Full wwPDB EM Validation Report ⓘ

Oct 5, 2022 – 12:25 PM JST

PDB ID	:	6LXV
EMDB ID	:	EMD-30007
Title	:	Cryo-EM structure of phosphoketolase from Bifidobacterium longum
Authors	:	Nakata, K.; Miyazaki, N.; Yamaguchi, H.; Hirose, M.; Miyano, H.; Mizukoshi, T.; Kashiwagi, T.; Iwasaki, K.
Deposited on	:	2020-02-12
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

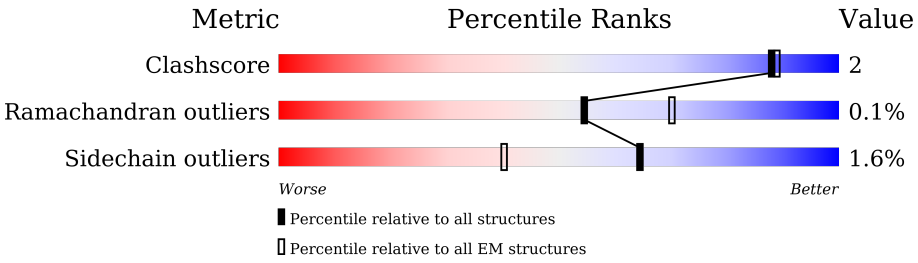
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	831	87% 9%
1	B	831	88% 9%
1	C	831	88% 9%
1	D	831	88% 9%
1	E	831	88% 8%
1	F	831	88% 8%
1	G	831	88% 8%
1	H	831	88% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 54924 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 Phosphoketolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	806	Total 6472	C 4107	N 1108	O 1238	S 19	7	0
1	B	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0
1	C	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0
1	D	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0
1	E	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0
1	F	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0
1	G	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0
1	H	806	Total 6467	C 4102	N 1108	O 1238	S 19	6	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	826	HIS	-	expression tag	UNP D6D942
A	827	HIS	-	expression tag	UNP D6D942
A	828	HIS	-	expression tag	UNP D6D942
A	829	HIS	-	expression tag	UNP D6D942
A	830	HIS	-	expression tag	UNP D6D942
A	831	HIS	-	expression tag	UNP D6D942
B	826	HIS	-	expression tag	UNP D6D942
B	827	HIS	-	expression tag	UNP D6D942
B	828	HIS	-	expression tag	UNP D6D942
B	829	HIS	-	expression tag	UNP D6D942
B	830	HIS	-	expression tag	UNP D6D942
B	831	HIS	-	expression tag	UNP D6D942
C	826	HIS	-	expression tag	UNP D6D942
C	827	HIS	-	expression tag	UNP D6D942

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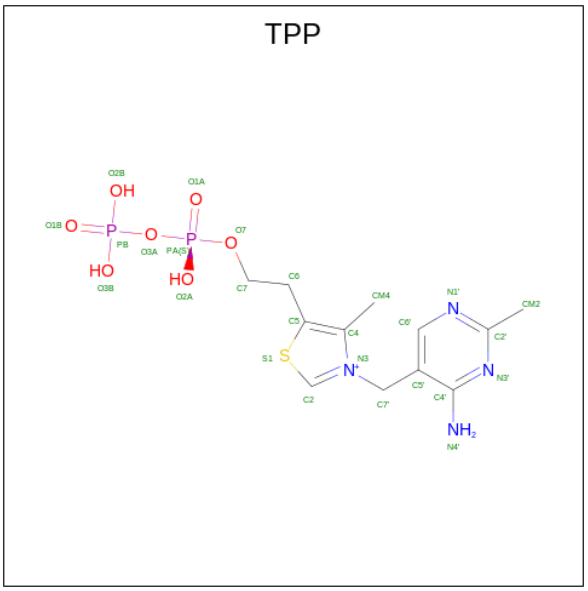
Chain	Residue	Modelled	Actual	Comment	Reference
C	828	HIS	-	expression tag	UNP D6D942
C	829	HIS	-	expression tag	UNP D6D942
C	830	HIS	-	expression tag	UNP D6D942
C	831	HIS	-	expression tag	UNP D6D942
D	826	HIS	-	expression tag	UNP D6D942
D	827	HIS	-	expression tag	UNP D6D942
D	828	HIS	-	expression tag	UNP D6D942
D	829	HIS	-	expression tag	UNP D6D942
D	830	HIS	-	expression tag	UNP D6D942
D	831	HIS	-	expression tag	UNP D6D942
E	826	HIS	-	expression tag	UNP D6D942
E	827	HIS	-	expression tag	UNP D6D942
E	828	HIS	-	expression tag	UNP D6D942
E	829	HIS	-	expression tag	UNP D6D942
E	830	HIS	-	expression tag	UNP D6D942
E	831	HIS	-	expression tag	UNP D6D942
F	826	HIS	-	expression tag	UNP D6D942
F	827	HIS	-	expression tag	UNP D6D942
F	828	HIS	-	expression tag	UNP D6D942
F	829	HIS	-	expression tag	UNP D6D942
F	830	HIS	-	expression tag	UNP D6D942
F	831	HIS	-	expression tag	UNP D6D942
G	826	HIS	-	expression tag	UNP D6D942
G	827	HIS	-	expression tag	UNP D6D942
G	828	HIS	-	expression tag	UNP D6D942
G	829	HIS	-	expression tag	UNP D6D942
G	830	HIS	-	expression tag	UNP D6D942
G	831	HIS	-	expression tag	UNP D6D942
H	826	HIS	-	expression tag	UNP D6D942
H	827	HIS	-	expression tag	UNP D6D942
H	828	HIS	-	expression tag	UNP D6D942
H	829	HIS	-	expression tag	UNP D6D942
H	830	HIS	-	expression tag	UNP D6D942
H	831	HIS	-	expression tag	UNP D6D942

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	B	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	C	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	D	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	E	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	F	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	G	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	H	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total Ca 1 1	0
3	E	1	Total Ca 1 1	0
3	F	1	Total Ca 1 1	0
3	G	1	Total Ca 1 1	0
3	H	1	Total Ca 1 1	0

- Molecule 4 is water.

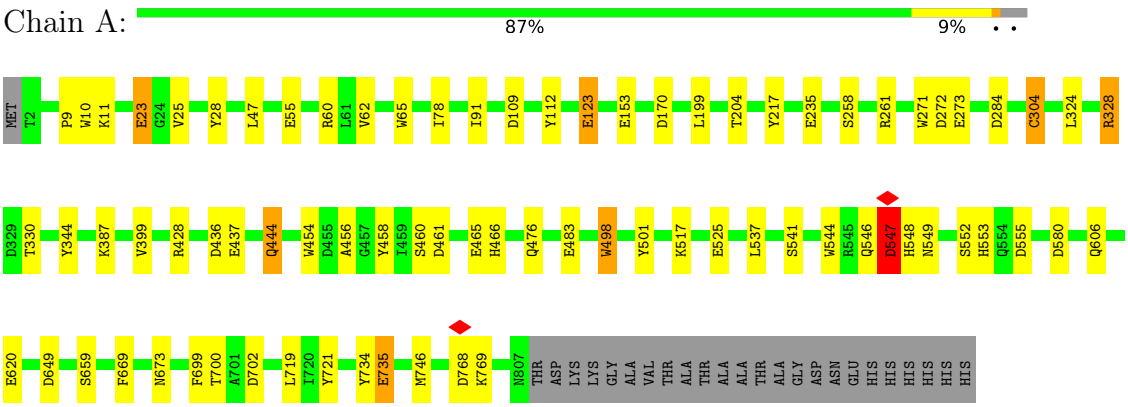
Mol	Chain	Residues	Atoms	AltConf
4	A	371	Total O 371 371	0
4	B	370	Total O 370 370	0
4	C	371	Total O 371 371	0
4	D	371	Total O 371 371	0
4	E	371	Total O 371 371	0
4	F	371	Total O 371 371	0
4	G	371	Total O 371 371	0
4	H	371	Total O 371 371	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

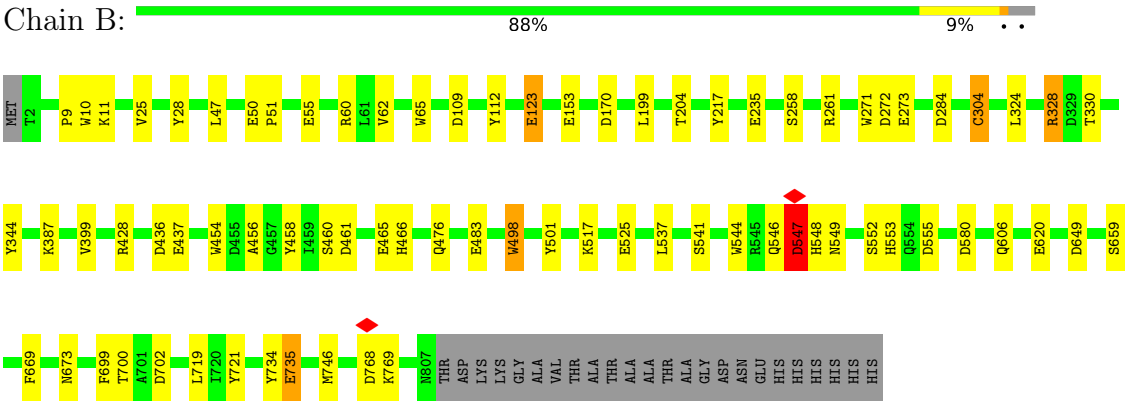
• Molecule 1: Phosphoketolase

Chain A:



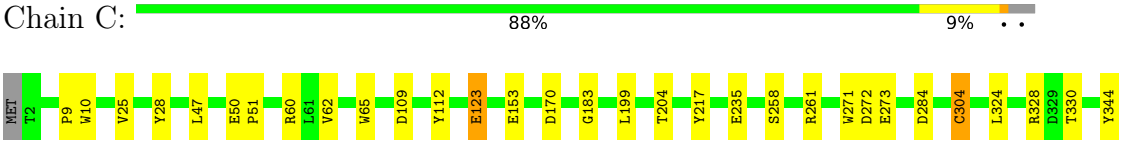
• Molecule 1: Phosphoketolase

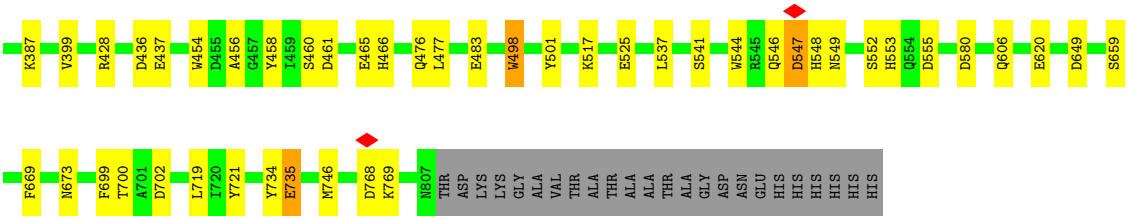
Chain B:



• Molecule 1: Phosphoketolase

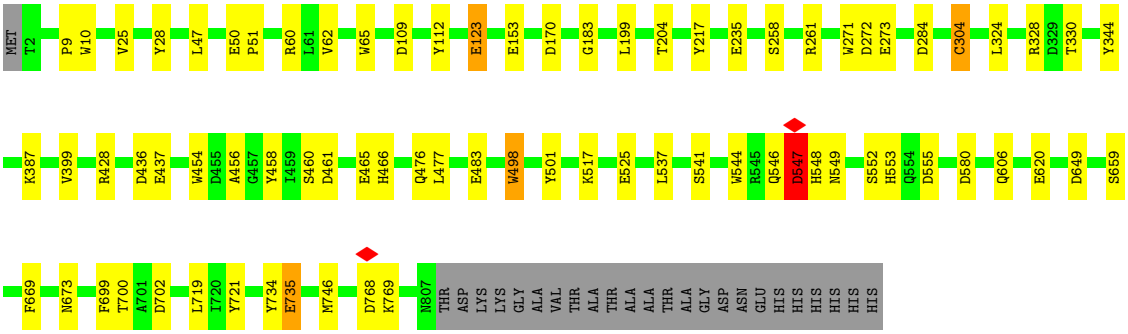
Chain C:





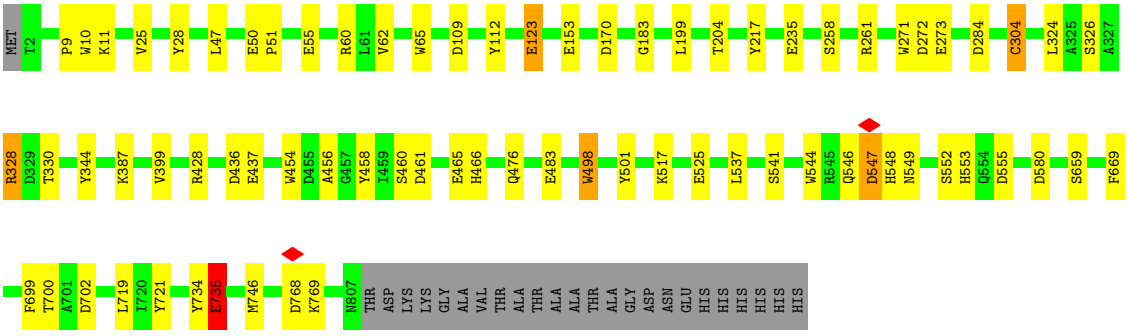
• Molecule 1: Phosphoketolase

Chain D:



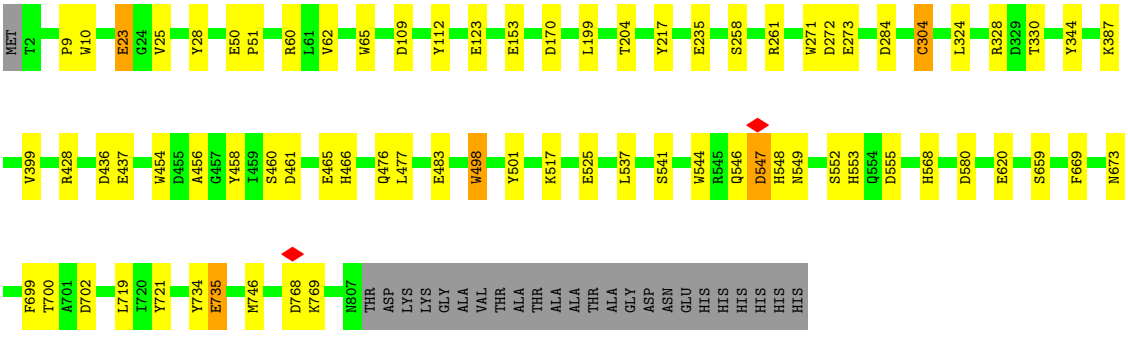
• Molecule 1: Phosphoketolase

Chain E:



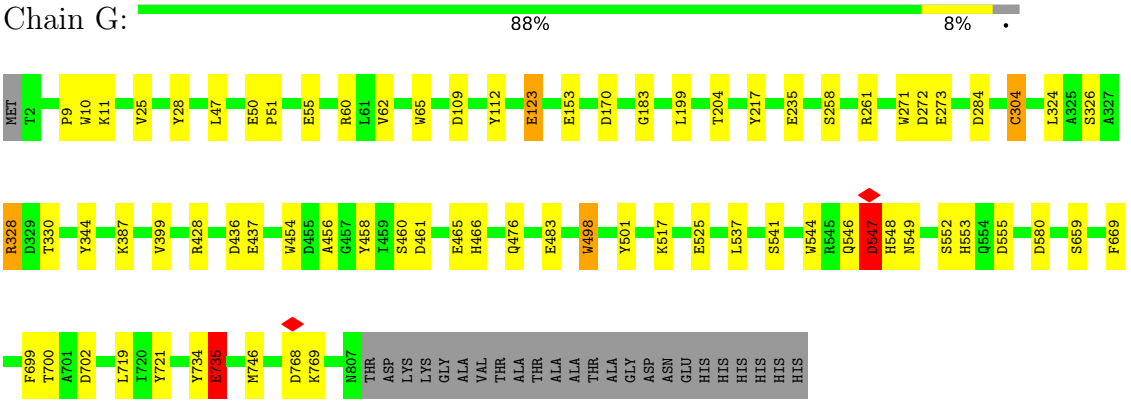
• Molecule 1: Phosphoketolase

Chain F:



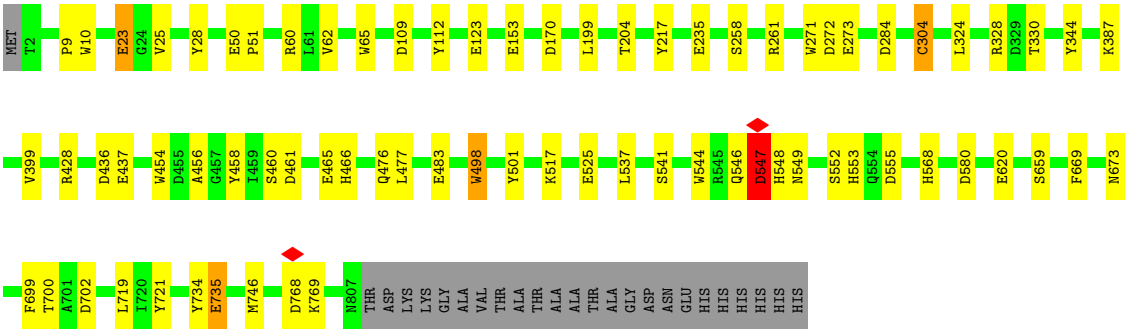
• Molecule 1: Phosphoketolase

Chain G:



• Molecule 1: Phosphoketolase

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	194517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.545	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	313.2, 313.2, 313.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.14	24/6654 (0.4%)	0.90	14/9049 (0.2%)
1	B	1.13	23/6646 (0.3%)	0.90	14/9038 (0.2%)
1	C	1.13	23/6646 (0.3%)	0.91	12/9038 (0.1%)
1	D	1.13	23/6646 (0.3%)	0.91	14/9038 (0.2%)
1	E	1.13	23/6646 (0.3%)	0.90	12/9038 (0.1%)
1	F	1.14	24/6646 (0.4%)	0.91	12/9038 (0.1%)
1	G	1.13	23/6646 (0.3%)	0.91	14/9038 (0.2%)
1	H	1.14	24/6646 (0.4%)	0.91	14/9038 (0.2%)
All	All	1.13	187/53176 (0.4%)	0.91	106/72315 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	TYR	CD1-CE1	-9.03	1.25	1.39
1	C	217	TYR	CD1-CE1	-8.99	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	217	TYR	CD1-CE1	-8.99	1.25	1.39
1	F	217	TYR	CD1-CE1	-8.98	1.25	1.39
1	A	217	TYR	CD1-CE1	-8.97	1.25	1.39
1	D	217	TYR	CD1-CE1	-8.97	1.25	1.39
1	G	217	TYR	CD1-CE1	-8.94	1.25	1.39
1	H	217	TYR	CD1-CE1	-8.94	1.25	1.39
1	A	28	TYR	CD1-CE1	-8.33	1.26	1.39
1	G	28	TYR	CD1-CE1	-8.31	1.26	1.39
1	H	28	TYR	CD1-CE1	-8.31	1.26	1.39
1	E	28	TYR	CD1-CE1	-8.30	1.26	1.39
1	B	28	TYR	CD1-CE1	-8.28	1.26	1.39
1	C	28	TYR	CD1-CE1	-8.28	1.26	1.39
1	D	28	TYR	CD1-CE1	-8.28	1.26	1.39
1	F	28	TYR	CD1-CE1	-8.22	1.27	1.39
1	A	23	GLU	CB-CG	-7.65	1.37	1.52
1	F	23	GLU	CB-CG	-7.61	1.37	1.52
1	H	23	GLU	CB-CG	-7.61	1.37	1.52
1	E	483	GLU	CD-OE2	-7.08	1.17	1.25
1	D	483	GLU	CD-OE2	-7.07	1.17	1.25
1	G	483	GLU	CD-OE2	-7.07	1.17	1.25
1	H	483	GLU	CD-OE2	-7.07	1.17	1.25
1	A	483	GLU	CD-OE2	-7.06	1.17	1.25
1	C	483	GLU	CD-OE2	-7.06	1.17	1.25
1	F	483	GLU	CD-OE2	-7.06	1.17	1.25
1	B	483	GLU	CD-OE2	-7.05	1.17	1.25
1	B	734	TYR	CD1-CE1	-6.65	1.29	1.39
1	D	399	VAL	CB-CG2	-6.63	1.39	1.52
1	G	399	VAL	CB-CG2	-6.63	1.39	1.52
1	B	399	VAL	CB-CG2	-6.62	1.39	1.52
1	D	734	TYR	CD1-CE1	-6.60	1.29	1.39
1	A	399	VAL	CB-CG2	-6.60	1.39	1.52
1	C	399	VAL	CB-CG2	-6.59	1.39	1.52
1	H	399	VAL	CB-CG2	-6.59	1.39	1.52
1	E	734	TYR	CD1-CE1	-6.58	1.29	1.39
1	F	734	TYR	CD1-CE1	-6.58	1.29	1.39
1	G	734	TYR	CD1-CE1	-6.58	1.29	1.39
1	F	399	VAL	CB-CG2	-6.58	1.39	1.52
1	A	734	TYR	CD1-CE1	-6.56	1.29	1.39
1	C	734	TYR	CD1-CE1	-6.56	1.29	1.39
1	E	399	VAL	CB-CG2	-6.55	1.39	1.52
1	H	734	TYR	CD1-CE1	-6.54	1.29	1.39
1	F	235	GLU	CB-CG	-6.51	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	GLU	CB-CG	-6.33	1.40	1.52
1	A	235	GLU	CB-CG	-6.32	1.40	1.52
1	C	235	GLU	CB-CG	-6.32	1.40	1.52
1	E	235	GLU	CB-CG	-6.32	1.40	1.52
1	G	235	GLU	CB-CG	-6.32	1.40	1.52
1	H	235	GLU	CB-CG	-6.31	1.40	1.52
1	B	235	GLU	CB-CG	-6.27	1.40	1.52
1	D	702	ASP	C-N	-6.24	1.19	1.34
1	G	702	ASP	C-N	-6.24	1.19	1.34
1	A	702	ASP	C-N	-6.21	1.19	1.34
1	B	702	ASP	C-N	-6.21	1.19	1.34
1	C	702	ASP	C-N	-6.21	1.19	1.34
1	E	702	ASP	C-N	-6.21	1.19	1.34
1	F	501	TYR	CD1-CE1	-6.21	1.30	1.39
1	F	702	ASP	C-N	-6.21	1.19	1.34
1	H	501	TYR	CD1-CE1	-6.21	1.30	1.39
1	H	702	ASP	C-N	-6.21	1.19	1.34
1	B	501	TYR	CD1-CE1	-6.18	1.30	1.39
1	D	501	TYR	CD1-CE1	-6.18	1.30	1.39
1	E	501	TYR	CD1-CE1	-6.18	1.30	1.39
1	G	501	TYR	CD1-CE1	-6.18	1.30	1.39
1	C	501	TYR	CD1-CE1	-6.14	1.30	1.39
1	A	501	TYR	CD1-CE1	-6.14	1.30	1.39
1	A	273	GLU	CB-CG	-6.13	1.40	1.52
1	B	273	GLU	CB-CG	-6.13	1.40	1.52
1	C	273	GLU	CB-CG	-6.13	1.40	1.52
1	E	273	GLU	CB-CG	-6.13	1.40	1.52
1	F	273	GLU	CB-CG	-6.13	1.40	1.52
1	G	273	GLU	CB-CG	-6.13	1.40	1.52
1	H	273	GLU	CB-CG	-6.13	1.40	1.52
1	D	273	GLU	CB-CG	-6.08	1.40	1.52
1	F	498	TRP	CB-CG	-6.00	1.39	1.50
1	C	498	TRP	CB-CG	-5.97	1.39	1.50
1	B	498	TRP	CB-CG	-5.96	1.39	1.50
1	D	498	TRP	CB-CG	-5.96	1.39	1.50
1	E	498	TRP	CB-CG	-5.96	1.39	1.50
1	A	498	TRP	CB-CG	-5.95	1.39	1.50
1	G	498	TRP	CB-CG	-5.95	1.39	1.50
1	H	498	TRP	CB-CG	-5.95	1.39	1.50
1	C	304	CYS	CB-SG	-5.76	1.72	1.81
1	E	304	CYS	CB-SG	-5.72	1.72	1.81
1	B	304	CYS	CB-SG	-5.71	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	721	TYR	CD1-CE1	-5.71	1.30	1.39
1	E	721	TYR	CD1-CE1	-5.71	1.30	1.39
1	A	304	CYS	CB-SG	-5.70	1.72	1.81
1	F	304	CYS	CB-SG	-5.70	1.72	1.81
1	G	304	CYS	CB-SG	-5.70	1.72	1.81
1	H	304	CYS	CB-SG	-5.70	1.72	1.81
1	H	735	GLU	CB-CG	-5.67	1.41	1.52
1	D	735	GLU	CB-CG	-5.65	1.41	1.52
1	C	735	GLU	CB-CG	-5.64	1.41	1.52
1	A	721	TYR	CD1-CE1	-5.63	1.30	1.39
1	C	721	TYR	CD1-CE1	-5.63	1.30	1.39
1	D	721	TYR	CD1-CE1	-5.63	1.30	1.39
1	G	721	TYR	CD1-CE1	-5.63	1.30	1.39
1	H	721	TYR	CD1-CE1	-5.63	1.30	1.39
1	E	735	GLU	CB-CG	-5.62	1.41	1.52
1	F	721	TYR	CD1-CE1	-5.62	1.30	1.39
1	A	735	GLU	CB-CG	-5.62	1.41	1.52
1	F	735	GLU	CB-CG	-5.61	1.41	1.52
1	B	735	GLU	CB-CG	-5.60	1.41	1.52
1	G	735	GLU	CB-CG	-5.59	1.41	1.52
1	D	304	CYS	CB-SG	-5.55	1.72	1.81
1	B	112	TYR	CD2-CE2	-5.46	1.31	1.39
1	C	112	TYR	CD2-CE2	-5.46	1.31	1.39
1	D	112	TYR	CD2-CE2	-5.46	1.31	1.39
1	E	112	TYR	CD2-CE2	-5.46	1.31	1.39
1	H	112	TYR	CD2-CE2	-5.46	1.31	1.39
1	A	112	TYR	CD2-CE2	-5.43	1.31	1.39
1	G	112	TYR	CD2-CE2	-5.41	1.31	1.39
1	F	112	TYR	CD2-CE2	-5.38	1.31	1.39
1	G	112	TYR	CD1-CE1	-5.35	1.31	1.39
1	D	460	SER	CB-OG	-5.35	1.35	1.42
1	G	460	SER	CB-OG	-5.35	1.35	1.42
1	H	460	SER	CB-OG	-5.35	1.35	1.42
1	A	112	TYR	CD1-CE1	-5.34	1.31	1.39
1	D	112	TYR	CD1-CE1	-5.34	1.31	1.39
1	D	25	VAL	CB-CG2	-5.33	1.41	1.52
1	A	460	SER	CB-OG	-5.33	1.35	1.42
1	C	460	SER	CB-OG	-5.33	1.35	1.42
1	E	460	SER	CB-OG	-5.33	1.35	1.42
1	F	460	SER	CB-OG	-5.33	1.35	1.42
1	B	112	TYR	CD1-CE1	-5.29	1.31	1.39
1	C	112	TYR	CD1-CE1	-5.29	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	25	VAL	CB-CG2	-5.29	1.41	1.52
1	A	25	VAL	CB-CG2	-5.29	1.41	1.52
1	B	460	SER	CB-OG	-5.29	1.35	1.42
1	E	25	VAL	CB-CG2	-5.29	1.41	1.52
1	F	25	VAL	CB-CG2	-5.28	1.41	1.52
1	G	25	VAL	CB-CG2	-5.28	1.41	1.52
1	E	112	TYR	CD1-CE1	-5.28	1.31	1.39
1	A	217	TYR	CD2-CE2	-5.26	1.31	1.39
1	G	217	TYR	CD2-CE2	-5.26	1.31	1.39
1	H	112	TYR	CD1-CE1	-5.25	1.31	1.39
1	B	25	VAL	CB-CG2	-5.24	1.41	1.52
1	H	25	VAL	CB-CG2	-5.23	1.41	1.52
1	F	112	TYR	CD1-CE1	-5.23	1.31	1.39
1	F	217	TYR	CD2-CE2	-5.22	1.31	1.39
1	B	217	TYR	CD2-CE2	-5.21	1.31	1.39
1	C	217	TYR	CD2-CE2	-5.21	1.31	1.39
1	H	217	TYR	CD2-CE2	-5.21	1.31	1.39
1	C	344	TYR	CD1-CE1	-5.19	1.31	1.39
1	E	344	TYR	CD1-CE1	-5.18	1.31	1.39
1	F	344	TYR	CD1-CE1	-5.17	1.31	1.39
1	D	217	TYR	CD2-CE2	-5.16	1.31	1.39
1	E	217	TYR	CD2-CE2	-5.16	1.31	1.39
1	D	271	TRP	CB-CG	-5.13	1.41	1.50
1	B	344	TYR	CD1-CE1	-5.12	1.31	1.39
1	D	344	TYR	CD1-CE1	-5.12	1.31	1.39
1	G	344	TYR	CD1-CE1	-5.12	1.31	1.39
1	A	437	GLU	CD-OE1	-5.11	1.20	1.25
1	B	437	GLU	CD-OE1	-5.11	1.20	1.25
1	C	437	GLU	CD-OE1	-5.11	1.20	1.25
1	D	437	GLU	CD-OE1	-5.11	1.20	1.25
1	E	437	GLU	CD-OE1	-5.11	1.20	1.25
1	F	437	GLU	CD-OE1	-5.11	1.20	1.25
1	G	437	GLU	CD-OE1	-5.11	1.20	1.25
1	H	437	GLU	CD-OE1	-5.11	1.20	1.25
1	A	271	TRP	CB-CG	-5.11	1.41	1.50
1	B	271	TRP	CB-CG	-5.11	1.41	1.50
1	C	271	TRP	CB-CG	-5.11	1.41	1.50
1	E	271	TRP	CB-CG	-5.11	1.41	1.50
1	F	271	TRP	CB-CG	-5.11	1.41	1.50
1	G	271	TRP	CB-CG	-5.11	1.41	1.50
1	H	271	TRP	CB-CG	-5.11	1.41	1.50
1	H	344	TYR	CD1-CE1	-5.11	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	B	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	C	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	D	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	E	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	F	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	G	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	H	458	TYR	CD1-CE1	-5.09	1.31	1.39
1	A	344	TYR	CD1-CE1	-5.06	1.31	1.39
1	B	544	TRP	CG-CD1	-5.04	1.29	1.36
1	H	544	TRP	CG-CD1	-5.04	1.29	1.36
1	A	544	TRP	CG-CD1	-5.03	1.29	1.36
1	C	544	TRP	CG-CD1	-5.03	1.29	1.36
1	D	544	TRP	CG-CD1	-5.03	1.29	1.36
1	E	544	TRP	CG-CD1	-5.03	1.29	1.36
1	F	544	TRP	CG-CD1	-5.03	1.29	1.36
1	G	544	TRP	CG-CD1	-5.03	1.29	1.36

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	109	ASP	CB-CG-OD1	9.43	126.78	118.30
1	H	109	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	109	ASP	CB-CG-OD1	9.40	126.77	118.30
1	B	109	ASP	CB-CG-OD1	9.40	126.76	118.30
1	E	109	ASP	CB-CG-OD1	9.39	126.75	118.30
1	C	109	ASP	CB-CG-OD1	9.37	126.73	118.30
1	G	109	ASP	CB-CG-OD1	9.36	126.73	118.30
1	F	109	ASP	CB-CG-OD1	9.34	126.71	118.30
1	A	436	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	D	436	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	G	436	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	H	436	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	F	436	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	C	436	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	B	436	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	E	436	ASP	CB-CG-OD2	-8.92	110.27	118.30
1	C	436	ASP	CB-CG-OD1	7.54	125.08	118.30
1	E	436	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	436	ASP	CB-CG-OD1	7.50	125.05	118.30
1	F	436	ASP	CB-CG-OD1	7.47	125.02	118.30
1	G	436	ASP	CB-CG-OD1	7.47	125.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	436	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	436	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	436	ASP	CB-CG-OD1	7.39	124.95	118.30
1	C	719	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	E	719	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	F	719	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	G	719	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	B	719	LEU	CB-CG-CD2	-6.78	99.48	111.00
1	D	719	LEU	CB-CG-CD2	-6.78	99.48	111.00
1	H	719	LEU	CB-CG-CD2	-6.78	99.48	111.00
1	A	719	LEU	CB-CG-CD2	-6.75	99.52	111.00
1	A	719	LEU	CA-CB-CG	6.74	130.81	115.30
1	G	719	LEU	CA-CB-CG	6.74	130.80	115.30
1	E	719	LEU	CA-CB-CG	6.74	130.80	115.30
1	F	719	LEU	CA-CB-CG	6.73	130.78	115.30
1	D	719	LEU	CA-CB-CG	6.73	130.77	115.30
1	B	719	LEU	CA-CB-CG	6.73	130.77	115.30
1	C	719	LEU	CA-CB-CG	6.73	130.77	115.30
1	H	719	LEU	CA-CB-CG	6.73	130.77	115.30
1	D	284	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	284	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	284	ASP	CB-CG-OD1	6.28	123.95	118.30
1	G	284	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	272	ASP	CB-CG-OD1	6.25	123.92	118.30
1	H	272	ASP	CB-CG-OD1	6.25	123.92	118.30
1	E	284	ASP	CB-CG-OD1	6.24	123.92	118.30
1	F	284	ASP	CB-CG-OD1	6.24	123.92	118.30
1	E	272	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	272	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	272	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	272	ASP	CB-CG-OD1	6.21	123.89	118.30
1	F	272	ASP	CB-CG-OD1	6.21	123.89	118.30
1	G	272	ASP	CB-CG-OD1	6.21	123.89	118.30
1	H	284	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	284	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	555	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	555	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	555	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	555	ASP	CB-CG-OD1	5.58	123.32	118.30
1	E	555	ASP	CB-CG-OD1	5.58	123.32	118.30
1	H	555	ASP	CB-CG-OD1	5.58	123.32	118.30
1	G	555	ASP	CB-CG-OD1	5.55	123.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	555	ASP	CB-CG-OD1	5.55	123.30	118.30
1	H	580	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	580	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	580	ASP	CB-CG-OD1	5.54	123.29	118.30
1	F	580	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	580	ASP	CB-CG-OD1	5.53	123.28	118.30
1	G	580	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	580	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	580	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	324	LEU	CB-CG-CD2	-5.46	101.73	111.00
1	D	324	LEU	CB-CG-CD2	-5.46	101.73	111.00
1	H	324	LEU	CB-CG-CD2	-5.46	101.73	111.00
1	C	324	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	A	324	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	E	324	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	F	324	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	G	324	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	A	328	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	C	328	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	328	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	D	461	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	461	ASP	CB-CG-OD1	5.11	122.89	118.30
1	H	461	ASP	CB-CG-OD1	5.11	122.89	118.30
1	E	328	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	G	328	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	D	328	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	E	461	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	461	ASP	CB-CG-OD1	5.08	122.87	118.30
1	G	461	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	547[A]	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	547[B]	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	547[A]	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	547[B]	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	461	ASP	CB-CG-OD1	5.04	122.83	118.30
1	F	328	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	H	328	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	G	547[A]	ASP	CB-CG-OD1	5.01	122.81	118.30
1	G	547[B]	ASP	CB-CG-OD1	5.01	122.81	118.30
1	H	547[A]	ASP	CB-CG-OD1	5.01	122.81	118.30
1	H	547[B]	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	547[A]	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	547[B]	ASP	CB-CG-OD1	5.01	122.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	461	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	699	PHE	Peptide
1	B	699	PHE	Peptide
1	C	699	PHE	Peptide
1	D	699	PHE	Peptide
1	E	699	PHE	Peptide
1	F	699	PHE	Peptide
1	G	699	PHE	Peptide
1	H	699	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6472	0	6154	27	0
1	B	6467	0	6143	26	0
1	C	6467	0	6143	26	0
1	D	6467	0	6143	26	0
1	E	6467	0	6143	27	0
1	F	6467	0	6143	24	0
1	G	6467	0	6143	27	0
1	H	6467	0	6143	24	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	1	0
2	E	26	0	16	1	0
2	F	26	0	16	1	0
2	G	26	0	16	1	0
2	H	26	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	371	0	0	3	0
4	B	370	0	0	2	0
4	C	371	0	0	2	0
4	D	371	0	0	2	0
4	E	371	0	0	2	0
4	F	371	0	0	2	0
4	G	371	0	0	2	0
4	H	371	0	0	2	0
All	All	54924	0	49283	193	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 2.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:SER:HA	1:B:517:LYS:HD3	1.70	0.73
1:A:517:LYS:HD3	1:B:552:SER:HA	1.70	0.73
1:E:517:LYS:HD3	1:F:552:SER:HA	1.70	0.73
1:G:517:LYS:HD3	1:H:552:SER:HA	1.70	0.73
1:G:552:SER:HA	1:H:517:LYS:HD3	1.70	0.72
1:E:552:SER:HA	1:F:517:LYS:HD3	1.70	0.72
1:C:517:LYS:HD3	1:D:552:SER:HA	1.70	0.71
1:C:552:SER:HA	1:D:517:LYS:HD3	1.70	0.71
1:E:548[A]:HIS:HA	1:F:62:VAL:HG13	1.79	0.65
1:G:548[A]:HIS:HA	1:H:62:VAL:HG13	1.79	0.65
1:A:548[A]:HIS:HA	1:B:62:VAL:HG13	1.79	0.64
1:A:62:VAL:HG13	1:B:548[A]:HIS:HA	1.79	0.64
1:C:62:VAL:HG13	1:D:548[A]:HIS:HA	1.79	0.64
1:C:548[A]:HIS:HA	1:D:62:VAL:HG13	1.79	0.64
1:E:62:VAL:HG13	1:F:548[A]:HIS:HA	1.79	0.64
1:G:62:VAL:HG13	1:H:548[A]:HIS:HA	1.79	0.63
1:A:261:ARG:NH2	4:A:1012:HOH:O	2.32	0.63
1:E:261:ARG:NH2	4:E:1011:HOH:O	2.32	0.63
1:B:261:ARG:NH2	4:B:1012:HOH:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ARG:NH2	4:G:1012:HOH:O	2.32	0.63
1:B:547[B]:ASP:HB3	1:B:746:MET:HG2	1.82	0.62
1:A:547[B]:ASP:HB3	1:A:746:MET:HG2	1.82	0.62
1:F:261:ARG:NH2	4:F:1012:HOH:O	2.32	0.62
1:D:261:ARG:NH2	4:D:1012:HOH:O	2.32	0.62
1:H:547[B]:ASP:HB3	1:H:746:MET:HG2	1.82	0.62
1:H:261:ARG:NH2	4:H:1012:HOH:O	2.32	0.62
1:C:261:ARG:NH2	4:C:1012:HOH:O	2.32	0.62
1:F:547[B]:ASP:HB3	1:F:746:MET:HG2	1.82	0.62
1:C:547[B]:ASP:HB3	1:C:746:MET:HG2	1.82	0.61
1:D:547[B]:ASP:HB3	1:D:746:MET:HG2	1.82	0.61
1:E:547[B]:ASP:HB3	1:E:746:MET:HG2	1.82	0.60
1:G:547[B]:ASP:HB3	1:G:746:MET:HG2	1.82	0.60
1:A:541:SER:O	1:A:546[B]:GLN:NE2	2.37	0.58
1:B:541:SER:O	1:B:546[B]:GLN:NE2	2.37	0.58
1:E:541:SER:O	1:E:546[B]:GLN:NE2	2.37	0.57
1:D:541:SER:O	1:D:546[B]:GLN:NE2	2.37	0.57
1:G:541:SER:O	1:G:546[B]:GLN:NE2	2.37	0.57
1:C:541:SER:O	1:C:546[B]:GLN:NE2	2.37	0.57
1:H:541:SER:O	1:H:546[B]:GLN:NE2	2.37	0.57
1:F:541:SER:O	1:F:546[B]:GLN:NE2	2.37	0.57
1:G:541:SER:O	1:G:546[A]:GLN:NE2	2.42	0.53
1:E:541:SER:O	1:E:546[A]:GLN:NE2	2.42	0.53
1:C:541:SER:O	1:C:546[A]:GLN:NE2	2.42	0.52
1:D:541:SER:O	1:D:546[A]:GLN:NE2	2.43	0.52
1:A:541:SER:O	1:A:546[A]:GLN:NE2	2.42	0.52
1:A:78:ILE:HG21	1:A:91[B]:ILE:HD11	1.91	0.52
1:B:541:SER:O	1:B:546[A]:GLN:NE2	2.42	0.52
1:F:541:SER:O	1:F:546[A]:GLN:NE2	2.42	0.51
1:H:541:SER:O	1:H:546[A]:GLN:NE2	2.42	0.51
1:B:153:GLU:OE1	4:B:1001:HOH:O	2.20	0.50
1:A:153:GLU:OE1	4:A:1001:HOH:O	2.20	0.50
1:C:153:GLU:OE1	4:C:1001:HOH:O	2.20	0.49
1:F:153:GLU:OE1	4:F:1001:HOH:O	2.20	0.49
1:D:153:GLU:OE1	4:D:1001:HOH:O	2.20	0.49
1:G:9:PRO:HB2	1:G:10:TRP:CD1	2.48	0.49
1:E:9:PRO:HB2	1:E:10:TRP:CD1	2.48	0.49
1:H:153:GLU:OE1	4:H:1001:HOH:O	2.20	0.49
2:H:900:TPP:C2	2:H:900:TPP:HN42	2.26	0.49
1:A:444:GLN:NE2	4:A:1029:HOH:O	2.44	0.49
2:F:900:TPP:HN42	2:F:900:TPP:C2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HB2	1:A:10:TRP:CD1	2.48	0.48
2:C:900:TPP:HN42	2:C:900:TPP:C2	2.26	0.48
1:B:9:PRO:HB2	1:B:10:TRP:CD1	2.48	0.48
2:B:900:TPP:HN42	2:B:900:TPP:C2	2.26	0.48
2:D:900:TPP:C2	2:D:900:TPP:HN42	2.26	0.48
2:G:900:TPP:HN42	2:G:900:TPP:C2	2.26	0.48
2:E:900:TPP:C2	2:E:900:TPP:HN42	2.26	0.48
1:G:153:GLU:OE1	4:G:1001:HOH:O	2.20	0.48
2:A:900:TPP:C2	2:A:900:TPP:HN42	2.26	0.48
1:F:9:PRO:HB2	1:F:10:TRP:CD1	2.48	0.48
1:H:9:PRO:HB2	1:H:10:TRP:CD1	2.48	0.48
1:H:170:ASP:OD1	1:H:428[A]:ARG:NH2	2.47	0.48
1:E:153:GLU:OE1	4:E:1001:HOH:O	2.20	0.48
1:F:170:ASP:OD1	1:F:428[A]:ARG:NH2	2.47	0.48
1:A:170:ASP:OD1	1:A:428[B]:ARG:NH2	2.47	0.48
1:B:170:ASP:OD1	1:B:428[A]:ARG:NH2	2.47	0.48
1:C:9:PRO:HB2	1:C:10:TRP:CD1	2.48	0.48
1:D:9:PRO:HB2	1:D:10:TRP:CD1	2.48	0.48
1:C:170:ASP:OD1	1:C:428[A]:ARG:NH2	2.47	0.47
1:D:170:ASP:OD1	1:D:428[A]:ARG:NH2	2.47	0.47
1:E:170:ASP:OD1	1:E:428[A]:ARG:NH2	2.47	0.47
1:G:170:ASP:OD1	1:G:428[A]:ARG:NH2	2.47	0.47
1:F:204:THR:HB	1:F:428[A]:ARG:NH2	2.31	0.46
1:E:11:LYS:HA	1:E:11:LYS:HD2	1.84	0.46
1:G:11:LYS:HA	1:G:11:LYS:HD2	1.84	0.46
1:C:204:THR:HB	1:C:428[A]:ARG:NH2	2.31	0.46
1:C:50:GLU:HA	1:C:51:PRO:HA	1.70	0.46
1:D:204:THR:HB	1:D:428[A]:ARG:NH2	2.31	0.46
1:H:204:THR:HB	1:H:428[A]:ARG:NH2	2.31	0.46
1:B:620:GLU:OE2	1:B:673:ASN:ND2	2.34	0.45
1:D:50:GLU:HA	1:D:51:PRO:HA	1.70	0.45
1:E:204:THR:HB	1:E:428[A]:ARG:NH2	2.31	0.45
1:G:204:THR:HB	1:G:428[A]:ARG:NH2	2.31	0.45
1:E:50:GLU:HA	1:E:51:PRO:HA	1.70	0.45
1:G:50:GLU:HA	1:G:51:PRO:HA	1.70	0.45
1:E:465:GLU:HG3	1:E:466:HIS:CD2	2.52	0.45
1:G:465:GLU:HG3	1:G:466:HIS:CD2	2.52	0.45
1:A:204:THR:HB	1:A:428[B]:ARG:NH2	2.31	0.45
1:A:620:GLU:OE2	1:A:673:ASN:ND2	2.34	0.45
1:B:204:THR:HB	1:B:428[A]:ARG:NH2	2.31	0.45
1:A:204:THR:HB	1:A:428[B]:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HB	1:B:428[A]:ARG:HH22	1.82	0.45
1:F:204:THR:HB	1:F:428[A]:ARG:HH22	1.82	0.45
1:F:465:GLU:HG3	1:F:466:HIS:CD2	2.52	0.45
1:H:465:GLU:HG3	1:H:466:HIS:CD2	2.52	0.45
1:A:199:LEU:HD11	1:A:476:GLN:HB2	1.99	0.45
1:B:199:LEU:HD11	1:B:476:GLN:HB2	1.99	0.45
1:H:204:THR:HB	1:H:428[A]:ARG:HH22	1.82	0.45
1:C:204:THR:HB	1:C:428[A]:ARG:HH22	1.82	0.44
1:D:204:THR:HB	1:D:428[A]:ARG:HH22	1.82	0.44
1:C:199:LEU:HD11	1:C:476:GLN:HB2	1.99	0.44
1:D:199:LEU:HD11	1:D:476:GLN:HB2	1.99	0.44
1:E:204:THR:HB	1:E:428[A]:ARG:HH22	1.82	0.44
1:A:11:LYS:HA	1:A:11:LYS:HD2	1.84	0.44
1:A:465:GLU:HG3	1:A:466:HIS:CD2	2.52	0.44
1:B:465:GLU:HG3	1:B:466:HIS:CD2	2.52	0.44
1:C:465:GLU:HG3	1:C:466:HIS:CD2	2.52	0.44
1:G:204:THR:HB	1:G:428[A]:ARG:HH22	1.82	0.44
1:B:11:LYS:HA	1:B:11:LYS:HD2	1.84	0.44
1:B:606:GLN:NE2	1:B:649:ASP:OD2	2.46	0.44
1:D:465:GLU:HG3	1:D:466:HIS:CD2	2.52	0.44
1:A:606:GLN:NE2	1:A:649:ASP:OD2	2.46	0.44
1:E:735:GLU:O	1:F:568[B]:HIS:NE2	2.49	0.44
1:F:199:LEU:HD11	1:F:476:GLN:HB2	1.99	0.44
1:F:620:GLU:OE2	1:F:673:ASN:ND2	2.34	0.43
1:H:199:LEU:HD11	1:H:476:GLN:HB2	1.99	0.43
1:G:735:GLU:O	1:H:568[B]:HIS:NE2	2.49	0.43
1:E:326:SER:O	1:E:326:SER:OG	2.30	0.43
1:G:326:SER:O	1:G:326:SER:OG	2.30	0.43
1:G:659:SER:HB2	1:G:669:PHE:CE1	2.53	0.43
1:E:659:SER:HB2	1:E:669:PHE:CE1	2.53	0.43
1:B:659:SER:HB2	1:B:669:PHE:CE1	2.53	0.43
1:C:659:SER:HB2	1:C:669:PHE:CE1	2.53	0.43
1:F:659:SER:HB2	1:F:669:PHE:CE1	2.53	0.43
1:G:199:LEU:HD11	1:G:476:GLN:HB2	1.99	0.43
1:H:659:SER:HB2	1:H:669:PHE:CE1	2.53	0.43
1:A:659:SER:HB2	1:A:669:PHE:CE1	2.53	0.43
1:D:659:SER:HB2	1:D:669:PHE:CE1	2.53	0.43
1:A:498:TRP:CE2	1:A:537:LEU:HD13	2.54	0.43
1:E:199:LEU:HD11	1:E:476:GLN:HB2	1.99	0.43
1:E:498:TRP:CE2	1:E:537:LEU:HD13	2.54	0.43
1:H:620:GLU:OE2	1:H:673:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:TRP:CE2	1:B:537:LEU:HD13	2.54	0.43
1:G:498:TRP:CE2	1:G:537:LEU:HD13	2.54	0.43
1:F:50:GLU:HA	1:F:51:PRO:HA	1.70	0.43
1:A:454:TRP:CZ2	1:A:456:ALA:HB3	2.54	0.42
1:B:454:TRP:CZ2	1:B:456:ALA:HB3	2.54	0.42
1:E:454:TRP:CZ2	1:E:456:ALA:HB3	2.54	0.42
1:G:454:TRP:CZ2	1:G:456:ALA:HB3	2.54	0.42
1:H:454:TRP:CZ2	1:H:456:ALA:HB3	2.54	0.42
1:C:498:TRP:CE2	1:C:537:LEU:HD13	2.54	0.42
1:D:620:GLU:OE2	1:D:673:ASN:ND2	2.34	0.42
1:E:55:GLU:OE1	1:E:328:ARG:NH1	2.52	0.42
1:F:454:TRP:CZ2	1:F:456:ALA:HB3	2.55	0.42
1:D:498:TRP:CE2	1:D:537:LEU:HD13	2.54	0.42
1:G:55:GLU:OE1	1:G:328:ARG:NH1	2.52	0.42
1:H:498:TRP:CE2	1:H:537:LEU:HD13	2.54	0.42
1:F:498:TRP:CE2	1:F:537:LEU:HD13	2.54	0.42
1:H:50:GLU:HA	1:H:51:PRO:HA	1.70	0.42
1:C:620:GLU:OE2	1:C:673:ASN:ND2	2.34	0.42
1:E:65:TRP:HE1	1:E:304:CYS:HB3	1.85	0.42
1:F:65:TRP:HE1	1:F:304:CYS:HB3	1.85	0.42
1:G:65:TRP:HE1	1:G:304:CYS:HB3	1.85	0.42
1:C:65:TRP:HE1	1:C:304:CYS:HB3	1.85	0.42
1:D:65:TRP:HE1	1:D:304:CYS:HB3	1.85	0.42
1:D:606:GLN:NE2	1:D:649:ASP:OD2	2.46	0.41
1:H:65:TRP:HE1	1:H:304:CYS:HB3	1.85	0.41
1:B:65:TRP:HE1	1:B:304:CYS:HB3	1.85	0.41
1:D:454:TRP:CZ2	1:D:456:ALA:HB3	2.54	0.41
1:C:454:TRP:CZ2	1:C:456:ALA:HB3	2.55	0.41
1:F:549[A]:ASN:HB3	1:F:553:HIS:CG	2.56	0.41
1:A:55:GLU:OE1	1:A:328:ARG:NH1	2.52	0.41
1:A:549[A]:ASN:HB3	1:A:553:HIS:CG	2.56	0.41
1:C:606:GLN:NE2	1:C:649:ASP:OD2	2.46	0.41
1:E:549[A]:ASN:HB3	1:E:553:HIS:CG	2.56	0.41
1:H:549[A]:ASN:HB3	1:H:553:HIS:CG	2.56	0.41
1:A:65:TRP:HE1	1:A:304:CYS:HB3	1.85	0.41
1:B:55:GLU:OE1	1:B:328:ARG:NH1	2.52	0.41
1:B:549[A]:ASN:HB3	1:B:553:HIS:CG	2.56	0.41
1:G:549[A]:ASN:HB3	1:G:553:HIS:CG	2.56	0.41
1:C:477:LEU:HD23	1:D:183:GLY:C	2.41	0.41
1:C:47:LEU:HD12	1:C:123:GLU:HG3	2.02	0.41
1:C:183:GLY:C	1:D:477:LEU:HD23	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:GLY:C	1:H:477:LEU:HD23	2.41	0.41
1:C:549[A]:ASN:HB3	1:C:553:HIS:CG	2.56	0.41
1:E:183:GLY:C	1:F:477:LEU:HD23	2.42	0.41
1:B:47:LEU:HD12	1:B:123:GLU:HG3	2.02	0.40
1:D:47:LEU:HD12	1:D:123:GLU:HG3	2.02	0.40
1:D:549[A]:ASN:HB3	1:D:553:HIS:CG	2.56	0.40
1:A:47:LEU:HD12	1:A:123:GLU:HG3	2.02	0.40
1:B:50:GLU:HA	1:B:51:PRO:HA	1.70	0.40
1:E:47:LEU:HD12	1:E:123:GLU:HG3	2.02	0.40
1:G:47:LEU:HD12	1:G:123:GLU:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	811/831 (98%)	780 (96%)	30 (4%)	1 (0%)	51	54
1	B	810/831 (98%)	780 (96%)	29 (4%)	1 (0%)	51	54
1	C	810/831 (98%)	779 (96%)	30 (4%)	1 (0%)	51	54
1	D	810/831 (98%)	779 (96%)	30 (4%)	1 (0%)	51	54
1	E	810/831 (98%)	779 (96%)	30 (4%)	1 (0%)	51	54
1	F	810/831 (98%)	779 (96%)	30 (4%)	1 (0%)	51	54
1	G	810/831 (98%)	780 (96%)	29 (4%)	1 (0%)	51	54
1	H	810/831 (98%)	780 (96%)	29 (4%)	1 (0%)	51	54
All	All	6481/6648 (98%)	6236 (96%)	237 (4%)	8 (0%)	54	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	700	THR
1	B	700	THR
1	C	700	THR
1	D	700	THR
1	E	700	THR
1	F	700	THR
1	G	700	THR
1	H	700	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	682/693 (98%)	669 (98%)	13 (2%)	57	63
1	B	681/693 (98%)	670 (98%)	11 (2%)	62	69
1	C	681/693 (98%)	670 (98%)	11 (2%)	62	69
1	D	681/693 (98%)	670 (98%)	11 (2%)	62	69
1	E	681/693 (98%)	670 (98%)	11 (2%)	62	69
1	F	681/693 (98%)	669 (98%)	12 (2%)	59	65
1	G	681/693 (98%)	670 (98%)	11 (2%)	62	69
1	H	681/693 (98%)	669 (98%)	12 (2%)	59	65
All	All	5449/5544 (98%)	5357 (98%)	92 (2%)	64	67

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	60	ARG
1	A	123	GLU
1	A	258	SER
1	A	330	THR
1	A	387	LYS
1	A	444	GLN
1	A	525	GLU

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Mol	Chain	Res	Type
1	A	547[A]	ASP
1	A	547[B]	ASP
1	A	735	GLU
1	A	768	ASP
1	A	769	LYS
1	B	60	ARG
1	B	123	GLU
1	B	258	SER
1	B	330	THR
1	B	387	LYS
1	B	525	GLU
1	B	547[A]	ASP
1	B	547[B]	ASP
1	B	735	GLU
1	B	768	ASP
1	B	769	LYS
1	C	60	ARG
1	C	123	GLU
1	C	258	SER
1	C	330	THR
1	C	387	LYS
1	C	525	GLU
1	C	547[A]	ASP
1	C	547[B]	ASP
1	C	735	GLU
1	C	768	ASP
1	C	769	LYS
1	D	60	ARG
1	D	123	GLU
1	D	258	SER
1	D	330	THR
1	D	387	LYS
1	D	525	GLU
1	D	547[A]	ASP
1	D	547[B]	ASP
1	D	735	GLU
1	D	768	ASP
1	D	769	LYS
1	E	60	ARG
1	E	123	GLU
1	E	258	SER
1	E	330	THR

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Mol	Chain	Res	Type
1	E	387	LYS
1	E	525	GLU
1	E	547[A]	ASP
1	E	547[B]	ASP
1	E	735	GLU
1	E	768	ASP
1	E	769	LYS
1	F	23	GLU
1	F	60	ARG
1	F	123	GLU
1	F	258	SER
1	F	330	THR
1	F	387	LYS
1	F	525	GLU
1	F	547[A]	ASP
1	F	547[B]	ASP
1	F	735	GLU
1	F	768	ASP
1	F	769	LYS
1	G	60	ARG
1	G	123	GLU
1	G	258	SER
1	G	330	THR
1	G	387	LYS
1	G	525	GLU
1	G	547[A]	ASP
1	G	547[B]	ASP
1	G	735	GLU
1	G	768	ASP
1	G	769	LYS
1	H	23	GLU
1	H	60	ARG
1	H	123	GLU
1	H	258	SER
1	H	330	THR
1	H	387	LYS
1	H	525	GLU
1	H	547[A]	ASP
1	H	547[B]	ASP
1	H	735	GLU
1	H	768	ASP
1	H	769	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	105	GLN
1	A	408	GLN
1	A	444	GLN
1	A	653	GLN
1	B	39	GLN
1	B	105	GLN
1	B	408	GLN
1	B	653	GLN
1	C	39	GLN
1	C	105	GLN
1	C	408	GLN
1	C	653	GLN
1	D	39	GLN
1	D	105	GLN
1	D	408	GLN
1	D	653	GLN
1	E	39	GLN
1	E	105	GLN
1	E	408	GLN
1	E	653	GLN
1	F	39	GLN
1	F	105	GLN
1	F	408	GLN
1	F	653	GLN
1	G	39	GLN
1	G	105	GLN
1	G	408	GLN
1	G	653	GLN
1	H	39	GLN
1	H	105	GLN
1	H	408	GLN
1	H	653	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPP	F	900	3	22,27,27	3.75	9 (40%)	29,40,40	2.23	7 (24%)
2	TPP	D	900	3	22,27,27	3.75	9 (40%)	29,40,40	2.22	7 (24%)
2	TPP	C	900	3	22,27,27	3.74	8 (36%)	29,40,40	2.28	11 (37%)
2	TPP	H	900	3	22,27,27	3.78	9 (40%)	29,40,40	2.28	11 (37%)
2	TPP	A	900	3	22,27,27	3.73	8 (36%)	29,40,40	2.30	11 (37%)
2	TPP	B	900	3	22,27,27	3.75	9 (40%)	29,40,40	2.22	7 (24%)
2	TPP	G	900	3	22,27,27	3.78	9 (40%)	29,40,40	2.22	7 (24%)
2	TPP	E	900	3	22,27,27	3.75	8 (36%)	29,40,40	2.28	11 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	F	900	3	-	2/16/17/17	0/2/2/2
2	TPP	D	900	3	-	2/16/17/17	0/2/2/2
2	TPP	C	900	3	-	5/16/17/17	0/2/2/2
2	TPP	H	900	3	-	5/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	900	3	-	5/16/17/17	0/2/2/2
2	TPP	B	900	3	-	2/16/17/17	0/2/2/2
2	TPP	G	900	3	-	2/16/17/17	0/2/2/2
2	TPP	E	900	3	-	5/16/17/17	0/2/2/2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	TPP	C4-N3	-13.02	1.28	1.39
2	F	900	TPP	C4-N3	-13.00	1.28	1.39
2	A	900	TPP	C4-N3	-12.99	1.28	1.39
2	H	900	TPP	C4-N3	-12.99	1.28	1.39
2	E	900	TPP	C4-N3	-12.95	1.28	1.39
2	B	900	TPP	C4-N3	-12.92	1.28	1.39
2	D	900	TPP	C4-N3	-12.92	1.28	1.39
2	C	900	TPP	C4-N3	-12.88	1.28	1.39
2	G	900	TPP	C6-C5	-7.88	1.47	1.50
2	H	900	TPP	C6-C5	-7.88	1.47	1.50
2	D	900	TPP	C6-C5	-7.66	1.47	1.50
2	E	900	TPP	C6-C5	-7.66	1.47	1.50
2	B	900	TPP	C6-C5	-7.61	1.47	1.50
2	C	900	TPP	C6-C5	-7.61	1.47	1.50
2	F	900	TPP	C6-C5	-7.49	1.47	1.50
2	A	900	TPP	C6-C5	-7.43	1.47	1.50
2	D	900	TPP	PB-O3B	-4.95	1.35	1.54
2	F	900	TPP	PB-O3B	-4.94	1.35	1.54
2	B	900	TPP	PB-O3B	-4.92	1.35	1.54
2	G	900	TPP	PB-O3B	-4.87	1.36	1.54
2	C	900	TPP	PB-O1B	-4.59	1.35	1.50
2	E	900	TPP	PB-O1B	-4.57	1.35	1.50
2	H	900	TPP	PB-O1B	-4.57	1.35	1.50
2	A	900	TPP	PB-O1B	-4.52	1.35	1.50
2	B	900	TPP	PB-O2B	-3.49	1.41	1.54
2	E	900	TPP	PB-O2B	-3.49	1.41	1.54
2	C	900	TPP	PB-O2B	-3.48	1.41	1.54
2	D	900	TPP	PB-O2B	-3.46	1.41	1.54
2	F	900	TPP	PB-O2B	-3.45	1.41	1.54
2	H	900	TPP	PB-O2B	-3.45	1.41	1.54
2	A	900	TPP	PB-O2B	-3.43	1.41	1.54
2	G	900	TPP	PB-O2B	-3.40	1.41	1.54
2	C	900	TPP	PA-O2A	-3.31	1.39	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	TPP	PA-O2A	-3.28	1.39	1.55
2	A	900	TPP	PA-O2A	-3.28	1.39	1.55
2	H	900	TPP	PA-O2A	-3.26	1.40	1.55
2	B	900	TPP	PA-O1A	-3.13	1.39	1.50
2	D	900	TPP	PA-O1A	-3.10	1.39	1.50
2	F	900	TPP	PA-O1A	-3.10	1.39	1.50
2	E	900	TPP	PB-O3B	-3.10	1.42	1.54
2	G	900	TPP	PA-O1A	-3.09	1.39	1.50
2	A	900	TPP	PB-O3B	-3.09	1.42	1.54
2	C	900	TPP	PB-O3B	-3.07	1.43	1.54
2	H	900	TPP	PB-O3B	-3.04	1.43	1.54
2	B	900	TPP	PA-O2A	-2.46	1.43	1.55
2	D	900	TPP	PA-O2A	-2.43	1.43	1.55
2	G	900	TPP	PA-O2A	-2.41	1.44	1.55
2	F	900	TPP	PA-O2A	-2.40	1.44	1.55
2	G	900	TPP	PB-O1B	-2.37	1.42	1.50
2	F	900	TPP	PB-O1B	-2.35	1.42	1.50
2	D	900	TPP	PB-O1B	-2.35	1.43	1.50
2	B	900	TPP	PB-O1B	-2.35	1.43	1.50
2	F	900	TPP	C5'-C4'	-2.30	1.39	1.42
2	B	900	TPP	C5'-C4'	-2.30	1.39	1.42
2	C	900	TPP	C5'-C4'	-2.30	1.39	1.42
2	D	900	TPP	C5'-C4'	-2.30	1.39	1.42
2	G	900	TPP	C5'-C4'	-2.30	1.39	1.42
2	H	900	TPP	C5'-C4'	-2.30	1.39	1.42
2	A	900	TPP	C5'-C4'	-2.28	1.39	1.42
2	E	900	TPP	C5'-C4'	-2.25	1.39	1.42
2	B	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	C	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	D	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	E	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	F	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	G	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	H	900	TPP	C4'-N4'	-2.22	1.28	1.34
2	A	900	TPP	C4'-N4'	-2.21	1.28	1.34
2	H	900	TPP	PA-O1A	-2.02	1.43	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	900	TPP	CM2-C2'-N1'	5.71	123.42	117.14
2	C	900	TPP	CM2-C2'-N1'	5.68	123.39	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	TPP	CM2-C2'-N1'	5.68	123.38	117.14
2	B	900	TPP	CM2-C2'-N1'	5.68	123.38	117.14
2	D	900	TPP	CM2-C2'-N1'	5.68	123.38	117.14
2	E	900	TPP	CM2-C2'-N1'	5.68	123.38	117.14
2	H	900	TPP	CM2-C2'-N1'	5.68	123.38	117.14
2	G	900	TPP	CM2-C2'-N1'	5.67	123.38	117.14
2	F	900	TPP	O7-PA-O1A	-5.29	88.40	109.07
2	D	900	TPP	O7-PA-O1A	-5.29	88.41	109.07
2	B	900	TPP	O7-PA-O1A	-5.27	88.49	109.07
2	G	900	TPP	O7-PA-O1A	-5.21	88.70	109.07
2	C	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	A	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	B	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	D	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	E	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	G	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	H	900	TPP	N1'-C2'-N3'	-5.01	116.92	125.54
2	F	900	TPP	N1'-C2'-N3'	-5.00	116.94	125.54
2	E	900	TPP	O2A-PA-O7	-4.17	88.39	107.75
2	C	900	TPP	O2A-PA-O7	-4.15	88.49	107.75
2	A	900	TPP	O2A-PA-O7	-4.14	88.51	107.75
2	H	900	TPP	O2A-PA-O7	-4.10	88.70	107.75
2	F	900	TPP	C6'-N1'-C2'	3.69	122.24	115.96
2	C	900	TPP	C6'-N1'-C2'	3.66	122.19	115.96
2	A	900	TPP	C6'-N1'-C2'	3.66	122.19	115.96
2	B	900	TPP	C6'-N1'-C2'	3.66	122.19	115.96
2	D	900	TPP	C6'-N1'-C2'	3.66	122.18	115.96
2	E	900	TPP	C6'-N1'-C2'	3.66	122.18	115.96
2	G	900	TPP	C6'-N1'-C2'	3.66	122.18	115.96
2	H	900	TPP	C6'-N1'-C2'	3.66	122.18	115.96
2	A	900	TPP	O3B-PB-O3A	3.42	116.11	104.64
2	C	900	TPP	O3B-PB-O3A	3.42	116.10	104.64
2	H	900	TPP	O3B-PB-O3A	3.40	116.04	104.64
2	E	900	TPP	O3B-PB-O3A	3.36	115.89	104.64
2	A	900	TPP	O3B-PB-O1B	-2.80	99.72	110.68
2	E	900	TPP	O3B-PB-O2B	2.79	118.30	107.64
2	A	900	TPP	O3B-PB-O2B	2.79	118.30	107.64
2	B	900	TPP	O3B-PB-O1B	-2.76	99.88	110.68
2	E	900	TPP	O3B-PB-O1B	-2.76	99.88	110.68
2	G	900	TPP	O3B-PB-O1B	-2.76	99.88	110.68
2	D	900	TPP	O3B-PB-O1B	-2.73	99.98	110.68
2	C	900	TPP	O3B-PB-O2B	2.73	118.08	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	900	TPP	O3B-PB-O1B	-2.72	100.02	110.68
2	H	900	TPP	O3B-PB-O1B	-2.72	100.02	110.68
2	H	900	TPP	O3B-PB-O2B	2.72	118.04	107.64
2	F	900	TPP	O3B-PB-O1B	-2.72	100.04	110.68
2	C	900	TPP	O7-PA-O1A	-2.54	99.13	109.07
2	A	900	TPP	O7-PA-O1A	-2.53	99.16	109.07
2	E	900	TPP	O7-PA-O1A	-2.53	99.18	109.07
2	H	900	TPP	O7-PA-O1A	-2.51	99.25	109.07
2	C	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	A	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	B	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	D	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	E	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	G	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	H	900	TPP	C2'-N3'-C4'	2.39	121.81	118.08
2	F	900	TPP	C2'-N3'-C4'	2.36	121.77	118.08
2	A	900	TPP	O2B-PB-O1B	-2.36	101.43	110.68
2	E	900	TPP	O2B-PB-O1B	-2.30	101.69	110.68
2	H	900	TPP	O2B-PB-O1B	-2.27	101.78	110.68
2	C	900	TPP	O2B-PB-O1B	-2.27	101.79	110.68
2	A	900	TPP	C7'-N3-C2	2.25	129.41	125.35
2	C	900	TPP	C7'-N3-C2	2.10	129.14	125.35
2	F	900	TPP	C7'-N3-C2	2.08	129.10	125.35
2	B	900	TPP	C7'-N3-C2	2.07	129.09	125.35
2	D	900	TPP	C7'-N3-C2	2.07	129.09	125.35
2	E	900	TPP	C7'-N3-C2	2.06	129.07	125.35
2	G	900	TPP	C7'-N3-C2	2.06	129.07	125.35
2	H	900	TPP	C7'-N3-C2	2.06	129.07	125.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	TPP	C4'-C5'-C7'-N3
2	A	900	TPP	PA-O3A-PB-O3B
2	B	900	TPP	C4'-C5'-C7'-N3
2	C	900	TPP	C4'-C5'-C7'-N3
2	C	900	TPP	PA-O3A-PB-O3B
2	D	900	TPP	C4'-C5'-C7'-N3
2	E	900	TPP	C4'-C5'-C7'-N3
2	E	900	TPP	PA-O3A-PB-O3B
2	F	900	TPP	C4'-C5'-C7'-N3

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Mol	Chain	Res	Type	Atoms
2	G	900	TPP	C4'-C5'-C7'-N3
2	H	900	TPP	C4'-C5'-C7'-N3
2	H	900	TPP	PA-O3A-PB-O3B
2	A	900	TPP	PB-O3A-PA-O1A
2	C	900	TPP	PB-O3A-PA-O1A
2	E	900	TPP	PB-O3A-PA-O1A
2	H	900	TPP	PB-O3A-PA-O1A
2	B	900	TPP	PA-O3A-PB-O1B
2	D	900	TPP	PA-O3A-PB-O1B
2	F	900	TPP	PA-O3A-PB-O1B
2	G	900	TPP	PA-O3A-PB-O1B
2	A	900	TPP	PB-O3A-PA-O2A
2	E	900	TPP	PB-O3A-PA-O2A
2	C	900	TPP	PB-O3A-PA-O2A
2	H	900	TPP	PB-O3A-PA-O2A
2	A	900	TPP	C7-O7-PA-O1A
2	C	900	TPP	C7-O7-PA-O1A
2	E	900	TPP	C7-O7-PA-O1A
2	H	900	TPP	C7-O7-PA-O1A

There are no ring outliers.

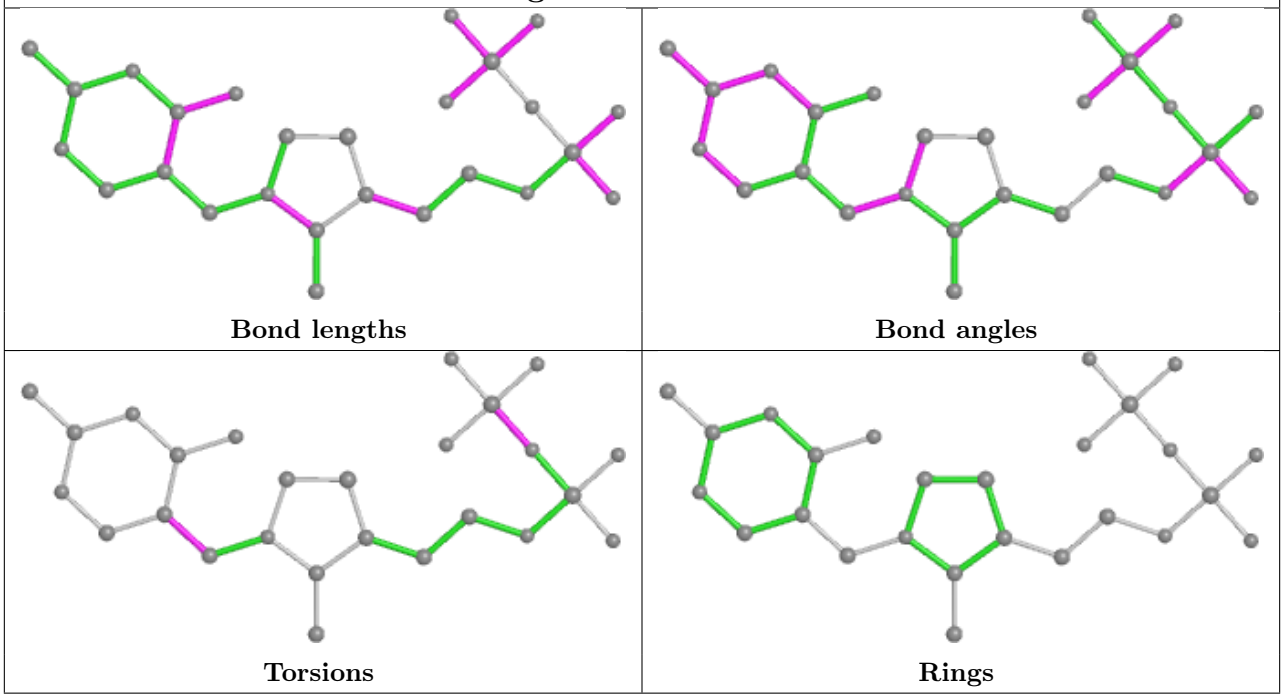
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	900	TPP	1	0
2	D	900	TPP	1	0
2	C	900	TPP	1	0
2	H	900	TPP	1	0
2	A	900	TPP	1	0
2	B	900	TPP	1	0
2	G	900	TPP	1	0
2	E	900	TPP	1	0

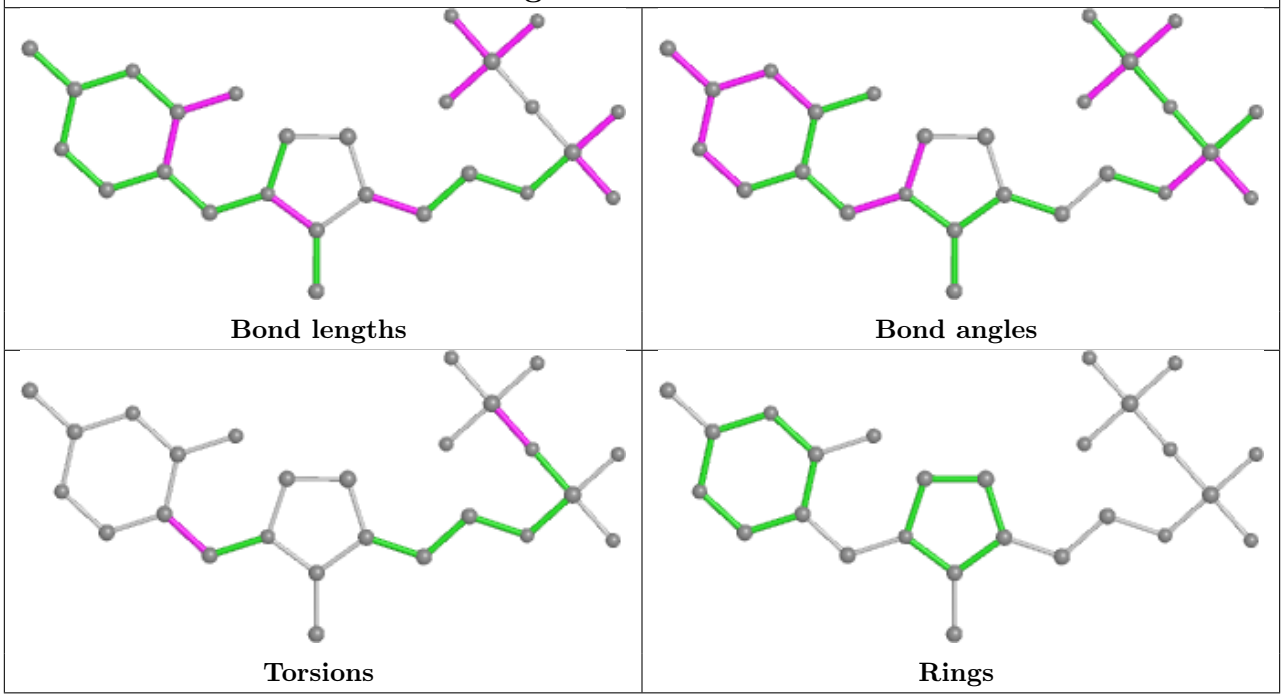
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

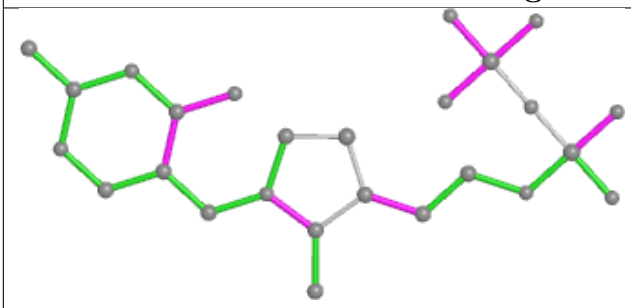
Ligand TPP F 900



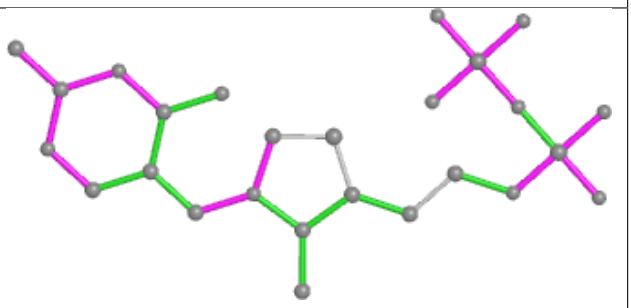
Ligand TPP D 900



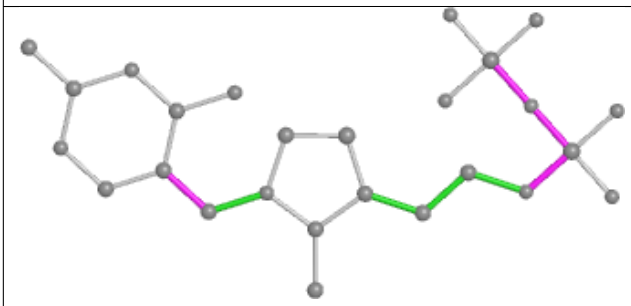
Ligand TPP C 900



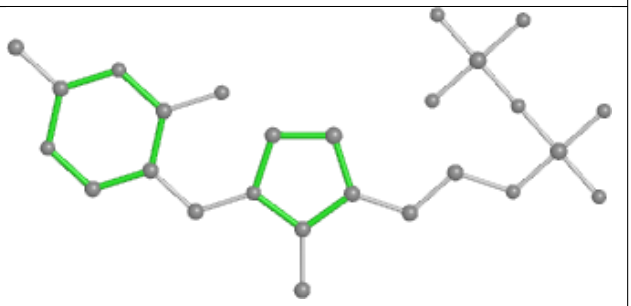
Bond lengths



Bond angles

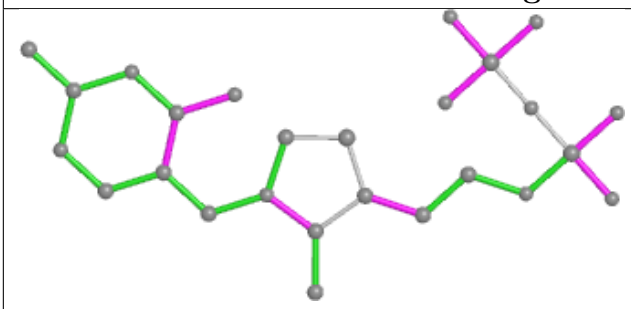


Torsions

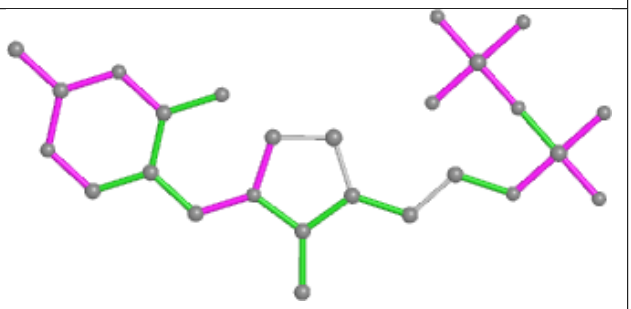


Rings

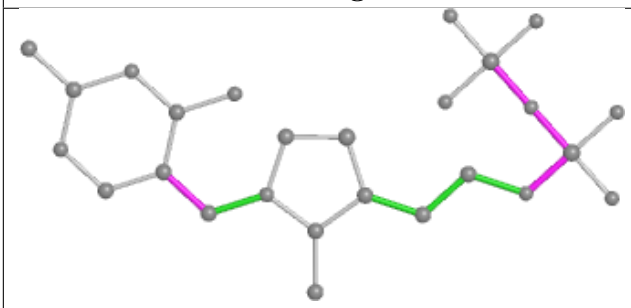
Ligand TPP H 900



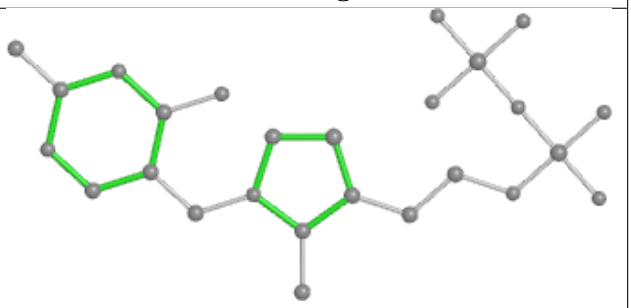
Bond lengths



Bond angles

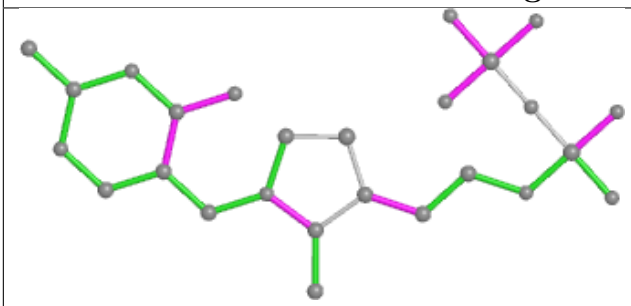


Torsions

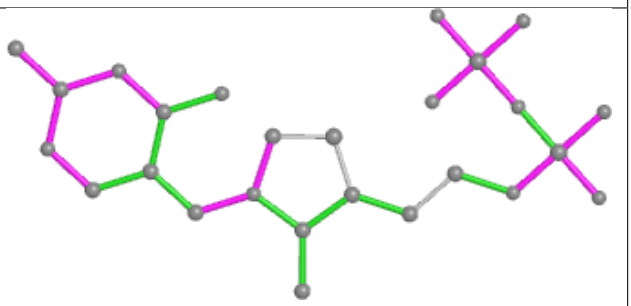


Rings

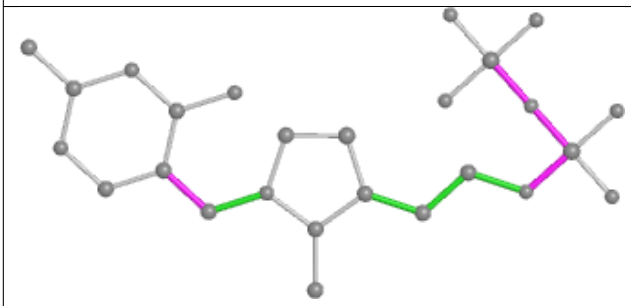
Ligand TPP A 900



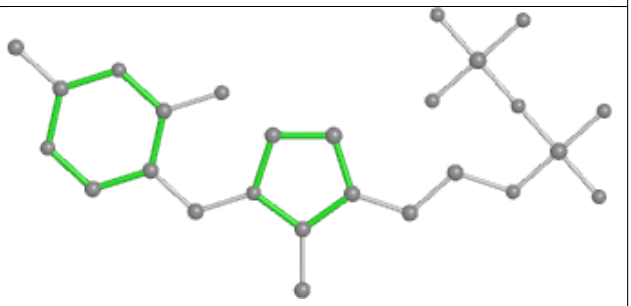
Bond lengths



Bond angles

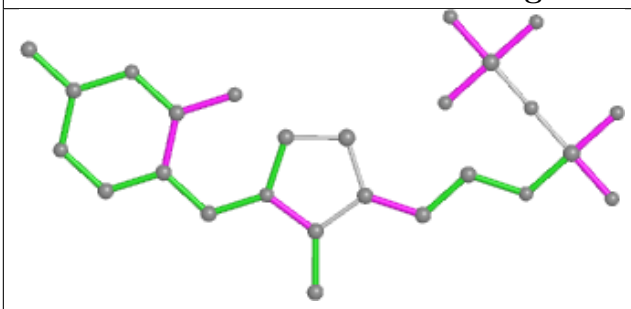


Torsions

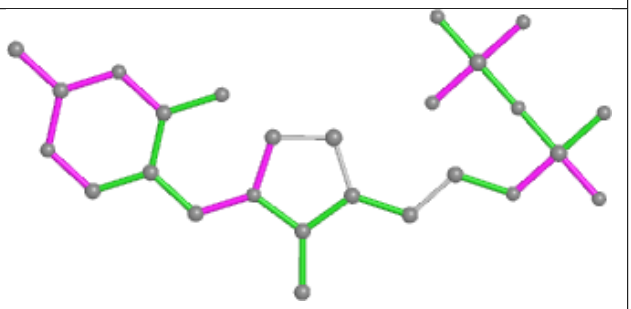


Rings

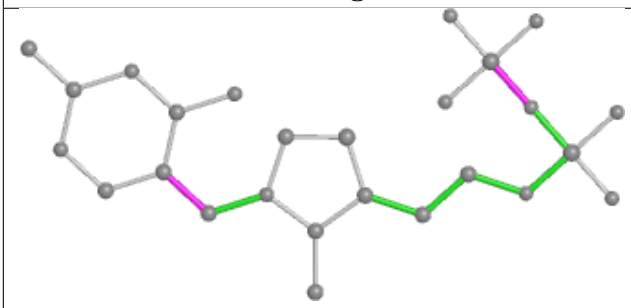
Ligand TPP B 900



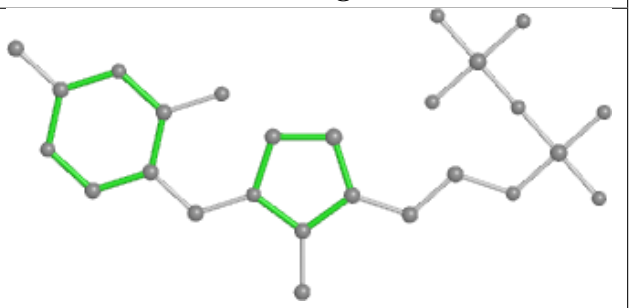
Bond lengths



Bond angles

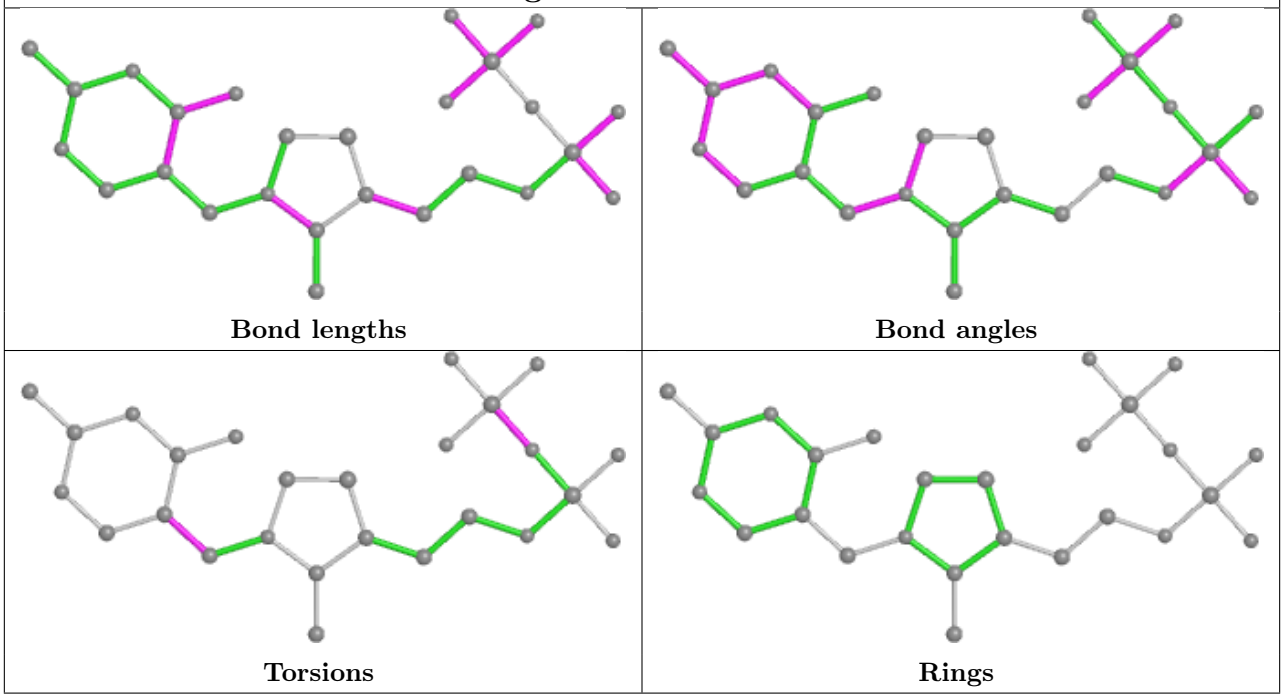


Torsions

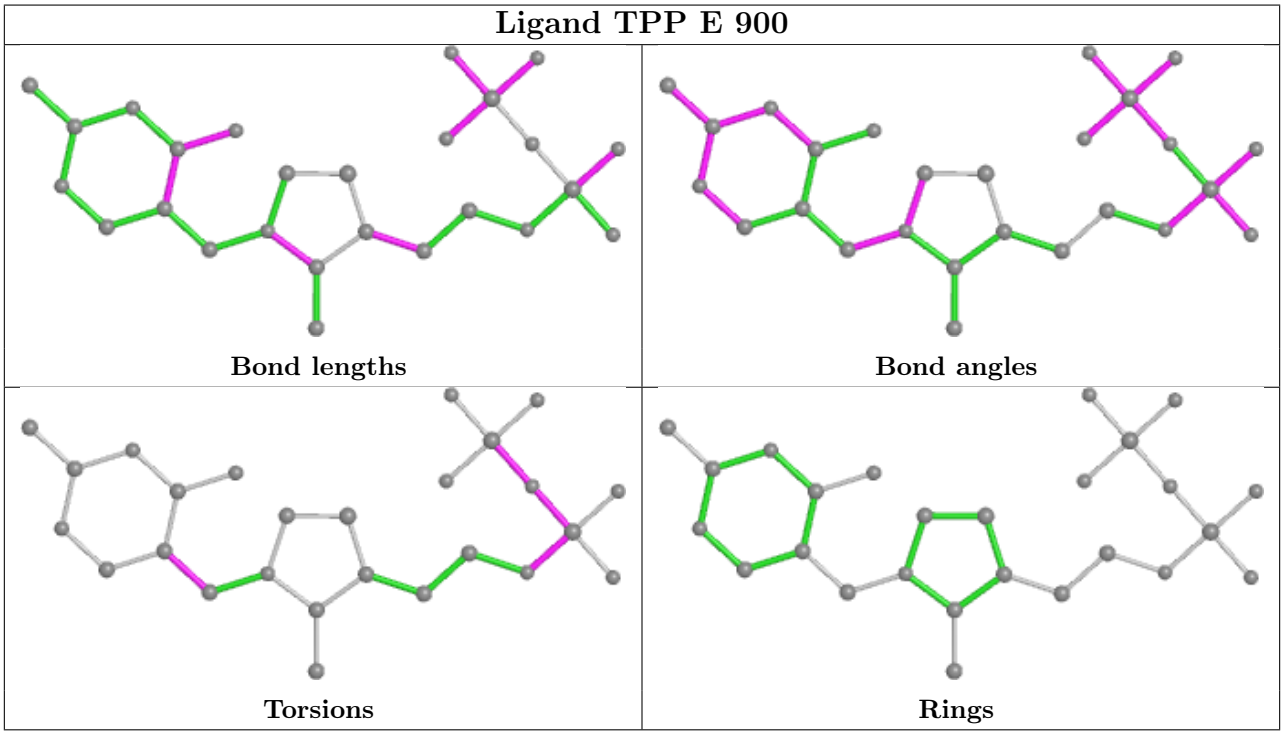


Rings

Ligand TPP G 900



Ligand TPP E 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1
1	E	1
1	F	1
1	G	1
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	702:ASP	C	703:LYS	N	1.19
1	B	702:ASP	C	703:LYS	N	1.19
1	C	702:ASP	C	703:LYS	N	1.19
1	D	702:ASP	C	703:LYS	N	1.19
1	E	702:ASP	C	703:LYS	N	1.19
1	F	702:ASP	C	703:LYS	N	1.19
1	G	702:ASP	C	703:LYS	N	1.19
1	H	702:ASP	C	703:LYS	N	1.19

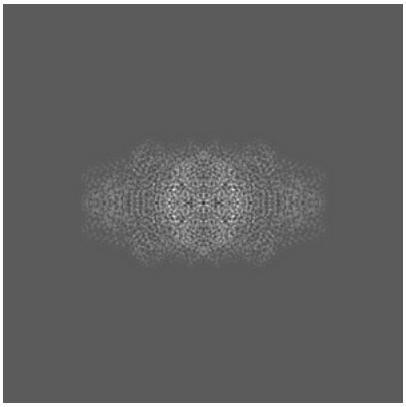
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30007. These allow visual inspection of the internal detail of the map and identification of artifacts.

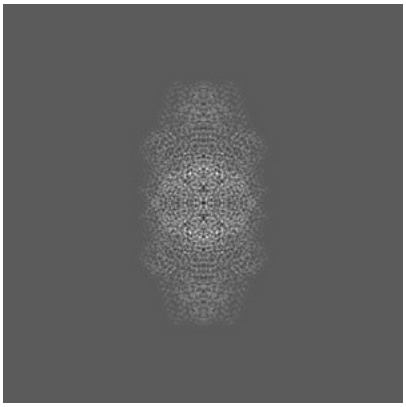
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



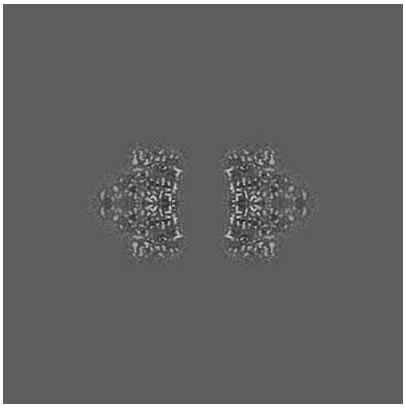
Y

Z

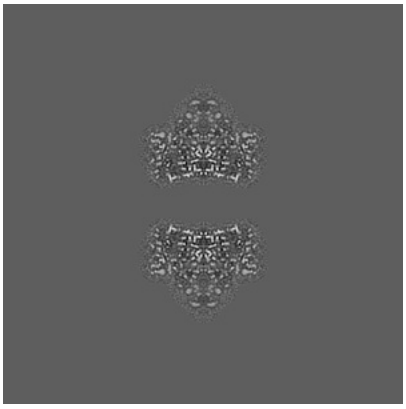
The images above show the map projected in three orthogonal directions.

6.2 Central slices

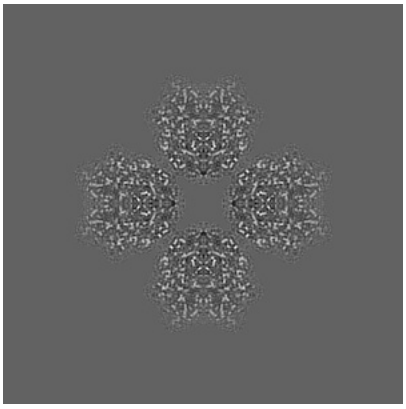
6.2.1 Primary map



X Index: 180



Y Index: 180

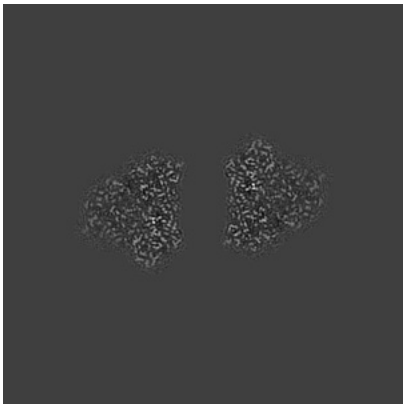


Z Index: 180

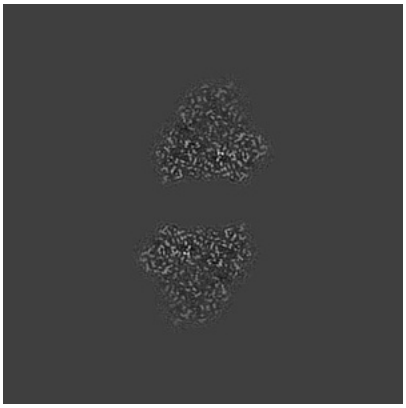
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

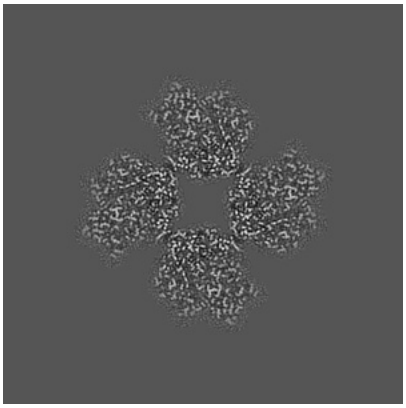
6.3.1 Primary map



X Index: 168



Y Index: 192

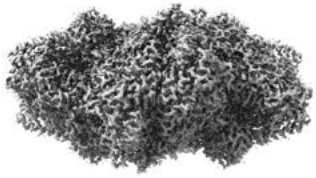


Z Index: 187

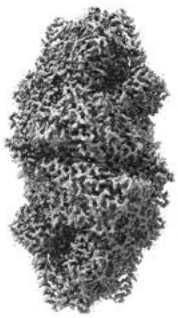
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

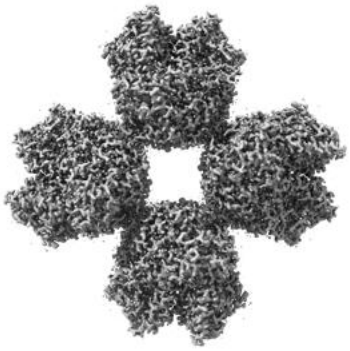
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

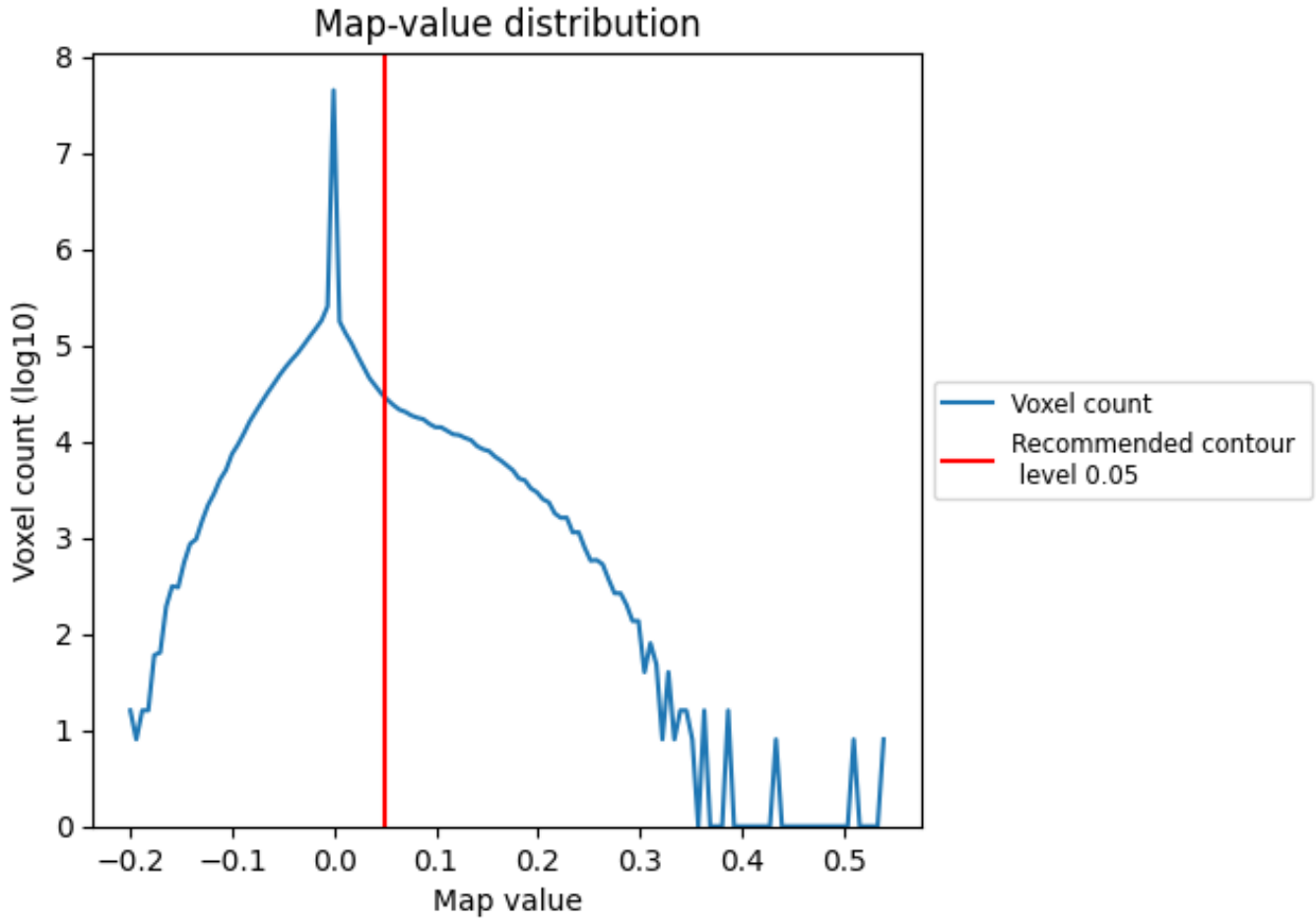
6.5 Mask visualisation (i)

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

7 Map analysis

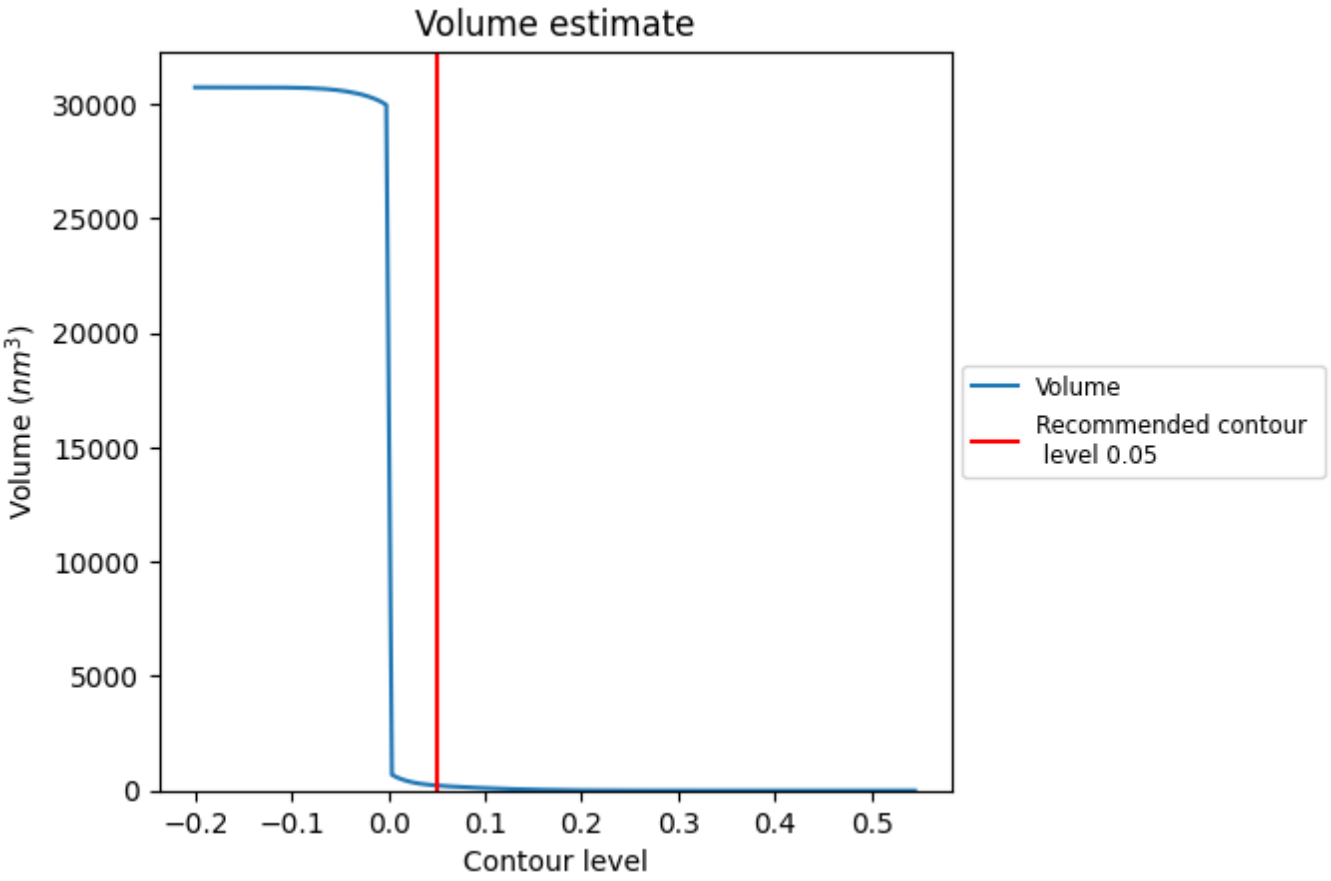
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

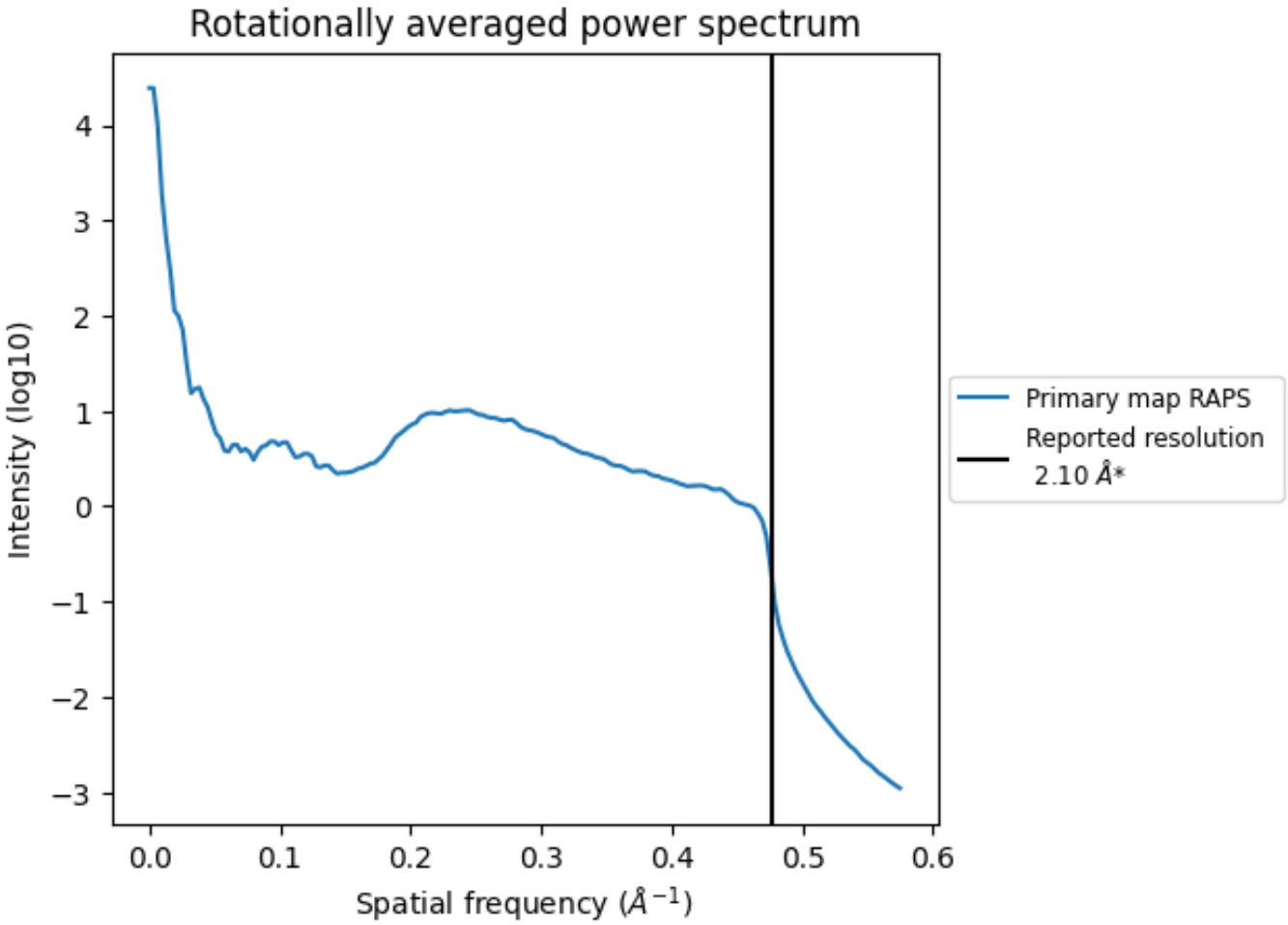
7.2 Volume estimate (i)



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 200 kDa.

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

7.3 Rotationally averaged power spectrum (i)

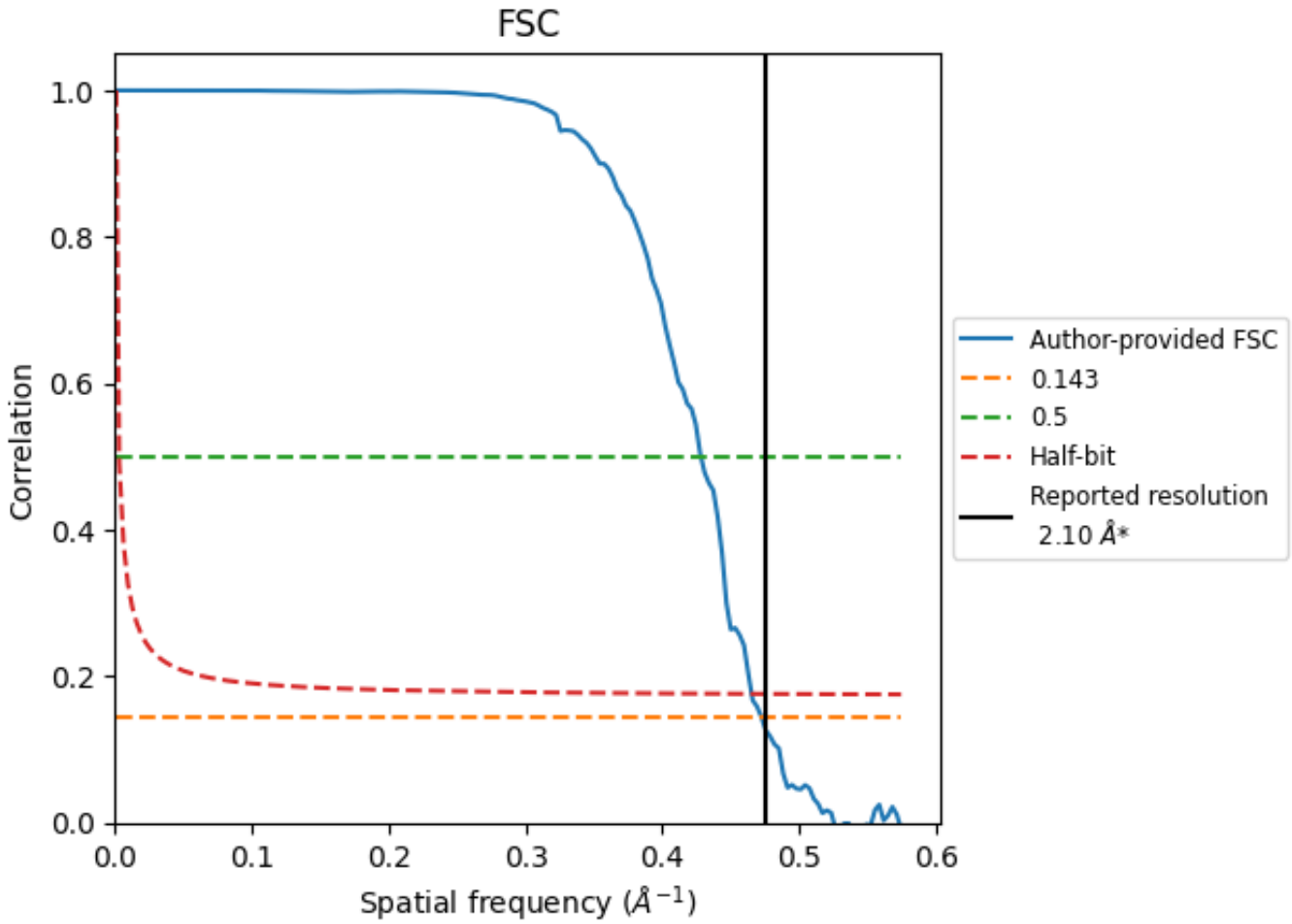


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8.2 Resolution estimates (i)

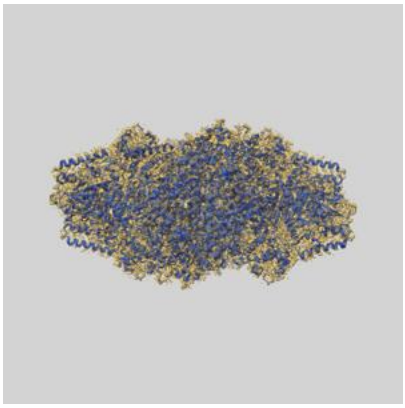
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	2.33	2.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

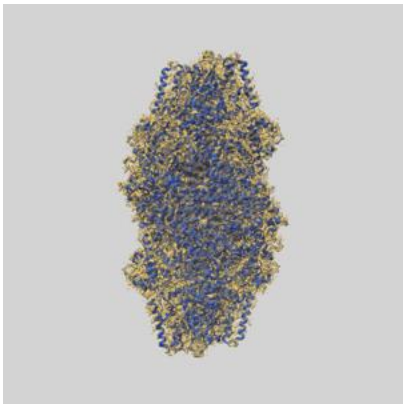
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30007 and PDB model 6LXV. Per-residue inclusion information can be found in section 3 on page 7.

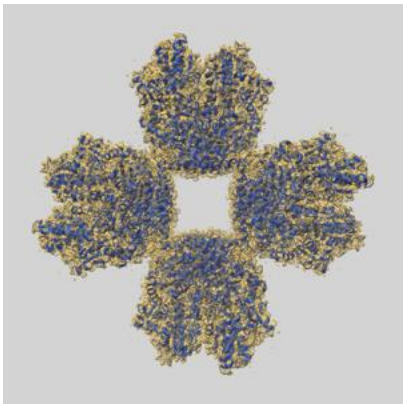
9.1 Map-model overlay



X



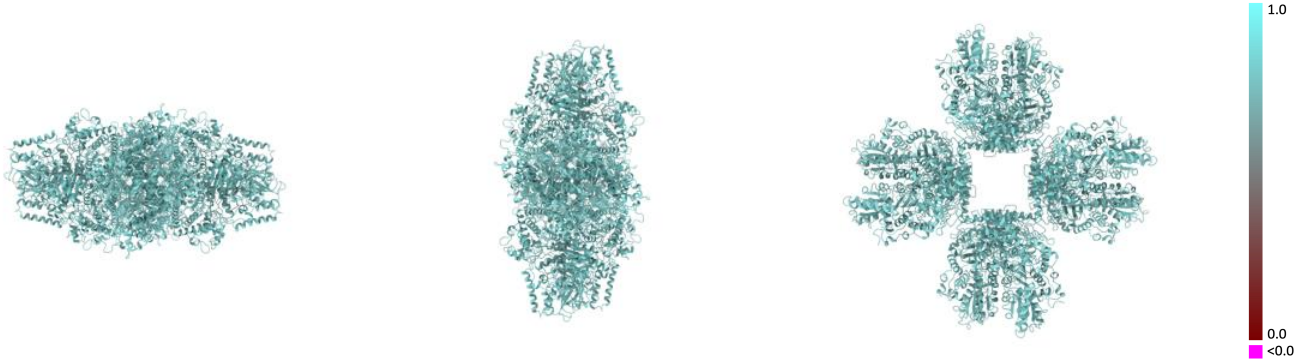
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

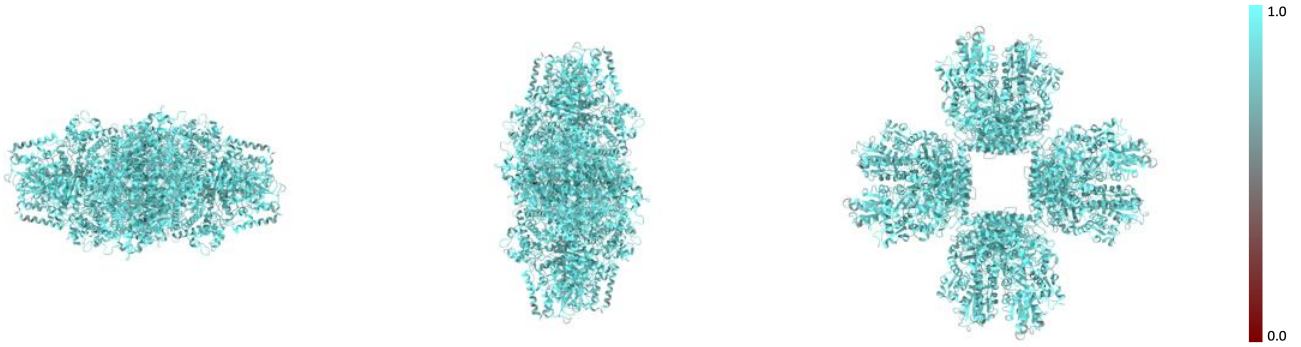
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

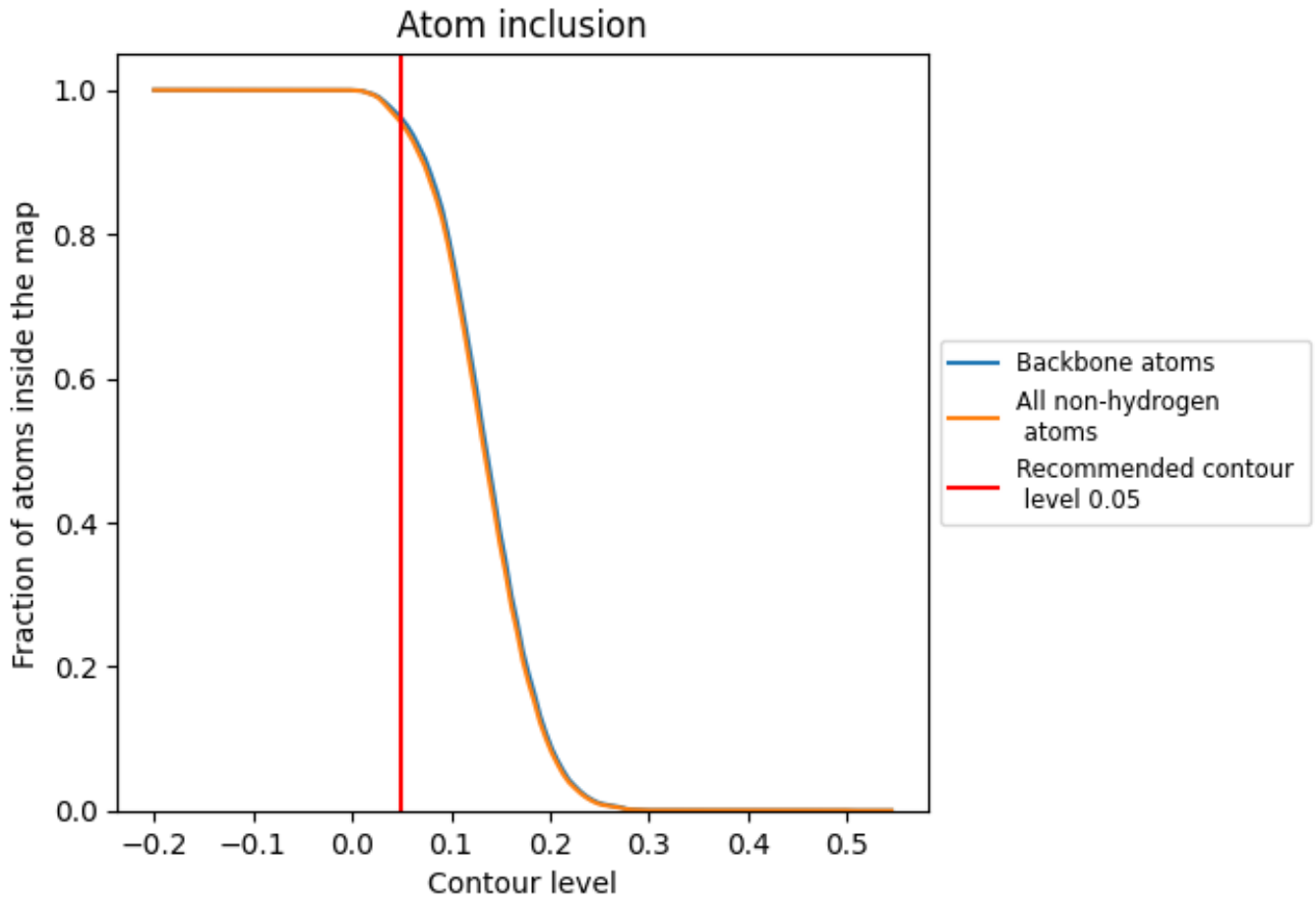
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9541	0.7630
A	0.9551	0.7630
B	0.9546	0.7620
C	0.9547	0.7630
D	0.9546	0.7620
E	0.9546	0.7620
F	0.9551	0.7630
G	0.9549	0.7620
H	0.9547	0.7630