



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:02 PM UTC

PDB ID : 7BVH / pdb_00007bvh
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

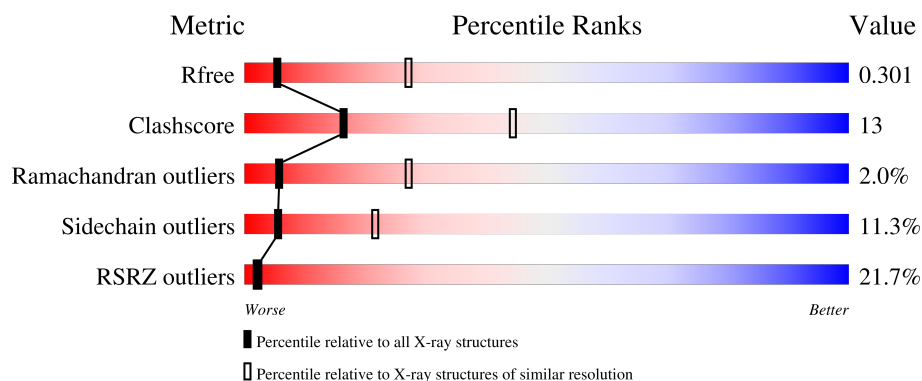
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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.



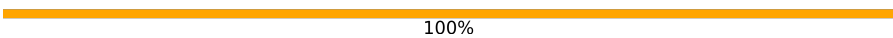
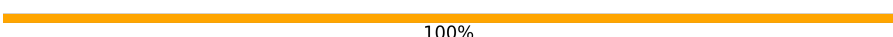
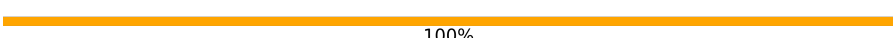
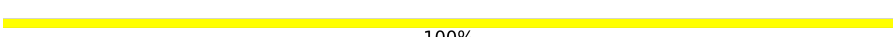
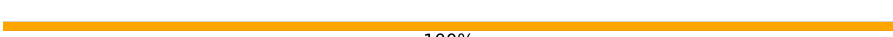
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	20% 61% 27% 5% • 7%
1	B	1113	21% 59% 29% • • 7%
2	C	99	19% 56% 28% • 15%
2	D	99	13% 65% 18% • 15%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	J	2	 50%50%
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.

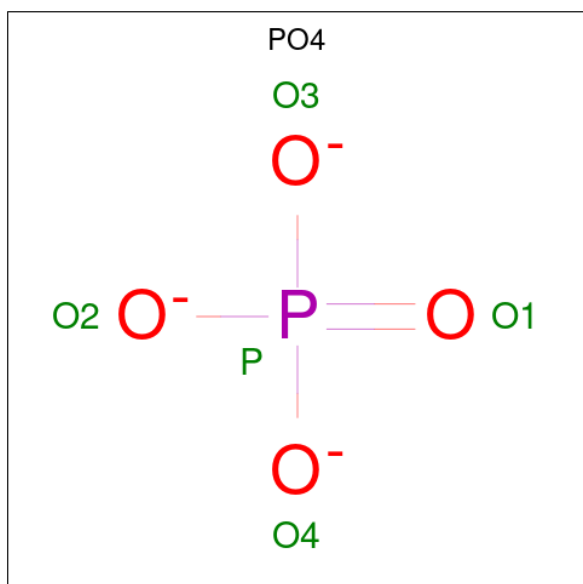


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	2	Total	C	O	0	0	0
			23	12	11			
4	G	2	Total	C	O	0	0	0
			23	12	11			
4	H	2	Total	C	O	0	0	0
			23	12	11			
4	I	2	Total	C	O	0	0	0
			23	12	11			
4	K	2	Total	C	O	0	0	0
			23	12	11			
4	L	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is CALCIUM ION (CCD ID: 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 (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



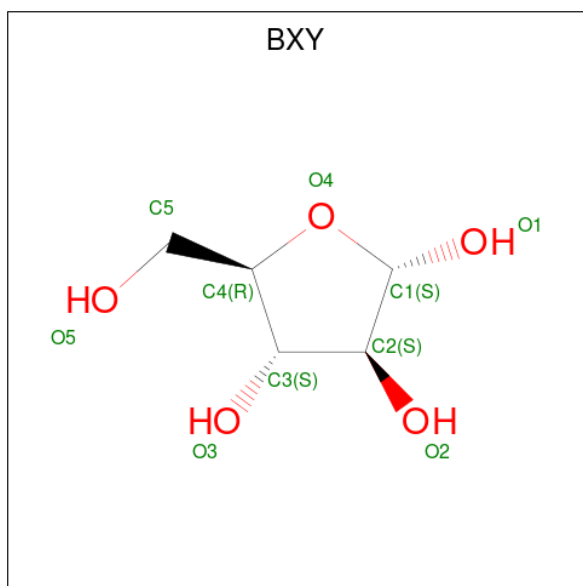
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 7 is alpha-D-arabinofuranose (CCD ID: BXY) (formula: $C_5H_{10}O_5$).

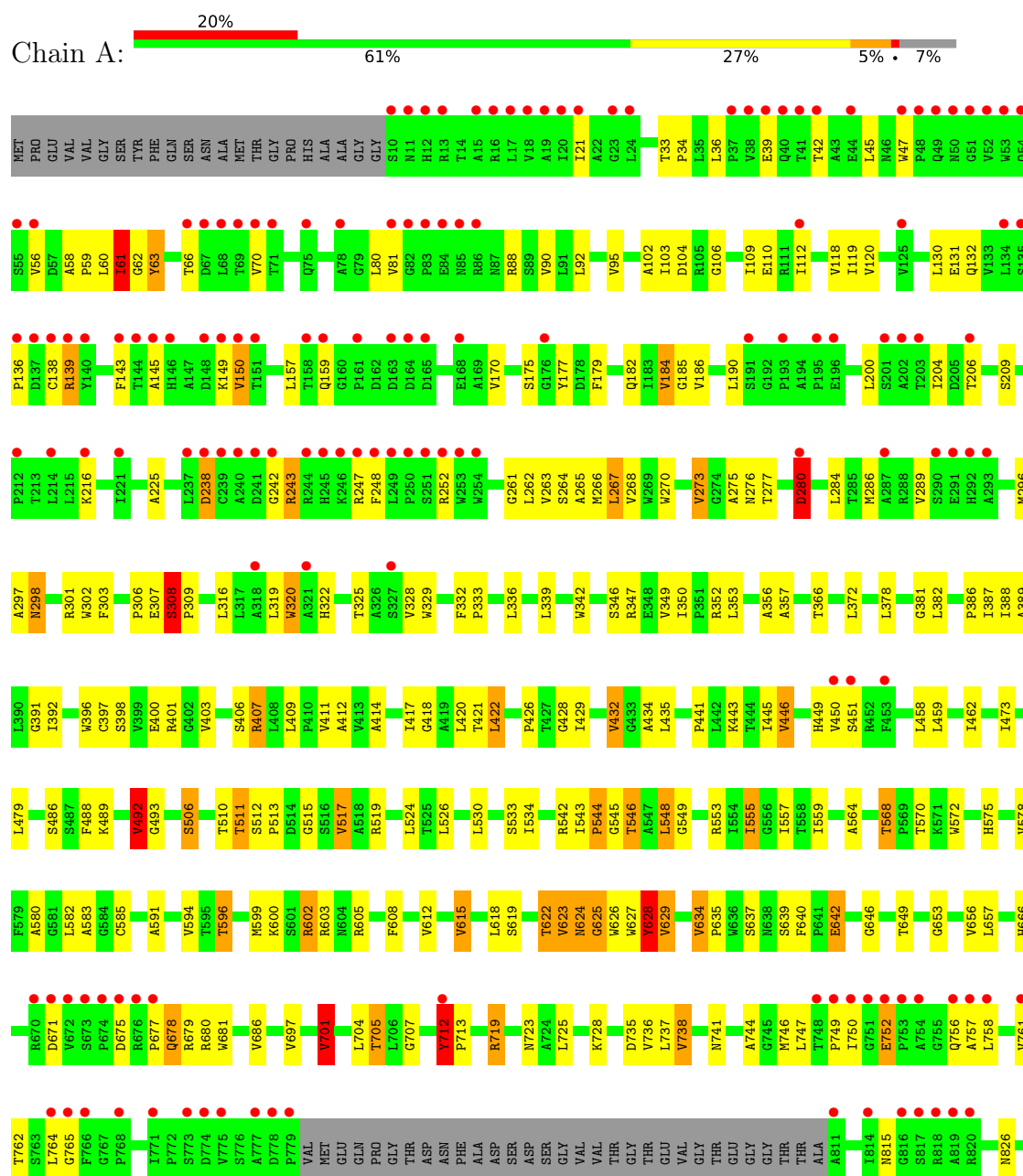


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	5	5		
7	A	1	Total	C	O	0	0
			10	5	5		
7	B	1	Total	C	O	0	0
			10	5	5		
7	B	1	Total	C	O	0	0
			10	5	5		

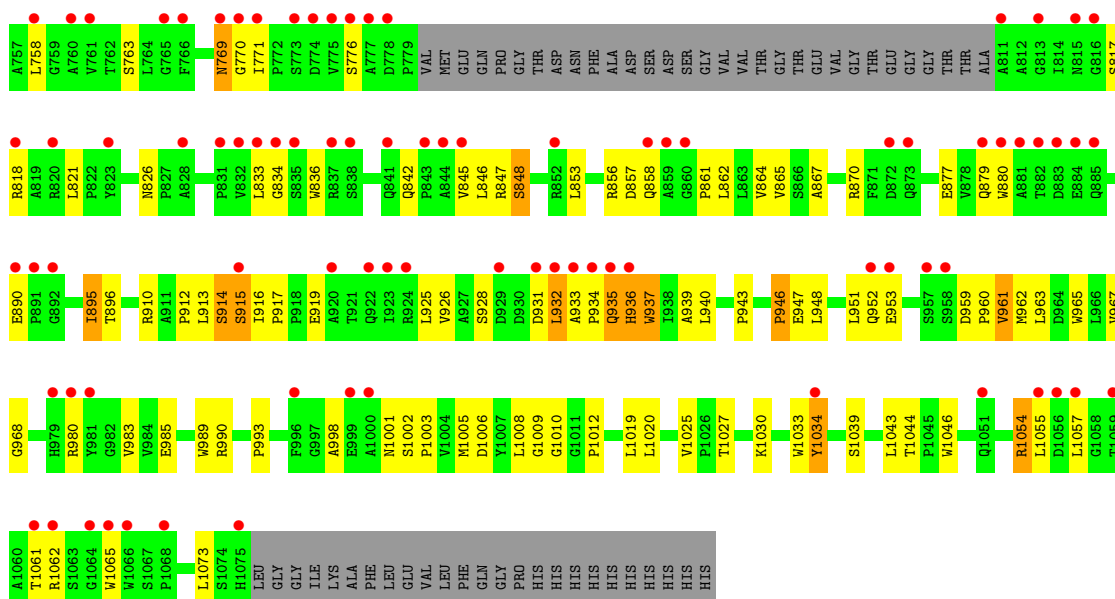
3 Residue-property plots [i](#)

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

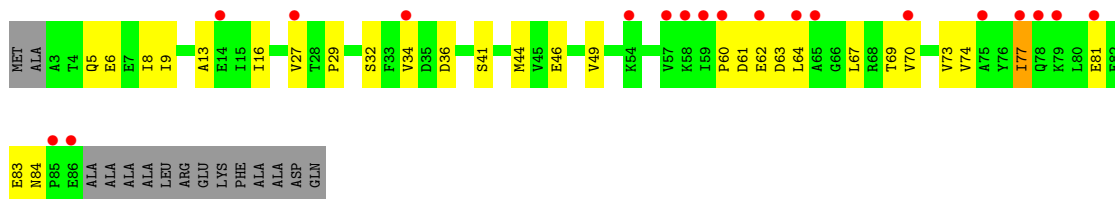
- Molecule 1: Integral membrane indolylacetyltransferase EmbC



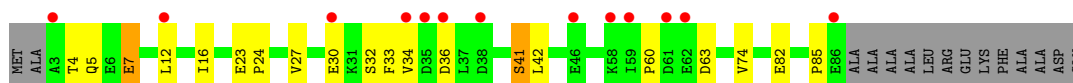




- Molecule 2: Meromycolate extension acyl carrier protein



- 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

Chain F:  100%

BGC1
GLC2

- 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 , 0.301	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: GLC, BXY, PO4, BGC, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	4/8124 (0.0%)	1.46	62/11137 (0.6%)
1	B	0.87	3/8124 (0.0%)	1.44	58/11137 (0.5%)
2	C	0.94	1/650 (0.2%)	1.54	4/884 (0.5%)
2	D	0.86	0/650	1.47	3/884 (0.3%)
All	All	0.88	8/17548 (0.0%)	1.45	127/24042 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	84	ASN	CA-C	6.63	1.58	1.53
1	B	350	ILE	CA-CB	6.37	1.57	1.54
1	A	568	THR	CA-C	6.32	1.59	1.53
1	A	625	GLY	CA-C	-5.85	1.48	1.52
1	A	752	GLU	CA-C	5.41	1.59	1.52
1	B	634	VAL	C-O	-5.38	1.18	1.25
1	B	712	TYR	N-CA	5.17	1.53	1.46
1	A	623	VAL	C-O	-5.17	1.17	1.24

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006	ASP	CA-CB-CG	8.79	121.39	112.60
1	A	1006	ASP	CA-CB-CG	7.82	120.42	112.60
1	B	81	VAL	CA-C-N	7.70	126.75	121.13
1	B	81	VAL	C-N-CA	7.70	126.75	121.13
1	B	61	ILE	N-CA-CB	6.95	119.47	110.57
1	B	506	SER	CA-C-N	6.93	130.85	120.31
1	B	506	SER	C-N-CA	6.93	130.85	120.31
1	A	627	TRP	N-CA-C	6.82	120.57	109.59
1	B	712	TYR	N-CA-C	6.66	124.52	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	TRP	CA-C-N	6.65	134.24	121.54
1	A	627	TRP	C-N-CA	6.65	134.24	121.54
1	A	625	GLY	N-CA-C	6.61	123.08	111.25
1	B	289	VAL	CA-C-N	6.43	129.73	120.79
1	B	289	VAL	C-N-CA	6.43	129.73	120.79
1	B	656	VAL	CA-C-N	6.38	128.74	120.44
1	B	656	VAL	C-N-CA	6.38	128.74	120.44
1	B	623	VAL	N-CA-CB	-6.36	101.78	110.56
1	A	106	GLY	N-CA-C	6.12	120.14	112.79
1	B	543	ILE	N-CA-CB	6.07	119.71	111.21
1	A	357	ALA	CA-C-N	6.05	128.38	120.28
1	A	357	ALA	C-N-CA	6.05	128.38	120.28
1	B	1033	TRP	N-CA-C	-6.00	102.61	110.53
1	A	289	VAL	CA-C-N	5.99	128.62	120.54
1	A	289	VAL	C-N-CA	5.99	128.62	120.54
1	A	238	ASP	N-CA-C	-5.93	106.18	113.41
1	B	640	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	596	THR	CA-C-N	5.81	128.34	120.44
1	A	596	THR	C-N-CA	5.81	128.34	120.44
1	B	362	ALA	N-CA-C	-5.79	105.05	111.36
1	B	959	ASP	CA-CB-CG	5.77	118.37	112.60
2	D	30	GLU	CA-C-N	5.74	130.52	121.56
2	D	30	GLU	C-N-CA	5.74	130.52	121.56
1	B	719	ARG	CA-C-N	5.71	127.93	120.28
1	B	719	ARG	C-N-CA	5.71	127.93	120.28
1	B	349	VAL	CA-C-N	5.70	125.90	120.43
1	B	349	VAL	C-N-CA	5.70	125.90	120.43
1	B	857	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	261	GLY	CA-C-N	5.65	127.86	120.28
1	A	261	GLY	C-N-CA	5.65	127.86	120.28
1	A	899	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	918	PRO	CA-C-N	5.62	127.81	120.28
1	A	918	PRO	C-N-CA	5.62	127.81	120.28
1	A	248	PHE	CA-C-N	5.59	127.08	120.09
1	A	248	PHE	C-N-CA	5.59	127.08	120.09
1	A	701	VAL	N-CA-CB	5.59	117.72	110.57
1	B	483	LEU	CA-C-N	5.56	127.67	120.44
1	B	483	LEU	C-N-CA	5.56	127.67	120.44
1	A	629	VAL	N-CA-C	-5.55	105.52	113.07
1	A	449	HIS	CA-CB-CG	5.55	119.35	113.80
1	A	675	ASP	CA-CB-CG	5.53	118.12	112.60
1	A	757	ALA	CA-C-N	5.51	127.92	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	757	ALA	C-N-CA	5.51	127.92	120.65
1	A	705	THR	N-CA-C	-5.50	104.14	111.24
1	A	765	GLY	CA-C-N	5.50	128.91	120.82
1	A	765	GLY	C-N-CA	5.50	128.91	120.82
1	B	298	ASN	N-CA-C	-5.50	100.14	108.67
1	B	46	ASN	CA-C-N	5.47	126.57	119.78
1	B	46	ASN	C-N-CA	5.47	126.57	119.78
2	C	81	GLU	CA-C-N	5.47	128.16	120.28
2	C	81	GLU	C-N-CA	5.47	128.16	120.28
1	A	725	LEU	CA-C-N	5.44	127.51	120.44
1	A	725	LEU	C-N-CA	5.44	127.51	120.44
1	B	94	THR	CA-C-N	5.42	129.33	121.68
1	B	94	THR	C-N-CA	5.42	129.33	121.68
1	B	265	ALA	CA-C-N	5.42	127.81	120.65
1	B	265	ALA	C-N-CA	5.42	127.81	120.65
1	A	61	ILE	N-CA-CB	5.39	117.47	110.57
1	A	628	TYR	CA-C-N	5.38	129.97	121.09
1	A	628	TYR	C-N-CA	5.38	129.97	121.09
1	A	978	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	357	ALA	CA-C-N	5.35	127.45	120.28
1	B	357	ALA	C-N-CA	5.35	127.45	120.28
1	B	946	PRO	N-CA-C	5.35	119.62	111.11
1	B	607	VAL	N-CA-CB	5.33	117.79	110.54
1	B	744	ALA	N-CA-C	5.33	116.77	111.07
1	A	624	ASN	N-CA-C	-5.31	105.98	113.20
1	A	298	ASN	N-CA-C	-5.31	100.44	108.67
1	A	1053	ALA	N-CA-C	5.31	117.38	110.43
1	B	417	ILE	CA-C-N	5.27	125.80	120.00
1	B	417	ILE	C-N-CA	5.27	125.80	120.00
1	A	707	GLY	CA-C-N	5.27	127.34	120.28
1	A	707	GLY	C-N-CA	5.27	127.34	120.28
1	B	281	GLY	CA-C-N	5.25	127.84	120.28
1	B	281	GLY	C-N-CA	5.25	127.84	120.28
1	A	1052	PRO	CA-C-N	5.23	129.71	120.87
1	A	1052	PRO	C-N-CA	5.23	129.71	120.87
1	B	769	ASN	CA-C-N	5.23	126.72	120.13
1	B	769	ASN	C-N-CA	5.23	126.72	120.13
1	A	225	ALA	CA-C-N	5.23	127.28	120.28
1	A	225	ALA	C-N-CA	5.23	127.28	120.28
1	A	627	TRP	CA-CB-CG	5.22	123.52	113.60
1	A	671	ASP	CA-C-N	5.22	127.61	120.46
1	A	671	ASP	C-N-CA	5.22	127.61	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ASP	CA-C-N	5.21	127.27	120.28
1	B	162	ASP	C-N-CA	5.21	127.27	120.28
1	B	622	THR	CB-CA-C	-5.21	100.84	113.19
1	A	307	GLU	N-CA-C	-5.21	106.92	113.28
1	A	858	GLN	CA-C-N	5.21	127.78	120.28
1	A	858	GLN	C-N-CA	5.21	127.78	120.28
1	A	677	PRO	CA-C-N	5.20	131.47	121.54
1	A	677	PRO	C-N-CA	5.20	131.47	121.54
1	B	307	GLU	N-CA-C	-5.19	99.50	108.52
1	B	286	MET	CA-C-N	5.17	128.17	120.31
1	B	286	MET	C-N-CA	5.17	128.17	120.31
1	B	734	ASN	CA-CB-CG	5.17	117.77	112.60
1	B	632	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	280	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	502	HIS	CA-C-N	5.15	127.04	120.56
1	B	502	HIS	C-N-CA	5.15	127.04	120.56
1	A	506	SER	CA-C-N	5.14	127.58	120.29
1	A	506	SER	C-N-CA	5.14	127.58	120.29
1	B	953	GLU	CA-C-N	5.13	127.11	120.70
1	B	953	GLU	C-N-CA	5.13	127.11	120.70
1	A	265	ALA	CA-C-N	5.10	127.07	120.44
1	A	265	ALA	C-N-CA	5.10	127.07	120.44
1	A	615	VAL	N-CA-CB	5.10	117.48	110.54
2	D	5	GLN	N-CA-C	-5.08	106.18	112.93
1	B	450	VAL	CA-C-N	5.07	127.03	120.44
1	B	450	VAL	C-N-CA	5.07	127.03	120.44
1	A	517	VAL	CA-C-N	5.05	127.36	120.54
1	A	517	VAL	C-N-CA	5.05	127.36	120.54
1	A	184	VAL	N-CA-C	-5.03	107.80	112.43
1	B	615	VAL	N-CA-CB	5.03	116.76	110.47
1	B	915	SER	N-CA-C	-5.02	107.14	114.12
1	A	627	TRP	O-C-N	5.02	129.58	123.21
2	C	83	GLU	CA-C-N	5.01	128.24	122.83
2	C	83	GLU	C-N-CA	5.01	128.24	122.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7900	0	7935	202	0
1	B	7900	0	7935	216	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	1	0
4	F	23	0	21	4	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	451	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 (451) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:BCY: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:BCY: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:320:TRP:HD1	1:B:330:MET:HE2	1.60	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:BCY:C2	4:G:2:GLC:C5	2.71	0.66
1:A:649:THR:HG21	7:A:1204:BCY:O3	1.96	0.66
1:A:286:MET:HE2	1:A:296:MET:HE2	1.75	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: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:B:216:LYS:HG2	1:B:220:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:BCY: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:330:MET:HE2	1:B:330:MET:HA	1.82	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:BCY: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: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:930:ASP:OD1	1:A:930:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:543:ILE:HD12	1:B:543:ILE:C	2.31	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
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:A:102:ALA:C	1:A:104:ASP:H	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:TRP:CD1	1:B:330:MET:HE2	2.44	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: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
1:A:286:MET:HE3	1:A:298:ASN:HA	1.95	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:A:962:MET:HE1	1:A:1013:LEU:HD12	1.95	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:A:489:LYS:HD2	4:F:2:GLC:HO2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:708:MET:HE1	1:B:722:LEU:HD11	1.97	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:B:936:HIS:ND1	1:B:936:HIS:C	2.72	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:B:266:MET:HE3	1:B:697:VAL: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:970:ALA:C	1:A:972:PRO:HD3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:623:VAL:C	1:A:625:GLY:H	2.25	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:279:ASP:CG	3:J:1:BCY:H5	2.44	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
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:426:PRO:C	1:A:428:GLY:H	2.27	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:320:TRP:HD1	1:B:330:MET:CE	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLY:CA	1:B:314:TYR:CD2	3.03	0.42
1:B:913:LEU:C	1:B:915:SER:H	2.28	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
1:B:594:VAL:HA	1:B:599:MET:HE3	2.01	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:962:MET:HE1	1:A:1013:LEU:CD1	2.51	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:286:MET:O	1:B:296:MET:HE1	2.21	0.40
1:B:301:ARG:HH21	1:B:493:GLY:HA2	1.80	0.40
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:B:83:PRO:C	1:B:85:ASN:H	2.30	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: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	28
1	B	1031/1113 (93%)	934 (91%)	77 (8%)	20 (2%)	6	28
2	C	82/99 (83%)	72 (88%)	7 (8%)	3 (4%)	2	17
2	D	82/99 (83%)	70 (85%)	10 (12%)	2 (2%)	4	24
All	All	2226/2424 (92%)	1991 (89%)	190 (8%)	45 (2%)	6	27

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
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

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Mol	Chain	Res	Type
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%)	733 (89%)	88 (11%)	6	24
1	B	821/880 (93%)	720 (88%)	101 (12%)	4	19
2	C	73/81 (90%)	68 (93%)	5 (7%)	14	42
2	D	73/81 (90%)	65 (89%)	8 (11%)	6	23
All	All	1788/1922 (93%)	1586 (89%)	202 (11%)	5	21

All (202) 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	56	VAL
1	A	61	ILE
1	A	92	LEU
1	A	103	ILE
1	A	112	ILE
1	A	119	ILE

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Mol	Chain	Res	Type
1	A	139	ARG
1	A	150	VAL
1	A	186	VAL
1	A	209	SER
1	A	267	LEU
1	A	273	VAL
1	A	276	ASN
1	A	280	ASP
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	411	VAL
1	A	420	LEU
1	A	422	LEU
1	A	432	VAL
1	A	443	LYS
1	A	446	VAL
1	A	458	LEU
1	A	486	SER
1	A	492	VAL
1	A	506	SER
1	A	511	THR
1	A	544	PRO
1	A	546	THR
1	A	548	LEU
1	A	555	ILE
1	A	570	THR
1	A	578	VAL
1	A	602	ARG
1	A	612	VAL
1	A	622	THR
1	A	629	VAL
1	A	634	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

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Mol	Chain	Res	Type
1	A	701	VAL
1	A	712	TYR
1	A	719	ARG
1	A	736	VAL
1	A	737	LEU
1	A	738	VAL
1	A	746	MET
1	A	747	LEU
1	A	750	ILE
1	A	758	LEU
1	A	762	THR
1	A	764	LEU
1	A	826	ASN
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
1	A	932	LEU
1	A	935	GLN
1	A	938	ILE
1	A	945	ILE
1	A	962	MET
1	A	969	LEU
1	A	974	GLN
1	A	984	VAL
1	A	988	LYS
1	A	991	ILE
1	A	994	ASP
1	A	1025	VAL
1	A	1039	SER
1	A	1044	THR
1	A	1054	ARG
1	B	17	LEU
1	B	33	THR
1	B	36	LEU
1	B	38	VAL
1	B	42	THR

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Mol	Chain	Res	Type
1	B	52	VAL
1	B	61	ILE
1	B	75	GLN
1	B	92	LEU
1	B	93	SER
1	B	94	THR
1	B	118	VAL
1	B	126	VAL
1	B	144	THR
1	B	146	HIS
1	B	157	LEU
1	B	190	LEU
1	B	198	LEU
1	B	200	LEU
1	B	245	HIS
1	B	249	LEU
1	B	263	VAL
1	B	267	LEU
1	B	268	VAL
1	B	286	MET
1	B	291	GLU
1	B	301	ARG
1	B	308	SER
1	B	328	VAL
1	B	348	GLU
1	B	388	ILE
1	B	394	LEU
1	B	398	SER
1	B	399	VAL
1	B	429	ILE
1	B	432	VAL
1	B	442	LEU
1	B	475	ARG
1	B	486	SER
1	B	542	ARG
1	B	543	ILE
1	B	544	PRO
1	B	597	THR
1	B	622	THR
1	B	623	VAL
1	B	634	VAL
1	B	642	GLU

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Mol	Chain	Res	Type
1	B	647	PHE
1	B	652	LEU
1	B	657	LEU
1	B	660	LEU
1	B	668	SER
1	B	670	ARG
1	B	672	VAL
1	B	676	ARG
1	B	681	TRP
1	B	689	LEU
1	B	698	ILE
1	B	701	VAL
1	B	704	LEU
1	B	706	LEU
1	B	712	TYR
1	B	716	SER
1	B	728	LYS
1	B	735	ASP
1	B	737	LEU
1	B	756	GLN
1	B	763	SER
1	B	817	SER
1	B	821	LEU
1	B	833	LEU
1	B	842	GLN
1	B	845	VAL
1	B	848	SER
1	B	853	LEU
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
1	B	952	GLN
1	B	961	VAL

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Mol	Chain	Res	Type
1	B	962	MET
1	B	967	VAL
1	B	990	ARG
1	B	1008	LEU
1	B	1019	LEU
1	B	1034	TYR
1	B	1039	SER
1	B	1044	THR
1	B	1054	ARG
1	B	1057	LEU
1	B	1062	ARG
1	B	1073	LEU
2	C	6	GLU
2	C	16	ILE
2	C	34	VAL
2	C	70	VAL
2	C	77	ILE
2	D	7	GLU
2	D	12	LEU
2	D	16	ILE
2	D	27	VAL
2	D	34	VAL
2	D	41	SER
2	D	74	VAL
2	D	82	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	12	HIS
1	A	40	GLN
1	A	98	GLN
1	A	132	GLN
1	A	245	HIS
1	A	292	HIS
1	A	298	ASN
1	A	322	HIS
1	A	484	GLN
1	A	666	HIS
1	A	710	ASN
1	A	741	ASN

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Mol	Chain	Res	Type
1	A	743	ASN
1	A	826	ASN
1	A	841	GLN
1	A	842	GLN
1	A	908	ASN
1	A	935	GLN
1	A	974	GLN
1	A	1075	HIS
1	B	46	ASN
1	B	54	GLN
1	B	87	ASN
1	B	113	ASN
1	B	146	HIS
1	B	159	GLN
1	B	235	HIS
1	B	298	ASN
1	B	322	HIS
1	B	484	GLN
1	B	575	HIS
1	B	624	ASN
1	B	631	ASN
1	B	638	ASN
1	B	678	GLN
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	889	ASN
1	B	908	ASN
1	B	979	HIS
1	B	1075	HIS
2	C	5	GLN
2	C	50	GLN
2	C	84	ASN

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	0.78	0	13,14,14	1.06	1 (7%)
3	BXY	E	2	3	9,9,10	0.47	0	11,12,14	0.90	1 (9%)
4	BGC	F	1	4	12,12,12	1.58	4 (33%)	17,17,17	2.31	6 (35%)
4	GLC	F	2	4	11,11,12	1.48	2 (18%)	15,15,17	2.33	6 (40%)
4	BGC	G	1	4	12,12,12	1.42	2 (16%)	17,17,17	2.37	8 (47%)
4	GLC	G	2	4	11,11,12	1.67	3 (27%)	15,15,17	1.79	4 (26%)
4	BGC	H	1	4	12,12,12	1.30	3 (25%)	17,17,17	1.64	4 (23%)
4	GLC	H	2	4	11,11,12	2.16	4 (36%)	15,15,17	3.04	6 (40%)
4	BGC	I	1	4	12,12,12	1.33	2 (16%)	17,17,17	1.61	2 (11%)
4	GLC	I	2	4	11,11,12	2.26	3 (27%)	15,15,17	2.60	5 (33%)
3	BXY	J	1	3	10,10,10	0.71	0	13,14,14	1.36	2 (15%)
3	BXY	J	2	3	9,9,10	0.44	0	11,12,14	0.90	1 (9%)
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	2.16	2 (18%)	15,15,17	2.88	8 (53%)
4	BGC	L	1	4	12,12,12	1.19	1 (8%)	17,17,17	0.82	0
4	GLC	L	2	4	11,11,12	1.68	2 (18%)	15,15,17	0.80	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	-5.82	1.43	1.52
4	H	2	GLC	O5-C1	4.98	1.52	1.43
4	I	2	GLC	O5-C1	4.69	1.51	1.43
4	L	2	GLC	O5-C1	4.37	1.51	1.43
4	I	2	GLC	C2-C3	-4.21	1.46	1.52
4	H	2	GLC	C2-C3	-3.98	1.46	1.52
4	G	2	GLC	O5-C1	3.59	1.49	1.43
4	F	2	GLC	C2-C3	-3.25	1.47	1.52
4	G	2	GLC	C2-C3	-3.21	1.47	1.52
4	I	2	GLC	C4-C3	-3.14	1.44	1.52
4	K	2	GLC	C4-C3	-3.01	1.44	1.52
4	L	1	BGC	O5-C1	2.99	1.50	1.42
4	G	1	BGC	O5-C1	2.95	1.50	1.42
4	I	1	BGC	O5-C1	2.77	1.49	1.42
4	F	1	BGC	C1-C2	-2.57	1.46	1.52
4	G	1	BGC	O5-C5	2.48	1.50	1.44
4	K	1	BGC	O5-C1	2.46	1.48	1.42
4	F	2	GLC	O5-C1	2.46	1.47	1.43
4	F	1	BGC	C4-C3	-2.46	1.46	1.52
4	F	1	BGC	C3-C2	-2.39	1.46	1.52
4	K	1	BGC	C4-C3	-2.35	1.46	1.52
4	I	1	BGC	C4-C3	-2.33	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	BGC	O5-C1	2.32	1.48	1.42
4	H	1	BGC	O5-C1	2.28	1.48	1.42
4	H	1	BGC	C1-C2	-2.23	1.47	1.52
4	G	2	GLC	C4-C3	-2.22	1.46	1.52
4	L	2	GLC	C2-C3	-2.15	1.49	1.52
4	H	2	GLC	O5-C5	2.07	1.47	1.43
4	H	2	GLC	C4-C3	-2.06	1.47	1.52
4	H	1	BGC	C4-C3	-2.06	1.47	1.52
4	K	1	BGC	O5-C5	2.03	1.49	1.44

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	GLC	C3-C4-C5	-8.37	95.06	110.23
4	I	2	GLC	C1-O5-C5	7.62	122.40	112.19
4	H	2	GLC	C2-C3-C4	-7.25	98.10	110.86
4	F	2	GLC	C3-C4-C5	-5.82	99.68	110.23
4	F	1	BGC	O4-C4-C3	-5.51	97.39	110.38
4	H	2	GLC	C3-C4-C5	-4.90	101.36	110.23
4	H	2	GLC	O4-C4-C3	4.71	121.49	110.38
4	I	1	BGC	C3-C4-C5	-4.61	101.87	110.23
4	G	2	GLC	C1-C2-C3	4.43	116.09	109.64
4	G	1	BGC	C4-C3-C2	-4.28	103.31	110.83
4	F	1	BGC	C3-C4-C5	4.03	117.53	110.23
4	G	1	BGC	O5-C5-C4	4.02	116.94	109.70
4	H	2	GLC	O5-C5-C6	3.82	115.10	107.66
4	K	1	BGC	C4-C3-C2	-3.80	104.16	110.83
4	F	1	BGC	O3-C3-C4	-3.61	101.86	110.38
4	G	1	BGC	O4-C4-C5	-3.61	100.44	109.32
4	H	1	BGC	O2-C2-C1	-3.59	100.96	109.25
4	K	1	BGC	C1-C2-C3	-3.54	103.14	110.36
4	F	2	GLC	O4-C4-C3	3.24	118.02	110.38
4	F	2	GLC	O3-C3-C2	-3.24	103.45	110.05
4	I	2	GLC	C6-C5-C4	-3.17	105.24	113.02
4	K	2	GLC	C2-C3-C4	-3.12	105.38	110.86
3	J	1	BXY	O4-C4-C5	3.08	115.73	109.22
4	H	1	BGC	C1-C2-C3	2.96	116.39	110.36
4	G	1	BGC	C1-C2-C3	-2.96	104.32	110.36
4	F	1	BGC	O3-C3-C2	-2.94	103.44	110.38
4	H	2	GLC	C6-C5-C4	-2.94	105.81	113.02
4	H	2	GLC	O2-C2-C1	2.92	115.91	109.22
4	G	1	BGC	C1-O5-C5	2.90	119.26	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	GLC	C1-C2-C3	2.90	113.86	109.64
4	K	2	GLC	O2-C2-C3	-2.87	104.21	110.15
4	F	2	GLC	C1-C2-C3	2.74	113.64	109.64
4	I	1	BGC	O5-C1-C2	2.60	114.87	110.30
4	K	2	GLC	O4-C4-C5	2.48	115.43	109.32
4	G	1	BGC	C6-C5-C4	-2.47	106.95	113.02
4	K	2	GLC	O2-C2-C1	2.46	114.86	109.22
3	E	1	BXY	C5-C4-C3	-2.45	109.32	115.10
4	F	2	GLC	O2-C2-C1	-2.43	103.65	109.22
4	G	1	BGC	O4-C4-C3	2.43	116.10	110.38
4	H	1	BGC	O4-C4-C3	-2.41	104.69	110.38
4	F	1	BGC	C4-C3-C2	2.41	115.06	110.83
4	K	2	GLC	O3-C3-C2	-2.39	105.18	110.05
4	F	2	GLC	O3-C3-C4	2.37	115.95	110.38
4	H	1	BGC	O5-C5-C4	2.34	113.92	109.70
3	J	2	BXY	O4-C4-C3	2.27	106.73	104.63
4	I	2	GLC	O2-C2-C3	-2.24	105.50	110.15
4	G	1	BGC	O3-C3-C4	2.20	115.56	110.38
4	K	2	GLC	O5-C1-C2	2.19	116.02	110.79
4	K	2	GLC	C1-C2-C3	2.18	112.82	109.64
4	G	2	GLC	O3-C3-C2	-2.18	105.60	110.05
4	F	1	BGC	C1-O5-C5	2.18	117.86	113.65
4	G	2	GLC	O3-C3-C4	-2.08	105.48	110.38
4	I	2	GLC	O2-C2-C1	2.07	113.96	109.22
3	E	2	BXY	C5-C4-C3	-2.04	110.29	115.10
3	J	1	BXY	C1-C2-C3	2.03	104.78	102.29
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	K	1	BGC	O5-C5-C6-O6
4	F	1	BGC	O5-C5-C6-O6
3	J	1	BXY	O4-C4-C5-O5
4	K	1	BGC	C4-C5-C6-O6
3	J	2	BXY	C3-C4-C5-O5
4	I	2	GLC	C4-C5-C6-O6

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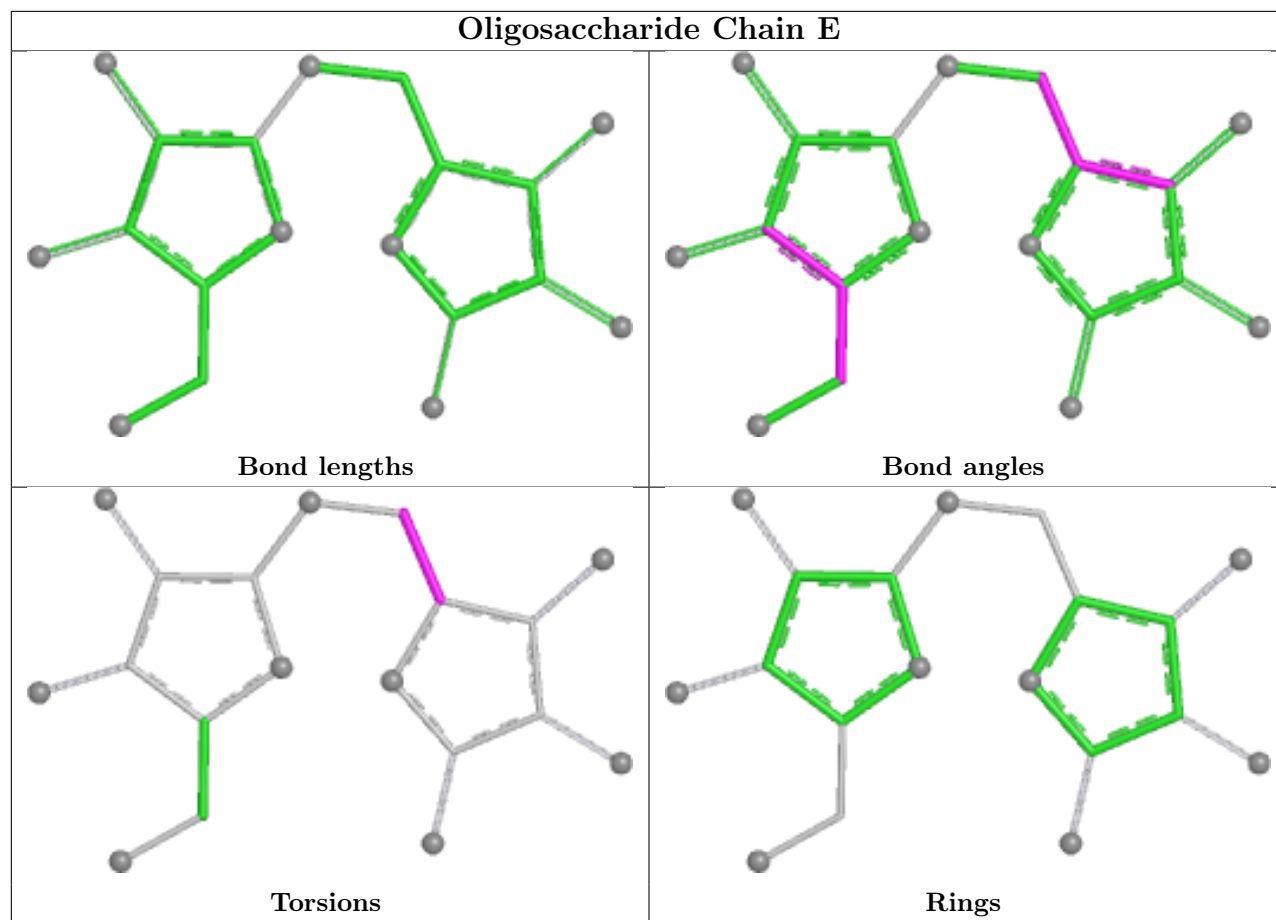
Mol	Chain	Res	Type	Atoms
4	L	1	BGC	C4-C5-C6-O6
3	J	1	BXY	C3-C4-C5-O5
4	F	1	BGC	C4-C5-C6-O6
4	L	2	GLC	O5-C5-C6-O6
4	G	1	BGC	O5-C5-C6-O6
4	H	2	GLC	O5-C5-C6-O6
4	I	2	GLC	O5-C5-C6-O6

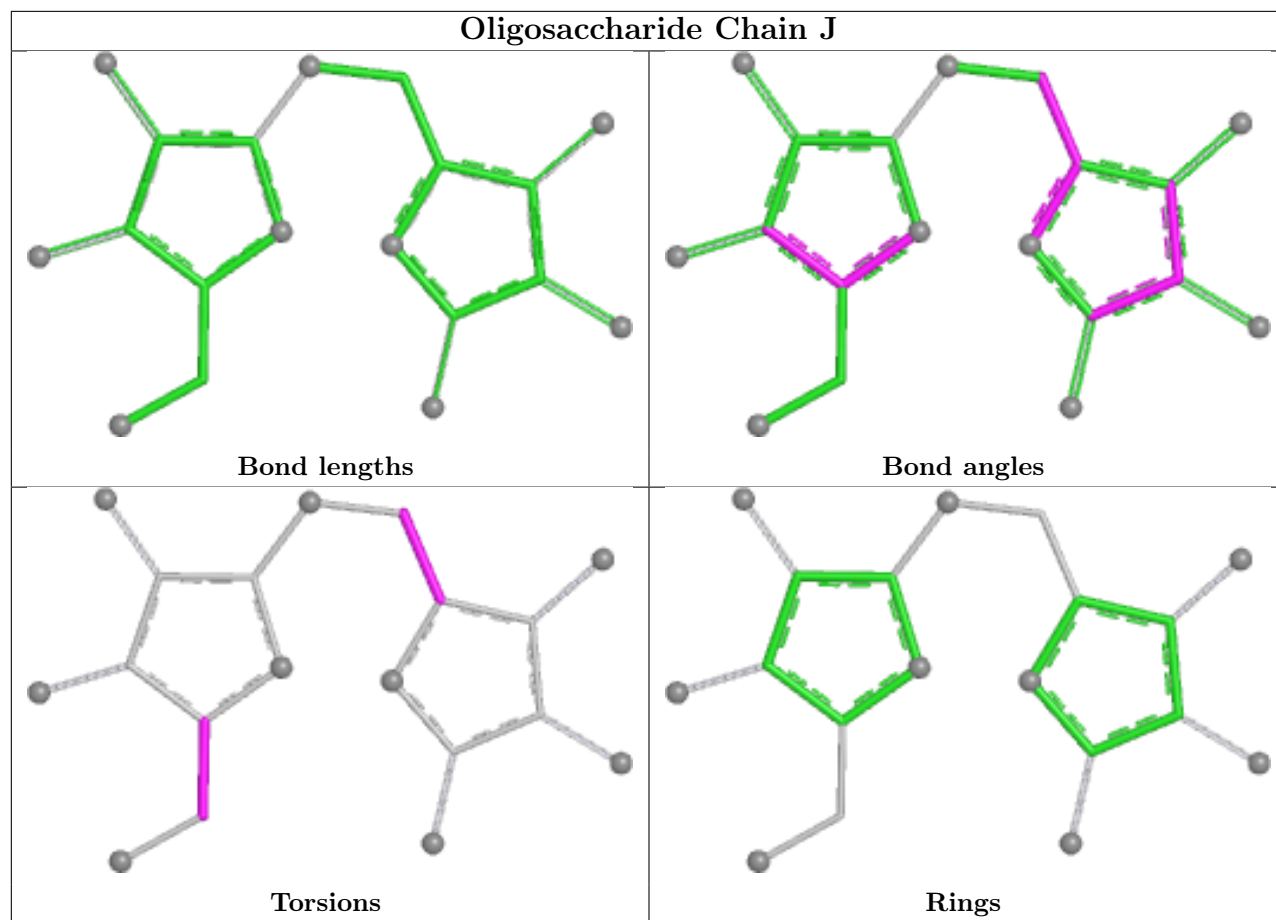
There are no ring outliers.

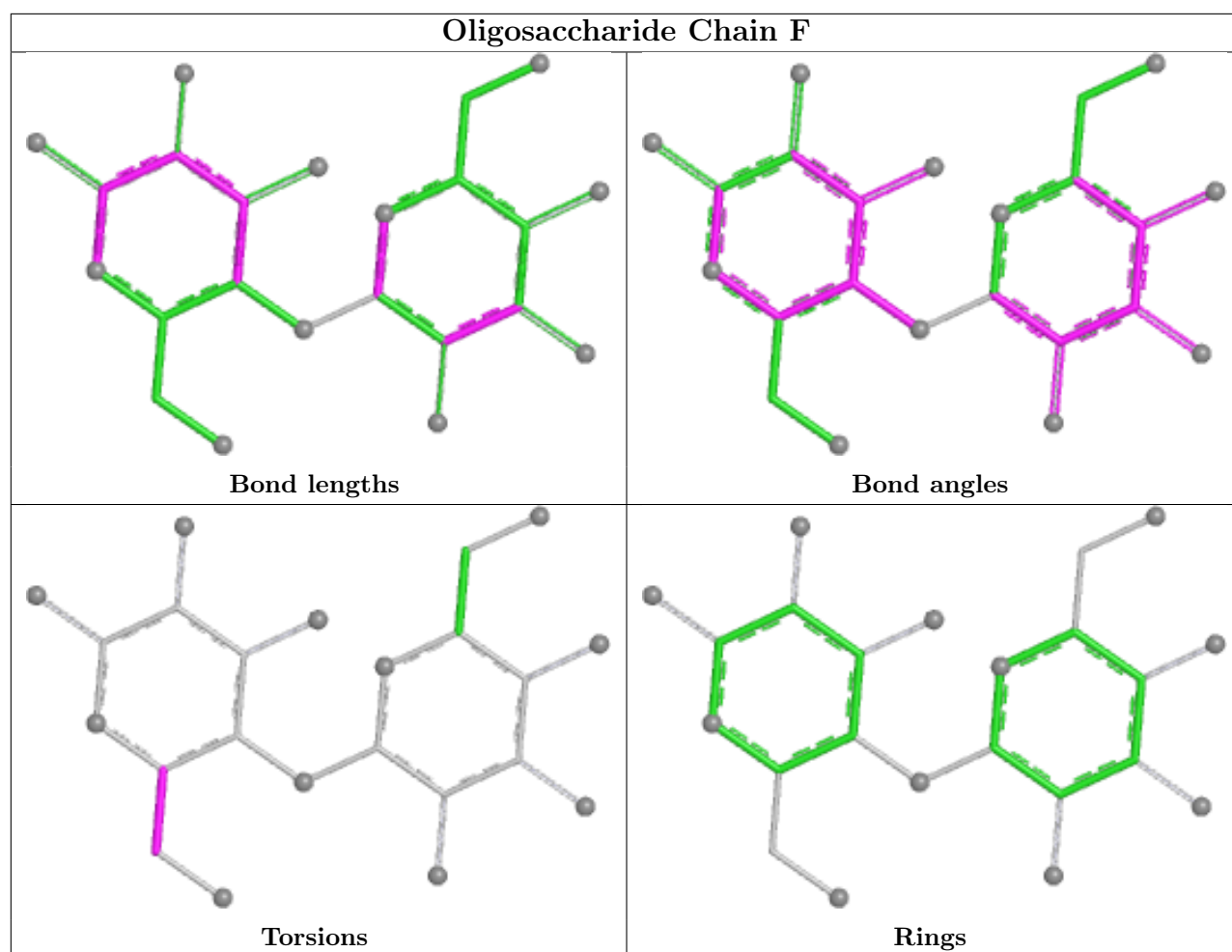
10 monomers are involved in 27 short contacts:

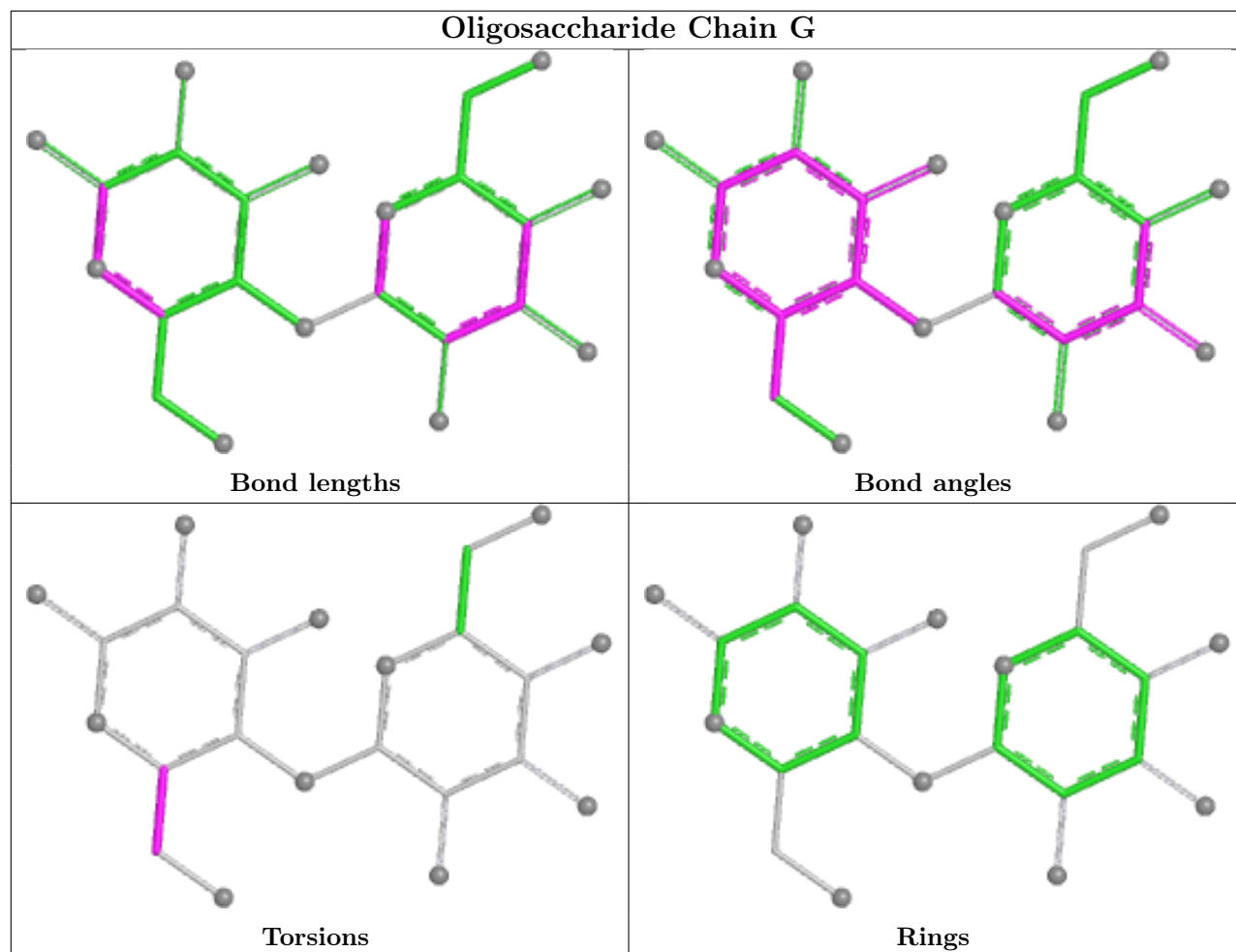
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	GLC	1	0
4	I	2	GLC	1	0
4	L	1	BGC	2	0
3	J	1	BXY	1	0
4	F	1	BGC	2	0
4	H	1	BGC	1	0
4	G	2	GLC	12	0
4	F	2	GLC	4	0
4	I	1	BGC	1	0
4	L	2	GLC	6	0

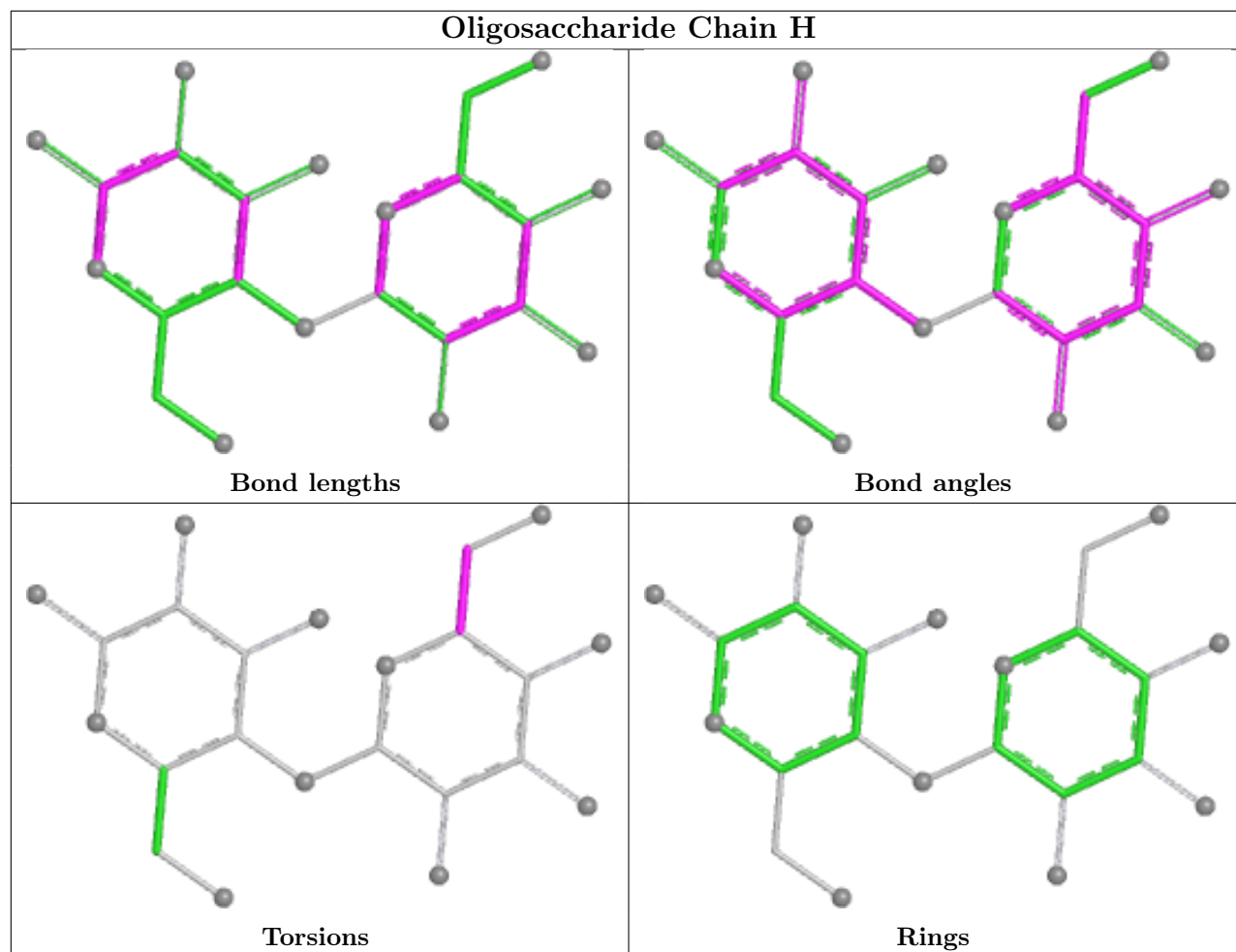
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

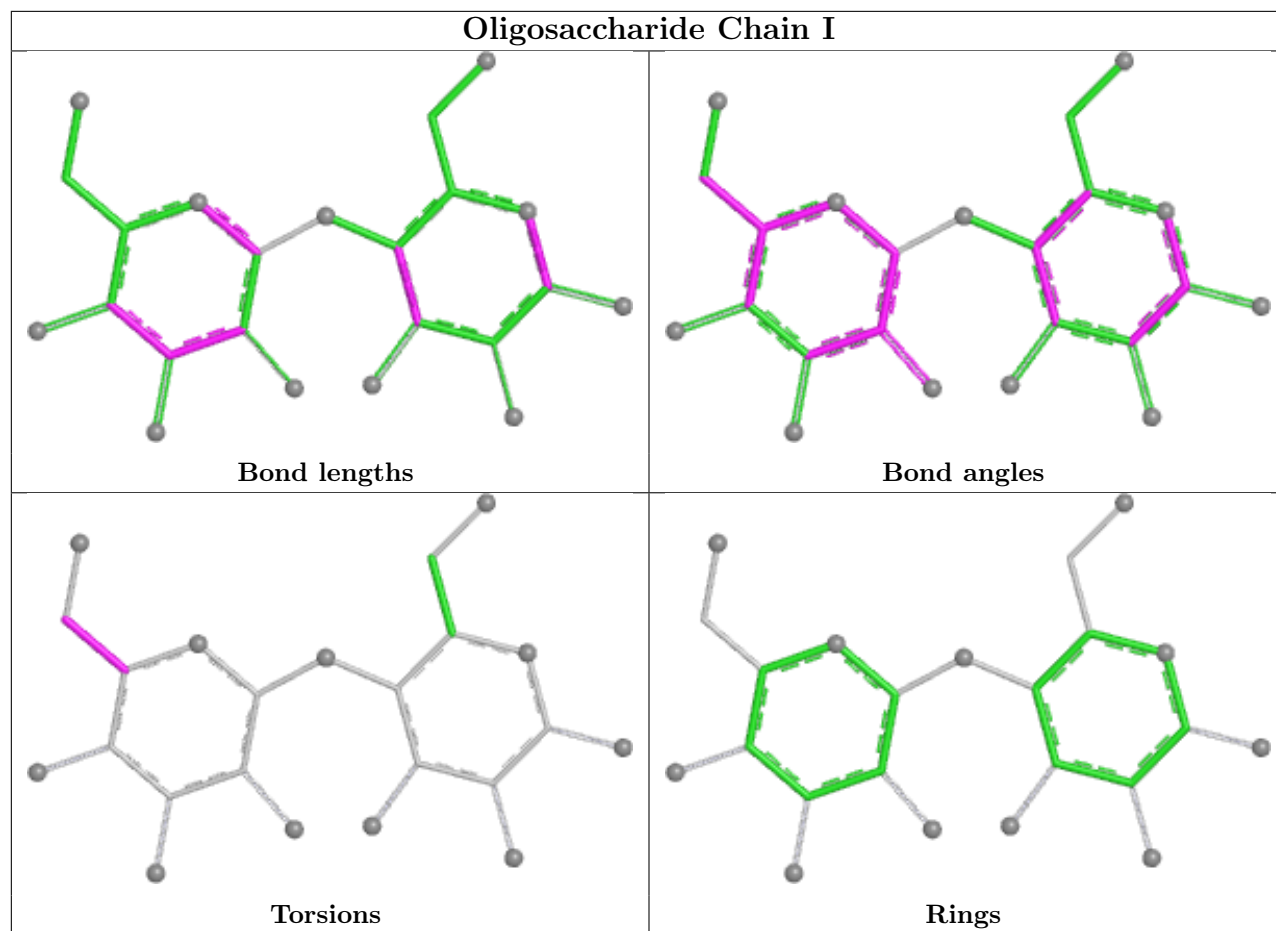


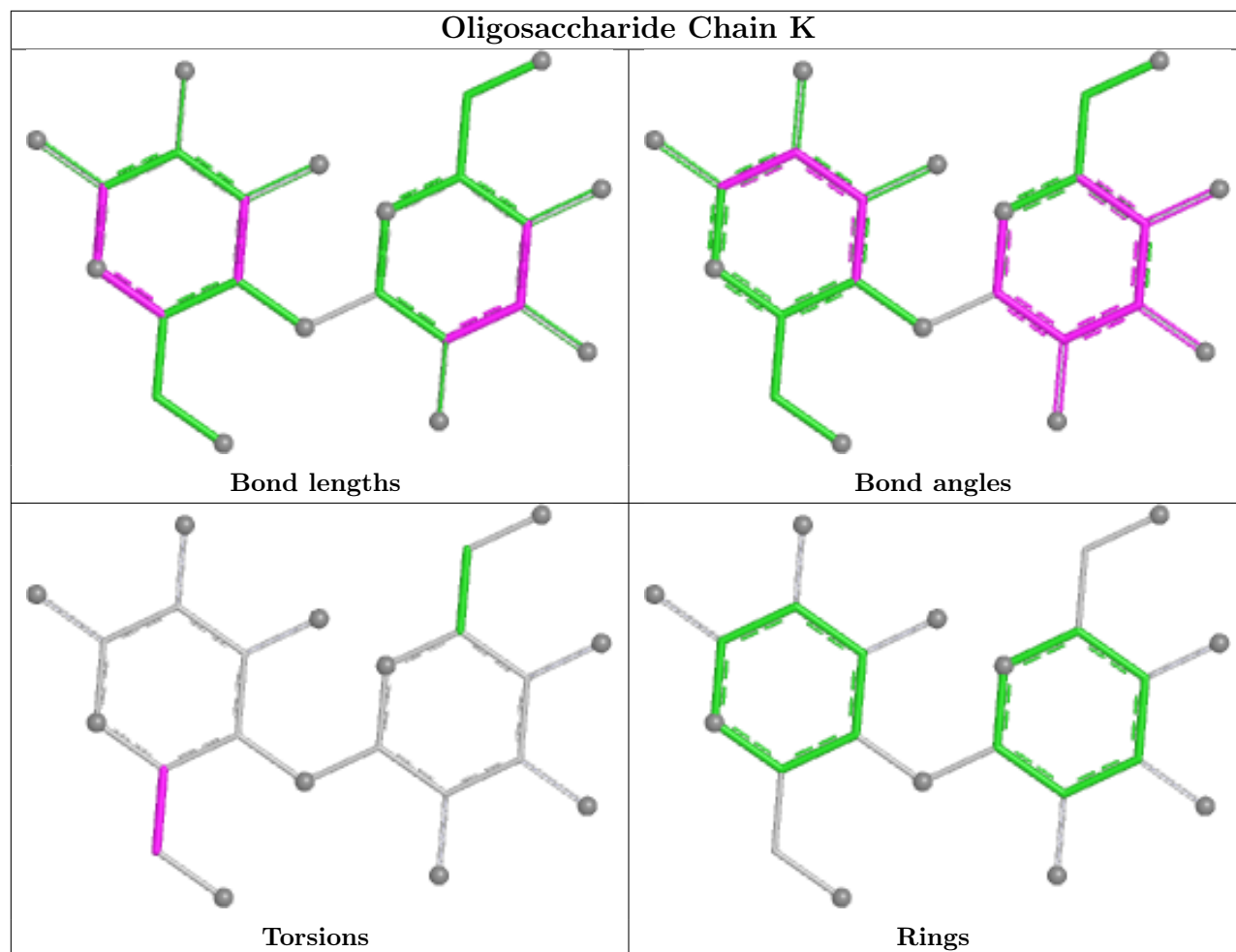


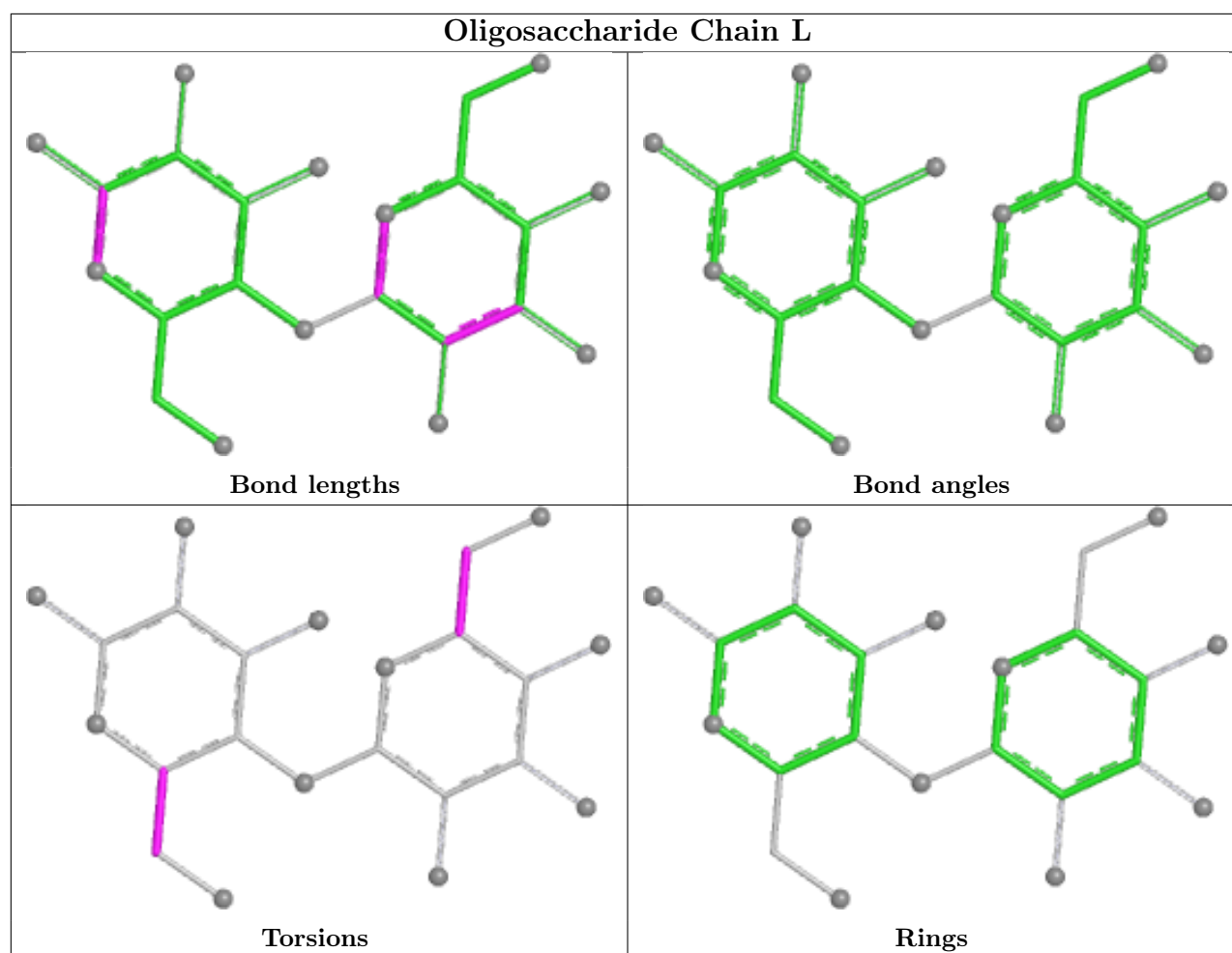












5.6 Ligand geometry [i](#)

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	A	1203	-	10,10,10	6.38	8 (80%)	13,14,14	3.49	8 (61%)
6	PO4	A	1202	-	4,4,4	2.56	2 (50%)	6,6,6	0.59	0
7	BXY	B	1203	-	10,10,10	5.05	7 (70%)	13,14,14	2.32	5 (38%)
7	BXY	A	1204	-	10,10,10	2.78	5 (50%)	13,14,14	1.80	3 (23%)
7	BXY	B	1204	-	10,10,10	3.61	7 (70%)	13,14,14	1.46	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	B	1202	-	4,4,4	2.59	2 (50%)	6,6,6	0.49	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	1203	-	-	2/2/18/18	0/1/1/1
7	BXY	B	1204	-	-	2/2/18/18	0/1/1/1
7	BXY	A	1204	-	-	0/2/18/18	0/1/1/1
7	BXY	B	1203	-	-	1/2/18/18	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1203	BXY	C1-C2	-12.78	1.38	1.52
7	B	1203	BXY	C1-C2	-12.70	1.38	1.52
7	A	1203	BXY	O4-C1	-8.75	1.32	1.43
7	B	1204	BXY	C1-C2	-7.52	1.44	1.52
7	A	1203	BXY	C3-C4	-6.69	1.36	1.53
7	A	1203	BXY	O2-C2	-6.40	1.27	1.43
7	B	1203	BXY	O4-C1	-5.93	1.35	1.43
7	A	1203	BXY	O4-C4	-5.48	1.32	1.45
7	B	1204	BXY	O4-C1	-4.84	1.37	1.43
7	A	1203	BXY	C2-C3	-4.76	1.40	1.53
7	A	1204	BXY	O4-C4	-4.67	1.34	1.45
7	B	1203	BXY	O2-C2	-4.55	1.31	1.43
7	B	1204	BXY	O4-C4	-4.40	1.35	1.45
6	B	1202	PO4	P-O1	4.28	1.60	1.50
6	A	1202	PO4	P-O1	4.25	1.60	1.50
7	A	1204	BXY	O4-C1	-3.78	1.38	1.43
7	A	1204	BXY	O3-C3	-3.77	1.33	1.43
7	A	1203	BXY	O1-C1	-3.59	1.28	1.39
7	A	1203	BXY	O3-C3	-3.55	1.34	1.43
7	B	1203	BXY	O4-C4	-3.15	1.38	1.45
7	B	1203	BXY	O1-C1	-3.08	1.29	1.39
7	A	1204	BXY	O2-C2	-3.03	1.35	1.43
7	A	1204	BXY	C3-C4	-2.91	1.45	1.53
7	B	1203	BXY	C3-C4	-2.86	1.45	1.53
7	B	1204	BXY	O3-C3	-2.79	1.36	1.43
7	B	1204	BXY	C3-C4	-2.78	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1204	BXY	O2-C2	-2.70	1.36	1.43
7	B	1203	BXY	O3-C3	-2.65	1.36	1.43
7	B	1204	BXY	C2-C3	-2.44	1.46	1.53
6	B	1202	PO4	P-O3	2.05	1.60	1.54
6	A	1202	PO4	P-O4	2.01	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	-6.90	89.27	102.61
7	A	1203	BXY	O1-C1-O4	-6.51	102.82	111.12
7	B	1203	BXY	C1-C2-C3	-4.76	96.44	102.29
7	A	1203	BXY	O4-C4-C5	4.69	119.13	109.22
7	A	1203	BXY	C1-C2-C3	-3.88	97.52	102.29
7	A	1204	BXY	O1-C1-O4	-3.55	106.60	111.12
7	B	1203	BXY	O3-C3-C4	-3.43	101.22	111.08
7	A	1204	BXY	O5-C5-C4	-3.15	100.62	111.33
7	B	1203	BXY	O1-C1-O4	-3.09	107.19	111.12
7	B	1204	BXY	O4-C4-C5	2.89	115.33	109.22
7	A	1203	BXY	O5-C5-C4	-2.82	101.73	111.33
7	B	1203	BXY	C2-C3-C4	-2.79	97.22	102.61
7	B	1203	BXY	O2-C2-C1	-2.75	104.20	111.85
7	A	1203	BXY	O4-C4-C3	-2.71	99.77	105.15
7	A	1203	BXY	O1-C1-C2	-2.57	98.46	110.25
7	A	1204	BXY	O2-C2-C3	-2.25	104.62	111.82
7	B	1204	BXY	O2-C2-C1	-2.24	105.60	111.85
7	A	1203	BXY	O2-C2-C1	-2.12	105.95	111.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

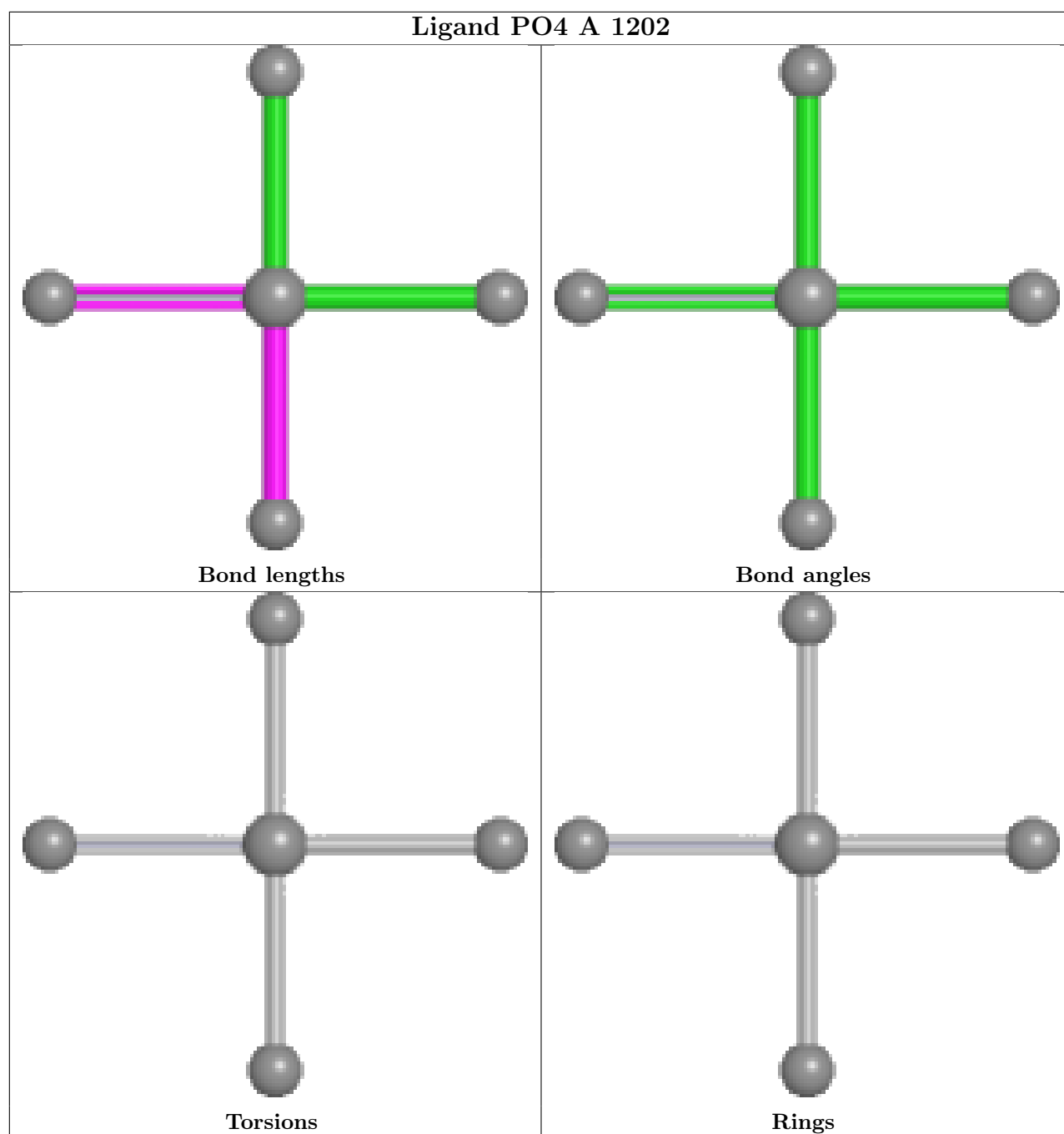
Mol	Chain	Res	Type	Atoms
7	B	1204	BXY	O4-C4-C5-O5
7	B	1204	BXY	C3-C4-C5-O5
7	A	1203	BXY	O4-C4-C5-O5
7	A	1203	BXY	C3-C4-C5-O5
7	B	1203	BXY	O4-C4-C5-O5

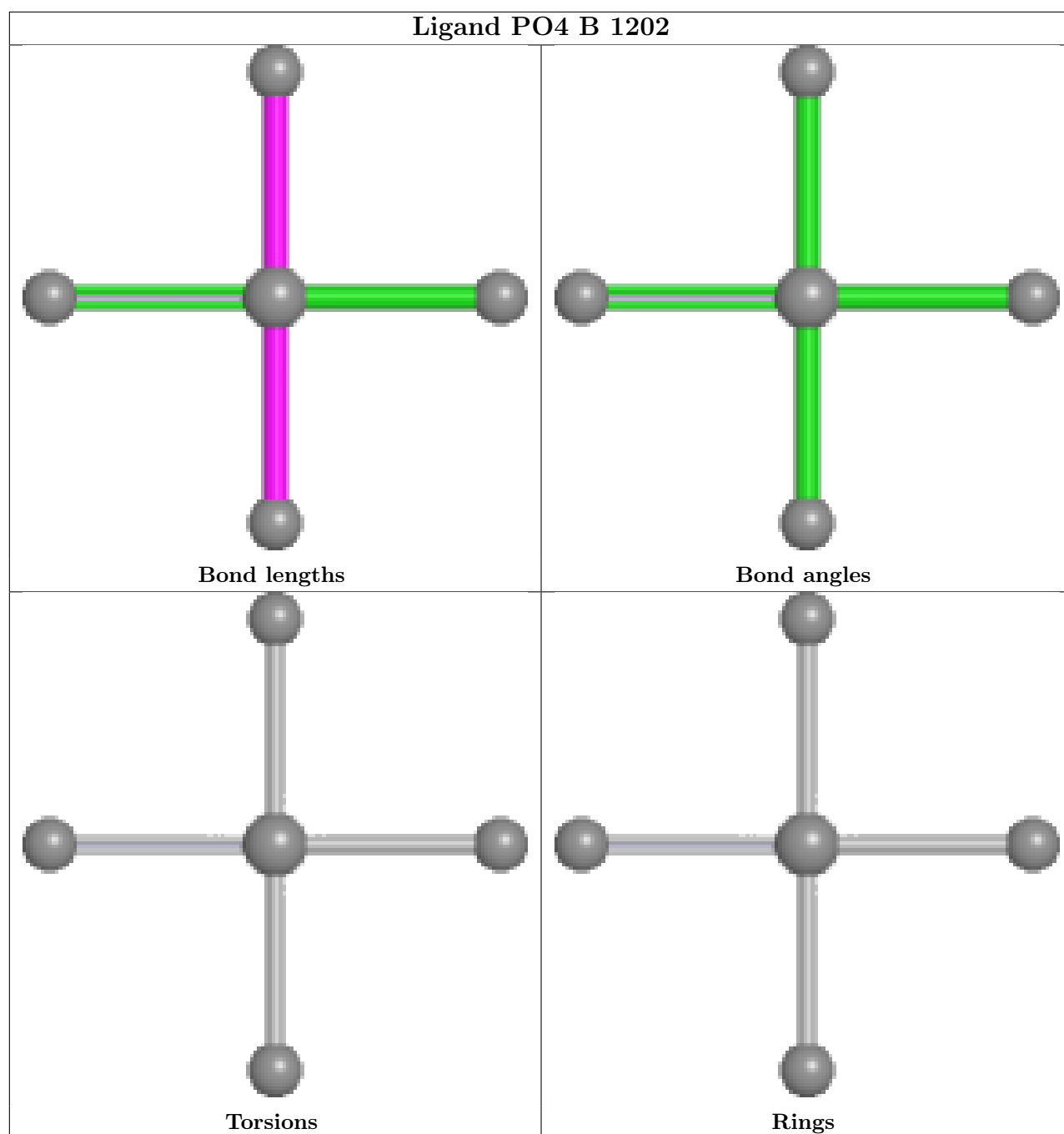
There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1203	BXY	2	0
7	A	1204	BXY	2	0
7	B	1204	BXY	13	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%)	1.07	221 (21%)  	4, 68, 160, 198	0
1	B	1035/1113 (92%)	1.12	233 (22%)  	5, 68, 173, 221	0
2	C	84/99 (84%)	1.49	19 (22%)  	44, 82, 125, 147	0
2	D	84/99 (84%)	1.24	13 (15%)  	45, 87, 126, 144	0
All	All	2238/2424 (92%)	1.12	486 (21%)  	4, 71, 164, 221	0

All (486) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	LEU	10.7
1	B	249	LEU	9.2
1	B	127	SER	9.0
1	A	40	GLN	8.6
1	A	291	GLU	7.3
1	B	163	ASP	7.2
1	A	67	ASP	7.0
1	B	110	GLU	6.7
1	B	111	ARG	6.5
1	B	171	ARG	6.4
1	B	113	ASN	6.4
1	B	115	ASP	6.3
1	B	164	ASP	6.2
1	A	250	PRO	6.2
1	B	117	THR	6.2
1	A	756	GLN	6.1
1	A	1062	ARG	6.0
1	A	1061	THR	6.0
1	A	915	SER	6.0
1	A	82	GLY	5.9
1	B	253	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	291	GLU	5.9
1	A	916	ILE	5.8
1	B	293	ALA	5.8
1	B	170	VAL	5.8
1	A	135	SER	5.7
1	B	712	TYR	5.7
1	B	1059	THR	5.7
1	B	873	GLN	5.6
1	B	292	HIS	5.5
1	A	677	PRO	5.4
1	A	912	PRO	5.4
1	B	242	GLY	5.2
1	B	778	ASP	5.2
1	B	680	ARG	5.2
1	B	246	LYS	5.2
1	B	209	SER	5.2
2	C	62	GLU	5.2
1	B	250	PRO	5.1
1	B	42	THR	5.1
1	B	10	SER	5.1
1	A	75	GLN	5.1
1	B	152	GLY	5.1
1	B	214	LEU	5.1
1	A	146	HIS	5.0
1	B	159	GLN	5.0
1	B	82	GLY	5.0
1	A	253	TRP	5.0
1	B	932	LEU	4.9
1	B	777	ALA	4.9
2	C	77	ILE	4.8
1	A	914	SER	4.8
1	B	81	VAL	4.8
1	A	779	PRO	4.8
1	B	776	SER	4.7
1	B	84	GLU	4.7
1	A	280	ASP	4.7
1	B	1057	LEU	4.6
1	B	240	ALA	4.5
1	A	145	ALA	4.5
1	B	172	GLY	4.5
1	B	1075	HIS	4.4
1	A	1060	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	675	ASP	4.4
1	B	161	PRO	4.4
1	B	294	GLY	4.4
1	B	215	LEU	4.4
2	C	14	GLU	4.4
1	A	895	ILE	4.4
1	B	674	PRO	4.4
1	B	153	GLU	4.3
1	B	140	TYR	4.3
1	B	892	GLY	4.3
1	A	999	GLU	4.3
1	A	775	VAL	4.3
1	B	142	THR	4.2
1	B	112	ILE	4.2
1	B	128	ALA	4.2
1	A	246	LYS	4.1
1	A	251	SER	4.1
1	B	254	TRP	4.1
1	B	881	ALA	4.1
1	B	85	ASN	4.1
1	B	14	THR	4.1
1	A	293	ALA	4.0
1	B	838	SER	4.0
1	A	163	ASP	4.0
1	A	899	ASP	4.0
1	B	774	ASP	4.0
1	A	48	PRO	3.9
1	A	676	ARG	3.9
1	B	154	PHE	3.9
1	B	126	VAL	3.9
1	A	49	GLN	3.9
1	A	1021	ARG	3.9
1	A	144	THR	3.9
1	A	894	SER	3.9
1	B	134	LEU	3.9
1	B	981	TYR	3.8
1	B	891	PRO	3.8
1	A	85	ASN	3.8
1	B	952	GLN	3.8
1	B	173	GLU	3.8
1	B	935	GLN	3.7
1	A	292	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1056	ASP	3.7
2	C	86	GLU	3.7
1	A	38	VAL	3.7
1	A	1023	SER	3.7
1	B	673	SER	3.7
2	C	85	PRO	3.7
2	D	3	ALA	3.7
1	B	11	ASN	3.7
1	B	996	PHE	3.7
1	A	164	ASP	3.6
1	B	1062	ARG	3.6
1	A	216	LYS	3.6
1	B	156	GLY	3.6
1	B	669	GLY	3.6
1	A	244	ARG	3.6
1	A	933	ALA	3.6
1	A	752	GLU	3.6
1	A	671	ASP	3.6
1	B	52	VAL	3.6
1	A	214	LEU	3.6
1	B	83	PRO	3.5
1	A	51	GLY	3.5
1	B	193	PRO	3.5
1	A	858	GLN	3.5
1	B	929	ASP	3.5
1	B	168	GLU	3.5
1	B	135	SER	3.5
1	B	686	VAL	3.5
1	A	995	ARG	3.5
1	B	684	LEU	3.5
1	A	840	THR	3.4
1	B	89	SER	3.4
1	A	318	ALA	3.4
1	A	835	SER	3.4
1	B	957	SER	3.4
1	A	176	GLY	3.4
1	B	890	GLU	3.4
1	A	980	ARG	3.4
2	C	64	LEU	3.4
1	B	109	ILE	3.4
1	A	125	VAL	3.3
1	A	670	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	149	LYS	3.3
1	B	169	ALA	3.3
1	A	880	TRP	3.3
1	B	831	PRO	3.3
1	B	41	THR	3.3
1	A	766	PHE	3.3
1	B	766	PHE	3.3
1	A	817	SER	3.3
1	A	54	GLN	3.3
1	B	754	ALA	3.3
1	A	148	ASP	3.3
1	A	932	LEU	3.3
1	B	160	GLY	3.3
1	A	451	SER	3.2
1	A	1046	TRP	3.2
1	B	53	TRP	3.2
1	B	683	ARG	3.2
1	A	1063	SER	3.2
1	B	75	GLN	3.2
1	A	254	TRP	3.2
1	A	66	THR	3.2
1	A	206	THR	3.2
1	A	861	PRO	3.2
1	A	247	ARG	3.2
1	B	872	ASP	3.2
1	A	240	ALA	3.2
1	A	811	ALA	3.2
1	A	248	PHE	3.2
1	B	87	ASN	3.1
1	B	885	GLN	3.1
1	A	69	THR	3.1
1	A	887	ALA	3.1
1	A	935	GLN	3.1
1	B	859	ALA	3.1
1	A	237	LEU	3.1
1	A	290	SER	3.1
1	A	673	SER	3.1
1	B	131	GLU	3.1
1	A	996	PHE	3.1
1	B	114	ASN	3.1
1	A	859	ALA	3.1
1	B	979	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	24	LEU	3.1
1	B	845	VAL	3.1
1	B	49	GLN	3.1
1	B	770	GLY	3.1
1	A	150	VAL	3.1
1	A	761	VAL	3.1
1	A	136	PRO	3.1
1	A	771	ILE	3.1
1	A	81	VAL	3.0
1	A	1066	TRP	3.0
1	A	1031	ASP	3.0
1	B	145	ALA	3.0
1	B	841	GLN	3.0
1	B	882	THR	3.0
1	A	453	PHE	3.0
1	A	47	TRP	3.0
1	B	752	GLU	3.0
1	B	670	ARG	3.0
1	A	161	PRO	3.0
1	A	193	PRO	3.0
1	A	10	SER	3.0
1	A	888	ALA	3.0
1	B	43	ALA	3.0
1	A	748	THR	3.0
1	A	674	PRO	3.0
1	B	915	SER	3.0
1	B	137	ASP	3.0
1	B	883	ASP	3.0
1	A	997	GLY	3.0
1	A	841	GLN	3.0
1	A	890	GLU	2.9
1	B	197	GLY	2.9
2	C	58	LYS	2.9
1	A	753	PRO	2.9
1	B	147	ALA	2.9
1	A	18	VAL	2.9
1	B	51	GLY	2.9
1	A	925	LEU	2.9
1	A	15	ALA	2.9
1	B	672	VAL	2.9
2	D	86	GLU	2.9
1	A	16	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	17	LEU	2.9
1	B	17	LEU	2.9
1	A	12	HIS	2.8
1	B	308	SER	2.8
2	D	30	GLU	2.8
1	B	980	ARG	2.8
1	A	860	GLY	2.8
1	A	55	SER	2.8
1	A	778	ASP	2.8
1	B	999	GLU	2.8
1	A	1030	LYS	2.8
1	B	80	LEU	2.8
1	A	239	CYS	2.8
1	A	159	GLN	2.8
1	B	78	ALA	2.8
2	C	75	ALA	2.8
1	B	166	PRO	2.8
1	B	247	ARG	2.8
1	A	134	LEU	2.8
1	A	758	LEU	2.8
1	B	1064	GLY	2.8
1	A	321	ALA	2.8
1	A	873	GLN	2.8
1	A	922	GLN	2.8
1	A	139	ARG	2.8
1	A	891	PRO	2.8
1	B	201	SER	2.8
1	B	775	VAL	2.8
1	A	39	GLU	2.8
1	B	1066	TRP	2.8
2	D	36	ASP	2.8
1	A	898	GLY	2.8
2	D	34	VAL	2.8
1	A	923	ILE	2.8
1	B	750	ILE	2.8
1	A	1065	TRP	2.7
1	A	241	ASP	2.7
1	A	994	ASP	2.7
1	A	764	LEU	2.7
1	B	248	PHE	2.7
1	B	295	TYR	2.7
1	A	768	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	203	THR	2.7
1	A	1033	TRP	2.7
1	B	818	ARG	2.7
1	A	1034	TYR	2.7
1	B	828	ALA	2.7
1	B	129	PRO	2.7
1	A	138	CYS	2.7
1	A	41	THR	2.7
1	B	820	ARG	2.7
2	D	61	ASP	2.7
1	A	52	VAL	2.7
1	B	116	LEU	2.7
1	B	1068	PRO	2.7
1	B	852	ARG	2.7
1	B	668	SER	2.7
1	B	481	ALA	2.7
1	B	760	ALA	2.7
1	A	137	ASP	2.7
1	A	11	ASN	2.7
1	A	50	ASN	2.7
1	A	842	GLN	2.6
2	D	59	ILE	2.6
1	B	244	ARG	2.6
1	B	252	ARG	2.6
1	A	196	GLU	2.6
1	A	919	GLU	2.6
1	A	71	THR	2.6
1	A	672	VAL	2.6
1	B	811	ALA	2.6
1	B	920	ALA	2.6
1	B	933	ALA	2.6
1	A	750	ILE	2.6
1	A	814	ILE	2.6
1	B	136	PRO	2.6
1	B	815	ASN	2.6
1	B	843	PRO	2.6
1	B	466	GLY	2.6
1	A	862	LEU	2.6
1	B	681	TRP	2.6
1	A	83	PRO	2.6
1	B	682	GLN	2.6
1	B	931	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	130	LEU	2.6
1	B	141	LEU	2.6
1	A	140	TYR	2.6
1	A	195	PRO	2.6
1	B	677	PRO	2.6
2	C	78	GLN	2.6
1	B	167	GLY	2.6
1	A	245	HIS	2.6
1	B	211	SER	2.6
1	B	132	GLN	2.6
1	A	165	ASP	2.6
1	A	56	VAL	2.6
1	A	252	ARG	2.6
1	A	201	SER	2.5
1	B	858	GLN	2.5
1	B	479	LEU	2.5
1	A	777	ALA	2.5
1	A	1028	TYR	2.5
1	B	1034	TYR	2.5
1	B	138	CYS	2.5
1	B	79	GLY	2.5
1	B	751	GLY	2.5
1	A	837	ARG	2.5
1	A	68	LEU	2.5
1	B	922	GLN	2.5
1	B	1051	GLN	2.5
1	B	769	ASN	2.5
1	B	151	THR	2.5
1	B	97	LYS	2.5
1	A	765	GLY	2.5
1	B	21	ILE	2.5
1	B	162	ASP	2.5
1	A	818	ARG	2.5
1	B	934	PRO	2.5
1	A	874	GLY	2.5
1	B	289	VAL	2.5
1	A	191	SER	2.4
1	B	884	GLU	2.4
1	B	178	ASP	2.4
2	C	79	LYS	2.4
1	A	19	ALA	2.4
1	B	1000	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	46	GLU	2.4
1	A	221	ILE	2.4
1	A	749	PRO	2.4
1	A	242	GLY	2.4
1	B	727	GLY	2.4
1	B	823	TYR	2.4
1	B	86	ARG	2.4
1	A	877	GLU	2.4
1	B	773	SER	2.4
1	A	892	GLY	2.4
1	B	765	GLY	2.4
1	A	754	ALA	2.4
1	B	844	ALA	2.4
1	A	44	GLU	2.4
1	B	39	GLU	2.4
1	B	44	GLU	2.4
1	A	1039	SER	2.4
1	A	1022	PRO	2.4
1	B	1065	TRP	2.4
1	B	15	ALA	2.3
1	B	835	SER	2.3
1	B	880	TRP	2.3
1	B	860	GLY	2.3
2	D	35	ASP	2.3
1	B	953	GLU	2.3
1	A	450	VAL	2.3
1	A	37	PRO	2.3
1	A	820	ARG	2.3
1	B	713	PRO	2.3
1	A	819	ALA	2.3
1	B	290	SER	2.3
1	A	863	LEU	2.3
1	A	84	GLU	2.3
2	C	70	VAL	2.3
1	A	53	TRP	2.3
1	B	958	SER	2.3
1	A	238	ASP	2.3
1	B	756	GLN	2.3
1	B	462	ILE	2.3
2	C	59	ILE	2.3
1	A	327	SER	2.3
1	B	40	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	678	GLN	2.3
1	B	104	ASP	2.3
1	A	911	ALA	2.2
1	A	42	THR	2.2
1	B	936	HIS	2.2
1	B	149	LYS	2.2
2	D	58	LYS	2.2
1	B	761	VAL	2.2
1	A	20	ILE	2.2
1	A	112	ILE	2.2
1	B	204	ILE	2.2
1	A	757	ALA	2.2
1	A	151	THR	2.2
1	A	13	ARG	2.2
1	B	837	ARG	2.2
1	B	125	VAL	2.2
2	C	27	VAL	2.2
2	C	57	VAL	2.2
1	A	875	GLU	2.2
1	A	751	GLY	2.2
1	B	69	THR	2.2
1	A	773	SER	2.2
1	B	199	GLN	2.2
1	A	21	ILE	2.2
1	B	32	ALA	2.2
1	B	671	ASP	2.2
1	A	86	ARG	2.2
2	C	34	VAL	2.2
1	A	958	SER	2.2
1	A	1051	GLN	2.2
1	A	881	ALA	2.2
1	B	675	ASP	2.2
1	A	836	TRP	2.2
1	A	896	THR	2.1
1	B	923	ILE	2.1
1	A	202	ALA	2.1
2	D	62	GLU	2.1
1	B	646	GLY	2.1
1	B	813	GLY	2.1
2	C	60	PRO	2.1
1	A	931	ASP	2.1
1	B	832	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	158	THR	2.1
1	B	210	THR	2.1
1	B	771	ILE	2.1
1	B	879	GLN	2.1
1	A	287	ALA	2.1
1	A	168	GLU	2.1
1	A	143	PHE	2.1
1	B	143	PHE	2.1
1	A	774	ASP	2.1
1	B	150	VAL	2.1
1	B	245	HIS	2.1
1	A	1044	THR	2.1
1	B	478	THR	2.1
1	B	758	LEU	2.1
1	B	1061	THR	2.1
1	A	882	THR	2.1
1	A	23	GLY	2.1
1	A	816	GLY	2.1
1	B	133	VAL	2.1
2	C	54	LYS	2.1
1	A	1057	LEU	2.1
1	A	979	HIS	2.1
1	B	196	GLU	2.1
2	C	81	GLU	2.1
1	A	848	SER	2.0
1	A	78	ALA	2.0
1	A	712	TYR	2.0
1	B	205	ASP	2.0
1	B	816	GLY	2.0
1	A	904	PRO	2.0
1	B	155	VAL	2.0
1	B	924	ARG	2.0
1	B	1055	LEU	2.0
1	A	936	HIS	2.0
2	C	65	ALA	2.0
1	B	165	ASP	2.0
2	D	38	ASP	2.0
1	A	893	GLY	2.0
1	B	834	GLY	2.0
1	A	212	PRO	2.0
1	B	484	GLN	2.0
1	A	70	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	348	GLU	2.0
1	B	833	LEU	2.0
2	D	12	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

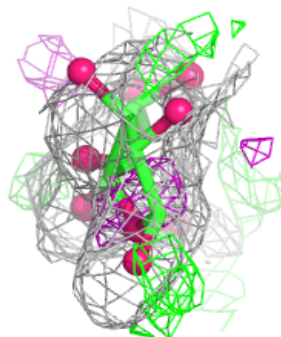
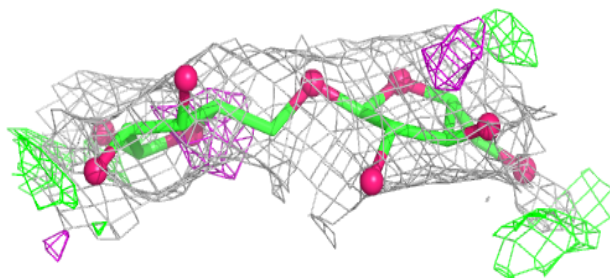
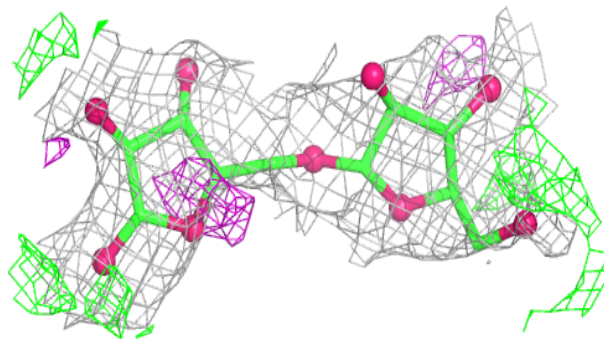
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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

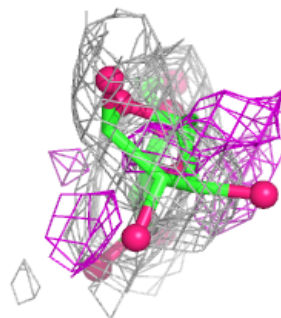
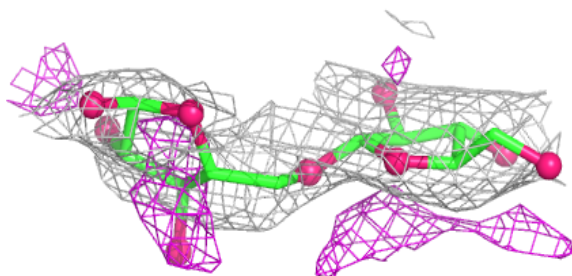
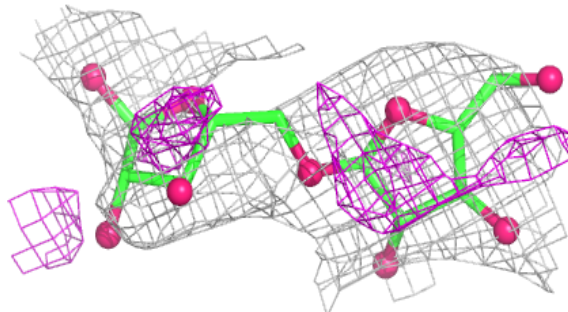
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

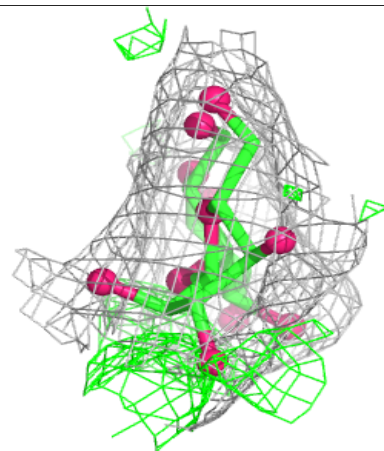
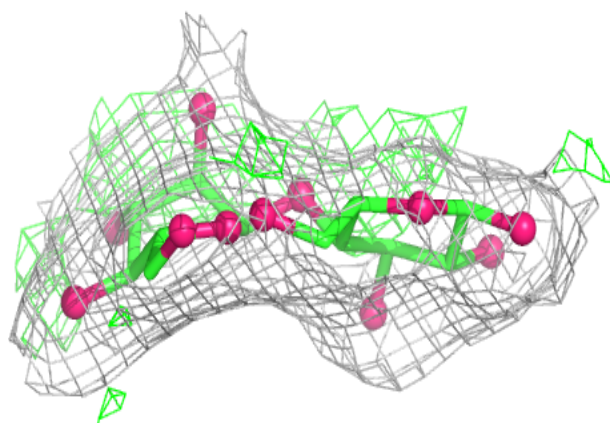
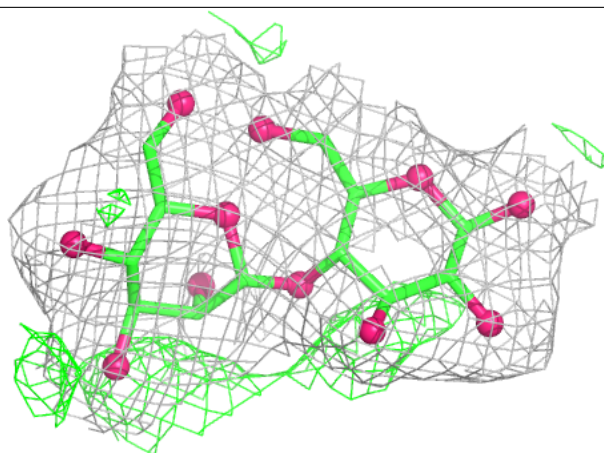
**Electron density around Chain J:**

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

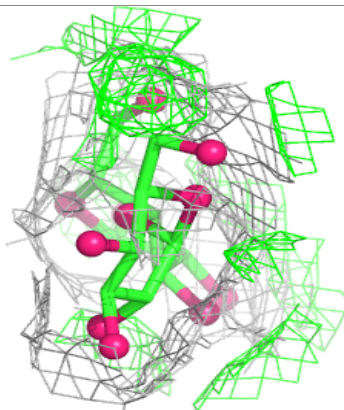
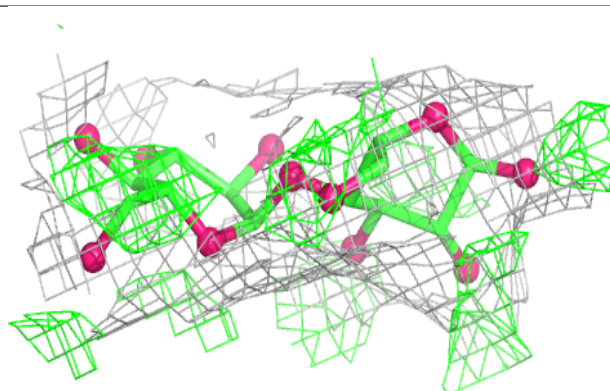
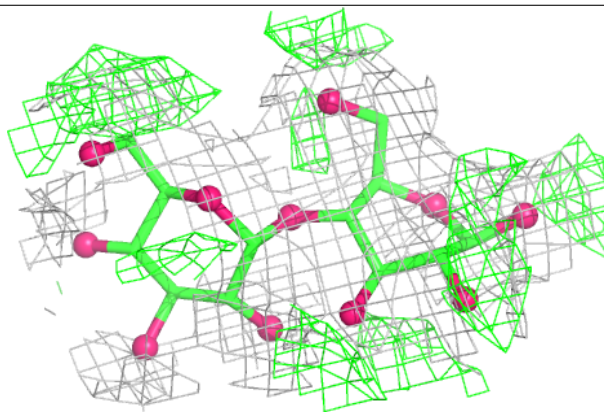


Electron density around Chain F:

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

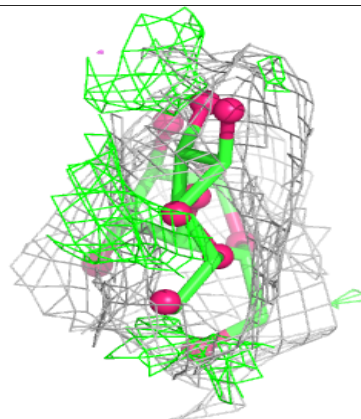
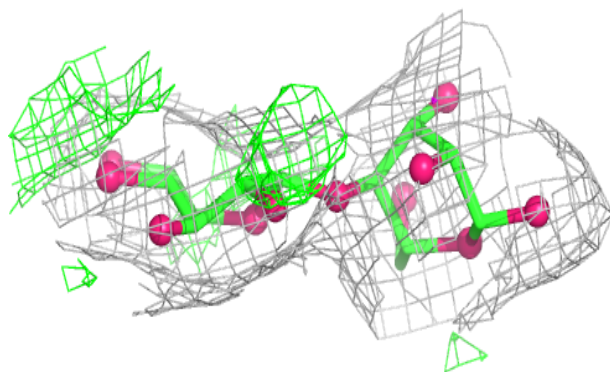
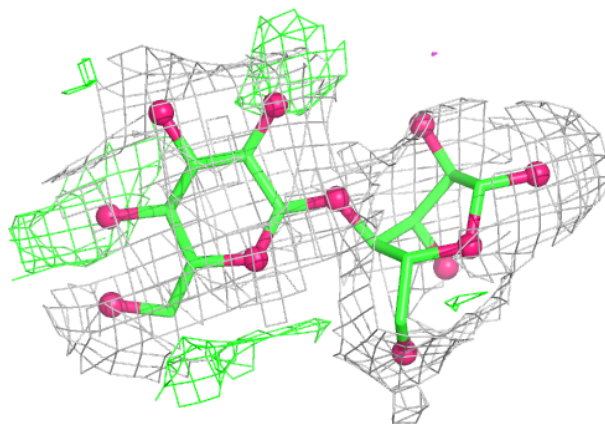
**Electron density around Chain G:**

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



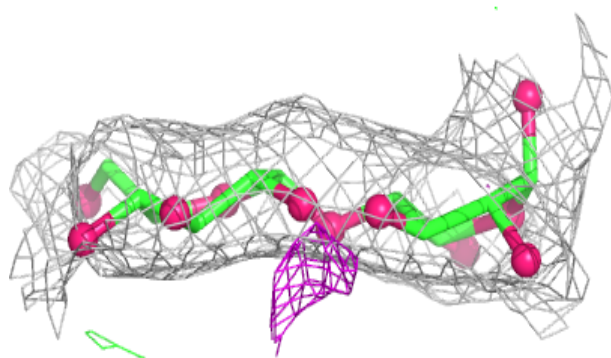
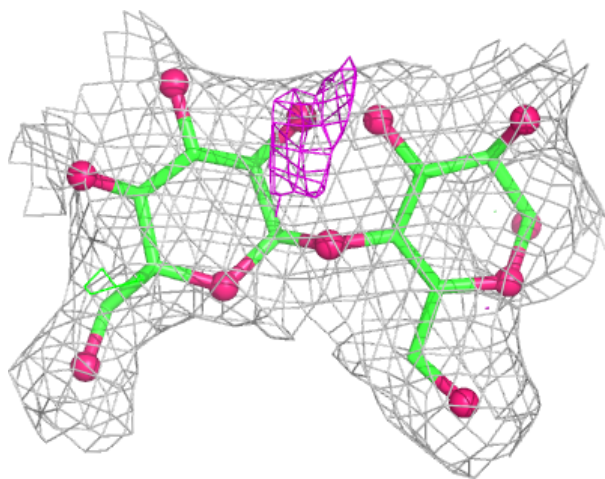
Electron density around Chain H:

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



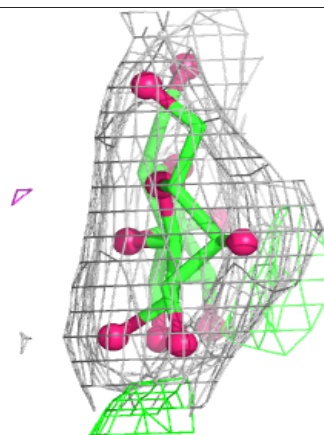
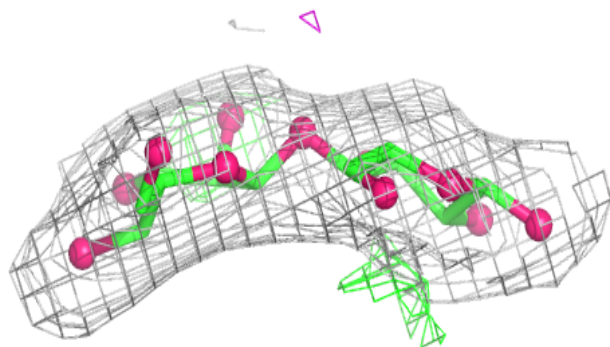
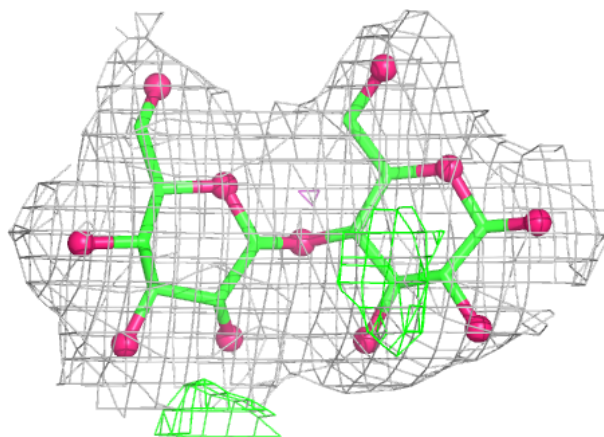
Electron density around Chain I:

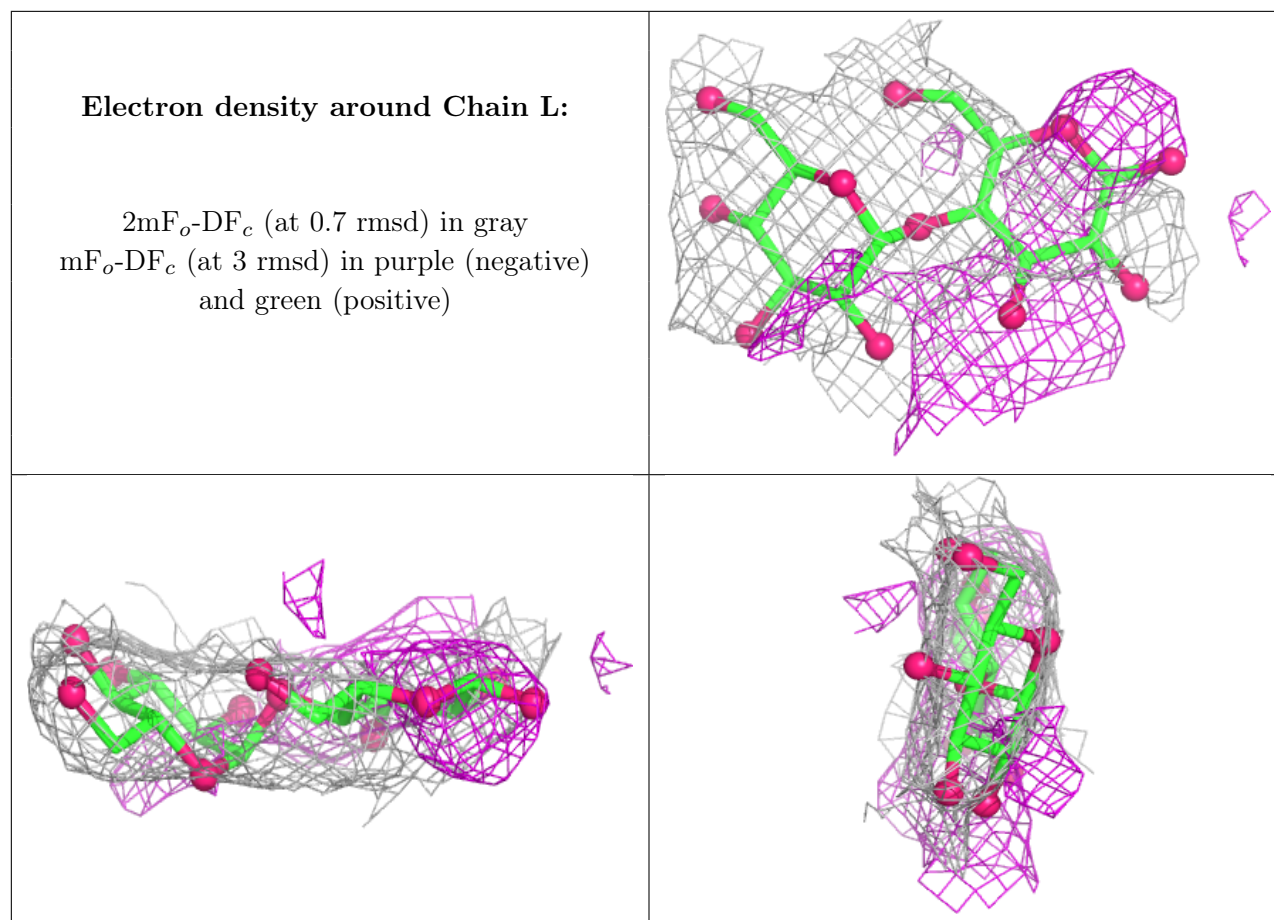
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.

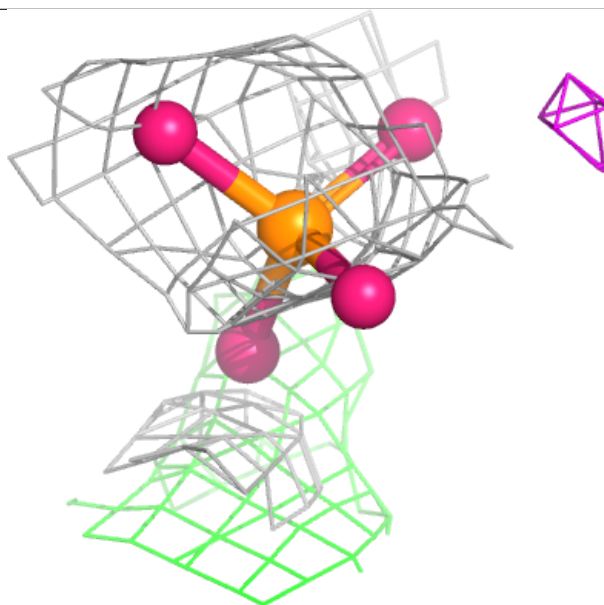
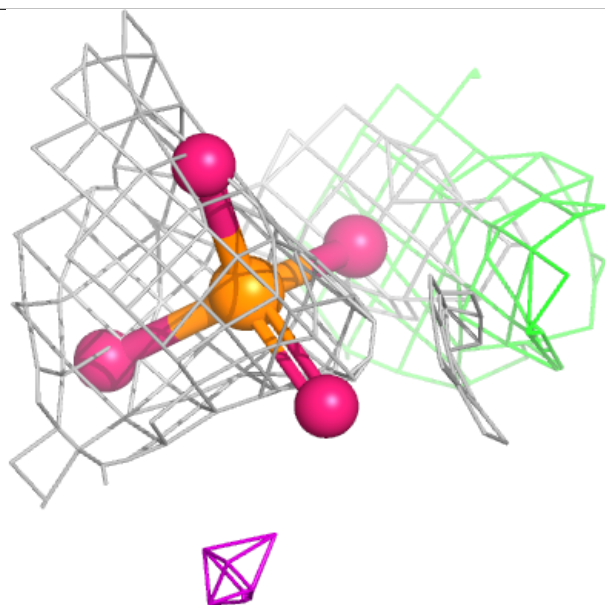
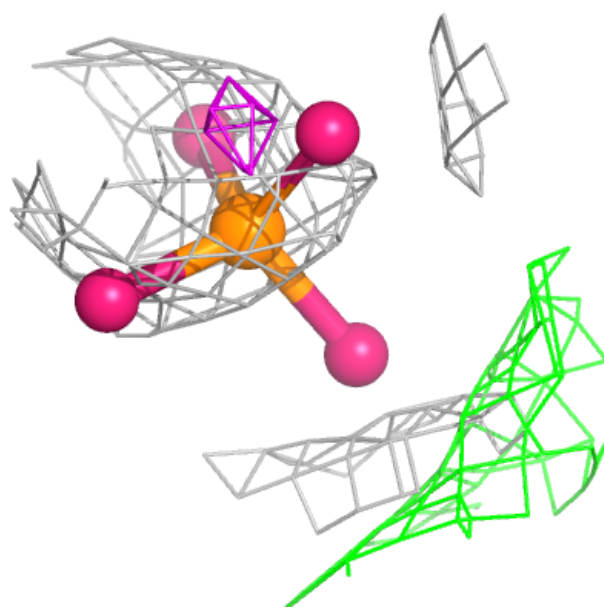
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BXY	B	1203	10/10	0.69	0.27	82,84,85,86	0
6	PO4	B	1202	5/5	0.70	0.38	150,153,153,157	0
7	BXY	A	1204	10/10	0.77	0.17	92,95,98,102	0
7	BXY	B	1204	10/10	0.80	0.16	106,111,113,114	0
6	PO4	A	1202	5/5	0.82	0.35	159,159,160,162	0
7	BXY	A	1203	10/10	0.84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

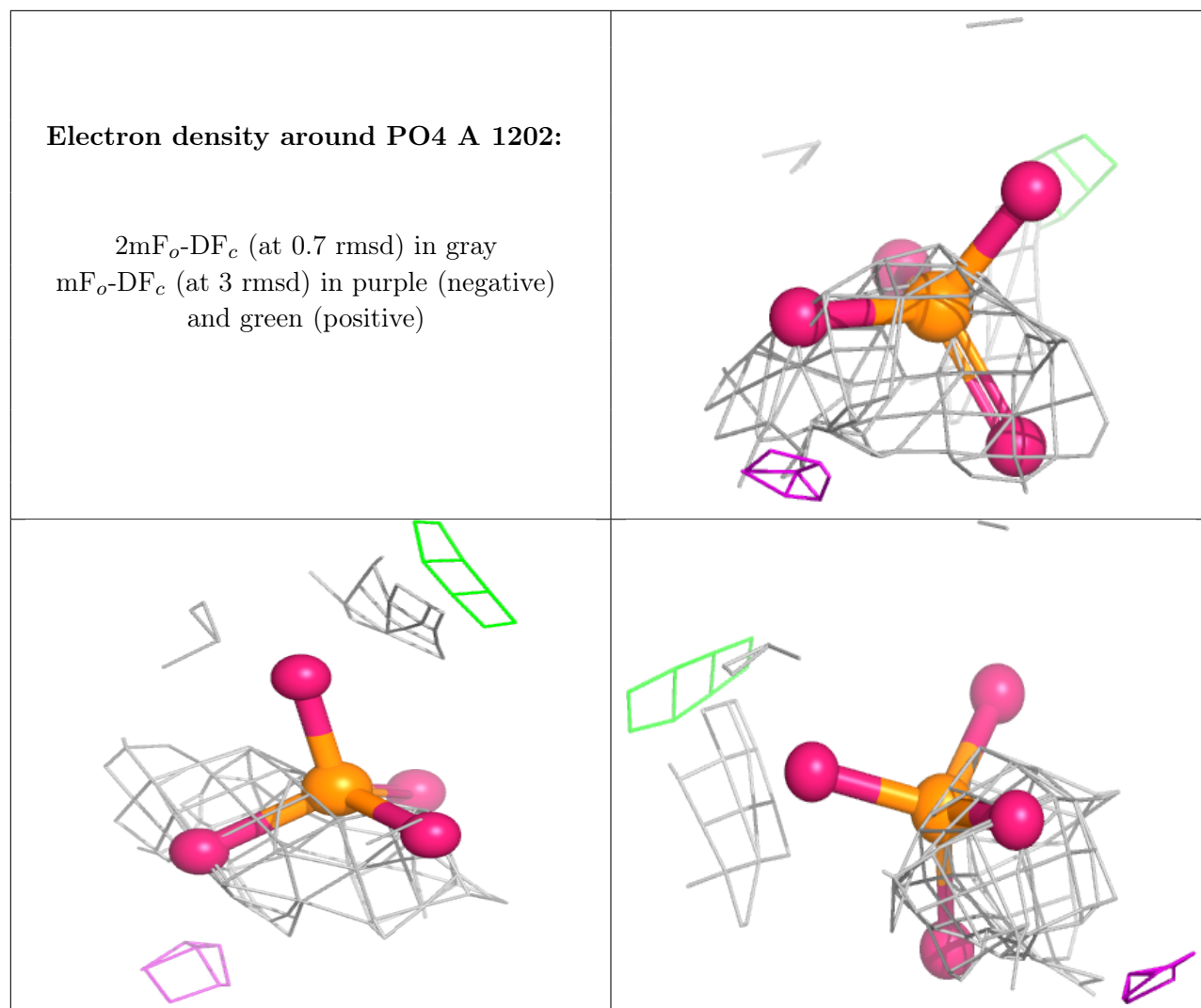
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

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.