



## Full wwPDB EM Validation Report ⓘ

Aug 21, 2025 – 06:57 pm BST

PDB ID : 9H4P / pdb\_00009h4p  
EMDB ID : EMD-51866  
Title : Tail of full Haloferax tailed virus 1  
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.  
Deposited on : 2024-10-21  
Resolution : 2.44 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

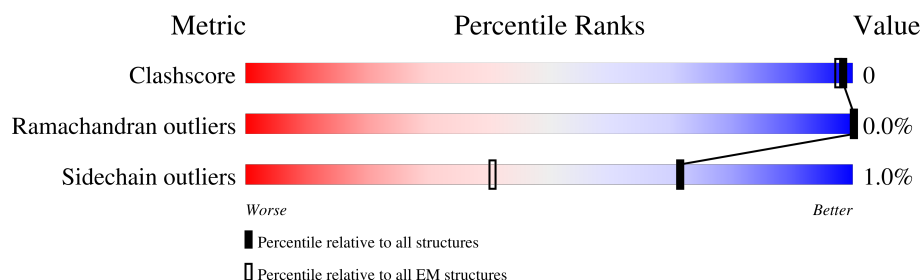
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.44 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.




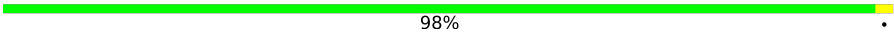
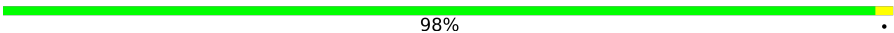
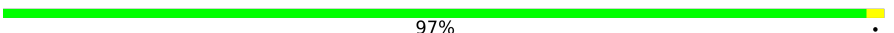
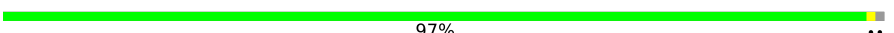
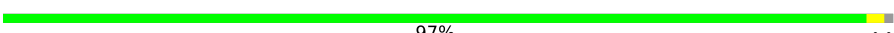
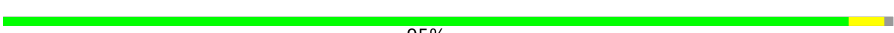








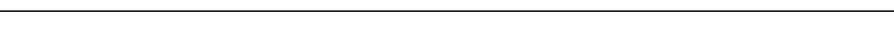
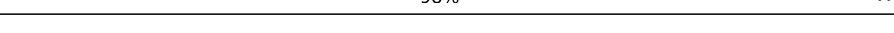
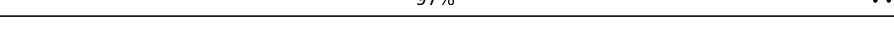
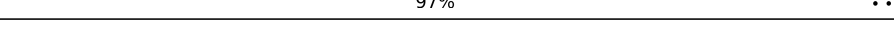
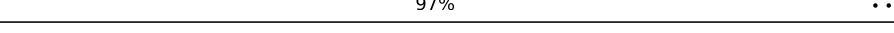
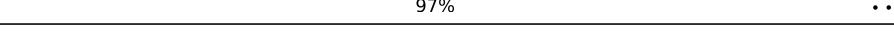
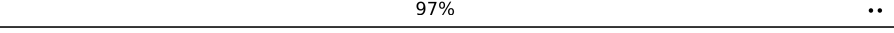
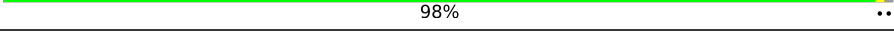
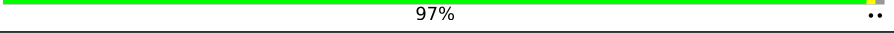
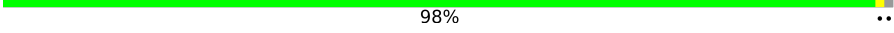
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	BD	954	 97%
1	BE	954	 96%
1	BF	954	 17% 96%
2	QE	341	 16% 93% 6%
2	QF	341	 18% 88% 7% 5%
2	QG	341	 17% 94%
2	QH	341	 16% 88% 7% 5%
2	QI	341	 16% 92% 7%

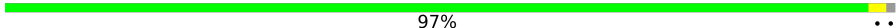
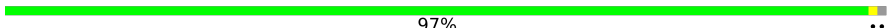
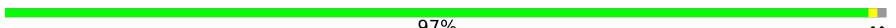
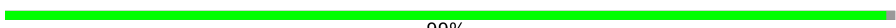
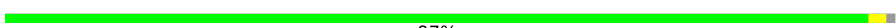








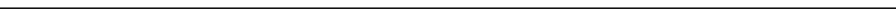

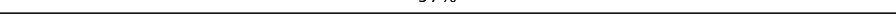
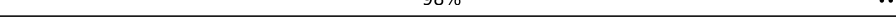
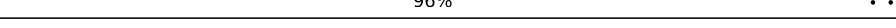
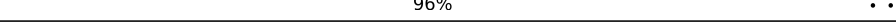
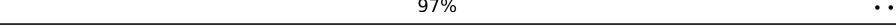
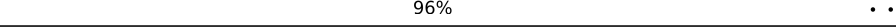
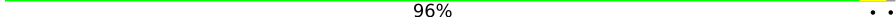
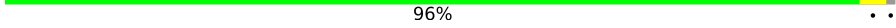
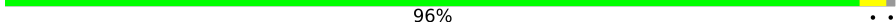
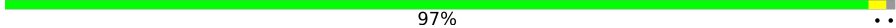
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Mol	Chain	Length	Quality of chain
2	QJ	341	 16% 89% 6% 5%
3	BA	285	 98%
3	BB	285	 98%
3	BC	285	 97%
4	B1	158	 97% ..
4	B2	158	 97% ..
4	B3	158	 95% . .
4	B4	158	 97% ..
4	B5	158	 97% ..
4	B6	158	 94% . .
4	P1	158	 97% ...
4	P2	158	 97% ..
4	P3	158	 97% ..
4	P4	158	 98% ..
4	P5	158	 98% ..
4	P6	158	 98% ..
4	S1	158	 97% ..
4	S2	158	 97% ..
4	SA	158	 97% ..
4	SB	158	 97% ..
4	SC	158	 97% ..
4	SD	158	 98% ..
4	SE	158	 97% ..
4	SF	158	 98% ..
4	SG	158	 97% ..

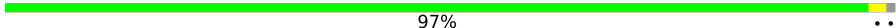
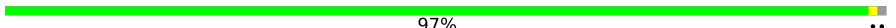
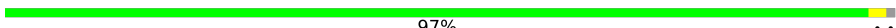
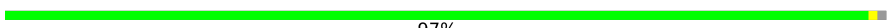
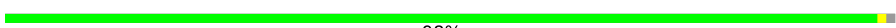








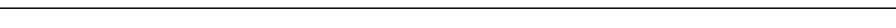

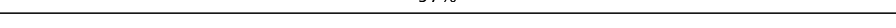
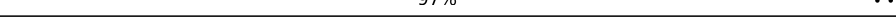
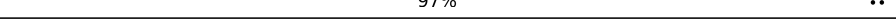
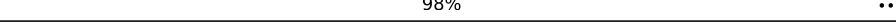
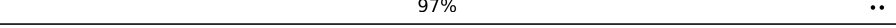
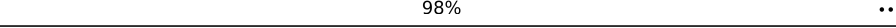
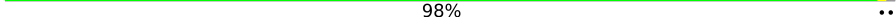
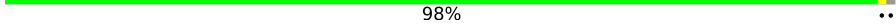
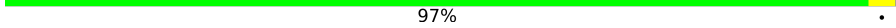
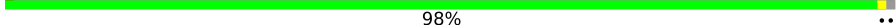
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Mol	Chain	Length	Quality of chain
4	SH	158	 97% ..
4	SI	158	 97% ..
4	SJ	158	 97% ..
4	SK	158	 99% .
4	SL	158	 97% ..
4	SM	158	 98% ..
4	SN	158	 96% ..
4	SO	158	 98% ..
4	SP	158	 99% .
4	SQ	158	 97% ..
4	SR	158	 97% ..
4	SS	158	 98% ..
4	ST	158	 96% ..
4	SU	158	 99% .
4	SV	158	 97% ..
4	SW	158	 98% ..
4	SX	158	 96% ..
4	SY	158	 96% ..
4	SZ	158	 97% ..
4	Sa	158	 96% ..
4	Sb	158	 96% ..
4	Sc	158	 96% ..
4	Sd	158	 96% ..
4	Se	158	 97% ..
4	Sf	158	 97% ..

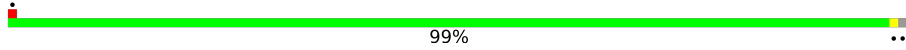
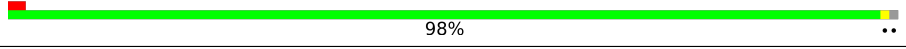
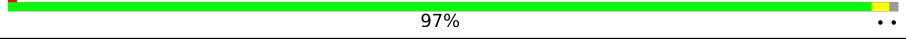
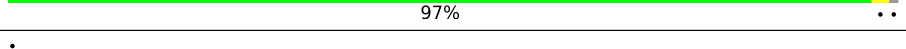
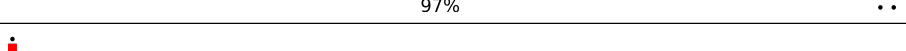
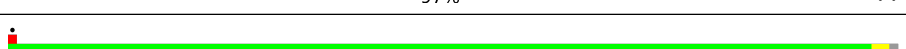
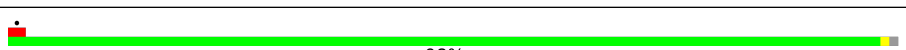
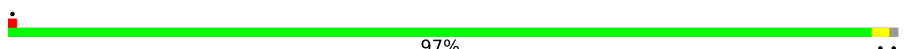
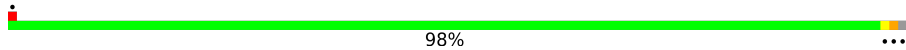
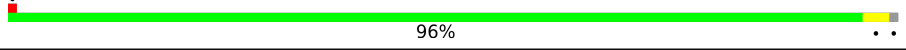
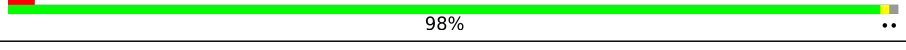
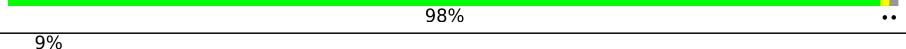
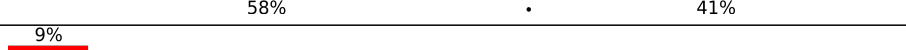

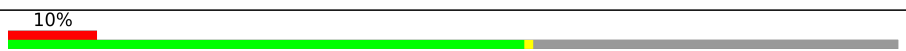



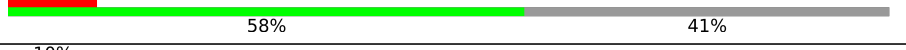






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Mol	Chain	Length	Quality of chain
4	Sg	158	 97% ..
4	Sh	158	 97% ..
4	Si	158	 97% ..
4	Sj	158	 97% ..
4	Sk	158	 98% ..
4	Sl	158	 97% ..
4	Sm	158	 96% ..
4	Sn	158	 98% ..
4	So	158	 97% ..
4	Sp	158	 97% ..
4	Sq	158	 97% ..
4	Sr	158	 97% ..
4	Ss	158	 97% ...
4	St	158	 98% ..
4	Su	158	 97% ..
4	Sv	158	 97% ..
4	Sw	158	 97% ..
4	Sx	158	 98% ..
4	Sy	158	 97% ..
4	Sz	158	 98% ..
5	Pa	157	 98% ..
5	Pb	157	 98% ..
5	Pc	157	 97% ..
5	Pd	157	 98% ..
5	Pe	157	 97% ..

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Mol	Chain	Length	Quality of chain
5	Pf	157	 99% ..
6	PM	141	 98% ..
6	PN	141	 97% ..
6	PO	141	 97% ..
6	PP	141	 97% ..
6	PQ	141	 97% ..
6	PR	141	 97% ..
6	PS	141	 98% ..
6	PT	141	 97% ..
6	PU	141	 98% ...
6	PV	141	 96% ..
6	PW	141	 98% ..
6	PX	141	 98% ..
7	PA	675	 9% 58% 41%
7	PB	675	 9% 58% 41%
7	PC	675	 9% 58% 41%
7	PD	675	 10% 58% 41%
7	PE	675	 10% 58% 41%
7	PF	675	 9% 58% 41%
7	PG	675	 9% 58% 41%
7	PH	675	 10% 58% 41%
7	PI	675	 10% 58% 41%
7	PJ	675	 10% 58% 41%
7	PK	675	 10% 58% 41%
7	PL	675	 11% 58% 41%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 179352 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 Baseplate hub.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BD	953	Total	C	N	O	S	0	0
			7212	4427	1207	1573	5		
1	BE	953	Total	C	N	O	S	0	0
			7212	4427	1207	1573	5		
1	BF	953	Total	C	N	O	S	0	0
			7212	4427	1207	1573	5		

- Molecule 2 is a protein called Phate tail tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	QG	337	Total	C	N	O	S	0	0
			2498	1541	427	522	8		
2	QH	324	Total	C	N	O	S	0	0
			2409	1485	411	505	8		
2	QI	337	Total	C	N	O	S	0	0
			2498	1541	427	522	8		
2	QJ	324	Total	C	N	O	S	0	0
			2409	1485	411	505	8		
2	QE	337	Total	C	N	O	S	0	0
			2498	1541	427	522	8		
2	QF	324	Total	C	N	O	S	0	0
			2409	1485	411	505	8		

- Molecule 3 is a protein called Baseplate to tube adapter protein gp41.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	BA	284	Total	C	N	O	0	0
			2136	1332	375	429		
3	BB	284	Total	C	N	O	0	0
			2136	1332	375	429		
3	BC	284	Total	C	N	O	0	0
			2136	1332	375	429		

- Molecule 4 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SG	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SH	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SI	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SJ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SK	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SL	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SS	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	ST	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SU	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SV	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SW	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SX	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SM	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SN	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SO	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SP	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SQ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SR	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SB	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SA	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SC	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SD	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	SE	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SF	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sk	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sl	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sm	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sn	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	So	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sp	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Se	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sf	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sg	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sh	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Si	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sj	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SY	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	SZ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sa	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sb	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sc	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sd	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	B1	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	B3	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	B4	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	B5	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	B6	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sw	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sx	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sy	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sz	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	S1	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	S2	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sq	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sr	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Ss	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	St	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Su	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	Sv	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	P1	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	P2	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	P3	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	P4	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P5	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
4	P6	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

- Molecule 5 is a protein called SPP1 gp17-like tail completion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Pa	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
5	Pb	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
5	Pc	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
5	Pd	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
5	Pe	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
5	Pf	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		

- Molecule 6 is a protein called HK97 gp6-like/SPP1 gp15-like head-tail connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	PT	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PM	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PN	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PO	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PP	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PQ	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PR	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PS	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PU	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	PV	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PW	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
6	PX	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		

- Molecule 7 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	PA	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PB	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PC	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PD	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PE	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PF	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PG	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PH	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PI	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PJ	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PK	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		
7	PL	396	Total	C	N	O	P S	0	0
			3106	1925	528	640	3 10		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	BD	1	Total	Mg	0
			1	1	
8	BE	1	Total	Mg	0
			1	1	

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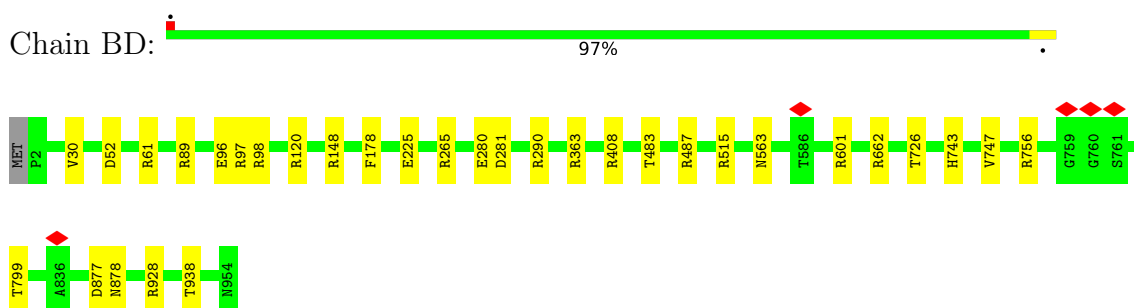
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Mol	Chain	Residues	Atoms		AltConf
8	BF	1	Total 1	Mg 1	0
8	PT	1	Total 1	Mg 1	0
8	PM	1	Total 1	Mg 1	0
8	PN	1	Total 1	Mg 1	0
8	PO	1	Total 1	Mg 1	0
8	PP	1	Total 1	Mg 1	0
8	PQ	1	Total 1	Mg 1	0
8	PR	1	Total 1	Mg 1	0
8	PS	1	Total 1	Mg 1	0
8	PU	2	Total 2	Mg 2	0
8	PV	1	Total 1	Mg 1	0
8	PW	1	Total 1	Mg 1	0

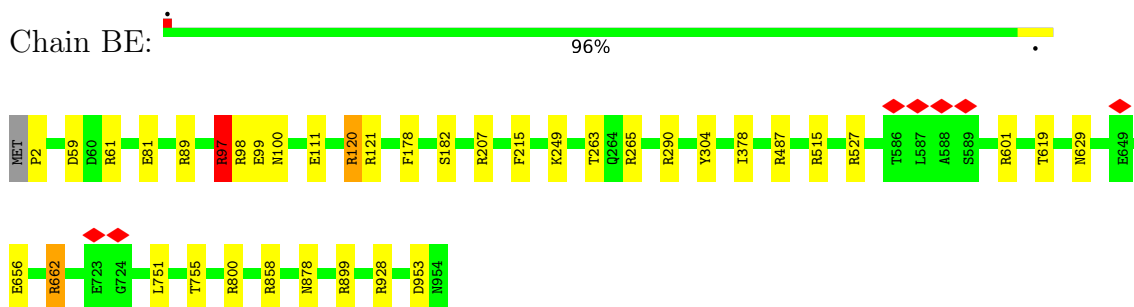
### 3 Residue-property plots

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.

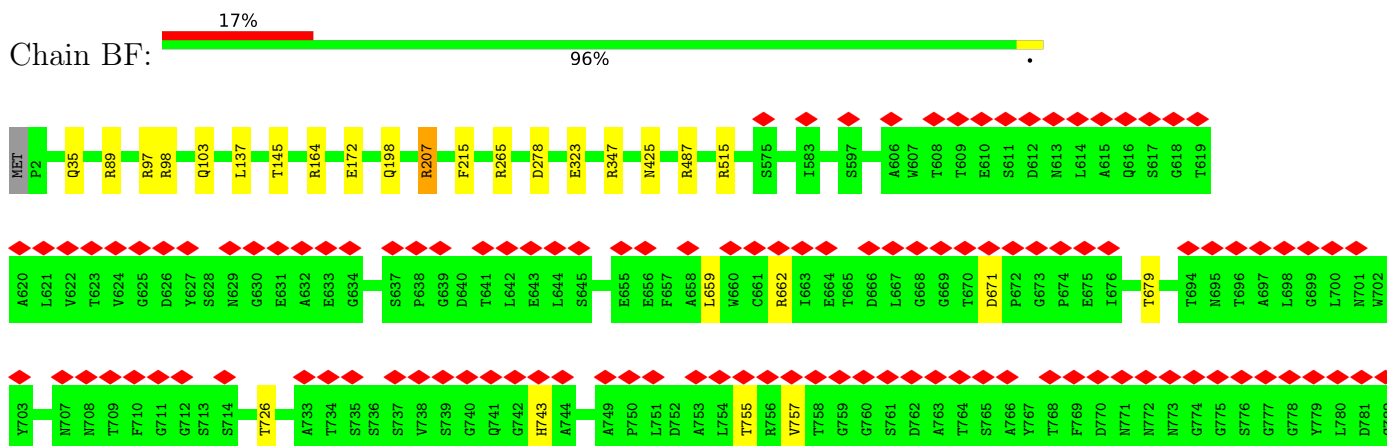
- Molecule 1: Baseplate hub

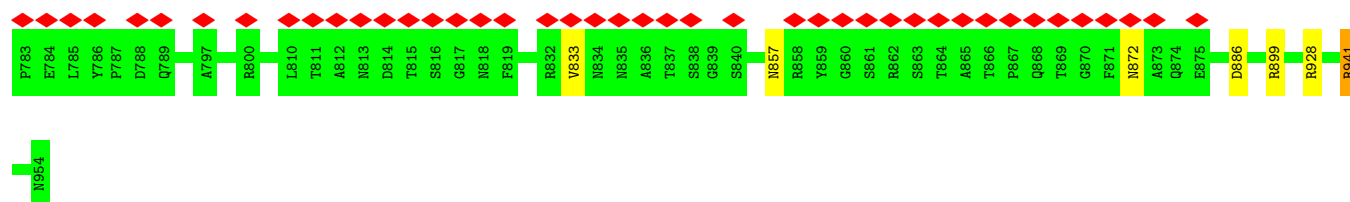


- Molecule 1: Baseplate hub

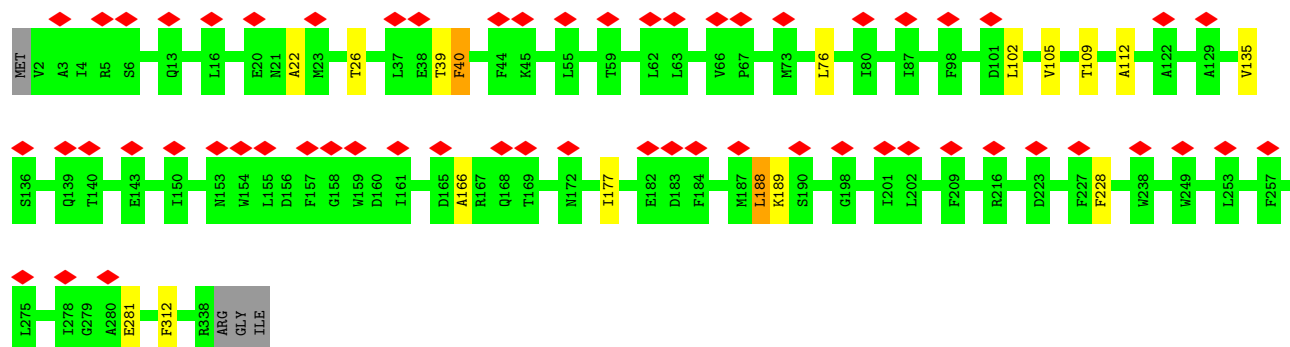


- Molecule 1: Baseplate hub

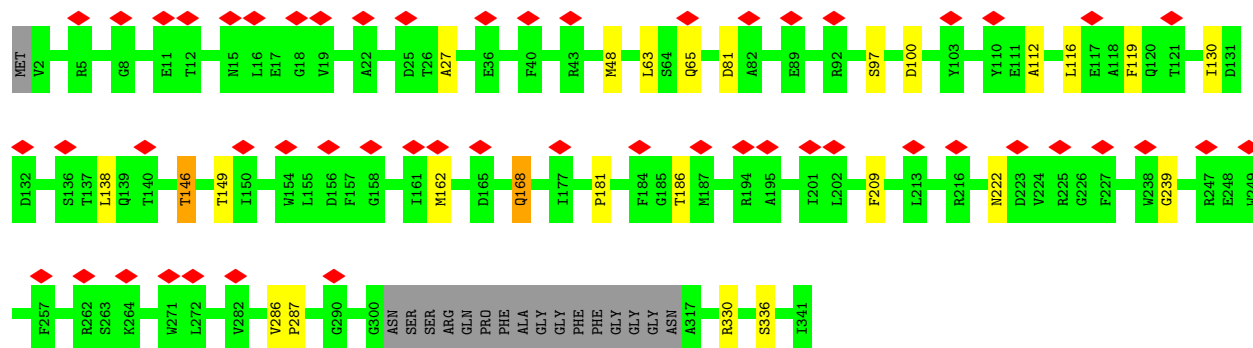
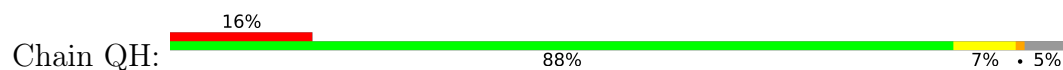




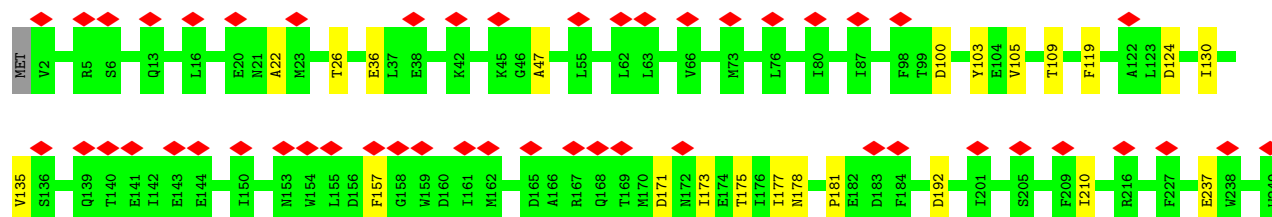
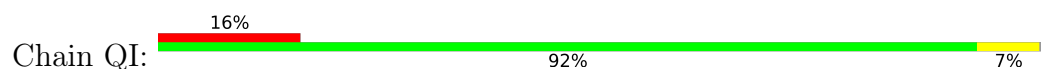
• Molecule 2: Phate tail tape measure protein

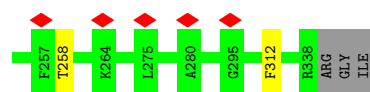


• Molecule 2: Phate tail tape measure protein



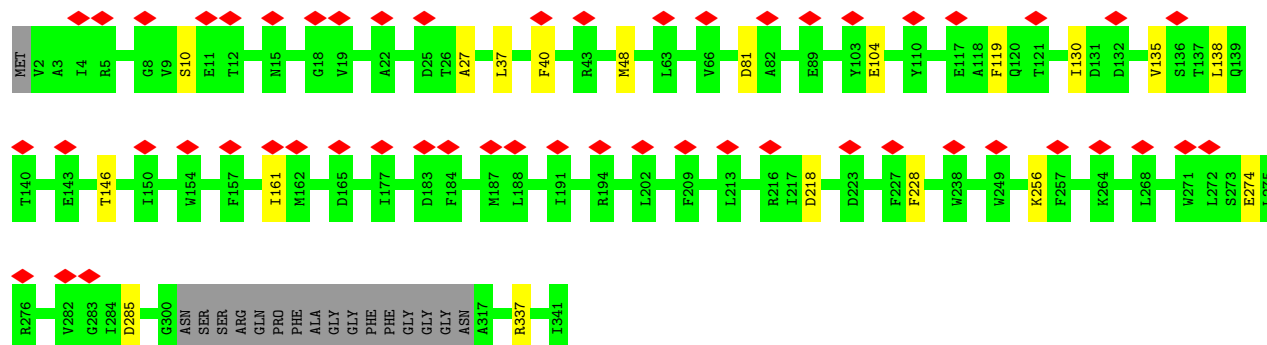
• Molecule 2: Phate tail tape measure protein





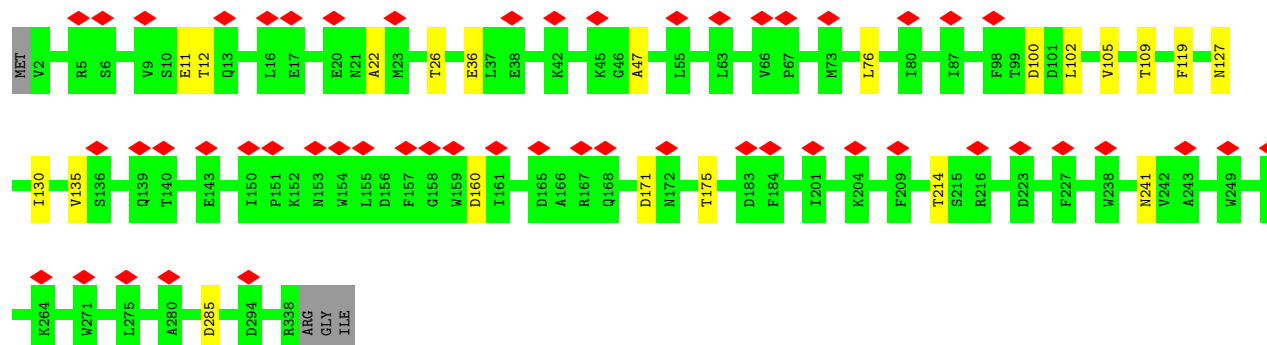
- Molecule 2: Phate tail tape measure protein

Chain QJ: 16% 89% 6% 5%



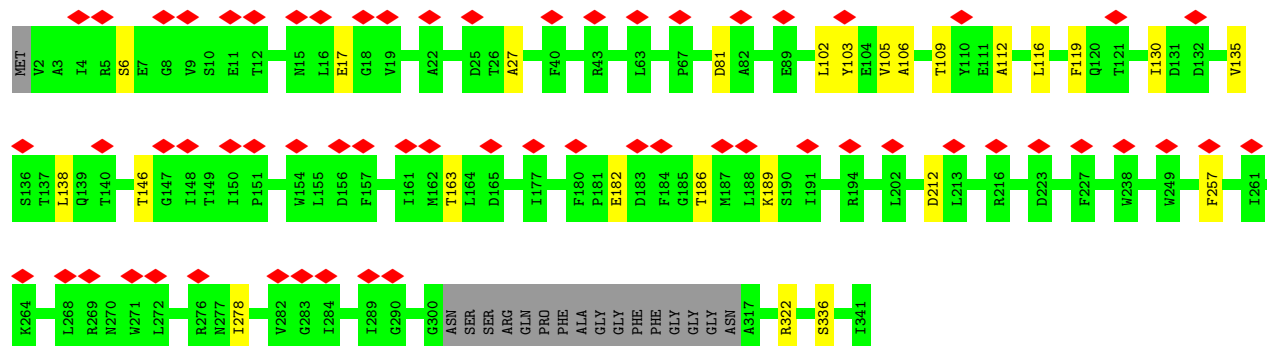
- Molecule 2: Phate tail tape measure protein

Chain QE: 16% 93% 6%



- Molecule 2: Phate tail tape measure protein

Chain QF: 18% 88% 7% 5%



- Molecule 3: Baseplate to tube adapter protein gp41



Chain BA:  98% .



- Molecule 3: Baseplate to tube adapter protein gp41

Chain BB:  98% .



- Molecule 3: Baseplate to tube adapter protein gp41

Chain BC:  97% .



- Molecule 4: Tail tube protein

Chain SG:  97% ..



- Molecule 4: Tail tube protein

Chain SH:  97% ..



- Molecule 4: Tail tube protein

Chain SI:  97% ..



- Molecule 4: Tail tube protein

Chain SJ:  97% ..



- Molecule 4: Tail tube protein

Chain SK:  99% .



- Molecule 4: Tail tube protein

Chain SL:  97% ..



- Molecule 4: Tail tube protein

Chain SS:  98% ..



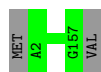
- Molecule 4: Tail tube protein

Chain ST:  96% ..



- Molecule 4: Tail tube protein

Chain SU:  99% .



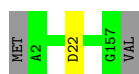
- Molecule 4: Tail tube protein

Chain SV:  97% ..



- Molecule 4: Tail tube protein

Chain SW:  98% ..



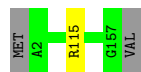
- Molecule 4: Tail tube protein

Chain SX:  96% ..



- Molecule 4: Tail tube protein

Chain SM:  98% ..



- Molecule 4: Tail tube protein

Chain SN:  96% ..



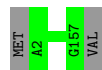
- Molecule 4: Tail tube protein

Chain SO:  98% ..



- Molecule 4: Tail tube protein

Chain SP:  99% ..



- Molecule 4: Tail tube protein

Chain SQ:  97% ..



- Molecule 4: Tail tube protein

Chain SR:  97% ..



- Molecule 4: Tail tube protein

Chain SB:  97% ..



- Molecule 4: Tail tube protein

Chain SA:  97% ..



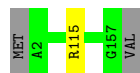
- Molecule 4: Tail tube protein

Chain SC:  97% ..



- Molecule 4: Tail tube protein

Chain SD:  98% ..



- Molecule 4: Tail tube protein

Chain SE:  97% ..



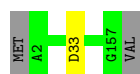
- Molecule 4: Tail tube protein

Chain SF:  98% ..



- Molecule 4: Tail tube protein

Chain Sk:  98% ..



- Molecule 4: Tail tube protein

Chain Sl:  97% ..



- Molecule 4: Tail tube protein

Chain Sm:  96% ..



- Molecule 4: Tail tube protein

Chain Sn:  98% ..



- Molecule 4: Tail tube protein

Chain So:  97% ..



- Molecule 4: Tail tube protein

Chain Sp:  97% ..



- Molecule 4: Tail tube protein

Chain Se:  97% ..



- Molecule 4: Tail tube protein

Chain Sf:  97% ..



- Molecule 4: Tail tube protein

Chain Sg:  97% ..



- Molecule 4: Tail tube protein

Chain Sh:  97% ..



- Molecule 4: Tail tube protein

Chain Si:  97% ..

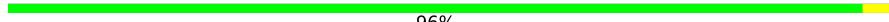


- Molecule 4: Tail tube protein

Chain Sj:  97% ..



- Molecule 4: Tail tube protein

Chain SY:  96% ..



- Molecule 4: Tail tube protein

Chain SZ:  97% ..



- Molecule 4: Tail tube protein

Chain Sa:  96% ..



- Molecule 4: Tail tube protein

Chain Sb:  96% ..



- Molecule 4: Tail tube protein

Chain Sc:  96% ..



- Molecule 4: Tail tube protein

Chain Sd:  96% ..



- Molecule 4: Tail tube protein

Chain B1:  97% ..



- Molecule 4: Tail tube protein

Chain B2:  97% ..



- Molecule 4: Tail tube protein

Chain B3:  95% ..



- Molecule 4: Tail tube protein

Chain B4:  97% ..



- Molecule 4: Tail tube protein

Chain B5:  97% ..



- Molecule 4: Tail tube protein

Chain B6:  94% ..



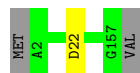
- Molecule 4: Tail tube protein

Chain Sw:  97% ..



- Molecule 4: Tail tube protein

Chain Sx:  98% ..



- Molecule 4: Tail tube protein

Chain Sy:  97% ..



- Molecule 4: Tail tube protein

Chain Sz:  98% ..



- Molecule 4: Tail tube protein

Chain S1:  97% ..



- Molecule 4: Tail tube protein



Chain S2:  97% ..



- Molecule 4: Tail tube protein

Chain Sq:  97% ..



- Molecule 4: Tail tube protein

Chain Sr:  97% ..



- Molecule 4: Tail tube protein

Chain Ss:  97% ...



- Molecule 4: Tail tube protein

Chain St:  98% ..



- Molecule 4: Tail tube protein

Chain Su:  97% ..



- Molecule 4: Tail tube protein

Chain Sv:  97% ..



- Molecule 4: Tail tube protein

Chain P1:  97% ...



- Molecule 4: Tail tube protein

Chain P2:  97% ..



- Molecule 4: Tail tube protein

Chain P3:  97% ..



- Molecule 4: Tail tube protein

Chain P4:  98% ..



- Molecule 4: Tail tube protein

Chain P5:  98% ..



- Molecule 4: Tail tube protein

Chain P6:  98% ..



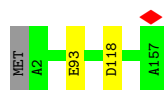
- Molecule 5: SPP1 gp17-like tail completion protein

Chain Pa:  98% ..



- Molecule 5: SPP1 gp17-like tail completion protein

Chain Pb:  98% ..



- Molecule 5: SPP1 gp17-like tail completion protein

Chain Pc:  97% ..



- Molecule 5: SPP1 gp17-like tail completion protein

Chain Pd:  98% ..



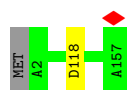
- Molecule 5: SPP1 gp17-like tail completion protein

Chain Pe:  97% ..



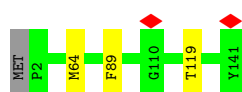
- Molecule 5: SPP1 gp17-like tail completion protein

Chain Pf:  99% ..



- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PT:  97% ..



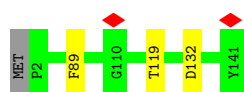
- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PM:  98% ..



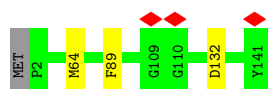
- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PN:  97% ..



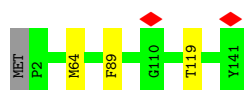
- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PO:  97% ..



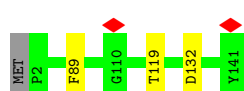
- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PP:  97% ..



- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PQ:  97% ..



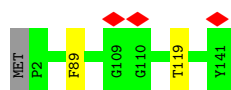
- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PR:  97% ..



- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PS:  98% ..

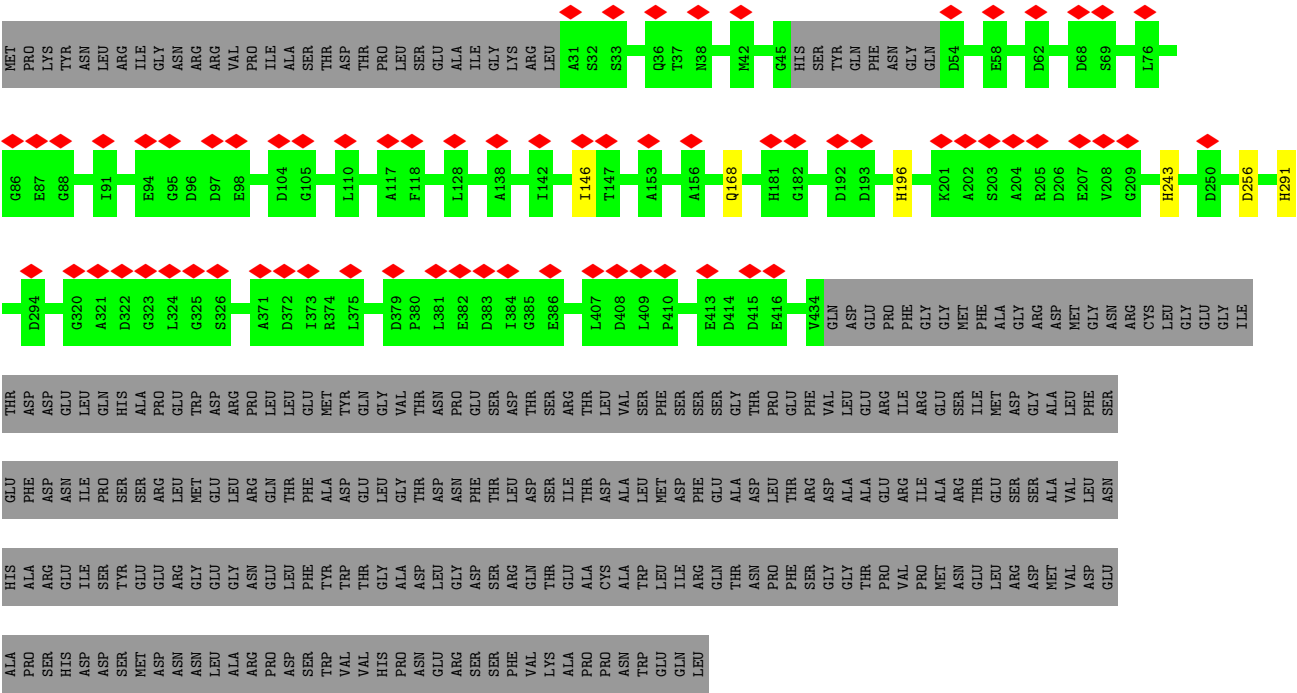


- Molecule 6: HK97 gp6-like/SPP1 gp15-like head-tail connector

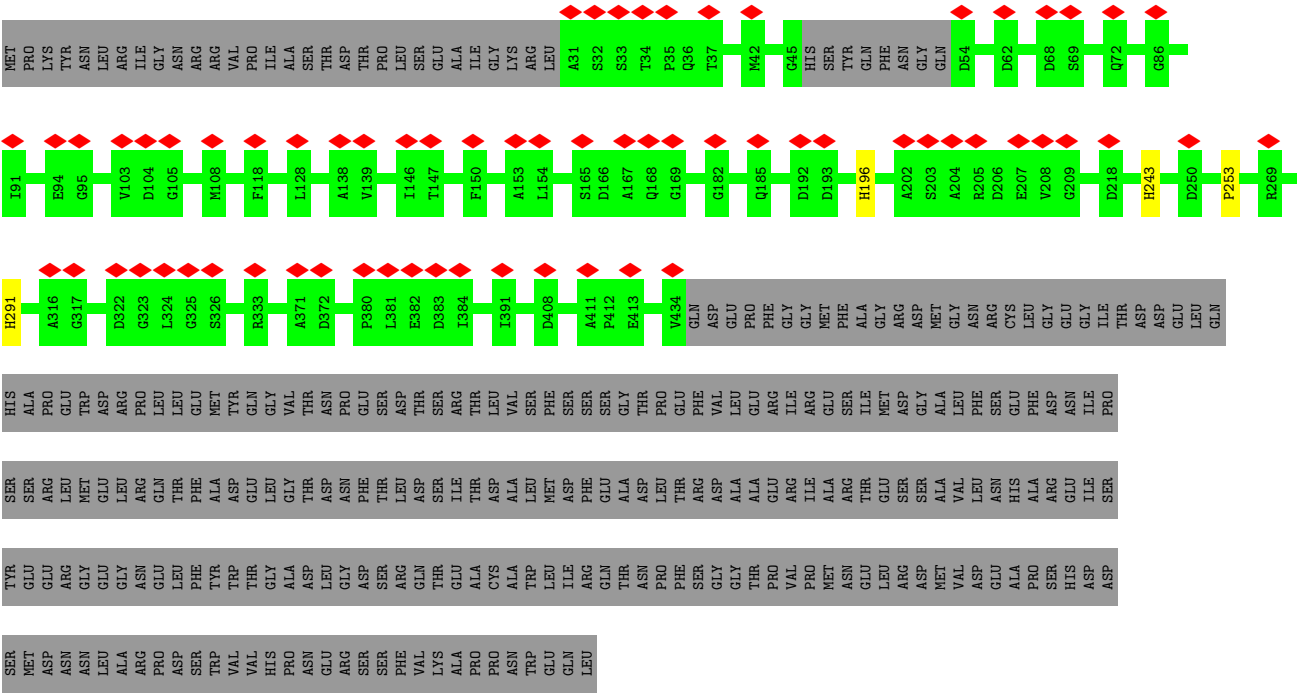
Chain PU:  98% ...







• Molecule 7: Portal protein



• Molecule 7: Portal protein

- Molecule 7: Portal protein

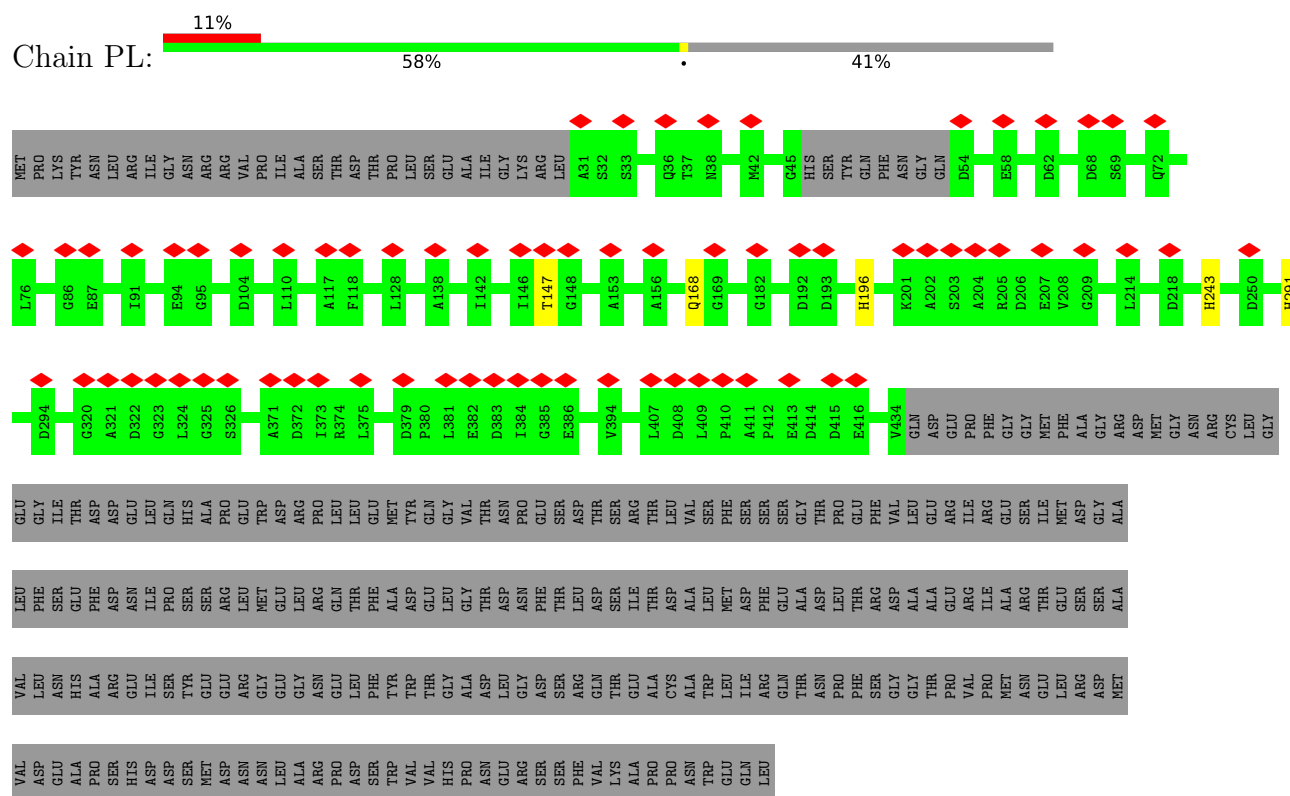
- Molecule 7: Portal protein



- Molecule 7: Portal protein

- Molecule 7: Portal protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116880	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 ( $e^-/\text{\AA}^2$ )	50, 54.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k), 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	0.006	Depositor
Map size ( $\text{\AA}$ )	899.328, 899.328, 899.328	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.171, 1.171, 1.171	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	BD	0.70	0/7332	1.25	21/10023 (0.2%)
1	BE	0.71	0/7332	1.26	22/10023 (0.2%)
1	BF	0.75	0/7332	1.30	17/10023 (0.2%)
2	QE	0.54	0/2534	1.28	3/3428 (0.1%)
2	QF	0.53	0/2440	1.29	5/3299 (0.2%)
2	QG	0.53	0/2534	1.29	1/3428 (0.0%)
2	QH	0.53	0/2440	1.29	9/3299 (0.3%)
2	QI	0.54	0/2534	1.27	3/3428 (0.1%)
2	QJ	0.53	0/2440	1.29	8/3299 (0.2%)
3	BA	0.58	0/2175	0.95	0/2970
3	BB	0.59	0/2175	0.97	2/2970 (0.1%)
3	BC	0.58	0/2175	0.97	0/2970
4	B1	0.57	0/1224	0.88	1/1672 (0.1%)
4	B2	0.58	0/1224	0.92	1/1672 (0.1%)
4	B3	0.57	0/1224	0.91	1/1672 (0.1%)
4	B4	0.57	0/1224	0.91	1/1672 (0.1%)
4	B5	0.58	0/1224	0.92	4/1672 (0.2%)
4	B6	0.58	0/1224	0.93	3/1672 (0.2%)
4	P1	0.57	0/1224	0.92	2/1672 (0.1%)
4	P2	0.57	0/1224	0.92	1/1672 (0.1%)
4	P3	0.57	0/1224	0.94	1/1672 (0.1%)
4	P4	0.57	0/1224	0.93	1/1672 (0.1%)
4	P5	0.57	0/1224	0.92	1/1672 (0.1%)
4	P6	0.57	0/1224	0.93	1/1672 (0.1%)
4	S1	0.59	0/1224	0.92	2/1672 (0.1%)
4	S2	0.58	0/1224	0.90	1/1672 (0.1%)
4	SA	0.57	0/1224	0.93	2/1672 (0.1%)
4	SB	0.58	0/1224	0.93	2/1672 (0.1%)
4	SC	0.58	0/1224	0.93	1/1672 (0.1%)
4	SD	0.57	0/1224	0.92	0/1672
4	SE	0.57	0/1224	0.92	1/1672 (0.1%)
4	SF	0.57	0/1224	0.91	0/1672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	SG	0.58	0/1224	0.91	1/1672 (0.1%)
4	SH	0.58	0/1224	0.91	2/1672 (0.1%)
4	SI	0.58	0/1224	0.90	1/1672 (0.1%)
4	SJ	0.58	0/1224	0.90	1/1672 (0.1%)
4	SK	0.58	0/1224	0.90	0/1672
4	SL	0.58	0/1224	0.90	1/1672 (0.1%)
4	SM	0.59	0/1224	0.90	0/1672
4	SN	0.58	0/1224	0.90	1/1672 (0.1%)
4	SO	0.58	0/1224	0.89	1/1672 (0.1%)
4	SP	0.59	0/1224	0.90	0/1672
4	SQ	0.59	0/1224	0.91	1/1672 (0.1%)
4	SR	0.58	0/1224	0.90	1/1672 (0.1%)
4	SS	0.58	0/1224	0.91	0/1672
4	ST	0.58	0/1224	0.90	2/1672 (0.1%)
4	SU	0.58	0/1224	0.89	0/1672
4	SV	0.58	0/1224	0.89	1/1672 (0.1%)
4	SW	0.58	0/1224	0.91	1/1672 (0.1%)
4	SX	0.58	0/1224	0.90	2/1672 (0.1%)
4	SY	0.58	0/1224	0.91	1/1672 (0.1%)
4	SZ	0.58	0/1224	0.92	2/1672 (0.1%)
4	Sa	0.58	0/1224	0.89	1/1672 (0.1%)
4	Sb	0.58	0/1224	0.92	2/1672 (0.1%)
4	Sc	0.59	0/1224	0.92	2/1672 (0.1%)
4	Sd	0.58	0/1224	0.90	1/1672 (0.1%)
4	Se	0.58	0/1224	0.92	2/1672 (0.1%)
4	Sf	0.58	0/1224	0.91	1/1672 (0.1%)
4	Sg	0.58	0/1224	0.92	2/1672 (0.1%)
4	Sh	0.58	0/1224	0.91	1/1672 (0.1%)
4	Si	0.58	0/1224	0.92	2/1672 (0.1%)
4	Sj	0.57	0/1224	0.93	1/1672 (0.1%)
4	Sk	0.58	0/1224	0.91	1/1672 (0.1%)
4	Sl	0.59	0/1224	0.92	1/1672 (0.1%)
4	Sm	0.57	0/1224	0.92	2/1672 (0.1%)
4	Sn	0.58	0/1224	0.91	0/1672
4	So	0.58	0/1224	0.91	2/1672 (0.1%)
4	Sp	0.59	0/1224	0.90	1/1672 (0.1%)
4	Sq	0.59	0/1224	0.92	1/1672 (0.1%)
4	Sr	0.58	0/1224	0.92	0/1672
4	Ss	0.59	0/1224	0.95	3/1672 (0.2%)
4	St	0.59	0/1224	0.90	0/1672
4	Su	0.59	0/1224	0.92	1/1672 (0.1%)
4	Sv	0.59	0/1224	0.92	2/1672 (0.1%)
4	Sw	0.59	0/1224	0.93	2/1672 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	Sx	0.59	0/1224	0.90	1/1672 (0.1%)
4	Sy	0.58	0/1224	0.89	1/1672 (0.1%)
4	Sz	0.58	0/1224	0.90	1/1672 (0.1%)
5	Pa	0.55	0/1248	1.04	0/1709
5	Pb	0.55	0/1248	1.06	1/1709 (0.1%)
5	Pc	0.56	0/1248	1.04	1/1709 (0.1%)
5	Pd	0.56	0/1248	1.05	1/1709 (0.1%)
5	Pe	0.56	0/1248	1.07	0/1709
5	Pf	0.55	0/1248	1.05	1/1709 (0.1%)
6	PM	0.53	0/1105	1.15	1/1492 (0.1%)
6	PN	0.54	0/1105	1.14	1/1492 (0.1%)
6	PO	0.54	0/1105	1.13	1/1492 (0.1%)
6	PP	0.56	0/1105	1.15	1/1492 (0.1%)
6	PQ	0.54	0/1105	1.15	1/1492 (0.1%)
6	PR	0.54	0/1105	1.13	1/1492 (0.1%)
6	PS	0.53	0/1105	1.11	1/1492 (0.1%)
6	PT	0.55	0/1105	1.14	1/1492 (0.1%)
6	PU	0.54	0/1105	1.14	1/1492 (0.1%)
6	PV	0.55	0/1105	1.14	1/1492 (0.1%)
6	PW	0.53	0/1105	1.12	1/1492 (0.1%)
6	PX	0.54	0/1105	1.15	1/1492 (0.1%)
7	PA	0.56	0/3117	1.14	0/4226
7	PB	0.56	0/3117	1.15	0/4226
7	PC	0.56	0/3117	1.13	0/4226
7	PD	0.56	0/3117	1.14	1/4226 (0.0%)
7	PE	0.56	0/3117	1.14	0/4226
7	PF	0.56	0/3117	1.15	0/4226
7	PG	0.56	0/3117	1.13	0/4226
7	PH	0.56	0/3117	1.14	0/4226
7	PI	0.57	0/3117	1.14	0/4226
7	PJ	0.56	0/3117	1.14	0/4226
7	PK	0.56	0/3117	1.13	0/4226
7	PL	0.56	0/3117	1.15	0/4226
All	All	0.59	0/182379	1.07	188/248382 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	BE	0	3
1	BF	0	3
6	PO	0	1
6	PT	0	1
6	PV	0	1
All	All	0	10

There are no bond length outliers.

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	QH	81	ASP	CA-CB-CG	7.31	119.91	112.60
2	QJ	285	ASP	CA-C-N	7.06	125.98	120.33
2	QJ	285	ASP	C-N-CA	7.06	125.98	120.33
1	BD	756	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	BF	662	ARG	NE-CZ-NH2	6.86	125.37	119.20
1	BF	198	GLN	N-CA-C	6.72	114.27	108.22
2	QJ	81	ASP	CA-CB-CG	6.56	119.16	112.60
1	BD	877	ASP	CA-CB-CG	6.55	119.15	112.60
2	QJ	119	PHE	CA-CB-CG	6.47	120.27	113.80
2	QF	119	PHE	CA-CB-CG	6.47	120.27	113.80
1	BE	120	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	BE	858	ARG	NE-CZ-NH2	6.20	124.78	119.20
6	PX	89	PHE	CA-CB-CG	6.16	119.96	113.80
1	BF	857	ASN	CA-CB-CG	6.11	118.71	112.60
1	BD	928	ARG	NE-CZ-NH2	6.06	124.66	119.20
2	QH	119	PHE	CA-CB-CG	6.06	119.86	113.80
1	BF	98	ARG	NE-CZ-NH2	6.05	124.65	119.20
6	PO	89	PHE	CA-CB-CG	6.04	119.84	113.80
1	BF	265	ARG	NE-CZ-NH2	6.03	124.63	119.20
6	PR	89	PHE	CA-CB-CG	6.01	119.81	113.80
2	QF	212	ASP	CA-CB-CG	6.01	118.61	112.60
1	BD	265	ARG	NE-CZ-NH2	6.01	124.61	119.20
4	P3	22	ASP	CA-CB-CG	5.94	118.54	112.60
6	PP	89	PHE	CA-CB-CG	5.93	119.73	113.80
1	BD	662	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	BE	97	ARG	NE-CZ-NH2	5.89	124.50	119.20
6	PT	89	PHE	CA-CB-CG	5.88	119.68	113.80
4	P6	22	ASP	CA-CB-CG	5.88	118.47	112.60
1	BE	265	ARG	NE-CZ-NH2	5.87	124.49	119.20
1	BD	290	ARG	NE-CZ-NH2	5.87	124.48	119.20
4	Sc	33	ASP	CA-CB-CG	5.85	118.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BE	2	PRO	CA-N-CD	-5.84	103.82	112.00
4	P4	22	ASP	CA-CB-CG	5.83	118.43	112.60
4	Ss	33	ASP	CA-CB-CG	5.82	118.42	112.60
2	QG	228	PHE	CA-CB-CG	5.81	119.61	113.80
1	BD	601	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	QF	81	ASP	CA-CB-CG	5.80	118.40	112.60
1	BF	928	ARG	NE-CZ-NH2	5.77	124.39	119.20
6	PV	89	PHE	CA-CB-CG	5.77	119.57	113.80
1	BD	89	ARG	NE-CZ-NH2	5.76	124.38	119.20
4	B6	33	ASP	CA-CB-CG	5.71	118.31	112.60
1	BF	886	ASP	CA-CB-CG	5.71	118.31	112.60
4	Sy	22	ASP	CA-CB-CG	5.68	118.28	112.60
1	BE	290	ARG	NE-CZ-NH2	5.66	124.30	119.20
2	QF	257	PHE	CA-CB-CG	5.66	119.45	113.80
4	B3	22	ASP	CA-CB-CG	5.64	118.24	112.60
2	QI	157	PHE	CA-CB-CG	5.63	119.43	113.80
4	Sx	22	ASP	CA-CB-CG	5.62	118.22	112.60
4	Sm	33	ASP	CA-CB-CG	5.62	118.22	112.60
4	ST	22	ASP	CA-CB-CG	5.62	118.22	112.60
1	BE	928	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	BF	347	ARG	NE-CZ-NH2	5.60	124.24	119.20
4	Ss	115	ARG	CG-CD-NE	5.59	124.30	112.00
1	BE	89	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	BF	487	ARG	NE-CZ-NH2	5.59	124.23	119.20
6	PN	89	PHE	CA-CB-CG	5.59	119.39	113.80
1	BF	164	ARG	NE-CZ-NH2	5.55	124.19	119.20
4	SO	33	ASP	CA-CB-CG	5.55	118.15	112.60
4	So	33	ASP	CA-CB-CG	5.54	118.14	112.60
1	BF	515	ARG	CA-C-N	5.54	126.35	121.58
1	BF	515	ARG	C-N-CA	5.54	126.35	121.58
4	P2	22	ASP	CA-CB-CG	5.54	118.14	112.60
1	BD	363	ARG	NE-CZ-NH2	5.53	124.17	119.20
4	SQ	33	ASP	CA-CB-CG	5.53	118.13	112.60
4	Sg	33	ASP	CA-CB-CG	5.52	118.12	112.60
4	SX	22	ASP	CA-CB-CG	5.52	118.12	112.60
4	SC	22	ASP	CA-CB-CG	5.52	118.12	112.60
1	BE	487	ARG	NE-CZ-NH2	5.52	124.16	119.20
4	Sb	22	ASP	CA-CB-CG	5.51	118.11	112.60
1	BE	953	ASP	CA-CB-CG	5.50	118.10	112.60
4	SE	22	ASP	CA-CB-CG	5.50	118.10	112.60
1	BD	515	ARG	NE-CZ-NH2	5.49	124.14	119.20
4	SB	33	ASP	CA-CB-CG	5.49	118.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Sq	22	ASP	CA-CB-CG	5.49	118.09	112.60
1	BD	515	ARG	CA-C-N	5.47	126.29	121.58
1	BD	515	ARG	C-N-CA	5.47	126.29	121.58
4	SA	22	ASP	CA-CB-CG	5.46	118.06	112.60
4	Sm	22	ASP	CA-CB-CG	5.46	118.06	112.60
1	BF	89	ARG	NE-CZ-NH2	5.45	124.11	119.20
2	QE	285	ASP	CA-C-N	5.45	124.69	120.33
2	QE	285	ASP	C-N-CA	5.45	124.69	120.33
4	SR	33	ASP	CA-CB-CG	5.44	118.04	112.60
4	B5	22	ASP	CA-CB-CG	5.44	118.04	112.60
4	SZ	22	ASP	CA-CB-CG	5.43	118.03	112.60
4	Sw	22	ASP	CA-CB-CG	5.42	118.02	112.60
2	QJ	40	PHE	CA-CB-CG	5.42	119.22	113.80
4	SY	22	ASP	CA-CB-CG	5.42	118.02	112.60
4	SW	22	ASP	CA-CB-CG	5.41	118.01	112.60
1	BD	487	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	QJ	104	GLU	CB-CG-CD	5.39	121.77	112.60
4	Ss	22	ASP	CA-CB-CG	5.38	117.98	112.60
4	P1	22	ASP	CA-CB-CG	5.38	117.98	112.60
4	Su	22	ASP	CA-CB-CG	5.37	117.97	112.60
4	Sj	54	ASP	CB-CA-C	5.37	118.07	109.27
4	P5	22	ASP	CA-CB-CG	5.37	117.97	112.60
4	S1	22	ASP	CA-CB-CG	5.36	117.96	112.60
4	B6	22	ASP	CA-CB-CG	5.36	117.96	112.60
4	Sv	33	ASP	CA-CB-CG	5.35	117.95	112.60
1	BE	98	ARG	NE-CZ-NH2	5.35	124.01	119.20
3	BB	3	ASP	CA-CB-CG	5.35	117.95	112.60
4	Sz	22	ASP	CA-CB-CG	5.35	117.95	112.60
4	SB	22	ASP	CA-CB-CG	5.34	117.94	112.60
4	S2	22	ASP	CA-CB-CG	5.33	117.94	112.60
4	So	22	ASP	CA-CB-CG	5.32	117.92	112.60
4	Si	22	ASP	CA-CB-CG	5.30	117.90	112.60
4	SV	22	ASP	CA-CB-CG	5.29	117.89	112.60
6	PM	89	PHE	CA-CB-CG	5.29	119.09	113.80
4	Sc	22	ASP	CA-CB-CG	5.28	117.88	112.60
1	BE	515	ARG	CA-C-N	5.28	125.67	121.61
1	BE	515	ARG	C-N-CA	5.28	125.67	121.61
4	Sg	22	ASP	CA-CB-CG	5.27	117.87	112.60
4	Se	33	ASP	CA-CB-CG	5.27	117.87	112.60
1	BD	408	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	BE	662	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	Sf	22	ASP	CA-CB-CG	5.26	117.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	PW	89	PHE	CA-CB-CG	5.26	119.06	113.80
4	S1	33	ASP	CA-CB-CG	5.26	117.86	112.60
2	QI	119	PHE	CA-CB-CG	5.25	119.05	113.80
4	SJ	22	ASP	CA-CB-CG	5.25	117.85	112.60
4	Se	22	ASP	CA-CB-CG	5.25	117.85	112.60
1	BE	178	PHE	CA-CB-CG	5.24	119.04	113.80
1	BF	425	ASN	CA-CB-CG	5.24	117.84	112.60
5	Pd	118	ASP	CA-CB-CG	5.24	117.84	112.60
4	SH	33	ASP	CA-CB-CG	5.23	117.83	112.60
4	SH	22	ASP	CA-CB-CG	5.23	117.83	112.60
2	QI	192	ASP	CA-CB-CG	5.23	117.83	112.60
1	BF	97	ARG	NE-CZ-NH2	5.22	123.90	119.20
4	Sk	33	ASP	CA-CB-CG	5.21	117.81	112.60
4	SZ	33	ASP	CA-CB-CG	5.21	117.81	112.60
4	Sw	33	ASP	CA-CB-CG	5.21	117.81	112.60
5	Pb	118	ASP	CA-CB-CG	5.20	117.80	112.60
4	B5	33	ASP	CA-CB-CG	5.20	117.80	112.60
5	Pf	118	ASP	CA-CB-CG	5.20	117.80	112.60
4	Sv	22	ASP	CA-CB-CG	5.20	117.80	112.60
1	BE	527	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	BD	938	THR	N-CA-C	5.19	119.10	112.87
2	QE	119	PHE	CA-CB-CG	5.19	118.99	113.80
6	PU	89	PHE	CA-CB-CG	5.18	118.98	113.80
4	B4	22	ASP	CA-CB-CG	5.18	117.78	112.60
4	Sa	22	ASP	CA-CB-CG	5.18	117.78	112.60
2	QJ	228	PHE	CA-CB-CG	5.17	118.97	113.80
5	Pc	118	ASP	CA-CB-CG	5.17	117.77	112.60
1	BF	743	HIS	CB-CG-CD2	-5.16	124.49	131.20
2	QH	100	ASP	CA-C-N	5.16	127.51	120.54
2	QH	100	ASP	C-N-CA	5.16	127.51	120.54
2	QF	278	ILE	CB-CA-C	5.16	118.95	111.88
4	SN	33	ASP	CA-CB-CG	5.16	117.76	112.60
4	B5	47	THR	CA-C-N	5.15	128.60	120.47
4	B5	47	THR	C-N-CA	5.15	128.60	120.47
2	QJ	218	ASP	CA-CB-CG	5.15	117.75	112.60
6	PQ	89	PHE	CA-CB-CG	5.14	118.94	113.80
1	BD	178	PHE	CA-CB-CG	5.14	118.94	113.80
1	BE	878	ASN	CA-CB-CG	5.13	117.73	112.60
1	BE	120	ARG	CD-NE-CZ	5.13	131.58	124.40
1	BE	121	ARG	NE-CZ-NH2	5.13	123.81	119.20
4	B6	59	TYR	CB-CA-C	5.12	120.60	110.42
4	SG	22	ASP	CA-CB-CG	5.11	117.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	SI	22	ASP	CA-CB-CG	5.11	117.71	112.60
1	BE	601	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	BD	98	ARG	NE-CZ-NH2	5.10	123.79	119.20
4	Sh	22	ASP	CA-CB-CG	5.10	117.70	112.60
1	BE	207	ARG	NE-CZ-NH2	5.08	123.77	119.20
2	QH	209	PHE	CA-CB-CG	5.08	118.88	113.80
4	Sd	22	ASP	CA-CB-CG	5.08	117.68	112.60
4	P1	33	ASP	CA-CB-CG	5.08	117.68	112.60
1	BD	52	ASP	CA-CB-CG	5.08	117.68	112.60
2	QH	162	MET	CA-C-N	5.07	127.04	120.44
2	QH	162	MET	C-N-CA	5.07	127.04	120.44
4	B1	22	ASP	CA-CB-CG	5.07	117.67	112.60
6	PS	89	PHE	CA-CB-CG	5.06	118.86	113.80
1	BD	97	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	BD	120	ARG	NE-CZ-NH2	5.06	123.75	119.20
7	PD	256	ASP	CA-CB-CG	5.06	117.66	112.60
1	BF	103	GLN	OE1-CD-NE2	-5.05	117.55	122.60
4	ST	33	ASP	CA-CB-CG	5.05	117.65	112.60
3	BB	16	PRO	N-CA-C	5.05	122.87	112.47
2	QH	65	GLN	CA-C-N	5.04	124.36	120.33
2	QH	65	GLN	C-N-CA	5.04	124.36	120.33
4	SL	130	ASP	CA-CB-CG	5.04	117.64	112.60
4	SX	33	ASP	CA-CB-CG	5.04	117.64	112.60
4	SA	130	ASP	CA-CB-CG	5.04	117.64	112.60
4	B2	22	ASP	CA-CB-CG	5.03	117.63	112.60
1	BE	515	ARG	NE-CZ-NH2	5.03	123.72	119.20
4	Sl	22	ASP	CA-CB-CG	5.02	117.62	112.60
4	Si	33	ASP	CA-CB-CG	5.01	117.61	112.60
4	Sb	33	ASP	CA-CB-CG	5.01	117.61	112.60
4	Sp	33	ASP	CA-CB-CG	5.00	117.60	112.60
1	BD	61	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BD	148	ARG	Sidechain
1	BE	304	TYR	Sidechain
1	BE	662	ARG	Sidechain
1	BE	97	ARG	Sidechain
1	BF	207	ARG	Sidechain
1	BF	899	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	BF	941	ARG	Sidechain
6	PO	64	MET	Peptide
6	PT	64	MET	Peptide
6	PV	64	MET	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BD	7212	0	6782	4	0
1	BE	7212	0	6784	11	0
1	BF	7212	0	6784	1	0
2	QE	2498	0	2395	9	0
2	QF	2409	0	2324	10	0
2	QG	2498	0	2395	11	0
2	QH	2409	0	2322	14	0
2	QI	2498	0	2395	11	0
2	QJ	2409	0	2324	6	0
3	BA	2136	0	2127	2	0
3	BB	2136	0	2127	0	0
3	BC	2136	0	2127	3	0
4	B1	1196	0	1094	0	0
4	B2	1196	0	1094	1	0
4	B3	1196	0	1094	3	0
4	B4	1196	0	1094	0	0
4	B5	1196	0	1094	0	0
4	B6	1196	0	1094	2	0
4	P1	1196	0	1094	0	0
4	P2	1196	0	1094	0	0
4	P3	1196	0	1094	0	0
4	P4	1196	0	1094	0	0
4	P5	1196	0	1094	0	0
4	P6	1196	0	1094	0	0
4	S1	1196	0	1094	0	0
4	S2	1196	0	1094	1	0
4	SA	1196	0	1094	0	0
4	SB	1196	0	1094	0	0
4	SC	1196	0	1094	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	SD	1196	0	1094	0	0
4	SE	1196	0	1094	0	0
4	SF	1196	0	1094	0	0
4	SG	1196	0	1094	0	0
4	SH	1196	0	1094	0	0
4	SI	1196	0	1094	0	0
4	SJ	1196	0	1094	0	0
4	SK	1196	0	1094	0	0
4	SL	1196	0	1094	0	0
4	SM	1196	0	1094	0	0
4	SN	1196	0	1094	1	0
4	SO	1196	0	1094	0	0
4	SP	1196	0	1094	0	0
4	SQ	1196	0	1094	0	0
4	SR	1196	0	1094	0	0
4	SS	1196	0	1094	0	0
4	ST	1196	0	1094	1	0
4	SU	1196	0	1094	0	0
4	SV	1196	0	1094	0	0
4	SW	1196	0	1094	0	0
4	SX	1196	0	1094	0	0
4	SY	1196	0	1094	1	0
4	SZ	1196	0	1094	0	0
4	Sa	1196	0	1094	1	0
4	Sb	1196	0	1094	1	0
4	Sc	1196	0	1094	1	0
4	Sd	1196	0	1094	2	0
4	Se	1196	0	1094	0	0
4	Sf	1196	0	1094	0	0
4	Sg	1196	0	1094	0	0
4	Sh	1196	0	1094	0	0
4	Si	1196	0	1094	0	0
4	Sj	1196	0	1094	0	0
4	Sk	1196	0	1094	0	0
4	Sl	1196	0	1094	0	0
4	Sm	1196	0	1094	0	0
4	Sn	1196	0	1094	0	0
4	So	1196	0	1094	0	0
4	Sp	1196	0	1094	0	0
4	Sq	1196	0	1094	0	0
4	Sr	1196	0	1094	2	0
4	Ss	1196	0	1094	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	St	1196	0	1094	0	0
4	Su	1196	0	1094	0	0
4	Sv	1196	0	1094	0	0
4	Sw	1196	0	1094	0	0
4	Sx	1196	0	1094	0	0
4	Sy	1196	0	1094	1	0
4	Sz	1196	0	1094	0	0
5	Pa	1220	0	1118	0	0
5	Pb	1220	0	1118	0	0
5	Pc	1220	0	1118	1	0
5	Pd	1220	0	1118	0	0
5	Pe	1220	0	1118	0	0
5	Pf	1220	0	1118	0	0
6	PM	1087	0	1018	0	0
6	PN	1087	0	1018	0	0
6	PO	1087	0	1018	0	0
6	PP	1087	0	1018	0	0
6	PQ	1087	0	1018	0	0
6	PR	1087	0	1018	1	0
6	PS	1087	0	1018	0	0
6	PT	1087	0	1018	0	0
6	PU	1087	0	1018	1	0
6	PV	1087	0	1018	1	0
6	PW	1087	0	1018	0	0
6	PX	1087	0	1018	0	0
7	PA	3106	0	2943	0	0
7	PB	3106	0	2943	0	0
7	PC	3106	0	2943	0	0
7	PD	3106	0	2943	0	0
7	PE	3106	0	2943	1	0
7	PF	3106	0	2943	1	0
7	PG	3106	0	2943	0	0
7	PH	3106	0	2943	0	0
7	PI	3106	0	2943	1	0
7	PJ	3106	0	2943	0	0
7	PK	3106	0	2943	0	0
7	PL	3106	0	2943	0	0
8	BD	1	0	0	0	0
8	BE	1	0	0	0	0
8	BF	1	0	0	0	0
8	PM	1	0	0	0	0
8	PN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	PO	1	0	0	0	0
8	PP	1	0	0	0	0
8	PQ	1	0	0	0	0
8	PR	1	0	0	0	0
8	PS	1	0	0	0	0
8	PT	1	0	0	0	0
8	PU	2	0	0	0	0
8	PV	1	0	0	0	0
8	PW	1	0	0	0	0
All	All	179352	0	167330	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (72) 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:BD:225:GLU:OE2	2:QJ:337:ARG:NH1	1.91	1.03
1:BD:96:GLU:OE2	2:QH:330:ARG:NH1	2.32	0.63
5:Pe:136:THR:HG21	6:PR:37:TRP:HA	1.79	0.63
2:QG:166:ALA:HB2	2:QH:168:GLN:HG2	1.84	0.59
1:BD:281:ASP:OD2	1:BE:800:ARG:NH1	2.33	0.59
2:QE:130:ILE:HG23	2:QF:135:VAL:CG2	2.32	0.59
2:QI:130:ILE:HG23	2:QJ:135:VAL:CG2	2.34	0.57
2:QI:105:VAL:O	2:QI:109:THR:HG23	2.07	0.55
2:QJ:48:MET:HG2	2:QE:47:ALA:HB2	1.88	0.54
2:QG:188:LEU:HD21	2:QH:186:THR:HB	1.89	0.54
1:BD:280:GLU:HG3	1:BE:378:ILE:HG13	1.91	0.53
2:QE:105:VAL:O	2:QE:109:THR:HG23	2.10	0.52
2:QH:27:ALA:HA	2:QI:26:THR:HG22	1.92	0.51
2:QE:171:ASP:O	2:QE:175:THR:HG23	2.11	0.51
2:QE:22:ALA:O	2:QE:26:THR:HG23	2.12	0.50
1:BE:111:GLU:CD	2:QF:322:ARG:HH12	2.20	0.50
4:Sr:130:ASP:HA	4:Ss:115:ARG:NH1	2.27	0.49
2:QH:181:PRO:HG2	2:QI:175:THR:HG22	1.95	0.49
4:Sd:13:GLY:HA2	4:Sd:106:THR:HG22	1.94	0.49
2:QG:22:ALA:O	2:QG:26:THR:HG23	2.13	0.48
2:QG:105:VAL:O	2:QG:109:THR:HG23	2.12	0.48
4:B6:44:GLU:HG3	4:B6:53:ARG:HD2	1.96	0.47
2:QI:171:ASP:O	2:QI:175:THR:HG23	2.15	0.47
2:QF:112:ALA:O	2:QF:116:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B3:47:THR:HG23	4:B3:54:ASP:HB2	1.96	0.47
1:BE:215:PHE:CE1	3:BA:38:ARG:HG3	2.50	0.46
2:QH:146:THR:HA	2:QH:149:THR:HG23	1.96	0.46
2:QI:22:ALA:O	2:QI:26:THR:HG23	2.16	0.46
1:BE:656:GLU:OE1	1:BE:755:THR:HG22	2.15	0.45
2:QG:166:ALA:CB	2:QH:168:GLN:HG2	2.47	0.45
2:QE:241:ASN:HD22	2:QE:241:ASN:C	2.25	0.45
1:BE:249:LYS:CE	1:BE:263:THR:HG22	2.47	0.45
4:Sa:13:GLY:HA2	4:Sa:106:THR:HG22	1.98	0.45
6:PU:132:ASP:OD2	7:PE:253:PRO:HD3	2.16	0.45
1:BE:59:ASP:OD1	3:BA:185:ARG:NH2	2.49	0.45
7:PF:424:PRO:HA	7:PF:427:MET:HE3	1.98	0.44
1:BE:81:GLU:OE1	3:BC:234:ARG:NH1	2.47	0.44
1:BE:111:GLU:OE1	2:QF:322:ARG:NH1	2.50	0.44
2:QH:48:MET:HG2	2:QI:47:ALA:HB2	2.00	0.44
4:Sr:130:ASP:HA	4:Ss:115:ARG:HH11	1.82	0.44
2:QI:258:THR:HG21	2:QJ:256:LYS:O	2.18	0.43
2:QH:97:SER:HB2	2:QI:100:ASP:OD2	2.19	0.43
2:QJ:37:LEU:HD21	2:QE:36:GLU:H	1.83	0.43
2:QJ:27:ALA:HA	2:QE:26:THR:HG22	2.01	0.43
2:QG:135:VAL:O	2:QG:135:VAL:HG12	2.18	0.42
2:QH:239:GLY:HA2	2:QI:237:GLU:HG3	2.01	0.42
2:QG:112:ALA:HB3	2:QH:116:LEU:HD13	2.02	0.42
6:PV:129:VAL:HG12	6:PV:129:VAL:O	2.20	0.42
3:BC:157:VAL:HG13	3:BC:237:VAL:HG11	2.02	0.42
4:ST:13:GLY:HA2	4:ST:106:THR:HG22	2.01	0.42
4:B6:13:GLY:HA2	4:B6:106:THR:HG22	2.01	0.42
2:QH:286:VAL:N	2:QH:287:PRO:HD3	2.35	0.41
7:PI:424:PRO:HA	7:PI:427:MET:HE3	2.01	0.41
2:QG:112:ALA:CB	2:QH:116:LEU:HD13	2.49	0.41
2:QE:102:LEU:HD13	2:QF:106:ALA:HB2	2.01	0.41
2:QF:103:TYR:O	2:QF:106:ALA:HB3	2.20	0.41
2:QF:105:VAL:O	2:QF:109:THR:HG23	2.20	0.41
1:BE:99:GLU:C	1:BE:100:ASN:HD22	2.28	0.41
2:QG:26:THR:HG22	2:QF:27:ALA:HA	2.03	0.41
1:BE:111:GLU:CD	2:QF:322:ARG:NH1	2.79	0.41
2:QH:112:ALA:O	2:QH:116:LEU:HG	2.20	0.41
4:Sc:91:SER:HB2	4:Sd:148:SER:HB2	2.03	0.41
4:Sb:13:GLY:HA2	4:Sb:106:THR:HG22	2.01	0.41
4:B2:91:SER:HB2	4:B3:148:SER:HB2	2.03	0.41
4:Sy:148:SER:HB2	4:S2:91:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:215:PHE:CD1	3:BC:38:ARG:HG2	2.56	0.41
4:B3:13:GLY:HA2	4:B3:106:THR:HG22	2.03	0.40
2:QG:189:LYS:HE3	2:QF:189:LYS:HD3	2.03	0.40
2:QI:177:ILE:O	2:QI:181:PRO:HD2	2.20	0.40
4:SY:13:GLY:HA2	4:SY:106:THR:HG22	2.04	0.40
2:QG:40:PHE:CD1	2:QG:40:PHE:C	2.99	0.40
4:SN:13:GLY:HA2	4:SN:106:THR:HG22	2.04	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	BD	951/954 (100%)	895 (94%)	56 (6%)	0	100	100
1	BE	951/954 (100%)	911 (96%)	40 (4%)	0	100	100
1	BF	951/954 (100%)	893 (94%)	58 (6%)	0	100	100
2	QE	335/341 (98%)	323 (96%)	11 (3%)	1 (0%)	37	44
2	QF	320/341 (94%)	296 (92%)	24 (8%)	0	100	100
2	QG	335/341 (98%)	317 (95%)	18 (5%)	0	100	100
2	QH	320/341 (94%)	302 (94%)	18 (6%)	0	100	100
2	QI	335/341 (98%)	318 (95%)	17 (5%)	0	100	100
2	QJ	320/341 (94%)	300 (94%)	20 (6%)	0	100	100
3	BA	282/285 (99%)	272 (96%)	10 (4%)	0	100	100
3	BB	282/285 (99%)	272 (96%)	10 (4%)	0	100	100
3	BC	282/285 (99%)	273 (97%)	9 (3%)	0	100	100
4	B1	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
4	B2	154/158 (98%)	150 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B3	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	B4	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	B5	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
4	B6	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	P1	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
4	P2	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	P3	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
4	P4	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	P5	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	P6	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	S1	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	S2	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SA	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	SB	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SC	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SD	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	SE	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SF	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	SG	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SH	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	SI	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	SJ	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SK	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SL	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SM	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SN	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	SO	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	SP	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	SQ	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SR	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	SS	154/158 (98%)	151 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	ST	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	SU	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	SV	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SW	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SX	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	SY	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	SZ	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	Sa	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	Sb	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sc	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sd	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Se	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sf	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sg	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sh	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Si	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sj	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sk	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
4	Sl	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sm	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sn	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
4	So	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sp	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
4	Sq	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sr	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Ss	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	St	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Su	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sv	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sw	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
4	Sx	154/158 (98%)	150 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Sy	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
4	Sz	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
5	Pa	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
5	Pb	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
5	Pc	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
5	Pd	154/157 (98%)	152 (99%)	2 (1%)	0	100	100
5	Pe	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
5	Pf	154/157 (98%)	151 (98%)	3 (2%)	0	100	100
6	PM	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
6	PN	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
6	PO	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
6	PP	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
6	PQ	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
6	PR	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
6	PS	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
6	PT	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
6	PU	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
6	PV	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
6	PW	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
6	PX	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
7	PA	389/675 (58%)	379 (97%)	10 (3%)	0	100	100
7	PB	389/675 (58%)	382 (98%)	7 (2%)	0	100	100
7	PC	389/675 (58%)	376 (97%)	13 (3%)	0	100	100
7	PD	389/675 (58%)	380 (98%)	9 (2%)	0	100	100
7	PE	389/675 (58%)	379 (97%)	10 (3%)	0	100	100
7	PF	389/675 (58%)	377 (97%)	12 (3%)	0	100	100
7	PG	389/675 (58%)	377 (97%)	12 (3%)	0	100	100
7	PH	389/675 (58%)	377 (97%)	12 (3%)	0	100	100
7	PI	389/675 (58%)	377 (97%)	12 (3%)	0	100	100
7	PJ	389/675 (58%)	379 (97%)	10 (3%)	0	100	100
7	PK	389/675 (58%)	375 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	PL	389/675 (58%)	381 (98%)	8 (2%)	0	100	100
All	All	23076/26925 (86%)	22362 (97%)	713 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QE	127	ASN

### 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	BD	799/800 (100%)	791 (99%)	8 (1%)	73	82
1	BE	799/800 (100%)	791 (99%)	8 (1%)	73	82
1	BF	799/800 (100%)	783 (98%)	16 (2%)	50	63
2	QE	259/262 (99%)	252 (97%)	7 (3%)	40	52
2	QF	251/262 (96%)	241 (96%)	10 (4%)	27	36
2	QG	259/262 (99%)	251 (97%)	8 (3%)	35	47
2	QH	251/262 (96%)	244 (97%)	7 (3%)	38	51
2	QI	259/262 (99%)	251 (97%)	8 (3%)	35	47
2	QJ	251/262 (96%)	245 (98%)	6 (2%)	44	57
3	BA	238/239 (100%)	234 (98%)	4 (2%)	56	69
3	BB	238/239 (100%)	235 (99%)	3 (1%)	65	77
3	BC	238/239 (100%)	235 (99%)	3 (1%)	65	77
4	B1	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	B2	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	B3	129/131 (98%)	129 (100%)	0	100	100
4	B4	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	B5	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B6	129/131 (98%)	129 (100%)	0	100	100
4	P1	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	P2	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	P3	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	P4	129/131 (98%)	129 (100%)	0	100	100
4	P5	129/131 (98%)	129 (100%)	0	100	100
4	P6	129/131 (98%)	129 (100%)	0	100	100
4	S1	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	S2	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SA	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SB	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SC	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SD	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SE	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SF	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SG	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SH	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SI	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SJ	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SK	129/131 (98%)	129 (100%)	0	100	100
4	SL	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	SM	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SN	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SO	129/131 (98%)	129 (100%)	0	100	100
4	SP	129/131 (98%)	129 (100%)	0	100	100
4	SQ	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SR	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SS	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	ST	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	SU	129/131 (98%)	129 (100%)	0	100	100
4	SV	129/131 (98%)	128 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SW	129/131 (98%)	129 (100%)	0	100	100
4	SX	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	SY	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	SZ	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sa	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	Sb	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sc	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	Sd	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Se	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sf	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	Sg	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sh	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Si	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sj	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sk	129/131 (98%)	129 (100%)	0	100	100
4	Sl	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sm	129/131 (98%)	127 (98%)	2 (2%)	58	71
4	Sn	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	So	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sp	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sq	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sr	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Ss	129/131 (98%)	129 (100%)	0	100	100
4	St	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Su	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sv	129/131 (98%)	128 (99%)	1 (1%)	79	87
4	Sw	129/131 (98%)	129 (100%)	0	100	100
4	Sx	129/131 (98%)	129 (100%)	0	100	100
4	Sy	129/131 (98%)	129 (100%)	0	100	100
4	Sz	129/131 (98%)	129 (100%)	0	100	100
5	Pa	135/136 (99%)	133 (98%)	2 (2%)	60	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Pb	135/136 (99%)	134 (99%)	1 (1%)	81	89
5	Pc	135/136 (99%)	133 (98%)	2 (2%)	60	73
5	Pd	135/136 (99%)	134 (99%)	1 (1%)	81	89
5	Pe	135/136 (99%)	131 (97%)	4 (3%)	36	48
5	Pf	135/136 (99%)	135 (100%)	0	100	100
6	PM	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PN	116/117 (99%)	114 (98%)	2 (2%)	56	69
6	PO	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PP	116/117 (99%)	114 (98%)	2 (2%)	56	69
6	PQ	116/117 (99%)	114 (98%)	2 (2%)	56	69
6	PR	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PS	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PT	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PU	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PV	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PW	116/117 (99%)	115 (99%)	1 (1%)	75	85
6	PX	116/117 (99%)	115 (99%)	1 (1%)	75	85
7	PA	327/568 (58%)	326 (100%)	1 (0%)	91	95
7	PB	327/568 (58%)	323 (99%)	4 (1%)	67	79
7	PC	327/568 (58%)	325 (99%)	2 (1%)	84	90
7	PD	327/568 (58%)	325 (99%)	2 (1%)	84	90
7	PE	327/568 (58%)	327 (100%)	0	100	100
7	PF	327/568 (58%)	325 (99%)	2 (1%)	84	90
7	PG	327/568 (58%)	324 (99%)	3 (1%)	75	85
7	PH	327/568 (58%)	327 (100%)	0	100	100
7	PI	327/568 (58%)	327 (100%)	0	100	100
7	PJ	327/568 (58%)	324 (99%)	3 (1%)	75	85
7	PK	327/568 (58%)	326 (100%)	1 (0%)	91	95
7	PL	327/568 (58%)	325 (99%)	2 (1%)	84	90
All	All	19281/22371 (86%)	19091 (99%)	190 (1%)	71	82

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BD	30	VAL
1	BD	483	THR
1	BD	563	ASN
1	BD	726	THR
1	BD	743	HIS
1	BD	747	VAL
1	BD	799	THR
1	BD	878	ASN
1	BE	61	ARG
1	BE	97	ARG
1	BE	120	ARG
1	BE	182	SER
1	BE	619	THR
1	BE	629	ASN
1	BE	751	LEU
1	BE	899	ARG
1	BF	35	GLN
1	BF	137	LEU
1	BF	145	THR
1	BF	172	GLU
1	BF	207	ARG
1	BF	278	ASP
1	BF	323	GLU
1	BF	659	LEU
1	BF	671	ASP
1	BF	679	THR
1	BF	726	THR
1	BF	755	THR
1	BF	757	VAL
1	BF	833	VAL
1	BF	872	ASN
1	BF	941	ARG
2	QG	39	THR
2	QG	40	PHE
2	QG	76	LEU
2	QG	102	LEU
2	QG	177	ILE
2	QG	188	LEU
2	QG	281	GLU
2	QG	312	PHE
2	QH	63	LEU
2	QH	130	ILE
2	QH	138	LEU

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Mol	Chain	Res	Type
2	QH	146	THR
2	QH	168	GLN
2	QH	222	ASN
2	QH	336	SER
2	QI	36	GLU
2	QI	103	TYR
2	QI	124	ASP
2	QI	135	VAL
2	QI	173	ILE
2	QI	178	ASN
2	QI	210	ILE
2	QI	312	PHE
2	QJ	10	SER
2	QJ	130	ILE
2	QJ	138	LEU
2	QJ	146	THR
2	QJ	161	ILE
2	QJ	274	GLU
2	QE	11	GLU
2	QE	12	THR
2	QE	76	LEU
2	QE	100	ASP
2	QE	135	VAL
2	QE	160	ASP
2	QE	214	THR
2	QF	6	SER
2	QF	17	GLU
2	QF	102	LEU
2	QF	130	ILE
2	QF	138	LEU
2	QF	146	THR
2	QF	163	THR
2	QF	182	GLU
2	QF	186	THR
2	QF	336	SER
3	BA	3	ASP
3	BA	26	LEU
3	BA	126	LEU
3	BA	190	GLN
3	BB	152	THR
3	BB	237	VAL
3	BB	284	ASN

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Mol	Chain	Res	Type
3	BC	3	ASP
3	BC	68	SER
3	BC	152	THR
4	SG	115	ARG
4	SH	74	LEU
4	SI	115	ARG
4	SJ	115	ARG
4	SL	62	ASN
4	SL	115	ARG
4	SS	115	ARG
4	ST	115	ARG
4	SV	115	ARG
4	SX	62	ASN
4	SX	115	ARG
4	SM	115	ARG
4	SN	115	ARG
4	SQ	115	ARG
4	SR	115	ARG
4	SB	115	ARG
4	SA	115	ARG
4	SC	115	ARG
4	SD	115	ARG
4	SE	115	ARG
4	SF	115	ARG
4	SI	115	ARG
4	Sm	66	GLU
4	Sm	115	ARG
4	Sn	115	ARG
4	So	115	ARG
4	Sp	115	ARG
4	Se	115	ARG
4	Sf	54	ASP
4	Sf	115	ARG
4	Sg	115	ARG
4	Sh	115	ARG
4	Si	115	ARG
4	Sj	115	ARG
4	SY	33	ASP
4	SY	115	ARG
4	SZ	115	ARG
4	Sa	62	ASN
4	Sa	115	ARG

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Mol	Chain	Res	Type
4	Sb	115	ARG
4	Sc	62	ASN
4	Sc	115	ARG
4	Sd	115	ARG
4	B1	115	ARG
4	B2	115	ARG
4	B4	115	ARG
4	S1	115	ARG
4	S2	115	ARG
4	Sq	115	ARG
4	Sr	115	ARG
4	St	115	ARG
4	Su	115	ARG
4	Sv	115	ARG
4	P1	33	ASP
4	P2	31	VAL
4	P3	49	ASP
4	P3	155	THR
5	Pa	73	VAL
5	Pa	90	THR
5	Pb	93	GLU
5	Pc	89	GLU
5	Pc	90	THR
5	Pd	110	ASN
5	Pe	43	GLU
5	Pe	73	VAL
5	Pe	90	THR
5	Pe	110	ASN
6	PT	119	THR
6	PM	119	THR
6	PN	119	THR
6	PN	132	ASP
6	PO	132	ASP
6	PP	64	MET
6	PP	119	THR
6	PQ	119	THR
6	PQ	132	ASP
6	PR	119	THR
6	PS	119	THR
6	PU	132	ASP
6	PV	119	THR
6	PW	119	THR

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Mol	Chain	Res	Type
6	PX	119	THR
7	PA	168	GLN
7	PB	39	VAL
7	PB	60	LEU
7	PB	168	GLN
7	PB	299	HIS
7	PC	205	ARG
7	PC	423	SER
7	PD	146	ILE
7	PD	168	GLN
7	PF	168	GLN
7	PF	212	GLU
7	PG	60	LEU
7	PG	146	ILE
7	PG	299	HIS
7	PJ	60	LEU
7	PJ	241	GLN
7	PJ	258	ASP
7	PK	299	HIS
7	PL	147	THR
7	PL	168	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196) such sidechains are listed below:

Mol	Chain	Res	Type
1	BD	37	ASN
1	BD	103	GLN
1	BD	204	HIS
1	BD	253	GLN
1	BD	367	GLN
1	BD	382	ASN
1	BD	425	ASN
1	BD	581	ASN
1	BD	695	ASN
1	BD	802	ASN
1	BD	835	ASN
1	BD	868	GLN
1	BE	100	ASN
1	BE	103	GLN
1	BE	160	GLN
1	BE	173	ASN
1	BE	198	GLN

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Mol	Chain	Res	Type
1	BE	409	ASN
1	BE	420	ASN
1	BE	425	ASN
1	BE	572	GLN
1	BE	789	GLN
1	BE	868	GLN
1	BE	954	ASN
1	BF	36	ASN
1	BF	37	ASN
1	BF	131	ASN
1	BF	198	GLN
1	BF	420	ASN
1	BF	741	GLN
1	BF	772	ASN
1	BF	802	ASN
1	BF	818	ASN
1	BF	857	ASN
2	QG	178	ASN
2	QG	316	ASN
2	QG	323	GLN
2	QH	14	GLN
2	QI	120	GLN
2	QI	153	ASN
2	QI	241	ASN
2	QI	270	ASN
2	QI	316	ASN
2	QI	323	GLN
2	QJ	13	GLN
2	QJ	139	GLN
2	QJ	270	ASN
2	QJ	277	ASN
2	QE	13	GLN
2	QE	211	ASN
2	QE	241	ASN
2	QF	65	GLN
2	QF	139	GLN
3	BA	36	ASN
3	BA	181	ASN
3	BA	203	ASN
3	BA	221	ASN
3	BA	262	GLN
3	BB	181	ASN

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Mol	Chain	Res	Type
3	BB	190	GLN
3	BB	203	ASN
3	BB	262	GLN
3	BC	262	GLN
4	SH	104	ASN
4	SI	104	ASN
4	SK	104	ASN
4	SL	104	ASN
4	SS	62	ASN
4	SS	64	ASN
4	SS	151	ASN
4	SU	104	ASN
4	SU	151	ASN
4	SV	151	ASN
4	SM	104	ASN
4	SN	104	ASN
4	SN	151	ASN
4	SO	62	ASN
4	SO	104	ASN
4	SO	151	ASN
4	SP	104	ASN
4	SQ	104	ASN
4	SR	62	ASN
4	SA	104	ASN
4	SC	104	ASN
4	SD	104	ASN
4	SE	104	ASN
4	SF	104	ASN
4	Sk	104	ASN
4	Sl	62	ASN
4	Sl	64	ASN
4	Sl	104	ASN
4	Sm	104	ASN
4	Sn	104	ASN
4	So	104	ASN
4	Sp	104	ASN
4	Se	104	ASN
4	Sf	104	ASN
4	Sg	104	ASN
4	Sh	104	ASN
4	Si	104	ASN
4	Sj	104	ASN

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Mol	Chain	Res	Type
4	SY	104	ASN
4	SZ	104	ASN
4	Sa	62	ASN
4	Sa	151	ASN
4	Sb	104	ASN
4	Sc	62	ASN
4	Sc	104	ASN
4	B1	104	ASN
4	B2	104	ASN
4	B5	104	ASN
4	Sw	104	ASN
4	Sw	151	ASN
4	Sx	151	ASN
4	Sy	151	ASN
4	Sz	104	ASN
4	S1	62	ASN
4	S1	64	ASN
4	S1	151	ASN
4	S2	151	ASN
4	Sq	104	ASN
4	Ss	62	ASN
4	St	62	ASN
4	St	64	ASN
4	St	104	ASN
4	St	151	ASN
4	Sv	151	ASN
4	P1	104	ASN
4	P2	104	ASN
4	P5	104	ASN
4	P6	151	ASN
5	Pa	77	ASN
5	Pa	113	GLN
5	Pa	156	ASN
5	Pc	77	ASN
5	Pd	29	GLN
5	Pd	77	ASN
5	Pd	110	ASN
5	Pe	11	GLN
5	Pe	110	ASN
6	PT	28	GLN
6	PN	28	GLN
6	PN	133	ASN

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Mol	Chain	Res	Type
6	PO	28	GLN
6	PP	133	ASN
6	PR	28	GLN
6	PR	95	GLN
6	PR	133	ASN
6	PU	28	GLN
6	PU	95	GLN
6	PV	133	ASN
6	PW	28	GLN
6	PX	63	ASN
6	PX	133	ASN
7	PA	392	GLN
7	PA	393	GLN
7	PB	400	ASN
7	PC	72	GLN
7	PC	168	GLN
7	PC	185	GLN
7	PC	281	GLN
7	PC	392	GLN
7	PC	393	GLN
7	PC	400	ASN
7	PD	168	GLN
7	PD	185	GLN
7	PE	185	GLN
7	PE	392	GLN
7	PE	393	GLN
7	PE	400	ASN
7	PF	72	GLN
7	PF	181	HIS
7	PF	305	ASN
7	PG	72	GLN
7	PG	181	HIS
7	PG	185	GLN
7	PG	392	GLN
7	PH	185	GLN
7	PH	274	ASN
7	PH	392	GLN
7	PI	392	GLN
7	PI	393	GLN
7	PI	400	ASN
7	PJ	72	GLN
7	PJ	185	GLN

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Mol	Chain	Res	Type
7	PJ	400	ASN
7	PK	72	GLN
7	PK	75	GLN
7	PK	274	ASN
7	PK	305	ASN
7	PK	392	GLN
7	PL	168	GLN
7	PL	200	ASN
7	PL	305	ASN
7	PL	392	GLN
7	PL	393	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

36 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	HIP	PB	196	7	10,14,15	1.53	3 (30%)	6,20,22	1.71	2 (33%)
7	HIP	PA	243	7	10,14,15	1.70	4 (40%)	6,20,22	1.57	2 (33%)
7	HIP	PC	196	7	10,14,15	1.50	3 (30%)	6,20,22	1.74	2 (33%)
7	HIP	PG	243	7	10,14,15	1.72	4 (40%)	6,20,22	1.57	2 (33%)
7	HIP	PK	196	7	10,14,15	1.59	3 (30%)	6,20,22	1.68	2 (33%)
7	HIP	PE	196	7	10,14,15	1.55	3 (30%)	6,20,22	1.81	3 (50%)
7	HIP	PB	291	7	10,14,15	1.50	3 (30%)	6,20,22	1.56	2 (33%)
7	HIP	PD	196	7	10,14,15	1.51	3 (30%)	6,20,22	1.73	2 (33%)
7	HIP	PC	243	7	10,14,15	1.74	4 (40%)	6,20,22	1.55	2 (33%)
7	HIP	PJ	196	7	10,14,15	1.49	3 (30%)	6,20,22	1.77	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	HIP	PF	196	7	10,14,15	1.54	3 (30%)	6,20,22	1.72	2 (33%)
7	HIP	PG	291	7	10,14,15	1.49	3 (30%)	6,20,22	1.66	3 (50%)
7	HIP	PD	243	7	10,14,15	1.72	4 (40%)	6,20,22	1.52	2 (33%)
7	HIP	PI	243	7	10,14,15	1.73	4 (40%)	6,20,22	1.55	2 (33%)
7	HIP	PI	291	7	10,14,15	1.58	3 (30%)	6,20,22	1.77	2 (33%)
7	HIP	PJ	243	7	10,14,15	1.73	4 (40%)	6,20,22	1.51	2 (33%)
7	HIP	PJ	291	7	10,14,15	1.60	3 (30%)	6,20,22	1.53	1 (16%)
7	HIP	PH	243	7	10,14,15	1.71	4 (40%)	6,20,22	1.57	2 (33%)
7	HIP	PH	291	7	10,14,15	1.45	3 (30%)	6,20,22	1.53	2 (33%)
7	HIP	PF	243	7	10,14,15	1.72	4 (40%)	6,20,22	1.50	2 (33%)
7	HIP	PF	291	7	10,14,15	1.59	3 (30%)	6,20,22	1.59	2 (33%)
7	HIP	PK	291	7	10,14,15	1.58	3 (30%)	6,20,22	1.57	2 (33%)
7	HIP	PI	196	7	10,14,15	1.56	3 (30%)	6,20,22	1.70	2 (33%)
7	HIP	PL	243	7	10,14,15	1.70	4 (40%)	6,20,22	1.52	2 (33%)
7	HIP	PL	291	7	10,14,15	1.58	3 (30%)	6,20,22	1.68	2 (33%)
7	HIP	PH	196	7	10,14,15	1.56	3 (30%)	6,20,22	1.65	2 (33%)
7	HIP	PD	291	7	10,14,15	1.59	3 (30%)	6,20,22	1.78	2 (33%)
7	HIP	PC	291	7	10,14,15	1.56	3 (30%)	6,20,22	1.71	3 (50%)
7	HIP	PK	243	7	10,14,15	1.78	4 (40%)	6,20,22	1.58	2 (33%)
7	HIP	PB	243	7	10,14,15	1.72	4 (40%)	6,20,22	1.55	2 (33%)
7	HIP	PE	291	7	10,14,15	1.65	4 (40%)	6,20,22	1.69	3 (50%)
7	HIP	PL	196	7	10,14,15	1.52	3 (30%)	6,20,22	1.68	3 (50%)
7	HIP	PA	196	7	10,14,15	1.53	3 (30%)	6,20,22	1.72	2 (33%)
7	HIP	PE	243	7	10,14,15	1.77	4 (40%)	6,20,22	1.55	2 (33%)
7	HIP	PA	291	7	10,14,15	1.62	3 (30%)	6,20,22	1.73	2 (33%)
7	HIP	PG	196	7	10,14,15	1.52	3 (30%)	6,20,22	1.87	3 (50%)

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
7	HIP	PB	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PA	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PC	196	7	-	2/5/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HIP	PG	243	7	-	2/5/12/14	0/1/1/1
7	HIP	PK	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PE	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PB	291	7	-	2/5/12/14	0/1/1/1
7	HIP	PD	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PC	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PJ	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PF	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PG	291	7	-	2/5/12/14	0/1/1/1
7	HIP	PD	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PI	243	7	-	0/5/12/14	0/1/1/1
7	HIP	PI	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PJ	243	7	-	1/5/12/14	0/1/1/1
7	HIP	PJ	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PH	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PH	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PF	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PF	291	7	-	2/5/12/14	0/1/1/1
7	HIP	PK	291	7	-	2/5/12/14	0/1/1/1
7	HIP	PI	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PL	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PL	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PH	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PD	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PC	291	7	-	1/5/12/14	0/1/1/1
7	HIP	PK	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PB	243	7	-	3/5/12/14	0/1/1/1
7	HIP	PE	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PL	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PA	196	7	-	2/5/12/14	0/1/1/1
7	HIP	PE	243	7	-	1/5/12/14	0/1/1/1
7	HIP	PA	291	7	-	0/5/12/14	0/1/1/1
7	HIP	PG	196	7	-	2/5/12/14	0/1/1/1

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	PK	243	HIP	P-O1P	3.83	1.50	1.47
7	PE	243	HIP	P-O1P	3.81	1.50	1.47
7	PB	243	HIP	P-O1P	3.62	1.50	1.47
7	PJ	243	HIP	P-O1P	3.52	1.50	1.47
7	PI	243	HIP	P-O1P	3.51	1.50	1.47
7	PH	243	HIP	P-O1P	3.50	1.50	1.47
7	PC	243	HIP	P-O1P	3.47	1.50	1.47
7	PF	291	HIP	P-O1P	3.42	1.50	1.47
7	PD	243	HIP	P-O1P	3.41	1.50	1.47
7	PF	243	HIP	P-O1P	3.40	1.50	1.47
7	PA	243	HIP	P-O1P	3.39	1.50	1.47
7	PG	243	HIP	P-O1P	3.35	1.50	1.47
7	PL	243	HIP	P-O1P	3.31	1.50	1.47
7	PC	291	HIP	P-O1P	3.17	1.50	1.47
7	PK	291	HIP	P-O1P	3.12	1.50	1.47
7	PJ	291	HIP	P-O1P	3.09	1.50	1.47
7	PL	291	HIP	P-O1P	3.09	1.50	1.47
7	PK	196	HIP	P-O1P	3.07	1.50	1.47
7	PE	291	HIP	P-O1P	3.01	1.49	1.47
7	PI	291	HIP	P-O1P	2.98	1.49	1.47
7	PI	196	HIP	P-O1P	2.98	1.49	1.47
7	PA	291	HIP	P-O1P	2.94	1.49	1.47
7	PB	291	HIP	P-O1P	2.92	1.49	1.47
7	PH	196	HIP	P-O1P	2.91	1.49	1.47
7	PD	291	HIP	P-O1P	2.84	1.49	1.47
7	PG	291	HIP	P-O1P	2.79	1.49	1.47
7	PL	196	HIP	P-O1P	2.75	1.49	1.47
7	PE	196	HIP	P-O1P	2.73	1.49	1.47
7	PA	196	HIP	P-O1P	2.70	1.49	1.47
7	PD	196	HIP	P-O1P	2.66	1.49	1.47
7	PF	196	HIP	P-O1P	2.65	1.49	1.47
7	PB	196	HIP	P-O1P	2.63	1.49	1.47
7	PH	291	HIP	P-O1P	2.60	1.49	1.47
7	PG	196	HIP	P-O1P	2.54	1.49	1.47
7	PG	243	HIP	CG-ND1	2.49	1.40	1.37
7	PF	196	HIP	P-O3P	-2.46	1.49	1.54
7	PA	291	HIP	P-O3P	-2.46	1.49	1.54
7	PE	291	HIP	P-O3P	-2.45	1.49	1.54
7	PI	291	HIP	P-O3P	-2.45	1.49	1.54
7	PJ	196	HIP	P-O1P	2.45	1.49	1.47
7	PD	291	HIP	P-O3P	-2.44	1.49	1.54
7	PC	243	HIP	CG-ND1	2.42	1.40	1.37
7	PB	196	HIP	P-O3P	-2.42	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	PC	196	HIP	P-O3P	-2.39	1.49	1.54
7	PC	196	HIP	P-O1P	2.39	1.49	1.47
7	PG	196	HIP	P-O3P	-2.38	1.49	1.54
7	PJ	196	HIP	P-O3P	-2.37	1.50	1.54
7	PD	243	HIP	CG-ND1	2.37	1.40	1.37
7	PG	196	HIP	P-O2P	-2.35	1.50	1.54
7	PE	196	HIP	P-O3P	-2.34	1.50	1.54
7	PD	196	HIP	P-O3P	-2.33	1.50	1.54
7	PA	196	HIP	P-O3P	-2.33	1.50	1.54
7	PL	196	HIP	P-O3P	-2.32	1.50	1.54
7	PL	243	HIP	CG-ND1	2.32	1.40	1.37
7	PA	196	HIP	P-O2P	-2.32	1.50	1.54
7	PH	196	HIP	P-O3P	-2.31	1.50	1.54
7	PJ	196	HIP	P-O2P	-2.31	1.50	1.54
7	PI	243	HIP	CG-ND1	2.30	1.40	1.37
7	PJ	291	HIP	P-O3P	-2.30	1.50	1.54
7	PL	291	HIP	P-O3P	-2.30	1.50	1.54
7	PF	243	HIP	CG-ND1	2.29	1.40	1.37
7	PK	291	HIP	P-O2P	-2.28	1.50	1.54
7	PG	291	HIP	P-O2P	-2.28	1.50	1.54
7	PI	196	HIP	P-O3P	-2.28	1.50	1.54
7	PD	196	HIP	P-O2P	-2.27	1.50	1.54
7	PE	243	HIP	CG-ND1	2.26	1.40	1.37
7	PK	291	HIP	P-O3P	-2.26	1.50	1.54
7	PK	243	HIP	CG-ND1	2.26	1.40	1.37
7	PA	243	HIP	CG-ND1	2.25	1.40	1.37
7	PH	243	HIP	CG-ND1	2.25	1.40	1.37
7	PF	243	HIP	P-O2P	-2.24	1.50	1.54
7	PG	291	HIP	P-O3P	-2.24	1.50	1.54
7	PC	196	HIP	P-O2P	-2.24	1.50	1.54
7	PL	243	HIP	P-O2P	-2.24	1.50	1.54
7	PE	196	HIP	P-O2P	-2.24	1.50	1.54
7	PH	291	HIP	P-O2P	-2.23	1.50	1.54
7	PC	291	HIP	P-O3P	-2.23	1.50	1.54
7	PJ	291	HIP	P-O2P	-2.23	1.50	1.54
7	PK	196	HIP	P-O3P	-2.22	1.50	1.54
7	PD	243	HIP	P-O2P	-2.22	1.50	1.54
7	PD	291	HIP	P-O2P	-2.22	1.50	1.54
7	PJ	243	HIP	P-O3P	-2.22	1.50	1.54
7	PA	243	HIP	P-O2P	-2.21	1.50	1.54
7	PJ	243	HIP	P-O2P	-2.21	1.50	1.54
7	PB	291	HIP	P-O2P	-2.21	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	PF	196	HIP	P-O2P	-2.20	1.50	1.54
7	PF	243	HIP	P-O3P	-2.20	1.50	1.54
7	PB	243	HIP	P-O3P	-2.19	1.50	1.54
7	PA	291	HIP	P-O2P	-2.19	1.50	1.54
7	PC	243	HIP	P-O3P	-2.19	1.50	1.54
7	PI	196	HIP	P-O2P	-2.19	1.50	1.54
7	PK	196	HIP	P-O2P	-2.19	1.50	1.54
7	PH	196	HIP	P-O2P	-2.18	1.50	1.54
7	PB	196	HIP	P-O2P	-2.18	1.50	1.54
7	PJ	243	HIP	CG-ND1	2.17	1.40	1.37
7	PC	291	HIP	P-O2P	-2.16	1.50	1.54
7	PI	243	HIP	P-O2P	-2.16	1.50	1.54
7	PL	196	HIP	P-O2P	-2.16	1.50	1.54
7	PL	243	HIP	P-O3P	-2.16	1.50	1.54
7	PC	243	HIP	P-O2P	-2.15	1.50	1.54
7	PG	243	HIP	P-O3P	-2.15	1.50	1.54
7	PE	291	HIP	P-O2P	-2.15	1.50	1.54
7	PE	243	HIP	P-O3P	-2.15	1.50	1.54
7	PA	243	HIP	P-O3P	-2.15	1.50	1.54
7	PK	243	HIP	P-O3P	-2.15	1.50	1.54
7	PG	243	HIP	P-O2P	-2.13	1.50	1.54
7	PB	291	HIP	P-O3P	-2.13	1.50	1.54
7	PD	243	HIP	P-O3P	-2.13	1.50	1.54
7	PI	243	HIP	P-O3P	-2.13	1.50	1.54
7	PB	243	HIP	CG-ND1	2.12	1.40	1.37
7	PF	291	HIP	P-O2P	-2.12	1.50	1.54
7	PE	291	HIP	CG-ND1	2.12	1.40	1.37
7	PH	243	HIP	P-O3P	-2.11	1.50	1.54
7	PH	243	HIP	P-O2P	-2.10	1.50	1.54
7	PF	291	HIP	P-O3P	-2.08	1.50	1.54
7	PH	291	HIP	P-O3P	-2.08	1.50	1.54
7	PL	291	HIP	P-O2P	-2.06	1.50	1.54
7	PI	291	HIP	P-O2P	-2.06	1.50	1.54
7	PE	243	HIP	P-O2P	-2.05	1.50	1.54
7	PK	243	HIP	P-O2P	-2.05	1.50	1.54
7	PB	243	HIP	P-O2P	-2.04	1.50	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	PD	291	HIP	CB-CA-C	2.80	116.73	111.47
7	PI	291	HIP	CB-CA-C	2.80	116.71	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	PK	196	HIP	CD2-NE2-CE1	2.65	109.92	105.78
7	PG	196	HIP	CD2-NE2-CE1	2.65	109.91	105.78
7	PK	243	HIP	CD2-NE2-CE1	2.65	109.91	105.78
7	PH	243	HIP	CD2-NE2-CE1	2.64	109.89	105.78
7	PC	196	HIP	CD2-NE2-CE1	2.62	109.87	105.78
7	PA	291	HIP	CB-CA-C	2.61	116.36	111.47
7	PE	243	HIP	CD2-NE2-CE1	2.60	109.84	105.78
7	PH	196	HIP	CD2-NE2-CE1	2.59	109.83	105.78
7	PA	243	HIP	CD2-NE2-CE1	2.59	109.82	105.78
7	PD	243	HIP	CD2-NE2-CE1	2.58	109.80	105.78
7	PJ	243	HIP	CD2-NE2-CE1	2.57	109.79	105.78
7	PB	196	HIP	CD2-NE2-CE1	2.57	109.78	105.78
7	PG	243	HIP	CD2-NE2-CE1	2.56	109.78	105.78
7	PE	196	HIP	CD2-NE2-CE1	2.55	109.76	105.78
7	PB	243	HIP	CD2-NE2-CE1	2.55	109.76	105.78
7	PJ	196	HIP	CD2-NE2-CE1	2.54	109.74	105.78
7	PL	196	HIP	CD2-NE2-CE1	2.54	109.74	105.78
7	PF	196	HIP	CD2-NE2-CE1	2.53	109.73	105.78
7	PL	291	HIP	CD2-NE2-CE1	2.53	109.72	105.78
7	PG	291	HIP	CD2-NE2-CE1	2.51	109.70	105.78
7	PA	196	HIP	CD2-NE2-CE1	2.51	109.70	105.78
7	PC	291	HIP	CD2-NE2-CE1	2.51	109.69	105.78
7	PD	196	HIP	CD2-NE2-CE1	2.50	109.68	105.78
7	PI	196	HIP	CD2-NE2-CE1	2.50	109.68	105.78
7	PI	291	HIP	CD2-NE2-CE1	2.50	109.68	105.78
7	PF	291	HIP	CD2-NE2-CE1	2.50	109.67	105.78
7	PI	243	HIP	CD2-NE2-CE1	2.47	109.64	105.78
7	PI	243	HIP	O2P-P-O1P	-2.47	108.10	113.44
7	PL	291	HIP	CB-CA-C	2.45	116.07	111.47
7	PH	291	HIP	CD2-NE2-CE1	2.43	109.57	105.78
7	PF	243	HIP	O2P-P-O1P	-2.43	108.19	113.44
7	PL	243	HIP	CD2-NE2-CE1	2.42	109.56	105.78
7	PE	291	HIP	CB-CA-C	2.42	116.01	111.47
7	PB	291	HIP	CD2-NE2-CE1	2.42	109.56	105.78
7	PC	243	HIP	CD2-NE2-CE1	2.40	109.53	105.78
7	PC	243	HIP	O2P-P-O1P	-2.40	108.25	113.44
7	PH	243	HIP	O2P-P-O1P	-2.40	108.25	113.44
7	PB	243	HIP	O2P-P-O1P	-2.39	108.27	113.44
7	PD	291	HIP	CD2-NE2-CE1	2.39	109.51	105.78
7	PJ	291	HIP	CD2-NE2-CE1	2.39	109.51	105.78
7	PA	291	HIP	CD2-NE2-CE1	2.38	109.50	105.78
7	PF	243	HIP	CD2-NE2-CE1	2.38	109.50	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	PL	243	HIP	O2P-P-O1P	-2.38	108.29	113.44
7	PE	243	HIP	O2P-P-O1P	-2.38	108.30	113.44
7	PE	291	HIP	CD2-NE2-CE1	2.38	109.49	105.78
7	PK	291	HIP	CD2-NE2-CE1	2.35	109.44	105.78
7	PA	243	HIP	O2P-P-O1P	-2.33	108.40	113.44
7	PC	291	HIP	CB-CA-C	2.32	115.82	111.47
7	PG	196	HIP	CB-CA-C	2.31	115.80	111.47
7	PJ	243	HIP	O2P-P-O1P	-2.29	108.49	113.44
7	PD	243	HIP	O2P-P-O1P	-2.28	108.50	113.44
7	PK	243	HIP	O2P-P-O1P	-2.28	108.52	113.44
7	PK	196	HIP	O2P-P-O1P	-2.28	108.52	113.44
7	PG	243	HIP	O2P-P-O1P	-2.26	108.56	113.44
7	PJ	196	HIP	O2P-P-O1P	-2.26	108.56	113.44
7	PA	196	HIP	O2P-P-O1P	-2.25	108.59	113.44
7	PC	291	HIP	O2P-P-O1P	-2.22	108.65	113.44
7	PG	291	HIP	CB-CA-C	2.20	115.60	111.47
7	PL	196	HIP	O2P-P-O1P	-2.20	108.69	113.44
7	PH	291	HIP	O2P-P-O1P	-2.19	108.71	113.44
7	PE	196	HIP	CB-CA-C	2.19	115.57	111.47
7	PF	291	HIP	O2P-P-O1P	-2.19	108.71	113.44
7	PF	196	HIP	O2P-P-O1P	-2.18	108.72	113.44
7	PG	196	HIP	O2P-P-O1P	-2.18	108.74	113.44
7	PB	291	HIP	O2P-P-O1P	-2.17	108.75	113.44
7	PI	196	HIP	O2P-P-O1P	-2.17	108.75	113.44
7	PB	196	HIP	O2P-P-O1P	-2.14	108.81	113.44
7	PG	291	HIP	O2P-P-O1P	-2.13	108.83	113.44
7	PK	291	HIP	O2P-P-O1P	-2.13	108.84	113.44
7	PD	196	HIP	O2P-P-O1P	-2.12	108.85	113.44
7	PC	196	HIP	O2P-P-O1P	-2.09	108.92	113.44
7	PH	196	HIP	O2P-P-O1P	-2.08	108.95	113.44
7	PE	196	HIP	O2P-P-O1P	-2.08	108.95	113.44
7	PE	291	HIP	O2P-P-O1P	-2.07	108.96	113.44
7	PL	196	HIP	O3P-P-O1P	-2.02	109.08	113.44

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	PA	243	HIP	O-C-CA-CB
7	PB	243	HIP	O-C-CA-CB
7	PC	243	HIP	O-C-CA-CB
7	PD	243	HIP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
7	PE	243	HIP	O-C-CA-CB
7	PF	243	HIP	O-C-CA-CB
7	PG	243	HIP	O-C-CA-CB
7	PH	243	HIP	O-C-CA-CB
7	PJ	196	HIP	C-CA-CB-CG
7	PJ	243	HIP	O-C-CA-CB
7	PK	243	HIP	O-C-CA-CB
7	PL	243	HIP	O-C-CA-CB
7	PB	243	HIP	CA-CB-CG-CD2
7	PC	291	HIP	CA-CB-CG-CD2
7	PL	243	HIP	CA-CB-CG-CD2
7	PA	243	HIP	CA-CB-CG-ND1
7	PB	243	HIP	CA-CB-CG-ND1
7	PC	243	HIP	CA-CB-CG-ND1
7	PF	243	HIP	CA-CB-CG-ND1
7	PH	243	HIP	CA-CB-CG-ND1
7	PK	243	HIP	CA-CB-CG-ND1
7	PL	243	HIP	CA-CB-CG-ND1
7	PA	196	HIP	C-CA-CB-CG
7	PB	196	HIP	C-CA-CB-CG
7	PC	196	HIP	C-CA-CB-CG
7	PD	196	HIP	C-CA-CB-CG
7	PE	196	HIP	C-CA-CB-CG
7	PF	196	HIP	C-CA-CB-CG
7	PG	196	HIP	C-CA-CB-CG
7	PH	196	HIP	C-CA-CB-CG
7	PI	196	HIP	C-CA-CB-CG
7	PK	196	HIP	C-CA-CB-CG
7	PL	196	HIP	C-CA-CB-CG
7	PA	196	HIP	N-CA-CB-CG
7	PB	196	HIP	N-CA-CB-CG
7	PC	196	HIP	N-CA-CB-CG
7	PD	196	HIP	N-CA-CB-CG
7	PE	196	HIP	N-CA-CB-CG
7	PF	196	HIP	N-CA-CB-CG
7	PG	196	HIP	N-CA-CB-CG
7	PH	196	HIP	N-CA-CB-CG
7	PI	196	HIP	N-CA-CB-CG
7	PJ	196	HIP	N-CA-CB-CG
7	PK	196	HIP	N-CA-CB-CG
7	PL	196	HIP	N-CA-CB-CG
7	PA	243	HIP	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
7	PB	291	HIP	CA-CB-CG-CD2
7	PC	243	HIP	CA-CB-CG-CD2
7	PD	243	HIP	CA-CB-CG-CD2
7	PF	243	HIP	CA-CB-CG-CD2
7	PF	291	HIP	CA-CB-CG-CD2
7	PG	243	HIP	CA-CB-CG-CD2
7	PG	291	HIP	CA-CB-CG-CD2
7	PH	243	HIP	CA-CB-CG-CD2
7	PK	243	HIP	CA-CB-CG-CD2
7	PK	291	HIP	CA-CB-CG-CD2
7	PB	291	HIP	CA-CB-CG-ND1
7	PD	243	HIP	CA-CB-CG-ND1
7	PF	291	HIP	CA-CB-CG-ND1
7	PG	291	HIP	CA-CB-CG-ND1
7	PK	291	HIP	CA-CB-CG-ND1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

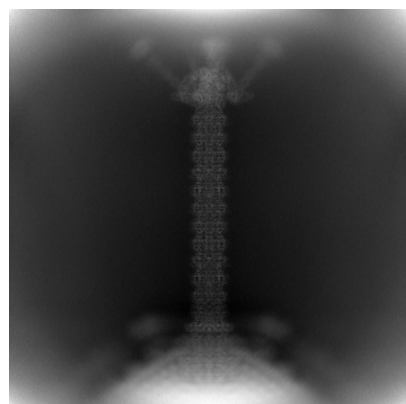
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51866. These allow visual inspection of the internal detail of the map and identification of artifacts.

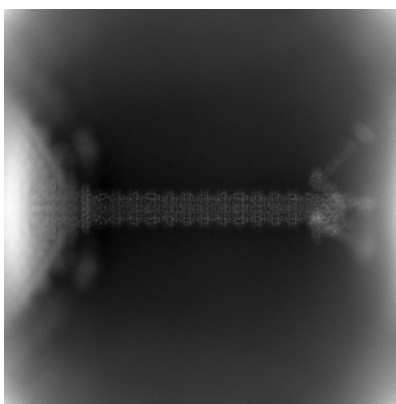
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

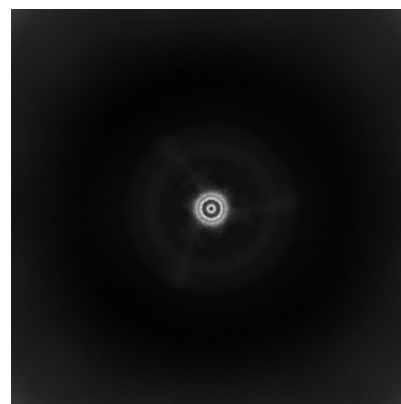
#### 6.1.1 Primary map



X

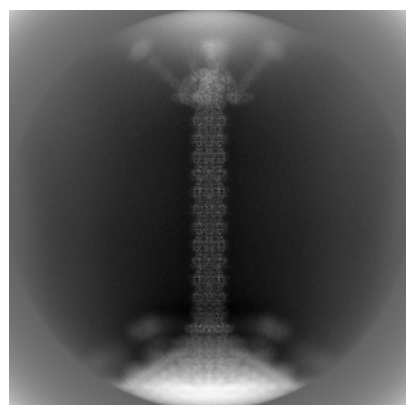


Y

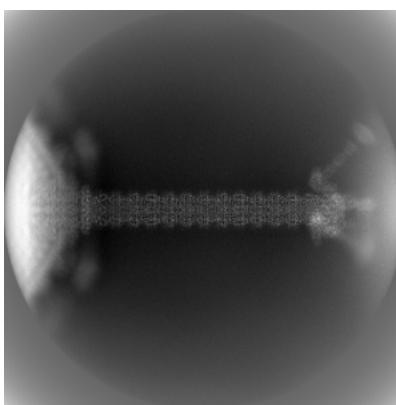


Z

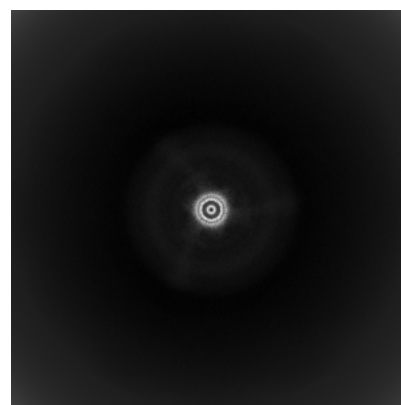
#### 6.1.2 Raw map



X



Y

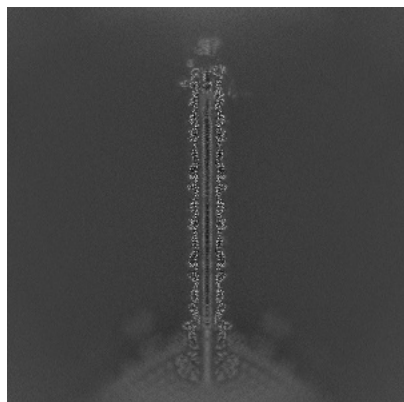


Z

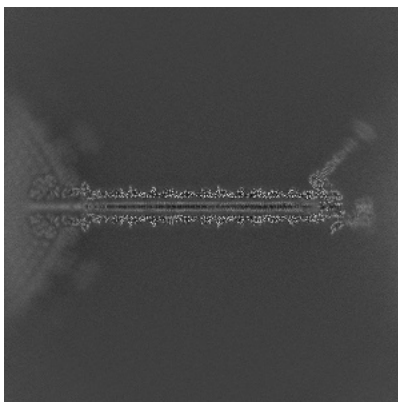
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

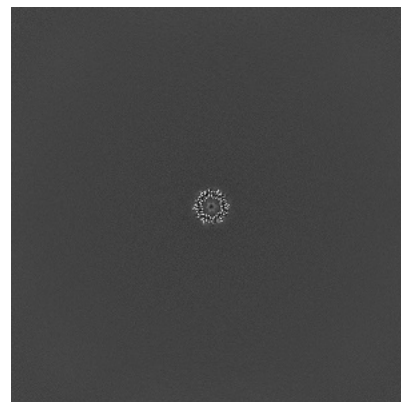
### 6.2.1 Primary map



X Index: 384

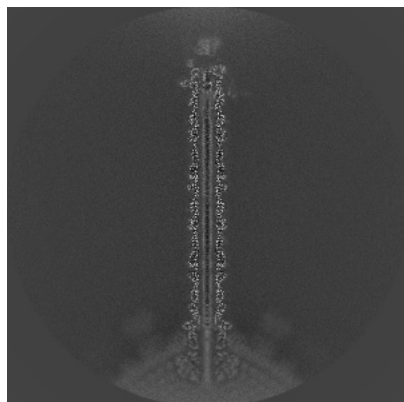


Y Index: 384



Z Index: 384

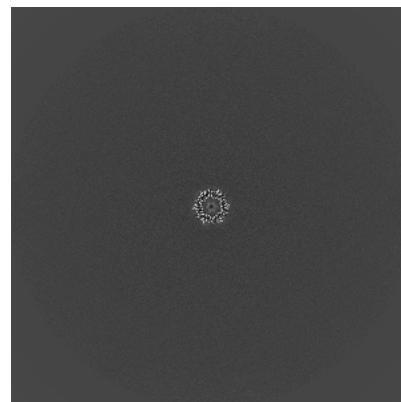
### 6.2.2 Raw map



X Index: 384



Y Index: 384



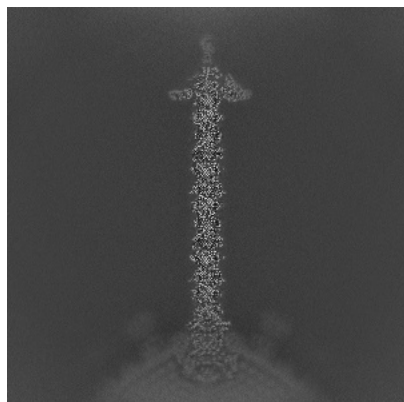
Z Index: 384

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

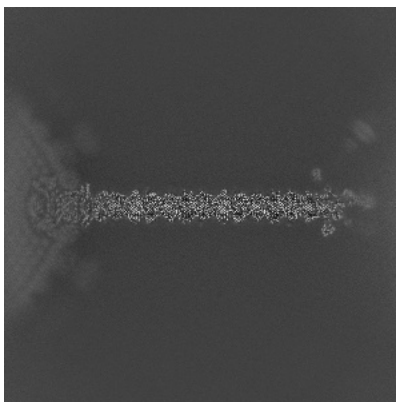


## 6.3 Largest variance slices [i](#)

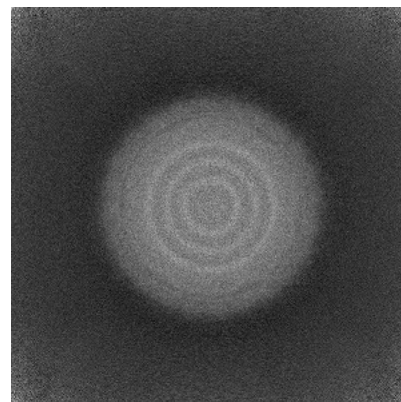
### 6.3.1 Primary map



X Index: 365

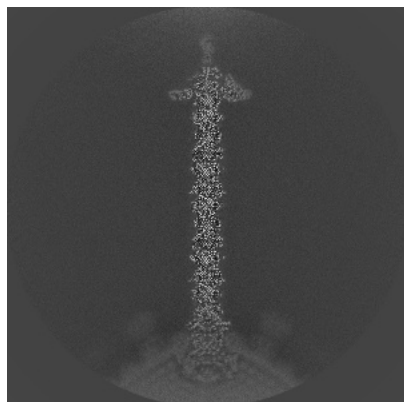


Y Index: 403

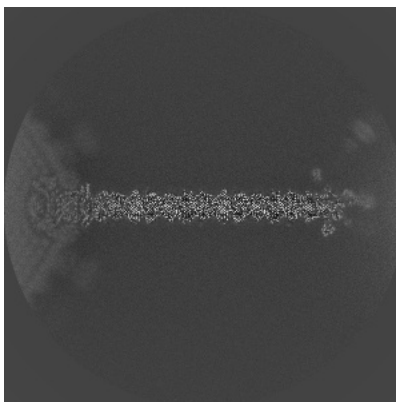


Z Index: 24

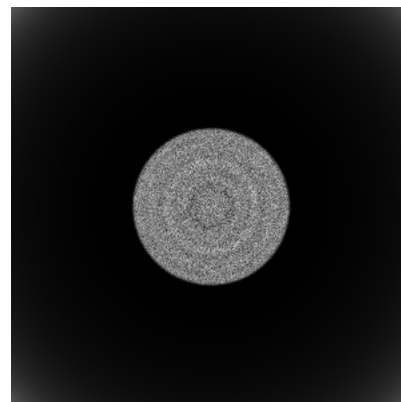
### 6.3.2 Raw map



X Index: 365



Y Index: 403



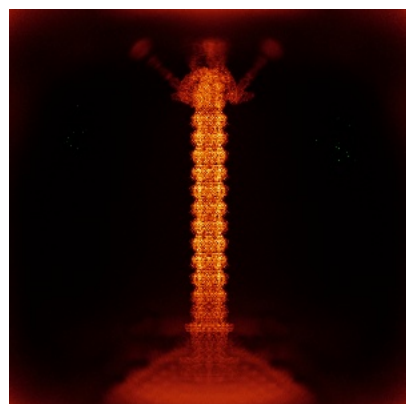
Z Index: 29

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

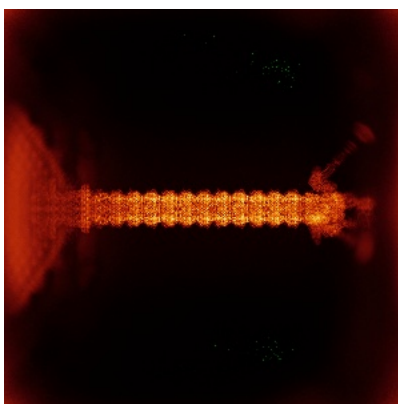


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

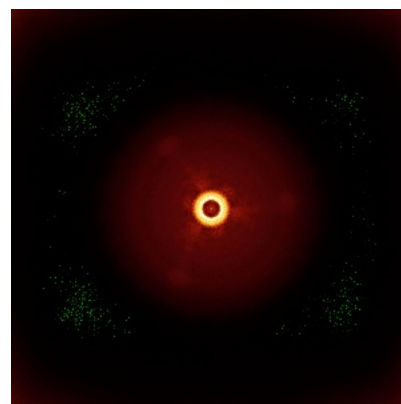
### 6.4.1 Primary map



X

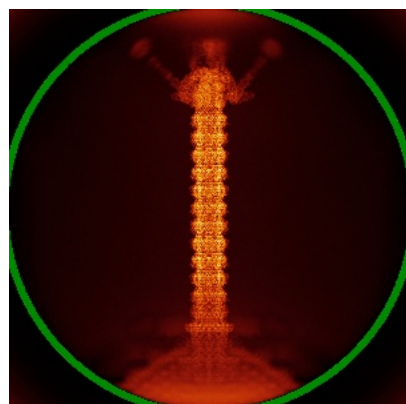


Y

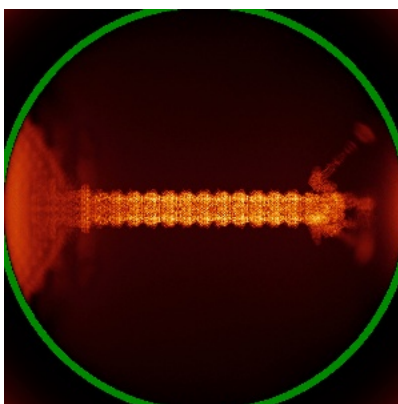


Z

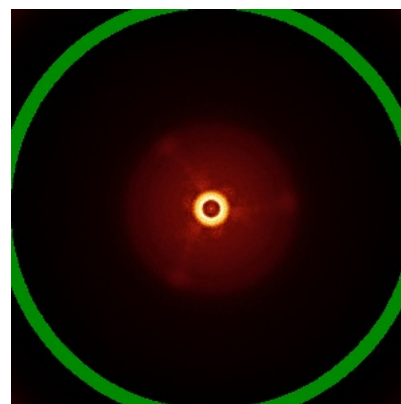
### 6.4.2 Raw map



X



Y

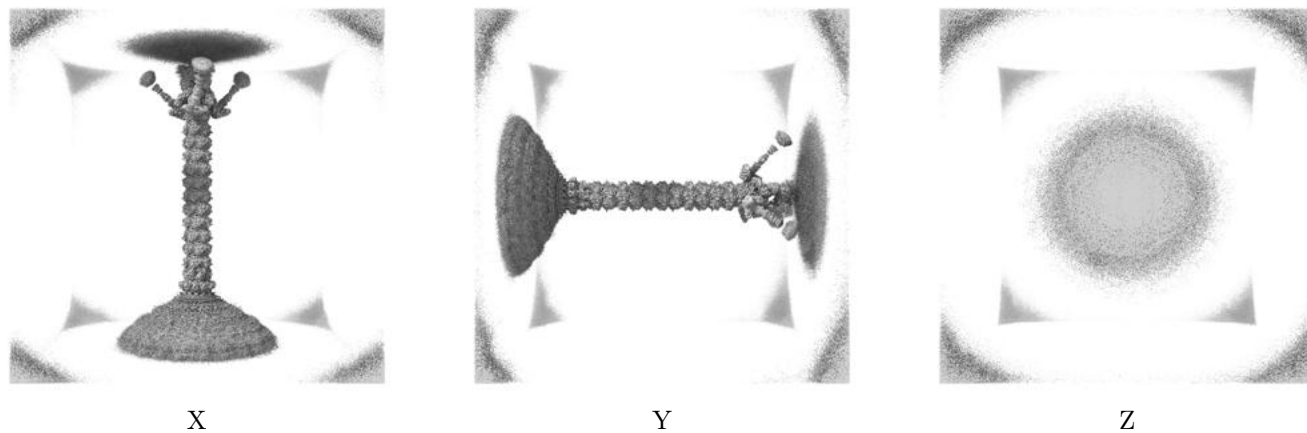


Z

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.

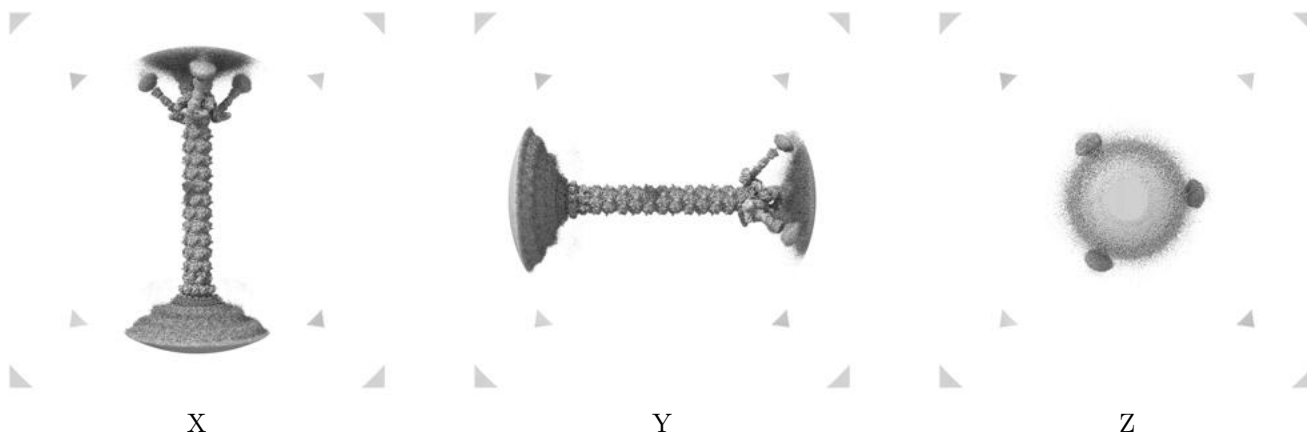
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

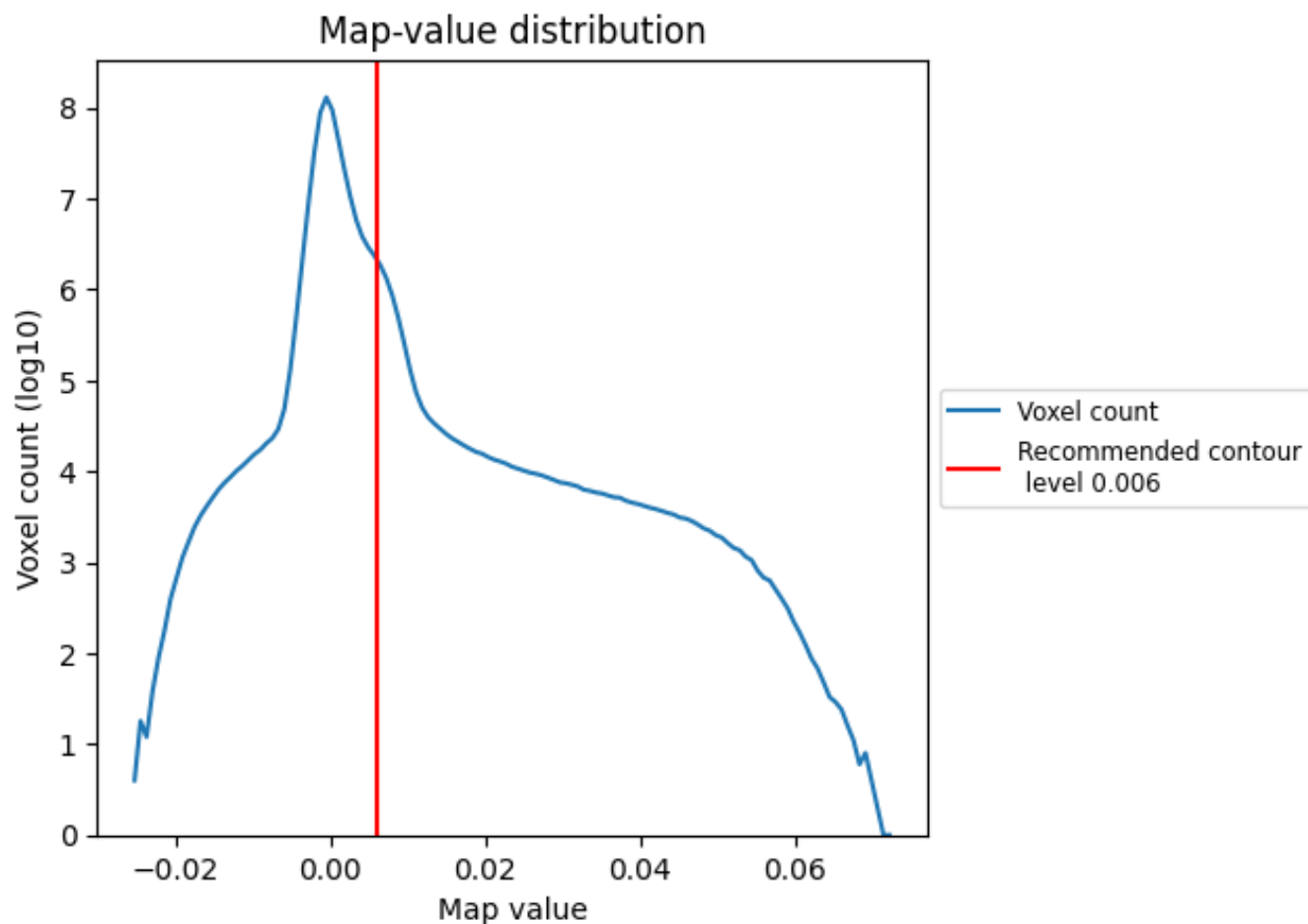
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

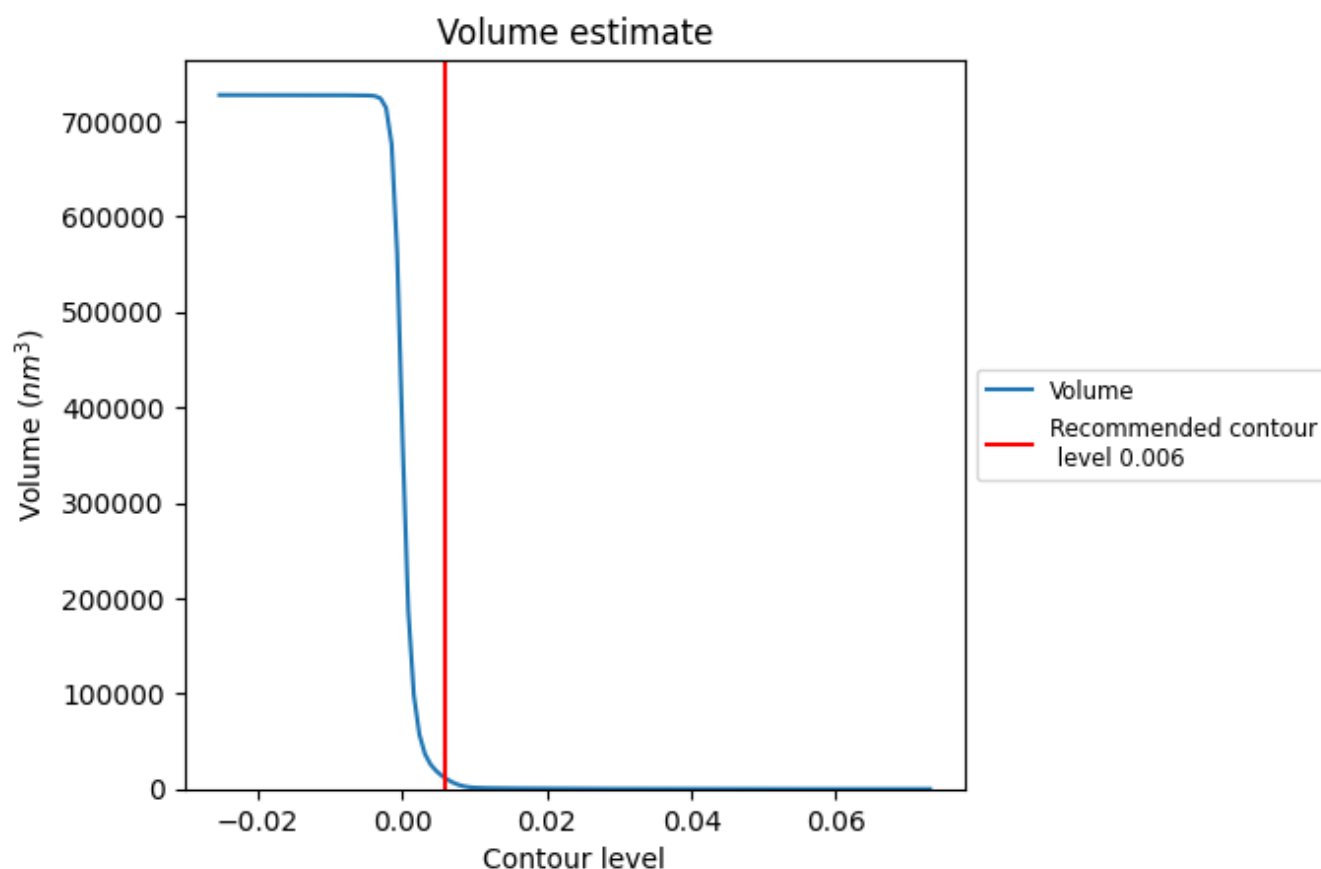
This section contains the results of statistical analysis of the map.

### 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.

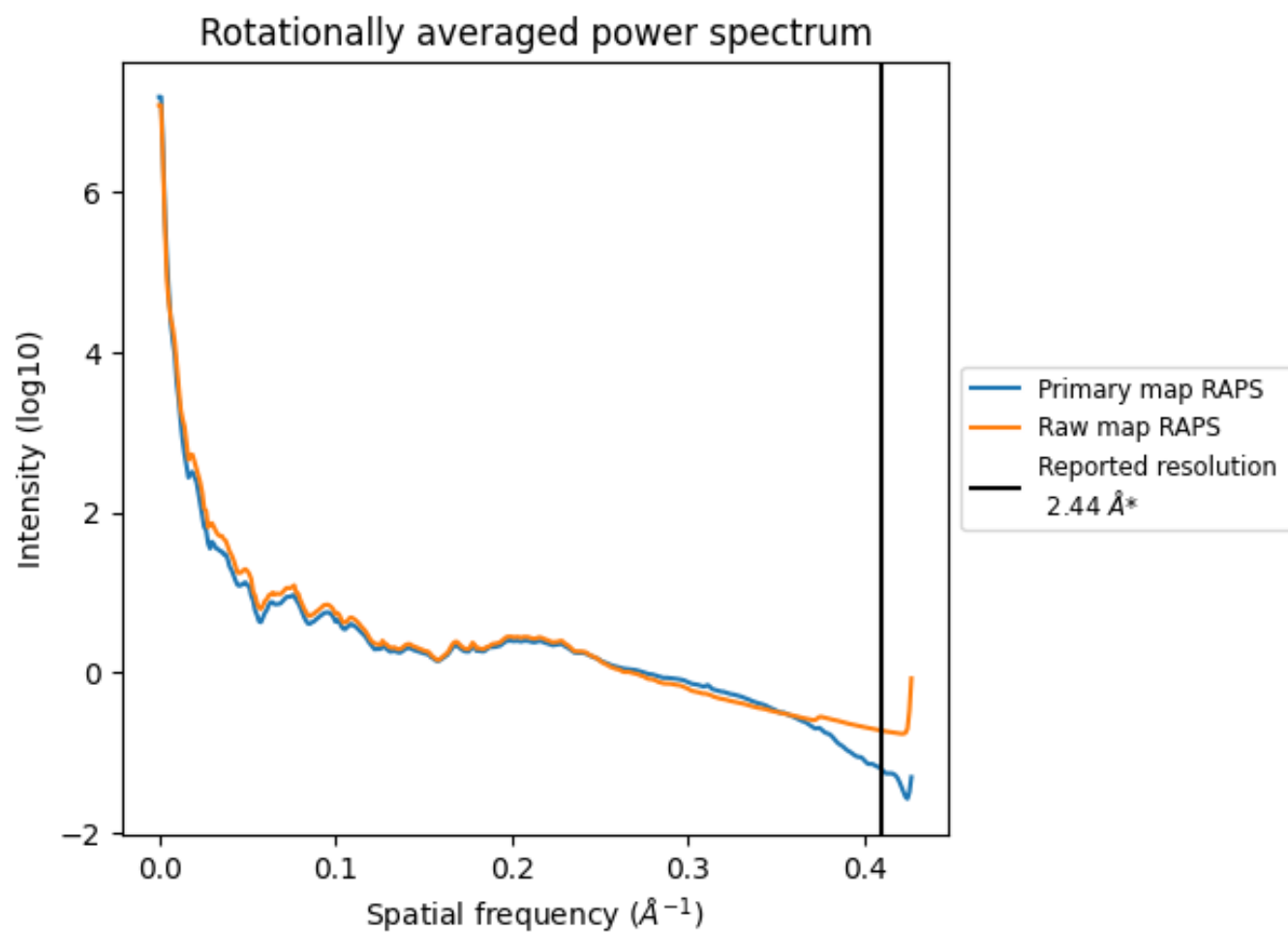
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11001  $\text{nm}^3$ ; this corresponds to an approximate mass of 9938 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 ⓘ

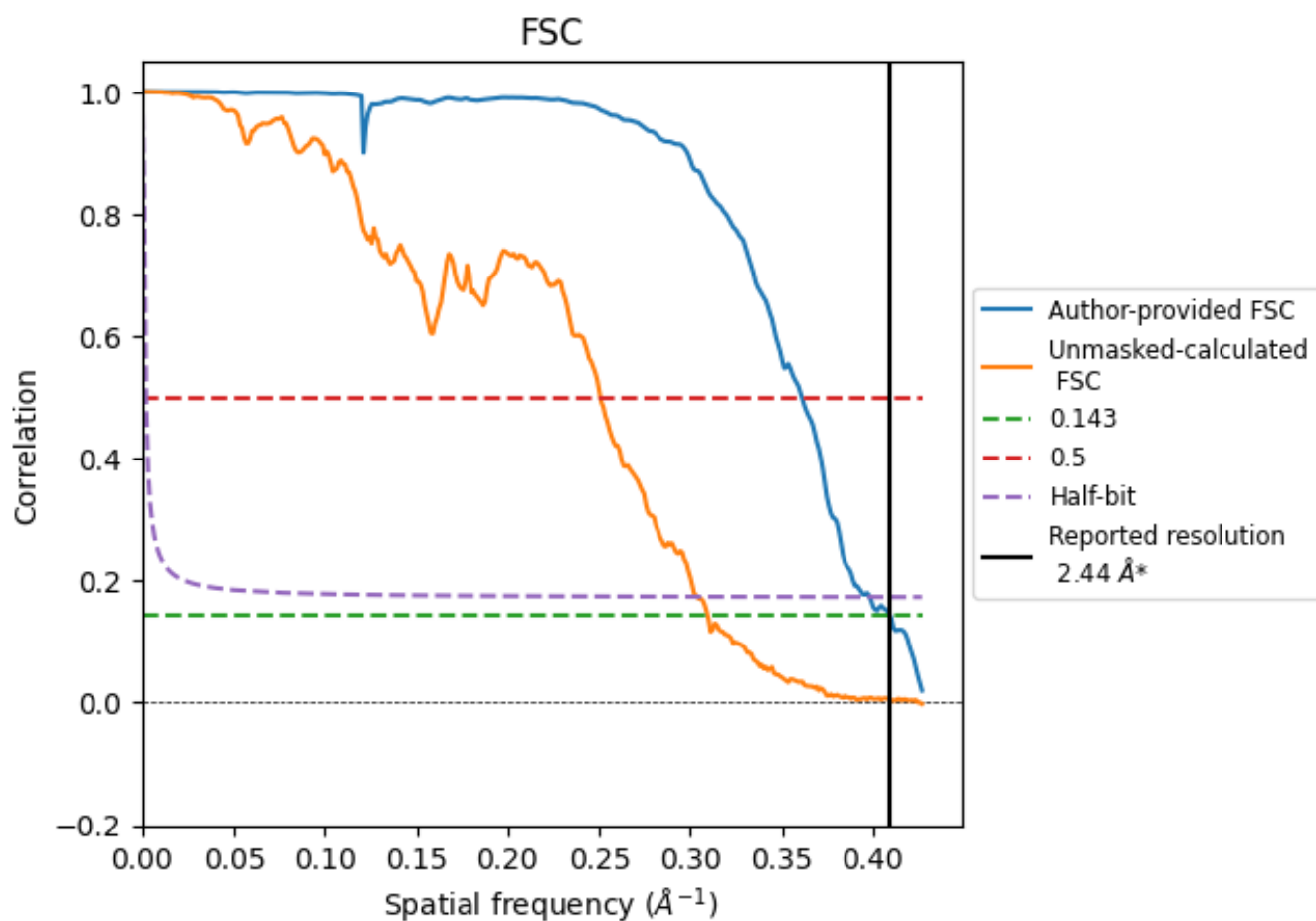


\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.77	2.51
Unmasked-calculated*	3.23	3.99	3.29

\*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 3.23 differs from the reported value 2.44 by more than 10 %

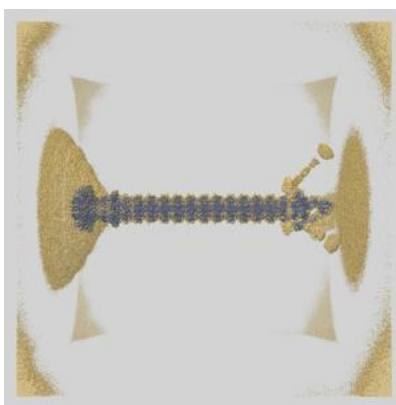
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51866 and PDB model 9H4P. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

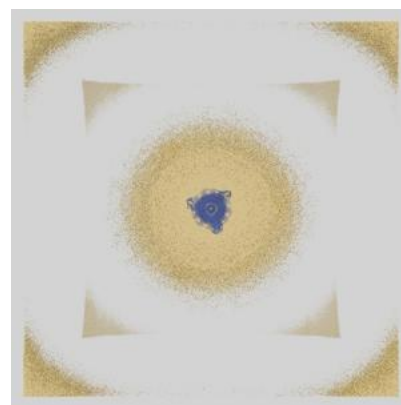
### 9.1 Map-model overlay [i](#)



X



Y

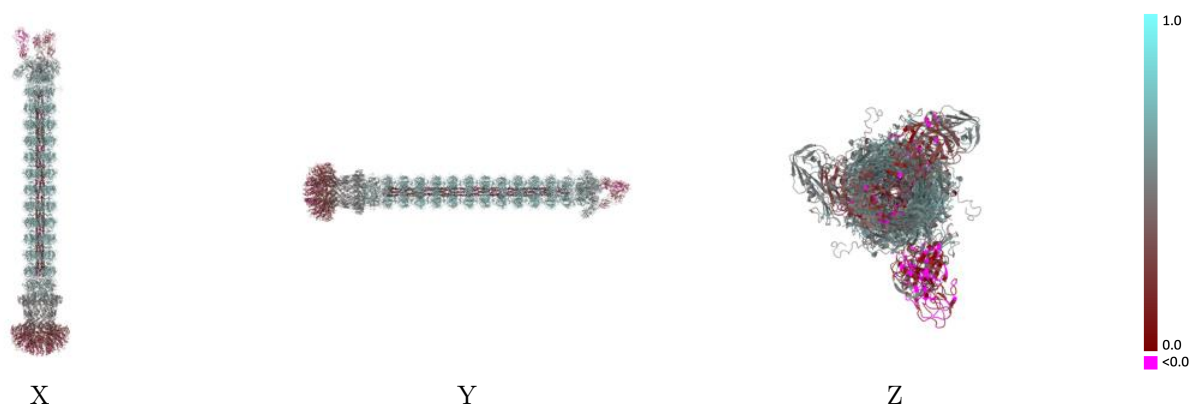


Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

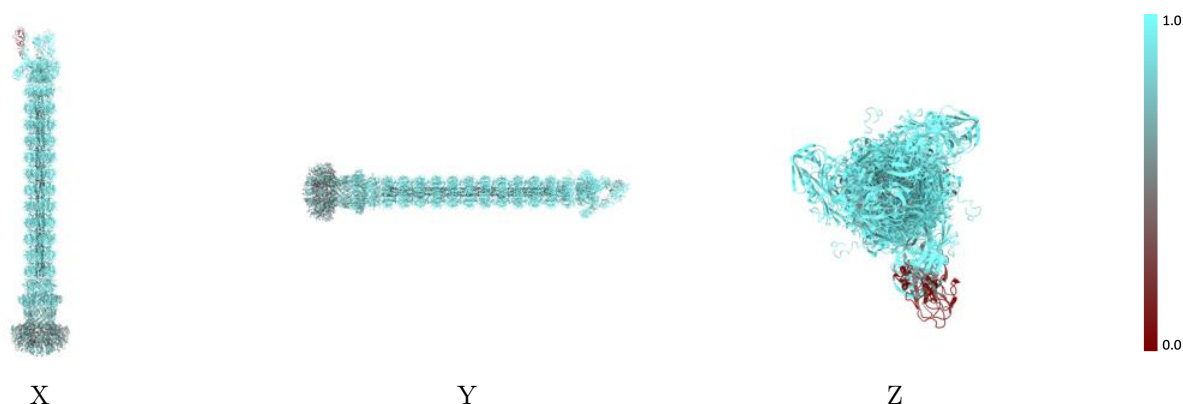


## 9.2 Q-score mapped to coordinate model [i](#)



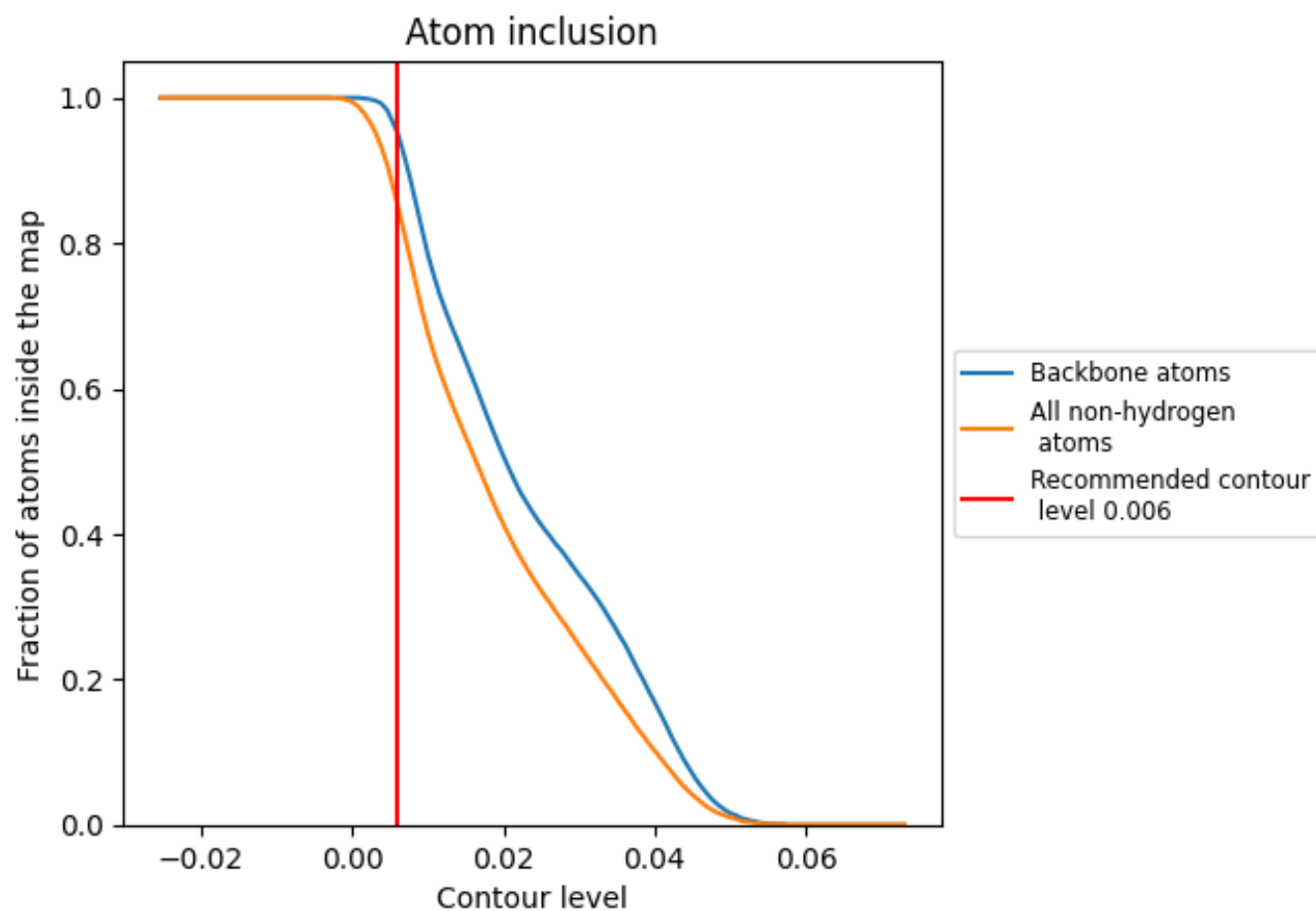
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.4710
B1	 0.9670	 0.6070
B2	 0.9670	 0.6060
B3	 0.9620	 0.6040
B4	 0.9660	 0.6050
B5	 0.9670	 0.6070
B6	 0.9600	 0.6020
BA	 0.9600	 0.5820
BB	 0.9590	 0.5790
BC	 0.9560	 0.5800
BD	 0.9410	 0.4300
BE	 0.9320	 0.4390
BF	 0.7990	 0.3740
P1	 0.9450	 0.5830
P2	 0.9470	 0.5820
P3	 0.9470	 0.5810
P4	 0.9490	 0.5860
P5	 0.9470	 0.5800
P6	 0.9490	 0.5810
PA	 0.6330	 0.2710
PB	 0.6410	 0.2690
PC	 0.6250	 0.2740
PD	 0.6320	 0.2670
PE	 0.6320	 0.2700
PF	 0.6450	 0.2710
PG	 0.6300	 0.2770
PH	 0.6320	 0.2700
PI	 0.6320	 0.2660
PJ	 0.6430	 0.2690
PK	 0.6270	 0.2700
PL	 0.6270	 0.2650
PM	 0.8400	 0.4800
PN	 0.8500	 0.4800
PO	 0.8490	 0.4740
PP	 0.8440	 0.4690



































































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Chain	Atom inclusion	Q-score
PQ	 0.8510	 0.4760
PR	 0.8430	 0.4720
PS	 0.8460	 0.4780
PT	 0.8490	 0.4790
PU	 0.8440	 0.4700
PV	 0.8410	 0.4710
PW	 0.8400	 0.4740
PX	 0.8510	 0.4780
Pa	 0.9170	 0.5390
Pb	 0.9240	 0.5450
Pc	 0.9210	 0.5430
Pd	 0.9240	 0.5460
Pe	 0.9200	 0.5420
Pf	 0.9250	 0.5420
QE	 0.6750	 0.2290
QF	 0.6690	 0.2400
QG	 0.6770	 0.2340
QH	 0.6850	 0.2450
QI	 0.6720	 0.2270
QJ	 0.6860	 0.2450
S1	 0.9680	 0.6140
S2	 0.9690	 0.6160
SA	 0.9610	 0.6010
SB	 0.9640	 0.5990
SC	 0.9610	 0.5990
SD	 0.9590	 0.6010
SE	 0.9610	 0.6000
SF	 0.9630	 0.5990
SG	 0.9680	 0.6100
SH	 0.9690	 0.6090
SI	 0.9680	 0.6090
SJ	 0.9710	 0.6110
SK	 0.9680	 0.6080
SL	 0.9640	 0.6100
SM	 0.9690	 0.6130
SN	 0.9670	 0.6130
SO	 0.9680	 0.6110
SP	 0.9680	 0.6120
SQ	 0.9720	 0.6110
SR	 0.9650	 0.6100
SS	 0.9740	 0.6160
ST	 0.9690	 0.6160

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Chain	Atom inclusion	Q-score
SU	 0.9750	 0.6150
SV	 0.9680	 0.6150
SW	 0.9750	 0.6130
SX	 0.9700	 0.6140
SY	 0.9720	 0.6110
SZ	 0.9720	 0.6150
Sa	 0.9720	 0.6140
Sb	 0.9720	 0.6150
Sc	 0.9730	 0.6150
Sd	 0.9690	 0.6130
Se	 0.9720	 0.6140
Sf	 0.9750	 0.6140
Sg	 0.9690	 0.6120
Sh	 0.9730	 0.6140
Si	 0.9730	 0.6140
Sj	 0.9730	 0.6120
Sk	 0.9740	 0.6130
Sl	 0.9700	 0.6140
Sm	 0.9690	 0.6140
Sn	 0.9690	 0.6150
So	 0.9710	 0.6110
Sp	 0.9700	 0.6150
Sq	 0.9720	 0.6150
Sr	 0.9710	 0.6130
Ss	 0.9680	 0.6130
St	 0.9700	 0.6150
Su	 0.9690	 0.6140
Sv	 0.9690	 0.6140
Sw	 0.9670	 0.6150
Sx	 0.9690	 0.6140
Sy	 0.9720	 0.6150
Sz	 0.9680	 0.6130