



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:33 PM UTC

PDB ID : 9WD8 / pdb_00009wd8
EMDB ID : EMD-20967
Title : structure of human KCNQ1-KCNE3-CaM complex with two PIP2
Authors : Cui, C.; Sun, J.
Deposited on : 2025-08-18
Resolution : 3.90 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:

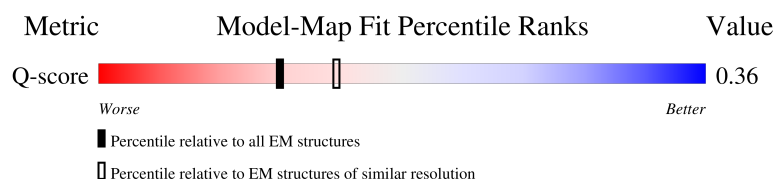
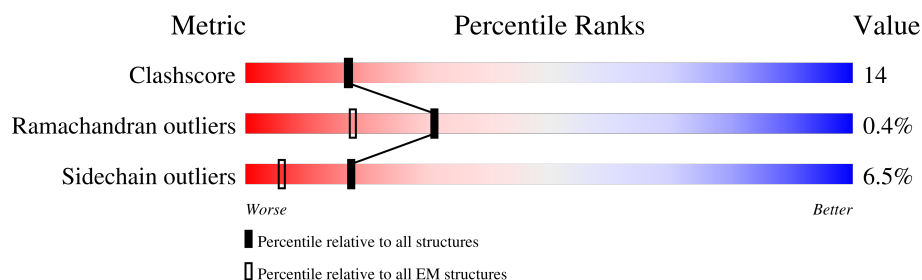
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.90 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	8855 (3.40 - 4.40)

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	B	149	50% 93% 5%
1	E	149	55% 92% 5%
1	H	149	60% 92% 5%
1	K	149	54% 92% 5%

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Mol	Chain	Length	Quality of chain
2	C	106	
2	F	106	
2	I	106	
2	L	106	
3	A	546	
3	D	546	
3	G	546	
3	J	546	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15660 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	144	Total	C	N	O	S	0	0
			828	520	154	152	2		
1	E	144	Total	C	N	O	S	0	0
			828	520	154	152	2		
1	H	144	Total	C	N	O	S	0	0
			828	520	154	152	2		
1	K	144	Total	C	N	O	S	0	0
			828	520	154	152	2		

- Molecule 2 is a protein called Potassium voltage-gated channel subfamily E member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	40	Total	C	N	O	S	0	0
			304	198	50	54	2		
2	F	40	Total	C	N	O	S	0	0
			304	198	50	54	2		
2	I	40	Total	C	N	O	S	0	0
			304	198	50	54	2		
2	L	40	Total	C	N	O	S	0	0
			304	198	50	54	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	104	SER	-	expression tag	UNP Q9Y6H6
C	105	ASN	-	expression tag	UNP Q9Y6H6
C	106	SER	-	expression tag	UNP Q9Y6H6
F	104	SER	-	expression tag	UNP Q9Y6H6
F	105	ASN	-	expression tag	UNP Q9Y6H6
F	106	SER	-	expression tag	UNP Q9Y6H6
I	104	SER	-	expression tag	UNP Q9Y6H6
I	105	ASN	-	expression tag	UNP Q9Y6H6
I	106	SER	-	expression tag	UNP Q9Y6H6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	104	SER	-	expression tag	UNP Q9Y6H6
L	105	ASN	-	expression tag	UNP Q9Y6H6
L	106	SER	-	expression tag	UNP Q9Y6H6

- Molecule 3 is a protein called Potassium voltage-gated channel subfamily KQT member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	331	Total	C	N	O	S	0	0
			2682	1762	470	439	11		
3	D	331	Total	C	N	O	S	0	0
			2682	1762	470	439	11		
3	G	331	Total	C	N	O	S	0	0
			2682	1762	470	439	11		
3	J	331	Total	C	N	O	S	0	0
			2682	1762	470	439	11		

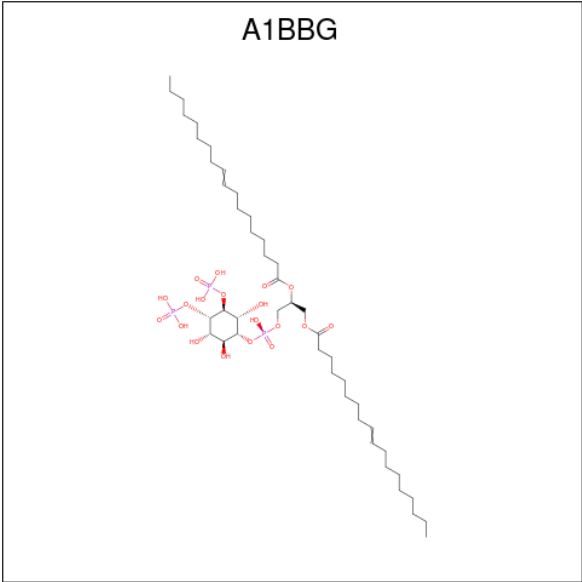
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	initiating methionine	UNP P51787
D	75	MET	-	initiating methionine	UNP P51787
G	75	MET	-	initiating methionine	UNP P51787
J	75	MET	-	initiating methionine	UNP P51787

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Ca	0
			2	2	
4	E	2	Total	Ca	0
			2	2	
4	H	2	Total	Ca	0
			2	2	
4	K	2	Total	Ca	0
			2	2	

- Molecule 5 is (2R)-3-[[[(S)-hydroxy{[(1R,2R,3S,4R,5R,6S)-2,3,6-trihydroxy-4,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl di[(9Z)-octadec-9-enoate] (CCD ID: A1BBG) (formula: C₄₅H₈₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).

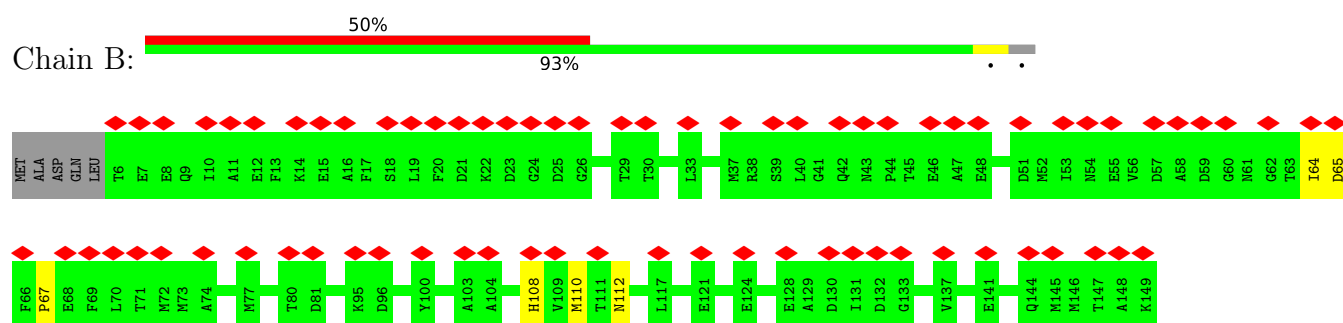


Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			45	23	19	3	
5	A	1	Total	C	O	P	0
			54	32	19	3	
5	D	1	Total	C	O	P	0
			54	32	19	3	
5	G	1	Total	C	O	P	0
			54	32	19	3	
5	J	1	Total	C	O	P	0
			54	32	19	3	
5	F	1	Total	C	O	P	0
			45	23	19	3	
5	I	1	Total	C	O	P	0
			45	23	19	3	
5	L	1	Total	C	O	P	0
			45	23	19	3	

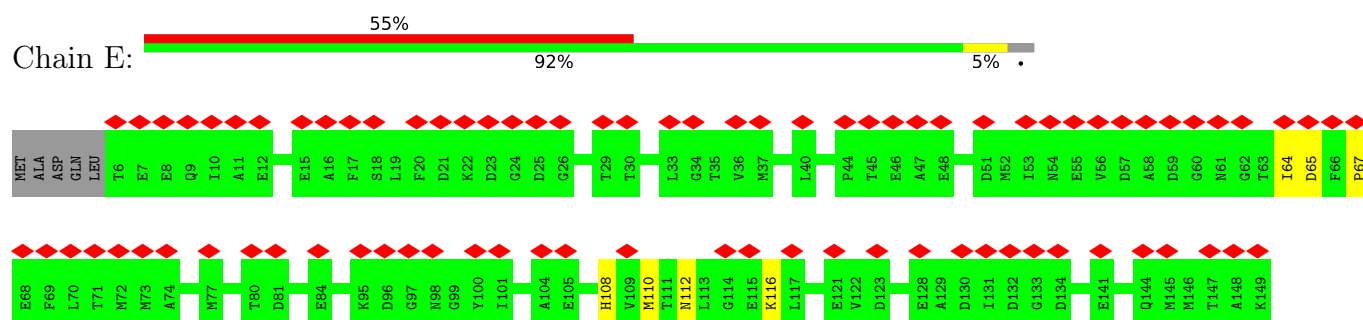
3 Residue-property plots [i](#)

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.

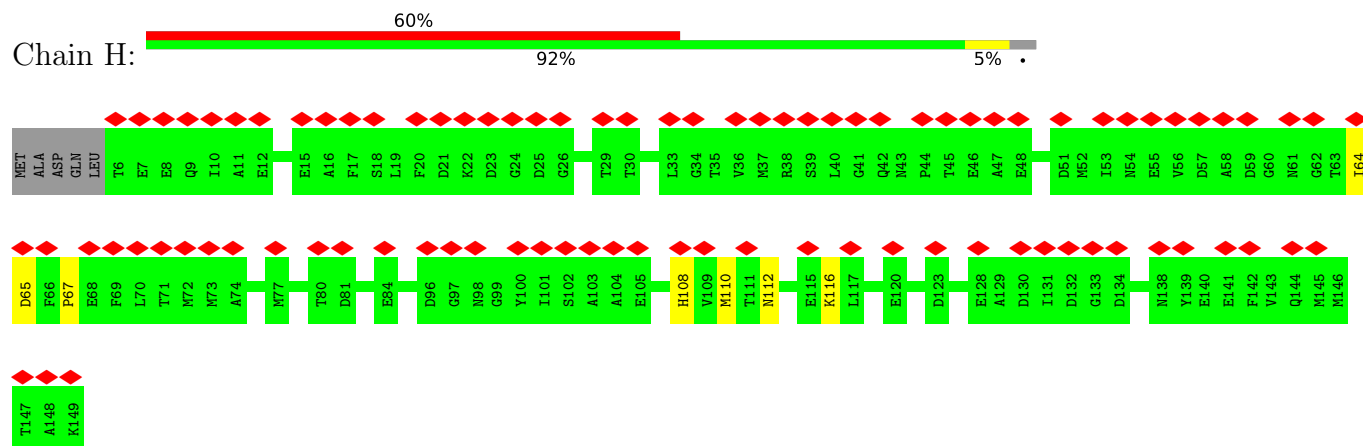
• Molecule 1: Calmodulin-1



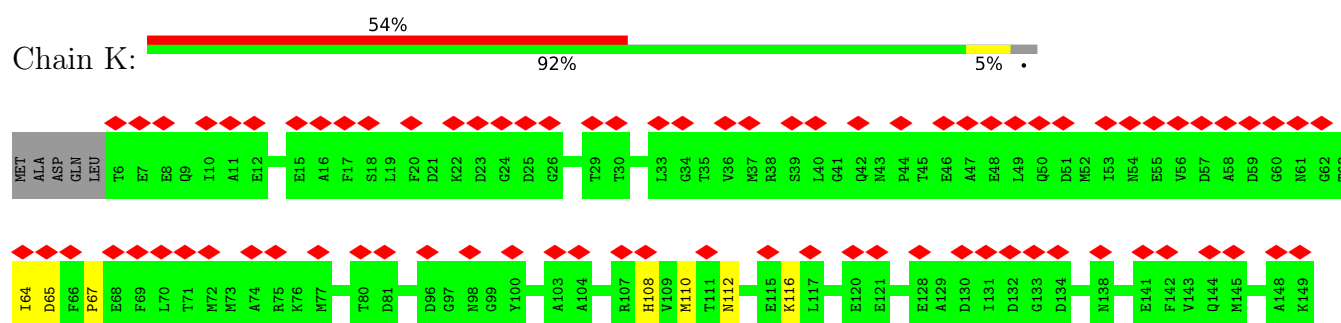
• Molecule 1: Calmodulin-1



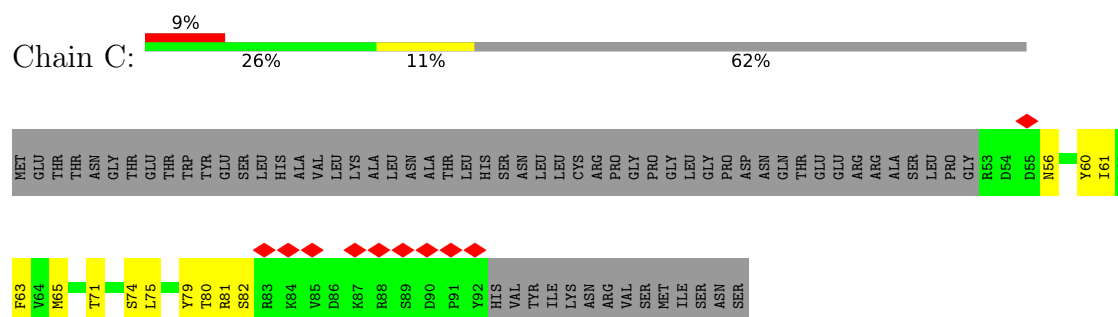
• Molecule 1: Calmodulin-1



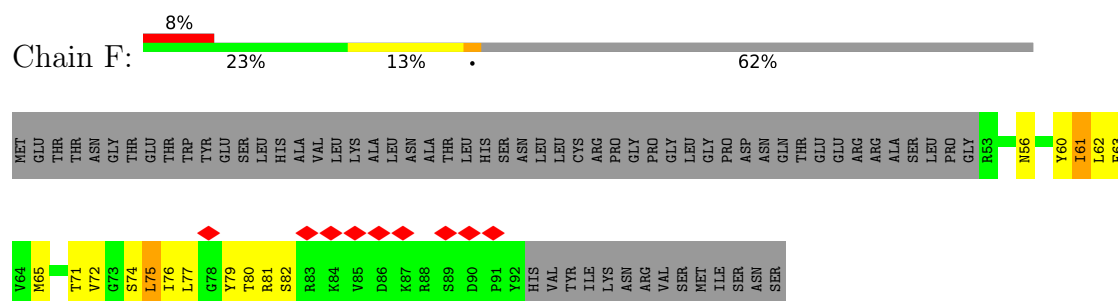
• Molecule 1: Calmodulin-1



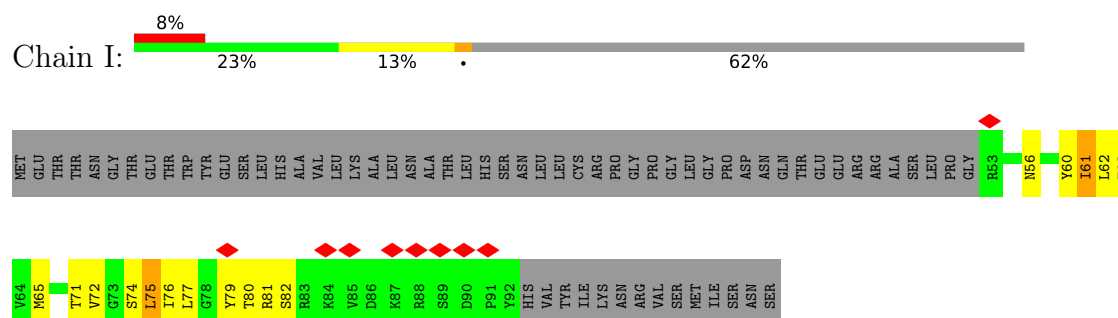
- Molecule 2: Potassium voltage-gated channel subfamily E member 3



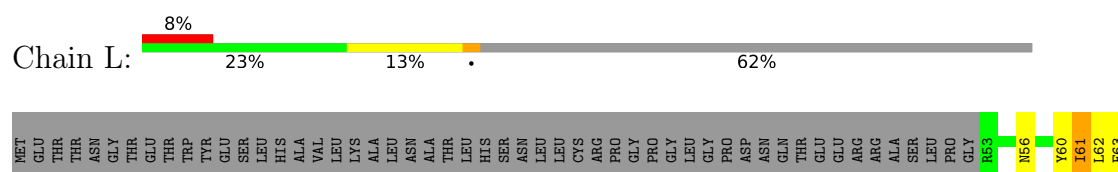
- Molecule 2: Potassium voltage-gated channel subfamily E member 3

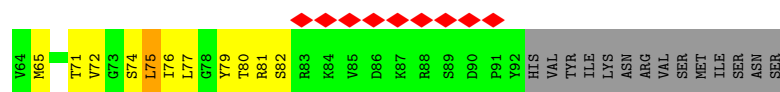


- Molecule 2: Potassium voltage-gated channel subfamily E member 3

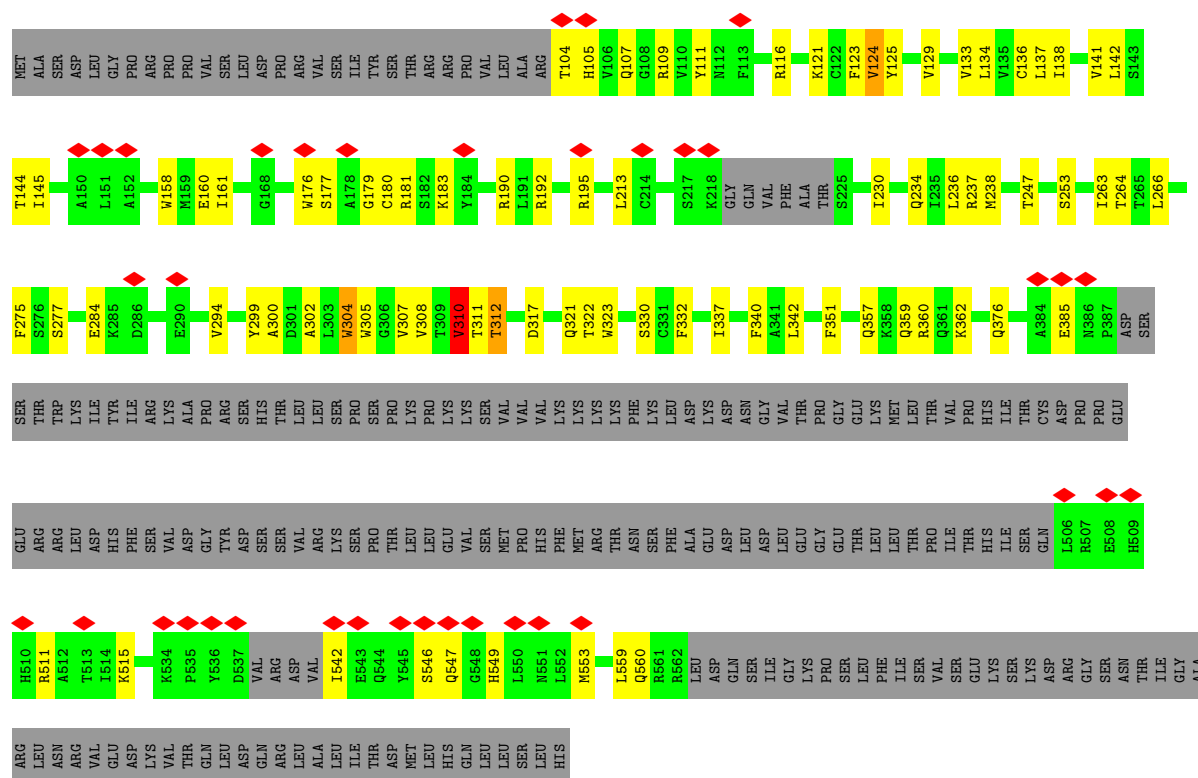


- Molecule 2: Potassium voltage-gated channel subfamily E member 3

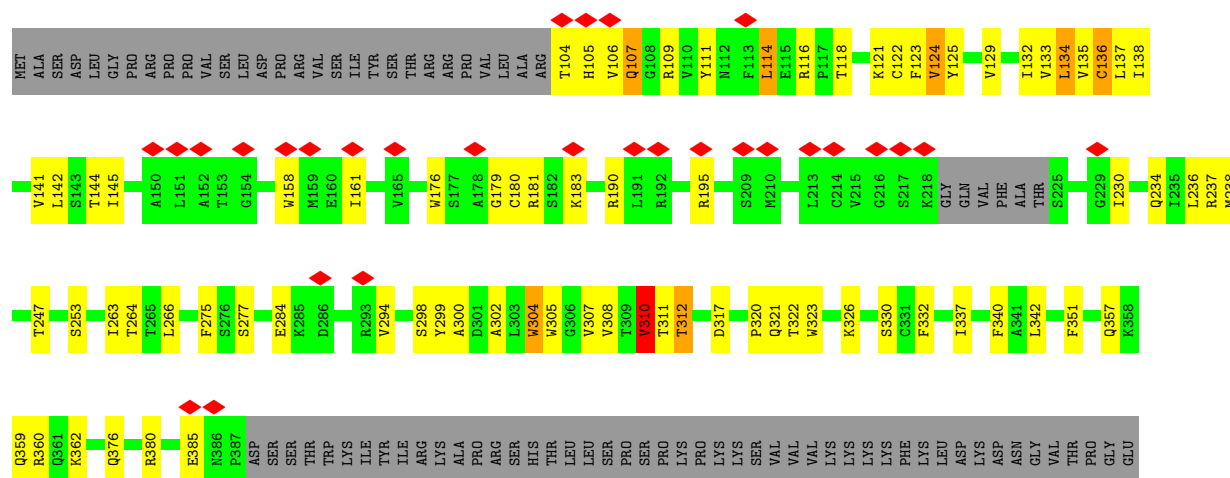




• Molecule 3: Potassium voltage-gated channel subfamily KQT member 1



• Molecule 3: Potassium voltage-gated channel subfamily KQT member 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	94	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.234	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	327.0, 327.0, 327.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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: CA, A1BBG

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	B	0.21	0/838	0.54	2/1152 (0.2%)
1	E	0.21	0/838	0.54	2/1152 (0.2%)
1	H	0.21	0/838	0.54	2/1152 (0.2%)
1	K	0.21	0/838	0.55	2/1152 (0.2%)
2	C	0.87	0/310	1.23	0/420
2	F	0.87	0/310	1.23	0/420
2	I	0.87	0/310	1.23	0/420
2	L	0.87	0/310	1.23	0/420
3	A	0.58	2/2748 (0.1%)	0.71	4/3715 (0.1%)
3	D	0.58	2/2748 (0.1%)	0.71	4/3715 (0.1%)
3	G	0.58	2/2748 (0.1%)	0.71	4/3715 (0.1%)
3	J	0.58	2/2748 (0.1%)	0.71	4/3715 (0.1%)
All	All	0.55	8/15584 (0.1%)	0.74	24/21148 (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
3	A	0	1
3	D	0	1
3	G	0	1
3	J	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	305	TRP	C-O	-6.37	1.16	1.24
3	A	305	TRP	C-O	-6.32	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	305	TRP	C-O	-6.32	1.16	1.24
3	G	305	TRP	C-O	-6.31	1.16	1.24
3	A	304	TRP	C-O	-5.33	1.17	1.24
3	D	304	TRP	C-O	-5.31	1.18	1.24
3	G	304	TRP	C-O	-5.31	1.18	1.24
3	J	304	TRP	C-O	-5.28	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	TRP	N-CA-C	-9.01	101.45	111.28
3	D	304	TRP	N-CA-C	-8.98	101.49	111.28
3	G	304	TRP	N-CA-C	-8.98	101.49	111.28
3	J	304	TRP	N-CA-C	-8.98	101.49	111.28
3	D	312	THR	N-CA-C	6.03	120.21	112.86
3	J	312	THR	N-CA-C	6.03	120.21	112.86
3	G	312	THR	N-CA-C	5.97	120.15	112.86
3	A	312	THR	N-CA-C	5.96	120.13	112.86
3	D	310	VAL	CA-C-N	-5.46	114.00	122.67
3	D	310	VAL	C-N-CA	-5.46	114.00	122.67
3	J	310	VAL	CA-C-N	-5.46	114.00	122.67
3	J	310	VAL	C-N-CA	-5.46	114.00	122.67
3	G	310	VAL	CA-C-N	-5.45	114.01	122.67
3	G	310	VAL	C-N-CA	-5.45	114.01	122.67
3	A	310	VAL	CA-C-N	-5.44	114.02	122.67
3	A	310	VAL	C-N-CA	-5.44	114.02	122.67
1	E	65	ASP	CA-C-N	5.38	130.72	124.21
1	E	65	ASP	C-N-CA	5.38	130.72	124.21
1	K	65	ASP	CA-C-N	5.38	130.72	124.21
1	K	65	ASP	C-N-CA	5.38	130.72	124.21
1	B	65	ASP	CA-C-N	5.33	130.66	124.21
1	B	65	ASP	C-N-CA	5.33	130.66	124.21
1	H	65	ASP	CA-C-N	5.32	130.65	124.21
1	H	65	ASP	C-N-CA	5.32	130.65	124.21

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	109	ARG	Sidechain
3	D	109	ARG	Sidechain
3	G	109	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	J	109	ARG	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	B	828	0	548	3	0
1	E	828	0	548	4	0
1	H	828	0	548	4	0
1	K	828	0	548	4	0
2	C	304	0	283	26	0
2	F	304	0	283	28	0
2	I	304	0	283	27	0
2	L	304	0	283	27	0
3	A	2682	0	2753	119	0
3	D	2682	0	2753	121	0
3	G	2682	0	2753	123	0
3	J	2682	0	2753	125	0
4	B	2	0	0	0	0
4	E	2	0	0	0	0
4	H	2	0	0	0	0
4	K	2	0	0	0	0
5	A	54	0	0	9	0
5	C	45	0	0	0	0
5	D	54	0	0	9	0
5	F	45	0	0	0	0
5	G	54	0	0	9	0
5	I	45	0	0	0	0
5	J	54	0	0	8	0
5	L	45	0	0	0	0
All	All	15660	0	14336	416	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 14.

All (416) 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)
3:A:141:VAL:HG21	3:J:299:TYR:CD2	1.40	1.55
3:A:299:TYR:CD2	3:D:141:VAL:HG21	1.40	1.54
3:G:299:TYR:CD2	3:J:141:VAL:HG21	1.40	1.52
3:D:299:TYR:CD2	3:G:141:VAL:HG21	1.40	1.52
3:G:299:TYR:CD2	3:J:141:VAL:CG2	1.98	1.44
3:A:141:VAL:CG2	3:J:299:TYR:CD2	1.98	1.44
3:D:299:TYR:CD2	3:G:141:VAL:CG2	1.98	1.43
3:A:299:TYR:CD2	3:D:141:VAL:CG2	1.98	1.42
3:A:141:VAL:HG23	3:J:299:TYR:CG	1.74	1.23
3:D:299:TYR:CG	3:G:141:VAL:HG23	1.74	1.22
3:A:299:TYR:CG	3:D:141:VAL:HG23	1.74	1.22
3:G:299:TYR:CG	3:J:141:VAL:HG23	1.74	1.22
3:A:264:THR:HG23	3:D:247:THR:HG23	1.36	1.08
3:A:247:THR:HG23	3:J:264:THR:HG23	1.36	1.07
3:G:264:THR:HG23	3:J:247:THR:HG23	1.36	1.07
3:D:264:THR:HG23	3:G:247:THR:HG23	1.36	1.04
3:G:299:TYR:CB	3:J:141:VAL:HG23	1.90	1.02
3:D:299:TYR:CB	3:G:141:VAL:HG23	1.90	1.01
3:A:299:TYR:CB	3:D:141:VAL:HG23	1.90	1.00
3:A:141:VAL:HG23	3:J:299:TYR:CD2	1.88	1.00
3:A:141:VAL:HG23	3:J:299:TYR:CB	1.90	1.00
3:A:299:TYR:CD2	3:D:141:VAL:HG23	1.88	0.99
3:G:299:TYR:CG	3:J:141:VAL:CG2	2.43	0.92
3:A:299:TYR:CG	3:D:141:VAL:CG2	2.43	0.92
3:G:299:TYR:CD2	3:J:141:VAL:HG23	1.88	0.92
3:A:141:VAL:CG2	3:J:299:TYR:CG	2.43	0.90
3:D:330:SER:HG	2:L:63:PHE:HE2	1.23	0.85
3:D:310:VAL:HG11	3:D:340:PHE:CE2	2.12	0.85
3:G:310:VAL:HG11	3:G:340:PHE:CE2	2.12	0.85
3:A:310:VAL:HG11	3:A:340:PHE:CE2	2.12	0.85
3:J:310:VAL:HG11	3:J:340:PHE:CE2	2.12	0.84
3:D:299:TYR:CG	3:G:141:VAL:CG2	2.43	0.83
3:A:299:TYR:HD2	3:D:141:VAL:HG21	0.99	0.81
3:A:141:VAL:HG21	3:J:299:TYR:HD2	0.99	0.81
3:J:136:CYS:HB3	3:J:234:GLN:HE21	1.45	0.80
3:A:136:CYS:HB3	3:A:234:GLN:HE21	1.46	0.80
3:D:299:TYR:HD2	3:G:141:VAL:HG21	0.99	0.80
3:G:136:CYS:HB3	3:G:234:GLN:HE21	1.46	0.80
3:G:299:TYR:HD2	3:J:141:VAL:HG21	0.99	0.79
3:A:134:LEU:HA	3:A:238:MET:HE1	1.65	0.79
3:D:136:CYS:HB3	3:D:234:GLN:HE21	1.45	0.79
2:C:63:PHE:CE2	3:G:330:SER:OG	2.36	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:LEU:HA	3:D:238:MET:HE1	1.65	0.78
3:J:134:LEU:HA	3:J:238:MET:HE1	1.65	0.78
3:G:134:LEU:HA	3:G:238:MET:HE1	1.65	0.78
3:A:141:VAL:HG23	3:J:299:TYR:HB3	1.65	0.78
3:G:310:VAL:CG1	3:G:340:PHE:CD2	2.66	0.78
3:D:310:VAL:CG1	3:D:340:PHE:CD2	2.66	0.78
3:A:307:VAL:HB	2:F:60:TYR:OH	1.84	0.78
3:D:299:TYR:HB3	3:G:141:VAL:CG2	2.14	0.78
3:D:307:VAL:HB	2:I:60:TYR:OH	1.84	0.78
3:G:299:TYR:HB3	3:J:141:VAL:CG2	2.14	0.78
3:A:310:VAL:CG1	3:A:340:PHE:CD2	2.66	0.78
3:J:330:SER:OG	2:F:63:PHE:CE2	2.36	0.78
2:C:60:TYR:OH	3:J:307:VAL:HB	1.84	0.78
3:J:310:VAL:CG1	3:J:340:PHE:CD2	2.66	0.77
3:A:141:VAL:CG2	3:J:299:TYR:HB3	2.14	0.77
3:A:299:TYR:HB3	3:D:141:VAL:HG23	1.66	0.77
3:D:330:SER:OG	2:L:63:PHE:CE2	2.36	0.77
3:A:330:SER:OG	2:I:63:PHE:CE2	2.36	0.77
3:D:299:TYR:CE2	3:G:141:VAL:HG21	2.18	0.77
3:G:307:VAL:HB	2:L:60:TYR:OH	1.84	0.76
3:A:141:VAL:HG21	3:J:299:TYR:CE2	2.18	0.76
3:A:263:ILE:HG22	2:F:75:LEU:HD13	1.66	0.76
3:A:299:TYR:HB3	3:D:141:VAL:CG2	2.14	0.76
3:G:299:TYR:HB3	3:J:141:VAL:HG23	1.66	0.76
3:G:263:ILE:HG22	2:L:75:LEU:HD13	1.66	0.76
2:C:75:LEU:HD13	3:J:263:ILE:HG22	1.66	0.76
3:D:299:TYR:HB3	3:G:141:VAL:HG23	1.65	0.76
3:G:310:VAL:HG23	3:G:332:PHE:CZ	2.21	0.76
3:J:310:VAL:HG23	3:J:332:PHE:CZ	2.21	0.76
3:D:263:ILE:HG22	2:I:75:LEU:HD13	1.66	0.75
5:A:801:A1BBG:O16	5:A:801:A1BBG:O26	2.05	0.75
3:A:310:VAL:HG23	3:A:332:PHE:CZ	2.21	0.75
5:J:801:A1BBG:O26	5:J:801:A1BBG:O16	2.05	0.75
3:G:299:TYR:HD2	3:J:141:VAL:CG2	1.66	0.75
5:D:801:A1BBG:O26	5:D:801:A1BBG:O16	2.05	0.74
3:D:310:VAL:HG23	3:D:332:PHE:CZ	2.21	0.74
5:G:801:A1BBG:O26	5:G:801:A1BBG:O16	2.05	0.74
3:A:299:TYR:CE2	3:D:141:VAL:HG21	2.19	0.74
3:A:542:ILE:HA	3:J:357:GLN:HE22	1.53	0.73
3:D:299:TYR:CB	3:G:141:VAL:CG2	2.66	0.73
3:A:310:VAL:HG13	3:A:340:PHE:CD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:357:GLN:HE22	3:J:542:ILE:HA	1.54	0.73
3:D:357:GLN:HE22	3:G:542:ILE:HA	1.53	0.72
3:A:330:SER:OG	2:I:63:PHE:HE2	1.72	0.72
3:J:310:VAL:HG13	3:J:340:PHE:CD2	2.23	0.72
2:C:63:PHE:HE2	3:G:330:SER:OG	1.72	0.72
3:G:310:VAL:HG13	3:G:340:PHE:CD2	2.23	0.72
3:G:299:TYR:CB	3:J:141:VAL:CG2	2.66	0.72
3:D:330:SER:OG	2:L:63:PHE:HE2	1.72	0.72
3:D:310:VAL:HG13	3:D:340:PHE:CD2	2.23	0.72
3:A:357:GLN:HE22	3:D:542:ILE:HA	1.54	0.72
3:J:330:SER:OG	2:F:63:PHE:HE2	1.72	0.72
3:A:136:CYS:HB3	3:A:234:GLN:NE2	2.06	0.71
3:J:136:CYS:HB3	3:J:234:GLN:NE2	2.06	0.71
3:A:263:ILE:CG2	2:F:75:LEU:HD13	2.21	0.71
3:A:299:TYR:CB	3:D:141:VAL:CG2	2.66	0.71
3:D:263:ILE:CG2	2:I:75:LEU:HD13	2.21	0.71
3:D:299:TYR:HD2	3:G:141:VAL:CG2	1.65	0.70
3:G:263:ILE:CG2	2:L:75:LEU:HD13	2.21	0.70
2:C:75:LEU:HD13	3:J:263:ILE:CG2	2.21	0.70
3:D:136:CYS:HB3	3:D:234:GLN:NE2	2.06	0.70
3:A:330:SER:HG	2:I:63:PHE:HE2	1.39	0.70
3:G:136:CYS:HB3	3:G:234:GLN:NE2	2.06	0.70
3:A:299:TYR:HD2	3:D:141:VAL:CG2	1.66	0.69
3:D:549:HIS:HE1	3:G:549:HIS:CE1	2.10	0.69
3:G:266:LEU:HB3	2:L:71:THR:HG21	1.74	0.69
3:A:549:HIS:HE1	3:D:549:HIS:CE1	2.10	0.68
3:A:549:HIS:CE1	3:J:549:HIS:HE1	2.10	0.68
3:G:549:HIS:HE1	3:J:549:HIS:CE1	2.10	0.68
3:A:266:LEU:HB3	2:F:71:THR:HG21	1.74	0.68
3:D:266:LEU:HB3	2:I:71:THR:HG21	1.74	0.68
2:C:71:THR:HG21	3:J:266:LEU:HB3	1.74	0.68
3:A:141:VAL:CG2	3:J:299:TYR:HD2	1.65	0.68
3:G:299:TYR:CE2	3:J:141:VAL:HG21	2.18	0.67
1:B:64:ILE:HB	1:B:67:PRO:HD2	1.79	0.65
1:H:64:ILE:HB	1:H:67:PRO:HD2	1.79	0.65
1:K:64:ILE:HB	1:K:67:PRO:HD2	1.79	0.64
3:D:357:GLN:NE2	3:G:542:ILE:HA	2.13	0.64
1:E:64:ILE:HB	1:E:67:PRO:HD2	1.79	0.64
3:A:357:GLN:NE2	3:D:542:ILE:HA	2.13	0.64
3:A:547:GLN:HG3	3:J:360:ARG:HE	1.63	0.64
3:G:357:GLN:NE2	3:J:542:ILE:HA	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:TYR:CE2	3:J:304:TRP:HA	2.34	0.63
3:D:304:TRP:HA	2:I:60:TYR:CE2	2.34	0.63
3:G:304:TRP:HA	2:L:60:TYR:CE2	2.34	0.63
3:G:310:VAL:CG1	3:G:340:PHE:CE2	2.81	0.63
3:A:542:ILE:HA	3:J:357:GLN:NE2	2.13	0.63
3:J:183:LYS:HG3	5:J:801:A1BBG:O24	1.99	0.63
3:A:310:VAL:CG1	3:A:340:PHE:CE2	2.81	0.62
3:A:304:TRP:HA	2:F:60:TYR:CE2	2.34	0.62
3:G:183:LYS:HG3	5:G:801:A1BBG:O24	1.99	0.62
3:J:330:SER:HG	2:F:63:PHE:HE2	1.38	0.62
3:G:360:ARG:HE	3:J:547:GLN:HG3	1.63	0.62
3:D:183:LYS:HG3	5:D:801:A1BBG:O24	1.99	0.62
3:A:183:LYS:HG3	5:A:801:A1BBG:O24	1.99	0.62
3:A:360:ARG:HE	3:D:547:GLN:HG3	1.63	0.61
2:C:63:PHE:HE2	3:G:330:SER:HG	1.38	0.61
3:D:360:ARG:HE	3:G:547:GLN:HG3	1.63	0.61
3:J:310:VAL:CG1	3:J:340:PHE:CE2	2.81	0.61
3:A:549:HIS:CE1	3:J:549:HIS:CE1	2.89	0.61
3:A:549:HIS:CE1	3:D:549:HIS:CE1	2.89	0.60
3:D:549:HIS:CE1	3:G:549:HIS:CE1	2.89	0.60
3:G:549:HIS:CE1	3:J:549:HIS:CE1	2.89	0.60
3:A:107:GLN:HB3	3:A:180:CYS:SG	2.42	0.60
3:D:310:VAL:CG1	3:D:340:PHE:CE2	2.81	0.60
3:D:107:GLN:HB3	3:D:180:CYS:SG	2.42	0.60
3:A:141:VAL:CG2	3:J:299:TYR:CB	2.66	0.60
3:G:107:GLN:HB3	3:G:180:CYS:SG	2.42	0.60
3:G:195:ARG:NH1	5:G:801:A1BBG:O50	2.35	0.60
3:J:107:GLN:HB3	3:J:180:CYS:SG	2.42	0.60
3:J:181:ARG:HG3	3:J:183:LYS:H	1.67	0.60
3:D:195:ARG:NH1	5:D:801:A1BBG:O50	2.35	0.60
3:A:181:ARG:HG3	3:A:183:LYS:H	1.67	0.59
3:D:181:ARG:HG3	3:D:183:LYS:H	1.67	0.59
3:J:195:ARG:NH1	5:J:801:A1BBG:O50	2.35	0.59
3:A:195:ARG:NH1	5:A:801:A1BBG:O50	2.35	0.59
3:G:181:ARG:HG3	3:G:183:LYS:H	1.67	0.59
3:G:116:ARG:HA	2:I:79:TYR:HE2	1.68	0.59
3:G:181:ARG:NH2	5:G:801:A1BBG:C11	2.66	0.59
3:J:181:ARG:NH2	5:J:801:A1BBG:C11	2.66	0.59
3:D:181:ARG:NH2	5:D:801:A1BBG:C11	2.66	0.58
3:A:181:ARG:NH2	5:A:801:A1BBG:C11	2.66	0.58
2:C:79:TYR:HE2	3:A:116:ARG:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:116:ARG:HA	2:L:79:TYR:HE2	1.68	0.58
3:D:116:ARG:HA	2:F:79:TYR:HE2	1.68	0.58
3:D:323:TRP:HB3	2:L:56:ASN:C	2.30	0.56
3:A:323:TRP:HB3	2:I:56:ASN:C	2.30	0.56
3:A:323:TRP:HB3	2:I:56:ASN:O	2.05	0.56
3:D:323:TRP:HB3	2:L:56:ASN:O	2.05	0.56
3:A:236:LEU:HD22	3:J:275:PHE:CE1	2.41	0.56
3:J:323:TRP:HB3	2:F:56:ASN:C	2.30	0.56
2:C:56:ASN:C	3:G:323:TRP:HB3	2.30	0.56
3:D:275:PHE:CE1	3:G:236:LEU:HD22	2.41	0.56
3:J:323:TRP:HB3	2:F:56:ASN:O	2.05	0.56
2:C:56:ASN:O	3:G:323:TRP:HB3	2.05	0.56
3:G:275:PHE:CE1	3:J:236:LEU:HD22	2.41	0.55
3:D:357:GLN:HE22	3:G:542:ILE:CA	2.19	0.55
3:A:104:THR:O	3:A:105:HIS:C	2.49	0.55
3:A:275:PHE:CE1	3:D:236:LEU:HD22	2.41	0.55
3:G:357:GLN:HE22	3:J:542:ILE:CA	2.20	0.55
3:J:116:ARG:HD3	5:J:801:A1BBG:O20	2.07	0.54
3:J:104:THR:O	3:J:105:HIS:C	2.49	0.54
2:C:80:THR:C	2:C:82:SER:H	2.16	0.54
3:A:357:GLN:HE22	3:D:542:ILE:CA	2.20	0.54
3:G:560:GLN:HG2	3:J:559:LEU:HD13	1.90	0.54
3:A:559:LEU:HD13	3:J:560:GLN:HG2	1.90	0.54
2:F:80:THR:C	2:F:82:SER:H	2.16	0.54
2:L:80:THR:C	2:L:82:SER:H	2.16	0.54
3:A:542:ILE:CA	3:J:357:GLN:HE22	2.19	0.53
3:G:116:ARG:HD3	5:G:801:A1BBG:O20	2.08	0.53
3:A:560:GLN:HG2	3:D:559:LEU:HD13	1.90	0.53
3:D:138:ILE:HG12	2:F:65:MET:HG3	1.90	0.53
3:J:138:ILE:HG12	2:L:65:MET:HG3	1.90	0.53
3:A:116:ARG:HD3	5:A:801:A1BBG:O20	2.08	0.53
3:D:385:GLU:O	3:D:511:ARG:NH1	2.42	0.53
3:G:104:THR:O	3:G:105:HIS:C	2.49	0.53
2:I:80:THR:C	2:I:82:SER:H	2.16	0.53
3:D:104:THR:O	3:D:105:HIS:C	2.49	0.53
3:D:116:ARG:HD3	5:D:801:A1BBG:O20	2.07	0.53
3:D:560:GLN:HG2	3:G:559:LEU:HD13	1.90	0.53
3:A:385:GLU:O	3:A:511:ARG:NH1	2.42	0.52
3:G:300:ALA:HB2	2:L:61:ILE:CD1	2.39	0.52
2:C:65:MET:HG3	3:A:138:ILE:HG12	1.90	0.52
3:G:138:ILE:HG12	2:I:65:MET:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:300:ALA:HB2	2:I:61:ILE:CD1	2.39	0.52
2:C:61:ILE:CD1	3:J:300:ALA:HB2	2.39	0.52
3:A:330:SER:HB2	2:I:60:TYR:HE1	1.75	0.52
3:G:385:GLU:O	3:G:511:ARG:NH1	2.42	0.52
5:G:801:A1BBG:O16	5:G:801:A1BBG:O08	2.28	0.52
5:J:801:A1BBG:O16	5:J:801:A1BBG:O08	2.28	0.52
3:A:300:ALA:HB2	2:F:61:ILE:CD1	2.39	0.52
3:J:385:GLU:O	3:J:511:ARG:NH1	2.42	0.51
2:C:60:TYR:HE1	3:G:330:SER:HB2	1.75	0.51
3:A:158:TRP:HA	3:A:161:ILE:HG22	1.93	0.51
3:D:330:SER:HB2	2:L:60:TYR:HE1	1.75	0.51
5:A:801:A1BBG:O16	5:A:801:A1BBG:O08	2.28	0.51
3:D:134:LEU:CA	3:D:238:MET:HE1	2.39	0.50
5:D:801:A1BBG:O16	5:D:801:A1BBG:O08	2.28	0.50
3:G:230:ILE:O	3:G:234:GLN:HB2	2.11	0.50
3:J:330:SER:HB2	2:F:60:TYR:HE1	1.75	0.50
3:A:124:VAL:O	3:A:125:TYR:C	2.55	0.50
3:G:134:LEU:CA	3:G:238:MET:HE1	2.39	0.50
3:J:230:ILE:O	3:J:234:GLN:HB2	2.11	0.50
3:A:230:ILE:O	3:A:234:GLN:HB2	2.11	0.50
3:D:158:TRP:HA	3:D:161:ILE:HG22	1.93	0.50
3:D:230:ILE:O	3:D:234:GLN:HB2	2.12	0.50
3:J:158:TRP:HA	3:J:161:ILE:HG22	1.93	0.50
3:G:176:TRP:O	3:G:190:ARG:NH1	2.45	0.50
3:G:158:TRP:HA	3:G:161:ILE:HG22	1.92	0.50
3:A:176:TRP:O	3:A:190:ARG:NH1	2.45	0.49
3:J:176:TRP:O	3:J:190:ARG:NH1	2.45	0.49
3:G:124:VAL:O	3:G:125:TYR:C	2.55	0.49
1:B:110:MET:O	3:A:376:GLN:NE2	2.45	0.49
1:E:110:MET:O	3:D:376:GLN:NE2	2.45	0.49
1:K:110:MET:O	3:J:376:GLN:NE2	2.45	0.49
3:A:307:VAL:CB	2:F:60:TYR:OH	2.59	0.49
3:D:307:VAL:CB	2:I:60:TYR:OH	2.59	0.49
3:A:299:TYR:HB3	3:D:141:VAL:HG22	1.94	0.49
1:H:110:MET:O	3:G:376:GLN:NE2	2.45	0.49
3:D:176:TRP:O	3:D:190:ARG:NH1	2.45	0.49
3:J:323:TRP:CZ3	2:F:60:TYR:HB2	2.48	0.49
3:D:277:SER:OG	3:D:302:ALA:O	2.30	0.49
3:G:299:TYR:HB3	3:J:141:VAL:HG22	1.93	0.48
3:G:317:ASP:N	3:G:317:ASP:OD1	2.46	0.48
3:A:141:VAL:O	3:A:144:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:275:PHE:CZ	3:D:236:LEU:HD22	2.48	0.48
3:A:323:TRP:CZ3	2:I:60:TYR:HB2	2.48	0.48
3:D:284:GLU:OE2	3:D:322:THR:N	2.41	0.48
2:C:60:TYR:HB2	3:G:323:TRP:CZ3	2.48	0.48
3:D:275:PHE:CZ	3:G:236:LEU:HD22	2.48	0.48
3:G:275:PHE:CZ	3:J:236:LEU:HD22	2.48	0.48
3:A:284:GLU:OE2	3:A:322:THR:N	2.41	0.48
3:D:141:VAL:O	3:D:144:THR:HG22	2.13	0.48
3:D:317:ASP:OD1	3:D:317:ASP:N	2.46	0.48
3:J:142:LEU:O	3:J:145:ILE:HG12	2.14	0.48
3:A:192:ARG:HD2	3:A:192:ARG:HA	1.70	0.48
3:A:134:LEU:CA	3:A:238:MET:HE1	2.39	0.48
3:A:236:LEU:HD22	3:J:275:PHE:CZ	2.48	0.48
3:D:323:TRP:HZ3	2:L:60:TYR:HB2	1.79	0.48
3:G:141:VAL:O	3:G:144:THR:HG22	2.13	0.48
3:D:323:TRP:CZ3	2:L:60:TYR:HB2	2.48	0.48
3:J:134:LEU:CA	3:J:238:MET:HE1	2.39	0.48
3:A:141:VAL:HG22	3:J:299:TYR:HB3	1.94	0.47
3:D:312:THR:HG22	3:D:337:ILE:CD1	2.44	0.47
3:J:309:THR:O	3:J:309:THR:OG1	2.31	0.47
3:A:323:TRP:HZ3	2:I:60:TYR:HB2	1.79	0.47
3:J:124:VAL:O	3:J:125:TYR:C	2.55	0.47
3:J:141:VAL:O	3:J:144:THR:HG22	2.13	0.47
3:A:312:THR:HG22	3:A:337:ILE:CD1	2.44	0.47
3:D:124:VAL:O	3:D:125:TYR:C	2.55	0.47
3:J:323:TRP:HZ3	2:F:60:TYR:HB2	1.79	0.47
3:A:179:GLY:H	3:A:190:ARG:HH11	1.62	0.47
3:D:142:LEU:O	3:D:145:ILE:HG12	2.14	0.47
3:G:142:LEU:O	3:G:145:ILE:HG12	2.14	0.47
3:A:142:LEU:O	3:A:145:ILE:HG12	2.14	0.47
3:G:179:GLY:H	3:G:190:ARG:HH11	1.62	0.47
3:G:277:SER:OG	3:G:302:ALA:O	2.30	0.47
1:E:108:HIS:O	1:E:112:ASN:ND2	2.48	0.47
1:K:108:HIS:O	1:K:112:ASN:ND2	2.48	0.47
3:G:312:THR:HG22	3:G:337:ILE:CD1	2.44	0.47
3:J:181:ARG:NH2	5:J:801:A1BBG:O22	2.46	0.47
3:J:312:THR:HG22	3:J:337:ILE:CD1	2.44	0.47
2:C:60:TYR:HB2	3:G:323:TRP:HZ3	1.79	0.47
1:H:108:HIS:O	1:H:112:ASN:ND2	2.48	0.47
3:A:111:TYR:OH	5:A:801:A1BBG:O19	2.29	0.47
3:A:277:SER:OG	3:A:302:ALA:O	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:179:GLY:H	3:D:190:ARG:HH11	1.62	0.47
3:D:299:TYR:HB3	3:G:141:VAL:HG22	1.94	0.46
3:J:277:SER:OG	3:J:302:ALA:O	2.30	0.46
3:J:323:TRP:CB	2:F:56:ASN:C	2.88	0.46
3:D:323:TRP:CB	2:L:56:ASN:C	2.88	0.46
3:J:317:ASP:OD1	3:J:317:ASP:N	2.46	0.46
3:J:179:GLY:H	3:J:190:ARG:HH11	1.62	0.46
2:I:80:THR:C	2:I:82:SER:N	2.73	0.46
3:A:310:VAL:CG2	3:A:332:PHE:CZ	2.97	0.46
2:C:56:ASN:C	3:G:323:TRP:CB	2.88	0.46
3:A:317:ASP:OD1	3:A:317:ASP:N	2.46	0.46
3:J:192:ARG:HA	3:J:192:ARG:HD2	1.70	0.46
2:L:80:THR:C	2:L:82:SER:N	2.73	0.46
3:A:121:LYS:HA	3:A:121:LYS:HD3	1.70	0.46
3:A:137:LEU:O	3:A:141:VAL:HG12	2.16	0.46
3:A:181:ARG:NH2	5:A:801:A1BBG:O22	2.46	0.46
3:A:323:TRP:CB	2:I:56:ASN:C	2.88	0.46
3:G:111:TYR:OH	5:G:801:A1BBG:O19	2.29	0.46
1:B:108:HIS:O	1:B:112:ASN:ND2	2.48	0.45
3:G:137:LEU:O	3:G:141:VAL:HG12	2.16	0.45
3:G:181:ARG:NH2	5:G:801:A1BBG:O22	2.46	0.45
3:A:359:GLN:HE22	3:A:362:LYS:HD3	1.81	0.45
3:J:137:LEU:O	3:J:141:VAL:HG12	2.17	0.45
3:J:359:GLN:HE22	3:J:362:LYS:HD3	1.81	0.45
3:D:137:LEU:O	3:D:141:VAL:HG12	2.17	0.45
3:G:310:VAL:CG2	3:G:332:PHE:CZ	2.97	0.45
2:F:75:LEU:HD12	2:F:75:LEU:HA	1.76	0.45
2:F:80:THR:C	2:F:82:SER:N	2.73	0.45
3:D:181:ARG:NH2	5:D:801:A1BBG:O22	2.46	0.45
3:D:359:GLN:HE22	3:D:362:LYS:HD3	1.81	0.45
3:G:307:VAL:CB	2:L:60:TYR:OH	2.59	0.44
3:D:360:ARG:HE	3:G:547:GLN:CG	2.29	0.44
3:G:359:GLN:HE22	3:G:362:LYS:HD3	1.81	0.44
3:D:528:LYS:HD3	3:D:528:LYS:HA	1.82	0.44
3:G:360:ARG:HE	3:J:547:GLN:CG	2.29	0.44
3:J:562:ARG:HA	3:J:562:ARG:HD2	1.82	0.44
3:G:177:SER:O	3:G:177:SER:OG	2.36	0.44
3:G:192:ARG:HA	3:G:192:ARG:HD2	1.70	0.44
3:J:310:VAL:CG2	3:J:332:PHE:CZ	2.97	0.43
2:I:75:LEU:HD12	2:I:75:LEU:HA	1.76	0.43
3:A:177:SER:O	3:A:177:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:THR:C	2:C:82:SER:N	2.73	0.43
3:A:234:GLN:HG3	3:A:237:ARG:HH11	1.84	0.43
3:D:234:GLN:HG3	3:D:237:ARG:HH11	1.84	0.43
3:D:284:GLU:OE2	3:D:321:GLN:N	2.52	0.43
3:D:310:VAL:CG2	3:D:332:PHE:CZ	2.97	0.43
2:L:75:LEU:HD12	2:L:75:LEU:HA	1.76	0.43
3:A:263:ILE:HD12	2:F:74:SER:HB2	2.01	0.43
3:D:121:LYS:HA	3:D:121:LYS:HD3	1.70	0.43
2:C:75:LEU:HD12	2:C:75:LEU:HA	1.76	0.42
3:A:330:SER:CB	2:I:63:PHE:CE2	3.02	0.42
3:D:330:SER:CB	2:L:63:PHE:CE2	3.02	0.42
3:J:177:SER:O	3:J:177:SER:OG	2.36	0.42
3:J:284:GLU:OE2	3:J:322:THR:N	2.41	0.42
2:C:74:SER:HB2	3:J:263:ILE:HD12	2.01	0.42
3:A:360:ARG:HE	3:D:547:GLN:CG	2.29	0.42
3:D:114:LEU:HD13	3:D:114:LEU:HA	1.76	0.42
3:D:320:PRO:O	3:D:326:LYS:NZ	2.40	0.42
3:G:121:LYS:HA	3:G:121:LYS:HD3	1.70	0.42
3:J:234:GLN:HG3	3:J:237:ARG:HH11	1.84	0.42
2:C:61:ILE:HD11	3:J:300:ALA:HB2	2.02	0.42
3:G:263:ILE:HD12	2:L:74:SER:HB2	2.01	0.42
3:J:263:ILE:HD13	3:J:263:ILE:HA	1.88	0.42
2:C:60:TYR:OH	3:J:307:VAL:CB	2.59	0.42
3:A:284:GLU:OE2	3:A:321:GLN:N	2.52	0.42
3:G:284:GLU:OE2	3:G:322:THR:N	2.41	0.42
3:G:552:LEU:HD12	3:G:552:LEU:HA	1.90	0.42
3:A:300:ALA:HB2	2:F:61:ILE:HD11	2.02	0.42
3:G:129:VAL:O	3:G:133:VAL:HG23	2.20	0.42
3:G:183:LYS:HA	3:G:183:LYS:HD3	1.92	0.42
3:G:284:GLU:OE2	3:G:321:GLN:N	2.52	0.42
3:G:528:LYS:HA	3:G:528:LYS:HD3	1.82	0.42
3:J:129:VAL:O	3:J:133:VAL:HG23	2.20	0.42
3:G:234:GLN:HG3	3:G:237:ARG:HH11	1.84	0.42
3:G:266:LEU:CB	2:L:71:THR:HG21	2.47	0.42
3:D:129:VAL:O	3:D:133:VAL:HG23	2.20	0.41
3:J:284:GLU:OE2	3:J:321:GLN:N	2.52	0.41
3:D:263:ILE:HD12	2:I:74:SER:HB2	2.01	0.41
3:G:300:ALA:HB2	2:L:61:ILE:HD11	2.02	0.41
3:J:330:SER:CB	2:F:63:PHE:CE2	3.02	0.41
3:D:123:PHE:HB2	2:F:80:THR:HG21	2.02	0.41
2:C:61:ILE:HD12	3:J:300:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:63:PHE:CE2	3:G:330:SER:CB	3.02	0.41
3:G:243:ARG:HD3	3:G:243:ARG:HA	1.92	0.41
3:A:515:LYS:H	3:A:515:LYS:HG3	1.70	0.41
3:A:351:PHE:CD2	3:J:342:LEU:HD21	2.56	0.41
3:A:547:GLN:CG	3:J:360:ARG:HE	2.29	0.41
3:J:121:LYS:HD3	3:J:121:LYS:HA	1.70	0.41
3:A:129:VAL:O	3:A:133:VAL:HG23	2.20	0.41
3:D:380:ARG:O	3:D:518:ARG:NH1	2.50	0.41
3:A:310:VAL:CG1	3:A:310:VAL:O	2.68	0.41
3:D:111:TYR:OH	5:D:801:A1BBG:O19	2.29	0.41
3:D:300:ALA:HB2	2:I:61:ILE:HD12	2.02	0.41
3:G:298:SER:HB2	3:J:145:ILE:HA	2.03	0.41
3:J:183:LYS:HA	3:J:183:LYS:HD3	1.92	0.41
5:A:801:A1BBG:O08	5:A:801:A1BBG:P23	2.79	0.41
3:D:263:ILE:HD13	3:D:263:ILE:HA	1.88	0.41
3:G:123:PHE:O	3:G:124:VAL:C	2.64	0.41
2:C:74:SER:HB2	3:J:263:ILE:CD1	2.51	0.40
3:A:160:GLU:HG3	3:A:213:LEU:HD11	2.03	0.40
3:A:342:LEU:HD21	3:D:351:PHE:CD2	2.56	0.40
3:D:123:PHE:O	3:D:124:VAL:C	2.64	0.40
3:D:300:ALA:HB2	2:I:61:ILE:HD11	2.02	0.40
3:G:264:THR:HG23	3:J:247:THR:CG2	2.27	0.40
3:J:553:MET:H	3:J:553:MET:HG3	1.72	0.40
1:K:116:LYS:O	3:J:380:ARG:NH2	2.55	0.40
3:A:263:ILE:CD1	2:F:74:SER:HB2	2.51	0.40
3:D:183:LYS:HA	3:D:183:LYS:HD3	1.92	0.40
3:G:123:PHE:HB2	2:I:80:THR:HG21	2.02	0.40
3:J:213:LEU:HD23	3:J:213:LEU:HA	1.90	0.40
1:H:116:LYS:O	3:G:380:ARG:NH2	2.54	0.40
3:A:123:PHE:O	3:A:124:VAL:C	2.64	0.40
3:D:298:SER:HB2	3:G:145:ILE:HA	2.03	0.40
3:G:300:ALA:HB2	2:L:61:ILE:HD12	2.02	0.40
5:G:801:A1BBG:O08	5:G:801:A1BBG:P23	2.79	0.40
3:J:160:GLU:HG3	3:J:213:LEU:HD11	2.03	0.40
1:E:116:LYS:O	3:D:380:ARG:NH2	2.55	0.40
3:A:263:ILE:HG13	2:F:74:SER:HB3	2.04	0.40
3:A:263:ILE:HG21	2:F:75:LEU:HD13	2.01	0.40
3:D:263:ILE:HG21	2:I:75:LEU:HD13	2.01	0.40
3:D:342:LEU:HD21	3:G:351:PHE:CD2	2.56	0.40
3:G:342:LEU:HD21	3:J:351:PHE:CD2	2.56	0.40
3:A:247:THR:CG2	3:J:264:THR:HG23	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:299:TYR:HB2	3:G:144:THR:HG21	2.03	0.40
5:D:801:A1BBG:O08	5:D:801:A1BBG:P23	2.79	0.40
3:J:123:PHE:O	3:J:124:VAL:C	2.64	0.40
3:J:123:PHE:HB2	2:L:80:THR:HG21	2.02	0.40
5:J:801:A1BBG:O08	5:J:801:A1BBG:P23	2.79	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	B	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
1	E	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
1	H	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
1	K	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
2	C	38/106 (36%)	33 (87%)	4 (10%)	1 (3%)	4	28
2	F	38/106 (36%)	33 (87%)	4 (10%)	1 (3%)	4	28
2	I	38/106 (36%)	33 (87%)	4 (10%)	1 (3%)	4	28
2	L	38/106 (36%)	33 (87%)	4 (10%)	1 (3%)	4	28
3	A	323/546 (59%)	308 (95%)	14 (4%)	1 (0%)	36	69
3	D	323/546 (59%)	308 (95%)	14 (4%)	1 (0%)	36	69
3	G	323/546 (59%)	308 (95%)	14 (4%)	1 (0%)	36	69
3	J	323/546 (59%)	308 (95%)	14 (4%)	1 (0%)	36	69
All	All	2012/3204 (63%)	1896 (94%)	108 (5%)	8 (0%)	31	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	ARG
2	F	81	ARG
2	I	81	ARG
2	L	81	ARG
3	A	124	VAL
3	D	124	VAL
3	G	124	VAL
3	J	124	VAL

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	H	11/127 (9%)	11 (100%)	0	100	100
2	F	30/94 (32%)	24 (80%)	6 (20%)	1	9
2	I	30/94 (32%)	24 (80%)	6 (20%)	1	9
2	L	30/94 (32%)	24 (80%)	6 (20%)	1	9
3	A	183/480 (38%)	176 (96%)	7 (4%)	29	52
3	D	281/480 (58%)	265 (94%)	16 (6%)	18	44
3	G	281/480 (58%)	265 (94%)	16 (6%)	18	44
3	J	281/480 (58%)	265 (94%)	16 (6%)	18	44
All	All	1127/2329 (48%)	1054 (94%)	73 (6%)	17	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	253	SER
3	A	294	VAL
3	A	308	VAL
3	A	310	VAL
3	A	311	THR
3	A	546	SER
3	A	553	MET
3	D	106	VAL

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Mol	Chain	Res	Type
3	D	107	GLN
3	D	114	LEU
3	D	118	THR
3	D	122	CYS
3	D	132	ILE
3	D	134	LEU
3	D	135	VAL
3	D	136	CYS
3	D	253	SER
3	D	294	VAL
3	D	308	VAL
3	D	310	VAL
3	D	311	THR
3	D	546	SER
3	D	553	MET
3	G	106	VAL
3	G	107	GLN
3	G	114	LEU
3	G	118	THR
3	G	122	CYS
3	G	132	ILE
3	G	134	LEU
3	G	135	VAL
3	G	136	CYS
3	G	253	SER
3	G	294	VAL
3	G	308	VAL
3	G	310	VAL
3	G	311	THR
3	G	546	SER
3	G	553	MET
3	J	106	VAL
3	J	107	GLN
3	J	114	LEU
3	J	118	THR
3	J	122	CYS
3	J	132	ILE
3	J	134	LEU
3	J	135	VAL
3	J	136	CYS
3	J	253	SER
3	J	294	VAL

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Mol	Chain	Res	Type
3	J	308	VAL
3	J	310	VAL
3	J	311	THR
3	J	546	SER
3	J	553	MET
2	F	61	ILE
2	F	62	LEU
2	F	72	VAL
2	F	75	LEU
2	F	76	ILE
2	F	77	LEU
2	I	61	ILE
2	I	62	LEU
2	I	72	VAL
2	I	75	LEU
2	I	76	ILE
2	I	77	LEU
2	L	61	ILE
2	L	62	LEU
2	L	72	VAL
2	L	75	LEU
2	L	76	ILE
2	L	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	356	GLN
3	A	357	GLN
3	A	359	GLN
3	A	365	ASN
3	A	376	GLN
3	A	547	GLN
3	A	549	HIS
3	D	112	ASN
3	D	126	HIS
3	D	356	GLN
3	D	357	GLN
3	D	359	GLN
3	D	365	ASN
3	D	376	GLN
3	D	547	GLN

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Mol	Chain	Res	Type
3	D	549	HIS
3	G	112	ASN
3	G	126	HIS
3	G	356	GLN
3	G	357	GLN
3	G	359	GLN
3	G	365	ASN
3	G	376	GLN
3	G	530	GLN
3	G	547	GLN
3	G	549	HIS
3	J	112	ASN
3	J	126	HIS
3	J	356	GLN
3	J	357	GLN
3	J	359	GLN
3	J	365	ASN
3	J	376	GLN
3	J	547	GLN
3	J	549	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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
5	A1BBG	I	201	-	45,45,67	0.66	1 (2%)	60,63,85	0.53	0
5	A1BBG	A	801	-	54,54,67	1.22	5 (9%)	69,72,85	1.14	8 (11%)
5	A1BBG	J	801	-	54,54,67	1.22	5 (9%)	69,72,85	1.14	8 (11%)
5	A1BBG	D	801	-	54,54,67	1.22	5 (9%)	69,72,85	1.14	8 (11%)
5	A1BBG	F	201	-	45,45,67	0.66	1 (2%)	60,63,85	0.53	0
5	A1BBG	C	201	-	45,45,67	0.66	1 (2%)	60,63,85	0.53	0
5	A1BBG	G	801	-	54,54,67	1.22	5 (9%)	69,72,85	1.14	8 (11%)
5	A1BBG	L	201	-	45,45,67	0.66	1 (2%)	60,63,85	0.53	0

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
5	A1BBG	I	201	-	-	12/42/66/88	0/1/1/1
5	A1BBG	A	801	-	-	19/51/75/88	0/1/1/1
5	A1BBG	J	801	-	-	19/51/75/88	0/1/1/1
5	A1BBG	D	801	-	-	19/51/75/88	0/1/1/1
5	A1BBG	F	201	-	-	12/42/66/88	0/1/1/1
5	A1BBG	C	201	-	-	12/42/66/88	0/1/1/1
5	A1BBG	G	801	-	-	19/51/75/88	0/1/1/1
5	A1BBG	L	201	-	-	12/42/66/88	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	A1BBG	C41-C40	-4.82	1.32	1.52
5	G	801	A1BBG	C41-C40	-4.82	1.32	1.52
5	D	801	A1BBG	C41-C40	-4.82	1.32	1.52
5	J	801	A1BBG	C41-C40	-4.82	1.32	1.52
5	A	801	A1BBG	C35-C34	-3.83	1.32	1.51
5	D	801	A1BBG	C35-C34	-3.83	1.32	1.51
5	G	801	A1BBG	C35-C34	-3.83	1.32	1.51
5	J	801	A1BBG	C35-C34	-3.83	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	801	A1BBG	C37-C38	-3.29	1.32	1.50
5	A	801	A1BBG	C37-C38	-3.29	1.32	1.50
5	D	801	A1BBG	C37-C38	-3.29	1.32	1.50
5	J	801	A1BBG	C37-C38	-3.28	1.32	1.50
5	A	801	A1BBG	C39-C38	3.26	1.50	1.31
5	G	801	A1BBG	C39-C38	3.26	1.50	1.31
5	D	801	A1BBG	C39-C38	3.26	1.50	1.31
5	J	801	A1BBG	C39-C38	3.24	1.50	1.31
5	D	801	A1BBG	C44-C43	-3.14	1.32	1.51
5	J	801	A1BBG	C44-C43	-3.14	1.32	1.51
5	A	801	A1BBG	C44-C43	-3.13	1.32	1.51
5	G	801	A1BBG	C44-C43	-3.13	1.32	1.51
5	L	201	A1BBG	C35-C34	-3.07	1.32	1.51
5	C	201	A1BBG	C35-C34	-3.07	1.32	1.51
5	F	201	A1BBG	C35-C34	-3.07	1.32	1.51
5	I	201	A1BBG	C35-C34	-3.07	1.32	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	A1BBG	P23-O22-C11	3.52	132.83	123.43
5	J	801	A1BBG	P23-O22-C11	3.52	132.83	123.43
5	A	801	A1BBG	P23-O22-C11	3.51	132.80	123.43
5	G	801	A1BBG	P23-O22-C11	3.50	132.78	123.43
5	A	801	A1BBG	C35-C34-C33	3.50	132.07	114.37
5	G	801	A1BBG	C35-C34-C33	3.50	132.07	114.37
5	D	801	A1BBG	C35-C34-C33	3.50	132.06	114.37
5	J	801	A1BBG	C35-C34-C33	3.50	132.04	114.37
5	G	801	A1BBG	C36-C37-C38	2.64	127.37	112.60
5	A	801	A1BBG	C36-C37-C38	2.63	127.34	112.60
5	D	801	A1BBG	C36-C37-C38	2.63	127.32	112.60
5	J	801	A1BBG	C36-C37-C38	2.62	127.30	112.60
5	A	801	A1BBG	C36-C35-C34	2.57	127.34	114.37
5	G	801	A1BBG	C36-C35-C34	2.57	127.34	114.37
5	D	801	A1BBG	C36-C35-C34	2.56	127.32	114.37
5	J	801	A1BBG	C36-C35-C34	2.56	127.32	114.37
5	D	801	A1BBG	C41-C40-C39	2.51	126.68	112.60
5	J	801	A1BBG	C41-C40-C39	2.51	126.68	112.60
5	A	801	A1BBG	C41-C40-C39	2.51	126.66	112.60
5	G	801	A1BBG	C41-C40-C39	2.51	126.66	112.60
5	D	801	A1BBG	C42-C41-C40	2.36	125.22	113.86
5	J	801	A1BBG	C42-C41-C40	2.36	125.21	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	A1BBG	C42-C41-C40	2.35	125.18	113.86
5	G	801	A1BBG	C42-C41-C40	2.35	125.18	113.86
5	G	801	A1BBG	C10-C11-C12	2.24	116.75	111.72
5	A	801	A1BBG	C10-C11-C12	2.23	116.74	111.72
5	D	801	A1BBG	C10-C11-C12	2.23	116.74	111.72
5	J	801	A1BBG	C10-C11-C12	2.23	116.74	111.72
5	A	801	A1BBG	C11-C10-C09	2.16	113.48	109.11
5	G	801	A1BBG	C11-C10-C09	2.16	113.48	109.11
5	D	801	A1BBG	C11-C10-C09	2.14	113.45	109.11
5	J	801	A1BBG	C11-C10-C09	2.14	113.45	109.11

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	A1BBG	C14-C09-O08-P05
5	C	201	A1BBG	C10-C09-O08-P05
5	C	201	A1BBG	C03-O04-P05-O07
5	C	201	A1BBG	C09-O08-P05-O04
5	A	801	A1BBG	C10-C11-O22-P23
5	D	801	A1BBG	C10-C11-O22-P23
5	G	801	A1BBG	C10-C11-O22-P23
5	J	801	A1BBG	C10-C11-O22-P23
5	F	201	A1BBG	C14-C09-O08-P05
5	F	201	A1BBG	C10-C09-O08-P05
5	F	201	A1BBG	C03-O04-P05-O07
5	F	201	A1BBG	C09-O08-P05-O04
5	I	201	A1BBG	C14-C09-O08-P05
5	I	201	A1BBG	C10-C09-O08-P05
5	I	201	A1BBG	C03-O04-P05-O07
5	I	201	A1BBG	C09-O08-P05-O04
5	L	201	A1BBG	C14-C09-O08-P05
5	L	201	A1BBG	C10-C09-O08-P05
5	L	201	A1BBG	C03-O04-P05-O07
5	L	201	A1BBG	C09-O08-P05-O04
5	A	801	A1BBG	C33-C34-C35-C36
5	D	801	A1BBG	C33-C34-C35-C36
5	G	801	A1BBG	C33-C34-C35-C36
5	J	801	A1BBG	C33-C34-C35-C36
5	A	801	A1BBG	C42-C43-C44-C45
5	D	801	A1BBG	C42-C43-C44-C45
5	G	801	A1BBG	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
5	J	801	A1BBG	C42-C43-C44-C45
5	L	201	A1BBG	C33-C34-C35-C36
5	A	801	A1BBG	C31-C32-C33-C34
5	D	801	A1BBG	C31-C32-C33-C34
5	G	801	A1BBG	C31-C32-C33-C34
5	J	801	A1BBG	C31-C32-C33-C34
5	C	201	A1BBG	C33-C34-C35-C36
5	F	201	A1BBG	C33-C34-C35-C36
5	I	201	A1BBG	C33-C34-C35-C36
5	C	201	A1BBG	C31-C29-O28-C02
5	F	201	A1BBG	C31-C29-O28-C02
5	I	201	A1BBG	C31-C29-O28-C02
5	L	201	A1BBG	C31-C29-O28-C02
5	C	201	A1BBG	C49-C51-C52-C53
5	F	201	A1BBG	C49-C51-C52-C53
5	I	201	A1BBG	C49-C51-C52-C53
5	L	201	A1BBG	C49-C51-C52-C53
5	A	801	A1BBG	C32-C33-C34-C35
5	D	801	A1BBG	C32-C33-C34-C35
5	G	801	A1BBG	C32-C33-C34-C35
5	J	801	A1BBG	C32-C33-C34-C35
5	A	801	A1BBG	C35-C36-C37-C38
5	D	801	A1BBG	C35-C36-C37-C38
5	G	801	A1BBG	C35-C36-C37-C38
5	J	801	A1BBG	C35-C36-C37-C38
5	C	201	A1BBG	O30-C29-O28-C02
5	F	201	A1BBG	O30-C29-O28-C02
5	I	201	A1BBG	O30-C29-O28-C02
5	L	201	A1BBG	O30-C29-O28-C02
5	C	201	A1BBG	C29-C31-C32-C33
5	F	201	A1BBG	C29-C31-C32-C33
5	I	201	A1BBG	C29-C31-C32-C33
5	L	201	A1BBG	C29-C31-C32-C33
5	A	801	A1BBG	O48-C01-C02-C03
5	D	801	A1BBG	O48-C01-C02-C03
5	G	801	A1BBG	O48-C01-C02-C03
5	J	801	A1BBG	O48-C01-C02-C03
5	A	801	A1BBG	O48-C01-C02-O28
5	D	801	A1BBG	O48-C01-C02-O28
5	G	801	A1BBG	O48-C01-C02-O28
5	J	801	A1BBG	O48-C01-C02-O28
5	A	801	A1BBG	C13-C12-O17-P18

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Mol	Chain	Res	Type	Atoms
5	D	801	A1BBG	C13-C12-O17-P18
5	G	801	A1BBG	C13-C12-O17-P18
5	J	801	A1BBG	C13-C12-O17-P18
5	C	201	A1BBG	C31-C32-C33-C34
5	F	201	A1BBG	C31-C32-C33-C34
5	L	201	A1BBG	C31-C32-C33-C34
5	A	801	A1BBG	C11-C12-O17-P18
5	D	801	A1BBG	C11-C12-O17-P18
5	G	801	A1BBG	C11-C12-O17-P18
5	J	801	A1BBG	C11-C12-O17-P18
5	I	201	A1BBG	C31-C32-C33-C34
5	A	801	A1BBG	C01-C02-C03-O04
5	D	801	A1BBG	C01-C02-C03-O04
5	G	801	A1BBG	C01-C02-C03-O04
5	J	801	A1BBG	C01-C02-C03-O04
5	A	801	A1BBG	O28-C02-C03-O04
5	D	801	A1BBG	O28-C02-C03-O04
5	G	801	A1BBG	O28-C02-C03-O04
5	J	801	A1BBG	O28-C02-C03-O04
5	C	201	A1BBG	C03-C02-O28-C29
5	F	201	A1BBG	C03-C02-O28-C29
5	I	201	A1BBG	C03-C02-O28-C29
5	L	201	A1BBG	C03-C02-O28-C29
5	D	801	A1BBG	O28-C29-C31-C32
5	J	801	A1BBG	O28-C29-C31-C32
5	A	801	A1BBG	O28-C29-C31-C32
5	G	801	A1BBG	O28-C29-C31-C32
5	A	801	A1BBG	O48-C49-C51-C52
5	G	801	A1BBG	O48-C49-C51-C52
5	D	801	A1BBG	O48-C49-C51-C52
5	J	801	A1BBG	O48-C49-C51-C52
5	A	801	A1BBG	C12-C11-O22-P23
5	D	801	A1BBG	C12-C11-O22-P23
5	G	801	A1BBG	C12-C11-O22-P23
5	J	801	A1BBG	C12-C11-O22-P23
5	A	801	A1BBG	C36-C37-C38-C39
5	D	801	A1BBG	C36-C37-C38-C39
5	G	801	A1BBG	C36-C37-C38-C39
5	J	801	A1BBG	C36-C37-C38-C39
5	C	201	A1BBG	C09-O08-P05-O06
5	A	801	A1BBG	C09-O08-P05-O06
5	A	801	A1BBG	C09-O08-P05-O07

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Mol	Chain	Res	Type	Atoms
5	D	801	A1BBG	C09-O08-P05-O06
5	D	801	A1BBG	C09-O08-P05-O07
5	G	801	A1BBG	C09-O08-P05-O06
5	G	801	A1BBG	C09-O08-P05-O07
5	J	801	A1BBG	C09-O08-P05-O06
5	J	801	A1BBG	C09-O08-P05-O07
5	F	201	A1BBG	C09-O08-P05-O06
5	I	201	A1BBG	C09-O08-P05-O06
5	L	201	A1BBG	C09-O08-P05-O06
5	A	801	A1BBG	C14-C09-O08-P05
5	D	801	A1BBG	C14-C09-O08-P05
5	G	801	A1BBG	C14-C09-O08-P05
5	J	801	A1BBG	C14-C09-O08-P05

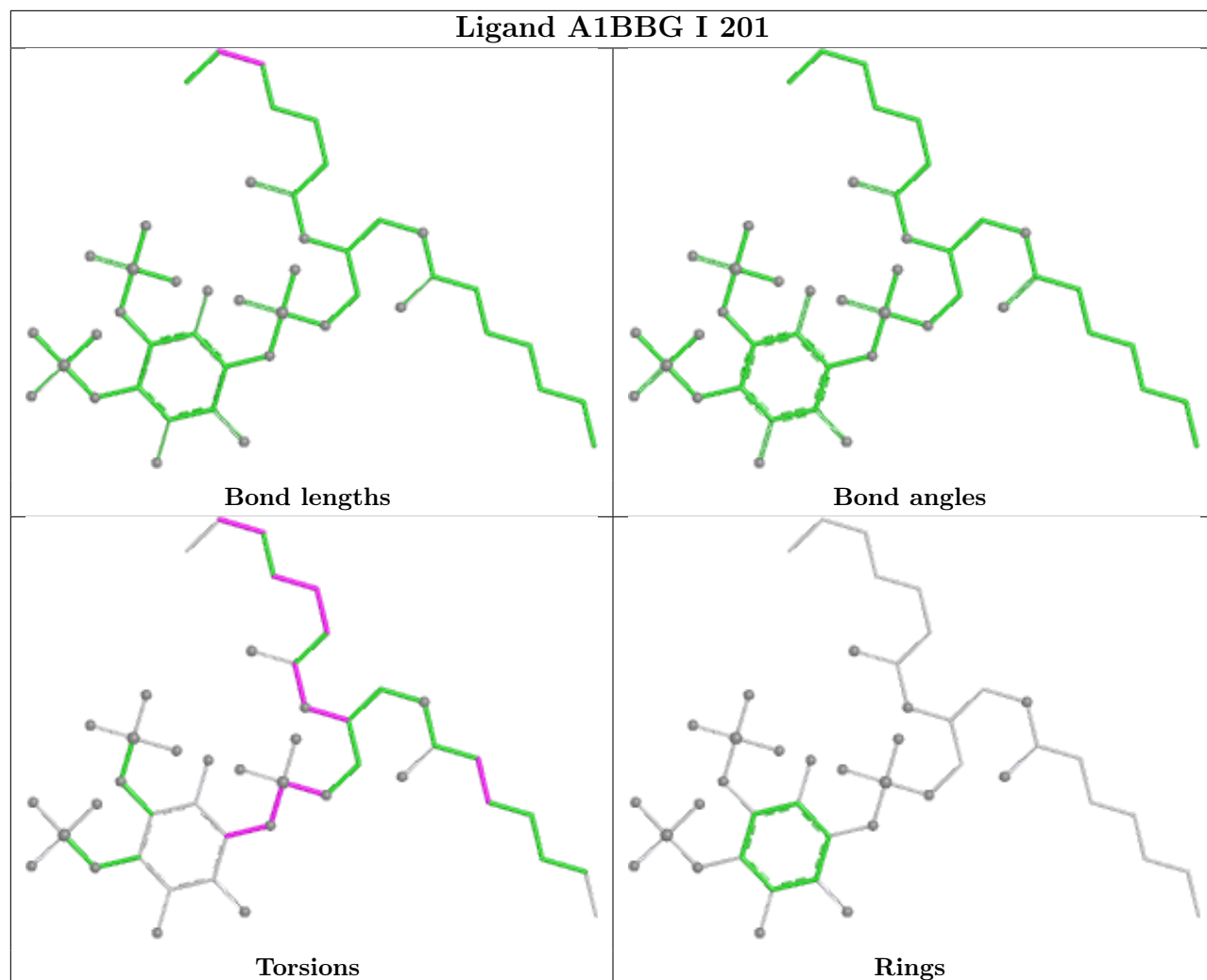
There are no ring outliers.

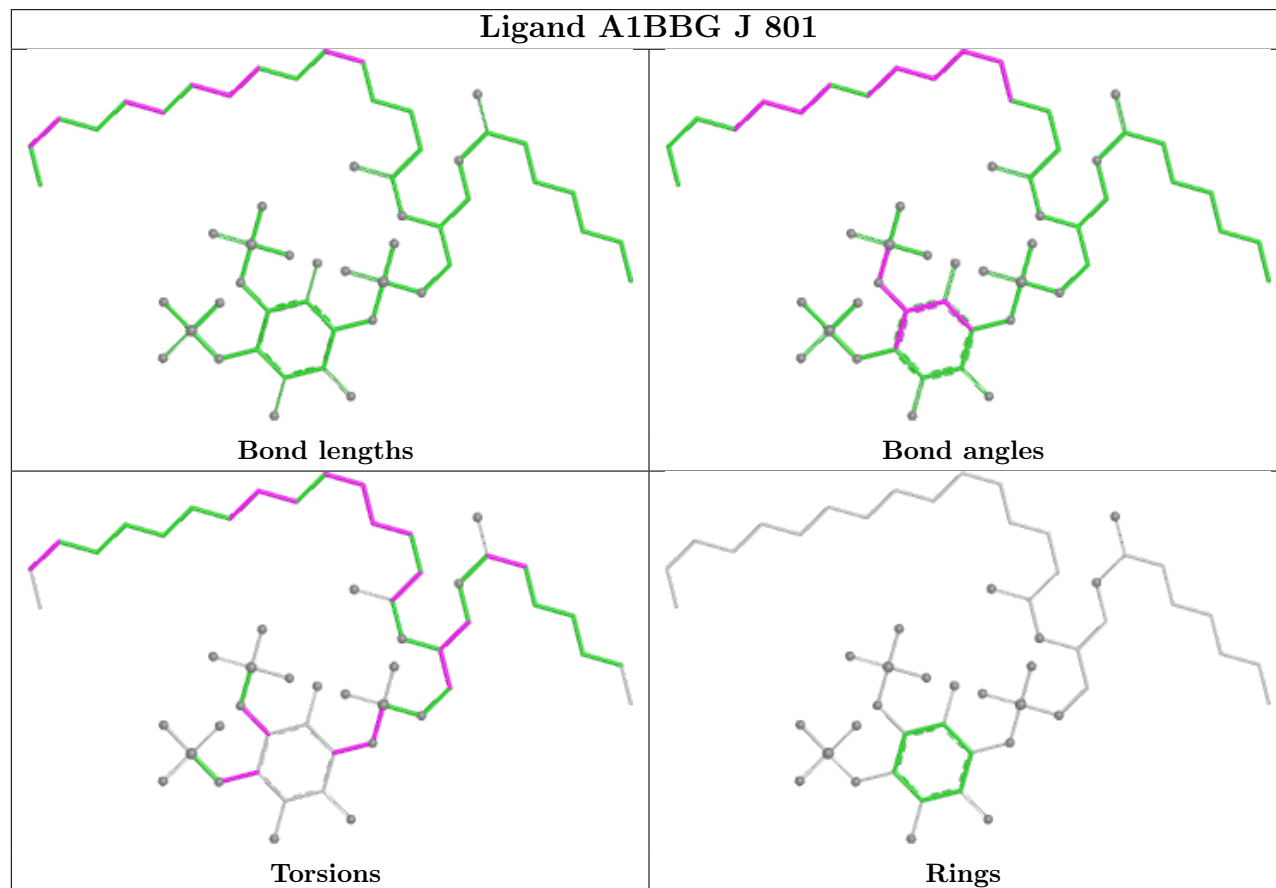
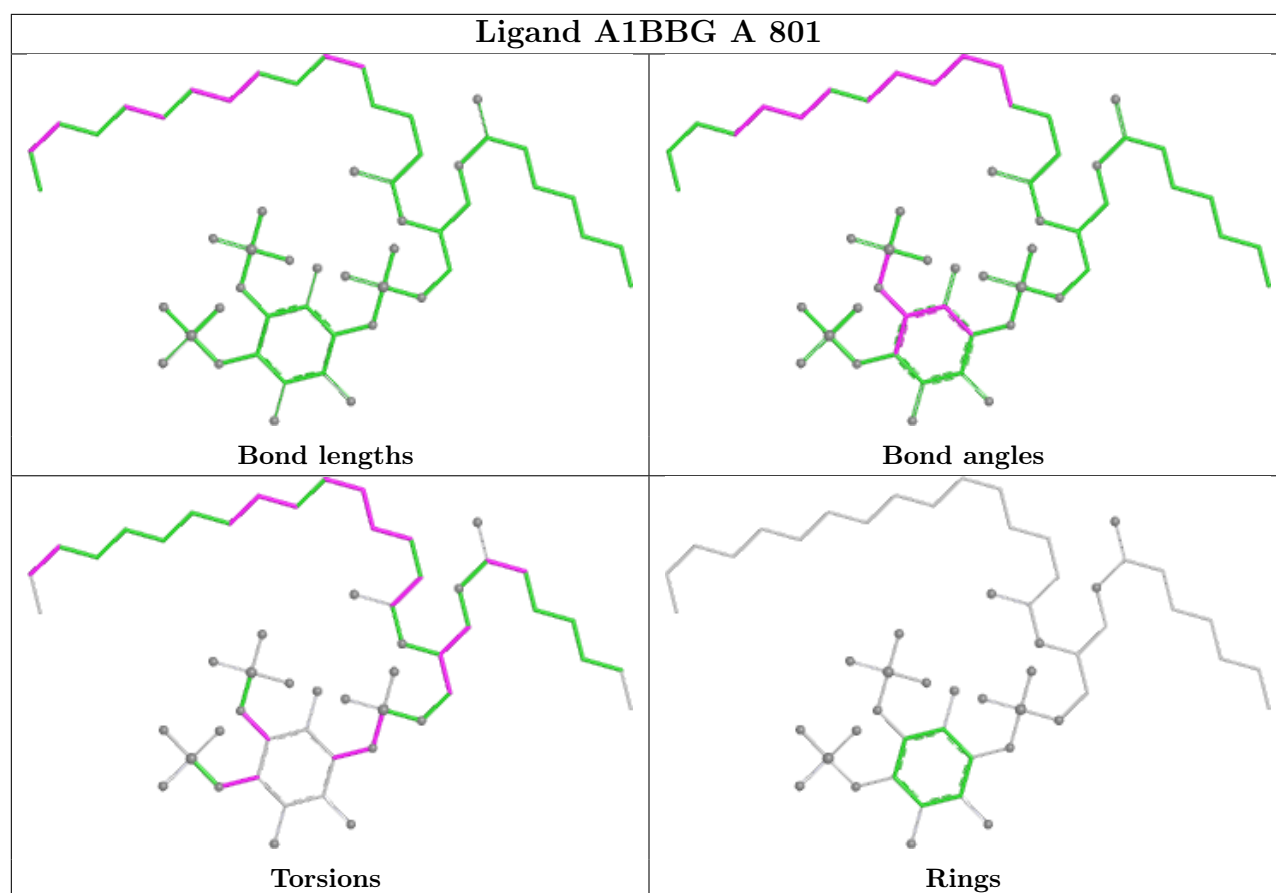
4 monomers are involved in 35 short contacts:

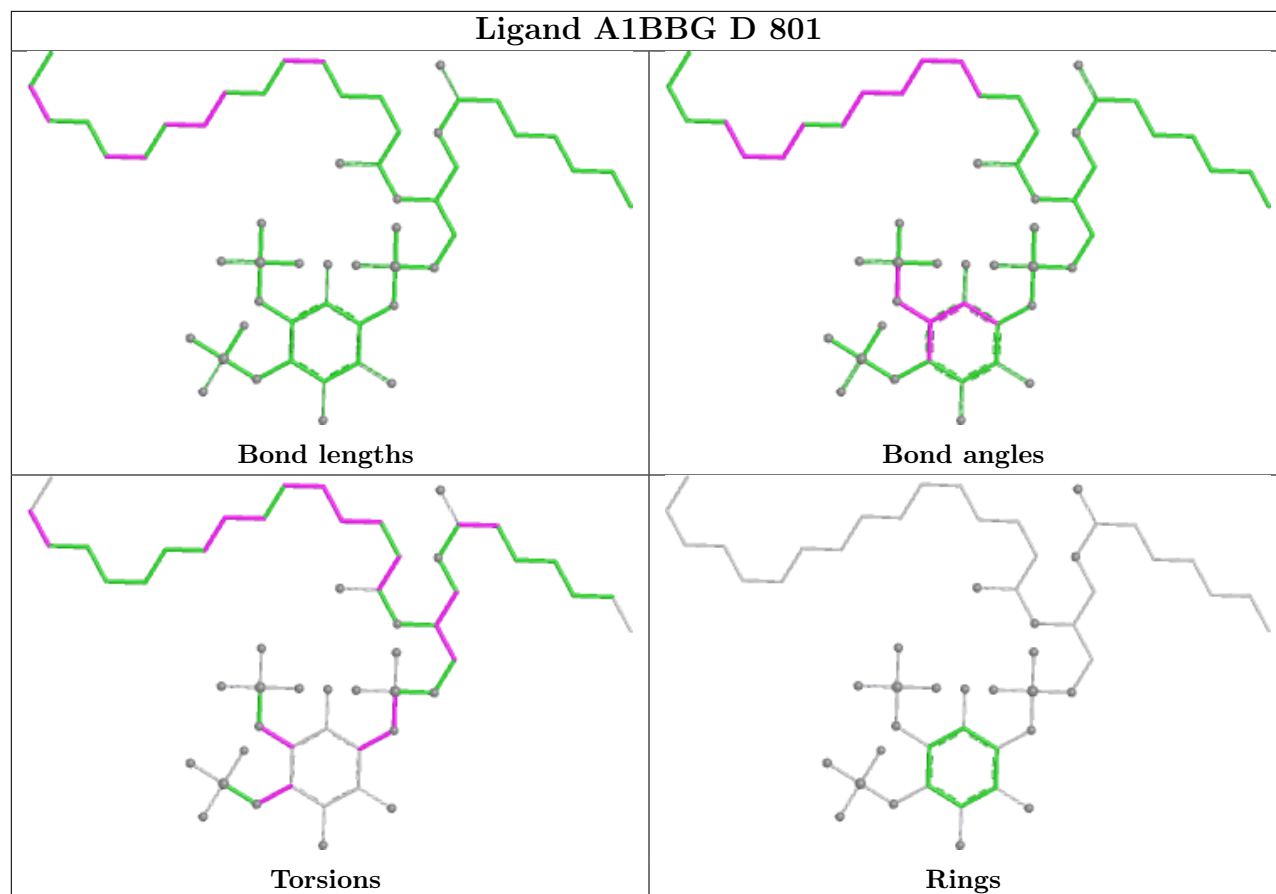
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	A1BBG	9	0
5	J	801	A1BBG	8	0
5	D	801	A1BBG	9	0
5	G	801	A1BBG	9	0

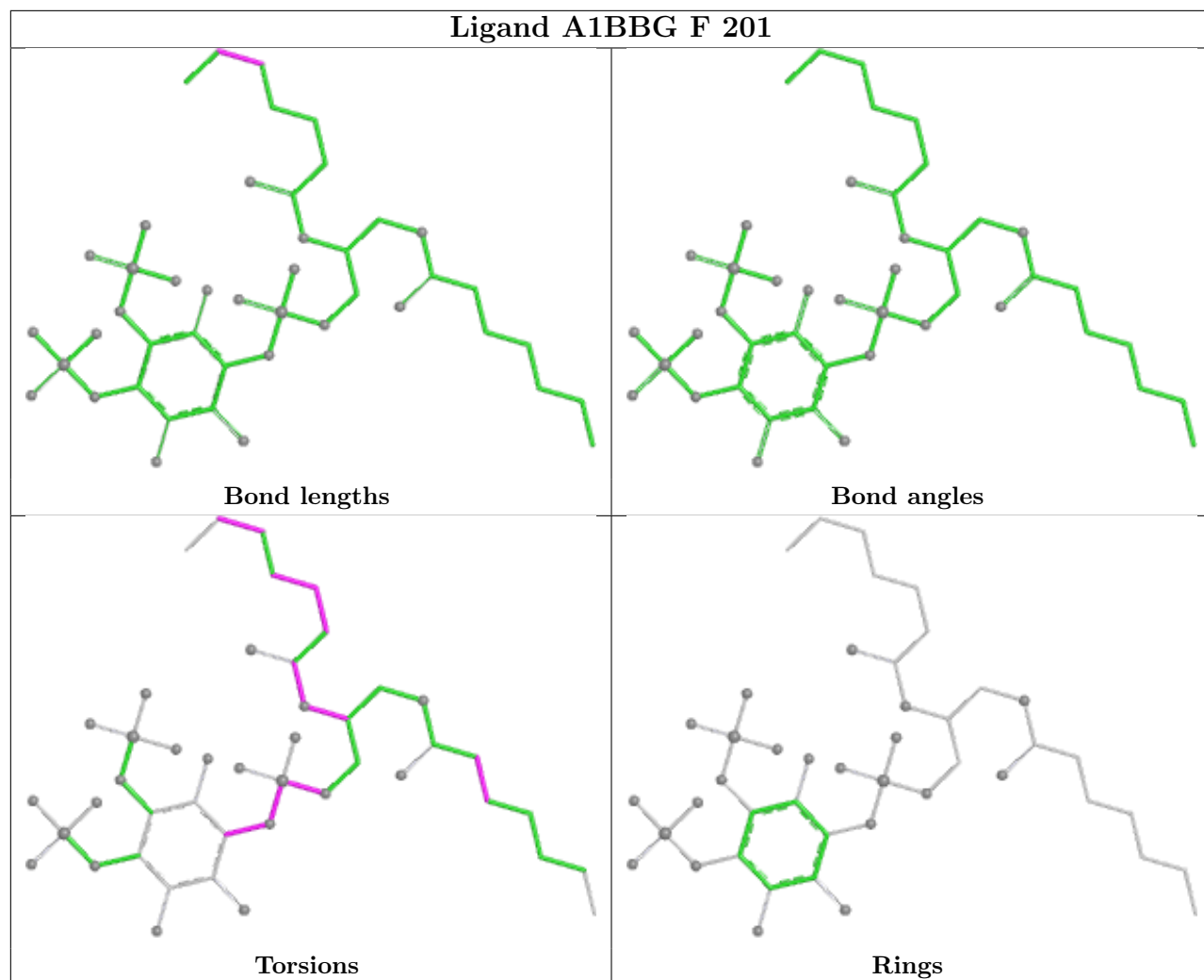
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

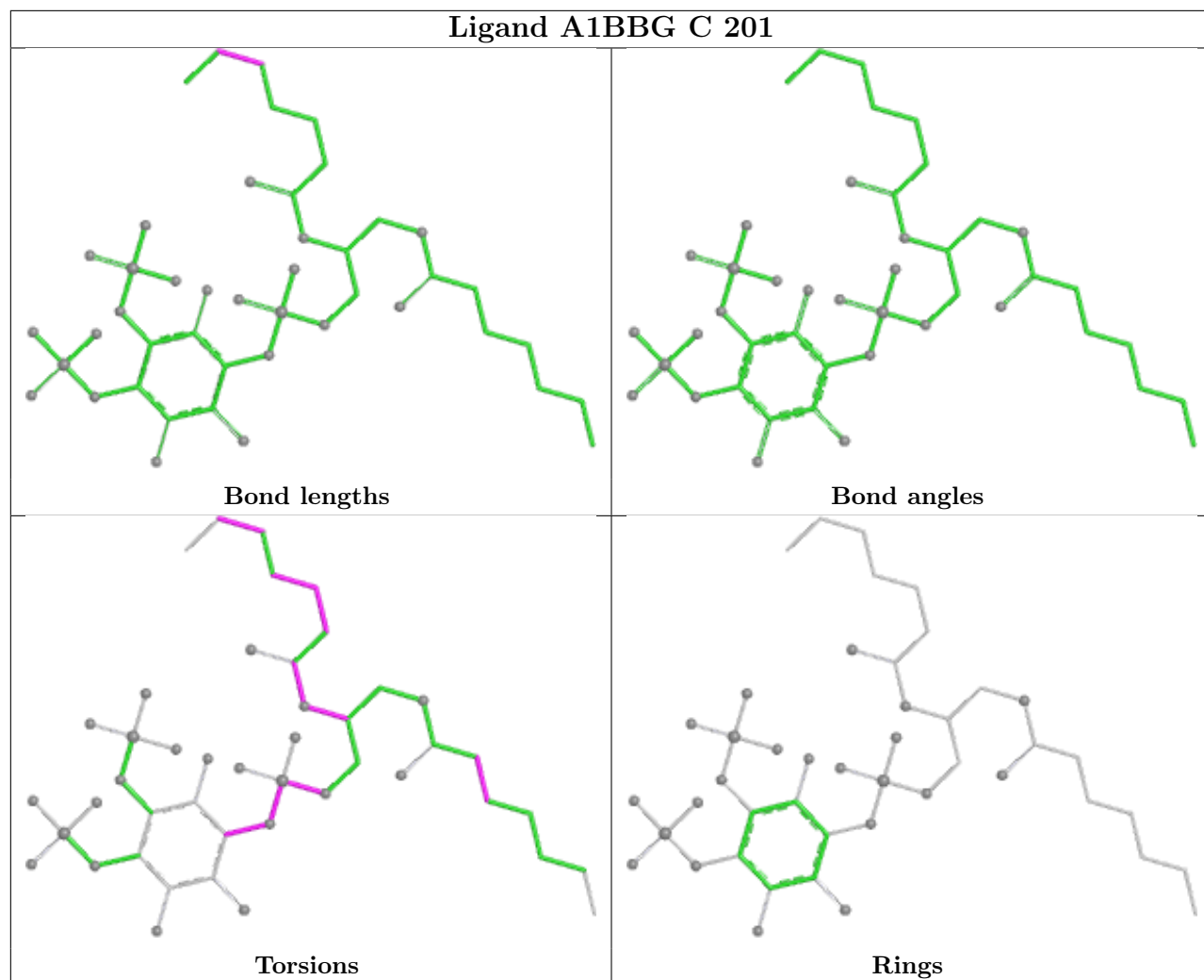
Ligand A1BBG I 201

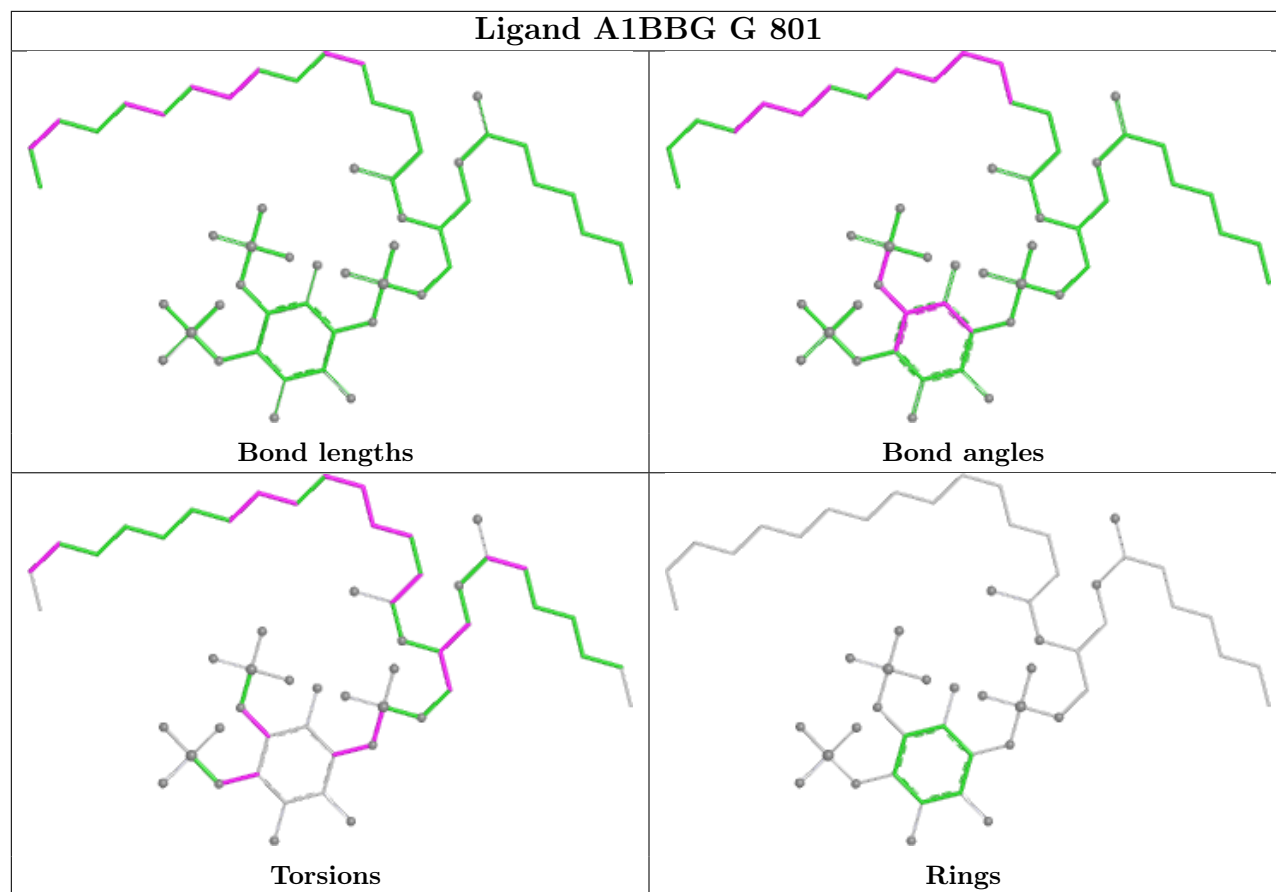


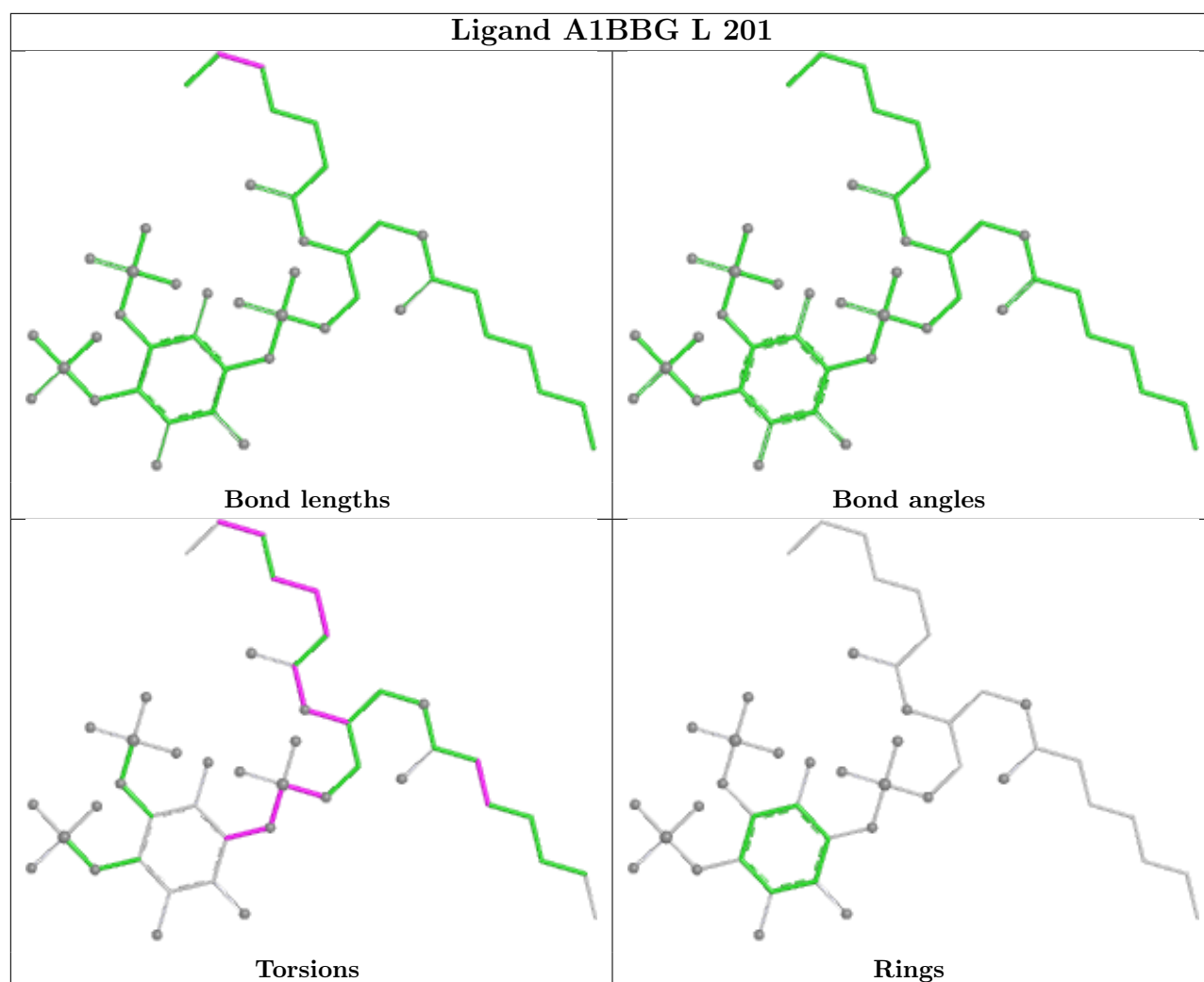












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

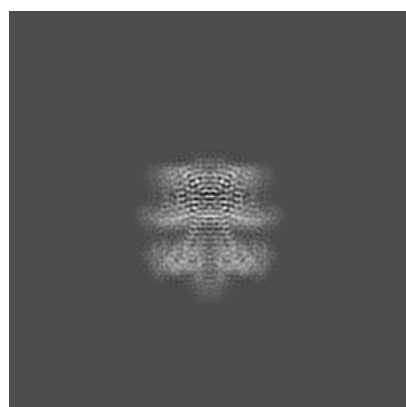
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20967. These allow visual inspection of the internal detail of the map and identification of artifacts.

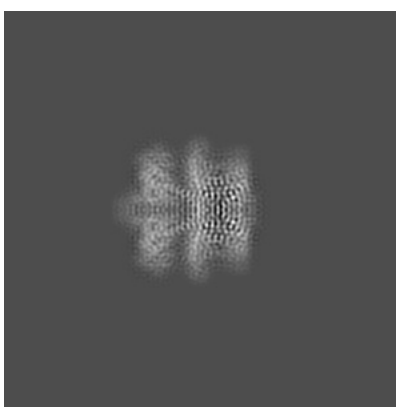
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

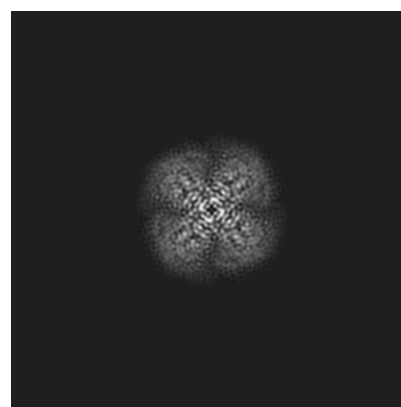
6.1.1 Primary map



X



Y



Z

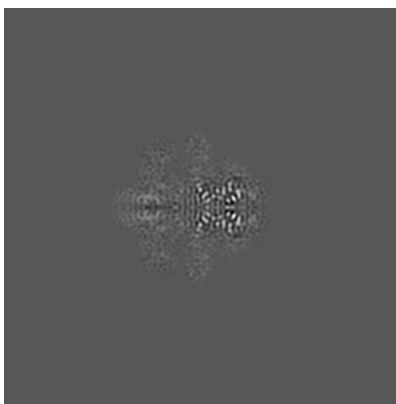
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

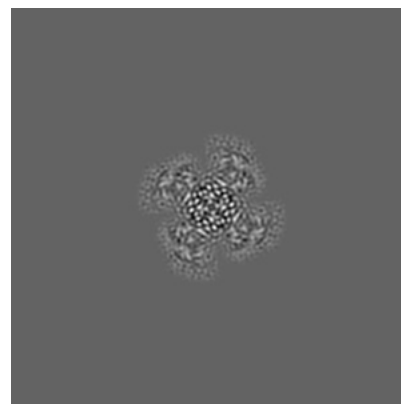
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

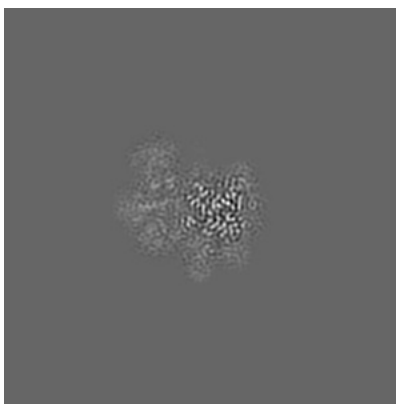
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

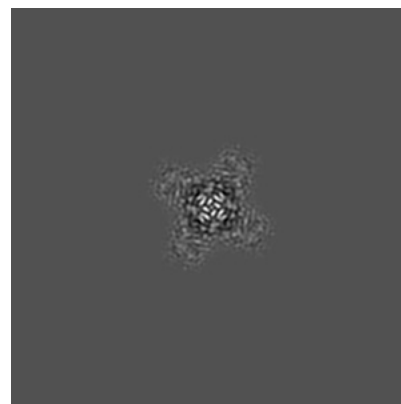
6.3.1 Primary map



X Index: 158



Y Index: 158

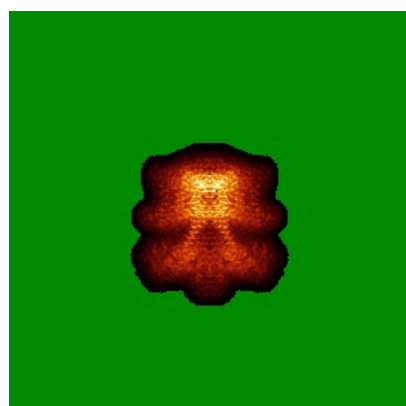


Z Index: 168

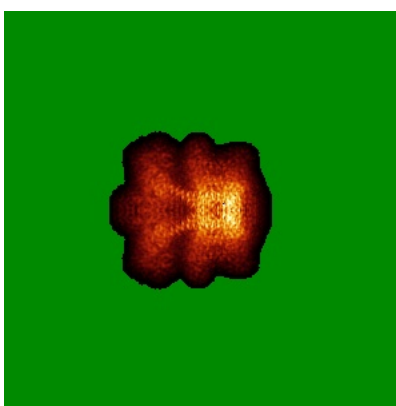
The images above show the largest variance slices of the map in three orthogonal directions.

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

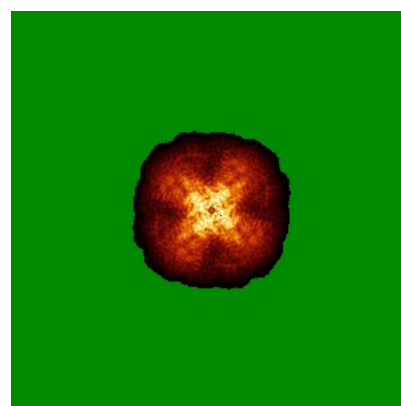
6.4.1 Primary map



X



Y

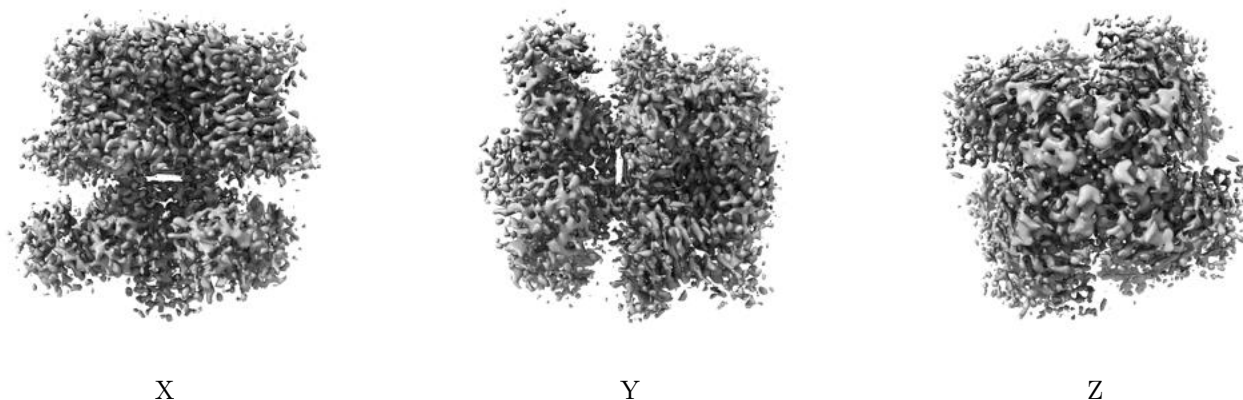


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

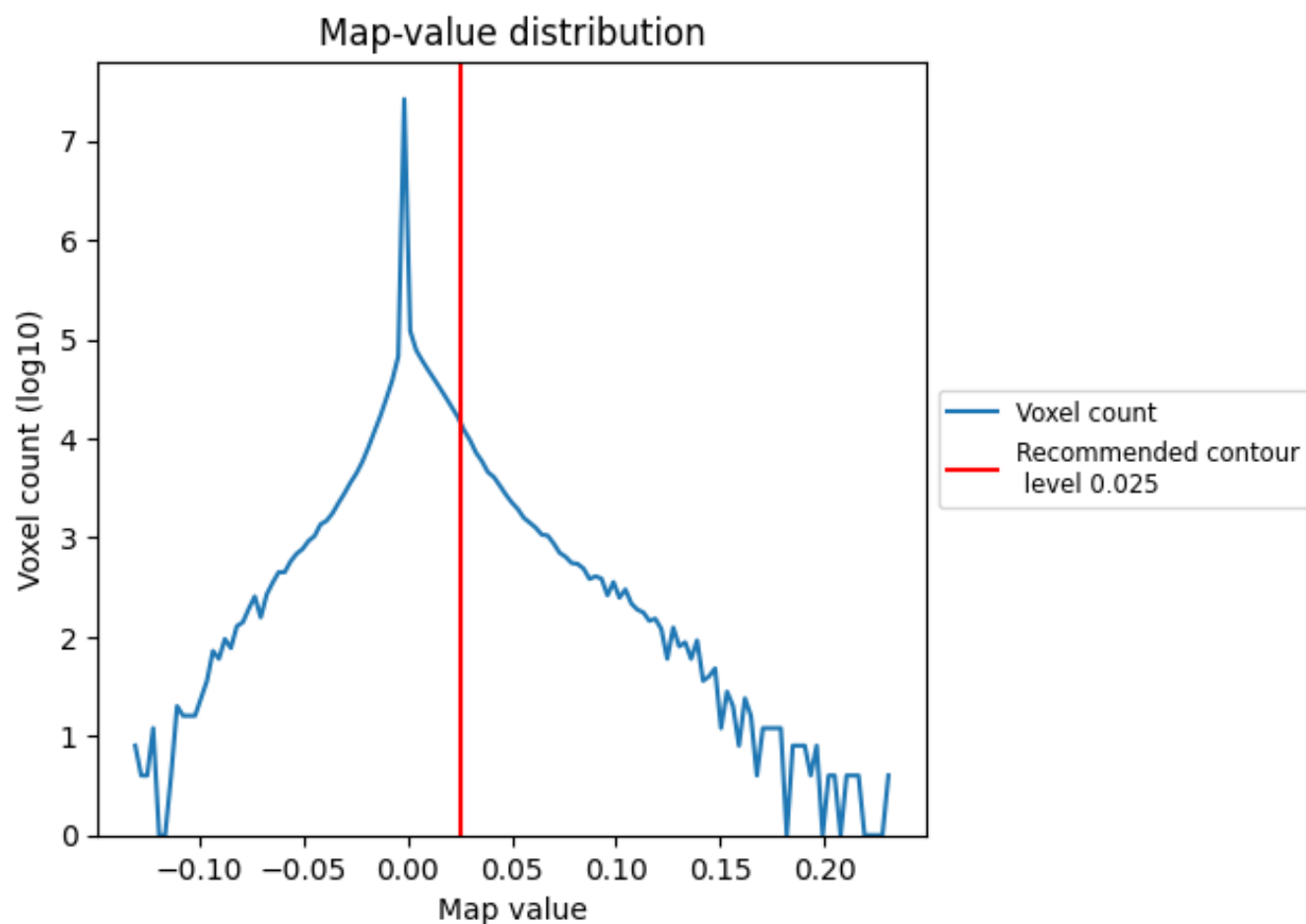
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

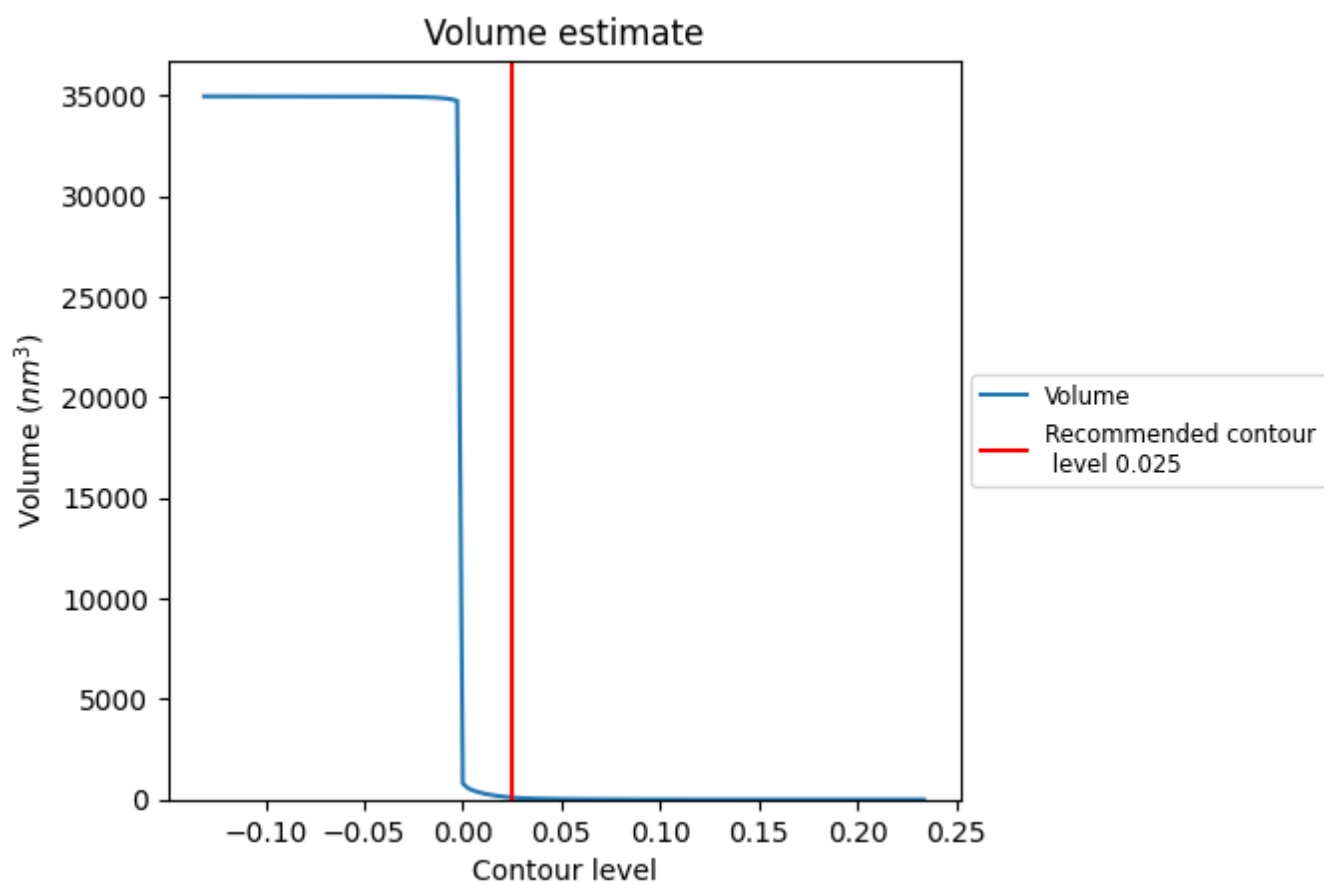
This section contains the results of statistical analysis of the map.

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.

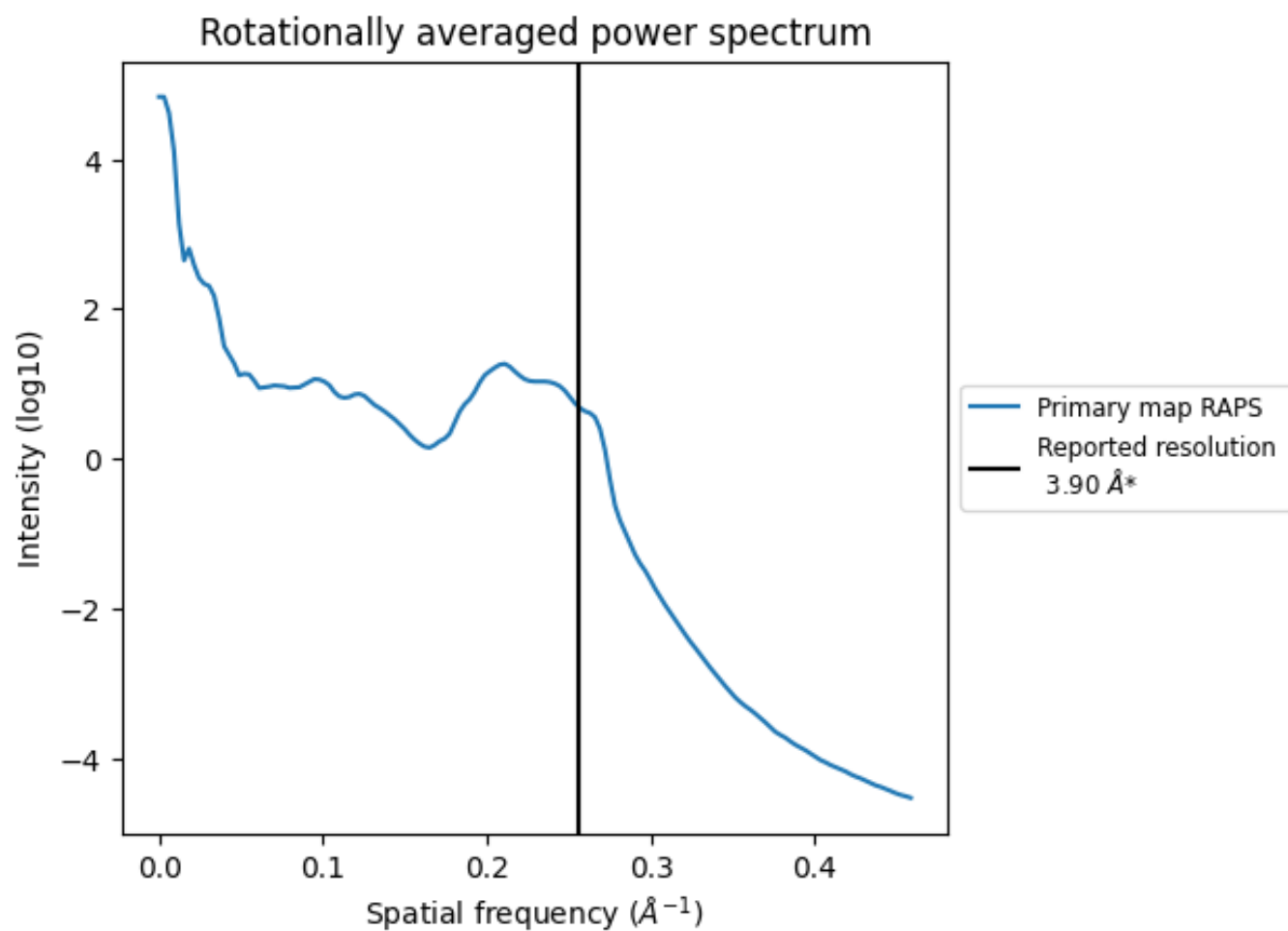
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 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 0.256 Å⁻¹

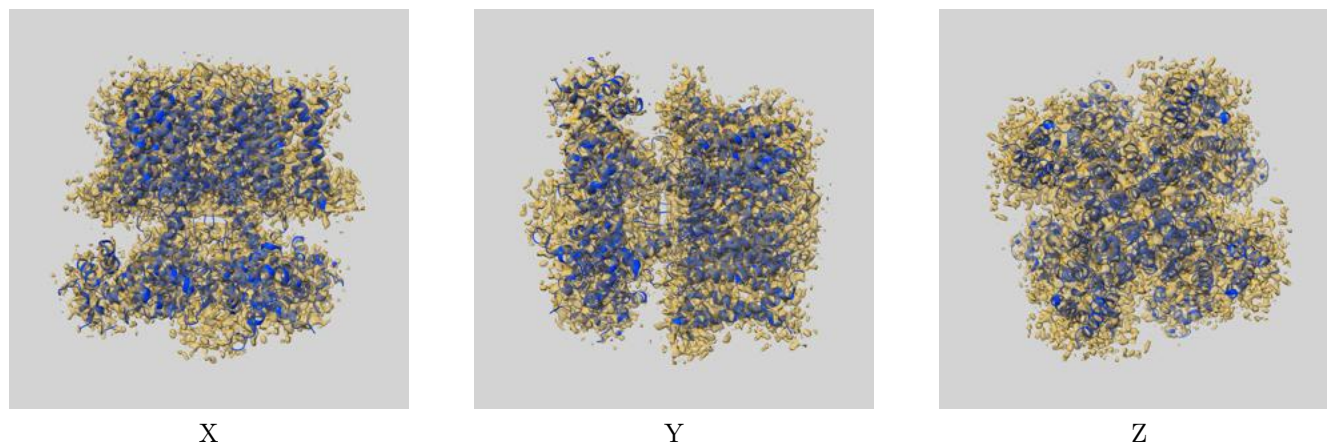
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

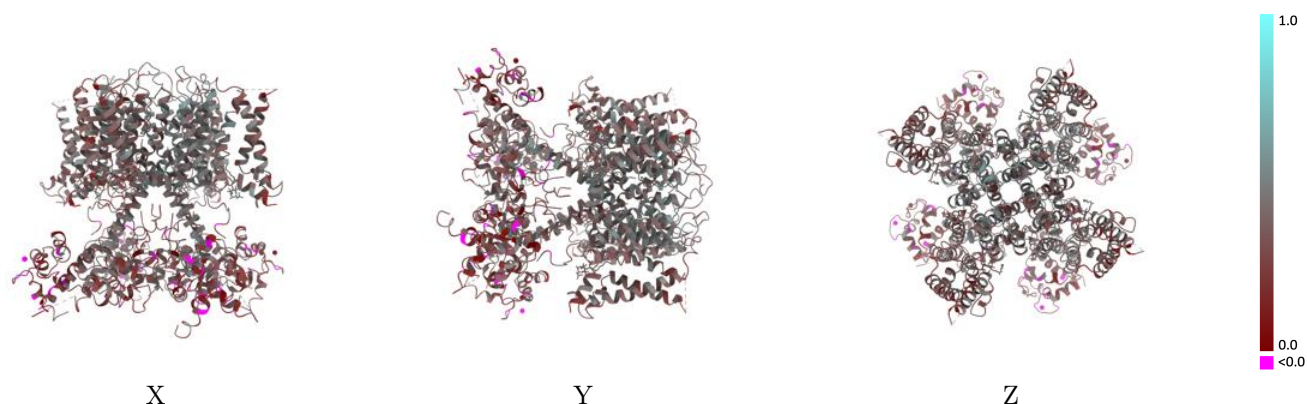
This section contains information regarding the fit between EMDB map EMD-20967 and PDB model 9WD8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



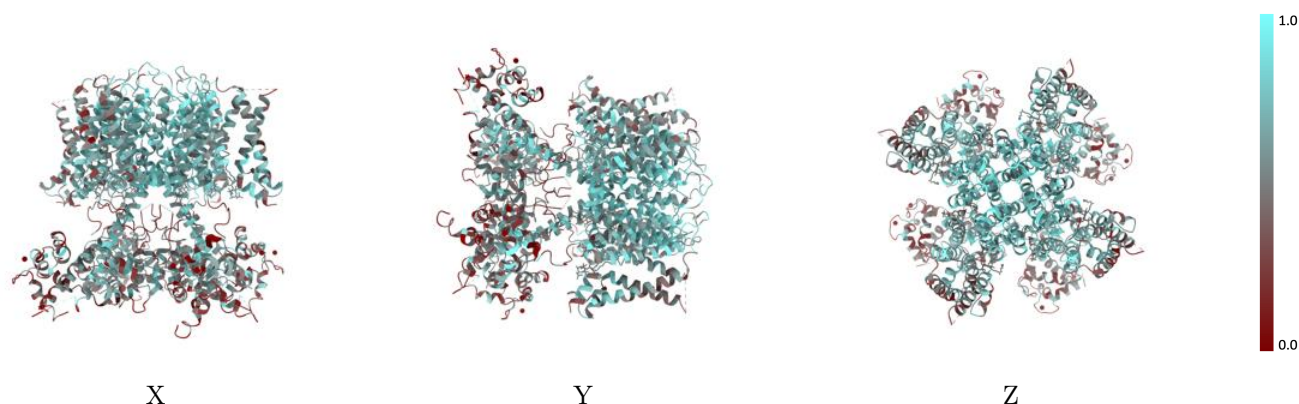
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



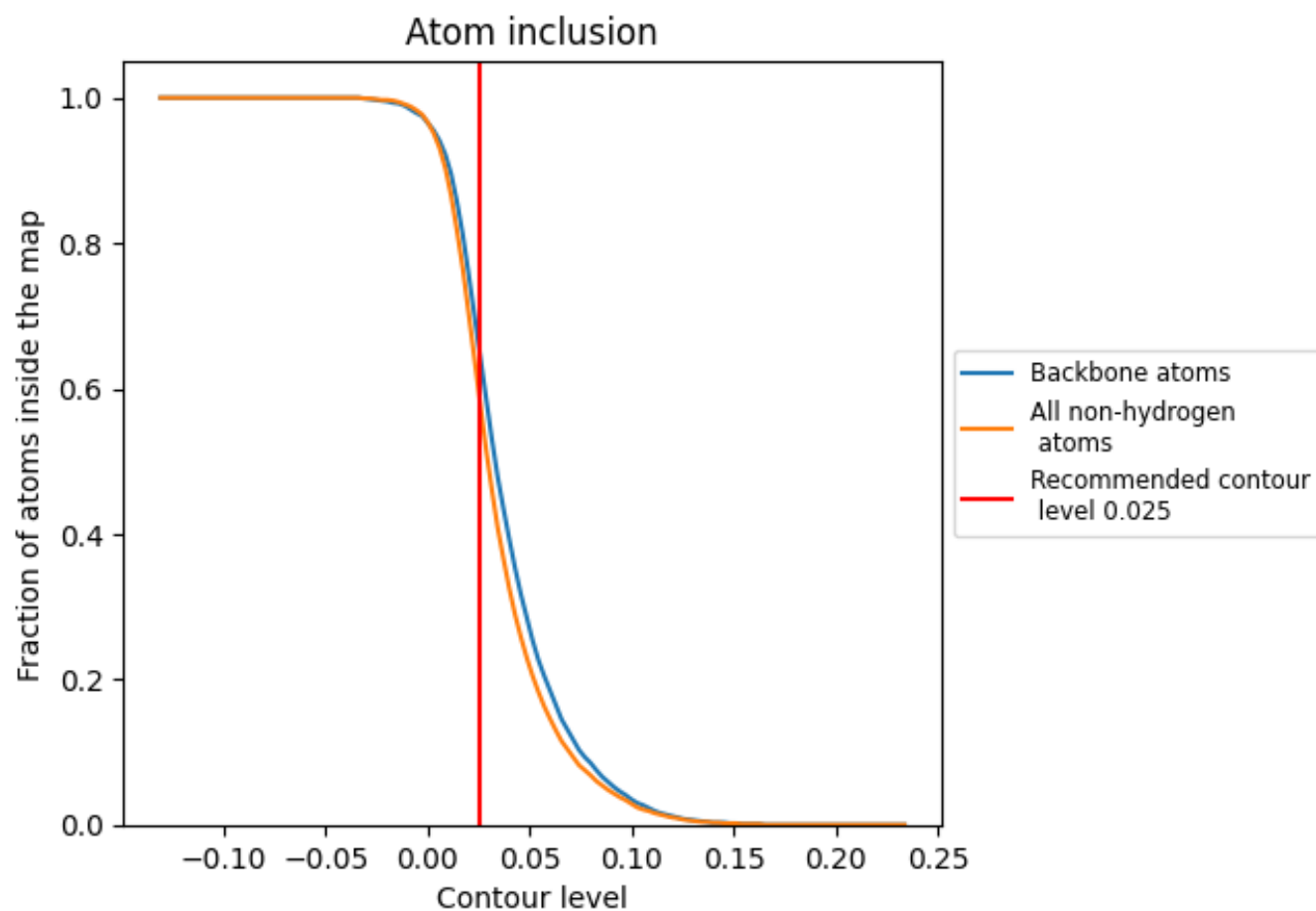
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5930	0.3600
A	0.6770	0.4170
B	0.4440	0.2990
C	0.6030	0.4350
D	0.6410	0.3780
E	0.4300	0.2770
F	0.6000	0.3820
G	0.6230	0.3480
H	0.3910	0.2460
I	0.5620	0.3480
J	0.6470	0.3840
K	0.4260	0.2740
L	0.5850	0.3970

