



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:13 AM UTC

PDB ID : 7MTA / pdb_00007mta
EMDB ID : EMD-23979
Title : Rhodopsin kinase (GRK1)-S5E/S488E/T489E in complex with rhodopsin and Fab1
Authors : Chen, Q.; Chen, C.-L.; Tesmer, J.J.G.
Deposited on : 2021-05-13
Resolution : 4.10 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

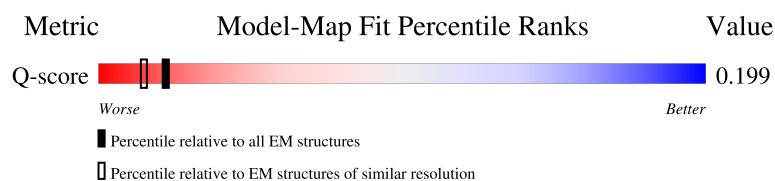
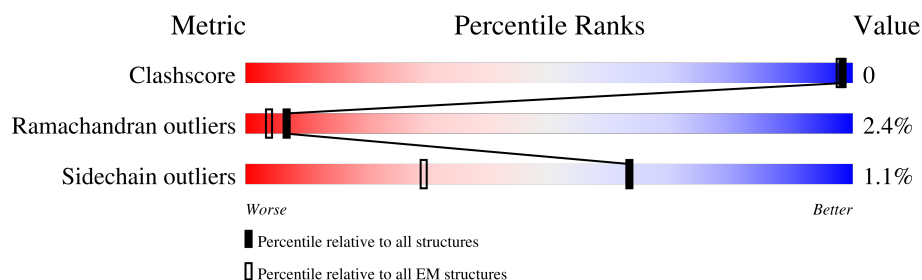
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



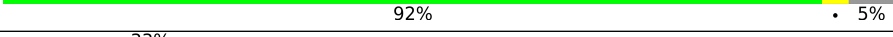
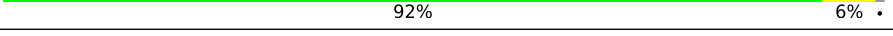
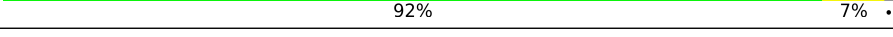
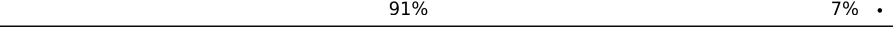
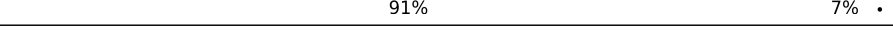
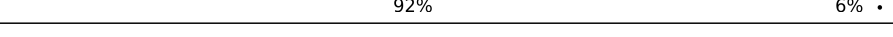
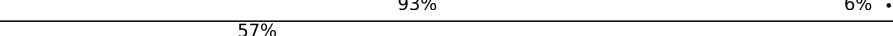
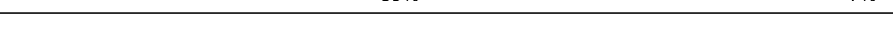
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-G	543	21% 60% 36%
1	2-G	543	60% 36%
1	3-G	543	61% 36%
1	4-G	543	61% 36%

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Mol	Chain	Length	Quality of chain
1	5-G	543	
1	6-G	543	
2	1-H	234	
2	2-H	234	
2	3-H	234	
2	4-H	234	
2	5-H	234	
2	6-H	234	
3	1-L	217	
3	2-L	217	
3	3-L	217	
3	4-L	217	
3	5-L	217	
3	6-L	217	
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 52194 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
			2746	1756	470	507	13		
1	3-G	346	Total	C	N	O	S	0	0
			2746	1756	470	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 Fab1 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	3-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	4-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	5-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	6-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		

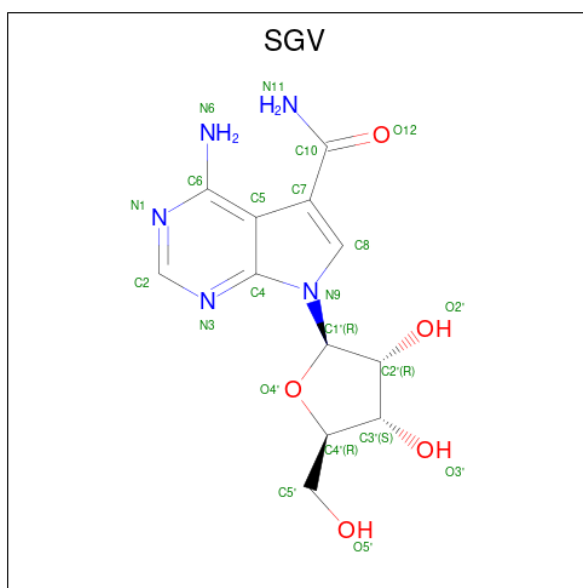
- Molecule 3 is a protein called Fab1 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	2-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	3-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	4-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	5-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	6-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		

- Molecule 4 is a protein called Rhodopsin.

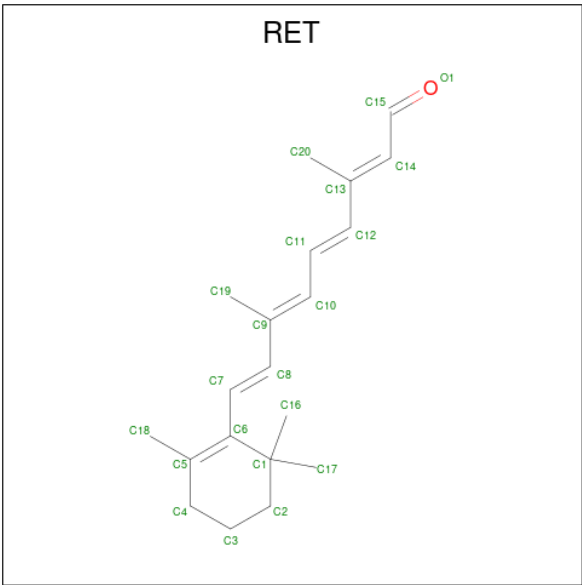
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	2-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	3-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	4-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	5-R	324	Total	C	N	O	S	0	0
			2575	1715	396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

- Molecule 5 is SANGIVAMYCIN (CCD ID: SGV) (formula: $C_{12}H_{15}N_5O_5$).



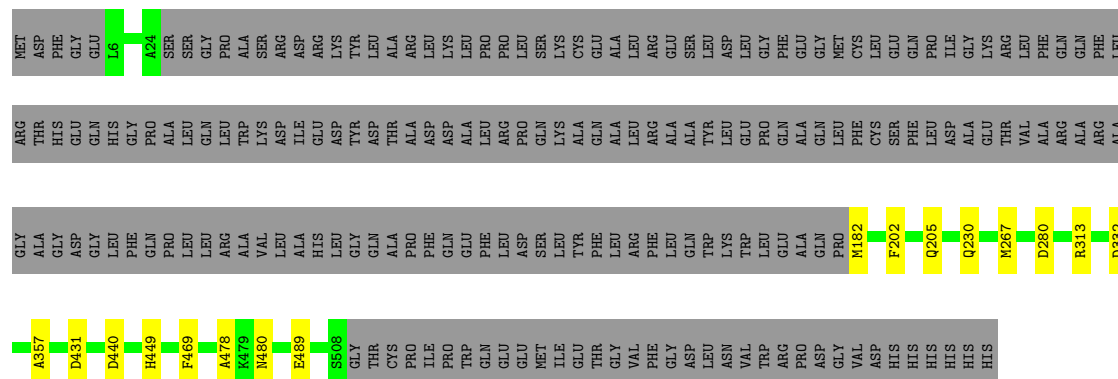
Mol	Chain	Residues	Atoms				AltConf
5	1-G	1	Total	C	N	O	0
			22	12	5	5	
5	2-G	1	Total	C	N	O	0
			22	12	5	5	
5	3-G	1	Total	C	N	O	0
			22	12	5	5	
5	4-G	1	Total	C	N	O	0
			22	12	5	5	
5	5-G	1	Total	C	N	O	0
			22	12	5	5	
5	6-G	1	Total	C	N	O	0
			22	12	5	5	

- Molecule 6 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).

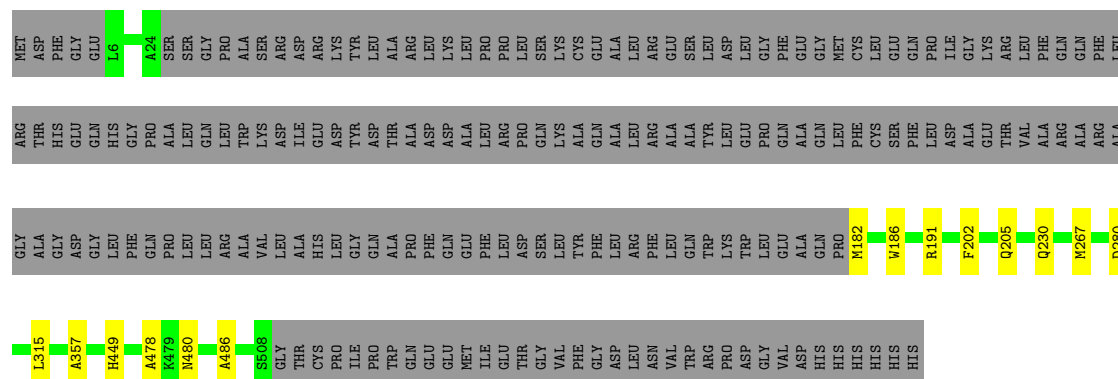


Mol	Chain	Residues	Atoms	AltConf
6	1-R	1	Total C 20 20	0
6	2-R	1	Total C 20 20	0
6	3-R	1	Total C 20 20	0
6	4-R	1	Total C 20 20	0
6	5-R	1	Total C 20 20	0
6	6-R	1	Total C 20 20	0

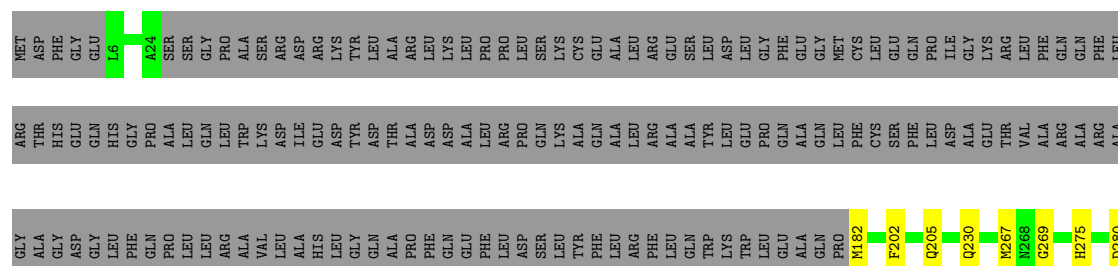
- Molecule 1: Rhodopsin kinase GRK1



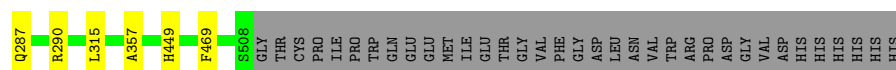
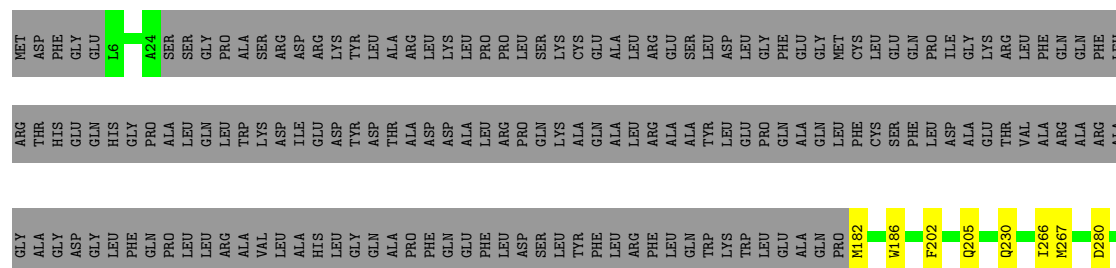
- Molecule 1: Rhodopsin kinase GRK1



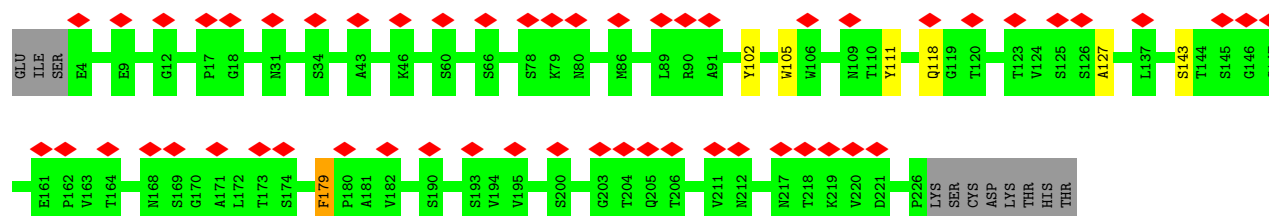
- Molecule 1: Rhodopsin kinase GRK1



- Molecule 1: Rhodopsin kinase GRK1



- Molecule 2: Fab1 Heavy chain



- Molecule 2: Fab1 Heavy chain



- Molecule 2: Fab1 Heavy chain



- Molecule 2: Fab1 Heavy chain





- Molecule 2: Fab1 Heavy chain

Chain 5-H: 91% 5% 5%



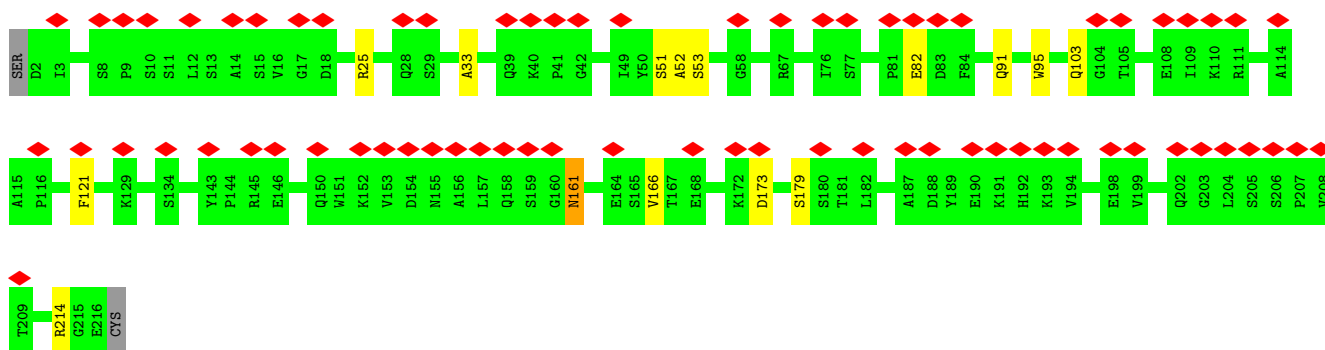
- Molecule 2: Fab1 Heavy chain

Chain 6-H: 92% 5%



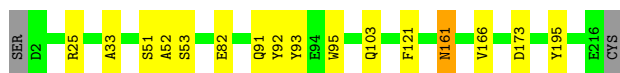
- Molecule 3: Fab1 Light chain

Chain 1-L: 33% 92% 6%



- Molecule 3: Fab1 Light chain

Chain 2-L: 92% 7%



- Molecule 3: Fab1 Light chain

Chain 3-L: 91% 7%



- Molecule 3: Fab1 Light chain

Chain 4-L: 91% 7%



- Molecule 3: Fab1 Light chain

Chain 5-L: 92% 6% .



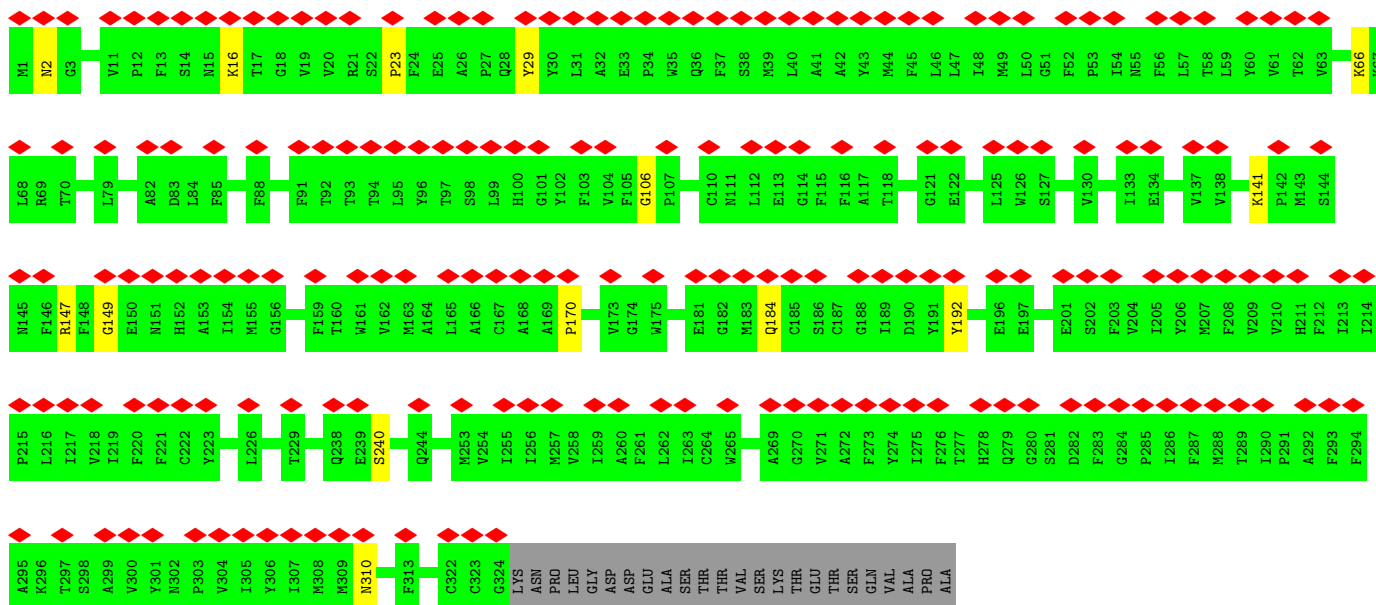
- Molecule 3: Fab1 Light chain

Chain 6-L: 93% 6% .



- Molecule 4: Rhodopsin

Chain 1-R: 57% 89% 7% .



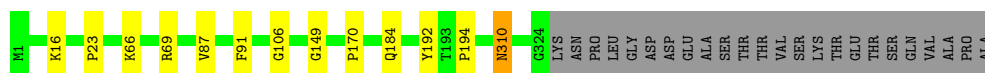
- Molecule 4: Rhodopsin

Chain 2-R: 90% 7% .



- Molecule 4: Rhodopsin

Chain 3-R: 89% 7% .



- Molecule 4: Rhodopsin

Chain 4-R: 89% 7%



- Molecule 4: Rhodopsin

Chain 5-R: 89% 7%



- Molecule 4: Rhodopsin

Chain 6-R: 89% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	310363	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 ($e^-/\text{\AA}^2$)	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	2.583	Depositor
Minimum map value	-2.566	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.49	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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.02	0/2803	1.16	7/3771 (0.2%)
1	2-G	1.02	0/2803	1.16	7/3771 (0.2%)
1	3-G	1.02	0/2803	1.16	7/3771 (0.2%)
1	4-G	1.02	0/2803	1.16	7/3771 (0.2%)
1	5-G	1.02	0/2803	1.16	7/3771 (0.2%)
1	6-G	1.02	0/2803	1.16	7/3771 (0.2%)
2	1-H	1.06	0/1722	1.03	3/2354 (0.1%)
2	2-H	1.06	0/1722	1.03	3/2354 (0.1%)
2	3-H	1.06	0/1722	1.03	3/2354 (0.1%)
2	4-H	1.06	0/1722	1.03	3/2354 (0.1%)
2	5-H	1.06	0/1722	1.03	3/2354 (0.1%)
2	6-H	1.06	0/1722	1.03	3/2354 (0.1%)
3	1-L	1.07	0/1697	1.01	0/2304
3	2-L	1.07	0/1697	1.01	0/2304
3	3-L	1.07	0/1697	1.01	0/2304
3	4-L	1.07	0/1697	1.01	0/2304
3	5-L	1.07	0/1697	1.01	0/2304
3	6-L	1.07	0/1697	1.01	0/2304
4	1-R	0.99	0/2657	1.29	7/3621 (0.2%)
4	2-R	0.99	0/2657	1.29	7/3621 (0.2%)
4	3-R	0.99	0/2657	1.29	7/3621 (0.2%)
4	4-R	0.99	0/2657	1.29	7/3621 (0.2%)
4	5-R	0.99	0/2657	1.29	7/3621 (0.2%)
4	6-R	0.99	0/2657	1.29	7/3621 (0.2%)
All	All	1.03	0/53274	1.15	102/72300 (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	1
1	2-G	0	1
1	3-G	0	1
1	4-G	0	1
1	5-G	0	1
1	6-G	0	1
2	1-H	0	1
2	2-H	0	1
2	3-H	0	1
2	4-H	0	1
2	5-H	0	2
2	6-H	0	1
3	1-L	0	1
3	2-L	0	3
3	3-L	0	1
3	4-L	0	2
3	5-L	0	1
3	6-L	0	1
4	4-R	0	1
4	6-R	0	1
All	All	0	24

There are no bond length outliers.

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-H	179	PHE	CA-CB-CG	-6.29	107.51	113.80
2	2-H	179	PHE	CA-CB-CG	-6.29	107.51	113.80
2	3-H	179	PHE	CA-CB-CG	-6.29	107.51	113.80
2	4-H	179	PHE	CA-CB-CG	-6.29	107.51	113.80
2	5-H	179	PHE	CA-CB-CG	-6.29	107.51	113.80
2	6-H	179	PHE	CA-CB-CG	-6.29	107.51	113.80
4	1-R	310	ASN	CA-C-N	6.00	128.64	120.54
4	1-R	310	ASN	C-N-CA	6.00	128.64	120.54
4	2-R	310	ASN	CA-C-N	6.00	128.64	120.54
4	2-R	310	ASN	C-N-CA	6.00	128.64	120.54
4	3-R	310	ASN	CA-C-N	6.00	128.64	120.54
4	3-R	310	ASN	C-N-CA	6.00	128.64	120.54
4	4-R	310	ASN	CA-C-N	6.00	128.64	120.54
4	4-R	310	ASN	C-N-CA	6.00	128.64	120.54
4	5-R	310	ASN	CA-C-N	6.00	128.64	120.54
4	5-R	310	ASN	C-N-CA	6.00	128.64	120.54
4	6-R	310	ASN	CA-C-N	6.00	128.64	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6-R	310	ASN	C-N-CA	6.00	128.64	120.54
4	1-R	106	GLY	CA-C-N	5.70	125.37	119.05
4	1-R	106	GLY	C-N-CA	5.70	125.37	119.05
4	2-R	106	GLY	CA-C-N	5.70	125.37	119.05
4	2-R	106	GLY	C-N-CA	5.70	125.37	119.05
4	3-R	106	GLY	CA-C-N	5.70	125.37	119.05
4	3-R	106	GLY	C-N-CA	5.70	125.37	119.05
4	4-R	106	GLY	CA-C-N	5.70	125.37	119.05
4	4-R	106	GLY	C-N-CA	5.70	125.37	119.05
4	5-R	106	GLY	CA-C-N	5.70	125.37	119.05
4	5-R	106	GLY	C-N-CA	5.70	125.37	119.05
4	6-R	106	GLY	CA-C-N	5.70	125.37	119.05
4	6-R	106	GLY	C-N-CA	5.70	125.37	119.05
1	1-G	357	ALA	CA-C-N	5.67	125.14	119.24
1	1-G	357	ALA	C-N-CA	5.67	125.14	119.24
1	2-G	357	ALA	CA-C-N	5.67	125.14	119.24
1	2-G	357	ALA	C-N-CA	5.67	125.14	119.24
1	3-G	357	ALA	CA-C-N	5.67	125.14	119.24
1	3-G	357	ALA	C-N-CA	5.67	125.14	119.24
1	4-G	357	ALA	CA-C-N	5.67	125.14	119.24
1	4-G	357	ALA	C-N-CA	5.67	125.14	119.24
1	5-G	357	ALA	CA-C-N	5.67	125.14	119.24
1	5-G	357	ALA	C-N-CA	5.67	125.14	119.24
1	6-G	357	ALA	CA-C-N	5.67	125.14	119.24
1	6-G	357	ALA	C-N-CA	5.67	125.14	119.24
1	1-G	205	GLN	CA-C-N	5.42	128.47	120.82
1	1-G	205	GLN	C-N-CA	5.42	128.47	120.82
1	2-G	205	GLN	CA-C-N	5.42	128.47	120.82
1	2-G	205	GLN	C-N-CA	5.42	128.47	120.82
1	3-G	205	GLN	CA-C-N	5.42	128.47	120.82
1	3-G	205	GLN	C-N-CA	5.42	128.47	120.82
1	4-G	205	GLN	CA-C-N	5.42	128.47	120.82
1	4-G	205	GLN	C-N-CA	5.42	128.47	120.82
1	5-G	205	GLN	CA-C-N	5.42	128.47	120.82
1	5-G	205	GLN	C-N-CA	5.42	128.47	120.82
1	6-G	205	GLN	CA-C-N	5.42	128.47	120.82
1	6-G	205	GLN	C-N-CA	5.42	128.47	120.82
4	1-R	170	PRO	N-CA-C	5.34	117.21	110.70
4	2-R	170	PRO	N-CA-C	5.34	117.21	110.70
4	3-R	170	PRO	N-CA-C	5.34	117.21	110.70
4	4-R	170	PRO	N-CA-C	5.34	117.21	110.70
4	5-R	170	PRO	N-CA-C	5.34	117.21	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6-R	170	PRO	N-CA-C	5.34	117.21	110.70
4	1-R	149	GLY	CA-C-N	5.23	127.55	120.38
4	1-R	149	GLY	C-N-CA	5.23	127.55	120.38
4	2-R	149	GLY	CA-C-N	5.23	127.55	120.38
4	2-R	149	GLY	C-N-CA	5.23	127.55	120.38
4	3-R	149	GLY	CA-C-N	5.23	127.55	120.38
4	3-R	149	GLY	C-N-CA	5.23	127.55	120.38
4	4-R	149	GLY	CA-C-N	5.23	127.55	120.38
4	4-R	149	GLY	C-N-CA	5.23	127.55	120.38
4	5-R	149	GLY	CA-C-N	5.23	127.55	120.38
4	5-R	149	GLY	C-N-CA	5.23	127.55	120.38
4	6-R	149	GLY	CA-C-N	5.23	127.55	120.38
4	6-R	149	GLY	C-N-CA	5.23	127.55	120.38
2	1-H	143	SER	CA-C-N	5.11	128.86	120.63
2	1-H	143	SER	C-N-CA	5.11	128.86	120.63
2	2-H	143	SER	CA-C-N	5.11	128.86	120.63
2	2-H	143	SER	C-N-CA	5.11	128.86	120.63
2	3-H	143	SER	CA-C-N	5.11	128.86	120.63
2	3-H	143	SER	C-N-CA	5.11	128.86	120.63
2	4-H	143	SER	CA-C-N	5.11	128.86	120.63
2	4-H	143	SER	C-N-CA	5.11	128.86	120.63
2	5-H	143	SER	CA-C-N	5.11	128.86	120.63
2	5-H	143	SER	C-N-CA	5.11	128.86	120.63
2	6-H	143	SER	CA-C-N	5.11	128.86	120.63
2	6-H	143	SER	C-N-CA	5.11	128.86	120.63
1	1-G	449	HIS	CA-C-N	5.06	124.72	119.56
1	1-G	449	HIS	C-N-CA	5.06	124.72	119.56
1	2-G	449	HIS	CA-C-N	5.06	124.72	119.56
1	2-G	449	HIS	C-N-CA	5.06	124.72	119.56
1	3-G	449	HIS	CA-C-N	5.06	124.72	119.56
1	3-G	449	HIS	C-N-CA	5.06	124.72	119.56
1	4-G	449	HIS	CA-C-N	5.06	124.72	119.56
1	4-G	449	HIS	C-N-CA	5.06	124.72	119.56
1	5-G	449	HIS	CA-C-N	5.06	124.72	119.56
1	5-G	449	HIS	C-N-CA	5.06	124.72	119.56
1	6-G	449	HIS	CA-C-N	5.06	124.72	119.56
1	6-G	449	HIS	C-N-CA	5.06	124.72	119.56
1	1-G	267	MET	N-CA-C	-5.01	100.12	110.80
1	2-G	267	MET	N-CA-C	-5.01	100.12	110.80
1	3-G	267	MET	N-CA-C	-5.01	100.12	110.80
1	4-G	267	MET	N-CA-C	-5.01	100.12	110.80
1	5-G	267	MET	N-CA-C	-5.01	100.12	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-G	267	MET	N-CA-C	-5.01	100.12	110.80

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-G	182	MET	Peptide
2	1-H	102	TYR	Sidechain
3	1-L	95	TRP	Peptide
1	2-G	182	MET	Peptide
2	2-H	102	TYR	Sidechain
3	2-L	195	TYR	Sidechain
3	2-L	92	TYR	Sidechain
3	2-L	95	TRP	Peptide
1	3-G	182	MET	Peptide
2	3-H	102	TYR	Sidechain
3	3-L	95	TRP	Peptide
1	4-G	182	MET	Peptide
2	4-H	102	TYR	Sidechain
3	4-L	92	TYR	Sidechain
3	4-L	95	TRP	Peptide
4	4-R	10	TYR	Sidechain
1	5-G	182	MET	Peptide
2	5-H	102	TYR	Sidechain
2	5-H	58	TYR	Sidechain
3	5-L	95	TRP	Peptide
1	6-G	182	MET	Peptide
2	6-H	102	TYR	Sidechain
3	6-L	95	TRP	Peptide
4	6-R	10	TYR	Sidechain

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	1-G	2746	0	2727	3	0
1	2-G	2746	0	2727	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-G	2746	0	2727	1	0
1	4-G	2746	0	2727	1	0
1	5-G	2746	0	2727	2	0
1	6-G	2746	0	2727	1	0
2	1-H	1676	0	1613	1	0
2	2-H	1676	0	1613	1	0
2	3-H	1676	0	1613	1	0
2	4-H	1676	0	1613	0	0
2	5-H	1676	0	1613	0	0
2	6-H	1676	0	1613	0	0
3	1-L	1660	0	1611	1	0
3	2-L	1660	0	1611	0	0
3	3-L	1660	0	1611	1	0
3	4-L	1660	0	1611	1	0
3	5-L	1660	0	1611	0	0
3	6-L	1660	0	1611	0	0
4	1-R	2575	0	2550	3	0
4	2-R	2575	0	2550	1	0
4	3-R	2575	0	2550	3	0
4	4-R	2575	0	2550	1	0
4	5-R	2575	0	2550	4	0
4	6-R	2575	0	2550	1	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	2	0
6	4-R	20	0	27	1	0
6	5-R	20	0	27	2	0
6	6-R	20	0	27	2	0
All	All	52194	0	51258	35	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 (35) 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	1.78	0.64
6:R:401:RET:H181	6:R:401:RET:C8	2.33	0.57
6:R:401:RET:H181	6:R:401:RET:C8	2.35	0.56
6:R:401:RET:H181	6:R:401:RET:C8	2.35	0.56
6:R:401:RET:H181	6:R:401:RET:C8	2.36	0.55
6:R:401:RET:H181	6:R:401:RET:H8	1.89	0.55
6:R:401:RET:H181	6:R:401:RET:H8	1.89	0.54
6:R:401:RET:H181	6:R:401:RET:C8	2.36	0.54
4:R:66:LYS:H	4:R:66:LYS:HD2	1.74	0.52
6:R:401:RET:H181	6:R:401:RET:C8	2.39	0.52
1:G:489:GLU:H	4:R:69:ARG:HH11	1.59	0.50
4:R:195:HIS:H	4:R:200:ASN:HD22	1.59	0.50
6:R:401:RET:H181	6:R:401:RET:H8	1.94	0.49
6:R:401:RET:H181	6:R:401:RET:H8	1.95	0.49
4:R:66:LYS:HD3	4:R:66:LYS:H	1.78	0.48
4:R:33:GLU:H	4:R:36:GLN:HE21	1.60	0.48
1:G:474:ARG:HE	4:R:237:GLN:HE22	1.59	0.48
1:G:187:PHE:HB2	4:R:147:ARG:HE	1.79	0.47
3:L:3:ILE:H	3:L:3:ILE:HD13	1.80	0.46
4:R:66:LYS:H	4:R:66:LYS:CD	2.29	0.46
4:R:66:LYS:H	4:R:66:LYS:HD2	1.82	0.45
1:G:191:ARG:HE	1:G:480:ASN:HA	1.83	0.44
2:H:39:TRP:CE2	2:H:84:LEU:HB2	2.54	0.42
1:G:243:HIS:CE1	1:G:249:SER:HA	2.55	0.42
4:R:87:VAL:HA	4:R:91:PHE:CD2	2.55	0.41
1:G:269:GLY:O	1:G:275:HIS:CE1	2.73	0.41
1:G:191:ARG:HE	1:G:480:ASN:HD22	1.68	0.41
1:G:243:HIS:CE1	1:G:250:LEU:H	2.39	0.41
2:H:179:PHE:CE2	3:L:179:SER:HB2	2.56	0.41
4:R:66:LYS:HD3	4:R:66:LYS:H	1.86	0.41
4:R:87:VAL:HA	4:R:91:PHE:CD2	2.55	0.41
4:R:87:VAL:HA	4:R:91:PHE:CD2	2.56	0.41
2:H:179:PHE:CE2	3:L:179:SER:HB2	2.57	0.40
1:G:287:GLN:H	1:G:290:ARG:HH21	1.68	0.40
1:G:360:LEU:HD23	1:G:366:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	315 (92%)	17 (5%)	10 (3%)	3	26
1	2-G	342/543 (63%)	314 (92%)	19 (6%)	9 (3%)	4	28
1	3-G	342/543 (63%)	315 (92%)	19 (6%)	8 (2%)	5	31
1	4-G	342/543 (63%)	321 (94%)	16 (5%)	5 (2%)	8	39
1	5-G	342/543 (63%)	320 (94%)	16 (5%)	6 (2%)	6	35
1	6-G	342/543 (63%)	316 (92%)	21 (6%)	5 (2%)	8	39
2	1-H	221/234 (94%)	201 (91%)	17 (8%)	3 (1%)	9	39
2	2-H	221/234 (94%)	203 (92%)	14 (6%)	4 (2%)	6	35
2	3-H	221/234 (94%)	208 (94%)	10 (4%)	3 (1%)	9	39
2	4-H	221/234 (94%)	200 (90%)	16 (7%)	5 (2%)	5	31
2	5-H	221/234 (94%)	202 (91%)	13 (6%)	6 (3%)	4	28
2	6-H	221/234 (94%)	208 (94%)	9 (4%)	4 (2%)	6	35
3	1-L	213/217 (98%)	191 (90%)	14 (7%)	8 (4%)	2	21
3	2-L	213/217 (98%)	191 (90%)	14 (7%)	8 (4%)	2	21
3	3-L	213/217 (98%)	188 (88%)	15 (7%)	10 (5%)	2	19
3	4-L	213/217 (98%)	194 (91%)	10 (5%)	9 (4%)	2	20
3	5-L	213/217 (98%)	192 (90%)	12 (6%)	9 (4%)	2	20
3	6-L	213/217 (98%)	190 (89%)	16 (8%)	7 (3%)	3	24
4	1-R	322/348 (92%)	290 (90%)	25 (8%)	7 (2%)	5	31
4	2-R	322/348 (92%)	296 (92%)	21 (6%)	5 (2%)	7	37
4	3-R	322/348 (92%)	298 (92%)	19 (6%)	5 (2%)	7	37
4	4-R	322/348 (92%)	294 (91%)	19 (6%)	9 (3%)	4	27
4	5-R	322/348 (92%)	296 (92%)	21 (6%)	5 (2%)	7	37
4	6-R	322/348 (92%)	301 (94%)	15 (5%)	6 (2%)	6	34
All	All	6588/8052 (82%)	6044 (92%)	388 (6%)	156 (2%)	7	30

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-G	280	ASP
1	1-G	315	LEU
1	1-G	483	ASP
2	1-H	111	TYR
2	1-H	127	ALA
3	1-L	53	SER
3	1-L	82	GLU
4	1-R	2	ASN
1	2-G	280	ASP
1	2-G	478	ALA
1	2-G	482	GLN
2	2-H	111	TYR
3	2-L	33	ALA
3	2-L	53	SER
3	2-L	82	GLU
3	2-L	93	TYR
3	2-L	173	ASP
1	3-G	440	ASP
2	3-H	111	TYR
3	3-L	53	SER
3	3-L	82	GLU
3	3-L	93	TYR
3	3-L	173	ASP
4	3-R	310	ASN
1	4-G	280	ASP
1	4-G	315	LEU
1	4-G	478	ALA
2	4-H	111	TYR
3	4-L	53	SER
3	4-L	93	TYR
3	4-L	214	ARG
4	4-R	310	ASN
1	5-G	315	LEU
3	5-L	53	SER
3	5-L	93	TYR
3	5-L	173	ASP
1	6-G	315	LEU
2	6-H	111	TYR
3	6-L	33	ALA
3	6-L	93	TYR
4	6-R	16	LYS
3	1-L	173	ASP

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Mol	Chain	Res	Type
1	2-G	185	ASP
1	2-G	315	LEU
2	2-H	127	ALA
4	2-R	310	ASN
1	3-G	280	ASP
1	3-G	431	ASP
1	3-G	469	PHE
1	3-G	478	ALA
2	3-H	108	ALA
3	3-L	33	ALA
1	4-G	486	ALA
2	4-H	106	TRP
3	4-L	33	ALA
3	4-L	52	ALA
1	5-G	280	ASP
1	5-G	346	THR
2	5-H	109	ASN
2	5-H	111	TYR
2	5-H	127	ALA
1	6-G	280	ASP
2	6-H	127	ALA
3	6-L	53	SER
3	6-L	173	ASP
1	1-G	441	GLY
2	1-H	105	TRP
3	1-L	33	ALA
3	1-L	214	ARG
4	1-R	16	LYS
4	1-R	29	TYR
1	2-G	184	GLU
1	2-G	469	PHE
3	2-L	51	SER
3	2-L	52	ALA
4	2-R	29	TYR
4	2-R	184	GLN
3	3-L	52	ALA
4	3-R	16	LYS
1	4-G	186	TRP
2	4-H	109	ASN
3	4-L	51	SER
3	4-L	173	ASP
4	4-R	2	ASN

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Mol	Chain	Res	Type
4	4-R	16	LYS
4	4-R	20	VAL
4	4-R	184	GLN
3	5-L	33	ALA
3	5-L	51	SER
3	5-L	52	ALA
4	5-R	16	LYS
4	5-R	29	TYR
4	5-R	184	GLN
2	6-H	109	ASN
3	6-L	214	ARG
4	6-R	29	TYR
4	6-R	184	GLN
4	6-R	239	GLU
1	1-G	186	TRP
1	1-G	257	LYS
1	1-G	266	ILE
1	1-G	267	MET
1	1-G	440	ASP
1	1-G	482	GLN
3	1-L	51	SER
3	1-L	52	ALA
4	1-R	141	LYS
4	1-R	184	GLN
4	1-R	240	SER
4	2-R	16	LYS
1	3-G	313	ARG
2	3-H	109	ASN
3	3-L	51	SER
3	3-L	214	ARG
4	3-R	184	GLN
2	4-H	88	SER
2	4-H	105	TRP
3	4-L	161	ASN
4	4-R	29	TYR
4	4-R	145	ASN
4	4-R	285	PRO
1	5-G	440	ASP
2	5-H	105	TRP
1	6-G	186	TRP
3	6-L	161	ASN
3	6-L	168	GLU

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Mol	Chain	Res	Type
3	2-L	161	ASN
1	3-G	480	ASN
3	3-L	161	ASN
3	5-L	67	ARG
3	5-L	161	ASN
3	5-L	214	ARG
4	5-R	145	ASN
4	5-R	310	ASN
1	6-G	469	PHE
4	6-R	237	GLN
3	1-L	161	ASN
4	1-R	23	PRO
1	2-G	431	ASP
2	2-H	5	VAL
1	3-G	332	ASP
1	5-G	394	GLU
1	5-G	431	ASP
2	5-H	88	SER
3	3-L	206	SER
4	4-R	23	PRO
4	3-R	23	PRO
4	3-R	194	PRO
3	4-L	102	GLY
1	6-G	266	ILE
1	2-G	468	PRO
4	6-R	23	PRO
4	2-R	23	PRO
2	5-H	162	PRO
2	2-H	162	PRO
2	6-H	162	PRO

5.3.2 Protein sidechains ⓘ

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%)	284 (99%)	2 (1%)	76 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-G	286/449 (64%)	284 (99%)	2 (1%)	76	79
1	3-G	286/449 (64%)	284 (99%)	2 (1%)	76	79
1	4-G	286/449 (64%)	284 (99%)	2 (1%)	76	79
1	5-G	286/449 (64%)	284 (99%)	2 (1%)	76	79
1	6-G	286/449 (64%)	284 (99%)	2 (1%)	76	79
2	1-H	184/195 (94%)	183 (100%)	1 (0%)	81	82
2	2-H	184/195 (94%)	183 (100%)	1 (0%)	81	82
2	3-H	184/195 (94%)	183 (100%)	1 (0%)	81	82
2	4-H	184/195 (94%)	183 (100%)	1 (0%)	81	82
2	5-H	184/195 (94%)	183 (100%)	1 (0%)	81	82
2	6-H	184/195 (94%)	183 (100%)	1 (0%)	81	82
3	1-L	190/192 (99%)	184 (97%)	6 (3%)	34	56
3	2-L	190/192 (99%)	184 (97%)	6 (3%)	34	56
3	3-L	190/192 (99%)	184 (97%)	6 (3%)	34	56
3	4-L	190/192 (99%)	184 (97%)	6 (3%)	34	56
3	5-L	190/192 (99%)	184 (97%)	6 (3%)	34	56
3	6-L	190/192 (99%)	184 (97%)	6 (3%)	34	56
4	1-R	276/296 (93%)	275 (100%)	1 (0%)	84	83
4	2-R	276/296 (93%)	275 (100%)	1 (0%)	84	83
4	3-R	276/296 (93%)	275 (100%)	1 (0%)	84	83
4	4-R	276/296 (93%)	275 (100%)	1 (0%)	84	83
4	5-R	276/296 (93%)	275 (100%)	1 (0%)	84	83
4	6-R	276/296 (93%)	275 (100%)	1 (0%)	84	83
All	All	5616/6792 (83%)	5556 (99%)	60 (1%)	63	74

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-G	202	PHE
1	1-G	230	GLN
2	1-H	118	GLN
3	1-L	25	ARG
3	1-L	91	GLN
3	1-L	103	GLN

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Mol	Chain	Res	Type
3	1-L	121	PHE
3	1-L	161	ASN
3	1-L	166	VAL
4	1-R	192	TYR
1	2-G	202	PHE
1	2-G	230	GLN
2	2-H	118	GLN
3	2-L	25	ARG
3	2-L	91	GLN
3	2-L	103	GLN
3	2-L	121	PHE
3	2-L	161	ASN
3	2-L	166	VAL
4	2-R	192	TYR
1	3-G	202	PHE
1	3-G	230	GLN
2	3-H	118	GLN
3	3-L	25	ARG
3	3-L	91	GLN
3	3-L	103	GLN
3	3-L	121	PHE
3	3-L	161	ASN
3	3-L	166	VAL
4	3-R	192	TYR
1	4-G	202	PHE
1	4-G	230	GLN
2	4-H	118	GLN
3	4-L	25	ARG
3	4-L	91	GLN
3	4-L	103	GLN
3	4-L	121	PHE
3	4-L	161	ASN
3	4-L	166	VAL
4	4-R	192	TYR
1	5-G	202	PHE
1	5-G	230	GLN
2	5-H	118	GLN
3	5-L	25	ARG
3	5-L	91	GLN
3	5-L	103	GLN
3	5-L	121	PHE
3	5-L	161	ASN

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Mol	Chain	Res	Type
3	5-L	166	VAL
4	5-R	192	TYR
1	6-G	202	PHE
1	6-G	230	GLN
2	6-H	118	GLN
3	6-L	25	ARG
3	6-L	91	GLN
3	6-L	103	GLN
3	6-L	121	PHE
3	6-L	161	ASN
3	6-L	166	VAL
4	6-R	192	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-G	243	HIS
1	1-G	268	ASN
1	1-G	275	HIS
1	1-G	283	ASN
1	1-G	343	GLN
1	1-G	408	GLN
1	1-G	480	ASN
2	1-H	6	GLN
2	1-H	87	ASN
3	1-L	7	GLN
3	1-L	38	GLN
3	1-L	80	GLN
3	1-L	90	GLN
3	1-L	103	GLN
3	1-L	192	HIS
4	1-R	15	ASN
4	1-R	28	GLN
4	1-R	100	HIS
4	1-R	145	ASN
4	1-R	184	GLN
4	1-R	238	GLN
4	1-R	244	GLN
4	1-R	278	HIS
4	1-R	315	ASN
1	2-G	243	HIS
1	2-G	304	HIS

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Mol	Chain	Res	Type
1	2-G	306	HIS
1	2-G	309	ASN
1	2-G	343	GLN
1	2-G	459	GLN
2	2-H	85	GLN
2	2-H	118	GLN
2	2-H	177	HIS
2	2-H	212	ASN
3	2-L	39	GLN
3	2-L	80	GLN
3	2-L	192	HIS
3	2-L	201	HIS
4	2-R	15	ASN
4	2-R	28	GLN
4	2-R	36	GLN
4	2-R	65	HIS
4	2-R	100	HIS
4	2-R	145	ASN
4	2-R	152	HIS
4	2-R	184	GLN
4	2-R	278	HIS
4	2-R	310	ASN
1	3-G	205	GLN
1	3-G	275	HIS
1	3-G	278	ASN
1	3-G	429	GLN
2	3-H	6	GLN
2	3-H	16	GLN
2	3-H	42	GLN
2	3-H	87	ASN
2	3-H	109	ASN
2	3-H	118	GLN
3	3-L	7	GLN
3	3-L	38	GLN
3	3-L	161	ASN
3	3-L	169	GLN
3	3-L	192	HIS
4	3-R	15	ASN
4	3-R	28	GLN
4	3-R	64	GLN
4	3-R	65	HIS
4	3-R	100	HIS

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Mol	Chain	Res	Type
4	3-R	111	ASN
4	3-R	184	GLN
4	3-R	238	GLN
4	3-R	278	HIS
1	4-G	275	HIS
1	4-G	278	ASN
1	4-G	283	ASN
1	4-G	306	HIS
1	4-G	403	GLN
2	4-H	85	GLN
2	4-H	87	ASN
2	4-H	118	GLN
2	4-H	205	GLN
2	4-H	212	ASN
3	4-L	7	GLN
3	4-L	28	GLN
3	4-L	38	GLN
3	4-L	39	GLN
3	4-L	80	GLN
3	4-L	90	GLN
3	4-L	140	ASN
3	4-L	141	ASN
3	4-L	150	GLN
3	4-L	161	ASN
3	4-L	169	GLN
3	4-L	201	HIS
3	4-L	213	ASN
4	4-R	2	ASN
4	4-R	15	ASN
4	4-R	28	GLN
4	4-R	36	GLN
4	4-R	64	GLN
4	4-R	65	HIS
4	4-R	100	HIS
4	4-R	238	GLN
4	4-R	244	GLN
4	4-R	278	HIS
4	4-R	279	GLN
1	5-G	243	HIS
1	5-G	275	HIS
1	5-G	278	ASN
1	5-G	403	GLN

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Mol	Chain	Res	Type
2	5-H	16	GLN
2	5-H	42	GLN
2	5-H	87	ASN
2	5-H	118	GLN
2	5-H	212	ASN
3	5-L	4	GLN
3	5-L	28	GLN
3	5-L	80	GLN
3	5-L	163	GLN
3	5-L	169	GLN
3	5-L	192	HIS
4	5-R	36	GLN
4	5-R	64	GLN
4	5-R	65	HIS
4	5-R	145	ASN
4	5-R	151	ASN
4	5-R	237	GLN
4	5-R	278	HIS
4	5-R	279	GLN
4	5-R	310	ASN
1	6-G	219	ASN
1	6-G	275	HIS
1	6-G	449	HIS
2	6-H	85	GLN
2	6-H	87	ASN
2	6-H	109	ASN
3	6-L	7	GLN
3	6-L	28	GLN
3	6-L	90	GLN
3	6-L	169	GLN
3	6-L	192	HIS
3	6-L	201	HIS
4	6-R	28	GLN
4	6-R	100	HIS
4	6-R	145	ASN
4	6-R	184	GLN
4	6-R	195	HIS
4	6-R	278	HIS

5.3.3 RNA ⓘ

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](#)

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	1-R	401	-	20,20,21	2.66	3 (15%)	27,27,28	0.88	0
5	SGV	1-G	601	-	24,24,24	0.87	1 (4%)	34,36,36	1.01	2 (5%)
6	RET	3-R	401	-	20,20,21	2.67	4 (20%)	27,27,28	0.86	0
6	RET	5-R	401	-	20,20,21	2.64	3 (15%)	27,27,28	0.92	0
5	SGV	3-G	601	-	24,24,24	0.82	1 (4%)	34,36,36	1.02	2 (5%)
6	RET	4-R	401	-	20,20,21	2.63	4 (20%)	27,27,28	0.89	0
5	SGV	2-G	601	-	24,24,24	0.83	1 (4%)	34,36,36	1.02	2 (5%)
5	SGV	5-G	601	-	24,24,24	0.84	1 (4%)	34,36,36	1.06	3 (8%)
6	RET	2-R	401	-	20,20,21	2.65	4 (20%)	27,27,28	0.98	1 (3%)
6	RET	6-R	401	-	20,20,21	2.66	4 (20%)	27,27,28	0.93	0
5	SGV	6-G	601	-	24,24,24	0.87	1 (4%)	34,36,36	0.94	2 (5%)
5	SGV	4-G	601	-	24,24,24	0.83	1 (4%)	34,36,36	0.99	2 (5%)

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	1-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	1-G	601	-	-	0/10/26/26	0/3/3/3
6	RET	3-R	401	-	-	0/13/30/31	0/1/1/1
6	RET	5-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	3-G	601	-	-	0/10/26/26	0/3/3/3
6	RET	4-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	2-G	601	-	-	0/10/26/26	0/3/3/3
5	SGV	5-G	601	-	-	1/10/26/26	0/3/3/3
6	RET	2-R	401	-	-	0/13/30/31	0/1/1/1
6	RET	6-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	6-G	601	-	-	0/10/26/26	0/3/3/3
5	SGV	4-G	601	-	-	0/10/26/26	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-R	401	RET	C14-C13	10.45	1.40	1.33
6	3-R	401	RET	C14-C13	10.43	1.40	1.33
6	6-R	401	RET	C14-C13	10.39	1.40	1.33
6	5-R	401	RET	C14-C13	10.34	1.40	1.33
6	2-R	401	RET	C14-C13	10.28	1.40	1.33
6	4-R	401	RET	C14-C13	10.24	1.40	1.33
6	1-R	401	RET	C15-C14	-3.29	1.37	1.49
6	4-R	401	RET	C15-C14	-3.29	1.37	1.49
6	2-R	401	RET	C15-C14	-3.28	1.37	1.49
6	6-R	401	RET	C15-C14	-3.28	1.37	1.49
6	5-R	401	RET	C15-C14	-3.27	1.37	1.49
6	3-R	401	RET	C15-C14	-3.27	1.37	1.49
6	1-R	401	RET	C12-C13	-2.59	1.40	1.46
6	5-R	401	RET	C12-C13	-2.56	1.40	1.46
6	2-R	401	RET	C12-C13	-2.56	1.40	1.46
6	3-R	401	RET	C12-C13	-2.55	1.40	1.46
6	6-R	401	RET	C12-C13	-2.53	1.40	1.46
6	4-R	401	RET	C12-C13	-2.53	1.40	1.46
5	1-G	601	SGV	C6-N6	2.36	1.40	1.34
5	6-G	601	SGV	C6-N6	2.36	1.40	1.34
6	2-R	401	RET	C1-C6	2.30	1.56	1.53
6	4-R	401	RET	C1-C6	2.26	1.56	1.53
5	3-G	601	SGV	C6-N6	2.25	1.40	1.34
5	4-G	601	SGV	C6-N6	2.25	1.40	1.34
5	2-G	601	SGV	C6-N6	2.23	1.39	1.34
5	5-G	601	SGV	C6-N6	2.23	1.39	1.34
6	3-R	401	RET	C1-C6	2.10	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6-R	401	RET	C1-C6	2.07	1.56	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1-G	601	SGV	C7-C8-N9	-3.75	108.97	110.54
5	6-G	601	SGV	C7-C8-N9	-3.38	109.12	110.54
5	3-G	601	SGV	C7-C8-N9	-3.26	109.17	110.54
5	5-G	601	SGV	C7-C8-N9	-3.25	109.18	110.54
5	4-G	601	SGV	C7-C8-N9	-3.20	109.20	110.54
5	2-G	601	SGV	C7-C8-N9	-3.12	109.23	110.54
5	3-G	601	SGV	C4-N9-C8	2.74	109.21	108.08
5	2-G	601	SGV	C4-N9-C8	2.71	109.20	108.08
5	5-G	601	SGV	C4-N9-C8	2.67	109.18	108.08
5	4-G	601	SGV	C4-N9-C8	2.63	109.17	108.08
5	1-G	601	SGV	C4-N9-C8	2.38	109.06	108.08
5	5-G	601	SGV	C5'-C4'-C3'	-2.25	109.78	115.10
5	6-G	601	SGV	C4-N9-C8	2.24	109.00	108.08
6	2-R	401	RET	C2-C1-C6	2.19	113.62	110.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	5-G	601	SGV	O4'-C1'-N9-C8

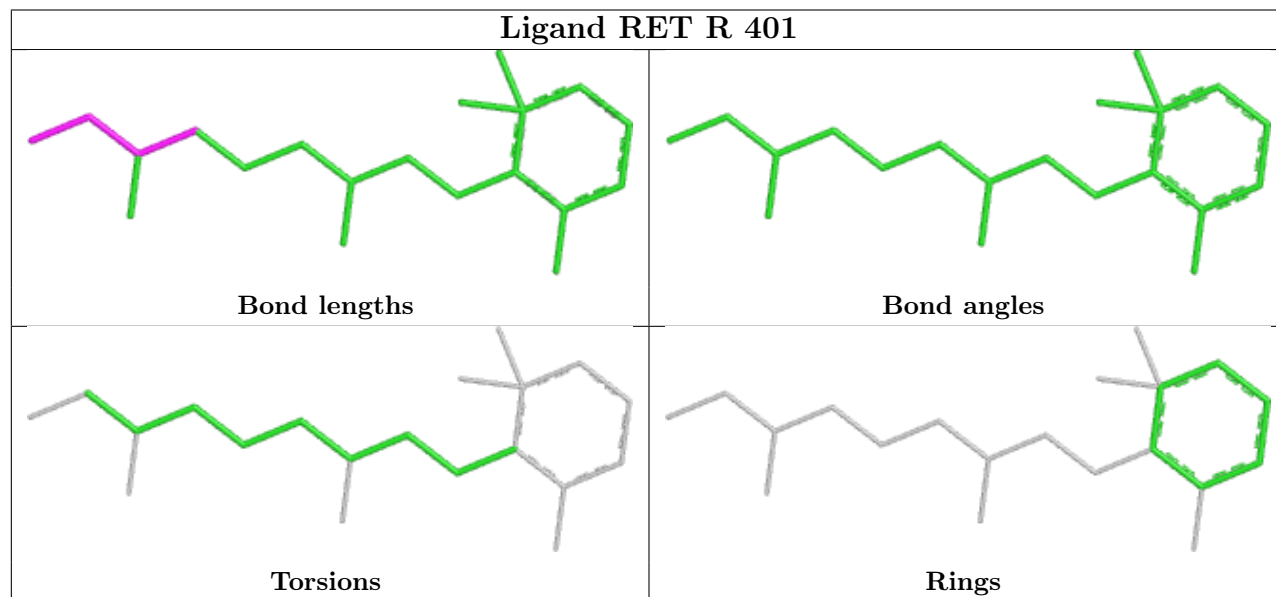
There are no ring outliers.

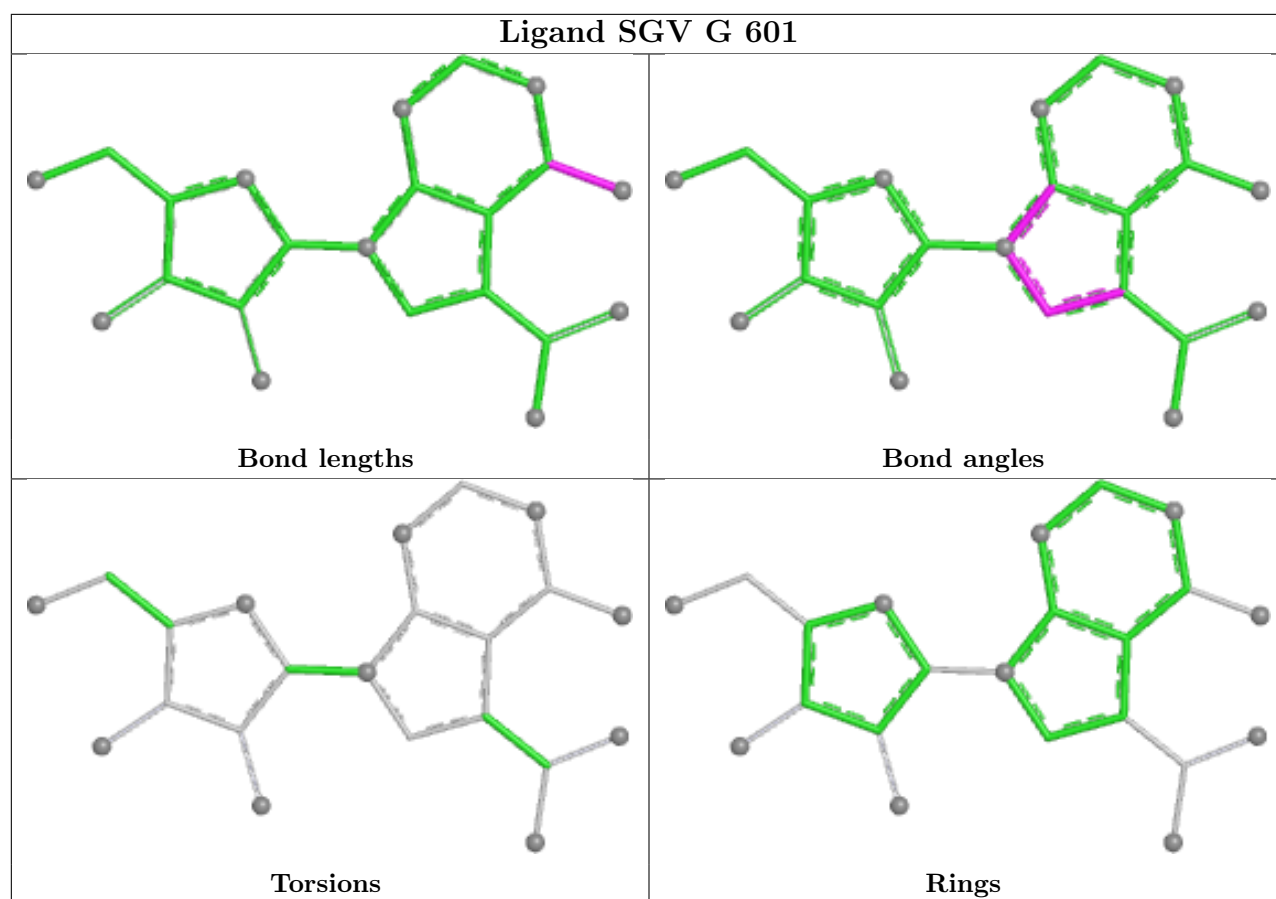
6 monomers are involved in 11 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23979. 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 [i](#)

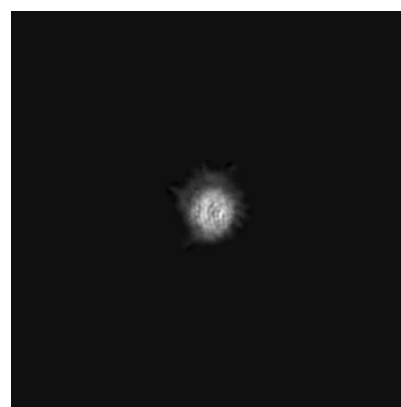
6.1.1 Primary map



X



Y

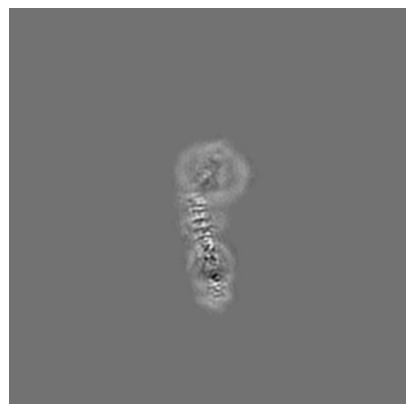


Z

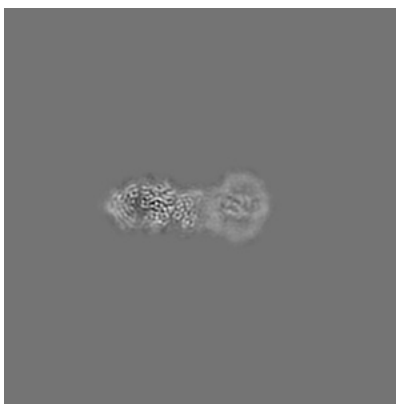
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

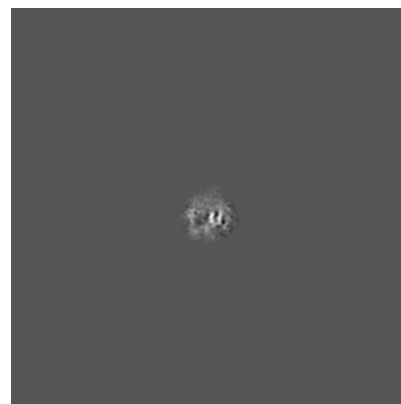
6.2.1 Primary map



X Index: 200



Y Index: 200

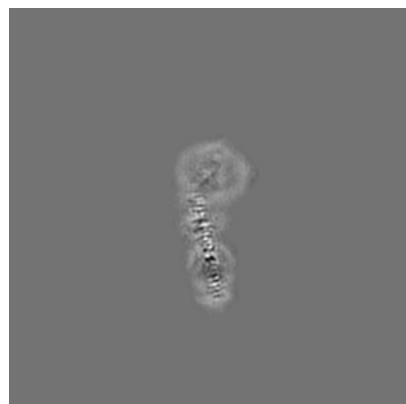


Z Index: 200

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

6.3 Largest variance slices [i](#)

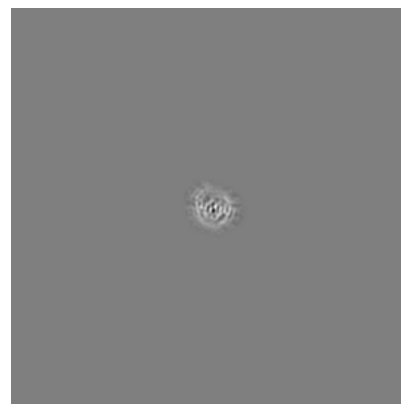
6.3.1 Primary map



X Index: 199



Y Index: 197

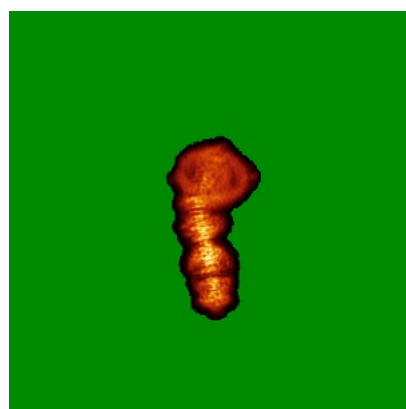


Z Index: 152

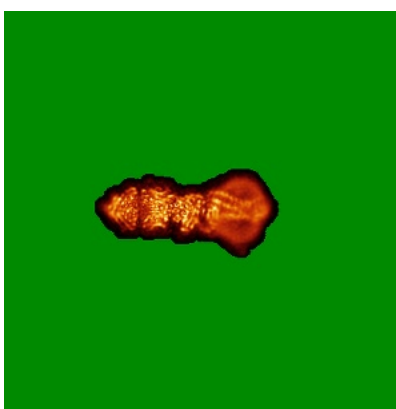
The images above show the largest variance slices of the map in three orthogonal directions.

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

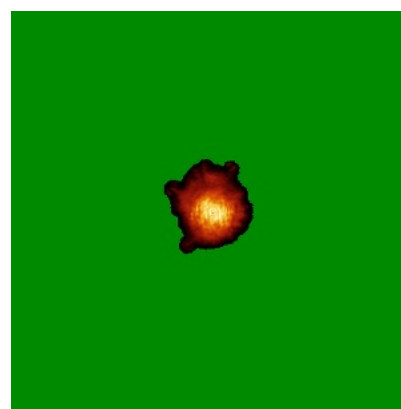
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

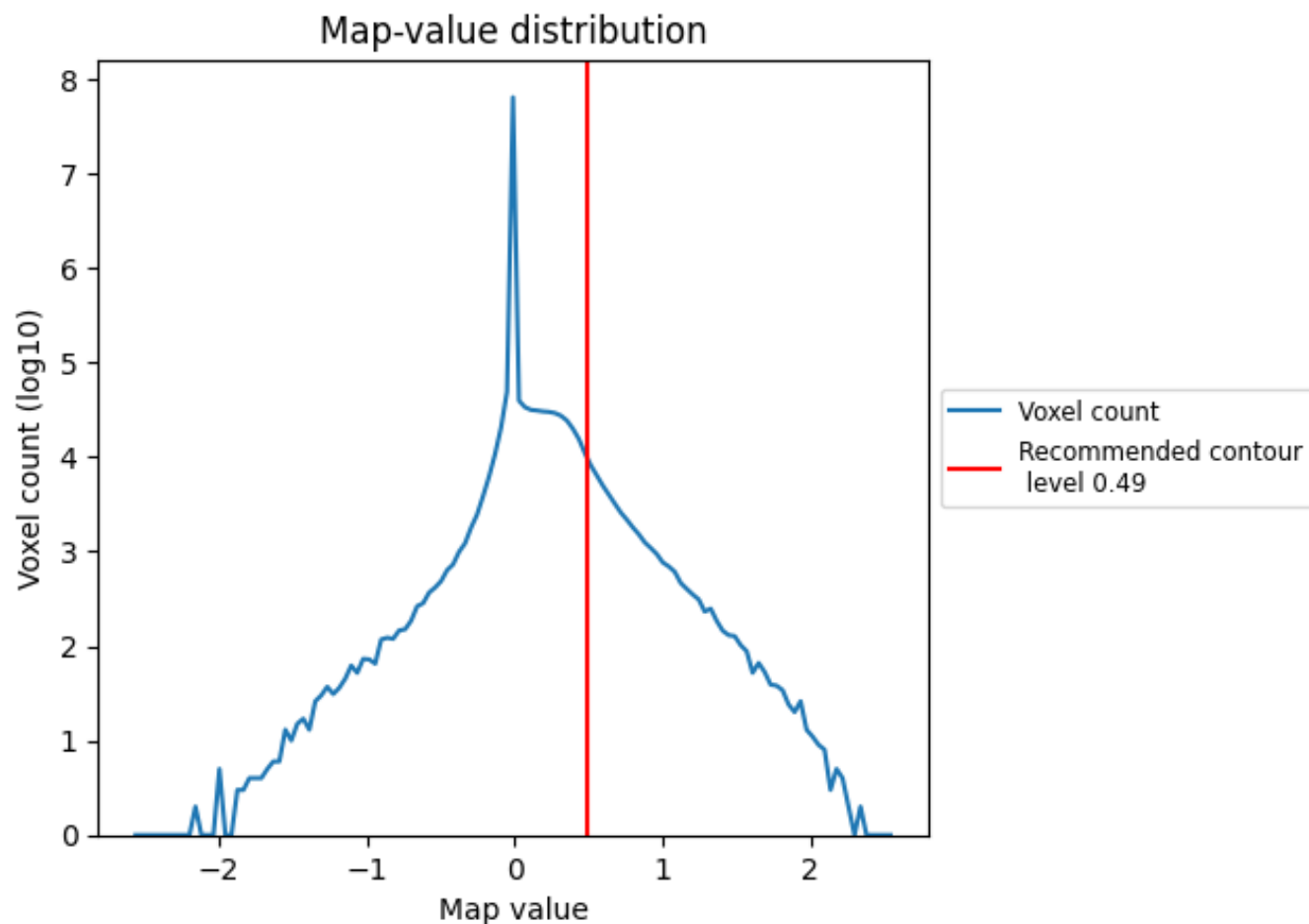
6.6 Mask visualisation

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

7 Map analysis [i](#)

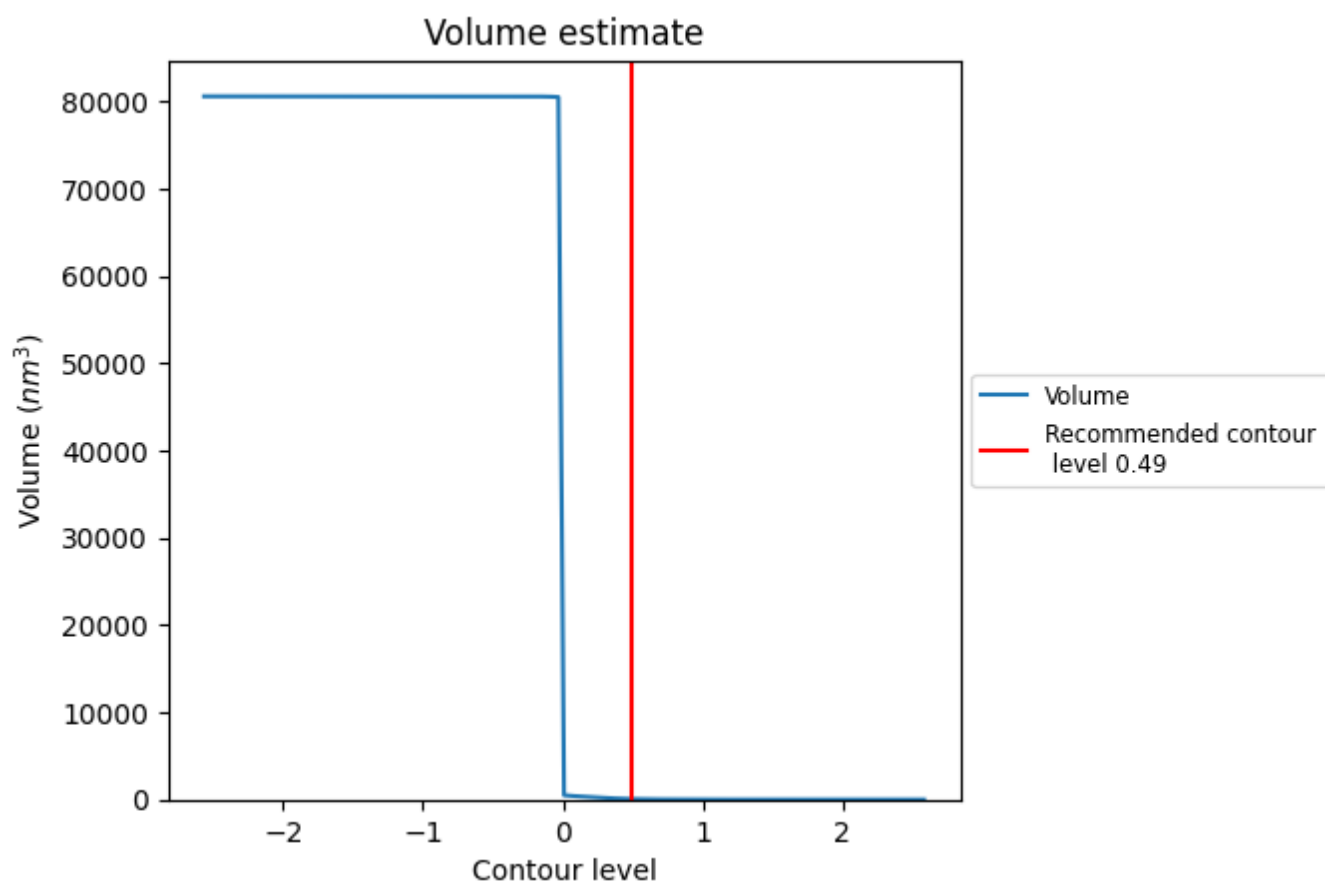
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

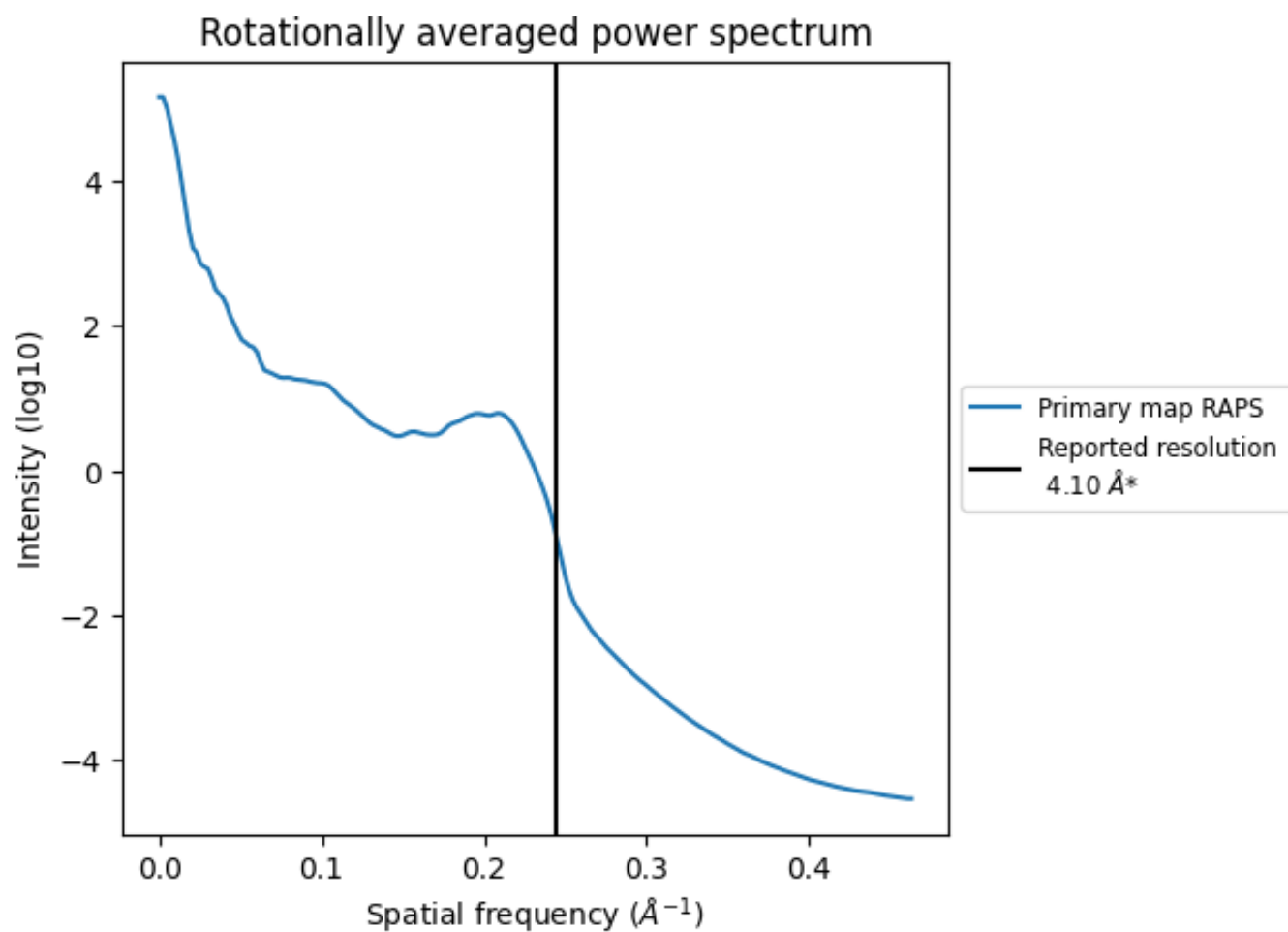
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm^3 ; this corresponds to an approximate mass of 56 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

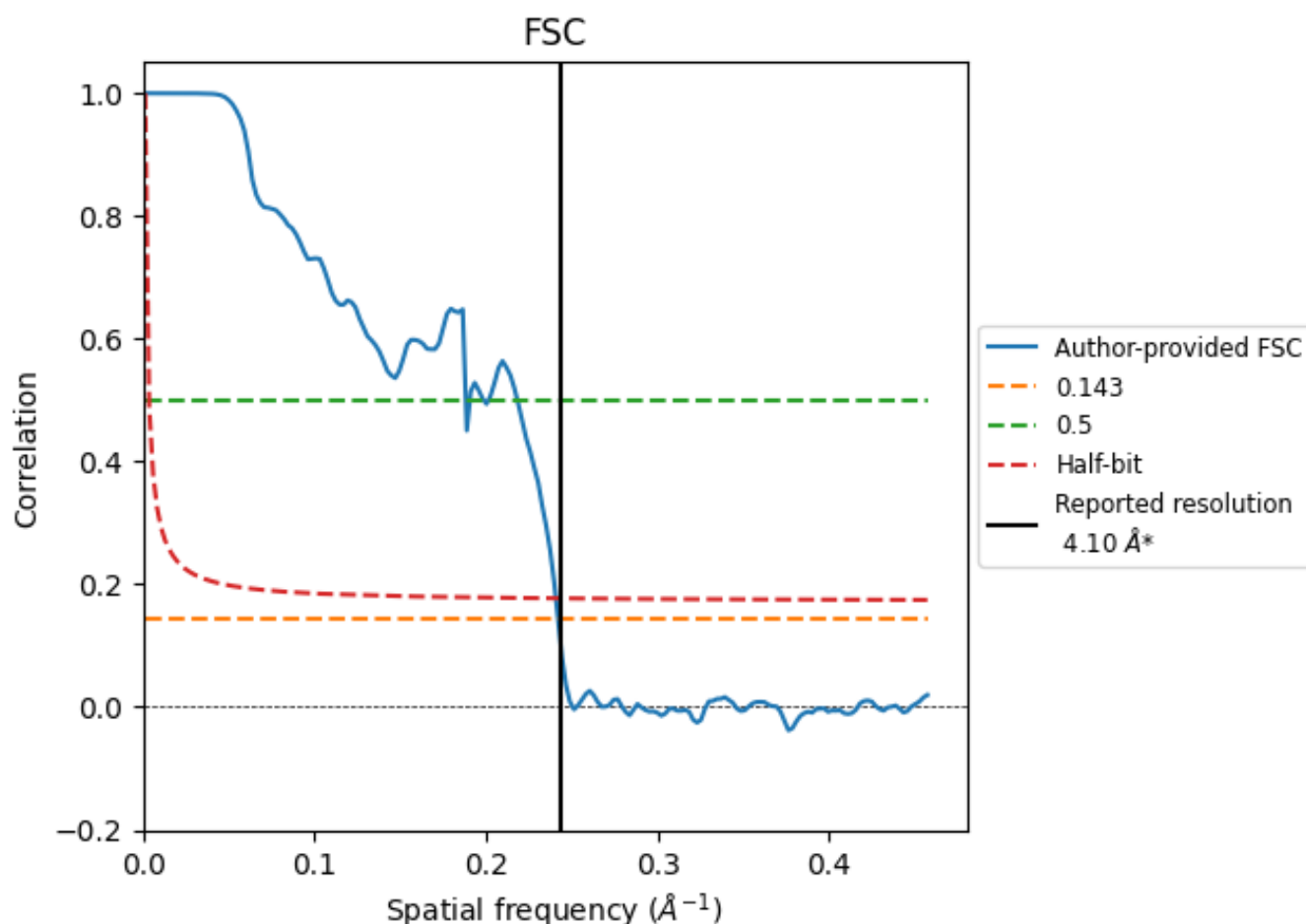


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	5.32	4.16
Unmasked-calculated*	-	-	-

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

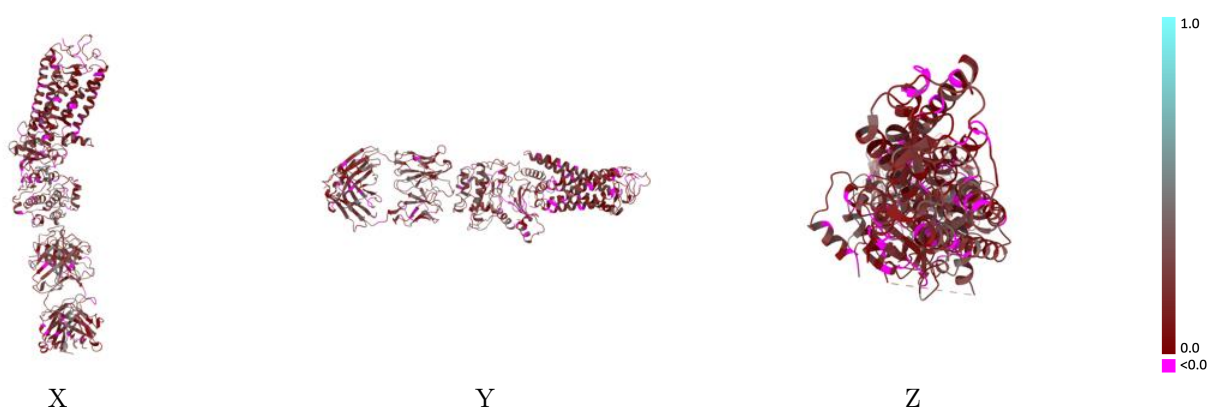
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23979 and PDB model 7MTA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

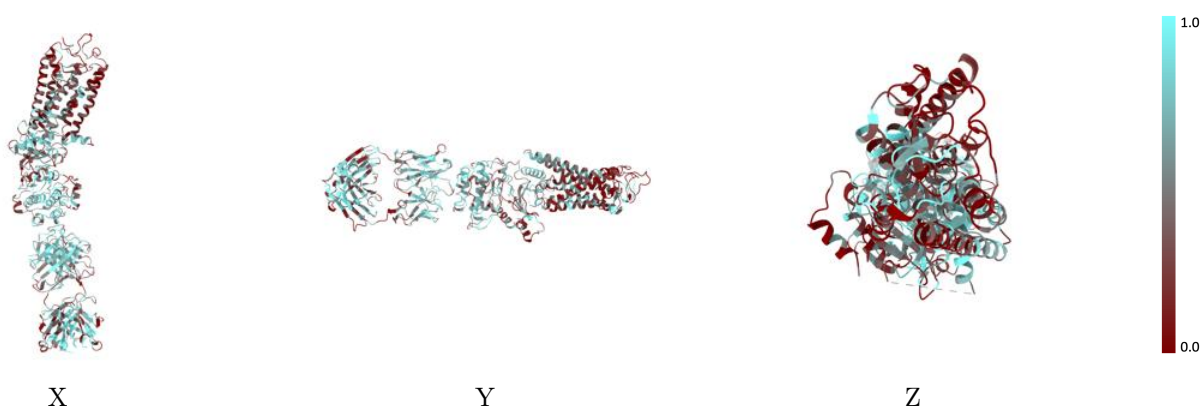
This section was not generated.

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



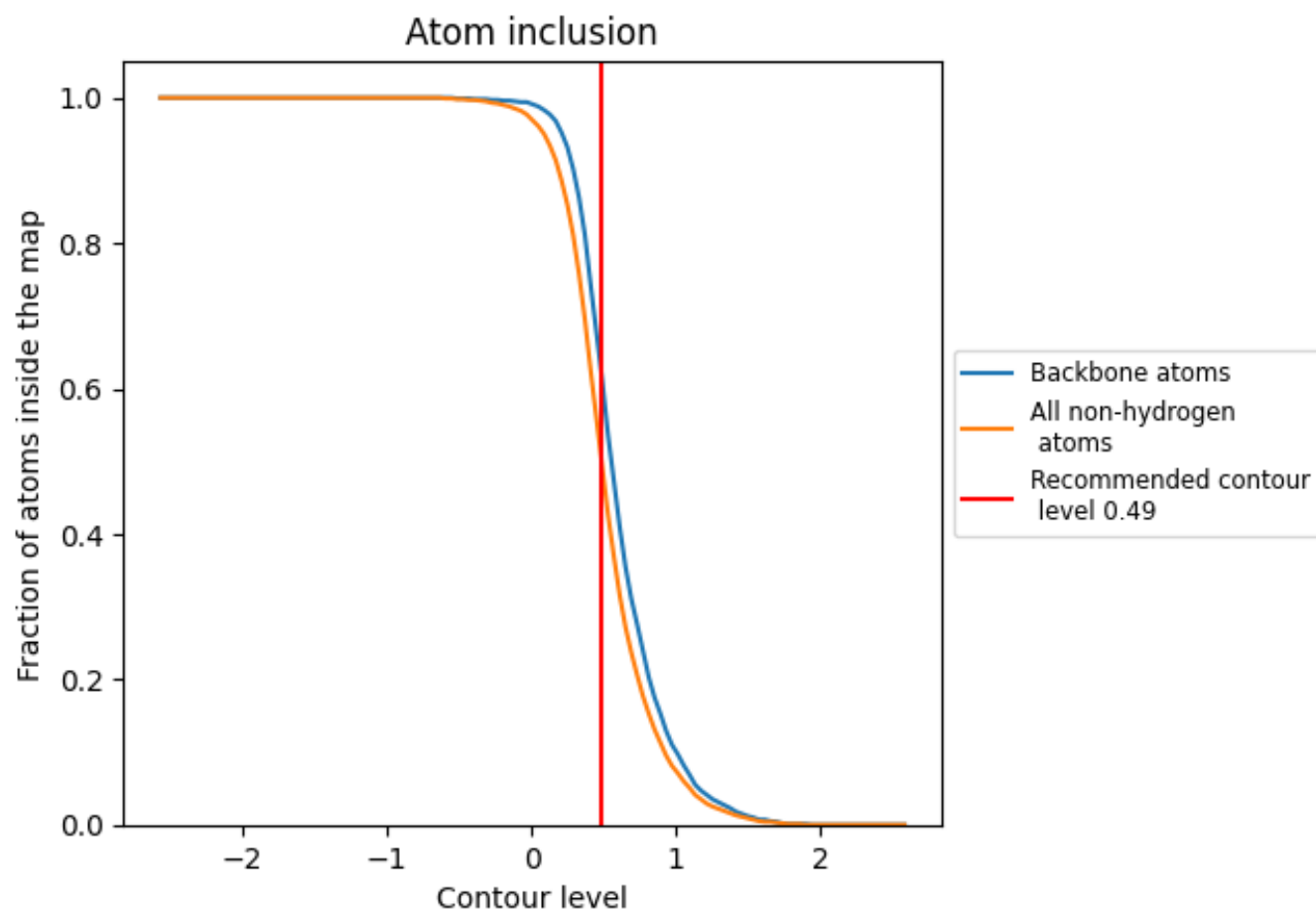
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.49).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 49% 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 (0.49) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.1990
G	0.5330	0.2090
H	0.6000	0.2450
L	0.5430	0.2290
R	0.3540	0.1410

