



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:03 PM UTC

PDB ID : 7PHK / pdb_00007phk
EMDB ID : EMD-13418
Title : Human voltage-gated potassium channel Kv3.1 in dimeric state (with Zn)
Authors : Chi, G.; Qian, P.; Castro-Hartmann, P.; Venkaya, S.; Singh, N.K.; McKinley, G.; Mukhopadhyay, S.M.M.; Marsden, B.; MacLean, E.M.; Fernandez-Cid, A.; Pike, A.C.W.; Sader, K.; Burgess-Brown, N.A.; Duerr, K.L.
Deposited on : 2021-08-17
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

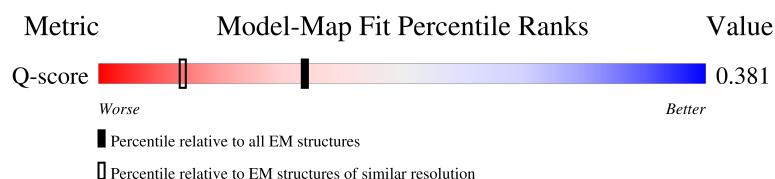
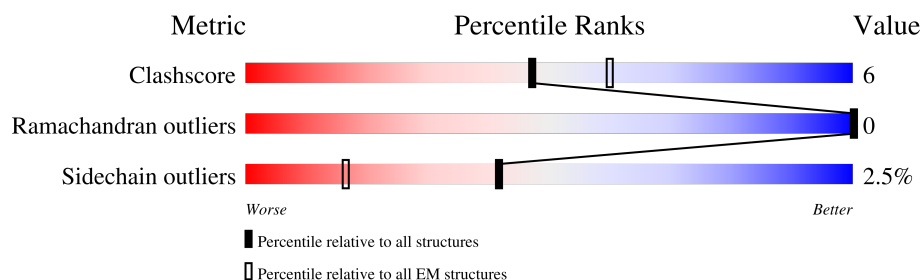
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	518	
1	B	518	
1	C	518	
1	D	518	

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Mol	Chain	Length	Quality of chain
1	E	518	42% 64% 12% 24%
1	F	518	42% 64% 12% 24%
1	G	518	42% 64% 12% 24%
1	H	518	42% 64% 12% 24%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25404 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 Potassium voltage-gated channel, Shaw-related subfamily, member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	392	Total	C	N	O	S	0	0
			3095	2023	525	530	17		
1	C	392	Total	C	N	O	S	0	0
			3095	2023	525	530	17		
1	B	392	Total	C	N	O	S	0	0
			3095	2023	525	530	17		
1	D	392	Total	C	N	O	S	0	0
			3095	2023	525	530	17		
1	E	393	Total	C	N	O	S	0	0
			3098	2025	525	531	17		
1	G	393	Total	C	N	O	S	0	0
			3098	2025	525	531	17		
1	F	393	Total	C	N	O	S	0	0
			3098	2025	525	531	17		
1	H	393	Total	C	N	O	S	0	0
			3098	2025	525	531	17		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	512	ALA	-	expression tag	UNP Q3KNS8
A	513	GLU	-	expression tag	UNP Q3KNS8
A	514	ASN	-	expression tag	UNP Q3KNS8
A	515	LEU	-	expression tag	UNP Q3KNS8
A	516	TYR	-	expression tag	UNP Q3KNS8
A	517	PHE	-	expression tag	UNP Q3KNS8
A	518	GLN	-	expression tag	UNP Q3KNS8
C	512	ALA	-	expression tag	UNP Q3KNS8
C	513	GLU	-	expression tag	UNP Q3KNS8
C	514	ASN	-	expression tag	UNP Q3KNS8
C	515	LEU	-	expression tag	UNP Q3KNS8
C	516	TYR	-	expression tag	UNP Q3KNS8
C	517	PHE	-	expression tag	UNP Q3KNS8

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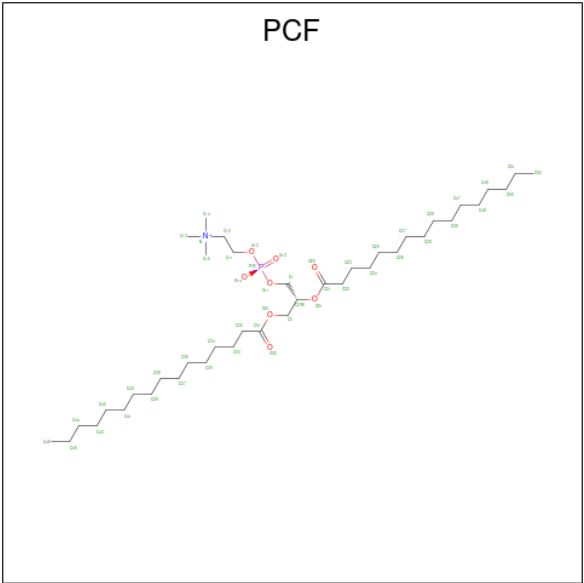
Chain	Residue	Modelled	Actual	Comment	Reference
C	518	GLN	-	expression tag	UNP Q3KNS8
B	512	ALA	-	expression tag	UNP Q3KNS8
B	513	GLU	-	expression tag	UNP Q3KNS8
B	514	ASN	-	expression tag	UNP Q3KNS8
B	515	LEU	-	expression tag	UNP Q3KNS8
B	516	TYR	-	expression tag	UNP Q3KNS8
B	517	PHE	-	expression tag	UNP Q3KNS8
B	518	GLN	-	expression tag	UNP Q3KNS8
D	512	ALA	-	expression tag	UNP Q3KNS8
D	513	GLU	-	expression tag	UNP Q3KNS8
D	514	ASN	-	expression tag	UNP Q3KNS8
D	515	LEU	-	expression tag	UNP Q3KNS8
D	516	TYR	-	expression tag	UNP Q3KNS8
D	517	PHE	-	expression tag	UNP Q3KNS8
D	518	GLN	-	expression tag	UNP Q3KNS8
E	512	ALA	-	expression tag	UNP Q3KNS8
E	513	GLU	-	expression tag	UNP Q3KNS8
E	514	ASN	-	expression tag	UNP Q3KNS8
E	515	LEU	-	expression tag	UNP Q3KNS8
E	516	TYR	-	expression tag	UNP Q3KNS8
E	517	PHE	-	expression tag	UNP Q3KNS8
E	518	GLN	-	expression tag	UNP Q3KNS8
G	512	ALA	-	expression tag	UNP Q3KNS8
G	513	GLU	-	expression tag	UNP Q3KNS8
G	514	ASN	-	expression tag	UNP Q3KNS8
G	515	LEU	-	expression tag	UNP Q3KNS8
G	516	TYR	-	expression tag	UNP Q3KNS8
G	517	PHE	-	expression tag	UNP Q3KNS8
G	518	GLN	-	expression tag	UNP Q3KNS8
F	512	ALA	-	expression tag	UNP Q3KNS8
F	513	GLU	-	expression tag	UNP Q3KNS8
F	514	ASN	-	expression tag	UNP Q3KNS8
F	515	LEU	-	expression tag	UNP Q3KNS8
F	516	TYR	-	expression tag	UNP Q3KNS8
F	517	PHE	-	expression tag	UNP Q3KNS8
F	518	GLN	-	expression tag	UNP Q3KNS8
H	512	ALA	-	expression tag	UNP Q3KNS8
H	513	GLU	-	expression tag	UNP Q3KNS8
H	514	ASN	-	expression tag	UNP Q3KNS8
H	515	LEU	-	expression tag	UNP Q3KNS8
H	516	TYR	-	expression tag	UNP Q3KNS8
H	517	PHE	-	expression tag	UNP Q3KNS8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	518	GLN	-	expression tag	UNP Q3KNS8

- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	D	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	E	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	E	1	Total	C	N	O	P	0
			32	22	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	G	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	F	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	H	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	H	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	

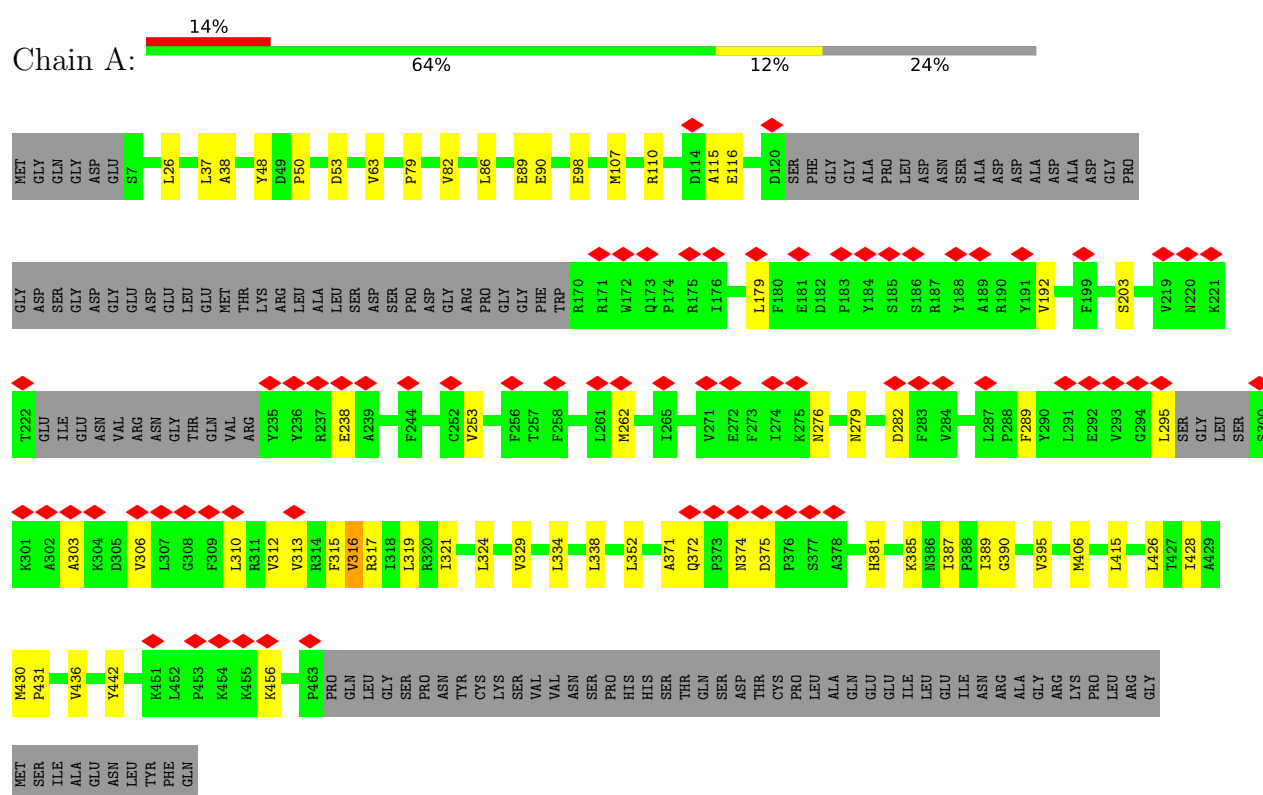
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

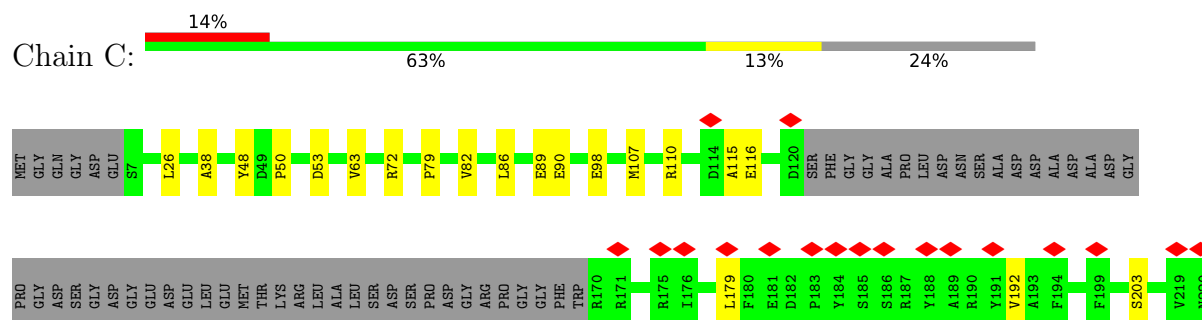
3 Residue-property plots

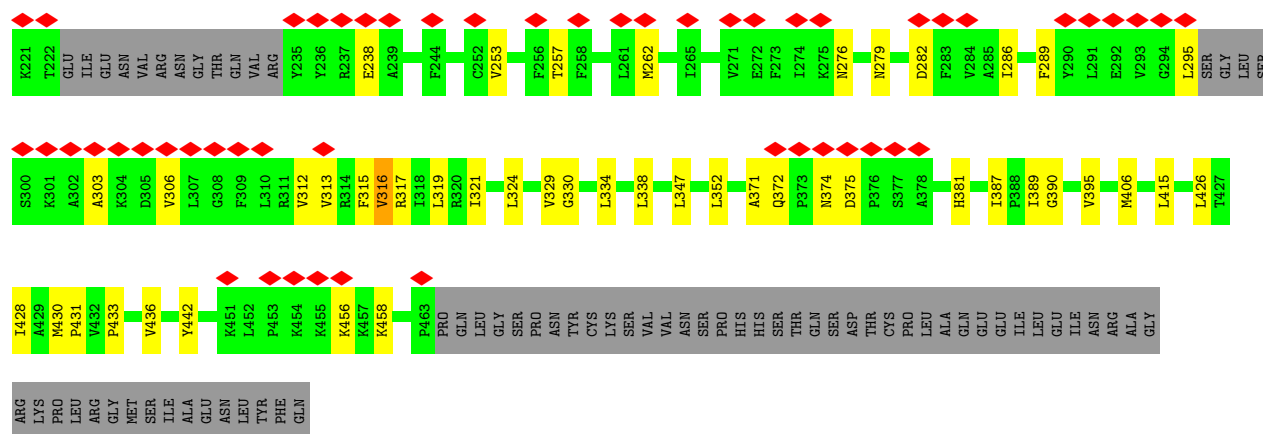
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Potassium voltage-gated channel, Shaw-related subfamily, member 1

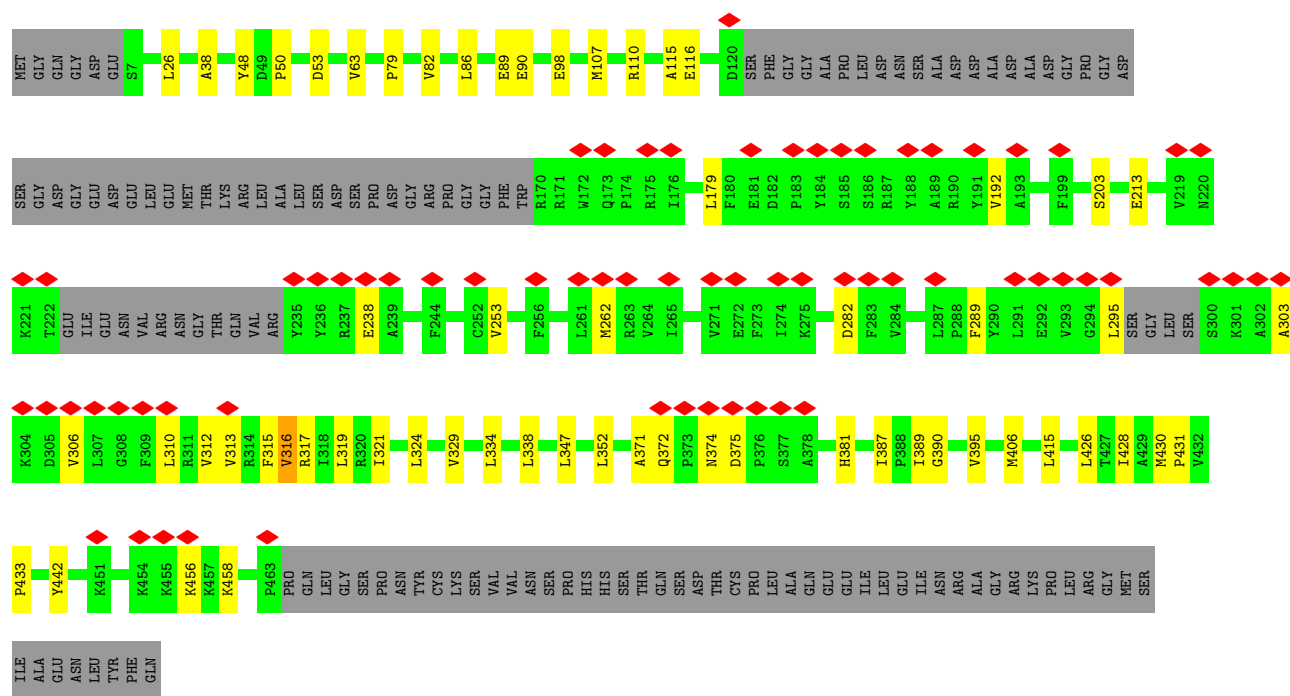


- Molecule 1: Potassium voltage-gated channel, Shaw-related subfamily, member 1

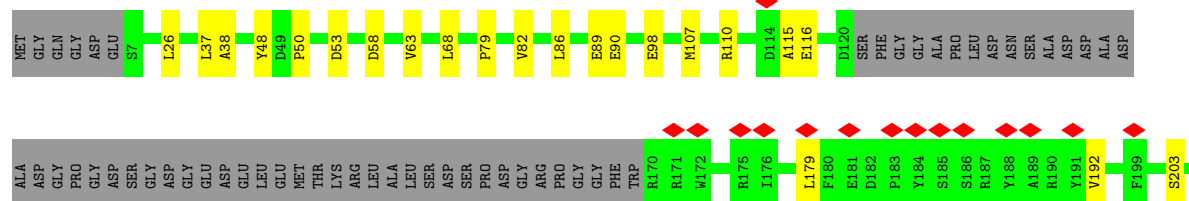


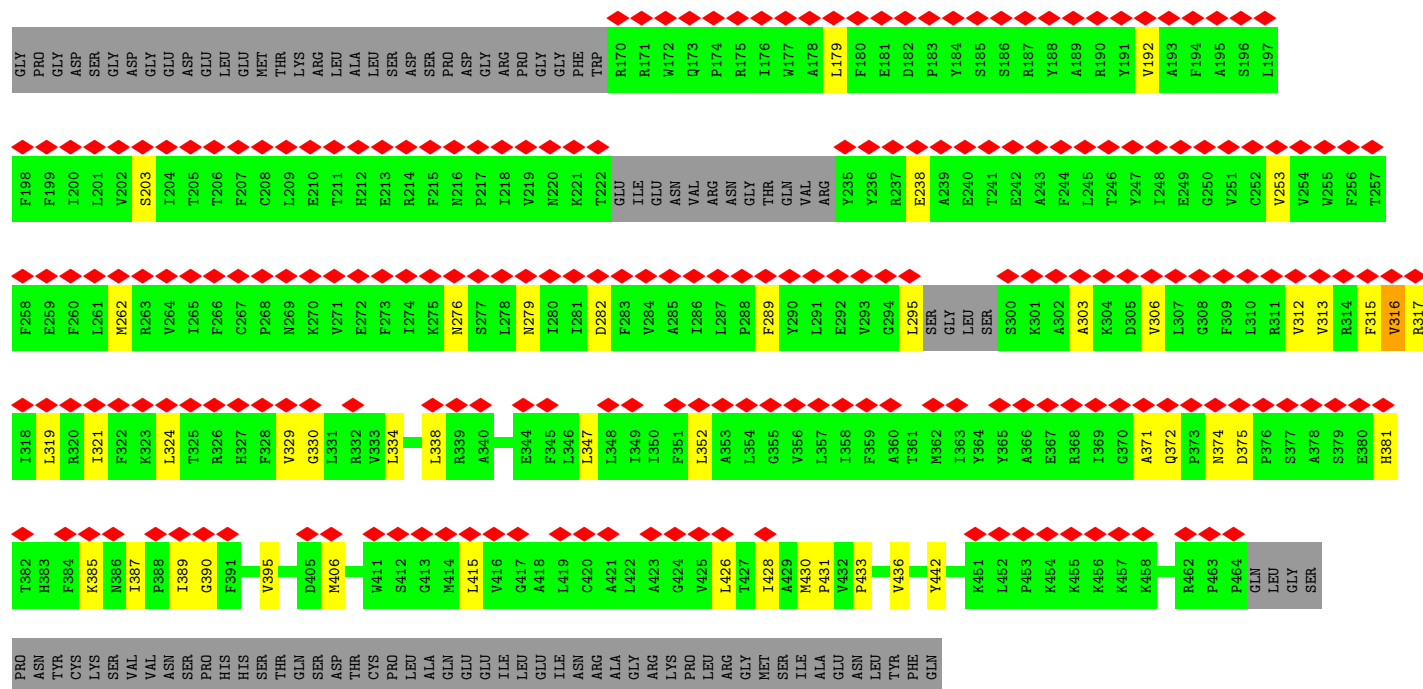


• Molecule 1: Potassium voltage-gated channel, Shaw-related subfamily, member 1

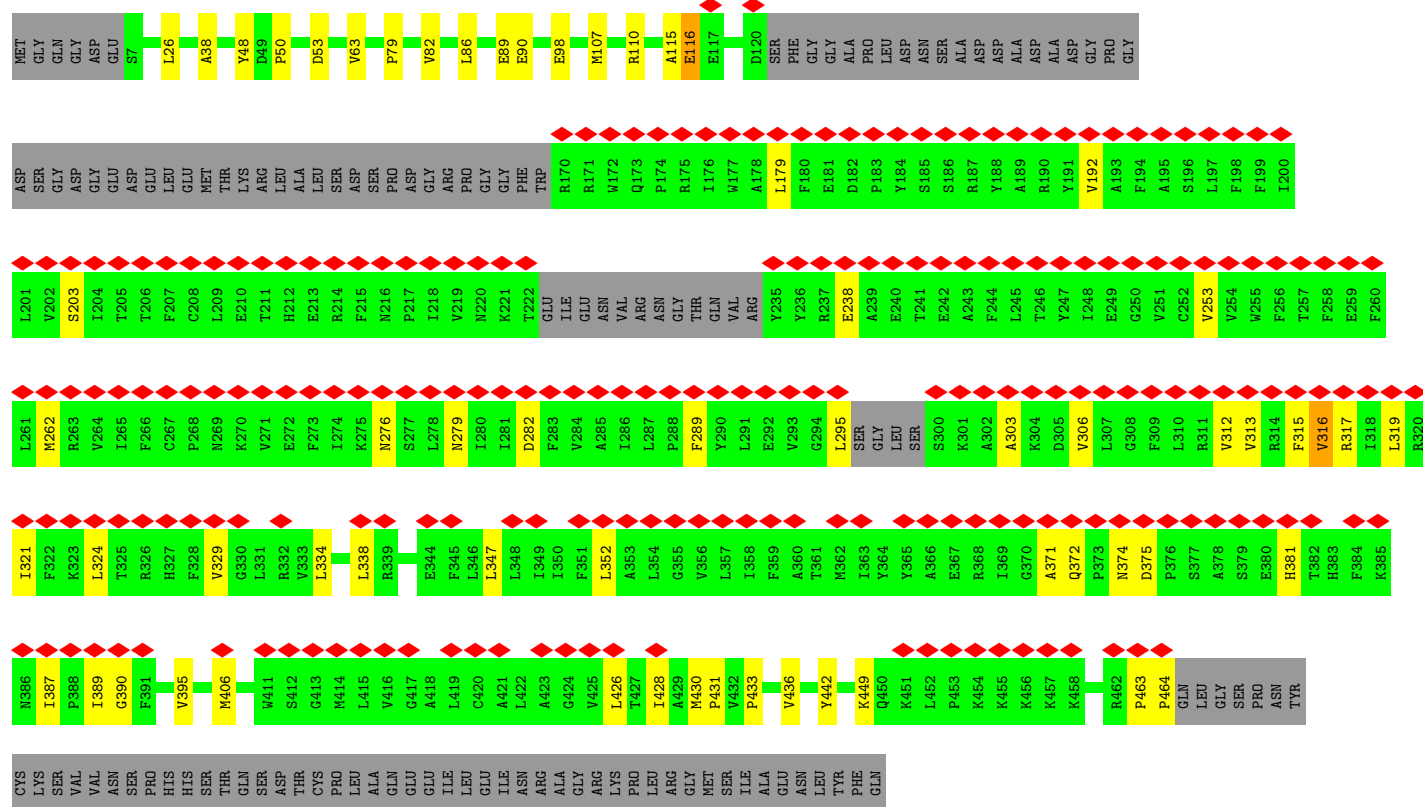
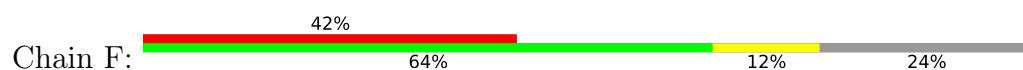


• Molecule 1: Potassium voltage-gated channel, Shaw-related subfamily, member 1





- Molecule 1: Potassium voltage-gated channel, Shaw-related subfamily, member 1



- Molecule 1: Potassium voltage-gated channel, Shaw-related subfamily, member 1



MET	GLY	GLN	GLY	ASP	GLU	S7	L26	L37	A38	Y48	D49	P50	D53	D58	V63	L68	P79	V82	L86	E89	E90	E98	M107	R110	A115	E116	E117	D120	SER	PHE	GLY	GLY	ALA	PRO	LEU	ASP	ASN	SER	ALA	ASP	ALA	ASP																		
ALA	ASP	GLY	PRO	GLY	ASP	SER	GLY	GLY	GLU	ASP	GLU	MET	THR	LYS	ARG	LEU	ALA	LEU	ASP	SER	PRO	ASP	GLY	GLY	ARG	PRO	GLY	PHE	TRP	R170	R171	W172	Q173	P174	R175	I176	W177	A178	L179	F180	E181	D182	P183	Y184	S185	S186	R187	Y188	A189	R190	Y191	V192	A193	F194	A195					
S196	L197	F198	F199	I200	L201	V202	S203	I204	T205	T206	F207	C208	L209	E210	T211	H212	E213	R214	F215	N216	P217	I218	V219	N220	K221	T222	GLU	ILE	GLU	ASN	VAL	ARG	ASN	THR	GLY	THR	GLN	VAL	ARG	Y235	Y236	R237	E238	A239	E240	T241	E242	A243	F244	L245	T246	Y247	I248	E249	G250	V251	C252	V253	V254	W255
F256	T257	F258	E259	F260	L261	M262	R263	V264	I265	F266	C267	P268	N269	K270	V271	E272	F273	I274	K275	N276	S277	L278	N279	I280	I281	D282	F283	V284	A285	I286	L287	P288	F289	Y290	L291	E292	V293	G294	L295	SER	GLY	LEU	SER	S300	K301	A302	A303	K304	D305	V306	L307	G308	F309	L310	R311	V312	V313	R314	F315	
V316	R317	I318	L319	R320	I321	F322	K323	L324	T325	R326	H327	F328	V329	G330	L331	R332	V333	L334	L338	R339	E344	F345	I349	I350	F351	L352	A353	L354	G355	V356	L357	I358	F359	A360	T361	M362	I363	Y364	Y365	A366	E367	R368	I369	G370	A371	Q372	P373	N374	D375	P376	S377	A378	E380	H381	T382					
H383	F384	K385	N386	I387	F388	I389	G390	F391	V395	M406	Y407	P408	W411	S412	C413	M414	L415	V416	G417	A418	L419	C420	A421	L422	A423	G424	V425	L426	T427	I428	A429	M430	P431	W432	P433	V436	Y442	M447	K451	L452	P453	K454	K455	K456	K457	K458	R462	P463	P464	GLN	LEU									
GLY	SER	PRO	ASN	TYR	LYS	SER	VAL	VAL	ASN	SER	PRO	HIS	HIS	SER	THR	GLN	SER	ASP	THR	CYS	PRO	LEU	ALA	GLN	GLU	ILE	LEU	ILE	ASN	ARG	ALA	GLY	ARG	LYS	PRO	LEU	GLY	MET	SER	ILE	ALA	ASN	LEU	TYR	PHE	GLN														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	72764	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 ($e^-/\text{\AA}^2$)	47.59	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	2.912	Depositor
Minimum map value	-1.820	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: PCF, K, ZN

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	0.17	0/3186	0.31	0/4343
1	B	0.17	0/3186	0.30	0/4343
1	C	0.17	0/3186	0.30	0/4343
1	D	0.17	0/3186	0.31	0/4343
1	E	0.17	0/3190	0.30	0/4351
1	F	0.17	0/3190	0.30	0/4351
1	G	0.17	0/3190	0.30	0/4351
1	H	0.17	0/3190	0.30	0/4351
All	All	0.17	0/25504	0.30	0/34776

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	3095	0	2985	36	0
1	B	3095	0	2985	34	0
1	C	3095	0	2984	39	0
1	D	3095	0	2985	41	0
1	E	3098	0	2981	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3098	0	2981	35	0
1	G	3098	0	2981	39	0
1	H	3098	0	2981	38	0
2	A	77	0	102	4	0
2	B	77	0	102	6	0
2	C	77	0	102	6	0
2	D	77	0	102	5	0
2	E	77	0	102	5	0
2	F	77	0	102	5	0
2	G	77	0	102	5	0
2	H	77	0	102	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	4	0	0	0	0
4	E	4	0	0	0	0
All	All	25404	0	24679	298	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 6.

All (298) 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:B:115:ALA:HA	1:B:442:TYR:HE1	1.65	0.62
1:G:115:ALA:HA	1:G:442:TYR:HE1	1.65	0.62
1:H:115:ALA:HA	1:H:442:TYR:HE1	1.65	0.62
1:C:115:ALA:HA	1:C:442:TYR:HE1	1.65	0.62
1:C:50:PRO:HB2	1:H:50:PRO:HB2	1.82	0.61
1:E:115:ALA:HA	1:E:442:TYR:HE1	1.65	0.61
1:A:115:ALA:HA	1:A:442:TYR:HE1	1.65	0.61
1:D:115:ALA:HA	1:D:442:TYR:HE1	1.65	0.61
1:C:456:LYS:HE2	1:C:458:LYS:HD3	1.82	0.60
1:F:115:ALA:HA	1:F:442:TYR:HE1	1.65	0.60
1:B:352:LEU:HD21	1:B:428:ILE:HD11	1.84	0.60
1:G:352:LEU:HD21	1:G:428:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:LEU:HD21	1:F:428:ILE:HD11	1.84	0.60
1:A:63:VAL:HG21	1:A:90:GLU:HG3	1.84	0.59
1:E:63:VAL:HG21	1:E:90:GLU:HG3	1.84	0.59
1:A:395:VAL:HG21	2:D:602:PCF:H291	1.83	0.59
1:C:352:LEU:HD21	1:C:428:ILE:HD11	1.84	0.59
1:F:63:VAL:HG21	1:F:90:GLU:HG3	1.84	0.59
1:C:63:VAL:HG21	1:C:90:GLU:HG3	1.84	0.58
1:G:63:VAL:HG21	1:G:90:GLU:HG3	1.84	0.58
1:D:352:LEU:HD21	1:D:428:ILE:HD11	1.84	0.58
1:D:63:VAL:HG21	1:D:90:GLU:HG3	1.84	0.58
1:A:352:LEU:HD21	1:A:428:ILE:HD11	1.84	0.58
1:B:63:VAL:HG21	1:B:90:GLU:HG3	1.84	0.58
1:E:352:LEU:HD21	1:E:428:ILE:HD11	1.84	0.58
1:H:352:LEU:HD21	1:H:428:ILE:HD11	1.84	0.57
1:A:456:LYS:O	1:A:456:LYS:HG2	2.04	0.57
1:H:63:VAL:HG21	1:H:90:GLU:HG3	1.84	0.57
1:B:50:PRO:HB2	1:E:50:PRO:HB2	1.85	0.57
2:E:601:PCF:H291	1:F:395:VAL:HG21	1.86	0.56
1:C:433:PRO:HG2	1:D:436:VAL:HG11	1.89	0.55
1:D:203:SER:OG	1:D:317:ARG:NH1	2.38	0.55
1:A:203:SER:OG	1:A:317:ARG:NH1	2.38	0.54
1:E:203:SER:OG	1:E:317:ARG:NH1	2.38	0.54
1:E:436:VAL:HG11	1:H:433:PRO:HG2	1.90	0.53
1:H:203:SER:OG	1:H:317:ARG:NH1	2.38	0.53
1:B:456:LYS:HE2	1:B:458:LYS:HD3	1.91	0.53
1:C:203:SER:OG	1:C:317:ARG:NH1	2.38	0.53
1:B:203:SER:OG	1:B:317:ARG:NH1	2.38	0.52
1:D:456:LYS:HG2	1:D:456:LYS:O	2.10	0.52
1:A:48:TYR:OH	1:A:53:ASP:OD1	2.27	0.52
1:A:371:ALA:HA	1:A:381:HIS:HE1	1.75	0.52
1:E:389:ILE:HD12	1:E:406:MET:HE1	1.92	0.52
1:G:436:VAL:HG11	1:F:433:PRO:HG2	1.91	0.51
1:F:371:ALA:HA	1:F:381:HIS:HE1	1.75	0.51
1:D:389:ILE:HD12	1:D:406:MET:HE1	1.93	0.51
1:A:389:ILE:HD12	1:A:406:MET:HE1	1.92	0.51
1:B:371:ALA:HA	1:B:381:HIS:HE1	1.75	0.51
1:G:389:ILE:HD12	1:G:406:MET:HE1	1.92	0.51
1:C:389:ILE:HD12	1:C:406:MET:HE1	1.92	0.51
1:F:203:SER:OG	1:F:317:ARG:NH1	2.38	0.51
1:H:389:ILE:HD12	1:H:406:MET:HE1	1.92	0.51
1:D:203:SER:HG	1:D:317:ARG:HH11	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ILE:HD12	1:B:406:MET:HE1	1.92	0.51
1:C:395:VAL:HG21	2:B:602:PCF:H291	1.92	0.51
1:E:48:TYR:OH	1:E:53:ASP:OD1	2.27	0.51
1:G:179:LEU:HG	1:G:192:VAL:HG11	1.93	0.51
1:G:371:ALA:HA	1:G:381:HIS:HE1	1.75	0.51
1:F:389:ILE:HD12	1:F:406:MET:HE1	1.92	0.51
1:F:179:LEU:HG	1:F:192:VAL:HG11	1.93	0.51
1:E:371:ALA:HA	1:E:381:HIS:HE1	1.75	0.50
1:B:48:TYR:OH	1:B:53:ASP:OD1	2.27	0.50
1:B:179:LEU:HG	1:B:192:VAL:HG11	1.93	0.50
1:G:203:SER:OG	1:G:317:ARG:NH1	2.38	0.50
1:G:321:ILE:HD12	1:G:324:LEU:HD12	1.93	0.50
1:D:371:ALA:HA	1:D:381:HIS:HE1	1.75	0.50
1:C:179:LEU:HG	1:C:192:VAL:HG11	1.93	0.50
1:H:321:ILE:HD12	1:H:324:LEU:HD12	1.94	0.50
1:A:179:LEU:HG	1:A:192:VAL:HG11	1.93	0.50
1:D:48:TYR:OH	1:D:53:ASP:OD1	2.27	0.50
1:H:371:ALA:HA	1:H:381:HIS:HE1	1.75	0.50
1:C:312:VAL:O	1:C:315:PHE:HB3	2.12	0.49
1:C:321:ILE:HD12	1:C:324:LEU:HD12	1.94	0.49
1:D:321:ILE:HD12	1:D:324:LEU:HD12	1.94	0.49
1:G:312:VAL:O	1:G:315:PHE:HB3	2.12	0.49
1:F:312:VAL:O	1:F:315:PHE:HB3	2.12	0.49
1:A:312:VAL:O	1:A:315:PHE:HB3	2.12	0.49
1:E:179:LEU:HG	1:E:192:VAL:HG11	1.93	0.49
1:E:430:MET:HB2	1:E:431:PRO:HD3	1.95	0.49
1:H:179:LEU:HG	1:H:192:VAL:HG11	1.93	0.49
1:H:312:VAL:O	1:H:315:PHE:HB3	2.12	0.49
1:E:321:ILE:HD12	1:E:324:LEU:HD12	1.94	0.49
1:F:430:MET:HB2	1:F:431:PRO:HD3	1.95	0.49
1:A:430:MET:HB2	1:A:431:PRO:HD3	1.95	0.49
1:C:371:ALA:HA	1:C:381:HIS:HE1	1.75	0.49
1:D:179:LEU:HG	1:D:192:VAL:HG11	1.93	0.49
1:D:312:VAL:O	1:D:315:PHE:HB3	2.12	0.49
1:F:321:ILE:HD12	1:F:324:LEU:HD12	1.94	0.49
1:A:321:ILE:HD12	1:A:324:LEU:HD12	1.94	0.49
1:B:321:ILE:HD12	1:B:324:LEU:HD12	1.94	0.49
1:B:430:MET:HB2	1:B:431:PRO:HD3	1.95	0.49
1:E:312:VAL:O	1:E:315:PHE:HB3	2.12	0.48
1:B:312:VAL:O	1:B:315:PHE:HB3	2.12	0.48
1:H:430:MET:HB2	1:H:431:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:PCF:H132	2:C:602:PCF:H111	1.70	0.48
1:G:430:MET:HB2	1:G:431:PRO:HD3	1.95	0.48
1:D:430:MET:HB2	1:D:431:PRO:HD3	1.95	0.48
2:C:601:PCF:H291	1:D:395:VAL:HG21	1.95	0.48
1:A:385:LYS:HB3	1:B:213:GLU:OE2	2.13	0.47
1:G:395:VAL:HG21	2:F:602:PCF:H291	1.96	0.47
1:H:48:TYR:OH	1:H:53:ASP:OD1	2.27	0.47
1:E:303:ALA:HA	1:E:306:VAL:HG22	1.97	0.47
1:A:303:ALA:HA	1:A:306:VAL:HG22	1.97	0.47
1:C:430:MET:HB2	1:C:431:PRO:HD3	1.95	0.47
1:G:347:LEU:HD13	1:H:330:GLY:HA3	1.95	0.47
2:G:601:PCF:H291	1:H:395:VAL:HG21	1.96	0.47
1:A:50:PRO:HB2	1:F:50:PRO:HB2	1.95	0.47
1:F:48:TYR:OH	1:F:53:ASP:OD1	2.27	0.47
1:C:436:VAL:HG11	1:B:433:PRO:HG2	1.97	0.47
1:D:303:ALA:HA	1:D:306:VAL:HG22	1.97	0.47
1:E:179:LEU:HB3	1:E:262:MET:HE1	1.97	0.47
1:F:303:ALA:HA	1:F:306:VAL:HG22	1.97	0.47
2:A:601:PCF:H291	1:B:395:VAL:HG21	1.96	0.46
1:H:303:ALA:HA	1:H:306:VAL:HG22	1.97	0.46
1:G:48:TYR:OH	1:G:53:ASP:OD1	2.27	0.46
1:G:387:ILE:O	1:G:390:GLY:N	2.48	0.46
1:H:179:LEU:HB3	1:H:262:MET:HE1	1.97	0.46
1:F:179:LEU:HB3	1:F:262:MET:HE1	1.97	0.46
1:B:303:ALA:HA	1:B:306:VAL:HG22	1.97	0.46
1:B:387:ILE:O	1:B:390:GLY:N	2.48	0.46
2:D:602:PCF:H152	2:D:602:PCF:H112	1.70	0.46
2:A:602:PCF:H132	2:A:602:PCF:H111	1.70	0.46
1:G:433:PRO:HG2	1:H:436:VAL:HG11	1.97	0.46
1:F:116:GLU:OE1	1:F:449:LYS:NZ	2.42	0.46
1:H:387:ILE:O	1:H:390:GLY:N	2.49	0.46
1:C:48:TYR:OH	1:C:53:ASP:OD1	2.27	0.46
1:C:303:ALA:HA	1:C:306:VAL:HG22	1.97	0.46
1:G:303:ALA:HA	1:G:306:VAL:HG22	1.97	0.46
1:A:387:ILE:O	1:A:390:GLY:N	2.49	0.46
1:G:179:LEU:HB3	1:G:262:MET:HE1	1.97	0.46
1:F:387:ILE:O	1:F:390:GLY:N	2.49	0.46
2:F:602:PCF:H152	2:F:602:PCF:H112	1.70	0.46
1:D:387:ILE:O	1:D:390:GLY:N	2.49	0.46
1:A:82:VAL:HB	1:A:86:LEU:HD23	1.98	0.45
1:A:179:LEU:HB3	1:A:262:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:SER:HG	1:G:317:ARG:HH11	1.63	0.45
1:C:387:ILE:O	1:C:390:GLY:N	2.49	0.45
1:D:179:LEU:HB3	1:D:262:MET:HE1	1.97	0.45
1:A:372:GLN:HG3	1:A:374:ASN:H	1.82	0.45
1:B:372:GLN:HG3	1:B:374:ASN:H	1.82	0.45
1:F:82:VAL:HB	1:F:86:LEU:HD23	1.98	0.45
1:C:179:LEU:HB3	1:C:262:MET:HE1	1.97	0.45
1:C:334:LEU:O	1:C:338:LEU:HG	2.17	0.45
2:G:602:PCF:H132	2:G:602:PCF:H111	1.70	0.45
1:B:82:VAL:HB	1:B:86:LEU:HD23	1.98	0.45
1:A:334:LEU:O	1:A:338:LEU:HG	2.17	0.45
1:E:387:ILE:O	1:E:390:GLY:N	2.48	0.45
1:D:426:LEU:O	1:D:430:MET:HG2	2.17	0.45
1:G:372:GLN:HG3	1:G:374:ASN:H	1.82	0.45
1:G:426:LEU:O	1:G:430:MET:HG2	2.17	0.45
1:C:372:GLN:HG3	1:C:374:ASN:H	1.82	0.45
1:B:426:LEU:O	1:B:430:MET:HG2	2.17	0.45
2:B:602:PCF:H272	2:B:602:PCF:H302	1.84	0.45
1:D:372:GLN:HG3	1:D:374:ASN:H	1.82	0.45
1:E:82:VAL:HB	1:E:86:LEU:HD23	1.98	0.45
2:H:602:PCF:H321	2:H:602:PCF:H352	1.88	0.45
1:F:372:GLN:HG3	1:F:374:ASN:H	1.82	0.45
1:H:334:LEU:O	1:H:338:LEU:HG	2.17	0.45
1:D:82:VAL:HB	1:D:86:LEU:HD23	1.98	0.45
1:E:334:LEU:O	1:E:338:LEU:HG	2.17	0.45
1:A:426:LEU:O	1:A:430:MET:HG2	2.17	0.44
1:B:179:LEU:HB3	1:B:262:MET:HE1	1.97	0.44
1:E:426:LEU:O	1:E:430:MET:HG2	2.17	0.44
1:F:334:LEU:O	1:F:338:LEU:HG	2.17	0.44
1:G:334:LEU:O	1:G:338:LEU:HG	2.17	0.44
1:H:426:LEU:O	1:H:430:MET:HG2	2.17	0.44
1:A:26:LEU:HB2	1:A:38:ALA:HB2	1.99	0.44
1:C:426:LEU:O	1:C:430:MET:HG2	2.17	0.44
1:D:26:LEU:HB2	1:D:38:ALA:HB2	1.99	0.44
1:C:82:VAL:HB	1:C:86:LEU:HD23	1.98	0.44
1:E:26:LEU:HB2	1:E:38:ALA:HB2	1.99	0.44
1:H:82:VAL:HB	1:H:86:LEU:HD23	1.98	0.44
1:E:372:GLN:HG3	1:E:374:ASN:H	1.82	0.44
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.80	0.44
1:D:334:LEU:O	1:D:338:LEU:HG	2.17	0.44
1:G:82:VAL:HB	1:G:86:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:LEU:HB2	1:H:38:ALA:HB2	2.00	0.44
1:B:334:LEU:O	1:B:338:LEU:HG	2.17	0.44
2:F:602:PCF:H272	2:F:602:PCF:H302	1.84	0.44
1:H:372:GLN:HG3	1:H:374:ASN:H	1.82	0.44
1:F:426:LEU:O	1:F:430:MET:HG2	2.17	0.43
1:F:26:LEU:HB2	1:F:38:ALA:HB2	1.99	0.43
1:A:436:VAL:HG11	1:D:433:PRO:HG2	1.99	0.43
2:C:601:PCF:H272	2:C:601:PCF:H302	1.84	0.43
1:D:98:GLU:OE1	1:D:110:ARG:NH2	2.52	0.43
1:F:463:PRO:HA	1:F:464:PRO:HD3	1.92	0.43
1:H:98:GLU:OE1	1:H:110:ARG:NH2	2.52	0.43
1:C:347:LEU:HD13	1:D:330:GLY:HA3	2.00	0.43
1:B:26:LEU:HB2	1:B:38:ALA:HB2	1.99	0.43
2:B:603:PCF:H132	2:B:603:PCF:H111	1.70	0.43
1:D:179:LEU:HD13	1:D:262:MET:SD	2.59	0.43
1:E:37:LEU:HD23	1:E:37:LEU:HA	1.80	0.43
2:E:602:PCF:H132	2:E:602:PCF:H111	1.70	0.43
1:F:98:GLU:OE1	1:F:110:ARG:NH2	2.52	0.43
1:C:26:LEU:HB2	1:C:38:ALA:HB2	1.99	0.43
1:D:79:PRO:HG2	1:D:82:VAL:HG22	2.01	0.43
2:H:602:PCF:H272	2:H:602:PCF:H302	1.84	0.43
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.80	0.43
1:C:79:PRO:HG2	1:C:82:VAL:HG22	2.01	0.43
2:F:603:PCF:H132	2:F:603:PCF:H111	1.70	0.43
1:C:179:LEU:HD13	1:C:262:MET:SD	2.59	0.42
1:C:389:ILE:HD11	2:B:602:PCF:H133	2.01	0.42
1:G:179:LEU:HD13	1:G:262:MET:SD	2.59	0.42
2:G:601:PCF:H152	2:G:601:PCF:H112	1.70	0.42
1:F:179:LEU:HD13	1:F:262:MET:SD	2.59	0.42
1:A:179:LEU:HD13	1:A:262:MET:SD	2.59	0.42
1:C:98:GLU:OE1	1:C:110:ARG:NH2	2.52	0.42
1:H:179:LEU:HD13	1:H:262:MET:SD	2.59	0.42
1:D:253:VAL:HG11	1:D:289:PHE:CD1	2.55	0.42
1:G:26:LEU:HB2	1:G:38:ALA:HB2	1.99	0.42
1:A:79:PRO:HG2	1:A:82:VAL:HG22	2.01	0.42
1:A:98:GLU:OE1	1:A:110:ARG:NH2	2.52	0.42
2:B:602:PCF:H152	2:B:602:PCF:H112	1.70	0.42
1:E:98:GLU:OE1	1:E:110:ARG:NH2	2.52	0.42
2:G:601:PCF:H321	2:G:601:PCF:H352	1.89	0.42
1:C:253:VAL:HG11	1:C:289:PHE:CD1	2.55	0.42
2:C:601:PCF:H133	1:D:389:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HD12	1:D:68:LEU:HA	1.88	0.42
1:E:179:LEU:HD13	1:E:262:MET:SD	2.59	0.42
1:G:253:VAL:HG11	1:G:289:PHE:CD1	2.55	0.42
1:B:98:GLU:OE1	1:B:110:ARG:NH2	2.52	0.42
1:B:313:VAL:O	1:B:316:VAL:HG22	2.20	0.42
1:F:253:VAL:HG11	1:F:289:PHE:CD1	2.55	0.42
1:F:313:VAL:O	1:F:316:VAL:HG22	2.20	0.42
1:H:253:VAL:HG11	1:H:289:PHE:CD1	2.55	0.42
1:C:330:GLY:HA3	1:B:347:LEU:HD13	2.01	0.42
1:B:79:PRO:HG2	1:B:82:VAL:HG22	2.01	0.42
1:D:50:PRO:HB2	1:G:50:PRO:HB2	2.01	0.42
1:G:72:ARG:NE	1:H:58:ASP:OD1	2.53	0.42
1:F:276:ASN:HB3	1:F:279:ASN:HD22	1.85	0.42
1:A:276:ASN:HB3	1:A:279:ASN:HD22	1.85	0.42
1:A:316:VAL:HB	1:A:319:LEU:HD12	2.02	0.42
1:C:313:VAL:O	1:C:316:VAL:HG22	2.20	0.42
1:B:253:VAL:HG11	1:B:289:PHE:CD1	2.55	0.42
1:D:107:MET:HA	1:D:107:MET:HE2	2.02	0.42
1:E:253:VAL:HG11	1:E:289:PHE:CD1	2.55	0.42
1:A:253:VAL:HG11	1:A:289:PHE:CD1	2.55	0.42
1:C:72:ARG:NE	1:D:58:ASP:OD1	2.53	0.42
1:E:313:VAL:O	1:E:316:VAL:HG22	2.20	0.42
1:G:79:PRO:HG2	1:G:82:VAL:HG22	2.01	0.42
1:G:98:GLU:OE1	1:G:110:ARG:NH2	2.52	0.42
1:G:313:VAL:O	1:G:316:VAL:HG22	2.20	0.42
1:H:79:PRO:HG2	1:H:82:VAL:HG22	2.01	0.42
1:H:313:VAL:O	1:H:316:VAL:HG22	2.20	0.42
1:B:179:LEU:HD13	1:B:262:MET:SD	2.59	0.41
1:H:371:ALA:HA	1:H:381:HIS:CE1	2.55	0.41
1:D:415:LEU:HD23	2:D:602:PCF:H271	2.02	0.41
1:H:37:LEU:HD23	1:H:37:LEU:HA	1.80	0.41
1:A:313:VAL:O	1:A:316:VAL:HG22	2.20	0.41
1:E:79:PRO:HG2	1:E:82:VAL:HG22	2.01	0.41
1:E:433:PRO:HG2	1:F:436:VAL:HG11	2.01	0.41
1:H:68:LEU:HD12	1:H:68:LEU:HA	1.88	0.41
1:D:313:VAL:O	1:D:316:VAL:HG22	2.20	0.41
2:E:601:PCF:H152	2:E:601:PCF:H112	1.70	0.41
1:H:310:LEU:HD23	1:H:310:LEU:HA	1.96	0.41
1:E:276:ASN:HB3	1:E:279:ASN:HD22	1.85	0.41
1:H:107:MET:HE2	1:H:107:MET:HA	2.02	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ASN:HB3	1:D:279:ASN:HD22	1.85	0.41
1:G:389:ILE:HD11	2:F:602:PCF:H133	2.03	0.41
1:F:107:MET:HA	1:F:107:MET:HE2	2.02	0.41
1:H:415:LEU:HD23	2:H:602:PCF:H271	2.02	0.41
1:E:316:VAL:HB	1:E:319:LEU:HD12	2.02	0.41
1:E:415:LEU:HD23	2:E:601:PCF:H271	2.02	0.41
1:G:385:LYS:HB3	1:H:213:GLU:OE2	2.20	0.41
1:F:316:VAL:HB	1:F:319:LEU:HD12	2.02	0.41
2:D:602:PCF:H272	2:D:602:PCF:H302	1.84	0.41
1:E:463:PRO:HA	1:E:464:PRO:HD3	1.92	0.41
1:G:316:VAL:HB	1:G:319:LEU:HD12	2.02	0.41
1:A:107:MET:HA	1:A:107:MET:HE2	2.02	0.41
1:C:276:ASN:HB3	1:C:279:ASN:HD22	1.85	0.41
1:C:316:VAL:HB	1:C:319:LEU:HD12	2.02	0.41
1:C:415:LEU:HD23	2:C:601:PCF:H271	2.02	0.41
1:B:107:MET:HE2	1:B:107:MET:HA	2.02	0.41
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.96	0.41
1:D:316:VAL:HB	1:D:319:LEU:HD12	2.02	0.41
1:F:371:ALA:HA	1:F:381:HIS:CE1	2.55	0.41
1:H:276:ASN:HB3	1:H:279:ASN:HD22	1.85	0.41
1:A:415:LEU:HD23	2:A:601:PCF:H271	2.02	0.41
1:C:433:PRO:HG2	1:D:436:VAL:CG1	2.50	0.41
2:C:601:PCF:H152	2:C:601:PCF:H112	1.70	0.41
2:E:601:PCF:H321	2:E:601:PCF:H352	1.89	0.41
1:F:79:PRO:HG2	1:F:82:VAL:HG22	2.01	0.41
1:B:316:VAL:HB	1:B:319:LEU:HD12	2.02	0.40
2:D:602:PCF:H321	2:D:602:PCF:H352	1.89	0.40
2:A:601:PCF:H272	2:A:601:PCF:H302	1.84	0.40
1:C:107:MET:HE2	1:C:107:MET:HA	2.02	0.40
1:B:415:LEU:HD23	2:B:602:PCF:H271	2.02	0.40
1:E:107:MET:HE2	1:E:107:MET:HA	2.02	0.40
1:G:37:LEU:HA	1:G:37:LEU:HD23	1.80	0.40
1:G:276:ASN:HB3	1:G:279:ASN:HD22	1.85	0.40
1:G:330:GLY:HA3	1:F:347:LEU:HD13	2.03	0.40
1:D:257:THR:HB	1:D:286:ILE:HD11	2.04	0.40
1:E:371:ALA:HA	1:E:381:HIS:CE1	2.55	0.40
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.95	0.40
1:C:257:THR:HB	1:C:286:ILE:HD11	2.04	0.40
1:G:107:MET:HA	1:G:107:MET:HE2	2.02	0.40
1:G:415:LEU:HD23	2:G:601:PCF:H271	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/518 (74%)	375 (98%)	9 (2%)	0	100	100
1	B	384/518 (74%)	375 (98%)	9 (2%)	0	100	100
1	C	384/518 (74%)	375 (98%)	9 (2%)	0	100	100
1	D	384/518 (74%)	375 (98%)	9 (2%)	0	100	100
1	E	385/518 (74%)	376 (98%)	9 (2%)	0	100	100
1	F	385/518 (74%)	376 (98%)	9 (2%)	0	100	100
1	G	385/518 (74%)	376 (98%)	9 (2%)	0	100	100
1	H	385/518 (74%)	376 (98%)	9 (2%)	0	100	100
All	All	3076/4144 (74%)	3004 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	316/442 (72%)	308 (98%)	8 (2%)	42	69
1	B	316/442 (72%)	308 (98%)	8 (2%)	42	69
1	C	316/442 (72%)	308 (98%)	8 (2%)	42	69
1	D	316/442 (72%)	308 (98%)	8 (2%)	42	69
1	E	316/442 (72%)	308 (98%)	8 (2%)	42	69
1	F	316/442 (72%)	308 (98%)	8 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	316/442 (72%)	308 (98%)	8 (2%)	42	69
1	H	316/442 (72%)	308 (98%)	8 (2%)	42	69
All	All	2528/3536 (72%)	2464 (98%)	64 (2%)	42	69

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	116	GLU
1	A	238	GLU
1	A	282	ASP
1	A	295	LEU
1	A	316	VAL
1	A	329	VAL
1	A	375	ASP
1	C	89	GLU
1	C	116	GLU
1	C	238	GLU
1	C	282	ASP
1	C	295	LEU
1	C	316	VAL
1	C	329	VAL
1	C	375	ASP
1	B	89	GLU
1	B	116	GLU
1	B	238	GLU
1	B	282	ASP
1	B	295	LEU
1	B	316	VAL
1	B	329	VAL
1	B	375	ASP
1	D	89	GLU
1	D	116	GLU
1	D	238	GLU
1	D	282	ASP
1	D	295	LEU
1	D	316	VAL
1	D	329	VAL
1	D	375	ASP
1	E	89	GLU
1	E	116	GLU

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Mol	Chain	Res	Type
1	E	238	GLU
1	E	282	ASP
1	E	295	LEU
1	E	316	VAL
1	E	329	VAL
1	E	375	ASP
1	G	89	GLU
1	G	116	GLU
1	G	238	GLU
1	G	282	ASP
1	G	295	LEU
1	G	316	VAL
1	G	329	VAL
1	G	375	ASP
1	F	89	GLU
1	F	116	GLU
1	F	238	GLU
1	F	282	ASP
1	F	295	LEU
1	F	316	VAL
1	F	329	VAL
1	F	375	ASP
1	H	89	GLU
1	H	116	GLU
1	H	238	GLU
1	H	282	ASP
1	H	295	LEU
1	H	316	VAL
1	H	329	VAL
1	H	375	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	C	19	HIS
1	B	19	HIS
1	B	381	HIS
1	D	19	HIS
1	E	19	HIS
1	E	381	HIS
1	G	19	HIS

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Mol	Chain	Res	Type
1	G	381	HIS
1	F	19	HIS
1	F	381	HIS
1	H	19	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 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\# Z > 2$
2	PCF	F	602	-	44,44,49	1.16	4 (9%)	50,52,57	1.05	2 (4%)
2	PCF	E	602	-	31,31,49	1.35	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	D	603	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	E	601	-	44,44,49	1.16	4 (9%)	50,52,57	1.05	2 (4%)
2	PCF	B	603	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	G	601	-	44,44,49	1.16	4 (9%)	50,52,57	1.04	2 (4%)
2	PCF	H	602	-	44,44,49	1.16	4 (9%)	50,52,57	1.04	2 (4%)
2	PCF	A	601	-	44,44,49	1.17	4 (9%)	50,52,57	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PCF	D	602	-	44,44,49	1.16	4 (9%)	50,52,57	1.05	2 (4%)
2	PCF	A	602	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	C	601	-	44,44,49	1.16	4 (9%)	50,52,57	1.05	2 (4%)
2	PCF	H	603	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	G	602	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	B	602	-	44,44,49	1.16	4 (9%)	50,52,57	1.04	2 (4%)
2	PCF	C	602	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)
2	PCF	F	603	-	31,31,49	1.34	3 (9%)	37,39,57	1.03	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCF	F	602	-	-	26/48/48/53	-
2	PCF	E	602	-	-	16/35/35/53	-
2	PCF	D	603	-	-	16/35/35/53	-
2	PCF	E	601	-	-	26/48/48/53	-
2	PCF	B	603	-	-	16/35/35/53	-
2	PCF	G	601	-	-	26/48/48/53	-
2	PCF	H	602	-	-	26/48/48/53	-
2	PCF	A	601	-	-	26/48/48/53	-
2	PCF	D	602	-	-	26/48/48/53	-
2	PCF	A	602	-	-	16/35/35/53	-
2	PCF	C	601	-	-	26/48/48/53	-
2	PCF	H	603	-	-	16/35/35/53	-
2	PCF	G	602	-	-	16/35/35/53	-
2	PCF	B	602	-	-	26/48/48/53	-
2	PCF	C	602	-	-	16/35/35/53	-
2	PCF	F	603	-	-	16/35/35/53	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	603	PCF	O21-C21	3.43	1.44	1.34
2	D	603	PCF	O21-C21	3.43	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	PCF	O21-C21	3.43	1.44	1.34
2	E	602	PCF	O21-C21	3.41	1.43	1.34
2	G	602	PCF	O21-C21	3.41	1.43	1.34
2	A	602	PCF	O21-C21	3.40	1.43	1.34
2	C	602	PCF	O21-C21	3.40	1.43	1.34
2	H	603	PCF	O21-C21	3.38	1.43	1.34
2	H	602	PCF	O21-C21	3.14	1.43	1.34
2	D	602	PCF	O21-C21	3.14	1.43	1.34
2	G	601	PCF	O21-C21	3.12	1.43	1.34
2	F	602	PCF	O21-C21	3.12	1.43	1.34
2	A	601	PCF	O21-C21	3.11	1.43	1.34
2	E	601	PCF	O21-C21	3.11	1.43	1.34
2	B	602	PCF	O21-C21	3.11	1.43	1.34
2	C	601	PCF	O21-C21	3.11	1.43	1.34
2	E	601	PCF	O31-C31	3.09	1.42	1.33
2	A	601	PCF	O31-C31	3.07	1.42	1.33
2	B	602	PCF	O31-C31	3.07	1.42	1.33
2	C	601	PCF	O31-C31	3.06	1.42	1.33
2	F	602	PCF	O31-C31	3.06	1.42	1.33
2	G	601	PCF	O31-C31	3.06	1.42	1.33
2	D	602	PCF	O31-C31	3.03	1.42	1.33
2	H	602	PCF	O31-C31	3.03	1.42	1.33
2	C	602	PCF	O31-C31	2.99	1.42	1.33
2	D	603	PCF	O31-C31	2.99	1.42	1.33
2	G	602	PCF	O31-C31	2.97	1.42	1.33
2	E	602	PCF	O31-C31	2.97	1.42	1.33
2	F	603	PCF	O31-C31	2.97	1.42	1.33
2	A	602	PCF	O31-C31	2.97	1.42	1.33
2	B	603	PCF	O31-C31	2.97	1.42	1.33
2	H	603	PCF	O31-C31	2.96	1.42	1.33
2	H	602	PCF	O21-C2	-2.17	1.41	1.46
2	D	602	PCF	O21-C2	-2.16	1.41	1.46
2	A	601	PCF	O21-C2	-2.16	1.41	1.46
2	F	602	PCF	O21-C2	-2.16	1.41	1.46
2	G	601	PCF	O21-C2	-2.14	1.41	1.46
2	C	601	PCF	O21-C2	-2.12	1.41	1.46
2	B	602	PCF	O21-C2	-2.12	1.41	1.46
2	E	601	PCF	O21-C2	-2.11	1.41	1.46
2	E	602	PCF	C22-C21	2.08	1.56	1.50
2	A	601	PCF	C22-C21	2.08	1.56	1.50
2	B	602	PCF	C22-C21	2.07	1.56	1.50
2	G	602	PCF	C22-C21	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	PCF	C22-C21	2.06	1.56	1.50
2	C	601	PCF	C22-C21	2.06	1.56	1.50
2	E	601	PCF	C22-C21	2.05	1.56	1.50
2	F	602	PCF	C22-C21	2.05	1.56	1.50
2	H	602	PCF	C22-C21	2.05	1.56	1.50
2	H	603	PCF	C22-C21	2.05	1.56	1.50
2	D	603	PCF	C22-C21	2.05	1.56	1.50
2	D	602	PCF	C22-C21	2.05	1.56	1.50
2	C	602	PCF	C22-C21	2.05	1.56	1.50
2	G	601	PCF	C22-C21	2.04	1.56	1.50
2	F	603	PCF	C22-C21	2.02	1.56	1.50
2	B	603	PCF	C22-C21	2.01	1.56	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	PCF	O21-C21-C22	3.79	119.69	111.48
2	C	601	PCF	O21-C21-C22	3.78	119.67	111.48
2	F	602	PCF	O21-C21-C22	3.78	119.66	111.48
2	D	602	PCF	O21-C21-C22	3.78	119.66	111.48
2	A	601	PCF	O21-C21-C22	3.78	119.66	111.48
2	B	602	PCF	O21-C21-C22	3.78	119.66	111.48
2	G	601	PCF	O21-C21-C22	3.77	119.64	111.48
2	H	602	PCF	O21-C21-C22	3.77	119.63	111.48
2	B	603	PCF	O21-C21-C22	3.13	118.25	111.48
2	C	602	PCF	O21-C21-C22	3.13	118.25	111.48
2	F	603	PCF	O21-C21-C22	3.13	118.25	111.48
2	A	602	PCF	O21-C21-C22	3.12	118.24	111.48
2	H	603	PCF	O21-C21-C22	3.12	118.22	111.48
2	D	603	PCF	O21-C21-C22	3.11	118.22	111.48
2	G	602	PCF	O21-C21-C22	3.11	118.21	111.48
2	E	602	PCF	O21-C21-C22	3.10	118.19	111.48
2	C	601	PCF	O31-C31-C32	2.79	120.36	111.83
2	D	602	PCF	O31-C31-C32	2.79	120.35	111.83
2	F	602	PCF	O31-C31-C32	2.79	120.34	111.83
2	E	601	PCF	O31-C31-C32	2.78	120.32	111.83
2	G	601	PCF	O31-C31-C32	2.78	120.31	111.83
2	B	602	PCF	O31-C31-C32	2.78	120.30	111.83
2	H	602	PCF	O31-C31-C32	2.77	120.29	111.83
2	A	601	PCF	O31-C31-C32	2.77	120.29	111.83
2	G	602	PCF	O31-C31-C32	2.73	120.17	111.83
2	F	603	PCF	O31-C31-C32	2.73	120.15	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	PCF	O31-C31-C32	2.72	120.14	111.83
2	C	602	PCF	O31-C31-C32	2.72	120.14	111.83
2	E	602	PCF	O31-C31-C32	2.72	120.13	111.83
2	B	603	PCF	O31-C31-C32	2.72	120.12	111.83
2	H	603	PCF	O31-C31-C32	2.72	120.12	111.83
2	D	603	PCF	O31-C31-C32	2.71	120.09	111.83

There are no chirality outliers.

All (336) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PCF	C1-O11-P-O12
2	A	601	PCF	C1-O11-P-O13
2	A	601	PCF	O13-C11-C12-N
2	A	601	PCF	O11-C1-C2-O21
2	A	602	PCF	C1-O11-P-O12
2	A	602	PCF	C1-O11-P-O13
2	A	602	PCF	C1-O11-P-O14
2	A	602	PCF	C11-O13-P-O11
2	A	602	PCF	C11-O13-P-O12
2	A	602	PCF	O13-C11-C12-N
2	C	601	PCF	C1-O11-P-O12
2	C	601	PCF	C1-O11-P-O13
2	C	601	PCF	O13-C11-C12-N
2	C	601	PCF	O11-C1-C2-O21
2	C	602	PCF	C1-O11-P-O12
2	C	602	PCF	C1-O11-P-O13
2	C	602	PCF	C1-O11-P-O14
2	C	602	PCF	C11-O13-P-O11
2	C	602	PCF	C11-O13-P-O12
2	C	602	PCF	O13-C11-C12-N
2	B	602	PCF	C1-O11-P-O12
2	B	602	PCF	C1-O11-P-O13
2	B	602	PCF	O13-C11-C12-N
2	B	602	PCF	O11-C1-C2-O21
2	B	603	PCF	C1-O11-P-O12
2	B	603	PCF	C1-O11-P-O13
2	B	603	PCF	C1-O11-P-O14
2	B	603	PCF	C11-O13-P-O11
2	B	603	PCF	C11-O13-P-O12
2	B	603	PCF	O13-C11-C12-N
2	D	602	PCF	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
2	D	602	PCF	C1-O11-P-O13
2	D	602	PCF	O13-C11-C12-N
2	D	602	PCF	O11-C1-C2-O21
2	D	603	PCF	C1-O11-P-O12
2	D	603	PCF	C1-O11-P-O13
2	D	603	PCF	C1-O11-P-O14
2	D	603	PCF	C11-O13-P-O11
2	D	603	PCF	C11-O13-P-O12
2	D	603	PCF	O13-C11-C12-N
2	E	601	PCF	C1-O11-P-O12
2	E	601	PCF	C1-O11-P-O13
2	E	601	PCF	O13-C11-C12-N
2	E	601	PCF	O11-C1-C2-O21
2	E	602	PCF	C1-O11-P-O12
2	E	602	PCF	C1-O11-P-O13
2	E	602	PCF	C1-O11-P-O14
2	E	602	PCF	C11-O13-P-O11
2	E	602	PCF	C11-O13-P-O12
2	E	602	PCF	O13-C11-C12-N
2	G	601	PCF	C1-O11-P-O12
2	G	601	PCF	C1-O11-P-O13
2	G	601	PCF	O13-C11-C12-N
2	G	601	PCF	O11-C1-C2-O21
2	G	602	PCF	C1-O11-P-O12
2	G	602	PCF	C1-O11-P-O13
2	G	602	PCF	C1-O11-P-O14
2	G	602	PCF	C11-O13-P-O11
2	G	602	PCF	C11-O13-P-O12
2	G	602	PCF	O13-C11-C12-N
2	F	602	PCF	C1-O11-P-O12
2	F	602	PCF	C1-O11-P-O13
2	F	602	PCF	O13-C11-C12-N
2	F	602	PCF	O11-C1-C2-O21
2	F	603	PCF	C1-O11-P-O12
2	F	603	PCF	C1-O11-P-O13
2	F	603	PCF	C1-O11-P-O14
2	F	603	PCF	C11-O13-P-O11
2	F	603	PCF	C11-O13-P-O12
2	F	603	PCF	O13-C11-C12-N
2	H	602	PCF	C1-O11-P-O12
2	H	602	PCF	C1-O11-P-O13
2	H	602	PCF	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
2	H	602	PCF	O11-C1-C2-O21
2	H	603	PCF	C1-O11-P-O12
2	H	603	PCF	C1-O11-P-O13
2	H	603	PCF	C1-O11-P-O14
2	H	603	PCF	C11-O13-P-O11
2	H	603	PCF	C11-O13-P-O12
2	H	603	PCF	O13-C11-C12-N
2	A	601	PCF	O32-C31-O31-C3
2	C	601	PCF	O32-C31-O31-C3
2	B	602	PCF	O32-C31-O31-C3
2	D	602	PCF	O32-C31-O31-C3
2	E	601	PCF	O32-C31-O31-C3
2	G	601	PCF	O32-C31-O31-C3
2	F	602	PCF	O32-C31-O31-C3
2	H	602	PCF	O32-C31-O31-C3
2	A	601	PCF	C32-C31-O31-C3
2	C	601	PCF	C32-C31-O31-C3
2	B	602	PCF	C32-C31-O31-C3
2	D	602	PCF	C32-C31-O31-C3
2	E	601	PCF	C32-C31-O31-C3
2	G	601	PCF	C32-C31-O31-C3
2	F	602	PCF	C32-C31-O31-C3
2	H	602	PCF	C32-C31-O31-C3
2	A	601	PCF	C11-C12-N-C15
2	C	601	PCF	C11-C12-N-C15
2	B	602	PCF	C11-C12-N-C15
2	D	602	PCF	C11-C12-N-C15
2	E	601	PCF	C11-C12-N-C15
2	G	601	PCF	C11-C12-N-C15
2	F	602	PCF	C11-C12-N-C15
2	H	602	PCF	C11-C12-N-C15
2	A	601	PCF	C11-C12-N-C13
2	C	601	PCF	C11-C12-N-C13
2	B	602	PCF	C11-C12-N-C13
2	D	602	PCF	C11-C12-N-C13
2	E	601	PCF	C11-C12-N-C13
2	G	601	PCF	C11-C12-N-C13
2	F	602	PCF	C11-C12-N-C13
2	H	602	PCF	C11-C12-N-C13
2	A	602	PCF	C21-C22-C23-C24
2	C	602	PCF	C21-C22-C23-C24
2	B	603	PCF	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	D	603	PCF	C21-C22-C23-C24
2	E	602	PCF	C21-C22-C23-C24
2	G	602	PCF	C21-C22-C23-C24
2	F	603	PCF	C21-C22-C23-C24
2	H	603	PCF	C21-C22-C23-C24
2	A	601	PCF	C27-C28-C29-C30
2	C	601	PCF	C27-C28-C29-C30
2	B	602	PCF	C27-C28-C29-C30
2	D	602	PCF	C27-C28-C29-C30
2	E	601	PCF	C27-C28-C29-C30
2	G	601	PCF	C27-C28-C29-C30
2	F	602	PCF	C27-C28-C29-C30
2	H	602	PCF	C27-C28-C29-C30
2	A	602	PCF	C11-C12-N-C13
2	A	602	PCF	C11-C12-N-C14
2	A	602	PCF	C11-C12-N-C15
2	C	602	PCF	C11-C12-N-C13
2	C	602	PCF	C11-C12-N-C14
2	C	602	PCF	C11-C12-N-C15
2	B	603	PCF	C11-C12-N-C13
2	B	603	PCF	C11-C12-N-C14
2	B	603	PCF	C11-C12-N-C15
2	D	603	PCF	C11-C12-N-C13
2	D	603	PCF	C11-C12-N-C14
2	D	603	PCF	C11-C12-N-C15
2	E	602	PCF	C11-C12-N-C13
2	E	602	PCF	C11-C12-N-C14
2	E	602	PCF	C11-C12-N-C15
2	G	602	PCF	C11-C12-N-C13
2	G	602	PCF	C11-C12-N-C14
2	G	602	PCF	C11-C12-N-C15
2	F	603	PCF	C11-C12-N-C13
2	F	603	PCF	C11-C12-N-C14
2	F	603	PCF	C11-C12-N-C15
2	H	603	PCF	C11-C12-N-C13
2	H	603	PCF	C11-C12-N-C14
2	H	603	PCF	C11-C12-N-C15
2	A	601	PCF	C11-C12-N-C14
2	C	601	PCF	C11-C12-N-C14
2	B	602	PCF	C11-C12-N-C14
2	D	602	PCF	C11-C12-N-C14
2	E	601	PCF	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
2	G	601	PCF	C11-C12-N-C14
2	F	602	PCF	C11-C12-N-C14
2	H	602	PCF	C11-C12-N-C14
2	D	602	PCF	C23-C24-C25-C26
2	E	601	PCF	C23-C24-C25-C26
2	G	601	PCF	C23-C24-C25-C26
2	H	602	PCF	C23-C24-C25-C26
2	A	601	PCF	C23-C24-C25-C26
2	C	601	PCF	C23-C24-C25-C26
2	B	602	PCF	C23-C24-C25-C26
2	F	602	PCF	C23-C24-C25-C26
2	A	601	PCF	C22-C23-C24-C25
2	C	601	PCF	C22-C23-C24-C25
2	B	602	PCF	C22-C23-C24-C25
2	D	602	PCF	C22-C23-C24-C25
2	E	601	PCF	C22-C23-C24-C25
2	G	601	PCF	C22-C23-C24-C25
2	F	602	PCF	C22-C23-C24-C25
2	H	602	PCF	C22-C23-C24-C25
2	C	601	PCF	C24-C25-C26-C27
2	D	602	PCF	C24-C25-C26-C27
2	F	602	PCF	C24-C25-C26-C27
2	A	601	PCF	C24-C25-C26-C27
2	B	602	PCF	C24-C25-C26-C27
2	E	601	PCF	C24-C25-C26-C27
2	G	601	PCF	C24-C25-C26-C27
2	H	602	PCF	C24-C25-C26-C27
2	A	601	PCF	C28-C29-C30-C47
2	B	602	PCF	C28-C29-C30-C47
2	G	601	PCF	C28-C29-C30-C47
2	C	601	PCF	C28-C29-C30-C47
2	D	602	PCF	C28-C29-C30-C47
2	E	601	PCF	C28-C29-C30-C47
2	F	602	PCF	C28-C29-C30-C47
2	H	602	PCF	C28-C29-C30-C47
2	G	601	PCF	C34-C35-C36-C37
2	C	601	PCF	C34-C35-C36-C37
2	B	602	PCF	C34-C35-C36-C37
2	A	601	PCF	C34-C35-C36-C37
2	A	602	PCF	C32-C33-C34-C35
2	C	602	PCF	C32-C33-C34-C35
2	B	603	PCF	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	D	602	PCF	C34-C35-C36-C37
2	D	603	PCF	C32-C33-C34-C35
2	E	601	PCF	C34-C35-C36-C37
2	E	602	PCF	C32-C33-C34-C35
2	G	602	PCF	C32-C33-C34-C35
2	F	602	PCF	C34-C35-C36-C37
2	H	602	PCF	C34-C35-C36-C37
2	H	603	PCF	C32-C33-C34-C35
2	A	601	PCF	O11-C1-C2-C3
2	C	601	PCF	O11-C1-C2-C3
2	B	602	PCF	O11-C1-C2-C3
2	D	602	PCF	O11-C1-C2-C3
2	E	601	PCF	O11-C1-C2-C3
2	G	601	PCF	O11-C1-C2-C3
2	F	602	PCF	O11-C1-C2-C3
2	H	602	PCF	O11-C1-C2-C3
2	F	603	PCF	C32-C33-C34-C35
2	G	601	PCF	C32-C33-C34-C35
2	A	601	PCF	C32-C33-C34-C35
2	C	601	PCF	C32-C33-C34-C35
2	B	602	PCF	C32-C33-C34-C35
2	D	602	PCF	C32-C33-C34-C35
2	E	601	PCF	C32-C33-C34-C35
2	F	602	PCF	C32-C33-C34-C35
2	H	602	PCF	C32-C33-C34-C35
2	A	601	PCF	C1-O11-P-O14
2	A	601	PCF	C11-O13-P-O11
2	A	601	PCF	C11-O13-P-O12
2	A	601	PCF	C11-O13-P-O14
2	A	602	PCF	C11-O13-P-O14
2	C	601	PCF	C1-O11-P-O14
2	C	601	PCF	C11-O13-P-O11
2	C	601	PCF	C11-O13-P-O12
2	C	601	PCF	C11-O13-P-O14
2	C	602	PCF	C11-O13-P-O14
2	B	602	PCF	C1-O11-P-O14
2	B	602	PCF	C11-O13-P-O11
2	B	602	PCF	C11-O13-P-O12
2	B	602	PCF	C11-O13-P-O14
2	B	603	PCF	C11-O13-P-O14
2	D	602	PCF	C1-O11-P-O14
2	D	602	PCF	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
2	D	602	PCF	C11-O13-P-O12
2	D	602	PCF	C11-O13-P-O14
2	D	603	PCF	C11-O13-P-O14
2	E	601	PCF	C1-O11-P-O14
2	E	601	PCF	C11-O13-P-O11
2	E	601	PCF	C11-O13-P-O12
2	E	601	PCF	C11-O13-P-O14
2	E	602	PCF	C11-O13-P-O14
2	G	601	PCF	C1-O11-P-O14
2	G	601	PCF	C11-O13-P-O11
2	G	601	PCF	C11-O13-P-O12
2	G	601	PCF	C11-O13-P-O14
2	G	602	PCF	C11-O13-P-O14
2	F	602	PCF	C1-O11-P-O14
2	F	602	PCF	C11-O13-P-O11
2	F	602	PCF	C11-O13-P-O12
2	F	602	PCF	C11-O13-P-O14
2	F	603	PCF	C11-O13-P-O14
2	H	602	PCF	C1-O11-P-O14
2	H	602	PCF	C11-O13-P-O11
2	H	602	PCF	C11-O13-P-O12
2	H	602	PCF	C11-O13-P-O14
2	H	603	PCF	C11-O13-P-O14
2	A	601	PCF	C21-C22-C23-C24
2	D	602	PCF	C21-C22-C23-C24
2	E	601	PCF	C21-C22-C23-C24
2	G	601	PCF	C21-C22-C23-C24
2	F	602	PCF	C21-C22-C23-C24
2	H	602	PCF	C21-C22-C23-C24
2	B	602	PCF	C21-C22-C23-C24
2	C	601	PCF	C21-C22-C23-C24
2	B	602	PCF	C22-C21-O21-C2
2	A	601	PCF	C22-C21-O21-C2
2	C	601	PCF	C22-C21-O21-C2
2	E	601	PCF	C22-C21-O21-C2
2	G	601	PCF	C22-C21-O21-C2
2	F	602	PCF	C22-C21-O21-C2
2	F	602	PCF	C37-C38-C39-C40
2	C	601	PCF	C37-C38-C39-C40
2	B	602	PCF	C37-C38-C39-C40
2	E	601	PCF	C37-C38-C39-C40
2	H	602	PCF	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
2	A	601	PCF	C37-C38-C39-C40
2	D	602	PCF	C37-C38-C39-C40
2	G	601	PCF	C37-C38-C39-C40
2	D	602	PCF	C22-C21-O21-C2
2	H	602	PCF	C22-C21-O21-C2
2	A	601	PCF	C33-C34-C35-C36
2	C	601	PCF	C33-C34-C35-C36
2	E	601	PCF	C33-C34-C35-C36
2	F	602	PCF	C33-C34-C35-C36
2	B	602	PCF	C33-C34-C35-C36
2	D	602	PCF	C33-C34-C35-C36
2	G	601	PCF	C33-C34-C35-C36
2	H	602	PCF	C33-C34-C35-C36
2	A	602	PCF	C3-C2-O21-C21
2	C	602	PCF	C3-C2-O21-C21
2	B	603	PCF	C3-C2-O21-C21
2	D	603	PCF	C3-C2-O21-C21
2	E	602	PCF	C3-C2-O21-C21
2	G	602	PCF	C3-C2-O21-C21
2	F	603	PCF	C3-C2-O21-C21
2	H	603	PCF	C3-C2-O21-C21
2	E	602	PCF	C22-C23-C24-C25
2	A	602	PCF	C22-C23-C24-C25
2	B	603	PCF	C22-C23-C24-C25
2	F	603	PCF	C22-C23-C24-C25
2	H	603	PCF	C22-C23-C24-C25
2	C	602	PCF	C22-C23-C24-C25
2	D	603	PCF	C22-C23-C24-C25
2	G	602	PCF	C22-C23-C24-C25
2	C	601	PCF	O22-C21-O21-C2
2	B	602	PCF	O22-C21-O21-C2
2	D	602	PCF	O22-C21-O21-C2
2	E	601	PCF	O22-C21-O21-C2
2	G	601	PCF	O22-C21-O21-C2
2	H	602	PCF	O22-C21-O21-C2
2	F	602	PCF	O22-C21-O21-C2
2	A	601	PCF	O22-C21-O21-C2
2	A	602	PCF	O31-C31-C32-C33
2	C	602	PCF	O31-C31-C32-C33
2	B	603	PCF	O31-C31-C32-C33
2	D	603	PCF	O31-C31-C32-C33
2	E	602	PCF	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	G	602	PCF	O31-C31-C32-C33
2	F	603	PCF	O31-C31-C32-C33
2	H	603	PCF	O31-C31-C32-C33
2	A	602	PCF	O32-C31-C32-C33
2	C	602	PCF	O32-C31-C32-C33
2	D	603	PCF	O32-C31-C32-C33
2	E	602	PCF	O32-C31-C32-C33
2	G	602	PCF	O32-C31-C32-C33
2	F	603	PCF	O32-C31-C32-C33
2	H	603	PCF	O32-C31-C32-C33
2	B	603	PCF	O32-C31-C32-C33

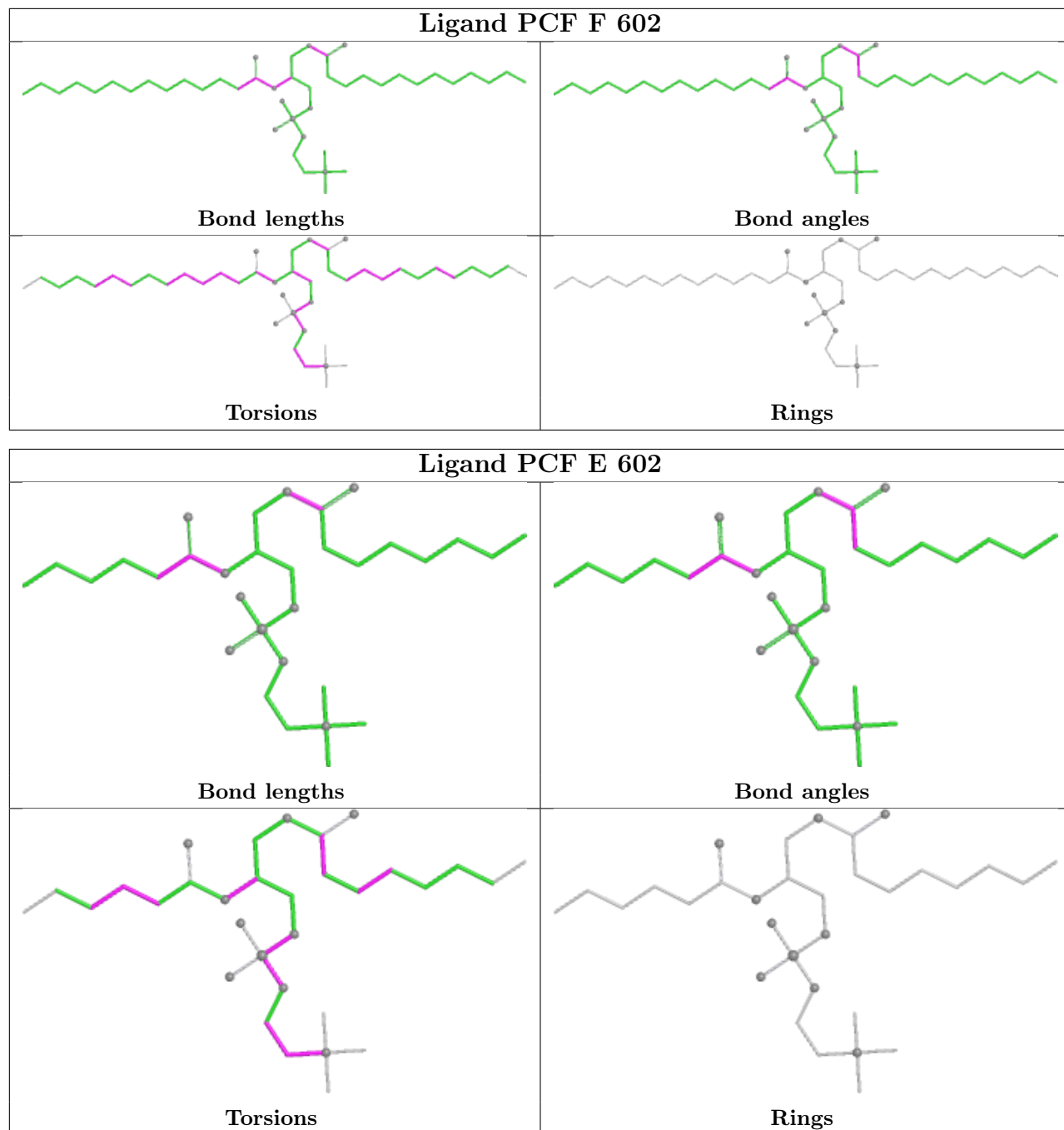
There are no ring outliers.

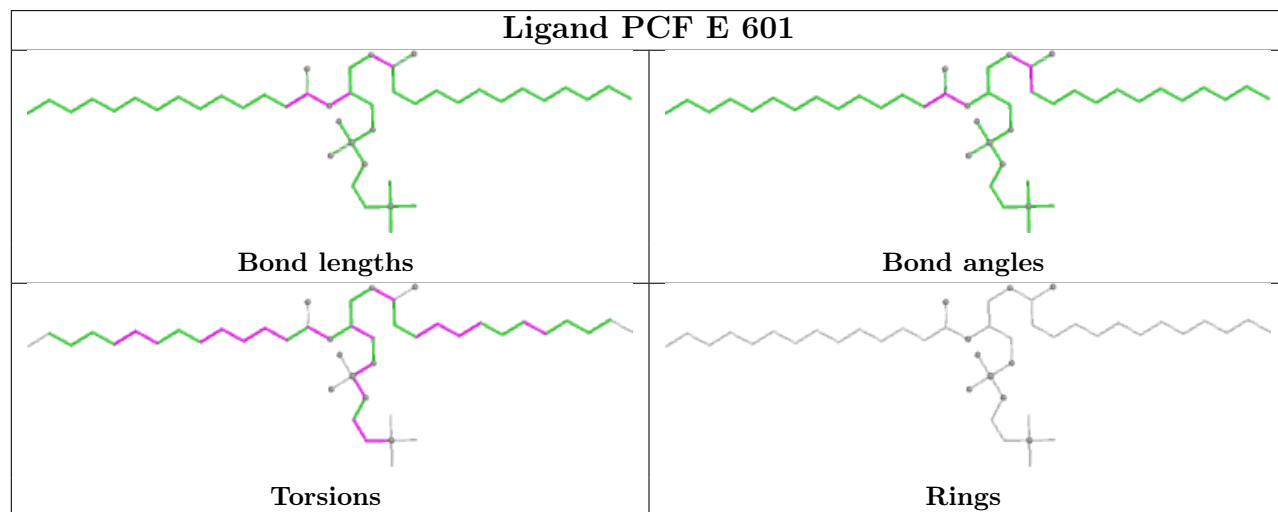
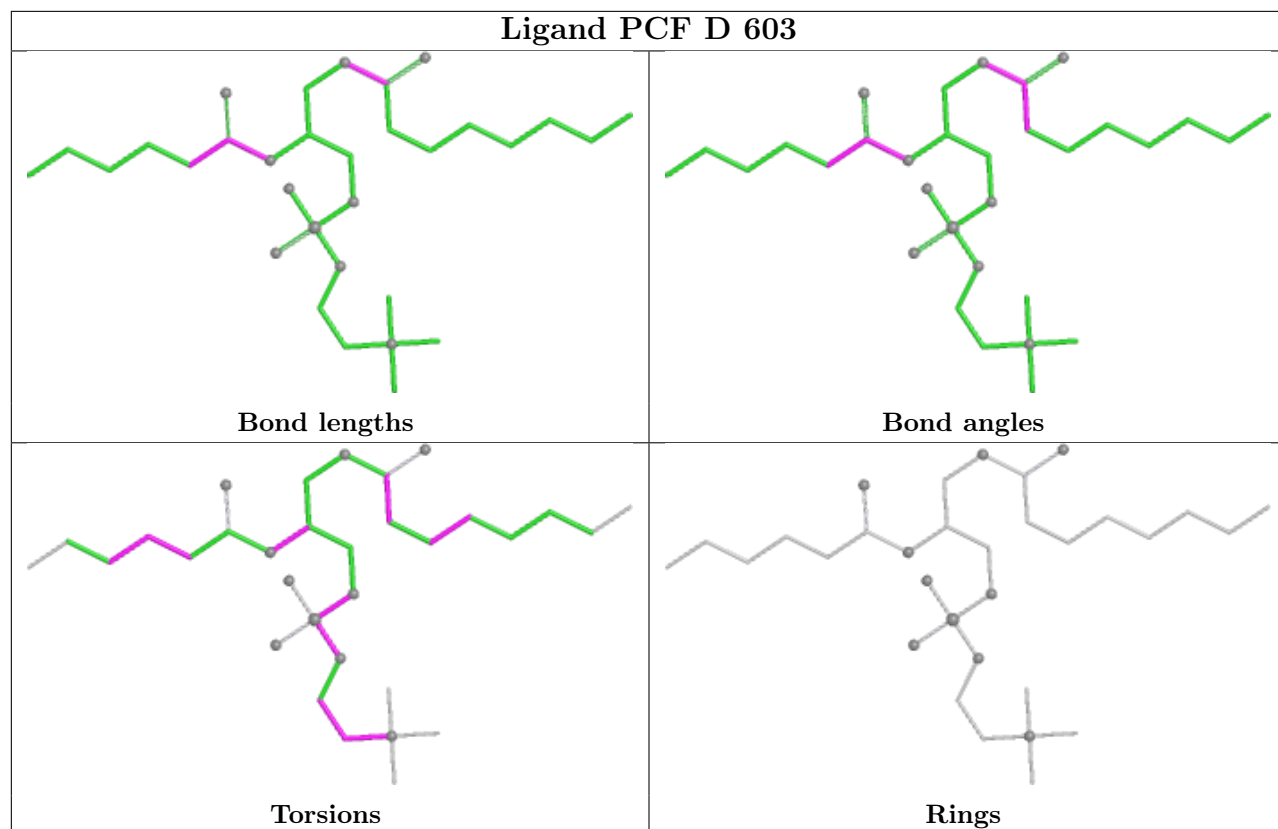
14 monomers are involved in 39 short contacts:

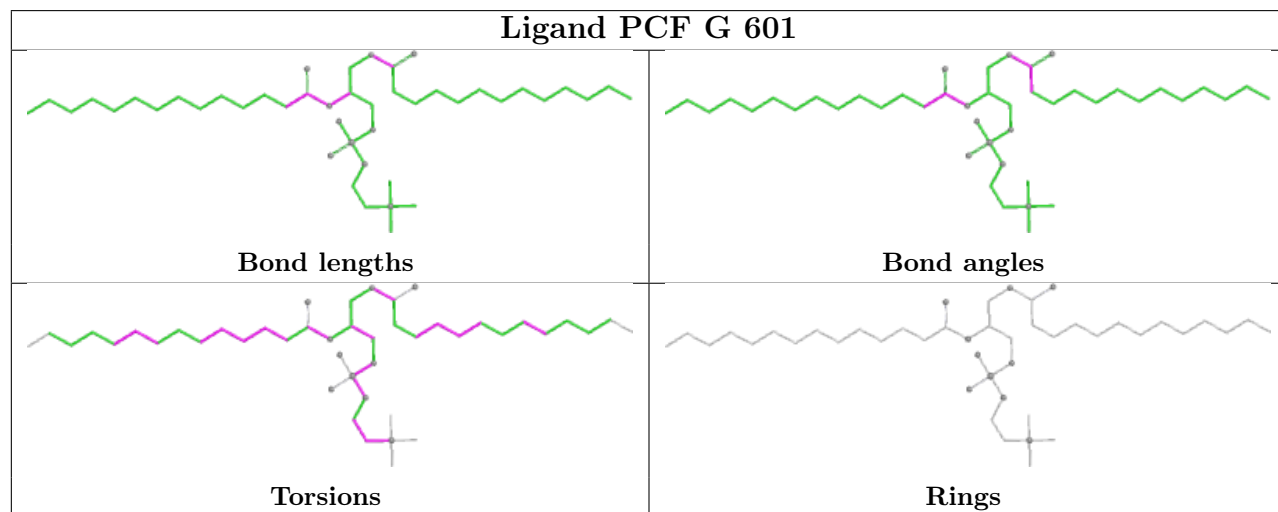
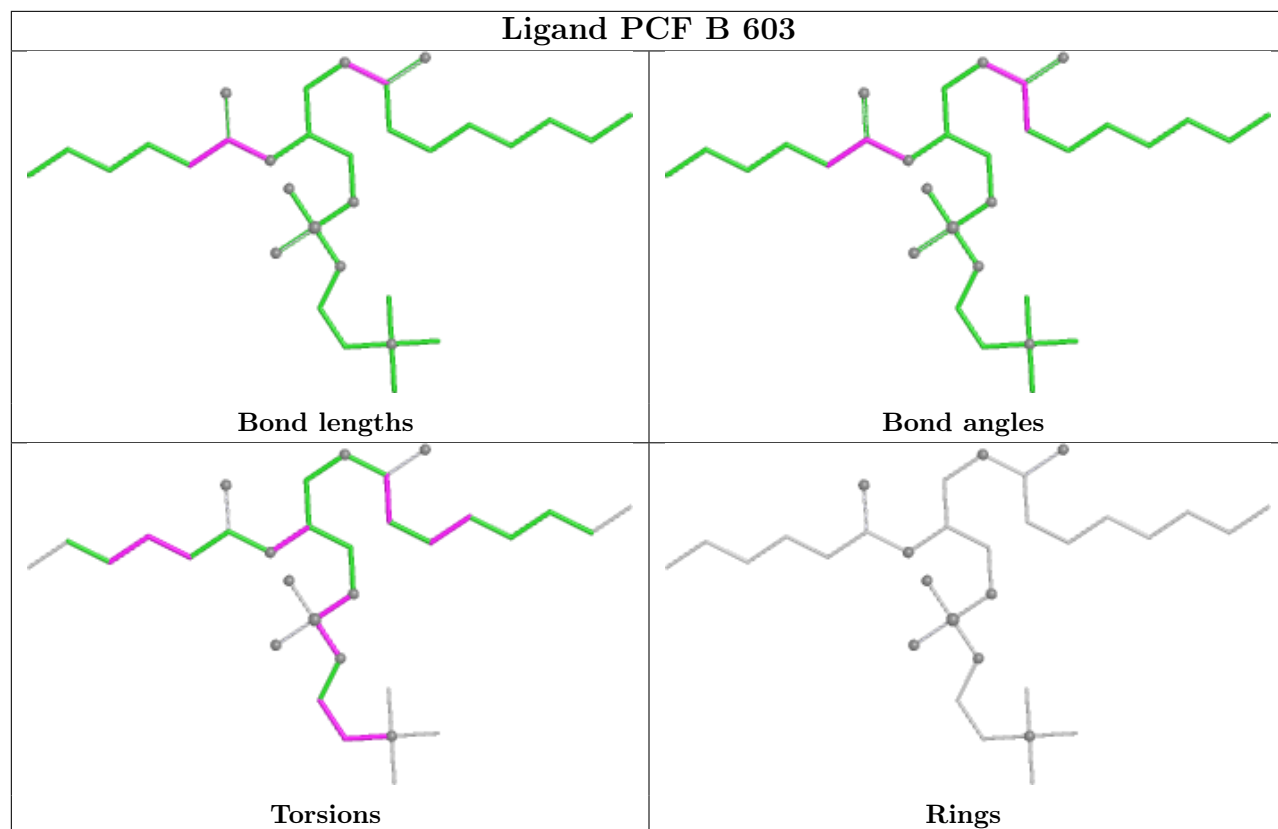
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	602	PCF	4	0
2	E	602	PCF	1	0
2	E	601	PCF	4	0
2	B	603	PCF	1	0
2	G	601	PCF	4	0
2	H	602	PCF	3	0
2	A	601	PCF	3	0
2	D	602	PCF	5	0
2	A	602	PCF	1	0
2	C	601	PCF	5	0
2	G	602	PCF	1	0
2	B	602	PCF	5	0
2	C	602	PCF	1	0
2	F	603	PCF	1	0

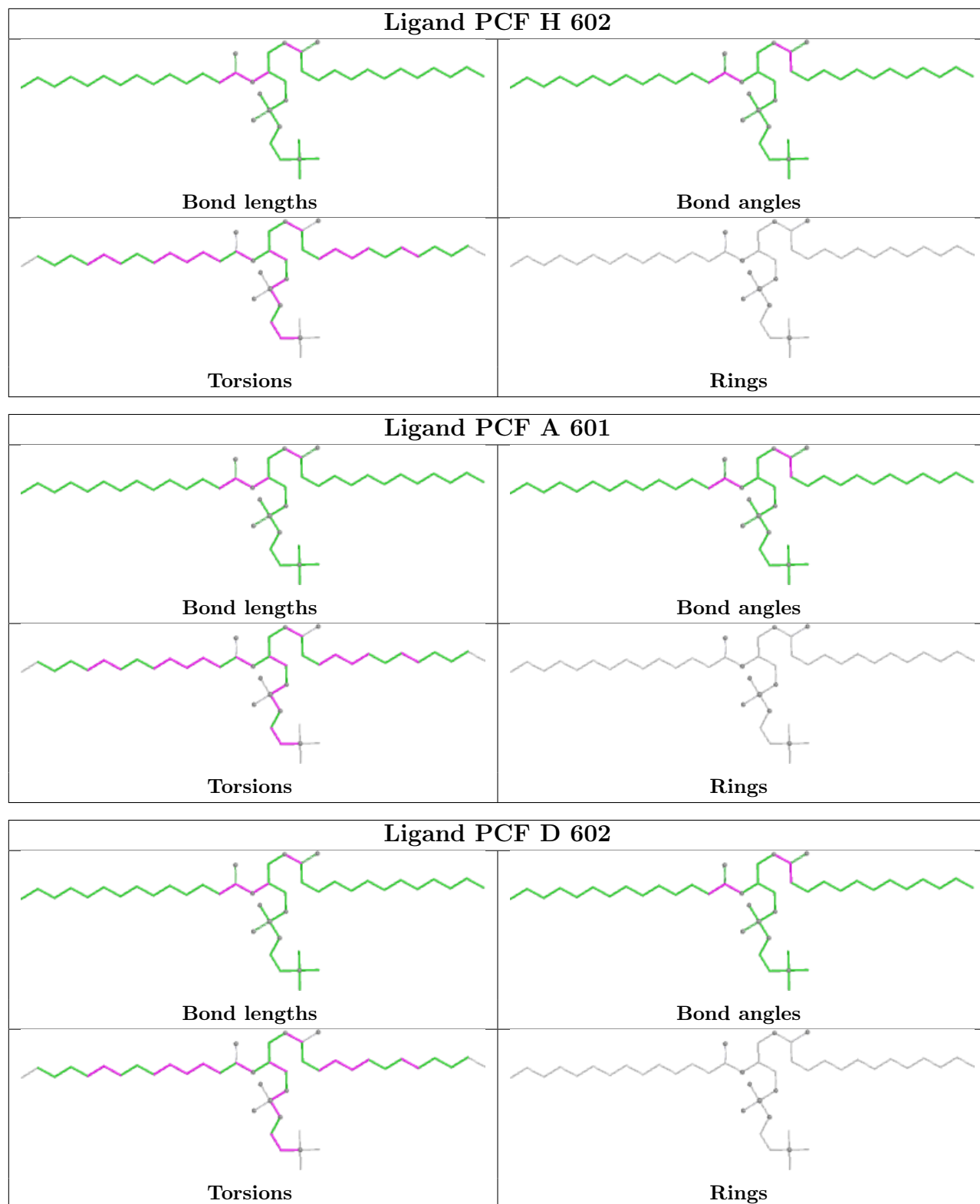
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

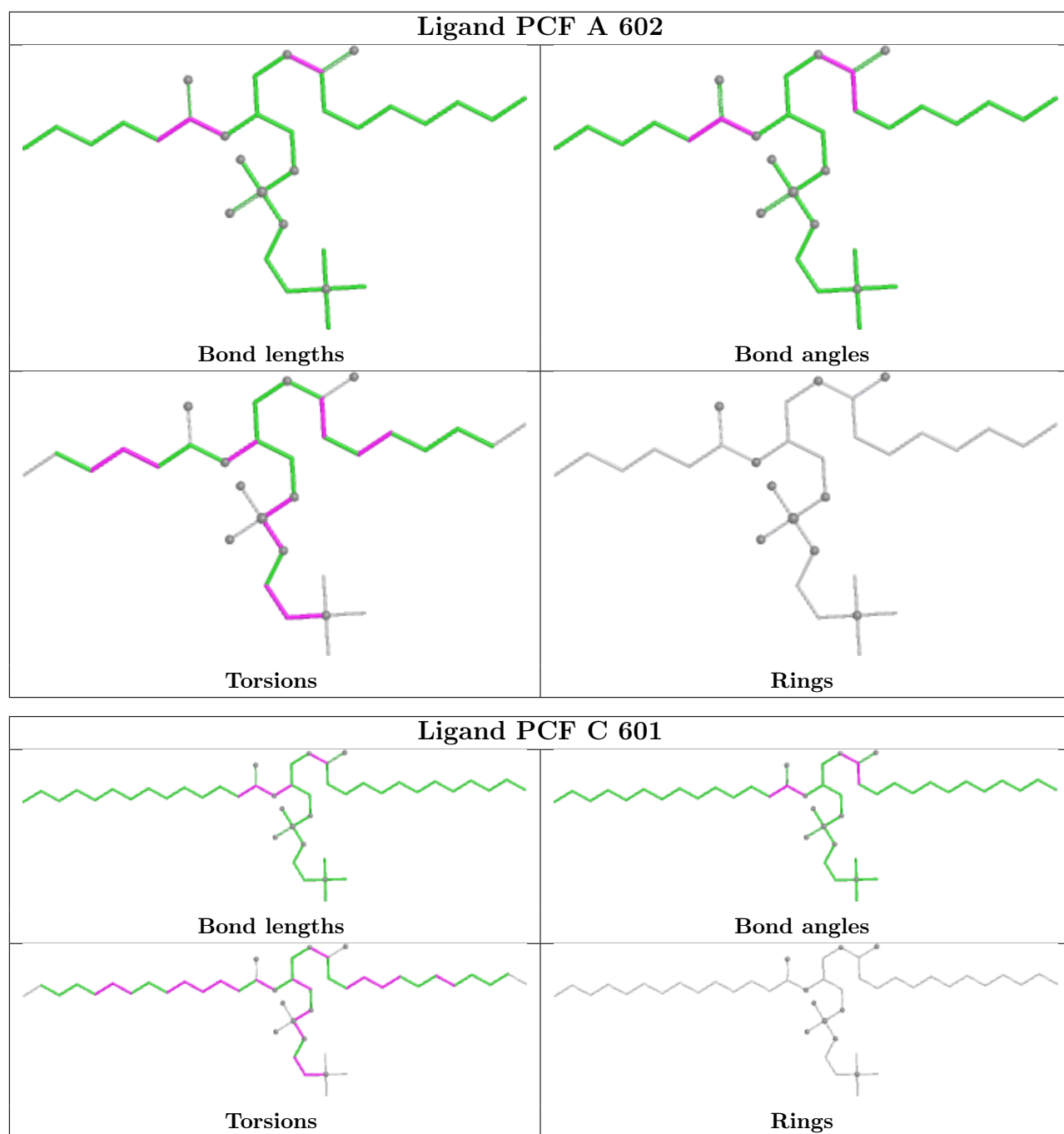
equivalents in the CSD to analyse the geometry.

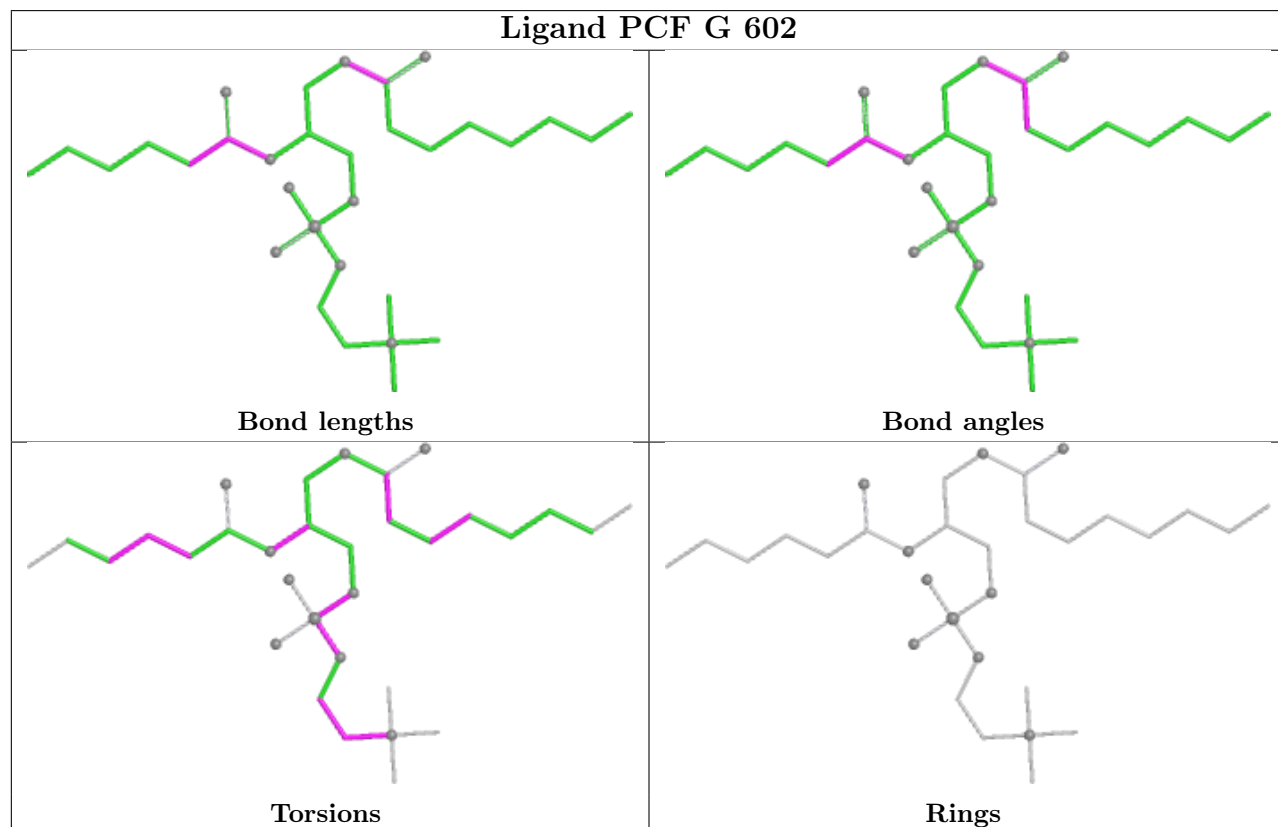
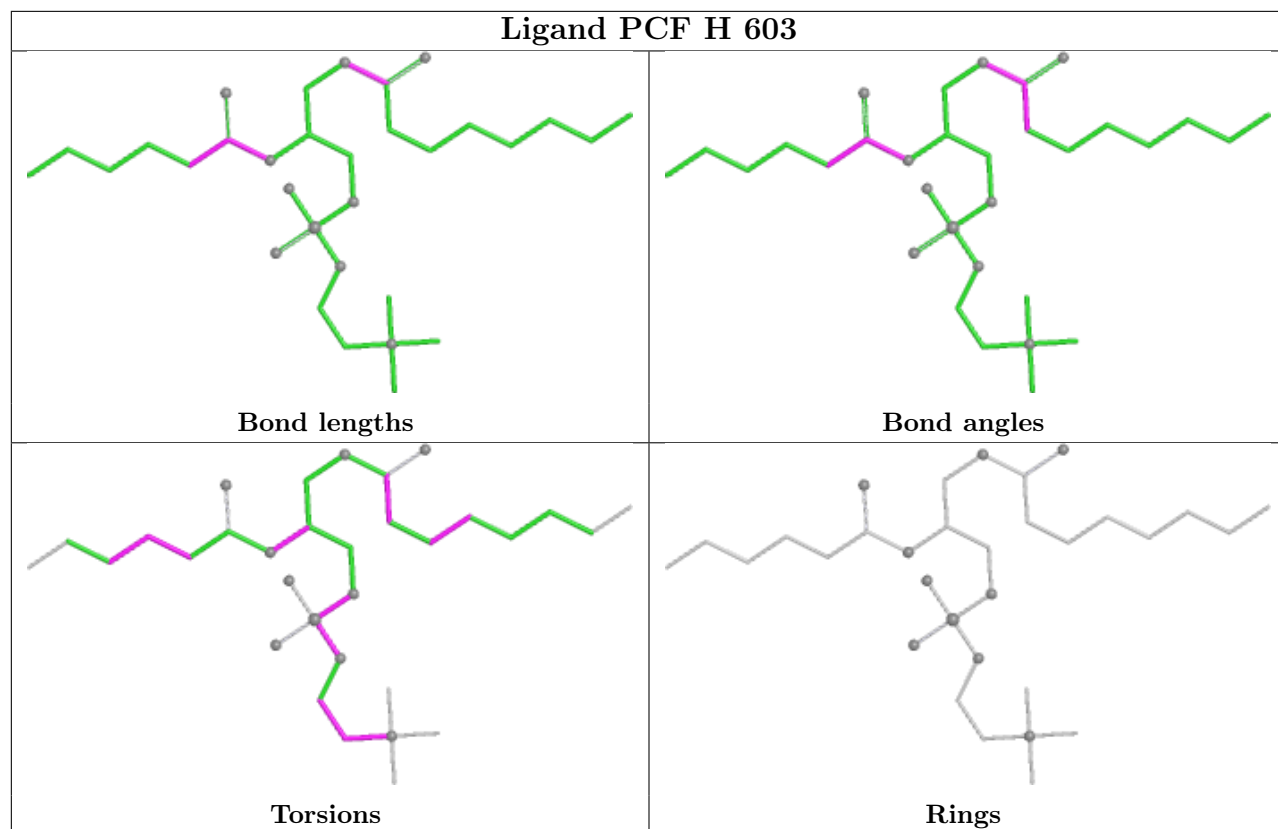


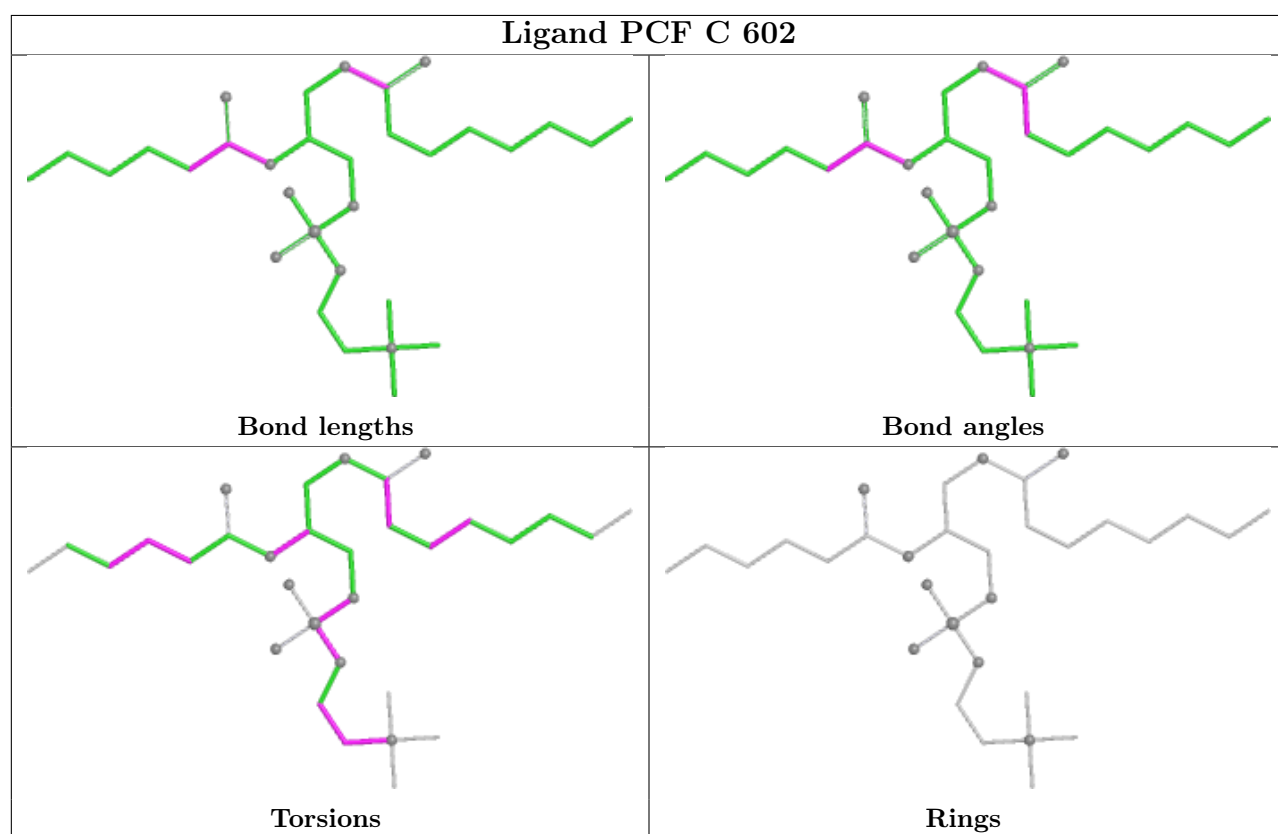
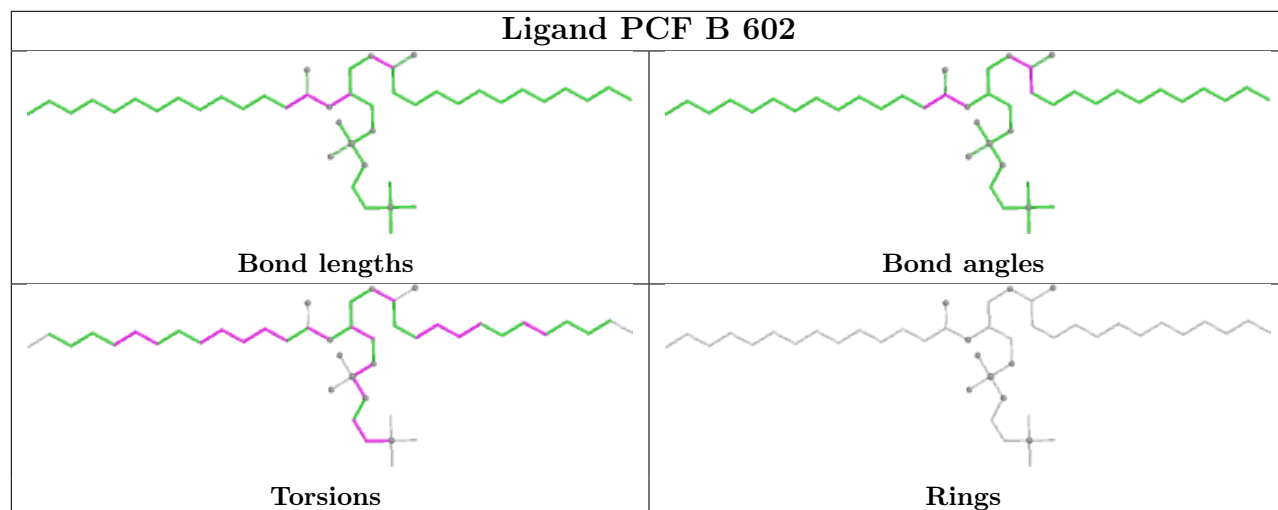


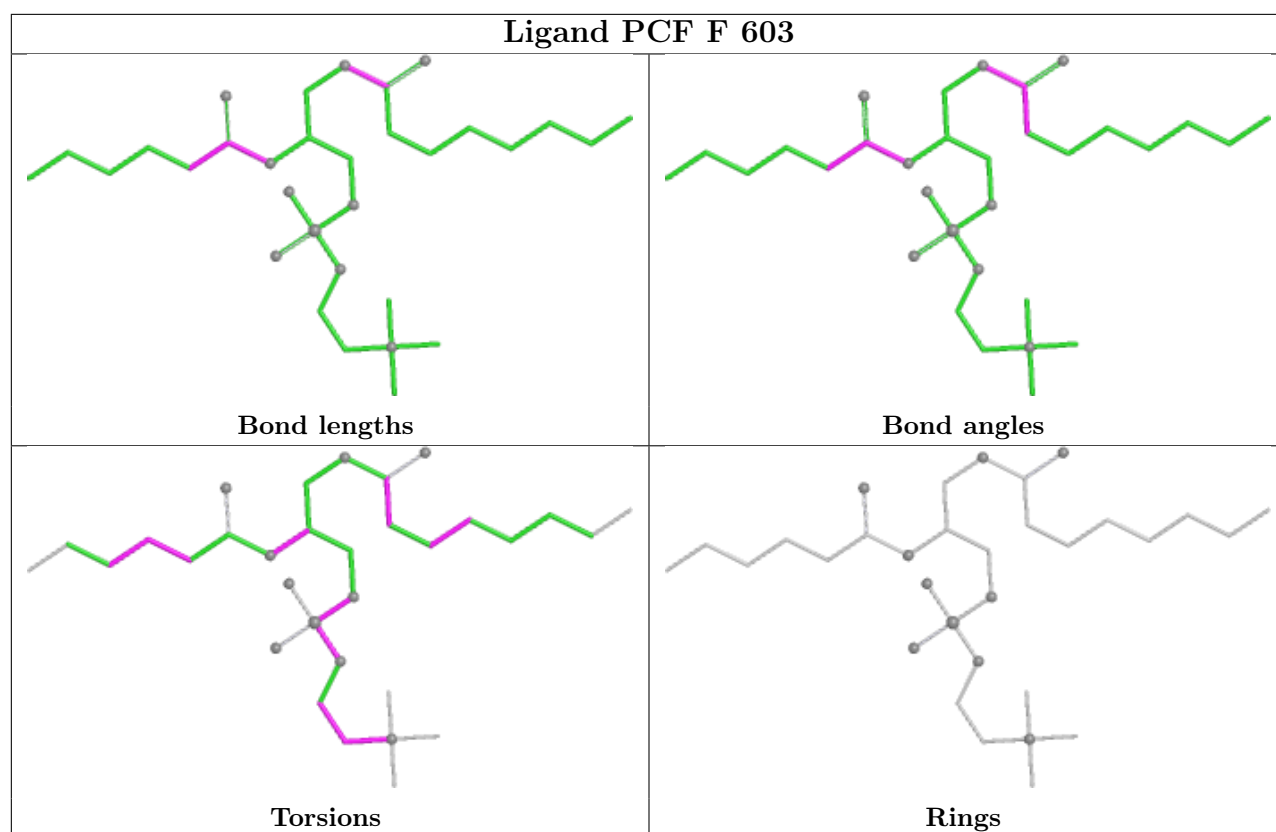












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

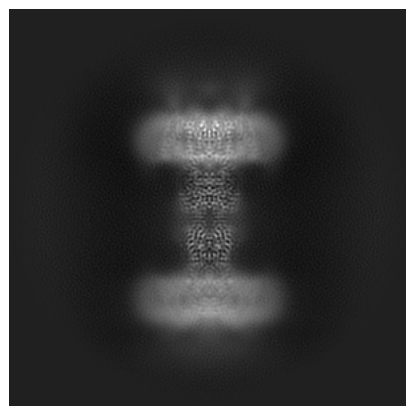
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13418. These allow visual inspection of the internal detail of the map and identification of artifacts.

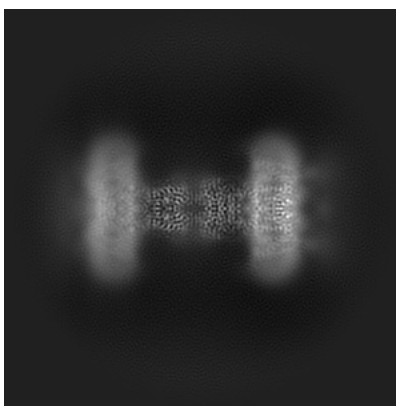
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

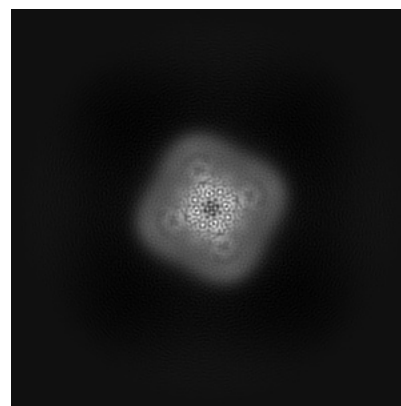
6.1.1 Primary map



X

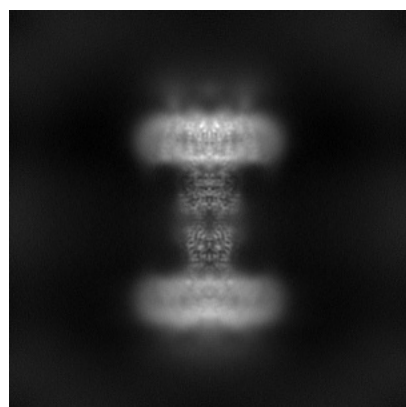


Y

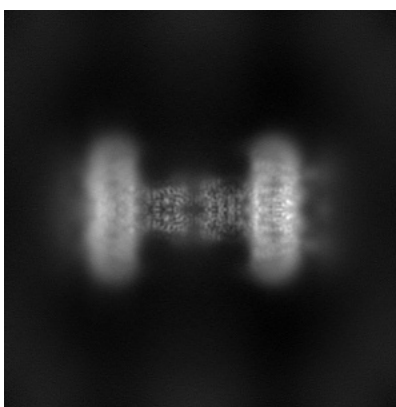


Z

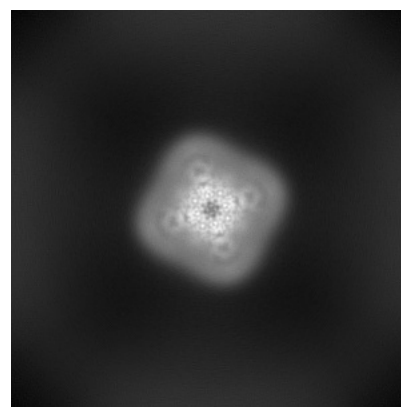
6.1.2 Raw map



X



Y

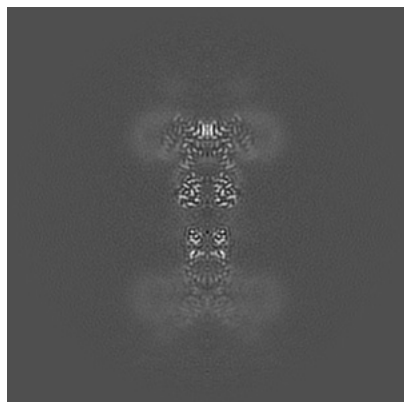


Z

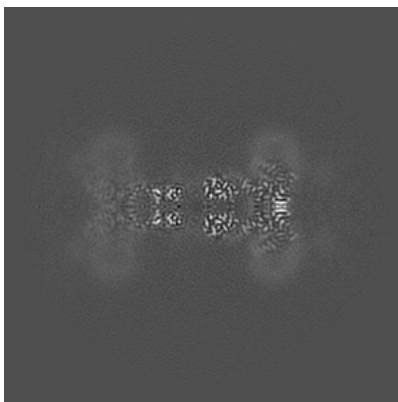
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

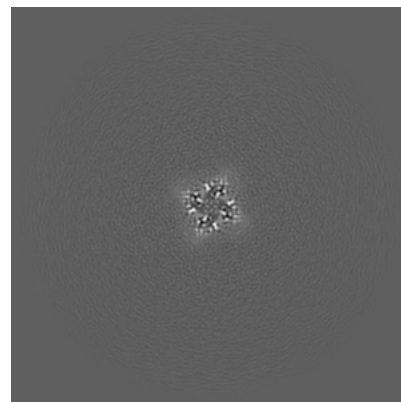
6.2.1 Primary map



X Index: 225

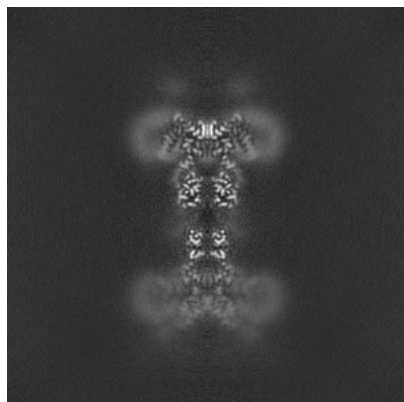


Y Index: 225

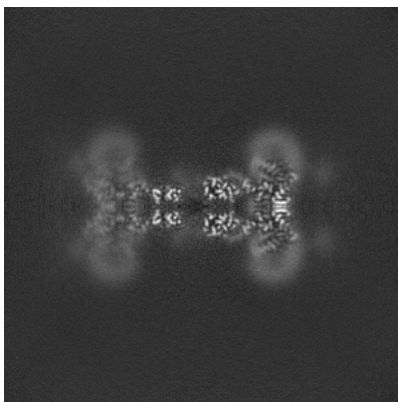


Z Index: 225

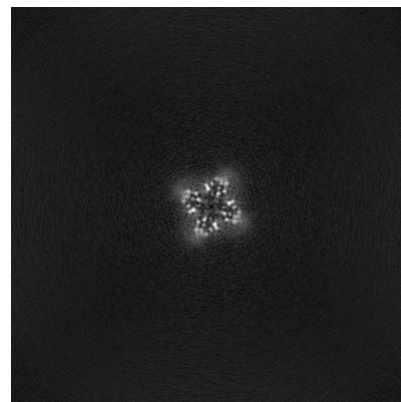
6.2.2 Raw map



X Index: 225



Y Index: 225

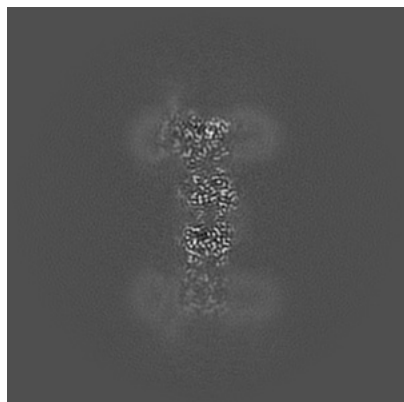


Z Index: 225

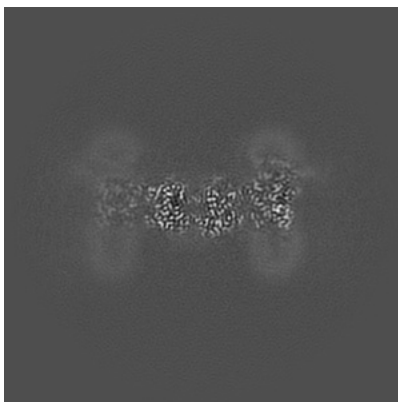
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

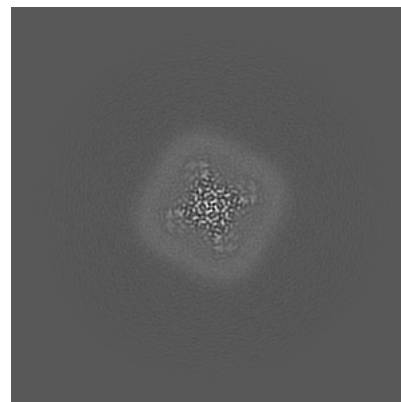
6.3.1 Primary map



X Index: 235

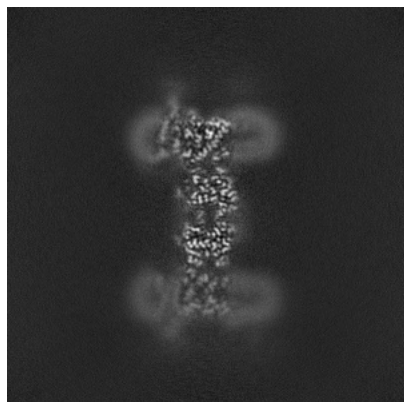


Y Index: 235

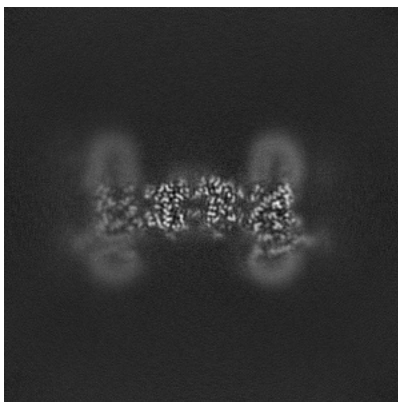


Z Index: 314

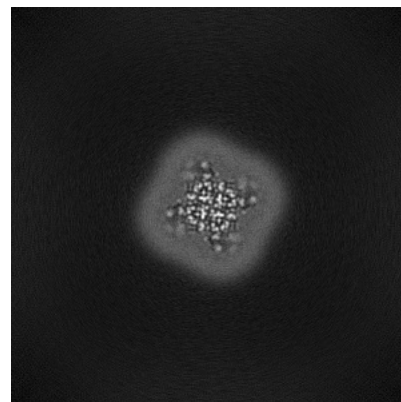
6.3.2 Raw map



X Index: 235



Y Index: 215

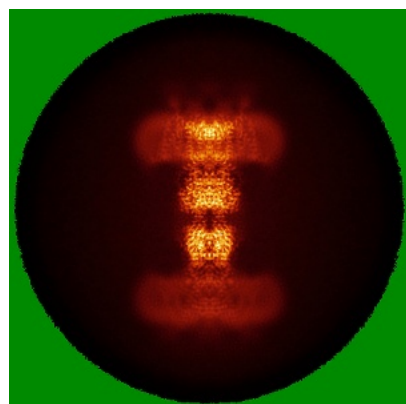


Z Index: 318

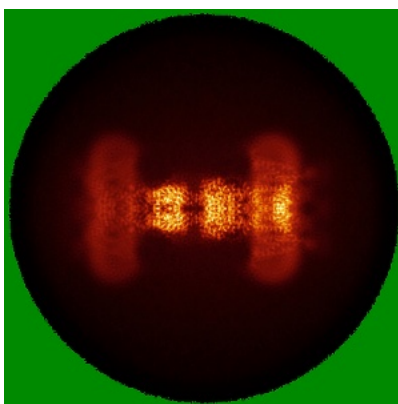
The images above show the largest variance slices of the map in three orthogonal directions.

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

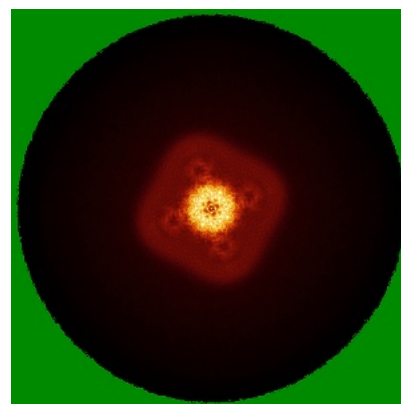
6.4.1 Primary map



X

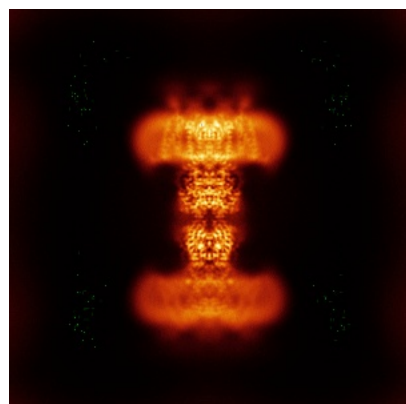


Y

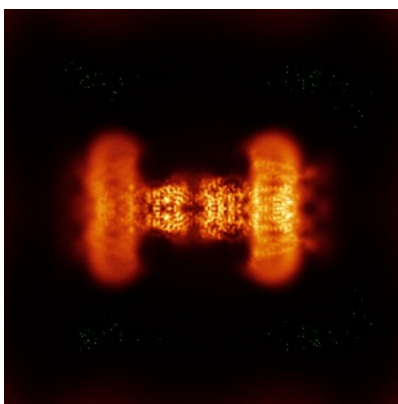


Z

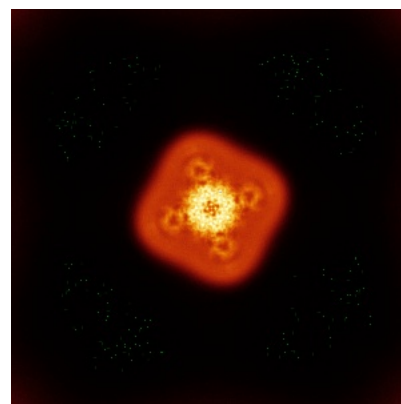
6.4.2 Raw map



X



Y

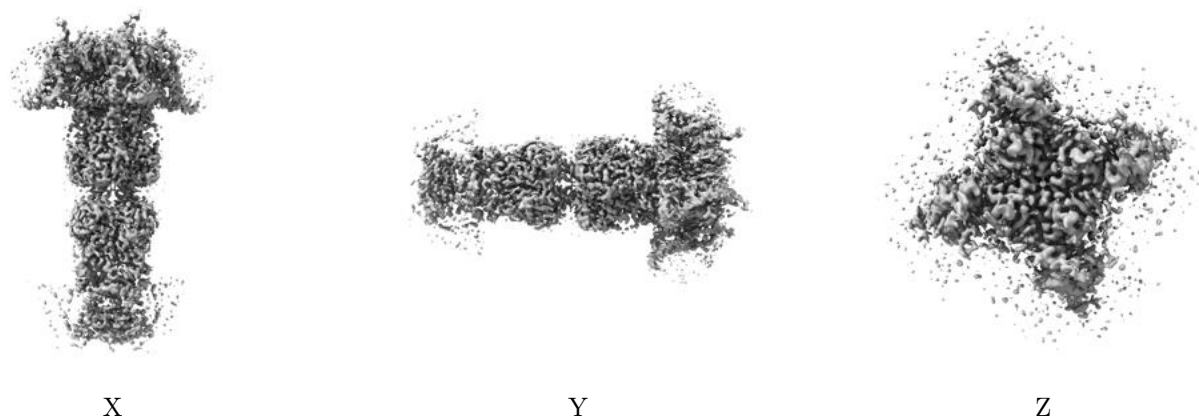


Z

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.

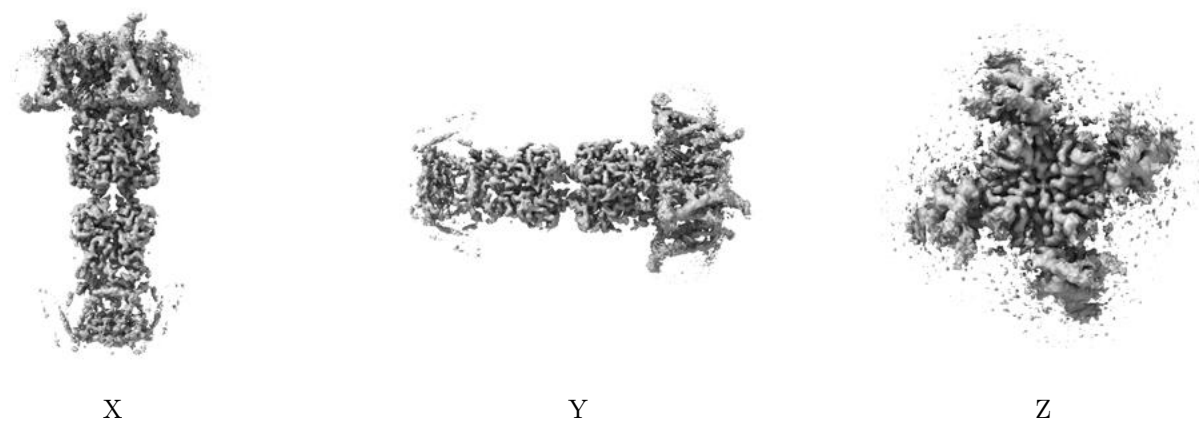
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

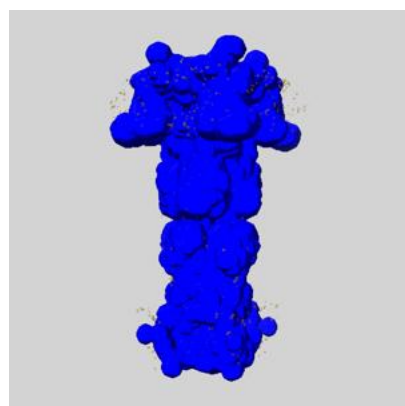
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

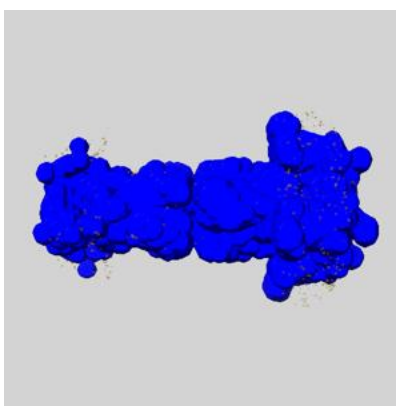
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

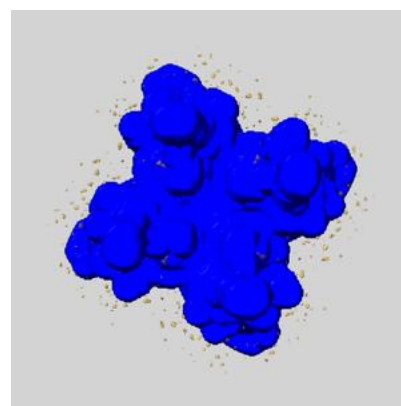
6.6.1 emd_13418_msk_1.map [i](#)



X



Y

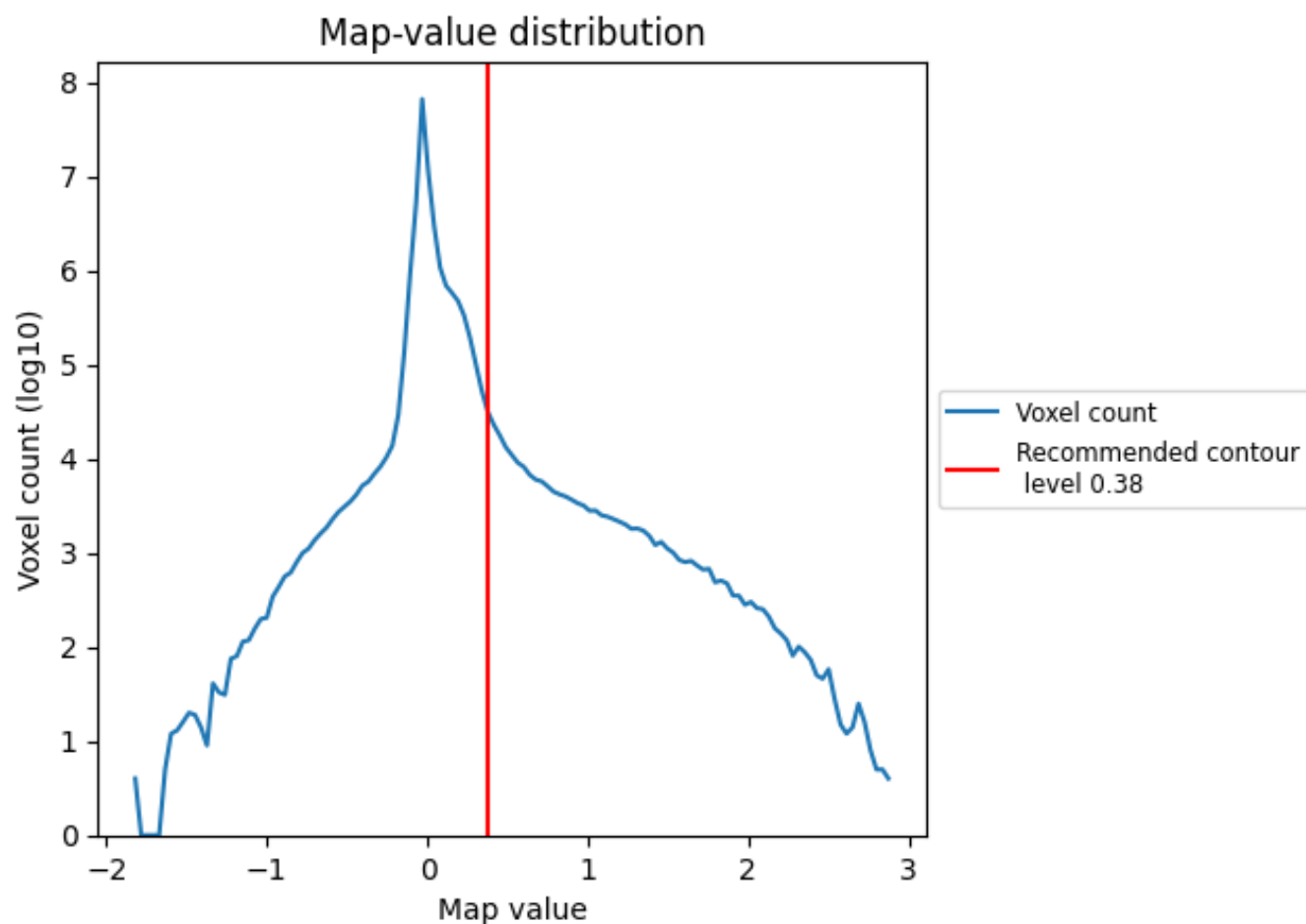


Z

7 Map analysis [i](#)

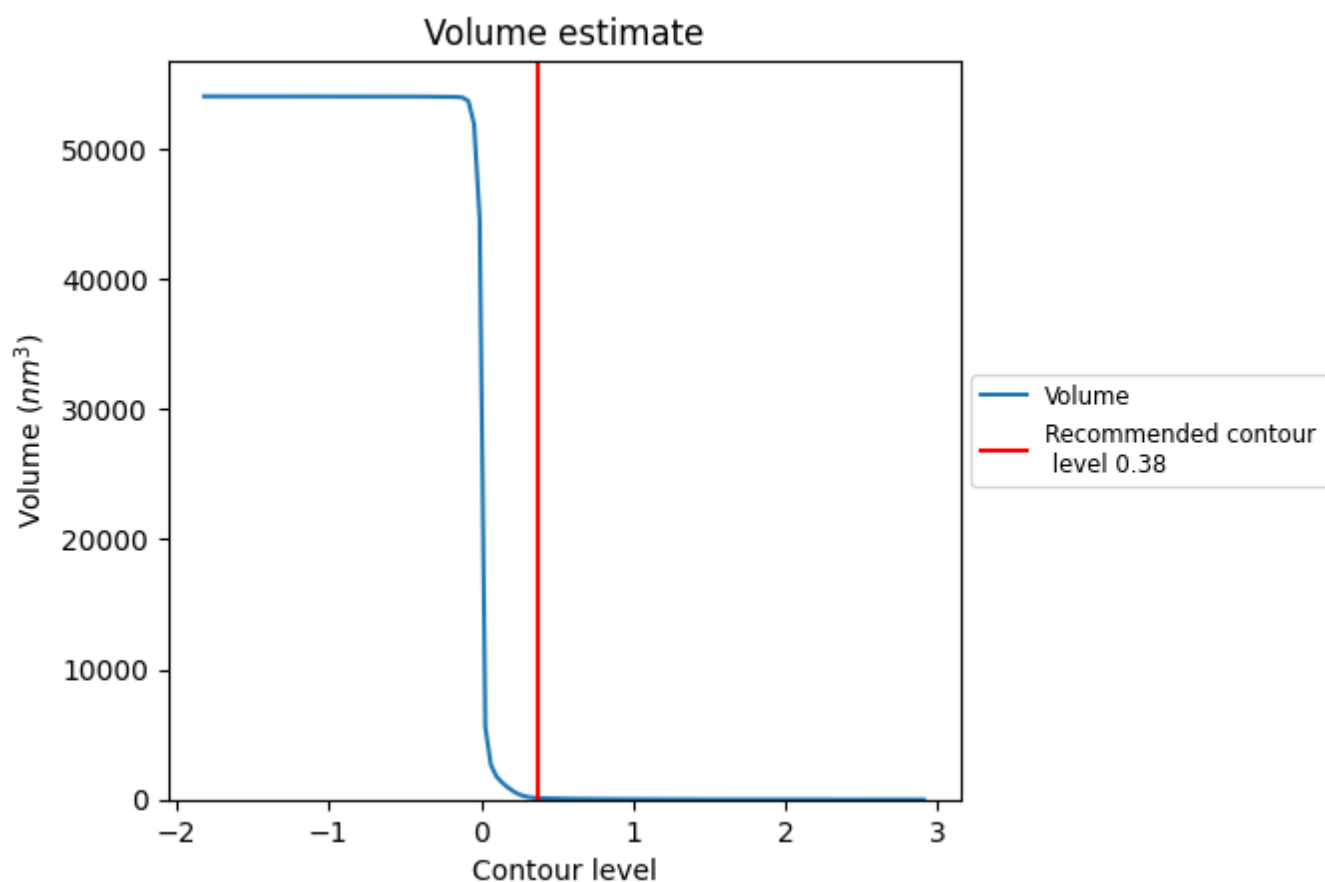
This section contains the results of statistical analysis of the map.

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.

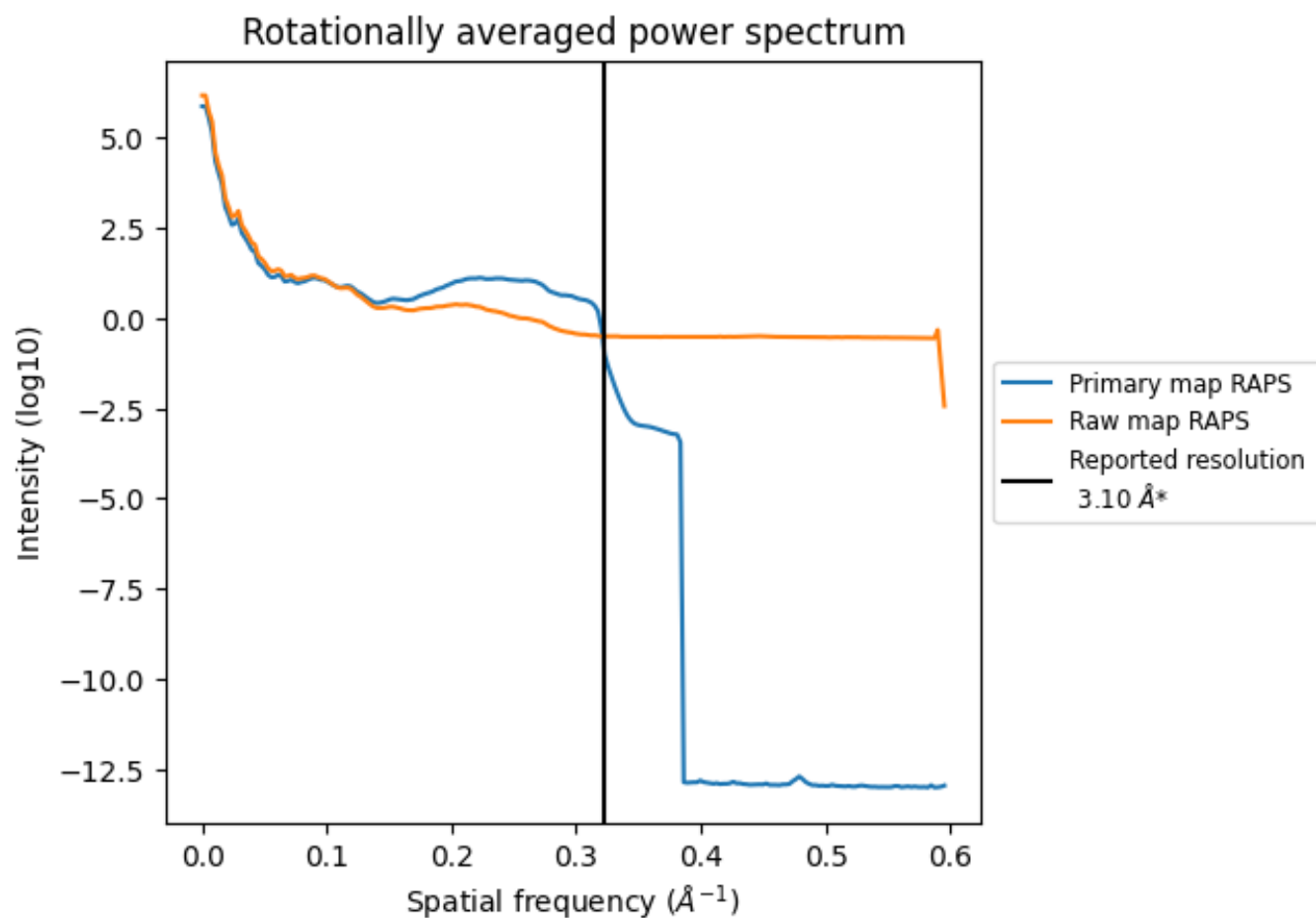
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 106 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

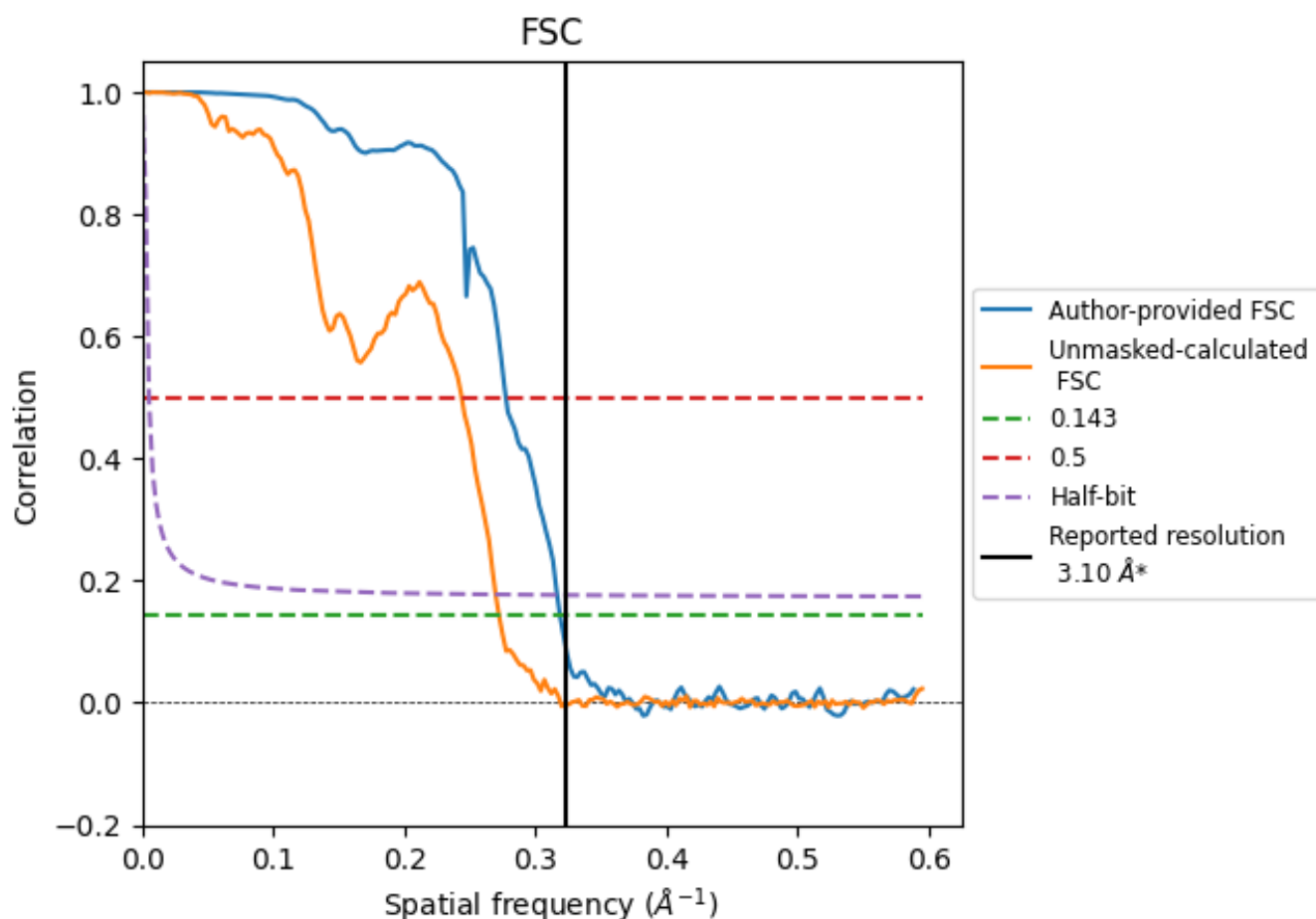


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

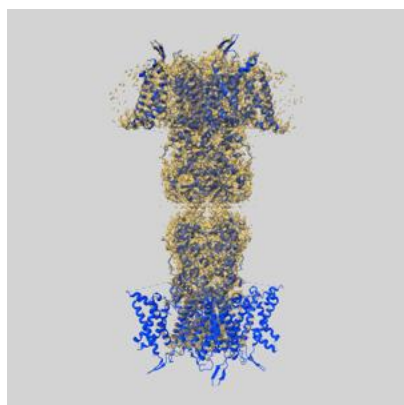
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.60	3.16
Unmasked-calculated*	3.67	4.10	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 3.1 by more than 10 %

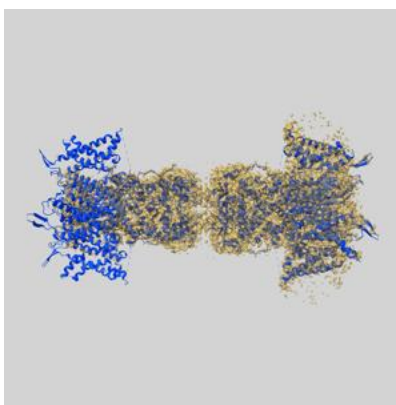
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13418 and PDB model 7PHK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

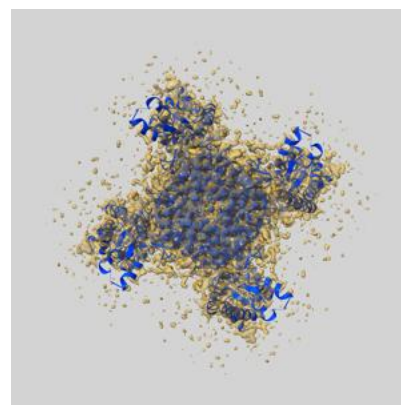
9.1 Map-model overlay [i](#)



X



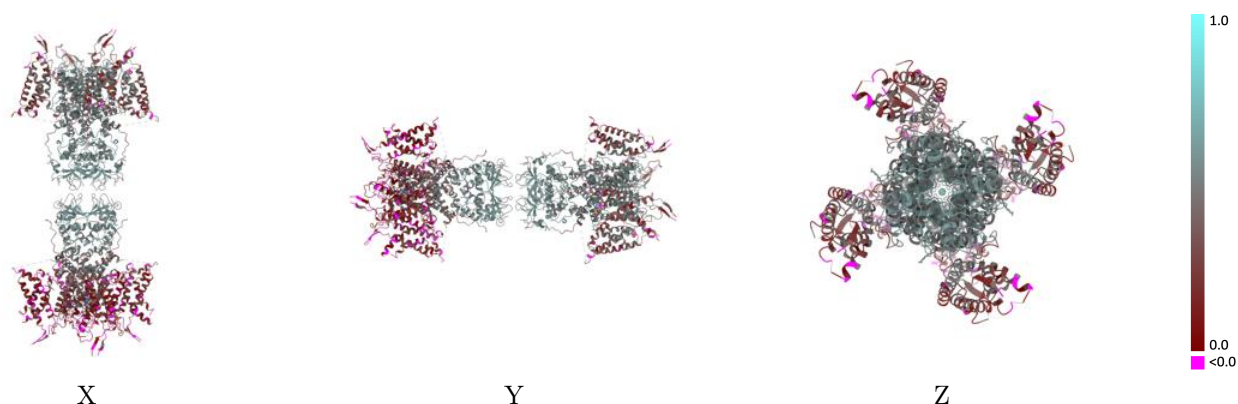
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.38 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](#)

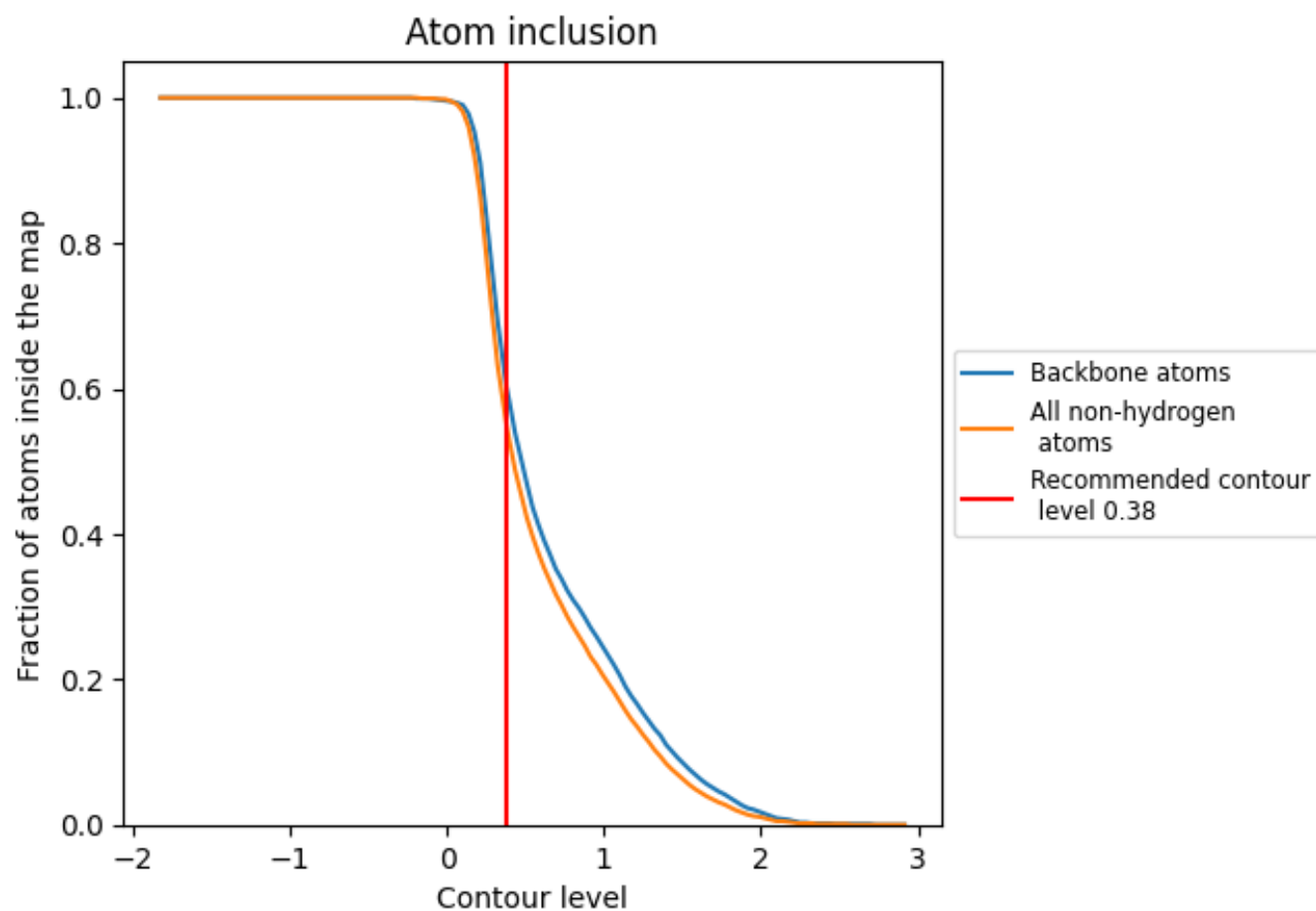


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 55% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5510	0.3810
A	0.7150	0.4520
B	0.7160	0.4520
C	0.7160	0.4540
D	0.7150	0.4530
E	0.3860	0.3100
F	0.3860	0.3100
G	0.3870	0.3110
H	0.3900	0.3090

