



## Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 07:44 AM EST

PDB ID : 7MT9  
EMDB ID : EMD-23978  
Title : Rhodopsin kinase (GRK1) in complex with rhodopsin  
Authors : Chen, Q.; Chen, C.-L.; Tesmer, J.J.G.  
Deposited on : 2021-05-13  
Resolution : 7.00 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](mailto: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>.

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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

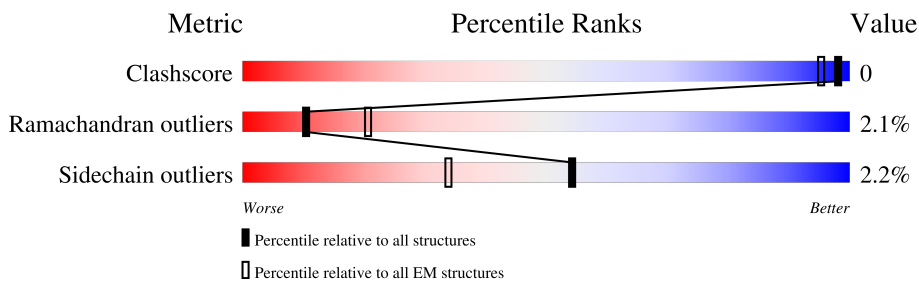
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.00 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  $\geq 3$ , 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	
1	2-G	543	
1	3-G	543	
1	4-G	543	
1	5-G	543	
1	6-G	543	
2	1-R	348	
2	2-R	348	

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Mol	Chain	Length	Quality of chain
2	3-R	348	 89% 5% 7%
2	4-R	348	 88% 5% 7%
2	5-R	348	 89% 5% 7%
2	6-R	348	 90% 5% 7%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 32147 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
			Total	C	N	O	S		
1	1-G	346	2741	1753	470	505	13	0	0
1	2-G	346	2741	1753	470	505	13	0	0
1	3-G	346	2740	1753	469	505	13	0	0
1	4-G	346	2741	1753	470	505	13	0	0
1	5-G	346	2741	1753	470	505	13	0	0
1	6-G	346	2741	1753	470	505	13	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 Rhodopsin.

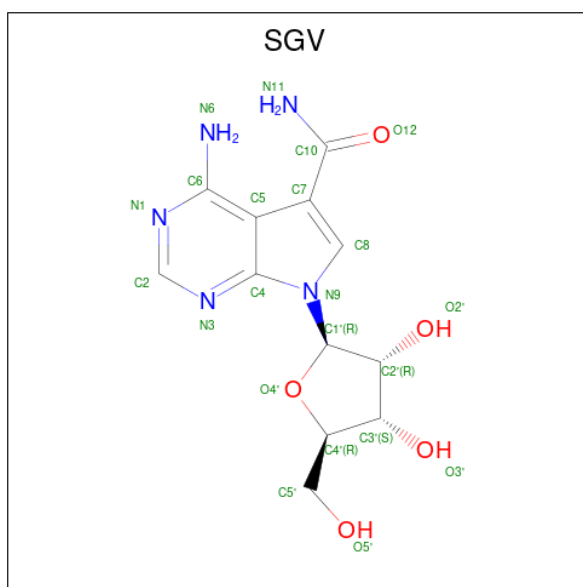
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1-R	324	2575	1715	396	438	26	0	0
2	2-R	324	2575	1715	396	438	26	0	0
2	3-R	324	2575	1715	396	438	26	0	0

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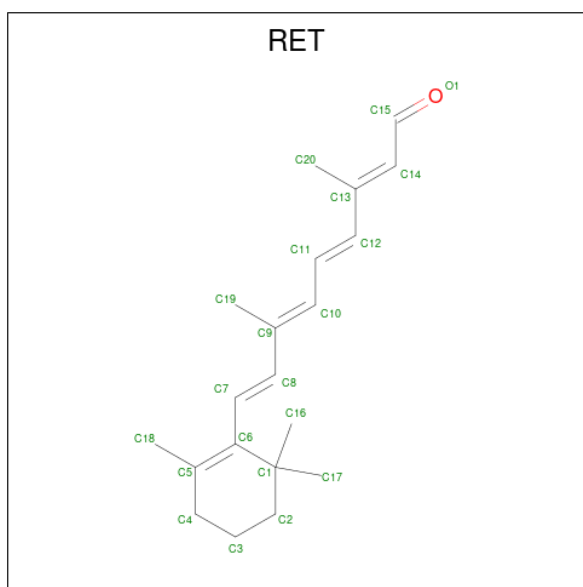
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
2	5-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
2	6-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		

- Molecule 3 is SANGIVAMYCIN (three-letter code: SGV) (formula:  $C_{12}H_{15}N_5O_5$ ).



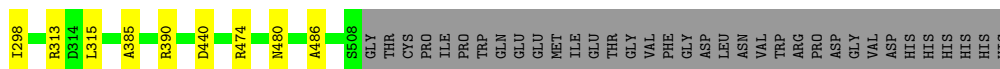
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	1-G	1	Total	C	N	O	0
			22	12	5	5	
3	2-G	1	Total	C	N	O	0
			22	12	5	5	
3	3-G	1	Total	C	N	O	0
			22	12	5	5	
3	4-G	1	Total	C	N	O	0
			22	12	5	5	
3	5-G	1	Total	C	N	O	0
			22	12	5	5	
3	6-G	1	Total	C	N	O	0
			22	12	5	5	

- Molecule 4 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).

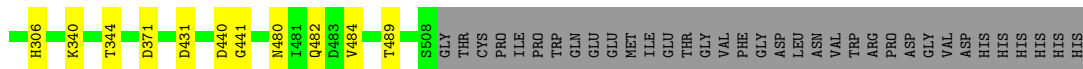
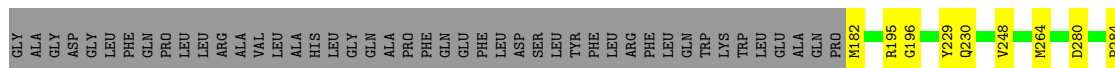
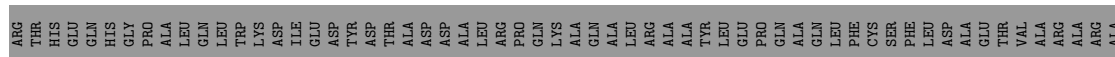
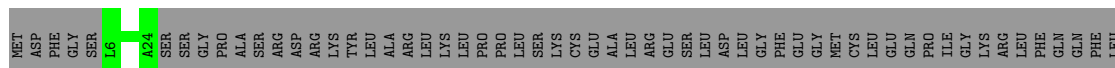


Mol	Chain	Residues	Atoms	AltConf
4	1-R	1	Total C 20 20	0
4	2-R	1	Total C 20 20	0
4	3-R	1	Total C 20 20	0
4	4-R	1	Total C 20 20	0
4	5-R	1	Total C 20 20	0
4	6-R	1	Total C 20 20	0

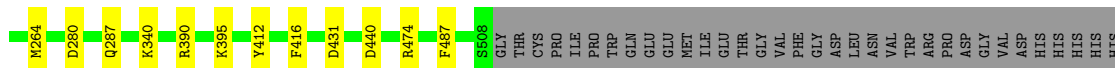
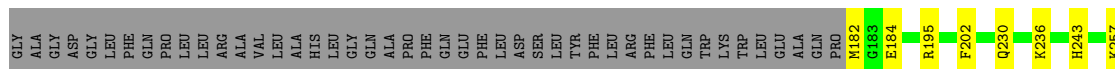
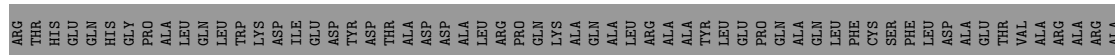
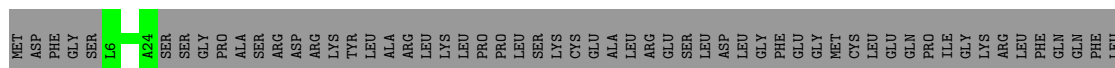




• Molecule 1: Rhodopsin kinase GRK1

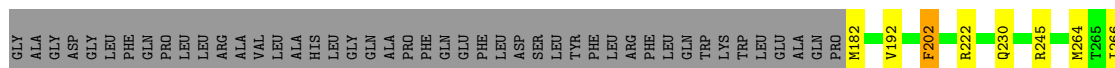
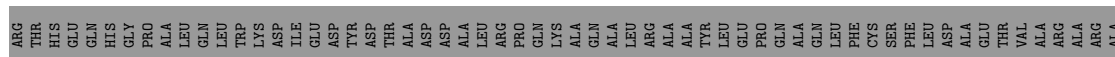
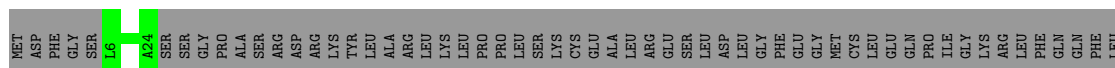


• Molecule 1: Rhodopsin kinase GRK1



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• Molecule 1: Rhodopsin kinase GRK1

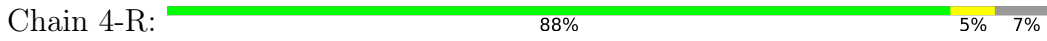








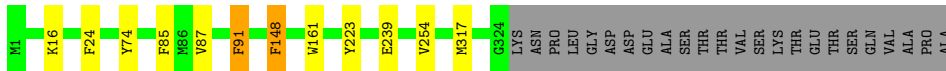
• Molecule 2: Rhodopsin



• Molecule 2: Rhodopsin



• Molecule 2: Rhodopsin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183717	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	0.278	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0435	Depositor
Map size (Å)	216.00002, 216.00002, 216.00002	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.16, 2.16, 2.16	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	0/2798	1.00	0/3765
1	2-G	0.93	0/2798	1.00	1/3765 (0.0%)
1	3-G	0.92	0/2797	0.98	2/3763 (0.1%)
1	4-G	0.93	0/2798	1.00	2/3765 (0.1%)
1	5-G	0.92	0/2798	1.00	3/3765 (0.1%)
1	6-G	0.92	0/2798	1.00	0/3765
2	1-R	0.87	0/2657	0.94	7/3621 (0.2%)
2	2-R	0.88	0/2657	0.96	5/3621 (0.1%)
2	3-R	0.88	0/2657	0.94	6/3621 (0.2%)
2	4-R	0.87	0/2657	0.95	7/3621 (0.2%)
2	5-R	0.87	0/2657	0.93	5/3621 (0.1%)
2	6-R	0.88	0/2657	0.93	6/3621 (0.2%)
All	All	0.90	0/32729	0.97	44/44314 (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	2
1	5-G	0	2
1	6-G	0	1
All	All	0	8

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-R	91	PHE	CB-CG-CD1	6.40	125.28	120.80
2	5-R	74	TYR	CB-CG-CD1	6.36	124.82	121.00
2	3-R	74	TYR	CB-CG-CD1	6.26	124.76	121.00
1	5-G	202	PHE	CB-CG-CD1	6.20	125.14	120.80
2	6-R	74	TYR	CB-CG-CD1	6.16	124.69	121.00
2	4-R	74	TYR	CB-CG-CD1	6.05	124.63	121.00
2	1-R	74	TYR	CB-CG-CD2	-6.02	117.39	121.00
2	3-R	91	PHE	CB-CG-CD2	-6.00	116.60	120.80
2	4-R	74	TYR	CB-CG-CD2	-5.99	117.40	121.00
2	1-R	74	TYR	CB-CG-CD1	5.99	124.59	121.00
2	3-R	74	TYR	CB-CG-CD2	-5.99	117.41	121.00
2	6-R	74	TYR	CB-CG-CD2	-5.97	117.42	121.00
2	2-R	220	PHE	CB-CG-CD2	5.94	124.96	120.80
2	6-R	85	PHE	CB-CG-CD1	5.94	124.96	120.80
2	5-R	74	TYR	CB-CG-CD2	-5.91	117.46	121.00
2	2-R	74	TYR	CB-CG-CD2	5.89	124.53	121.00
2	3-R	220	PHE	CB-CG-CD1	5.84	124.89	120.80
2	6-R	91	PHE	CB-CG-CD1	5.82	124.88	120.80
2	4-R	220	PHE	CB-CG-CD1	5.82	124.88	120.80
2	5-R	220	PHE	CB-CG-CD1	5.80	124.86	120.80
2	1-R	91	PHE	CB-CG-CD1	5.78	124.84	120.80
2	6-R	85	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	5-G	202	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	2-R	74	TYR	CB-CG-CD1	-5.65	117.61	121.00
2	2-R	220	PHE	CB-CG-CD1	-5.59	116.89	120.80
2	4-R	91	PHE	CB-CG-CD1	5.53	124.67	120.80
2	1-R	220	PHE	CB-CG-CD1	5.50	124.65	120.80
2	5-R	220	PHE	CB-CG-CD2	-5.49	116.95	120.80
2	4-R	220	PHE	CB-CG-CD2	-5.48	116.96	120.80
2	2-R	91	PHE	CB-CG-CD1	5.48	124.64	120.80
2	3-R	220	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	4-G	416	PHE	CB-CG-CD2	5.43	124.61	120.80
2	5-R	91	PHE	CB-CG-CD1	5.40	124.58	120.80
2	4-R	148	PHE	CB-CG-CD1	5.39	124.58	120.80
2	6-R	91	PHE	CB-CG-CD2	-5.34	117.06	120.80
2	1-R	91	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	5-G	440	ASP	N-CA-CB	5.14	119.85	110.60
2	1-R	220	PHE	CB-CG-CD2	-5.12	117.22	120.80
2	1-R	148	PHE	CB-CG-CD2	5.06	124.34	120.80
1	3-G	229	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	4-G	416	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	3-G	195	ARG	N-CA-C	-5.03	97.41	111.00
2	4-R	91	PHE	CB-CG-CD2	-5.03	117.28	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-G	385	ALA	N-CA-CB	5.00	117.11	110.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-G	182	MET	Peptide
1	2-G	182	MET	Peptide
1	3-G	182	MET	Peptide
1	4-G	182	MET	Peptide
1	4-G	412	TYR	Sidechain
1	5-G	182	MET	Peptide
1	5-G	222	ARG	Sidechain
1	6-G	182	MET	Peptide

## 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	2741	0	2727	0	0
1	2-G	2741	0	2727	2	0
1	3-G	2740	0	2726	1	0
1	4-G	2741	0	2727	0	0
1	5-G	2741	0	2727	1	0
1	6-G	2741	0	2727	0	0
2	1-R	2575	0	2550	0	0
2	2-R	2575	0	2550	1	0
2	3-R	2575	0	2550	1	0
2	4-R	2575	0	2550	1	0
2	5-R	2575	0	2550	0	0
2	6-R	2575	0	2550	2	0
3	1-G	22	0	15	0	0
3	2-G	22	0	15	0	0
3	3-G	22	0	15	0	0
3	4-G	22	0	15	0	0
3	5-G	22	0	15	0	0
3	6-G	22	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1-R	20	0	27	2	0
4	2-R	20	0	27	2	0
4	3-R	20	0	27	2	0
4	4-R	20	0	27	2	0
4	5-R	20	0	27	2	0
4	6-R	20	0	27	2	0
All	All	32147	0	31913	21	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 (21) 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)
4:R:401:RET:H181	4:R:401:RET:C8	2.33	0.58
4:R:401:RET:H181	4:R:401:RET:C8	2.34	0.57
4:R:401:RET:H181	4:R:401:RET:C8	2.36	0.56
4:R:401:RET:H181	4:R:401:RET:H8	1.88	0.56
4:R:401:RET:H181	4:R:401:RET:C8	2.36	0.55
4:R:401:RET:H181	4:R:401:RET:C8	2.36	0.55
4:R:401:RET:H181	4:R:401:RET:C8	2.37	0.54
1:G:256:THR:HG22	1:G:257:LYS:H	1.75	0.51
4:R:401:RET:H181	4:R:401:RET:H8	1.92	0.51
4:R:401:RET:H181	4:R:401:RET:H8	1.94	0.48
1:G:298:ILE:HG21	1:G:315:LEU:HD21	1.96	0.47
4:R:401:RET:H181	4:R:401:RET:H8	1.94	0.47
2:R:146:PHE:HA	2:R:152:HIS:CE1	2.53	0.44
2:R:87:VAL:HG22	2:R:91:PHE:CE2	2.53	0.44
4:R:401:RET:H181	4:R:401:RET:H8	1.98	0.43
2:R:223:TYR:HB3	2:R:254:VAL:HG13	2.01	0.43
4:R:401:RET:H181	4:R:401:RET:H8	1.98	0.43
2:R:223:TYR:HB3	2:R:254:VAL:HG13	2.00	0.42
2:R:223:TYR:HB3	2:R:254:VAL:HG13	2.02	0.42
1:G:192:VAL:HG22	1:G:481:ILE:HA	2.02	0.41
1:G:306:HIS:CE1	1:G:371:ASP:OD1	2.74	0.41

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%)	310 (91%)	26 (8%)	6 (2%)	8	40
1	2-G	342/543 (63%)	310 (91%)	26 (8%)	6 (2%)	8	40
1	3-G	342/543 (63%)	311 (91%)	20 (6%)	11 (3%)	4	26
1	4-G	342/543 (63%)	315 (92%)	22 (6%)	5 (2%)	10	46
1	5-G	342/543 (63%)	313 (92%)	20 (6%)	9 (3%)	5	31
1	6-G	342/543 (63%)	317 (93%)	20 (6%)	5 (2%)	10	46
2	1-R	322/348 (92%)	298 (92%)	15 (5%)	9 (3%)	5	30
2	2-R	322/348 (92%)	298 (92%)	16 (5%)	8 (2%)	5	32
2	3-R	322/348 (92%)	300 (93%)	16 (5%)	6 (2%)	8	38
2	4-R	322/348 (92%)	300 (93%)	16 (5%)	6 (2%)	8	38
2	5-R	322/348 (92%)	299 (93%)	16 (5%)	7 (2%)	6	35
2	6-R	322/348 (92%)	299 (93%)	19 (6%)	4 (1%)	13	50
All	All	3984/5346 (74%)	3670 (92%)	232 (6%)	82 (2%)	10	36

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-G	280	ASP
1	1-G	431	ASP
1	2-G	280	ASP
1	3-G	280	ASP
1	4-G	280	ASP
1	4-G	395	LYS
1	4-G	487	PHE
2	4-R	148	PHE
1	5-G	280	ASP
1	5-G	332	ASP
1	5-G	440	ASP
1	5-G	482	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6-G	440	ASP
2	6-R	148	PHE
1	1-G	392	ARG
2	1-R	176	SER
2	1-R	239	GLU
2	2-R	176	SER
1	3-G	484	VAL
2	3-R	143	MET
2	3-R	176	SER
1	6-G	431	ASP
2	6-R	239	GLU
1	1-G	478	ALA
2	1-R	2	ASN
2	1-R	16	LYS
2	1-R	285	PRO
1	2-G	480	ASN
1	2-G	486	ALA
2	2-R	16	LYS
1	3-G	196	GLY
1	3-G	344	THR
1	3-G	441	GLY
1	3-G	489	THR
2	3-R	16	LYS
2	3-R	29	TYR
2	3-R	184	GLN
2	4-R	16	LYS
2	4-R	237	GLN
1	5-G	396	VAL
1	5-G	411	THR
2	5-R	2	ASN
2	5-R	16	LYS
1	6-G	186	TRP
1	6-G	280	ASP
2	6-R	16	LYS
1	1-G	346	THR
1	1-G	486	ALA
2	1-R	29	TYR
2	1-R	145	ASN
1	2-G	208	ALA
1	2-G	440	ASP
2	2-R	24	PHE
2	2-R	29	TYR

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Mol	Chain	Res	Type
2	2-R	145	ASN
1	3-G	480	ASN
1	4-G	440	ASP
2	4-R	29	TYR
2	4-R	184	GLN
1	5-G	313	ARG
1	5-G	487	PHE
2	5-R	8	ASN
2	5-R	29	TYR
2	5-R	184	GLN
2	1-R	142	PRO
1	2-G	313	ARG
1	3-G	440	ASP
1	4-G	431	ASP
1	5-G	266	ILE
1	6-G	395	LYS
2	6-R	24	PHE
2	1-R	194	PRO
2	2-R	142	PRO
2	2-R	184	GLN
2	3-R	323	CYS
2	4-R	194	PRO
1	3-G	431	ASP
2	2-R	20	VAL
1	3-G	248	VAL
2	5-R	142	PRO
2	5-R	7	PRO
1	3-G	284	PRO

### 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	286/449 (64%)	281 (98%)	5 (2%)	60	78
1	3-G	285/449 (64%)	281 (99%)	4 (1%)	67	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-G	286/449 (64%)	274 (96%)	12 (4%)	30	54
1	5-G	286/449 (64%)	278 (97%)	8 (3%)	43	65
1	6-G	286/449 (64%)	279 (98%)	7 (2%)	49	69
2	1-R	276/296 (93%)	271 (98%)	5 (2%)	59	77
2	2-R	276/296 (93%)	268 (97%)	8 (3%)	42	64
2	3-R	276/296 (93%)	271 (98%)	5 (2%)	59	77
2	4-R	276/296 (93%)	267 (97%)	9 (3%)	38	61
2	5-R	276/296 (93%)	272 (99%)	4 (1%)	67	80
2	6-R	276/296 (93%)	273 (99%)	3 (1%)	73	84
All	All	3371/4470 (75%)	3296 (98%)	75 (2%)	54	71

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-G	6	LEU
1	1-G	245	ARG
1	1-G	264	MET
1	1-G	390	ARG
1	1-G	482	GLN
2	1-R	8	ASN
2	1-R	66	LYS
2	1-R	70	THR
2	1-R	161	TRP
2	1-R	228	PHE
1	2-G	195	ARG
1	2-G	230	GLN
1	2-G	264	MET
1	2-G	390	ARG
1	2-G	474	ARG
2	2-R	1	MET
2	2-R	67	LYS
2	2-R	78	ASN
2	2-R	141	LYS
2	2-R	228	PHE
2	2-R	247	GLU
2	2-R	254	VAL
2	2-R	311	LYS
1	3-G	230	GLN
1	3-G	264	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	3-G	340	LYS
1	3-G	482	GLN
2	3-R	31	LEU
2	3-R	228	PHE
2	3-R	254	VAL
2	3-R	289	THR
2	3-R	311	LYS
1	4-G	184	GLU
1	4-G	195	ARG
1	4-G	202	PHE
1	4-G	230	GLN
1	4-G	236	LYS
1	4-G	243	HIS
1	4-G	257	LYS
1	4-G	264	MET
1	4-G	287	GLN
1	4-G	340	LYS
1	4-G	390	ARG
1	4-G	474	ARG
2	4-R	2	ASN
2	4-R	31	LEU
2	4-R	67	LYS
2	4-R	70	THR
2	4-R	73	ASN
2	4-R	143	MET
2	4-R	148	PHE
2	4-R	228	PHE
2	4-R	289	THR
1	5-G	202	PHE
1	5-G	230	GLN
1	5-G	245	ARG
1	5-G	264	MET
1	5-G	287	GLN
1	5-G	293	PHE
1	5-G	390	ARG
1	5-G	474	ARG
2	5-R	70	THR
2	5-R	228	PHE
2	5-R	247	GLU
2	5-R	254	VAL
1	6-G	191	ARG
1	6-G	221	LYS

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Mol	Chain	Res	Type
1	6-G	245	ARG
1	6-G	264	MET
1	6-G	287	GLN
1	6-G	430	LYS
1	6-G	482	GLN
2	6-R	148	PHE
2	6-R	161	TRP
2	6-R	317	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-G	306	HIS
2	1-R	28	GLN
2	1-R	65	HIS
2	1-R	100	HIS
2	1-R	195	HIS
2	1-R	211	HIS
2	1-R	312	GLN
1	2-G	275	HIS
2	2-R	15	ASN
2	2-R	28	GLN
2	2-R	279	GLN
2	2-R	310	ASN
1	3-G	275	HIS
1	3-G	482	GLN
2	3-R	65	HIS
2	3-R	78	ASN
2	3-R	152	HIS
2	3-R	312	GLN
1	4-G	306	HIS
2	4-R	65	HIS
2	4-R	195	HIS
2	4-R	312	GLN
1	5-G	307	GLN
2	5-R	111	ASN
2	5-R	195	HIS
2	5-R	211	HIS
2	5-R	310	ASN
2	6-R	195	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
4	RET	3-R	401	-	20,20,21	2.46	4 (20%)	27,27,28	0.95	0
4	RET	2-R	401	-	20,20,21	2.45	4 (20%)	27,27,28	0.92	0
4	RET	4-R	401	-	20,20,21	2.45	4 (20%)	27,27,28	0.96	0
4	RET	6-R	401	-	20,20,21	2.45	4 (20%)	27,27,28	0.93	0
3	SGV	5-G	601	-	22,24,24	1.28	4 (18%)	23,36,36	1.04	1 (4%)
3	SGV	4-G	601	-	22,24,24	1.32	4 (18%)	23,36,36	0.96	2 (8%)
3	SGV	2-G	601	-	22,24,24	1.32	4 (18%)	23,36,36	0.94	1 (4%)
3	SGV	6-G	601	-	22,24,24	1.32	4 (18%)	23,36,36	0.93	0
4	RET	1-R	401	-	20,20,21	2.46	4 (20%)	27,27,28	0.96	1 (3%)
3	SGV	1-G	601	-	22,24,24	1.35	4 (18%)	23,36,36	1.03	2 (8%)
4	RET	5-R	401	-	20,20,21	2.43	3 (15%)	27,27,28	0.94	0
3	SGV	3-G	601	-	22,24,24	1.31	4 (18%)	23,36,36	0.97	2 (8%)

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

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-R	401	RET	C14-C13	9.34	1.40	1.33
4	3-R	401	RET	C14-C13	9.32	1.40	1.33
4	4-R	401	RET	C14-C13	9.30	1.40	1.33
4	6-R	401	RET	C14-C13	9.29	1.40	1.33
4	2-R	401	RET	C14-C13	9.29	1.40	1.33
4	5-R	401	RET	C14-C13	9.17	1.40	1.33
4	4-R	401	RET	C15-C14	-3.24	1.37	1.49
4	5-R	401	RET	C15-C14	-3.22	1.37	1.49
4	6-R	401	RET	C15-C14	-3.20	1.37	1.49
4	1-R	401	RET	C15-C14	-3.20	1.37	1.49
4	2-R	401	RET	C15-C14	-3.19	1.37	1.49
4	3-R	401	RET	C15-C14	-3.17	1.37	1.49
3	2-G	601	SGV	C7-C10	-2.91	1.45	1.50
3	4-G	601	SGV	C7-C10	-2.90	1.45	1.50
3	6-G	601	SGV	C7-C10	-2.76	1.45	1.50
3	3-G	601	SGV	C7-C10	-2.71	1.46	1.50
3	1-G	601	SGV	C7-C10	-2.71	1.46	1.50
3	1-G	601	SGV	C10-N11	2.67	1.38	1.33
3	6-G	601	SGV	C10-N11	2.64	1.38	1.33
3	3-G	601	SGV	C10-N11	2.60	1.37	1.33
3	2-G	601	SGV	C10-N11	2.56	1.37	1.33
3	1-G	601	SGV	O4'-C1'	2.55	1.44	1.41
3	4-G	601	SGV	C10-N11	2.55	1.37	1.33
3	5-G	601	SGV	C10-N11	2.53	1.37	1.33
4	6-R	401	RET	C12-C13	-2.52	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6-G	601	SGV	C2-N3	2.51	1.36	1.32
3	4-G	601	SGV	C2-N3	2.49	1.36	1.32
3	2-G	601	SGV	C2-N3	2.49	1.36	1.32
3	3-G	601	SGV	C2-N3	2.48	1.36	1.32
3	5-G	601	SGV	C7-C10	-2.47	1.46	1.50
4	4-R	401	RET	C12-C13	-2.47	1.40	1.45
4	1-R	401	RET	C12-C13	-2.47	1.40	1.45
4	5-R	401	RET	C12-C13	-2.46	1.40	1.45
3	1-G	601	SGV	C2-N3	2.46	1.36	1.32
4	2-R	401	RET	C12-C13	-2.46	1.40	1.45
3	5-G	601	SGV	C2-N3	2.41	1.36	1.32
4	3-R	401	RET	C12-C13	-2.41	1.40	1.45
3	6-G	601	SGV	O4'-C1'	2.40	1.44	1.41
3	4-G	601	SGV	O4'-C1'	2.37	1.44	1.41
3	3-G	601	SGV	O4'-C1'	2.36	1.44	1.41
3	2-G	601	SGV	O4'-C1'	2.28	1.44	1.41
3	5-G	601	SGV	O4'-C1'	2.26	1.44	1.41
4	1-R	401	RET	C1-C6	2.17	1.56	1.53
4	4-R	401	RET	C1-C6	2.11	1.56	1.53
4	3-R	401	RET	C1-C6	2.11	1.56	1.53
4	2-R	401	RET	C1-C6	2.11	1.56	1.53
4	6-R	401	RET	C1-C6	2.04	1.56	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-G	601	SGV	O12-C10-C7	2.27	122.89	120.22
3	4-G	601	SGV	C7-C10-N11	-2.25	114.86	118.28
3	2-G	601	SGV	C7-C10-N11	-2.11	115.06	118.28
3	3-G	601	SGV	O12-C10-C7	2.10	122.70	120.22
4	1-R	401	RET	C2-C1-C6	2.09	113.71	110.48
3	1-G	601	SGV	O12-C10-C7	2.07	122.66	120.22
3	3-G	601	SGV	C7-C10-N11	-2.07	115.13	118.28
3	1-G	601	SGV	C7-C10-N11	-2.05	115.16	118.28
3	4-G	601	SGV	O12-C10-C7	2.01	122.59	120.22

There are no chirality outliers.

There are no torsion outliers.

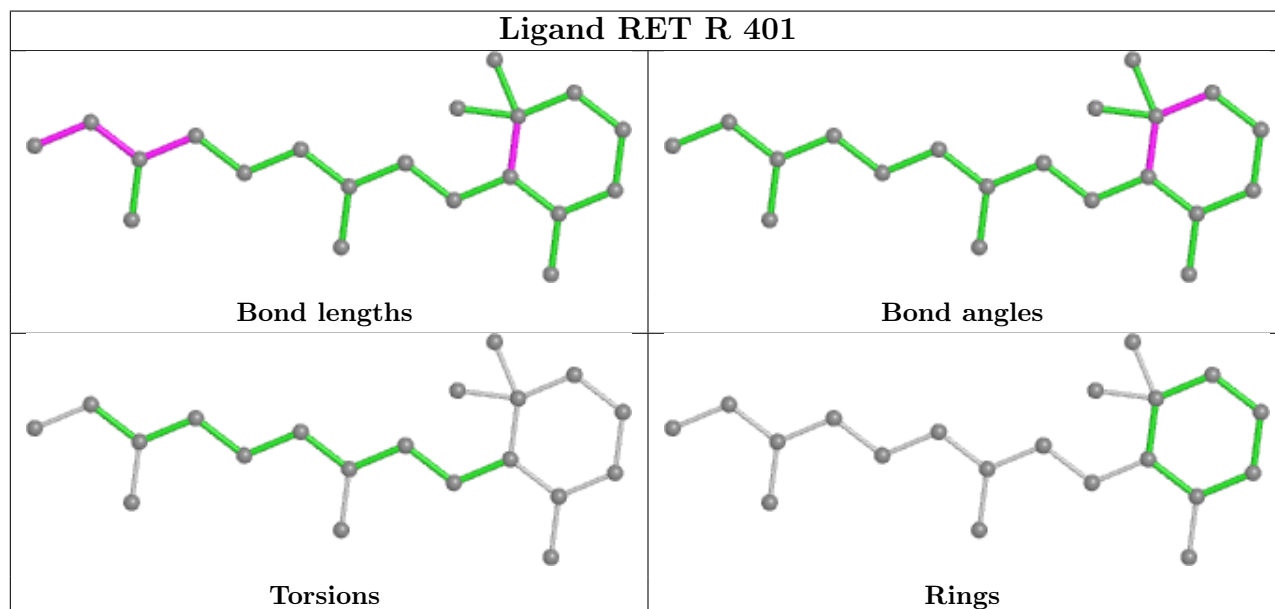
There are no ring outliers.

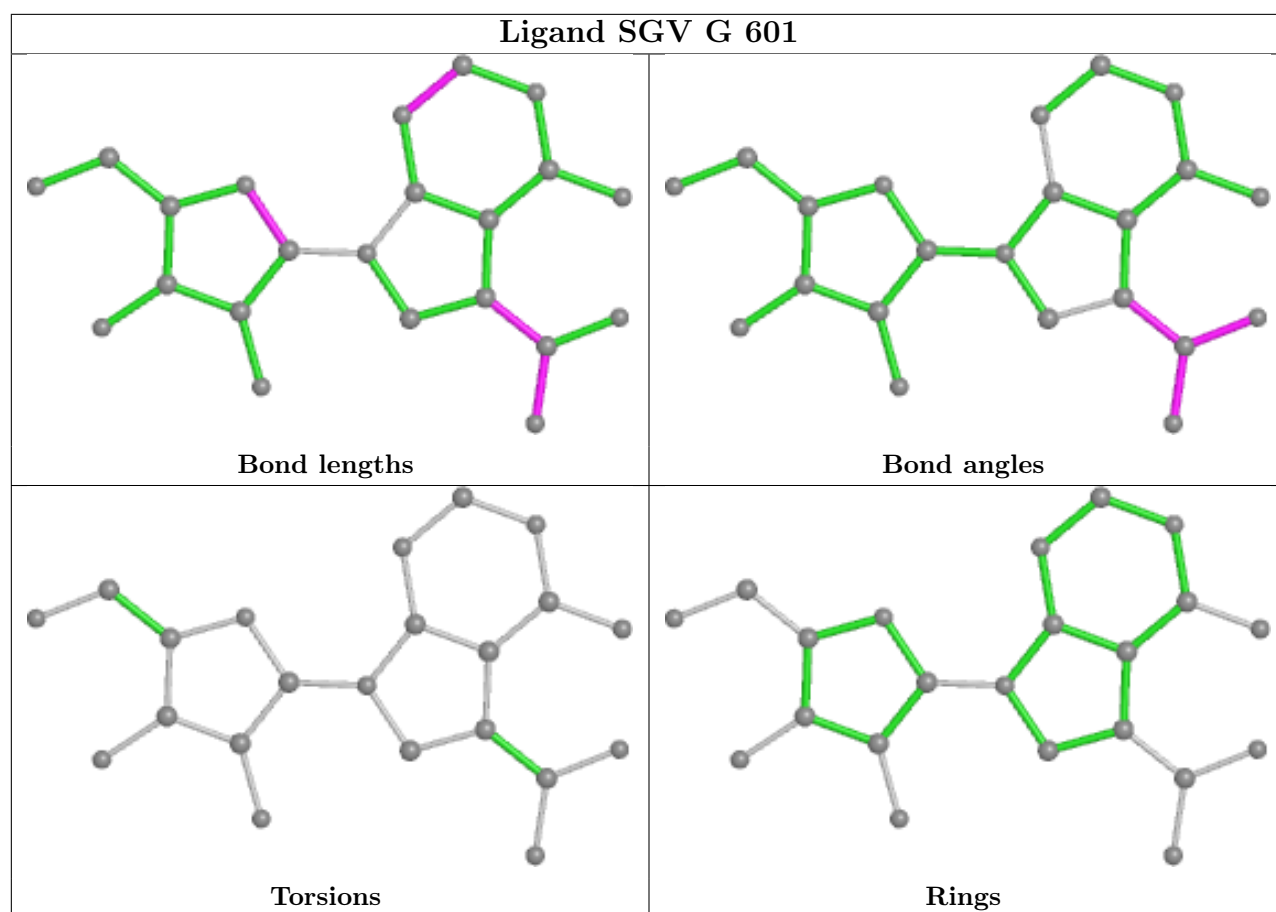
6 monomers are involved in 12 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3-R	401	RET	2	0
4	2-R	401	RET	2	0
4	4-R	401	RET	2	0
4	6-R	401	RET	2	0
4	1-R	401	RET	2	0
4	5-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-23978. 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: 50



Y Index: 50



Z Index: 50

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: 48



Y Index: 50



Z Index: 52

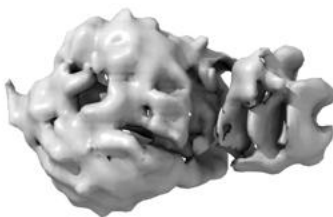
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.0435. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

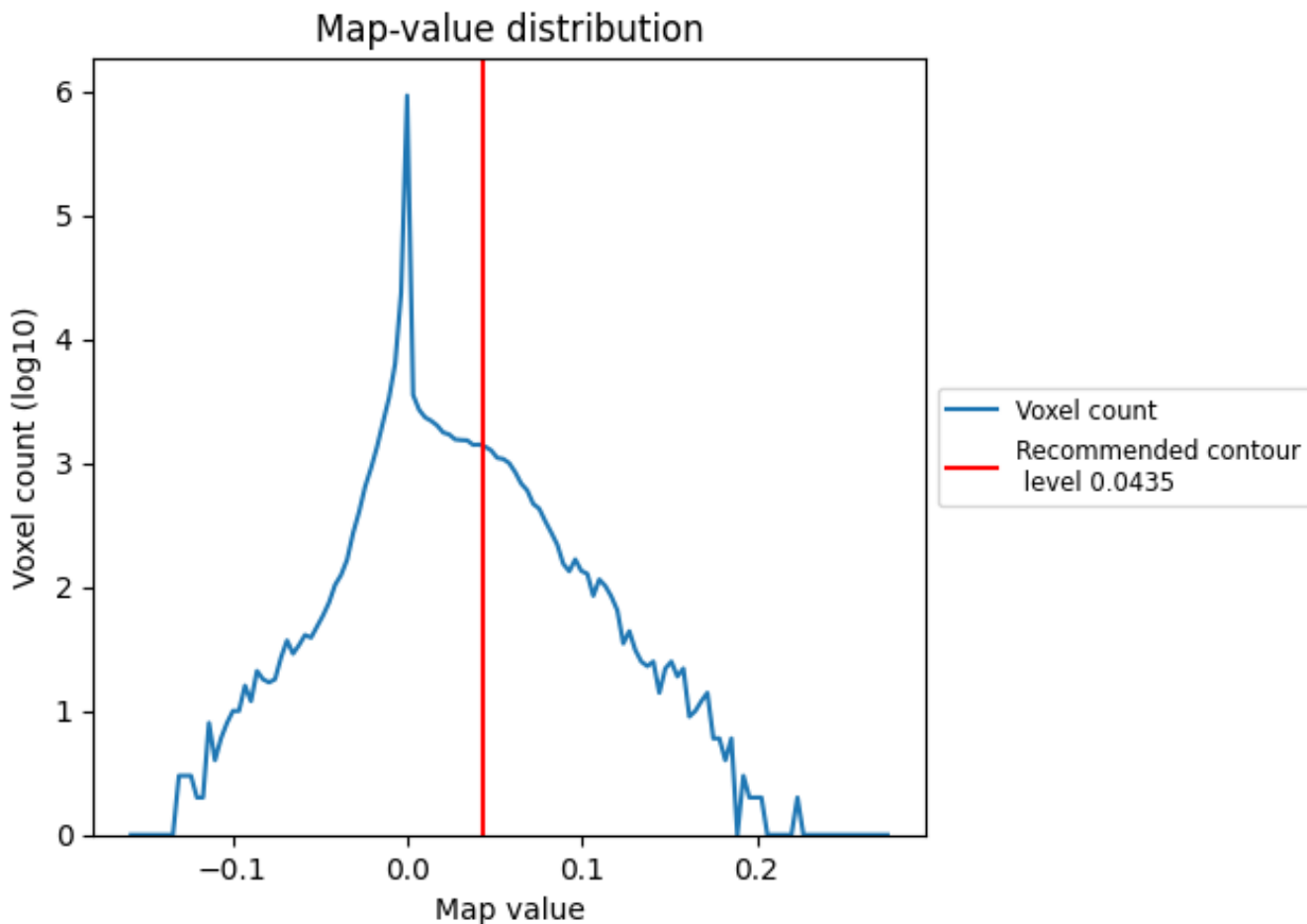
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

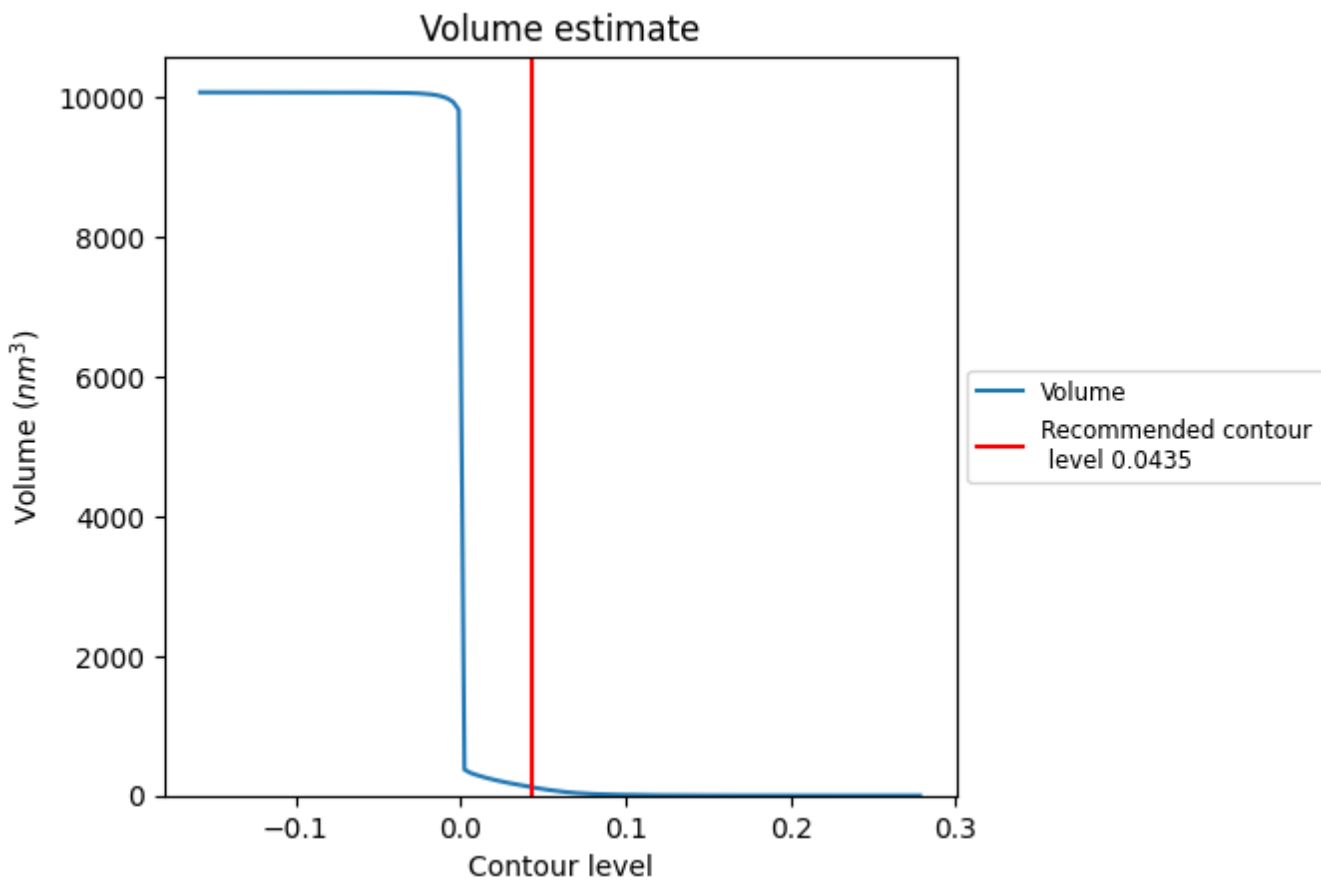
This section contains the results of statistical analysis of the map.

### 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.

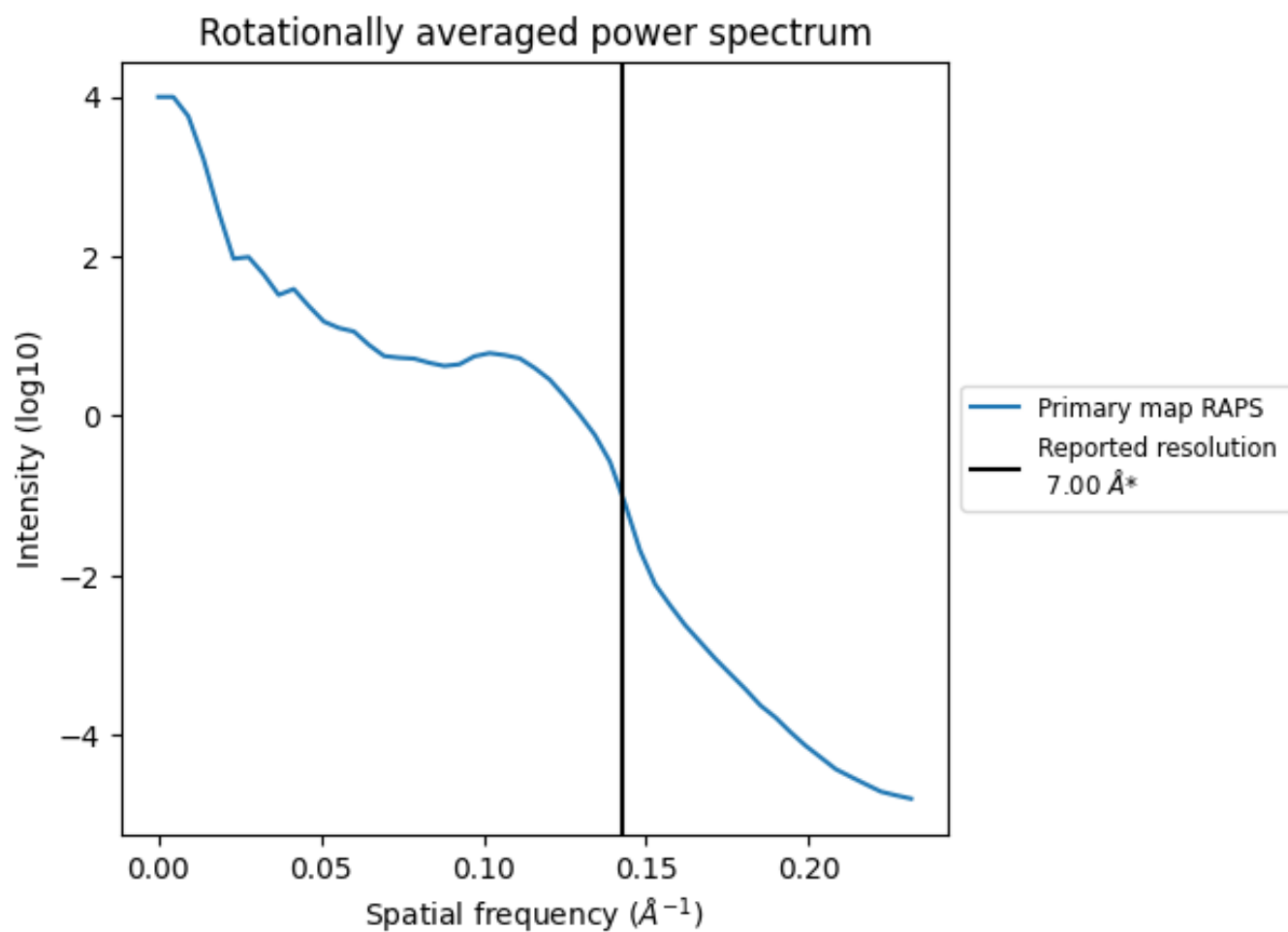
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm<sup>3</sup>; this corresponds to an approximate mass of 106 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](#)



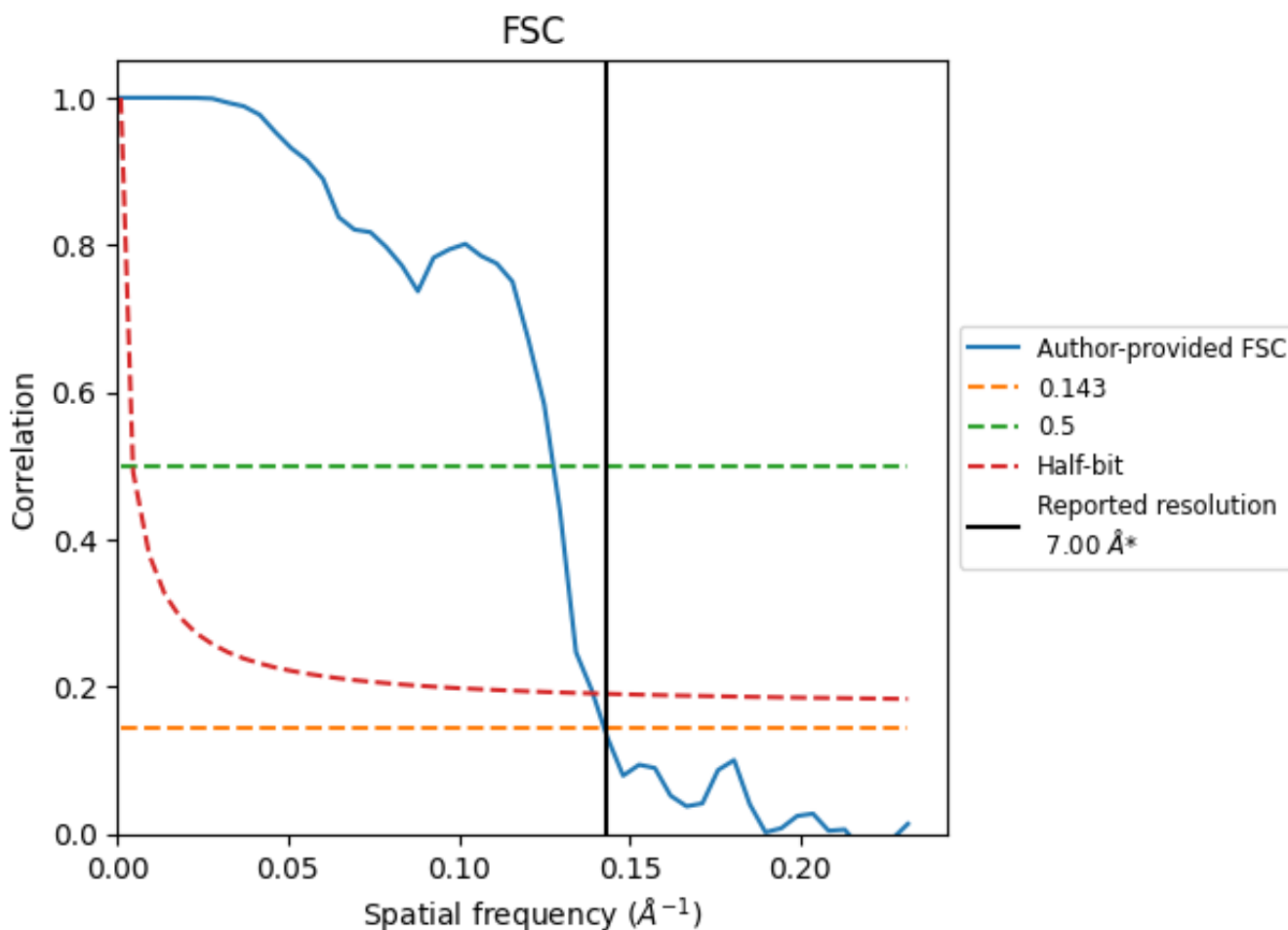
\*Reported resolution corresponds to spatial frequency of 0.143 Å<sup>-1</sup>



## 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 0.143 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

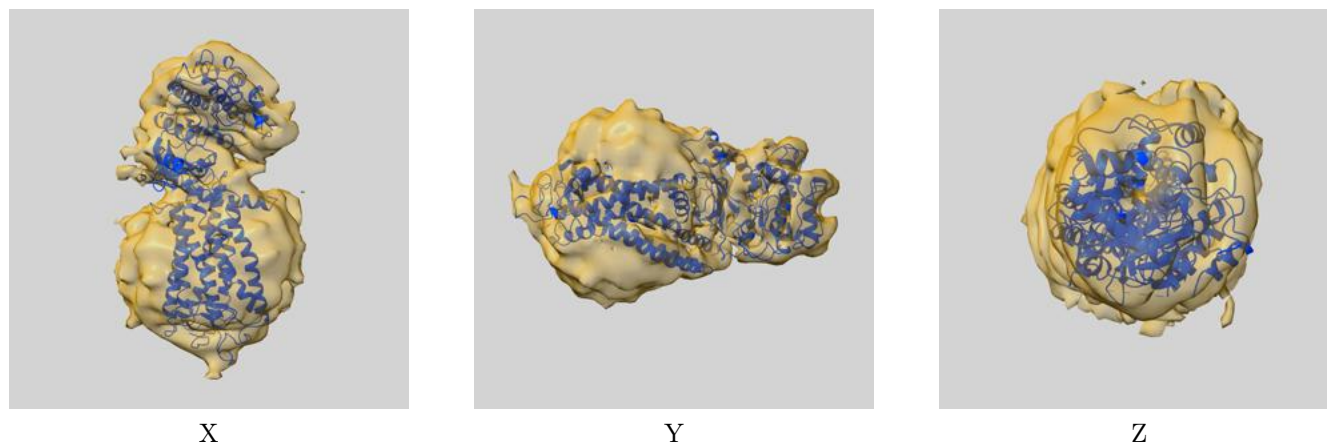
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	7.01	7.83	7.18
Unmasked-calculated*	-	-	-

\*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-23978 and PDB model 7MT9. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)

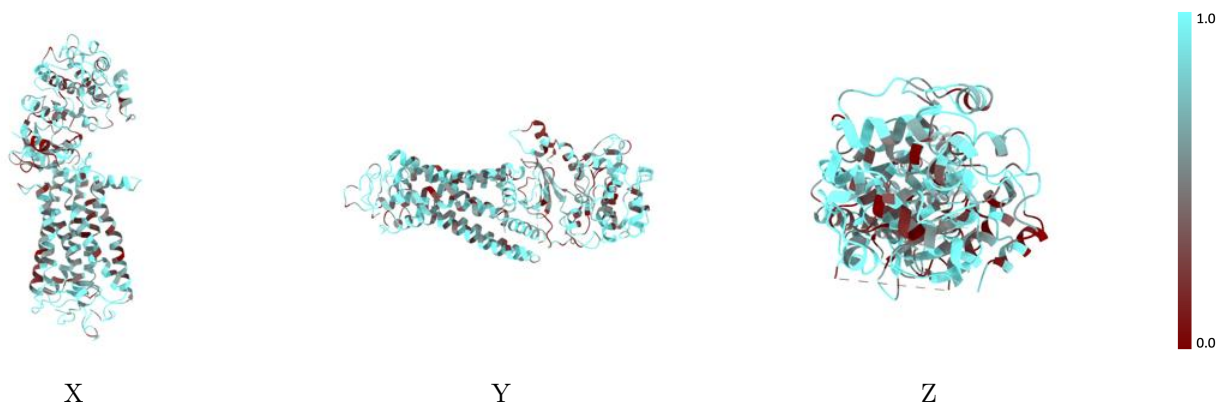


The images above show the 3D surface view of the map at the recommended contour level 0.0435 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

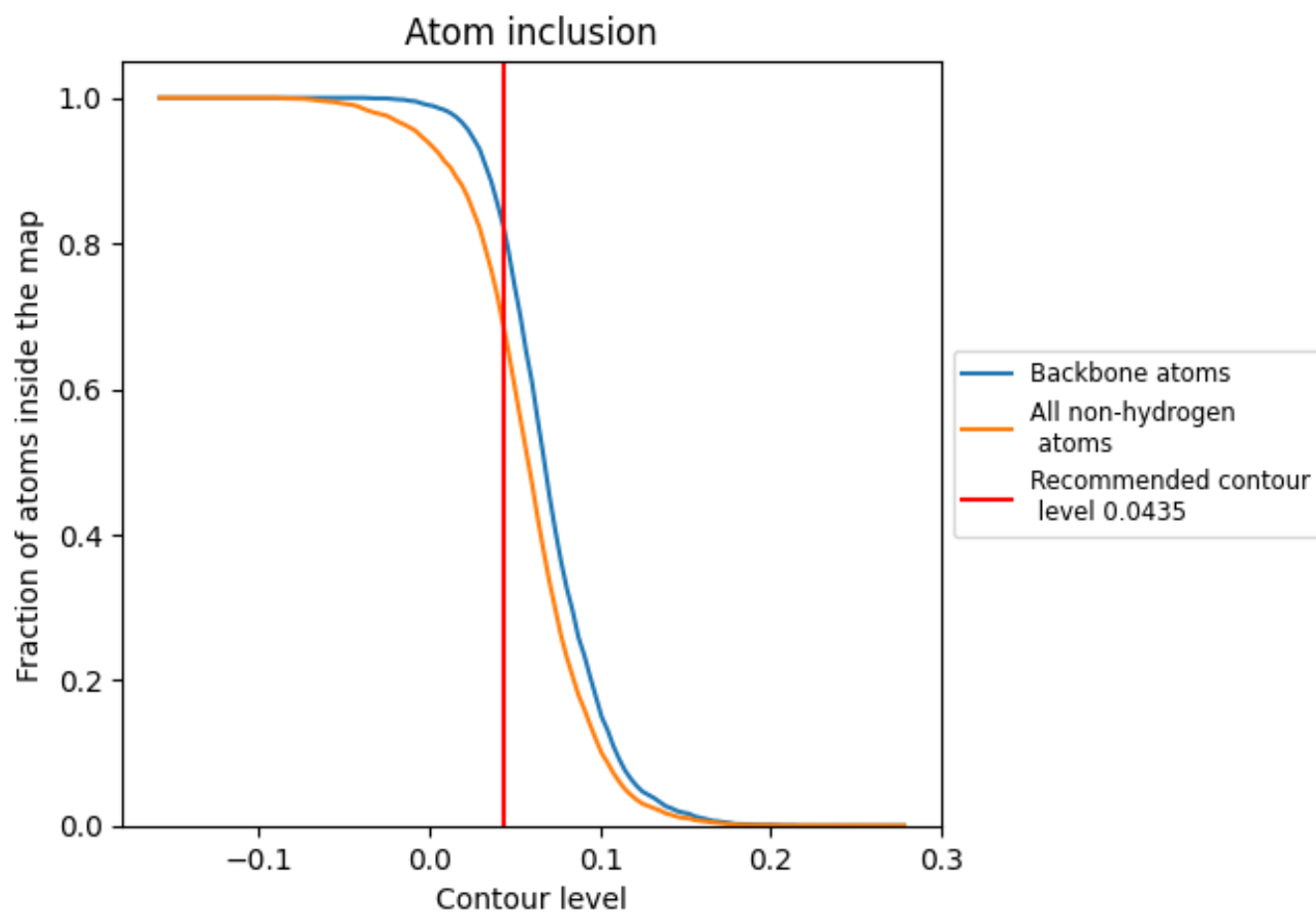
This section was not generated.

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



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 (0.0435).




## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0435) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.6846
G	 0.6681
R	 0.7021

