



# Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:24 PM JST

PDB ID : 7BYL  
EMDB ID : EMD-30244  
Title : Cryo-EM structure of human KCNQ4  
Authors : Shen, H.; Li, T.; Yue, Z.  
Deposited on : 2020-04-23  
Resolution : 2.50 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>.

---

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) : 2.31.3

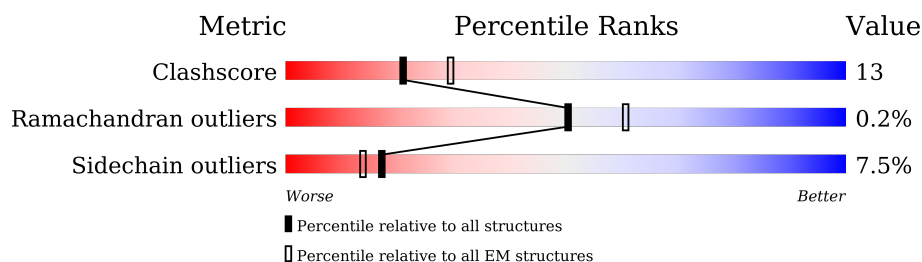
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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	A	979	
1	C	979	
1	E	979	
1	G	979	
2	B	149	
2	D	149	
2	F	149	
2	H	149	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16332 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 Green fluorescent protein,Potassium voltage-gated channel subfamily KQT member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	354	Total	C	N	O	S	0	0
			2872	1882	501	475	14		
1	C	354	Total	C	N	O	S	0	0
			2872	1882	501	475	14		
1	E	354	Total	C	N	O	S	0	0
			2872	1882	501	475	14		
1	G	354	Total	C	N	O	S	0	0
			2872	1882	501	475	14		

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-283	MET	-	expression tag	UNP P42212
A	-282	HIS	-	expression tag	UNP P42212
A	-281	HIS	-	expression tag	UNP P42212
A	-280	HIS	-	expression tag	UNP P42212
A	-279	HIS	-	expression tag	UNP P42212
A	-278	HIS	-	expression tag	UNP P42212
A	-277	HIS	-	expression tag	UNP P42212
A	-276	HIS	-	expression tag	UNP P42212
A	-275	HIS	-	expression tag	UNP P42212
A	-274	ALA	-	expression tag	UNP P42212
A	-273	ALA	-	expression tag	UNP P42212
A	-272	ASP	-	expression tag	UNP P42212
A	-271	TYR	-	expression tag	UNP P42212
A	-270	LYS	-	expression tag	UNP P42212
A	-269	ASP	-	expression tag	UNP P42212
A	-268	HIS	-	expression tag	UNP P42212
A	-267	ASP	-	expression tag	UNP P42212
A	-266	ILE	-	expression tag	UNP P42212
A	-265	ASP	-	expression tag	UNP P42212
A	-264	TYR	-	expression tag	UNP P42212
A	-263	LYS	-	expression tag	UNP P42212

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-262	ASP	-	expression tag	UNP P42212
A	-261	ASP	-	expression tag	UNP P42212
A	-260	ASP	-	expression tag	UNP P42212
A	-259	ASP	-	expression tag	UNP P42212
A	-258	LYS	-	expression tag	UNP P42212
A	-257	SER	-	expression tag	UNP P42212
A	-256	ALA	-	expression tag	UNP P42212
A	-255	MET	-	expression tag	UNP P42212
A	-254	VAL	-	expression tag	UNP P42212
A	-191	LEU	PHE	engineered mutation	UNP P42212
A	-190	THR	SER	engineered mutation	UNP P42212
A	-148	THR	LYS	engineered mutation	UNP P42212
A	-49	LYS	ALA	engineered mutation	UNP P42212
A	-24	LEU	HIS	engineered mutation	UNP P42212
A	-16	SER	-	linker	UNP P42212
A	-15	GLY	-	linker	UNP P42212
A	-14	LEU	-	linker	UNP P42212
A	-13	ARG	-	linker	UNP P42212
A	-12	SER	-	linker	UNP P42212
A	-11	GLY	-	linker	UNP P42212
A	-10	LEU	-	linker	UNP P42212
A	-9	GLU	-	linker	UNP P42212
A	-8	VAL	-	linker	UNP P42212
A	-7	LEU	-	linker	UNP P42212
A	-6	PHE	-	linker	UNP P42212
A	-5	GLN	-	linker	UNP P42212
A	-4	GLY	-	linker	UNP P42212
A	-3	PRO	-	linker	UNP P42212
A	-2	GLY	-	linker	UNP P42212
A	-1	GLY	-	linker	UNP P42212
A	0	ARG	-	linker	UNP P42212
C	-283	MET	-	expression tag	UNP P42212
C	-282	HIS	-	expression tag	UNP P42212
C	-281	HIS	-	expression tag	UNP P42212
C	-280	HIS	-	expression tag	UNP P42212
C	-279	HIS	-	expression tag	UNP P42212
C	-278	HIS	-	expression tag	UNP P42212
C	-277	HIS	-	expression tag	UNP P42212
C	-276	HIS	-	expression tag	UNP P42212
C	-275	HIS	-	expression tag	UNP P42212
C	-274	ALA	-	expression tag	UNP P42212
C	-273	ALA	-	expression tag	UNP P42212

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-272	ASP	-	expression tag	UNP P42212
C	-271	TYR	-	expression tag	UNP P42212
C	-270	LYS	-	expression tag	UNP P42212
C	-269	ASP	-	expression tag	UNP P42212
C	-268	HIS	-	expression tag	UNP P42212
C	-267	ASP	-	expression tag	UNP P42212
C	-266	ILE	-	expression tag	UNP P42212
C	-265	ASP	-	expression tag	UNP P42212
C	-264	TYR	-	expression tag	UNP P42212
C	-263	LYS	-	expression tag	UNP P42212
C	-262	ASP	-	expression tag	UNP P42212
C	-261	ASP	-	expression tag	UNP P42212
C	-260	ASP	-	expression tag	UNP P42212
C	-259	ASP	-	expression tag	UNP P42212
C	-258	LYS	-	expression tag	UNP P42212
C	-257	SER	-	expression tag	UNP P42212
C	-256	ALA	-	expression tag	UNP P42212
C	-255	MET	-	expression tag	UNP P42212
C	-254	VAL	-	expression tag	UNP P42212
C	-191	LEU	PHE	engineered mutation	UNP P42212
C	-190	THR	SER	engineered mutation	UNP P42212
C	-148	THR	LYS	engineered mutation	UNP P42212
C	-49	LYS	ALA	engineered mutation	UNP P42212
C	-24	LEU	HIS	engineered mutation	UNP P42212
C	-16	SER	-	linker	UNP P42212
C	-15	GLY	-	linker	UNP P42212
C	-14	LEU	-	linker	UNP P42212
C	-13	ARG	-	linker	UNP P42212
C	-12	SER	-	linker	UNP P42212
C	-11	GLY	-	linker	UNP P42212
C	-10	LEU	-	linker	UNP P42212
C	-9	GLU	-	linker	UNP P42212
C	-8	VAL	-	linker	UNP P42212
C	-7	LEU	-	linker	UNP P42212
C	-6	PHE	-	linker	UNP P42212
C	-5	GLN	-	linker	UNP P42212
C	-4	GLY	-	linker	UNP P42212
C	-3	PRO	-	linker	UNP P42212
C	-2	GLY	-	linker	UNP P42212
C	-1	GLY	-	linker	UNP P42212
C	0	ARG	-	linker	UNP P42212
E	-283	MET	-	expression tag	UNP P42212

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-282	HIS	-	expression tag	UNP P42212
E	-281	HIS	-	expression tag	UNP P42212
E	-280	HIS	-	expression tag	UNP P42212
E	-279	HIS	-	expression tag	UNP P42212
E	-278	HIS	-	expression tag	UNP P42212
E	-277	HIS	-	expression tag	UNP P42212
E	-276	HIS	-	expression tag	UNP P42212
E	-275	HIS	-	expression tag	UNP P42212
E	-274	ALA	-	expression tag	UNP P42212
E	-273	ALA	-	expression tag	UNP P42212
E	-272	ASP	-	expression tag	UNP P42212
E	-271	TYR	-	expression tag	UNP P42212
E	-270	LYS	-	expression tag	UNP P42212
E	-269	ASP	-	expression tag	UNP P42212
E	-268	HIS	-	expression tag	UNP P42212
E	-267	ASP	-	expression tag	UNP P42212
E	-266	ILE	-	expression tag	UNP P42212
E	-265	ASP	-	expression tag	UNP P42212
E	-264	TYR	-	expression tag	UNP P42212
E	-263	LYS	-	expression tag	UNP P42212
E	-262	ASP	-	expression tag	UNP P42212
E	-261	ASP	-	expression tag	UNP P42212
E	-260	ASP	-	expression tag	UNP P42212
E	-259	ASP	-	expression tag	UNP P42212
E	-258	LYS	-	expression tag	UNP P42212
E	-257	SER	-	expression tag	UNP P42212
E	-256	ALA	-	expression tag	UNP P42212
E	-255	MET	-	expression tag	UNP P42212
E	-254	VAL	-	expression tag	UNP P42212
E	-191	LEU	PHE	engineered mutation	UNP P42212
E	-190	THR	SER	engineered mutation	UNP P42212
E	-148	THR	LYS	engineered mutation	UNP P42212
E	-49	LYS	ALA	engineered mutation	UNP P42212
E	-24	LEU	HIS	engineered mutation	UNP P42212
E	-16	SER	-	linker	UNP P42212
E	-15	GLY	-	linker	UNP P42212
E	-14	LEU	-	linker	UNP P42212
E	-13	ARG	-	linker	UNP P42212
E	-12	SER	-	linker	UNP P42212
E	-11	GLY	-	linker	UNP P42212
E	-10	LEU	-	linker	UNP P42212
E	-9	GLU	-	linker	UNP P42212

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	VAL	-	linker	UNP P42212
E	-7	LEU	-	linker	UNP P42212
E	-6	PHE	-	linker	UNP P42212
E	-5	GLN	-	linker	UNP P42212
E	-4	GLY	-	linker	UNP P42212
E	-3	PRO	-	linker	UNP P42212
E	-2	GLY	-	linker	UNP P42212
E	-1	GLY	-	linker	UNP P42212
E	0	ARG	-	linker	UNP P42212
G	-283	MET	-	expression tag	UNP P42212
G	-282	HIS	-	expression tag	UNP P42212
G	-281	HIS	-	expression tag	UNP P42212
G	-280	HIS	-	expression tag	UNP P42212
G	-279	HIS	-	expression tag	UNP P42212
G	-278	HIS	-	expression tag	UNP P42212
G	-277	HIS	-	expression tag	UNP P42212
G	-276	HIS	-	expression tag	UNP P42212
G	-275	HIS	-	expression tag	UNP P42212
G	-274	ALA	-	expression tag	UNP P42212
G	-273	ALA	-	expression tag	UNP P42212
G	-272	ASP	-	expression tag	UNP P42212
G	-271	TYR	-	expression tag	UNP P42212
G	-270	LYS	-	expression tag	UNP P42212
G	-269	ASP	-	expression tag	UNP P42212
G	-268	HIS	-	expression tag	UNP P42212
G	-267	ASP	-	expression tag	UNP P42212
G	-266	ILE	-	expression tag	UNP P42212
G	-265	ASP	-	expression tag	UNP P42212
G	-264	TYR	-	expression tag	UNP P42212
G	-263	LYS	-	expression tag	UNP P42212
G	-262	ASP	-	expression tag	UNP P42212
G	-261	ASP	-	expression tag	UNP P42212
G	-260	ASP	-	expression tag	UNP P42212
G	-259	ASP	-	expression tag	UNP P42212
G	-258	LYS	-	expression tag	UNP P42212
G	-257	SER	-	expression tag	UNP P42212
G	-256	ALA	-	expression tag	UNP P42212
G	-255	MET	-	expression tag	UNP P42212
G	-254	VAL	-	expression tag	UNP P42212
G	-191	LEU	PHE	engineered mutation	UNP P42212
G	-190	THR	SER	engineered mutation	UNP P42212
G	-148	THR	LYS	engineered mutation	UNP P42212

*Continued on next page...*

*Continued from previous page...*

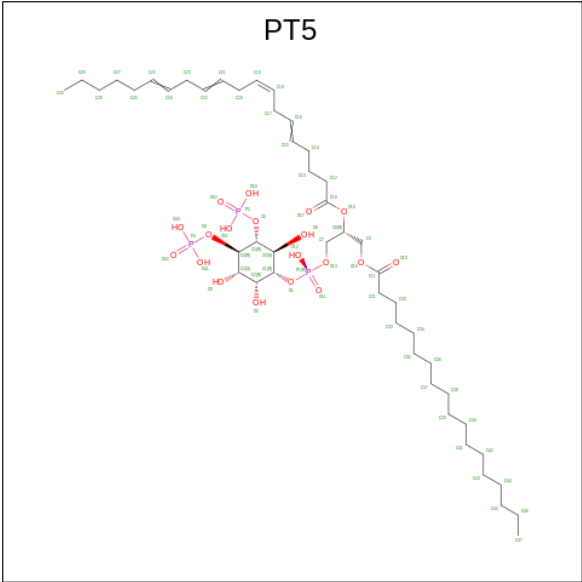
Chain	Residue	Modelled	Actual	Comment	Reference
G	-49	LYS	ALA	engineered mutation	UNP P42212
G	-24	LEU	HIS	engineered mutation	UNP P42212
G	-16	SER	-	linker	UNP P42212
G	-15	GLY	-	linker	UNP P42212
G	-14	LEU	-	linker	UNP P42212
G	-13	ARG	-	linker	UNP P42212
G	-12	SER	-	linker	UNP P42212
G	-11	GLY	-	linker	UNP P42212
G	-10	LEU	-	linker	UNP P42212
G	-9	GLU	-	linker	UNP P42212
G	-8	VAL	-	linker	UNP P42212
G	-7	LEU	-	linker	UNP P42212
G	-6	PHE	-	linker	UNP P42212
G	-5	GLN	-	linker	UNP P42212
G	-4	GLY	-	linker	UNP P42212
G	-3	PRO	-	linker	UNP P42212
G	-2	GLY	-	linker	UNP P42212
G	-1	GLY	-	linker	UNP P42212
G	0	ARG	-	linker	UNP P42212

- Molecule 2 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	146	Total	C	N	O	S	0	0
			1151	705	185	252	9		
2	D	146	Total	C	N	O	S	0	0
			1151	705	185	252	9		
2	F	146	Total	C	N	O	S	0	0
			1151	705	185	252	9		
2	H	146	Total	C	N	O	S	0	0
			1151	705	185	252	9		

- Molecule 3 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: C<sub>47</sub>H<sub>85</sub>O<sub>19</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	P
			56	34	19	3
3	C	1	Total	C	O	P
			56	34	19	3
3	E	1	Total	C	O	P
			56	34	19	3
3	G	1	Total	C	O	P
			56	34	19	3

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	K	0
			4	4	

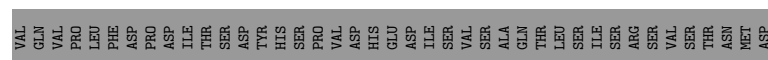
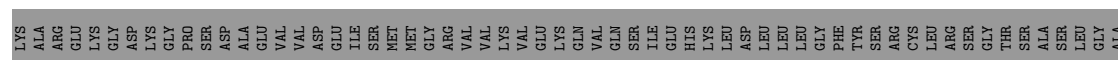
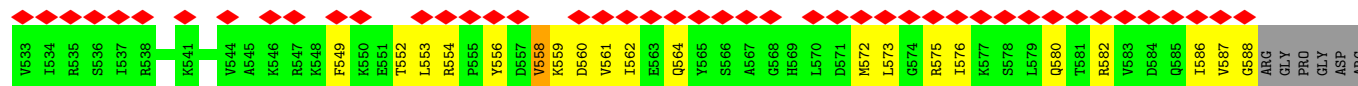
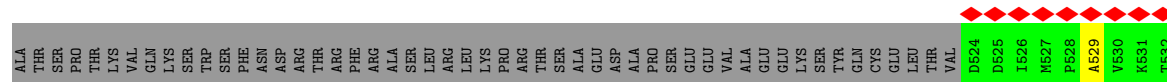
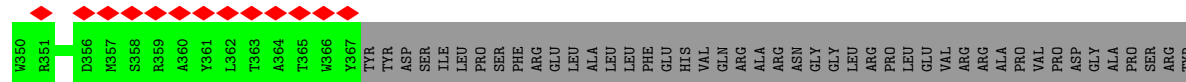
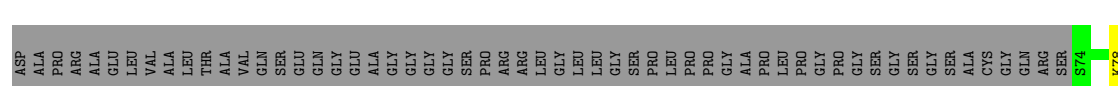
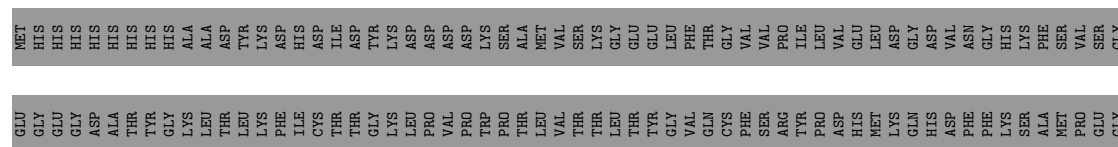
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	O	0
			3	3	
5	C	3	Total	O	0
			3	3	
5	E	3	Total	O	0
			3	3	
5	G	3	Total	O	0
			3	3	

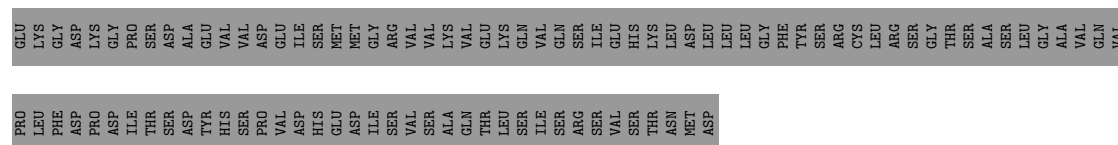
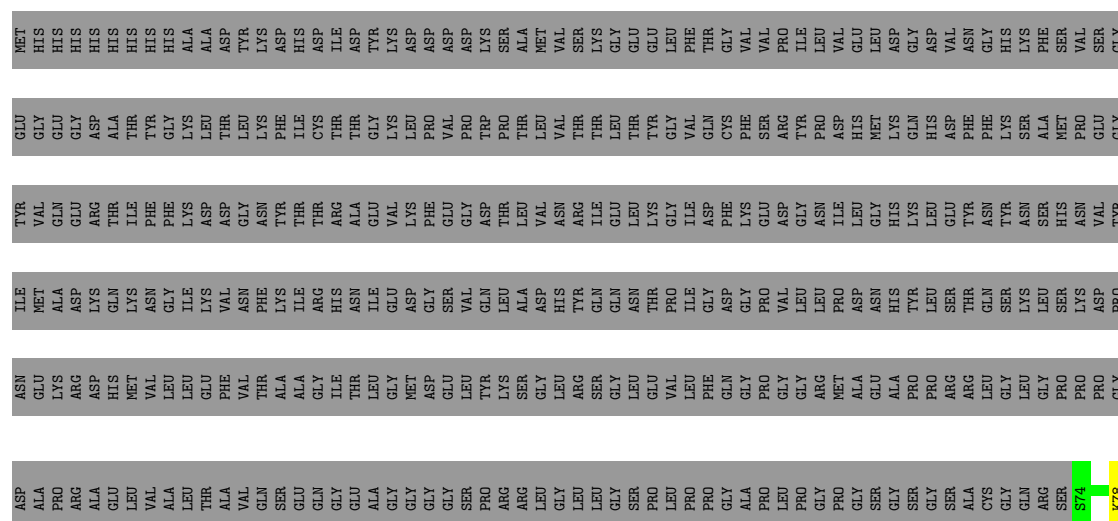




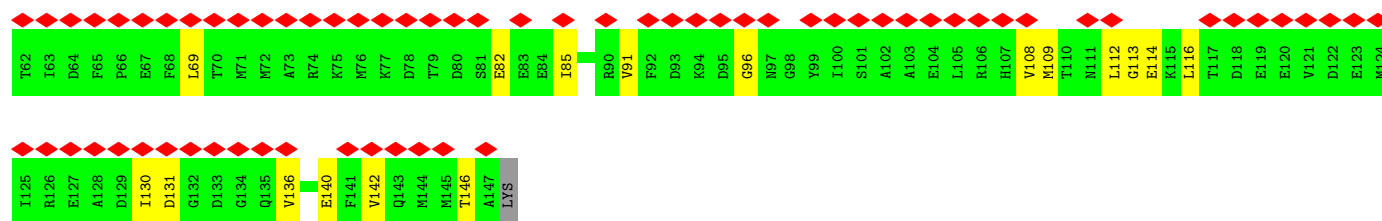
- Molecule 1: Green fluorescent protein, Potassium voltage-gated channel subfamily KQT member 4



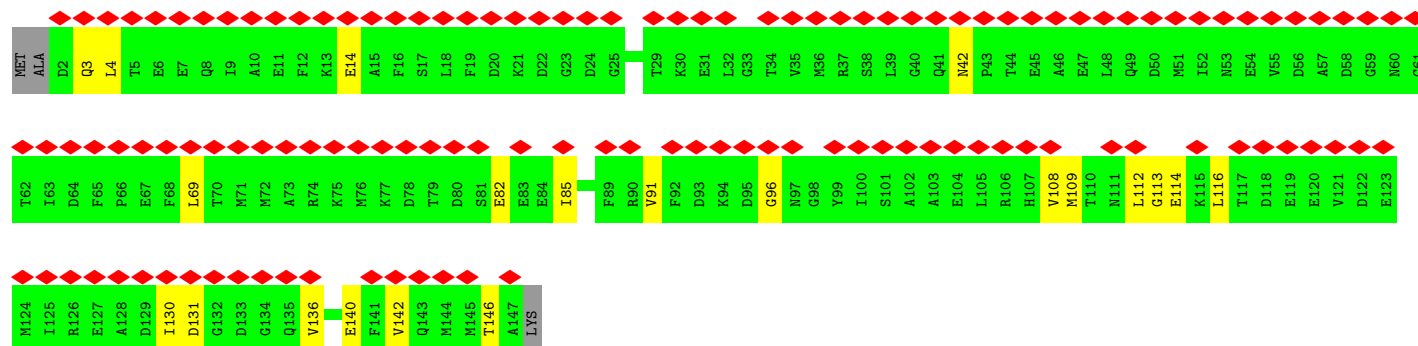
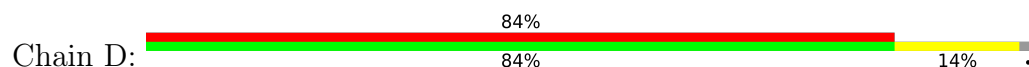
- Molecule 1: Green fluorescent protein, Potassium voltage-gated channel subfamily KQT member 4



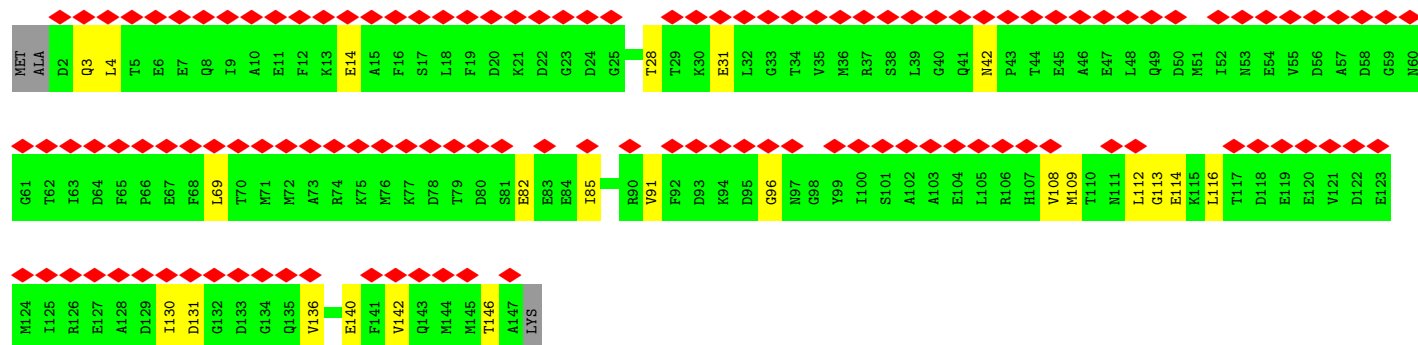
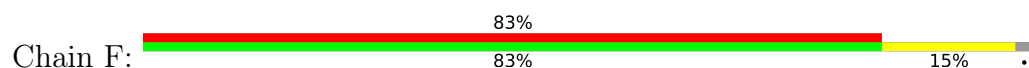
MET	D2	Q3	L4	T5	E6	E7	Q8	I9	A10	E11	F12	K13	E14	A15	F16	S17	L18	F19	D20	K21	D22	G23	D24	G25	T29	K30	E31	L32	G33	T34	V35	M36	R37	S38	S39	L39	G40	Q41	N42	P43	T44	E45	A46	E47	L48	Q49	D50	M51	I52	N53	E54	M55	V56	D57	A58	G59	M60	C61
-----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



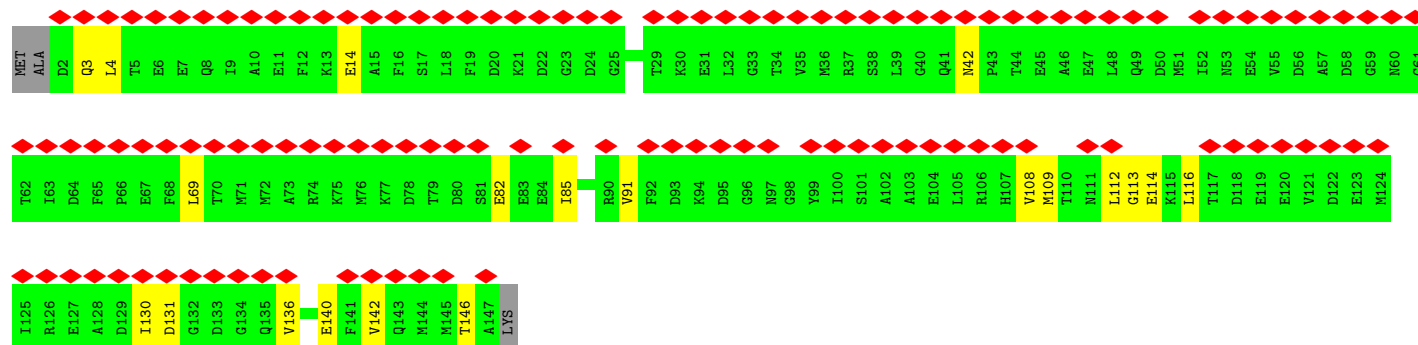
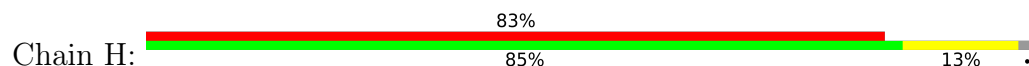
• Molecule 2: Calmodulin-3



• Molecule 2: Calmodulin-3



• Molecule 2: Calmodulin-3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192507	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0129	Depositor
Map size ( $\text{\AA}$ )	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.087, 1.087, 1.087	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: PT5, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/2944	0.48	0/3983
1	C	0.39	0/2944	0.48	0/3983
1	E	0.39	0/2944	0.48	0/3983
1	G	0.39	0/2944	0.48	0/3983
2	B	0.39	0/1163	0.55	0/1562
2	D	0.39	0/1163	0.55	0/1562
2	F	0.39	0/1163	0.55	0/1562
2	H	0.39	0/1163	0.55	0/1562
All	All	0.39	0/16428	0.50	0/22180

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	A	2872	0	2934	107	0
1	C	2872	0	2934	114	0
1	E	2872	0	2934	118	0
1	G	2872	0	2934	111	0
2	B	1151	0	1075	28	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1151	0	1075	33	0
2	F	1151	0	1075	33	0
2	H	1151	0	1075	29	0
3	A	56	0	50	17	0
3	C	56	0	50	18	0
3	E	56	0	50	16	0
3	G	56	0	50	17	0
4	A	4	0	0	0	0
5	A	3	0	0	2	0
5	C	3	0	0	2	0
5	E	3	0	0	2	0
5	G	3	0	0	2	0
All	All	16332	0	16236	431	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 13.

All (431) 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)
1:A:341:PRO:HG2	1:A:552:THR:CG2	1.48	1.42
1:G:341:PRO:HG2	1:G:552:THR:CG2	1.50	1.42
1:E:341:PRO:HG2	1:E:552:THR:CG2	1.48	1.40
1:A:338:ARG:O	1:A:341:PRO:HD2	1.32	1.28
1:E:341:PRO:CG	1:E:552:THR:HG21	1.64	1.27
1:G:338:ARG:O	1:G:341:PRO:HD2	1.32	1.25
1:A:341:PRO:CG	1:A:552:THR:HG21	1.66	1.24
1:C:338:ARG:O	1:C:341:PRO:HD2	1.32	1.23
1:E:338:ARG:O	1:E:341:PRO:HD2	1.32	1.23
1:C:341:PRO:HG2	1:C:552:THR:CG2	1.68	1.22
1:G:341:PRO:CG	1:G:552:THR:HG21	1.70	1.21
1:C:338:ARG:HH21	2:D:91:VAL:CG2	1.56	1.18
1:A:338:ARG:HH21	2:B:91:VAL:CG2	1.56	1.18
1:E:338:ARG:HH21	2:F:91:VAL:CG2	1.56	1.17
1:G:338:ARG:HH21	2:H:91:VAL:CG2	1.56	1.16
1:C:341:PRO:HG2	1:C:552:THR:HG21	1.14	1.15
1:C:150:ARG:HD3	5:C:801:HOH:O	1.52	1.10
1:A:338:ARG:HH21	2:B:91:VAL:HG22	0.92	1.09
1:G:150:ARG:HD3	5:G:801:HOH:O	1.52	1.09
1:A:150:ARG:HD3	5:A:801:HOH:O	1.52	1.09
1:E:150:ARG:HD3	5:E:801:HOH:O	1.52	1.08

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG22	3:A:701:PT5:H26	1.34	1.08
1:G:338:ARG:HH21	2:H:91:VAL:HG22	0.92	1.06
1:C:338:ARG:HH21	2:D:91:VAL:HG22	0.92	1.05
1:E:103:VAL:HG22	3:E:701:PT5:H26	1.34	1.05
1:C:103:VAL:HG22	3:C:701:PT5:H26	1.34	1.04
1:G:103:VAL:HG22	3:G:701:PT5:H26	1.34	1.04
1:E:338:ARG:HH21	2:F:91:VAL:HG22	0.92	1.03
1:A:338:ARG:NH2	2:B:91:VAL:HG22	1.76	1.00
1:A:158:CYS:SG	2:B:140:GLU:HG2	2.00	1.00
1:C:338:ARG:NH2	2:D:91:VAL:HG22	1.76	1.00
1:C:338:ARG:O	1:C:341:PRO:CD	2.09	1.00
1:G:338:ARG:O	1:G:341:PRO:CD	2.09	1.00
1:G:338:ARG:NH2	2:H:91:VAL:HG22	1.76	1.00
1:E:338:ARG:O	1:E:341:PRO:CD	2.09	0.99
1:E:338:ARG:NH2	2:F:91:VAL:HG22	1.76	0.99
1:E:158:CYS:SG	2:F:140:GLU:HG2	2.01	0.99
1:A:338:ARG:O	1:A:341:PRO:CD	2.09	0.99
1:C:158:CYS:SG	2:D:140:GLU:HG2	2.03	0.98
1:C:341:PRO:CG	1:C:552:THR:HG21	1.93	0.98
1:G:341:PRO:CG	1:G:552:THR:CG2	2.37	0.97
1:G:342:ALA:HB2	1:G:549:PHE:HE1	1.34	0.93
1:C:342:ALA:HB2	1:C:549:PHE:HE1	1.33	0.92
1:E:342:ALA:HB2	1:E:549:PHE:HE1	1.34	0.91
1:A:342:ALA:HB2	1:A:549:PHE:HE1	1.33	0.91
1:E:341:PRO:CG	1:E:552:THR:CG2	2.36	0.89
1:G:341:PRO:HG2	1:G:552:THR:HG21	0.89	0.88
1:A:339:ARG:HH22	2:B:112:LEU:CD2	1.89	0.86
1:A:341:PRO:CG	1:A:552:THR:CG2	2.35	0.86
1:E:339:ARG:HH22	2:F:112:LEU:CD2	1.89	0.86
1:C:339:ARG:HH22	2:D:112:LEU:CD2	1.89	0.85
1:G:339:ARG:HH22	2:H:112:LEU:CD2	1.89	0.85
1:C:341:PRO:CG	1:C:552:THR:CG2	2.55	0.84
1:C:92:GLU:CD	5:C:802:HOH:O	2.17	0.84
1:E:92:GLU:CD	5:E:802:HOH:O	2.17	0.83
2:D:4:LEU:HD21	2:D:69:LEU:HD11	1.61	0.83
1:A:341:PRO:HG2	1:A:552:THR:HG21	0.84	0.83
3:C:701:PT5:H32	3:C:701:PT5:H27	1.60	0.83
2:B:4:LEU:HD21	2:B:69:LEU:HD11	1.61	0.83
1:A:92:GLU:CD	5:A:802:HOH:O	2.17	0.83
2:F:4:LEU:HD21	2:F:69:LEU:HD11	1.61	0.83
3:E:701:PT5:H27	3:E:701:PT5:H32	1.61	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:GLU:CD	5:G:802:HOH:O	2.17	0.82
1:C:342:ALA:HB2	1:C:549:PHE:CE1	2.14	0.82
1:A:342:ALA:HB2	1:A:549:PHE:CE1	2.15	0.82
1:A:586:ILE:HG21	1:C:587:VAL:CG1	2.10	0.82
2:H:4:LEU:HD21	2:H:69:LEU:HD11	1.61	0.82
1:C:586:ILE:HG21	1:E:587:VAL:CG1	2.10	0.82
3:A:701:PT5:H32	3:A:701:PT5:H27	1.60	0.81
1:C:338:ARG:NH2	2:D:91:VAL:CG2	2.38	0.81
3:G:701:PT5:H32	3:G:701:PT5:H27	1.60	0.81
1:G:342:ALA:HB2	1:G:549:PHE:CE1	2.16	0.81
1:E:586:ILE:HG21	1:G:587:VAL:CG1	2.11	0.81
1:G:341:PRO:HG2	1:G:552:THR:HG22	1.62	0.80
1:E:342:ALA:HB2	1:E:549:PHE:CE1	2.16	0.80
1:C:103:VAL:CG2	3:C:701:PT5:H26	2.12	0.80
1:E:338:ARG:NH2	2:F:91:VAL:CG2	2.38	0.80
1:E:103:VAL:CG2	3:E:701:PT5:H26	2.12	0.79
1:A:338:ARG:NH2	2:B:91:VAL:CG2	2.38	0.79
1:G:103:VAL:CG2	3:G:701:PT5:H26	2.12	0.79
1:A:341:PRO:HG2	1:A:552:THR:HG22	1.64	0.78
1:C:575:ARG:NH1	1:E:573:LEU:HD11	1.97	0.78
1:E:575:ARG:NH1	1:G:573:LEU:HD11	1.99	0.78
1:G:338:ARG:NH2	2:H:91:VAL:CG2	2.38	0.77
1:A:587:VAL:CG1	1:G:586:ILE:HG21	2.15	0.77
1:A:103:VAL:CG2	3:A:701:PT5:H26	2.12	0.77
1:A:561:VAL:HG12	1:C:562:ILE:HG13	1.68	0.76
1:A:339:ARG:HH22	2:B:112:LEU:HD21	1.51	0.75
1:A:562:ILE:HG13	1:G:561:VAL:HG12	1.69	0.75
3:A:701:PT5:H28	3:A:701:PT5:H22	1.69	0.75
1:C:339:ARG:HH22	2:D:112:LEU:HD21	1.51	0.75
3:C:701:PT5:H28	3:C:701:PT5:H22	1.69	0.75
3:E:701:PT5:H28	3:E:701:PT5:H22	1.69	0.74
3:G:701:PT5:H32	3:G:701:PT5:C16	2.17	0.74
3:E:701:PT5:H32	3:E:701:PT5:C16	2.17	0.74
3:A:701:PT5:H32	3:A:701:PT5:C16	2.17	0.74
3:G:701:PT5:H22	3:G:701:PT5:H28	1.69	0.74
1:E:339:ARG:HH22	2:F:112:LEU:HD21	1.51	0.74
3:C:701:PT5:H32	3:C:701:PT5:C16	2.17	0.74
1:G:339:ARG:NH2	2:H:112:LEU:CD1	2.51	0.74
1:G:339:ARG:HH22	2:H:112:LEU:HD21	1.51	0.73
1:C:339:ARG:NH2	2:D:112:LEU:CD1	2.51	0.73
1:G:158:CYS:SG	2:H:140:GLU:HG2	2.28	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:CG	3:A:701:PT5:O11	2.37	0.73
1:E:338:ARG:HA	1:E:552:THR:HB	1.71	0.73
1:G:94:PRO:CG	3:G:701:PT5:O11	2.37	0.73
1:C:341:PRO:HG2	1:C:552:THR:HG22	1.67	0.73
1:E:339:ARG:NH2	2:F:112:LEU:CD1	2.51	0.73
1:A:573:LEU:HD11	1:G:575:ARG:NH1	2.04	0.73
1:A:339:ARG:NH2	2:B:112:LEU:CD1	2.51	0.72
1:C:94:PRO:CG	3:C:701:PT5:O11	2.37	0.72
1:E:341:PRO:HG2	1:E:552:THR:HG21	0.77	0.72
1:E:94:PRO:CG	3:E:701:PT5:O11	2.37	0.72
1:A:575:ARG:NH1	1:C:573:LEU:HD11	2.03	0.72
1:A:338:ARG:HA	1:A:552:THR:HB	1.70	0.71
1:E:339:ARG:NH2	2:F:112:LEU:CD2	2.54	0.71
1:E:586:ILE:HG21	1:G:587:VAL:HG12	1.73	0.71
1:C:586:ILE:HG21	1:E:587:VAL:HG11	1.72	0.71
1:A:339:ARG:NH2	2:B:112:LEU:CD2	2.54	0.71
1:G:338:ARG:HA	1:G:552:THR:HB	1.70	0.70
1:G:339:ARG:NH2	2:H:112:LEU:CD2	2.54	0.70
1:C:216:ARG:O	3:C:701:PT5:H2	1.91	0.70
1:C:339:ARG:NH2	2:D:112:LEU:CD2	2.54	0.70
1:E:216:ARG:O	3:E:701:PT5:H2	1.91	0.70
2:D:130:ILE:HD12	2:D:136:VAL:HG22	1.73	0.70
2:B:130:ILE:HD12	2:B:136:VAL:HG22	1.73	0.70
1:C:340:MET:HE3	2:D:113:GLY:H	1.57	0.70
1:G:216:ARG:O	3:G:701:PT5:H2	1.91	0.70
1:A:216:ARG:O	3:A:701:PT5:H2	1.91	0.69
1:A:587:VAL:HG12	1:G:586:ILE:HG21	1.75	0.69
2:F:130:ILE:HD12	2:F:136:VAL:HG22	1.73	0.69
1:C:342:ALA:CB	1:C:549:PHE:CE1	2.76	0.69
2:H:130:ILE:HD12	2:H:136:VAL:HG22	1.73	0.68
1:E:94:PRO:CD	3:E:701:PT5:O11	2.42	0.68
1:A:342:ALA:CB	1:A:549:PHE:CE1	2.76	0.68
1:A:586:ILE:HG21	1:C:587:VAL:HG11	1.74	0.68
1:C:342:ALA:HA	1:C:549:PHE:CD1	2.29	0.68
1:A:586:ILE:HG21	1:C:587:VAL:HG12	1.76	0.68
1:C:219:ARG:HB3	3:C:701:PT5:H53	1.76	0.67
1:E:342:ALA:CB	1:E:549:PHE:CE1	2.77	0.67
1:G:78:LYS:HE3	2:H:131:ASP:OD1	1.94	0.67
1:G:94:PRO:CD	3:G:701:PT5:O11	2.42	0.67
1:G:219:ARG:HB3	3:G:701:PT5:H53	1.76	0.67
1:A:219:ARG:HB3	3:A:701:PT5:H53	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:CD	3:A:701:PT5:O11	2.42	0.67
1:C:94:PRO:CD	3:C:701:PT5:O11	2.42	0.67
1:E:219:ARG:HB3	3:E:701:PT5:H53	1.77	0.67
1:A:94:PRO:HG3	3:A:701:PT5:O11	1.95	0.67
1:C:339:ARG:NH2	2:D:112:LEU:HD13	2.10	0.67
1:A:339:ARG:NH2	2:B:112:LEU:HD13	2.10	0.67
1:C:586:ILE:HG21	1:E:587:VAL:HG12	1.77	0.67
1:G:342:ALA:CB	1:G:549:PHE:CE1	2.77	0.66
1:G:94:PRO:HG3	3:G:701:PT5:O11	1.95	0.66
1:G:342:ALA:HA	1:G:549:PHE:CD1	2.31	0.66
1:G:339:ARG:NH2	2:H:112:LEU:HD13	2.10	0.66
1:A:342:ALA:HA	1:A:549:PHE:CD1	2.31	0.66
1:C:94:PRO:HG3	3:C:701:PT5:O11	1.95	0.65
1:E:529:ALA:HB2	2:F:14:GLU:HG3	1.78	0.65
1:C:529:ALA:HB2	2:D:14:GLU:HG3	1.78	0.65
1:E:339:ARG:NH2	2:F:112:LEU:HD13	2.10	0.65
1:E:94:PRO:HG3	3:E:701:PT5:O11	1.95	0.65
1:C:561:VAL:HG12	1:E:562:ILE:HG13	1.79	0.65
1:E:342:ALA:HA	1:E:549:PHE:CD1	2.32	0.65
1:E:561:VAL:HG12	1:G:562:ILE:HG13	1.78	0.65
1:G:529:ALA:HB2	2:H:14:GLU:HG3	1.78	0.65
1:E:586:ILE:HG21	1:G:587:VAL:HG11	1.78	0.64
1:E:340:MET:HE3	2:F:113:GLY:H	1.61	0.64
1:A:529:ALA:HB2	2:B:14:GLU:HG3	1.78	0.64
1:G:341:PRO:CB	1:G:552:THR:HG21	2.26	0.63
1:A:341:PRO:CB	1:A:552:THR:HG21	2.26	0.63
1:A:339:ARG:HH22	2:B:112:LEU:CD1	2.12	0.62
1:G:339:ARG:HH22	2:H:112:LEU:CD1	2.12	0.62
1:E:341:PRO:HG2	1:E:552:THR:HG22	1.72	0.62
1:C:78:LYS:CD	2:D:131:ASP:OD1	2.47	0.62
1:A:322:PHE:HB3	1:C:237:GLU:HG2	1.82	0.62
1:C:284:ILE:HD11	1:E:308:ILE:HD11	1.81	0.62
1:C:564:GLN:HE22	1:E:562:ILE:HA	1.65	0.62
1:E:339:ARG:NH2	2:F:112:LEU:HD22	2.16	0.61
1:C:339:ARG:HH22	2:D:112:LEU:CD1	2.12	0.61
1:C:339:ARG:NH2	2:D:112:LEU:HD22	2.16	0.61
1:E:339:ARG:HH22	2:F:112:LEU:CD1	2.12	0.60
1:E:341:PRO:CB	1:E:552:THR:HG21	2.31	0.60
1:C:338:ARG:HA	1:C:552:THR:HB	1.82	0.60
1:A:339:ARG:NH2	2:B:112:LEU:HD22	2.16	0.59
1:C:558:VAL:O	1:C:558:VAL:HG13	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:MET:CE	2:H:113:GLY:H	2.14	0.59
1:G:339:ARG:NH2	2:H:112:LEU:HD22	2.16	0.59
2:H:108:VAL:HG13	2:H:112:LEU:HD12	1.85	0.59
1:A:340:MET:CE	2:B:113:GLY:H	2.14	0.59
1:C:340:MET:CE	2:D:113:GLY:H	2.14	0.59
1:E:340:MET:CE	2:F:113:GLY:H	2.14	0.59
1:C:78:LYS:HE3	2:D:131:ASP:OD1	2.02	0.59
1:G:558:VAL:HG13	1:G:558:VAL:O	2.02	0.59
1:A:587:VAL:HG11	1:G:586:ILE:HG21	1.83	0.59
2:B:108:VAL:HG13	2:B:112:LEU:HD12	1.85	0.58
2:F:108:VAL:HG13	2:F:112:LEU:HD12	1.85	0.58
1:A:558:VAL:HG13	1:A:558:VAL:O	2.02	0.58
1:E:558:VAL:O	1:E:558:VAL:HG13	2.02	0.57
2:D:108:VAL:HG13	2:D:112:LEU:HD12	1.85	0.57
1:E:78:LYS:CD	2:F:131:ASP:OD1	2.52	0.57
1:E:564:GLN:HE22	1:G:562:ILE:HA	1.69	0.57
1:C:342:ALA:CB	1:C:549:PHE:HE1	2.09	0.56
1:A:340:MET:HE3	2:B:113:GLY:H	1.69	0.56
1:C:278:THR:O	1:C:282:THR:HG22	2.06	0.56
1:C:188:VAL:HG13	1:C:203:LEU:HD22	1.88	0.56
1:G:278:THR:O	1:G:282:THR:HG22	2.06	0.56
1:E:158:CYS:HG	2:F:140:GLU:HG2	1.68	0.56
1:A:278:THR:O	1:A:282:THR:HG22	2.06	0.55
1:C:78:LYS:CE	2:D:131:ASP:OD1	2.55	0.55
1:E:188:VAL:HG13	1:E:203:LEU:HD22	1.88	0.55
1:E:278:THR:O	1:E:282:THR:HG22	2.06	0.55
1:G:188:VAL:HG13	1:G:203:LEU:HD22	1.88	0.55
1:A:188:VAL:HG13	1:A:203:LEU:HD22	1.88	0.55
1:A:588:GLY:O	1:G:586:ILE:HD13	2.06	0.55
2:D:82:GLU:HB2	2:D:146:THR:HG21	1.89	0.55
1:C:219:ARG:CB	3:C:701:PT5:H53	2.37	0.55
1:G:78:LYS:CE	2:H:131:ASP:OD1	2.54	0.55
1:C:341:PRO:CB	1:C:552:THR:HG21	2.37	0.55
1:E:219:ARG:CB	3:E:701:PT5:H53	2.37	0.55
2:B:82:GLU:HB2	2:B:146:THR:HG21	1.89	0.54
1:G:219:ARG:CB	3:G:701:PT5:H53	2.37	0.54
1:A:219:ARG:CB	3:A:701:PT5:H53	2.37	0.54
2:F:82:GLU:HB2	2:F:146:THR:HG21	1.89	0.54
1:A:237:GLU:HG2	1:G:322:PHE:HB3	1.89	0.54
1:A:564:GLN:HE22	1:C:562:ILE:HA	1.73	0.54
2:H:82:GLU:HB2	2:H:146:THR:HG21	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:ARG:HG3	1:E:576:ILE:HG21	1.91	0.53
1:E:586:ILE:HD13	1:G:588:GLY:O	2.08	0.53
1:E:322:PHE:HB3	1:G:237:GLU:HG2	1.90	0.52
1:E:553:LEU:C	1:E:553:LEU:HD13	2.30	0.52
1:C:575:ARG:HH12	1:E:573:LEU:HD11	1.74	0.52
1:G:553:LEU:HD13	1:G:553:LEU:C	2.30	0.52
1:A:117:VAL:O	1:A:120:THR:OG1	2.27	0.52
1:E:78:LYS:HE3	2:F:131:ASP:OD1	2.10	0.52
1:E:339:ARG:C	1:E:341:PRO:HD2	2.30	0.52
1:G:339:ARG:C	1:G:341:PRO:HD2	2.30	0.52
1:G:340:MET:HE3	2:H:113:GLY:H	1.75	0.51
1:A:553:LEU:HD13	1:A:553:LEU:C	2.31	0.51
1:C:282:THR:O	1:C:283:THR:OG1	2.27	0.51
1:C:564:GLN:NE2	1:E:562:ILE:HA	2.25	0.51
1:A:339:ARG:C	1:A:341:PRO:HD2	2.30	0.51
1:C:553:LEU:C	1:C:553:LEU:HD13	2.31	0.51
1:E:553:LEU:O	1:E:553:LEU:HD22	2.11	0.51
1:A:562:ILE:CG1	1:G:561:VAL:HG12	2.40	0.51
1:G:553:LEU:O	1:G:553:LEU:HD22	2.11	0.51
1:C:339:ARG:C	1:C:341:PRO:HD2	2.30	0.51
1:E:582:ARG:HD2	1:G:580:GLN:NE2	2.26	0.51
1:E:117:VAL:O	1:E:120:THR:OG1	2.27	0.50
1:A:553:LEU:O	1:A:553:LEU:HD22	2.11	0.50
1:G:117:VAL:O	1:G:120:THR:OG1	2.27	0.50
1:C:575:ARG:NH1	1:E:573:LEU:CD1	2.70	0.50
1:A:158:CYS:SG	2:B:140:GLU:CG	2.89	0.50
1:C:117:VAL:O	1:C:120:THR:OG1	2.27	0.50
1:C:556:TYR:CE2	1:C:560:ASP:HB2	2.47	0.50
1:E:556:TYR:CE2	1:E:560:ASP:HB2	2.47	0.49
1:E:575:ARG:NH1	1:G:573:LEU:CD1	2.74	0.49
1:C:582:ARG:HD2	1:E:580:GLN:NE2	2.27	0.49
1:A:562:ILE:HA	1:G:564:GLN:HE22	1.77	0.49
1:A:556:TYR:CE2	1:A:560:ASP:HB2	2.47	0.49
1:C:342:ALA:CA	1:C:549:PHE:CD1	2.95	0.49
1:G:556:TYR:CE2	1:G:560:ASP:HB2	2.47	0.49
1:C:344:ASN:OD1	2:D:114:GLU:HG2	2.13	0.49
1:C:582:ARG:HD2	1:E:580:GLN:HE22	1.77	0.49
3:E:701:PT5:C16	3:E:701:PT5:C20	2.89	0.49
1:C:85:ASN:O	1:C:89:ASN:ND2	2.47	0.48
3:C:701:PT5:C16	3:C:701:PT5:C20	2.89	0.48
1:A:282:THR:O	1:A:283:THR:OG1	2.27	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:ASN:O	1:G:89:ASN:ND2	2.47	0.48
1:G:338:ARG:CA	1:G:552:THR:HB	2.43	0.48
1:E:582:ARG:HD2	1:G:580:GLN:HE22	1.79	0.48
1:A:344:ASN:OD1	2:B:114:GLU:HG2	2.13	0.48
1:E:78:LYS:CE	2:F:131:ASP:OD1	2.62	0.48
1:A:575:ARG:HG3	1:C:576:ILE:HG21	1.95	0.48
1:C:553:LEU:O	1:C:553:LEU:HD22	2.12	0.48
1:E:282:THR:O	1:E:283:THR:OG1	2.27	0.48
1:A:342:ALA:HA	1:A:549:PHE:CE1	2.49	0.48
1:A:564:GLN:NE2	1:C:562:ILE:HA	2.29	0.48
1:E:85:ASN:O	1:E:89:ASN:ND2	2.47	0.48
1:E:93:ARG:NH1	2:F:96:GLY:O	2.47	0.48
1:G:282:THR:O	1:G:282:THR:OG1	2.32	0.48
1:A:85:ASN:O	1:A:89:ASN:ND2	2.47	0.48
1:A:174:PHE:HB3	3:A:701:PT5:O53	2.14	0.47
1:C:342:ALA:HA	1:C:549:PHE:CE1	2.48	0.47
1:E:564:GLN:NE2	1:G:562:ILE:HA	2.29	0.47
1:G:342:ALA:CA	1:G:549:PHE:CD1	2.97	0.47
1:G:344:ASN:OD1	2:H:114:GLU:HG2	2.13	0.47
1:A:338:ARG:CA	1:A:552:THR:HB	2.43	0.47
1:E:344:ASN:OD1	2:F:114:GLU:HG2	2.13	0.47
1:C:93:ARG:NH1	2:D:96:GLY:O	2.47	0.47
1:E:339:ARG:NH2	2:F:112:LEU:HD11	2.30	0.47
1:G:342:ALA:HA	1:G:549:PHE:CE1	2.49	0.47
1:A:339:ARG:HB3	1:A:340:MET:H	1.55	0.47
1:A:569:HIS:NE2	1:G:572:MET:HG2	2.30	0.47
1:C:174:PHE:HB3	3:C:701:PT5:O53	2.15	0.47
1:E:174:PHE:HB3	3:E:701:PT5:O53	2.15	0.47
1:G:174:PHE:HB3	3:G:701:PT5:O53	2.15	0.47
1:A:282:THR:O	1:A:282:THR:OG1	2.32	0.46
1:A:118:LEU:HD23	1:A:121:ILE:HD12	1.97	0.46
3:A:701:PT5:C16	3:A:701:PT5:C20	2.89	0.46
1:E:282:THR:O	1:E:282:THR:OG1	2.32	0.46
1:A:342:ALA:CA	1:A:549:PHE:CD1	2.97	0.46
1:E:118:LEU:HD23	1:E:121:ILE:HD12	1.97	0.46
1:E:342:ALA:HA	1:E:549:PHE:CE1	2.49	0.46
1:E:575:ARG:HH12	1:G:573:LEU:HD11	1.78	0.46
1:G:338:ARG:O	1:G:341:PRO:CG	2.64	0.46
1:A:134:ILE:H	1:A:134:ILE:HG13	1.60	0.46
3:G:701:PT5:C16	3:G:701:PT5:C20	2.89	0.46
1:G:118:LEU:HD23	1:G:121:ILE:HD12	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ALA:CA	1:E:549:PHE:CD1	2.98	0.45
1:A:580:GLN:NE2	1:G:582:ARG:HD2	2.30	0.45
1:C:123:GLU:OE1	1:C:124:HIS:NE2	2.49	0.45
1:E:123:GLU:OE1	1:E:124:HIS:NE2	2.49	0.45
1:G:113:LEU:O	1:G:116:SER:OG	2.33	0.45
1:G:123:GLU:OE1	1:G:124:HIS:NE2	2.50	0.45
1:C:322:PHE:HB3	1:E:237:GLU:HG2	1.98	0.45
1:C:118:LEU:HD23	1:C:121:ILE:HD12	1.97	0.45
1:A:123:GLU:OE1	1:A:124:HIS:NE2	2.49	0.45
1:G:339:ARG:HB3	1:G:340:MET:H	1.56	0.45
1:A:339:ARG:HH22	2:B:112:LEU:HD11	1.82	0.45
1:C:78:LYS:HD2	2:D:131:ASP:OD1	2.17	0.45
1:C:339:ARG:NH2	2:D:112:LEU:HD11	2.29	0.45
1:E:575:ARG:HG3	1:G:576:ILE:HG21	1.99	0.45
1:G:339:ARG:HH22	2:H:112:LEU:HD11	1.82	0.45
1:E:339:ARG:HH22	2:F:112:LEU:HD11	1.82	0.45
1:C:189:ILE:HA	1:C:189:ILE:HD12	1.65	0.45
1:C:586:ILE:CG2	1:E:587:VAL:CG1	2.91	0.45
1:C:282:THR:O	1:C:282:THR:OG1	2.32	0.44
1:E:89:ASN:HA	1:E:93:ARG:HG2	1.99	0.44
3:C:701:PT5:H22	3:C:701:PT5:C17	2.45	0.44
1:E:338:ARG:O	1:E:341:PRO:CG	2.64	0.44
1:A:89:ASN:HA	1:A:93:ARG:HG2	2.00	0.44
1:C:338:ARG:O	1:C:341:PRO:CG	2.64	0.44
1:C:339:ARG:HH22	2:D:112:LEU:HD11	1.82	0.44
1:C:582:ARG:HH11	1:E:580:GLN:HE21	1.65	0.44
1:G:340:MET:HE1	2:H:113:GLY:H	1.79	0.44
1:A:93:ARG:NH1	2:B:96:GLY:O	2.50	0.44
1:A:240:THR:HG23	1:G:223:THR:HB	1.99	0.44
1:C:89:ASN:HA	1:C:93:ARG:HG2	1.99	0.44
1:G:89:ASN:HA	1:G:93:ARG:HG2	2.00	0.44
1:G:219:ARG:HD2	3:G:701:PT5:H56	1.99	0.44
1:A:561:VAL:HG12	1:C:562:ILE:CG1	2.43	0.44
1:A:586:ILE:HD13	1:C:588:GLY:O	2.18	0.44
1:A:338:ARG:O	1:A:341:PRO:CG	2.64	0.44
1:C:78:LYS:CG	2:D:131:ASP:OD1	2.66	0.44
1:C:134:ILE:H	1:C:134:ILE:HG13	1.60	0.44
1:A:339:ARG:NH2	2:B:112:LEU:HD11	2.29	0.44
1:A:582:ARG:HD2	1:C:580:GLN:HE22	1.82	0.44
1:C:219:ARG:HD2	3:C:701:PT5:H56	1.99	0.44
1:A:219:ARG:HD2	3:A:701:PT5:H56	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:CYS:SG	2:F:140:GLU:CG	2.90	0.43
1:C:342:ALA:CA	1:C:549:PHE:CE1	3.01	0.43
1:E:219:ARG:HD2	3:E:701:PT5:H56	1.99	0.43
1:E:223:THR:HB	1:G:240:THR:HG23	2.01	0.43
1:A:586:ILE:CG2	1:C:587:VAL:CG1	2.91	0.43
1:G:189:ILE:HD12	1:G:189:ILE:HA	1.65	0.43
1:C:261:LYS:H	1:C:261:LYS:HG2	1.61	0.43
1:E:189:ILE:HD12	1:E:189:ILE:HA	1.65	0.43
1:A:580:GLN:HE22	1:G:582:ARG:HD2	1.84	0.43
1:A:342:ALA:CA	1:A:549:PHE:CE1	3.02	0.43
1:C:586:ILE:HD13	1:E:588:GLY:O	2.19	0.43
1:E:219:ARG:HB3	3:E:701:PT5:C32	2.47	0.42
1:E:586:ILE:CG2	1:G:587:VAL:CG1	2.91	0.42
3:A:701:PT5:H22	3:A:701:PT5:C17	2.45	0.42
1:C:158:CYS:SG	2:D:140:GLU:CG	2.93	0.42
1:A:582:ARG:HD2	1:C:580:GLN:NE2	2.34	0.42
1:A:126:GLU:O	1:A:130:GLU:HG2	2.20	0.42
2:B:85:ILE:HG22	2:B:142:VAL:HG22	2.01	0.42
2:F:85:ILE:HG22	2:F:142:VAL:HG22	2.01	0.42
2:H:85:ILE:HG22	2:H:142:VAL:HG22	2.01	0.42
1:A:588:GLY:O	1:G:586:ILE:CD1	2.68	0.42
1:C:282:THR:OG1	1:E:308:ILE:HD13	2.19	0.42
1:G:282:THR:O	1:G:283:THR:OG1	2.27	0.42
1:G:339:ARG:NH2	2:H:112:LEU:HD11	2.29	0.42
1:A:261:LYS:H	1:A:261:LYS:HG2	1.61	0.42
1:A:562:ILE:HA	1:G:564:GLN:NE2	2.34	0.42
1:G:97:TRP:O	1:G:100:VAL:HG22	2.20	0.42
2:F:28:THR:OG1	2:F:31:GLU:OE1	2.22	0.42
1:E:126:GLU:O	1:E:130:GLU:HG2	2.20	0.42
1:E:261:LYS:H	1:E:261:LYS:HG2	1.62	0.42
1:G:126:GLU:O	1:G:130:GLU:HG2	2.20	0.42
2:D:85:ILE:HG22	2:D:142:VAL:HG22	2.01	0.42
2:H:109:MET:HB3	2:H:116:LEU:HD12	2.02	0.42
1:E:134:ILE:H	1:E:134:ILE:HG13	1.60	0.42
1:G:342:ALA:CA	1:G:549:PHE:CE1	3.02	0.42
1:E:97:TRP:O	1:E:100:VAL:HG22	2.20	0.41
1:G:78:LYS:CD	2:H:131:ASP:OD1	2.67	0.41
1:C:344:ASN:ND2	2:D:113:GLY:CA	2.83	0.41
1:C:126:GLU:O	1:C:130:GLU:HG2	2.20	0.41
1:C:339:ARG:HB3	1:C:340:MET:H	1.56	0.41
1:A:97:TRP:O	1:A:100:VAL:HG22	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:VAL:CG1	1:G:586:ILE:CG2	2.94	0.41
1:E:342:ALA:CB	1:E:549:PHE:HE1	2.11	0.41
1:E:344:ASN:ND2	2:F:113:GLY:CA	2.83	0.41
3:E:701:PT5:O2	3:E:701:PT5:P1	2.79	0.41
1:G:240:THR:O	1:G:244:ILE:HG12	2.21	0.41
1:C:126:GLU:CD	1:C:126:GLU:H	2.23	0.41
1:E:240:THR:O	1:E:244:ILE:HG12	2.21	0.41
2:D:109:MET:HB3	2:D:116:LEU:HD12	2.02	0.41
1:C:97:TRP:O	1:C:100:VAL:HG22	2.20	0.41
1:C:340:MET:N	1:C:341:PRO:CD	2.84	0.41
1:C:344:ASN:HD21	2:D:113:GLY:HA2	1.86	0.41
1:E:344:ASN:HD21	2:F:113:GLY:HA2	1.85	0.41
1:E:572:MET:HG2	1:G:569:HIS:NE2	2.36	0.41
1:E:586:ILE:CD1	1:G:588:GLY:O	2.68	0.41
1:G:126:GLU:CD	1:G:126:GLU:H	2.23	0.41
1:E:340:MET:N	1:E:341:PRO:CD	2.84	0.41
1:E:342:ALA:CA	1:E:549:PHE:CE1	3.03	0.41
1:G:344:ASN:ND2	2:H:113:GLY:CA	2.83	0.41
1:C:575:ARG:CZ	1:E:573:LEU:HD11	2.48	0.41
1:E:126:GLU:CD	1:E:126:GLU:H	2.23	0.41
1:E:339:ARG:HB3	1:E:340:MET:H	1.56	0.41
2:B:109:MET:HB3	2:B:116:LEU:HD12	2.02	0.41
2:F:109:MET:HB3	2:F:116:LEU:HD12	2.02	0.41
1:A:94:PRO:HD2	3:A:701:PT5:O11	2.21	0.41
1:C:356:ASP:OD1	1:C:535:ARG:NH2	2.44	0.40
3:C:701:PT5:O17	3:C:701:PT5:H15	2.21	0.40
3:G:701:PT5:H22	3:G:701:PT5:C17	2.45	0.40
3:G:701:PT5:O2	3:G:701:PT5:P1	2.79	0.40
1:A:219:ARG:HB3	3:A:701:PT5:C32	2.47	0.40
1:G:219:ARG:HB3	3:G:701:PT5:C32	2.47	0.40
1:G:340:MET:N	1:G:341:PRO:CD	2.84	0.40
1:A:126:GLU:H	1:A:126:GLU:CD	2.23	0.40
1:A:340:MET:N	1:A:341:PRO:CD	2.84	0.40
1:A:344:ASN:ND2	2:B:113:GLY:CA	2.83	0.40
3:C:701:PT5:O2	3:C:701:PT5:P1	2.79	0.40
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.91	0.40
1:G:356:ASP:OD1	1:G:535:ARG:NH2	2.44	0.40
1:A:78:LYS:CD	2:B:131:ASP:OD1	2.69	0.40
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.90	0.40
1:C:219:ARG:HB3	3:C:701:PT5:C32	2.47	0.40
1:E:113:LEU:O	1:E:116:SER:OG	2.33	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/979 (36%)	343 (99%)	4 (1%)	1 (0%)	41	61
1	C	348/979 (36%)	343 (99%)	4 (1%)	1 (0%)	41	61
1	E	348/979 (36%)	343 (99%)	4 (1%)	1 (0%)	41	61
1	G	348/979 (36%)	343 (99%)	4 (1%)	1 (0%)	41	61
2	B	144/149 (97%)	141 (98%)	3 (2%)	0	100	100
2	D	144/149 (97%)	141 (98%)	3 (2%)	0	100	100
2	F	144/149 (97%)	141 (98%)	3 (2%)	0	100	100
2	H	144/149 (97%)	141 (98%)	3 (2%)	0	100	100
All	All	1968/4512 (44%)	1936 (98%)	28 (1%)	4 (0%)	50	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ARG
1	C	339	ARG
1	E	339	ARG
1	G	339	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/828 (36%)	269 (90%)	30 (10%)	7	15
1	C	299/828 (36%)	270 (90%)	29 (10%)	8	16
1	E	299/828 (36%)	269 (90%)	30 (10%)	7	15
1	G	299/828 (36%)	269 (90%)	30 (10%)	7	15
2	B	125/127 (98%)	123 (98%)	2 (2%)	62	84
2	D	125/127 (98%)	123 (98%)	2 (2%)	62	84
2	F	125/127 (98%)	123 (98%)	2 (2%)	62	84
2	H	125/127 (98%)	123 (98%)	2 (2%)	62	84
All	All	1696/3820 (44%)	1569 (92%)	127 (8%)	17	26

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	93	ARG
1	A	97	TRP
1	A	111	SER
1	A	126	GLU
1	A	129	ASN
1	A	140	ILE
1	A	153	SER
1	A	160	TYR
1	A	163	TRP
1	A	185	SER
1	A	189	ILE
1	A	200	THR
1	A	206	MET
1	A	211	ILE
1	A	235	SER
1	A	261	LYS
1	A	262	ASP
1	A	268	SER
1	A	273	SER
1	A	282	THR
1	A	331	ARG
1	A	333	LYS
1	A	335	PHE
1	A	337	LYS
1	A	339	ARG
1	A	340	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	554	ARG
1	A	558	VAL
1	A	559	LYS
1	C	81	ARG
1	C	93	ARG
1	C	97	TRP
1	C	111	SER
1	C	126	GLU
1	C	129	ASN
1	C	140	ILE
1	C	153	SER
1	C	160	TYR
1	C	163	TRP
1	C	185	SER
1	C	189	ILE
1	C	200	THR
1	C	206	MET
1	C	211	ILE
1	C	235	SER
1	C	261	LYS
1	C	262	ASP
1	C	268	SER
1	C	273	SER
1	C	282	THR
1	C	331	ARG
1	C	333	LYS
1	C	337	LYS
1	C	339	ARG
1	C	340	MET
1	C	554	ARG
1	C	558	VAL
1	C	559	LYS
1	E	81	ARG
1	E	93	ARG
1	E	97	TRP
1	E	111	SER
1	E	126	GLU
1	E	129	ASN
1	E	140	ILE
1	E	153	SER
1	E	160	TYR
1	E	163	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	185	SER
1	E	189	ILE
1	E	200	THR
1	E	206	MET
1	E	211	ILE
1	E	235	SER
1	E	261	LYS
1	E	262	ASP
1	E	268	SER
1	E	273	SER
1	E	282	THR
1	E	331	ARG
1	E	333	LYS
1	E	335	PHE
1	E	337	LYS
1	E	339	ARG
1	E	340	MET
1	E	554	ARG
1	E	558	VAL
1	E	559	LYS
1	G	81	ARG
1	G	93	ARG
1	G	97	TRP
1	G	111	SER
1	G	126	GLU
1	G	129	ASN
1	G	140	ILE
1	G	153	SER
1	G	160	TYR
1	G	163	TRP
1	G	185	SER
1	G	189	ILE
1	G	200	THR
1	G	206	MET
1	G	211	ILE
1	G	235	SER
1	G	261	LYS
1	G	262	ASP
1	G	268	SER
1	G	273	SER
1	G	282	THR
1	G	329	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	331	ARG
1	G	333	LYS
1	G	337	LYS
1	G	339	ARG
1	G	340	MET
1	G	554	ARG
1	G	558	VAL
1	G	559	LYS
2	B	3	GLN
2	B	42	ASN
2	D	3	GLN
2	D	42	ASN
2	F	3	GLN
2	F	42	ASN
2	H	3	GLN
2	H	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	125	GLN
1	A	210	GLN
1	A	234	HIS
1	A	329	GLN
1	A	564	GLN
1	A	580	GLN
1	C	84	GLN
1	C	125	GLN
1	C	210	GLN
1	C	234	HIS
1	C	329	GLN
1	C	564	GLN
1	C	580	GLN
1	E	84	GLN
1	E	125	GLN
1	E	210	GLN
1	E	234	HIS
1	E	329	GLN
1	E	564	GLN
1	E	580	GLN
1	G	84	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	G	125	GLN
1	G	210	GLN
1	G	234	HIS
1	G	580	GLN

### 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
3	PT5	A	701	-	56,56,69	0.44	0	69,74,87	0.44	0
3	PT5	G	701	-	56,56,69	0.44	0	69,74,87	0.44	0
3	PT5	C	701	-	56,56,69	0.44	0	69,74,87	0.44	0
3	PT5	E	701	-	56,56,69	0.44	0	69,74,87	0.44	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
3	PT5	A	701	-	-	30/53/77/90	0/1/1/1
3	PT5	G	701	-	-	29/53/77/90	0/1/1/1
3	PT5	C	701	-	-	29/53/77/90	0/1/1/1
3	PT5	E	701	-	-	29/53/77/90	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	PT5	C7-O13-P1-O12
3	A	701	PT5	C7-O13-P1-O11
3	A	701	PT5	C7-O13-P1-O1
3	A	701	PT5	C1-O1-P1-O13
3	A	701	PT5	C6-C1-O1-P1
3	A	701	PT5	C2-C1-O1-P1
3	A	701	PT5	C5-O5-P5-O52
3	A	701	PT5	C16-C17-C18-C19
3	A	701	PT5	C19-C20-C21-C22
3	C	701	PT5	C7-O13-P1-O12
3	C	701	PT5	C7-O13-P1-O11
3	C	701	PT5	C7-O13-P1-O1
3	C	701	PT5	C1-O1-P1-O13
3	C	701	PT5	C6-C1-O1-P1
3	C	701	PT5	C2-C1-O1-P1
3	C	701	PT5	C5-O5-P5-O52
3	C	701	PT5	C16-C17-C18-C19
3	C	701	PT5	C19-C20-C21-C22
3	E	701	PT5	C7-O13-P1-O12
3	E	701	PT5	C7-O13-P1-O11
3	E	701	PT5	C7-O13-P1-O1
3	E	701	PT5	C1-O1-P1-O13
3	E	701	PT5	C6-C1-O1-P1
3	E	701	PT5	C2-C1-O1-P1
3	E	701	PT5	C5-O5-P5-O52
3	E	701	PT5	C16-C17-C18-C19
3	E	701	PT5	C19-C20-C21-C22
3	G	701	PT5	C7-O13-P1-O12
3	G	701	PT5	C7-O13-P1-O11
3	G	701	PT5	C7-O13-P1-O1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	G	701	PT5	C1-O1-P1-O13
3	G	701	PT5	C6-C1-O1-P1
3	G	701	PT5	C2-C1-O1-P1
3	G	701	PT5	C5-O5-P5-O52
3	G	701	PT5	C16-C17-C18-C19
3	G	701	PT5	C19-C20-C21-C22
3	A	701	PT5	C14-C15-C16-C17
3	A	701	PT5	C20-C21-C22-C23
3	C	701	PT5	C14-C15-C16-C17
3	C	701	PT5	C20-C21-C22-C23
3	E	701	PT5	C14-C15-C16-C17
3	E	701	PT5	C20-C21-C22-C23
3	G	701	PT5	C14-C15-C16-C17
3	G	701	PT5	C20-C21-C22-C23
3	C	701	PT5	C11-C31-C32-C33
3	E	701	PT5	C11-C31-C32-C33
3	G	701	PT5	C11-C31-C32-C33
3	A	701	PT5	C11-C31-C32-C33
3	A	701	PT5	C31-C11-O18-C9
3	C	701	PT5	C31-C11-O18-C9
3	E	701	PT5	C31-C11-O18-C9
3	G	701	PT5	C31-C11-O18-C9
3	A	701	PT5	O19-C11-O18-C9
3	C	701	PT5	O19-C11-O18-C9
3	E	701	PT5	O19-C11-O18-C9
3	G	701	PT5	O19-C11-O18-C9
3	A	701	PT5	C36-C37-C38-C39
3	E	701	PT5	C36-C37-C38-C39
3	C	701	PT5	C36-C37-C38-C39
3	G	701	PT5	C36-C37-C38-C39
3	A	701	PT5	C12-C10-O16-C8
3	C	701	PT5	C12-C10-O16-C8
3	E	701	PT5	C12-C10-O16-C8
3	G	701	PT5	C12-C10-O16-C8
3	A	701	PT5	C34-C35-C36-C37
3	C	701	PT5	C34-C35-C36-C37
3	E	701	PT5	C34-C35-C36-C37
3	G	701	PT5	C34-C35-C36-C37
3	A	701	PT5	C12-C13-C14-C15
3	C	701	PT5	C12-C13-C14-C15
3	E	701	PT5	C12-C13-C14-C15
3	G	701	PT5	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	701	PT5	O17-C10-O16-C8
3	C	701	PT5	O17-C10-O16-C8
3	E	701	PT5	O17-C10-O16-C8
3	G	701	PT5	O17-C10-O16-C8
3	A	701	PT5	C37-C38-C39-C40
3	C	701	PT5	C37-C38-C39-C40
3	E	701	PT5	C37-C38-C39-C40
3	G	701	PT5	C37-C38-C39-C40
3	A	701	PT5	C6-C5-O5-P5
3	C	701	PT5	C6-C5-O5-P5
3	E	701	PT5	C6-C5-O5-P5
3	G	701	PT5	C6-C5-O5-P5
3	A	701	PT5	C13-C14-C15-C16
3	C	701	PT5	C13-C14-C15-C16
3	E	701	PT5	C13-C14-C15-C16
3	G	701	PT5	C13-C14-C15-C16
3	A	701	PT5	C1-O1-P1-O11
3	C	701	PT5	C1-O1-P1-O11
3	E	701	PT5	C1-O1-P1-O11
3	G	701	PT5	C1-O1-P1-O11
3	A	701	PT5	C21-C22-C23-C24
3	C	701	PT5	C21-C22-C23-C24
3	E	701	PT5	C21-C22-C23-C24
3	G	701	PT5	C21-C22-C23-C24
3	A	701	PT5	C4-C5-O5-P5
3	C	701	PT5	C4-C5-O5-P5
3	E	701	PT5	C4-C5-O5-P5
3	G	701	PT5	C4-C5-O5-P5
3	A	701	PT5	C8-C7-O13-P1
3	C	701	PT5	C8-C7-O13-P1
3	E	701	PT5	C8-C7-O13-P1
3	G	701	PT5	C8-C7-O13-P1
3	C	701	PT5	C33-C34-C35-C36
3	A	701	PT5	C33-C34-C35-C36
3	G	701	PT5	C33-C34-C35-C36
3	E	701	PT5	C33-C34-C35-C36
3	A	701	PT5	C5-O5-P5-O53
3	E	701	PT5	O18-C11-C31-C32
3	G	701	PT5	O18-C11-C31-C32
3	A	701	PT5	O18-C11-C31-C32
3	C	701	PT5	O18-C11-C31-C32
3	E	701	PT5	O19-C11-C31-C32

*Continued on next page...*

*Continued from previous page...*

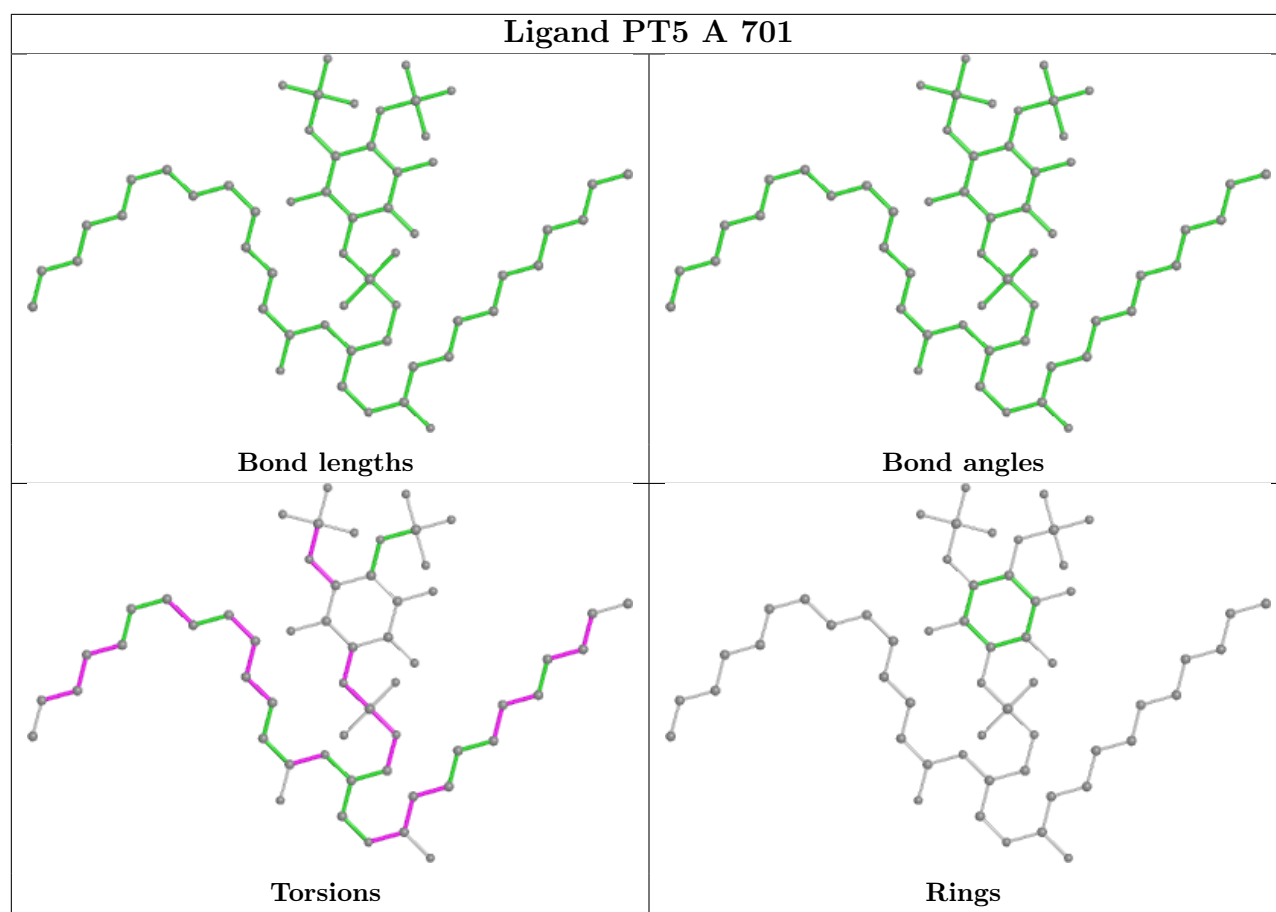
Mol	Chain	Res	Type	Atoms
3	G	701	PT5	O19-C11-C31-C32
3	A	701	PT5	O19-C11-C31-C32
3	C	701	PT5	O19-C11-C31-C32

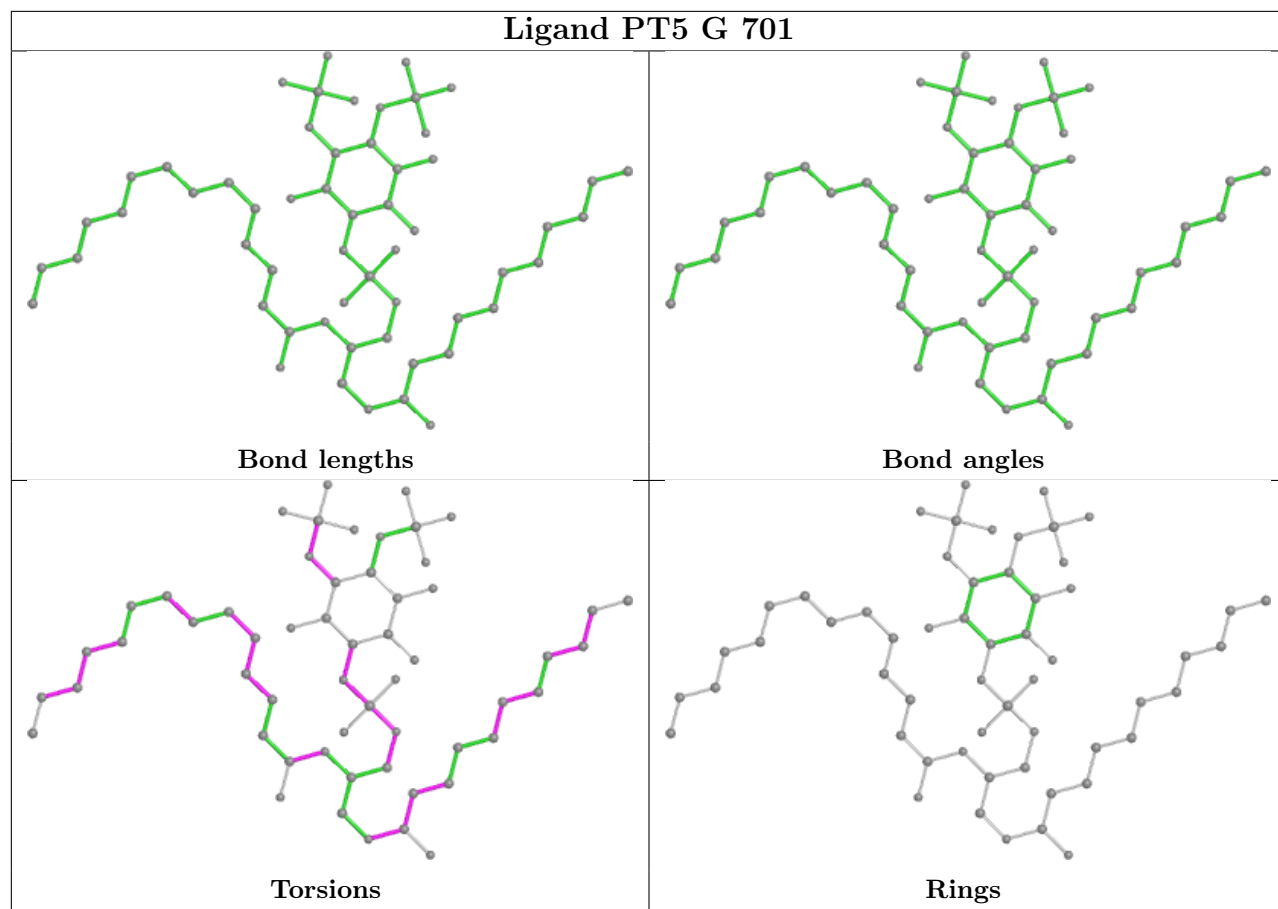
There are no ring outliers.

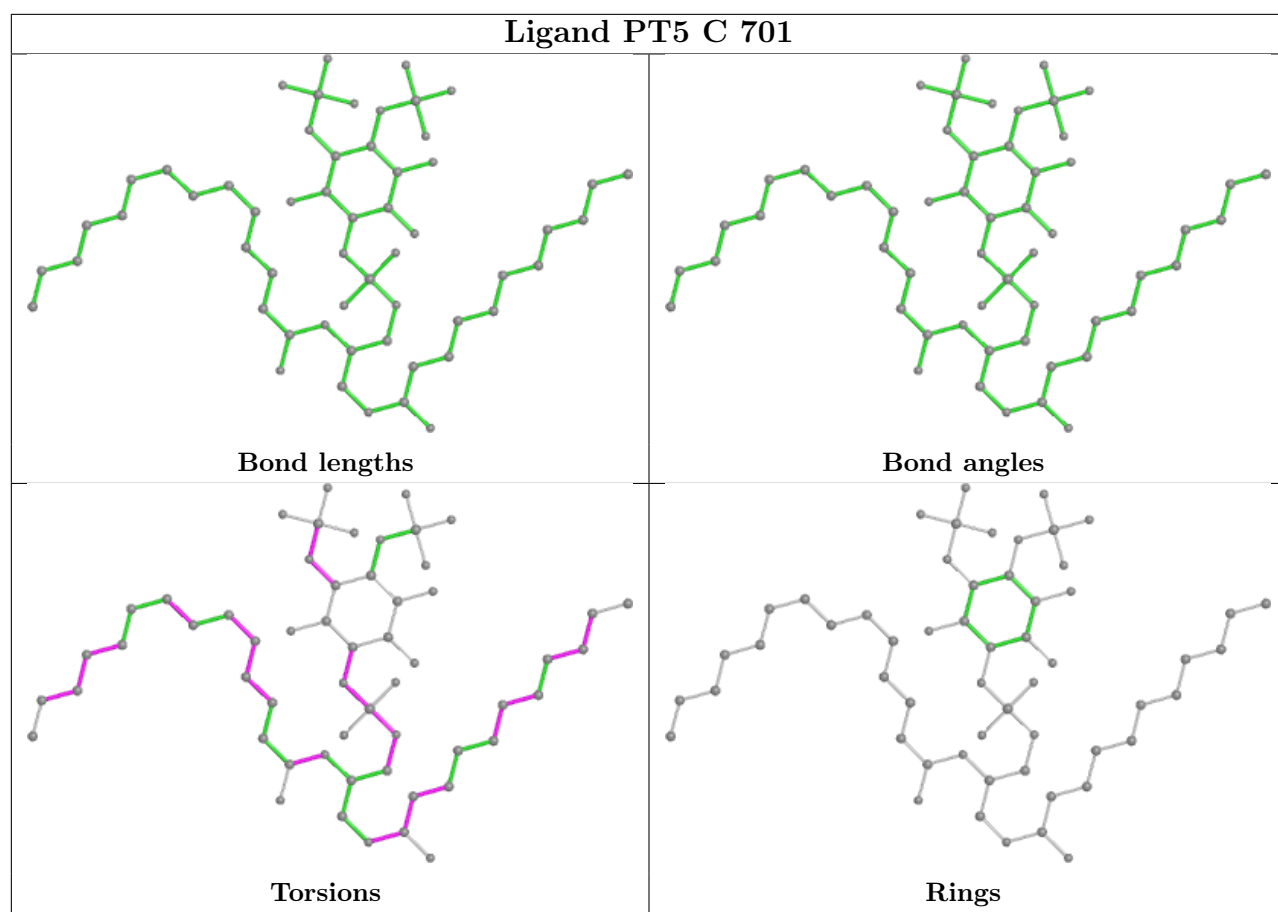
4 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	PT5	17	0
3	G	701	PT5	17	0
3	C	701	PT5	18	0
3	E	701	PT5	16	0

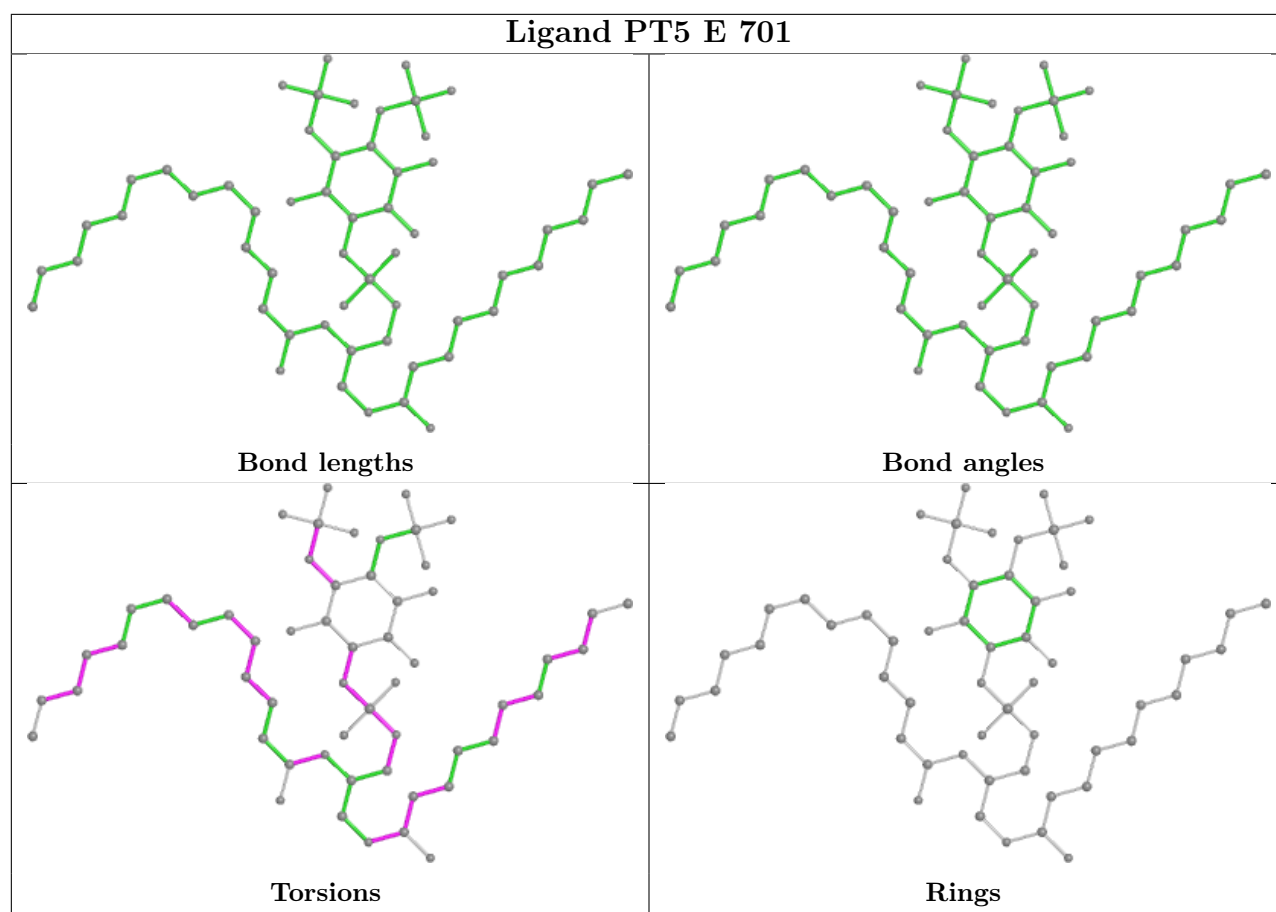
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

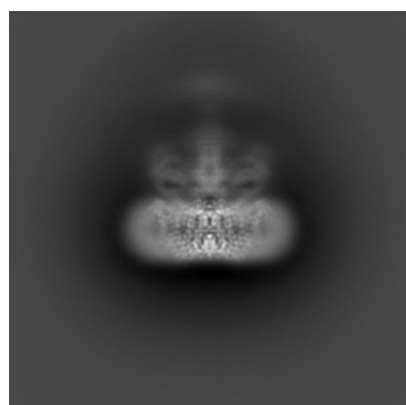
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30244. These allow visual inspection of the internal detail of the map and identification of artifacts.

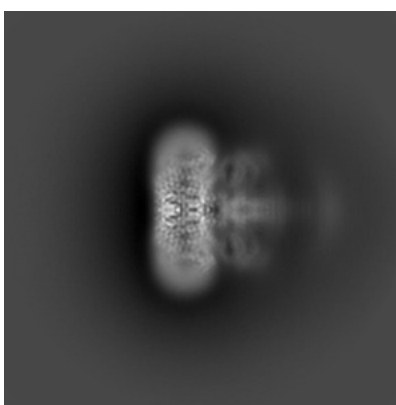
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

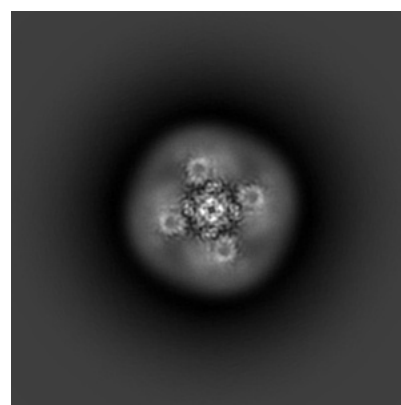
#### 6.1.1 Primary map



X



Y

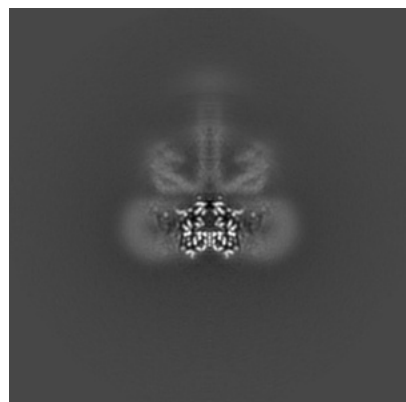


Z

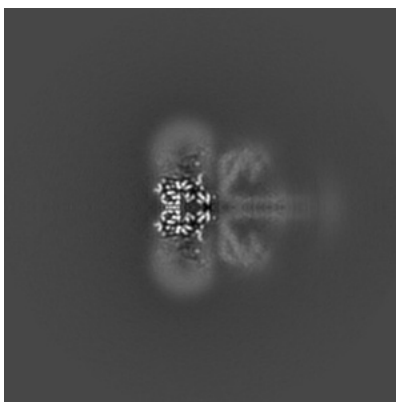
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

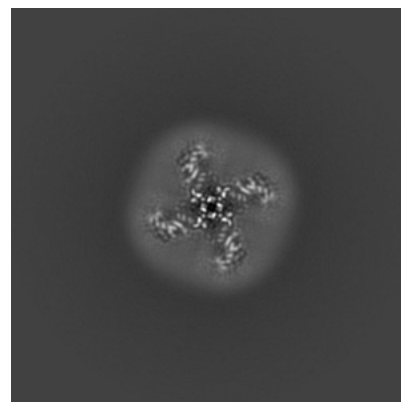
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

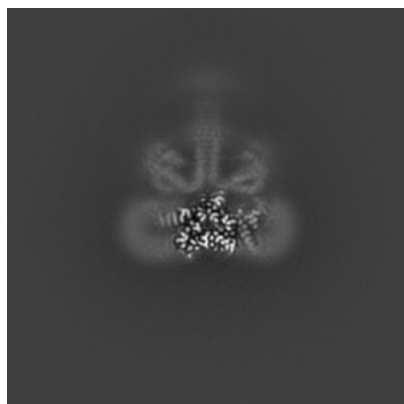


Z Index: 160

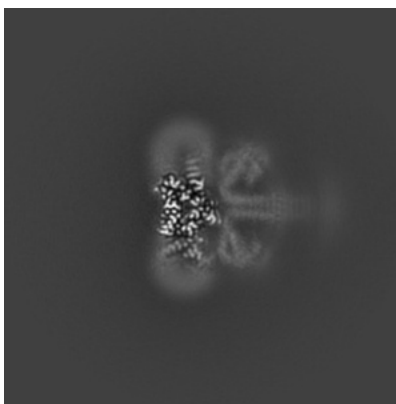
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

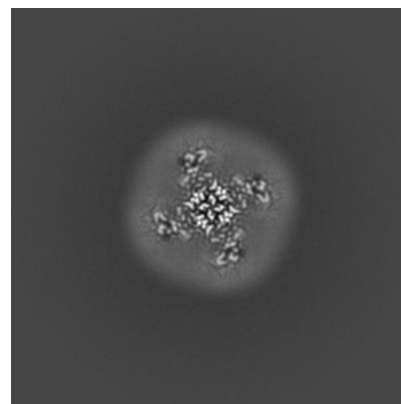
### 6.3.1 Primary map



X Index: 157



Y Index: 157



Z Index: 158

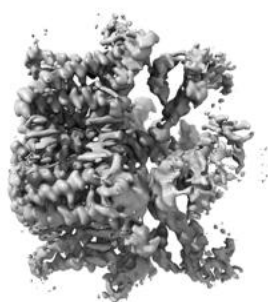
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

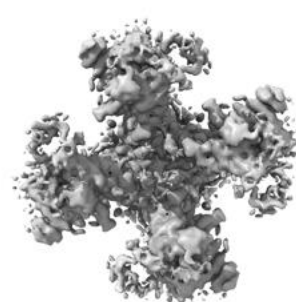
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

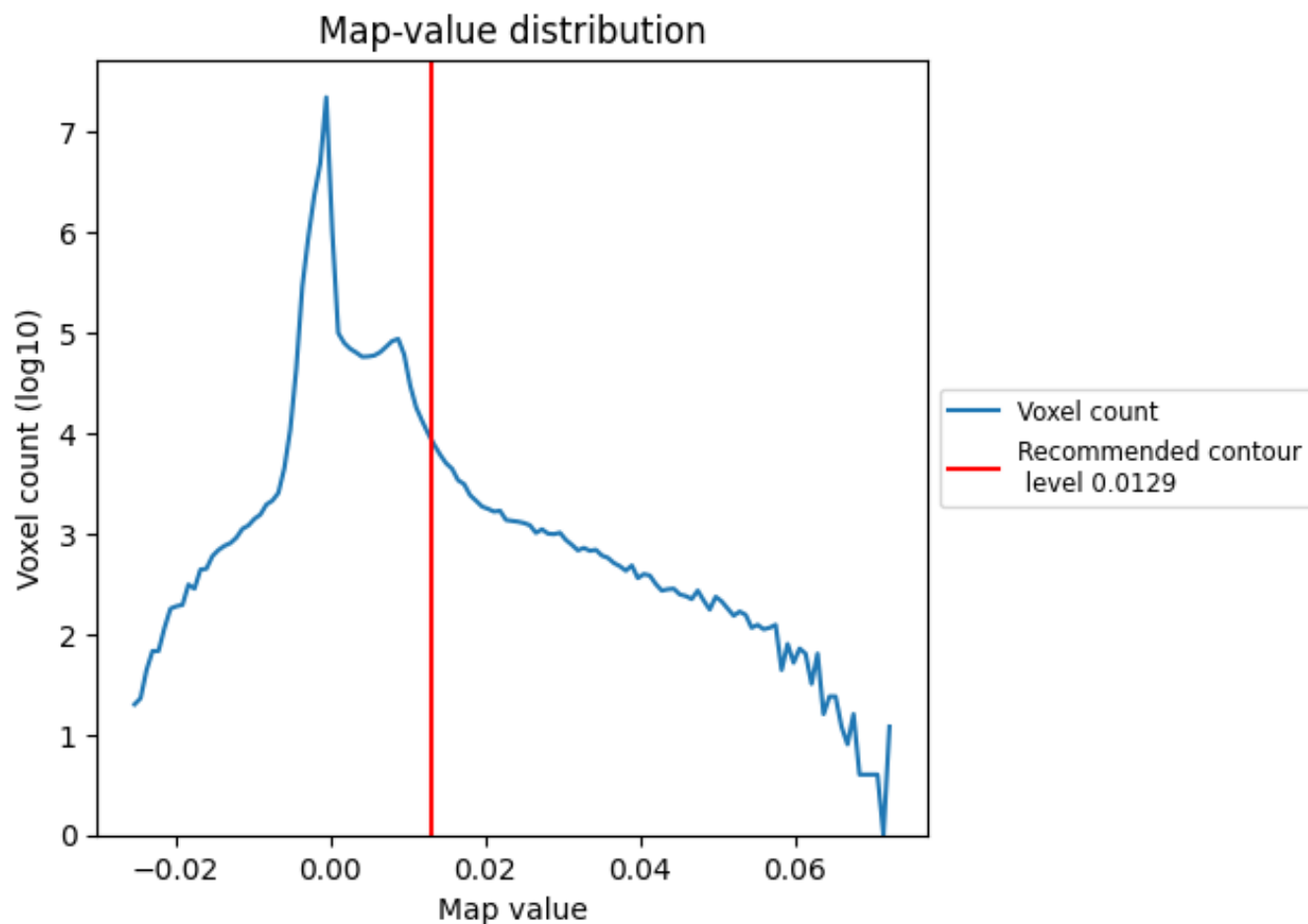
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

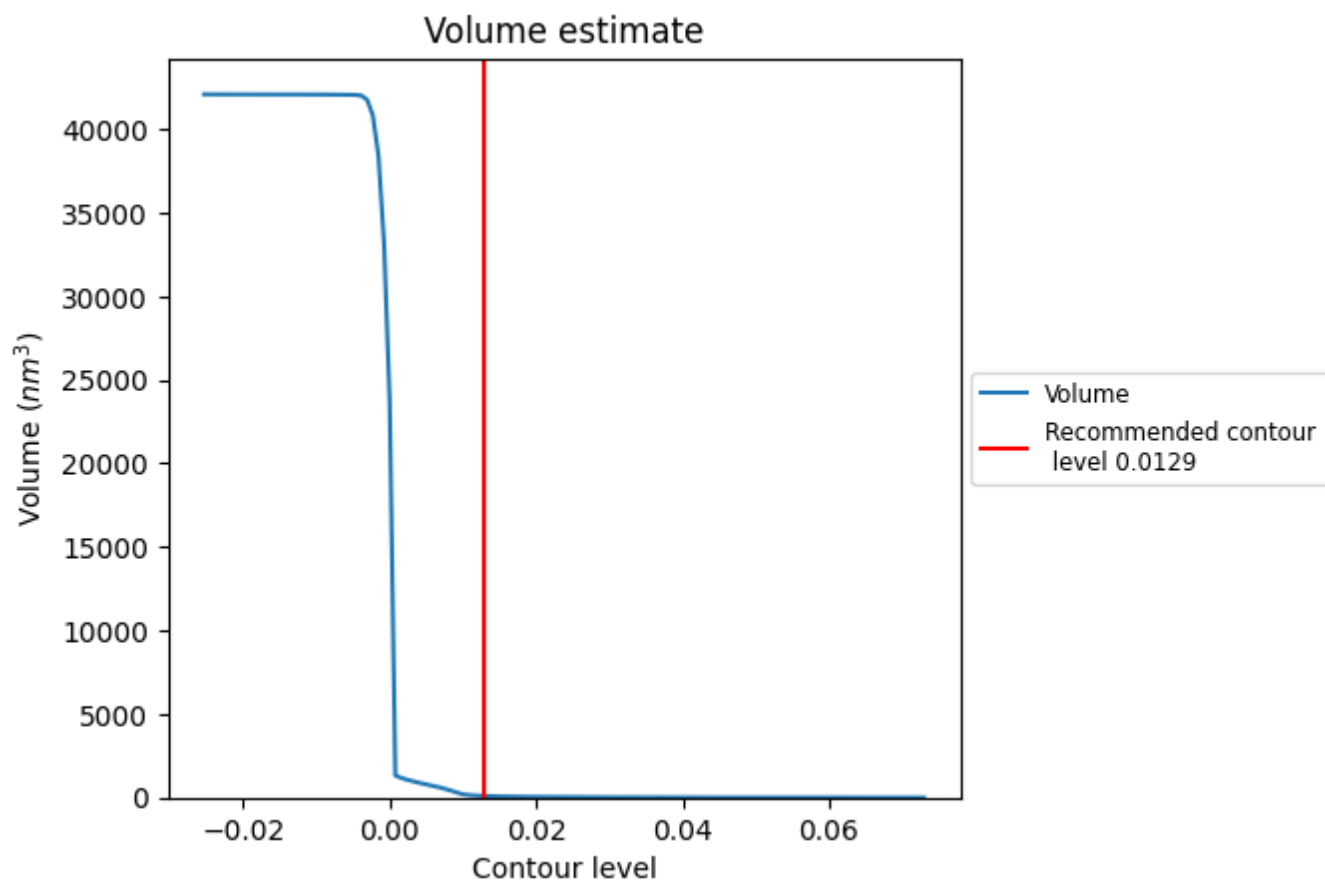
This section contains the results of statistical analysis of the map.

### 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.

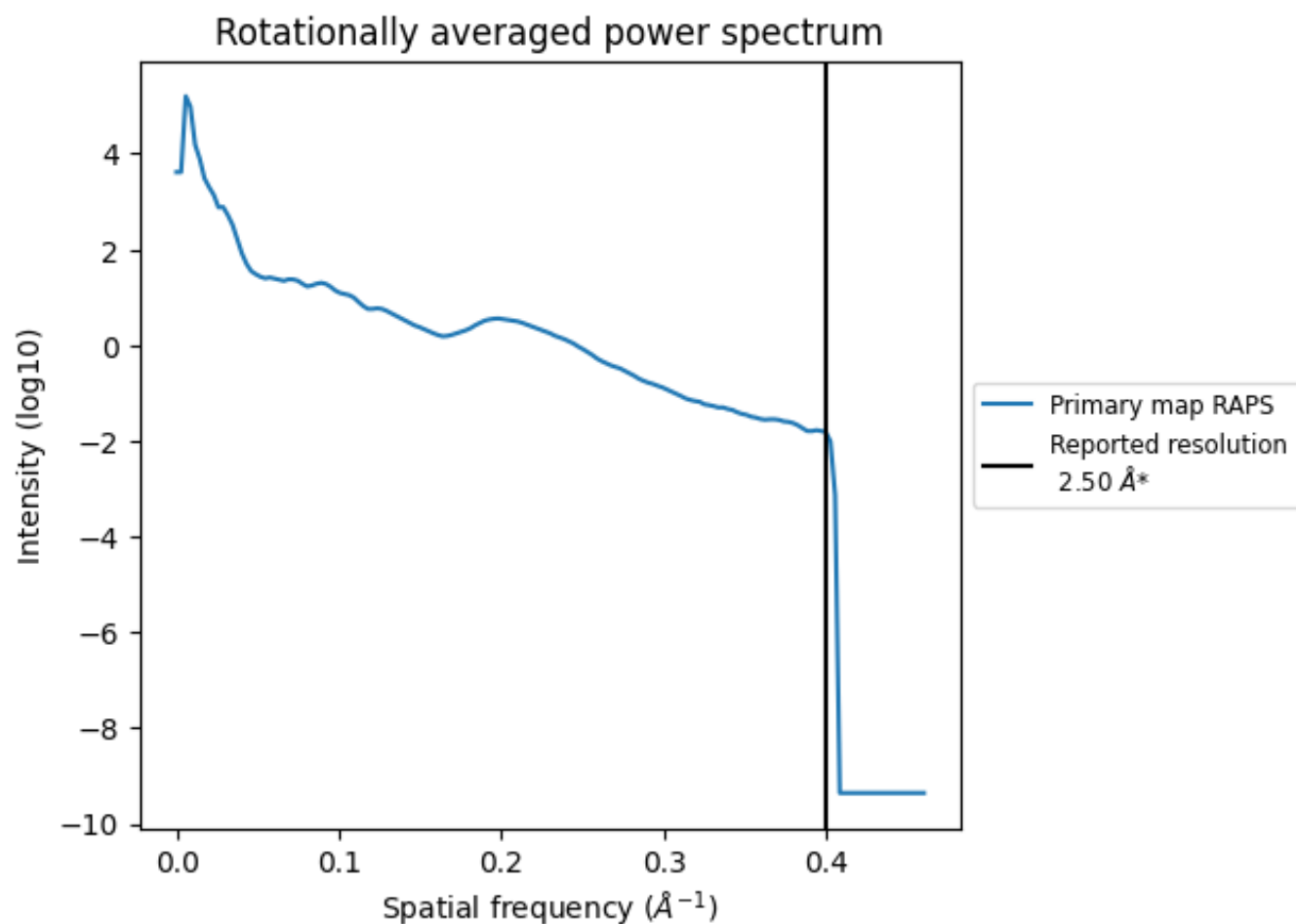
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93  $\text{nm}^3$ ; this corresponds to an approximate mass of 84 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 0.400 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

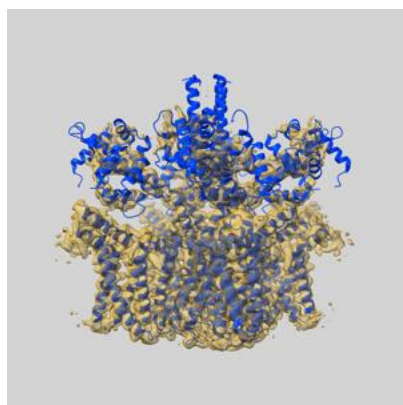
This section was not generated. No FSC curve or half-maps provided.



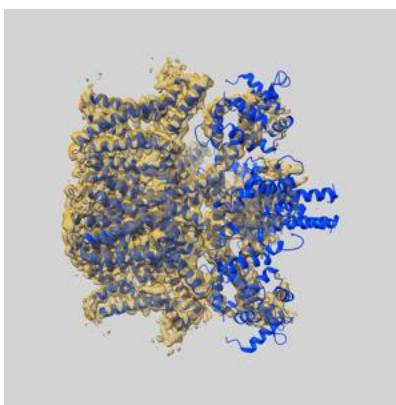
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30244 and PDB model 7BYL. Per-residue inclusion information can be found in section 3 on page 10.

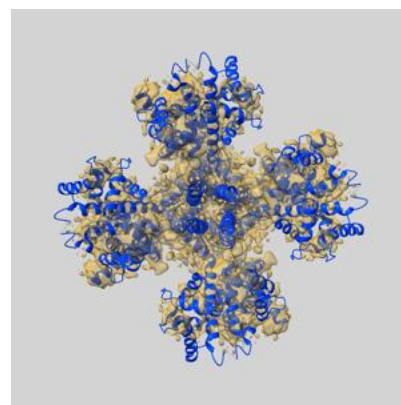
### 9.1 Map-model overlay [i](#)



X



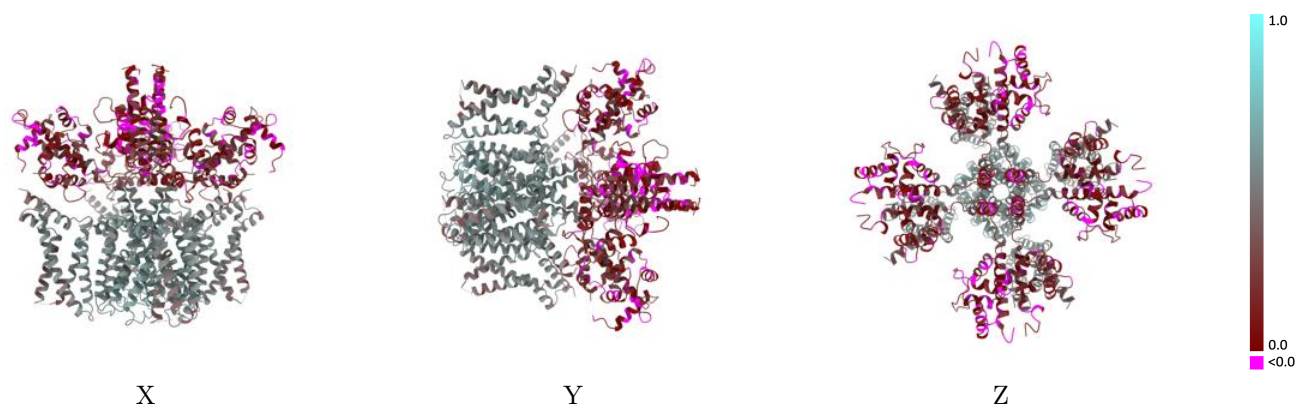
Y



Z

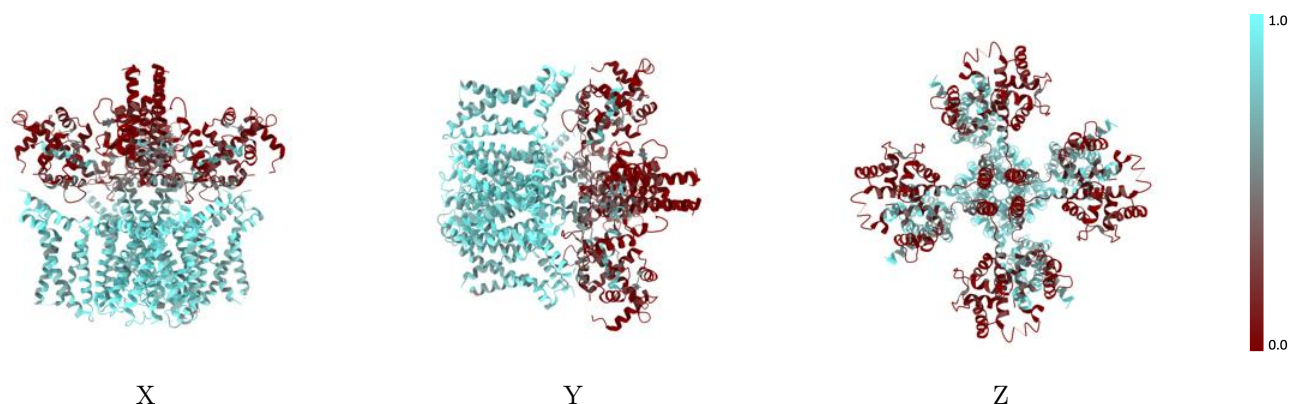
The images above show the 3D surface view of the map at the recommended contour level 0.0129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



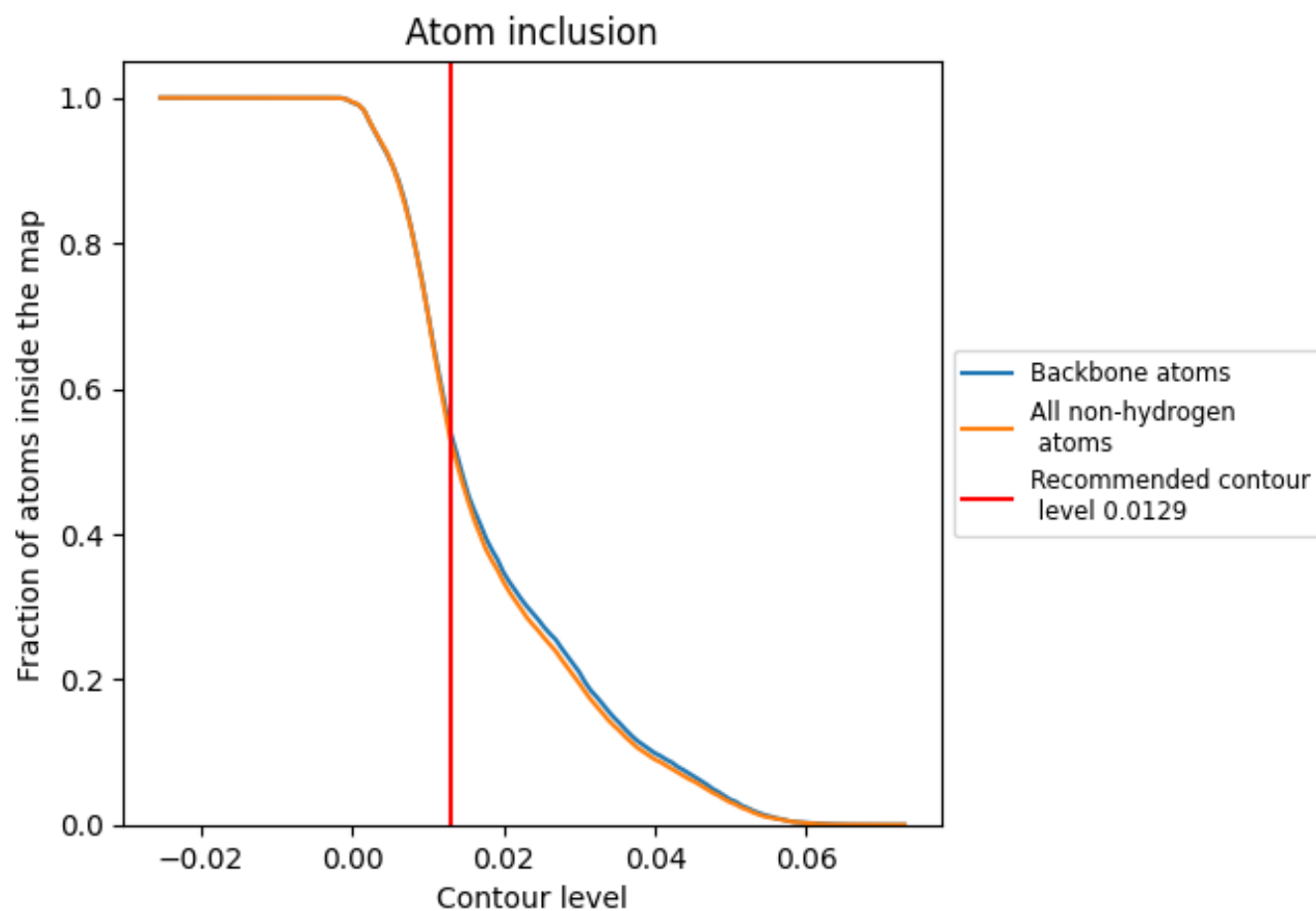
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0129).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 53% 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 (0.0129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5333	<div></div> 0.3260
A	<div></div> 0.6949	<div></div> 0.4140
B	<div></div> 0.1557	<div></div> 0.1070
C	<div></div> 0.6920	<div></div> 0.4130
D	<div></div> 0.1539	<div></div> 0.1080
E	<div></div> 0.6973	<div></div> 0.4110
F	<div></div> 0.1566	<div></div> 0.1070
G	<div></div> 0.6941	<div></div> 0.4120
H	<div></div> 0.1548	<div></div> 0.1060

