Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 07:56 AM EST

PDB ID	:	7MTB
EMDB ID	:	EMD-23980
Title	:	Rhodopsin kinase (GRK1)-S5E/S488E/T489E in complex with rhodopsin and Fab6
Authors	:	Chen, Q.; Chen, C.-L.; Tesmer, J.J.G.
Deposited on	:	2021-05-13
Resolution	:	4.00 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:

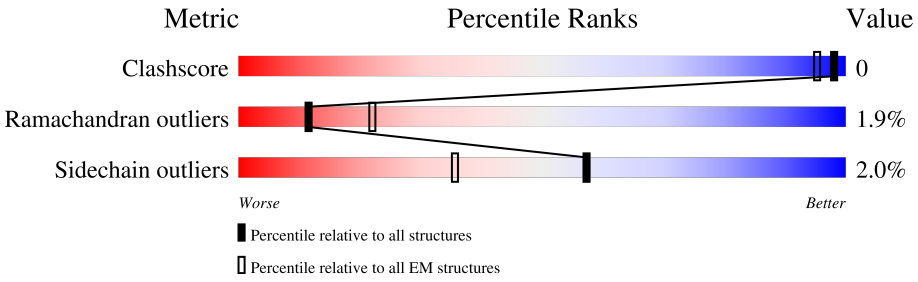
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1-G	543	16% 62% · 36%
1	2-G	543	61% · 36%
1	3-G	543	61% · 36%
1	4-G	543	61% · 36%
1	5-G	543	60% · 36%
1	6-G	543	61% · 36%
2	1-H	234	8% 92% · ·
2	2-H	234	91% · ·

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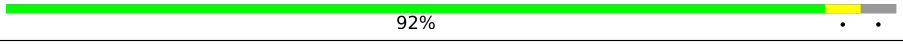
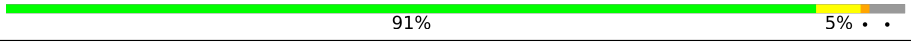
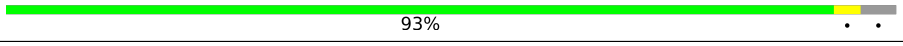
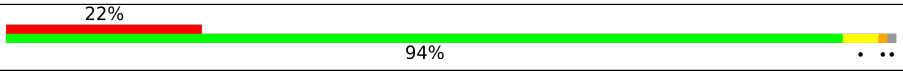
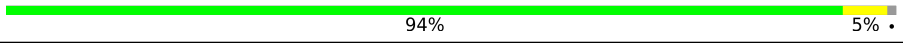
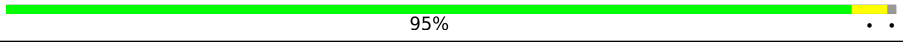
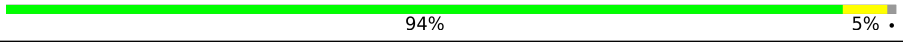
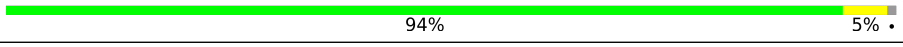
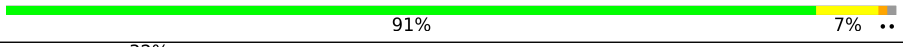
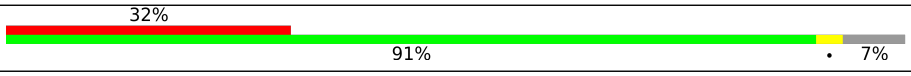
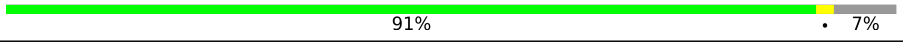
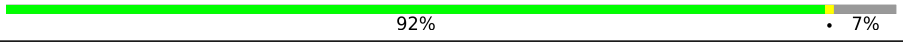
Mol	Chain	Length	Quality of chain
2	3-H	234	
2	4-H	234	
2	5-H	234	
2	6-H	234	
3	1-L	216	
3	2-L	216	
3	3-L	216	
3	4-L	216	
3	5-L	216	
3	6-L	216	
4	1-R	348	
4	2-R	348	
4	3-R	348	
4	4-R	348	
4	5-R	348	
4	6-R	348	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 52240 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 Rhodopsin kinase GRK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-G	346	Total	C	N	O	S	0	0
			2746	1756	470	507	13		
1	2-G	346	Total	C	N	O	S	0	0
			2745	1756	469	507	13		
1	3-G	346	Total	C	N	O	S	0	0
			2745	1756	469	507	13		
1	4-G	346	Total	C	N	O	S	0	0
			2746	1756	470	507	13		
1	5-G	346	Total	C	N	O	S	0	0
			2746	1756	470	507	13		
1	6-G	346	Total	C	N	O	S	0	0
			2746	1756	470	507	13		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	GLU	SER	engineered mutation	UNP P28327
G	488	GLU	SER	engineered mutation	UNP P28327
G	489	GLU	THR	engineered mutation	UNP P28327
G	536	VAL	-	expression tag	UNP P28327
G	537	ASP	-	expression tag	UNP P28327
G	538	HIS	-	expression tag	UNP P28327
G	539	HIS	-	expression tag	UNP P28327
G	540	HIS	-	expression tag	UNP P28327
G	541	HIS	-	expression tag	UNP P28327
G	542	HIS	-	expression tag	UNP P28327
G	543	HIS	-	expression tag	UNP P28327

- Molecule 2 is a protein called Fab6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-H	225	Total	C	N	O	S	0	0
			1704	1081	284	334	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2-H	225	Total	C	N	O	S	0	0
			1704	1081	284	334	5		
2	3-H	225	Total	C	N	O	S	0	0
			1704	1081	284	334	5		
2	4-H	225	Total	C	N	O	S	0	0
			1704	1081	284	334	5		
2	5-H	225	Total	C	N	O	S	0	0
			1704	1081	284	334	5		
2	6-H	225	Total	C	N	O	S	0	0
			1704	1081	284	334	5		

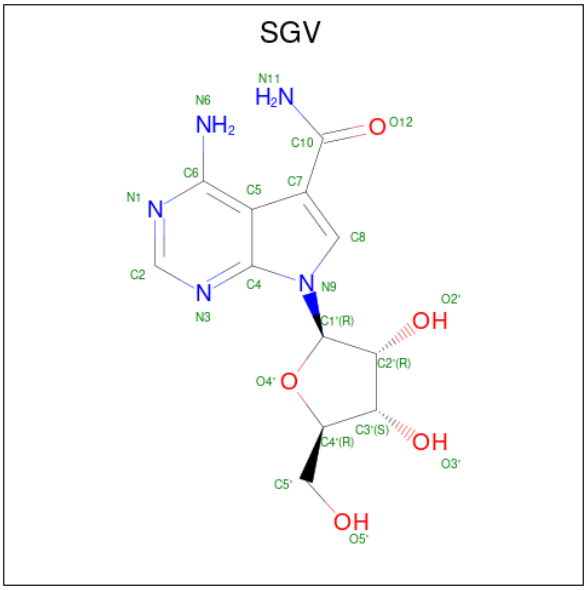
- Molecule 3 is a protein called Fab6 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-L	214	Total	C	N	O	S	0	0
			1640	1027	275	333	5		
3	2-L	214	Total	C	N	O	S	0	0
			1640	1027	275	333	5		
3	3-L	214	Total	C	N	O	S	0	0
			1640	1027	275	333	5		
3	4-L	214	Total	C	N	O	S	0	0
			1640	1027	275	333	5		
3	5-L	214	Total	C	N	O	S	0	0
			1640	1027	275	333	5		
3	6-L	214	Total	C	N	O	S	0	0
			1640	1027	275	333	5		

- Molecule 4 is a protein called Rhodopsin.

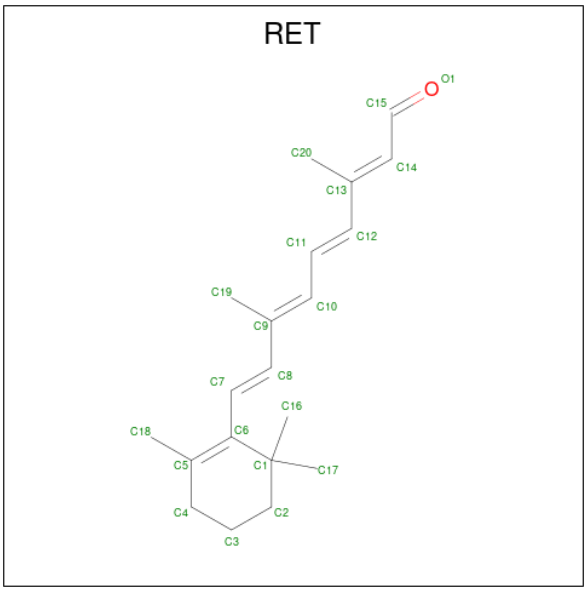
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	2-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	3-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	4-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	5-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	6-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		

- Molecule 5 is SANGIVAMYCIN (three-letter code: SGV) (formula: $C_{12}H_{15}N_5O_5$).



Mol	Chain	Residues	Atoms				AltConf
5	1-G	1	Total	C	N	O	0
			22	12	5	5	
5	2-G	1	Total	C	N	O	0
			22	12	5	5	
5	3-G	1	Total	C	N	O	0
			22	12	5	5	
5	4-G	1	Total	C	N	O	0
			22	12	5	5	
5	5-G	1	Total	C	N	O	0
			22	12	5	5	
5	6-G	1	Total	C	N	O	0
			22	12	5	5	

- Molecule 6 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



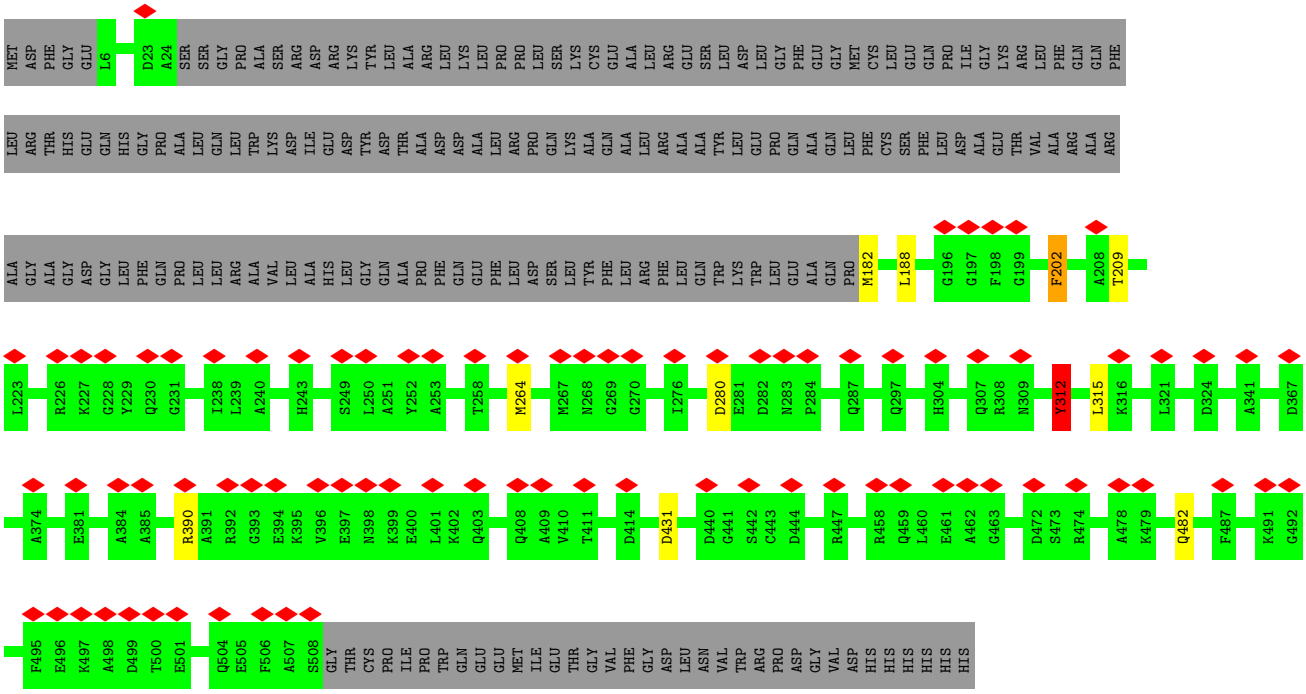
Mol	Chain	Residues	Atoms	AltConf
6	1-R	1	Total C 20 20	0
6	2-R	1	Total C 20 20	0
6	3-R	1	Total C 20 20	0
6	4-R	1	Total C 20 20	0
6	5-R	1	Total C 20 20	0
6	6-R	1	Total C 20 20	0

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.

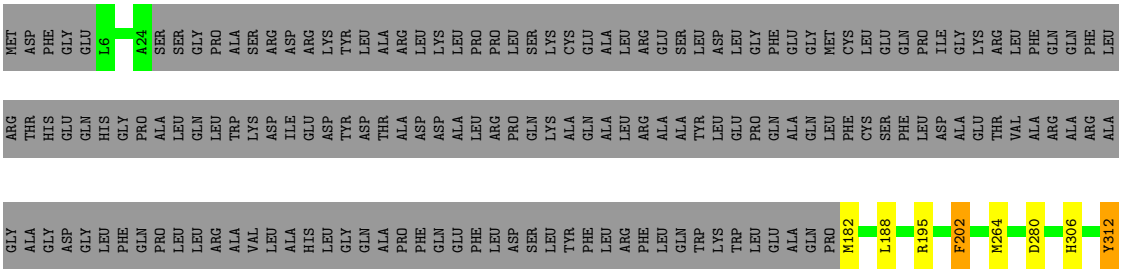
• Molecule 1: Rhodopsin kinase GRK1

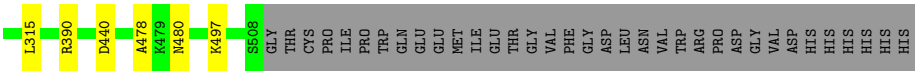
Chain 1-G:



• Molecule 1: Rhodopsin kinase GRK1

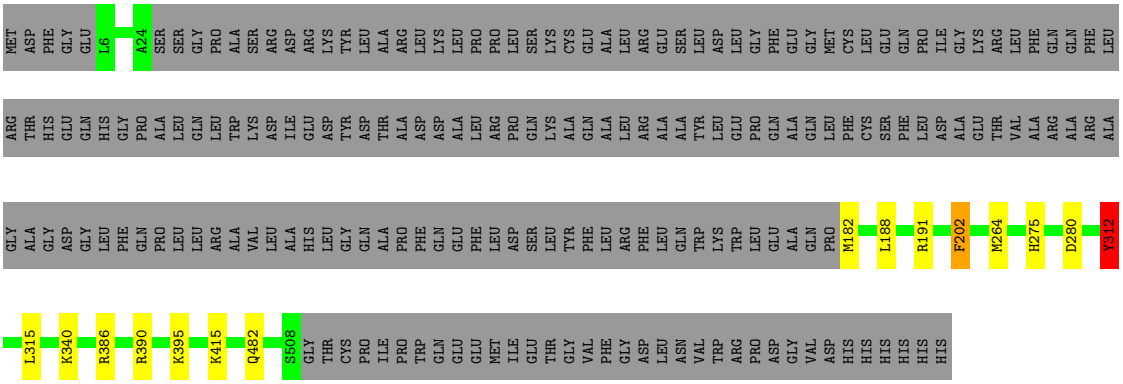
Chain 2-G:





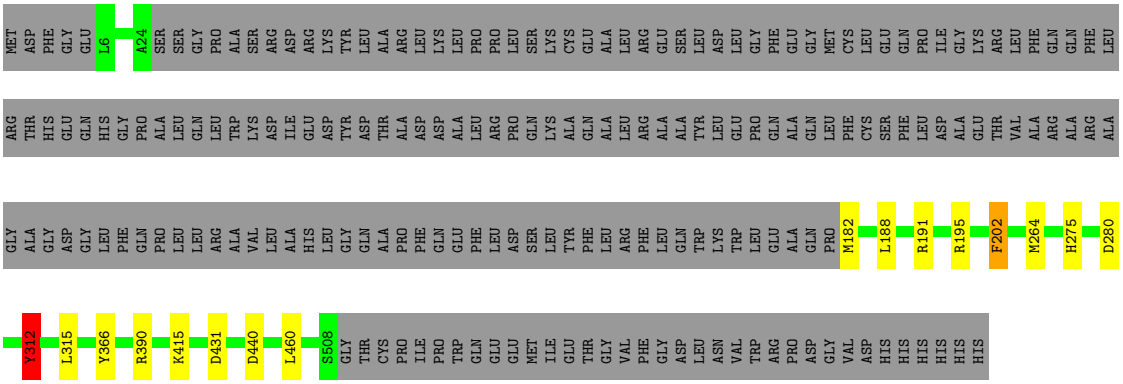
• Molecule 1: Rhodopsin kinase GRK1

Chain 3-G:



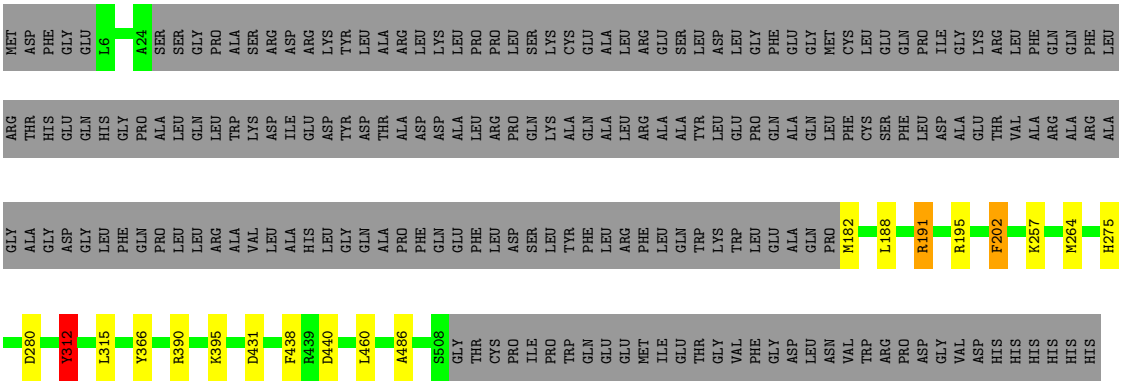
• Molecule 1: Rhodopsin kinase GRK1

Chain 4-G:



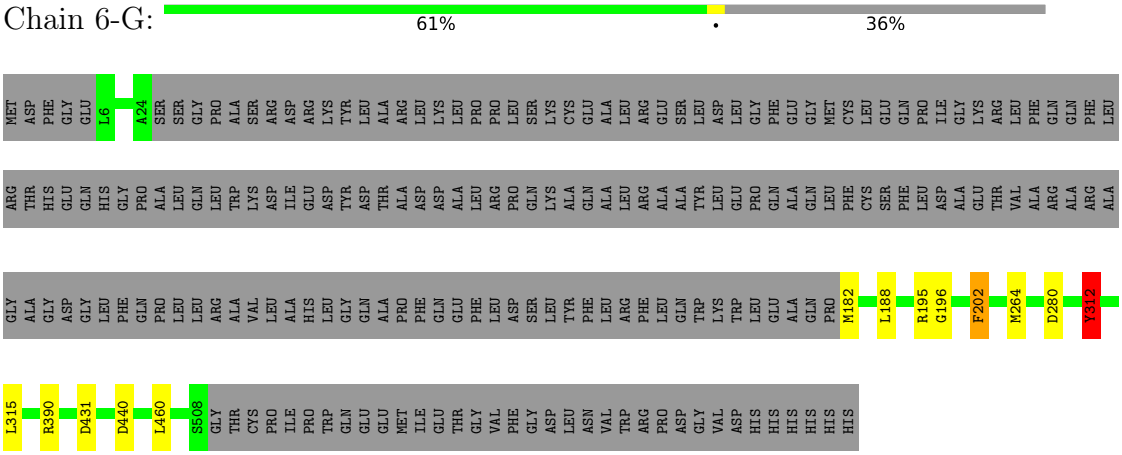
• Molecule 1: Rhodopsin kinase GRK1

Chain 5-G:



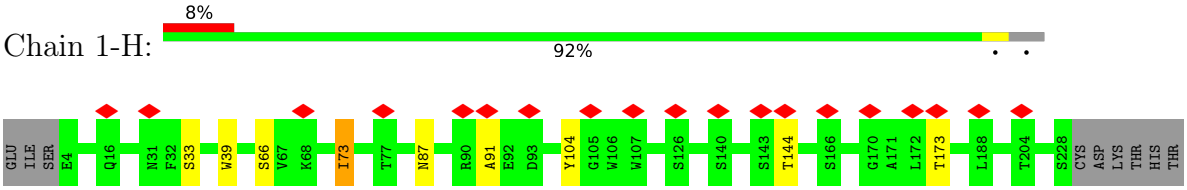
• Molecule 1: Rhodopsin kinase GRK1

Chain 6-G:



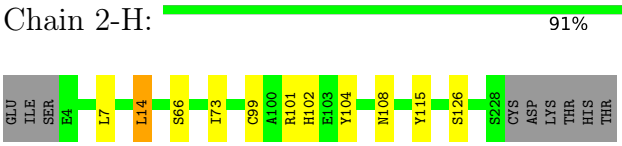
• Molecule 2: Fab6 heavy chain

Chain 1-H:



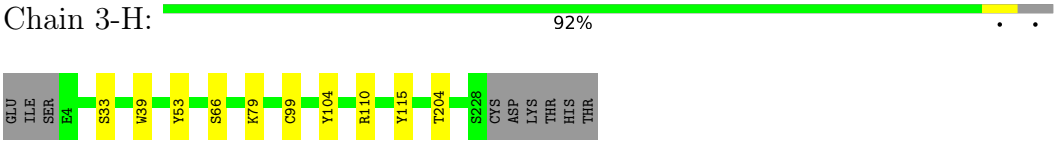
• Molecule 2: Fab6 heavy chain

Chain 2-H:



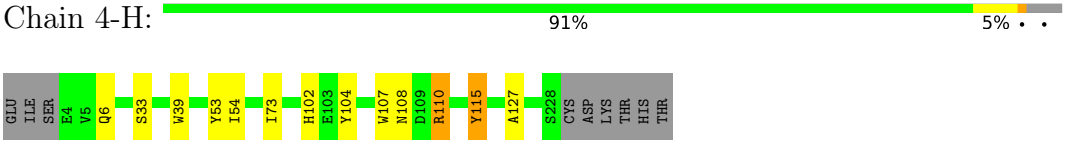
• Molecule 2: Fab6 heavy chain

Chain 3-H:



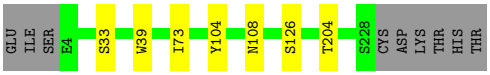
• Molecule 2: Fab6 heavy chain

Chain 4-H:

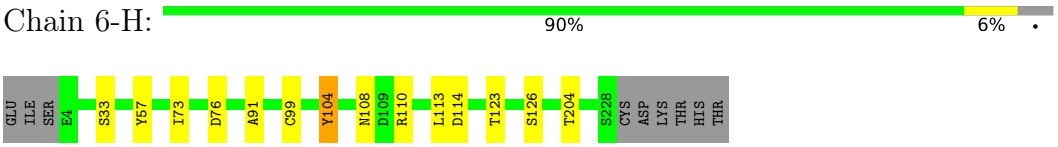


• Molecule 2: Fab6 heavy chain

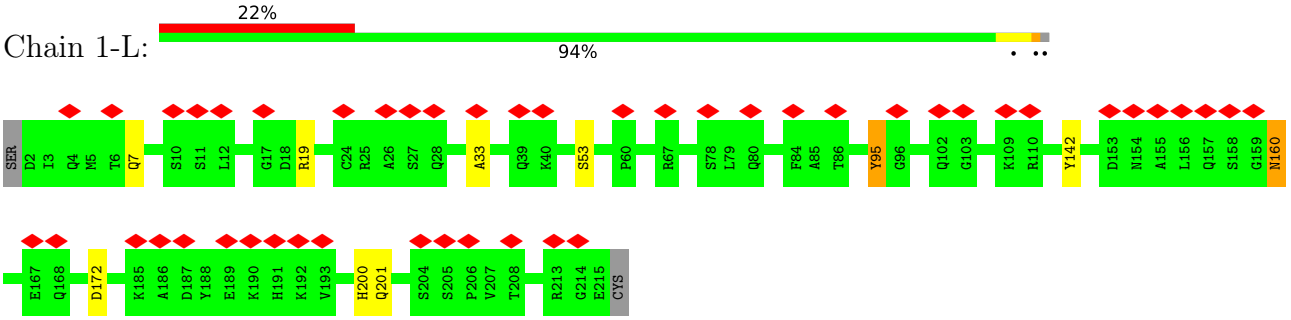
Chain 5-H:



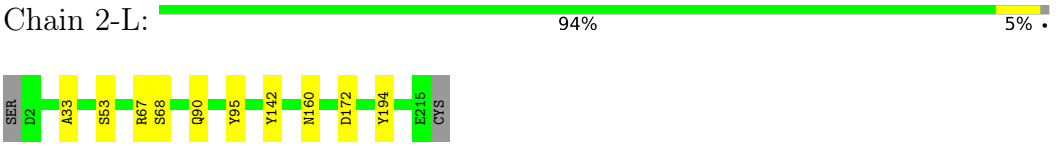
• Molecule 2: Fab6 heavy chain



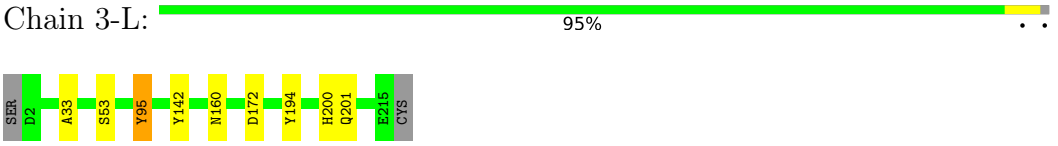
• Molecule 3: Fab6 light chain



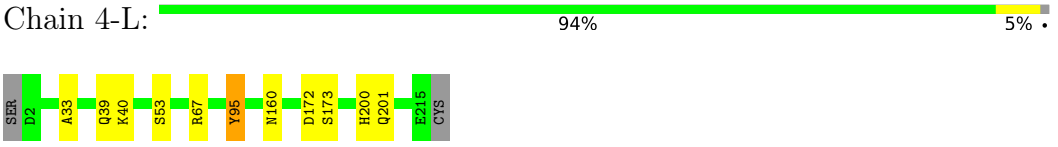
• Molecule 3: Fab6 light chain



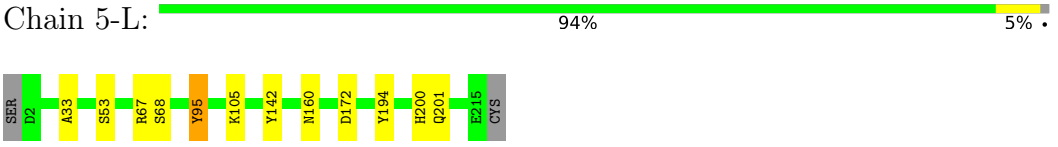
• Molecule 3: Fab6 light chain



• Molecule 3: Fab6 light chain

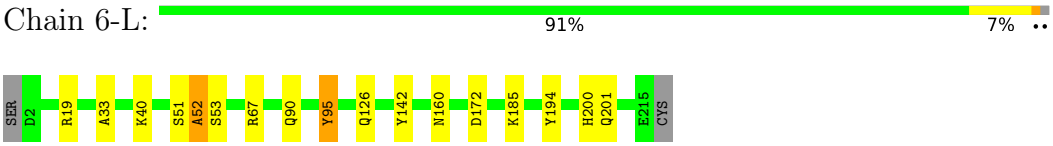


• Molecule 3: Fab6 light chain



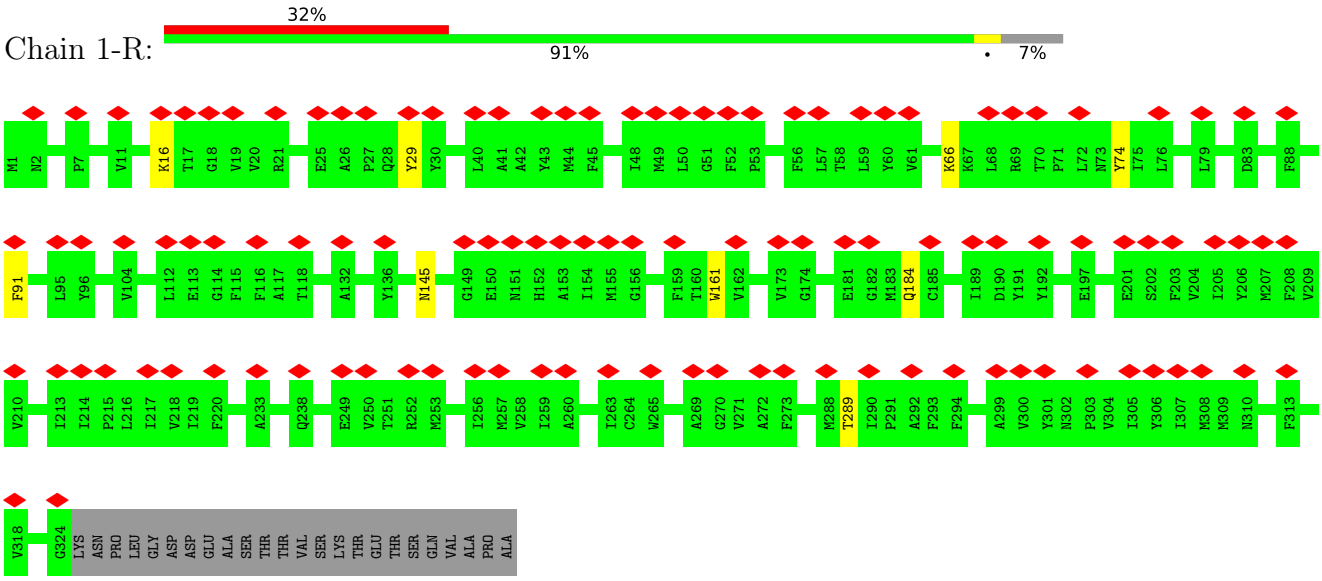
• Molecule 3: Fab6 light chain

Chain 6-L:



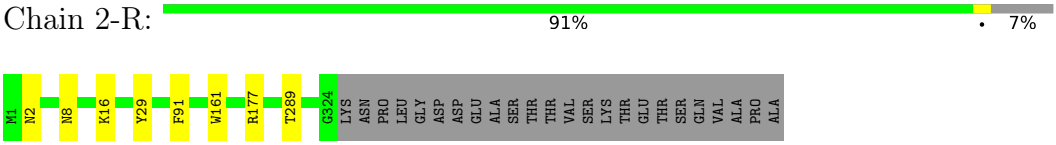
• Molecule 4: Rhodopsin

Chain 1-R:



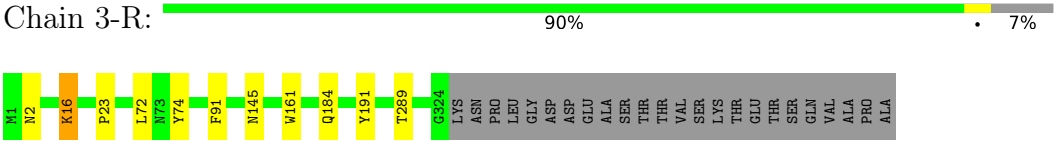
• Molecule 4: Rhodopsin

Chain 2-R:



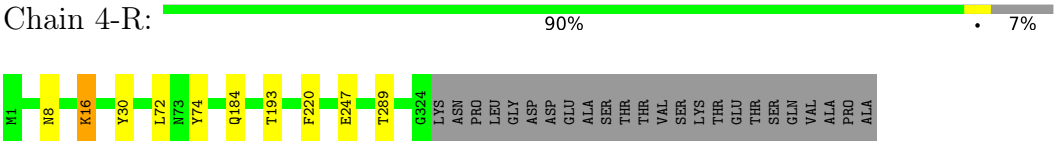
• Molecule 4: Rhodopsin

Chain 3-R:



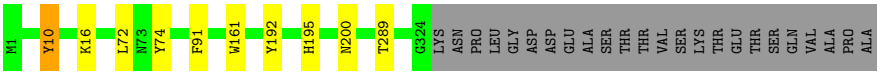
• Molecule 4: Rhodopsin

Chain 4-R:



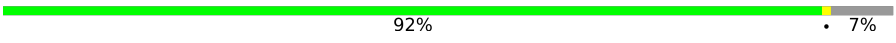
• Molecule 4: Rhodopsin

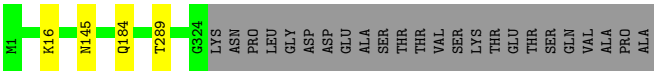
Chain 5-R:



• Molecule 4: Rhodopsin

Chain 6-R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250547	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.220	Depositor
Minimum map value	-2.412	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, SGV

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	1-G	0.92	0/2803	1.00	4/3771 (0.1%)
1	2-G	0.92	0/2802	1.00	4/3769 (0.1%)
1	3-G	0.91	0/2802	1.01	4/3769 (0.1%)
1	4-G	0.92	0/2803	1.00	4/3771 (0.1%)
1	5-G	0.91	0/2803	1.00	4/3771 (0.1%)
1	6-G	0.92	0/2803	1.00	4/3771 (0.1%)
2	1-H	0.91	0/1752	1.02	2/2391 (0.1%)
2	2-H	0.91	0/1752	1.03	2/2391 (0.1%)
2	3-H	0.92	0/1752	1.00	2/2391 (0.1%)
2	4-H	0.91	0/1752	1.03	1/2391 (0.0%)
2	5-H	0.92	0/1752	1.01	2/2391 (0.1%)
2	6-H	0.91	0/1752	1.01	2/2391 (0.1%)
3	1-L	0.91	0/1677	1.01	0/2277
3	2-L	0.91	0/1677	1.02	0/2277
3	3-L	0.91	0/1677	1.00	0/2277
3	4-L	0.91	0/1677	1.01	0/2277
3	5-L	0.91	0/1677	1.01	0/2277
3	6-L	0.91	0/1677	1.02	1/2277 (0.0%)
4	1-R	0.87	0/2657	0.91	3/3621 (0.1%)
4	2-R	0.87	0/2657	0.90	1/3621 (0.0%)
4	3-R	0.87	0/2657	0.90	3/3621 (0.1%)
4	4-R	0.87	0/2657	0.92	3/3621 (0.1%)
4	5-R	0.87	0/2657	0.91	6/3621 (0.2%)
4	6-R	0.87	0/2657	0.88	0/3621
All	All	0.90	0/53332	0.98	52/72356 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-G	0	2
1	2-G	0	1
1	3-G	0	3
1	4-G	0	3
1	5-G	0	4
1	6-G	0	2
2	4-H	0	1
2	6-H	0	1
3	1-L	0	1
3	2-L	0	2
3	3-L	0	2
3	5-L	0	2
3	6-L	0	2
All	All	0	26

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-G	312	TYR	CB-CG-CD2	-8.14	116.11	121.00
1	6-G	312	TYR	CB-CG-CD2	-8.11	116.14	121.00
1	3-G	312	TYR	CB-CG-CD2	-7.99	116.20	121.00
1	4-G	312	TYR	CB-CG-CD2	-7.89	116.27	121.00
1	3-G	312	TYR	CB-CG-CD1	7.79	125.67	121.00
1	2-G	312	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	6-G	312	TYR	CB-CG-CD1	7.73	125.64	121.00
1	1-G	312	TYR	CB-CG-CD1	7.66	125.60	121.00
1	4-G	312	TYR	CB-CG-CD1	7.63	125.58	121.00
1	2-G	312	TYR	CB-CG-CD1	7.40	125.44	121.00
1	3-G	202	PHE	CB-CG-CD1	7.26	125.88	120.80
1	6-G	202	PHE	CB-CG-CD1	6.96	125.67	120.80
1	1-G	202	PHE	CB-CG-CD1	6.96	125.67	120.80
1	5-G	202	PHE	CB-CG-CD1	6.84	125.59	120.80
1	4-G	202	PHE	CB-CG-CD1	6.72	125.51	120.80
1	5-G	312	TYR	CB-CG-CD2	-6.62	117.03	121.00
2	6-H	104	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	3-G	202	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	2-G	202	PHE	CB-CG-CD1	6.46	125.32	120.80
1	1-G	202	PHE	CB-CG-CD2	-6.42	116.30	120.80
1	5-G	312	TYR	CB-CG-CD1	6.42	124.85	121.00
2	3-H	104	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	6-G	202	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	5-G	202	PHE	CB-CG-CD2	-6.20	116.46	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	4-G	202	PHE	CB-CG-CD2	-6.15	116.50	120.80
2	6-H	104	TYR	CB-CG-CD2	5.94	124.57	121.00
1	2-G	202	PHE	CB-CG-CD2	-5.91	116.66	120.80
3	6-L	52	ALA	N-CA-CB	5.87	118.32	110.10
2	2-H	104	TYR	CB-CG-CD1	-5.70	117.58	121.00
2	3-H	104	TYR	CB-CG-CD2	5.68	124.41	121.00
4	4-R	74	TYR	CB-CG-CD1	-5.62	117.63	121.00
2	5-H	104	TYR	CB-CG-CD1	-5.62	117.63	121.00
4	5-R	192	TYR	CB-CG-CD2	-5.61	117.63	121.00
4	1-R	74	TYR	CB-CG-CD1	-5.55	117.67	121.00
4	4-R	74	TYR	CB-CG-CD2	5.54	124.33	121.00
4	3-R	91	PHE	CB-CG-CD1	5.50	124.65	120.80
4	3-R	74	TYR	CB-CG-CD2	-5.49	117.70	121.00
4	1-R	74	TYR	CB-CG-CD2	5.46	124.28	121.00
2	5-H	104	TYR	CB-CG-CD2	5.41	124.25	121.00
2	2-H	104	TYR	CB-CG-CD2	5.41	124.24	121.00
2	4-H	115	TYR	CB-CG-CD2	-5.38	117.77	121.00
4	5-R	74	TYR	CB-CG-CD2	-5.35	117.79	121.00
2	1-H	104	TYR	CB-CG-CD1	-5.33	117.80	121.00
4	3-R	74	TYR	CB-CG-CD1	5.28	124.17	121.00
4	5-R	192	TYR	CB-CG-CD1	5.18	124.11	121.00
2	1-H	104	TYR	CB-CG-CD2	5.17	124.10	121.00
4	2-R	91	PHE	CB-CG-CD1	5.16	124.41	120.80
4	1-R	91	PHE	CB-CG-CD1	5.16	124.41	120.80
4	5-R	10	TYR	CB-CG-CD2	-5.16	117.91	121.00
4	4-R	220	PHE	CB-CG-CD2	5.07	124.35	120.80
4	5-R	91	PHE	CB-CG-CD1	5.05	124.34	120.80
4	5-R	74	TYR	CB-CG-CD1	5.02	124.01	121.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-G	182	MET	Peptide
1	1-G	312	TYR	Sidechain
3	1-L	142	TYR	Sidechain
1	2-G	182	MET	Peptide
3	2-L	142	TYR	Sidechain
3	2-L	194	TYR	Sidechain
1	3-G	182	MET	Peptide
1	3-G	191	ARG	Sidechain
1	3-G	312	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	3-L	142	TYR	Sidechain
3	3-L	194	TYR	Sidechain
1	4-G	182	MET	Peptide
1	4-G	312	TYR	Sidechain
1	4-G	366	TYR	Sidechain
2	4-H	104	TYR	Sidechain
1	5-G	182	MET	Peptide
1	5-G	191	ARG	Sidechain
1	5-G	312	TYR	Sidechain
1	5-G	366	TYR	Sidechain
3	5-L	142	TYR	Sidechain
3	5-L	194	TYR	Sidechain
1	6-G	182	MET	Peptide
1	6-G	312	TYR	Sidechain
2	6-H	104	TYR	Sidechain
3	6-L	142	TYR	Sidechain
3	6-L	194	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-G	2746	0	2727	0	0
1	2-G	2745	0	2726	0	0
1	3-G	2745	0	2726	0	0
1	4-G	2746	0	2727	0	0
1	5-G	2746	0	2727	0	0
1	6-G	2746	0	2727	0	0
2	1-H	1704	0	1634	1	0
2	2-H	1704	0	1634	2	0
2	3-H	1704	0	1634	0	0
2	4-H	1704	0	1634	1	0
2	5-H	1704	0	1634	0	0
2	6-H	1704	0	1634	0	0
3	1-L	1640	0	1589	1	0
3	2-L	1640	0	1589	0	0
3	3-L	1640	0	1589	1	0
3	4-L	1640	0	1589	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5-L	1640	0	1589	1	0
3	6-L	1640	0	1589	1	0
4	1-R	2575	0	2550	0	0
4	2-R	2575	0	2550	0	0
4	3-R	2575	0	2550	1	0
4	4-R	2575	0	2550	0	0
4	5-R	2575	0	2550	1	0
4	6-R	2575	0	2550	0	0
5	1-G	22	0	15	0	0
5	2-G	22	0	15	0	0
5	3-G	22	0	15	0	0
5	4-G	22	0	15	0	0
5	5-G	22	0	15	0	0
5	6-G	22	0	15	0	0
6	1-R	20	0	27	2	0
6	2-R	20	0	27	2	0
6	3-R	20	0	27	3	0
6	4-R	20	0	27	2	0
6	5-R	20	0	27	4	0
6	6-R	20	0	27	3	0
All	All	52240	0	51250	27	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 0.

All (27) 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)
6:R:401:RET:H181	6:R:401:RET:H8	1.68	0.76
6:R:401:RET:H181	6:R:401:RET:H8	1.74	0.69
6:R:401:RET:H181	6:R:401:RET:H8	1.74	0.68
6:R:401:RET:H181	6:R:401:RET:H8	1.76	0.68
6:R:401:RET:H181	6:R:401:RET:H8	1.79	0.65
6:R:401:RET:H181	6:R:401:RET:H8	1.79	0.64
6:R:401:RET:H181	6:R:401:RET:C8	2.31	0.60
6:R:401:RET:H181	6:R:401:RET:C8	2.32	0.60
6:R:401:RET:H181	6:R:401:RET:C8	2.30	0.59
6:R:401:RET:H181	6:R:401:RET:C8	2.33	0.58
6:R:401:RET:H181	6:R:401:RET:C8	2.33	0.56
6:R:401:RET:H181	6:R:401:RET:C8	2.30	0.55
3:L:200:HIS:CD2	3:L:201:GLN:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:200:HIS:CD2	3:L:201:GLN:H	2.25	0.54
3:L:200:HIS:CD2	3:L:201:GLN:H	2.29	0.50
3:L:200:HIS:CD2	3:L:201:GLN:H	2.32	0.47
4:R:72:LEU:H	4:R:72:LEU:HD23	1.80	0.46
3:L:200:HIS:CD2	3:L:201:GLN:H	2.35	0.44
2:H:110:ARG:HD3	2:H:110:ARG:H	1.83	0.44
2:H:73:ILE:HD13	2:H:73:ILE:H	1.83	0.43
4:R:195:HIS:H	4:R:200:ASN:HB2	1.85	0.42
2:H:73:ILE:HD12	2:H:73:ILE:H	1.86	0.41
6:R:401:RET:H11	6:R:401:RET:H191	1.91	0.41
6:R:401:RET:H11	6:R:401:RET:H191	1.93	0.41
6:R:401:RET:H8	6:R:401:RET:C18	2.48	0.41
6:R:401:RET:H8	6:R:401:RET:C18	2.47	0.41
2:H:14:LEU:H	2:H:14:LEU:HD23	1.87	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	1-G	342/543 (63%)	319 (93%)	18 (5%)	5 (2%)	10	45
1	2-G	342/543 (63%)	323 (94%)	14 (4%)	5 (2%)	10	45
1	3-G	342/543 (63%)	315 (92%)	22 (6%)	5 (2%)	10	45
1	4-G	342/543 (63%)	318 (93%)	20 (6%)	4 (1%)	13	49
1	5-G	342/543 (63%)	319 (93%)	16 (5%)	7 (2%)	7	40
1	6-G	342/543 (63%)	319 (93%)	18 (5%)	5 (2%)	10	45
2	1-H	223/234 (95%)	199 (89%)	20 (9%)	4 (2%)	8	41
2	2-H	223/234 (95%)	193 (86%)	24 (11%)	6 (3%)	5	34
2	3-H	223/234 (95%)	198 (89%)	20 (9%)	5 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4-H	223/234 (95%)	198 (89%)	18 (8%)	7 (3%)	4	31
2	5-H	223/234 (95%)	201 (90%)	18 (8%)	4 (2%)	8	41
2	6-H	223/234 (95%)	199 (89%)	16 (7%)	8 (4%)	3	28
3	1-L	212/216 (98%)	197 (93%)	10 (5%)	5 (2%)	6	36
3	2-L	212/216 (98%)	200 (94%)	6 (3%)	6 (3%)	5	33
3	3-L	212/216 (98%)	198 (93%)	9 (4%)	5 (2%)	6	36
3	4-L	212/216 (98%)	198 (93%)	7 (3%)	7 (3%)	4	30
3	5-L	212/216 (98%)	201 (95%)	4 (2%)	7 (3%)	4	30
3	6-L	212/216 (98%)	199 (94%)	5 (2%)	8 (4%)	3	27
4	1-R	322/348 (92%)	299 (93%)	19 (6%)	4 (1%)	13	49
4	2-R	322/348 (92%)	300 (93%)	19 (6%)	3 (1%)	17	55
4	3-R	322/348 (92%)	298 (92%)	18 (6%)	6 (2%)	8	40
4	4-R	322/348 (92%)	303 (94%)	17 (5%)	2 (1%)	25	63
4	5-R	322/348 (92%)	299 (93%)	22 (7%)	1 (0%)	41	75
4	6-R	322/348 (92%)	304 (94%)	15 (5%)	3 (1%)	17	55
All	All	6594/8046 (82%)	6097 (92%)	375 (6%)	122 (2%)	11	40

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-G	315	LEU
1	1-G	431	ASP
1	1-G	482	GLN
1	2-G	315	LEU
2	2-H	66	SER
2	2-H	102	HIS
2	2-H	115	TYR
3	2-L	33	ALA
3	2-L	172	ASP
2	3-H	33	SER
2	3-H	66	SER
2	3-H	115	TYR
3	3-L	33	ALA
3	3-L	172	ASP
1	4-G	315	LEU
2	4-H	33	SER
2	4-H	115	TYR

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Mol	Chain	Res	Type
3	4-L	33	ALA
1	5-G	280	ASP
1	5-G	315	LEU
1	5-G	440	ASP
2	5-H	33	SER
2	5-H	108	ASN
3	5-L	33	ALA
3	5-L	172	ASP
2	6-H	33	SER
3	6-L	33	ALA
3	6-L	52	ALA
3	6-L	172	ASP
2	1-H	33	SER
1	2-G	280	ASP
1	2-G	478	ALA
2	2-H	108	ASN
1	3-G	280	ASP
1	3-G	315	LEU
4	3-R	184	GLN
2	4-H	102	HIS
4	4-R	184	GLN
1	5-G	395	LYS
1	5-G	438	PHE
1	6-G	315	LEU
1	6-G	431	ASP
2	1-H	66	SER
2	1-H	91	ALA
3	1-L	53	SER
3	1-L	172	ASP
4	1-R	16	LYS
4	1-R	184	GLN
1	2-G	440	ASP
1	2-G	480	ASN
2	2-H	126	SER
3	2-L	53	SER
3	2-L	67	ARG
4	2-R	2	ASN
4	2-R	16	LYS
1	3-G	386	ARG
1	3-G	395	LYS
1	3-G	415	LYS
3	3-L	53	SER

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Mol	Chain	Res	Type
4	3-R	2	ASN
4	3-R	145	ASN
1	4-G	280	ASP
1	4-G	431	ASP
1	4-G	440	ASP
2	4-H	53	TYR
2	4-H	107	TRP
2	4-H	127	ALA
3	4-L	53	SER
3	4-L	172	ASP
4	4-R	16	LYS
1	5-G	486	ALA
2	5-H	126	SER
2	5-H	204	THR
3	5-L	53	SER
4	5-R	16	LYS
1	6-G	280	ASP
1	6-G	440	ASP
2	6-H	57	TYR
2	6-H	91	ALA
2	6-H	108	ASN
2	6-H	114	ASP
2	6-H	204	THR
3	6-L	53	SER
3	6-L	160	ASN
4	6-R	16	LYS
4	6-R	184	GLN
1	1-G	209	THR
4	1-R	145	ASN
2	2-H	101	ARG
3	2-L	160	ASN
3	3-L	95	TYR
3	3-L	160	ASN
4	3-R	16	LYS
4	3-R	191	TYR
2	4-H	108	ASN
3	4-L	160	ASN
3	4-L	173	SER
3	5-L	67	ARG
3	5-L	68	SER
3	5-L	95	TYR
3	5-L	160	ASN

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Mol	Chain	Res	Type
2	6-H	126	SER
3	6-L	95	TYR
4	6-R	145	ASN
3	1-L	33	ALA
3	1-L	95	TYR
3	1-L	160	ASN
4	1-R	29	TYR
3	2-L	68	SER
2	3-H	53	TYR
2	3-H	204	THR
3	4-L	67	ARG
3	4-L	95	TYR
2	6-H	76	ASP
1	1-G	280	ASP
2	1-H	87	ASN
4	2-R	29	TYR
1	5-G	257	LYS
3	6-L	51	SER
3	6-L	67	ARG
4	3-R	23	PRO
1	6-G	196	GLY

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	1-G	286/449 (64%)	281 (98%)	5 (2%)	60	78
1	2-G	285/449 (64%)	277 (97%)	8 (3%)	43	65
1	3-G	285/449 (64%)	277 (97%)	8 (3%)	43	65
1	4-G	286/449 (64%)	276 (96%)	10 (4%)	36	61
1	5-G	286/449 (64%)	276 (96%)	10 (4%)	36	61
1	6-G	286/449 (64%)	279 (98%)	7 (2%)	49	69
2	1-H	187/196 (95%)	183 (98%)	4 (2%)	53	72
2	2-H	187/196 (95%)	184 (98%)	3 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	3-H	187/196 (95%)	183 (98%)	4 (2%)	53 72
2	4-H	187/196 (95%)	182 (97%)	5 (3%)	44 66
2	5-H	187/196 (95%)	185 (99%)	2 (1%)	73 85
2	6-H	187/196 (95%)	182 (97%)	5 (3%)	44 66
3	1-L	188/190 (99%)	184 (98%)	4 (2%)	53 72
3	2-L	188/190 (99%)	186 (99%)	2 (1%)	73 85
3	3-L	188/190 (99%)	187 (100%)	1 (0%)	88 93
3	4-L	188/190 (99%)	185 (98%)	3 (2%)	62 79
3	5-L	188/190 (99%)	186 (99%)	2 (1%)	73 85
3	6-L	188/190 (99%)	182 (97%)	6 (3%)	39 62
4	1-R	276/296 (93%)	273 (99%)	3 (1%)	73 85
4	2-R	276/296 (93%)	272 (99%)	4 (1%)	67 81
4	3-R	276/296 (93%)	273 (99%)	3 (1%)	73 85
4	4-R	276/296 (93%)	269 (98%)	7 (2%)	47 68
4	5-R	276/296 (93%)	272 (99%)	4 (1%)	67 81
4	6-R	276/296 (93%)	275 (100%)	1 (0%)	91 94
All	All	5620/6786 (83%)	5509 (98%)	111 (2%)	57 73

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-G	188	LEU
1	1-G	202	PHE
1	1-G	264	MET
1	1-G	312	TYR
1	1-G	390	ARG
2	1-H	39	TRP
2	1-H	73	ILE
2	1-H	144	THR
2	1-H	173	THR
3	1-L	7	GLN
3	1-L	19	ARG
3	1-L	95	TYR
3	1-L	160	ASN
4	1-R	66	LYS
4	1-R	161	TRP

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Mol	Chain	Res	Type
4	1-R	289	THR
1	2-G	188	LEU
1	2-G	195	ARG
1	2-G	202	PHE
1	2-G	264	MET
1	2-G	306	HIS
1	2-G	312	TYR
1	2-G	390	ARG
1	2-G	497	LYS
2	2-H	7	LEU
2	2-H	14	LEU
2	2-H	99	CYS
3	2-L	90	GLN
3	2-L	95	TYR
4	2-R	8	ASN
4	2-R	161	TRP
4	2-R	177	ARG
4	2-R	289	THR
1	3-G	188	LEU
1	3-G	202	PHE
1	3-G	264	MET
1	3-G	275	HIS
1	3-G	312	TYR
1	3-G	340	LYS
1	3-G	390	ARG
1	3-G	482	GLN
2	3-H	39	TRP
2	3-H	79	LYS
2	3-H	99	CYS
2	3-H	110	ARG
3	3-L	95	TYR
4	3-R	16	LYS
4	3-R	161	TRP
4	3-R	289	THR
1	4-G	188	LEU
1	4-G	191	ARG
1	4-G	195	ARG
1	4-G	202	PHE
1	4-G	264	MET
1	4-G	275	HIS
1	4-G	312	TYR
1	4-G	390	ARG

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Mol	Chain	Res	Type
1	4-G	415	LYS
1	4-G	460	LEU
2	4-H	6	GLN
2	4-H	39	TRP
2	4-H	54	ILE
2	4-H	73	ILE
2	4-H	110	ARG
3	4-L	39	GLN
3	4-L	40	LYS
3	4-L	95	TYR
4	4-R	8	ASN
4	4-R	16	LYS
4	4-R	30	TYR
4	4-R	72	LEU
4	4-R	193	THR
4	4-R	247	GLU
4	4-R	289	THR
1	5-G	188	LEU
1	5-G	191	ARG
1	5-G	195	ARG
1	5-G	202	PHE
1	5-G	264	MET
1	5-G	275	HIS
1	5-G	312	TYR
1	5-G	390	ARG
1	5-G	431	ASP
1	5-G	460	LEU
2	5-H	39	TRP
2	5-H	73	ILE
3	5-L	95	TYR
3	5-L	105	LYS
4	5-R	10	TYR
4	5-R	72	LEU
4	5-R	161	TRP
4	5-R	289	THR
1	6-G	188	LEU
1	6-G	195	ARG
1	6-G	202	PHE
1	6-G	264	MET
1	6-G	312	TYR
1	6-G	390	ARG
1	6-G	460	LEU

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Mol	Chain	Res	Type
2	6-H	73	ILE
2	6-H	99	CYS
2	6-H	110	ARG
2	6-H	113	LEU
2	6-H	123	THR
3	6-L	19	ARG
3	6-L	40	LYS
3	6-L	90	GLN
3	6-L	95	TYR
3	6-L	126	GLN
3	6-L	185	LYS
4	6-R	289	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-G	243	HIS
1	1-G	275	HIS
1	1-G	306	HIS
1	1-G	319	ASN
3	1-L	7	GLN
3	1-L	90	GLN
3	1-L	157	GLN
3	1-L	160	ASN
3	1-L	191	HIS
4	1-R	28	GLN
4	1-R	100	HIS
1	2-G	306	HIS
3	2-L	90	GLN
4	2-R	73	ASN
4	2-R	152	HIS
4	2-R	211	HIS
1	3-G	275	HIS
1	3-G	306	HIS
3	3-L	200	HIS
3	3-L	212	ASN
4	3-R	28	GLN
4	3-R	73	ASN
4	3-R	111	ASN
1	4-G	243	HIS
2	4-H	177	HIS
3	4-L	191	HIS

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Mol	Chain	Res	Type
4	4-R	100	HIS
4	4-R	211	HIS
1	5-G	243	HIS
1	5-G	275	HIS
1	5-G	297	GLN
1	5-G	306	HIS
1	5-G	327	ASN
3	5-L	90	GLN
1	6-G	243	HIS
1	6-G	275	HIS
1	6-G	306	HIS
1	6-G	327	ASN
2	6-H	177	HIS
3	6-L	90	GLN
4	6-R	28	GLN
4	6-R	211	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	RET	2-R	401	-	20,20,21	2.44	4 (20%)	27,27,28	0.91	0
6	RET	5-R	401	-	20,20,21	2.44	4 (20%)	27,27,28	0.92	0
6	RET	3-R	401	-	20,20,21	2.44	4 (20%)	27,27,28	1.02	1 (3%)
6	RET	4-R	401	-	20,20,21	2.47	4 (20%)	27,27,28	0.92	1 (3%)
5	SGV	2-G	601	-	22,24,24	1.32	5 (22%)	23,36,36	0.92	1 (4%)
5	SGV	1-G	601	-	22,24,24	1.32	4 (18%)	23,36,36	1.02	1 (4%)
6	RET	1-R	401	-	20,20,21	2.46	4 (20%)	27,27,28	0.84	0
5	SGV	3-G	601	-	22,24,24	1.31	4 (18%)	23,36,36	0.96	0
5	SGV	6-G	601	-	22,24,24	1.30	4 (18%)	23,36,36	0.90	0
6	RET	6-R	401	-	20,20,21	2.49	4 (20%)	27,27,28	0.82	0
5	SGV	5-G	601	-	22,24,24	1.33	5 (22%)	23,36,36	0.93	1 (4%)
5	SGV	4-G	601	-	22,24,24	1.33	4 (18%)	23,36,36	0.95	1 (4%)

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	RET	2-R	401	-	-	0/13/30/31	0/1/1/1
6	RET	5-R	401	-	-	2/13/30/31	0/1/1/1
6	RET	3-R	401	-	-	2/13/30/31	0/1/1/1
6	RET	4-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	2-G	601	-	-	0/3/26/26	0/3/3/3
5	SGV	1-G	601	-	-	0/3/26/26	0/3/3/3
6	RET	1-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	3-G	601	-	-	0/3/26/26	0/3/3/3
5	SGV	6-G	601	-	-	0/3/26/26	0/3/3/3
6	RET	6-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	5-G	601	-	-	0/3/26/26	0/3/3/3
5	SGV	4-G	601	-	-	0/3/26/26	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6-R	401	RET	C14-C13	9.44	1.41	1.33
6	4-R	401	RET	C14-C13	9.25	1.40	1.33
6	1-R	401	RET	C14-C13	9.24	1.40	1.33
6	2-R	401	RET	C14-C13	9.17	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5-R	401	RET	C14-C13	9.14	1.40	1.33
6	3-R	401	RET	C14-C13	9.11	1.40	1.33
6	2-R	401	RET	C15-C14	-3.25	1.37	1.49
6	4-R	401	RET	C15-C14	-3.24	1.37	1.49
6	5-R	401	RET	C15-C14	-3.24	1.37	1.49
6	3-R	401	RET	C15-C14	-3.22	1.37	1.49
6	1-R	401	RET	C15-C14	-3.20	1.37	1.49
6	6-R	401	RET	C15-C14	-3.17	1.37	1.49
5	4-G	601	SGV	C7-C10	-2.74	1.46	1.50
5	3-G	601	SGV	C7-C10	-2.66	1.46	1.50
5	2-G	601	SGV	C10-N11	2.66	1.38	1.33
5	6-G	601	SGV	C7-C10	-2.65	1.46	1.50
5	1-G	601	SGV	C10-N11	2.65	1.38	1.33
5	4-G	601	SGV	C10-N11	2.64	1.38	1.33
5	5-G	601	SGV	C10-N11	2.64	1.38	1.33
5	3-G	601	SGV	C10-N11	2.62	1.38	1.33
5	5-G	601	SGV	C7-C10	-2.61	1.46	1.50
5	2-G	601	SGV	C7-C10	-2.60	1.46	1.50
5	1-G	601	SGV	C7-C10	-2.60	1.46	1.50
5	6-G	601	SGV	C10-N11	2.58	1.37	1.33
6	4-R	401	RET	C12-C13	-2.56	1.40	1.45
6	1-R	401	RET	C12-C13	-2.53	1.40	1.45
6	2-R	401	RET	C12-C13	-2.51	1.40	1.45
6	5-R	401	RET	C12-C13	-2.51	1.40	1.45
6	3-R	401	RET	C12-C13	-2.46	1.40	1.45
5	6-G	601	SGV	C2-N3	2.45	1.36	1.32
5	5-G	601	SGV	C2-N3	2.44	1.36	1.32
5	1-G	601	SGV	C2-N3	2.43	1.36	1.32
5	3-G	601	SGV	C2-N3	2.42	1.36	1.32
6	6-R	401	RET	C12-C13	-2.41	1.40	1.45
5	4-G	601	SGV	O4'-C1'	2.41	1.44	1.41
5	4-G	601	SGV	C2-N3	2.40	1.36	1.32
5	1-G	601	SGV	O4'-C1'	2.39	1.44	1.41
5	5-G	601	SGV	O4'-C1'	2.39	1.44	1.41
5	3-G	601	SGV	O4'-C1'	2.39	1.44	1.41
5	2-G	601	SGV	C2-N3	2.38	1.35	1.32
5	2-G	601	SGV	O4'-C1'	2.34	1.44	1.41
6	3-R	401	RET	C1-C6	2.30	1.56	1.53
6	4-R	401	RET	C1-C6	2.28	1.56	1.53
6	6-R	401	RET	C1-C6	2.24	1.56	1.53
5	6-G	601	SGV	O4'-C1'	2.23	1.44	1.41
6	1-R	401	RET	C1-C6	2.20	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5-R	401	RET	C1-C6	2.11	1.56	1.53
6	2-R	401	RET	C1-C6	2.07	1.56	1.53
5	5-G	601	SGV	C7-C5	2.03	1.44	1.42
5	2-G	601	SGV	C7-C5	2.00	1.44	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5-G	601	SGV	O12-C10-C7	2.23	122.84	120.22
5	1-G	601	SGV	O12-C10-C7	2.08	122.68	120.22
6	4-R	401	RET	C2-C1-C6	2.08	113.69	110.48
5	2-G	601	SGV	O12-C10-C7	2.08	122.67	120.22
6	3-R	401	RET	C2-C1-C6	2.08	113.68	110.48
5	4-G	601	SGV	O12-C10-C7	2.06	122.64	120.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	3-R	401	RET	C5-C6-C7-C8
6	5-R	401	RET	C5-C6-C7-C8
6	5-R	401	RET	C1-C6-C7-C8
6	3-R	401	RET	C1-C6-C7-C8

There are no ring outliers.

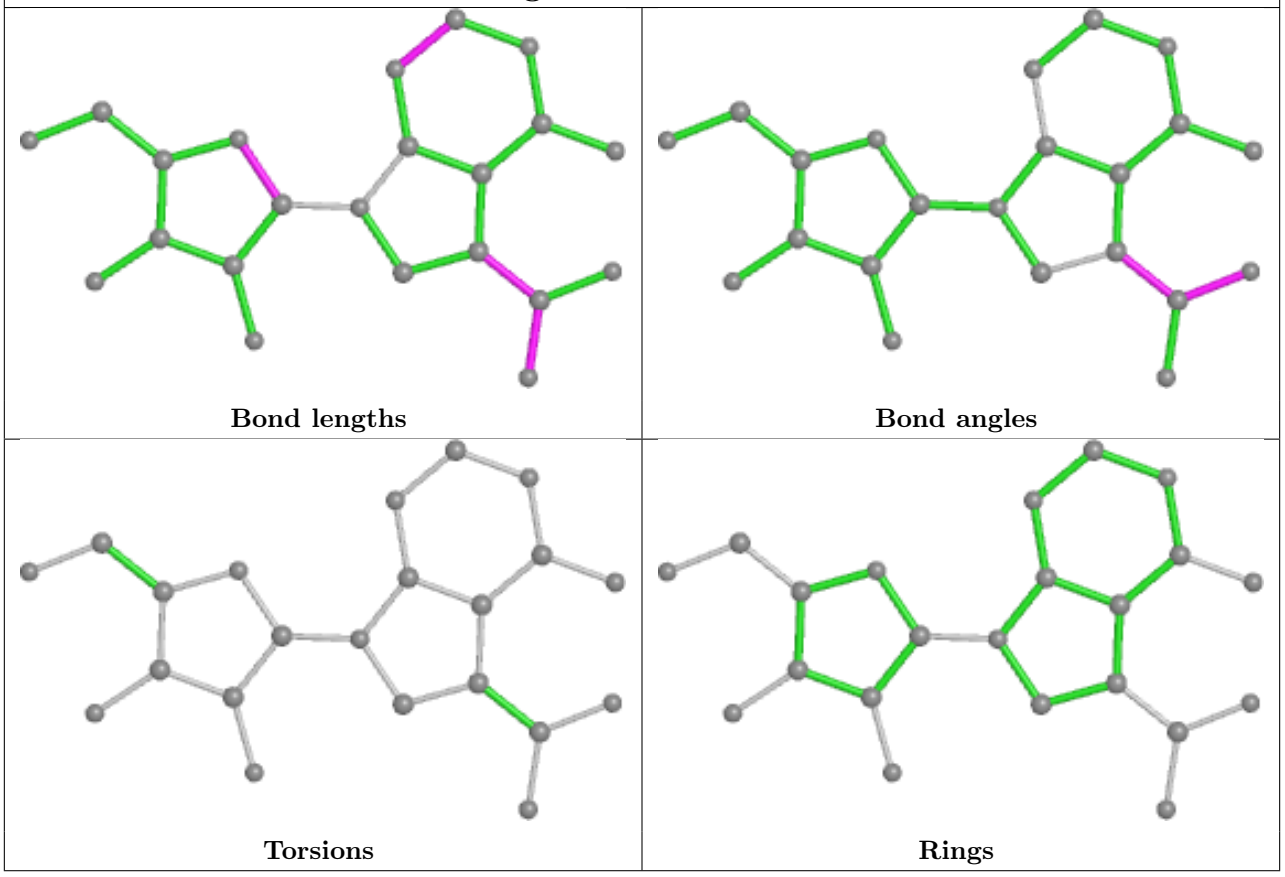
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2-R	401	RET	2	0
6	5-R	401	RET	4	0
6	3-R	401	RET	3	0
6	4-R	401	RET	2	0
6	1-R	401	RET	2	0
6	6-R	401	RET	3	0

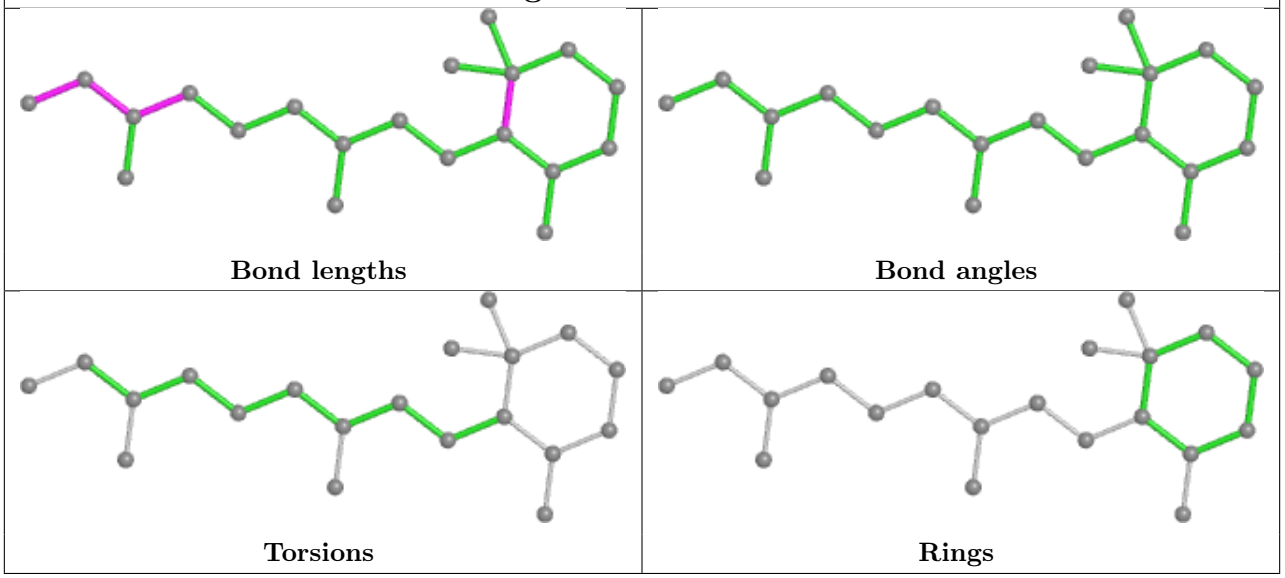
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand RET 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.

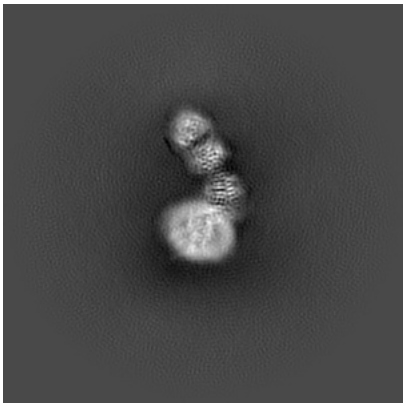
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23980. These allow visual inspection of the internal detail of the map and identification of artifacts.

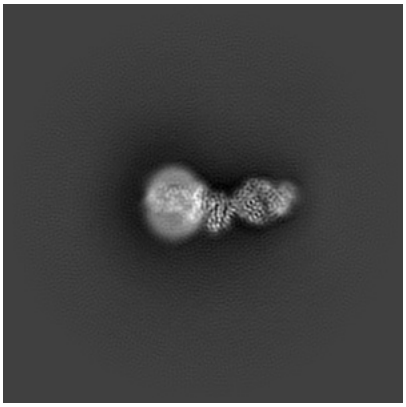
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

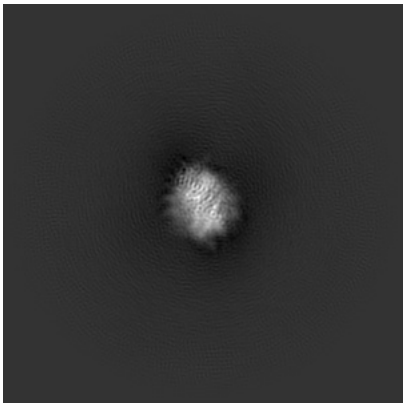
6.1.1 Primary map



X



Y

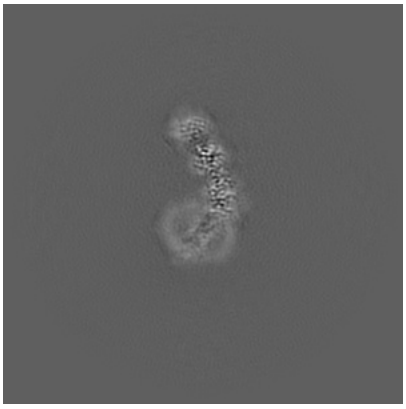


Z

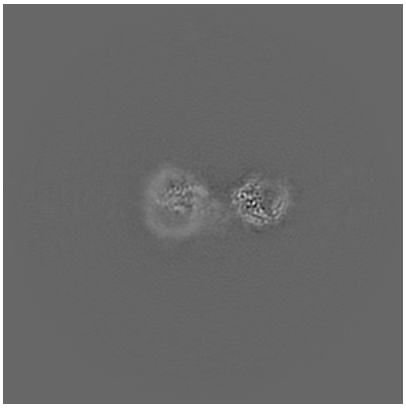
The images above show the map projected in three orthogonal directions.

6.2 Central slices

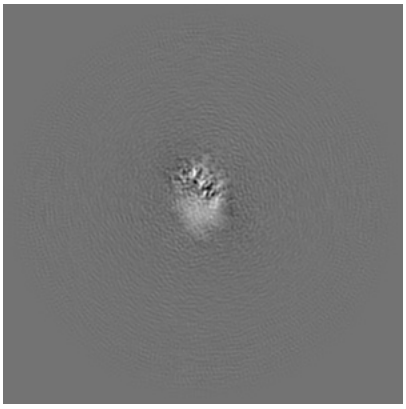
6.2.1 Primary map



X Index: 200



Y Index: 200

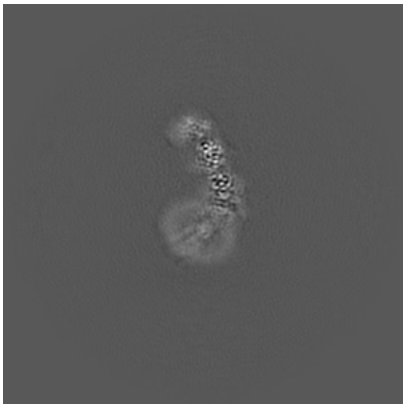


Z Index: 200

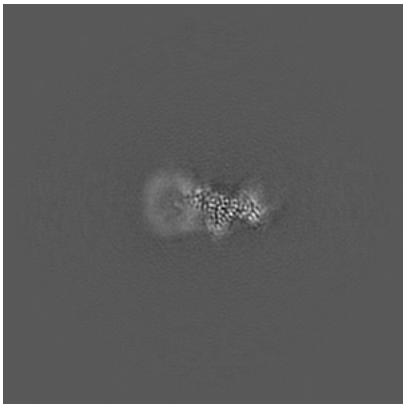
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

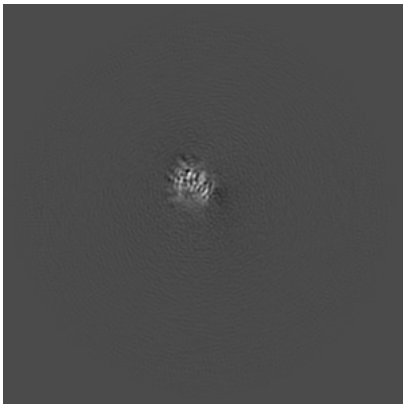
6.3.1 Primary map



X Index: 195



Y Index: 214



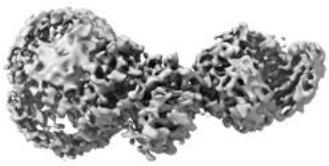
Z Index: 210

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

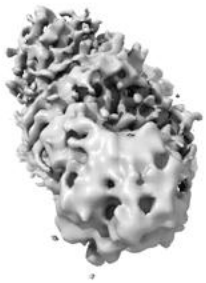
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

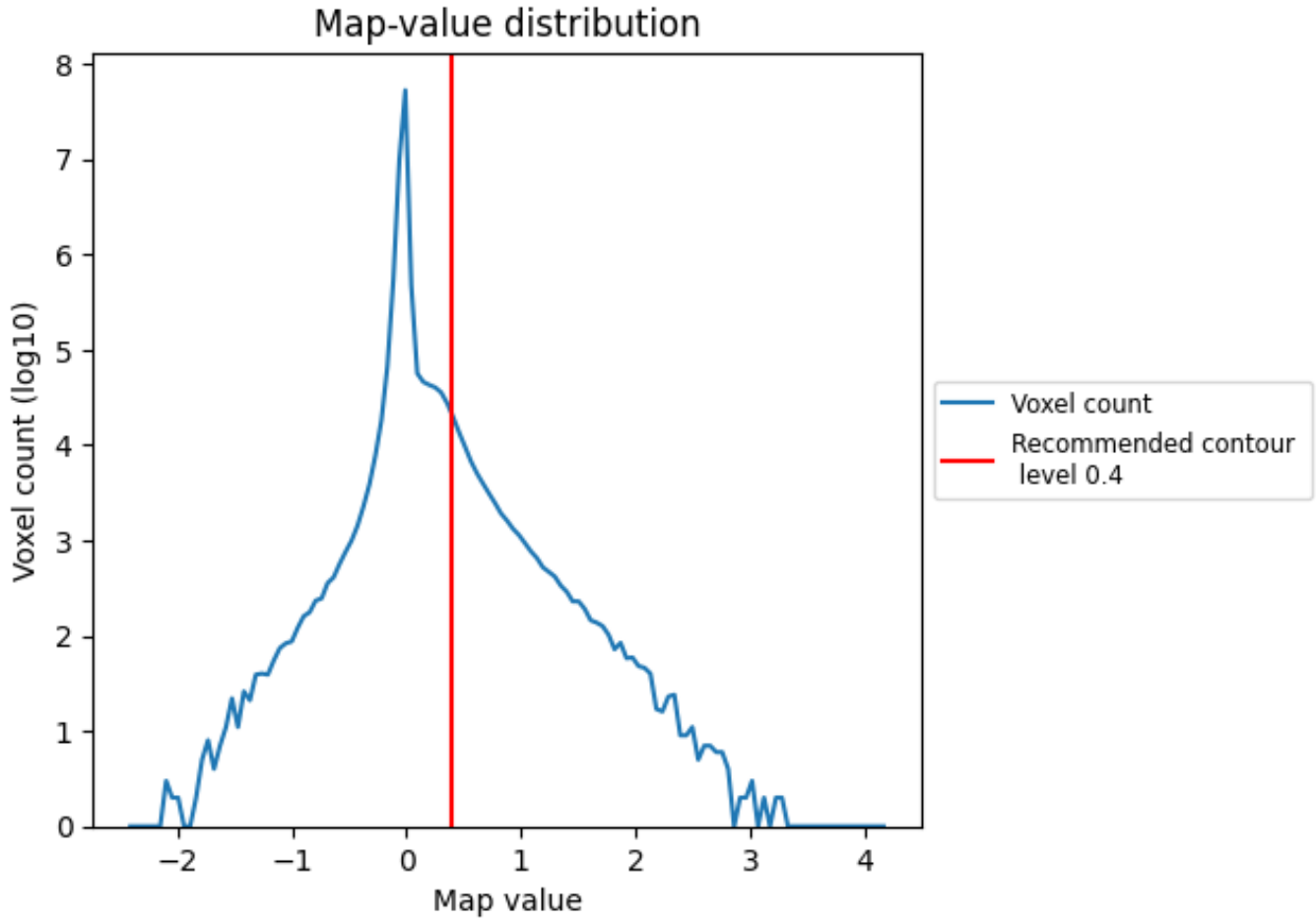
6.5 Mask visualisation (i)

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

7 Map analysis

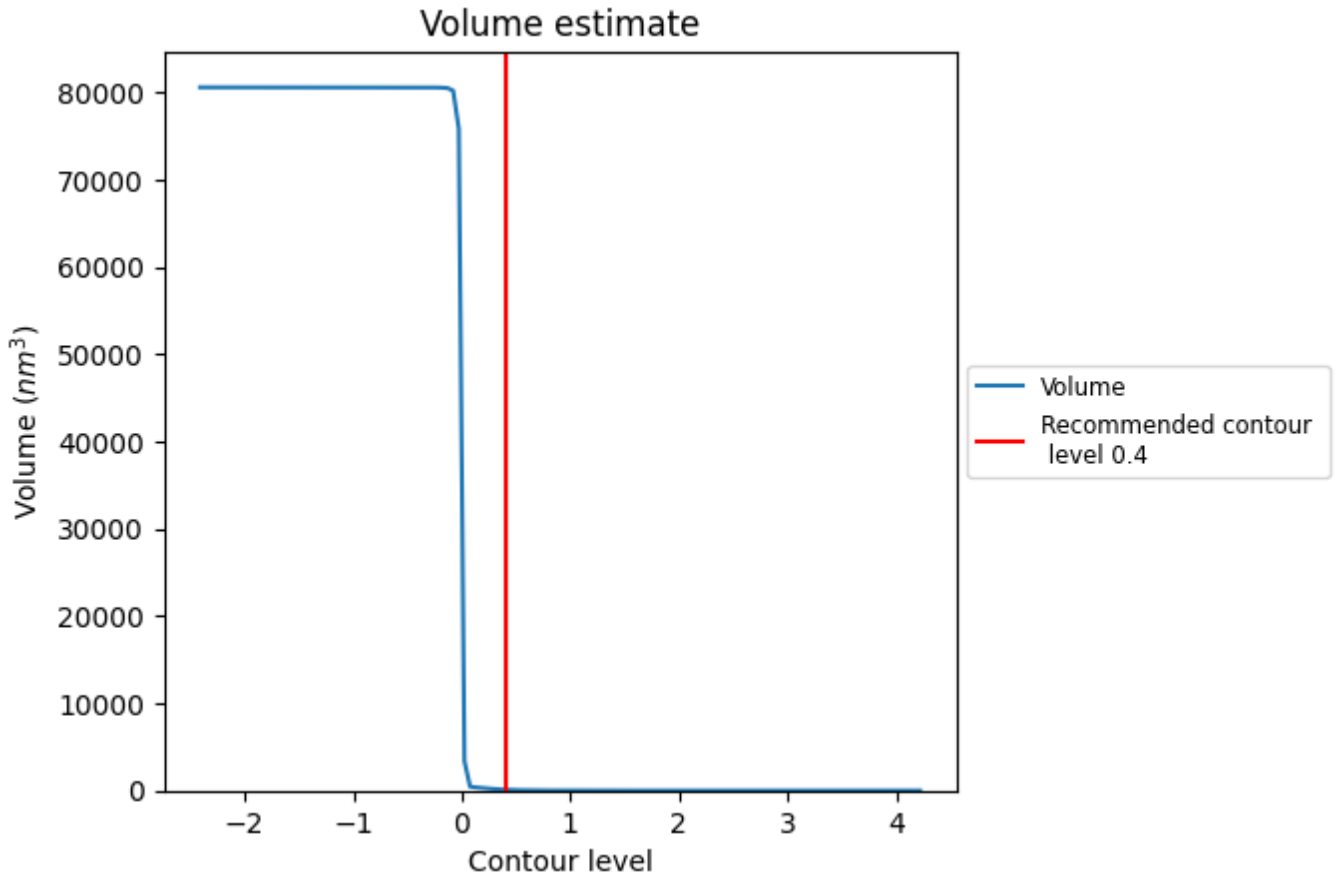
This section contains the results of statistical analysis of the map.

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.

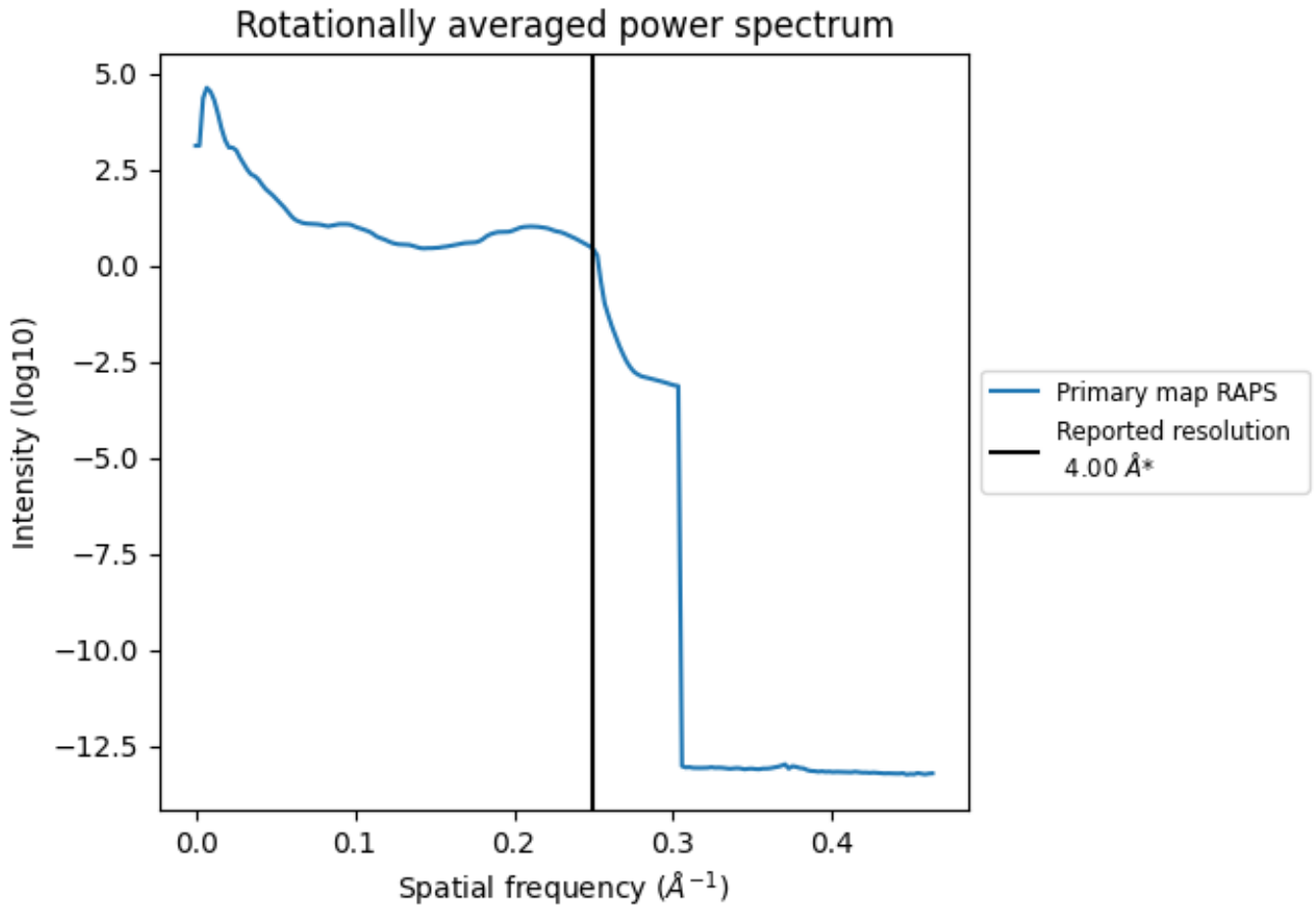
7.2 Volume estimate



The volume at the recommended contour level is 101 nm^3; this corresponds to an approximate mass of 91 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)

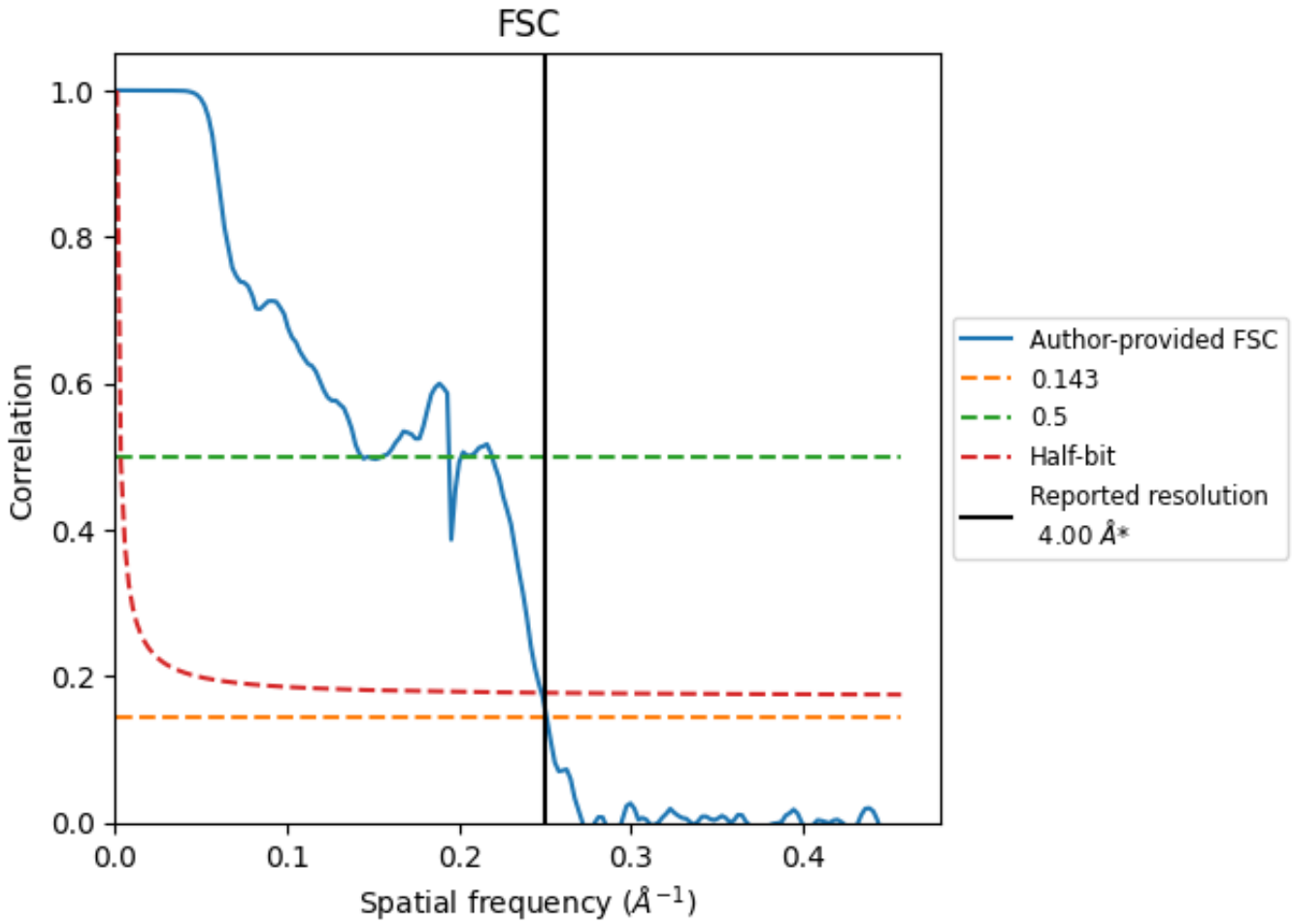


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

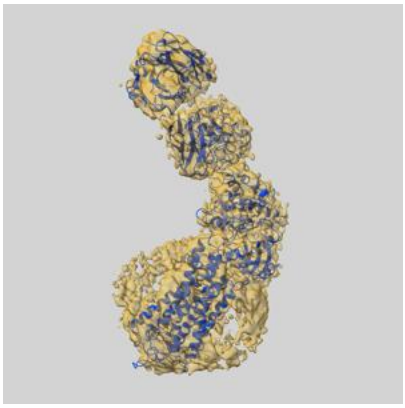
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	6.97	4.03
Unmasked-calculated*	-	-	-

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

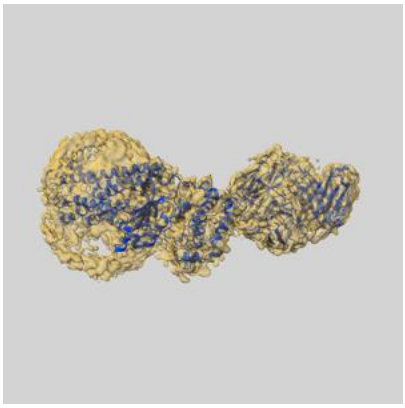
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23980 and PDB model 7MTB. Per-residue inclusion information can be found in section 3 on page 8.

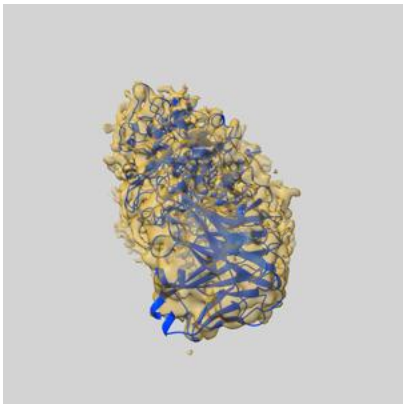
9.1 Map-model overlay



X



Y



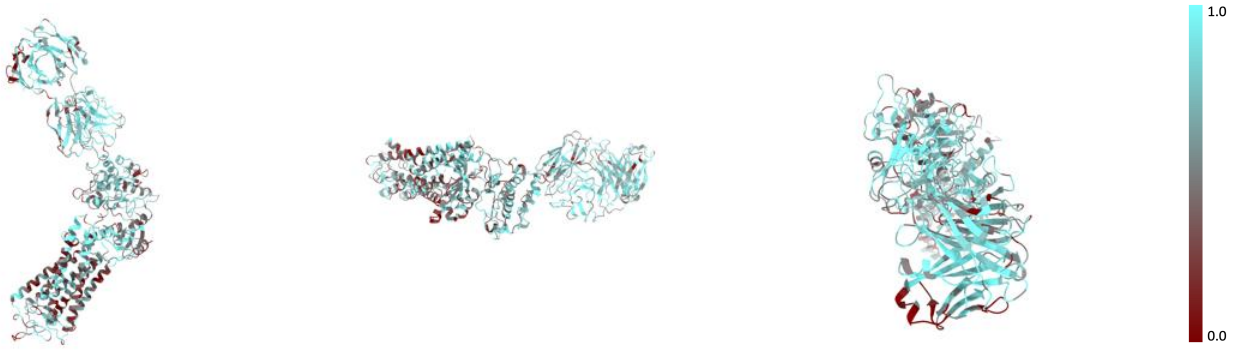
Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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)

This section was not generated.

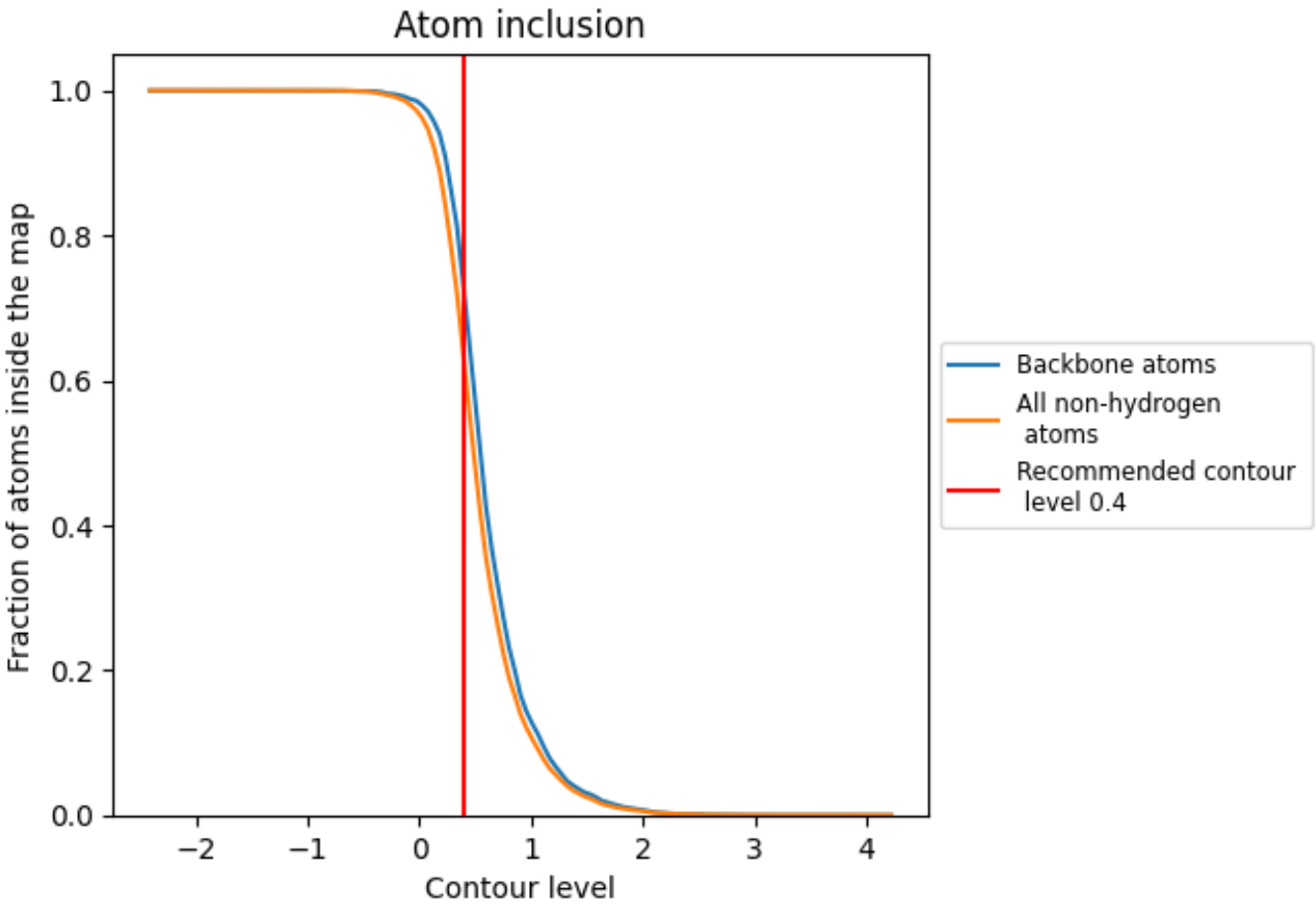
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6214
G	0.6160
H	0.7319
L	0.6398
R	0.5434