



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 02:52 PM UTC

PDB ID : 8AA2 / pdb_00008aa2
EMDB ID : EMD-15291
Title : Inactive levan utilisation machinery (utilisome) in the presence of levan fructo-oligosaccharides DP 15-25
Authors : White, J.B.R.; Silale, A.; Ranson, N.A.; van den Berg, B.
Deposited on : 2022-06-29
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

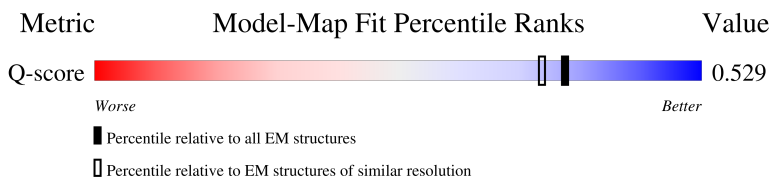
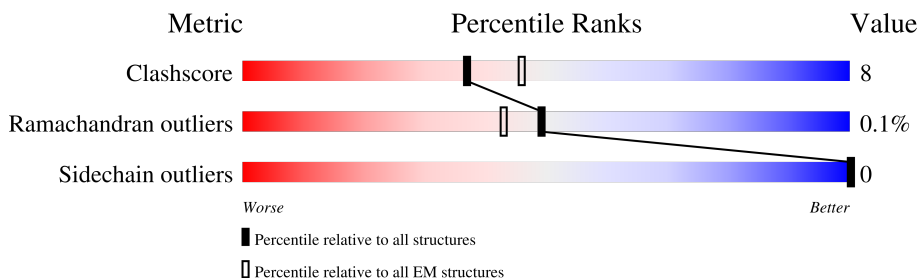
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.10 Å.

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




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

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

Mol	Chain	Length	Quality of chain
1	E	523	
1	M	523	
2	G	467	
2	T	467	

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Mol	Chain	Length	Quality of chain
3	B	570	 81% 16%
3	J	570	 82% 15%
4	A	1041	 75% 14% 11%
4	I	1041	 76% 13% 11%
5	H	13	 46% 100%
6	F	5	 40% 100%
6	N	5	 60% 100%
7	C	7	 100%
7	K	7	 14% 100%
8	D	4	 25% 100%
8	L	4	 25% 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FRU	H	13	X	-	-	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 35942 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 Glycoside hydrolase family 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	497	Total	C	N	O	S	0	0
			3979	2528	658	773	20		
1	M	497	Total	C	N	O	S	0	0
			3979	2528	658	773	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	ALA	ASP	conflict	UNP Q8A6W6
M	42	ALA	ASP	conflict	UNP Q8A6W6

- Molecule 2 is a protein called DUF4960 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	93	Total	C	N	O	S	0	0
			721	455	117	146	3		
2	G	435	Total	C	N	O	S	0	0
			3351	2127	547	666	11		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	439	HIS	-	expression tag	UNP Q8A6W5
T	440	HIS	-	expression tag	UNP Q8A6W5
T	441	HIS	-	expression tag	UNP Q8A6W5
T	442	HIS	-	expression tag	UNP Q8A6W5
T	443	HIS	-	expression tag	UNP Q8A6W5
T	444	HIS	-	expression tag	UNP Q8A6W5
G	439	HIS	-	expression tag	UNP Q8A6W5
G	440	HIS	-	expression tag	UNP Q8A6W5
G	441	HIS	-	expression tag	UNP Q8A6W5
G	442	HIS	-	expression tag	UNP Q8A6W5
G	443	HIS	-	expression tag	UNP Q8A6W5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	444	HIS	-	expression tag	UNP Q8A6W5

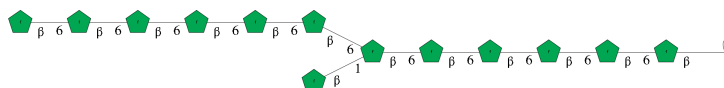
- Molecule 3 is a protein called SusD homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	551	4436	2810	736	870	20	0	0
3	J	551	4436	2810	736	870	20	0	0

- Molecule 4 is a protein called SusC homolog.

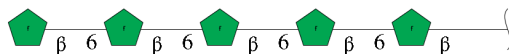
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	924	7267	4586	1248	1412	21	0	0
4	I	924	7267	4586	1248	1412	21	0	0

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



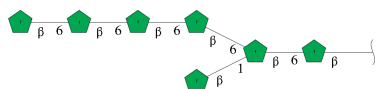
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
5	H	13	144	78	66	0	0

- Molecule 6 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



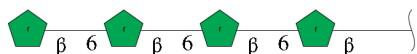
Mol	Chain	Residues	Atoms			AltConf	Trace
6	F	5	Total	C	O	0	0
			56	30	26		
6	N	5	Total	C	O	0	0
			56	30	26		

- Molecule 7 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
7	C	7	Total	C	O	0	0
			78	42	36		
7	K	7	Total	C	O	0	0
			78	42	36		

- Molecule 8 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
8	D	4	Total	C	O	0	0
			45	24	21		
8	L	4	Total	C	O	0	0
			45	24	21		

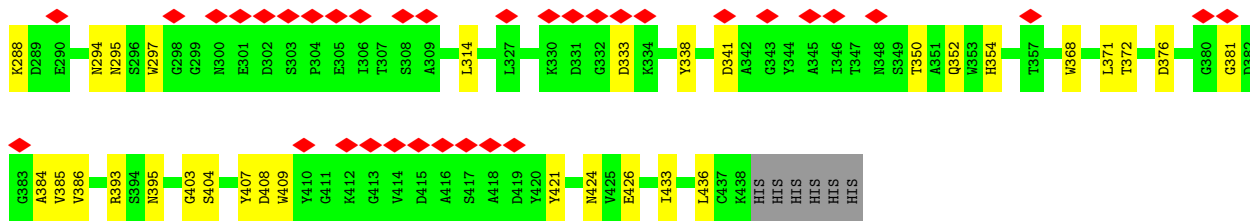
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total	Mg	0
			1	1	
9	A	1	Total	Mg	0
			1	1	
9	J	1	Total	Mg	0
			1	1	

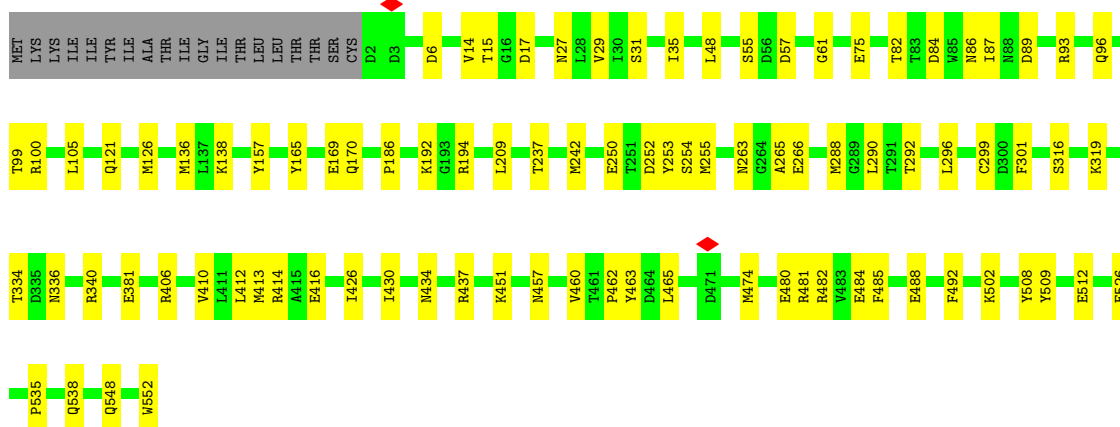
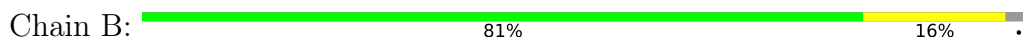
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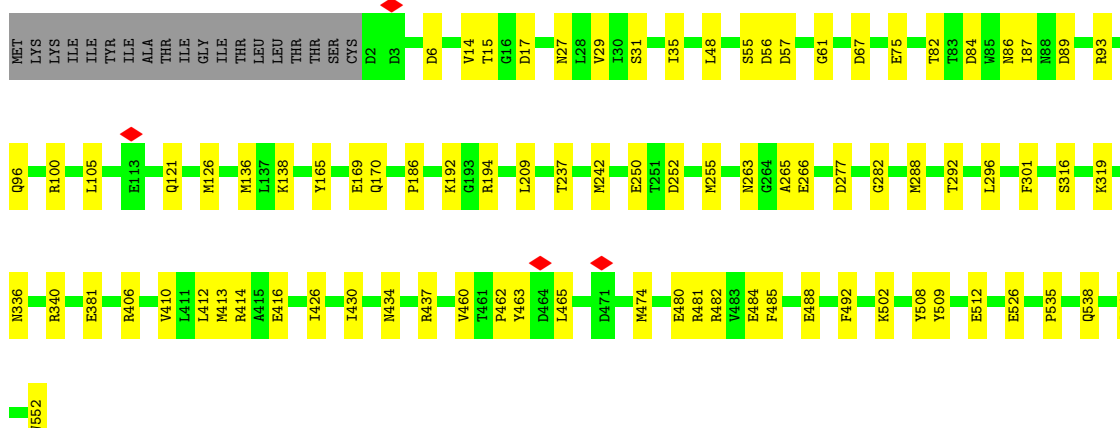
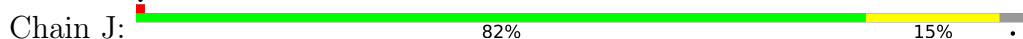
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	I	1	1	1	0



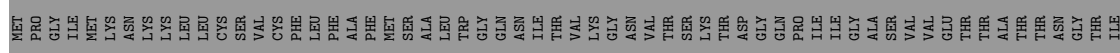
• Molecule 3: SusD homolog

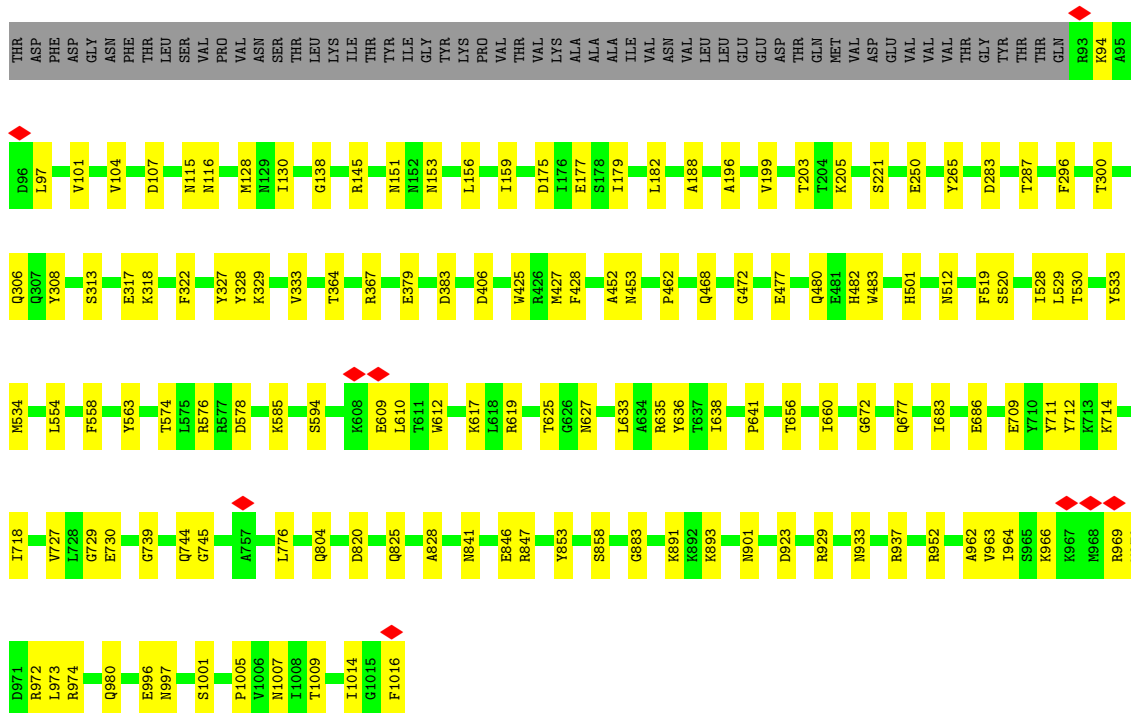


• Molecule 3: SusD homolog

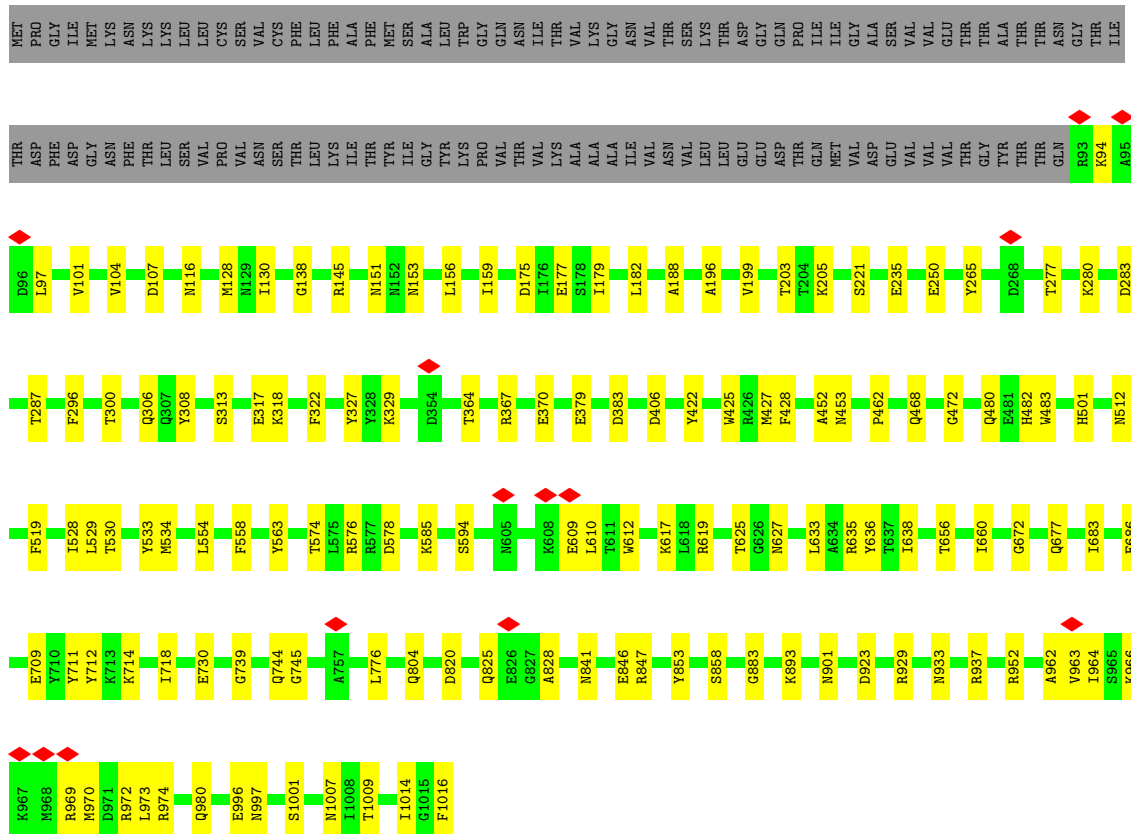
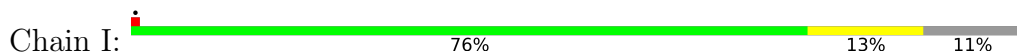


• Molecule 4: SusC homolog





• Molecule 4: SusC homolog



- Molecule 5: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain H: 



- Molecule 6: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain F: 



- Molecule 6: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain N: 



- Molecule 7: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain C: 



- Molecule 7: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain K: 



- Molecule 8: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



- Molecule 8: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27310	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 ($e^-/\text{\AA}^2$)	37.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0425	Depositor
Map size (Å)	319.50003, 319.50003, 319.50003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: MG, FRU

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	E	0.12	0/4088	0.29	0/5543
1	M	0.12	0/4088	0.29	0/5543
2	G	0.10	0/3431	0.27	0/4686
2	T	0.12	0/731	0.33	0/992
3	B	0.14	0/4542	0.25	0/6163
3	J	0.14	0/4542	0.25	0/6163
4	A	0.14	0/7440	0.27	0/10085
4	I	0.14	0/7440	0.27	0/10085
All	All	0.13	0/36302	0.27	0/49260

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3979	0	3745	59	0
1	M	3979	0	3745	61	0
2	G	3351	0	3218	58	0
2	T	721	0	715	17	0
3	B	4436	0	4205	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	4436	0	4205	55	0
4	A	7267	0	6960	92	0
4	I	7267	0	6960	90	0
5	H	144	0	118	28	0
6	F	56	0	46	9	0
6	N	56	0	46	9	0
7	C	78	0	64	15	0
7	K	78	0	64	16	0
8	D	45	0	37	6	0
8	L	45	0	37	6	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
All	All	35942	0	34165	532	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 8.

All (532) 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)
8:D:4:FRU:O5	8:D:4:FRU:C2	1.64	1.31
5:H:9:FRU:O5	5:H:9:FRU:C2	1.64	1.30
5:H:12:FRU:O5	5:H:12:FRU:C2	1.64	1.30
5:H:4:FRU:O5	5:H:4:FRU:C2	1.64	1.29
7:C:5:FRU:O5	7:C:5:FRU:C2	1.64	1.29
6:N:5:FRU:O5	6:N:5:FRU:C2	1.64	1.29
5:H:8:FRU:C2	5:H:8:FRU:O5	1.64	1.29
6:N:1:FRU:O5	6:N:1:FRU:C2	1.64	1.29
6:F:2:FRU:O5	6:F:2:FRU:C2	1.64	1.28
8:L:4:FRU:O5	8:L:4:FRU:C2	1.64	1.28
8:D:1:FRU:O5	8:D:1:FRU:C2	1.64	1.28
7:K:3:FRU:C2	7:K:3:FRU:O5	1.64	1.28
7:C:3:FRU:O5	7:C:3:FRU:C2	1.64	1.28
6:F:1:FRU:C2	6:F:1:FRU:O5	1.64	1.26
8:D:3:FRU:O5	8:D:3:FRU:C2	1.64	1.26
6:F:5:FRU:O5	6:F:5:FRU:C2	1.64	1.26
5:H:10:FRU:O5	5:H:10:FRU:C2	1.64	1.26
7:K:4:FRU:O5	7:K:4:FRU:C2	1.64	1.26
5:H:3:FRU:O5	5:H:3:FRU:C2	1.64	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6:FRU:C2	5:H:6:FRU:O5	1.64	1.25
7:C:2:FRU:O5	7:C:2:FRU:C2	1.64	1.25
5:H:1:FRU:O5	5:H:1:FRU:C2	1.64	1.24
8:L:3:FRU:O5	8:L:3:FRU:C2	1.64	1.24
5:H:13:FRU:O5	5:H:13:FRU:C2	1.63	1.23
6:F:4:FRU:O5	6:F:4:FRU:C2	1.64	1.23
6:N:2:FRU:O5	6:N:2:FRU:C2	1.64	1.22
7:C:1:FRU:O5	7:C:1:FRU:C2	1.64	1.22
7:C:7:FRU:O5	7:C:7:FRU:C2	1.64	1.22
8:L:1:FRU:O5	8:L:1:FRU:C2	1.64	1.22
8:L:2:FRU:O5	8:L:2:FRU:C2	1.64	1.22
7:K:7:FRU:O5	7:K:7:FRU:C2	1.64	1.21
5:H:2:FRU:O5	5:H:2:FRU:C2	1.64	1.20
7:K:6:FRU:O5	7:K:6:FRU:C2	1.64	1.20
7:K:5:FRU:O5	7:K:5:FRU:C2	1.64	1.20
5:H:7:FRU:O5	5:H:7:FRU:C2	1.64	1.20
5:H:11:FRU:O5	5:H:11:FRU:C2	1.63	1.20
6:N:4:FRU:O5	6:N:4:FRU:C2	1.64	1.20
5:H:5:FRU:O5	5:H:5:FRU:C2	1.64	1.19
7:K:2:FRU:O5	7:K:2:FRU:C2	1.64	1.18
6:F:3:FRU:O5	6:F:3:FRU:C2	1.64	1.17
7:C:6:FRU:C2	7:C:6:FRU:O5	1.64	1.16
7:K:1:FRU:O5	7:K:1:FRU:C2	1.64	1.15
6:N:3:FRU:O5	6:N:3:FRU:C2	1.64	1.14
7:C:4:FRU:O5	7:C:4:FRU:C2	1.64	1.12
8:D:2:FRU:O5	8:D:2:FRU:C2	1.64	1.12
2:T:9:LEU:HD21	4:I:235:GLU:HB2	1.51	0.92
5:H:13:FRU:O5	5:H:13:FRU:C1	2.25	0.84
1:E:111:ASN:HD21	1:E:203:LEU:HD12	1.47	0.80
1:M:111:ASN:HD21	1:M:203:LEU:HD12	1.47	0.80
1:M:246:LYS:HD3	1:M:276:MET:HE1	1.65	0.79
1:E:246:LYS:HD3	1:E:276:MET:HE1	1.65	0.77
1:E:133:ASN:HD22	1:E:157:LYS:HD2	1.50	0.75
1:M:133:ASN:HD22	1:M:157:LYS:HD2	1.50	0.74
4:I:972:ARG:HH21	4:I:974:ARG:HD2	1.53	0.74
4:A:972:ARG:HH21	4:A:974:ARG:HD2	1.53	0.73
2:T:45:ASP:O	2:T:47:THR:N	2.22	0.71
1:M:466:ILE:HB	1:M:470:LEU:HB3	1.73	0.70
4:I:627:ASN:HB3	4:I:686:GLU:HB3	1.73	0.70
5:H:8:FRU:H62	5:H:9:FRU:O5	1.93	0.69
4:A:627:ASN:HB3	4:A:686:GLU:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ILE:HB	1:E:470:LEU:HB3	1.73	0.69
4:A:177:GLU:HG2	4:A:205:LYS:HA	1.75	0.69
1:E:197:GLU:HB2	1:E:212:PHE:HB2	1.77	0.67
4:I:177:GLU:HG2	4:I:205:LYS:HA	1.75	0.67
3:J:35:ILE:HB	3:J:100:ARG:HD2	1.76	0.67
1:M:197:GLU:HB2	1:M:212:PHE:HB2	1.76	0.67
3:B:35:ILE:HB	3:B:100:ARG:HD2	1.76	0.67
3:J:138:LYS:NZ	3:J:170:GLN:OE1	2.28	0.67
3:B:138:LYS:NZ	3:B:170:GLN:OE1	2.28	0.66
8:L:2:FRU:H62	8:L:3:FRU:O5	1.95	0.66
5:H:9:FRU:H62	5:H:10:FRU:O5	1.95	0.66
4:A:529:LEU:HA	4:A:534:MET:HE3	1.78	0.66
5:H:3:FRU:H62	5:H:4:FRU:O5	1.96	0.65
8:D:2:FRU:H62	8:D:3:FRU:O5	1.95	0.65
3:B:61:GLY:HA3	3:B:301:PHE:HA	1.78	0.65
7:K:5:FRU:H61	7:K:6:FRU:O5	1.97	0.65
4:I:529:LEU:HA	4:I:534:MET:HE3	1.78	0.65
3:B:82:THR:N	4:A:846:GLU:OE2	2.30	0.65
4:A:427:MET:HE3	4:I:427:MET:HE3	1.79	0.65
2:T:53:GLU:OE2	2:T:55:ASN:ND2	2.29	0.64
3:J:61:GLY:HA3	3:J:301:PHE:HA	1.78	0.64
2:T:9:LEU:HB3	2:T:11:LEU:HG	1.79	0.64
3:J:502:LYS:HE3	3:J:526:GLU:HG3	1.80	0.64
1:M:327:LEU:HD22	1:M:335:LEU:HD22	1.80	0.64
3:J:96:GLN:HE21	4:I:730:GLU:HB3	1.62	0.64
1:E:327:LEU:HD22	1:E:335:LEU:HD22	1.80	0.63
7:C:5:FRU:H61	7:C:6:FRU:O5	1.97	0.63
1:E:321:ASN:OD1	1:E:475:ARG:NH1	2.32	0.63
1:M:321:ASN:OD1	1:M:475:ARG:NH1	2.32	0.63
4:A:482:HIS:HE1	4:I:453:ASN:HD21	1.46	0.63
3:J:82:THR:N	4:I:846:GLU:OE2	2.31	0.63
3:B:502:LYS:HE3	3:B:526:GLU:HG3	1.80	0.62
4:I:453:ASN:OD1	4:I:480:GLN:NE2	2.26	0.62
1:M:314:VAL:HG23	1:M:315:GLU:H	1.64	0.62
1:E:314:VAL:HG23	1:E:315:GLU:H	1.64	0.62
4:A:453:ASN:OD1	4:A:480:GLN:NE2	2.26	0.61
4:I:633:LEU:O	4:I:677:GLN:NE2	2.34	0.61
4:A:633:LEU:O	4:A:677:GLN:NE2	2.34	0.61
4:A:453:ASN:HD21	4:I:482:HIS:HE1	1.48	0.61
1:M:481:LYS:NZ	4:I:820:ASP:OD2	2.31	0.61
4:A:462:PRO:HB3	4:A:472:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:97:LEU:O	4:A:617:LYS:NZ	2.29	0.61
7:K:1:FRU:H61	7:K:2:FRU:O5	2.00	0.61
1:E:358:LYS:NZ	1:E:362:MET:SD	2.64	0.60
4:A:825:GLN:HG2	4:A:828:ALA:HB2	1.83	0.60
1:E:19:THR:O	1:E:381:ARG:NH2	2.34	0.60
1:E:152:ARG:HD2	2:G:70:ILE:HD12	1.82	0.60
1:M:176:THR:OG1	1:M:178:ASP:OD1	2.17	0.60
4:I:462:PRO:HB3	4:I:472:GLY:HA2	1.82	0.60
7:C:1:FRU:H61	7:C:2:FRU:O5	2.00	0.60
1:E:176:THR:OG1	1:E:178:ASP:OD1	2.17	0.60
2:G:114:ASP:OD1	2:G:119:THR:OG1	2.16	0.59
4:I:825:GLN:HG2	4:I:828:ALA:HB2	1.84	0.59
1:E:34:LYS:HB2	1:E:321:ASN:HD22	1.67	0.59
1:M:34:LYS:HB2	1:M:321:ASN:HD22	1.67	0.59
2:G:264:TYR:CZ	2:G:269:GLY:HA3	2.38	0.59
4:A:901:ASN:OD1	7:C:4:FRU:O3	2.19	0.59
3:J:316:SER:HA	3:J:336:ASN:HD22	1.68	0.59
2:G:350:THR:OG1	2:G:403:GLY:O	2.21	0.58
3:J:209:LEU:HD22	3:J:413:MET:HG3	1.84	0.58
1:E:159:ASP:HB3	1:E:165:LYS:HG2	1.85	0.58
2:T:82:ASN:OD1	2:T:83:GLY:N	2.35	0.58
3:B:209:LEU:HD22	3:B:413:MET:HG3	1.84	0.58
1:E:261:THR:HG23	1:E:268:ILE:HB	1.85	0.58
2:G:288:LYS:NZ	3:B:334:THR:O	2.30	0.58
1:M:358:LYS:NZ	1:M:362:MET:SD	2.64	0.58
1:M:261:THR:HG23	1:M:268:ILE:HB	1.85	0.58
3:B:316:SER:HA	3:B:336:ASN:HD22	1.68	0.58
2:G:62:ALA:HB1	2:G:78:LEU:HD11	1.84	0.58
2:G:338:TYR:O	2:G:424:ASN:ND2	2.37	0.57
4:I:452:ALA:HB3	4:I:483:TRP:HB2	1.85	0.57
4:I:901:ASN:OD1	7:K:4:FRU:O3	2.15	0.57
1:E:111:ASN:ND2	1:E:203:LEU:HD12	2.18	0.57
2:G:63:SER:OG	2:G:79:THR:OG1	2.22	0.57
4:A:383:ASP:OD2	7:C:7:FRU:O4	2.22	0.57
1:E:481:LYS:NZ	4:A:820:ASP:OD2	2.31	0.57
3:B:237:THR:HG23	3:B:414:ARG:HH11	1.70	0.56
4:A:970:MET:HB2	4:A:1016:PHE:HA	1.87	0.56
1:M:159:ASP:HB3	1:M:165:LYS:HG2	1.85	0.56
4:A:452:ALA:HB3	4:A:483:TRP:HB2	1.85	0.56
1:E:44:MET:HE2	1:E:105:THR:HA	1.88	0.56
1:M:19:THR:O	1:M:381:ARG:NH2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:237:THR:HG23	3:J:414:ARG:HH11	1.70	0.56
2:G:352:GLN:HG3	2:G:384:ALA:HB1	1.88	0.56
4:I:558:PHE:HB3	4:I:576:ARG:HG3	1.87	0.55
2:T:62:ALA:HB1	2:T:78:LEU:HD11	1.88	0.55
3:J:67:ASP:OD1	7:K:4:FRU:O3	2.24	0.55
4:I:970:MET:HB2	4:I:1016:PHE:HA	1.87	0.55
4:A:558:PHE:HB3	4:A:576:ARG:HG3	1.87	0.55
3:J:87:ILE:HG22	3:J:535:PRO:HG3	1.88	0.55
2:G:21:ARG:HB3	2:G:53:GLU:HG2	1.88	0.55
1:M:169:ARG:NH2	1:M:222:GLU:OE2	2.33	0.55
4:I:619:ARG:NH2	4:I:709:GLU:OE2	2.39	0.55
1:E:313:ASP:O	1:E:315:GLU:N	2.40	0.55
1:M:44:MET:HE2	1:M:105:THR:HA	1.88	0.55
3:J:416:GLU:HG3	3:J:474:MET:HE1	1.88	0.55
3:J:57:ASP:OD1	3:J:482:ARG:NH1	2.40	0.55
4:I:97:LEU:O	4:I:617:LYS:NZ	2.29	0.54
4:I:116:ASN:HB2	4:I:138:GLY:HA3	1.89	0.54
1:M:313:ASP:O	1:M:315:GLU:N	2.40	0.54
3:B:406:ARG:NH2	3:B:488:GLU:OE2	2.35	0.54
2:G:275:ARG:NH2	2:G:407:TYR:O	2.39	0.54
4:A:619:ARG:NH2	4:A:709:GLU:OE2	2.39	0.54
3:J:27:ASN:HB3	4:I:672:GLY:HA2	1.90	0.54
3:B:57:ASP:OD1	3:B:482:ARG:NH1	2.40	0.54
4:A:635:ARG:NH2	4:A:636:TYR:OH	2.41	0.54
3:J:121:GLN:HG2	3:J:186:PRO:HD3	1.89	0.54
1:M:111:ASN:ND2	1:M:203:LEU:HD12	2.18	0.54
3:B:165:TYR:HB3	3:B:169:GLU:HB2	1.90	0.54
4:A:116:ASN:HB2	4:A:138:GLY:HA3	1.90	0.54
3:B:416:GLU:HG3	3:B:474:MET:HE1	1.88	0.54
3:B:87:ILE:HG22	3:B:535:PRO:HG3	1.88	0.54
3:J:165:TYR:HB3	3:J:169:GLU:HB2	1.90	0.54
3:J:406:ARG:NH2	3:J:488:GLU:OE2	2.35	0.54
7:C:5:FRU:C6	7:C:6:FRU:O5	2.56	0.54
2:G:186:PHE:HB2	2:G:208:MET:SD	2.48	0.54
7:K:5:FRU:C6	7:K:6:FRU:O5	2.56	0.54
2:G:297:TRP:HE1	5:H:1:FRU:H4	1.73	0.53
1:E:134:ALA:HB3	1:E:166:ASN:HA	1.89	0.53
4:A:182:LEU:HB3	4:A:188:ALA:HB2	1.90	0.53
3:B:6:ASP:OD2	4:A:585:LYS:NZ	2.41	0.53
4:I:182:LEU:HB3	4:I:188:ALA:HB2	1.90	0.53
1:M:451:TYR:HA	1:M:467:ASN:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:997:ASN:OD1	4:A:1001:SER:OG	2.27	0.53
4:I:997:ASN:OD1	4:I:1001:SER:OG	2.27	0.53
1:E:451:TYR:HA	1:E:467:ASN:HD22	1.73	0.53
1:M:134:ALA:HB3	1:M:166:ASN:HA	1.89	0.53
1:M:86:SER:HB3	4:I:265:TYR:HB2	1.90	0.53
2:T:46:ILE:HA	2:T:49:MET:HE3	1.90	0.53
3:B:121:GLN:HG2	3:B:186:PRO:HD3	1.89	0.53
5:H:9:FRU:C6	5:H:10:FRU:O5	2.57	0.53
8:L:2:FRU:C6	8:L:3:FRU:O5	2.57	0.53
2:G:139:VAL:HG11	2:G:143:ALA:HB3	1.91	0.53
3:B:412:LEU:HD13	3:B:481:ARG:HG2	1.91	0.53
3:B:508:TYR:CE1	3:B:512:GLU:HG3	2.44	0.53
1:E:169:ARG:NH2	1:E:222:GLU:OE2	2.33	0.53
1:M:398:THR:O	1:M:490:LYS:NZ	2.39	0.53
5:H:8:FRU:C6	5:H:9:FRU:O5	2.56	0.53
2:T:42:TYR:O	2:T:95:ARG:NH2	2.41	0.52
3:J:412:LEU:HD13	3:J:481:ARG:HG2	1.91	0.52
3:J:535:PRO:HB2	3:J:538:GLN:HG2	1.92	0.52
8:D:2:FRU:C6	8:D:3:FRU:O5	2.57	0.52
3:B:437:ARG:NH1	3:B:480:GLU:OE1	2.41	0.52
1:E:43:PRO:HD3	1:E:299:TRP:HD1	1.74	0.52
4:A:313:SER:HB3	4:A:322:PHE:HD1	1.75	0.52
4:I:635:ARG:NH2	4:I:636:TYR:OH	2.41	0.52
5:H:7:FRU:H62	5:H:8:FRU:O5	2.09	0.52
2:T:45:ASP:C	2:T:47:THR:H	2.14	0.52
4:I:151:ASN:O	4:I:153:ASN:ND2	2.43	0.52
3:B:84:ASP:HB2	3:B:87:ILE:HD12	1.91	0.52
3:B:535:PRO:HB2	3:B:538:GLN:HG2	1.92	0.52
3:J:508:TYR:CE1	3:J:512:GLU:HG3	2.44	0.51
1:E:401:PHE:HB3	1:E:493:ILE:HG21	1.91	0.51
2:G:191:SER:OG	2:G:195:LEU:O	2.23	0.51
1:M:401:PHE:HB3	1:M:493:ILE:HG21	1.91	0.51
3:J:84:ASP:HB2	3:J:87:ILE:HD12	1.91	0.51
1:M:100:ASP:HB3	1:M:138:MET:SD	2.51	0.51
4:A:151:ASN:O	4:A:153:ASN:ND2	2.43	0.51
2:G:113:VAL:HG13	2:G:120:ILE:HG13	1.92	0.51
3:B:27:ASN:HB3	4:A:672:GLY:HA2	1.91	0.51
5:H:4:FRU:H62	5:H:5:FRU:O5	2.11	0.51
2:G:273:LEU:HB3	2:G:277:ALA:O	2.10	0.51
4:I:313:SER:HB3	4:I:322:PHE:HD1	1.75	0.51
1:E:100:ASP:HB3	1:E:138:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:43:PRO:HD3	1:M:299:TRP:HD1	1.74	0.50
3:B:31:SER:HA	4:A:656:THR:HG23	1.92	0.50
4:I:145:ARG:HD2	4:I:711:TYR:CZ	2.46	0.50
4:I:367:ARG:HG3	4:I:425:TRP:CZ2	2.46	0.50
2:T:36:ILE:HB	2:T:91:ILE:HG13	1.92	0.50
2:G:105:LEU:HD21	2:G:133:LEU:HD13	1.93	0.50
2:G:238:TRP:HB3	2:G:273:LEU:HD23	1.93	0.50
3:J:31:SER:HA	4:I:656:THR:HG23	1.92	0.50
5:H:3:FRU:C6	5:H:4:FRU:O5	2.58	0.50
2:G:242:ALA:H	2:G:276:TYR:HD2	1.59	0.50
4:A:221:SER:HB2	4:A:1009:THR:HG23	1.93	0.50
1:E:308:ASN:OD1	1:E:477:TYR:N	2.38	0.50
2:G:376:ASP:OD1	2:G:376:ASP:N	2.44	0.50
1:M:394:THR:HG22	1:M:493:ILE:HG22	1.94	0.50
4:A:841:ASN:HD22	4:A:847:ARG:HH21	1.58	0.50
3:J:437:ARG:NH1	3:J:480:GLU:OE1	2.41	0.50
4:I:221:SER:HB2	4:I:1009:THR:HG23	1.94	0.50
4:I:841:ASN:HD22	4:I:847:ARG:HH21	1.58	0.50
1:E:86:SER:HB3	4:A:265:TYR:HB2	1.93	0.50
4:A:477:GLU:OE2	4:A:520:SER:OG	2.21	0.50
3:J:250:GLU:HG2	3:J:266:GLU:HB2	1.94	0.50
7:C:1:FRU:C6	7:C:2:FRU:O5	2.59	0.50
7:K:1:FRU:C6	7:K:2:FRU:O5	2.59	0.50
2:G:132:GLN:HA	2:G:152:ILE:HG23	1.93	0.50
3:B:29:VAL:HG13	3:B:126:MET:HE3	1.94	0.50
4:A:145:ARG:HD2	4:A:711:TYR:CZ	2.47	0.50
3:J:29:VAL:HG13	3:J:126:MET:HE3	1.94	0.50
4:I:933:ASN:O	4:I:937:ARG:NH2	2.43	0.50
2:T:34:LYS:HE3	2:T:87:MET:HE3	1.94	0.50
2:G:187:VAL:HG21	2:G:261:PHE:HZ	1.77	0.50
4:A:367:ARG:HG3	4:A:425:TRP:CZ2	2.46	0.50
5:H:7:FRU:C6	5:H:8:FRU:O5	2.59	0.50
1:E:394:THR:HG22	1:E:493:ILE:HG22	1.94	0.49
3:B:288:MET:HG3	3:B:381:GLU:HB2	1.94	0.49
2:G:147:PRO:HB3	2:G:153:GLN:HE22	1.77	0.49
4:I:718:ILE:HB	4:I:739:GLY:HA3	1.95	0.49
4:A:196:ALA:HA	4:A:625:THR:HG21	1.95	0.49
1:E:142:SER:HB2	1:E:148:TRP:CD2	2.48	0.49
2:G:368:TRP:O	2:G:372:THR:OG1	2.29	0.49
4:A:250:GLU:OE1	4:A:929:ARG:NE	2.45	0.49
3:J:250:GLU:OE2	3:J:265:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:250:GLU:OE1	4:I:929:ARG:NE	2.45	0.49
1:M:215:MET:HE2	1:M:221:TYR:HB2	1.95	0.49
3:B:502:LYS:HG3	3:B:526:GLU:HA	1.95	0.49
3:J:15:THR:OG1	3:J:17:ASP:OD1	2.29	0.49
4:I:635:ARG:HB3	4:I:683:ILE:HD11	1.95	0.49
2:T:70:ILE:HG12	1:M:152:ARG:HD2	1.93	0.48
2:G:64:ILE:HG13	2:G:78:LEU:HD13	1.95	0.48
1:M:383:LYS:O	1:M:386:ASN:ND2	2.37	0.48
3:B:55:SER:HB3	3:B:492:PHE:HB2	1.95	0.48
3:B:340:ARG:NH1	3:B:484:GLU:OE1	2.46	0.48
3:J:288:MET:HG3	3:J:381:GLU:HB2	1.94	0.48
4:I:923:ASP:OD1	4:I:923:ASP:N	2.46	0.48
1:E:215:MET:HE2	1:E:221:TYR:HB2	1.95	0.48
3:B:250:GLU:HG2	3:B:266:GLU:HB2	1.94	0.48
2:G:270:ASN:HB3	2:G:436:LEU:HD22	1.95	0.48
3:B:437:ARG:HH21	3:B:460:VAL:HG23	1.78	0.48
1:M:142:SER:HB2	1:M:148:TRP:CD2	2.48	0.48
3:J:84:ASP:HB3	3:J:86:ASN:OD1	2.14	0.48
3:J:340:ARG:NH1	3:J:484:GLU:OE1	2.46	0.48
3:J:437:ARG:HH21	3:J:460:VAL:HG23	1.78	0.48
1:E:216:MET:SD	1:E:262:THR:OG1	2.72	0.48
3:B:75:GLU:O	3:B:509:TYR:OH	2.26	0.48
1:E:383:LYS:O	1:E:386:ASN:ND2	2.37	0.48
3:B:292:THR:HB	3:B:296:LEU:HD12	1.96	0.48
3:J:242:MET:HE3	3:J:410:VAL:HG11	1.96	0.48
3:J:252:ASP:HB3	3:J:255:MET:HG3	1.95	0.48
5:H:4:FRU:C6	5:H:5:FRU:O5	2.62	0.48
3:J:6:ASP:OD2	4:I:585:LYS:NZ	2.44	0.48
3:J:55:SER:HB3	3:J:492:PHE:HB2	1.95	0.48
7:C:4:FRU:H62	7:C:5:FRU:O5	2.14	0.48
3:B:250:GLU:OE2	3:B:265:ALA:N	2.46	0.47
3:B:252:ASP:OD2	3:B:254:SER:OG	2.26	0.47
4:A:635:ARG:HB3	4:A:683:ILE:HD11	1.95	0.47
4:A:973:LEU:HD13	4:A:1014:ILE:HG12	1.96	0.47
7:K:4:FRU:H62	7:K:5:FRU:O5	2.14	0.47
4:I:196:ALA:HA	4:I:625:THR:HG21	1.95	0.47
4:I:364:THR:HG22	4:I:428:PHE:HB3	1.96	0.47
2:G:205:ALA:O	2:G:209:MET:HG2	2.14	0.47
3:B:48:LEU:HD11	3:B:136:MET:HG3	1.97	0.47
3:J:292:THR:HB	3:J:296:LEU:HD12	1.96	0.47
3:J:502:LYS:HG3	3:J:526:GLU:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:952:ARG:HH22	4:I:996:GLU:CD	2.22	0.47
3:B:15:THR:OG1	3:B:17:ASP:OD1	2.29	0.47
4:A:712:TYR:HD2	4:A:744:GLN:HG2	1.80	0.47
4:A:952:ARG:HH22	4:A:996:GLU:CD	2.22	0.47
4:A:718:ILE:HB	4:A:739:GLY:HA3	1.95	0.47
4:A:963:VAL:HG13	4:A:964:ILE:HD12	1.96	0.47
1:E:362:MET:HB3	1:E:371:LEU:HG	1.97	0.47
1:M:383:LYS:HD2	1:M:502:THR:HG21	1.97	0.47
3:B:84:ASP:HB3	3:B:86:ASN:OD1	2.14	0.47
3:B:89:ASP:O	3:B:93:ARG:HG3	2.15	0.47
3:B:252:ASP:HB3	3:B:255:MET:HG3	1.95	0.47
4:I:973:LEU:HD13	4:I:1014:ILE:HG12	1.96	0.47
1:M:216:MET:SD	1:M:262:THR:OG1	2.72	0.47
1:M:362:MET:HB3	1:M:371:LEU:HG	1.97	0.47
4:A:711:TYR:CZ	4:A:745:GLY:HA3	2.49	0.47
3:J:89:ASP:O	3:J:93:ARG:HG3	2.15	0.47
2:G:238:TRP:CE2	2:G:240:PHE:HB2	2.50	0.47
2:G:341:ASP:HB2	2:G:421:TYR:HD2	1.79	0.47
3:B:412:LEU:HD12	3:B:485:PHE:HE2	1.80	0.47
4:I:711:TYR:CZ	4:I:745:GLY:HA3	2.49	0.47
3:J:412:LEU:HD12	3:J:485:PHE:HE2	1.80	0.47
2:T:81:LYS:HZ3	4:I:277:THR:HG21	1.79	0.46
3:B:14:VAL:HG22	4:I:528:ILE:HD11	1.98	0.46
3:B:194:ARG:HG2	4:A:660:ILE:HD11	1.97	0.46
3:J:48:LEU:HD11	3:J:136:MET:HG3	1.97	0.46
4:A:980:GLN:HB2	4:A:1007:ASN:HB2	1.98	0.46
4:I:101:VAL:HG22	4:I:182:LEU:HD13	1.97	0.46
3:B:242:MET:HE3	3:B:410:VAL:HG11	1.96	0.46
4:A:128:MET:HE2	4:A:130:ILE:HD11	1.97	0.46
4:I:712:TYR:HD2	4:I:744:GLN:HG2	1.80	0.46
4:I:963:VAL:HG13	4:I:964:ILE:HD12	1.96	0.46
2:G:333:ASP:OD1	2:G:333:ASP:N	2.49	0.46
4:A:804:GLN:HB2	4:A:853:TYR:HB3	1.98	0.46
4:I:574:THR:HG22	4:I:594:SER:HB2	1.98	0.46
4:A:101:VAL:HG22	4:A:182:LEU:HD13	1.97	0.46
4:A:156:LEU:HB3	4:A:199:VAL:HG22	1.97	0.46
4:A:177:GLU:N	4:A:203:THR:O	2.47	0.46
4:A:364:THR:HG22	4:A:428:PHE:HB3	1.96	0.46
4:A:574:THR:HG22	4:A:594:SER:HB2	1.98	0.46
3:J:316:SER:HA	3:J:336:ASN:ND2	2.30	0.46
4:I:980:GLN:HB2	4:I:1007:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:LYS:HD2	1:E:502:THR:HG21	1.97	0.46
2:G:42:TYR:HA	2:G:95:ARG:HB3	1.98	0.46
4:A:512:ASN:HB2	4:A:554:LEU:HB2	1.98	0.46
2:G:395:ASN:H	3:B:451:LYS:NZ	2.14	0.46
1:M:187:THR:OG1	1:M:188:ARG:N	2.49	0.46
3:J:194:ARG:HG2	4:I:660:ILE:HD11	1.98	0.46
7:C:3:FRU:C6	7:C:4:FRU:O5	2.64	0.46
3:J:75:GLU:O	3:J:509:TYR:OH	2.26	0.45
4:A:317:GLU:HG2	4:A:318:LYS:HG2	1.98	0.45
2:G:395:ASN:H	3:B:451:LYS:HZ1	1.65	0.45
4:I:177:GLU:N	4:I:203:THR:O	2.47	0.45
4:I:128:MET:HE2	4:I:130:ILE:HD11	1.97	0.45
4:I:317:GLU:HG2	4:I:318:LYS:HG2	1.97	0.45
2:T:23:ASP:OD2	2:T:44:TYR:OH	2.31	0.45
4:A:933:ASN:O	4:A:937:ARG:NH2	2.43	0.45
4:I:501:HIS:HB3	4:I:563:TYR:HE1	1.81	0.45
2:G:294:ASN:HD21	2:G:354:HIS:HB3	1.81	0.45
3:B:96:GLN:HG2	4:A:730:GLU:N	2.32	0.45
2:T:14:ASP:HA	4:I:280:LYS:HE2	1.99	0.45
4:I:512:ASN:HB2	4:I:554:LEU:HB2	1.98	0.45
5:H:6:FRU:H62	5:H:7:FRU:H12	1.51	0.45
7:K:3:FRU:C6	7:K:4:FRU:O5	2.64	0.45
1:E:388:ILE:HG13	1:E:500:VAL:HG22	1.99	0.45
4:A:296:PHE:O	4:A:300:THR:OG1	2.25	0.45
4:A:969:ARG:NH1	4:A:969:ARG:HA	2.32	0.45
1:E:187:THR:OG1	1:E:188:ARG:N	2.49	0.45
1:E:222:GLU:HB2	1:E:238:SER:HB2	1.99	0.45
1:M:71:HIS:ND1	6:N:4:FRU:O1	2.46	0.45
4:A:501:HIS:HB3	4:A:563:TYR:HE1	1.82	0.45
2:G:96:ASP:OD2	2:G:167:SER:OG	2.34	0.45
1:M:244:MET:O	1:M:246:LYS:HG3	2.17	0.45
3:B:93:ARG:HA	3:B:96:GLN:HE21	1.82	0.45
4:I:156:LEU:HB3	4:I:199:VAL:HG22	1.97	0.45
2:G:61:LYS:HB2	2:G:61:LYS:HE2	1.73	0.44
2:G:223:VAL:HB	2:G:230:LEU:HD11	1.98	0.44
1:M:222:GLU:HB2	1:M:238:SER:HB2	1.99	0.44
4:I:633:LEU:HB2	4:I:638:ILE:HD11	1.99	0.44
4:I:804:GLN:HB2	4:I:853:TYR:HB3	1.98	0.44
4:A:519:PHE:CZ	4:I:480:GLN:HB2	2.52	0.44
2:G:276:TYR:OH	2:G:297:TRP:O	2.35	0.44
1:M:251:LYS:NZ	1:M:332:ASP:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:319:LYS:NZ	3:B:462:PRO:O	2.49	0.44
4:A:576:ARG:NH1	4:A:578:ASP:OD1	2.50	0.44
3:B:426:ILE:O	3:B:430:ILE:HG12	2.18	0.44
3:B:434:ASN:OD1	3:B:463:TYR:N	2.51	0.44
4:A:283:ASP:OD2	4:A:287:THR:OG1	2.36	0.44
3:J:434:ASN:OD1	3:J:463:TYR:N	2.51	0.44
1:E:58:TYR:HE1	1:E:76:VAL:HG23	1.83	0.44
2:G:148:ALA:HB3	2:G:151:SER:HB3	1.98	0.44
1:M:308:ASN:OD1	1:M:477:TYR:N	2.38	0.44
3:B:465:LEU:HD23	3:B:465:LEU:HA	1.85	0.44
3:J:96:GLN:HG2	4:I:730:GLU:N	2.32	0.44
3:J:192:LYS:HE2	3:J:263:ASN:HB3	2.00	0.44
3:J:426:ILE:O	3:J:430:ILE:HG12	2.18	0.44
2:G:393:ARG:O	3:B:457:ASN:ND2	2.39	0.44
1:M:172:PHE:HD2	1:M:184:LEU:HD12	1.82	0.44
1:M:262:THR:HA	1:M:266:ALA:HB3	1.99	0.44
1:M:388:ILE:HG13	1:M:500:VAL:HG22	1.99	0.44
4:I:159:ILE:HB	4:I:428:PHE:HE2	1.83	0.44
4:I:969:ARG:NH1	4:I:969:ARG:HA	2.32	0.44
2:G:260:LYS:HE3	2:G:260:LYS:HB3	1.68	0.44
1:E:189:LYS:HB3	1:E:194:HIS:CD2	2.53	0.44
3:B:316:SER:HA	3:B:336:ASN:ND2	2.30	0.44
1:E:251:LYS:NZ	1:E:332:ASP:O	2.50	0.43
1:M:63:ARG:HB2	1:M:64:PRO:HD3	2.00	0.43
1:M:189:LYS:HB3	1:M:194:HIS:CD2	2.53	0.43
4:A:923:ASP:OD1	4:A:923:ASP:N	2.46	0.43
4:I:379:GLU:OE1	4:I:893:LYS:HE3	2.18	0.43
1:E:244:MET:O	1:E:246:LYS:HG3	2.17	0.43
1:E:428:PHE:HB2	1:E:472:PHE:CE2	2.54	0.43
2:G:112:LYS:HB2	2:G:121:SER:OG	2.18	0.43
1:M:428:PHE:HB2	1:M:472:PHE:CE2	2.54	0.43
3:B:192:LYS:HE2	3:B:263:ASN:HB3	2.00	0.43
4:A:633:LEU:HB2	4:A:638:ILE:HD11	1.99	0.43
4:I:283:ASP:OD2	4:I:287:THR:OG1	2.35	0.43
4:I:576:ARG:NH1	4:I:578:ASP:OD1	2.50	0.43
2:T:65:ALA:N	2:T:68:GLU:OE2	2.40	0.43
4:A:574:THR:CG2	4:A:594:SER:HB2	2.49	0.43
4:I:296:PHE:O	4:I:300:THR:OG1	2.25	0.43
2:T:56:LEU:HD11	2:T:62:ALA:HB2	2.00	0.43
4:A:379:GLU:OE1	4:A:893:LYS:HE3	2.18	0.43
3:J:319:LYS:NZ	3:J:462:PRO:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LYS:HD3	1:E:145:PHE:CD2	2.54	0.43
1:E:262:THR:HA	1:E:266:ALA:HB3	1.99	0.43
1:E:394:THR:OG1	1:E:449:ASN:HB3	2.18	0.43
4:A:480:GLN:HB2	4:I:519:PHE:CZ	2.53	0.43
2:G:352:GLN:HB2	2:G:385:VAL:O	2.18	0.43
1:M:55:LYS:HD3	1:M:145:PHE:CD2	2.54	0.43
4:A:107:ASP:OD1	4:A:107:ASP:N	2.52	0.43
4:A:519:PHE:HZ	4:I:480:GLN:HB2	1.83	0.43
4:A:530:THR:HG23	4:A:533:TYR:H	1.84	0.43
1:E:63:ARG:HB2	1:E:64:PRO:HD3	2.01	0.43
2:G:120:ILE:HD13	2:G:174:VAL:HG22	1.99	0.43
3:B:165:TYR:HB2	3:B:170:GLN:HG3	2.00	0.43
4:A:159:ILE:HB	4:A:428:PHE:HE2	1.83	0.43
1:E:172:PHE:HD2	1:E:184:LEU:HD12	1.82	0.43
1:M:58:TYR:HE1	1:M:76:VAL:HG23	1.83	0.43
1:M:155:TYR:HB3	1:M:157:LYS:HE3	2.01	0.43
3:J:165:TYR:HB2	3:J:170:GLN:HG3	2.00	0.43
1:M:394:THR:OG1	1:M:449:ASN:HB3	2.18	0.43
3:B:105:LEU:HG	3:B:126:MET:HB3	2.01	0.43
1:E:136:VAL:HG11	1:E:155:TYR:HD1	1.84	0.43
2:G:275:ARG:NH2	2:G:408:ASP:HA	2.33	0.43
4:I:107:ASP:OD1	4:I:107:ASP:N	2.52	0.42
2:G:278:THR:O	2:G:281:ILE:HG12	2.20	0.42
4:I:530:THR:HG23	4:I:533:TYR:H	1.84	0.42
4:I:574:THR:CG2	4:I:594:SER:HB2	2.48	0.42
1:M:303:ARG:HB2	1:M:477:TYR:HE2	1.85	0.42
1:E:303:ARG:HB2	1:E:477:TYR:HE2	1.84	0.42
2:G:237:TRP:HD1	2:G:272:LEU:O	2.02	0.42
1:M:136:VAL:HG11	1:M:155:TYR:HD1	1.84	0.42
1:M:342:ALA:HA	1:M:345:ARG:HG2	2.00	0.42
3:J:105:LEU:HG	3:J:126:MET:HB3	2.01	0.42
4:I:383:ASP:OD2	7:K:7:FRU:O4	2.38	0.42
4:I:962:ALA:O	4:I:966:LYS:HG2	2.19	0.42
2:G:409:TRP:HZ3	2:G:426:GLU:HG3	1.84	0.42
4:A:406:ASP:OD1	4:A:406:ASP:N	2.52	0.42
3:J:548:GLN:HG3	3:J:552:TRP:HB2	2.02	0.42
4:I:612:TRP:CD1	4:I:612:TRP:H	2.37	0.42
2:G:294:ASN:OD1	2:G:295:ASN:N	2.52	0.42
4:A:480:GLN:HB2	4:I:519:PHE:HZ	1.84	0.42
4:A:714:LYS:HE3	4:A:776:LEU:HD12	2.01	0.42
2:G:295:ASN:ND2	5:H:3:FRU:O1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:612:TRP:H	4:A:612:TRP:CD1	2.37	0.42
1:E:342:ALA:HA	1:E:345:ARG:HG2	2.01	0.42
4:A:175:ASP:HA	4:A:205:LYS:HD2	2.02	0.42
4:I:858:SER:HB2	4:I:883:GLY:HA3	2.02	0.42
1:E:422:ASP:OD1	1:E:423:GLU:N	2.53	0.41
4:A:858:SER:HB2	4:A:883:GLY:HA3	2.02	0.41
4:A:962:ALA:O	4:A:966:LYS:HG2	2.19	0.41
4:I:104:VAL:HB	4:I:179:ILE:HB	2.01	0.41
4:I:306:GLN:HE21	4:I:329:LYS:HD3	1.84	0.41
1:E:71:HIS:ND1	6:F:4:FRU:O1	2.50	0.41
4:A:528:ILE:HD11	3:J:14:VAL:HG22	2.02	0.41
4:I:714:LYS:HE3	4:I:776:LEU:HD12	2.01	0.41
2:G:386:VAL:HB	2:G:404:SER:HB3	2.01	0.41
3:B:290:LEU:HA	3:B:299:CYS:HB3	2.03	0.41
1:E:398:THR:O	1:E:490:LYS:NZ	2.39	0.41
4:A:306:GLN:HE21	4:A:329:LYS:HD3	1.84	0.41
4:A:308:TYR:HD2	4:A:327:TYR:HD2	1.69	0.41
4:I:308:TYR:HD2	4:I:327:TYR:HD2	1.68	0.41
6:F:1:FRU:C6	6:F:2:FRU:O5	2.69	0.41
1:E:55:LYS:HD3	1:E:145:PHE:CE2	2.56	0.41
1:M:228:LYS:NZ	1:M:230:GLY:O	2.54	0.41
4:A:94:LYS:HD3	4:A:101:VAL:HB	2.03	0.41
4:I:370:GLU:OE1	4:I:422:TYR:OH	2.29	0.41
6:N:1:FRU:C6	6:N:2:FRU:O5	2.69	0.41
4:A:406:ASP:HB2	4:A:468:GLN:HE21	1.85	0.41
1:E:155:TYR:HB3	1:E:157:LYS:HE3	2.01	0.41
1:M:410:ASP:OD1	1:M:410:ASP:N	2.53	0.41
3:B:253:TYR:OH	3:B:484:GLU:O	2.38	0.41
3:J:277:ASP:OD1	3:J:282:GLY:HA2	2.21	0.41
1:E:120:PHE:HB2	1:E:173:LEU:HD11	2.03	0.41
2:G:229:ASP:OD1	2:G:229:ASP:N	2.49	0.41
2:G:288:LYS:HB2	2:G:371:LEU:O	2.21	0.41
2:G:314:LEU:HD22	2:G:381:GLY:HA2	2.02	0.41
1:M:124:ASN:OD1	1:M:135:GLN:HG2	2.21	0.41
1:M:422:ASP:OD1	1:M:423:GLU:N	2.53	0.41
4:A:333:VAL:HG11	4:A:1005:PRO:HB3	2.03	0.41
4:A:609:GLU:HG2	4:A:610:LEU:HD12	2.03	0.41
4:A:641:PRO:HG3	4:I:533:TYR:OH	2.21	0.41
3:J:56:ASP:OD1	3:J:56:ASP:N	2.44	0.41
1:E:124:ASN:ND2	6:F:4:FRU:H11	2.36	0.41
2:G:297:TRP:CD1	5:H:2:FRU:HO3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:433:ILE:HD13	2:G:433:ILE:HA	1.94	0.41
1:M:168:PHE:CE1	1:M:185:ILE:HG21	2.56	0.41
4:I:406:ASP:HB2	4:I:468:GLN:HE21	1.85	0.41
3:B:99:THR:OG1	4:A:729:GLY:HA3	2.21	0.40
4:I:94:LYS:HD3	4:I:101:VAL:HB	2.03	0.40
4:I:609:GLU:HG2	4:I:610:LEU:HD12	2.03	0.40
4:A:891:LYS:HE2	4:A:891:LYS:HB2	1.90	0.40
1:E:124:ASN:OD1	1:E:135:GLN:HG2	2.21	0.40
1:M:171:PRO:HA	1:M:185:ILE:HD13	2.04	0.40
3:B:548:GLN:HG3	3:B:552:TRP:HB2	2.02	0.40
3:J:465:LEU:HD23	3:J:465:LEU:HA	1.85	0.40
4:I:175:ASP:HA	4:I:205:LYS:HD2	2.02	0.40
6:N:3:FRU:C6	6:N:4:FRU:O5	2.70	0.40
4:A:104:VAL:HB	4:A:179:ILE:HB	2.01	0.40
1:E:228:LYS:NZ	1:E:230:GLY:O	2.54	0.40
2:G:184:THR:HG23	2:G:235:ALA:HB3	2.03	0.40
1:M:55:LYS:HD3	1:M:145:PHE:CE2	2.56	0.40
1:M:240:GLN:NE2	6:N:2:FRU:O3	2.54	0.40
3:B:157:TYR:HD2	4:A:727:VAL:HG23	1.86	0.40
4:A:115:ASN:HB2	4:A:328:TYR:CZ	2.57	0.40
6:F:3:FRU:C6	6:F:4:FRU:O5	2.70	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	E	495/523 (95%)	472 (95%)	22 (4%)	1 (0%)	43	73
1	M	495/523 (95%)	472 (95%)	22 (4%)	1 (0%)	43	73
2	G	433/467 (93%)	401 (93%)	32 (7%)	0	100	100
2	T	91/467 (20%)	86 (94%)	4 (4%)	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	549/570 (96%)	538 (98%)	11 (2%)	0	100	100
3	J	549/570 (96%)	538 (98%)	11 (2%)	0	100	100
4	A	922/1041 (89%)	899 (98%)	23 (2%)	0	100	100
4	I	922/1041 (89%)	898 (97%)	24 (3%)	0	100	100
All	All	4456/5202 (86%)	4304 (97%)	149 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	314	VAL
2	T	46	ILE
1	M	314	VAL

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	E	421/443 (95%)	421 (100%)	0	100	100
1	M	421/443 (95%)	421 (100%)	0	100	100
2	G	361/393 (92%)	361 (100%)	0	100	100
2	T	81/393 (21%)	81 (100%)	0	100	100
3	B	472/489 (96%)	472 (100%)	0	100	100
3	J	472/489 (96%)	472 (100%)	0	100	100
4	A	768/869 (88%)	768 (100%)	0	100	100
4	I	768/869 (88%)	768 (100%)	0	100	100
All	All	3764/4388 (86%)	3764 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	E	133	ASN
1	E	361	ASN
2	G	295	ASN
1	M	133	ASN
3	B	120	ASN
3	B	283	ASN
3	B	307	ASN
3	B	420	GLN
4	A	211	GLN
4	A	262	ASN
4	A	306	GLN
4	A	482	HIS
4	A	489	ASN
4	A	642	ASN
4	A	754	ASN
4	A	816	GLN
4	A	825	GLN
4	A	1013	ASN
3	J	96	GLN
3	J	120	ASN
3	J	283	ASN
3	J	307	ASN
3	J	420	GLN
4	I	211	GLN
4	I	262	ASN
4	I	306	GLN
4	I	417	ASN
4	I	482	HIS
4	I	642	ASN
4	I	680	ASN
4	I	754	ASN
4	I	816	GLN
4	I	1013	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

45 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FRU	C	1	7	11,12,12	4.74	6 (54%)	10,18,18	0.90	1 (10%)
7	FRU	C	2	7	11,11,12	4.10	6 (54%)	15,15,18	1.13	2 (13%)
7	FRU	C	3	7	11,11,12	4.12	6 (54%)	15,15,18	0.79	1 (6%)
7	FRU	C	4	7	11,11,12	4.13	6 (54%)	15,15,18	0.98	1 (6%)
7	FRU	C	5	7	11,11,12	4.11	6 (54%)	15,15,18	0.97	2 (13%)
7	FRU	C	6	7	11,11,12	4.10	6 (54%)	15,15,18	1.10	2 (13%)
7	FRU	C	7	7	11,11,12	4.14	6 (54%)	15,15,18	0.90	2 (13%)
8	FRU	D	1	8	11,12,12	4.76	6 (54%)	10,18,18	0.82	0
8	FRU	D	2	8	11,11,12	4.10	6 (54%)	15,15,18	0.94	1 (6%)
8	FRU	D	3	8	11,11,12	4.11	6 (54%)	15,15,18	1.12	2 (13%)
8	FRU	D	4	8	11,11,12	4.11	6 (54%)	15,15,18	0.97	1 (6%)
6	FRU	F	1	6	11,12,12	4.70	6 (54%)	10,18,18	0.91	1 (10%)
6	FRU	F	2	6	11,11,12	4.11	6 (54%)	15,15,18	1.08	2 (13%)
6	FRU	F	3	6	11,11,12	4.09	6 (54%)	15,15,18	1.06	1 (6%)
6	FRU	F	4	6	11,11,12	4.12	6 (54%)	15,15,18	1.01	1 (6%)
6	FRU	F	5	6	11,11,12	4.10	6 (54%)	15,15,18	1.09	2 (13%)
5	FRU	H	1	5	11,12,12	4.77	6 (54%)	10,18,18	0.82	0
5	FRU	H	10	5	11,11,12	4.10	6 (54%)	15,15,18	1.11	2 (13%)
5	FRU	H	11	5	11,11,12	4.09	6 (54%)	15,15,18	0.99	2 (13%)
5	FRU	H	12	5	11,11,12	4.10	6 (54%)	15,15,18	1.00	2 (13%)
5	FRU	H	13	5	11,11,12	4.06	6 (54%)	15,15,18	4.01	4 (26%)
5	FRU	H	2	5	11,11,12	4.12	6 (54%)	15,15,18	1.03	2 (13%)
5	FRU	H	3	5	11,11,12	4.11	6 (54%)	15,15,18	0.96	1 (6%)
5	FRU	H	4	5	11,11,12	4.10	6 (54%)	15,15,18	1.17	1 (6%)
5	FRU	H	5	5	11,11,12	4.10	6 (54%)	15,15,18	0.96	1 (6%)
5	FRU	H	6	5	11,11,12	4.06	6 (54%)	15,15,18	1.33	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FRU	H	7	5	11,11,12	4.13	6 (54%)	15,15,18	1.22	2 (13%)
5	FRU	H	8	5	11,11,12	4.12	6 (54%)	15,15,18	1.09	1 (6%)
5	FRU	H	9	5	11,11,12	4.09	6 (54%)	15,15,18	1.27	2 (13%)
7	FRU	K	1	7	11,12,12	4.74	6 (54%)	10,18,18	0.90	1 (10%)
7	FRU	K	2	7	11,11,12	4.10	6 (54%)	15,15,18	1.12	2 (13%)
7	FRU	K	3	7	11,11,12	4.12	6 (54%)	15,15,18	0.79	1 (6%)
7	FRU	K	4	7	11,11,12	4.14	6 (54%)	15,15,18	0.98	1 (6%)
7	FRU	K	5	7	11,11,12	4.13	6 (54%)	15,15,18	0.97	2 (13%)
7	FRU	K	6	7	11,11,12	4.11	6 (54%)	15,15,18	1.10	2 (13%)
7	FRU	K	7	7	11,11,12	4.14	6 (54%)	15,15,18	0.90	2 (13%)
8	FRU	L	1	8	11,12,12	4.76	6 (54%)	10,18,18	0.82	0
8	FRU	L	2	8	11,11,12	4.12	6 (54%)	15,15,18	0.94	1 (6%)
8	FRU	L	3	8	11,11,12	4.11	6 (54%)	15,15,18	1.12	1 (6%)
8	FRU	L	4	8	11,11,12	4.11	6 (54%)	15,15,18	0.97	1 (6%)
6	FRU	N	1	6	11,12,12	4.72	6 (54%)	10,18,18	0.91	1 (10%)
6	FRU	N	2	6	11,11,12	4.11	6 (54%)	15,15,18	1.08	2 (13%)
6	FRU	N	3	6	11,11,12	4.09	6 (54%)	15,15,18	1.06	1 (6%)
6	FRU	N	4	6	11,11,12	4.11	6 (54%)	15,15,18	1.01	1 (6%)
6	FRU	N	5	6	11,11,12	4.10	6 (54%)	15,15,18	1.08	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FRU	C	1	7	-	5/5/24/24	0/1/1/1
7	FRU	C	2	7	-	4/4/20/24	0/1/1/1
7	FRU	C	3	7	-	2/4/20/24	0/1/1/1
7	FRU	C	4	7	-	0/4/20/24	0/1/1/1
7	FRU	C	5	7	-	4/4/20/24	0/1/1/1
7	FRU	C	6	7	-	0/4/20/24	0/1/1/1
7	FRU	C	7	7	-	2/4/20/24	0/1/1/1
8	FRU	D	1	8	-	3/5/24/24	0/1/1/1
8	FRU	D	2	8	-	0/4/20/24	0/1/1/1
8	FRU	D	3	8	-	4/4/20/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FRU	D	4	8	-	2/4/20/24	0/1/1/1
6	FRU	F	1	6	-	3/5/24/24	0/1/1/1
6	FRU	F	2	6	-	4/4/20/24	0/1/1/1
6	FRU	F	3	6	-	2/4/20/24	0/1/1/1
6	FRU	F	4	6	-	2/4/20/24	0/1/1/1
6	FRU	F	5	6	-	2/4/20/24	0/1/1/1
5	FRU	H	1	5	-	2/5/24/24	0/1/1/1
5	FRU	H	10	5	-	4/4/20/24	0/1/1/1
5	FRU	H	11	5	-	4/4/20/24	0/1/1/1
5	FRU	H	12	5	-	2/4/20/24	0/1/1/1
5	FRU	H	13	5	1/1/4/4	4/4/20/24	0/1/1/1
5	FRU	H	2	5	-	1/4/20/24	0/1/1/1
5	FRU	H	3	5	-	4/4/20/24	0/1/1/1
5	FRU	H	4	5	-	4/4/20/24	0/1/1/1
5	FRU	H	5	5	-	4/4/20/24	0/1/1/1
5	FRU	H	6	5	-	2/4/20/24	0/1/1/1
5	FRU	H	7	5	-	2/4/20/24	0/1/1/1
5	FRU	H	8	5	-	4/4/20/24	0/1/1/1
5	FRU	H	9	5	-	2/4/20/24	0/1/1/1
7	FRU	K	1	7	-	5/5/24/24	0/1/1/1
7	FRU	K	2	7	-	4/4/20/24	0/1/1/1
7	FRU	K	3	7	-	2/4/20/24	0/1/1/1
7	FRU	K	4	7	-	0/4/20/24	0/1/1/1
7	FRU	K	5	7	-	4/4/20/24	0/1/1/1
7	FRU	K	6	7	-	0/4/20/24	0/1/1/1
7	FRU	K	7	7	-	2/4/20/24	0/1/1/1
8	FRU	L	1	8	-	3/5/24/24	0/1/1/1
8	FRU	L	2	8	-	0/4/20/24	0/1/1/1
8	FRU	L	3	8	-	4/4/20/24	0/1/1/1
8	FRU	L	4	8	-	2/4/20/24	0/1/1/1
6	FRU	N	1	6	-	3/5/24/24	0/1/1/1
6	FRU	N	2	6	-	4/4/20/24	0/1/1/1
6	FRU	N	3	6	-	2/4/20/24	0/1/1/1
6	FRU	N	4	6	-	2/4/20/24	0/1/1/1
6	FRU	N	5	6	-	2/4/20/24	0/1/1/1

All (270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	FRU	O5-C2	13.21	1.64	1.43
8	L	1	FRU	O5-C2	13.20	1.64	1.43
8	D	1	FRU	O5-C2	13.18	1.64	1.43
7	C	1	FRU	O5-C2	13.14	1.64	1.43
7	K	1	FRU	O5-C2	13.14	1.64	1.43
6	N	1	FRU	O5-C2	12.95	1.64	1.43
6	F	1	FRU	O5-C2	12.90	1.64	1.43
5	H	6	FRU	O5-C2	8.83	1.64	1.45
6	F	4	FRU	O5-C2	8.83	1.64	1.45
5	H	2	FRU	O5-C2	8.80	1.64	1.45
7	K	4	FRU	O5-C2	8.80	1.64	1.45
6	N	4	FRU	O5-C2	8.80	1.64	1.45
7	K	2	FRU	O5-C2	8.78	1.64	1.45
5	H	7	FRU	O5-C2	8.77	1.64	1.45
7	C	2	FRU	O5-C2	8.77	1.64	1.45
5	H	8	FRU	O5-C2	8.76	1.64	1.45
8	L	3	FRU	O5-C2	8.76	1.64	1.45
7	K	5	FRU	O5-C2	8.76	1.64	1.45
8	D	3	FRU	O5-C2	8.75	1.64	1.45
7	C	4	FRU	O5-C2	8.75	1.64	1.45
7	C	5	FRU	O5-C2	8.73	1.64	1.45
5	H	10	FRU	O5-C2	8.72	1.64	1.45
5	H	4	FRU	O5-C2	8.71	1.64	1.45
7	C	7	FRU	O5-C2	8.69	1.64	1.45
7	C	3	FRU	O5-C2	8.69	1.64	1.45
5	H	5	FRU	O5-C2	8.68	1.64	1.45
7	K	3	FRU	O5-C2	8.67	1.64	1.45
5	H	9	FRU	O5-C2	8.66	1.64	1.45
7	K	7	FRU	O5-C2	8.66	1.64	1.45
7	K	6	FRU	O5-C2	8.64	1.64	1.45
7	C	6	FRU	O5-C2	8.63	1.64	1.45
8	D	4	FRU	O5-C2	8.63	1.64	1.45
6	F	2	FRU	O5-C2	8.62	1.64	1.45
5	H	3	FRU	O5-C2	8.62	1.64	1.45
5	H	12	FRU	O5-C2	8.62	1.64	1.45
8	L	2	FRU	O5-C2	8.61	1.64	1.45
8	L	4	FRU	O5-C2	8.61	1.64	1.45
6	N	2	FRU	O5-C2	8.61	1.64	1.45
6	F	5	FRU	O5-C2	8.60	1.64	1.45
6	N	5	FRU	O5-C2	8.60	1.64	1.45
6	F	3	FRU	O5-C2	8.56	1.64	1.45
6	N	3	FRU	O5-C2	8.56	1.64	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2	FRU	O5-C2	8.56	1.64	1.45
5	H	11	FRU	O5-C2	8.51	1.63	1.45
5	H	13	FRU	O5-C2	8.44	1.63	1.45
7	K	7	FRU	C3-C2	-6.96	1.35	1.53
7	K	3	FRU	C3-C2	-6.95	1.35	1.53
7	C	7	FRU	C3-C2	-6.95	1.35	1.53
7	C	3	FRU	C3-C2	-6.93	1.35	1.53
8	L	2	FRU	C3-C2	-6.93	1.35	1.53
8	D	2	FRU	C3-C2	-6.91	1.35	1.53
5	H	3	FRU	C3-C2	-6.88	1.35	1.53
7	C	4	FRU	C3-C2	-6.86	1.35	1.53
7	K	4	FRU	C3-C2	-6.86	1.35	1.53
7	C	6	FRU	C3-C2	-6.84	1.35	1.53
8	L	4	FRU	C3-C2	-6.84	1.35	1.53
7	K	6	FRU	C3-C2	-6.83	1.35	1.53
8	D	4	FRU	C3-C2	-6.83	1.35	1.53
7	K	5	FRU	C3-C2	-6.81	1.35	1.53
7	C	5	FRU	C3-C2	-6.79	1.35	1.53
6	N	2	FRU	C3-C2	-6.78	1.35	1.53
6	F	3	FRU	C3-C2	-6.78	1.35	1.53
6	N	5	FRU	C3-C2	-6.77	1.35	1.53
6	F	2	FRU	C3-C2	-6.77	1.35	1.53
6	F	5	FRU	C3-C2	-6.76	1.35	1.53
5	H	8	FRU	C3-C2	-6.75	1.35	1.53
5	H	7	FRU	C3-C2	-6.74	1.35	1.53
6	N	3	FRU	C3-C2	-6.74	1.35	1.53
5	H	11	FRU	C3-C2	-6.72	1.35	1.53
5	H	12	FRU	C3-C2	-6.72	1.36	1.53
5	H	4	FRU	C3-C2	-6.71	1.36	1.53
5	H	2	FRU	C3-C2	-6.70	1.36	1.53
8	L	3	FRU	C3-C2	-6.67	1.36	1.53
8	D	3	FRU	C3-C2	-6.67	1.36	1.53
5	H	9	FRU	C3-C2	-6.66	1.36	1.53
7	C	2	FRU	C3-C2	-6.65	1.36	1.53
6	F	4	FRU	C3-C2	-6.65	1.36	1.53
7	K	2	FRU	C3-C2	-6.64	1.36	1.53
6	N	4	FRU	C3-C2	-6.62	1.36	1.53
5	H	10	FRU	C3-C2	-6.54	1.36	1.53
5	H	5	FRU	C3-C2	-6.51	1.36	1.53
5	H	13	FRU	C3-C2	-6.47	1.36	1.53
5	H	6	FRU	C3-C2	-6.26	1.37	1.53
5	H	5	FRU	O5-C5	-5.75	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	10	FRU	O5-C5	-5.73	1.32	1.45
8	L	3	FRU	O5-C5	-5.65	1.32	1.45
8	D	3	FRU	O5-C5	-5.65	1.32	1.45
5	H	11	FRU	O5-C5	-5.65	1.32	1.45
6	N	4	FRU	O5-C5	-5.64	1.32	1.45
5	H	7	FRU	O5-C5	-5.64	1.32	1.45
6	N	2	FRU	O5-C5	-5.63	1.32	1.45
6	F	2	FRU	O5-C5	-5.62	1.32	1.45
6	F	4	FRU	O5-C5	-5.62	1.32	1.45
7	K	4	FRU	O5-C5	-5.60	1.32	1.45
7	C	4	FRU	O5-C5	-5.60	1.32	1.45
5	H	12	FRU	O5-C5	-5.59	1.32	1.45
6	F	5	FRU	O5-C5	-5.59	1.32	1.45
6	N	3	FRU	O5-C5	-5.58	1.32	1.45
6	N	5	FRU	O5-C5	-5.58	1.32	1.45
7	K	5	FRU	O5-C5	-5.57	1.32	1.45
6	F	3	FRU	O5-C5	-5.56	1.32	1.45
5	H	8	FRU	O5-C5	-5.56	1.32	1.45
7	C	2	FRU	O5-C5	-5.55	1.32	1.45
7	C	5	FRU	O5-C5	-5.55	1.32	1.45
5	H	9	FRU	O5-C5	-5.55	1.32	1.45
7	K	2	FRU	O5-C5	-5.53	1.32	1.45
8	L	4	FRU	O5-C5	-5.52	1.32	1.45
5	H	4	FRU	O5-C5	-5.52	1.32	1.45
7	K	6	FRU	O5-C5	-5.52	1.32	1.45
5	H	2	FRU	O5-C5	-5.52	1.32	1.45
7	C	7	FRU	O5-C5	-5.51	1.32	1.45
8	L	2	FRU	O5-C5	-5.50	1.32	1.45
8	D	2	FRU	O5-C5	-5.49	1.32	1.45
7	C	6	FRU	O5-C5	-5.48	1.32	1.45
8	D	4	FRU	O5-C5	-5.48	1.32	1.45
7	K	7	FRU	O5-C5	-5.48	1.32	1.45
7	C	3	FRU	O5-C5	-5.46	1.32	1.45
5	H	3	FRU	O5-C5	-5.45	1.32	1.45
7	K	3	FRU	O5-C5	-5.45	1.32	1.45
5	H	6	FRU	O5-C5	-5.44	1.32	1.45
5	H	13	FRU	O5-C5	-5.28	1.33	1.45
6	N	1	FRU	O5-C5	-5.17	1.32	1.43
6	F	1	FRU	O5-C5	-5.15	1.32	1.43
5	H	1	FRU	O5-C5	-5.13	1.32	1.43
8	D	1	FRU	O5-C5	-5.03	1.32	1.43
8	L	1	FRU	O5-C5	-5.03	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1	FRU	O5-C5	-5.01	1.32	1.43
7	K	1	FRU	O5-C5	-4.98	1.32	1.43
7	K	3	FRU	O4-C4	-4.13	1.32	1.43
7	C	5	FRU	O4-C4	-4.13	1.32	1.43
7	C	3	FRU	O4-C4	-4.12	1.32	1.43
7	K	5	FRU	O4-C4	-4.10	1.32	1.43
7	K	4	FRU	O4-C4	-4.10	1.32	1.43
7	K	2	FRU	O4-C4	-4.10	1.32	1.43
7	C	4	FRU	O4-C4	-4.10	1.32	1.43
8	L	2	FRU	O4-C4	-4.09	1.32	1.43
8	L	1	FRU	O4-C4	-4.09	1.32	1.43
5	H	2	FRU	O4-C4	-4.08	1.32	1.43
7	C	2	FRU	O4-C4	-4.08	1.32	1.43
8	D	3	FRU	O4-C4	-4.08	1.32	1.43
5	H	5	FRU	O4-C4	-4.07	1.32	1.43
8	D	1	FRU	O4-C4	-4.07	1.32	1.43
6	N	3	FRU	O4-C4	-4.07	1.32	1.43
8	D	2	FRU	O4-C4	-4.07	1.32	1.43
5	H	6	FRU	O4-C4	-4.07	1.32	1.43
8	L	3	FRU	O4-C4	-4.07	1.32	1.43
5	H	8	FRU	O4-C4	-4.06	1.32	1.43
7	K	7	FRU	O4-C4	-4.05	1.32	1.43
7	C	7	FRU	O4-C4	-4.05	1.32	1.43
6	F	3	FRU	O4-C4	-4.05	1.32	1.43
6	F	4	FRU	O4-C4	-4.05	1.32	1.43
5	H	3	FRU	O4-C4	-4.04	1.32	1.43
5	H	7	FRU	O4-C4	-4.04	1.33	1.43
5	H	4	FRU	O4-C4	-4.04	1.33	1.43
5	H	1	FRU	O4-C4	-4.03	1.33	1.43
5	H	10	FRU	O4-C4	-4.03	1.33	1.43
8	D	4	FRU	O4-C4	-4.03	1.33	1.43
6	F	1	FRU	O4-C4	-4.03	1.33	1.43
8	L	4	FRU	O4-C4	-4.02	1.33	1.43
6	N	2	FRU	O4-C4	-4.02	1.33	1.43
5	H	11	FRU	O4-C4	-4.02	1.33	1.43
6	F	2	FRU	O4-C4	-4.02	1.33	1.43
5	H	9	FRU	O4-C4	-4.01	1.33	1.43
5	H	13	FRU	O4-C4	-4.01	1.33	1.43
7	C	1	FRU	O4-C4	-4.00	1.33	1.43
6	N	5	FRU	O4-C4	-4.00	1.33	1.43
6	N	1	FRU	O4-C4	-4.00	1.33	1.43
6	N	4	FRU	O4-C4	-3.99	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	1	FRU	O4-C4	-3.99	1.33	1.43
7	K	6	FRU	O4-C4	-3.99	1.33	1.43
6	F	5	FRU	O4-C4	-3.99	1.33	1.43
7	C	6	FRU	O4-C4	-3.98	1.33	1.43
5	H	12	FRU	O4-C4	-3.97	1.33	1.43
6	N	1	FRU	C1-C2	3.85	1.61	1.52
7	K	1	FRU	C1-C2	3.80	1.60	1.52
8	D	1	FRU	C1-C2	3.78	1.60	1.52
6	F	1	FRU	C1-C2	3.78	1.60	1.52
5	H	1	FRU	C1-C2	3.76	1.60	1.52
7	C	1	FRU	C1-C2	3.73	1.60	1.52
8	L	1	FRU	C1-C2	3.71	1.60	1.52
5	H	13	FRU	C4-C5	3.22	1.61	1.53
5	H	13	FRU	C1-C2	2.95	1.61	1.51
8	L	1	FRU	O2-C2	-2.80	1.35	1.40
8	D	1	FRU	O2-C2	-2.79	1.35	1.40
5	H	11	FRU	C1-C2	2.78	1.61	1.51
8	L	4	FRU	C4-C5	2.77	1.60	1.53
6	N	1	FRU	C4-C5	2.76	1.60	1.53
7	K	1	FRU	O2-C2	-2.76	1.35	1.40
8	D	4	FRU	C4-C5	2.76	1.60	1.53
5	H	3	FRU	C4-C5	2.76	1.60	1.53
5	H	12	FRU	C4-C5	2.75	1.60	1.53
6	F	1	FRU	C4-C5	2.75	1.60	1.53
7	K	7	FRU	C4-C5	2.74	1.59	1.53
7	C	7	FRU	C4-C5	2.74	1.59	1.53
5	H	12	FRU	C1-C2	2.74	1.61	1.51
6	N	1	FRU	O2-C2	-2.73	1.36	1.40
5	H	3	FRU	C1-C2	2.73	1.61	1.51
5	H	7	FRU	C1-C2	2.73	1.61	1.51
8	L	2	FRU	C4-C5	2.73	1.59	1.53
6	F	2	FRU	C4-C5	2.72	1.59	1.53
6	N	2	FRU	C4-C5	2.71	1.59	1.53
6	N	5	FRU	C4-C5	2.71	1.59	1.53
7	C	1	FRU	O2-C2	-2.70	1.36	1.40
6	N	3	FRU	C4-C5	2.70	1.59	1.53
7	C	1	FRU	C4-C5	2.70	1.59	1.53
7	K	6	FRU	C4-C5	2.70	1.59	1.53
6	N	3	FRU	C1-C2	2.70	1.60	1.51
8	D	4	FRU	C1-C2	2.69	1.60	1.51
6	F	3	FRU	C1-C2	2.69	1.60	1.51
7	K	1	FRU	C4-C5	2.69	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2	FRU	C4-C5	2.69	1.59	1.53
5	H	10	FRU	C1-C2	2.69	1.60	1.51
6	F	1	FRU	O2-C2	-2.69	1.36	1.40
7	C	6	FRU	C4-C5	2.69	1.59	1.53
8	L	4	FRU	C1-C2	2.69	1.60	1.51
6	F	3	FRU	C4-C5	2.69	1.59	1.53
7	C	2	FRU	C1-C2	2.68	1.60	1.51
7	K	7	FRU	C1-C2	2.68	1.60	1.51
6	N	5	FRU	C1-C2	2.68	1.60	1.51
5	H	6	FRU	C1-C2	2.68	1.60	1.51
7	K	2	FRU	C1-C2	2.68	1.60	1.51
7	K	6	FRU	C1-C2	2.68	1.60	1.51
7	C	5	FRU	C1-C2	2.67	1.60	1.51
5	H	11	FRU	C4-C5	2.67	1.59	1.53
5	H	2	FRU	C1-C2	2.67	1.60	1.51
8	L	3	FRU	C1-C2	2.67	1.60	1.51
5	H	5	FRU	C1-C2	2.67	1.60	1.51
6	F	5	FRU	C1-C2	2.67	1.60	1.51
5	H	9	FRU	C4-C5	2.67	1.59	1.53
5	H	8	FRU	C1-C2	2.66	1.60	1.51
7	C	7	FRU	C1-C2	2.66	1.60	1.51
5	H	1	FRU	O2-C2	-2.66	1.36	1.40
6	F	2	FRU	C1-C2	2.66	1.60	1.51
6	F	5	FRU	C4-C5	2.66	1.59	1.53
5	H	6	FRU	C4-C5	2.66	1.59	1.53
8	D	3	FRU	C1-C2	2.65	1.60	1.51
8	D	2	FRU	C1-C2	2.65	1.60	1.51
5	H	9	FRU	C1-C2	2.65	1.60	1.51
7	C	6	FRU	C1-C2	2.65	1.60	1.51
6	N	4	FRU	C1-C2	2.65	1.60	1.51
7	K	5	FRU	C1-C2	2.65	1.60	1.51
6	F	4	FRU	C1-C2	2.64	1.60	1.51
7	K	3	FRU	C1-C2	2.64	1.60	1.51
8	L	2	FRU	C1-C2	2.63	1.60	1.51
5	H	4	FRU	C1-C2	2.63	1.60	1.51
7	C	3	FRU	C1-C2	2.62	1.60	1.51
6	N	2	FRU	C1-C2	2.62	1.60	1.51
5	H	4	FRU	C4-C5	2.61	1.59	1.53
7	K	4	FRU	C1-C2	2.59	1.60	1.51
7	C	4	FRU	C1-C2	2.59	1.60	1.51
5	H	5	FRU	C4-C5	2.59	1.59	1.53
8	D	1	FRU	C4-C5	2.59	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1	FRU	C4-C5	2.58	1.59	1.53
7	K	3	FRU	C4-C5	2.57	1.59	1.53
5	H	10	FRU	C4-C5	2.57	1.59	1.53
5	H	1	FRU	C4-C5	2.56	1.59	1.53
5	H	2	FRU	C4-C5	2.55	1.59	1.53
7	C	3	FRU	C4-C5	2.55	1.59	1.53
5	H	7	FRU	C4-C5	2.51	1.59	1.53
5	H	8	FRU	C4-C5	2.51	1.59	1.53
7	K	5	FRU	C4-C5	2.50	1.59	1.53
6	F	4	FRU	C4-C5	2.50	1.59	1.53
7	K	2	FRU	C4-C5	2.50	1.59	1.53
7	C	2	FRU	C4-C5	2.50	1.59	1.53
6	N	4	FRU	C4-C5	2.49	1.59	1.53
7	C	5	FRU	C4-C5	2.48	1.59	1.53
8	D	3	FRU	C4-C5	2.47	1.59	1.53
8	L	3	FRU	C4-C5	2.46	1.59	1.53
7	C	4	FRU	C4-C5	2.43	1.59	1.53
7	K	4	FRU	C4-C5	2.40	1.59	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	13	FRU	O5-C2-C1	-10.11	87.84	109.22
5	H	13	FRU	C1-C2-C3	-9.93	91.65	115.10
5	H	13	FRU	O5-C2-C3	5.09	115.26	105.15
5	H	6	FRU	C1-C2-C3	-3.35	107.19	115.10
5	H	7	FRU	C1-C2-C3	-3.12	107.72	115.10
7	K	2	FRU	C1-C2-C3	-2.75	108.60	115.10
7	C	2	FRU	C1-C2-C3	-2.75	108.61	115.10
5	H	3	FRU	C1-C2-C3	-2.66	108.81	115.10
8	L	3	FRU	C1-C2-C3	-2.65	108.85	115.10
8	D	3	FRU	C1-C2-C3	-2.64	108.86	115.10
5	H	5	FRU	C1-C2-C3	-2.63	108.89	115.10
5	H	8	FRU	C1-C2-C3	-2.62	108.91	115.10
5	H	2	FRU	C1-C2-C3	-2.59	108.98	115.10
6	F	2	FRU	C1-C2-C3	-2.59	108.99	115.10
6	N	3	FRU	C1-C2-C3	-2.58	109.01	115.10
6	F	3	FRU	C1-C2-C3	-2.57	109.03	115.10
6	N	2	FRU	C1-C2-C3	-2.57	109.04	115.10
7	K	4	FRU	C1-C2-C3	-2.56	109.04	115.10
5	H	9	FRU	C1-C2-C3	-2.56	109.05	115.10
7	C	4	FRU	C1-C2-C3	-2.55	109.09	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	6	FRU	C4-C3-C2	2.52	107.48	102.61
7	K	6	FRU	C1-C2-C3	-2.51	109.17	115.10
7	C	6	FRU	C1-C2-C3	-2.51	109.17	115.10
6	N	4	FRU	C1-C2-C3	-2.48	109.23	115.10
6	N	5	FRU	C1-C2-C3	-2.48	109.25	115.10
6	F	4	FRU	C1-C2-C3	-2.48	109.25	115.10
6	F	5	FRU	C1-C2-C3	-2.48	109.25	115.10
7	K	5	FRU	C1-C2-C3	-2.41	109.40	115.10
7	C	5	FRU	C1-C2-C3	-2.41	109.41	115.10
5	H	10	FRU	C1-C2-C3	-2.40	109.42	115.10
8	L	4	FRU	C1-C2-C3	-2.37	109.50	115.10
8	D	4	FRU	C1-C2-C3	-2.36	109.53	115.10
8	D	2	FRU	C1-C2-C3	-2.35	109.54	115.10
8	L	2	FRU	C1-C2-C3	-2.34	109.57	115.10
5	H	4	FRU	C1-C2-C3	-2.33	109.59	115.10
5	H	10	FRU	C4-C3-C2	2.28	107.00	102.61
5	H	9	FRU	C4-C3-C2	2.21	106.88	102.61
5	H	12	FRU	C1-C2-C3	-2.19	109.92	115.10
7	K	6	FRU	C6-C5-C4	-2.19	109.93	115.10
5	H	12	FRU	C6-C5-C4	-2.19	109.94	115.10
7	C	6	FRU	C6-C5-C4	-2.18	109.95	115.10
7	K	7	FRU	C1-C2-C3	-2.18	109.96	115.10
5	H	11	FRU	C1-C2-C3	-2.17	109.96	115.10
7	C	7	FRU	C1-C2-C3	-2.17	109.97	115.10
7	K	3	FRU	C1-C2-C3	-2.16	110.00	115.10
7	C	3	FRU	C1-C2-C3	-2.16	110.00	115.10
7	C	7	FRU	C6-C5-C4	-2.13	110.07	115.10
7	K	7	FRU	C6-C5-C4	-2.11	110.11	115.10
5	H	7	FRU	C6-C5-C4	-2.10	110.14	115.10
5	H	13	FRU	C3-C4-C5	2.09	106.64	102.61
7	C	1	FRU	C6-C5-C4	-2.09	110.17	115.10
7	K	1	FRU	C6-C5-C4	-2.08	110.18	115.10
6	N	5	FRU	C6-C5-C4	-2.06	110.23	115.10
6	N	1	FRU	C6-C5-C4	-2.06	110.23	115.10
6	F	5	FRU	C6-C5-C4	-2.05	110.25	115.10
6	F	1	FRU	C6-C5-C4	-2.05	110.27	115.10
5	H	11	FRU	C6-C5-C4	-2.04	110.27	115.10
6	N	2	FRU	C6-C5-C4	-2.04	110.29	115.10
7	C	2	FRU	C6-C5-C4	-2.03	110.31	115.10
5	H	2	FRU	C6-C5-C4	-2.03	110.31	115.10
6	F	2	FRU	C6-C5-C4	-2.02	110.32	115.10
7	K	5	FRU	C6-C5-C4	-2.01	110.35	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	5	FRU	C6-C5-C4	-2.01	110.36	115.10
7	K	2	FRU	C6-C5-C4	-2.01	110.36	115.10
8	D	3	FRU	C6-C5-C4	-2.00	110.37	115.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	13	FRU	C2

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1	FRU	O1-C1-C2-C3
7	C	1	FRU	O1-C1-C2-O2
7	C	1	FRU	O1-C1-C2-O5
7	C	1	FRU	C4-C5-C6-O6
7	C	5	FRU	O1-C1-C2-C3
7	K	1	FRU	O1-C1-C2-C3
7	K	1	FRU	O1-C1-C2-O2
7	K	1	FRU	O1-C1-C2-O5
7	K	1	FRU	C4-C5-C6-O6
7	K	5	FRU	O1-C1-C2-C3
8	D	1	FRU	O1-C1-C2-C3
8	D	1	FRU	O1-C1-C2-O2
8	L	1	FRU	O1-C1-C2-C3
8	L	1	FRU	O1-C1-C2-O2
5	H	10	FRU	O5-C5-C6-O6
7	C	1	FRU	O5-C5-C6-O6
7	C	5	FRU	O1-C1-C2-O5
7	K	1	FRU	O5-C5-C6-O6
7	K	5	FRU	O1-C1-C2-O5
5	H	4	FRU	C4-C5-C6-O6
8	D	4	FRU	O1-C1-C2-C3
8	L	4	FRU	O1-C1-C2-C3
5	H	7	FRU	O1-C1-C2-O5
5	H	11	FRU	O1-C1-C2-O5
5	H	11	FRU	O5-C5-C6-O6
6	F	3	FRU	O5-C5-C6-O6
6	F	4	FRU	O1-C1-C2-O5
6	N	3	FRU	O5-C5-C6-O6
6	N	4	FRU	O1-C1-C2-O5
7	C	3	FRU	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	C	7	FRU	O1-C1-C2-O5
7	K	3	FRU	O5-C5-C6-O6
7	K	7	FRU	O1-C1-C2-O5
8	D	4	FRU	O1-C1-C2-O5
8	L	4	FRU	O1-C1-C2-O5
5	H	3	FRU	C4-C5-C6-O6
5	H	7	FRU	O1-C1-C2-C3
5	H	9	FRU	C4-C5-C6-O6
5	H	11	FRU	O1-C1-C2-C3
6	F	4	FRU	O1-C1-C2-C3
6	N	4	FRU	O1-C1-C2-C3
7	C	3	FRU	C4-C5-C6-O6
7	C	7	FRU	O1-C1-C2-C3
7	K	3	FRU	C4-C5-C6-O6
7	K	7	FRU	O1-C1-C2-C3
5	H	4	FRU	O1-C1-C2-O5
5	H	5	FRU	O1-C1-C2-O5
7	C	2	FRU	O5-C5-C6-O6
7	C	5	FRU	O5-C5-C6-O6
7	K	2	FRU	O5-C5-C6-O6
7	K	5	FRU	O5-C5-C6-O6
5	H	8	FRU	C4-C5-C6-O6
5	H	10	FRU	C4-C5-C6-O6
5	H	12	FRU	O1-C1-C2-C3
7	C	2	FRU	O1-C1-C2-C3
7	C	2	FRU	C4-C5-C6-O6
7	K	2	FRU	O1-C1-C2-C3
7	K	2	FRU	C4-C5-C6-O6
8	D	3	FRU	C4-C5-C6-O6
8	L	3	FRU	C4-C5-C6-O6
5	H	3	FRU	O5-C5-C6-O6
5	H	4	FRU	O5-C5-C6-O6
5	H	9	FRU	O5-C5-C6-O6
7	C	2	FRU	O1-C1-C2-O5
7	K	2	FRU	O1-C1-C2-O5
5	H	8	FRU	O1-C1-C2-C3
5	H	11	FRU	C4-C5-C6-O6
6	F	3	FRU	C4-C5-C6-O6
6	N	3	FRU	C4-C5-C6-O6
8	D	3	FRU	O1-C1-C2-C3
8	L	3	FRU	O1-C1-C2-C3
8	D	3	FRU	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	L	3	FRU	O5-C5-C6-O6
5	H	6	FRU	O1-C1-C2-C3
5	H	5	FRU	O5-C5-C6-O6
5	H	8	FRU	O1-C1-C2-O5
5	H	8	FRU	O5-C5-C6-O6
6	F	5	FRU	C4-C5-C6-O6
6	N	5	FRU	C4-C5-C6-O6
5	H	3	FRU	O1-C1-C2-O5
5	H	12	FRU	O1-C1-C2-O5
6	F	1	FRU	O1-C1-C2-O5
6	N	1	FRU	O1-C1-C2-O5
8	D	1	FRU	O1-C1-C2-O5
8	L	1	FRU	O1-C1-C2-O5
5	H	4	FRU	O1-C1-C2-C3
7	C	5	FRU	C4-C5-C6-O6
7	K	5	FRU	C4-C5-C6-O6
6	F	2	FRU	C4-C5-C6-O6
6	N	2	FRU	C4-C5-C6-O6
5	H	1	FRU	C4-C5-C6-O6
8	D	3	FRU	O1-C1-C2-O5
8	L	3	FRU	O1-C1-C2-O5
6	F	2	FRU	O1-C1-C2-C3
6	N	2	FRU	O1-C1-C2-C3
6	F	2	FRU	O5-C5-C6-O6
6	N	2	FRU	O5-C5-C6-O6
6	F	1	FRU	O1-C1-C2-C3
6	N	1	FRU	O1-C1-C2-C3
5	H	1	FRU	O5-C5-C6-O6
5	H	13	FRU	C4-C5-C6-O6
6	F	2	FRU	O1-C1-C2-O5
6	N	2	FRU	O1-C1-C2-O5
5	H	13	FRU	O5-C5-C6-O6
5	H	6	FRU	O1-C1-C2-O5
6	F	5	FRU	O5-C5-C6-O6
6	N	5	FRU	O5-C5-C6-O6
5	H	5	FRU	O1-C1-C2-C3
5	H	10	FRU	O1-C1-C2-C3
5	H	5	FRU	C4-C5-C6-O6
5	H	13	FRU	O1-C1-C2-C3
6	F	1	FRU	O1-C1-C2-O2
6	N	1	FRU	O1-C1-C2-O2
5	H	13	FRU	O1-C1-C2-O5

Continued on next page...

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Mol	Chain	Res	Type	Atoms
5	H	10	FRU	O1-C1-C2-O5
5	H	3	FRU	O1-C1-C2-C3
5	H	2	FRU	O1-C1-C2-C3

There are no ring outliers.

45 monomers are involved in 89 short contacts:

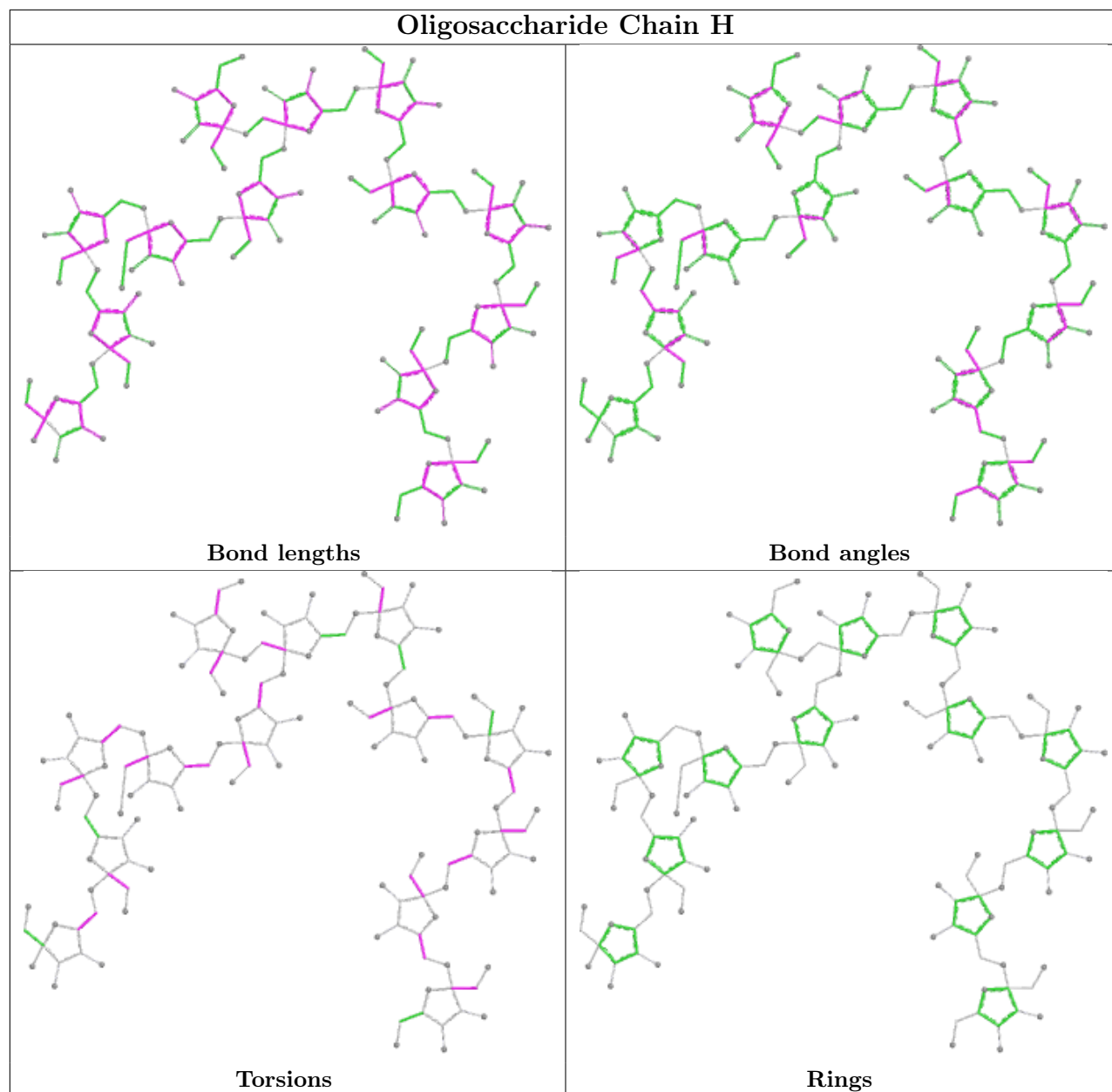
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	3	FRU	2	0
5	H	8	FRU	5	0
7	C	4	FRU	4	0
7	C	2	FRU	3	0
7	C	1	FRU	3	0
5	H	13	FRU	2	0
8	D	1	FRU	1	0
6	N	2	FRU	3	0
8	L	1	FRU	1	0
6	F	5	FRU	1	0
8	L	2	FRU	3	0
7	C	6	FRU	3	0
7	C	7	FRU	2	0
5	H	11	FRU	1	0
7	K	3	FRU	2	0
7	K	6	FRU	3	0
6	F	4	FRU	4	0
5	H	5	FRU	3	0
6	N	1	FRU	2	0
8	D	3	FRU	3	0
7	K	5	FRU	4	0
6	F	3	FRU	2	0
7	K	1	FRU	3	0
5	H	1	FRU	2	0
5	H	3	FRU	4	0
6	N	4	FRU	3	0
8	D	4	FRU	1	0
5	H	9	FRU	5	0
5	H	2	FRU	2	0
5	H	10	FRU	3	0
6	N	3	FRU	2	0
6	F	2	FRU	2	0
7	K	2	FRU	3	0
5	H	4	FRU	5	0

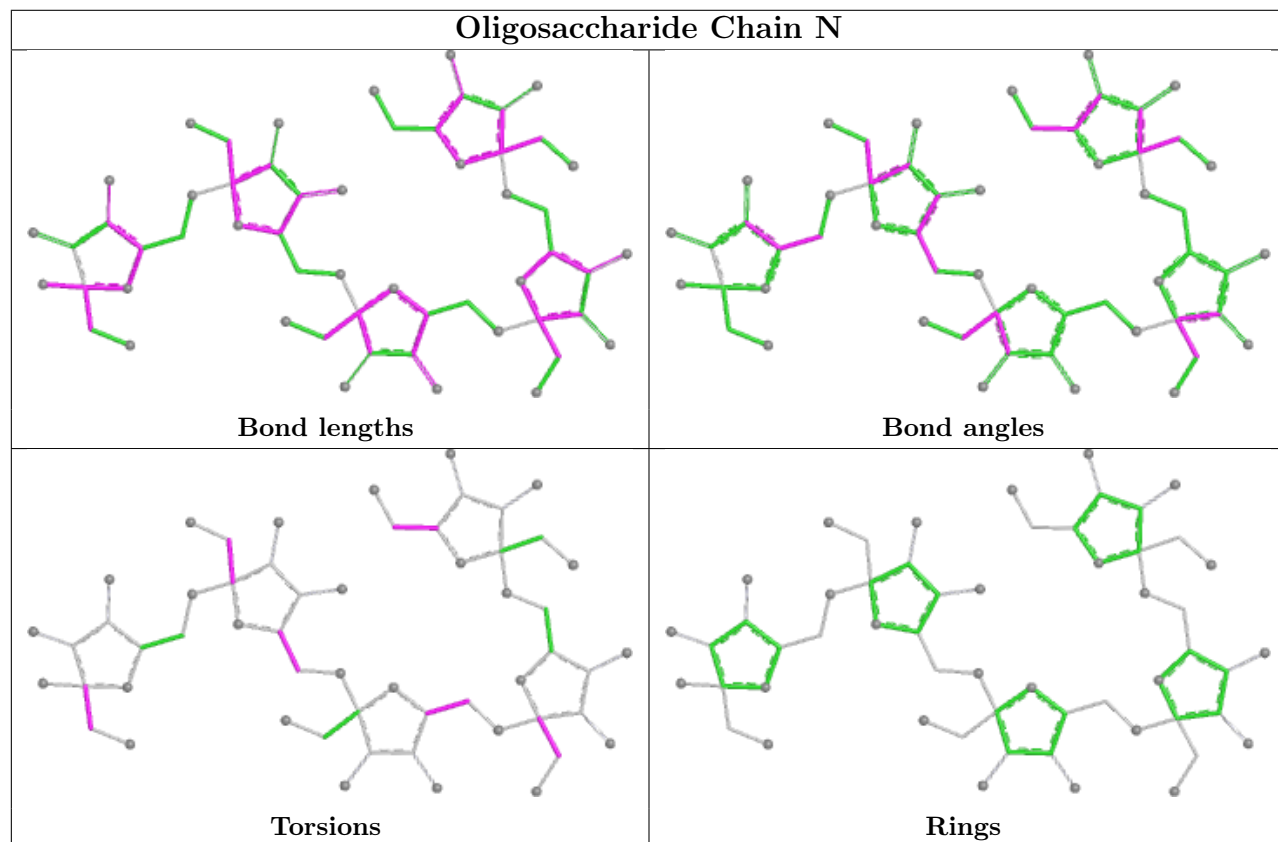
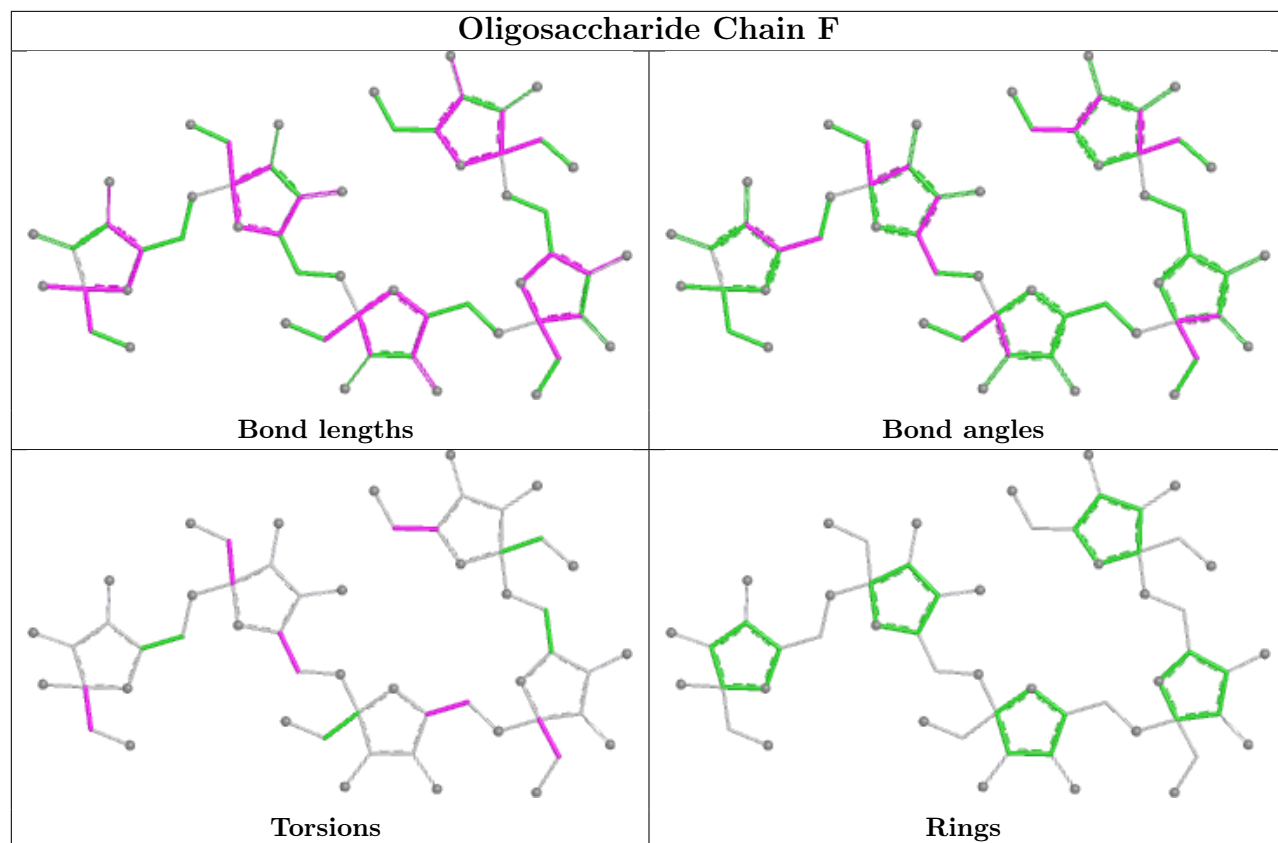
Continued on next page...

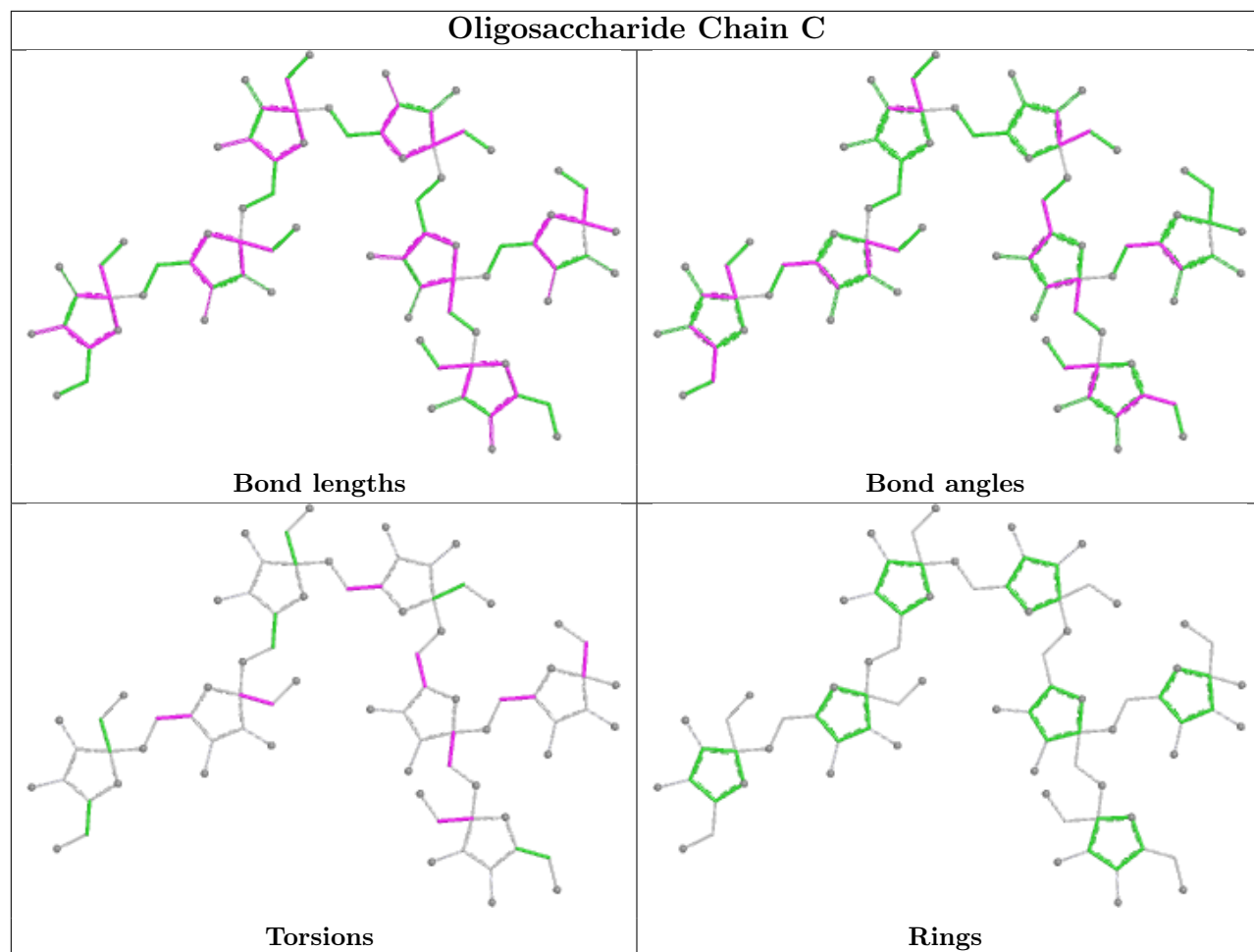
Continued from previous page...

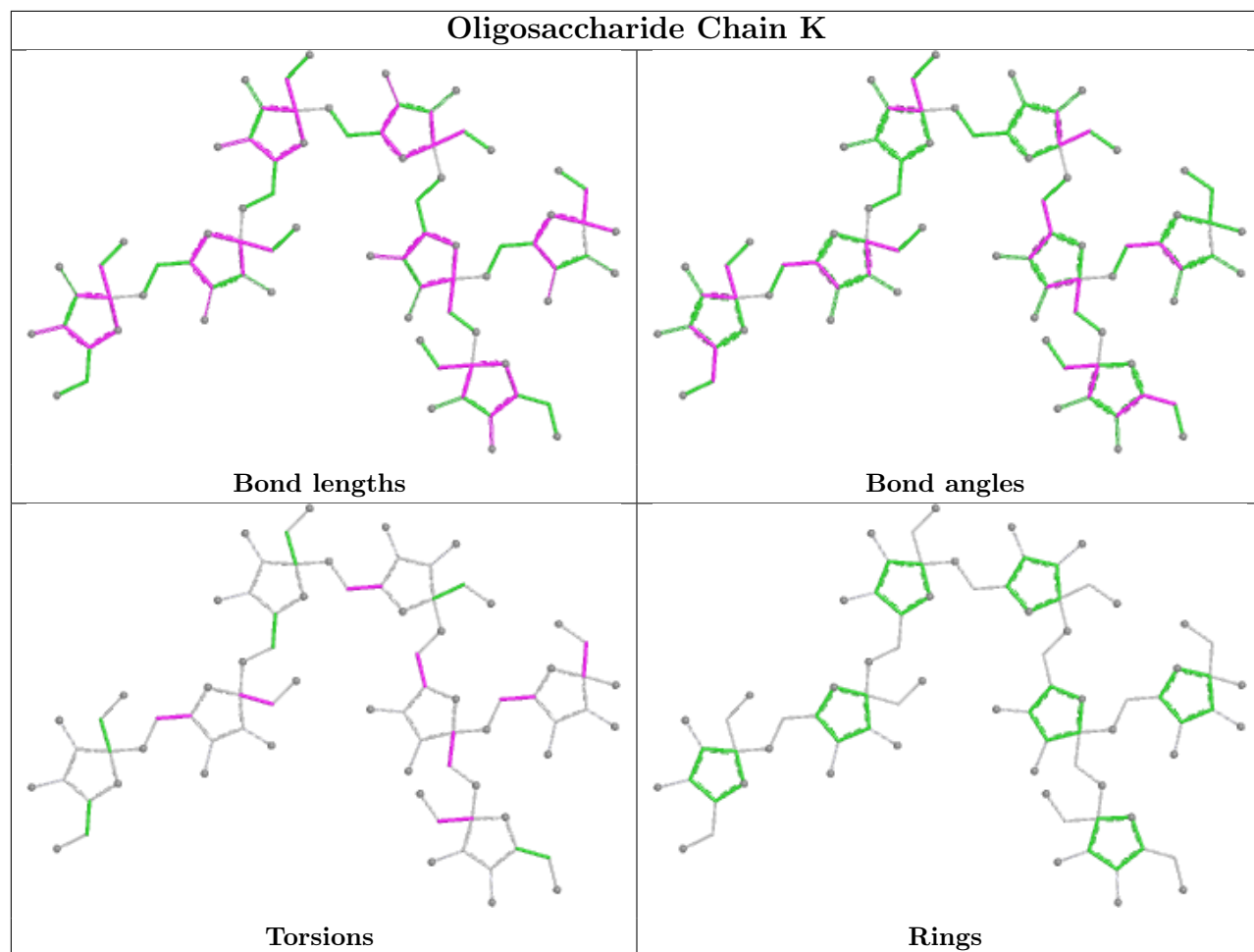
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	12	FRU	1	0
8	L	4	FRU	1	0
8	L	3	FRU	3	0
8	D	2	FRU	3	0
7	K	7	FRU	2	0
5	H	6	FRU	2	0
6	N	5	FRU	1	0
5	H	7	FRU	4	0
7	C	5	FRU	4	0
7	K	4	FRU	5	0
6	F	1	FRU	2	0

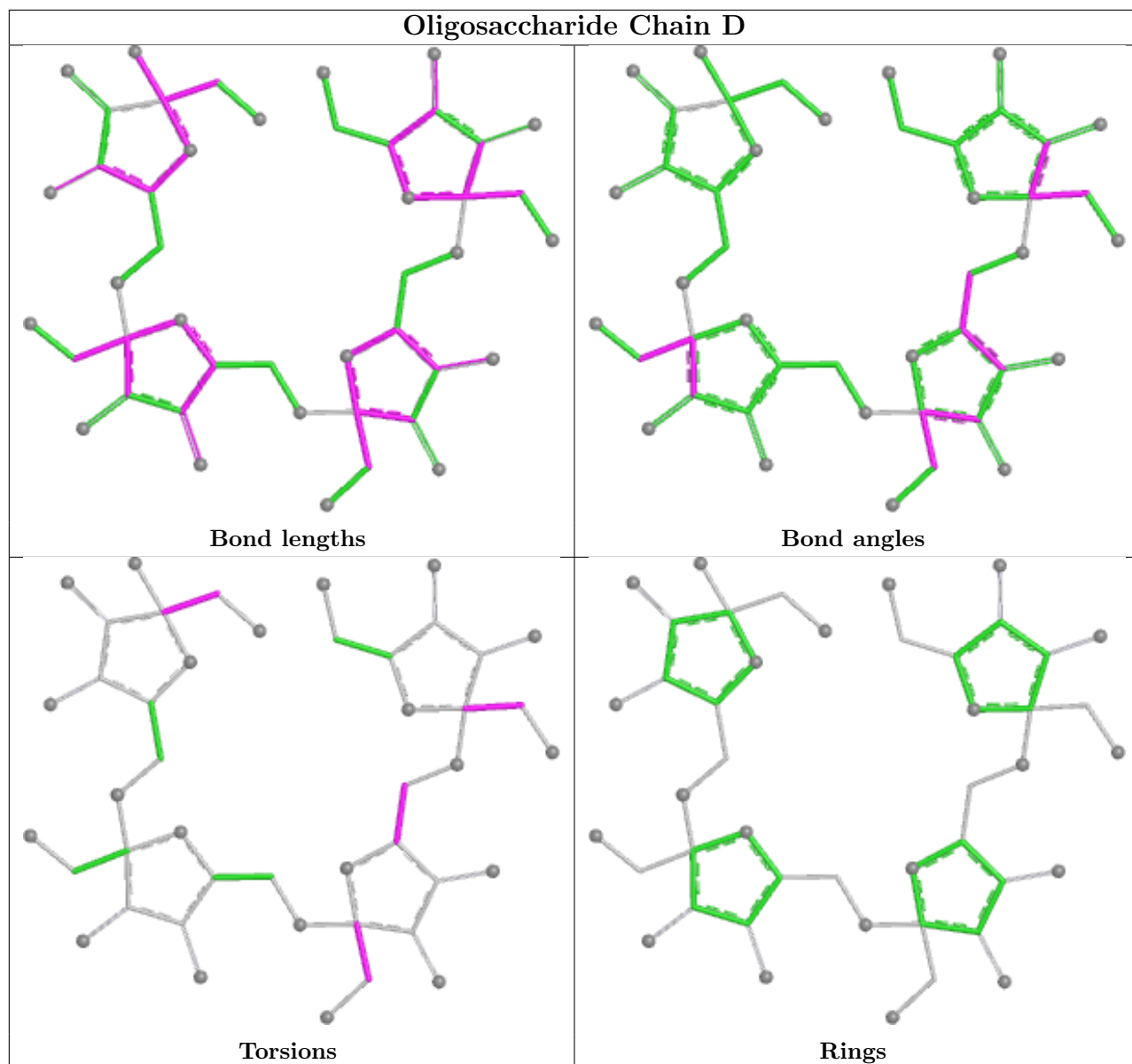
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

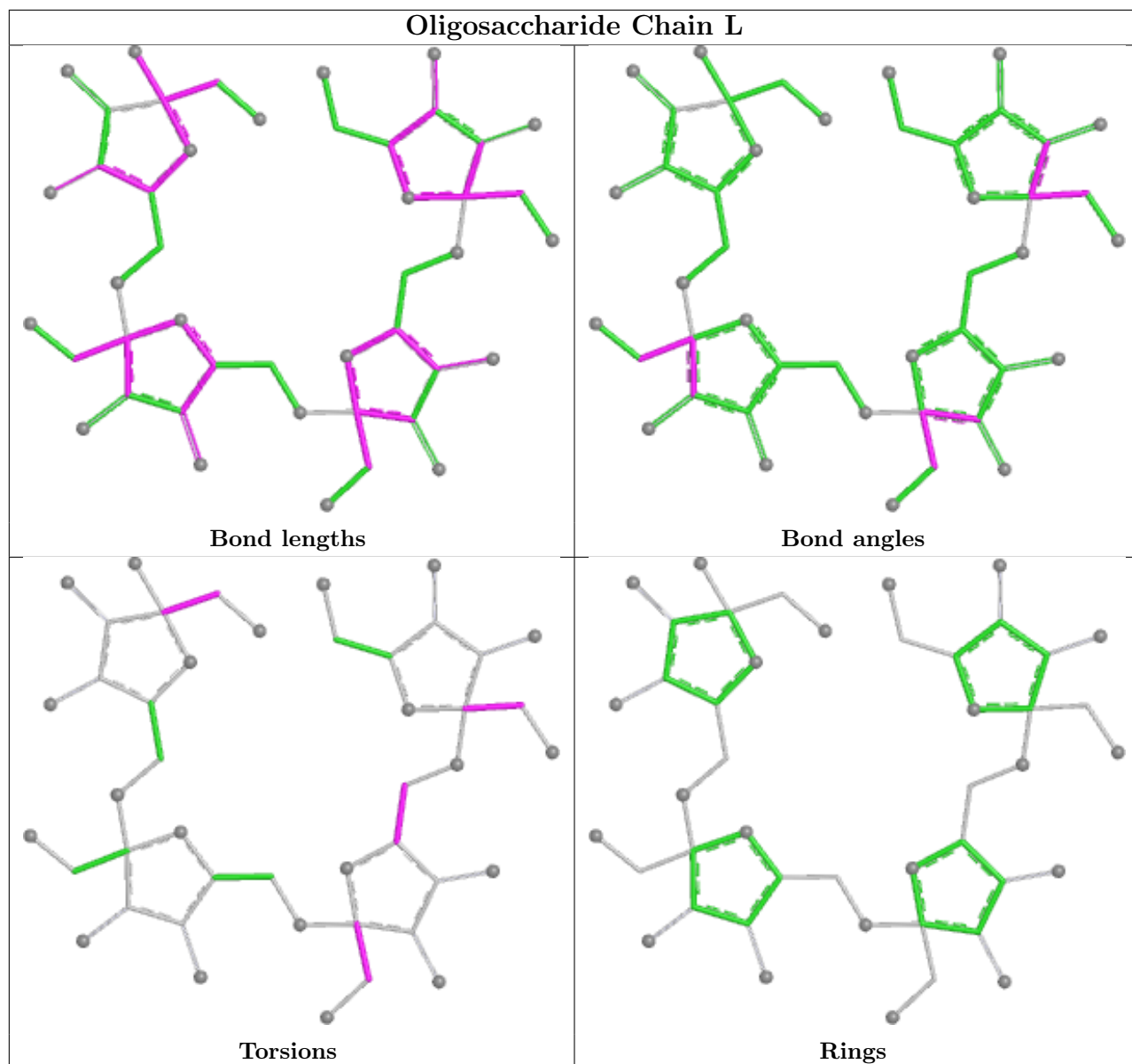












5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

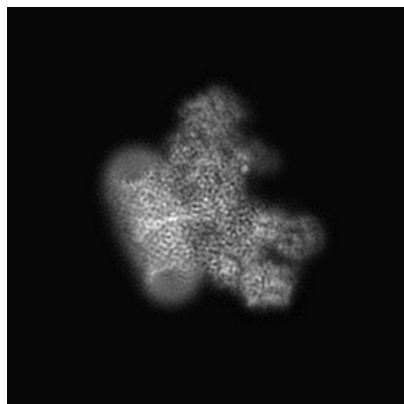
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15291. These allow visual inspection of the internal detail of the map and identification of artifacts.

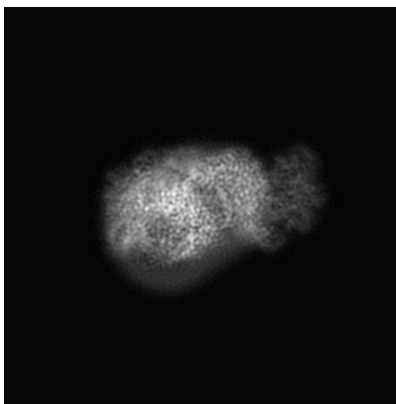
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

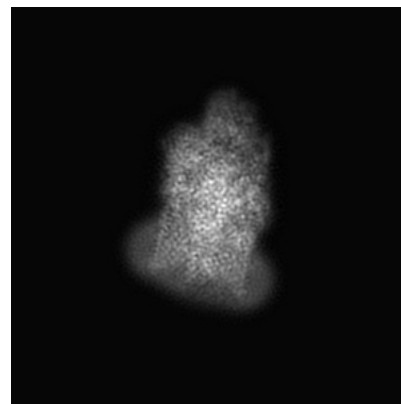
6.1.1 Primary map



X

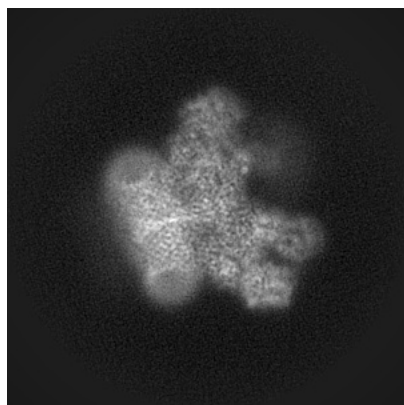


Y

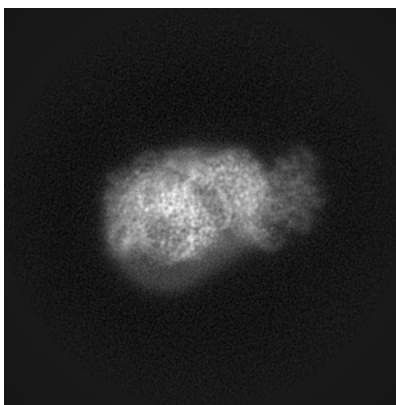


Z

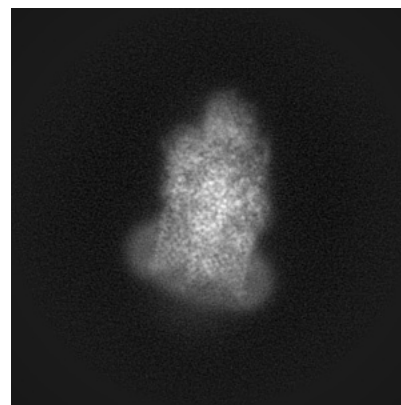
6.1.2 Raw map



X



Y

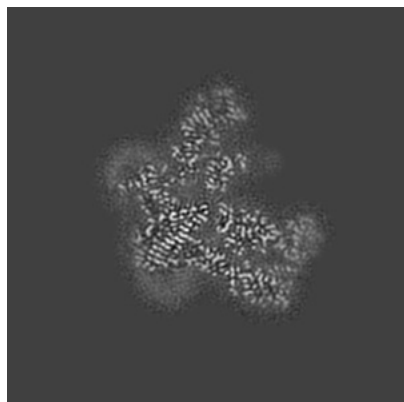


Z

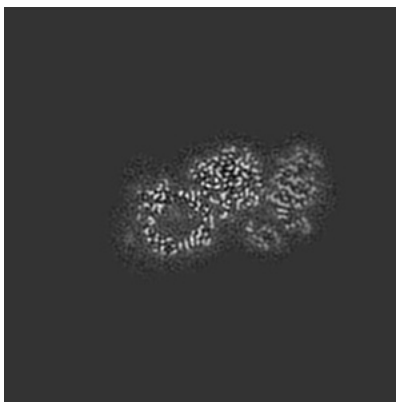
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

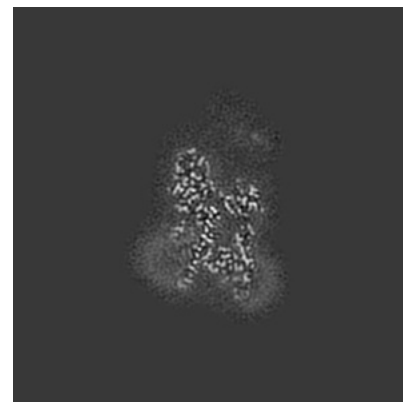
6.2.1 Primary map



X Index: 150

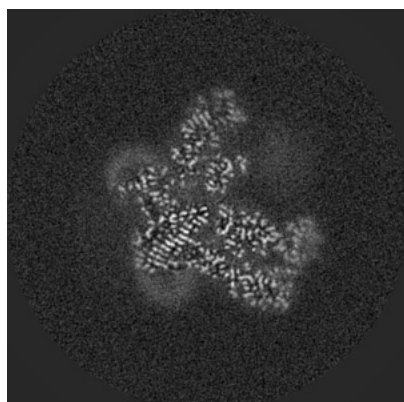


Y Index: 150

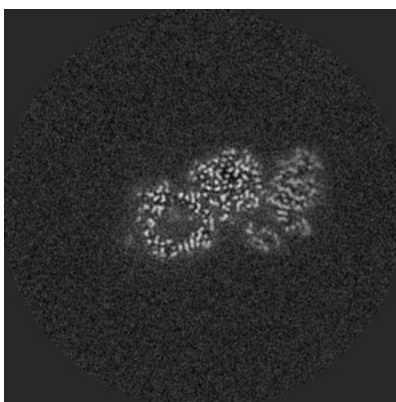


Z Index: 150

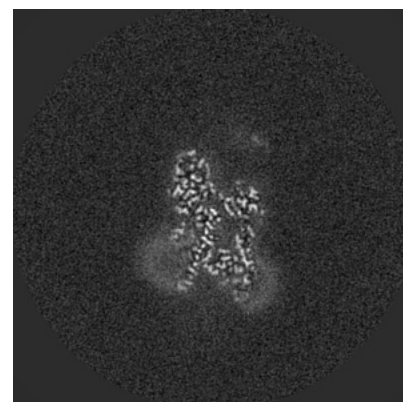
6.2.2 Raw map



X Index: 150



Y Index: 150

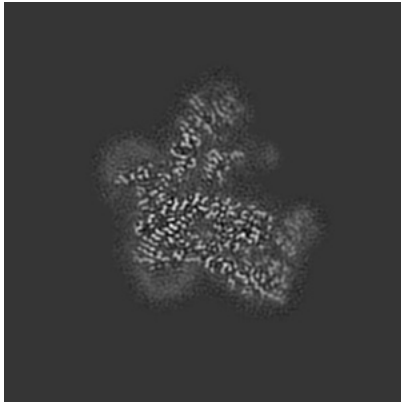


Z Index: 150

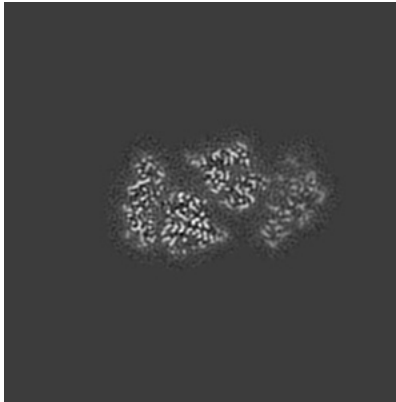
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

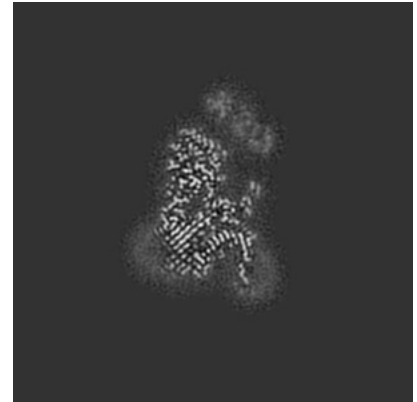
6.3.1 Primary map



X Index: 148

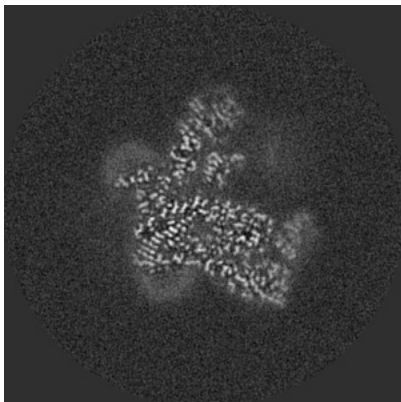


Y Index: 163

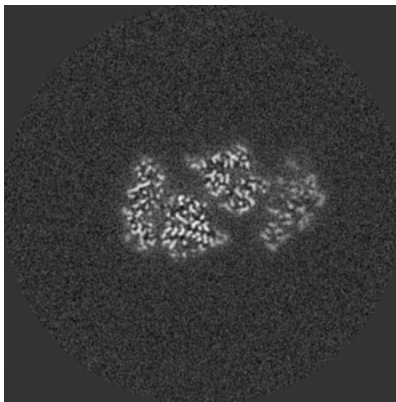


Z Index: 141

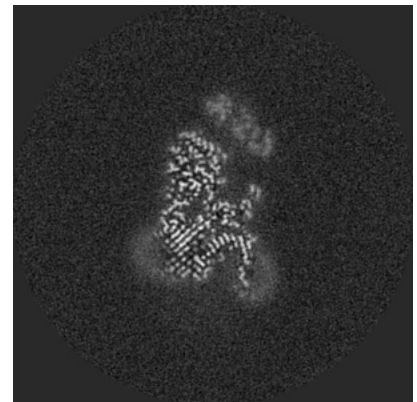
6.3.2 Raw map



X Index: 148



Y Index: 163

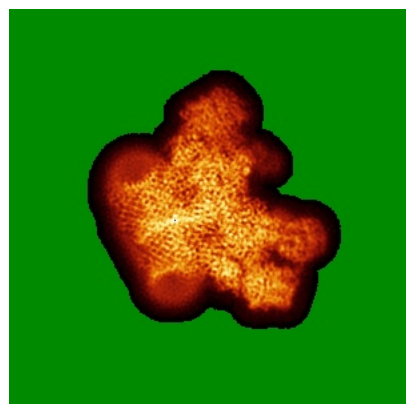


Z Index: 141

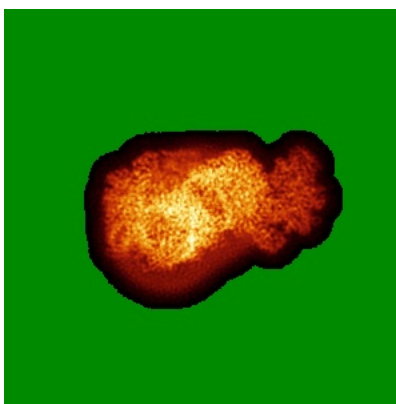
The images above show the largest variance slices of the map in three orthogonal directions.

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

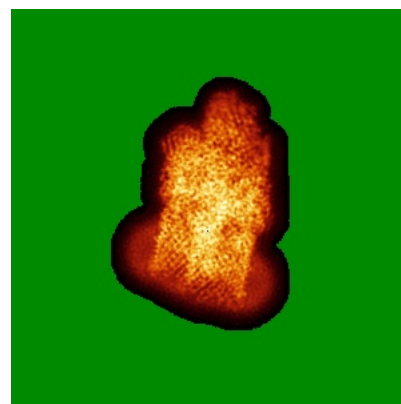
6.4.1 Primary map



X

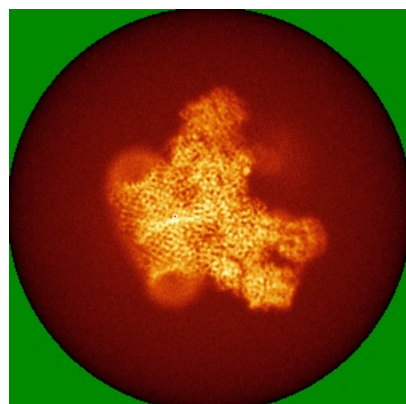


Y

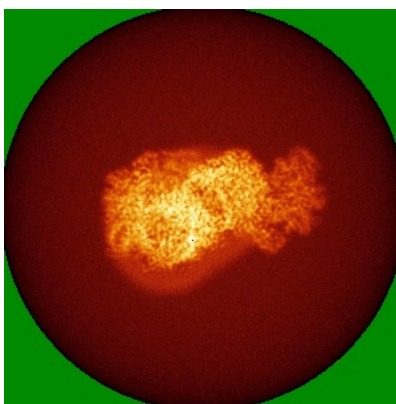


Z

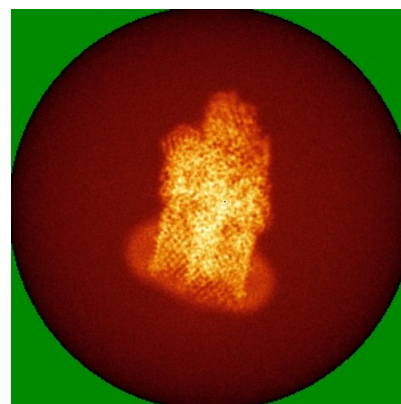
6.4.2 Raw map



X



Y

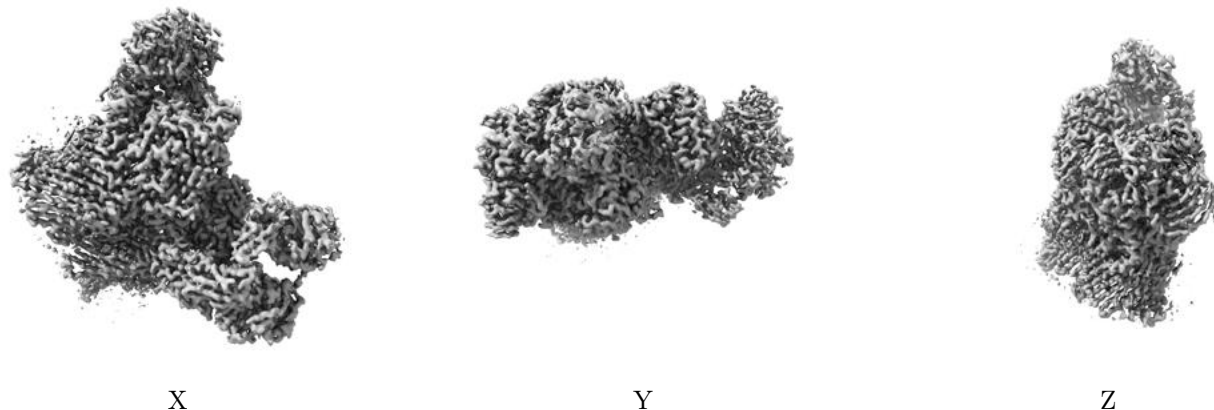


Z

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

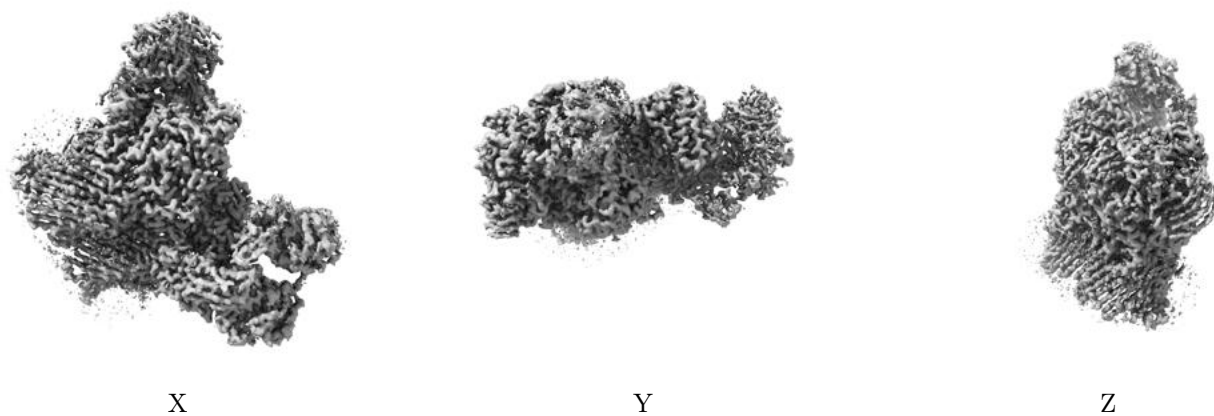
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0425. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

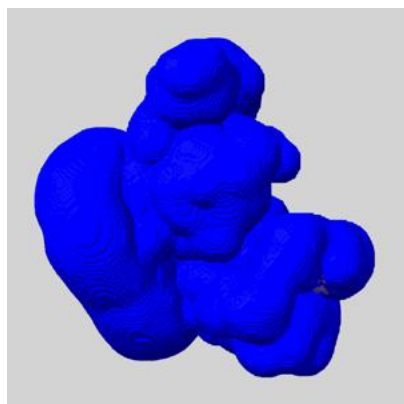
6.6 Mask visualisation [i](#)

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

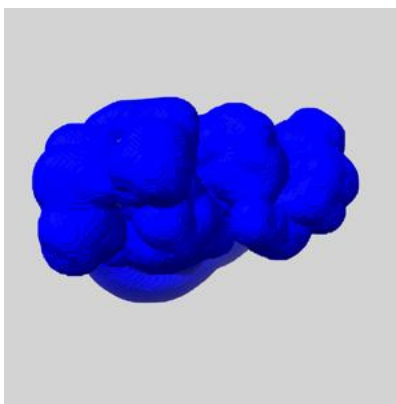
A mask typically either:

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

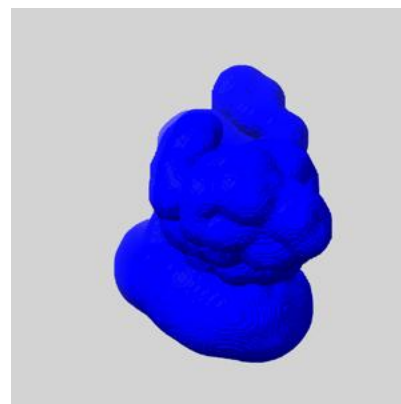
6.6.1 emd_15291_msk_1.map [i](#)



X



Y

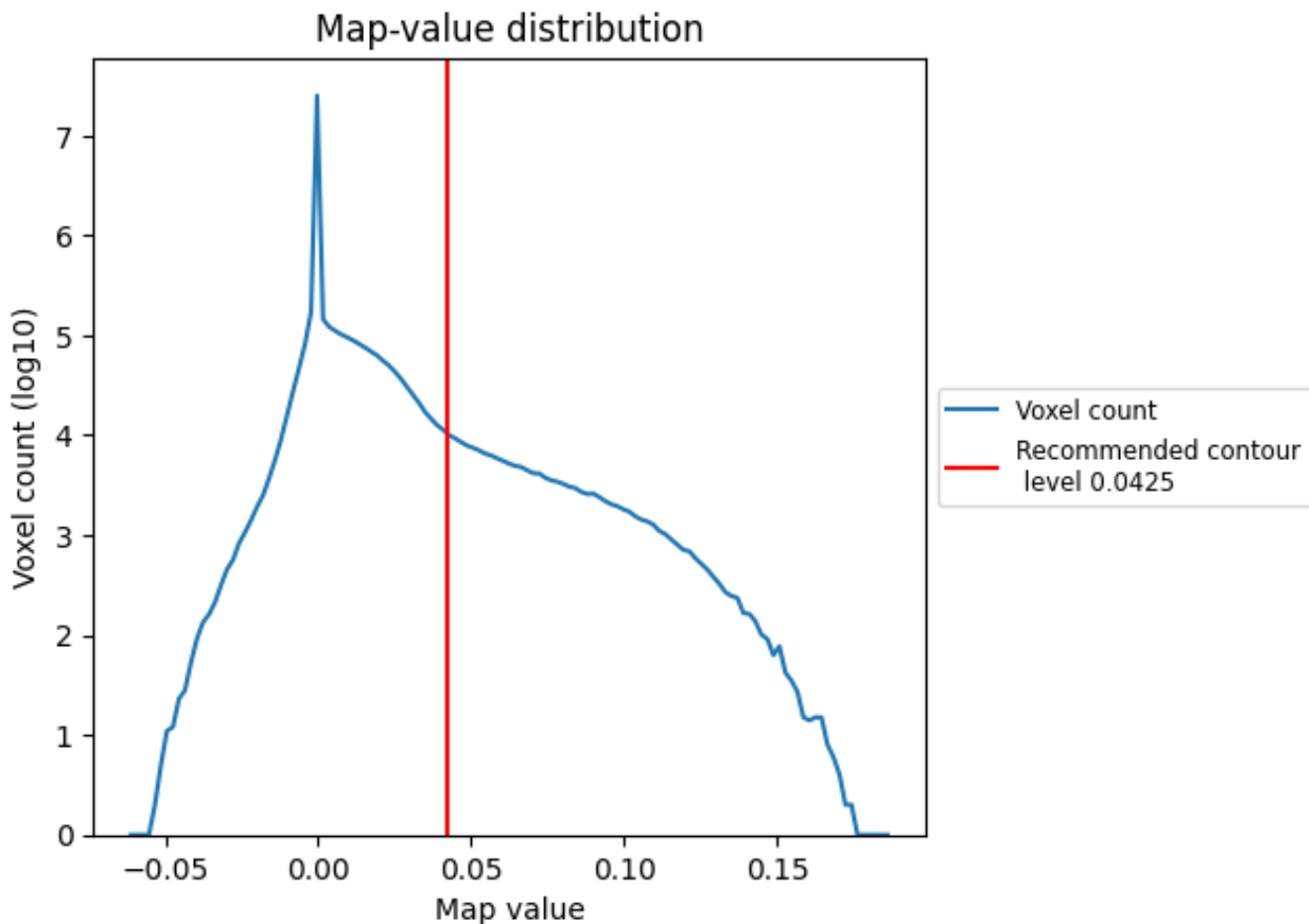


Z

7 Map analysis [i](#)

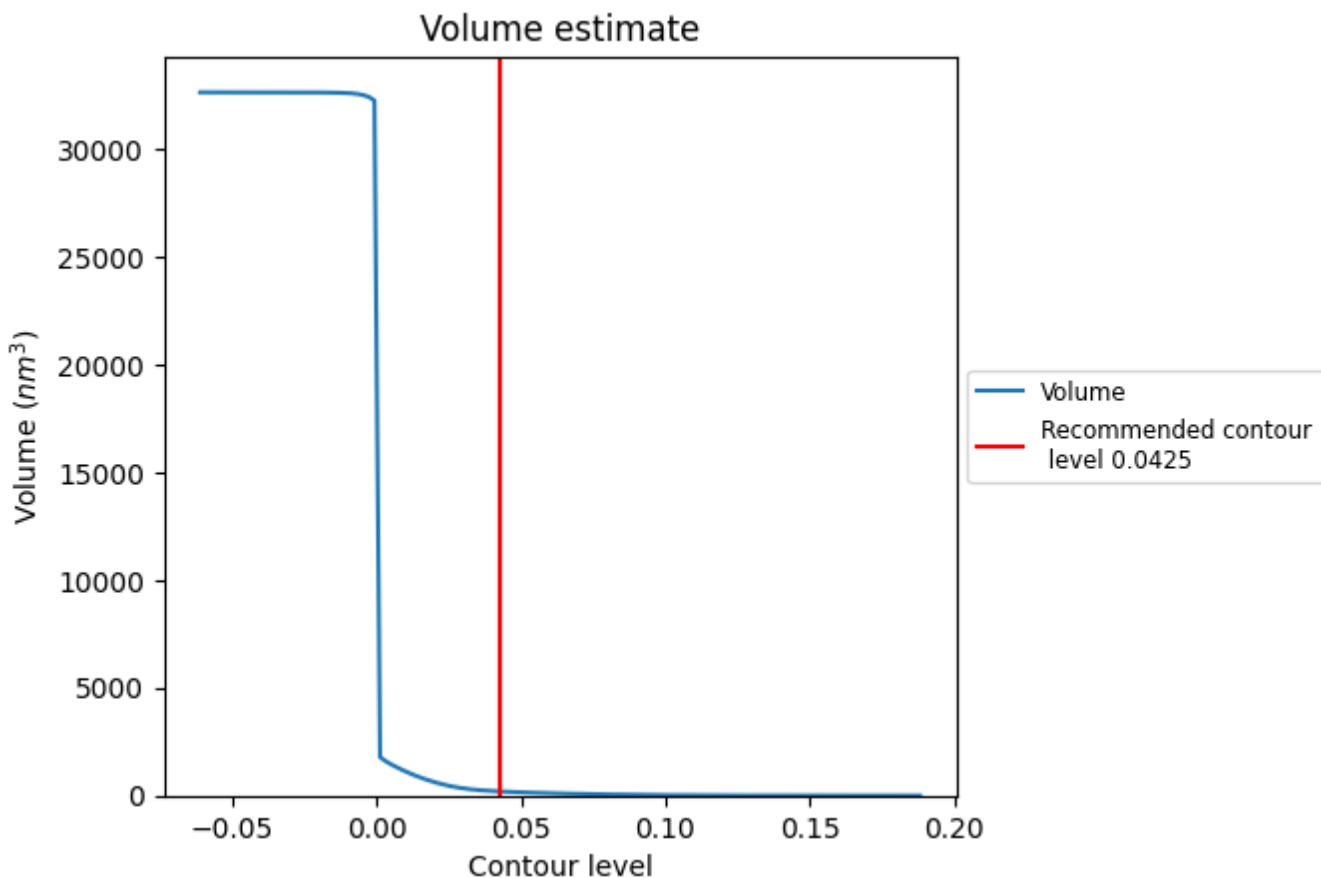
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

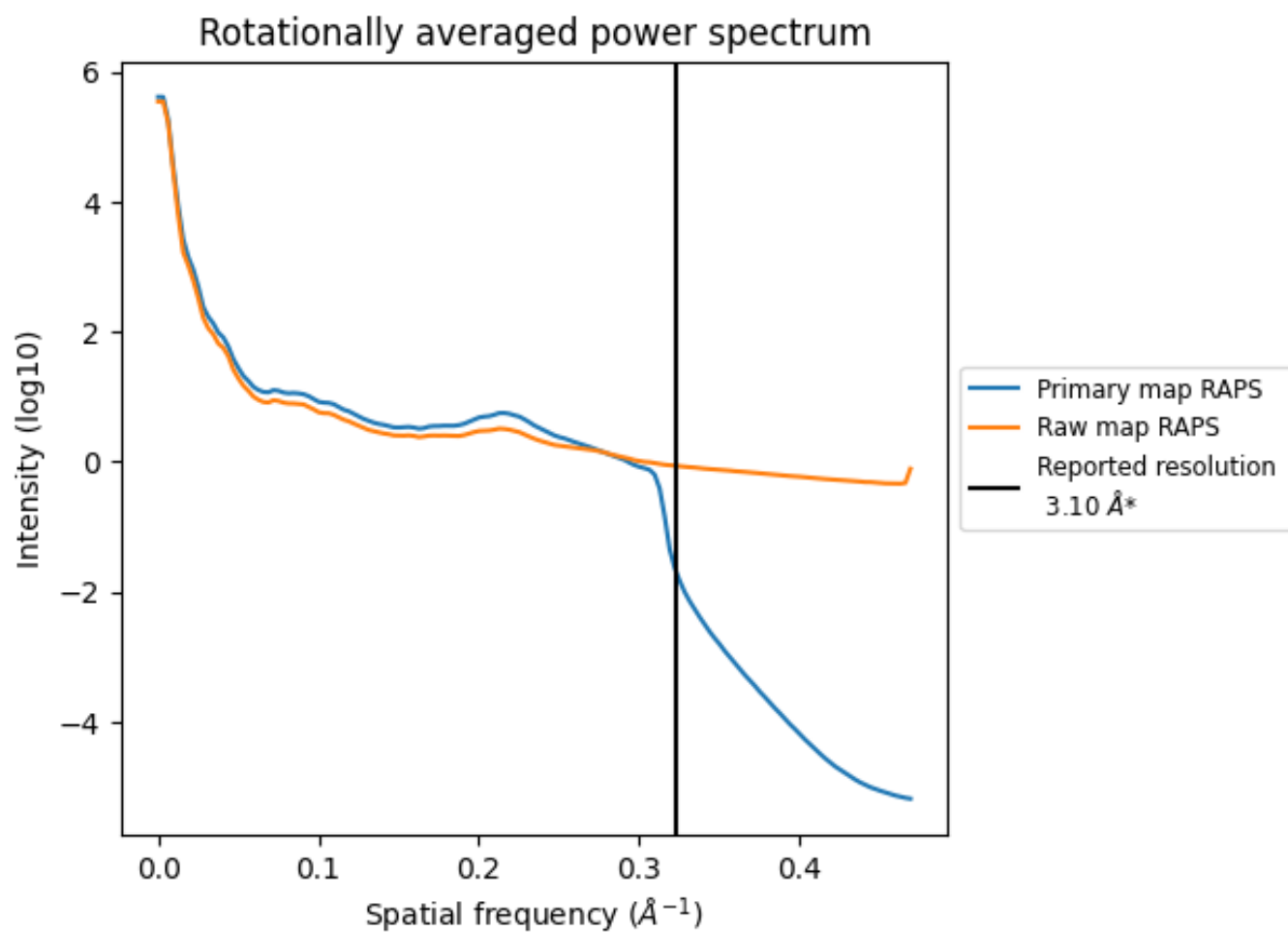
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 174 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](#)

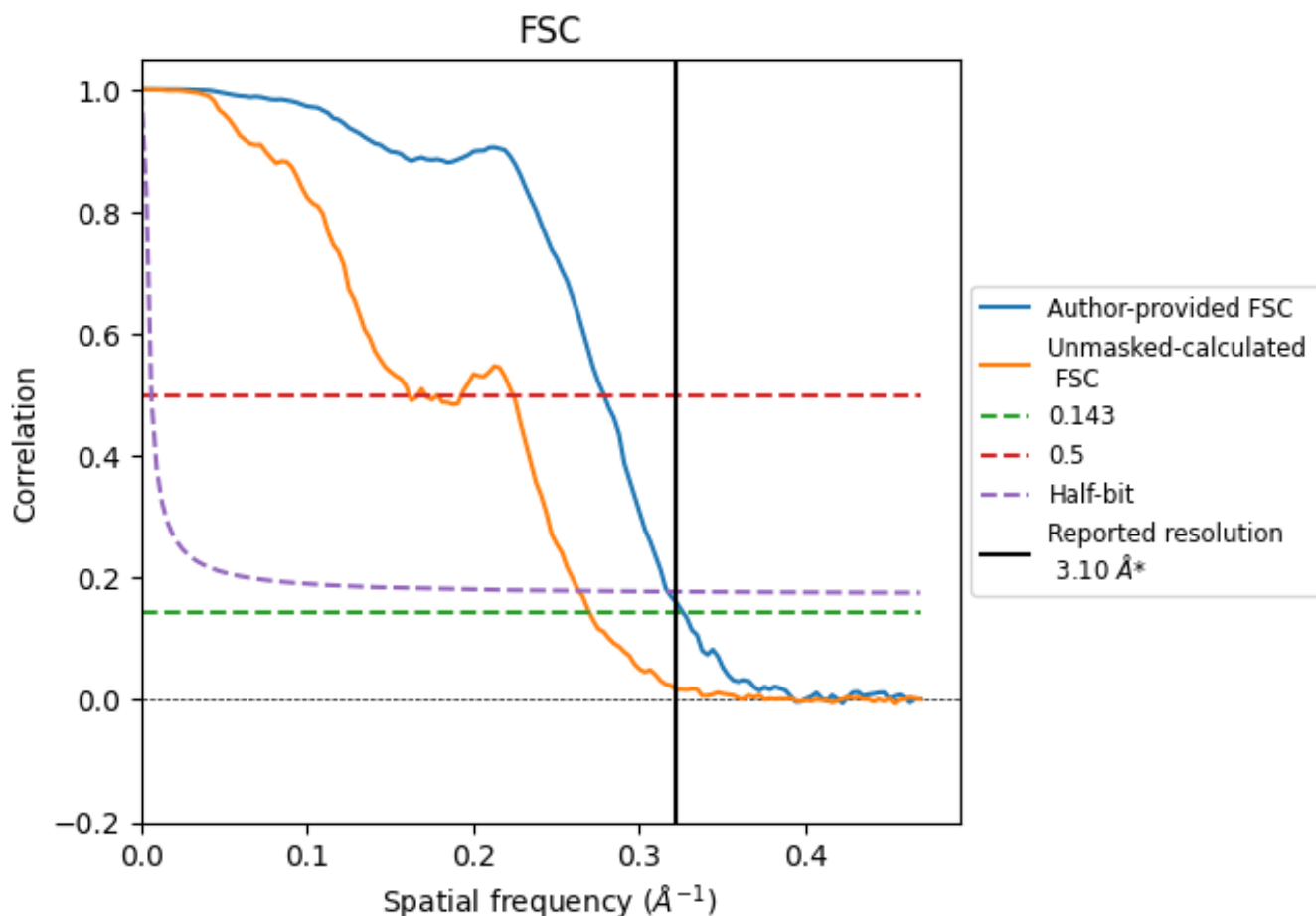


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

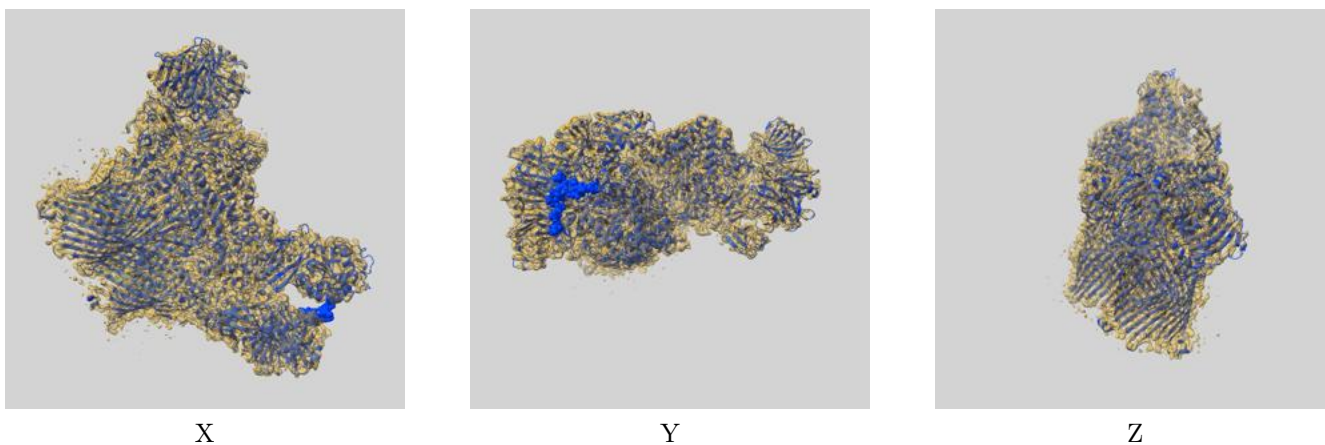
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.59	3.15
Unmasked-calculated*	3.70	6.19	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

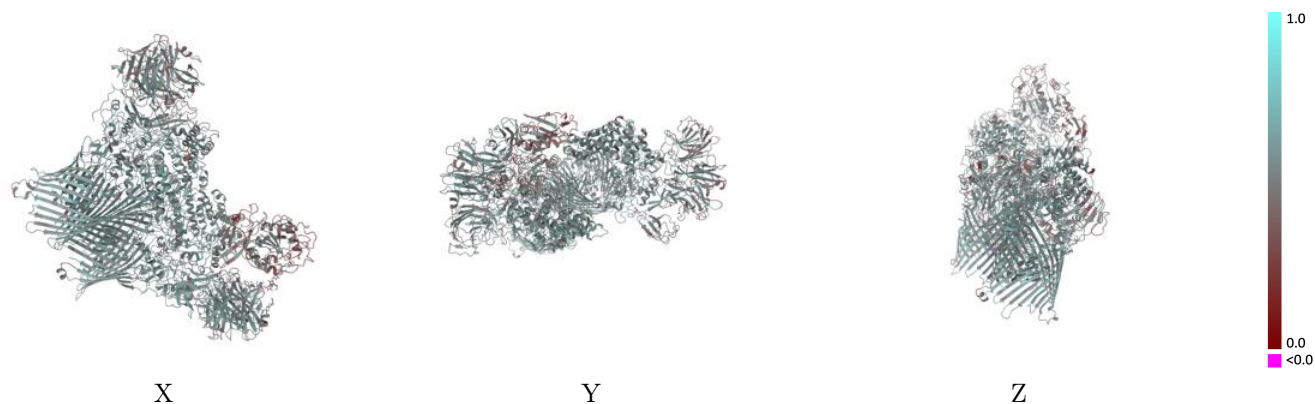
This section contains information regarding the fit between EMDB map EMD-15291 and PDB model 8AA2. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



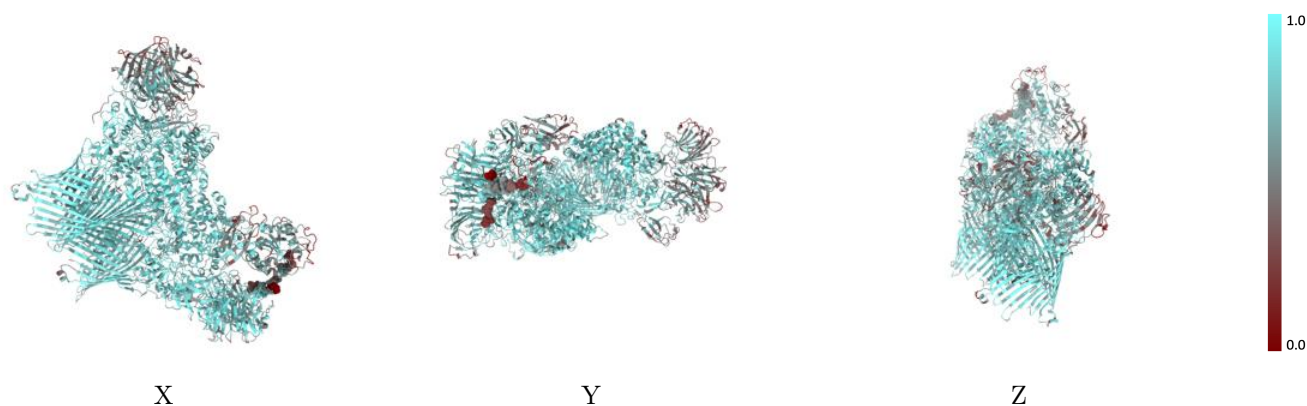
The images above show the 3D surface view of the map at the recommended contour level 0.0425 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



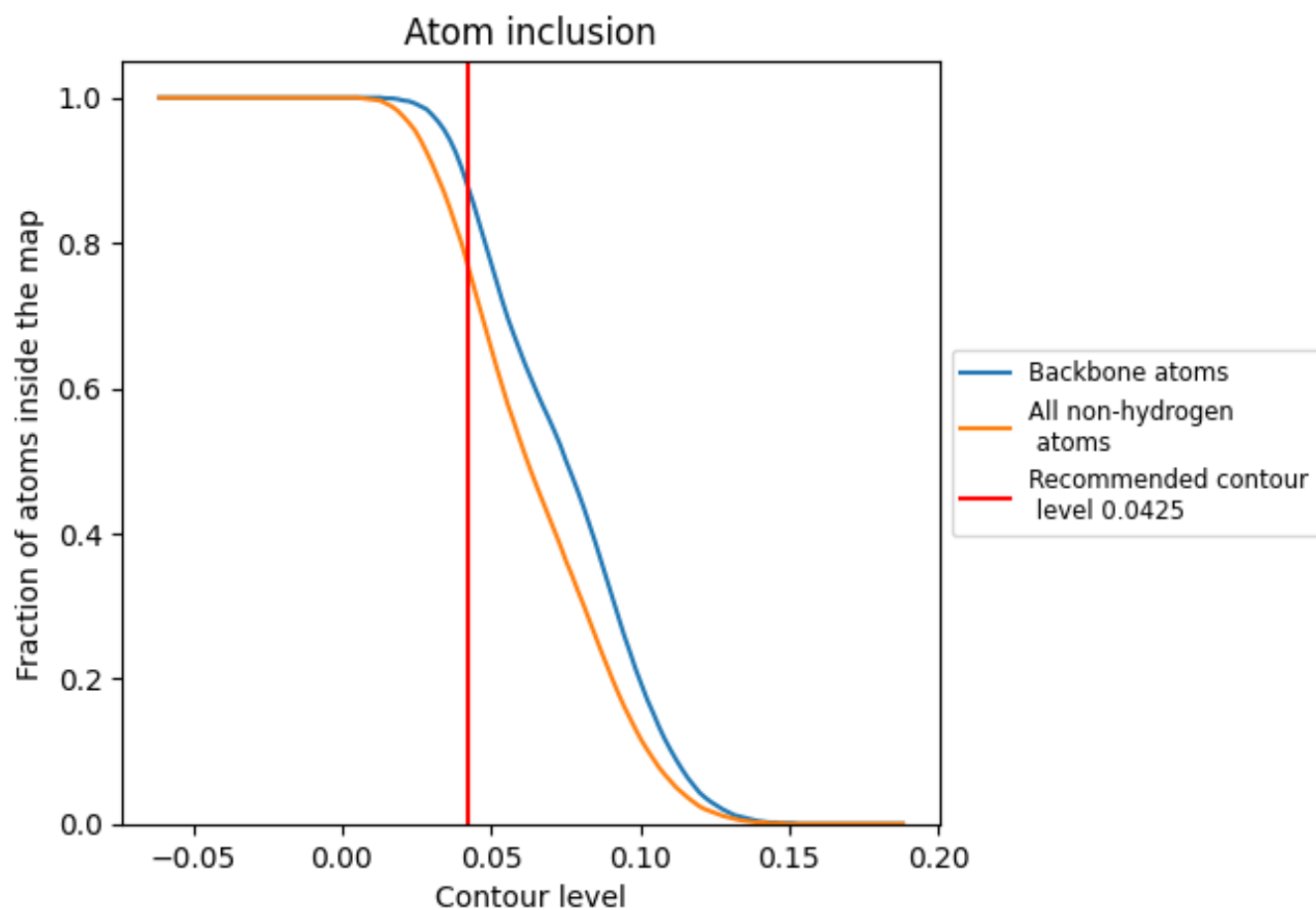
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0425).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (0.0425) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.5290
A	 0.8490	 0.5590
B	 0.8520	 0.5550
C	 0.7560	 0.4680
D	 0.6890	 0.5380
E	 0.7480	 0.5210
F	 0.4460	 0.4170
G	 0.5960	 0.4390
H	 0.4170	 0.3780
I	 0.8380	 0.5520
J	 0.8330	 0.5480
K	 0.7180	 0.4640
L	 0.6220	 0.5070
M	 0.5430	 0.4900
N	 0.2860	 0.4110
T	 0.5090	 0.4590

