P25116
R	460	SER	-	expression tag	UNP P25116
R	461	GLY	-	expression tag	UNP P25116
R	462	GLU	-	expression tag	UNP P25116
R	463	ASN	-	expression tag	UNP P25116
R	464	ALA	-	expression tag	UNP P25116
R	465	LEU	-	expression tag	UNP P25116
R	466	LYS	-	expression tag	UNP P25116
R	467	ILE	-	expression tag	UNP P25116
R	468	ASP	-	expression tag	UNP P25116
R	469	ILE	-	expression tag	UNP P25116
R	470	HIS	-	expression tag	UNP P25116
R	471	VAL	-	expression tag	UNP P25116
R	472	ILE	-	expression tag	UNP P25116
R	473	ILE	-	expression tag	UNP P25116
R	474	PRO	-	expression tag	UNP P25116
R	475	TYR	-	expression tag	UNP P25116
R	476	GLU	-	expression tag	UNP P25116

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Chain	Residue	Modelled	Actual	Comment	Reference
R	477	GLY	-	expression tag	UNP P25116
R	478	LEU	-	expression tag	UNP P25116
R	479	SER	-	expression tag	UNP P25116
R	480	ALA	-	expression tag	UNP P25116
R	481	ASP	-	expression tag	UNP P25116
R	482	GLN	-	expression tag	UNP P25116
R	483	MET	-	expression tag	UNP P25116
R	484	ALA	-	expression tag	UNP P25116
R	485	GLN	-	expression tag	UNP P25116
R	486	ILE	-	expression tag	UNP P25116
R	487	GLU	-	expression tag	UNP P25116
R	488	GLU	-	expression tag	UNP P25116
R	489	VAL	-	expression tag	UNP P25116
R	490	PHE	-	expression tag	UNP P25116
R	491	LYS	-	expression tag	UNP P25116
R	492	VAL	-	expression tag	UNP P25116
R	493	VAL	-	expression tag	UNP P25116
R	494	TYR	-	expression tag	UNP P25116
R	495	PRO	-	expression tag	UNP P25116
R	496	VAL	-	expression tag	UNP P25116
R	497	ASP	-	expression tag	UNP P25116
R	498	ASP	-	expression tag	UNP P25116
R	499	HIS	-	expression tag	UNP P25116
R	500	HIS	-	expression tag	UNP P25116
R	501	PHE	-	expression tag	UNP P25116
R	502	LYS	-	expression tag	UNP P25116
R	503	VAL	-	expression tag	UNP P25116
R	504	ILE	-	expression tag	UNP P25116
R	505	LEU	-	expression tag	UNP P25116
R	506	PRO	-	expression tag	UNP P25116
R	507	TYR	-	expression tag	UNP P25116
R	508	GLY	-	expression tag	UNP P25116
R	509	THR	-	expression tag	UNP P25116
R	510	LEU	-	expression tag	UNP P25116
R	511	VAL	-	expression tag	UNP P25116
R	512	ILE	-	expression tag	UNP P25116
R	513	ASP	-	expression tag	UNP P25116
R	514	GLY	-	expression tag	UNP P25116
R	515	VAL	-	expression tag	UNP P25116
R	516	THR	-	expression tag	UNP P25116
R	517	PRO	-	expression tag	UNP P25116
R	518	ASN	-	expression tag	UNP P25116

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Chain	Residue	Modelled	Actual	Comment	Reference
R	519	MET	-	expression tag	UNP P25116
R	520	LEU	-	expression tag	UNP P25116
R	521	ASN	-	expression tag	UNP P25116
R	522	TYR	-	expression tag	UNP P25116
R	523	PHE	-	expression tag	UNP P25116
R	524	GLY	-	expression tag	UNP P25116
R	525	ARG	-	expression tag	UNP P25116
R	526	PRO	-	expression tag	UNP P25116
R	527	TYR	-	expression tag	UNP P25116
R	528	GLU	-	expression tag	UNP P25116
R	529	GLY	-	expression tag	UNP P25116
R	530	ILE	-	expression tag	UNP P25116
R	531	ALA	-	expression tag	UNP P25116
R	532	VAL	-	expression tag	UNP P25116
R	533	PHE	-	expression tag	UNP P25116
R	534	ASP	-	expression tag	UNP P25116
R	535	GLY	-	expression tag	UNP P25116
R	536	LYS	-	expression tag	UNP P25116
R	537	LYS	-	expression tag	UNP P25116
R	538	ILE	-	expression tag	UNP P25116
R	539	THR	-	expression tag	UNP P25116
R	540	VAL	-	expression tag	UNP P25116
R	541	THR	-	expression tag	UNP P25116
R	542	GLY	-	expression tag	UNP P25116
R	543	THR	-	expression tag	UNP P25116
R	544	LEU	-	expression tag	UNP P25116
R	545	TRP	-	expression tag	UNP P25116
R	546	ASN	-	expression tag	UNP P25116
R	547	GLY	-	expression tag	UNP P25116
R	548	ASN	-	expression tag	UNP P25116
R	549	LYS	-	expression tag	UNP P25116
R	550	ILE	-	expression tag	UNP P25116
R	551	ILE	-	expression tag	UNP P25116
R	552	ASP	-	expression tag	UNP P25116
R	553	GLU	-	expression tag	UNP P25116
R	554	ARG	-	expression tag	UNP P25116
R	555	LEU	-	expression tag	UNP P25116
R	556	ILE	-	expression tag	UNP P25116
R	557	THR	-	expression tag	UNP P25116
R	558	PRO	-	expression tag	UNP P25116
R	559	ASP	-	expression tag	UNP P25116
R	560	GLY	-	expression tag	UNP P25116

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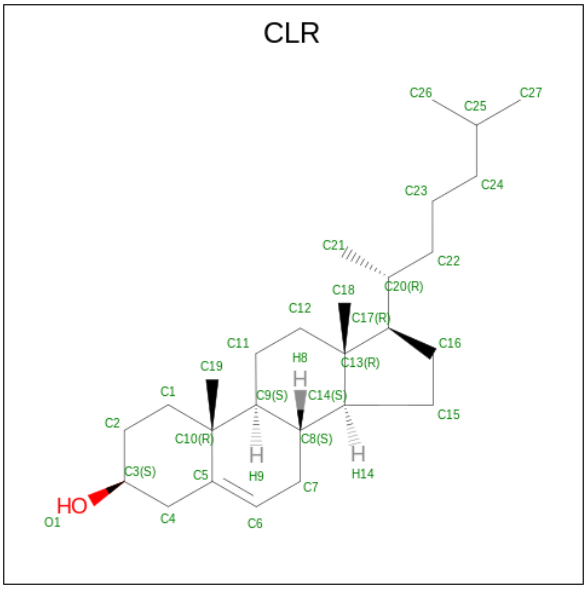
Chain	Residue	Modelled	Actual	Comment	Reference
R	561	SER	-	expression tag	UNP P25116
R	562	MET	-	expression tag	UNP P25116
R	563	LEU	-	expression tag	UNP P25116
R	564	PHE	-	expression tag	UNP P25116
R	565	ARG	-	expression tag	UNP P25116
R	566	VAL	-	expression tag	UNP P25116
R	567	THR	-	expression tag	UNP P25116
R	568	ILE	-	expression tag	UNP P25116
R	569	ASN	-	expression tag	UNP P25116
R	570	SER	-	expression tag	UNP P25116
R	571	GLY	-	expression tag	UNP P25116
R	572	GLY	-	expression tag	UNP P25116
R	573	SER	-	expression tag	UNP P25116

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



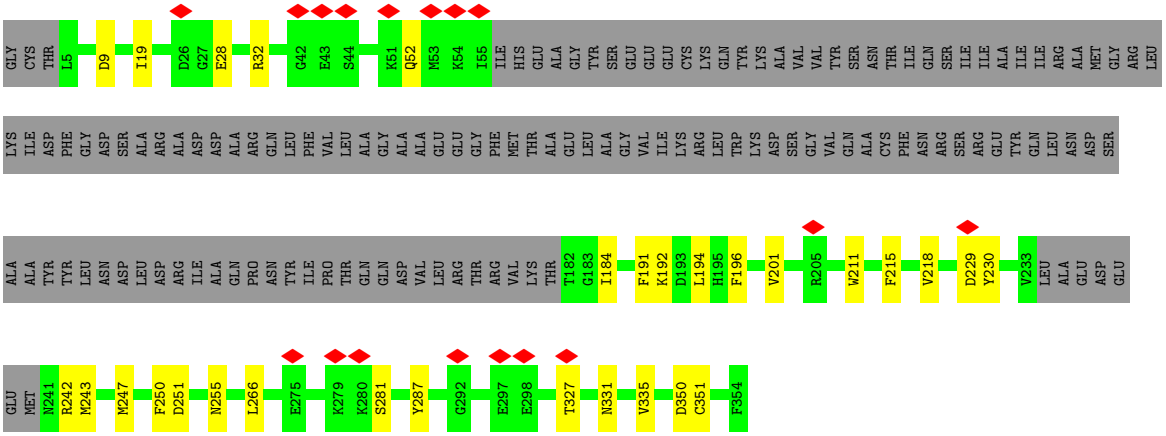
Mol	Chain	Residues	Atoms	AltConf
6	R	1	Total C O 28 27 1	0
6	R	1	Total C O 28 27 1	0

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.

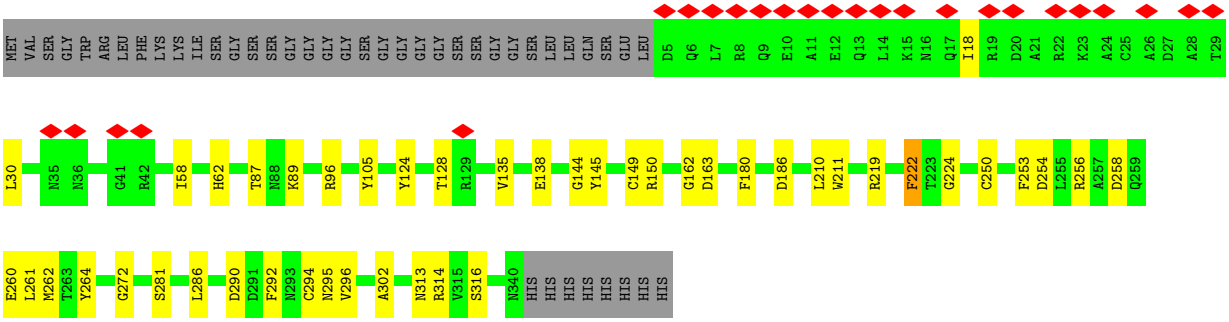
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



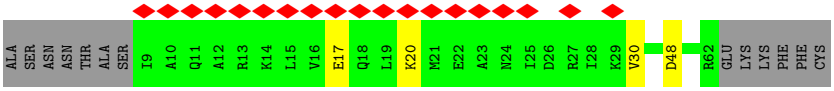
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



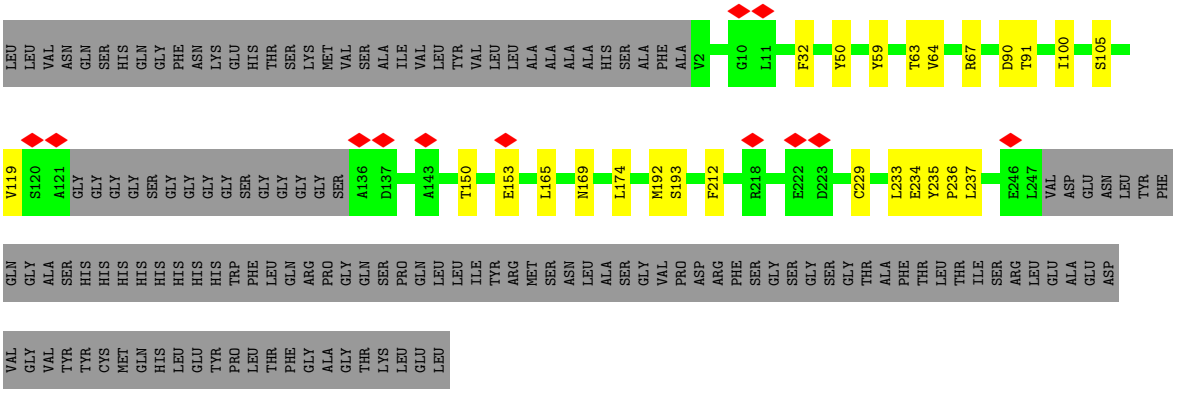
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



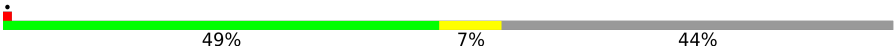
• Molecule 4: scFv16

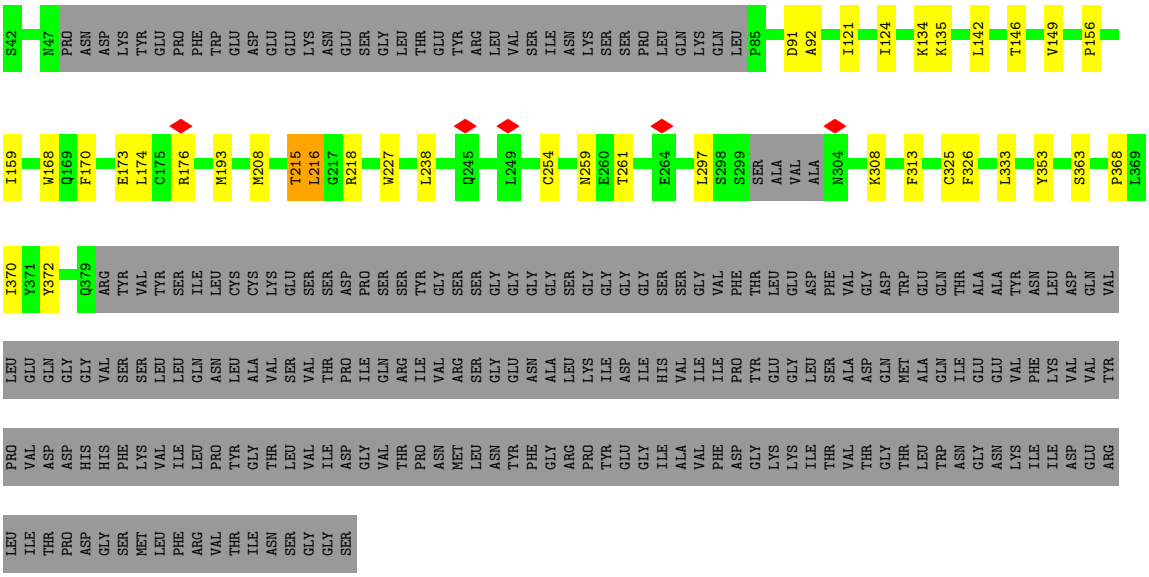
Chain E:



• Molecule 5: Proteinase-activated receptor 1 LgBiT

Chain R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162724	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 ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0207	Depositor
Map size (Å)	214.2, 214.2, 214.2	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.071, 1.071, 1.071	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

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	0.33	0/1781	0.48	0/2388
2	B	0.40	0/2624	0.55	0/3559
3	C	0.21	0/424	0.43	0/572
4	E	0.39	0/1825	0.66	0/2475
5	R	0.32	0/2398	0.51	0/3270
All	All	0.36	0/9052	0.55	0/12264

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	1752	0	1750	19	0
2	B	2577	0	2477	37	0
3	C	418	0	431	3	0
4	E	1781	0	1721	22	0
5	R	2335	0	2370	30	0
6	R	56	0	92	19	0
All	All	8919	0	8841	112	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 6.

All (112) 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:253:PHE:CE1	2:B:260:GLU:HG2	1.51	1.46
2:B:253:PHE:CE1	2:B:260:GLU:CG	2.20	1.24
2:B:253:PHE:HE1	2:B:260:GLU:CG	1.58	1.06
2:B:224:GLY:HA3	2:B:260:GLU:OE2	1.65	0.96
4:E:50:TYR:CD2	4:E:235:TYR:OH	2.24	0.89
2:B:253:PHE:HE1	2:B:260:GLU:HG3	1.39	0.87
2:B:253:PHE:CD1	2:B:260:GLU:HG2	2.16	0.81
4:E:50:TYR:CG	4:E:235:TYR:OH	2.38	0.75
2:B:253:PHE:CE1	2:B:260:GLU:HG3	2.17	0.74
2:B:224:GLY:CA	2:B:260:GLU:OE2	2.36	0.73
5:R:313:PHE:HB3	6:R:602:CLR:H72	1.76	0.67
4:E:235:TYR:O	4:E:237:LEU:HG	1.96	0.65
2:B:262:MET:HE2	2:B:302:ALA:HB2	1.79	0.64
4:E:234:GLU:HG2	4:E:236:PRO:HD2	1.79	0.64
2:B:96:ARG:NH2	2:B:138:GLU:OE2	2.29	0.62
5:R:170:PHE:HB3	5:R:174:LEU:HD12	1.82	0.60
1:A:247:MET:SD	1:A:287:TYR:OH	2.57	0.59
5:R:370:ILE:HD13	6:R:602:CLR:H232	1.85	0.58
5:R:142:LEU:HD21	6:R:601:CLR:H42	1.85	0.56
2:B:290:ASP:OD1	2:B:314:ARG:NH2	2.37	0.56
5:R:297:LEU:HD21	5:R:308:LYS:HB3	1.86	0.56
1:A:9:ASP:OD2	4:E:169:ASN:ND2	2.37	0.55
5:R:313:PHE:HB2	6:R:602:CLR:H191	1.89	0.55
1:A:230:TYR:OH	1:A:281:SER:OG	2.25	0.54
2:B:145:TYR:O	2:B:162:GLY:N	2.34	0.53
4:E:91:THR:HB	4:E:119:VAL:HG12	1.89	0.53
5:R:227:TRP:CE3	6:R:601:CLR:H241	2.43	0.53
5:R:227:TRP:CE2	6:R:601:CLR:H183	2.43	0.52
2:B:253:PHE:CD1	2:B:260:GLU:CG	2.85	0.52
4:E:63:THR:HG23	4:E:64:VAL:HG13	1.91	0.52
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.92	0.52
3:C:17:GLU:O	3:C:20:LYS:HG2	2.10	0.51
4:E:165:LEU:HA	4:E:233:LEU:HD22	1.92	0.51
2:B:286:LEU:HD13	2:B:296:VAL:HG22	1.93	0.51
1:A:19:ILE:HD11	2:B:89:LYS:HB3	1.92	0.50
1:A:194:LEU:HD23	1:A:196:PHE:CZ	2.47	0.50
4:E:235:TYR:N	4:E:236:PRO:HD2	2.26	0.50
1:A:194:LEU:HD22	5:R:208:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ASP:OD1	1:A:351:CYS:N	2.45	0.50
2:B:292:PHE:HB3	2:B:313:ASN:C	2.36	0.49
1:A:19:ILE:HD11	2:B:89:LYS:CB	2.42	0.49
2:B:281:SER:HB3	3:C:48:ASP:HB2	1.95	0.49
1:A:229:ASP:HB3	1:A:242:ARG:HD2	1.94	0.49
5:R:146:THR:HG21	6:R:601:CLR:H191	1.95	0.49
2:B:186:ASP:N	2:B:186:ASP:OD1	2.46	0.49
2:B:30:LEU:HD23	2:B:262:MET:SD	2.53	0.49
4:E:100:ILE:HG23	4:E:105:SER:OG	2.12	0.49
5:R:142:LEU:HD21	6:R:601:CLR:H22	1.95	0.48
4:E:150:THR:N	4:E:153:GLU:OE1	2.41	0.48
1:A:52:GLN:NE2	1:A:327:THR:HA	2.28	0.48
4:E:59:TYR:HD2	4:E:235:TYR:CZ	2.32	0.48
4:E:174:LEU:HD11	4:E:229:CYS:SG	2.53	0.48
2:B:62:HIS:CD2	2:B:105:TYR:H	2.32	0.48
6:R:601:CLR:H273	6:R:601:CLR:H232	1.67	0.47
5:R:193:MET:HE1	5:R:326:PHE:CE2	2.50	0.47
4:E:235:TYR:C	4:E:237:LEU:N	2.70	0.47
6:R:601:CLR:H213	6:R:601:CLR:H231	1.69	0.46
1:A:184:ILE:HD11	1:A:215:PHE:HZ	1.80	0.46
5:R:168:TRP:CZ2	5:R:170:PHE:HB2	2.51	0.46
1:A:230:TYR:HA	1:A:243:MET:HB2	1.97	0.46
2:B:224:GLY:HA3	2:B:260:GLU:CD	2.38	0.46
4:E:235:TYR:O	4:E:236:PRO:C	2.57	0.45
6:R:602:CLR:H25	6:R:602:CLR:H221	1.25	0.45
1:A:250:PHE:CE2	1:A:266:LEU:HD21	2.52	0.45
4:E:234:GLU:CG	4:E:236:PRO:HD2	2.45	0.45
5:R:333:LEU:HG	5:R:353:TYR:CE1	2.51	0.45
5:R:176:ARG:HD3	5:R:238:LEU:HA	1.99	0.44
2:B:222:PHE:HE2	2:B:258:ASP:HA	1.81	0.44
2:B:272:GLY:N	2:B:290:ASP:OD2	2.51	0.44
4:E:192:MET:HG3	4:E:193:SER:OG	2.17	0.44
5:R:313:PHE:HD2	6:R:602:CLR:H42	1.82	0.44
5:R:134:LYS:HG3	5:R:135:LYS:HG3	2.00	0.43
2:B:254:ASP:OD1	2:B:256:ARG:N	2.51	0.43
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.47	0.43
4:E:59:TYR:HD2	4:E:235:TYR:CE1	2.37	0.43
2:B:294:CYS:C	2:B:295:ASN:HD22	2.26	0.43
5:R:313:PHE:CD2	6:R:602:CLR:H42	2.54	0.43
4:E:32:PHE:CD2	4:E:100:ILE:HB	2.54	0.43
5:R:156:PRO:HA	5:R:159:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ILE:O	2:B:316:SER:OG	2.32	0.43
4:E:235:TYR:N	4:E:236:PRO:CD	2.81	0.43
5:R:368:PRO:HA	5:R:372:TYR:CD2	2.53	0.43
5:R:216:LEU:HA	5:R:216:LEU:HD23	1.65	0.42
2:B:286:LEU:CD1	2:B:296:VAL:HG22	2.49	0.42
1:A:201:VAL:HG21	1:A:211:TRP:CZ3	2.54	0.42
2:B:149:CYS:O	2:B:150:ARG:NH2	2.50	0.42
1:A:191:PHE:CD2	1:A:192:LYS:HG2	2.54	0.42
5:R:325:CYS:SG	5:R:363:SER:HB3	2.59	0.42
4:E:67:ARG:NH1	4:E:90:ASP:OD1	2.34	0.42
4:E:174:LEU:HD22	4:E:212:PHE:CG	2.54	0.42
6:R:601:CLR:H183	6:R:601:CLR:H20	1.80	0.42
2:B:210:LEU:HD23	2:B:219:ARG:HD2	2.01	0.42
2:B:180:PHE:HB3	2:B:211:TRP:CZ3	2.55	0.42
6:R:601:CLR:H182	6:R:601:CLR:H8	1.74	0.42
6:R:602:CLR:H212	6:R:602:CLR:H121	2.01	0.42
5:R:215:THR:HG23	5:R:218:ARG:HD2	2.01	0.41
1:A:28:GLU:O	1:A:32:ARG:NH2	2.53	0.41
2:B:124:TYR:CE1	2:B:135:VAL:HG22	2.56	0.41
5:R:121:ILE:HA	5:R:124:ILE:HG22	2.02	0.41
5:R:227:TRP:CZ3	6:R:601:CLR:H222	2.55	0.41
1:A:215:PHE:O	1:A:218:VAL:HG22	2.20	0.41
2:B:87:THR:HG22	2:B:87:THR:O	2.20	0.41
2:B:261:LEU:HD22	3:C:30:VAL:HG13	2.03	0.41
5:R:173:GLU:OE1	5:R:173:GLU:N	2.51	0.41
5:R:259:ASN:OD1	5:R:261:THR:N	2.53	0.41
6:R:602:CLR:H182	6:R:602:CLR:H8	1.82	0.41
1:A:331:ASN:O	1:A:335:VAL:HG23	2.21	0.40
5:R:91:ASP:OD1	5:R:92:ALA:N	2.54	0.40
2:B:144:GLY:HA3	2:B:163:ASP:H	1.86	0.40
2:B:250:CYS:HB2	2:B:264:TYR:HB2	2.04	0.40
5:R:176:ARG:NH2	5:R:238:LEU:O	2.48	0.40
5:R:142:LEU:HD11	6:R:601:CLR:H42	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/353 (60%)	206 (98%)	5 (2%)	0	100	100
2	B	334/379 (88%)	315 (94%)	19 (6%)	0	100	100
3	C	52/67 (78%)	51 (98%)	1 (2%)	0	100	100
4	E	228/375 (61%)	214 (94%)	14 (6%)	0	100	100
5	R	291/532 (55%)	279 (96%)	12 (4%)	0	100	100
All	All	1116/1706 (65%)	1065 (95%)	51 (5%)	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	194/305 (64%)	194 (100%)	0	100	100
2	B	278/310 (90%)	275 (99%)	3 (1%)	70	86
3	C	44/55 (80%)	44 (100%)	0	100	100
4	E	195/304 (64%)	195 (100%)	0	100	100
5	R	262/462 (57%)	258 (98%)	4 (2%)	60	81
All	All	973/1436 (68%)	966 (99%)	7 (1%)	80	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	18	ILE
2	B	128	THR
2	B	222	PHE
5	R	149	VAL
5	R	215	THR
5	R	216	LEU
5	R	254	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	322	HIS
2	B	62	HIS
2	B	220	GLN
2	B	239	ASN
2	B	259	GLN
2	B	268	ASN
2	B	295	ASN
4	E	13	GLN
4	E	183	GLN
5	R	250	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)

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	CLR	R	601	-	31,31,31	0.88	2 (6%)	48,48,48	1.52	7 (14%)
6	CLR	R	602	-	31,31,31	0.85	2 (6%)	48,48,48	1.39	8 (16%)

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	-	-	9/10/68/68	0/4/4/4
6	CLR	R	602	-	-	9/10/68/68	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	CLR	C10-C9	-2.36	1.52	1.56
6	R	602	CLR	C10-C9	-2.35	1.52	1.56
6	R	601	CLR	C13-C14	-2.13	1.50	1.55
6	R	602	CLR	C13-C14	-2.01	1.51	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	601	CLR	C13-C17-C20	-4.20	112.91	119.49
6	R	601	CLR	C13-C14-C8	-4.07	108.35	114.38
6	R	602	CLR	C13-C17-C20	-3.46	114.06	119.49
6	R	602	CLR	C13-C14-C8	-3.38	109.37	114.38
6	R	601	CLR	C17-C13-C14	3.08	103.72	100.07
6	R	602	CLR	C4-C5-C10	3.01	120.42	116.42
6	R	602	CLR	C7-C8-C9	2.99	113.34	109.71
6	R	601	CLR	C4-C5-C10	2.86	120.22	116.42
6	R	601	CLR	C11-C12-C13	-2.62	108.29	112.78
6	R	601	CLR	C7-C8-C9	2.52	112.77	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	602	CLR	C17-C13-C14	2.32	102.82	100.07
6	R	601	CLR	C3-C4-C5	-2.19	108.31	112.03
6	R	602	CLR	C14-C8-C9	-2.07	106.32	109.09
6	R	602	CLR	C10-C5-C6	-2.03	119.80	122.90
6	R	602	CLR	C11-C12-C13	-2.02	109.32	112.78

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	602	CLR	C22-C23-C24-C25
6	R	601	CLR	C21-C20-C22-C23
6	R	602	CLR	C17-C20-C22-C23
6	R	602	CLR	C21-C20-C22-C23
6	R	601	CLR	C17-C20-C22-C23
6	R	601	CLR	C20-C22-C23-C24
6	R	602	CLR	C20-C22-C23-C24
6	R	602	CLR	C23-C24-C25-C27
6	R	601	CLR	C13-C17-C20-C22
6	R	602	CLR	C23-C24-C25-C26
6	R	601	CLR	C22-C23-C24-C25
6	R	601	CLR	C13-C17-C20-C21
6	R	601	CLR	C16-C17-C20-C21
6	R	601	CLR	C16-C17-C20-C22
6	R	602	CLR	C13-C17-C20-C21
6	R	602	CLR	C13-C17-C20-C22
6	R	601	CLR	C23-C24-C25-C27
6	R	602	CLR	C16-C17-C20-C22

There are no ring outliers.

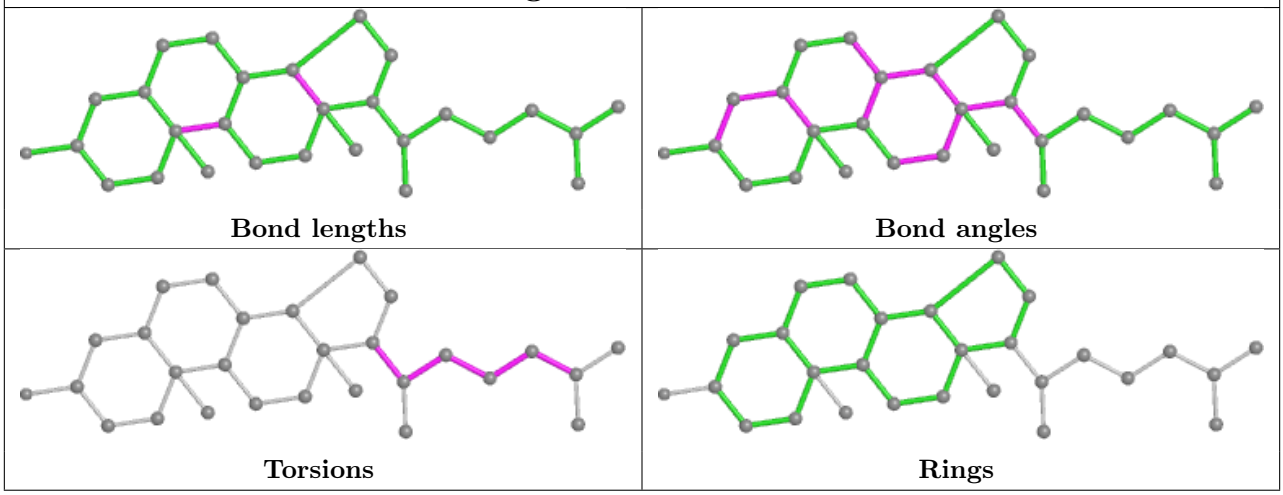
2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	601	CLR	11	0
6	R	602	CLR	8	0

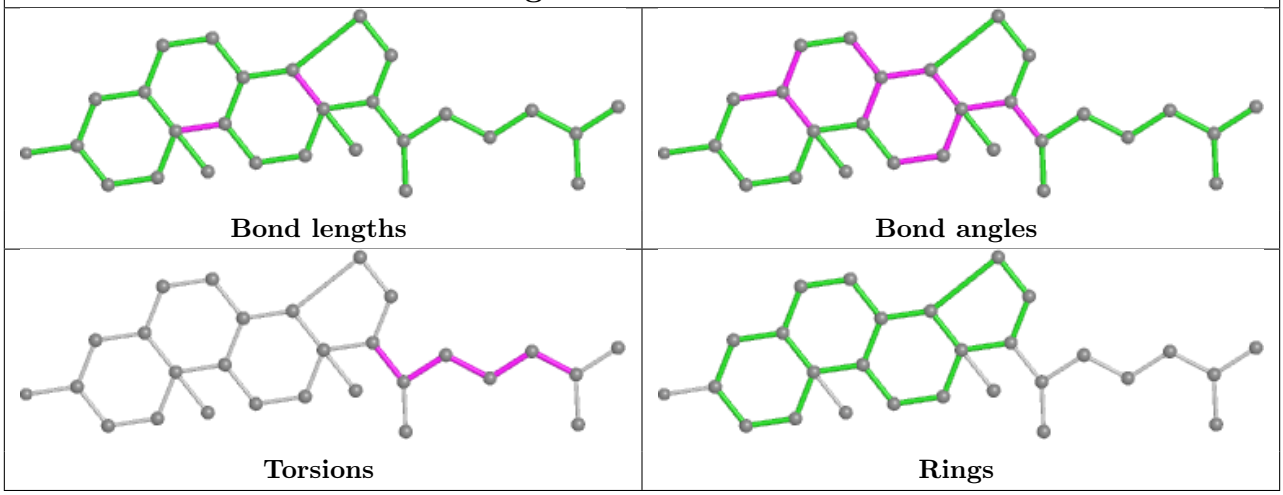
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 601



Ligand CLR R 602



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

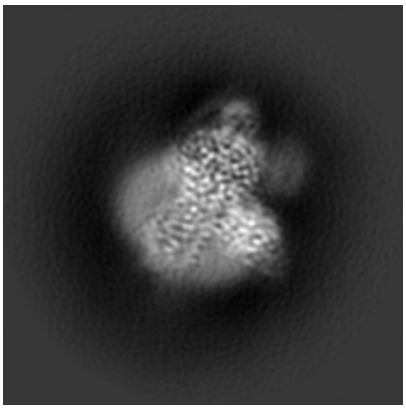
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38539. These allow visual inspection of the internal detail of the map and identification of artifacts.

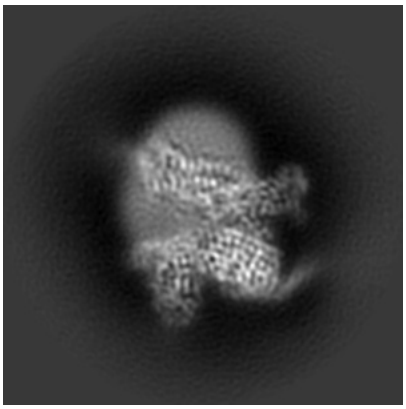
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

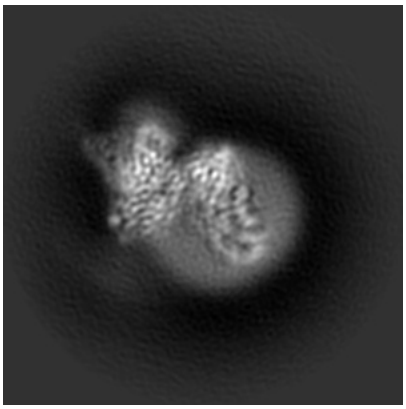
6.1.1 Primary map



X

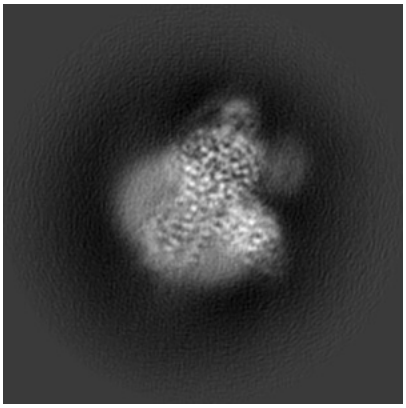


Y

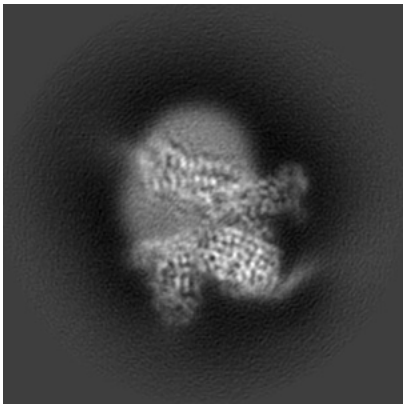


Z

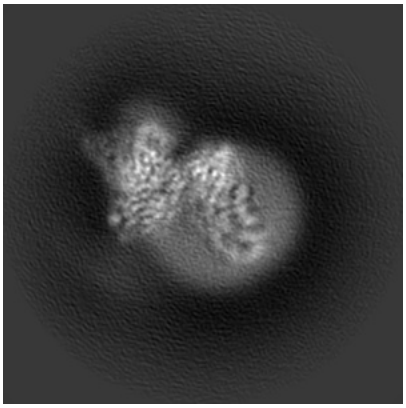
6.1.2 Raw map



X



Y

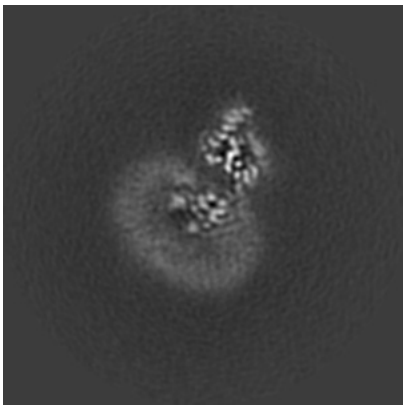


Z

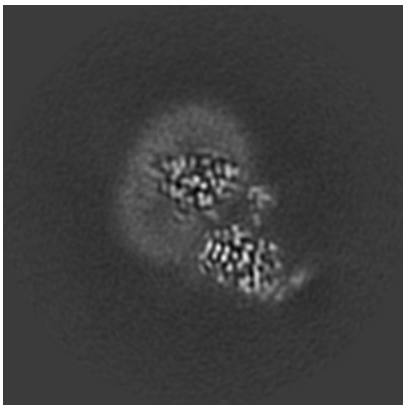
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

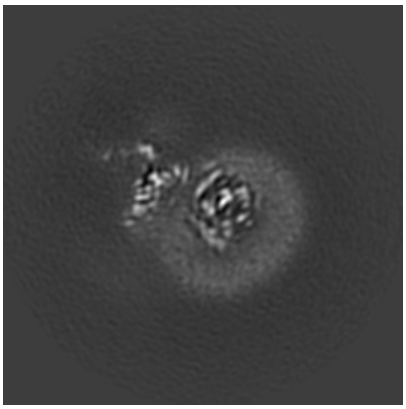
6.2.1 Primary map



X Index: 100

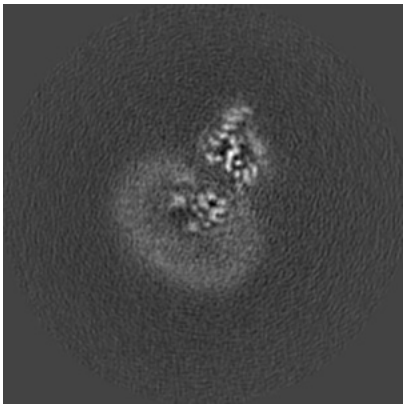


Y Index: 100

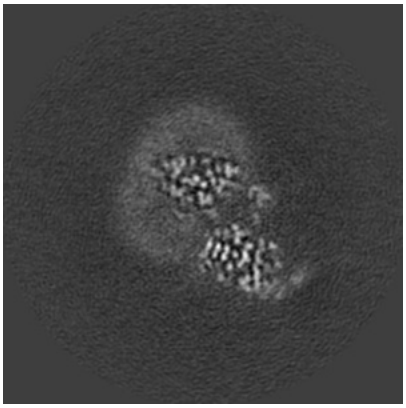


Z Index: 100

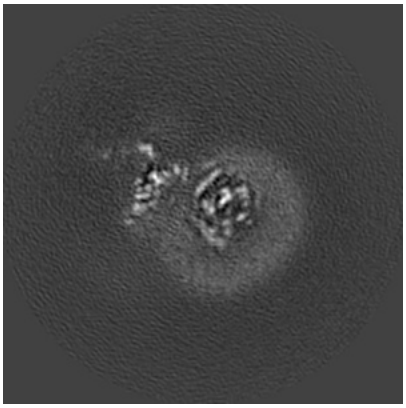
6.2.2 Raw map



X Index: 100



Y Index: 100

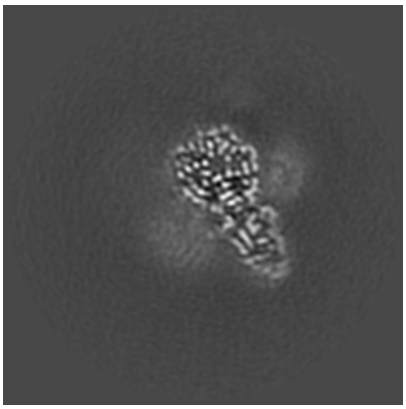


Z Index: 100

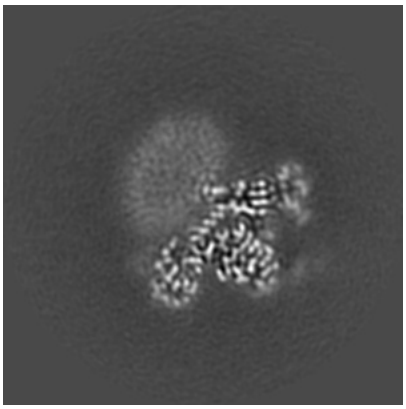
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

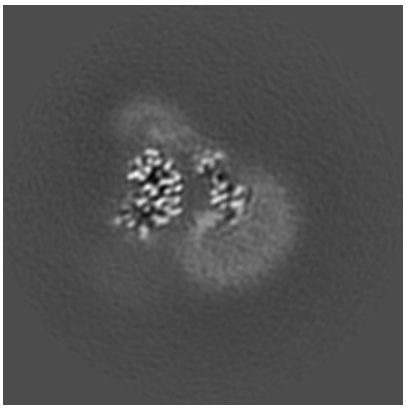
6.3.1 Primary map



X Index: 75

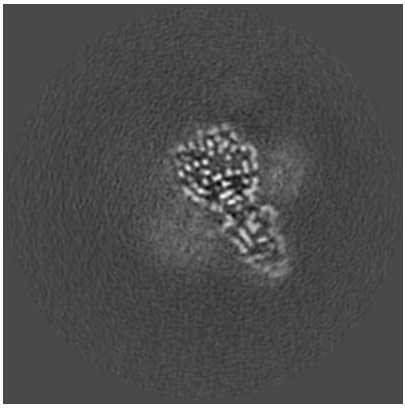


Y Index: 116

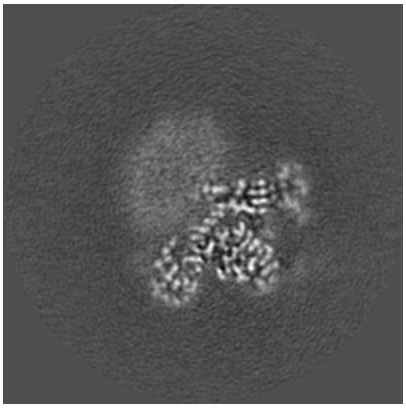


Z Index: 112

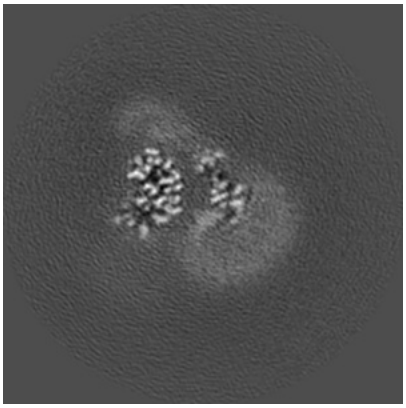
6.3.2 Raw map



X Index: 75



Y Index: 116

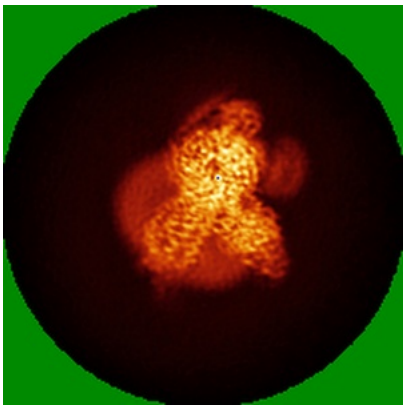


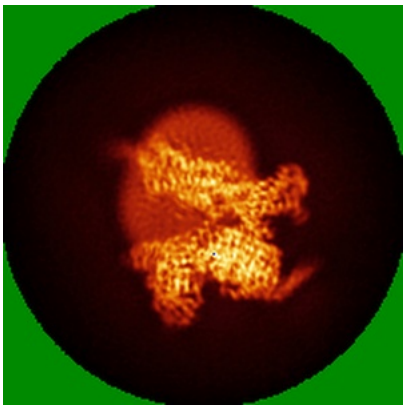
Z Index: 112

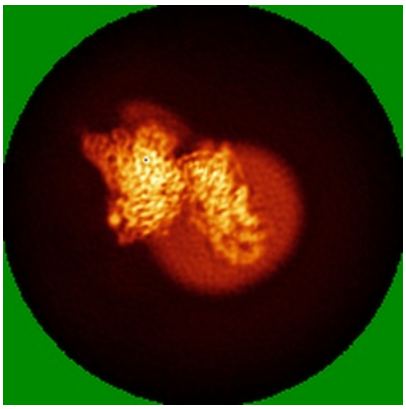
The images above show the largest variance slices of the map in three orthogonal directions.

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

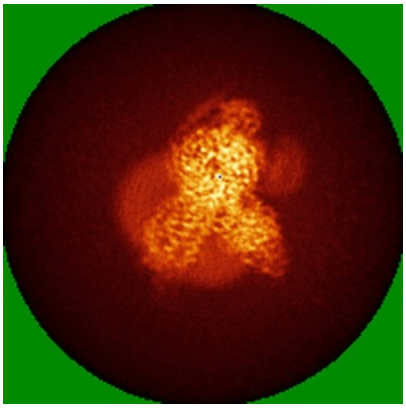
6.4.1 Primary map

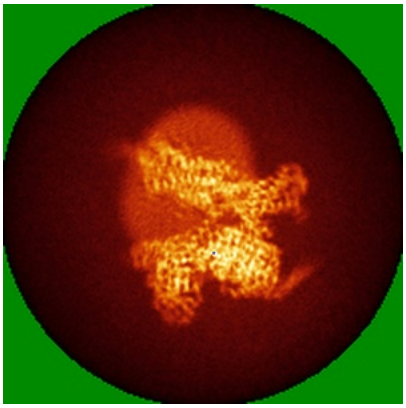

X

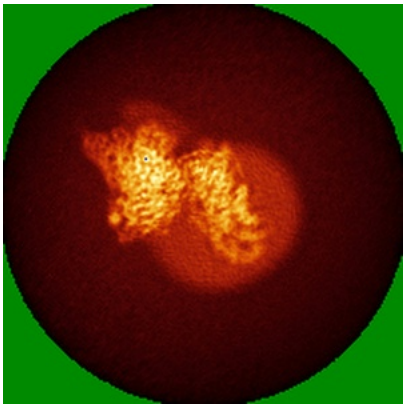

Y


Z

6.4.2 Raw map


X


Y

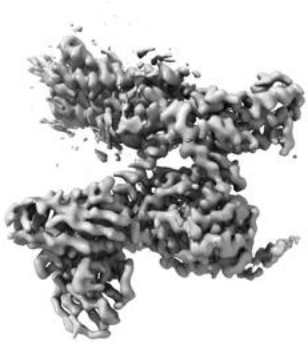

Z

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.

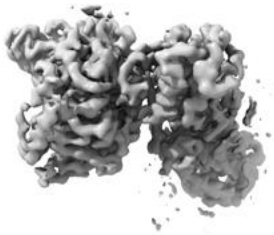
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y



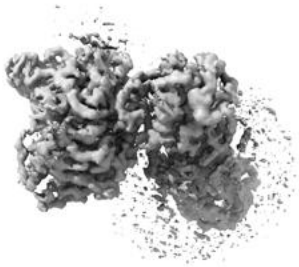
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0207. 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.

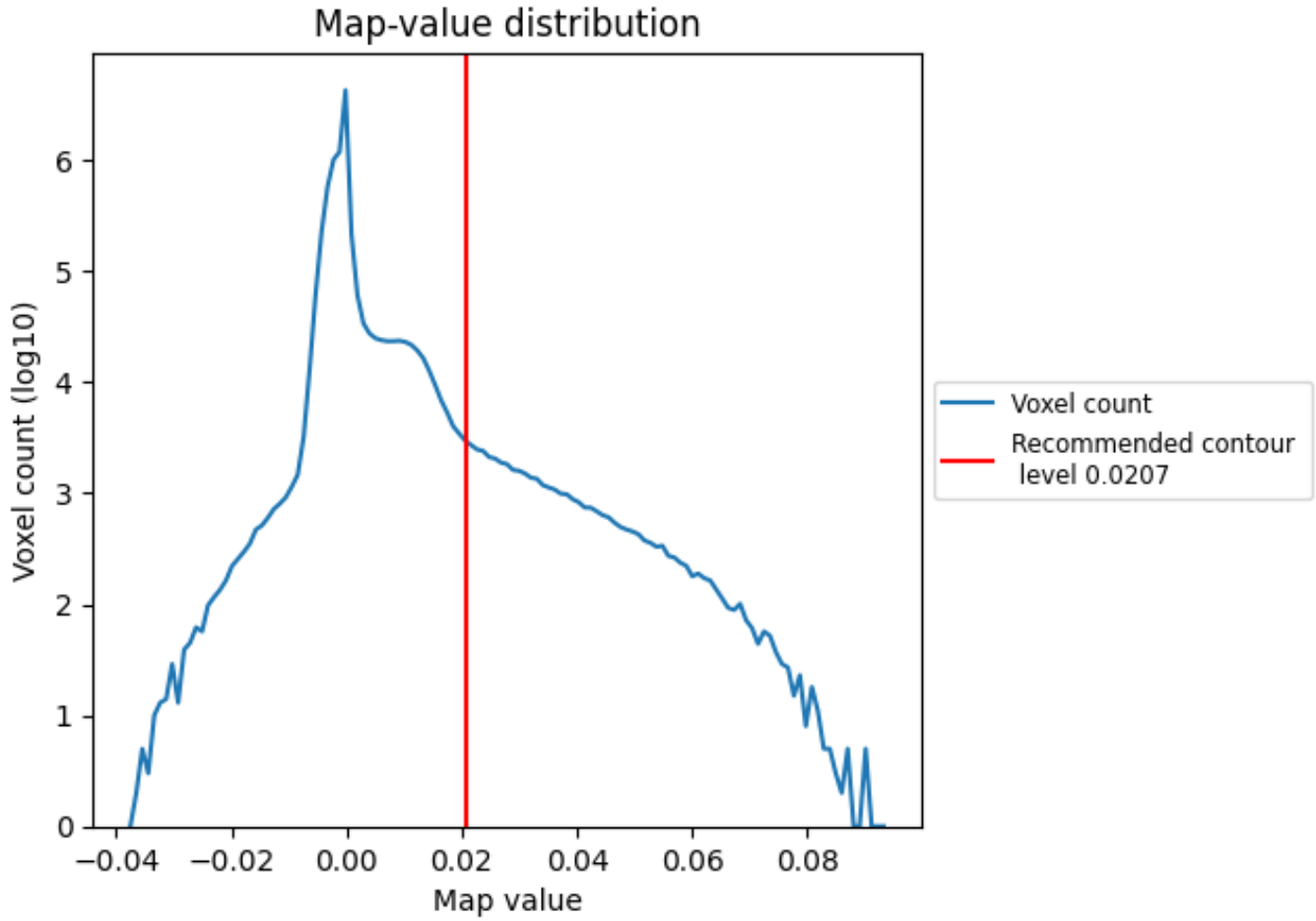
6.6 Mask visualisation (i)

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

7 Map analysis

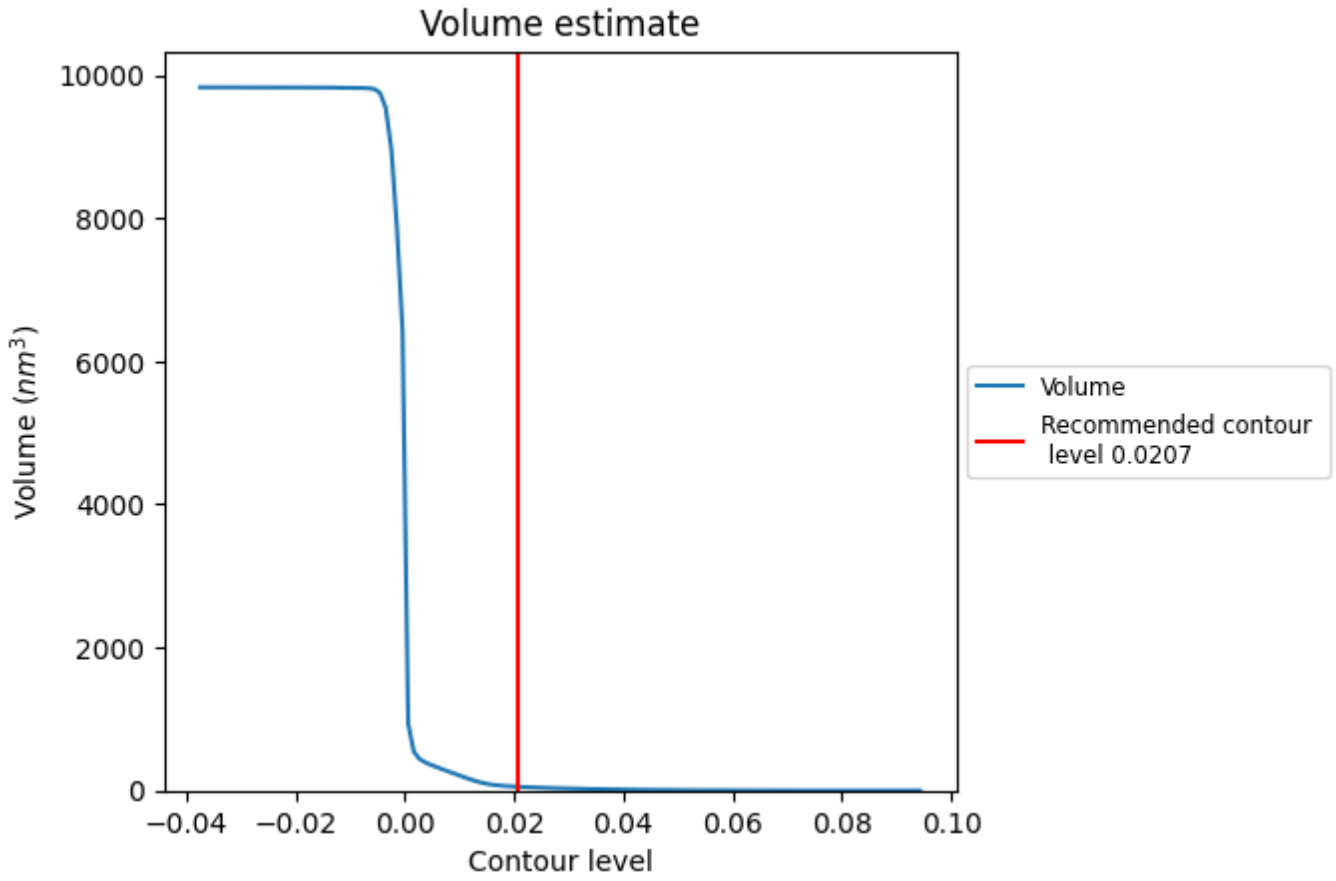
This section contains the results of statistical analysis of the map.

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.

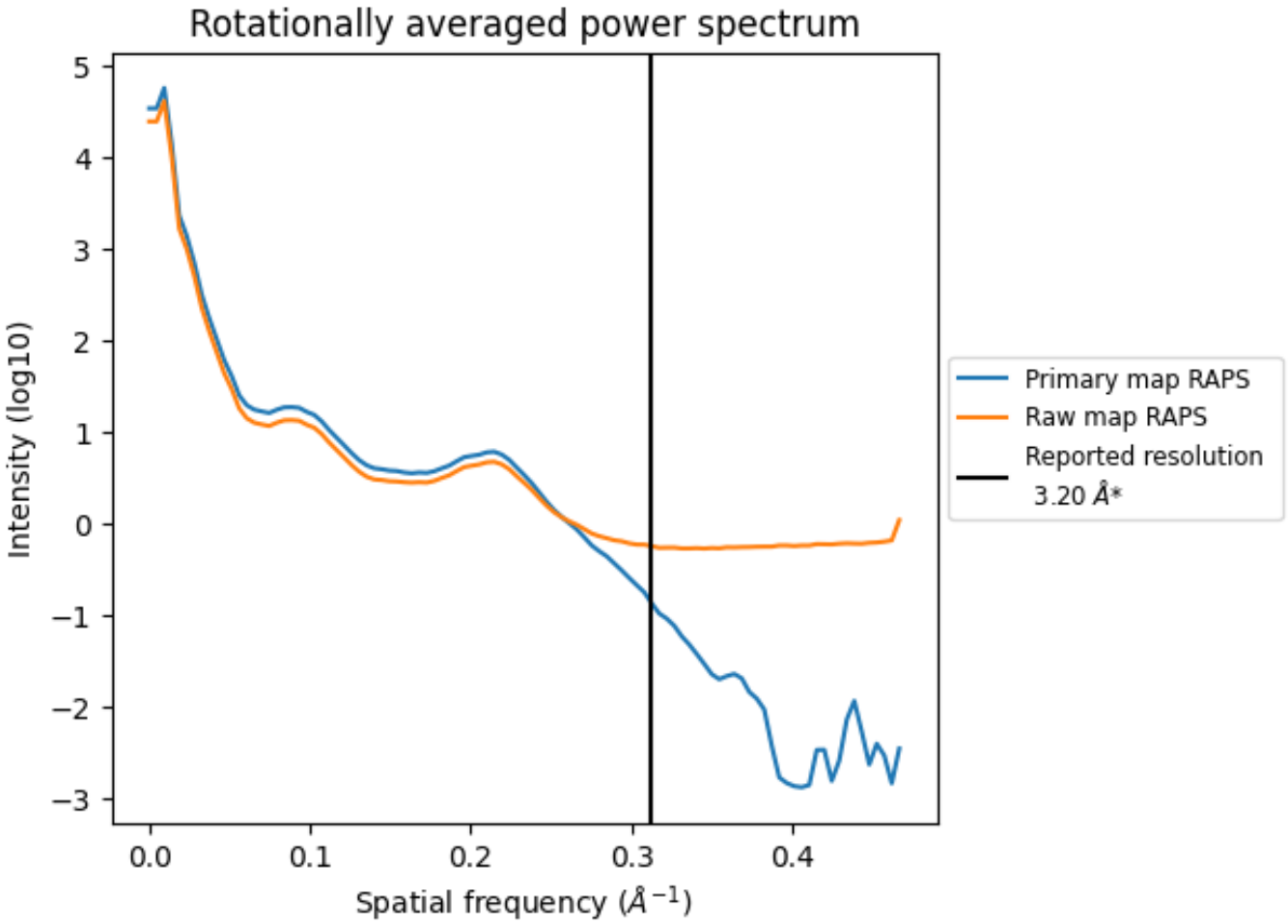
7.2 Volume estimate (i)



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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)

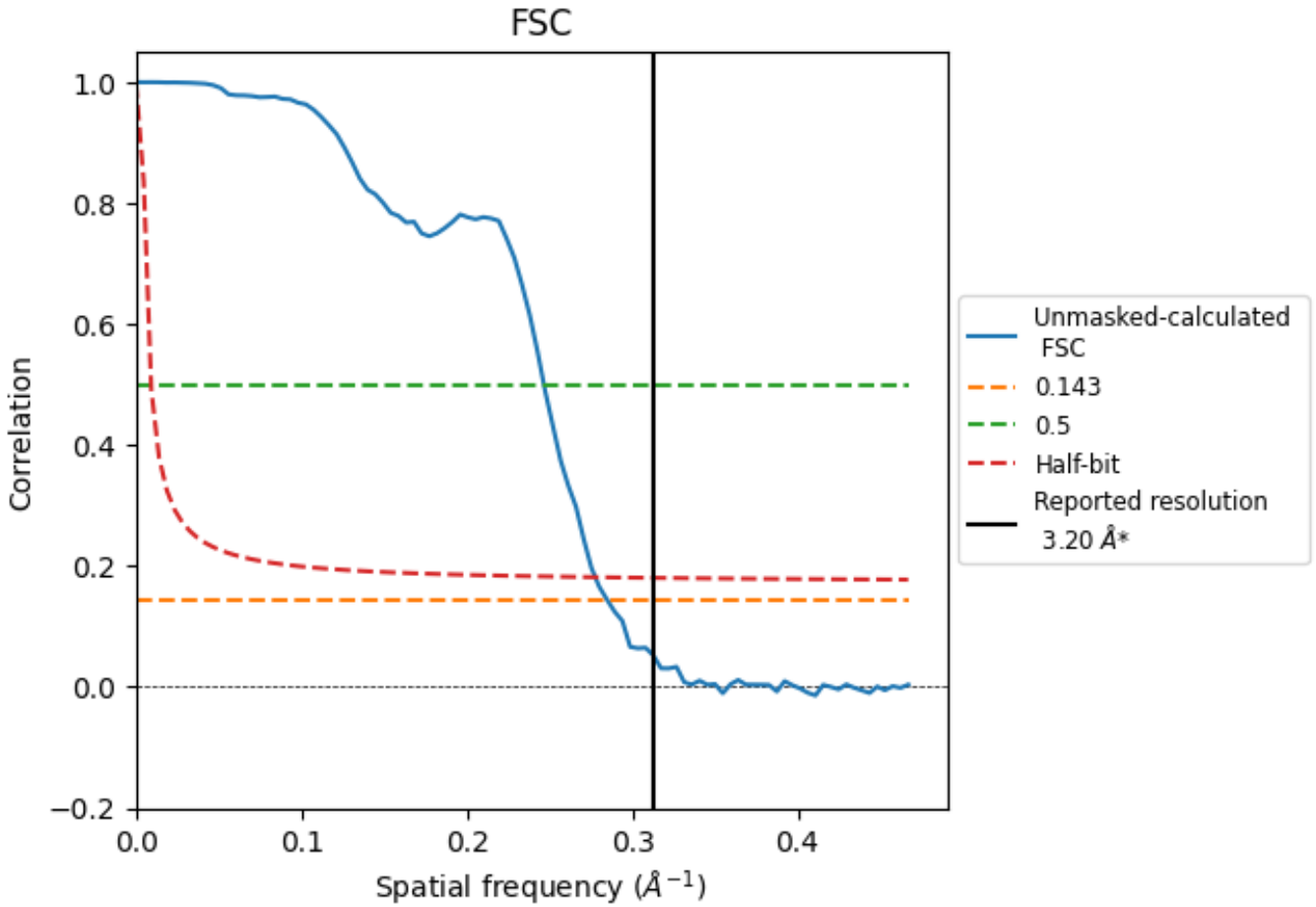


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

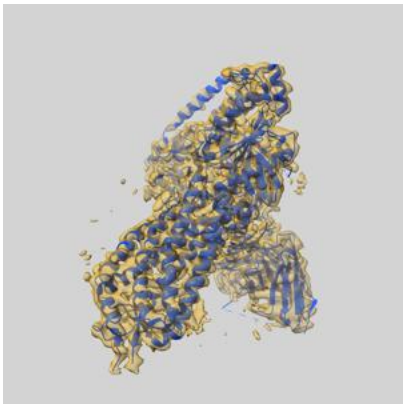
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.05	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

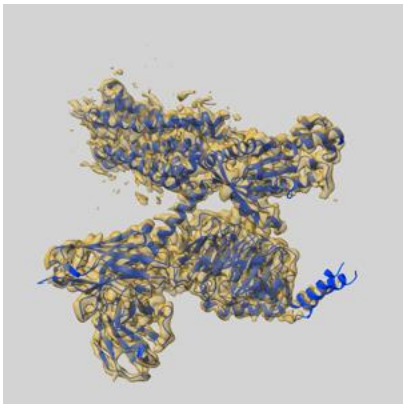
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38539 and PDB model 8XOS. Per-residue inclusion information can be found in section 3 on page 10.

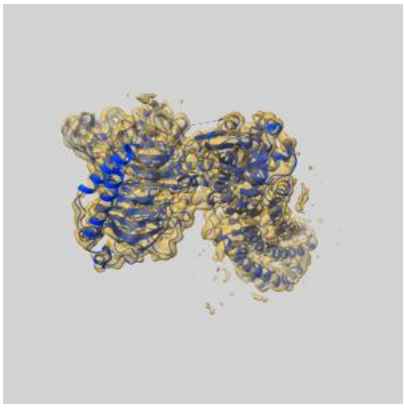
9.1 Map-model overlay



X



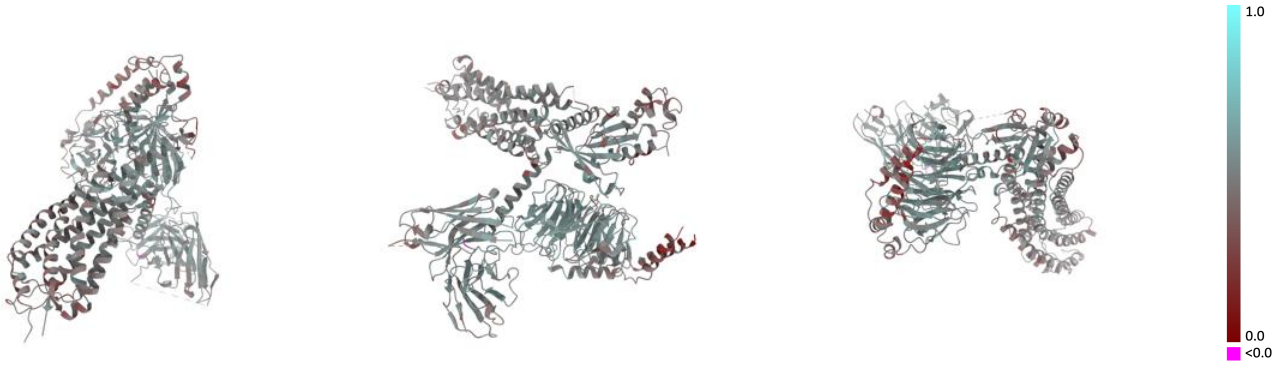
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0207 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.

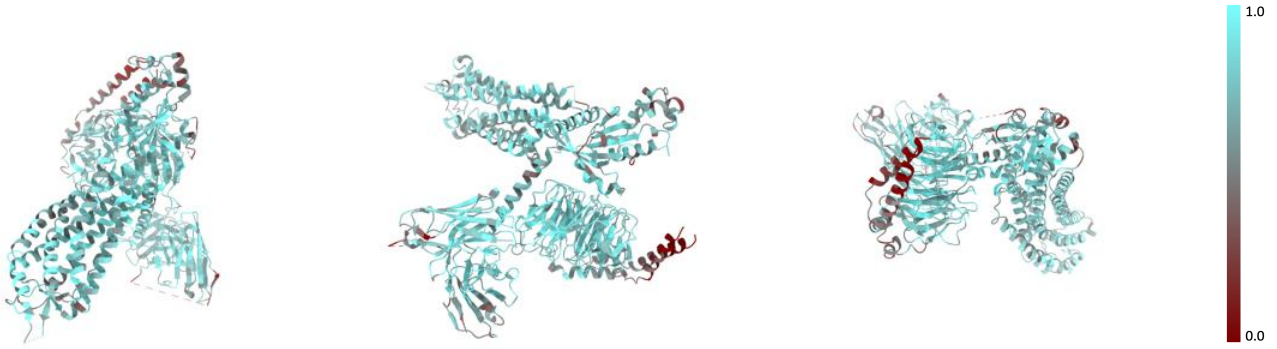
9.2 Q-score mapped to coordinate model (i)



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.

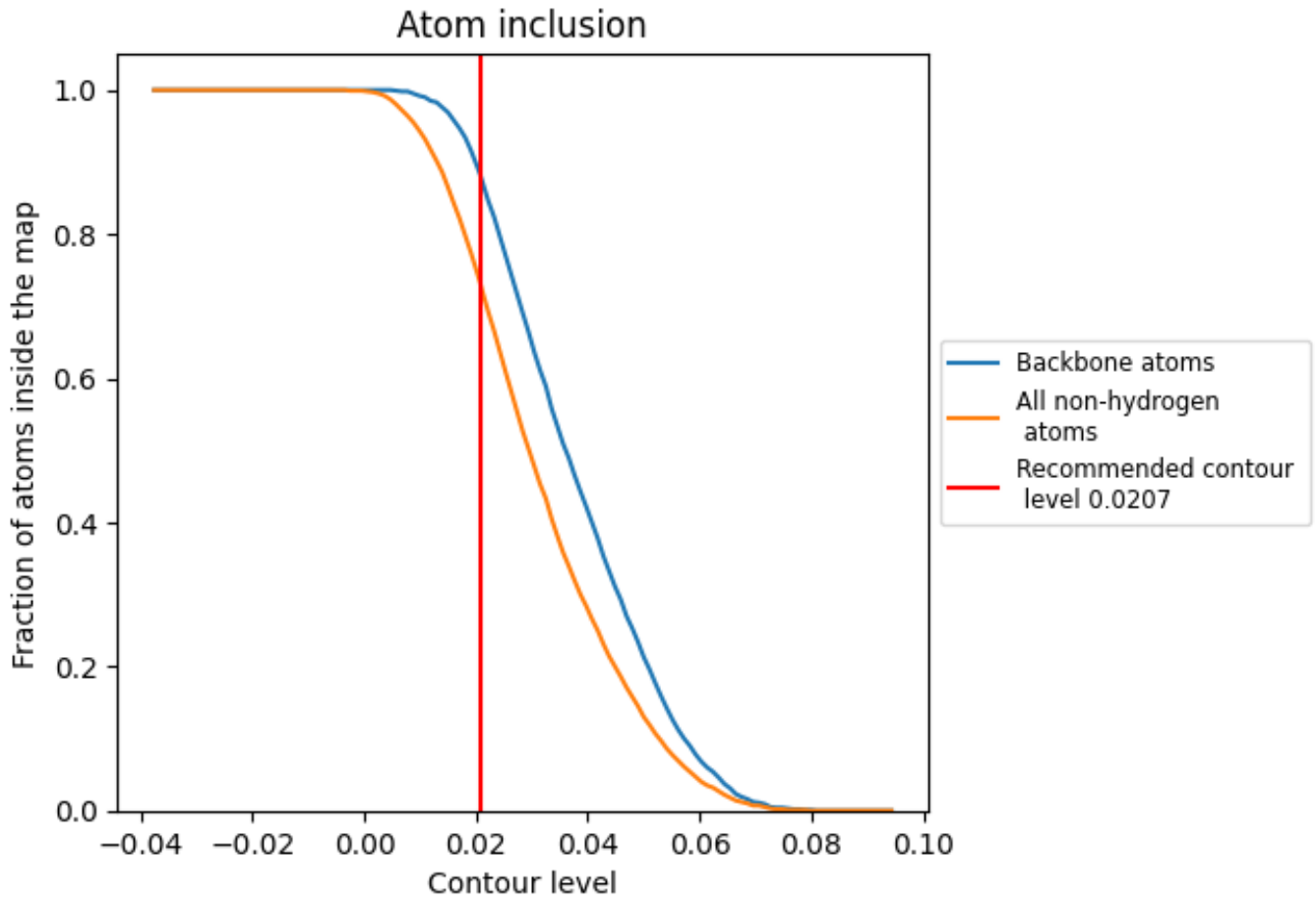
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0207).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 73% 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 (0.0207) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.4800
A	0.7190	0.4790
B	0.7610	0.5030
C	0.5060	0.4230
E	0.7570	0.4990
R	0.7380	0.4520