



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 06:35 AM UTC

PDB ID : 7YK5 / pdb_00007yk5
EMDB ID : EMD-33887
Title : Rubisco from Phaeodactylum tricornutum bound to PYCO1(452-592)
Authors : Oh, Z.G.; Ang, W.S.L.; Bhushan, S.; Mueller-Cajar, O.
Deposited on : 2022-07-21
Resolution : 2.00 Å(reported)
Based on initial model : 5MZ2

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

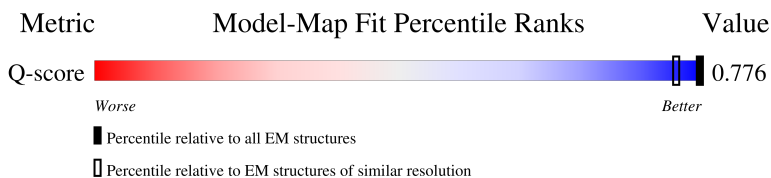
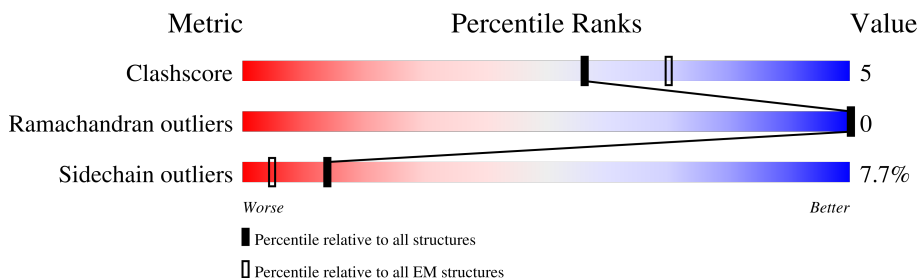
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.00 Å.

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



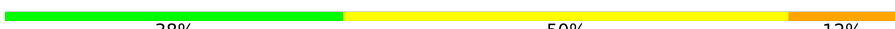
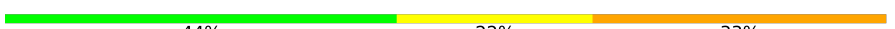
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1659 (1.50 - 2.50)

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

Mol	Chain	Length	Quality of chain
1	A	490	
1	B	490	
1	C	490	
1	D	490	

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Mol	Chain	Length	Quality of chain
1	E	490	 85% 11% ..
1	F	490	 85% 11% ..
1	G	490	 85% 11% ..
1	H	490	 84% 12% ..
2	I	139	 86% 10% .
2	J	139	 87% 9% .
2	K	139	 85% 12% .
2	L	139	 85% 11% .
2	M	139	 85% 12% .
2	N	139	 86% 11% .
2	O	139	 87% 10% .
2	P	139	 87% 10% .
3	i	8	 38% 50% 12%
3	j	8	 38% 50% 12%
3	k	8	 38% 50% 12%
3	l	8	 38% 50% 12%
4	a	9	 56% 44%
4	b	9	 56% 11% 33%
4	c	9	 67% 11% 22%
4	d	9	 56% 22% 22%
4	e	9	 44% 22% 33%
4	f	9	 56% 22% 22%
4	g	9	 44% 22% 33%
4	h	9	 56% 11% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 39948 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	B	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	C	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	D	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	E	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	F	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	G	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		
1	H	481	Total	C	N	O	S	0	0
			3746	2379	644	701	22		

- Molecule 2 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		
2	J	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		
2	K	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		
2	L	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		
2	M	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		
2	N	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		
2	O	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	139	Total	C	N	O	S	0	0
			1128	716	193	211	8		

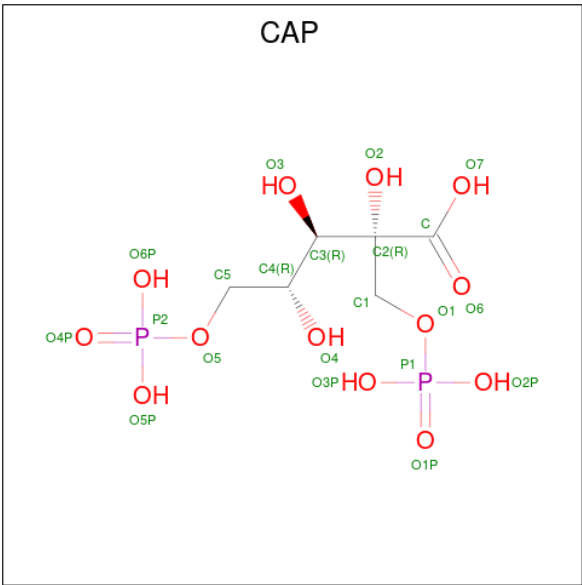
- Molecule 3 is a protein called PYCO1 SSU binding motif.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	8	Total	C	N	O		0	0
			61	38	13	10			
3	k	8	Total	C	N	O		0	0
			61	38	13	10			
3	j	8	Total	C	N	O		0	0
			61	38	13	10			
3	l	8	Total	C	N	O		0	0
			61	38	13	10			

- Molecule 4 is a protein called PYCO1 LSU binding motif.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	g	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	f	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	e	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	d	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	c	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	b	9	Total	C	N	O	S	0	0
			68	41	12	14	1		
4	a	9	Total	C	N	O	S	0	0
			68	41	12	14	1		

- Molecule 5 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).

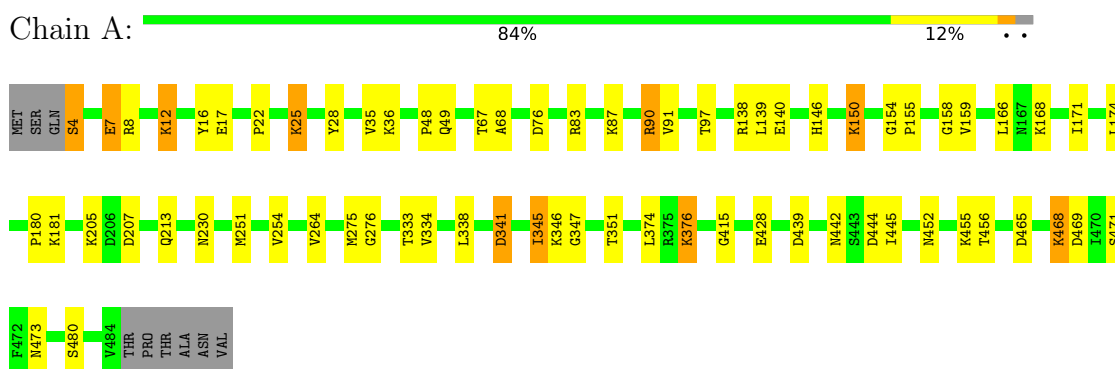


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			21	6	13	2	
5	B	1	Total	C	O	P	0
			21	6	13	2	
5	C	1	Total	C	O	P	0
			21	6	13	2	
5	D	1	Total	C	O	P	0
			21	6	13	2	
5	E	1	Total	C	O	P	0
			21	6	13	2	
5	F	1	Total	C	O	P	0
			21	6	13	2	
5	G	1	Total	C	O	P	0
			21	6	13	2	
5	H	1	Total	C	O	P	0
			21	6	13	2	

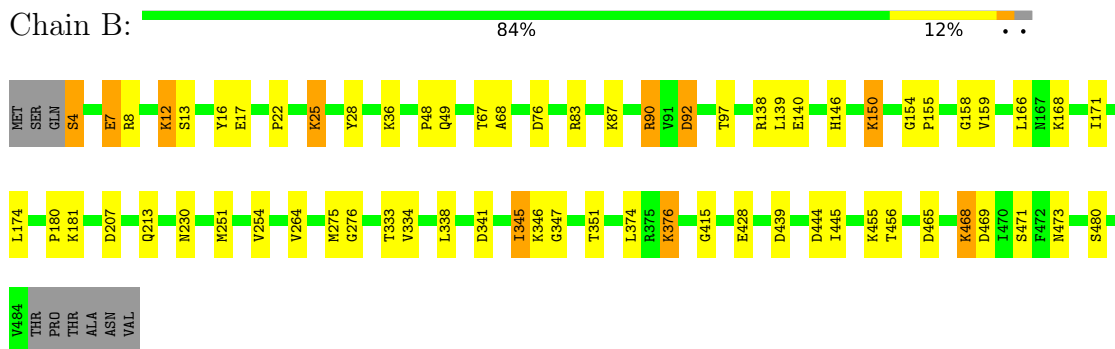
3 Residue-property plots

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.

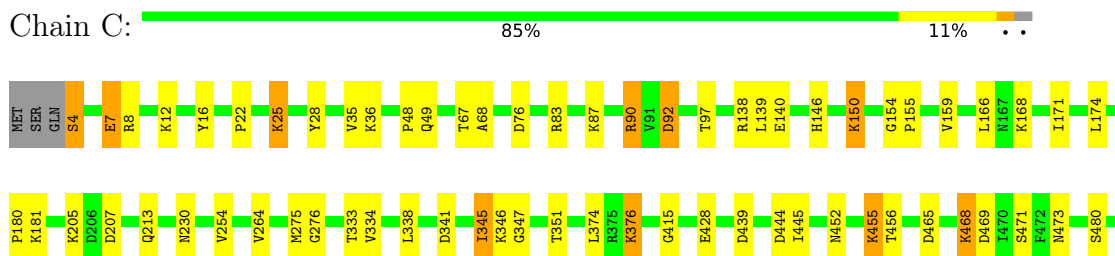
- Molecule 1: Ribulose biphosphate carboxylase large chain



- Molecule 1: Ribulose bisphosphate carboxylase large chain



- Molecule 1: Ribulose bisphosphate carboxylase large chain



V484
THR
PRO
THR
ALA
ASN
VAL

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain D:  84% 11% ..

MET SER GLN S4 E7 R8 K12 S13 Y16 E17 P22 K25 Y28 V35 K36 P48 Q49 T67 A68 D76 R83 R87 R90 V91 D92 T97 R138 L139 E140 H146 K150 G154 P155 G158 V159 L166 H167 K168 I171

L174 L180 P180 K181 D207 Q213 N230 Y254 V264 M275 G276 T333 V334 L338 D341 T345 K346 G347 T351 L374 R375 V91 G415 E428 I431 D439 D444 I445 T456 D465 K468 D469 L470 N473 S471 F472 H473 S480

V483
THR
PRO
THR
ALA
ASN
VAL

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E:  85% 11% ..

MET SER GLN S4 E7 R8 K12 Y16 P22 K25 Y28 V35 K36 P48 Q49 T67 A68 D76 R83 R87 R90 V91 D92 T97 R138 L139 E140 H146 K150 G154 P155 V159 L166 N167 K168 I171 L174

P180 K181 K205 D206 D207 Q213 N230 M251 V254 V264 M275 G276 T333 V334 L338 D341 I345 K346 G347 T351 L374 R375 V91 K376 G415 E428 D439 D444 I445 T456 K468 D469 I470 S471 N473 S480 V484 THR PRO

THR
ALA
ASN
VAL

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain F:  85% 11% ..

MET SER GLN S4 E7 R8 K12 Y16 P22 K25 Y28 V35 P48 Q49 T67 A68 D76 R83 R87 R90 V91 D92 T97 R138 L139 E140 H146 K150 G154 P155 V159 L166 N167 K168 I171 L174 P180

K181 D207 Q213 N230 M251 V254 V264 M275 G276 T333 V334 L338 D341 I345 K346 G347 T351 L374 R375 V91 G415 E428 D439 D444 I445 K455 T456 D465 K468 D469 I470 S471 N473 S480 V484 THR PRO

THR
ALA
ASN
VAL

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G:  85% 11% ..

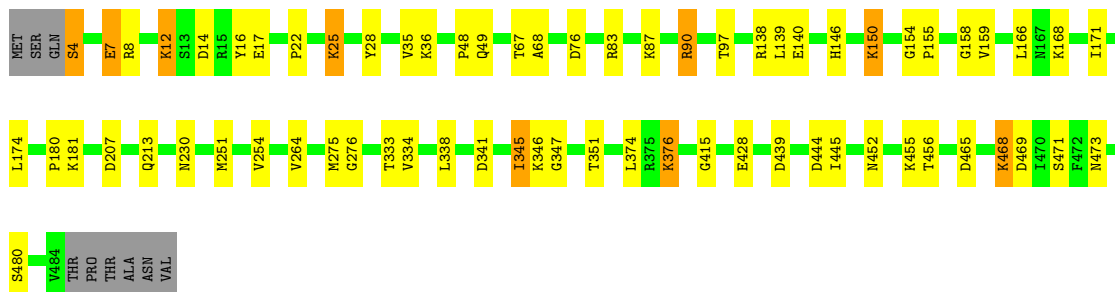
MET SER GLN S4 E7 R8 Y16 P22 K25 Y28 V35 K36 P48 Q49 T67 A68 D76 R83 R87 R90 V91 T97 R138 L139 E140 H146 K150 G154 P155 G158 V159 L166 N167 K168 I171 L174 P180 K181

L204 K205 D206 D207 N230 M251 V254 V264 M275 G276 T333 V334 L338 D341 I345 K346 G347 T351 L374 R375 V91 G415 E428 D439 D444 I445 K455 T456 D465 K468 S471 F472 N473 S480 V484 THR PRO THR

ALA
ASN
VAL

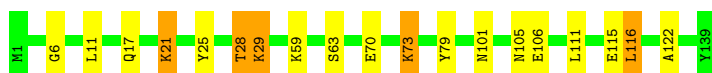
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain H:  84% 12% . .



- Molecule 2: Multifunctional fusion protein

Chain I:  86% 10% .



- Molecule 2: Multifunctional fusion protein

Chain J:  87% 9% .



- Molecule 2: Multifunctional fusion protein

Chain K:  85% 12% .



- Molecule 2: Multifunctional fusion protein

Chain L:  85% 11% .



- Molecule 2: Multifunctional fusion protein

Chain M:  85% 12% .



- Molecule 2: Multifunctional fusion protein

Chain N:  86% 11% .



- Molecule 2: Multifunctional fusion protein

Chain O:  87% 10% .

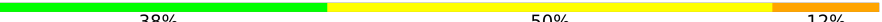


- Molecule 2: Multifunctional fusion protein

Chain P:  87% 10% .

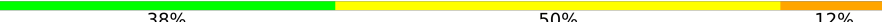


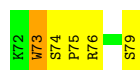
- Molecule 3: PYCO1 SSU binding motif

Chain i:  38% 50% 12%

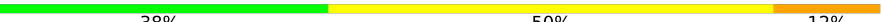


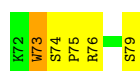
- Molecule 3: PYCO1 SSU binding motif

Chain k:  38% 50% 12%



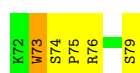
- Molecule 3: PYCO1 SSU binding motif

Chain j:  38% 50% 12%



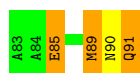
- Molecule 3: PYCO1 SSU binding motif

Chain l:  38% 50% 12%

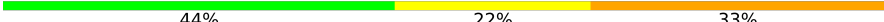


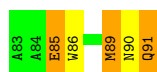
- Molecule 4: PYCO1 LSU binding motif

Chain h:  56% 11% 33%



- Molecule 4: PYCO1 LSU binding motif

Chain g:  44% 22% 33%

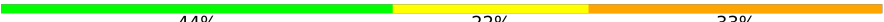


- Molecule 4: PYCO1 LSU binding motif

Chain f:  56% 22% 22%



- Molecule 4: PYCO1 LSU binding motif

Chain e:  44% 22% 33%



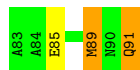
- Molecule 4: PYCO1 LSU binding motif

Chain d:  56% 22% 22%



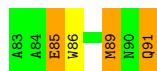
- Molecule 4: PYCO1 LSU binding motif

Chain c:  67% 11% 22%



- Molecule 4: PYCO1 LSU binding motif

Chain b:  56% 11% 33%



- Molecule 4: PYCO1 LSU binding motif



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	259796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.452	Depositor
Minimum map value	-0.273	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.0095	Depositor
Map size ($\text{\AA}$)	223.08, 223.08, 223.08	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.858, 0.858, 0.858	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, CAP, CSO, KCX, LYO, M3L, HLU

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	1.06	1/3745 (0.0%)	1.10	2/5072 (0.0%)
1	B	1.06	1/3745 (0.0%)	1.10	2/5072 (0.0%)
1	C	1.06	1/3745 (0.0%)	1.10	1/5072 (0.0%)
1	D	1.06	1/3745 (0.0%)	1.10	2/5072 (0.0%)
1	E	1.06	1/3745 (0.0%)	1.10	1/5072 (0.0%)
1	F	1.06	1/3745 (0.0%)	1.11	1/5072 (0.0%)
1	G	1.06	0/3745	1.10	2/5072 (0.0%)
1	H	1.06	1/3745 (0.0%)	1.10	2/5072 (0.0%)
2	I	1.03	0/1159	1.08	1/1570 (0.1%)
2	J	1.03	0/1159	1.08	1/1570 (0.1%)
2	K	1.03	0/1159	1.08	1/1570 (0.1%)
2	L	1.03	0/1159	1.09	1/1570 (0.1%)
2	M	1.03	0/1159	1.08	1/1570 (0.1%)
2	N	1.03	0/1159	1.09	1/1570 (0.1%)
2	O	1.03	0/1159	1.09	1/1570 (0.1%)
2	P	1.03	0/1159	1.09	1/1570 (0.1%)
3	i	0.94	0/63	1.03	0/83
3	j	0.93	0/63	1.03	0/83
3	k	0.94	0/63	1.03	0/83
3	l	0.92	0/63	0.98	0/83
4	a	0.88	0/69	1.09	0/92
4	b	0.90	0/69	0.99	0/92
4	c	0.88	0/69	0.98	0/92
4	d	0.89	0/69	0.99	0/92
4	e	0.88	0/69	0.99	0/92
4	f	0.89	0/69	0.99	0/92
4	g	0.88	0/69	0.99	0/92
4	h	0.89	0/69	0.99	0/92
All	All	1.05	7/40036 (0.0%)	1.10	21/54204 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLN	N-CA	5.15	1.49	1.46
1	C	213	GLN	N-CA	5.15	1.49	1.46
1	E	213	GLN	N-CA	5.11	1.49	1.46
1	D	213	GLN	N-CA	5.08	1.49	1.46
1	H	213	GLN	N-CA	5.08	1.49	1.46
1	B	213	GLN	N-CA	5.04	1.49	1.46
1	F	213	GLN	N-CA	5.04	1.49	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	6	GLY	CA-C-O	-6.23	117.96	122.45
2	M	6	GLY	CA-C-O	-6.21	117.98	122.45
2	N	6	GLY	CA-C-O	-6.21	117.98	122.45
2	I	6	GLY	CA-C-O	-6.20	117.98	122.45
2	O	6	GLY	CA-C-O	-6.20	117.98	122.45
2	K	6	GLY	CA-C-O	-6.19	118.00	122.45
2	L	6	GLY	CA-C-O	-6.18	118.00	122.45
2	J	6	GLY	CA-C-O	-6.17	118.01	122.45
1	A	415	GLY	CA-C-O	-5.97	118.15	122.45
1	F	415	GLY	CA-C-O	-5.96	118.16	122.45
1	G	415	GLY	CA-C-O	-5.95	118.17	122.45
1	E	415	GLY	CA-C-O	-5.94	118.17	122.45
1	D	415	GLY	CA-C-O	-5.89	118.21	122.45
1	H	415	GLY	CA-C-O	-5.89	118.21	122.45
1	C	415	GLY	CA-C-O	-5.81	118.26	122.45
1	B	415	GLY	CA-C-O	-5.78	118.29	122.45
1	A	158	GLY	CA-C-O	-5.04	117.86	122.24
1	B	158	GLY	CA-C-O	-5.04	117.86	122.24
1	D	158	GLY	CA-C-O	-5.04	117.86	122.24
1	G	158	GLY	CA-C-O	-5.04	117.86	122.24
1	H	158	GLY	CA-C-O	-5.04	117.86	122.24

There are no chirality outliers.

There are no planarity outliers.

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	A	3746	0	3685	34	0
1	B	3746	0	3685	34	0
1	C	3746	0	3685	38	0
1	D	3746	0	3685	37	0
1	E	3746	0	3685	39	0
1	F	3746	0	3685	32	0
1	G	3746	0	3685	31	0
1	H	3746	0	3685	33	0
2	I	1128	0	1077	10	0
2	J	1128	0	1077	11	0
2	K	1128	0	1077	11	0
2	L	1128	0	1077	12	0
2	M	1128	0	1077	11	0
2	N	1128	0	1077	12	0
2	O	1128	0	1077	9	0
2	P	1128	0	1077	11	0
3	i	61	0	58	15	0
3	j	61	0	58	16	0
3	k	61	0	58	16	0
3	l	61	0	58	16	0
4	a	68	0	56	3	0
4	b	68	0	56	6	0
4	c	68	0	56	5	0
4	d	68	0	56	12	0
4	e	68	0	56	12	0
4	f	68	0	56	12	0
4	g	68	0	56	8	0
4	h	68	0	56	5	0
5	A	21	0	9	0	0
5	B	21	0	9	0	0
5	C	21	0	9	0	0
5	D	21	0	9	0	0
5	E	21	0	9	0	0
5	F	21	0	9	0	0
5	G	21	0	9	0	0
5	H	21	0	9	0	0
All	All	39948	0	38848	388	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 5.

All (388) 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:D:90:ARG:HG3	4:e:89:MET:SD	1.43	1.54
1:B:90:ARG:CG	4:c:89:MET:HE1	1.43	1.48
1:B:90:ARG:HG3	4:c:89:MET:CE	1.41	1.47
1:E:90:ARG:HG3	4:f:89:MET:SD	1.69	1.32
1:C:90:ARG:HG3	4:d:89:MET:SD	1.73	1.29
1:D:90:ARG:CG	4:e:89:MET:SD	2.38	1.11
1:E:90:ARG:HD2	4:f:89:MET:HE1	1.33	1.10
1:G:90:ARG:HG3	4:h:89:MET:HE1	1.11	1.05
3:i:75:PRO:O	3:l:73:TRP:CZ2	2.16	0.99
4:f:86:TRP:CD1	4:f:89:MET:HE2	1.97	0.99
4:e:86:TRP:CD1	4:e:89:MET:HE2	1.97	0.99
4:g:86:TRP:CD1	4:g:89:MET:HE2	1.97	0.99
4:d:86:TRP:CD1	4:d:89:MET:HE2	1.97	0.98
1:C:90:ARG:HD2	4:d:89:MET:HE1	1.46	0.97
4:b:86:TRP:CD1	4:b:89:MET:HE2	1.99	0.97
3:k:75:PRO:O	3:j:73:TRP:CZ2	2.16	0.97
1:E:90:ARG:CG	4:f:89:MET:SD	2.54	0.96
3:k:79:SER:HB3	3:j:73:TRP:CD2	2.03	0.93
1:C:90:ARG:CG	4:d:89:MET:SD	2.55	0.93
1:E:90:ARG:HD2	4:f:89:MET:CE	1.99	0.93
1:G:90:ARG:CG	4:h:89:MET:HE1	1.99	0.92
3:i:79:SER:HB3	3:l:73:TRP:CD2	2.04	0.91
3:i:73:TRP:CZ2	3:j:75:PRO:O	2.23	0.90
1:E:90:ARG:CD	4:f:89:MET:HE1	2.02	0.89
1:H:90:ARG:HE	4:a:89:MET:HE1	1.36	0.89
3:k:73:TRP:CZ2	3:l:75:PRO:O	2.25	0.89
3:k:73:TRP:CD2	3:l:79:SER:HB3	2.06	0.89
1:C:90:ARG:CD	4:d:89:MET:HE1	2.03	0.86
1:C:90:ARG:HD2	4:d:89:MET:CE	2.07	0.85
3:i:73:TRP:CD2	3:j:79:SER:HB3	2.13	0.83
3:k:75:PRO:O	3:j:73:TRP:HZ2	1.65	0.79
3:k:79:SER:HB3	3:j:73:TRP:CG	2.19	0.77
3:i:79:SER:HB3	3:l:73:TRP:CG	2.21	0.76
2:K:70:GLU:HA	2:K:73:LYS:HD2	1.68	0.76
3:i:73:TRP:HZ2	3:j:75:PRO:O	1.66	0.76
1:B:90:ARG:CD	4:c:89:MET:HE1	2.14	0.76
2:M:70:GLU:HA	2:M:73:LYS:HD2	1.67	0.76
4:d:86:TRP:CD1	4:d:89:MET:CE	2.70	0.74
1:G:35:VAL:HG21	4:h:90:ASN:HA	1.69	0.74
2:J:70:GLU:HA	2:J:73:LYS:HD2	1.70	0.74
4:f:86:TRP:CD1	4:f:89:MET:CE	2.71	0.74
3:i:75:PRO:O	3:l:73:TRP:HZ2	1.66	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:VAL:HG21	1:F:275:MET:HE1	1.71	0.73
2:O:70:GLU:HA	2:O:73:LYS:HD2	1.71	0.73
3:k:73:TRP:HZ2	3:l:75:PRO:O	1.70	0.73
1:A:276:GLY:HA3	1:B:276:GLY:HA3	1.70	0.73
1:C:276:GLY:HA3	1:D:276:GLY:HA3	1.70	0.73
1:B:254:VAL:HG21	1:B:275:MET:HE1	1.71	0.73
1:H:254:VAL:HG21	1:H:275:MET:HE1	1.71	0.73
2:I:70:GLU:HA	2:I:73:LYS:HD2	1.71	0.73
1:D:254:VAL:HG21	1:D:275:MET:HE1	1.71	0.72
1:E:276:GLY:HA3	1:F:276:GLY:HA3	1.70	0.72
2:P:70:GLU:HA	2:P:73:LYS:HD2	1.71	0.72
1:G:276:GLY:HA3	1:H:276:GLY:HA3	1.70	0.72
4:g:86:TRP:HD1	4:g:89:MET:HE2	1.54	0.72
4:g:86:TRP:CD1	4:g:89:MET:CE	2.72	0.72
2:L:70:GLU:HA	2:L:73:LYS:HD2	1.71	0.72
4:e:86:TRP:CD1	4:e:89:MET:CE	2.72	0.72
4:e:86:TRP:HD1	4:e:89:MET:HE2	1.54	0.71
1:H:90:ARG:NE	4:a:89:MET:HE1	2.05	0.71
4:b:86:TRP:CD1	4:b:89:MET:CE	2.72	0.71
4:b:86:TRP:HD1	4:b:89:MET:HE2	1.56	0.69
1:F:90:ARG:NE	1:F:92:ASP:OD2	2.25	0.69
1:C:254:VAL:HG21	1:C:275:MET:HE1	1.75	0.68
1:E:254:VAL:HG21	1:E:275:MET:HE1	1.76	0.68
4:d:86:TRP:HD1	4:d:89:MET:HE2	1.54	0.68
1:B:230:ASN:HB3	2:J:111:LEU:HD21	1.76	0.68
1:F:230:ASN:HB3	2:N:111:LEU:HD21	1.76	0.67
1:G:230:ASN:HB3	2:O:111:LEU:HD21	1.76	0.67
1:G:254:VAL:HG21	1:G:275:MET:HE1	1.76	0.67
1:A:254:VAL:HG21	1:A:275:MET:HE1	1.77	0.67
3:k:73:TRP:CG	3:l:79:SER:HB3	2.29	0.67
1:C:230:ASN:HB3	2:K:111:LEU:HD21	1.77	0.67
4:f:86:TRP:HD1	4:f:89:MET:HE2	1.54	0.66
1:D:230:ASN:HB3	2:L:111:LEU:HD21	1.77	0.65
1:E:230:ASN:HB3	2:M:111:LEU:HD21	1.77	0.65
1:H:230:ASN:HB3	2:P:111:LEU:HD21	1.77	0.65
1:F:90:ARG:HD2	4:g:89:MET:HE1	1.79	0.65
1:A:230:ASN:HB3	2:I:111:LEU:HD21	1.77	0.64
1:C:90:ARG:NE	1:C:92:ASP:OD2	2.30	0.64
1:F:159:VAL:HB	1:F:376:LYS:HG3	1.80	0.64
1:G:159:VAL:HB	1:G:376:LYS:HG3	1.80	0.64
1:H:35:VAL:HG21	4:a:90:ASN:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:VAL:HB	1:E:376:LYS:HG3	1.80	0.63
3:i:73:TRP:CG	3:j:79:SER:HB3	2.34	0.62
1:F:35:VAL:HG21	4:g:90:ASN:HA	1.81	0.62
1:A:159:VAL:HB	1:A:376:LYS:HG3	1.80	0.62
1:D:159:VAL:HB	1:D:376:LYS:HG3	1.80	0.62
1:D:35:VAL:HG21	4:e:90:ASN:HA	1.81	0.62
1:H:159:VAL:HB	1:H:376:LYS:HG3	1.81	0.61
2:N:70:GLU:HA	2:N:73:LYS:HD2	1.80	0.61
1:B:159:VAL:HB	1:B:376:LYS:HG3	1.80	0.61
1:C:159:VAL:HB	1:C:376:LYS:HG3	1.80	0.61
1:B:90:ARG:NE	1:B:92:ASP:OD2	2.34	0.60
1:C:90:ARG:HD2	4:d:89:MET:SD	2.42	0.59
1:B:90:ARG:HG3	4:c:89:MET:HE1	0.64	0.58
1:E:90:ARG:HD2	4:f:89:MET:SD	2.44	0.58
1:C:22:PRO:HB2	1:C:25:LYS:HG3	1.86	0.58
1:A:22:PRO:HB2	1:A:25:LYS:HG3	1.86	0.57
1:B:22:PRO:HB2	1:B:25:LYS:HG3	1.86	0.57
1:D:22:PRO:HB2	1:D:25:LYS:HG3	1.86	0.57
1:A:154:GLY:HA3	1:A:374:LEU:HD22	1.87	0.57
1:D:154:GLY:HA3	1:D:374:LEU:HD22	1.87	0.57
1:G:154:GLY:HA3	1:G:374:LEU:HD22	1.86	0.57
2:M:17:GLN:O	2:M:21:LYS:HG3	2.05	0.57
1:E:154:GLY:HA3	1:E:374:LEU:HD22	1.87	0.57
1:G:22:PRO:HB2	1:G:25:LYS:HG3	1.86	0.57
1:E:22:PRO:HB2	1:E:25:LYS:HG3	1.86	0.57
2:J:105:ASN:ND2	3:i:79:SER:O	2.36	0.57
1:B:154:GLY:HA3	1:B:374:LEU:HD22	1.87	0.57
1:F:22:PRO:HB2	1:F:25:LYS:HG3	1.86	0.57
1:H:22:PRO:HB2	1:H:25:LYS:HG3	1.86	0.56
1:C:180:PRO:HB2	1:D:67:THR:OG1	2.06	0.56
1:E:180:PRO:HB2	1:F:67:THR:OG1	2.06	0.56
1:F:154:GLY:HA3	1:F:374:LEU:HD22	1.87	0.56
1:H:4:SER:O	1:H:7:GLU:HG3	2.06	0.56
1:E:4:SER:O	1:E:7:GLU:HG3	2.06	0.56
2:I:17:GLN:O	2:I:21:LYS:HG3	2.06	0.56
1:A:180:PRO:HB2	1:B:67:THR:OG1	2.06	0.56
1:G:180:PRO:HB2	1:H:67:THR:OG1	2.06	0.56
1:C:90:ARG:CD	4:d:89:MET:SD	2.93	0.56
1:C:154:GLY:HA3	1:C:374:LEU:HD22	1.88	0.56
1:C:4:SER:O	1:C:7:GLU:HG3	2.07	0.55
1:E:90:ARG:NE	1:E:92:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:GLU:OE1	2:M:11:LEU:HG	2.07	0.55
1:G:4:SER:O	1:G:7:GLU:HG3	2.06	0.55
1:H:428:GLU:OE1	2:P:11:LEU:HG	2.07	0.55
1:B:4:SER:O	1:B:7:GLU:HG3	2.07	0.55
1:F:428:GLU:OE1	2:N:11:LEU:HG	2.07	0.55
1:G:428:GLU:OE1	2:O:11:LEU:HG	2.07	0.55
1:A:4:SER:O	1:A:7:GLU:HG3	2.06	0.55
1:A:452:ASN:HA	1:A:455:LYS:HE3	1.89	0.55
1:E:254:VAL:CG2	1:E:275:MET:HE1	2.37	0.55
1:D:4:SER:O	1:D:7:GLU:HG3	2.06	0.54
1:D:90:ARG:CD	4:e:89:MET:HE1	2.37	0.54
1:E:90:ARG:CD	4:f:89:MET:SD	2.94	0.54
1:B:428:GLU:OE1	2:J:11:LEU:HG	2.07	0.54
1:C:90:ARG:CD	4:d:89:MET:CE	2.77	0.54
1:G:4:SER:O	1:G:8:ARG:HG3	2.07	0.54
1:G:254:VAL:CG2	1:G:275:MET:HE1	2.37	0.54
1:C:254:VAL:CG2	1:C:275:MET:HE1	2.37	0.54
1:C:428:GLU:OE1	2:K:11:LEU:HG	2.07	0.54
1:F:4:SER:O	1:F:8:ARG:HG3	2.08	0.54
1:F:4:SER:O	1:F:7:GLU:HG3	2.08	0.54
1:C:4:SER:O	1:C:8:ARG:HG3	2.08	0.54
1:D:428:GLU:OE1	2:L:11:LEU:HG	2.07	0.54
1:A:428:GLU:OE1	2:I:11:LEU:HG	2.07	0.54
1:H:154:GLY:HA3	1:H:374:LEU:HD22	1.90	0.54
1:A:254:VAL:CG2	1:A:275:MET:HE1	2.37	0.53
2:L:133:ASN:OD1	3:j:73:TRP:O	2.26	0.53
1:A:4:SER:O	1:A:8:ARG:HG3	2.07	0.53
1:B:4:SER:O	1:B:8:ARG:HG3	2.08	0.53
1:E:4:SER:O	1:E:8:ARG:HG3	2.08	0.53
1:D:4:SER:O	1:D:8:ARG:HG3	2.08	0.53
1:H:4:SER:O	1:H:8:ARG:HG3	2.08	0.52
1:D:90:ARG:HG3	4:e:89:MET:CE	2.35	0.52
1:A:22:PRO:HD2	1:A:25:LYS:HD3	1.92	0.52
2:L:105:ASN:ND2	3:j:79:SER:O	2.41	0.52
2:P:25:TYR:O	2:P:28:THR:HG22	2.10	0.52
1:D:22:PRO:HD2	1:D:25:LYS:HD3	1.92	0.52
2:M:25:TYR:O	2:M:28:THR:HG22	2.11	0.51
1:B:22:PRO:HD2	1:B:25:LYS:HD3	1.92	0.51
2:O:25:TYR:O	2:O:28:THR:HG22	2.10	0.51
1:C:22:PRO:HD2	1:C:25:LYS:HD3	1.92	0.51
2:J:25:TYR:O	2:J:28:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:452:ASN:HA	1:H:455:LYS:HE3	1.93	0.51
2:L:17:GLN:O	2:L:21:LYS:HG3	2.10	0.51
3:j:74:SER:N	3:j:75:PRO:CD	2.74	0.51
1:C:28:TYR:CZ	1:C:68:ALA:HB2	2.46	0.51
1:E:22:PRO:HD2	1:E:25:LYS:HD3	1.92	0.51
1:D:90:ARG:HD3	4:e:89:MET:HE1	1.92	0.51
1:H:22:PRO:HD2	1:H:25:LYS:HD3	1.92	0.51
3:i:74:SER:N	3:i:75:PRO:CD	2.74	0.51
3:k:74:SER:N	3:k:75:PRO:CD	2.74	0.50
2:K:25:TYR:O	2:K:28:THR:HG22	2.11	0.50
1:B:28:TYR:CZ	1:B:68:ALA:HB2	2.47	0.50
3:k:75:PRO:O	3:j:73:TRP:CH2	2.64	0.50
2:I:25:TYR:O	2:I:28:THR:HG22	2.11	0.50
2:N:25:TYR:O	2:N:28:THR:HG22	2.11	0.50
1:E:67:THR:OG1	1:F:180:PRO:HB2	2.12	0.50
2:L:25:TYR:O	2:L:28:THR:HG22	2.10	0.50
1:C:67:THR:OG1	1:D:180:PRO:HB2	2.12	0.50
1:E:28:TYR:CZ	1:E:68:ALA:HB2	2.46	0.50
1:E:90:ARG:CD	4:f:89:MET:CE	2.76	0.50
3:l:74:SER:N	3:l:75:PRO:CD	2.74	0.50
1:A:28:TYR:CZ	1:A:68:ALA:HB2	2.46	0.50
1:H:28:TYR:CZ	1:H:68:ALA:HB2	2.47	0.50
1:F:347:GLY:O	1:F:351:THR:HG23	2.12	0.49
1:G:67:THR:OG1	1:H:180:PRO:HB2	2.12	0.49
1:G:347:GLY:O	1:G:351:THR:HG23	2.12	0.49
3:i:75:PRO:O	3:l:73:TRP:CH2	2.62	0.49
1:A:347:GLY:O	1:A:351:THR:HG23	2.12	0.49
1:D:28:TYR:CZ	1:D:68:ALA:HB2	2.47	0.49
1:G:16:TYR:HE1	1:G:76:ASP:HB2	1.76	0.49
1:G:28:TYR:CZ	1:G:68:ALA:HB2	2.46	0.49
3:k:74:SER:N	3:k:75:PRO:HD2	2.28	0.49
1:A:67:THR:HA	1:B:181:LYS:HB2	1.94	0.49
1:D:347:GLY:O	1:D:351:THR:HG23	2.12	0.49
1:F:28:TYR:CZ	1:F:68:ALA:HB2	2.46	0.49
2:N:105:ASN:ND2	3:k:79:SER:O	2.36	0.49
1:A:67:THR:OG1	1:B:180:PRO:HB2	2.12	0.49
1:C:16:TYR:HE1	1:C:76:ASP:HB2	1.77	0.49
1:E:16:TYR:HE1	1:E:76:ASP:HB2	1.77	0.49
1:E:347:GLY:O	1:E:351:THR:HG23	2.12	0.49
3:i:74:SER:N	3:i:75:PRO:HD2	2.28	0.49
1:A:16:TYR:HE1	1:A:76:ASP:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:GLY:O	1:H:351:THR:HG23	2.12	0.49
1:C:347:GLY:O	1:C:351:THR:HG23	2.12	0.48
1:B:347:GLY:O	1:B:351:THR:HG23	2.12	0.48
1:C:67:THR:HA	1:D:181:LYS:HB2	1.94	0.48
1:E:67:THR:HA	1:F:181:LYS:HB2	1.94	0.48
3:l:74:SER:N	3:l:75:PRO:HD2	2.28	0.48
3:j:74:SER:N	3:j:75:PRO:HD2	2.28	0.48
1:G:67:THR:HA	1:H:181:LYS:HB2	1.94	0.48
1:E:146:HIS:CE1	1:E:150:LYO:HD1	2.49	0.48
1:C:181:LYS:HB2	1:D:67:THR:HA	1.96	0.48
1:F:146:HIS:CE1	1:F:150:LYO:HD1	2.49	0.48
1:G:146:HIS:CE1	1:G:150:LYO:HD1	2.49	0.48
1:H:146:HIS:CE1	1:H:150:LYO:HD1	2.49	0.48
1:H:16:TYR:HE1	1:H:76:ASP:HB2	1.78	0.48
1:A:181:LYS:HB2	1:B:67:THR:HA	1.95	0.48
1:A:439:ASP:HB3	1:A:445:ILE:HD13	1.96	0.48
1:B:146:HIS:CE1	1:B:150:LYO:HD1	2.49	0.48
1:C:146:HIS:CE1	1:C:150:LYO:HD1	2.49	0.48
1:G:90:ARG:HD3	1:G:91:VAL:N	2.28	0.48
3:k:73:TRP:CE2	3:l:79:SER:HB3	2.49	0.48
1:G:181:LYS:HB2	1:H:67:THR:HA	1.95	0.47
1:A:146:HIS:CE1	1:A:150:LYO:HD1	2.49	0.47
1:F:16:TYR:HE1	1:F:76:ASP:HB2	1.78	0.47
1:F:90:ARG:HD3	1:F:92:ASP:OD1	2.13	0.47
1:A:90:ARG:HG3	4:b:89:MET:SD	2.54	0.47
1:D:146:HIS:CE1	1:D:150:LYO:HD1	2.49	0.47
1:E:181:LYS:HB2	1:F:67:THR:HA	1.96	0.47
1:A:90:ARG:HD3	1:A:91:VAL:N	2.29	0.47
2:O:73:LYS:HE3	2:O:73:LYS:HB3	1.68	0.47
1:D:16:TYR:HE1	1:D:76:ASP:HB2	1.79	0.47
1:D:376:LYS:HE3	1:D:376:LYS:HB3	1.55	0.47
1:E:90:ARG:CZ	1:E:92:ASP:OD2	2.63	0.47
1:B:16:TYR:HE1	1:B:76:ASP:HB2	1.80	0.47
1:B:439:ASP:HB3	1:B:445:ILE:HD13	1.97	0.47
1:E:376:LYS:HB3	1:E:376:LYS:HE3	1.55	0.47
1:A:376:LYS:HE3	1:A:376:LYS:HB3	1.55	0.46
1:C:439:ASP:HB3	1:C:445:ILE:HD13	1.98	0.46
1:D:439:ASP:HB3	1:D:445:ILE:HD13	1.98	0.46
1:H:376:LYS:HE3	1:H:376:LYS:HB3	1.57	0.46
2:P:116:LEU:HD11	2:P:122:ALA:HB2	1.97	0.46
1:F:439:ASP:HB3	1:F:445:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:PRO:HD2	1:G:25:LYS:HD3	1.96	0.46
1:H:439:ASP:HB3	1:H:445:ILE:HD13	1.97	0.46
2:N:73:LYS:HB3	2:N:73:LYS:HE3	1.45	0.46
2:K:33:MET:HE3	2:K:33:MET:HB3	1.83	0.46
2:M:116:LEU:HD11	2:M:122:ALA:HB2	1.98	0.46
2:O:116:LEU:HD11	2:O:122:ALA:HB2	1.97	0.46
2:P:133:ASN:OD1	3:l:73:TRP:O	2.33	0.46
1:G:439:ASP:HB3	1:G:445:ILE:HD13	1.98	0.46
2:M:79:TYR:OH	2:M:106:GLU:HG3	2.16	0.46
1:F:22:PRO:HD2	1:F:25:LYS:HD3	1.97	0.46
1:E:439:ASP:HB3	1:E:445:ILE:HD13	1.98	0.46
2:O:79:TYR:OH	2:O:106:GLU:HG3	2.16	0.46
1:B:166:LEU:O	1:B:168:LYS:HG2	2.16	0.45
1:E:166:LEU:O	1:E:168:LYS:HG2	2.17	0.45
1:H:166:LEU:O	1:H:168:LYS:HG2	2.17	0.45
1:C:166:LEU:O	1:C:168:LYS:HG2	2.17	0.45
2:N:116:LEU:HD11	2:N:122:ALA:HB2	1.98	0.45
2:K:79:TYR:OH	2:K:106:GLU:HG3	2.16	0.45
2:M:17:GLN:CD	2:M:17:GLN:H	2.25	0.45
2:J:116:LEU:HD11	2:J:122:ALA:HB2	1.98	0.45
2:P:105:ASN:ND2	3:l:79:SER:O	2.37	0.45
2:K:17:GLN:CD	2:K:17:GLN:H	2.25	0.45
2:K:116:LEU:HD11	2:K:122:ALA:HB2	1.98	0.45
2:P:17:GLN:CD	2:P:17:GLN:H	2.25	0.45
4:g:91:GLN:HE21	4:g:91:GLN:HB2	1.55	0.45
2:L:116:LEU:HD11	2:L:122:ALA:HB2	1.98	0.45
2:N:25:TYR:O	2:N:29:LYS:HG2	2.17	0.45
2:N:133:ASN:OD1	3:k:73:TRP:O	2.35	0.44
4:f:91:GLN:HE21	4:f:91:GLN:HB2	1.55	0.44
1:A:166:LEU:O	1:A:168:LYS:HG2	2.17	0.44
2:N:17:GLN:H	2:N:17:GLN:CD	2.25	0.44
4:h:91:GLN:HE21	4:h:91:GLN:HB2	1.55	0.44
2:L:73:LYS:HE3	2:L:73:LYS:HB3	1.68	0.44
2:M:25:TYR:O	2:M:29:LYS:HG2	2.18	0.44
2:I:79:TYR:OH	2:I:106:GLU:HG3	2.16	0.44
2:K:25:TYR:O	2:K:29:LYS:HG2	2.18	0.44
2:O:25:TYR:O	2:O:29:LYS:HG2	2.18	0.44
1:E:468:LYS:HD3	1:E:469:ASP:CG	2.41	0.44
1:F:465:ASP:O	1:F:468:LYS:HG2	2.18	0.44
1:A:465:ASP:O	1:A:468:LYS:HG2	2.18	0.43
1:F:166:LEU:O	1:F:168:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:LYS:H	2:I:29:LYS:HG2	1.65	0.43
2:L:29:LYS:H	2:L:29:LYS:HG2	1.66	0.43
2:P:25:TYR:O	2:P:29:LYS:HG2	2.18	0.43
1:B:376:LYS:HE3	1:B:376:LYS:HB3	1.55	0.43
1:G:166:LEU:O	1:G:168:LYS:HG2	2.17	0.43
1:G:465:ASP:O	1:G:468:LYS:HG2	2.18	0.43
1:H:465:ASP:O	1:H:468:LYS:HG2	2.18	0.43
2:I:116:LEU:HD11	2:I:122:ALA:HB2	1.99	0.43
1:B:465:ASP:O	1:B:468:LYS:HG2	2.18	0.43
1:H:12:LYS:HA	1:H:17:GLU:OE1	2.18	0.43
2:J:25:TYR:O	2:J:29:LYS:HG2	2.18	0.43
1:D:166:LEU:O	1:D:168:LYS:HG2	2.17	0.43
4:b:85:GLU:H	4:b:85:GLU:HG2	1.51	0.43
3:k:74:SER:H	3:k:75:PRO:HD2	1.84	0.43
1:B:12:LYS:HA	1:B:17:GLU:OE1	2.19	0.43
1:C:376:LYS:HE3	1:C:376:LYS:HB3	1.54	0.43
4:e:85:GLU:H	4:e:85:GLU:HG2	1.51	0.43
2:I:73:LYS:HE3	2:I:73:LYS:HB3	1.67	0.43
2:L:25:TYR:O	2:L:29:LYS:HG2	2.18	0.43
1:D:90:ARG:CD	4:e:89:MET:SD	3.03	0.43
1:E:346:M3L:HD3	1:E:346:M3L:HA	1.79	0.43
1:A:346:M3L:HA	1:A:346:M3L:HD3	1.78	0.43
1:D:346:M3L:HA	1:D:346:M3L:HD3	1.79	0.42
1:D:468:LYS:HB2	1:D:468:LYS:HE2	1.70	0.42
2:I:25:TYR:O	2:I:29:LYS:HG2	2.18	0.42
3:l:74:SER:H	3:l:75:PRO:HD2	1.84	0.42
4:e:91:GLN:HE21	4:e:91:GLN:HB2	1.55	0.42
1:A:138:ARG:HD3	1:A:140:GLU:OE2	2.19	0.42
1:D:138:ARG:HD3	1:D:140:GLU:OE2	2.19	0.42
2:P:33:MET:HE3	2:P:33:MET:HB3	1.83	0.42
1:D:12:LYS:HA	1:D:17:GLU:OE1	2.19	0.42
1:B:138:ARG:HD3	1:B:140:GLU:OE2	2.19	0.42
1:D:376:LYS:H	1:D:376:LYS:HG2	1.64	0.42
1:F:374:LEU:HD23	1:F:374:LEU:HA	1.85	0.42
1:H:346:M3L:HD3	1:H:346:M3L:HA	1.79	0.42
2:N:33:MET:HE3	2:N:33:MET:HB3	1.83	0.42
4:h:85:GLU:H	4:h:85:GLU:HG2	1.51	0.42
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.85	0.42
1:C:138:ARG:HD3	1:C:140:GLU:OE2	2.19	0.42
1:C:374:LEU:HD23	1:C:374:LEU:HA	1.85	0.42
3:j:74:SER:H	3:j:75:PRO:CD	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:ASP:O	1:D:468:LYS:HG2	2.19	0.42
1:E:25:LYS:HE3	1:E:25:LYS:HB3	1.83	0.42
2:K:82:ILE:HD12	2:K:100:VAL:HG21	2.02	0.42
3:k:74:SER:H	3:k:75:PRO:CD	2.33	0.42
1:G:138:ARG:HD3	1:G:140:GLU:OE2	2.19	0.42
2:M:33:MET:HE3	2:M:33:MET:HB3	1.83	0.42
4:g:85:GLU:H	4:g:85:GLU:HG2	1.51	0.42
1:A:376:LYS:H	1:A:376:LYS:HG2	1.64	0.42
1:F:341:ASP:O	1:F:345:ILE:HG13	2.20	0.42
1:G:341:ASP:O	1:G:345:ILE:HG13	2.20	0.42
1:H:341:ASP:O	1:H:345:ILE:HG13	2.20	0.42
1:H:374:LEU:HD23	1:H:374:LEU:HA	1.85	0.42
2:O:33:MET:HE3	2:O:33:MET:HB3	1.83	0.42
1:C:465:ASP:O	1:C:468:LYS:HG2	2.20	0.42
1:E:138:ARG:HD3	1:E:140:GLU:OE2	2.19	0.42
1:E:341:ASP:O	1:E:345:ILE:HG13	2.20	0.42
1:F:138:ARG:HD3	1:F:140:GLU:OE2	2.19	0.42
1:H:138:ARG:HD3	1:H:140:GLU:OE2	2.19	0.42
1:B:341:ASP:O	1:B:345:ILE:HG13	2.20	0.41
2:J:73:LYS:HB3	2:J:73:LYS:HE3	1.67	0.41
3:i:74:SER:H	3:i:75:PRO:HD2	1.84	0.41
4:d:91:GLN:HE21	4:d:91:GLN:HB2	1.55	0.41
4:c:91:GLN:HE21	4:c:91:GLN:HB2	1.55	0.41
1:C:341:ASP:O	1:C:345:ILE:HG13	2.20	0.41
1:D:333:THR:O	1:D:334:VAL:HB	2.20	0.41
1:G:374:LEU:HD23	1:G:374:LEU:HA	1.86	0.41
4:b:91:GLN:HE21	4:b:91:GLN:HB2	1.55	0.41
3:i:73:TRP:CE2	3:j:79:SER:HB3	2.53	0.41
1:A:333:THR:O	1:A:334:VAL:HB	2.20	0.41
2:M:69:ARG:O	2:M:73:LYS:HE3	2.21	0.41
3:i:74:SER:H	3:i:75:PRO:CD	2.33	0.41
1:C:452:ASN:HA	1:C:455:LYS:HZ2	1.85	0.41
1:A:341:ASP:O	1:A:345:ILE:HG13	2.20	0.41
1:B:346:M3L:HA	1:B:346:M3L:HD3	1.79	0.41
1:D:341:ASP:O	1:D:345:ILE:HG13	2.20	0.41
3:l:74:SER:H	3:l:75:PRO:CD	2.33	0.41
1:B:333:THR:O	1:B:334:VAL:HB	2.20	0.41
1:E:333:THR:O	1:E:334:VAL:HB	2.20	0.41
1:F:376:LYS:HE3	1:F:376:LYS:HB3	1.55	0.41
2:N:29:LYS:HB3	2:N:29:LYS:HE2	1.76	0.41
3:j:74:SER:H	3:j:75:PRO:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:THR:O	1:H:334:VAL:HB	2.20	0.41
2:L:79:TYR:OH	2:L:106:GLU:HG3	2.21	0.41
1:C:333:THR:O	1:C:334:VAL:HB	2.20	0.40
1:C:346:M3L:HA	1:C:346:M3L:HD3	1.78	0.40
1:F:333:THR:O	1:F:334:VAL:HB	2.20	0.40
1:G:333:THR:O	1:G:334:VAL:HB	2.20	0.40
2:J:79:TYR:OH	2:J:106:GLU:HG3	2.21	0.40
2:K:111:LEU:HD12	2:K:111:LEU:HA	1.94	0.40
2:P:29:LYS:HG2	2:P:29:LYS:H	1.66	0.40
1:A:12:LYS:HA	1:A:17:GLU:OE1	2.20	0.40
2:J:29:LYS:HG2	2:J:29:LYS:H	1.65	0.40
1:D:171:ILE:HG22	1:D:431:ILE:HG13	2.03	0.40
1:G:251:MET:HG2	1:H:251:MET:HG2	2.04	0.40
1:A:251:MET:HG2	1:B:251:MET:HG2	2.03	0.40
1:E:251:MET:HG2	1:F:251:MET:HG2	2.04	0.40
1:F:90:ARG:HD2	4:g:89:MET:CE	2.47	0.40
2:J:111:LEU:HD12	2:J:111:LEU:HA	1.93	0.40
1:A:442:ASN:HB3	1:A:445:ILE:HD12	2.03	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	471/490 (96%)	453 (96%)	18 (4%)	0	100	100
1	B	471/490 (96%)	454 (96%)	17 (4%)	0	100	100
1	C	471/490 (96%)	454 (96%)	17 (4%)	0	100	100
1	D	471/490 (96%)	453 (96%)	18 (4%)	0	100	100
1	E	471/490 (96%)	454 (96%)	17 (4%)	0	100	100
1	F	471/490 (96%)	452 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	471/490 (96%)	453 (96%)	18 (4%)	0	100	100
1	H	471/490 (96%)	453 (96%)	18 (4%)	0	100	100
2	I	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	J	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	K	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	L	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	M	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	N	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	O	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
2	P	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
3	i	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
3	j	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
3	k	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
3	l	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
4	a	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	b	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	c	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	d	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	e	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	f	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	g	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	h	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	4944/5136 (96%)	4750 (96%)	194 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/390 (98%)	356 (93%)	26 (7%)	14	11
1	B	382/390 (98%)	355 (93%)	27 (7%)	13	10
1	C	382/390 (98%)	355 (93%)	27 (7%)	13	10
1	D	382/390 (98%)	355 (93%)	27 (7%)	13	10
1	E	382/390 (98%)	357 (94%)	25 (6%)	15	12
1	F	382/390 (98%)	356 (93%)	26 (7%)	14	11
1	G	382/390 (98%)	356 (93%)	26 (7%)	14	11
1	H	382/390 (98%)	357 (94%)	25 (6%)	15	12
2	I	119/119 (100%)	109 (92%)	10 (8%)	10	7
2	J	119/119 (100%)	109 (92%)	10 (8%)	10	7
2	K	119/119 (100%)	110 (92%)	9 (8%)	12	9
2	L	119/119 (100%)	108 (91%)	11 (9%)	8	5
2	M	119/119 (100%)	109 (92%)	10 (8%)	10	7
2	N	119/119 (100%)	110 (92%)	9 (8%)	12	9
2	O	119/119 (100%)	110 (92%)	9 (8%)	12	9
2	P	119/119 (100%)	111 (93%)	8 (7%)	15	11
3	i	6/6 (100%)	4 (67%)	2 (33%)	0	0
3	j	6/6 (100%)	4 (67%)	2 (33%)	0	0
3	k	6/6 (100%)	4 (67%)	2 (33%)	0	0
3	l	6/6 (100%)	4 (67%)	2 (33%)	0	0
4	a	6/6 (100%)	4 (67%)	2 (33%)	0	0
4	b	6/6 (100%)	3 (50%)	3 (50%)	0	0
4	c	6/6 (100%)	3 (50%)	3 (50%)	0	0
4	d	6/6 (100%)	3 (50%)	3 (50%)	0	0
4	e	6/6 (100%)	3 (50%)	3 (50%)	0	0
4	f	6/6 (100%)	3 (50%)	3 (50%)	0	0
4	g	6/6 (100%)	3 (50%)	3 (50%)	0	0
4	h	6/6 (100%)	3 (50%)	3 (50%)	0	0
All	All	4080/4144 (98%)	3764 (92%)	316 (8%)	14	8

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	7	GLU
1	A	12	LYS
1	A	25	LYS
1	A	35	VAL
1	A	36	LYS
1	A	49	GLN
1	A	83	ARG
1	A	87	LYS
1	A	90	ARG
1	A	97	THR
1	A	139	LEU
1	A	171	ILE
1	A	207	ASP
1	A	264	VAL
1	A	338	LEU
1	A	341	ASP
1	A	345	ILE
1	A	376	LYS
1	A	444	ASP
1	A	456	THR
1	A	468	LYS
1	A	469	ASP
1	A	471	SER
1	A	473	ASN
1	A	480	SER
1	B	4	SER
1	B	7	GLU
1	B	12	LYS
1	B	13	SER
1	B	25	LYS
1	B	36	LYS
1	B	49	GLN
1	B	83	ARG
1	B	87	LYS
1	B	90	ARG
1	B	92	ASP
1	B	97	THR
1	B	139	LEU
1	B	171	ILE
1	B	207	ASP
1	B	264	VAL
1	B	338	LEU

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Mol	Chain	Res	Type
1	B	345	ILE
1	B	376	LYS
1	B	444	ASP
1	B	455	LYS
1	B	456	THR
1	B	468	LYS
1	B	469	ASP
1	B	471	SER
1	B	473	ASN
1	B	480	SER
1	C	4	SER
1	C	7	GLU
1	C	12	LYS
1	C	25	LYS
1	C	35	VAL
1	C	36	LYS
1	C	49	GLN
1	C	83	ARG
1	C	87	LYS
1	C	90	ARG
1	C	92	ASP
1	C	97	THR
1	C	139	LEU
1	C	171	ILE
1	C	207	ASP
1	C	264	VAL
1	C	338	LEU
1	C	345	ILE
1	C	376	LYS
1	C	444	ASP
1	C	455	LYS
1	C	456	THR
1	C	468	LYS
1	C	469	ASP
1	C	471	SER
1	C	473	ASN
1	C	480	SER
1	D	4	SER
1	D	7	GLU
1	D	12	LYS
1	D	13	SER
1	D	25	LYS

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Mol	Chain	Res	Type
1	D	36	LYS
1	D	49	GLN
1	D	83	ARG
1	D	87	LYS
1	D	90	ARG
1	D	92	ASP
1	D	97	THR
1	D	139	LEU
1	D	171	ILE
1	D	207	ASP
1	D	264	VAL
1	D	338	LEU
1	D	341	ASP
1	D	345	ILE
1	D	376	LYS
1	D	444	ASP
1	D	456	THR
1	D	468	LYS
1	D	469	ASP
1	D	471	SER
1	D	473	ASN
1	D	480	SER
1	E	4	SER
1	E	7	GLU
1	E	12	LYS
1	E	25	LYS
1	E	35	VAL
1	E	36	LYS
1	E	49	GLN
1	E	83	ARG
1	E	87	LYS
1	E	90	ARG
1	E	92	ASP
1	E	97	THR
1	E	139	LEU
1	E	171	ILE
1	E	207	ASP
1	E	264	VAL
1	E	338	LEU
1	E	345	ILE
1	E	376	LYS
1	E	444	ASP

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Mol	Chain	Res	Type
1	E	456	THR
1	E	468	LYS
1	E	471	SER
1	E	473	ASN
1	E	480	SER
1	F	4	SER
1	F	7	GLU
1	F	12	LYS
1	F	25	LYS
1	F	49	GLN
1	F	83	ARG
1	F	87	LYS
1	F	90	ARG
1	F	92	ASP
1	F	97	THR
1	F	139	LEU
1	F	171	ILE
1	F	207	ASP
1	F	264	VAL
1	F	338	LEU
1	F	341	ASP
1	F	345	ILE
1	F	376	LYS
1	F	444	ASP
1	F	455	LYS
1	F	456	THR
1	F	468	LYS
1	F	469	ASP
1	F	471	SER
1	F	473	ASN
1	F	480	SER
1	G	4	SER
1	G	7	GLU
1	G	25	LYS
1	G	35	VAL
1	G	36	LYS
1	G	49	GLN
1	G	83	ARG
1	G	87	LYS
1	G	90	ARG
1	G	97	THR
1	G	139	LEU

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Mol	Chain	Res	Type
1	G	171	ILE
1	G	204	LEU
1	G	207	ASP
1	G	264	VAL
1	G	338	LEU
1	G	341	ASP
1	G	345	ILE
1	G	376	LYS
1	G	444	ASP
1	G	455	LYS
1	G	456	THR
1	G	468	LYS
1	G	471	SER
1	G	473	ASN
1	G	480	SER
1	H	4	SER
1	H	7	GLU
1	H	12	LYS
1	H	14	ASP
1	H	25	LYS
1	H	36	LYS
1	H	49	GLN
1	H	83	ARG
1	H	87	LYS
1	H	90	ARG
1	H	97	THR
1	H	139	LEU
1	H	171	ILE
1	H	207	ASP
1	H	264	VAL
1	H	338	LEU
1	H	345	ILE
1	H	376	LYS
1	H	444	ASP
1	H	456	THR
1	H	468	LYS
1	H	469	ASP
1	H	471	SER
1	H	473	ASN
1	H	480	SER
2	I	21	LYS
2	I	28	THR

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Mol	Chain	Res	Type
2	I	29	LYS
2	I	59	LYS
2	I	63	SER
2	I	73	LYS
2	I	101	ASN
2	I	105	ASN
2	I	115	GLU
2	I	116	LEU
2	J	28	THR
2	J	29	LYS
2	J	55	LEU
2	J	59	LYS
2	J	63	SER
2	J	73	LYS
2	J	101	ASN
2	J	105	ASN
2	J	115	GLU
2	J	116	LEU
2	K	28	THR
2	K	29	LYS
2	K	59	LYS
2	K	63	SER
2	K	73	LYS
2	K	101	ASN
2	K	105	ASN
2	K	115	GLU
2	K	116	LEU
2	L	21	LYS
2	L	28	THR
2	L	29	LYS
2	L	55	LEU
2	L	59	LYS
2	L	63	SER
2	L	73	LYS
2	L	101	ASN
2	L	105	ASN
2	L	115	GLU
2	L	116	LEU
2	M	21	LYS
2	M	28	THR
2	M	29	LYS
2	M	59	LYS

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Mol	Chain	Res	Type
2	M	63	SER
2	M	73	LYS
2	M	101	ASN
2	M	105	ASN
2	M	115	GLU
2	M	116	LEU
2	N	28	THR
2	N	29	LYS
2	N	55	LEU
2	N	59	LYS
2	N	63	SER
2	N	73	LYS
2	N	101	ASN
2	N	115	GLU
2	N	116	LEU
2	O	28	THR
2	O	29	LYS
2	O	59	LYS
2	O	63	SER
2	O	73	LYS
2	O	101	ASN
2	O	105	ASN
2	O	115	GLU
2	O	116	LEU
2	P	28	THR
2	P	29	LYS
2	P	59	LYS
2	P	63	SER
2	P	73	LYS
2	P	101	ASN
2	P	115	GLU
2	P	116	LEU
3	i	73	TRP
3	i	76	ARG
3	k	73	TRP
3	k	76	ARG
3	j	73	TRP
3	j	76	ARG
3	l	73	TRP
3	l	76	ARG
4	h	85	GLU
4	h	89	MET

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Mol	Chain	Res	Type
4	h	91	GLN
4	g	85	GLU
4	g	89	MET
4	g	91	GLN
4	f	85	GLU
4	f	89	MET
4	f	91	GLN
4	e	85	GLU
4	e	89	MET
4	e	91	GLN
4	d	85	GLU
4	d	89	MET
4	d	91	GLN
4	c	85	GLU
4	c	89	MET
4	c	91	GLN
4	b	85	GLU
4	b	89	MET
4	b	91	GLN
4	a	85	GLU
4	a	91	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	386	HIS
1	A	392	GLN
1	A	404	GLN
1	A	461	GLN
1	B	146	HIS
1	B	301	ASN
1	B	386	HIS
1	B	392	GLN
1	B	404	GLN
1	B	461	GLN
1	C	146	HIS
1	C	301	ASN
1	C	386	HIS
1	C	392	GLN
1	C	404	GLN
1	C	461	GLN

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Mol	Chain	Res	Type
1	D	146	HIS
1	D	386	HIS
1	D	392	GLN
1	D	404	GLN
1	D	461	GLN
1	E	146	HIS
1	E	301	ASN
1	E	386	HIS
1	E	404	GLN
1	F	146	HIS
1	F	301	ASN
1	F	386	HIS
1	F	404	GLN
1	G	146	HIS
1	G	301	ASN
1	G	386	HIS
1	G	392	GLN
1	G	404	GLN
1	H	146	HIS
1	H	301	ASN
1	H	386	HIS
1	H	404	GLN
2	I	101	ASN
2	I	114	GLN
2	J	101	ASN
2	J	114	GLN
2	J	133	ASN
2	K	101	ASN
2	K	114	GLN
2	L	101	ASN
2	L	114	GLN
2	L	133	ASN
2	M	101	ASN
2	M	114	GLN
2	N	101	ASN
2	N	114	GLN
2	N	133	ASN
2	O	101	ASN
2	O	114	GLN
2	P	101	ASN
2	P	114	GLN
2	P	133	ASN

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Mol	Chain	Res	Type
4	h	91	GLN
4	g	90	ASN
4	g	91	GLN
4	f	91	GLN
4	e	90	ASN
4	e	91	GLN
4	d	91	GLN
4	c	91	GLN
4	b	91	GLN
4	a	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

64 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
1	KCX	G	205	1	10,11,12	2.07	1 (10%)	6,12,14	3.06	1 (16%)
1	LYO	A	150	1	7,9,10	0.68	0	7,10,12	1.31	1 (14%)
1	HYP	G	48	1	7,8,9	0.49	0	5,10,12	1.19	1 (20%)
1	HYP	E	48	1	7,8,9	0.49	0	5,10,12	1.20	1 (20%)
1	KCX	H	205	1	10,11,12	0.49	0	6,12,14	0.27	0
1	HLU	F	174	1	7,8,9	0.59	0	7,10,12	1.78	2 (28%)
1	KCX	F	205	1	10,11,12	0.50	0	6,12,14	0.26	0
1	HYP	A	155	1	7,8,9	0.42	0	5,10,12	1.17	1 (20%)
1	M3L	D	346	1	10,11,12	0.45	0	9,14,16	0.13	0
1	LYO	F	198	1	7,9,10	0.72	0	7,10,12	0.96	0
1	LYO	B	198	1	7,9,10	0.72	0	7,10,12	0.97	0
1	HLU	A	174	1	7,8,9	0.60	0	7,10,12	1.78	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	G	155	1	7,8,9	0.42	0	5,10,12	1.18	1 (20%)
1	LYO	D	150	1	7,9,10	0.68	0	7,10,12	1.30	1 (14%)
1	LYO	A	198	1	7,9,10	0.72	0	7,10,12	0.97	0
1	M3L	E	346	1	10,11,12	0.45	0	9,14,16	0.13	0
1	CSO	E	109	1	3,6,7	0.83	0	1,6,8	0.53	0
1	CSO	G	109	1	3,6,7	0.82	0	1,6,8	0.54	0
1	LYO	G	150	1	7,9,10	0.68	0	7,10,12	1.29	1 (14%)
1	HYP	D	155	1	7,8,9	0.41	0	5,10,12	1.16	1 (20%)
1	KCX	C	205	1	10,11,12	2.09	1 (10%)	6,12,14	3.07	1 (16%)
1	HLU	C	174	1	7,8,9	0.58	0	7,10,12	1.72	2 (28%)
1	CSO	D	109	1	3,6,7	0.83	0	1,6,8	0.55	0
1	HYP	B	155	1	7,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	F	48	1	7,8,9	0.48	0	5,10,12	1.19	1 (20%)
1	LYO	H	150	1	7,9,10	0.68	0	7,10,12	1.29	1 (14%)
1	LYO	G	198	1	7,9,10	0.72	0	7,10,12	0.97	0
1	LYO	C	150	1	7,9,10	0.68	0	7,10,12	1.29	1 (14%)
1	HLU	D	174	1	7,8,9	0.58	0	7,10,12	1.78	2 (28%)
1	HYP	A	48	1	7,8,9	0.49	0	5,10,12	1.18	1 (20%)
1	HYP	F	155	1	7,8,9	0.41	0	5,10,12	1.16	1 (20%)
1	KCX	E	205	1	10,11,12	2.08	1 (10%)	6,12,14	3.05	1 (16%)
1	HYP	C	48	1	7,8,9	0.48	0	5,10,12	1.20	1 (20%)
1	CSO	F	109	1	3,6,7	0.82	0	1,6,8	0.54	0
1	M3L	F	346	1	10,11,12	0.46	0	9,14,16	0.13	0
1	CSO	B	109	1	3,6,7	0.82	0	1,6,8	0.55	0
1	M3L	B	346	1	10,11,12	0.45	0	9,14,16	0.13	0
1	HLU	H	174	1	7,8,9	0.58	0	7,10,12	1.78	2 (28%)
1	CSO	A	109	1	3,6,7	0.82	0	1,6,8	0.54	0
1	KCX	D	205	1	10,11,12	0.50	0	6,12,14	0.28	0
1	HYP	D	48	1	7,8,9	0.49	0	5,10,12	1.19	1 (20%)
1	M3L	A	346	1	10,11,12	0.46	0	9,14,16	0.14	0
1	HLU	B	174	1	7,8,9	0.59	0	7,10,12	1.78	2 (28%)
1	LYO	E	150	1	7,9,10	0.69	0	7,10,12	1.31	1 (14%)
1	LYO	H	198	1	7,9,10	0.72	0	7,10,12	0.97	0
1	HYP	C	155	1	7,8,9	0.42	0	5,10,12	1.18	1 (20%)
1	CSO	C	109	1	3,6,7	0.83	0	1,6,8	0.54	0
1	M3L	C	346	1	10,11,12	0.46	0	9,14,16	0.14	0
1	HYP	E	155	1	7,8,9	0.40	0	5,10,12	1.16	1 (20%)
1	M3L	G	346	1	10,11,12	0.46	0	9,14,16	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	H	48	1	7,8,9	0.49	0	5,10,12	1.19	1 (20%)
1	LYO	C	198	1	7,9,10	0.72	0	7,10,12	0.95	0
1	KCX	B	205	1	10,11,12	0.50	0	6,12,14	0.26	0
1	HYP	B	48	1	7,8,9	0.48	0	5,10,12	1.19	1 (20%)
1	HLU	G	174	1	7,8,9	0.60	0	7,10,12	1.78	2 (28%)
1	HLU	E	174	1	7,8,9	0.58	0	7,10,12	1.78	2 (28%)
1	LYO	E	198	1	7,9,10	0.71	0	7,10,12	0.96	0
1	KCX	A	205	1	10,11,12	2.07	1 (10%)	6,12,14	3.06	1 (16%)
1	M3L	H	346	1	10,11,12	0.45	0	9,14,16	0.14	0
1	LYO	B	150	1	7,9,10	0.67	0	7,10,12	1.31	1 (14%)
1	LYO	F	150	1	7,9,10	0.68	0	7,10,12	1.31	1 (14%)
1	HYP	H	155	1	7,8,9	0.41	0	5,10,12	1.16	1 (20%)
1	LYO	D	198	1	7,9,10	0.72	0	7,10,12	0.96	0
1	CSO	H	109	1	3,6,7	0.82	0	1,6,8	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	G	205	1	-	1/9/10/12	-
1	LYO	A	150	1	-	2/8/9/11	-
1	HYP	G	48	1	-	0/0/11/13	0/1/1/1
1	HYP	E	48	1	-	0/0/11/13	0/1/1/1
1	KCX	H	205	1	-	1/9/10/12	-
1	HLU	F	174	1	-	5/9/10/12	-
1	KCX	F	205	1	-	1/9/10/12	-
1	HYP	A	155	1	-	0/0/11/13	0/1/1/1
1	M3L	D	346	1	-	6/9/10/12	-
1	LYO	F	198	1	-	2/8/9/11	-
1	LYO	B	198	1	-	2/8/9/11	-
1	HLU	A	174	1	-	5/9/10/12	-
1	HYP	G	155	1	-	0/0/11/13	0/1/1/1
1	LYO	D	150	1	-	2/8/9/11	-
1	LYO	A	198	1	-	2/8/9/11	-
1	M3L	E	346	1	-	6/9/10/12	-
1	CSO	E	109	1	-	0/1/5/7	-
1	CSO	G	109	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYO	G	150	1	-	2/8/9/11	-
1	HYP	D	155	1	-	0/0/11/13	0/1/1/1
1	KCX	C	205	1	-	1/9/10/12	-
1	HLU	C	174	1	-	5/9/10/12	-
1	CSO	D	109	1	-	0/1/5/7	-
1	HYP	B	155	1	-	0/0/11/13	0/1/1/1
1	HYP	F	48	1	-	0/0/11/13	0/1/1/1
1	LYO	H	150	1	-	2/8/9/11	-
1	LYO	G	198	1	-	2/8/9/11	-
1	LYO	C	150	1	-	2/8/9/11	-
1	HLU	D	174	1	-	5/9/10/12	-
1	HYP	A	48	1	-	0/0/11/13	0/1/1/1
1	HYP	F	155	1	-	0/0/11/13	0/1/1/1
1	KCX	E	205	1	-	1/9/10/12	-
1	HYP	C	48	1	-	0/0/11/13	0/1/1/1
1	CSO	F	109	1	-	0/1/5/7	-
1	M3L	F	346	1	-	6/9/10/12	-
1	CSO	B	109	1	-	0/1/5/7	-
1	M3L	B	346	1	-	6/9/10/12	-
1	HLU	H	174	1	-	5/9/10/12	-
1	CSO	A	109	1	-	0/1/5/7	-
1	KCX	D	205	1	-	1/9/10/12	-
1	HYP	D	48	1	-	0/0/11/13	0/1/1/1
1	M3L	A	346	1	-	6/9/10/12	-
1	HLU	B	174	1	-	5/9/10/12	-
1	LYO	E	150	1	-	2/8/9/11	-
1	LYO	H	198	1	-	2/8/9/11	-
1	HYP	C	155	1	-	0/0/11/13	0/1/1/1
1	CSO	C	109	1	-	0/1/5/7	-
1	M3L	C	346	1	-	6/9/10/12	-
1	HYP	E	155	1	-	0/0/11/13	0/1/1/1
1	M3L	G	346	1	-	6/9/10/12	-
1	HYP	H	48	1	-	0/0/11/13	0/1/1/1
1	LYO	C	198	1	-	2/8/9/11	-
1	KCX	B	205	1	-	1/9/10/12	-
1	HYP	B	48	1	-	0/0/11/13	0/1/1/1
1	HLU	G	174	1	-	5/9/10/12	-
1	HLU	E	174	1	-	5/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYO	E	198	1	-	2/8/9/11	-
1	KCX	A	205	1	-	1/9/10/12	-
1	M3L	H	346	1	-	6/9/10/12	-
1	LYO	B	150	1	-	2/8/9/11	-
1	LYO	F	150	1	-	2/8/9/11	-
1	HYP	H	155	1	-	0/0/11/13	0/1/1/1
1	LYO	D	198	1	-	2/8/9/11	-
1	CSO	H	109	1	-	0/1/5/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	205	KCX	OQ1-CX	6.24	1.33	1.21
1	E	205	KCX	OQ1-CX	6.21	1.33	1.21
1	G	205	KCX	OQ1-CX	6.18	1.33	1.21
1	A	205	KCX	OQ1-CX	6.16	1.33	1.21

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	KCX	OQ1-CX-NZ	-7.51	113.51	124.92
1	A	205	KCX	OQ1-CX-NZ	-7.50	113.53	124.92
1	G	205	KCX	OQ1-CX-NZ	-7.50	113.53	124.92
1	E	205	KCX	OQ1-CX-NZ	-7.48	113.56	124.92
1	H	174	HLU	CD2-CG-CB	-2.95	106.42	111.23
1	B	174	HLU	CD2-CG-CB	-2.94	106.44	111.23
1	G	174	HLU	CD2-CG-CB	-2.93	106.44	111.23
1	A	174	HLU	CD2-CG-CB	-2.93	106.45	111.23
1	D	174	HLU	CD2-CG-CB	-2.92	106.46	111.23
1	E	174	HLU	CD2-CG-CB	-2.92	106.46	111.23
1	F	174	HLU	CD2-CG-CB	-2.92	106.47	111.23
1	C	174	HLU	CD2-CG-CB	-2.80	106.66	111.23
1	A	150	LYO	CB-CA-C	-2.68	106.87	110.99
1	B	150	LYO	CB-CA-C	-2.68	106.87	110.99
1	F	150	LYO	CB-CA-C	-2.68	106.87	110.99
1	E	150	LYO	CB-CA-C	-2.67	106.88	110.99
1	F	174	HLU	CG-CB-CA	2.66	119.20	113.61
1	D	150	LYO	CB-CA-C	-2.66	106.90	110.99
1	D	174	HLU	CG-CB-CA	2.65	119.17	113.61
1	E	174	HLU	CG-CB-CA	2.65	119.17	113.61
1	G	150	LYO	CB-CA-C	-2.65	106.92	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	150	LYO	CB-CA-C	-2.65	106.92	110.99
1	G	174	HLU	CG-CB-CA	2.64	119.16	113.61
1	A	174	HLU	CG-CB-CA	2.64	119.15	113.61
1	H	174	HLU	CG-CB-CA	2.64	119.15	113.61
1	B	174	HLU	CG-CB-CA	2.64	119.14	113.61
1	C	150	LYO	CB-CA-C	-2.63	106.94	110.99
1	C	48	HYP	O-C-CA	-2.54	118.23	124.77
1	E	48	HYP	O-C-CA	-2.54	118.25	124.77
1	D	48	HYP	O-C-CA	-2.53	118.27	124.77
1	H	48	HYP	O-C-CA	-2.53	118.28	124.77
1	C	174	HLU	CG-CB-CA	2.52	118.90	113.61
1	F	48	HYP	O-C-CA	-2.52	118.29	124.77
1	B	48	HYP	O-C-CA	-2.52	118.29	124.77
1	A	48	HYP	O-C-CA	-2.51	118.31	124.77
1	G	48	HYP	O-C-CA	-2.51	118.31	124.77
1	A	155	HYP	O-C-CA	-2.51	118.32	124.77
1	C	155	HYP	O-C-CA	-2.51	118.32	124.77
1	G	155	HYP	O-C-CA	-2.51	118.32	124.77
1	D	155	HYP	O-C-CA	-2.48	118.39	124.77
1	B	155	HYP	O-C-CA	-2.48	118.39	124.77
1	E	155	HYP	O-C-CA	-2.48	118.39	124.77
1	F	155	HYP	O-C-CA	-2.48	118.39	124.77
1	H	155	HYP	O-C-CA	-2.48	118.40	124.77

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	150	LYO	N-CA-CB-CG
1	A	150	LYO	CG-CD-CE-NZ
1	A	174	HLU	N-CA-CB-CG
1	A	174	HLU	C-CA-CB-CG
1	A	174	HLU	O-C-CA-CB
1	A	198	LYO	CG-CD-CE-NZ
1	B	150	LYO	N-CA-CB-CG
1	B	150	LYO	CG-CD-CE-NZ
1	B	174	HLU	N-CA-CB-CG
1	B	174	HLU	C-CA-CB-CG
1	B	174	HLU	O-C-CA-CB
1	B	198	LYO	CG-CD-CE-NZ
1	C	150	LYO	N-CA-CB-CG
1	C	150	LYO	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	C	174	HLU	N-CA-CB-CG
1	C	174	HLU	C-CA-CB-CG
1	C	174	HLU	O-C-CA-CB
1	C	198	LYO	CG-CD-CE-NZ
1	D	150	LYO	N-CA-CB-CG
1	D	150	LYO	CG-CD-CE-NZ
1	D	174	HLU	N-CA-CB-CG
1	D	174	HLU	C-CA-CB-CG
1	D	174	HLU	O-C-CA-CB
1	D	198	LYO	CE-CD-CG-OG
1	D	198	LYO	CG-CD-CE-NZ
1	E	150	LYO	N-CA-CB-CG
1	E	150	LYO	CG-CD-CE-NZ
1	E	174	HLU	N-CA-CB-CG
1	E	174	HLU	C-CA-CB-CG
1	E	174	HLU	O-C-CA-CB
1	E	198	LYO	CG-CD-CE-NZ
1	F	150	LYO	N-CA-CB-CG
1	F	150	LYO	CG-CD-CE-NZ
1	F	174	HLU	N-CA-CB-CG
1	F	174	HLU	C-CA-CB-CG
1	F	174	HLU	O-C-CA-CB
1	F	198	LYO	CG-CD-CE-NZ
1	G	150	LYO	N-CA-CB-CG
1	G	150	LYO	CG-CD-CE-NZ
1	G	174	HLU	N-CA-CB-CG
1	G	174	HLU	C-CA-CB-CG
1	G	174	HLU	O-C-CA-CB
1	G	198	LYO	CG-CD-CE-NZ
1	H	150	LYO	N-CA-CB-CG
1	H	150	LYO	CG-CD-CE-NZ
1	H	174	HLU	N-CA-CB-CG
1	H	174	HLU	C-CA-CB-CG
1	H	174	HLU	O-C-CA-CB
1	H	198	LYO	CG-CD-CE-NZ
1	A	346	M3L	CG-CD-CE-NZ
1	B	346	M3L	CG-CD-CE-NZ
1	C	346	M3L	CG-CD-CE-NZ
1	D	346	M3L	CG-CD-CE-NZ
1	E	346	M3L	CG-CD-CE-NZ
1	F	346	M3L	CG-CD-CE-NZ
1	G	346	M3L	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	H	346	M3L	CG-CD-CE-NZ
1	A	205	KCX	CG-CD-CE-NZ
1	B	205	KCX	CG-CD-CE-NZ
1	C	205	KCX	CG-CD-CE-NZ
1	D	205	KCX	CG-CD-CE-NZ
1	E	205	KCX	CG-CD-CE-NZ
1	F	205	KCX	CG-CD-CE-NZ
1	H	205	KCX	CG-CD-CE-NZ
1	G	205	KCX	CG-CD-CE-NZ
1	A	174	HLU	C-CA-CB-OH
1	B	174	HLU	C-CA-CB-OH
1	C	174	HLU	C-CA-CB-OH
1	D	174	HLU	C-CA-CB-OH
1	E	174	HLU	C-CA-CB-OH
1	F	174	HLU	C-CA-CB-OH
1	G	174	HLU	C-CA-CB-OH
1	H	174	HLU	C-CA-CB-OH
1	A	346	M3L	CE-CD-CG-CB
1	C	346	M3L	CE-CD-CG-CB
1	D	346	M3L	CE-CD-CG-CB
1	E	346	M3L	CE-CD-CG-CB
1	H	346	M3L	CE-CD-CG-CB
1	F	346	M3L	CE-CD-CG-CB
1	G	346	M3L	CE-CD-CG-CB
1	B	346	M3L	CE-CD-CG-CB
1	F	346	M3L	CA-CB-CG-CD
1	A	346	M3L	CD-CE-NZ-CM1
1	B	346	M3L	CD-CE-NZ-CM1
1	C	346	M3L	CD-CE-NZ-CM1
1	D	346	M3L	CD-CE-NZ-CM1
1	E	346	M3L	CD-CE-NZ-CM1
1	F	346	M3L	CD-CE-NZ-CM1
1	G	346	M3L	CD-CE-NZ-CM1
1	H	346	M3L	CD-CE-NZ-CM1
1	A	346	M3L	CA-CB-CG-CD
1	A	346	M3L	CD-CE-NZ-CM2
1	B	346	M3L	CD-CE-NZ-CM2
1	C	346	M3L	CD-CE-NZ-CM2
1	D	346	M3L	CD-CE-NZ-CM2
1	E	346	M3L	CD-CE-NZ-CM2
1	F	346	M3L	CD-CE-NZ-CM2
1	G	346	M3L	CD-CE-NZ-CM2

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Mol	Chain	Res	Type	Atoms
1	H	346	M3L	CD-CE-NZ-CM2
1	C	346	M3L	CA-CB-CG-CD
1	G	346	M3L	CA-CB-CG-CD
1	H	346	M3L	CA-CB-CG-CD
1	B	346	M3L	CA-CB-CG-CD
1	D	346	M3L	CA-CB-CG-CD
1	E	346	M3L	CA-CB-CG-CD
1	A	346	M3L	CD-CE-NZ-CM3
1	B	346	M3L	CD-CE-NZ-CM3
1	C	346	M3L	CD-CE-NZ-CM3
1	D	346	M3L	CD-CE-NZ-CM3
1	E	346	M3L	CD-CE-NZ-CM3
1	F	346	M3L	CD-CE-NZ-CM3
1	G	346	M3L	CD-CE-NZ-CM3
1	H	346	M3L	CD-CE-NZ-CM3
1	B	198	LYO	CE-CD-CG-OG
1	C	198	LYO	CE-CD-CG-OG
1	E	198	LYO	CE-CD-CG-OG
1	G	198	LYO	CE-CD-CG-OG
1	H	198	LYO	CE-CD-CG-OG
1	A	198	LYO	CE-CD-CG-OG
1	F	198	LYO	CE-CD-CG-OG
1	A	174	HLU	N-CA-CB-OH
1	B	174	HLU	N-CA-CB-OH
1	C	174	HLU	N-CA-CB-OH
1	D	174	HLU	N-CA-CB-OH
1	E	174	HLU	N-CA-CB-OH
1	F	174	HLU	N-CA-CB-OH
1	G	174	HLU	N-CA-CB-OH
1	H	174	HLU	N-CA-CB-OH

There are no ring outliers.

14 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	150	LYO	1	0
1	D	346	M3L	1	0
1	D	150	LYO	1	0
1	E	346	M3L	1	0
1	G	150	LYO	1	0
1	H	150	LYO	1	0
1	C	150	LYO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	346	M3L	1	0
1	A	346	M3L	1	0
1	E	150	LYO	1	0
1	C	346	M3L	1	0
1	H	346	M3L	1	0
1	B	150	LYO	1	0
1	F	150	LYO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands 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	$\# Z > 2$
5	CAP	A	501	-	18,20,20	0.85	0	23,31,31	1.14	1 (4%)
5	CAP	H	501	-	18,20,20	0.85	0	23,31,31	1.22	1 (4%)
5	CAP	C	501	-	18,20,20	0.86	0	23,31,31	1.13	1 (4%)
5	CAP	E	501	-	18,20,20	0.86	0	23,31,31	1.14	1 (4%)
5	CAP	G	501	-	18,20,20	0.87	0	23,31,31	1.14	1 (4%)
5	CAP	F	501	-	18,20,20	0.85	0	23,31,31	1.22	1 (4%)
5	CAP	B	501	-	18,20,20	0.84	0	23,31,31	1.22	1 (4%)
5	CAP	D	501	-	18,20,20	0.84	0	23,31,31	1.22	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CAP	A	501	-	-	15/29/29/29	-
5	CAP	H	501	-	-	14/29/29/29	-
5	CAP	C	501	-	-	15/29/29/29	-
5	CAP	E	501	-	-	15/29/29/29	-
5	CAP	G	501	-	-	15/29/29/29	-
5	CAP	F	501	-	-	14/29/29/29	-
5	CAP	B	501	-	-	14/29/29/29	-
5	CAP	D	501	-	-	14/29/29/29	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	CAP	O7-C-C2	4.05	120.84	114.06
5	F	501	CAP	O7-C-C2	4.03	120.80	114.06
5	B	501	CAP	O7-C-C2	4.02	120.80	114.06
5	D	501	CAP	O7-C-C2	4.02	120.80	114.06
5	A	501	CAP	O7-C-C2	3.59	120.06	114.06
5	C	501	CAP	O7-C-C2	3.58	120.06	114.06
5	E	501	CAP	O7-C-C2	3.58	120.06	114.06
5	G	501	CAP	O7-C-C2	3.58	120.06	114.06

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	CAP	O1-C1-C2-C3
5	A	501	CAP	O1-C1-C2-C
5	A	501	CAP	O1-C1-C2-O2
5	A	501	CAP	O7-C-C2-C1
5	A	501	CAP	O6-C-C2-O2
5	A	501	CAP	O7-C-C2-O2
5	A	501	CAP	C2-C3-C4-O4
5	A	501	CAP	O3-C3-C4-O4
5	A	501	CAP	C1-O1-P1-O2P
5	A	501	CAP	C1-O1-P1-O3P
5	B	501	CAP	O1-C1-C2-C3
5	B	501	CAP	O1-C1-C2-C
5	B	501	CAP	O1-C1-C2-O2
5	B	501	CAP	O6-C-C2-C1

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Mol	Chain	Res	Type	Atoms
5	B	501	CAP	O7-C-C2-C1
5	B	501	CAP	O6-C-C2-O2
5	B	501	CAP	O7-C-C2-O2
5	B	501	CAP	C2-C3-C4-O4
5	B	501	CAP	O3-C3-C4-O4
5	B	501	CAP	C1-O1-P1-O2P
5	B	501	CAP	C1-O1-P1-O3P
5	C	501	CAP	O1-C1-C2-C3
5	C	501	CAP	O1-C1-C2-C
5	C	501	CAP	O1-C1-C2-O2
5	C	501	CAP	O7-C-C2-C1
5	C	501	CAP	O6-C-C2-O2
5	C	501	CAP	O7-C-C2-O2
5	C	501	CAP	C2-C3-C4-O4
5	C	501	CAP	O3-C3-C4-O4
5	C	501	CAP	C1-O1-P1-O2P
5	C	501	CAP	C1-O1-P1-O3P
5	D	501	CAP	O1-C1-C2-C3
5	D	501	CAP	O1-C1-C2-C
5	D	501	CAP	O1-C1-C2-O2
5	D	501	CAP	O6-C-C2-C1
5	D	501	CAP	O7-C-C2-C1
5	D	501	CAP	O6-C-C2-O2
5	D	501	CAP	O7-C-C2-O2
5	D	501	CAP	C2-C3-C4-O4
5	D	501	CAP	O3-C3-C4-O4
5	D	501	CAP	C1-O1-P1-O2P
5	D	501	CAP	C1-O1-P1-O3P
5	E	501	CAP	O1-C1-C2-C3
5	E	501	CAP	O1-C1-C2-C
5	E	501	CAP	O1-C1-C2-O2
5	E	501	CAP	O7-C-C2-C1
5	E	501	CAP	O6-C-C2-O2
5	E	501	CAP	O7-C-C2-O2
5	E	501	CAP	C2-C3-C4-O4
5	E	501	CAP	O3-C3-C4-O4
5	E	501	CAP	C1-O1-P1-O2P
5	E	501	CAP	C1-O1-P1-O3P
5	F	501	CAP	O1-C1-C2-C3
5	F	501	CAP	O1-C1-C2-C
5	F	501	CAP	O1-C1-C2-O2
5	F	501	CAP	O6-C-C2-C1

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Mol	Chain	Res	Type	Atoms
5	F	501	CAP	O7-C-C2-C1
5	F	501	CAP	O6-C-C2-O2
5	F	501	CAP	O7-C-C2-O2
5	F	501	CAP	C2-C3-C4-O4
5	F	501	CAP	O3-C3-C4-O4
5	F	501	CAP	C1-O1-P1-O2P
5	F	501	CAP	C1-O1-P1-O3P
5	G	501	CAP	O1-C1-C2-C3
5	G	501	CAP	O1-C1-C2-C
5	G	501	CAP	O1-C1-C2-O2
5	G	501	CAP	O7-C-C2-C1
5	G	501	CAP	O6-C-C2-O2
5	G	501	CAP	O7-C-C2-O2
5	G	501	CAP	C2-C3-C4-O4
5	G	501	CAP	O3-C3-C4-O4
5	G	501	CAP	C1-O1-P1-O2P
5	G	501	CAP	C1-O1-P1-O3P
5	H	501	CAP	O1-C1-C2-C3
5	H	501	CAP	O1-C1-C2-C
5	H	501	CAP	O1-C1-C2-O2
5	H	501	CAP	O6-C-C2-C1
5	H	501	CAP	O7-C-C2-C1
5	H	501	CAP	O6-C-C2-O2
5	H	501	CAP	O7-C-C2-O2
5	H	501	CAP	C2-C3-C4-O4
5	H	501	CAP	O3-C3-C4-O4
5	H	501	CAP	C1-O1-P1-O2P
5	H	501	CAP	C1-O1-P1-O3P
5	B	501	CAP	C1-O1-P1-O1P
5	D	501	CAP	C1-O1-P1-O1P
5	F	501	CAP	C1-O1-P1-O1P
5	H	501	CAP	C1-O1-P1-O1P
5	A	501	CAP	O6-C-C2-C1
5	C	501	CAP	O6-C-C2-C1
5	E	501	CAP	O6-C-C2-C1
5	G	501	CAP	O6-C-C2-C1
5	A	501	CAP	O2-C2-C3-C4
5	B	501	CAP	O2-C2-C3-C4
5	C	501	CAP	O2-C2-C3-C4
5	D	501	CAP	O2-C2-C3-C4
5	E	501	CAP	O2-C2-C3-C4
5	F	501	CAP	O2-C2-C3-C4

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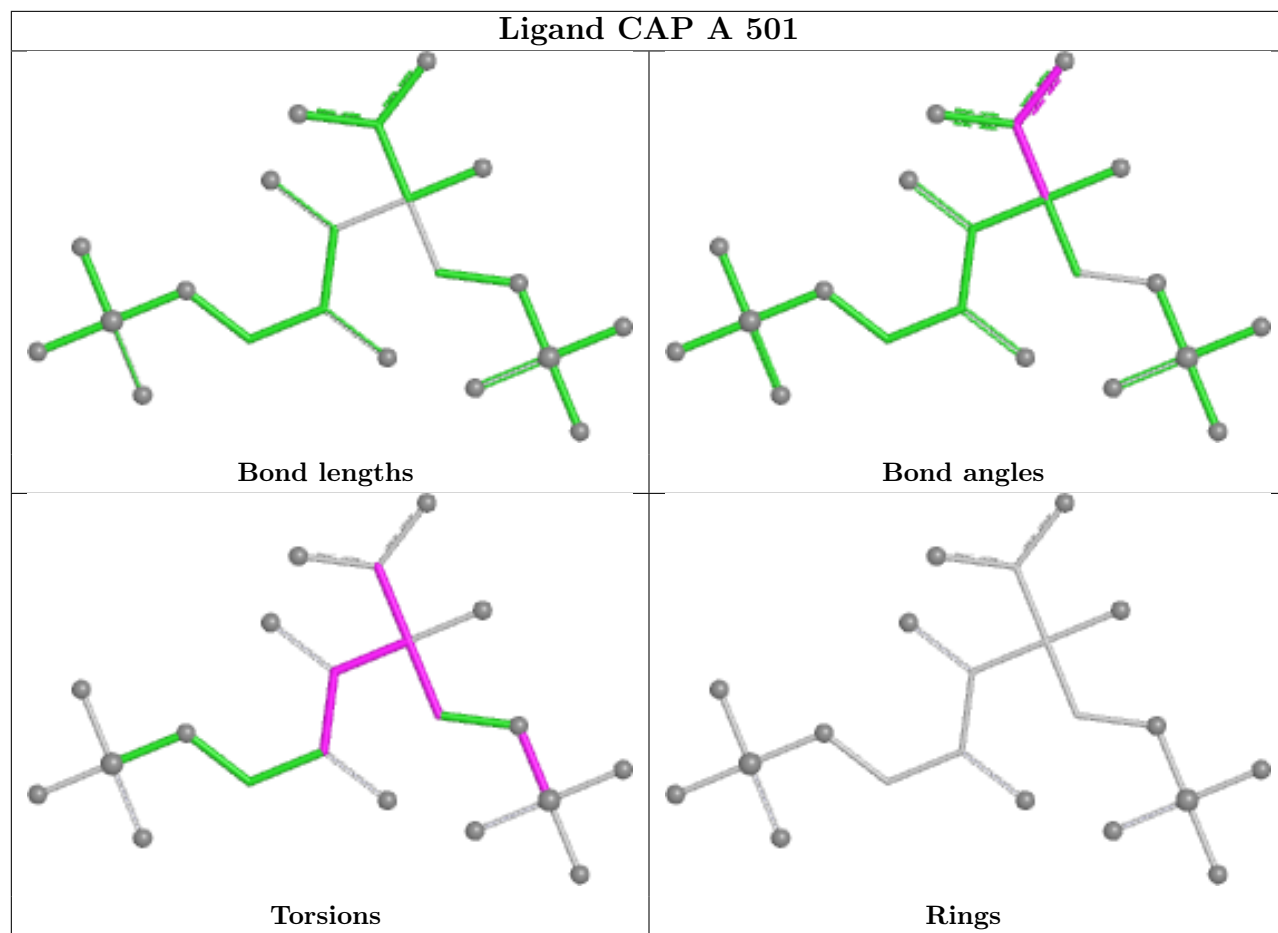
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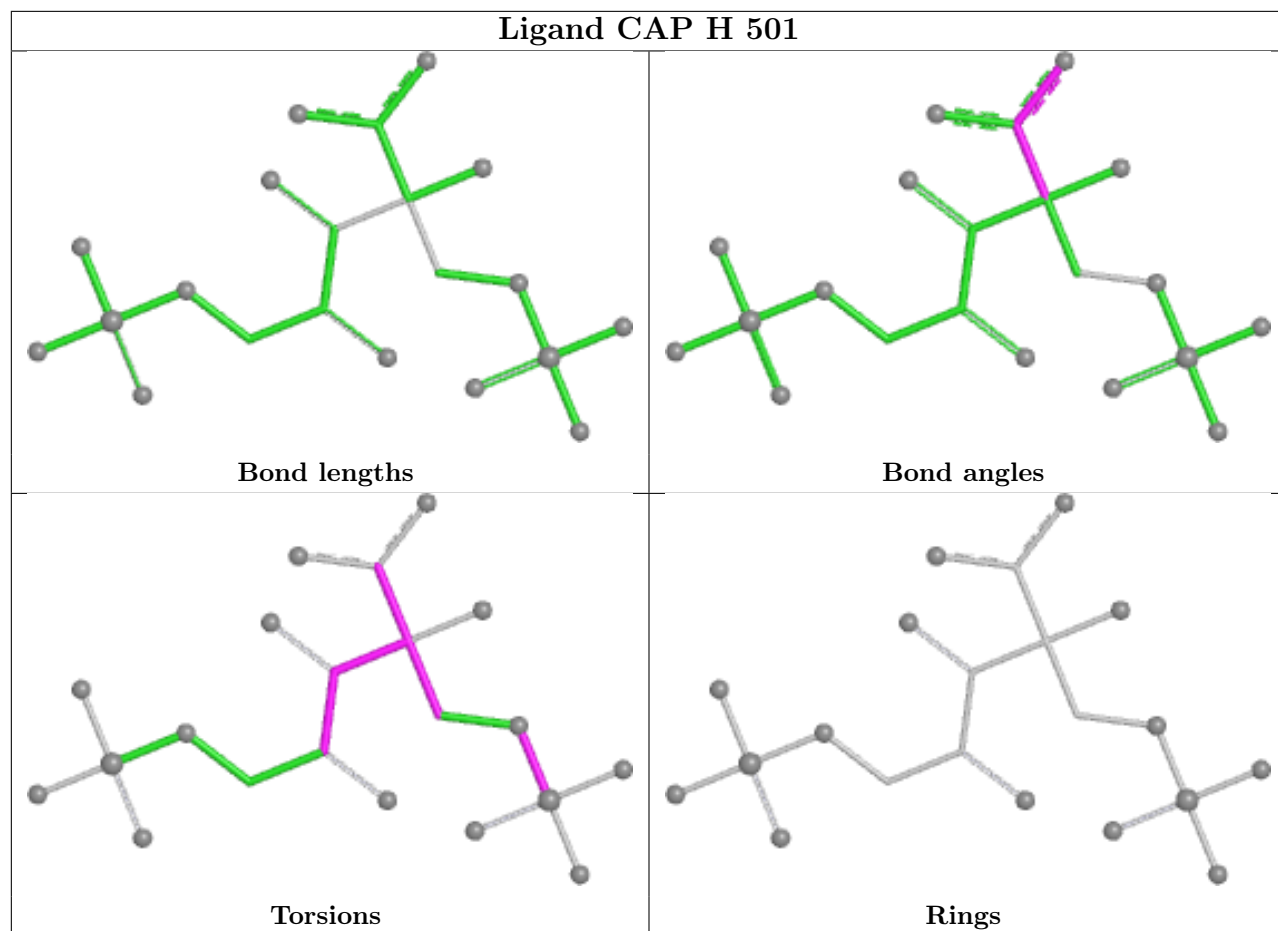
Mol	Chain	Res	Type	Atoms
5	G	501	CAP	O2-C2-C3-C4
5	H	501	CAP	O2-C2-C3-C4
5	A	501	CAP	O6-C-C2-C3
5	C	501	CAP	O6-C-C2-C3
5	E	501	CAP	O6-C-C2-C3
5	G	501	CAP	O6-C-C2-C3
5	A	501	CAP	C1-O1-P1-O1P
5	C	501	CAP	C1-O1-P1-O1P
5	E	501	CAP	C1-O1-P1-O1P
5	G	501	CAP	C1-O1-P1-O1P
5	A	501	CAP	C2-C3-C4-C5
5	B	501	CAP	C2-C3-C4-C5
5	C	501	CAP	C2-C3-C4-C5
5	D	501	CAP	C2-C3-C4-C5
5	E	501	CAP	C2-C3-C4-C5
5	F	501	CAP	C2-C3-C4-C5
5	G	501	CAP	C2-C3-C4-C5
5	H	501	CAP	C2-C3-C4-C5

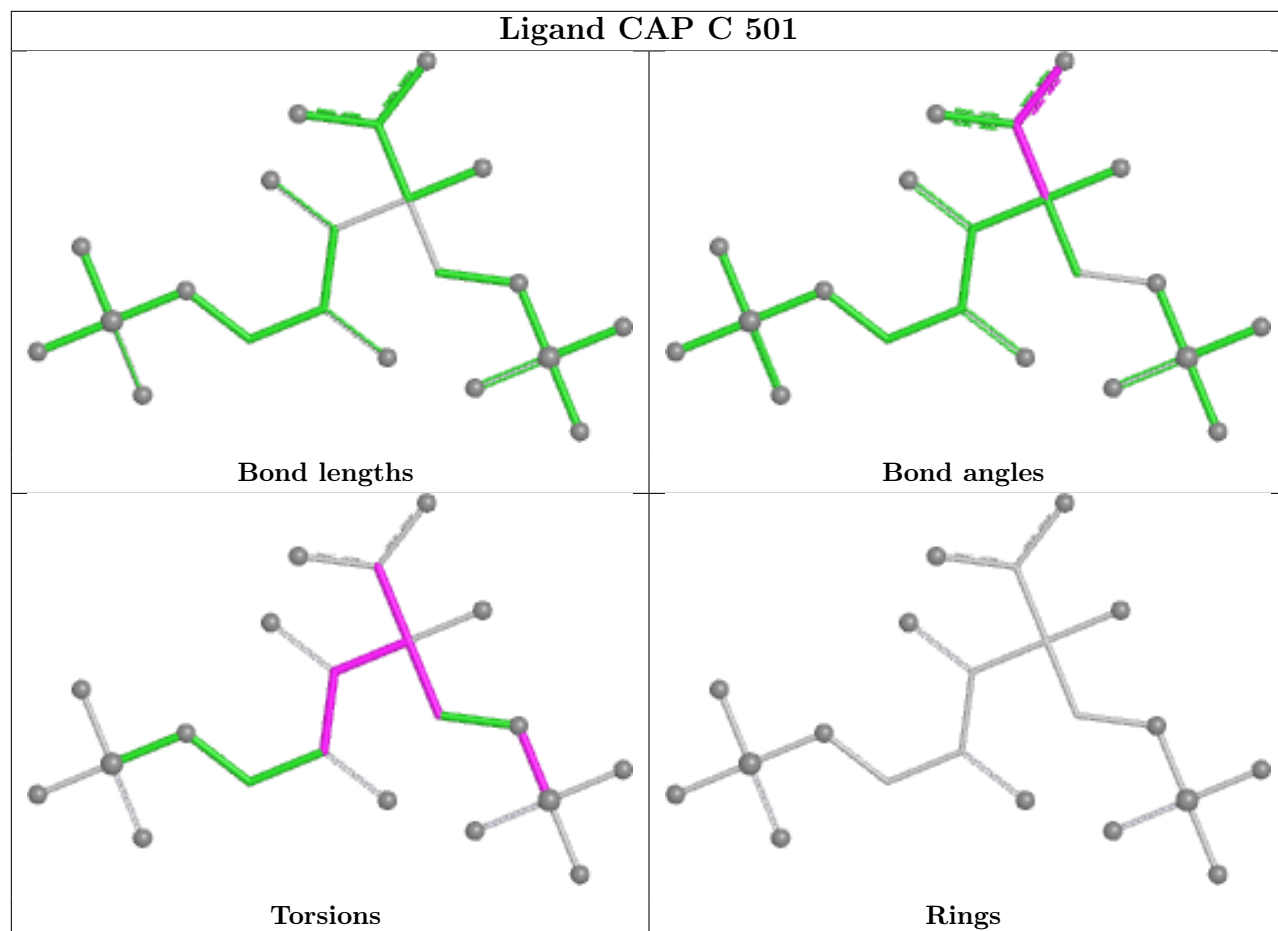
There are no ring outliers.

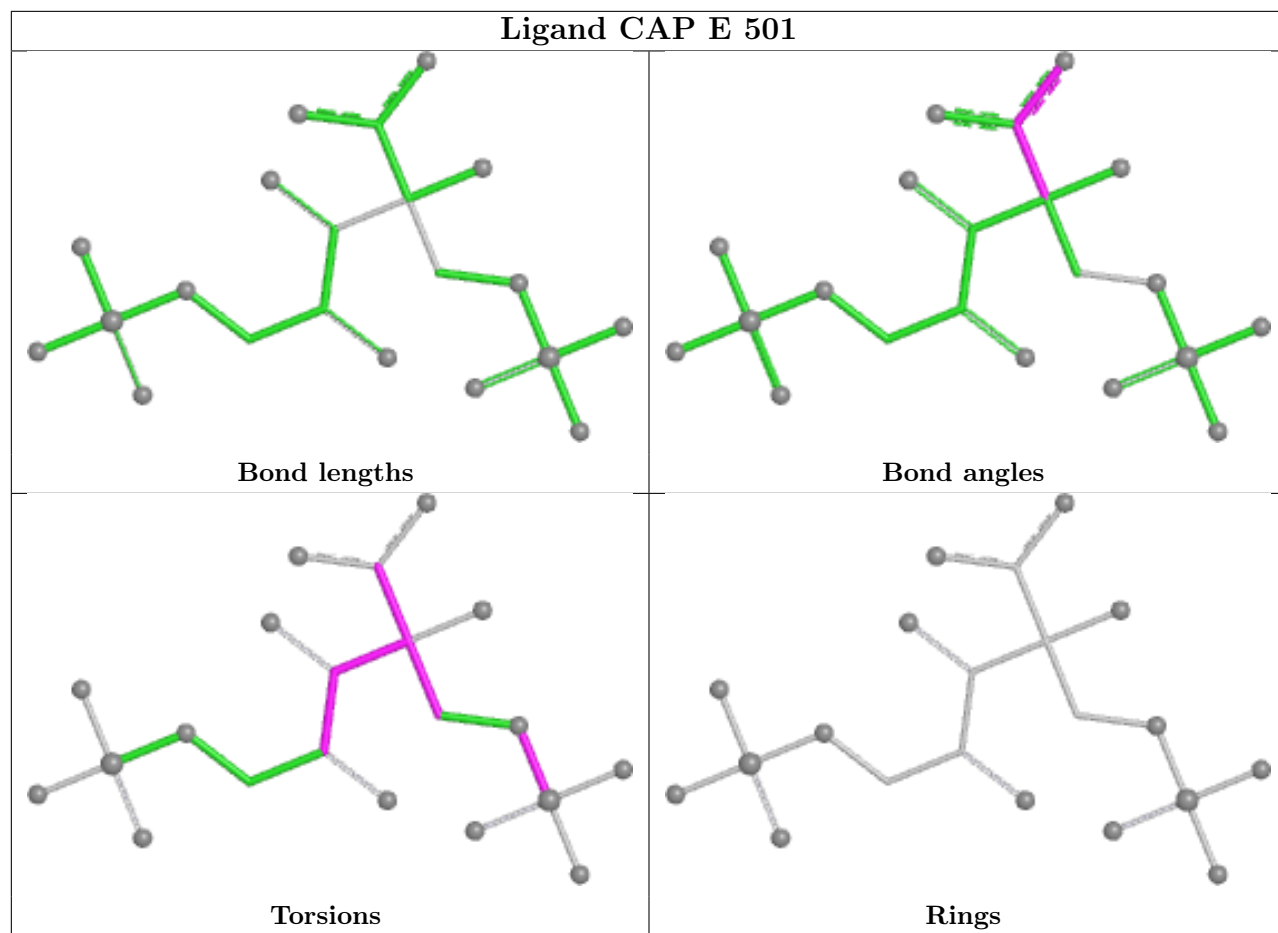
No monomer is involved in short contacts.

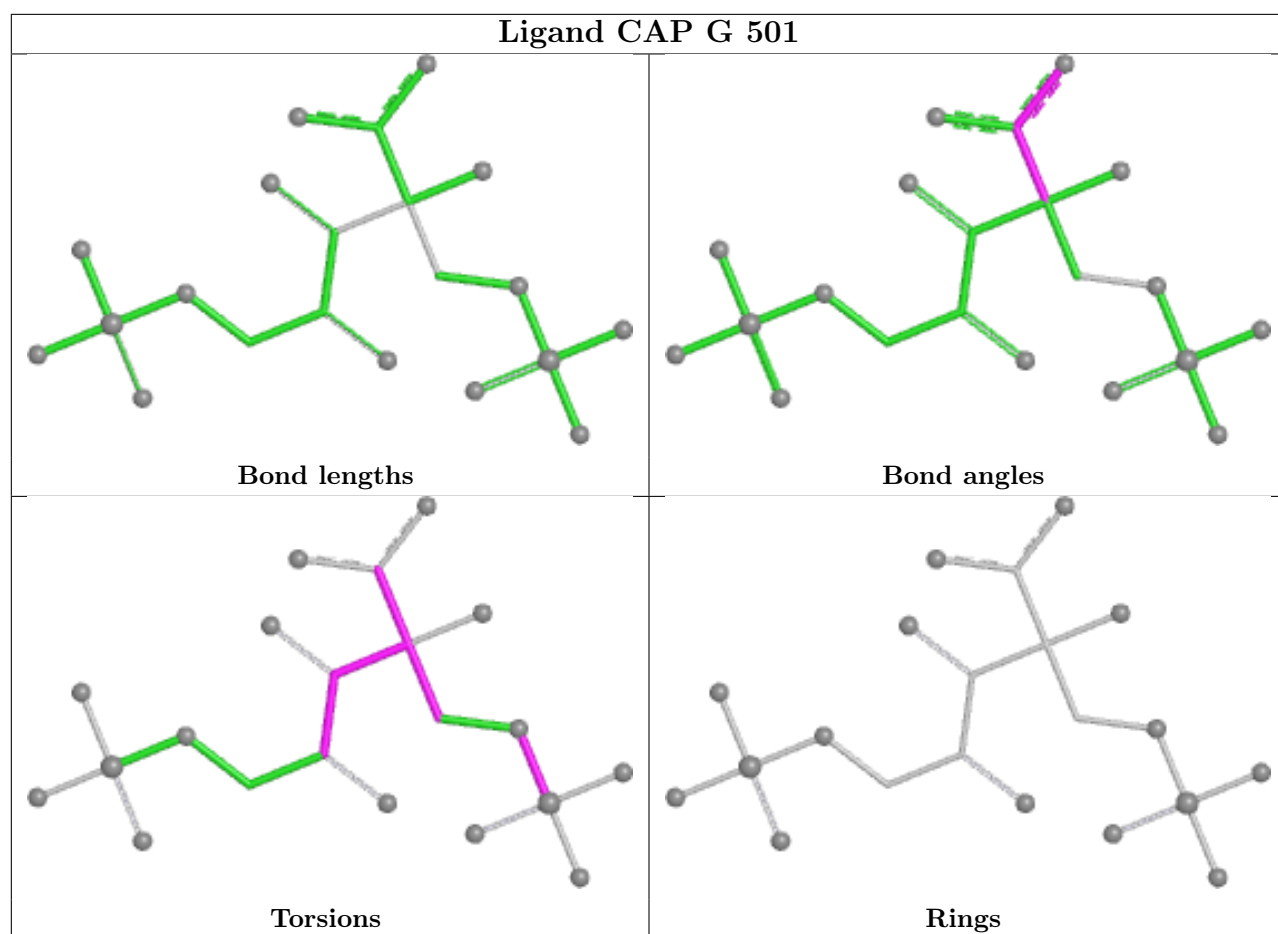
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

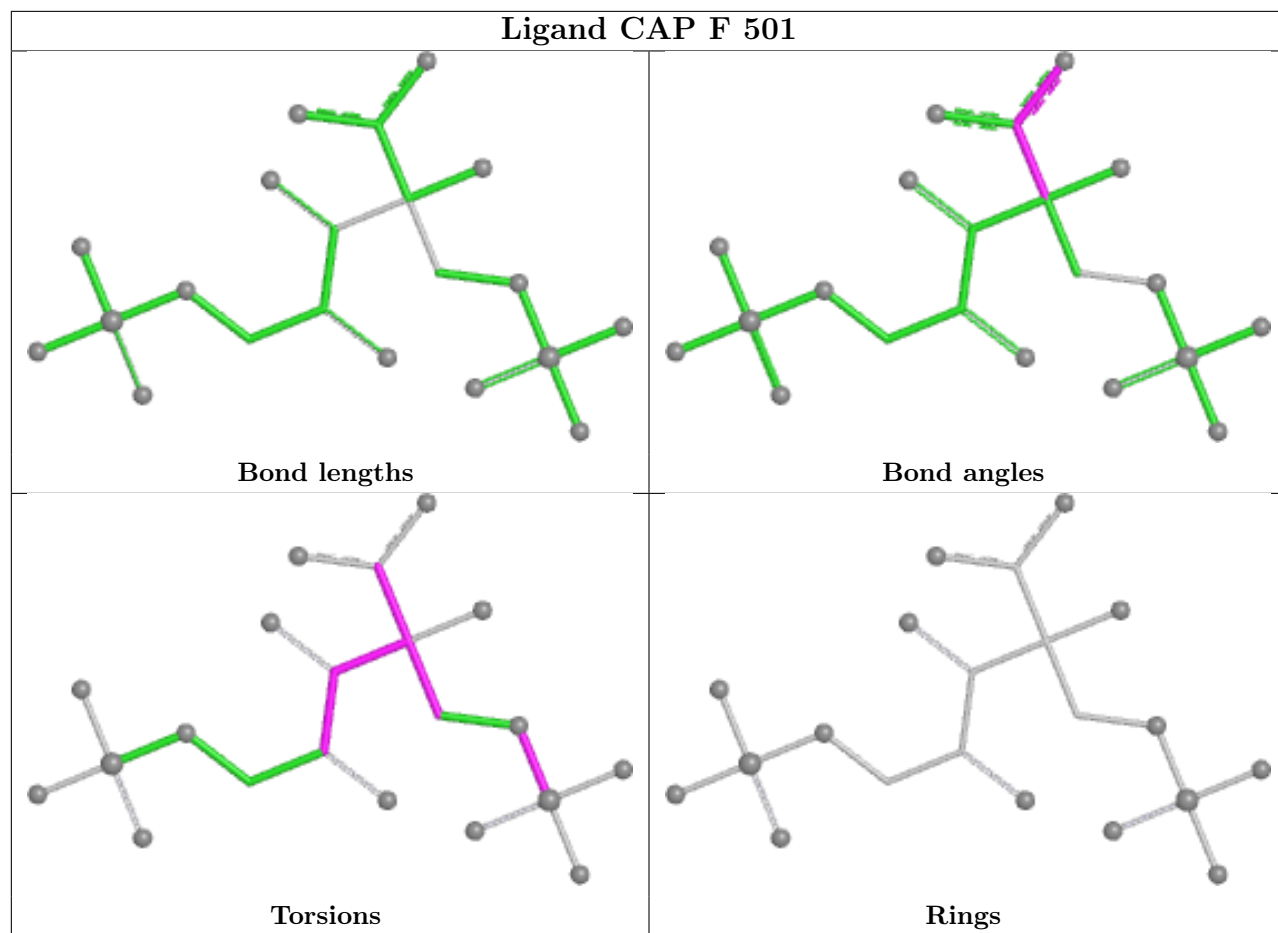


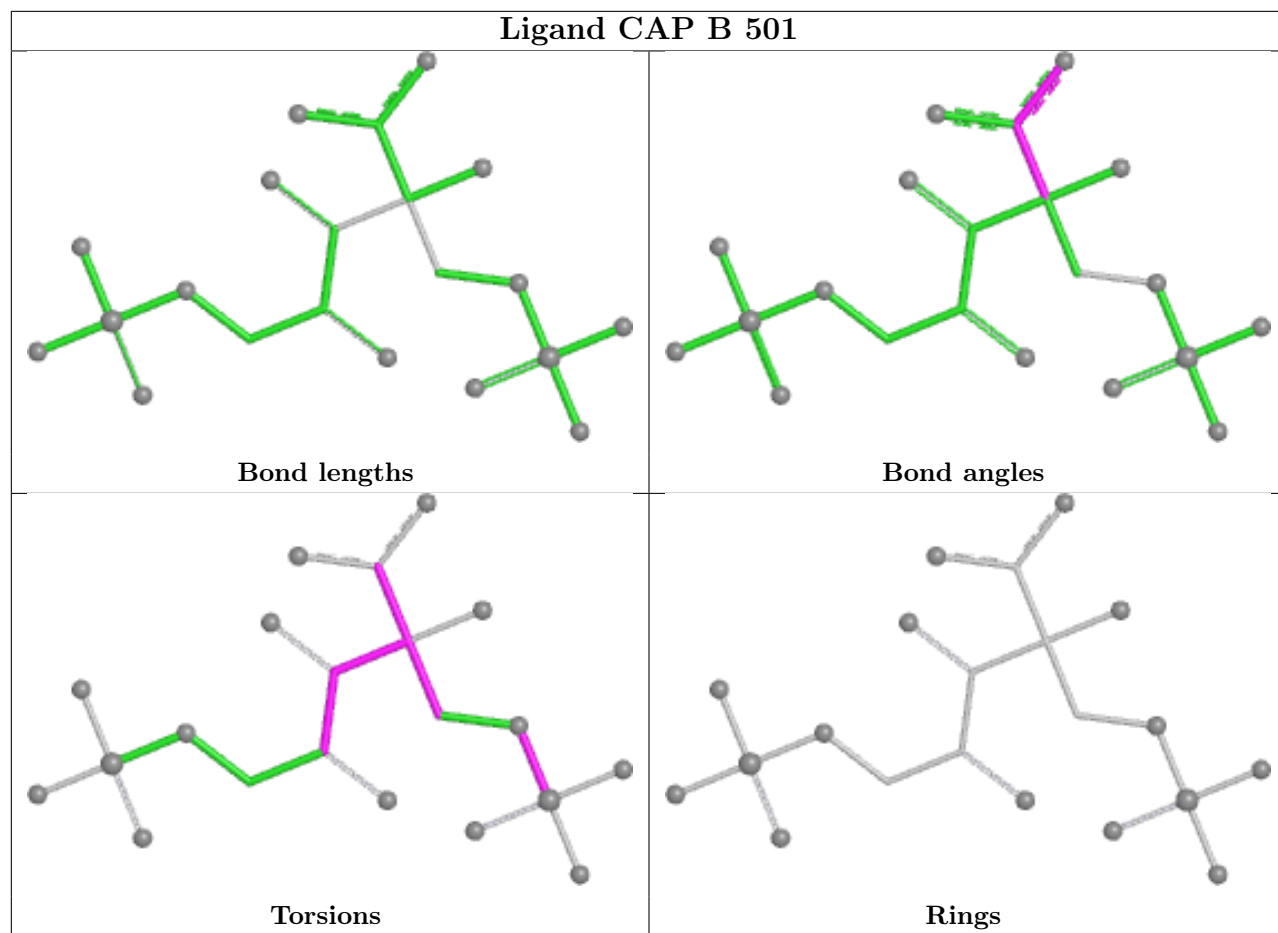


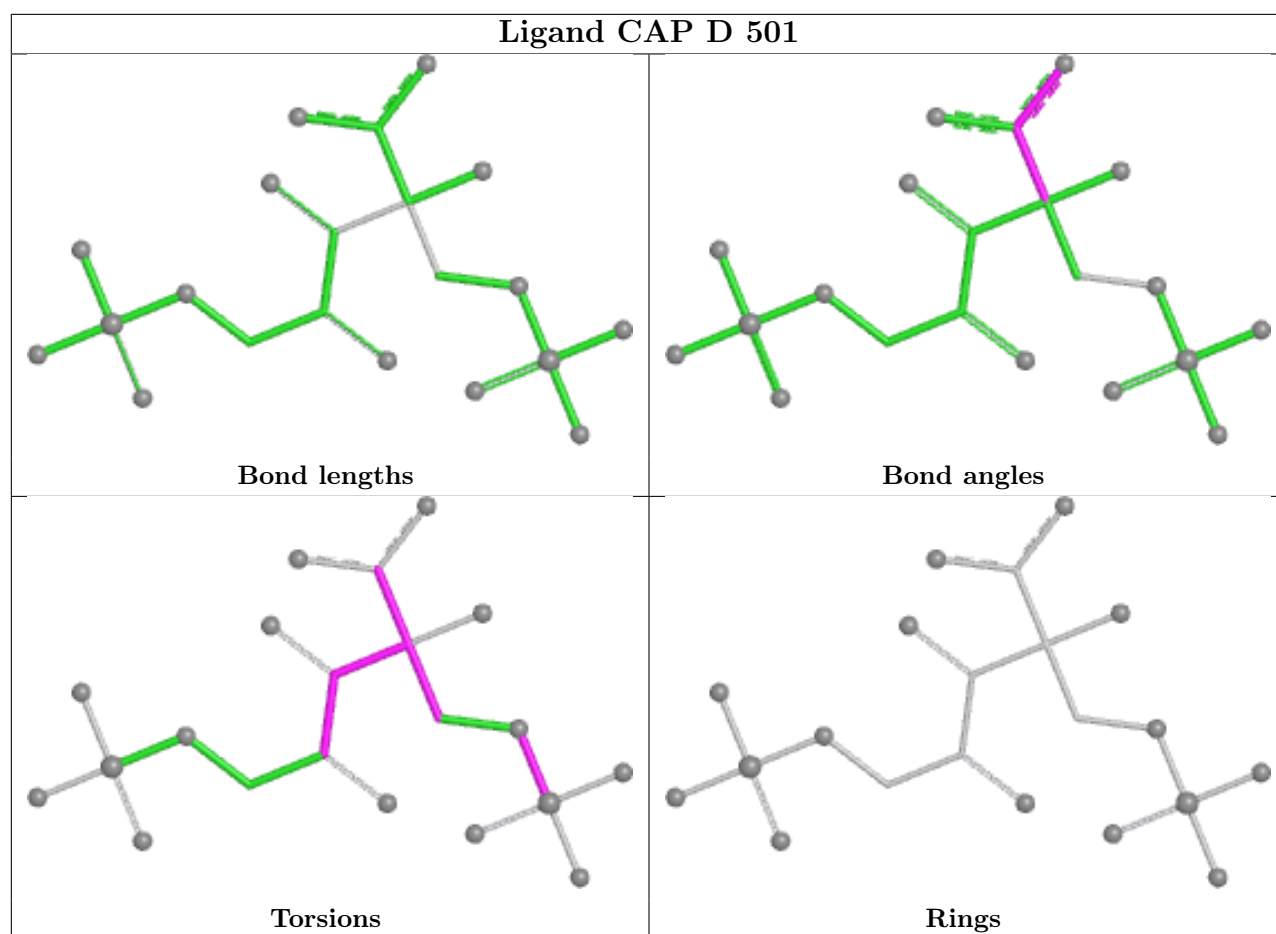












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

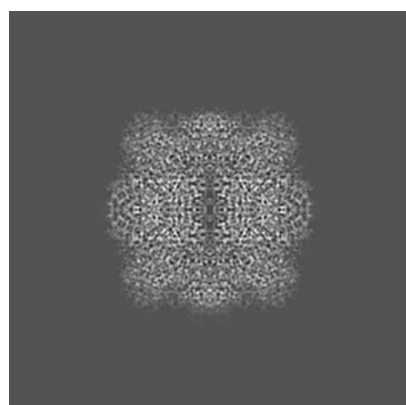
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33887. These allow visual inspection of the internal detail of the map and identification of artifacts.

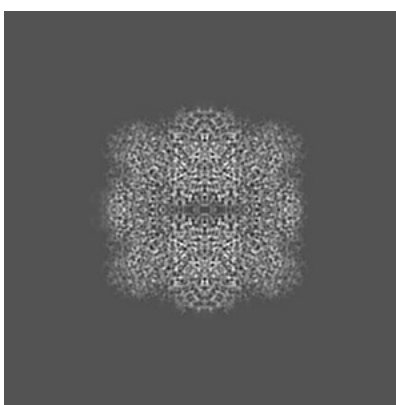
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

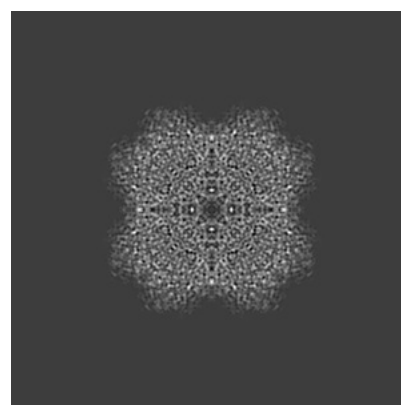
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

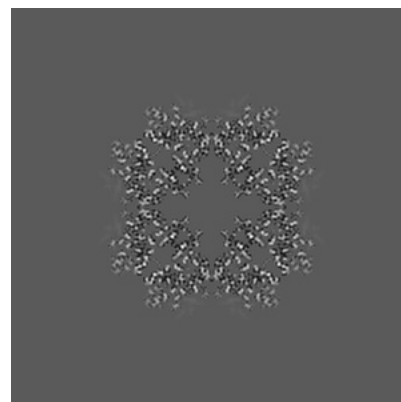
6.2.1 Primary map



X Index: 130



Y Index: 130

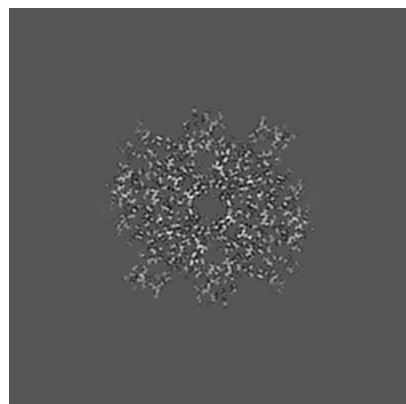


Z Index: 130

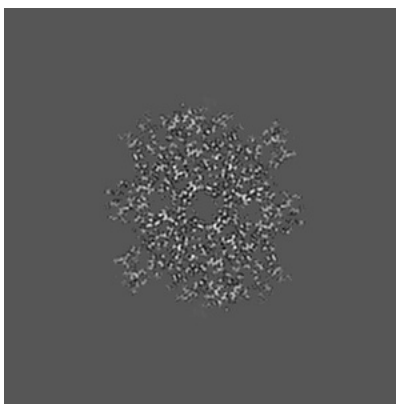
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

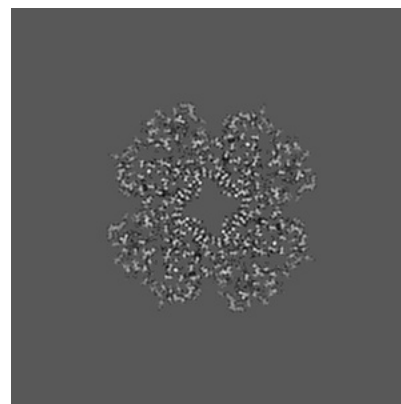
6.3.1 Primary map



X Index: 151



Y Index: 109

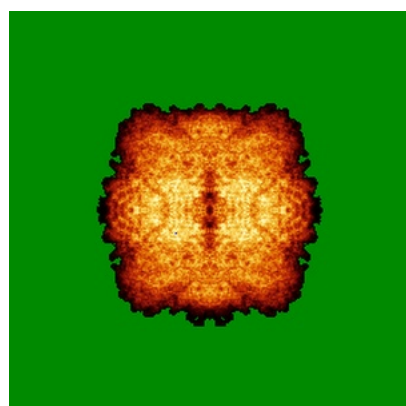


Z Index: 143

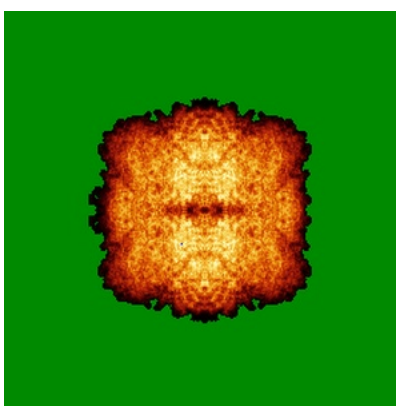
The images above show the largest variance slices of the map in three orthogonal directions.

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

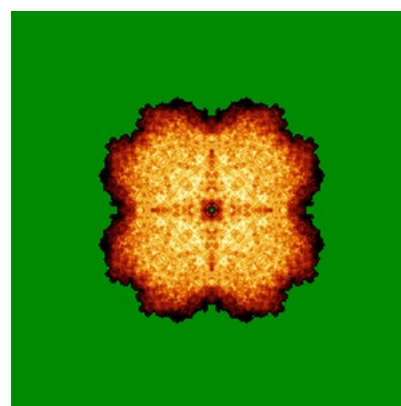
6.4.1 Primary map



X



Y

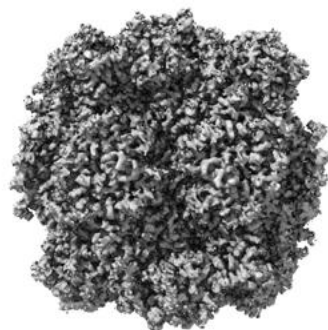


Z

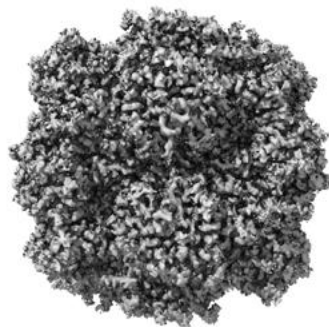
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

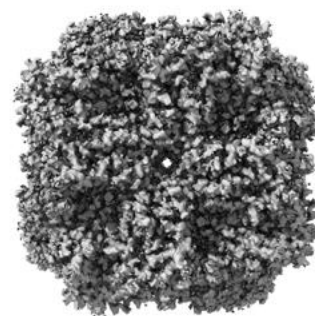
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

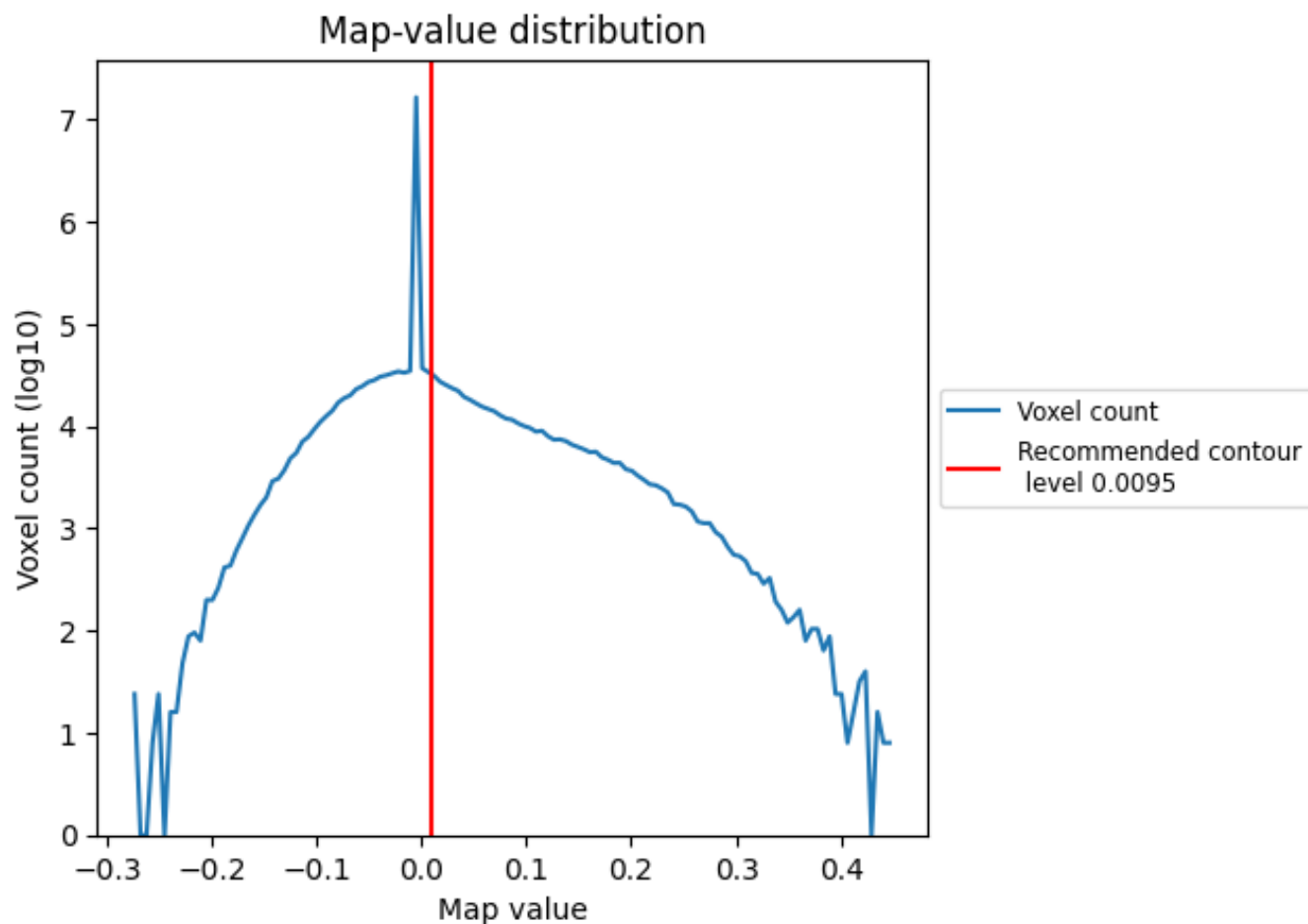
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

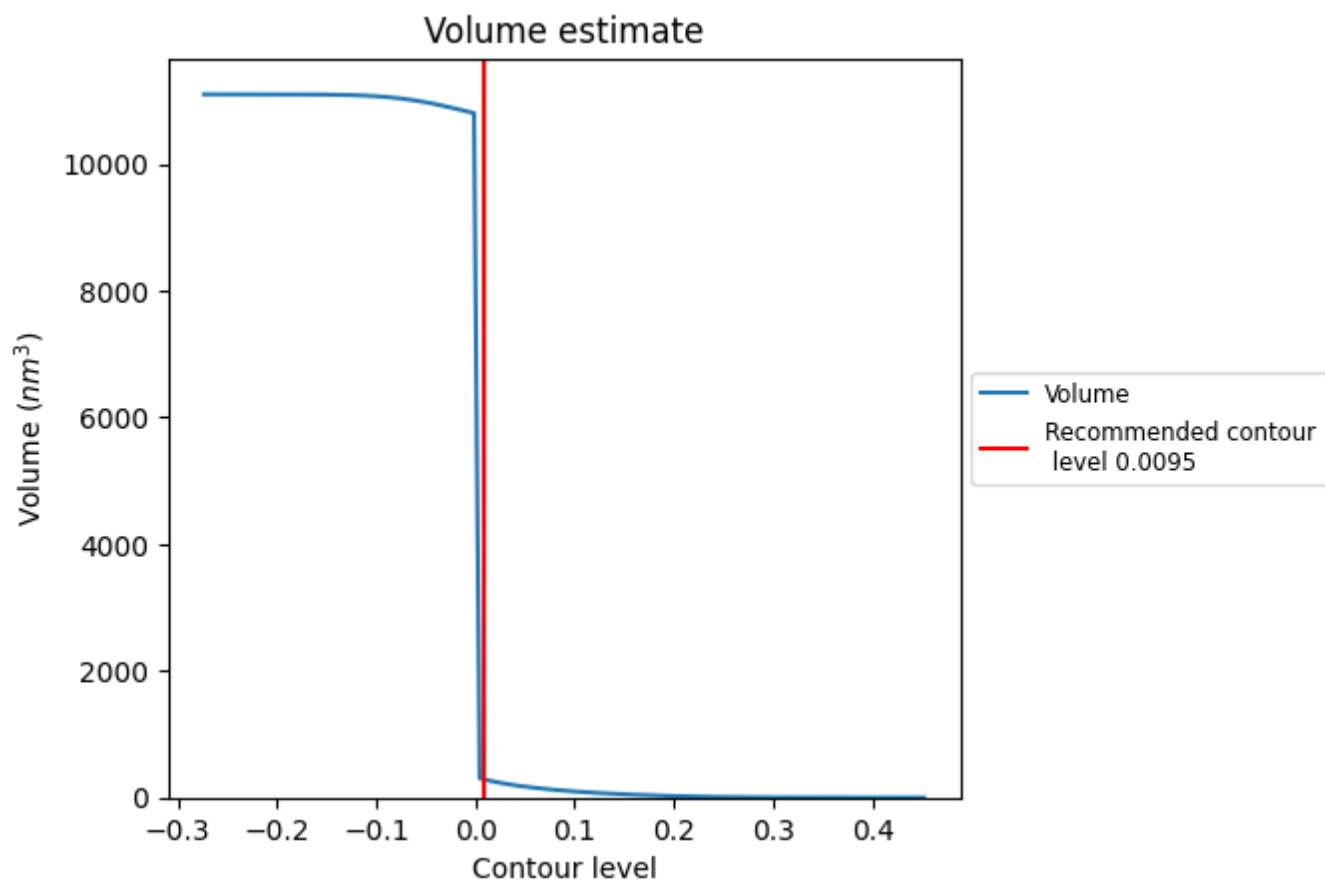
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

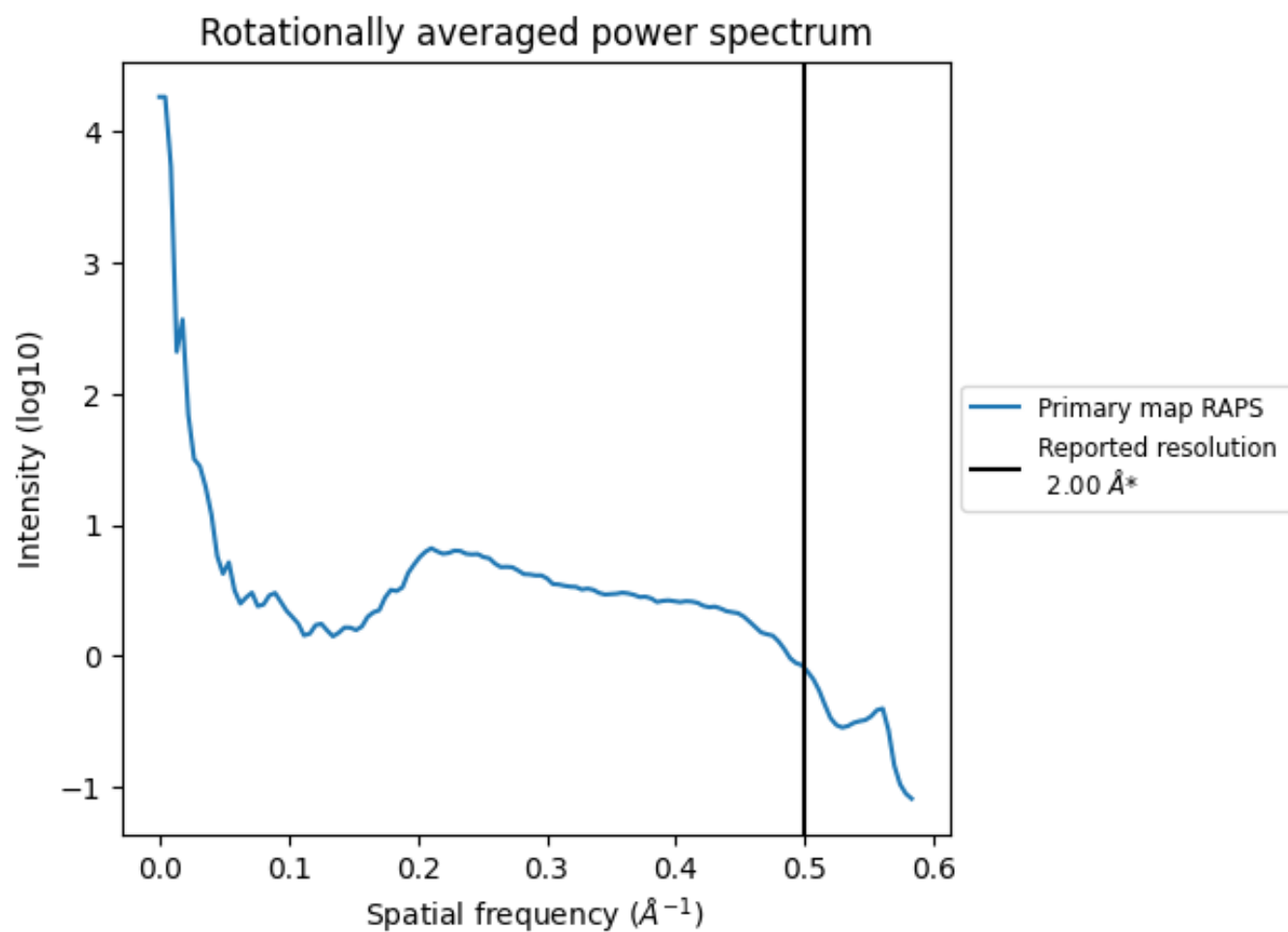
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 256 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 ⓘ

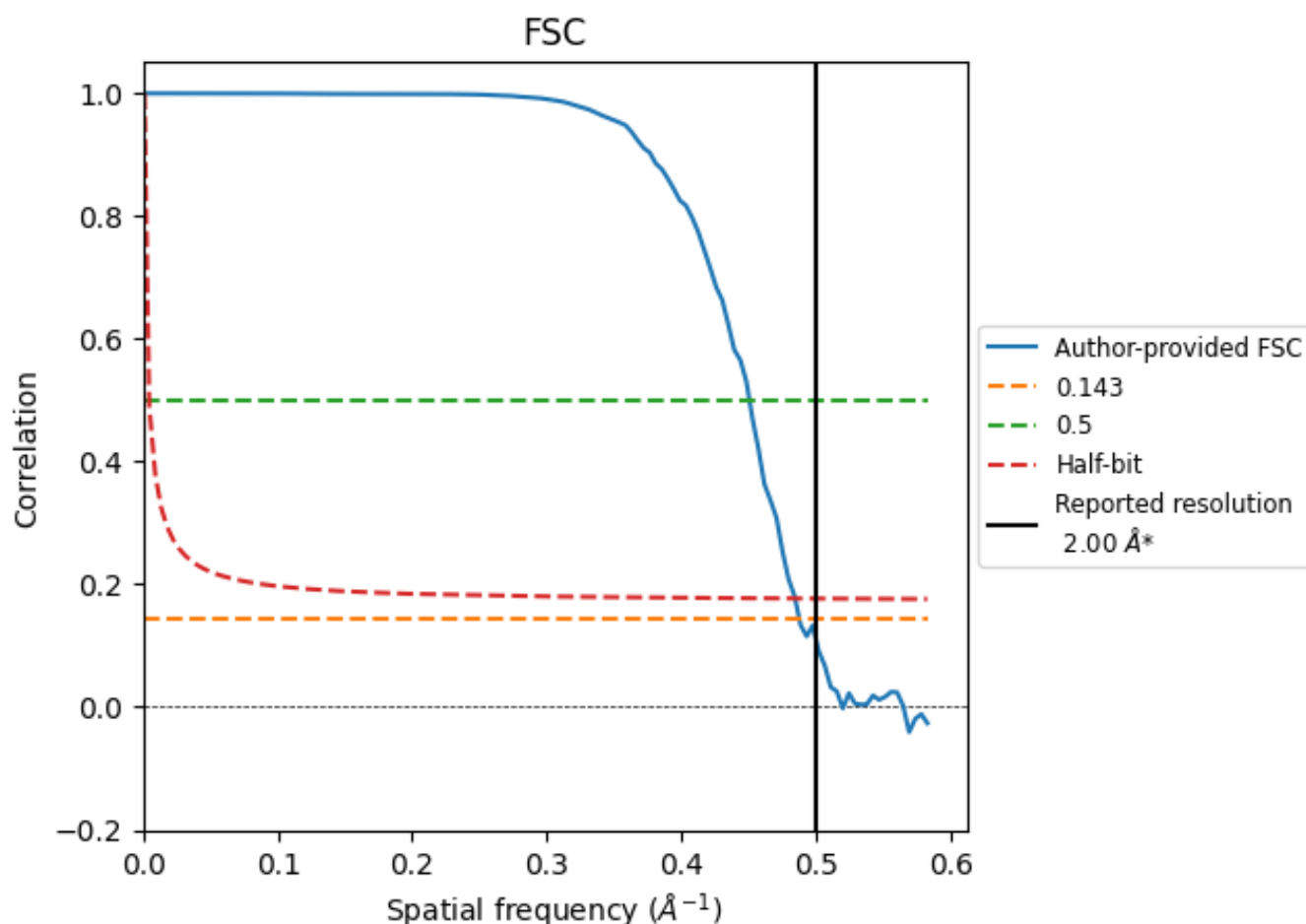


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

8.2 Resolution estimates [i](#)

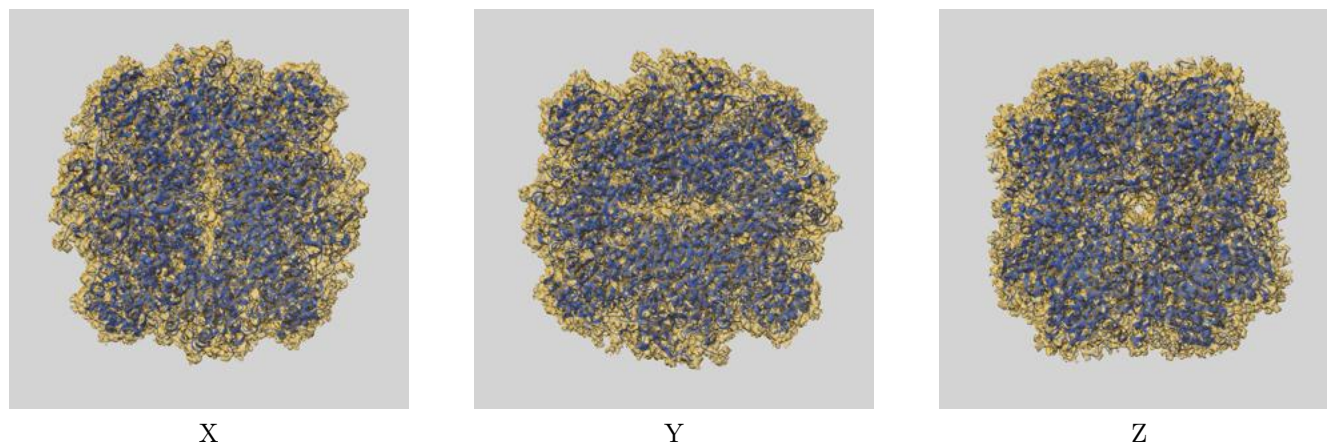
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.05	2.22	2.06
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

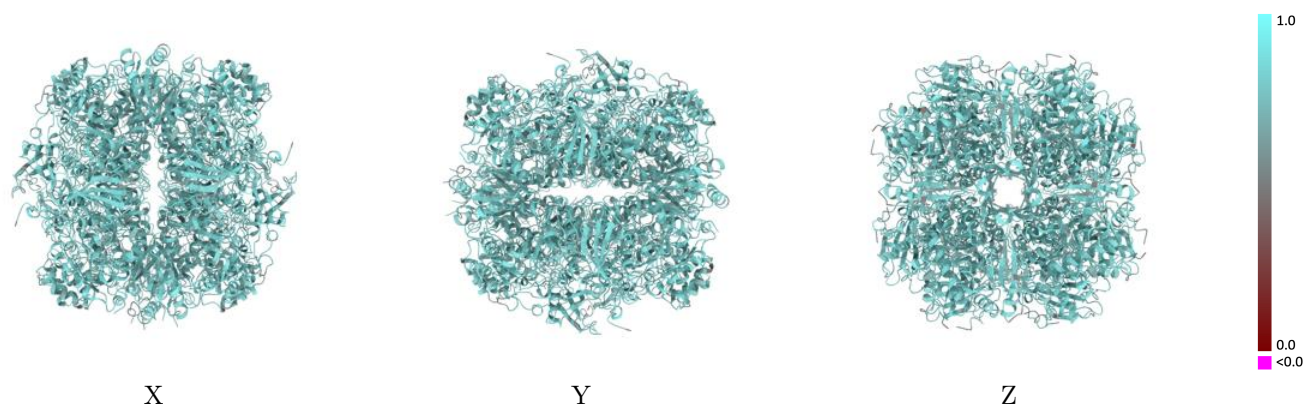
This section contains information regarding the fit between EMDB map EMD-33887 and PDB model 7YK5. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



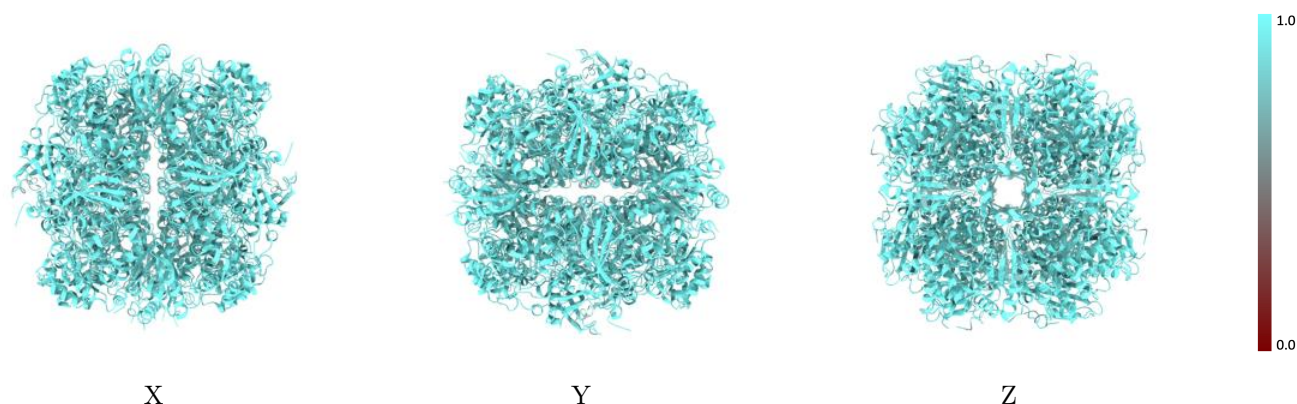
The images above show the 3D surface view of the map at the recommended contour level 0.0095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



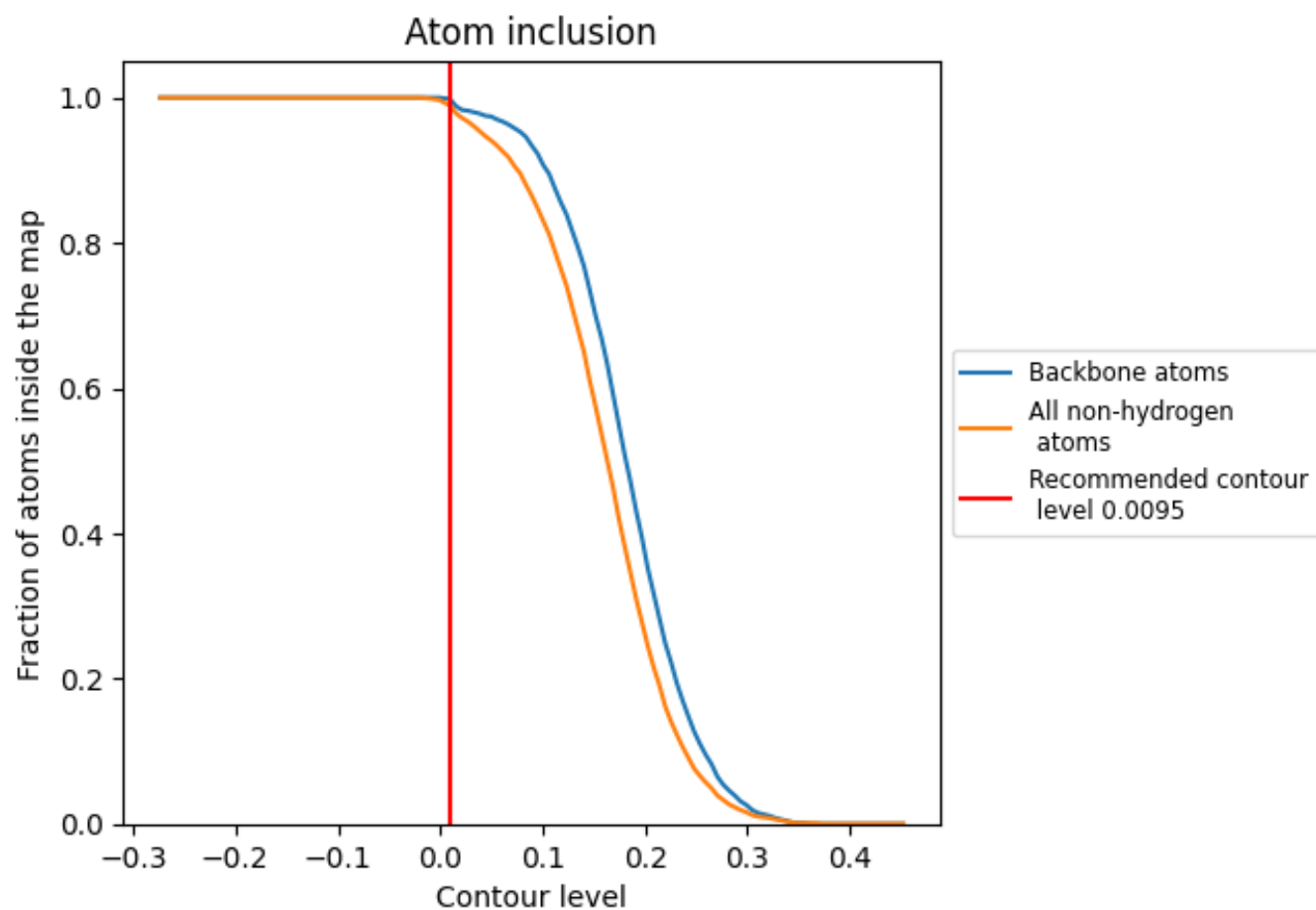
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0095).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.7760
A	 0.9940	 0.7840
B	 0.9920	 0.7830
C	 0.9930	 0.7830
D	 0.9930	 0.7840
E	 0.9930	 0.7850
F	 0.9920	 0.7830
G	 0.9930	 0.7850
H	 0.9940	 0.7830
I	 0.9870	 0.7670
J	 0.9900	 0.7710
K	 0.9880	 0.7680
L	 0.9880	 0.7700
M	 0.9880	 0.7680
N	 0.9910	 0.7720
O	 0.9880	 0.7690
P	 0.9900	 0.7700
a	 0.7610	 0.5570
b	 0.7910	 0.5870
c	 0.8210	 0.5770
d	 0.8060	 0.5900
e	 0.8060	 0.5850
f	 0.8060	 0.5900
g	 0.8060	 0.5830
h	 0.8210	 0.5680
i	 0.9660	 0.5690
j	 0.9660	 0.5680
k	 0.9660	 0.5610
l	 0.9480	 0.5560

