



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 12:39 AM JST

PDB ID : 7BVH
Title : Crystal structure of arabinosyltransferase EmbC2-AcpM2 complex from Mycobacterium smegmatis complexed with di-arabinose
Authors : Zhao, Y.; Zhang, L.; Wu, L.J.; Wang, Q.; Li, J.; Besra, G.S.; Rao, Z.H.
Deposited on : 2020-04-10
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

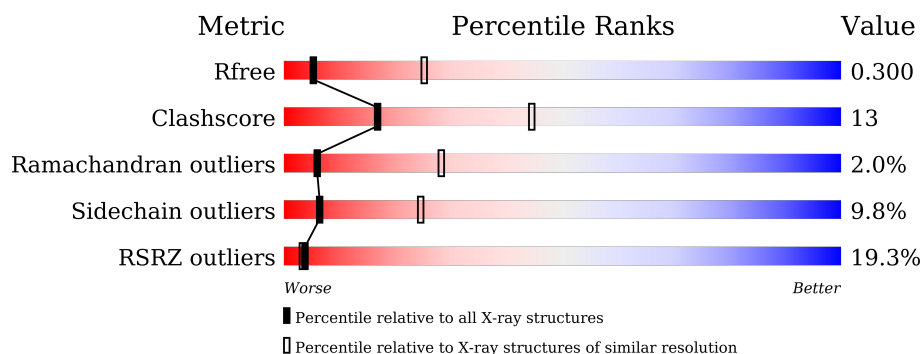
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1113	<div> <div>18%</div> <div>64%</div> <div>25%</div> <div>7%</div> </div>
1	B	1113	<div> <div>19%</div> <div>63%</div> <div>27%</div> <div>7%</div> </div>
2	C	99	<div> <div>15%</div> <div>62%</div> <div>22%</div> <div>15%</div> </div>
2	D	99	<div> <div>11%</div> <div>68%</div> <div>14%</div> <div>15%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>
3	J	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	G	2	 50% 50%
4	H	2	 100%
4	I	2	 100%
4	K	2	 100%
4	L	2	 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
4	GLC	G	2	-	-	X	-
4	GLC	L	2	-	-	X	-
7	BXY	A	1203	-	X	-	-
7	BXY	B	1204	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17316 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Integral membrane indolylacetylinsitol arabinosyltransferase EmbC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1035	Total	C	N	O	S	0	0	0
			7900	5101	1373	1400	26			
1	B	1035	Total	C	N	O	S	0	0	0
			7900	5101	1373	1400	26			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP I7FMU5
A	-11	PRO	-	expression tag	UNP I7FMU5
A	-10	GLU	-	expression tag	UNP I7FMU5
A	-9	VAL	-	expression tag	UNP I7FMU5
A	-8	VAL	-	expression tag	UNP I7FMU5
A	-7	GLY	-	expression tag	UNP I7FMU5
A	-6	SER	-	expression tag	UNP I7FMU5
A	-5	TYR	-	expression tag	UNP I7FMU5
A	-4	PHE	-	expression tag	UNP I7FMU5
A	-3	GLN	-	expression tag	UNP I7FMU5
A	-2	SER	-	expression tag	UNP I7FMU5
A	-1	ASN	-	expression tag	UNP I7FMU5
A	0	ALA	-	expression tag	UNP I7FMU5
A	1075	HIS	-	expression tag	UNP I7FMU5
A	1076	LEU	-	expression tag	UNP I7FMU5
A	1077	GLY	-	expression tag	UNP I7FMU5
A	1078	GLY	-	expression tag	UNP I7FMU5
A	1079	ILE	-	expression tag	UNP I7FMU5
A	1080	LYS	-	expression tag	UNP I7FMU5
A	1081	ALA	-	expression tag	UNP I7FMU5
A	1082	PHE	-	expression tag	UNP I7FMU5
A	1083	LEU	-	expression tag	UNP I7FMU5
A	1084	GLU	-	expression tag	UNP I7FMU5
A	1085	VAL	-	expression tag	UNP I7FMU5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1086	LEU	-	expression tag	UNP I7FMU5
A	1087	PHE	-	expression tag	UNP I7FMU5
A	1088	GLN	-	expression tag	UNP I7FMU5
A	1089	GLY	-	expression tag	UNP I7FMU5
A	1090	PRO	-	expression tag	UNP I7FMU5
A	1091	HIS	-	expression tag	UNP I7FMU5
A	1092	HIS	-	expression tag	UNP I7FMU5
A	1093	HIS	-	expression tag	UNP I7FMU5
A	1094	HIS	-	expression tag	UNP I7FMU5
A	1095	HIS	-	expression tag	UNP I7FMU5
A	1096	HIS	-	expression tag	UNP I7FMU5
A	1097	HIS	-	expression tag	UNP I7FMU5
A	1098	HIS	-	expression tag	UNP I7FMU5
A	1099	HIS	-	expression tag	UNP I7FMU5
A	1100	HIS	-	expression tag	UNP I7FMU5
B	-12	MET	-	initiating methionine	UNP I7FMU5
B	-11	PRO	-	expression tag	UNP I7FMU5
B	-10	GLU	-	expression tag	UNP I7FMU5
B	-9	VAL	-	expression tag	UNP I7FMU5
B	-8	VAL	-	expression tag	UNP I7FMU5
B	-7	GLY	-	expression tag	UNP I7FMU5
B	-6	SER	-	expression tag	UNP I7FMU5
B	-5	TYR	-	expression tag	UNP I7FMU5
B	-4	PHE	-	expression tag	UNP I7FMU5
B	-3	GLN	-	expression tag	UNP I7FMU5
B	-2	SER	-	expression tag	UNP I7FMU5
B	-1	ASN	-	expression tag	UNP I7FMU5
B	0	ALA	-	expression tag	UNP I7FMU5
B	1075	HIS	-	expression tag	UNP I7FMU5
B	1076	LEU	-	expression tag	UNP I7FMU5
B	1077	GLY	-	expression tag	UNP I7FMU5
B	1078	GLY	-	expression tag	UNP I7FMU5
B	1079	ILE	-	expression tag	UNP I7FMU5
B	1080	LYS	-	expression tag	UNP I7FMU5
B	1081	ALA	-	expression tag	UNP I7FMU5
B	1082	PHE	-	expression tag	UNP I7FMU5
B	1083	LEU	-	expression tag	UNP I7FMU5
B	1084	GLU	-	expression tag	UNP I7FMU5
B	1085	VAL	-	expression tag	UNP I7FMU5
B	1086	LEU	-	expression tag	UNP I7FMU5
B	1087	PHE	-	expression tag	UNP I7FMU5
B	1088	GLN	-	expression tag	UNP I7FMU5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1089	GLY	-	expression tag	UNP I7FMU5
B	1090	PRO	-	expression tag	UNP I7FMU5
B	1091	HIS	-	expression tag	UNP I7FMU5
B	1092	HIS	-	expression tag	UNP I7FMU5
B	1093	HIS	-	expression tag	UNP I7FMU5
B	1094	HIS	-	expression tag	UNP I7FMU5
B	1095	HIS	-	expression tag	UNP I7FMU5
B	1096	HIS	-	expression tag	UNP I7FMU5
B	1097	HIS	-	expression tag	UNP I7FMU5
B	1098	HIS	-	expression tag	UNP I7FMU5
B	1099	HIS	-	expression tag	UNP I7FMU5
B	1100	HIS	-	expression tag	UNP I7FMU5

- Molecule 2 is a protein called Meromycolate extension acyl carrier protein.

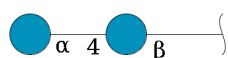
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	84	Total	C	N	O	S	0	0	0
			644	403	95	145	1			
2	D	84	Total	C	N	O	S	0	0	0
			644	403	95	145	1			

- Molecule 3 is an oligosaccharide called alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	E	2	Total	C O	0	0	0
			19 10 9				
3	J	2	Total	C O	0	0	0
			19 10 9				

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

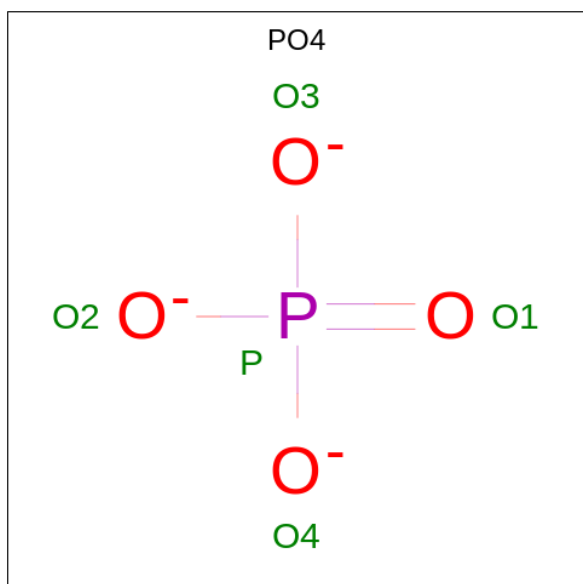


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	2	Total	C	O	0	0	0
			23	12	11			
4	G	2	Total	C	O	0	0	0
			23	12	11			
4	H	2	Total	C	O	0	0	0
			23	12	11			
4	I	2	Total	C	O	0	0	0
			23	12	11			
4	K	2	Total	C	O	0	0	0
			23	12	11			
4	L	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



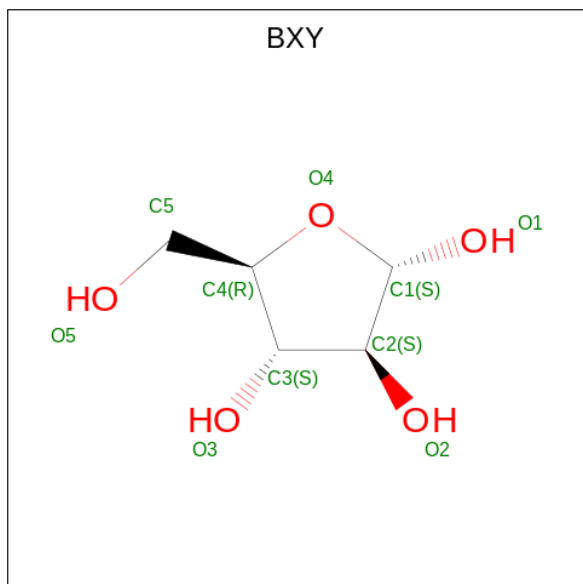
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

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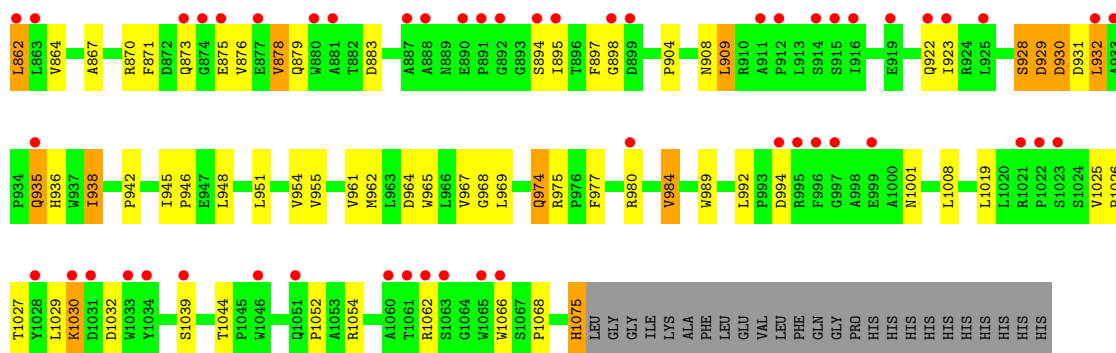
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

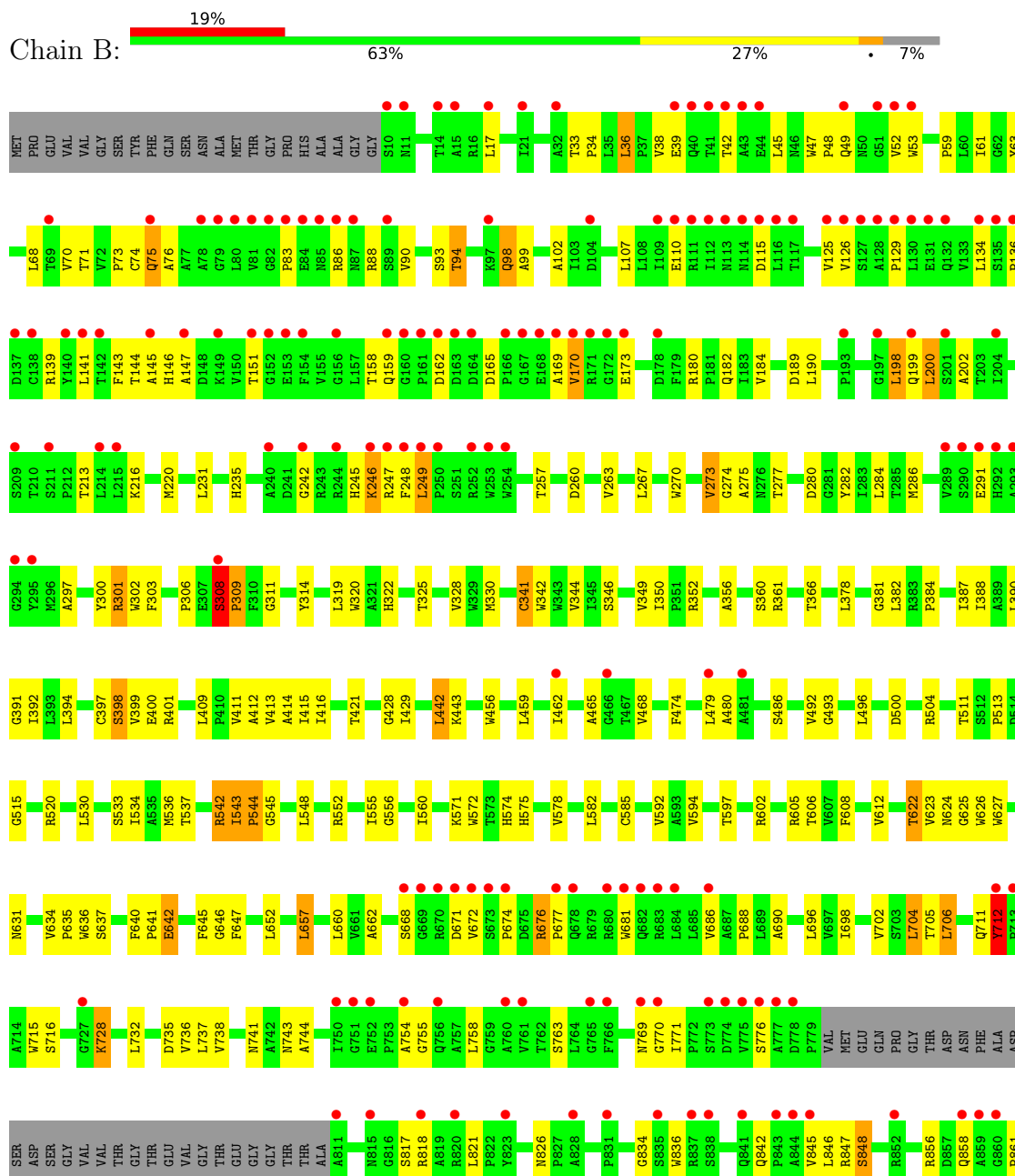
- Molecule 7 is alpha-D-arabinofuranose (three-letter code: BXY) (formula: C₅H₁₀O₅).

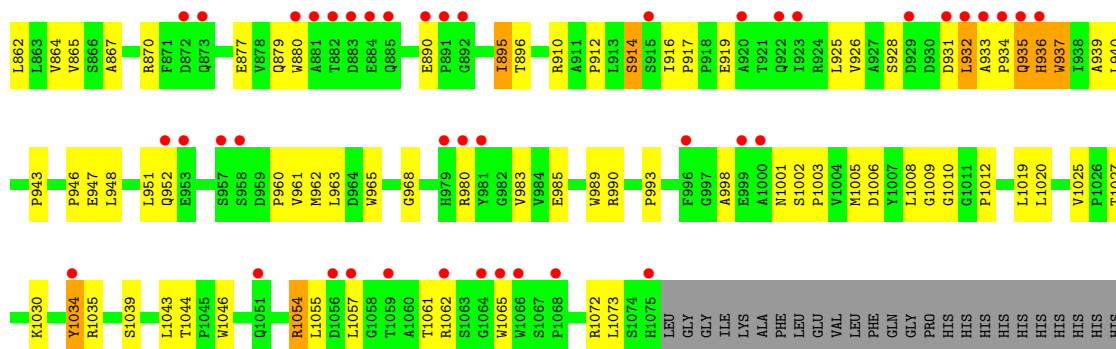


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	5	5		
7	A	1	Total	C	O	0	0
			10	5	5		
7	B	1	Total	C	O	0	0
			10	5	5		
7	B	1	Total	C	O	0	0
			10	5	5		

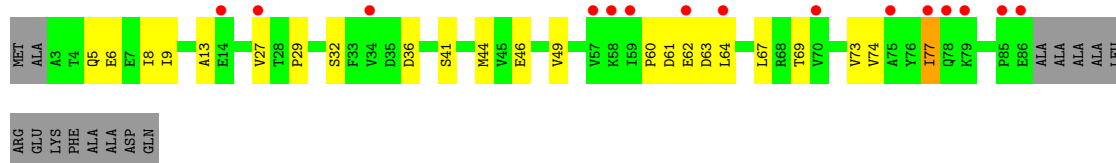


• Molecule 1: Integral membrane indolylacetyltransferase EmbC





- Molecule 2: Meromycolate extension acyl carrier protein



- Molecule 2: Meromycolate extension acyl carrier protein



- Molecule 3: alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose



- Molecule 3: alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose



- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:  50% 50%

BGC1
GLC2

- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

BGC1
GLC2

- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain I:  100%

BGC1
GLC2

- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain K:  100%

BGC1
GLC2

- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain L:  100%

BGC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.08Å 176.33Å 207.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.30 49.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.67-3.30) 100.0 (49.67-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.232 , 0.265 0.265 , 0.300	Depositor DCC
R_{free} test set	3362 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	17316	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, BGC, BXY, GLC, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	1/8124 (0.0%)	0.75	2/11137 (0.0%)
1	B	0.50	0/8124	0.74	1/11137 (0.0%)
2	C	0.48	0/650	0.71	0/884
2	D	0.47	0/650	0.68	0/884
All	All	0.51	1/17548 (0.0%)	0.74	3/24042 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	626	TRP	CB-CG	-5.37	1.40	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	TRP	CA-CB-CG	5.17	123.52	113.70
1	A	627	TRP	C-N-CA	5.01	134.24	121.70
1	B	712	TYR	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7900	0	7935	195	0
1	B	7900	0	7935	209	0
2	C	644	0	626	13	0
2	D	644	0	626	6	0
3	E	19	0	17	0	0
3	J	19	0	17	0	0
4	F	23	0	21	3	0
4	G	23	0	21	12	0
4	H	23	0	21	2	0
4	I	23	0	19	1	0
4	K	23	0	21	0	0
4	L	23	0	21	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	20	0	14	4	0
7	B	20	0	14	13	0
All	All	17316	0	17308	437	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 13.

All (437) 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)
7:B:1204:BXY:O2	4:G:2:GLC:H3	1.31	1.24
4:I:1:BGC:O3	4:I:2:GLC:O2	1.54	1.22
1:A:841:GLN:HG3	1:A:932:LEU:O	1.36	1.21
1:B:543:ILE:HD11	1:B:592:VAL:HG12	1.31	1.09
1:A:719:ARG:HG2	1:A:719:ARG:HH21	1.12	1.07
1:B:635:PRO:HA	4:L:2:GLC:O2	1.57	1.05
7:B:1204:BXY:C2	4:G:2:GLC:H5	1.91	0.99
1:A:628:TYR:OH	1:A:967:VAL:HG12	1.65	0.97
1:A:247:ARG:HB3	2:C:41:SER:HB2	1.43	0.96
1:A:600:LYS:H	7:A:1203:BXY:H1	1.30	0.94
1:A:320:TRP:HZ3	1:A:329:TRP:O	1.49	0.93
7:B:1204:BXY:O2	4:G:2:GLC:C3	2.17	0.93
1:A:841:GLN:CG	1:A:932:LEU:O	2.20	0.90
1:B:247:ARG:HB3	2:D:41:SER:HB2	1.54	0.90
4:F:1:BGC:O6	4:F:2:GLC:O6	1.88	0.89
1:B:635:PRO:CA	4:L:2:GLC:O2	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ARG:HH21	1:B:575:HIS:CD2	1.91	0.89
1:A:391:GLY:HA3	1:A:421:THR:HG21	1.59	0.84
1:B:738:VAL:HG12	1:B:1027:THR:HG22	1.58	0.84
1:A:712:TYR:HB2	1:A:713:PRO:HD3	1.57	0.84
1:B:515:GLY:O	1:B:622:THR:HG21	1.77	0.84
1:B:605:ARG:HH12	1:B:672:VAL:HG21	1.41	0.84
1:B:935:GLN:N	1:B:935:GLN:OE1	2.10	0.84
1:A:515:GLY:O	1:A:622:THR:HG21	1.79	0.83
7:B:1204:BXY:H2	4:G:2:GLC:H5	1.60	0.83
1:B:543:ILE:HD11	1:B:592:VAL:CG1	2.07	0.82
1:A:138:CYS:HB2	1:A:139:ARG:HH21	1.45	0.82
1:A:962:MET:HG2	1:A:977:PHE:HE1	1.42	0.82
1:B:635:PRO:HB3	4:L:2:GLC:O2	1.79	0.82
1:A:974:GLN:H	1:A:974:GLN:HE21	1.29	0.80
1:B:925:LEU:HD21	1:B:940:LEU:HD13	1.65	0.79
1:B:94:THR:HG22	1:B:107:LEU:H	1.47	0.78
1:A:719:ARG:HG2	1:A:719:ARG:NH2	1.92	0.78
7:A:1204:BXY:O2	4:H:1:BGC:H1	1.84	0.78
1:B:301:ARG:NH2	1:B:493:GLY:HA2	2.00	0.77
1:B:635:PRO:CB	4:L:2:GLC:O2	2.33	0.76
4:F:1:BGC:O6	4:F:2:GLC:O5	2.04	0.76
1:B:932:LEU:HD22	1:B:932:LEU:H	1.50	0.76
1:A:932:LEU:N	1:A:932:LEU:HD23	2.02	0.75
1:B:277:THR:HG22	1:B:381:GLY:HA3	1.68	0.74
1:B:932:LEU:H	1:B:932:LEU:HD13	1.52	0.74
1:A:302:TRP:HE1	1:A:493:GLY:HA3	1.53	0.74
1:B:605:ARG:NH1	1:B:672:VAL:HG21	2.03	0.73
1:B:847:ARG:HG2	1:B:926:VAL:HG12	1.69	0.73
7:B:1204:BXY:H2	4:G:2:GLC:C5	2.17	0.73
1:A:600:LYS:N	7:A:1203:BXY:H1	2.05	0.72
1:B:635:PRO:HB3	4:L:1:BGC:O3	1.90	0.72
1:B:758:LEU:HA	1:B:848:SER:HB2	1.72	0.71
1:A:302:TRP:HD1	1:A:492:VAL:HG13	1.55	0.71
1:B:847:ARG:CG	1:B:926:VAL:HG12	2.21	0.71
1:A:309:PRO:HA	1:A:473:ILE:HG23	1.70	0.71
1:B:932:LEU:HD13	1:B:932:LEU:N	2.06	0.70
1:A:301:ARG:HH21	1:A:493:GLY:HA2	1.54	0.70
1:A:280:ASP:HB3	1:A:382:LEU:H	1.58	0.69
1:B:520:ARG:NH1	1:B:622:THR:HG23	2.08	0.69
1:A:238:ASP:HB3	1:A:407:ARG:HH11	1.57	0.68
1:A:572:TRP:HB2	1:A:575:HIS:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG12	1:A:984:VAL:HG13	1.76	0.68
1:B:932:LEU:HD22	1:B:932:LEU:N	2.08	0.68
1:B:645:PHE:O	7:B:1204:BXY:O3	2.11	0.68
1:A:489:LYS:HD2	4:F:2:GLC:O2	1.94	0.68
1:B:246:LYS:HB3	1:B:249:LEU:HB3	1.77	0.67
1:A:761:VAL:HB	1:A:847:ARG:HB3	1.75	0.67
7:B:1204:BXY:O2	4:G:2:GLC:H5	1.95	0.67
1:A:242:GLY:O	1:A:243:ARG:HB2	1.94	0.66
1:B:392:ILE:HD13	1:B:582:LEU:HG	1.76	0.66
1:A:81:VAL:HG22	1:A:130:LEU:HD22	1.75	0.66
1:A:80:LEU:HB3	1:A:190:LEU:HD11	1.77	0.66
7:B:1204:BXY:C2	4:G:2:GLC:C5	2.71	0.66
1:A:649:THR:HG21	7:A:1204:BXY:O3	1.96	0.66
1:A:302:TRP:CD1	1:A:492:VAL:HG13	2.30	0.65
4:H:2:GLC:O6	4:H:2:GLC:O4	2.08	0.65
1:B:391:GLY:HA3	1:B:421:THR:HG21	1.78	0.65
1:B:480:ALA:HB2	1:B:1065:TRP:HA	1.77	0.65
1:B:330:MET:HA	1:B:330:MET:HE2	1.78	0.65
1:A:70:VAL:HG22	1:A:200:LEU:HD23	1.80	0.64
1:B:302:TRP:HE1	1:B:493:GLY:HA3	1.63	0.64
1:A:63:TYR:HB3	1:A:182:GLN:HG3	1.80	0.64
1:B:248:PHE:HB3	2:D:42:LEU:HB2	1.80	0.64
1:A:36:LEU:HD23	1:A:216:LYS:HA	1.80	0.64
1:A:511:THR:HA	1:A:622:THR:HG22	1.80	0.64
1:B:297:ALA:HA	1:B:306:PRO:HA	1.80	0.63
1:A:962:MET:HG2	1:A:977:PHE:CE1	2.30	0.63
1:A:403:VAL:HG11	1:A:553:ARG:HH12	1.63	0.63
1:B:397:CYS:O	1:B:401:ARG:HG2	1.99	0.63
1:B:235:HIS:HB2	1:B:409:LEU:HD13	1.81	0.62
1:B:352:ARG:HE	1:B:400:GLU:HG3	1.62	0.62
1:B:879:GLN:NE2	1:B:926:VAL:HG11	2.13	0.62
1:B:47:TRP:HB3	1:B:200:LEU:HB2	1.82	0.62
1:A:109:ILE:HG12	1:A:118:VAL:HG22	1.81	0.62
1:B:270:TRP:O	1:B:274:GLY:HA3	1.99	0.62
1:B:319:LEU:HA	1:B:322:HIS:CD2	2.34	0.62
1:B:624:ASN:O	1:B:637:SER:HA	2.00	0.62
1:B:744:ALA:HB1	1:B:947:GLU:HG3	1.82	0.61
1:A:264:SER:O	1:A:268:VAL:HG23	1.99	0.61
1:B:384:PRO:HA	1:B:387:ILE:HD13	1.82	0.61
1:A:320:TRP:CZ3	1:A:329:TRP:O	2.42	0.61
1:A:277:THR:HG22	1:A:381:GLY:HA3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:CYS:SG	1:B:139:ARG:HB2	2.41	0.61
1:B:159:GLN:HE21	1:B:162:ASP:HB3	1.66	0.61
1:A:352:ARG:HE	1:A:400:GLU:HG3	1.66	0.60
1:A:749:PRO:HA	1:A:851:TYR:HA	1.81	0.60
1:B:533:SER:HB3	1:B:555:ILE:HD11	1.82	0.60
7:B:1204:BXY:H2	4:G:2:GLC:H61	1.83	0.59
1:B:511:THR:HA	1:B:622:THR:HG22	1.83	0.59
1:B:626:TRP:H	1:B:631:ASN:ND2	2.01	0.59
1:B:70:VAL:HB	1:B:143:PHE:HB3	1.83	0.59
1:A:594:VAL:HG21	1:A:608:PHE:CD2	2.38	0.59
1:B:543:ILE:CD1	1:B:592:VAL:HG12	2.20	0.59
1:B:319:LEU:HA	1:B:322:HIS:HD2	1.67	0.59
1:B:865:VAL:HG12	1:B:943:PRO:HA	1.84	0.59
1:B:642:GLU:HA	1:B:646:GLY:HA2	1.84	0.58
7:B:1204:BXY:H2	4:G:2:GLC:C6	2.33	0.58
1:A:862:LEU:O	1:A:946:PRO:HD2	2.03	0.58
1:B:530:LEU:O	1:B:534:ILE:HG12	2.04	0.58
1:A:446:VAL:O	1:A:450:VAL:HB	2.04	0.58
1:A:897:PHE:HB3	1:A:909:LEU:HD12	1.85	0.58
1:B:496:LEU:HD23	1:B:500:ASP:HB3	1.83	0.58
1:B:398:SER:HB3	1:B:414:ALA:HB2	1.85	0.58
1:B:301:ARG:HH22	1:B:493:GLY:HA2	1.68	0.57
1:B:303:PHE:H	1:B:1010:GLY:HA3	1.68	0.57
1:B:686:VAL:O	1:B:688:PRO:HD3	2.05	0.57
1:B:937:TRP:N	1:B:937:TRP:CD1	2.73	0.57
1:A:930:ASP:OD1	1:A:930:ASP:N	2.36	0.57
1:A:965:TRP:CZ2	1:A:1001:ASN:HB3	2.40	0.57
1:A:626:TRP:CD1	1:A:626:TRP:N	2.73	0.57
1:B:993:PRO:HD2	1:B:998:ALA:HB2	1.85	0.57
1:B:870:ARG:HB2	1:B:936:HIS:HA	1.86	0.57
1:A:429:ILE:HD12	1:A:564:ALA:O	2.05	0.57
1:B:231:LEU:HD21	1:B:465:ALA:HB2	1.88	0.56
1:B:246:LYS:HB3	1:B:249:LEU:CB	2.36	0.56
1:A:407:ARG:HH21	1:A:409:LEU:H	1.54	0.56
1:B:870:ARG:HD2	1:B:935:GLN:O	2.05	0.56
1:A:429:ILE:O	1:A:432:VAL:HB	2.07	0.55
1:A:510:THR:O	1:A:515:GLY:HA3	2.06	0.55
1:A:870:ARG:HG3	1:A:904:PRO:HB3	1.88	0.55
1:B:115:ASP:HA	1:B:129:PRO:HA	1.88	0.55
1:A:412:ALA:HB2	1:A:462:ILE:HG22	1.88	0.55
1:A:835:SER:OG	1:A:929:ASP:OD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:ILE:HG23	2:C:77:ILE:HD11	1.88	0.55
1:B:39:GLU:HB3	1:B:1061:THR:HG22	1.88	0.55
1:B:711:GLN:NE2	1:B:715:TRP:O	2.39	0.55
1:B:879:GLN:NE2	1:B:926:VAL:CG1	2.69	0.55
1:A:273:VAL:HG21	1:A:705:THR:HA	1.89	0.55
1:A:59:PRO:HA	1:A:184:VAL:HA	1.89	0.54
1:A:712:TYR:HB2	1:A:713:PRO:CD	2.33	0.54
7:B:1204:BCY:O2	4:G:2:GLC:C4	2.56	0.54
1:A:302:TRP:HD1	1:A:492:VAL:CG1	2.20	0.54
1:A:530:LEU:O	1:A:534:ILE:HG12	2.07	0.54
1:B:556:GLY:O	1:B:560:ILE:HG12	2.08	0.54
1:A:42:THR:HA	1:A:206:THR:HG21	1.89	0.54
1:A:533:SER:HB3	1:A:555:ILE:HD11	1.89	0.54
1:A:623:VAL:HG23	1:A:625:GLY:H	1.73	0.54
1:B:302:TRP:HE1	1:B:493:GLY:CA	2.21	0.54
1:A:145:ALA:HA	1:A:150:VAL:HG23	1.90	0.53
1:A:572:TRP:HB2	1:A:575:HIS:HD2	1.71	0.53
2:C:32:SER:HA	2:C:69:THR:HA	1.90	0.53
1:B:257:THR:HG21	1:B:361:ARG:NH2	2.24	0.53
1:B:965:TRP:CZ2	1:B:1001:ASN:HB3	2.44	0.53
1:B:932:LEU:H	1:B:932:LEU:CD1	2.11	0.53
1:B:769:ASN:HD21	1:B:818:ARG:H	1.56	0.53
1:A:262:LEU:O	1:A:266:MET:HG2	2.09	0.53
1:B:608:PHE:O	1:B:612:VAL:HG23	2.09	0.53
1:B:738:VAL:CG1	1:B:1027:THR:HG22	2.36	0.53
2:C:13:ALA:HA	2:C:27:VAL:HG21	1.91	0.53
1:A:403:VAL:HA	1:A:445:ILE:HD11	1.91	0.53
1:B:320:TRP:HD1	1:B:330:MET:HE2	1.74	0.53
1:B:625:GLY:HA2	1:B:631:ASN:HD21	1.73	0.53
1:A:624:ASN:ND2	1:A:635:PRO:O	2.32	0.52
1:B:965:TRP:HZ2	1:B:1001:ASN:HB3	1.74	0.52
1:A:741:ASN:HB3	1:A:744:ALA:HB2	1.92	0.52
1:A:524:LEU:HD21	1:A:618:LEU:HD23	1.91	0.52
1:A:697:VAL:O	1:A:701:VAL:HG23	2.08	0.52
1:B:834:GLY:HA2	1:B:939:ALA:HA	1.91	0.52
1:A:406:SER:HB2	2:C:49:VAL:HG21	1.92	0.52
1:B:356:ALA:O	1:B:360:SER:HB2	2.10	0.52
1:A:284:LEU:HD22	1:A:969:LEU:HD12	1.91	0.52
1:A:517:VAL:HG22	1:A:619:SER:O	2.10	0.52
1:B:273:VAL:HG21	1:B:705:THR:HA	1.91	0.52
1:B:862:LEU:HB2	1:B:912:PRO:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG12	1:A:110:GLU:HB3	1.92	0.51
1:A:841:GLN:CB	1:A:932:LEU:O	2.57	0.51
1:A:860:GLY:HA2	1:A:948:LEU:HD12	1.92	0.51
1:B:263:VAL:HG11	1:B:342:TRP:CD1	2.45	0.51
1:A:62:GLY:HA2	1:A:303:PHE:HB3	1.93	0.51
1:B:917:PRO:HB2	1:B:919:GLU:HG2	1.93	0.51
1:A:349:VAL:HG11	1:A:585:CYS:SG	2.50	0.51
1:B:388:ILE:HG23	1:B:421:THR:HB	1.93	0.51
1:A:879:GLN:HG2	1:A:894:SER:HB3	1.93	0.51
1:B:36:LEU:HD23	1:B:216:LYS:HA	1.93	0.51
1:B:543:ILE:HD12	1:B:543:ILE:C	2.31	0.50
1:B:1005:MET:HB3	1:B:1012:PRO:HD2	1.94	0.50
1:A:965:TRP:HZ2	1:A:1001:ASN:HB3	1.76	0.50
1:B:388:ILE:HB	1:B:578:VAL:HG23	1.94	0.50
1:A:955:VAL:HG12	1:A:989:TRP:CD2	2.47	0.50
1:A:1062:ARG:HD3	1:A:1066:TRP:CH2	2.47	0.50
1:A:735:ASP:HB3	1:A:1030:LYS:HB2	1.94	0.50
1:A:878:VAL:HG23	1:A:895:ILE:HG23	1.93	0.50
1:A:850:TRP:HB3	1:A:922:GLN:HB3	1.94	0.49
2:C:8:ILE:HG21	2:C:74:VAL:HA	1.93	0.49
2:C:44:MET:HB3	2:C:64:LEU:HD22	1.94	0.49
1:B:606:THR:HB	1:B:662:ALA:HB2	1.93	0.49
1:A:308:SER:CB	1:A:309:PRO:HD3	2.43	0.49
1:A:599:MET:O	1:A:605:ARG:HD2	2.13	0.49
1:B:736:VAL:HG23	1:B:951:LEU:HB2	1.92	0.49
1:A:418:GLY:HA3	1:A:435:LEU:HD21	1.94	0.49
1:A:904:PRO:HG3	1:A:935:GLN:HE22	1.77	0.49
1:B:877:GLU:HG2	1:B:896:THR:HG22	1.94	0.49
1:A:302:TRP:NE1	1:A:493:GLY:HA3	2.24	0.49
1:A:389:ALA:HB1	1:A:580:ALA:HB3	1.95	0.49
1:B:636:TRP:H	4:L:2:GLC:C3	2.25	0.49
1:B:73:PRO:HG2	1:B:76:ALA:HB2	1.94	0.49
1:A:908:ASN:HD21	1:A:1026:PRO:HB3	1.78	0.49
1:B:68:LEU:HD13	1:B:202:ALA:HB2	1.95	0.49
1:B:125:VAL:HG13	1:B:126:VAL:HG23	1.94	0.49
1:B:657:LEU:HA	1:B:660:LEU:HD12	1.93	0.49
1:A:407:ARG:HH21	1:A:409:LEU:CB	2.26	0.48
1:A:642:GLU:CB	1:A:646:GLY:HA2	2.43	0.48
1:A:841:GLN:CB	1:A:932:LEU:HA	2.43	0.48
1:B:864:VAL:HG22	1:B:946:PRO:HD3	1.94	0.48
1:A:102:ALA:C	1:A:104:ASP:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TRP:HD1	1:A:557:ILE:HD12	1.78	0.48
1:B:537:THR:HG23	1:B:542:ARG:HA	1.95	0.48
1:A:273:VAL:CG2	1:A:705:THR:HA	2.43	0.48
1:A:429:ILE:HD11	1:A:568:THR:HG23	1.96	0.48
1:B:605:ARG:HH12	1:B:672:VAL:HG11	1.77	0.48
4:L:1:BGC:O6	4:L:2:GLC:H5	2.14	0.48
1:B:159:GLN:HB2	1:B:170:VAL:HG22	1.96	0.48
7:B:1204:BCY:O2	4:G:2:GLC:C5	2.61	0.48
1:B:961:VAL:HG22	1:B:963:LEU:HG	1.96	0.48
1:A:177:TYR:HB3	1:A:179:PHE:CE2	2.49	0.48
1:A:302:TRP:HE1	1:A:493:GLY:CA	2.26	0.48
1:B:743:ASN:HD21	1:B:826:ASN:H	1.60	0.48
1:B:847:ARG:HG3	1:B:926:VAL:HG12	1.93	0.48
1:A:392:ILE:HD13	1:A:582:LEU:HG	1.95	0.47
1:B:49:GLN:HB3	1:B:1054:ARG:HG3	1.96	0.47
1:B:983:VAL:HG21	1:B:1055:LEU:HD11	1.96	0.47
1:B:38:VAL:HG23	1:B:216:LYS:HD3	1.95	0.47
1:A:642:GLU:HB2	1:A:646:GLY:HA2	1.97	0.47
1:A:1008:LEU:HD21	1:A:1075:HIS:HD2	1.78	0.47
1:A:34:PRO:HB2	1:A:479:LEU:HB2	1.95	0.47
1:A:45:LEU:HB2	1:A:204:ILE:HD11	1.97	0.47
1:A:414:ALA:HA	1:A:417:ILE:HD12	1.96	0.47
1:B:548:LEU:HD11	1:B:552:ARG:HH21	1.79	0.47
1:B:366:THR:CG2	1:B:690:ALA:HB2	2.44	0.47
1:B:647:PHE:N	1:B:647:PHE:CD1	2.81	0.47
1:A:407:ARG:NH2	1:A:409:LEU:H	2.12	0.47
1:B:257:THR:H	1:B:260:ASP:HB2	1.79	0.47
1:A:864:VAL:HG22	1:A:946:PRO:HD3	1.97	0.47
1:B:151:THR:HG22	1:B:173:GLU:HG2	1.96	0.47
1:B:867:ALA:HB2	1:B:940:LEU:HD23	1.97	0.47
2:C:5:GLN:HG3	2:C:74:VAL:HG11	1.97	0.47
1:A:858:GLN:HG3	1:A:860:GLY:H	1.78	0.47
1:A:297:ALA:HA	1:A:306:PRO:HA	1.97	0.47
1:A:378:LEU:HD21	1:A:519:ARG:HG2	1.97	0.47
1:B:59:PRO:HA	1:B:184:VAL:HA	1.96	0.47
1:B:622:THR:O	1:B:640:PHE:HA	2.15	0.47
1:B:412:ALA:HA	1:B:415:ILE:HD12	1.97	0.46
1:A:263:VAL:HG11	1:A:342:TRP:CG	2.51	0.46
1:A:407:ARG:HH21	1:A:409:LEU:HB2	1.80	0.46
1:A:873:GLN:HE22	1:A:898:GLY:HA2	1.79	0.46
1:B:45:LEU:HB3	1:B:202:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:ASN:ND2	1:B:637:SER:HB2	2.30	0.46
1:B:280:ASP:HB3	1:B:382:LEU:H	1.80	0.46
1:A:120:VAL:HG21	1:A:143:PHE:CZ	2.50	0.46
1:A:149:LYS:HB3	1:A:175:SER:HB3	1.98	0.46
1:A:320:TRP:CH2	1:A:332:PHE:HB3	2.50	0.46
1:B:86:ARG:HD2	1:B:88:ARG:NH1	2.31	0.46
1:A:346:SER:HA	1:A:350:ILE:HD12	1.96	0.46
1:A:512:SER:HB2	1:A:513:PRO:HD2	1.96	0.46
1:A:603:ARG:HD2	1:A:666:HIS:HB2	1.97	0.46
1:B:83:PRO:HB3	1:B:86:ARG:HE	1.81	0.46
1:B:862:LEU:CD1	1:B:910:ARG:HB2	2.45	0.46
1:A:270:TRP:HE3	1:A:701:VAL:HG13	1.80	0.46
1:B:366:THR:HG22	1:B:690:ALA:N	2.31	0.46
1:B:933:ALA:HA	1:B:934:PRO:HD3	1.78	0.46
1:A:712:TYR:CB	1:A:713:PRO:HD3	2.38	0.45
1:B:63:TYR:HB3	1:B:182:GLN:HG3	1.98	0.45
1:B:862:LEU:HD11	1:B:910:ARG:HB2	1.97	0.45
1:A:267:LEU:HD22	1:A:372:LEU:HD21	1.97	0.45
1:A:623:VAL:HG23	1:A:623:VAL:O	2.16	0.45
1:B:284:LEU:HD11	1:B:325:THR:HG23	1.98	0.45
1:B:416:ILE:HG12	1:B:468:VAL:HG11	1.98	0.45
1:B:158:THR:HG22	1:B:169:ALA:H	1.81	0.45
2:D:4:THR:HG23	2:D:7:GLU:H	1.81	0.45
1:A:131:GLU:HG2	1:A:132:GLN:H	1.80	0.45
1:A:434:ALA:HA	1:A:557:ILE:HG12	1.98	0.45
1:A:831:PRO:HD2	1:A:942:PRO:HG3	1.98	0.45
1:B:572:TRP:H	1:B:575:HIS:CD2	2.35	0.45
1:B:572:TRP:H	1:B:575:HIS:HD2	1.63	0.45
1:B:702:VAL:O	1:B:706:LEU:HB2	2.16	0.45
1:B:960:PRO:HB3	1:B:985:GLU:OE1	2.17	0.45
2:D:60:PRO:HD2	2:D:63:ASP:HB2	1.99	0.45
1:A:184:VAL:HB	1:A:1019:LEU:HD13	1.98	0.45
1:B:513:PRO:HD2	1:B:627:TRP:CZ2	2.51	0.45
1:B:311:GLY:HA3	1:B:314:TYR:HD2	1.82	0.45
1:B:626:TRP:CD1	1:B:634:VAL:HG21	2.52	0.45
1:B:249:LEU:HG	1:B:401:ARG:HE	1.82	0.44
1:B:282:TYR:CD2	1:B:965:TRP:HB2	2.52	0.44
1:B:352:ARG:NE	1:B:400:GLU:HG3	2.32	0.44
1:B:861:PRO:HD2	1:B:948:LEU:HD12	1.99	0.44
1:A:622:THR:HB	1:A:623:VAL:H	1.39	0.44
1:B:88:ARG:HG2	1:B:189:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:TRP:HD1	1:B:330:MET:CE	2.30	0.44
1:B:846:LEU:O	1:B:926:VAL:HA	2.18	0.44
2:C:9:ILE:HD11	2:C:29:PRO:HG3	1.99	0.44
1:A:95:VAL:HG11	1:A:102:ALA:HA	1.99	0.44
1:A:320:TRP:HH2	1:A:332:PHE:HB3	1.82	0.44
1:A:336:LEU:HA	1:A:339:LEU:HD12	1.99	0.44
1:A:397:CYS:O	1:A:401:ARG:HG3	2.17	0.44
1:A:951:LEU:O	1:A:955:VAL:HG22	2.16	0.44
1:A:252:ARG:HD2	1:A:347:ARG:HB3	1.98	0.44
1:A:386:PRO:HG2	1:A:387:ILE:HD12	1.99	0.44
1:A:841:GLN:HB2	1:A:932:LEU:HA	1.99	0.44
1:B:311:GLY:CA	1:B:314:TYR:HD2	2.31	0.44
1:B:936:HIS:O	1:B:936:HIS:CG	2.70	0.44
1:A:908:ASN:ND2	1:A:1026:PRO:HB3	2.32	0.44
1:B:741:ASN:HB3	1:B:744:ALA:HB2	2.00	0.44
1:A:316:LEU:HA	1:A:319:LEU:HD12	2.00	0.44
1:A:845:VAL:HG12	1:A:928:SER:HA	2.00	0.44
1:B:910:ARG:HD2	1:B:1034:TYR:H	1.83	0.44
2:D:23:GLU:HG3	2:D:24:PRO:HD2	2.00	0.44
1:B:536:MET:HG3	1:B:543:ILE:HA	1.99	0.44
1:B:1020:LEU:HD22	1:B:1043:LEU:HB3	1.99	0.44
1:A:136:PRO:HB2	1:A:139:ARG:CZ	2.48	0.44
1:B:136:PRO:HG2	1:B:139:ARG:HD3	2.00	0.44
1:B:249:LEU:HA	1:B:401:ARG:HE	1.83	0.44
7:B:1204:BCY:C3	4:G:2:GLC:H5	2.43	0.43
1:A:634:VAL:HG22	1:A:637:SER:HB3	2.00	0.43
1:B:349:VAL:HG11	1:B:585:CYS:SG	2.58	0.43
1:A:356:ALA:HB2	1:A:545:GLY:HA3	2.00	0.43
1:A:534:ILE:CD1	1:A:559:ILE:HD11	2.47	0.43
1:B:737:LEU:HB3	1:B:948:LEU:HB3	2.00	0.43
1:A:88:ARG:HD3	1:A:190:LEU:HA	2.00	0.43
1:B:388:ILE:HD13	1:B:428:GLY:HA2	2.00	0.43
1:A:738:VAL:HG22	1:A:954:VAL:HG21	2.00	0.43
1:B:301:ARG:HG3	1:B:1009:GLY:O	2.18	0.43
1:A:139:ARG:HG2	1:A:157:LEU:HB2	2.00	0.43
1:A:159:GLN:HB2	1:A:170:VAL:HG22	2.00	0.43
1:B:626:TRP:O	1:B:631:ASN:HB2	2.18	0.43
2:C:46:GLU:HA	2:C:49:VAL:HG12	2.01	0.43
1:A:366:THR:HG21	1:A:591:ALA:HB2	2.01	0.43
1:A:841:GLN:HB2	1:A:932:LEU:CA	2.49	0.43
1:A:320:TRP:CZ3	1:A:333:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TRP:CD1	1:A:557:ILE:HD12	2.54	0.43
1:A:653:GLY:O	1:A:656:VAL:HG12	2.19	0.43
1:B:99:ALA:HB3	1:B:102:ALA:HB2	2.00	0.43
1:B:474:PHE:HE2	1:B:479:LEU:HA	1.83	0.43
2:D:32:SER:H	2:D:36:ASP:HB2	1.84	0.43
1:A:931:ASP:HB3	1:A:936:HIS:HB3	2.00	0.42
1:A:974:GLN:H	1:A:974:GLN:NE2	2.06	0.42
1:A:441:PRO:O	1:A:445:ILE:HG12	2.19	0.42
1:A:524:LEU:HB3	1:A:615:VAL:HB	2.01	0.42
1:A:602:ARG:HD2	1:A:602:ARG:HA	1.78	0.42
1:B:1002:SER:N	1:B:1003:PRO:CD	2.82	0.42
1:A:284:LEU:HD11	1:A:325:THR:HG23	2.00	0.42
1:B:776:SER:OG	1:B:937:TRP:HH2	2.02	0.42
1:B:879:GLN:HE21	1:B:926:VAL:HG13	1.84	0.42
1:A:967:VAL:HG23	1:A:967:VAL:O	2.19	0.42
1:B:34:PRO:HB3	1:B:474:PHE:CD2	2.54	0.42
1:B:671:ASP:HB3	1:B:674:PRO:HD2	2.00	0.42
1:B:848:SER:HB3	1:B:925:LEU:HB3	2.01	0.42
1:A:58:ALA:HB3	1:A:185:GLY:HA2	2.02	0.42
1:A:33:THR:HA	1:A:36:LEU:HD22	2.02	0.42
1:A:549:GLY:HA3	1:A:553:ARG:HH21	1.85	0.42
1:A:1029:LEU:HB3	1:A:1032:ASP:O	2.20	0.42
1:B:147:ALA:HA	1:B:180:ARG:HH21	1.85	0.42
1:B:770:GLY:O	1:B:836:TRP:HE3	2.02	0.42
1:A:459:LEU:O	1:A:462:ILE:HG13	2.20	0.42
1:B:311:GLY:CA	1:B:314:TYR:CD2	3.03	0.42
1:B:98:GLN:HG3	1:B:1046:TRP:CE3	2.55	0.42
1:B:771:ILE:HG21	1:B:939:ALA:HB2	2.01	0.42
2:C:63:ASP:O	2:C:67:LEU:HG	2.19	0.42
1:A:308:SER:HB2	1:A:309:PRO:HD3	2.02	0.42
1:B:53:TRP:CZ3	1:B:190:LEU:HD13	2.54	0.42
1:A:961:VAL:HG12	1:A:989:TRP:HB2	2.01	0.41
1:B:48:PRO:HG3	1:B:199:GLN:HA	2.01	0.41
1:B:94:THR:CG2	1:B:107:LEU:H	2.24	0.41
1:B:459:LEU:O	1:B:462:ILE:HG13	2.20	0.41
1:B:880:TRP:HZ3	1:B:895:ILE:HG23	1.85	0.41
2:C:67:LEU:HB3	2:C:73:VAL:HG22	2.02	0.41
1:A:422:LEU:HD11	1:A:432:VAL:HG23	2.02	0.41
1:B:300:TYR:HE1	1:B:963:LEU:O	2.04	0.41
2:C:32:SER:H	2:C:36:ASP:HB2	1.85	0.41
1:B:346:SER:HA	1:B:350:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ARG:CZ	1:B:676:ARG:HH11	2.33	0.41
1:B:769:ASN:ND2	1:B:818:ARG:H	2.19	0.41
1:A:60:LEU:HD22	1:A:204:ILE:HG23	2.01	0.41
1:A:871:PHE:HB2	1:A:875:GLU:HG3	2.02	0.41
1:B:71:THR:HA	1:B:141:LEU:O	2.20	0.41
1:B:308:SER:CB	1:B:309:PRO:HD3	2.49	0.41
1:B:320:TRP:CD1	1:B:330:MET:HE2	2.54	0.41
1:A:132:GLN:HB3	1:A:157:LEU:HD11	2.02	0.41
1:A:738:VAL:HG12	1:A:1027:THR:HG22	2.01	0.41
1:B:68:LEU:HB3	1:B:145:ALA:HB3	2.02	0.41
1:B:341:CYS:HA	1:B:390:LEU:HD13	2.02	0.41
1:B:344:VAL:O	1:B:349:VAL:HG23	2.20	0.41
1:B:366:THR:HG23	1:B:690:ALA:HB2	2.02	0.41
1:B:936:HIS:ND1	1:B:936:HIS:C	2.72	0.41
1:A:319:LEU:HA	1:A:322:HIS:CD2	2.55	0.41
1:A:356:ALA:CB	1:A:545:GLY:HA3	2.51	0.41
1:A:738:VAL:HG21	1:A:954:VAL:HG11	2.03	0.41
1:B:409:LEU:O	1:B:413:VAL:HG23	2.21	0.41
1:B:594:VAL:HG21	1:B:608:PHE:CD2	2.55	0.41
1:B:636:TRP:CD2	1:B:641:PRO:HA	2.55	0.41
1:A:488:PHE:O	1:A:492:VAL:HG12	2.21	0.41
1:A:622:THR:O	1:A:640:PHE:HA	2.20	0.41
1:A:961:VAL:HG22	1:A:975:ARG:O	2.21	0.41
1:B:594:VAL:O	1:B:594:VAL:HG22	2.21	0.41
1:B:935:GLN:OE1	1:B:935:GLN:CA	2.69	0.41
1:B:989:TRP:HZ3	1:B:1025:VAL:HG21	1.85	0.41
1:A:542:ARG:HG3	1:A:546:THR:HG22	2.03	0.41
1:A:543:ILE:O	1:A:546:THR:HB	2.21	0.41
1:A:679:ARG:HD2	1:A:681:TRP:HE1	1.86	0.41
1:A:723:ASN:HB3	1:A:728:LYS:HE3	2.03	0.41
1:A:867:ALA:HB3	1:A:909:LEU:HD23	2.03	0.41
1:B:275:ALA:H	1:B:704:LEU:HD22	1.86	0.41
1:B:378:LEU:HD22	1:B:574:HIS:HA	2.02	0.41
1:A:623:VAL:O	1:A:623:VAL:CG2	2.69	0.41
1:B:411:VAL:HG11	1:B:442:LEU:HB2	2.01	0.41
1:B:743:ASN:HD21	1:B:826:ASN:N	2.19	0.41
1:B:647:PHE:N	1:B:647:PHE:HD1	2.19	0.40
1:B:946:PRO:HB2	1:B:948:LEU:HG	2.03	0.40
1:A:275:ALA:H	1:A:704:LEU:HD13	1.86	0.40
1:A:388:ILE:HD13	1:A:428:GLY:HA2	2.03	0.40
1:B:301:ARG:HH21	1:B:493:GLY:HA2	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:HD13	1:B:696:LEU:HA	1.97	0.40
1:A:263:VAL:HG11	1:A:342:TRP:CD1	2.56	0.40
1:A:835:SER:HB3	1:A:938:ILE:H	1.86	0.40
1:B:71:THR:O	1:B:198:LEU:HA	2.20	0.40
1:A:526:LEU:HD13	1:A:583:ALA:HA	2.03	0.40
1:B:90:VAL:HG22	1:B:110:GLU:HB3	2.03	0.40
1:B:216:LYS:HG2	1:B:220:MET:HE2	2.04	0.40
1:A:303:PHE:HE1	1:A:492:VAL:HG21	1.87	0.40
1:A:756:GLN:HG3	1:A:815:ASN:ND2	2.36	0.40
1:B:75:GLN:HA	1:B:134:LEU:HD12	2.03	0.40
1:B:605:ARG:HH12	1:B:672:VAL:CG2	2.22	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 X-ray entries followed by that with respect to entries of similar resolution.

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	1031/1113 (93%)	915 (89%)	96 (9%)	20 (2%)	6	29
1	B	1031/1113 (93%)	934 (91%)	77 (8%)	20 (2%)	6	29
2	C	82/99 (83%)	72 (88%)	7 (8%)	3 (4%)	2	17
2	D	82/99 (83%)	70 (85%)	10 (12%)	2 (2%)	5	25
All	All	2226/2424 (92%)	1991 (89%)	190 (8%)	45 (2%)	6	28

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	243	ARG
1	A	308	SER
1	A	451	SER

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Mol	Chain	Res	Type
1	A	628	TYR
1	A	1030	LYS
1	B	544	PRO
1	B	712	TYR
1	B	1030	LYS
2	C	60	PRO
2	C	61	ASP
1	A	678	GLN
1	A	712	TYR
1	A	980	ARG
1	B	242	GLY
1	B	492	VAL
1	B	754	ALA
2	C	62	GLU
1	A	856	ARG
1	A	968	GLY
1	A	1068	PRO
1	B	728	LYS
1	B	755	GLY
2	D	33	PHE
1	A	66	THR
1	A	492	VAL
1	A	548	LEU
1	A	752	GLU
1	B	165	ASP
1	B	246	LYS
1	B	308	SER
1	B	914	SER
1	B	980	ARG
1	A	596	THR
1	A	857	ASP
1	B	309	PRO
1	B	677	PRO
1	A	544	PRO
1	B	170	VAL
1	B	213	THR
2	D	85	PRO
1	A	1052	PRO
1	B	273	VAL
1	B	545	GLY
1	B	968	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	821/880 (93%)	741 (90%)	80 (10%)	6	25
1	B	821/880 (93%)	736 (90%)	85 (10%)	5	22
2	C	73/81 (90%)	71 (97%)	2 (3%)	40	65
2	D	73/81 (90%)	65 (89%)	8 (11%)	5	20
All	All	1788/1922 (93%)	1613 (90%)	175 (10%)	6	24

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	39	GLU
1	A	47	TRP
1	A	61	ILE
1	A	97	LYS
1	A	115	ASP
1	A	119	ILE
1	A	139	ARG
1	A	150	VAL
1	A	209	SER
1	A	273	VAL
1	A	276	ASN
1	A	280	ASP
1	A	282	TYR
1	A	308	SER
1	A	320	TRP
1	A	328	VAL
1	A	353	LEU
1	A	398	SER
1	A	407	ARG
1	A	432	VAL
1	A	443	LYS
1	A	446	VAL
1	A	458	LEU

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Mol	Chain	Res	Type
1	A	486	SER
1	A	506	SER
1	A	511	THR
1	A	536	MET
1	A	542	ARG
1	A	544	PRO
1	A	546	THR
1	A	548	LEU
1	A	562	PHE
1	A	570	THR
1	A	578	VAL
1	A	602	ARG
1	A	612	VAL
1	A	622	THR
1	A	627	TRP
1	A	629	VAL
1	A	639	SER
1	A	642	GLU
1	A	657	LEU
1	A	678	GLN
1	A	680	ARG
1	A	686	VAL
1	A	701	VAL
1	A	712	TYR
1	A	719	ARG
1	A	735	ASP
1	A	736	VAL
1	A	737	LEU
1	A	738	VAL
1	A	746	MET
1	A	758	LEU
1	A	762	THR
1	A	764	LEU
1	A	862	LEU
1	A	876	VAL
1	A	878	VAL
1	A	883	ASP
1	A	909	LEU
1	A	923	ILE
1	A	928	SER
1	A	929	ASP
1	A	930	ASP

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Mol	Chain	Res	Type
1	A	932	LEU
1	A	935	GLN
1	A	938	ILE
1	A	945	ILE
1	A	964	ASP
1	A	974	GLN
1	A	984	VAL
1	A	992	LEU
1	A	994	ASP
1	A	1025	VAL
1	A	1039	SER
1	A	1044	THR
1	A	1054	ARG
1	A	1075	HIS
1	B	17	LEU
1	B	33	THR
1	B	36	LEU
1	B	42	THR
1	B	52	VAL
1	B	61	ILE
1	B	75	GLN
1	B	93	SER
1	B	94	THR
1	B	98	GLN
1	B	144	THR
1	B	146	HIS
1	B	198	LEU
1	B	200	LEU
1	B	245	HIS
1	B	249	LEU
1	B	267	LEU
1	B	286	MET
1	B	291	GLU
1	B	301	ARG
1	B	308	SER
1	B	328	VAL
1	B	341	CYS
1	B	394	LEU
1	B	398	SER
1	B	399	VAL
1	B	429	ILE
1	B	442	LEU

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Mol	Chain	Res	Type
1	B	443	LYS
1	B	456	TRP
1	B	486	SER
1	B	542	ARG
1	B	543	ILE
1	B	544	PRO
1	B	571	LYS
1	B	597	THR
1	B	622	THR
1	B	623	VAL
1	B	642	GLU
1	B	652	LEU
1	B	657	LEU
1	B	668	SER
1	B	676	ARG
1	B	681	TRP
1	B	698	ILE
1	B	704	LEU
1	B	706	LEU
1	B	712	TYR
1	B	716	SER
1	B	728	LYS
1	B	732	LEU
1	B	735	ASP
1	B	763	SER
1	B	817	SER
1	B	821	LEU
1	B	842	GLN
1	B	845	VAL
1	B	848	SER
1	B	856	ARG
1	B	858	GLN
1	B	890	GLU
1	B	895	ILE
1	B	914	SER
1	B	916	ILE
1	B	928	SER
1	B	931	ASP
1	B	932	LEU
1	B	935	GLN
1	B	936	HIS
1	B	937	TRP

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Mol	Chain	Res	Type
1	B	952	GLN
1	B	962	MET
1	B	990	ARG
1	B	1006	ASP
1	B	1008	LEU
1	B	1019	LEU
1	B	1034	TYR
1	B	1035	ARG
1	B	1039	SER
1	B	1044	THR
1	B	1054	ARG
1	B	1057	LEU
1	B	1062	ARG
1	B	1072	ARG
1	B	1073	LEU
2	C	6	GLU
2	C	77	ILE
2	D	7	GLU
2	D	12	LEU
2	D	16	ILE
2	D	34	VAL
2	D	41	SER
2	D	63	ASP
2	D	72	ASP
2	D	82	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	85	ASN
1	A	132	GLN
1	A	159	GLN
1	A	292	HIS
1	A	322	HIS
1	A	710	ASN
1	A	743	ASN
1	A	826	ASN
1	A	841	GLN
1	A	842	GLN
1	A	935	GLN
1	A	974	GLN

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Mol	Chain	Res	Type
1	A	1075	HIS
1	B	54	GLN
1	B	113	ASN
1	B	159	GLN
1	B	235	HIS
1	B	322	HIS
1	B	449	HIS
1	B	575	HIS
1	B	631	ASN
1	B	710	ASN
1	B	740	GLN
1	B	743	ASN
1	B	769	ASN
1	B	842	GLN
1	B	858	GLN
1	B	879	GLN
1	B	908	ASN
1	B	979	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	$\# Z > 2$
3	BXY	E	1	3	10,10,10	0.76	0	13,14,14	1.06	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BXY	E	2	3	9,9,10	0.49	0	10,12,14	0.88	0
4	BGC	F	1	4	12,12,12	1.58	4 (33%)	17,17,17	2.34	6 (35%)
4	GLC	F	2	4	11,11,12	1.54	2 (18%)	15,15,17	2.49	7 (46%)
4	BGC	G	1	4	12,12,12	1.42	2 (16%)	17,17,17	2.38	8 (47%)
4	GLC	G	2	4	11,11,12	1.73	3 (27%)	15,15,17	2.04	5 (33%)
4	BGC	H	1	4	12,12,12	1.29	3 (25%)	17,17,17	1.64	4 (23%)
4	GLC	H	2	4	11,11,12	2.24	3 (27%)	15,15,17	3.26	6 (40%)
4	BGC	I	1	4	12,12,12	1.33	2 (16%)	17,17,17	1.62	2 (11%)
4	GLC	I	2	4	11,11,12	2.35	3 (27%)	15,15,17	2.72	6 (40%)
3	BXY	J	1	3	10,10,10	0.70	0	13,14,14	1.39	2 (15%)
3	BXY	J	2	3	9,9,10	0.47	0	10,12,14	0.93	1 (10%)
4	BGC	K	1	4	12,12,12	1.51	3 (25%)	17,17,17	1.64	2 (11%)
4	GLC	K	2	4	11,11,12	2.24	3 (27%)	15,15,17	3.04	8 (53%)
4	BGC	L	1	4	12,12,12	1.19	1 (8%)	17,17,17	0.83	0
4	GLC	L	2	4	11,11,12	1.75	2 (18%)	15,15,17	0.90	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
3	BXY	E	1	3	-	2/2/18/18	0/1/1/1
3	BXY	E	2	3	-	0/2/15/18	0/1/1/1
4	BGC	F	1	4	-	2/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1
4	BGC	G	1	4	-	1/2/22/22	0/1/1/1
4	GLC	G	2	4	-	0/2/19/22	0/1/1/1
4	BGC	H	1	4	-	0/2/22/22	0/1/1/1
4	GLC	H	2	4	-	1/2/19/22	0/1/1/1
4	BGC	I	1	4	-	0/2/22/22	0/1/1/1
4	GLC	I	2	4	-	2/2/19/22	0/1/1/1
3	BXY	J	1	3	-	2/2/18/18	0/1/1/1
3	BXY	J	2	3	-	2/2/15/18	0/1/1/1
4	BGC	K	1	4	-	2/2/22/22	0/1/1/1
4	GLC	K	2	4	-	0/2/19/22	0/1/1/1
4	BGC	L	1	4	-	2/2/22/22	0/1/1/1
4	GLC	L	2	4	-	1/2/19/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	GLC	C2-C3	-6.07	1.43	1.52
4	H	2	GLC	O5-C1	5.22	1.52	1.43
4	I	2	GLC	O5-C1	4.92	1.51	1.43
4	L	2	GLC	O5-C1	4.58	1.51	1.43
4	I	2	GLC	C2-C3	-4.40	1.46	1.52
4	H	2	GLC	C2-C3	-4.15	1.46	1.52
4	G	2	GLC	O5-C1	3.76	1.49	1.43
4	F	2	GLC	C2-C3	-3.40	1.47	1.52
4	G	2	GLC	C2-C3	-3.36	1.47	1.52
4	I	2	GLC	C4-C3	-3.20	1.44	1.52
4	K	2	GLC	C4-C3	-3.06	1.44	1.52
4	L	1	BGC	O5-C1	2.92	1.50	1.42
4	G	1	BGC	O5-C1	2.88	1.50	1.42
4	I	1	BGC	O5-C1	2.70	1.49	1.42
4	F	2	GLC	O5-C1	2.57	1.47	1.43
4	G	1	BGC	O5-C5	2.51	1.50	1.44
4	F	1	BGC	C4-C3	-2.50	1.46	1.52
4	F	1	BGC	C1-C2	-2.46	1.46	1.52
4	F	1	BGC	C3-C2	-2.43	1.46	1.52
4	K	1	BGC	O5-C1	2.40	1.48	1.42
4	K	1	BGC	C4-C3	-2.40	1.46	1.52
4	I	1	BGC	C4-C3	-2.37	1.46	1.52
4	F	1	BGC	O5-C1	2.26	1.48	1.42
4	G	2	GLC	C4-C3	-2.26	1.46	1.52
4	L	2	GLC	C2-C3	-2.25	1.49	1.52
4	H	1	BGC	O5-C1	2.22	1.48	1.42
4	H	1	BGC	C1-C2	-2.13	1.47	1.52
4	H	2	GLC	C4-C3	-2.10	1.47	1.52
4	H	1	BGC	C4-C3	-2.10	1.47	1.52
4	K	1	BGC	O5-C5	2.06	1.49	1.44
4	K	2	GLC	O5-C1	2.04	1.47	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	GLC	C3-C4-C5	-8.51	95.06	110.24
4	I	2	GLC	C1-O5-C5	7.53	122.40	112.19
4	H	2	GLC	C2-C3-C4	-7.39	98.10	110.89
4	F	2	GLC	C3-C4-C5	-5.92	99.68	110.24
4	F	1	BGC	O4-C4-C3	-5.60	97.39	110.35
4	G	2	GLC	C1-C2-C3	5.23	116.09	109.67
4	H	2	GLC	O5-C5-C6	5.03	115.10	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	GLC	C3-C4-C5	-4.98	101.36	110.24
4	H	2	GLC	O4-C4-C3	4.82	121.49	110.35
4	I	1	BGC	C3-C4-C5	-4.69	101.87	110.24
4	G	1	BGC	C4-C3-C2	-4.30	103.31	110.82
4	F	1	BGC	C3-C4-C5	4.09	117.53	110.24
4	G	1	BGC	O5-C5-C4	3.99	116.94	109.69
4	K	1	BGC	C4-C3-C2	-3.82	104.16	110.82
4	F	1	BGC	O3-C3-C4	-3.67	101.86	110.35
4	G	1	BGC	O4-C4-C5	-3.57	100.44	109.30
4	H	1	BGC	O2-C2-C1	-3.54	100.96	109.16
4	K	1	BGC	C1-C2-C3	-3.46	103.14	110.31
4	F	2	GLC	O3-C3-C2	-3.42	103.45	109.99
4	I	2	GLC	C1-C2-C3	3.41	113.86	109.67
4	K	2	GLC	O5-C1-C2	3.40	116.02	110.77
4	F	2	GLC	O4-C4-C3	3.32	118.02	110.35
4	I	2	GLC	C6-C5-C4	-3.32	105.24	113.00
4	H	2	GLC	O2-C2-C1	3.30	115.91	109.15
4	F	2	GLC	C1-C2-C3	3.23	113.64	109.67
4	K	2	GLC	C2-C3-C4	-3.19	105.38	110.89
4	H	2	GLC	C6-C5-C4	-3.07	105.81	113.00
3	J	1	BXY	O4-C4-C5	3.01	115.73	109.21
4	F	1	BGC	O3-C3-C2	-2.99	103.44	110.35
4	G	1	BGC	C1-O5-C5	2.97	119.26	113.66
4	K	2	GLC	O2-C2-C3	-2.96	104.21	110.14
4	H	1	BGC	C1-C2-C3	2.93	116.39	110.31
4	G	1	BGC	C1-C2-C3	-2.89	104.32	110.31
4	K	2	GLC	O2-C2-C1	2.79	114.86	109.15
4	F	2	GLC	O2-C2-C1	-2.69	103.65	109.15
4	G	1	BGC	C6-C5-C4	-2.58	106.95	113.00
4	I	1	BGC	O5-C1-C2	2.57	114.87	110.28
4	K	2	GLC	C1-C2-C3	2.57	112.82	109.67
4	K	2	GLC	O3-C3-C2	-2.51	105.18	109.99
4	G	1	BGC	O4-C4-C3	2.49	116.10	110.35
4	K	2	GLC	O4-C4-C5	2.47	115.43	109.30
4	H	1	BGC	O4-C4-C3	-2.45	104.69	110.35
4	F	1	BGC	C4-C3-C2	2.43	115.06	110.82
4	F	2	GLC	O3-C3-C4	2.42	115.95	110.35
3	E	1	BXY	C5-C4-C3	-2.39	109.32	115.09
4	G	2	GLC	O5-C5-C6	2.37	110.92	107.20
4	I	2	GLC	O2-C2-C1	2.35	113.96	109.15
4	I	2	GLC	O5-C5-C6	2.35	110.88	107.20
4	H	1	BGC	O5-C5-C4	2.33	113.92	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	GLC	O2-C2-C3	-2.31	105.50	110.14
4	G	2	GLC	O3-C3-C2	-2.29	105.60	109.99
3	J	2	BXY	O4-C4-C3	2.29	106.73	104.70
4	G	1	BGC	O3-C3-C4	2.25	115.56	110.35
4	F	2	GLC	O5-C1-C2	-2.23	107.32	110.77
4	F	1	BGC	C1-O5-C5	2.23	117.86	113.66
4	G	2	GLC	O3-C3-C4	-2.11	105.48	110.35
3	J	1	BXY	O4-C1-C2	2.10	107.05	104.46
4	G	2	GLC	O5-C5-C4	-2.00	105.96	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	BXY	O4-C4-C5-O5
3	E	1	BXY	C3-C4-C5-O5
3	J	2	BXY	O4-C4-C5-O5
4	L	1	BGC	O5-C5-C6-O6
4	F	1	BGC	O5-C5-C6-O6
4	K	1	BGC	O5-C5-C6-O6
4	K	1	BGC	C4-C5-C6-O6
3	J	1	BXY	O4-C4-C5-O5
3	J	2	BXY	C3-C4-C5-O5
4	I	2	GLC	C4-C5-C6-O6
4	L	1	BGC	C4-C5-C6-O6
3	J	1	BXY	C3-C4-C5-O5
4	F	1	BGC	C4-C5-C6-O6
4	L	2	GLC	O5-C5-C6-O6
4	G	1	BGC	O5-C5-C6-O6
4	H	2	GLC	O5-C5-C6-O6
4	I	2	GLC	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 25 short contacts:

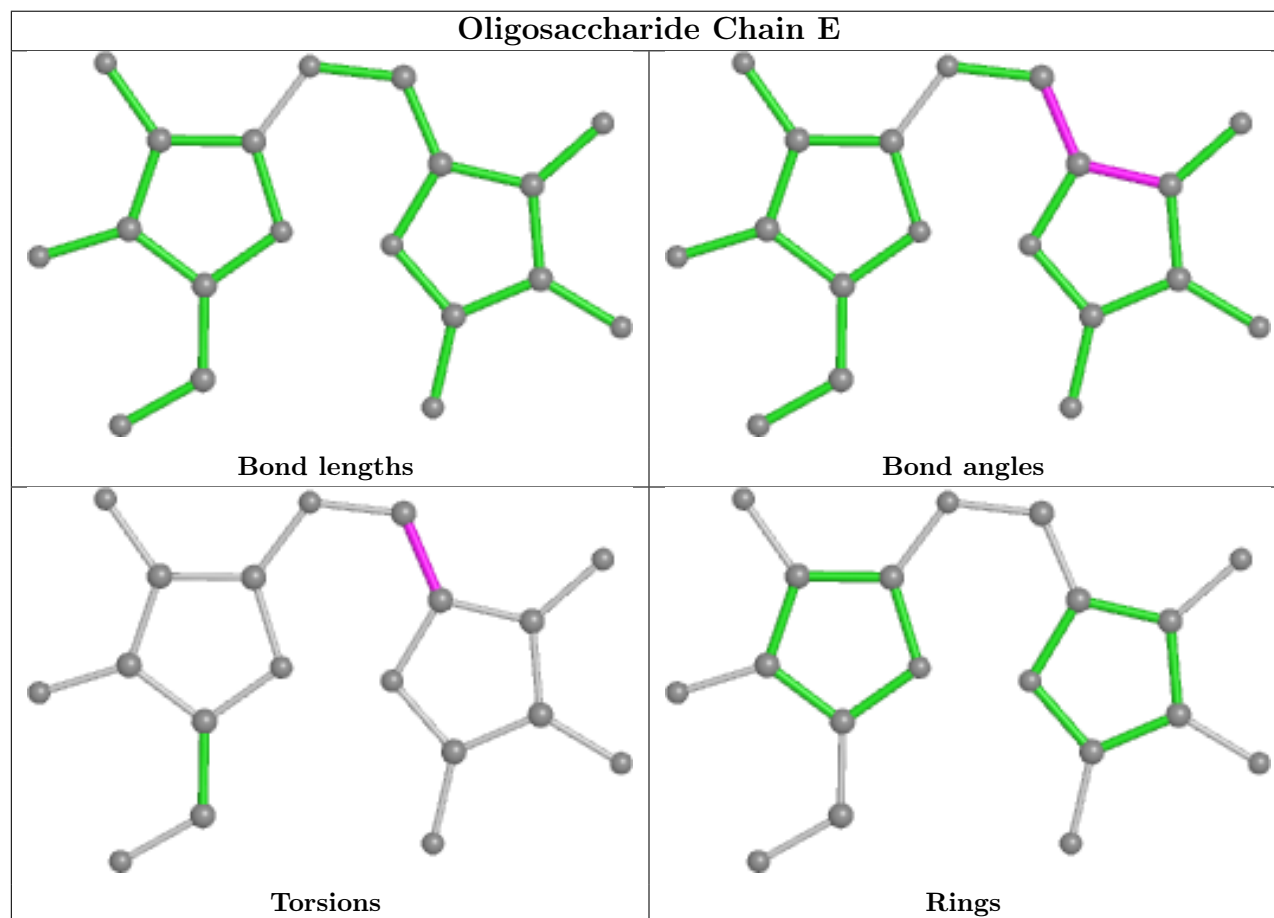
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	BGC	1	0
4	G	2	GLC	12	0
4	H	2	GLC	1	0
4	F	1	BGC	2	0
4	L	1	BGC	2	0

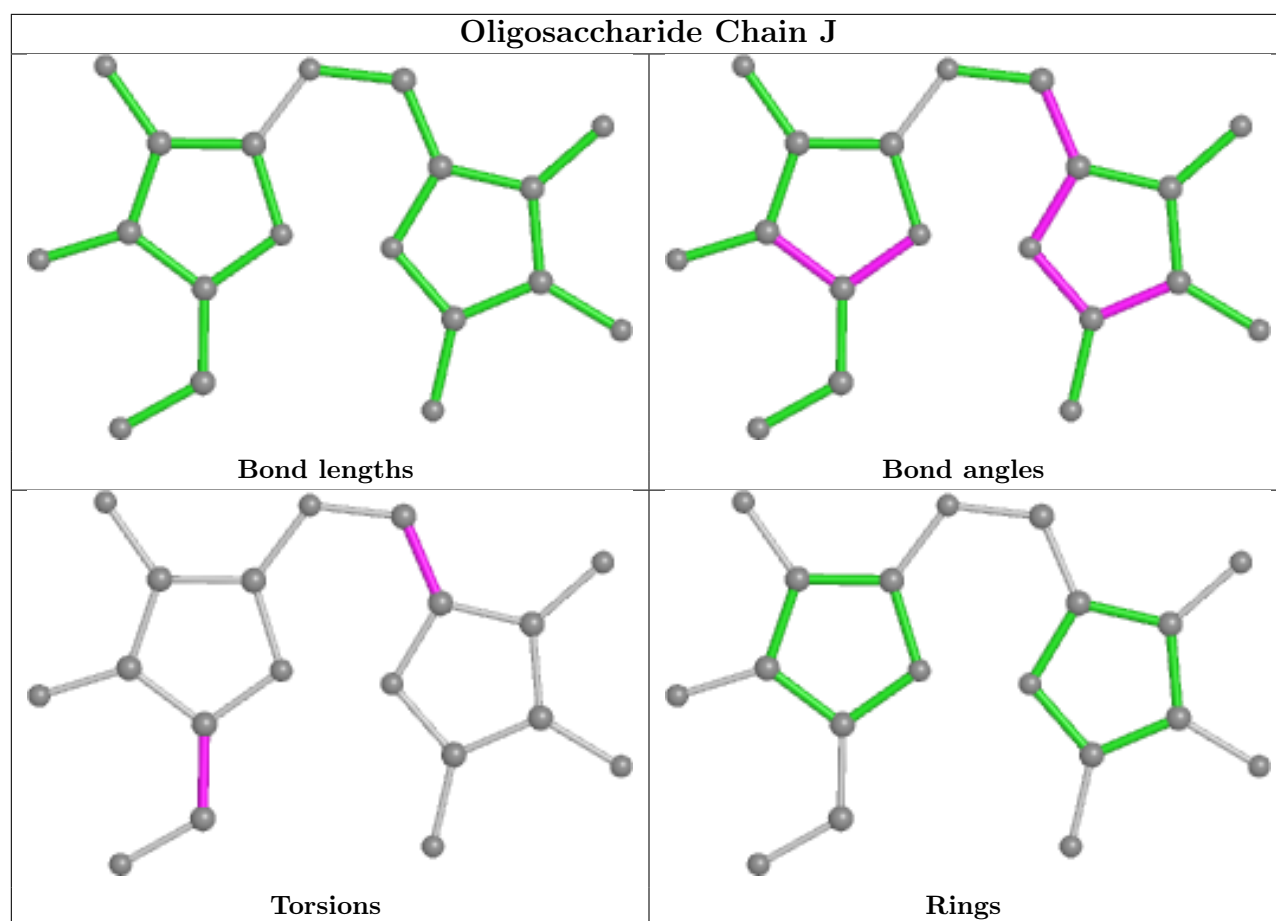
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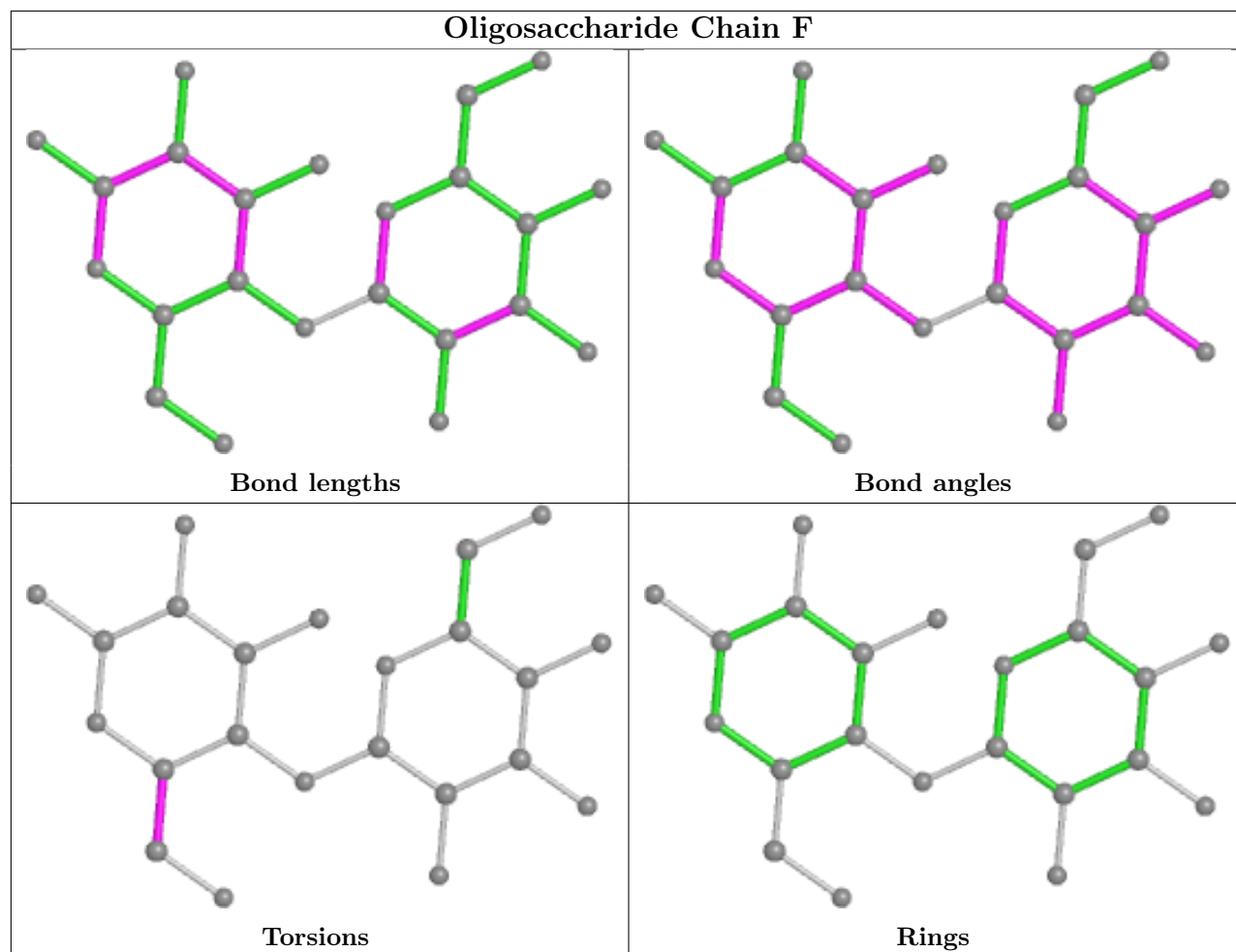
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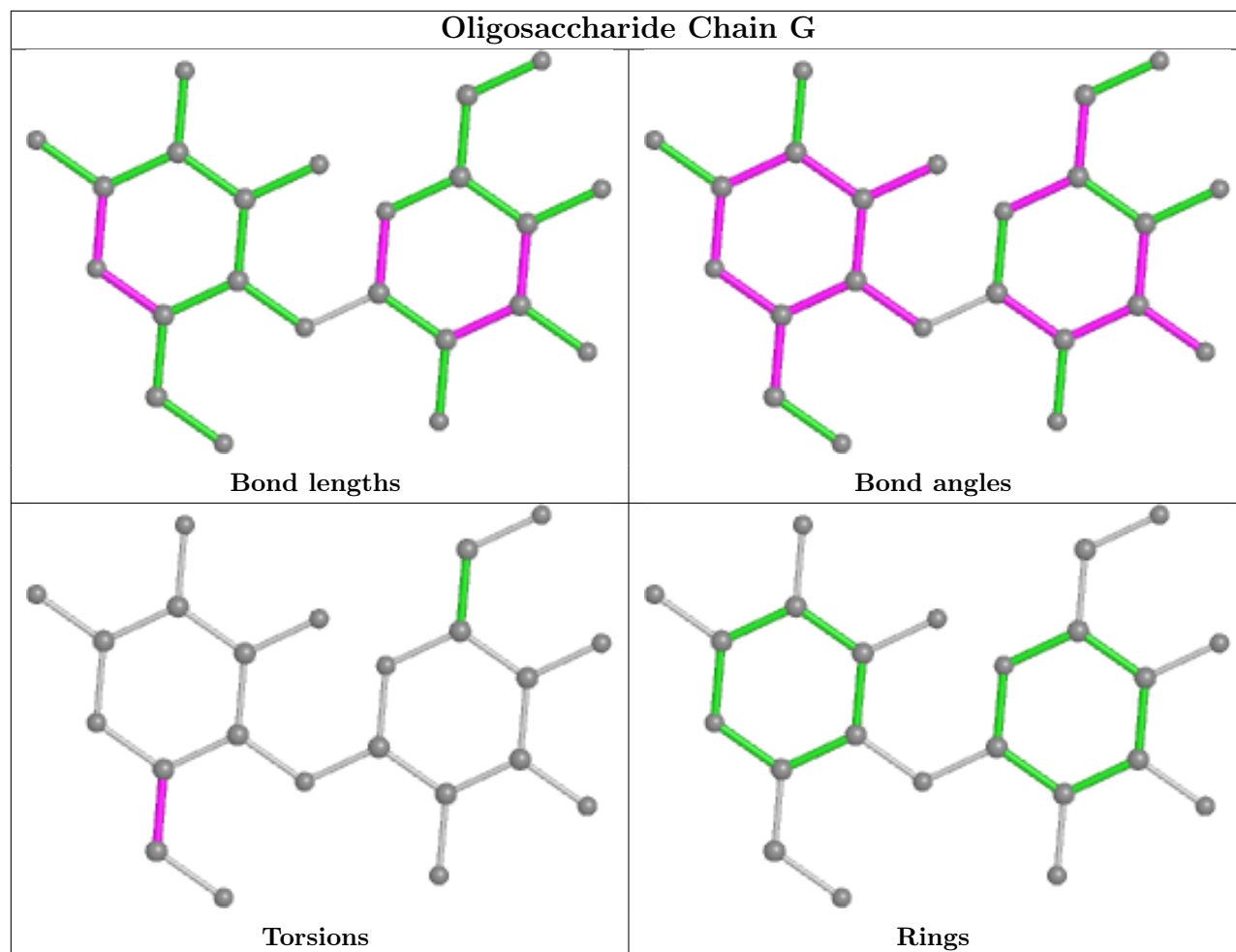
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	BGC	1	0
4	F	2	GLC	3	0
4	L	2	GLC	6	0
4	I	2	GLC	1	0

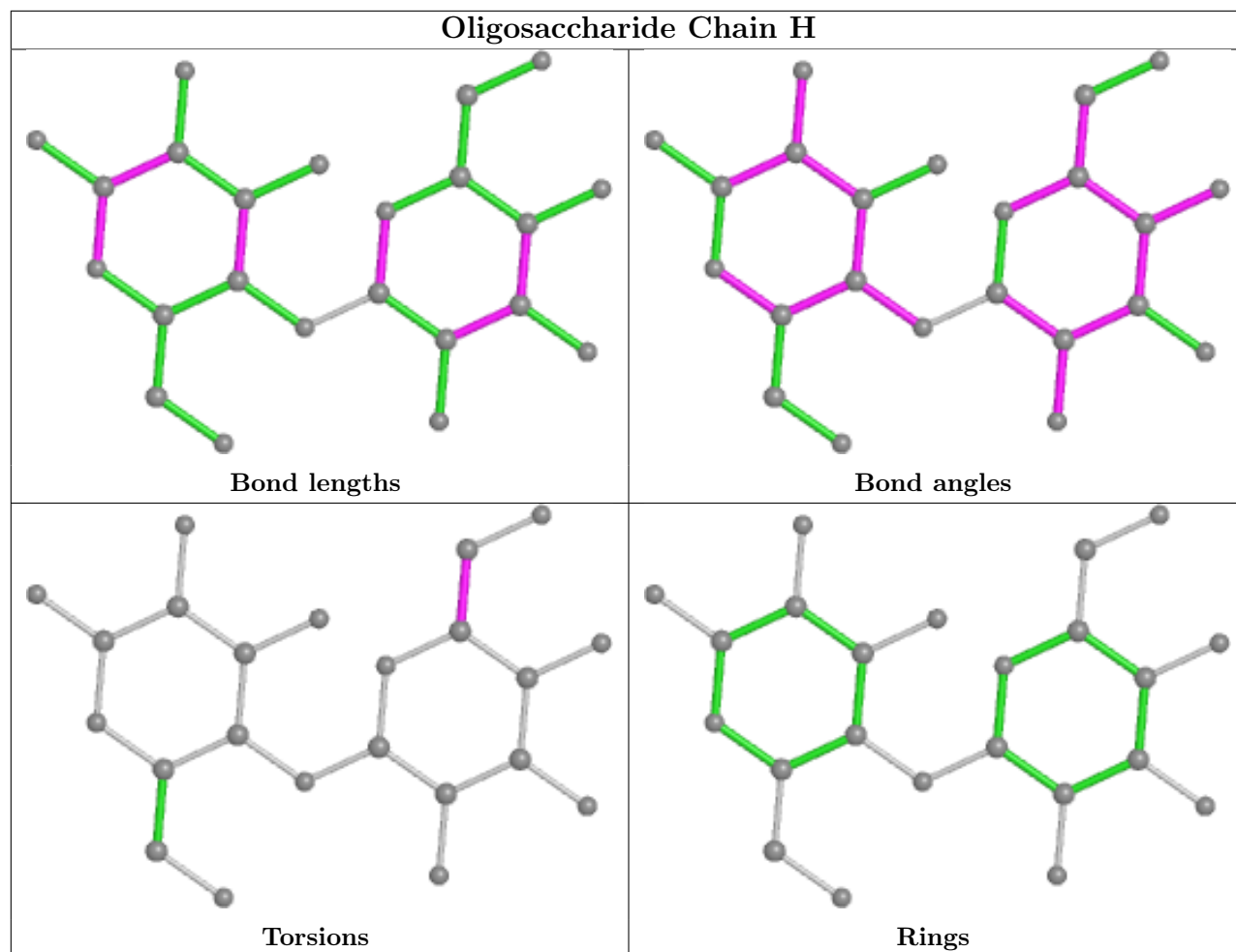
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

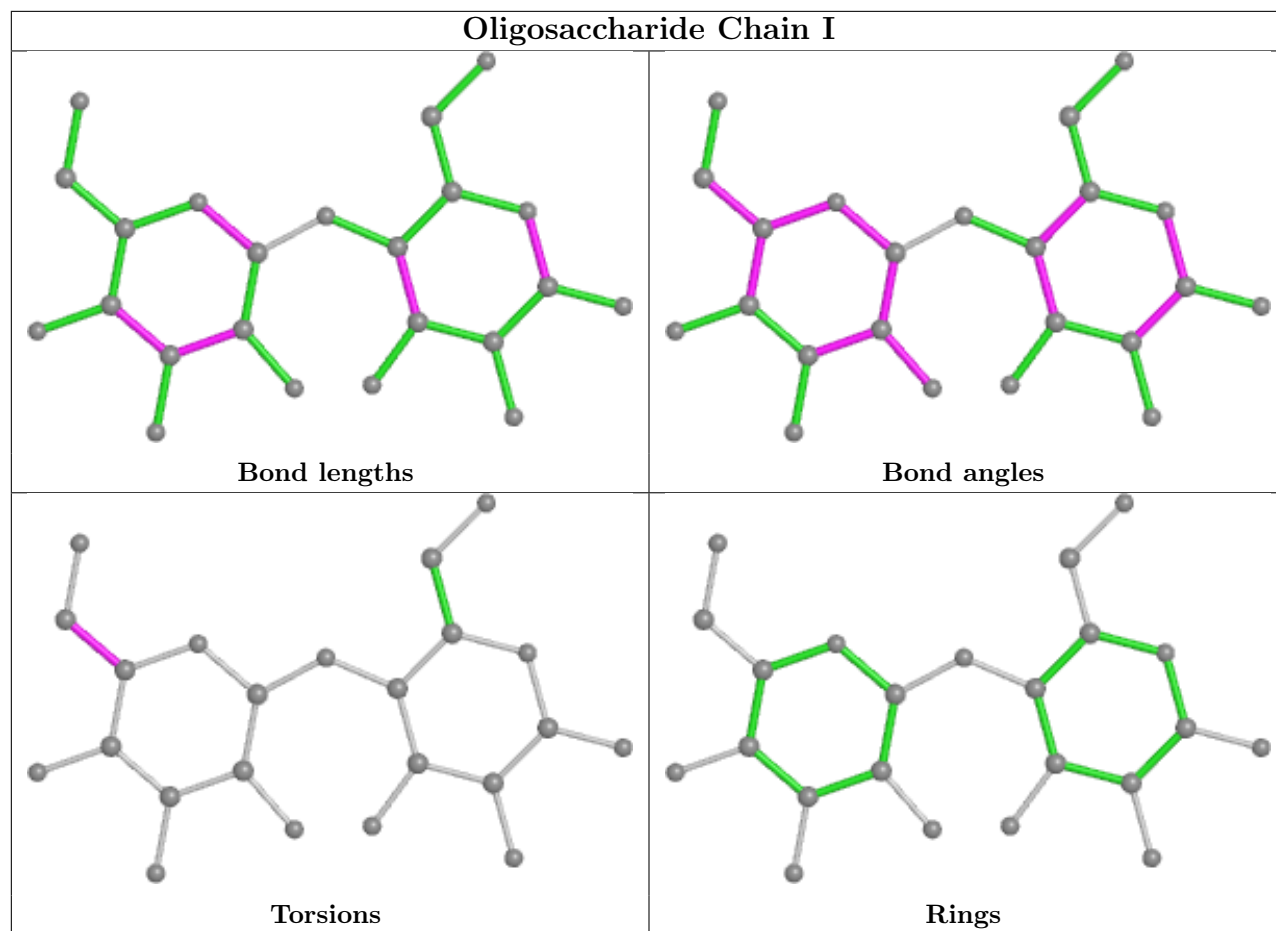


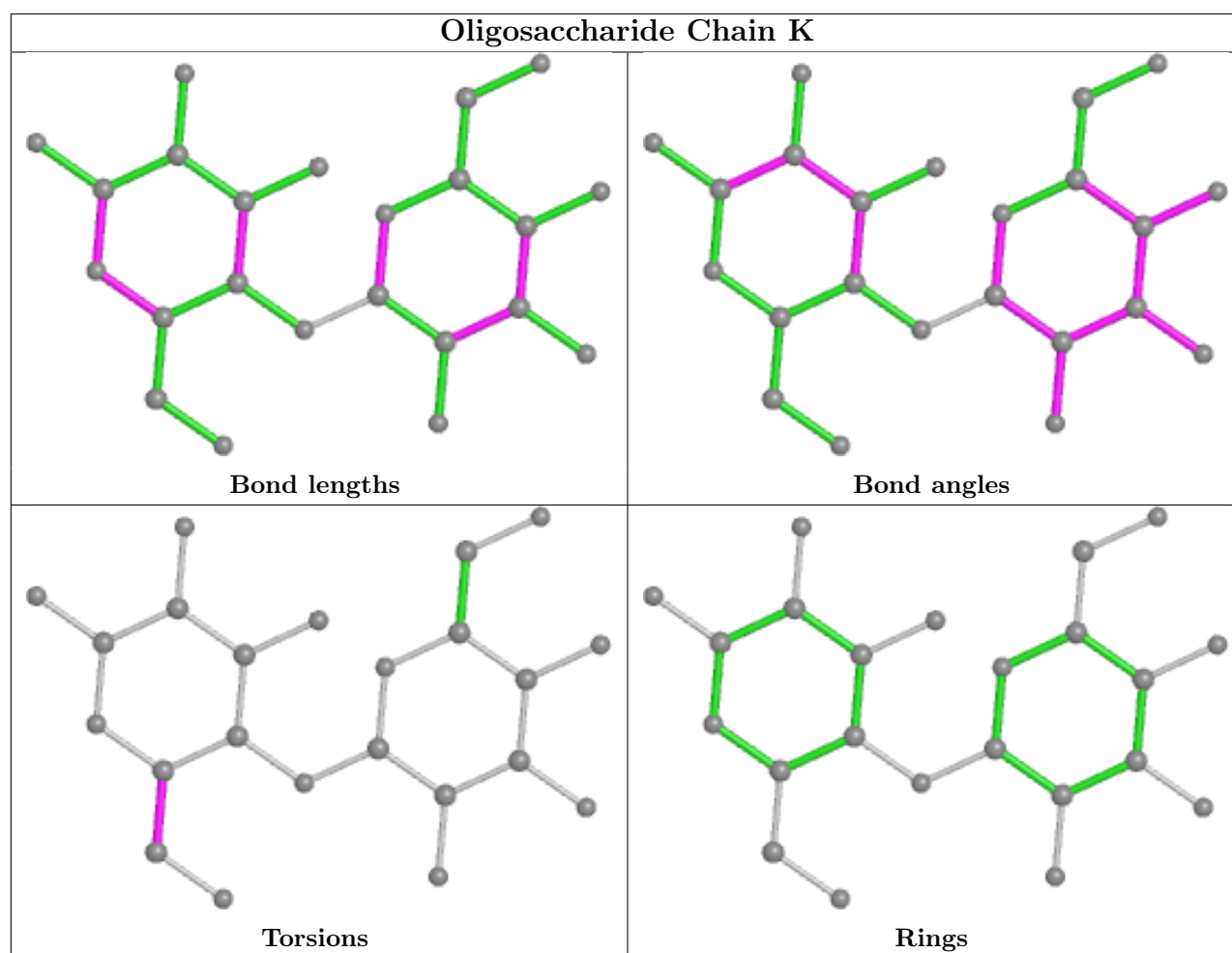


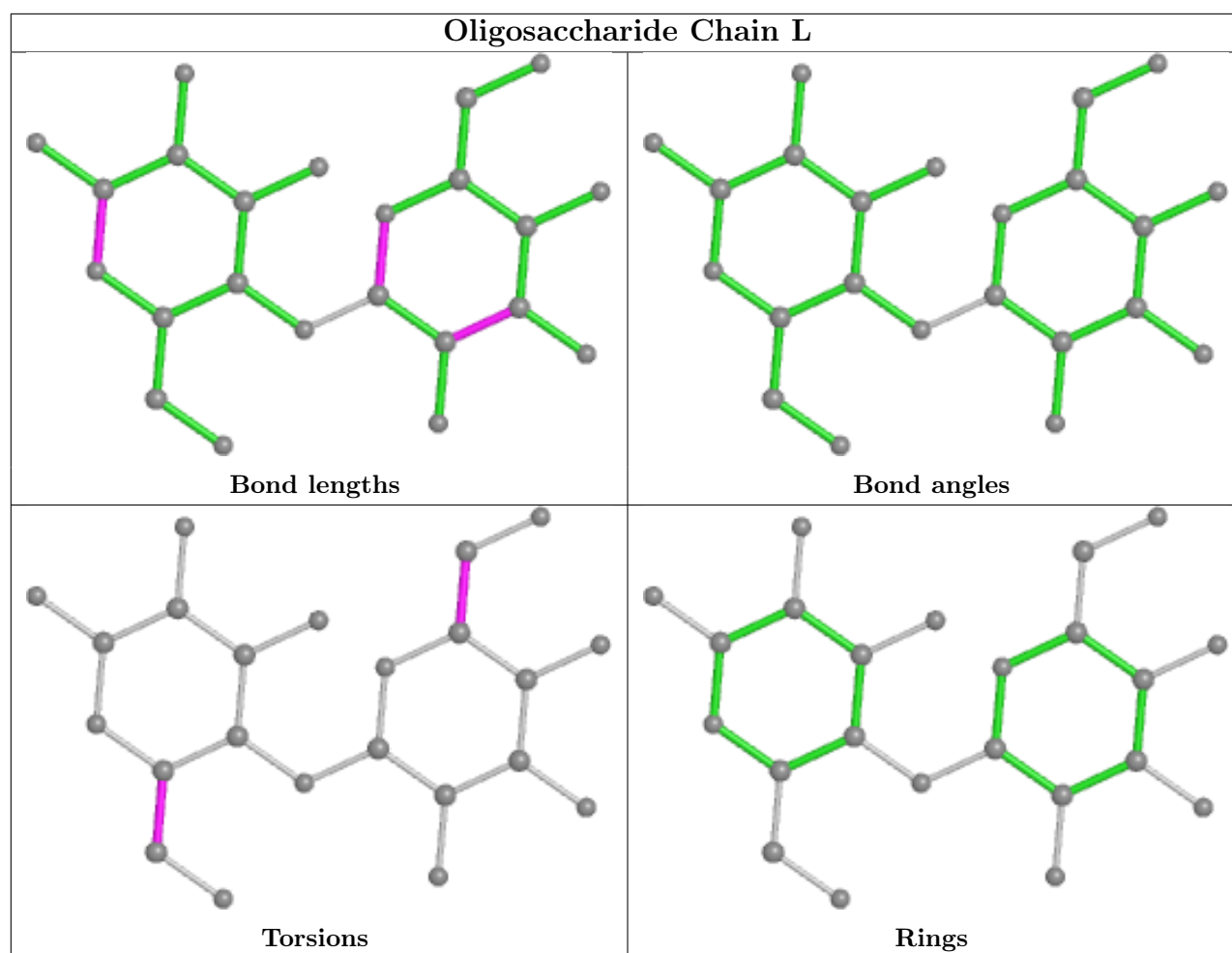












5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	BXY	B	1204	-	10,10,10	3.62	7 (70%)	13,14,14	1.48	2 (15%)
7	BXY	B	1203	-	10,10,10	5.04	7 (70%)	13,14,14	2.30	5 (38%)
7	BXY	A	1204	-	10,10,10	2.84	5 (50%)	13,14,14	1.80	3 (23%)
6	PO4	B	1202	-	4,4,4	2.50	2 (50%)	6,6,6	0.47	0
7	BXY	A	1203	-	10,10,10	6.39	8 (80%)	13,14,14	3.46	8 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	A	1202	-	4,4,4	2.47	1 (25%)	6,6,6	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
7	BXY	A	1204	-	-	0/2/18/18	0/1/1/1
7	BXY	B	1204	-	-	2/2/18/18	0/1/1/1
7	BXY	A	1203	-	-	2/2/18/18	0/1/1/1
7	BXY	B	1203	-	-	1/2/18/18	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1203	BXY	C1-C2	-12.56	1.38	1.52
7	B	1203	BXY	C1-C2	-12.48	1.38	1.52
7	A	1203	BXY	O4-C1	-8.94	1.32	1.43
7	B	1204	BXY	C1-C2	-7.39	1.44	1.52
7	A	1203	BXY	O2-C2	-6.74	1.27	1.43
7	A	1203	BXY	C3-C4	-6.64	1.36	1.53
7	B	1203	BXY	O4-C1	-6.10	1.35	1.43
7	A	1203	BXY	O4-C4	-5.45	1.32	1.45
7	B	1204	BXY	O4-C1	-5.00	1.37	1.43
7	B	1203	BXY	O2-C2	-4.79	1.31	1.43
7	A	1203	BXY	C2-C3	-4.71	1.40	1.53
7	A	1204	BXY	O4-C4	-4.65	1.34	1.45
7	B	1204	BXY	O4-C4	-4.38	1.35	1.45
6	B	1202	PO4	P-O1	4.13	1.60	1.50
6	A	1202	PO4	P-O1	4.10	1.60	1.50
7	A	1204	BXY	O3-C3	-3.97	1.33	1.43
7	A	1204	BXY	O4-C1	-3.93	1.38	1.43
7	A	1203	BXY	O3-C3	-3.74	1.34	1.43
7	A	1203	BXY	O1-C1	-3.53	1.28	1.39
7	A	1204	BXY	O2-C2	-3.20	1.35	1.43
7	B	1203	BXY	O4-C4	-3.13	1.38	1.45
7	B	1203	BXY	O1-C1	-3.03	1.29	1.39
7	B	1204	BXY	O3-C3	-2.94	1.36	1.43
7	A	1204	BXY	C3-C4	-2.88	1.45	1.53
7	B	1204	BXY	O2-C2	-2.85	1.36	1.43
7	B	1203	BXY	C3-C4	-2.84	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1203	BXY	O3-C3	-2.79	1.36	1.43
7	B	1204	BXY	C3-C4	-2.76	1.45	1.53
7	B	1204	BXY	C2-C3	-2.40	1.46	1.53
6	B	1202	PO4	P-O3	2.00	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1203	BXY	C2-C3-C4	-6.88	89.27	102.64
7	A	1203	BXY	O1-C1-O4	-6.49	102.82	111.13
7	B	1203	BXY	C1-C2-C3	-4.68	96.44	102.30
7	A	1203	BXY	O4-C4-C5	4.59	119.13	109.21
7	A	1203	BXY	C1-C2-C3	-3.82	97.52	102.30
7	A	1204	BXY	O1-C1-O4	-3.54	106.60	111.13
7	B	1203	BXY	O3-C3-C4	-3.40	101.22	111.05
7	A	1204	BXY	O5-C5-C4	-3.11	100.62	111.29
7	B	1203	BXY	O1-C1-O4	-3.08	107.19	111.13
7	B	1204	BXY	O4-C4-C5	2.83	115.33	109.21
7	B	1203	BXY	C2-C3-C4	-2.79	97.22	102.64
7	A	1203	BXY	O5-C5-C4	-2.79	101.73	111.29
7	B	1203	BXY	O2-C2-C1	-2.76	104.20	111.82
7	A	1203	BXY	O4-C4-C3	-2.70	99.77	105.11
7	A	1203	BXY	O1-C1-C2	-2.50	98.46	110.39
7	B	1204	BXY	O2-C2-C1	-2.25	105.60	111.82
7	A	1204	BXY	O2-C2-C3	-2.23	104.62	111.82
7	A	1203	BXY	O2-C2-C1	-2.13	105.95	111.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

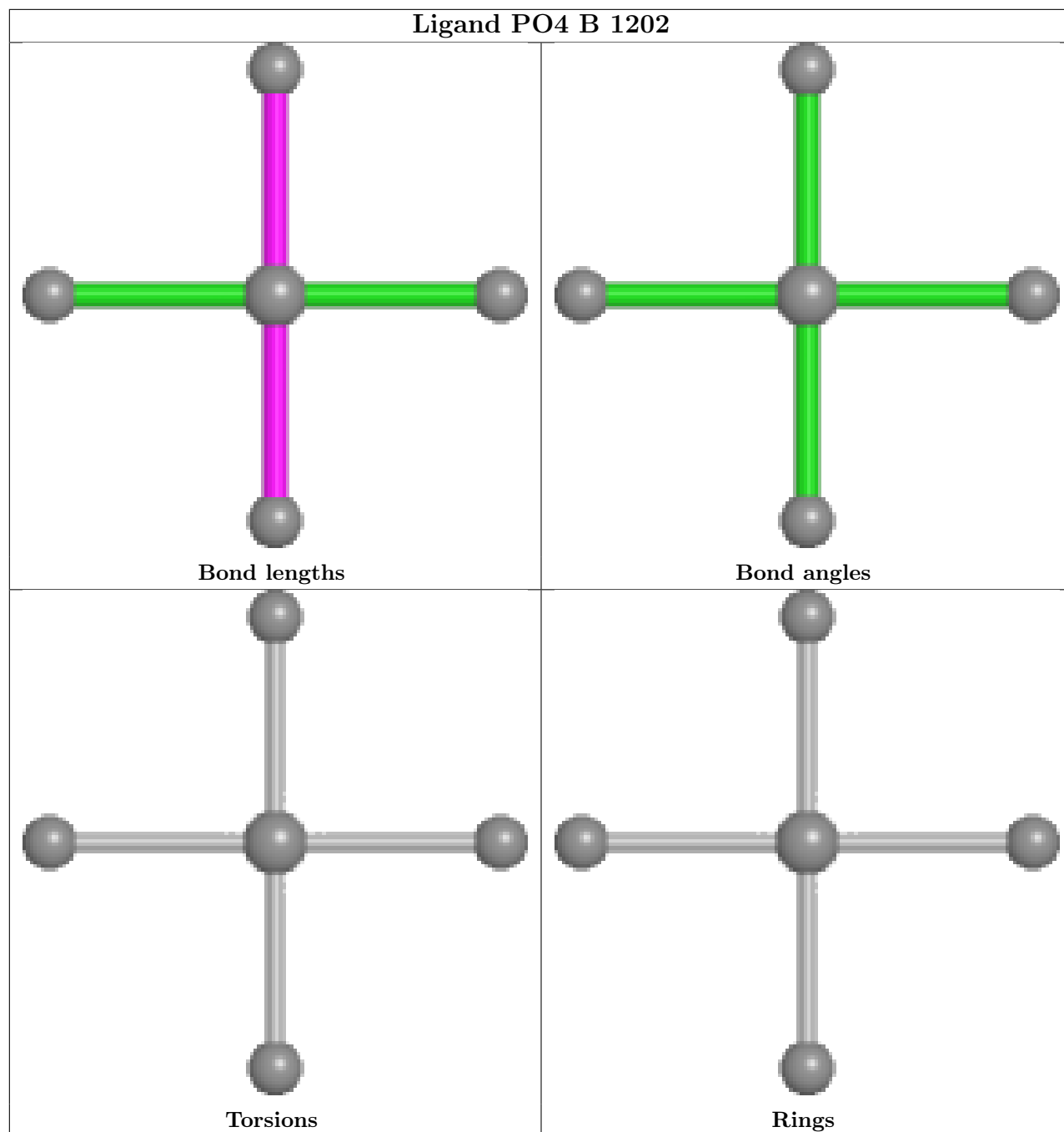
Mol	Chain	Res	Type	Atoms
7	B	1204	BXY	O4-C4-C5-O5
7	B	1204	BXY	C3-C4-C5-O5
7	A	1203	BXY	O4-C4-C5-O5
7	A	1203	BXY	C3-C4-C5-O5
7	B	1203	BXY	O4-C4-C5-O5

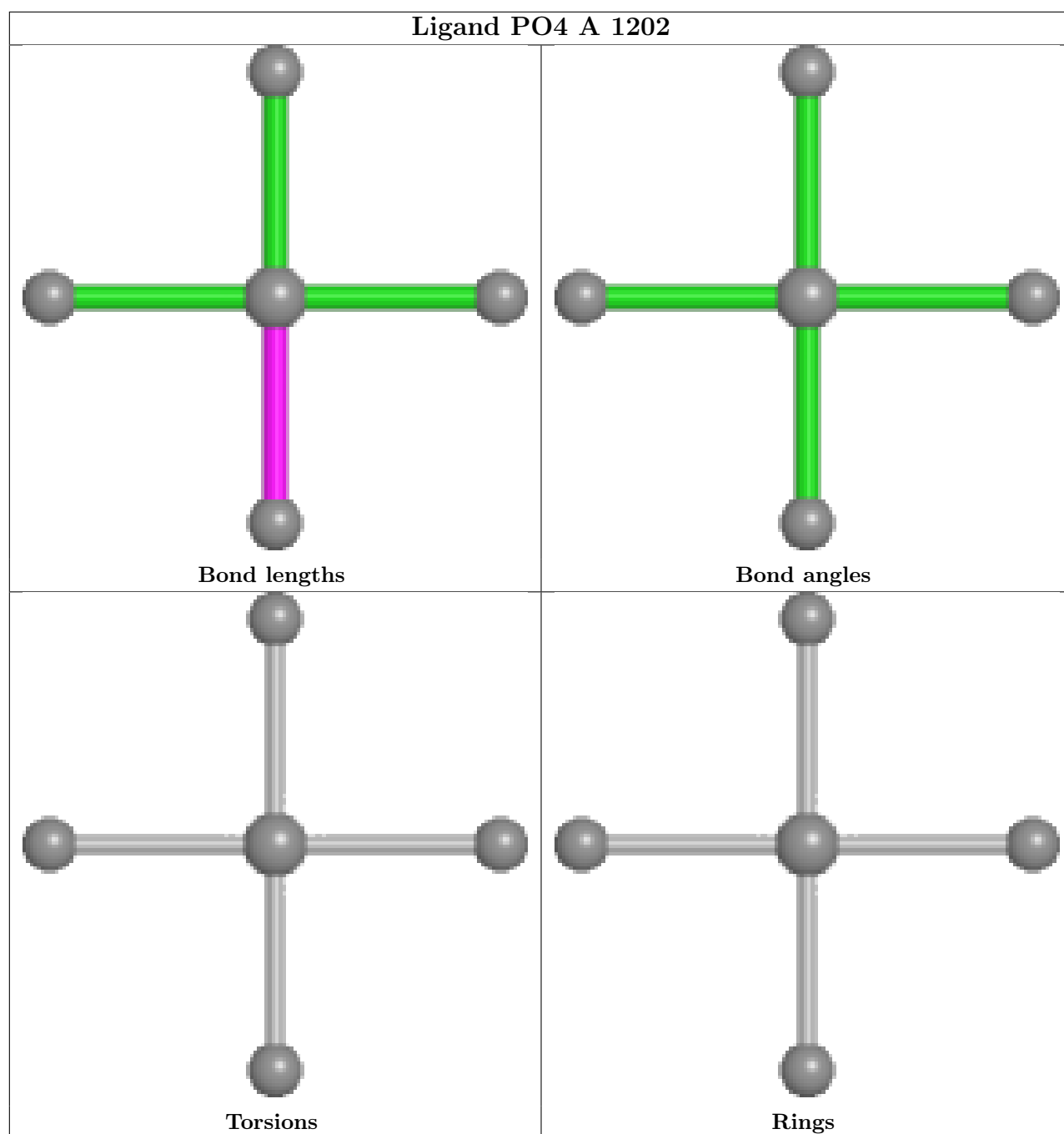
There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1204	BXY	13	0
7	A	1204	BXY	2	0
7	A	1203	BXY	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 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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1035/1113 (92%)	0.92	198 (19%) 4 3	4, 68, 160, 198	0
1	B	1035/1113 (92%)	0.98	208 (20%) 3 3	5, 68, 173, 221	0
2	C	84/99 (84%)	1.34	15 (17%) 4 4	44, 82, 125, 147	0
2	D	84/99 (84%)	1.09	11 (13%) 8 8	45, 87, 126, 144	0
All	All	2238/2424 (92%)	0.97	432 (19%) 4 3	4, 71, 164, 221	0

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	LEU	10.5
1	B	249	LEU	9.1
1	B	127	SER	8.8
1	A	40	GLN	8.6
1	A	291	GLU	7.3
1	B	163	ASP	7.0
1	A	67	ASP	6.8
1	B	110	GLU	6.7
1	B	111	ARG	6.5
1	B	171	ARG	6.4
1	B	113	ASN	6.3
1	B	115	ASP	6.1
1	B	164	ASP	6.1
1	B	117	THR	6.0
1	A	250	PRO	6.0
1	A	1062	ARG	6.0
1	A	756	GLN	5.9
1	A	1061	THR	5.9
1	A	915	SER	5.8
1	B	291	GLU	5.8
1	A	82	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	916	ILE	5.6
1	B	293	ALA	5.6
1	B	170	VAL	5.6
1	B	253	TRP	5.6
1	A	135	SER	5.5
1	B	712	TYR	5.5
1	B	1059	THR	5.5
1	B	873	GLN	5.5
1	B	292	HIS	5.3
1	A	677	PRO	5.2
1	A	912	PRO	5.2
1	B	680	ARG	5.1
1	B	246	LYS	5.1
2	C	62	GLU	5.1
1	B	242	GLY	5.1
1	B	778	ASP	5.0
1	B	42	THR	5.0
1	A	75	GLN	5.0
1	B	209	SER	5.0
1	B	250	PRO	4.9
1	B	10	SER	4.9
1	B	214	LEU	4.9
1	B	159	GLN	4.9
1	B	152	GLY	4.9
1	A	146	HIS	4.9
1	B	82	GLY	4.8
1	B	932	LEU	4.7
1	A	253	TRP	4.7
1	B	777	ALA	4.7
2	C	77	ILE	4.7
1	B	81	VAL	4.6
1	A	914	SER	4.6
1	B	84	GLU	4.6
1	A	779	PRO	4.6
1	B	776	SER	4.5
1	A	280	ASP	4.5
1	B	1057	LEU	4.5
1	B	240	ALA	4.4
1	A	145	ALA	4.4
1	B	172	GLY	4.3
1	A	1060	ALA	4.3
1	B	1075	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	14	GLU	4.3
1	A	675	ASP	4.3
1	B	153	GLU	4.2
1	B	215	LEU	4.2
1	B	294	GLY	4.2
1	B	161	PRO	4.2
1	A	895	ILE	4.2
1	A	999	GLU	4.2
1	B	674	PRO	4.2
1	B	140	TYR	4.1
1	A	775	VAL	4.1
1	B	892	GLY	4.1
1	B	142	THR	4.0
1	A	246	LYS	4.0
1	B	112	ILE	4.0
1	B	128	ALA	4.0
1	B	85	ASN	4.0
1	B	881	ALA	4.0
1	A	251	SER	3.9
1	B	14	THR	3.9
1	A	293	ALA	3.9
1	B	254	TRP	3.9
1	A	676	ARG	3.8
1	B	838	SER	3.8
1	A	163	ASP	3.8
1	A	899	ASP	3.8
1	B	774	ASP	3.8
1	A	1021	ARG	3.8
1	A	48	PRO	3.8
1	A	49	GLN	3.7
1	B	126	VAL	3.7
1	B	154	PHE	3.7
1	A	144	THR	3.7
1	B	134	LEU	3.7
1	A	894	SER	3.7
1	B	981	TYR	3.7
1	B	173	GLU	3.6
1	B	952	GLN	3.6
1	A	85	ASN	3.6
2	C	86	GLU	3.6
1	B	891	PRO	3.6
1	B	935	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	3.6
1	A	292	HIS	3.6
1	B	1056	ASP	3.6
1	B	1062	ARG	3.5
2	D	3	ALA	3.5
1	A	1023	SER	3.5
1	B	673	SER	3.5
1	A	216	LYS	3.5
1	B	11	ASN	3.5
1	A	244	ARG	3.5
2	C	85	PRO	3.5
1	A	164	ASP	3.5
1	A	752	GLU	3.5
1	B	156	GLY	3.5
1	B	996	PHE	3.5
1	A	933	ALA	3.4
1	B	669	GLY	3.4
1	B	52	VAL	3.4
1	A	214	LEU	3.4
1	A	671	ASP	3.4
1	B	168	GLU	3.4
1	A	995	ARG	3.4
1	A	858	GLN	3.4
1	B	83	PRO	3.4
1	A	51	GLY	3.4
1	B	193	PRO	3.3
1	B	686	VAL	3.3
1	B	929	ASP	3.3
1	B	684	LEU	3.3
1	B	135	SER	3.3
1	A	840	THR	3.3
1	A	980	ARG	3.3
1	A	318	ALA	3.3
1	B	890	GLU	3.3
1	B	89	SER	3.3
1	A	670	ARG	3.2
1	A	835	SER	3.2
1	B	957	SER	3.2
1	A	149	LYS	3.2
1	A	176	GLY	3.2
1	B	109	ILE	3.2
2	C	64	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	125	VAL	3.2
1	B	169	ALA	3.2
1	B	41	THR	3.2
1	A	54	GLN	3.1
1	B	754	ALA	3.1
1	B	683	ARG	3.1
1	B	831	PRO	3.1
1	A	817	SER	3.1
1	A	766	PHE	3.1
1	B	766	PHE	3.1
1	A	932	LEU	3.1
1	A	148	ASP	3.1
1	A	880	TRP	3.1
1	B	160	GLY	3.1
1	B	75	GLN	3.1
1	A	247	ARG	3.1
1	A	451	SER	3.1
1	A	1063	SER	3.0
1	A	66	THR	3.0
1	A	206	THR	3.0
1	A	240	ALA	3.0
1	A	811	ALA	3.0
1	A	1046	TRP	3.0
1	B	53	TRP	3.0
1	A	861	PRO	3.0
1	B	872	ASP	3.0
1	B	87	ASN	3.0
1	B	885	GLN	3.0
1	A	887	ALA	3.0
1	A	254	TRP	3.0
1	B	131	GLU	3.0
1	A	69	THR	3.0
1	A	248	PHE	3.0
1	A	935	GLN	3.0
1	B	859	ALA	3.0
1	A	237	LEU	3.0
1	A	859	ALA	3.0
1	B	114	ASN	3.0
1	A	24	LEU	2.9
1	B	845	VAL	2.9
1	A	290	SER	2.9
1	A	673	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	49	GLN	2.9
1	B	979	HIS	2.9
1	A	150	VAL	2.9
1	A	761	VAL	2.9
1	A	996	PHE	2.9
1	A	771	ILE	2.9
1	B	670	ARG	2.9
1	A	81	VAL	2.9
1	B	770	GLY	2.9
1	B	752	GLU	2.9
1	B	145	ALA	2.9
1	B	841	GLN	2.9
1	A	136	PRO	2.9
1	B	882	THR	2.9
1	A	1031	ASP	2.9
1	A	888	ALA	2.8
1	B	43	ALA	2.8
1	A	453	PHE	2.8
1	A	890	GLU	2.8
1	A	748	THR	2.8
1	A	841	GLN	2.8
1	A	10	SER	2.8
1	A	161	PRO	2.8
1	A	193	PRO	2.8
1	A	1066	TRP	2.8
2	C	58	LYS	2.8
1	A	997	GLY	2.8
1	A	674	PRO	2.8
1	B	137	ASP	2.8
1	B	883	ASP	2.8
1	B	915	SER	2.8
1	A	47	TRP	2.8
1	B	197	GLY	2.8
1	B	147	ALA	2.8
1	A	18	VAL	2.8
1	A	16	ARG	2.7
1	A	15	ALA	2.7
1	A	925	LEU	2.7
2	D	86	GLU	2.7
1	B	672	VAL	2.7
1	B	51	GLY	2.7
1	B	980	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	753	PRO	2.7
2	D	30	GLU	2.7
1	A	1030	LYS	2.7
1	A	17	LEU	2.7
1	B	17	LEU	2.7
1	B	999	GLU	2.7
1	B	247	ARG	2.7
1	A	12	HIS	2.7
1	A	139	ARG	2.7
1	B	308	SER	2.7
1	A	860	GLY	2.7
1	B	78	ALA	2.7
1	B	80	LEU	2.7
2	C	75	ALA	2.7
1	A	159	GLN	2.7
1	A	39	GLU	2.6
1	A	55	SER	2.6
1	A	778	ASP	2.6
1	A	134	LEU	2.6
1	A	321	ALA	2.6
1	A	758	LEU	2.6
1	A	873	GLN	2.6
1	A	922	GLN	2.6
1	B	775	VAL	2.6
1	A	239	CYS	2.6
1	B	1064	GLY	2.6
1	B	166	PRO	2.6
2	D	34	VAL	2.6
1	A	923	ILE	2.6
1	B	750	ILE	2.6
1	A	898	GLY	2.6
1	A	891	PRO	2.6
1	B	201	SER	2.6
2	D	36	ASP	2.6
1	B	818	ARG	2.6
1	A	764	LEU	2.6
1	A	241	ASP	2.6
1	A	994	ASP	2.6
1	B	820	ARG	2.6
1	B	828	ALA	2.6
1	B	852	ARG	2.6
1	A	203	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1066	TRP	2.5
1	B	248	PHE	2.5
1	B	295	TYR	2.5
1	B	244	ARG	2.5
1	B	252	ARG	2.5
1	A	768	PRO	2.5
1	A	52	VAL	2.5
1	A	41	THR	2.5
1	A	1065	TRP	2.5
1	B	116	LEU	2.5
1	A	1034	TYR	2.5
1	B	481	ALA	2.5
1	B	760	ALA	2.5
1	A	196	GLU	2.5
1	A	919	GLU	2.5
1	B	129	PRO	2.5
2	D	59	ILE	2.5
1	A	138	CYS	2.5
2	D	61	ASP	2.5
1	A	11	ASN	2.5
1	A	50	ASN	2.5
1	A	842	GLN	2.5
1	B	811	ALA	2.5
1	B	920	ALA	2.5
1	B	933	ALA	2.5
1	A	672	VAL	2.5
1	B	1068	PRO	2.5
1	A	750	ILE	2.5
1	A	814	ILE	2.5
1	A	71	THR	2.5
1	B	668	SER	2.5
1	A	137	ASP	2.5
1	A	1033	TRP	2.5
1	B	815	ASN	2.5
1	A	862	LEU	2.5
1	B	466	GLY	2.5
1	B	682	GLN	2.5
1	B	136	PRO	2.5
1	B	843	PRO	2.5
1	B	130	LEU	2.4
1	B	141	LEU	2.4
1	A	252	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	78	GLN	2.4
1	B	931	ASP	2.4
1	A	83	PRO	2.4
1	B	167	GLY	2.4
1	B	132	GLN	2.4
1	A	56	VAL	2.4
1	A	140	TYR	2.4
1	A	195	PRO	2.4
1	B	677	PRO	2.4
1	A	837	ARG	2.4
1	A	245	HIS	2.4
1	A	777	ALA	2.4
1	B	681	TRP	2.4
1	B	858	GLN	2.4
1	B	211	SER	2.4
1	A	165	ASP	2.4
1	B	479	LEU	2.4
1	A	201	SER	2.4
1	B	97	LYS	2.4
1	B	79	GLY	2.4
1	B	751	GLY	2.4
1	A	818	ARG	2.4
1	B	922	GLN	2.4
1	B	1051	GLN	2.4
1	A	68	LEU	2.3
1	A	1028	TYR	2.3
1	B	1034	TYR	2.3
1	B	769	ASN	2.3
1	B	138	CYS	2.3
1	B	151	THR	2.3
1	B	21	ILE	2.3
2	C	79	LYS	2.3
1	B	884	GLU	2.3
1	A	765	GLY	2.3
1	B	289	VAL	2.3
1	B	162	ASP	2.3
2	D	46	GLU	2.3
1	A	19	ALA	2.3
1	A	874	GLY	2.3
1	B	1000	ALA	2.3
1	B	934	PRO	2.3
1	B	86	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	191	SER	2.3
1	B	178	ASP	2.3
1	A	221	ILE	2.3
1	A	877	GLU	2.3
1	A	242	GLY	2.2
1	A	754	ALA	2.2
1	B	727	GLY	2.2
1	B	844	ALA	2.2
1	A	44	GLU	2.2
1	B	39	GLU	2.2
1	B	44	GLU	2.2
1	A	749	PRO	2.2
1	B	823	TYR	2.2
1	B	15	ALA	2.2
1	A	892	GLY	2.2
1	B	765	GLY	2.2
1	B	773	SER	2.2
1	A	820	ARG	2.2
1	B	953	GLU	2.2
1	A	1039	SER	2.2
1	A	1022	PRO	2.2
1	A	450	VAL	2.2
1	A	819	ALA	2.2
1	B	860	GLY	2.2
1	A	84	GLU	2.2
1	B	835	SER	2.2
1	A	863	LEU	2.2
2	C	70	VAL	2.2
2	D	35	ASP	2.2
1	A	37	PRO	2.1
1	B	713	PRO	2.1
1	B	1065	TRP	2.1
1	B	290	SER	2.1
1	B	756	GLN	2.1
1	B	462	ILE	2.1
2	C	59	ILE	2.1
1	B	149	LYS	2.1
2	D	58	LYS	2.1
1	B	880	TRP	2.1
1	B	958	SER	2.1
1	A	911	ALA	2.1
1	A	238	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	40	GLN	2.1
1	B	678	GLN	2.1
1	A	13	ARG	2.1
1	B	837	ARG	2.1
1	B	761	VAL	2.1
1	A	757	ALA	2.1
1	A	20	ILE	2.1
1	A	42	THR	2.1
1	A	112	ILE	2.1
1	A	327	SER	2.1
1	B	204	ILE	2.1
1	B	104	ASP	2.1
1	A	875	GLU	2.1
1	B	936	HIS	2.1
1	A	53	TRP	2.1
1	B	125	VAL	2.1
2	C	27	VAL	2.1
2	C	57	VAL	2.1
1	A	86	ARG	2.1
1	A	151	THR	2.1
1	A	21	ILE	2.0
1	B	32	ALA	2.0
1	A	751	GLY	2.0
1	B	69	THR	2.0
1	B	199	GLN	2.0
2	C	34	VAL	2.0
1	A	881	ALA	2.0
1	A	1051	GLN	2.0
1	A	773	SER	2.0
1	B	671	ASP	2.0
1	A	202	ALA	2.0
1	B	923	ILE	2.0
2	D	62	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

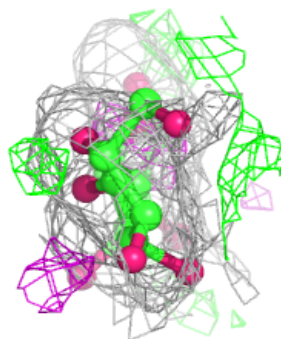
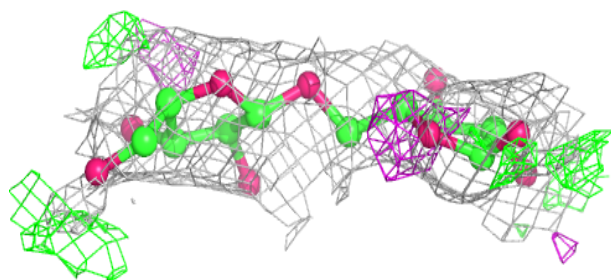
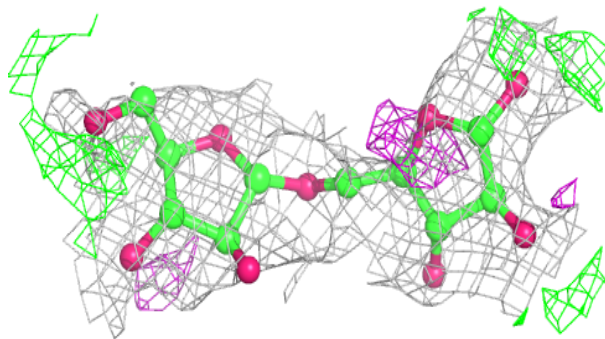
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	H	2	11/12	0.71	0.22	99,102,108,109	0
4	BGC	I	1	12/12	0.72	0.18	104,106,113,116	0
4	BGC	L	1	12/12	0.73	0.22	88,95,98,99	0
4	GLC	I	2	11/12	0.78	0.19	98,101,103,103	0
4	BGC	H	1	12/12	0.78	0.19	99,107,114,116	0
4	BGC	G	1	12/12	0.79	0.21	71,79,81,81	0
3	BXY	E	1	10/10	0.79	0.27	72,77,78,79	0
3	BXY	E	2	9/10	0.83	0.22	78,79,82,85	0
4	GLC	L	2	11/12	0.84	0.17	88,90,92,94	0
4	GLC	G	2	11/12	0.85	0.13	78,80,86,87	0
3	BXY	J	2	9/10	0.86	0.22	78,80,82,84	0
4	BGC	K	1	12/12	0.86	0.15	49,59,66,66	0
3	BXY	J	1	10/10	0.87	0.23	76,82,84,86	0
4	BGC	F	1	12/12	0.88	0.14	36,40,44,45	0
4	GLC	F	2	11/12	0.91	0.13	27,29,32,33	0
4	GLC	K	2	11/12	0.94	0.11	32,36,40,41	0

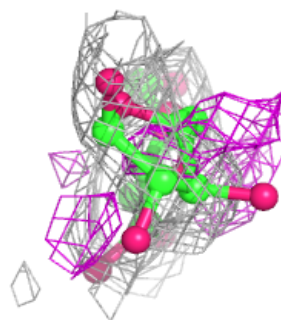
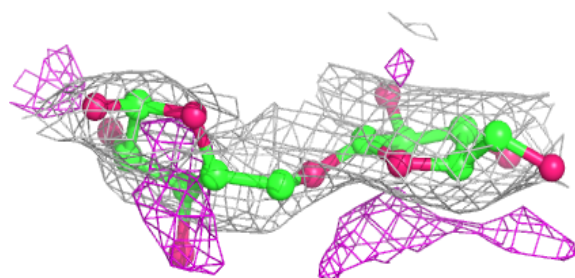
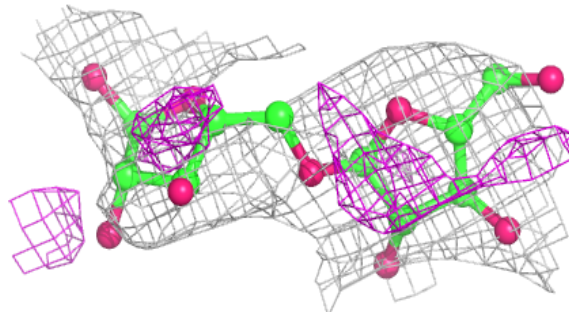
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

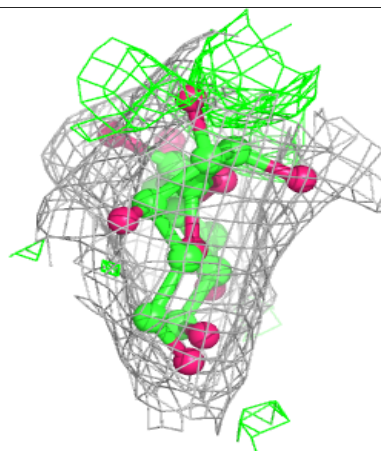
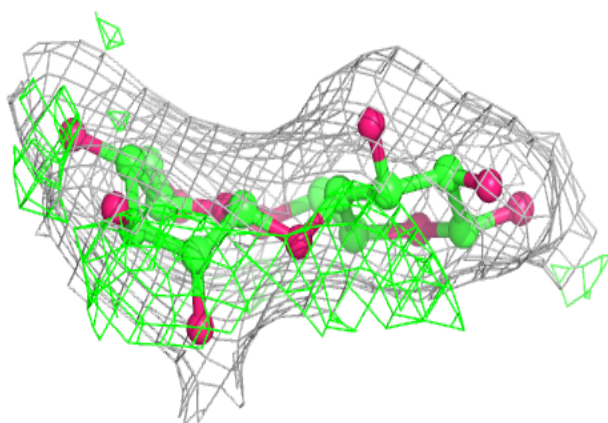
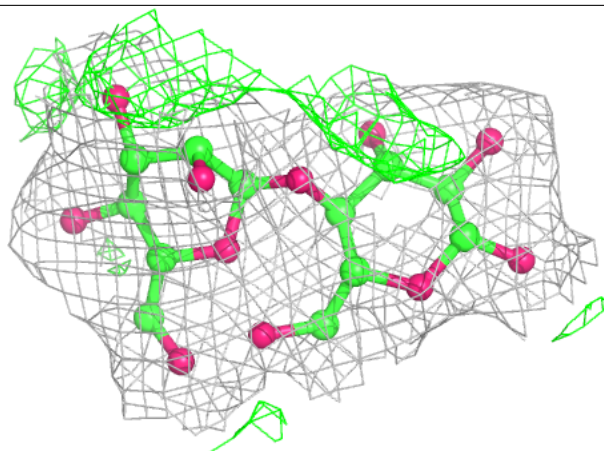
**Electron density around Chain J:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

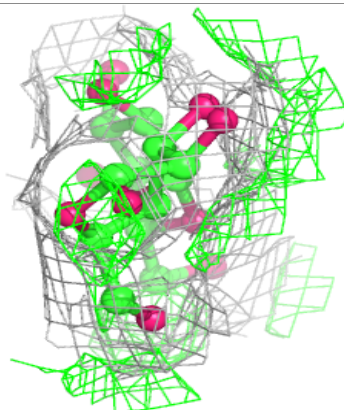
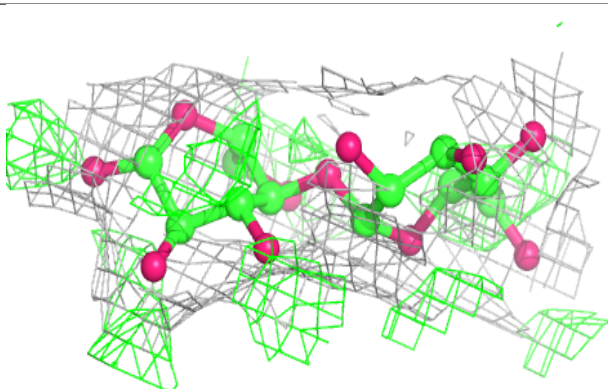
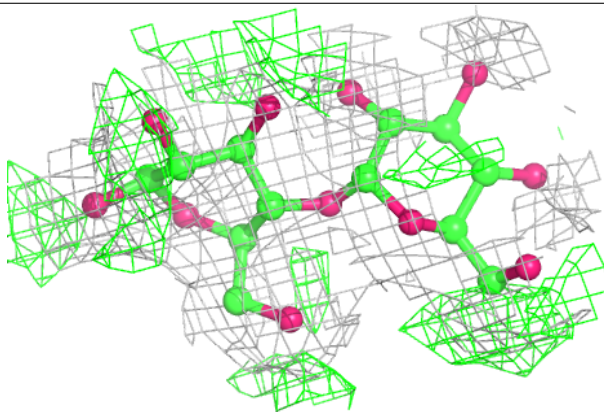


Electron density around Chain F:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

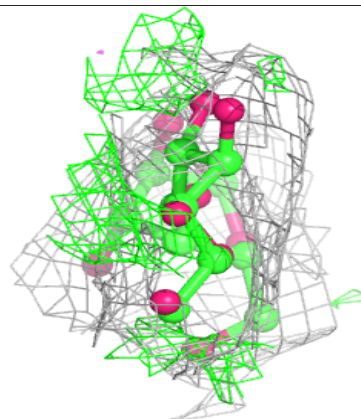
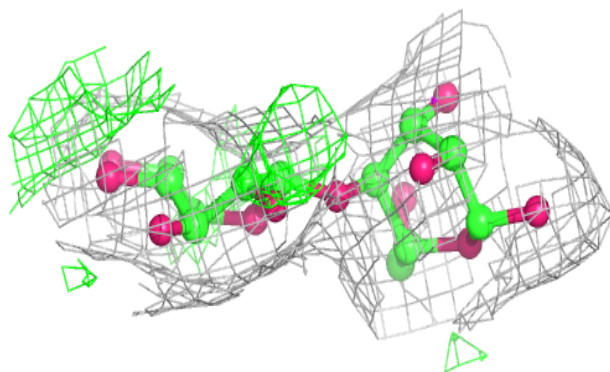
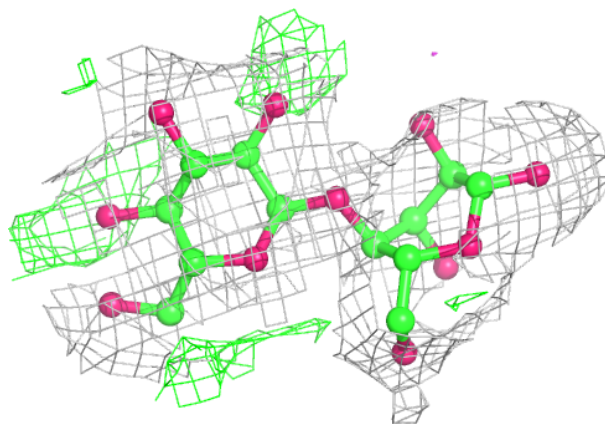
**Electron density around Chain G:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



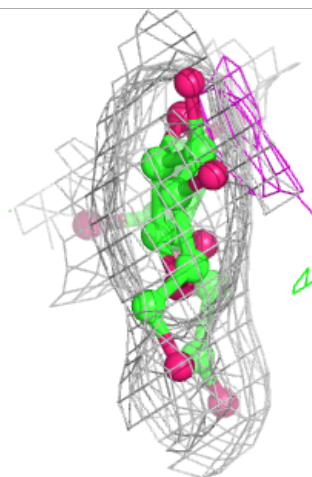
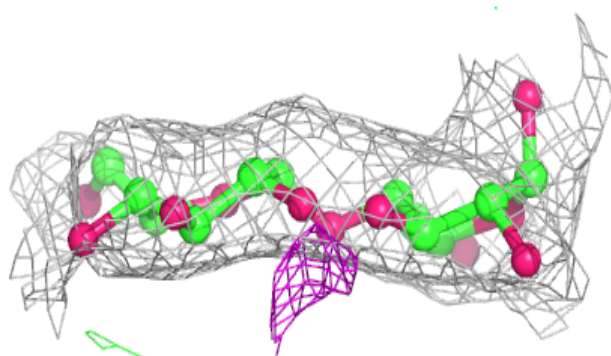
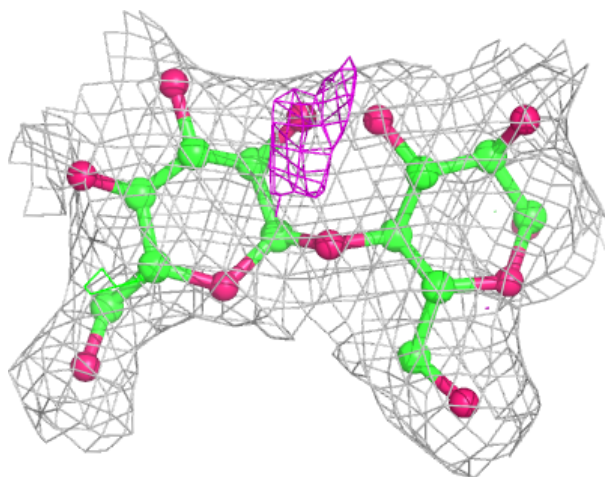
Electron density around Chain H:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



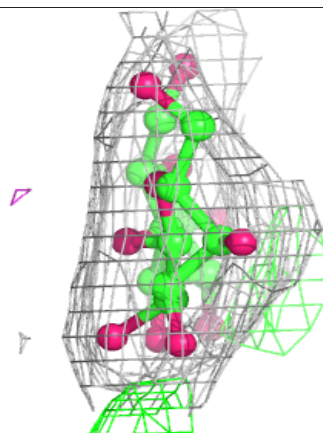
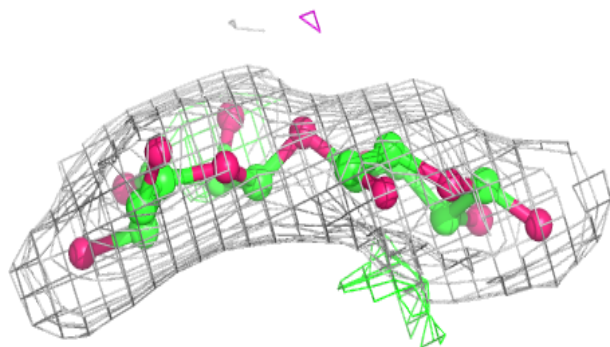
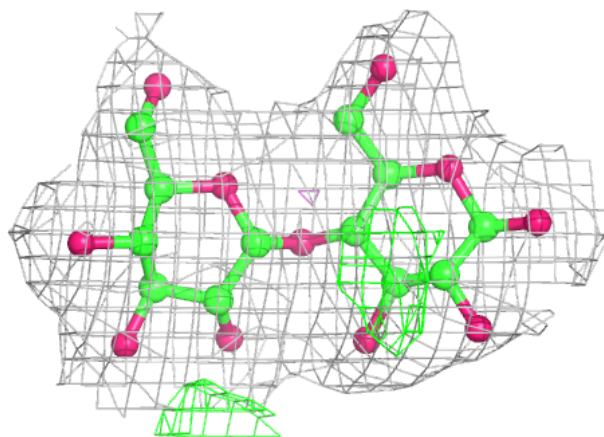
Electron density around Chain I:

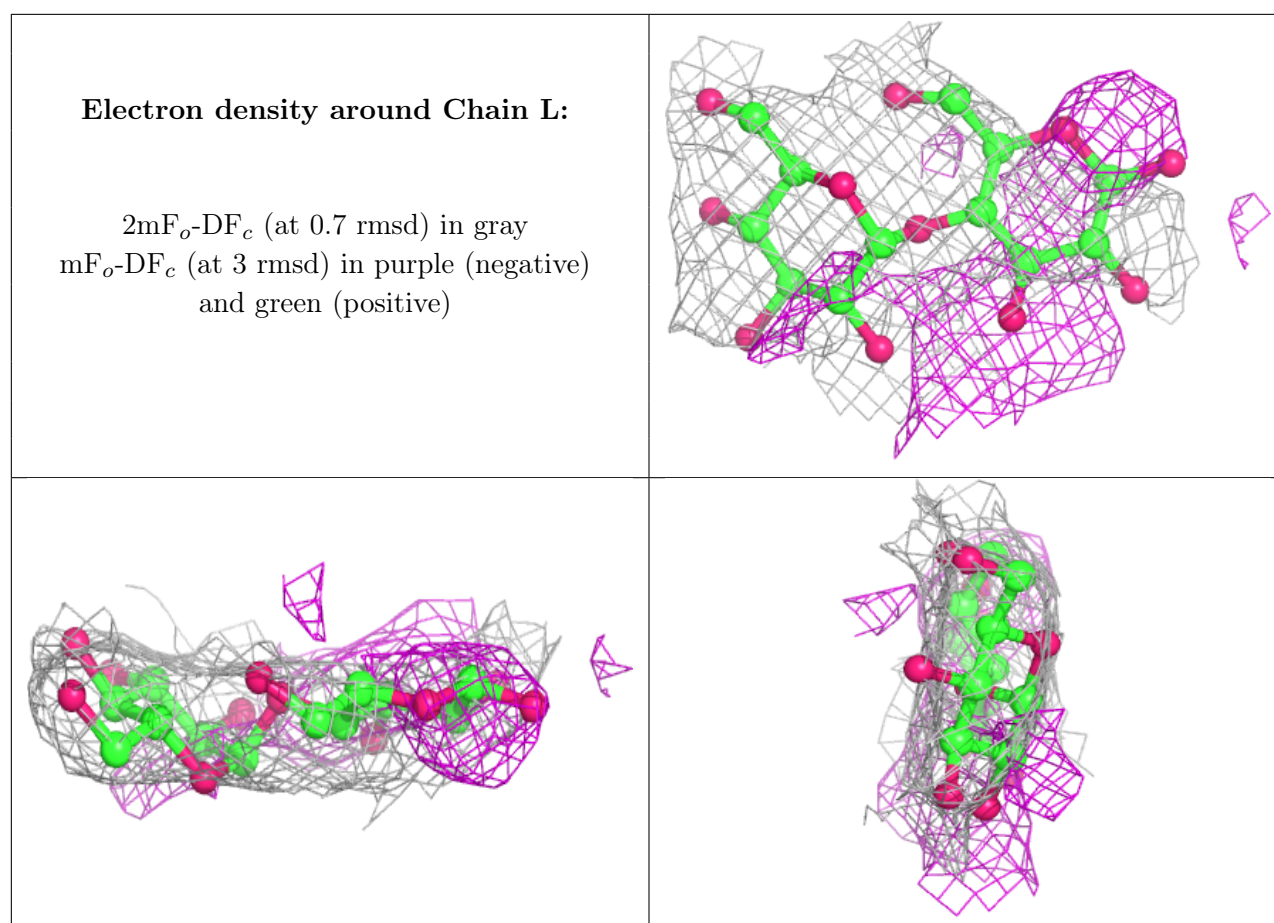
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

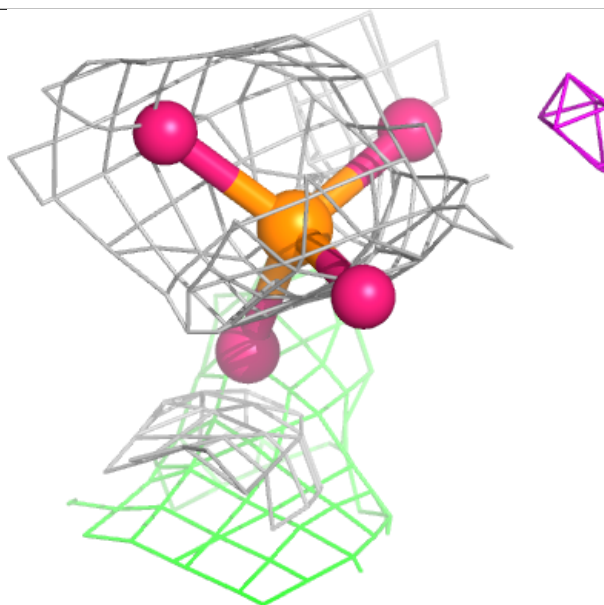
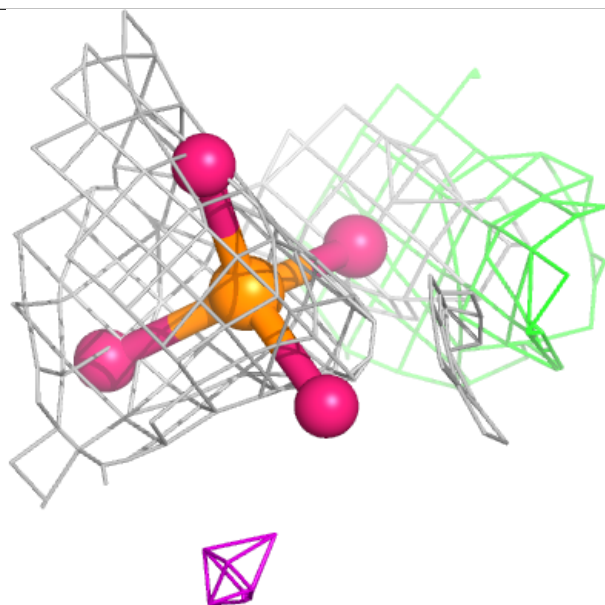
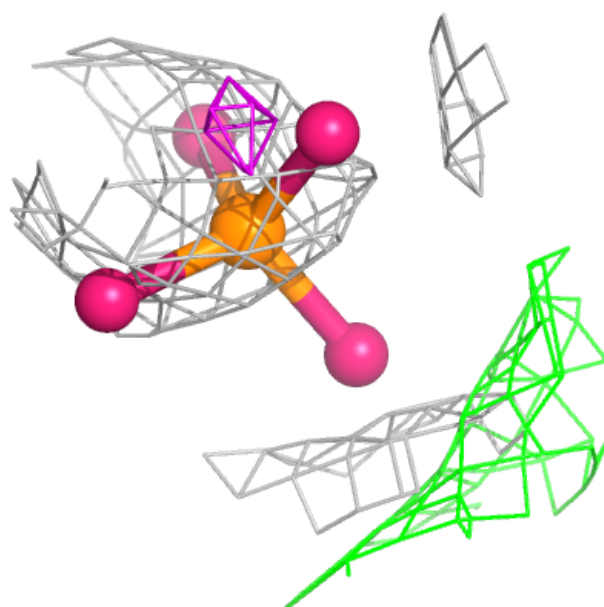
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BXY	B	1203	10/10	0.69	0.27	82,84,85,86	0
6	PO4	B	1202	5/5	0.70	0.38	150,153,153,157	0
7	BXY	A	1204	10/10	0.77	0.17	92,95,98,102	0
7	BXY	B	1204	10/10	0.80	0.16	106,111,113,114	0
6	PO4	A	1202	5/5	0.82	0.35	159,159,160,162	0
7	BXY	A	1203	10/10	0.84	0.16	52,57,59,61	0
5	CA	B	1201	1/1	0.87	0.18	109,109,109,109	0
5	CA	A	1201	1/1	0.90	0.21	88,88,88,88	0

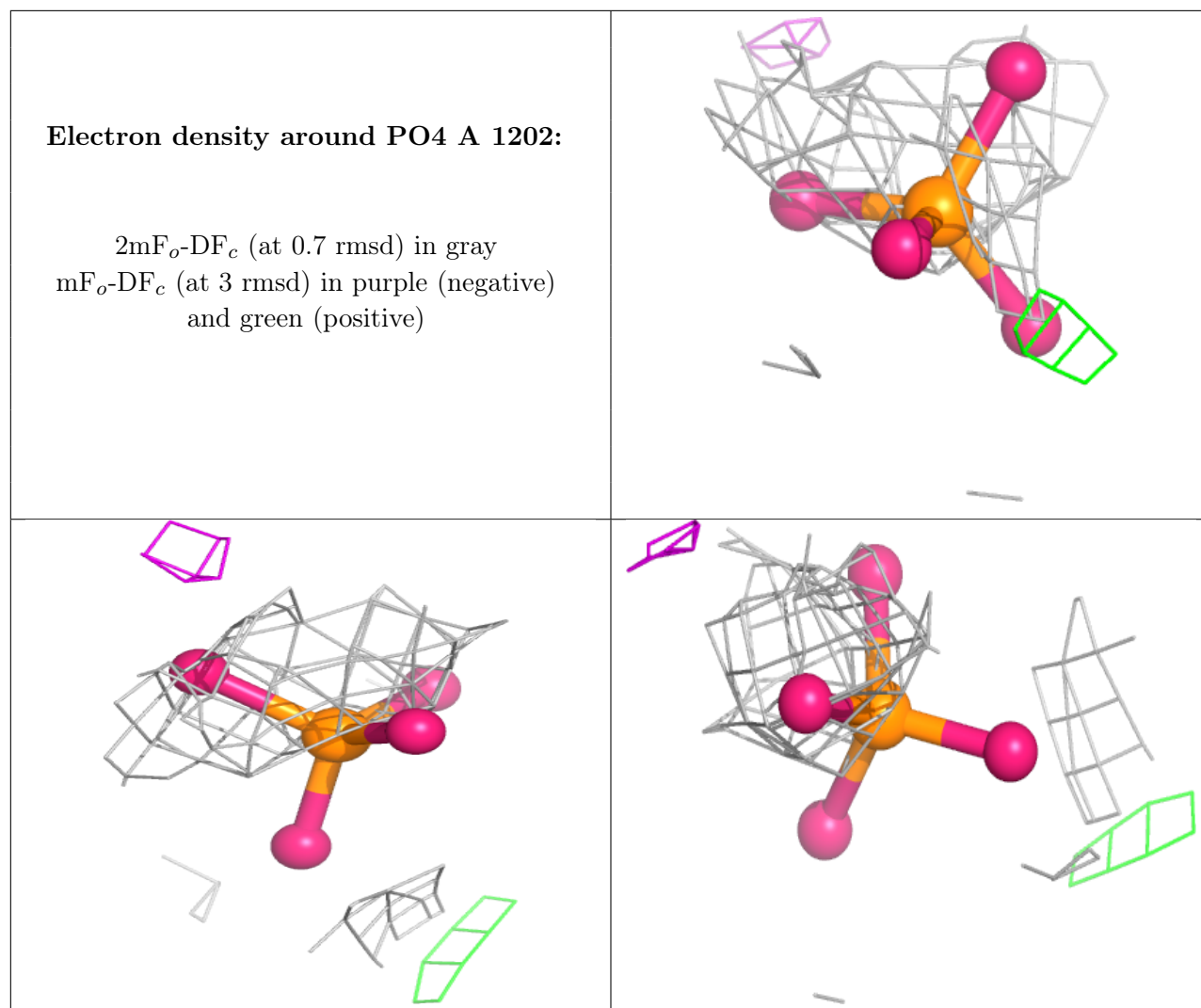
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around PO4 B 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.