



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:57 AM BST

PDB ID : 3T6X
Title : Crystal Structure of *Steccherinum ochraceum* Laccase obtained by multi-crystals composite data collection technique (20% dose)
Authors : Ferraroni, M.; Briganti, F.; Matera, I.; Kolomytseva, M.; Golovleva, L.; Scozzafava, A.; Chernykh, A.M.
Deposited on : 2011-07-29
Resolution : 2.15 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 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 : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

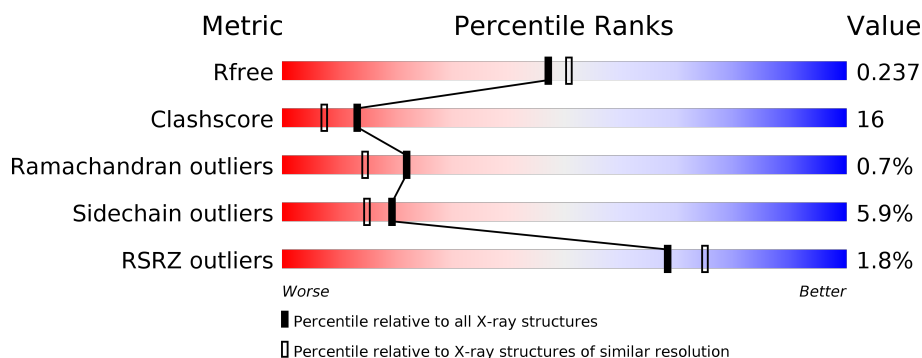
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	495	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	495	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
1	C	495	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
2	D	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%

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
2	NAG	G	2	-	-	-	X
4	SO4	B	506	-	-	X	-
4	SO4	C	505	-	-	X	-
5	GOL	A	508	-	-	X	-
5	GOL	B	508	-	-	X	-
5	GOL	C	506	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12916 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 Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	5	0
			3734	2360	626	729	19			
1	B	495	Total	C	N	O	S	0	5	0
			3728	2357	629	724	18			
1	C	495	Total	C	N	O	S	0	3	0
			3725	2354	629	725	17			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cu	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	0
			4	4		
3	C	4	Total	Cu	0	0
			4	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



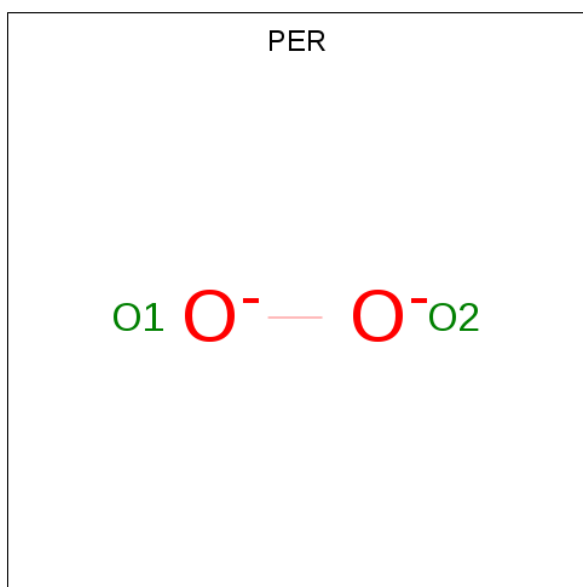
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



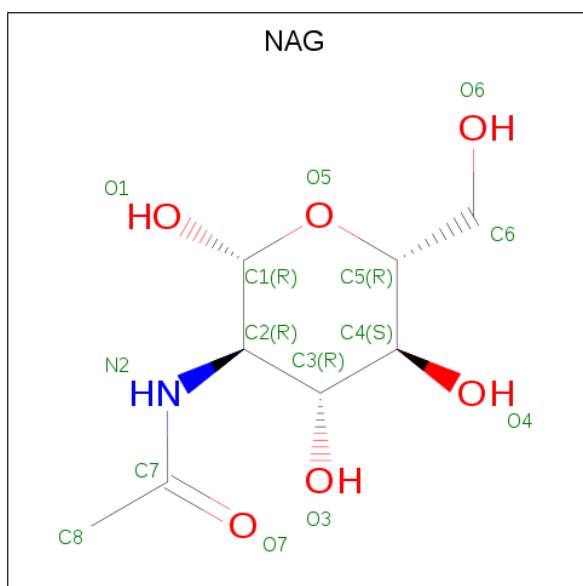
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	C	1	Total O 2 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

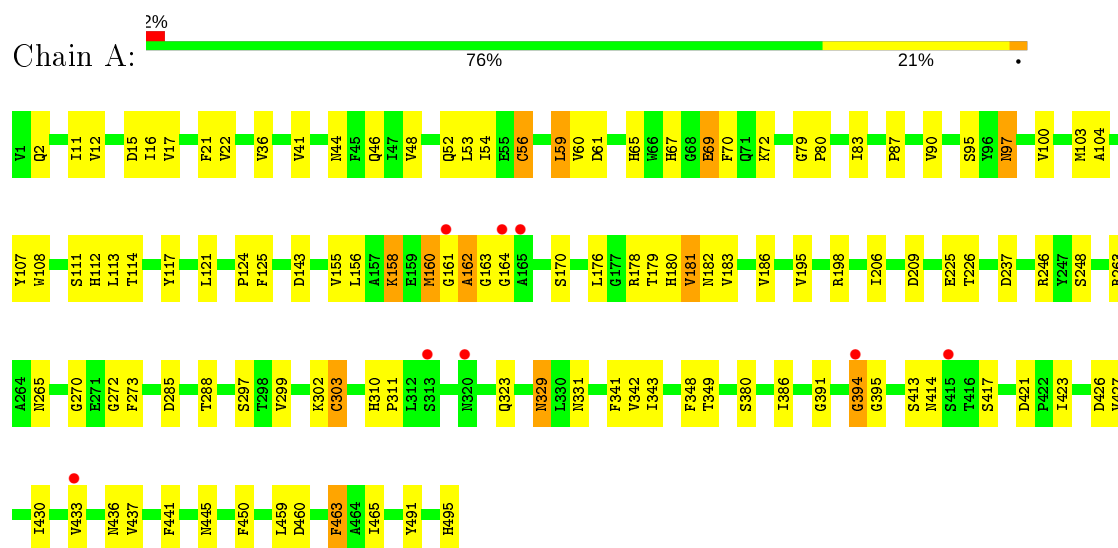
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	531	Total	O	0	0
			531	531		
8	B	465	Total	O	0	0
			465	465		
8	C	478	Total	O	0	0
			478	478		

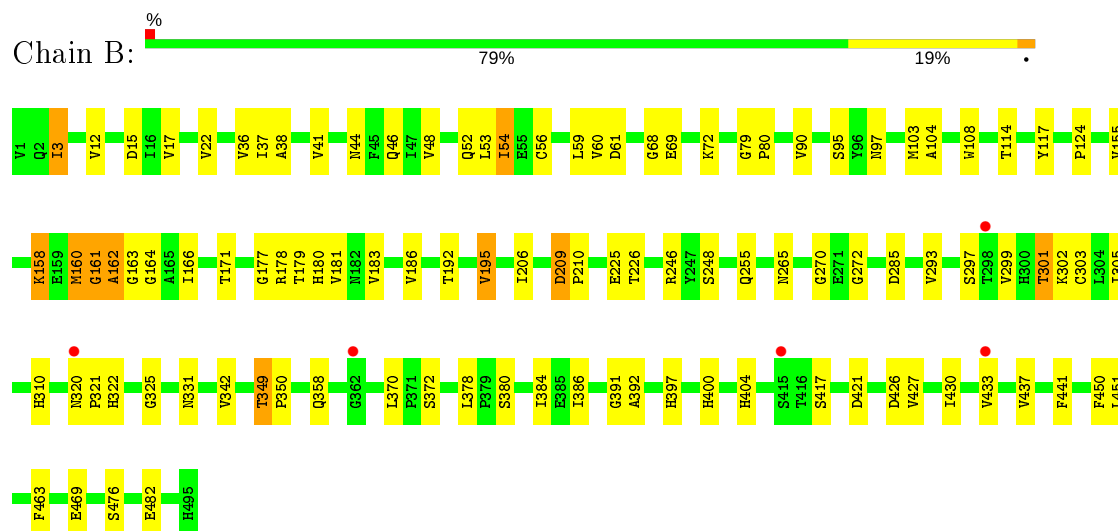
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

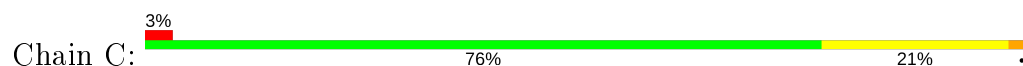
• Molecule 1: Laccase



• Molecule 1: Laccase



• Molecule 1: Laccase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.51Å 140.04Å 172.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.15 19.87 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.6 (19.87-2.15) 94.7 (19.87-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.236 0.178 , 0.237	Depositor DCC
R_{free} test set	4626 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12916	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: GOL, CU, NAG, PER, SO4

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	0.67	3/3857 (0.1%)	0.72	1/5296 (0.0%)
1	B	0.63	0/3851	0.69	1/5288 (0.0%)
1	C	0.63	2/3844 (0.1%)	0.71	1/5279 (0.0%)
All	All	0.64	5/11552 (0.0%)	0.71	3/15863 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56[A]	CYS	CB-SG	-5.46	1.73	1.81
1	C	56[B]	CYS	CB-SG	-5.46	1.73	1.81
1	A	56[A]	CYS	CB-SG	-5.24	1.73	1.81
1	A	56[B]	CYS	CB-SG	-5.24	1.73	1.81
1	A	303	CYS	CB-SG	-5.12	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	GLY	N-CA-C	-5.67	98.94	113.10
1	A	237	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	3	ILE	N-CA-C	-5.10	97.22	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	3734	0	3513	126	0
1	B	3728	0	3501	111	0
1	C	3725	0	3502	122	0
2	D	28	0	25	4	0
2	E	28	0	25	7	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	5	0
4	C	5	0	0	2	0
5	A	12	0	16	6	0
5	B	24	0	32	9	0
5	C	12	0	16	7	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	1	0
7	C	14	0	13	1	0
8	A	531	0	0	35	1
8	B	465	0	0	32	1
8	C	478	0	0	32	0
All	All	12916	0	10718	360	1

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 16.

All (360) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASN:HD21	2:D:1:NAG:C1	0.90	1.51
1:A:414:ASN:ND2	2:D:1:NAG:C1	1.72	1.42
1:A:436:ASN:ND2	2:E:1:NAG:C1	1.84	1.41
1:A:436:ASN:HD21	2:E:1:NAG:C1	1.31	1.38
1:A:161:GLY:HA2	1:A:162:ALA:CB	1.77	1.14
1:C:17:VAL:HG12	1:C:22:VAL:HA	1.38	1.06
1:B:161:GLY:CA	1:B:162:ALA:HB2	1.86	1.05
1:C:162:ALA:HB2	1:C:166:ILE:HD11	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ALA:HB2	1:C:166:ILE:CD1	1.91	1.00
1:C:358:GLN:HE22	1:C:370:LEU:H	1.03	1.00
1:C:59:LEU:HD11	1:C:114:THR:HG21	1.44	0.99
1:B:59:LEU:HD11	1:B:114:THR:HG21	1.45	0.98
1:C:17:VAL:HG12	1:C:22:VAL:CA	1.92	0.98
1:B:358:GLN:HE22	1:B:370:LEU:H	1.12	0.98
1:C:329:ASN:HD22	1:C:329:ASN:N	1.58	0.97
1:C:329:ASN:ND2	1:C:329:ASN:H	1.61	0.96
1:B:161:GLY:N	1:B:162:ALA:HB2	1.81	0.96
1:B:161:GLY:HA3	1:B:162:ALA:HB2	1.48	0.95
1:B:161:GLY:N	1:B:162:ALA:CB	2.30	0.95
1:A:331:ASN:HB2	8:A:1055:HOH:O	1.66	0.94
1:B:41:VAL:HG13	1:B:103:MET:O	1.66	0.94
1:A:112:HIS:HD1	5:A:508:GOL:H32	1.31	0.94
1:A:161:GLY:HA2	1:A:162:ALA:HB3	1.46	0.94
1:C:20:GLY:O	5:C:506:GOL:H31	1.67	0.94
1:B:265[A]:ASN:HD21	1:B:272:GLY:H	1.16	0.94
1:C:179:THR:O	1:C:183:VAL:HG22	1.69	0.93
1:C:48:VAL:HG23	8:C:686:HOH:O	1.68	0.93
1:B:36:VAL:HG22	1:B:124:PRO:HG2	1.48	0.92
5:C:506:GOL:H11	8:C:666:HOH:O	1.68	0.92
1:A:195:VAL:HG23	8:A:681:HOH:O	1.67	0.92
1:B:195:VAL:HG11	8:B:1004:HOH:O	1.70	0.92
1:B:342:VAL:HG23	8:B:761:HOH:O	1.69	0.92
1:C:164:GLY:HA2	1:C:165:ALA:HB3	1.52	0.91
1:A:59:LEU:CD1	1:A:114:THR:HG21	2.01	0.91
1:A:161:GLY:HA2	1:A:162:ALA:HB2	1.53	0.89
1:A:41:VAL:HB	8:A:1062:HOH:O	1.71	0.89
1:B:302:LYS:HD3	8:B:788:HOH:O	1.72	0.89
1:A:17:VAL:HG23	5:C:506:GOL:O1	1.73	0.88
1:A:310:HIS:HE1	8:A:856:HOH:O	1.58	0.87
1:A:59:LEU:HD11	1:A:114:THR:HG21	1.58	0.86
1:C:12:VAL:HG22	8:C:665:HOH:O	1.75	0.86
1:A:299:VAL:HB	8:A:1002:HOH:O	1.75	0.86
1:A:183:VAL:HG21	8:A:619:HOH:O	1.75	0.85
1:A:53:LEU:O	1:A:90:VAL:HG21	1.76	0.85
1:B:293:VAL:HG23	8:B:841:HOH:O	1.75	0.84
8:B:605:HOH:O	1:C:12:VAL:HG21	1.76	0.84
1:A:48:VAL:HG23	8:A:761:HOH:O	1.77	0.84
1:B:53:LEU:O	1:B:90:VAL:HG21	1.76	0.84
1:C:44:ASN:ND2	1:C:46:GLN:HE21	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG21	8:C:677:HOH:O	1.77	0.83
1:A:436:ASN:CG	2:E:1:NAG:C1	2.47	0.83
8:A:1131:HOH:O	2:E:2:NAG:H2	1.79	0.83
1:C:53:LEU:O	1:C:90:VAL:HG21	1.79	0.83
1:B:161:GLY:H	1:B:162:ALA:HB3	1.45	0.82
1:C:17:VAL:CG1	1:C:22:VAL:HA	2.10	0.81
1:B:12:VAL:HG22	8:B:646:HOH:O	1.79	0.81
1:A:44:ASN:HD21	1:A:46:GLN:HE21	1.29	0.80
1:A:112:HIS:ND1	5:A:508:GOL:H32	1.96	0.80
8:A:797:HOH:O	1:B:12:VAL:HG21	1.80	0.80
1:A:56[A]:CYS:SG	1:B:52:GLN:NE2	2.55	0.80
1:B:56[A]:CYS:SG	1:C:52:GLN:NE2	2.55	0.79
1:B:3:ILE:O	1:B:37:ILE:HA	1.82	0.79
1:A:329:ASN:ND2	1:A:329:ASN:H	1.81	0.79
1:A:160:MET:O	1:A:162:ALA:HB2	1.83	0.78
1:C:209:ASP:HB3	1:C:210:PRO:HD3	1.65	0.78
1:B:59:LEU:CD1	1:B:114:THR:HG21	2.14	0.78
1:A:161:GLY:CA	1:A:162:ALA:CB	2.61	0.78
1:A:17:VAL:HG12	1:A:22:VAL:N	1.98	0.78
1:A:162:ALA:H	1:A:163:GLY:HA2	1.48	0.77
1:B:179:THR:O	1:B:183:VAL:HG22	1.83	0.77
1:C:209:ASP:HB3	1:C:210:PRO:CD	2.14	0.77
1:C:61:ASP:OD2	8:C:1075:HOH:O	2.01	0.77
5:A:509:GOL:O2	1:B:17:VAL:HG23	1.85	0.77
1:C:451:LEU:HD12	1:C:465:ILE:HD11	1.66	0.77
1:B:72:LYS:N	5:B:508:GOL:H12	1.99	0.76
1:A:329:ASN:N	1:A:329:ASN:ND2	2.33	0.76
1:C:17:VAL:HG12	1:C:22:VAL:N	2.00	0.76
1:C:60:VAL:HG21	8:C:617:HOH:O	1.85	0.75
1:C:3:ILE:O	1:C:37:ILE:HA	1.87	0.75
1:A:52:GLN:NE2	1:C:56[A]:CYS:SG	2.60	0.75
1:C:155:VAL:HG23	8:C:871:HOH:O	1.87	0.74
1:C:70:PHE:H	1:C:103:MET:HE1	1.52	0.73
1:A:12:VAL:HG22	8:A:818:HOH:O	1.89	0.73
1:C:17:VAL:HG21	5:C:506:GOL:H2	1.69	0.73
1:A:36:VAL:HG22	1:A:124:PRO:HG2	1.71	0.73
1:C:59:LEU:HD11	1:C:114:THR:CG2	2.18	0.72
1:C:367:ALA:HA	8:C:1043:HOH:O	1.87	0.72
1:A:60:VAL:HG23	8:A:666:HOH:O	1.88	0.72
1:A:265:ASN:HD21	1:A:272:GLY:H	1.38	0.72
1:A:414:ASN:CG	2:D:1:NAG:C1	2.57	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:O	1:B:103:MET:HE1	1.90	0.72
1:B:160:MET:O	8:B:1054:HOH:O	2.08	0.71
1:A:17:VAL:HG12	1:A:22:VAL:CA	2.20	0.71
1:C:17:VAL:CG1	1:C:22:VAL:CA	2.68	0.71
1:A:459:LEU:HD21	5:A:508:GOL:H31	1.73	0.70
1:C:265[B]:ASN:HD21	1:C:272:GLY:H	1.37	0.70
1:A:170:SER:HB3	1:A:179:THR:HA	1.73	0.70
1:B:183:VAL:HG21	8:B:782:HOH:O	1.92	0.70
1:B:90:VAL:HG22	8:B:707:HOH:O	1.93	0.69
8:C:735:HOH:O	2:H:1:NAG:N2	2.24	0.69
1:C:329:ASN:HD22	1:C:329:ASN:H	0.79	0.69
1:A:329:ASN:N	1:A:329:ASN:HD22	1.90	0.69
1:A:342:VAL:HG23	8:A:662:HOH:O	1.93	0.69
1:A:60:VAL:HG21	8:A:978:HOH:O	1.93	0.69
1:B:60:VAL:HG23	8:B:726:HOH:O	1.93	0.68
1:C:162:ALA:HB1	1:C:163:GLY:HA2	1.75	0.68
1:A:323:GLN:OE1	8:A:1127:HOH:O	2.11	0.68
1:C:162:ALA:CB	1:C:166:ILE:HD11	2.21	0.68
4:B:506:SO4:O2	1:C:17:VAL:HG22	1.93	0.68
1:C:162:ALA:HB2	1:C:166:ILE:HD12	1.75	0.68
1:A:95:SER:HB3	8:A:689:HOH:O	1.95	0.67
1:B:161:GLY:CA	1:B:162:ALA:CB	2.56	0.67
1:A:17:VAL:CG2	4:B:506:SO4:O4	2.43	0.67
1:A:17:VAL:HG22	4:B:506:SO4:O4	1.95	0.67
1:A:310:HIS:HD2	1:A:421:ASP:O	1.78	0.67
1:A:426:ASP:OD1	1:A:427:VAL:HG23	1.94	0.67
1:C:426:ASP:OD1	1:C:427:VAL:HG23	1.94	0.67
1:B:161:GLY:H	1:B:162:ALA:CB	1.98	0.66
1:A:17:VAL:HG23	5:C:506:GOL:HO1	1.61	0.66
1:B:358:GLN:NE2	1:B:370:LEU:H	1.89	0.66
1:C:59:LEU:HD21	1:C:158[B]:LYS:HE3	1.76	0.66
1:A:69:GLU:HA	1:A:103:MET:HE1	1.78	0.66
1:C:17:VAL:HG23	8:C:650:HOH:O	1.94	0.66
1:A:386:ILE:CD1	1:A:441:PHE:HE1	2.09	0.66
1:B:61:ASP:OD2	8:B:1038:HOH:O	2.12	0.66
1:C:36:VAL:HG21	1:C:143:ASP:OD2	1.96	0.66
1:C:90:VAL:HG22	8:C:611:HOH:O	1.96	0.66
1:C:59:LEU:CD1	1:C:114:THR:CG2	2.75	0.65
1:B:72:LYS:H	5:B:508:GOL:H12	1.60	0.65
8:A:1063:HOH:O	2:E:1:NAG:H81	1.95	0.65
1:B:301:THR:HB	8:B:1014:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD12	1:A:114:THR:HG21	1.76	0.65
1:B:161:GLY:N	1:B:162:ALA:HB3	2.05	0.65
1:C:164:GLY:N	8:C:1076:HOH:O	2.30	0.65
1:A:70:PHE:H	1:A:103:MET:HE2	1.61	0.65
1:C:179:THR:HG22	8:C:621:HOH:O	1.97	0.65
1:B:17:VAL:HG12	1:B:22:VAL:N	2.12	0.64
1:A:90:VAL:HG22	8:A:792:HOH:O	1.96	0.64
1:C:164:GLY:CA	1:C:165:ALA:HB3	2.25	0.64
1:C:413:SER:HB2	8:C:1021:HOH:O	1.98	0.64
1:C:17:VAL:CG1	1:C:22:VAL:HB	2.27	0.64
1:C:36:VAL:HG22	1:C:124:PRO:HG2	1.78	0.64
1:B:162:ALA:HB1	8:B:839:HOH:O	1.98	0.63
1:A:158[B]:LYS:HE2	8:A:1016:HOH:O	1.98	0.63
1:B:378:LEU:HD22	1:B:384:ILE:HD12	1.81	0.62
1:C:374:SER:O	1:C:465:ILE:HG22	1.99	0.62
1:C:400:HIS:HB2	1:C:427:VAL:HG22	1.80	0.62
1:A:17:VAL:HG12	1:A:22:VAL:HA	1.80	0.62
1:C:60:VAL:HG23	8:C:614:HOH:O	1.98	0.62
1:B:426:ASP:OD1	1:B:427:VAL:HG23	1.98	0.62
1:A:161:GLY:CA	1:A:162:ALA:HB2	2.25	0.62
1:B:41:VAL:HG22	1:B:104:ALA:HB2	1.81	0.61
1:A:414:ASN:HD21	2:D:1:NAG:C2	1.96	0.61
1:A:391:GLY:HA2	1:A:433:VAL:HG22	1.81	0.61
1:A:288:THR:HG22	8:A:655:HOH:O	2.00	0.61
1:C:358:GLN:HE22	1:C:370:LEU:N	1.86	0.61
1:C:59:LEU:CD1	1:C:114:THR:HG21	2.25	0.60
1:A:386:ILE:HD11	1:A:441:PHE:HE1	1.66	0.60
1:B:36:VAL:HG23	8:B:867:HOH:O	2.01	0.60
1:C:359:ILE:HA	1:C:363:ALA:HB3	1.83	0.60
1:A:265:ASN:ND2	8:A:781:HOH:O	2.34	0.60
1:B:72:LYS:H	5:B:508:GOL:H2	1.67	0.60
1:B:255:GLN:NE2	8:B:892:HOH:O	2.34	0.59
1:A:41:VAL:HG22	1:A:103:MET:O	2.02	0.59
1:C:451:LEU:HD12	1:C:465:ILE:CD1	2.31	0.59
1:A:430:ILE:HA	1:A:437:VAL:HG21	1.85	0.59
1:B:293:VAL:HG22	8:B:983:HOH:O	2.00	0.59
1:A:41:VAL:HG13	1:A:103:MET:O	2.02	0.59
1:C:170:SER:HB3	1:C:179:THR:HA	1.85	0.59
1:B:358:GLN:HE22	1:B:370:LEU:N	1.93	0.58
1:C:54:ILE:HD13	8:C:629:HOH:O	2.02	0.58
1:C:167:THR:HG23	8:C:773:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LEU:HB3	1:C:465:ILE:HD12	1.86	0.57
1:C:70:PHE:H	1:C:103:MET:CE	2.17	0.57
1:A:53:LEU:O	1:A:90:VAL:CG2	2.49	0.57
1:B:36:VAL:HG22	1:B:124:PRO:CG	2.28	0.57
1:A:113:LEU:HG	1:A:114:THR:HG22	1.87	0.57
1:B:186:VAL:HG23	8:B:613:HOH:O	2.04	0.57
1:A:70:PHE:H	1:A:103:MET:CE	2.17	0.57
1:A:181:VAL:HG13	8:A:770:HOH:O	2.05	0.57
1:A:41:VAL:HG21	1:A:104:ALA:HB2	1.87	0.57
1:B:391:GLY:HA2	1:B:433:VAL:HG22	1.87	0.57
1:B:59:LEU:HD21	1:B:158[B]:LYS:HE3	1.88	0.56
1:B:265[A]:ASN:ND2	1:B:272:GLY:H	1.97	0.56
1:B:46:GLN:HA	1:B:97:ASN:HD22	1.71	0.56
1:A:413:SER:HB2	8:A:740:HOH:O	2.06	0.56
1:A:17:VAL:CG1	1:A:22:VAL:HA	2.36	0.56
1:A:195:VAL:HG22	8:A:965:HOH:O	2.06	0.55
1:A:225:GLU:HB3	1:A:248:SER:HB2	1.87	0.55
1:B:183:VAL:HG23	5:B:509:GOL:O3	2.07	0.55
1:A:11:ILE:HG22	1:A:53:LEU:HD21	1.89	0.55
1:A:112:HIS:HD1	5:A:508:GOL:C3	2.12	0.55
1:A:386:ILE:HD11	1:A:441:PHE:CE1	2.42	0.55
1:A:61:ASP:OD2	8:A:1082:HOH:O	2.18	0.54
1:C:3:ILE:O	1:C:38:ALA:N	2.40	0.54
1:A:17:VAL:CG1	1:A:22:VAL:CA	2.85	0.54
1:B:48:VAL:HG23	8:B:622:HOH:O	2.07	0.54
1:A:41:VAL:CG2	1:A:104:ALA:HB2	2.37	0.54
1:A:59:LEU:HD12	1:A:114:THR:CG2	2.37	0.54
1:B:44:ASN:ND2	1:B:46:GLN:HE21	2.05	0.54
1:B:17:VAL:HG12	1:B:22:VAL:CA	2.37	0.54
1:B:293:VAL:CG2	8:B:983:HOH:O	2.55	0.54
1:A:178:ARG:HG2	1:A:186:VAL:HG22	1.89	0.54
1:C:17:VAL:CG1	1:C:22:VAL:CB	2.85	0.54
1:A:162:ALA:H	1:A:164:GLY:HA3	1.73	0.53
1:A:343:ILE:HG21	1:A:465:ILE:HG12	1.90	0.53
1:A:179:THR:O	1:A:183:VAL:HG22	2.07	0.53
1:B:171:THR:O	1:B:177:GLY:HA3	2.09	0.53
5:B:511:GOL:H11	8:B:814:HOH:O	2.07	0.53
1:A:17:VAL:HG12	1:A:21:PHE:C	2.28	0.53
1:A:495:HIS:NE2	8:A:1082:HOH:O	1.96	0.53
1:B:320:ASN:HB2	1:B:325:GLY:HA3	1.91	0.53
1:B:3:ILE:O	1:B:38:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:CD1	1:B:114:THR:CG2	2.84	0.53
1:C:265[B]:ASN:ND2	1:C:272:GLY:H	2.05	0.53
1:A:59:LEU:CD1	1:A:114:THR:CG2	2.83	0.52
1:B:36:VAL:CG2	1:B:124:PRO:HG2	2.31	0.52
1:A:182:ASN:HD21	1:B:192:THR:H	1.57	0.52
1:A:112:HIS:CE1	5:A:508:GOL:H32	2.45	0.52
1:C:343:ILE:HD12	1:C:465:ILE:HG13	1.92	0.52
1:C:83:ILE:HD11	1:C:348:PHE:CZ	2.44	0.52
1:A:83:ILE:HD11	1:A:348:PHE:CZ	2.45	0.52
1:B:179:THR:HG23	1:B:183:VAL:HA	1.92	0.51
1:B:72:LYS:H	5:B:508:GOL:C1	2.23	0.51
1:C:293:VAL:HG21	8:C:1061:HOH:O	2.09	0.51
1:C:83:ILE:HD11	1:C:348:PHE:HZ	1.75	0.51
1:A:17:VAL:CG1	1:A:22:VAL:HB	2.41	0.51
1:B:225:GLU:HB3	1:B:248:SER:HB2	1.93	0.51
1:C:391:GLY:HA2	1:C:433:VAL:HG22	1.92	0.51
1:B:114:THR:H	5:B:510:GOL:C3	2.24	0.51
1:C:11:ILE:HG22	1:C:53:LEU:HD21	1.92	0.51
1:B:331:ASN:ND2	2:G:1:NAG:H3	2.25	0.51
1:C:183:VAL:HG21	8:C:634:HOH:O	2.11	0.51
1:B:17:VAL:HG22	4:B:506:SO4:O3	2.11	0.51
1:B:386:ILE:HD13	1:B:441:PHE:HE1	1.76	0.51
1:C:192:THR:HA	1:C:283:ARG:O	2.11	0.51
1:C:41:VAL:CG1	1:C:103:MET:O	2.59	0.51
1:C:225:GLU:HB3	1:C:248:SER:HB2	1.94	0.50
1:A:176:LEU:HD21	5:C:506:GOL:H32	1.93	0.50
1:C:17:VAL:HG11	1:C:22:VAL:HB	1.92	0.50
1:A:103:MET:HE3	8:A:935:HOH:O	2.11	0.50
1:C:342:VAL:HG23	8:C:612:HOH:O	2.11	0.50
1:A:178:ARG:HG2	1:A:186:VAL:CG2	2.41	0.50
1:B:79:GLY:N	1:B:80:PRO:HD2	2.27	0.50
1:C:305:ILE:HD13	8:C:841:HOH:O	2.10	0.50
1:A:302:LYS:HD3	8:A:1068:HOH:O	2.11	0.50
1:C:374:SER:C	1:C:465:ILE:HG22	2.32	0.49
1:B:195:VAL:HB	8:B:956:HOH:O	2.12	0.49
1:B:209:ASP:HB3	1:B:210:PRO:CD	2.42	0.49
1:B:72:LYS:H	5:B:508:GOL:C2	2.26	0.49
1:B:108:TRP:CE3	1:B:206:ILE:HG22	2.48	0.49
1:B:103:MET:HE3	8:B:875:HOH:O	2.12	0.49
4:B:506:SO4:O1	8:B:1039:HOH:O	2.18	0.48
1:C:44:ASN:HD21	1:C:46:GLN:HE21	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:HIS:CE1	1:C:244:ALA:HB1	2.48	0.48
1:B:310:HIS:HD2	1:B:421:ASP:O	1.96	0.48
1:B:320:ASN:HB3	1:B:322:HIS:CE1	2.49	0.48
1:C:183:VAL:HG23	5:C:507:GOL:O1	2.14	0.48
1:B:179:THR:CG2	1:B:183:VAL:HA	2.44	0.48
1:C:394:GLY:O	1:C:458:HIS:HE1	1.97	0.48
1:A:111:SER:HB2	1:A:121:LEU:HD13	1.96	0.48
5:B:511:GOL:H12	8:B:760:HOH:O	2.13	0.47
1:B:54:ILE:HG13	8:C:603:HOH:O	2.14	0.47
1:B:155:VAL:HG22	1:C:1:VAL:CG1	2.43	0.47
1:C:366:ALA:HB3	4:C:505:SO4:O3	2.14	0.47
1:B:59:LEU:HD21	1:B:158[B]:LYS:CE	2.43	0.47
1:A:2:GLN:NE2	8:A:1091:HOH:O	2.47	0.47
1:A:163:GLY:HA3	8:A:746:HOH:O	2.14	0.47
1:C:364:ASN:HB2	8:C:946:HOH:O	2.14	0.47
1:B:180:HIS:CD2	1:B:270:GLY:H	2.33	0.47
1:B:209:ASP:HB3	1:B:210:PRO:HD3	1.97	0.47
1:B:482:GLU:HG2	8:B:608:HOH:O	2.15	0.47
1:C:162:ALA:CB	1:C:163:GLY:HA2	2.37	0.47
1:B:178:ARG:HG2	1:B:186:VAL:HG22	1.96	0.47
1:C:179:THR:HG23	1:C:183:VAL:HA	1.97	0.46
1:A:65:HIS:NE2	1:A:67:HIS:HA	2.30	0.46
1:A:103:MET:CE	8:A:935:HOH:O	2.63	0.46
1:A:436:ASN:OD1	2:E:1:NAG:C1	2.64	0.46
1:C:301:THR:HB	8:C:755:HOH:O	2.16	0.46
1:A:155:VAL:HG13	8:A:702:HOH:O	2.15	0.46
1:A:198:ARG:HD3	8:A:1073:HOH:O	2.16	0.46
1:C:164:GLY:HA2	1:C:165:ALA:CB	2.27	0.46
1:C:2:GLN:HG2	1:C:36:VAL:HB	1.96	0.46
1:A:386:ILE:HD12	1:A:441:PHE:HE1	1.79	0.46
1:A:394:GLY:HA2	1:A:395:GLY:HA3	1.65	0.46
1:B:301:THR:HG21	8:B:927:HOH:O	2.17	0.45
1:A:36:VAL:HG21	1:A:143:ASP:OD2	2.16	0.45
1:A:100:VAL:HG23	1:A:100:VAL:O	2.16	0.45
1:A:323:GLN:HG2	8:A:1129:HOH:O	2.16	0.45
1:B:53:LEU:O	1:B:90:VAL:CG2	2.58	0.45
1:A:107:TYR:HB2	1:A:125:PHE:HB3	1.99	0.45
1:A:108:TRP:CE3	1:A:206:ILE:HG22	2.52	0.45
1:B:320:ASN:O	1:B:322:HIS:N	2.40	0.45
1:B:430:ILE:HA	1:B:437:VAL:HG21	1.99	0.45
8:A:1055:HOH:O	2:E:1:NAG:H62	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:O	1:C:90:VAL:CG2	2.59	0.44
1:B:68:GLY:O	1:B:103:MET:CE	2.62	0.44
1:C:366:ALA:HB3	4:C:505:SO4:S	2.57	0.44
1:C:162:ALA:CB	1:C:166:ILE:CD1	2.81	0.44
1:B:392:ALA:O	1:B:397:HIS:HE1	2.00	0.44
1:A:97:ASN:C	1:A:97:ASN:HD22	2.21	0.44
1:B:60:VAL:HG21	8:B:846:HOH:O	2.17	0.44
1:C:41:VAL:HG13	1:C:103:MET:O	2.18	0.44
1:B:342:VAL:CG2	8:B:761:HOH:O	2.47	0.43
1:B:158[B]:LYS:HE2	8:B:834:HOH:O	2.17	0.43
1:A:263:ARG:HB3	1:A:273:PHE:CE1	2.54	0.43
1:C:92:ASN:ND2	8:C:989:HOH:O	2.51	0.43
1:A:59:LEU:HD11	1:A:158[A]:LYS:HE2	2.00	0.43
1:C:111:SER:HB2	1:C:121:LEU:HD13	2.00	0.43
1:A:67:HIS:C	1:A:67:HIS:CD2	2.92	0.43
1:B:163:GLY:HA2	1:B:164:GLY:HA3	1.81	0.43
1:B:305:ILE:HD13	8:B:796:HOH:O	2.19	0.43
1:C:170:SER:HA	1:C:180:HIS:CE1	2.54	0.43
1:C:232:GLN:NE2	1:C:310:HIS:HB2	2.33	0.43
1:C:400:HIS:CD2	6:C:510:PER:O1	2.72	0.43
1:C:113:LEU:HG	1:C:114:THR:HG22	2.00	0.43
1:C:17:VAL:HG12	1:C:21:PHE:C	2.38	0.43
1:C:195:VAL:HG11	8:C:703:HOH:O	2.19	0.43
1:C:331:ASN:OD1	7:C:509:NAG:H5	2.19	0.42
1:A:79:GLY:N	1:A:80:PRO:HD2	2.34	0.42
1:B:17:VAL:HG12	1:B:22:VAL:HA	2.01	0.42
1:C:79:GLY:N	1:C:80:PRO:CD	2.82	0.42
1:B:22:VAL:CG2	8:C:642:HOH:O	2.67	0.42
1:B:303[A]:CYS:SG	8:B:706:HOH:O	2.48	0.42
1:C:186:VAL:HG23	8:C:714:HOH:O	2.20	0.42
1:C:209:ASP:HA	1:C:455:ILE:HG23	2.00	0.42
1:B:349:THR:HA	1:B:350:PRO:HD3	1.88	0.42
1:A:180:HIS:CD2	1:A:270:GLY:H	2.38	0.42
1:A:87:PRO:HG2	1:A:491:TYR:CE1	2.55	0.42
1:C:394:GLY:O	1:C:458:HIS:CE1	2.73	0.42
1:C:151:ASP:OD1	1:C:151:ASP:N	2.53	0.41
1:C:41:VAL:HG11	8:C:978:HOH:O	2.21	0.41
1:B:209:ASP:C	1:B:209:ASP:OD1	2.58	0.41
1:A:83:ILE:HD11	1:A:348:PHE:HZ	1.83	0.41
1:C:162:ALA:HA	1:C:164:GLY:HA3	2.03	0.41
1:C:16:ILE:HD11	1:C:152:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:OD1	1:C:448:PRO:HD2	2.20	0.41
1:A:162:ALA:HB3	8:A:1034:HOH:O	2.21	0.41
1:C:299:VAL:HG12	8:C:1026:HOH:O	2.19	0.41
1:A:160:MET:CE	1:A:160:MET:HA	2.51	0.41
1:B:178:ARG:HG2	1:B:186:VAL:CG2	2.51	0.41
1:B:400:HIS:HB2	1:B:427:VAL:HG22	2.03	0.41
1:C:164:GLY:CA	8:C:1076:HOH:O	2.66	0.41
1:B:386:ILE:CD1	1:B:441:PHE:HE1	2.34	0.41
1:B:95:SER:HB3	8:B:675:HOH:O	2.21	0.41
1:A:16:ILE:HG22	1:C:22:VAL:HG21	2.03	0.41
1:B:404:HIS:NE2	1:B:469:GLU:OE1	2.48	0.41
1:C:404:HIS:NE2	1:C:469:GLU:OE1	2.51	0.41
1:C:310:HIS:HD2	1:C:421:ASP:O	2.03	0.40
1:A:341:PHE:HB3	1:A:463:PHE:CD1	2.55	0.40
1:A:72:LYS:HA	1:A:445:ASN:OD1	2.21	0.40
1:A:160:MET:HE3	1:A:160:MET:HA	2.03	0.40
1:B:155:VAL:HG22	1:C:1:VAL:HG13	2.02	0.40
1:B:161:GLY:HA3	1:B:166:ILE:HD11	2.03	0.40
1:C:71:GLN:HE22	1:C:98:PHE:CB	2.34	0.40
1:A:311:PRO:HD3	1:A:423:ILE:HA	2.03	0.40
1:C:195:VAL:CG1	8:C:703:HOH:O	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:719:HOH:O	8:B:1004:HOH:O[1_655]	2.17	0.03

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	498/495 (101%)	474 (95%)	20 (4%)	4 (1%)	19	12
1	B	497/495 (100%)	473 (95%)	20 (4%)	4 (1%)	19	12
1	C	496/495 (100%)	473 (95%)	20 (4%)	3 (1%)	25	18
All	All	1491/1485 (100%)	1420 (95%)	60 (4%)	11 (1%)	22	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ALA
1	B	162	ALA
1	A	394	GLY
1	C	209	ASP
1	A	209	ASP
1	B	161	GLY
1	B	209	ASP
1	C	327	ASP
1	A	59	LEU
1	B	321	PRO
1	C	59	LEU

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	409/406 (101%)	387 (95%)	22 (5%)	22	18
1	B	406/406 (100%)	383 (94%)	23 (6%)	20	16
1	C	406/406 (100%)	377 (93%)	29 (7%)	14	9
All	All	1221/1218 (100%)	1147 (94%)	74 (6%)	19	14

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	54	ILE

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Mol	Chain	Res	Type
1	A	69	GLU
1	A	97	ASN
1	A	117	TYR
1	A	156	LEU
1	A	158[A]	LYS
1	A	158[B]	LYS
1	A	160	MET
1	A	181	VAL
1	A	226	THR
1	A	246	ARG
1	A	285	ASP
1	A	297	SER
1	A	303	CYS
1	A	329	ASN
1	A	349	THR
1	A	380	SER
1	A	417	SER
1	A	450	PHE
1	A	460	ASP
1	A	463	PHE
1	B	15	ASP
1	B	54	ILE
1	B	69	GLU
1	B	117	TYR
1	B	158[A]	LYS
1	B	158[B]	LYS
1	B	160	MET
1	B	181	VAL
1	B	195	VAL
1	B	226	THR
1	B	246	ARG
1	B	285	ASP
1	B	297	SER
1	B	299	VAL
1	B	301	THR
1	B	349	THR
1	B	372	SER
1	B	380	SER
1	B	417	SER
1	B	450	PHE
1	B	451	LEU
1	B	463	PHE

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Mol	Chain	Res	Type
1	B	476	SER
1	C	15	ASP
1	C	41	VAL
1	C	54	ILE
1	C	69	GLU
1	C	97	ASN
1	C	114	THR
1	C	117	TYR
1	C	156	LEU
1	C	158[A]	LYS
1	C	158[B]	LYS
1	C	160	MET
1	C	167	THR
1	C	195	VAL
1	C	226	THR
1	C	246	ARG
1	C	285	ASP
1	C	297	SER
1	C	302	LYS
1	C	303	CYS
1	C	314	ARG
1	C	329	ASN
1	C	331	ASN
1	C	349	THR
1	C	417	SER
1	C	450	PHE
1	C	451	LEU
1	C	460	ASP
1	C	463	PHE
1	C	465	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	44	ASN
1	A	52	GLN
1	A	71	GLN
1	A	92	ASN
1	A	97	ASN
1	A	180	HIS
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	265	ASN
1	A	310	HIS
1	A	320	ASN
1	A	323	GLN
1	A	329	ASN
1	A	414	ASN
1	A	486	ASN
1	B	44	ASN
1	B	52	GLN
1	B	92	ASN
1	B	97	ASN
1	B	116	GLN
1	B	180	HIS
1	B	182	ASN
1	B	255	GLN
1	B	310	HIS
1	B	358	GLN
1	B	397	HIS
1	B	486	ASN
1	C	2	GLN
1	C	44	ASN
1	C	52	GLN
1	C	71	GLN
1	C	85	GLN
1	C	92	ASN
1	C	136	ASN
1	C	180	HIS
1	C	232	GLN
1	C	310	HIS
1	C	329	ASN
1	C	358	GLN
1	C	473	ASN
1	C	486	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 ⓘ

10 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
2	NAG	D	1	2	14,14,15	1.20	1 (7%)	17,19,21	1.77	3 (17%)
2	NAG	D	2	2	14,14,15	1.39	2 (14%)	17,19,21	2.88	7 (41%)
2	NAG	E	1	2	14,14,15	1.41	4 (28%)	17,19,21	1.30	3 (17%)
2	NAG	E	2	2	14,14,15	0.93	0	17,19,21	1.63	4 (23%)
2	NAG	F	1	1,2	14,14,15	0.68	0	17,19,21	1.51	3 (17%)
2	NAG	F	2	2	14,14,15	0.69	0	17,19,21	3.05	7 (41%)
2	NAG	G	1	2	14,14,15	1.05	0	17,19,21	2.54	8 (47%)
2	NAG	G	2	2	14,14,15	1.17	2 (14%)	17,19,21	2.59	6 (35%)
2	NAG	H	1	1,2	14,14,15	2.73	2 (14%)	17,19,21	1.87	2 (11%)
2	NAG	H	2	2	14,14,15	2.71	4 (28%)	17,19,21	2.36	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	H	2	2	-	6/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O7-C7	9.34	1.44	1.23
2	H	2	NAG	O7-C7	8.76	1.43	1.23
2	D	1	NAG	O5-C1	-3.37	1.38	1.43
2	D	2	NAG	O5-C1	-2.88	1.39	1.43
2	H	1	NAG	C7-N2	2.80	1.44	1.34
2	G	2	NAG	C2-N2	-2.70	1.41	1.46
2	E	1	NAG	O7-C7	-2.55	1.17	1.23
2	G	2	NAG	O5-C1	-2.54	1.39	1.43
2	E	1	NAG	C2-N2	-2.37	1.42	1.46
2	D	2	NAG	C2-N2	-2.37	1.42	1.46
2	E	1	NAG	O5-C1	-2.30	1.40	1.43
2	H	2	NAG	C8-C7	2.17	1.55	1.50
2	H	2	NAG	O5-C5	-2.08	1.39	1.43
2	H	2	NAG	O5-C1	-2.03	1.40	1.43
2	E	1	NAG	O5-C5	-2.01	1.39	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C2-N2-C7	7.63	133.77	122.90
2	F	2	NAG	C1-O5-C5	6.90	121.53	112.19
2	F	2	NAG	C6-C5-C4	-6.83	97.01	113.00
2	D	2	NAG	C2-N2-C7	-5.96	114.41	122.90
2	D	2	NAG	C1-O5-C5	5.50	119.64	112.19
2	D	1	NAG	C1-O5-C5	5.29	119.36	112.19
2	G	1	NAG	O4-C4-C3	-5.21	98.30	110.35
2	H	1	NAG	C1-O5-C5	4.74	118.61	112.19
2	D	2	NAG	C4-C3-C2	4.29	117.30	111.02
2	F	2	NAG	O5-C5-C4	4.15	120.92	110.83
2	H	2	NAG	C1-C2-N2	4.14	117.56	110.49
2	G	2	NAG	C8-C7-N2	-4.08	109.19	116.10
2	G	1	NAG	O3-C3-C4	-3.86	101.41	110.35
2	D	2	NAG	O5-C5-C6	-3.84	101.18	107.20
2	H	2	NAG	C3-C4-C5	-3.67	103.69	110.24
2	G	1	NAG	C2-N2-C7	3.64	128.09	122.90
2	G	1	NAG	C1-O5-C5	3.63	117.11	112.19
2	H	2	NAG	O5-C1-C2	-3.55	105.68	111.29
2	H	2	NAG	C4-C3-C2	3.52	116.17	111.02
2	F	2	NAG	O3-C3-C4	-3.42	102.45	110.35
2	F	2	NAG	O5-C5-C6	3.37	112.48	107.20
2	G	1	NAG	C4-C3-C2	3.36	115.94	111.02
2	H	2	NAG	O3-C3-C2	-3.30	102.64	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C3-C4-C5	3.29	116.10	110.24
2	F	1	NAG	O5-C1-C2	-3.18	106.27	111.29
2	E	2	NAG	C1-C2-N2	-2.97	105.42	110.49
2	F	1	NAG	C4-C3-C2	2.95	115.34	111.02
2	D	2	NAG	O5-C1-C2	-2.93	106.66	111.29
2	F	2	NAG	C3-C4-C5	2.92	115.45	110.24
2	H	2	NAG	C1-O5-C5	2.80	115.98	112.19
2	D	1	NAG	O4-C4-C5	-2.79	102.38	109.30
2	H	1	NAG	C4-C3-C2	2.78	115.09	111.02
2	H	2	NAG	O7-C7-N2	-2.74	116.92	121.95
2	G	2	NAG	O7-C7-N2	2.73	126.98	121.95
2	F	2	NAG	O5-C1-C2	-2.63	107.13	111.29
2	E	1	NAG	C6-C5-C4	-2.51	107.12	113.00
2	E	2	NAG	C3-C4-C5	2.51	114.72	110.24
2	E	1	NAG	O5-C5-C6	2.47	111.07	107.20
2	G	1	NAG	C8-C7-N2	-2.41	112.01	116.10
2	G	2	NAG	O4-C4-C3	-2.35	104.93	110.35
2	E	2	NAG	C1-O5-C5	2.29	115.29	112.19
2	G	1	NAG	O3-C3-C2	2.29	114.20	109.47
2	G	2	NAG	O5-C1-C2	-2.29	107.68	111.29
2	H	2	NAG	C2-N2-C7	2.26	126.12	122.90
2	D	2	NAG	O4-C4-C3	-2.23	105.18	110.35
2	E	1	NAG	C8-C7-N2	2.22	119.86	116.10
2	G	1	NAG	C6-C5-C4	-2.21	107.84	113.00
2	G	2	NAG	O3-C3-C2	2.19	114.00	109.47
2	E	2	NAG	O3-C3-C4	-2.06	105.58	110.35
2	D	1	NAG	C2-N2-C7	-2.03	120.02	122.90
2	F	1	NAG	O3-C3-C2	-2.00	105.32	109.47

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C3-C2-N2-C7
2	H	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6

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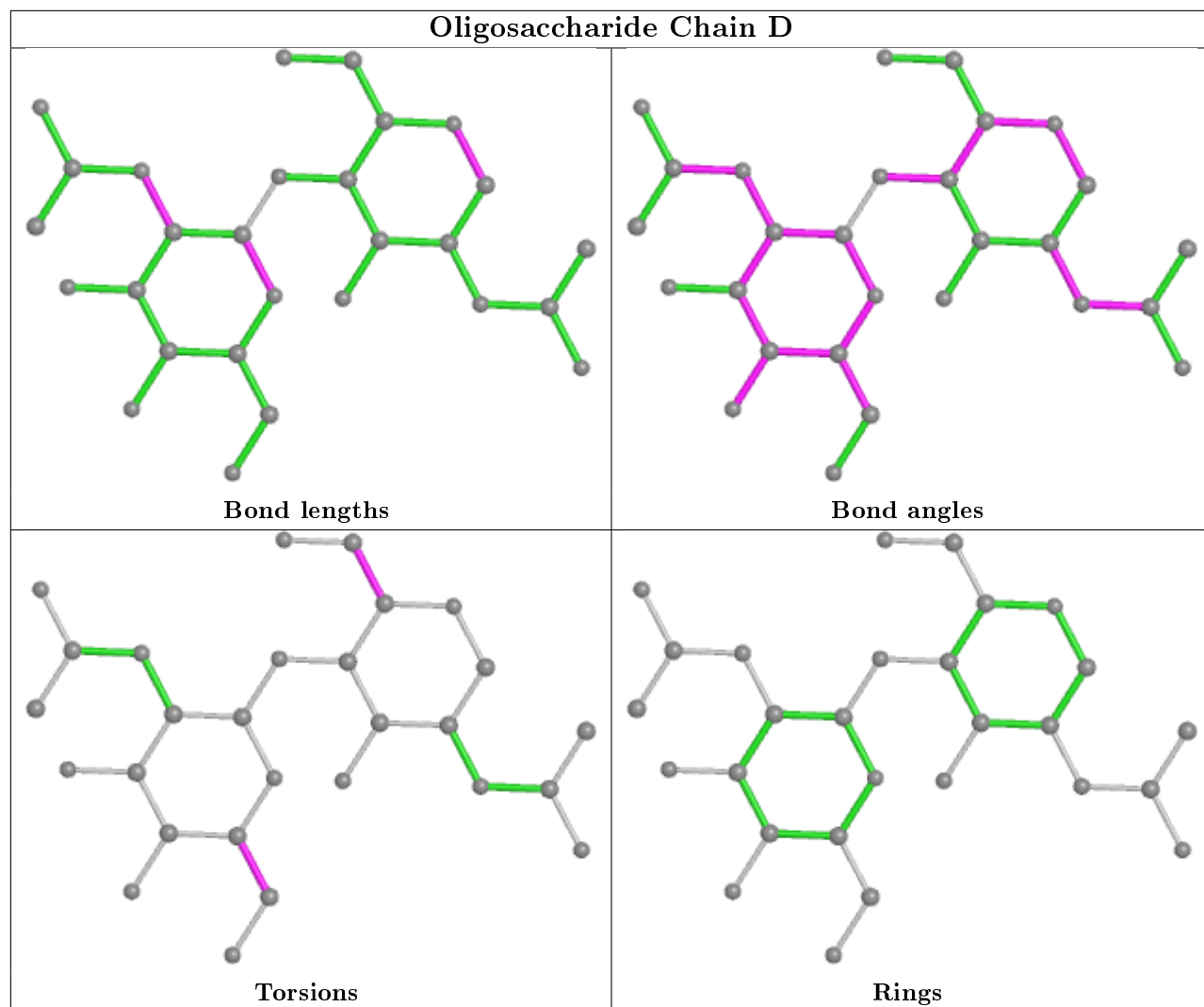
Mol	Chain	Res	Type	Atoms
2	H	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6

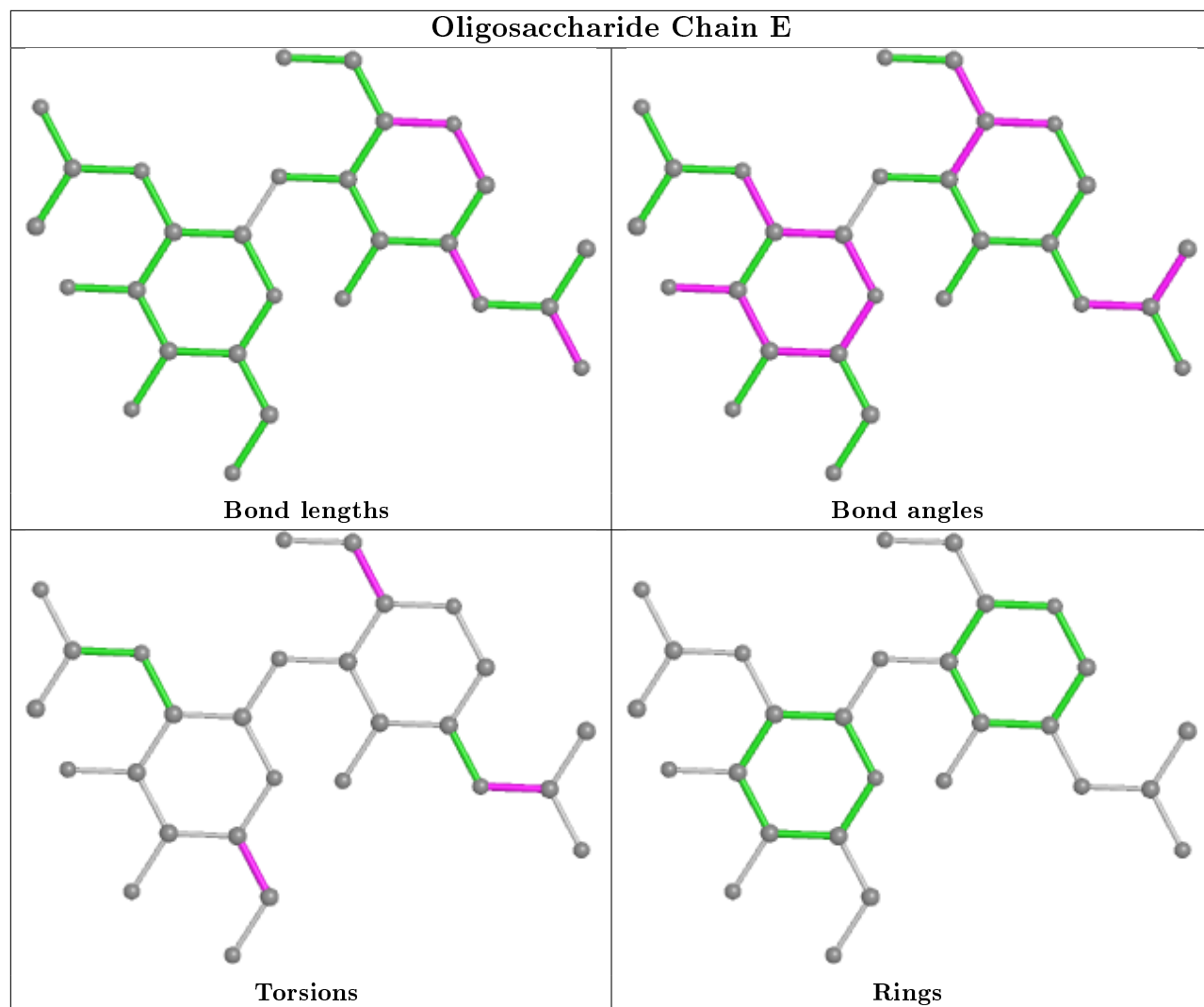
There are no ring outliers.

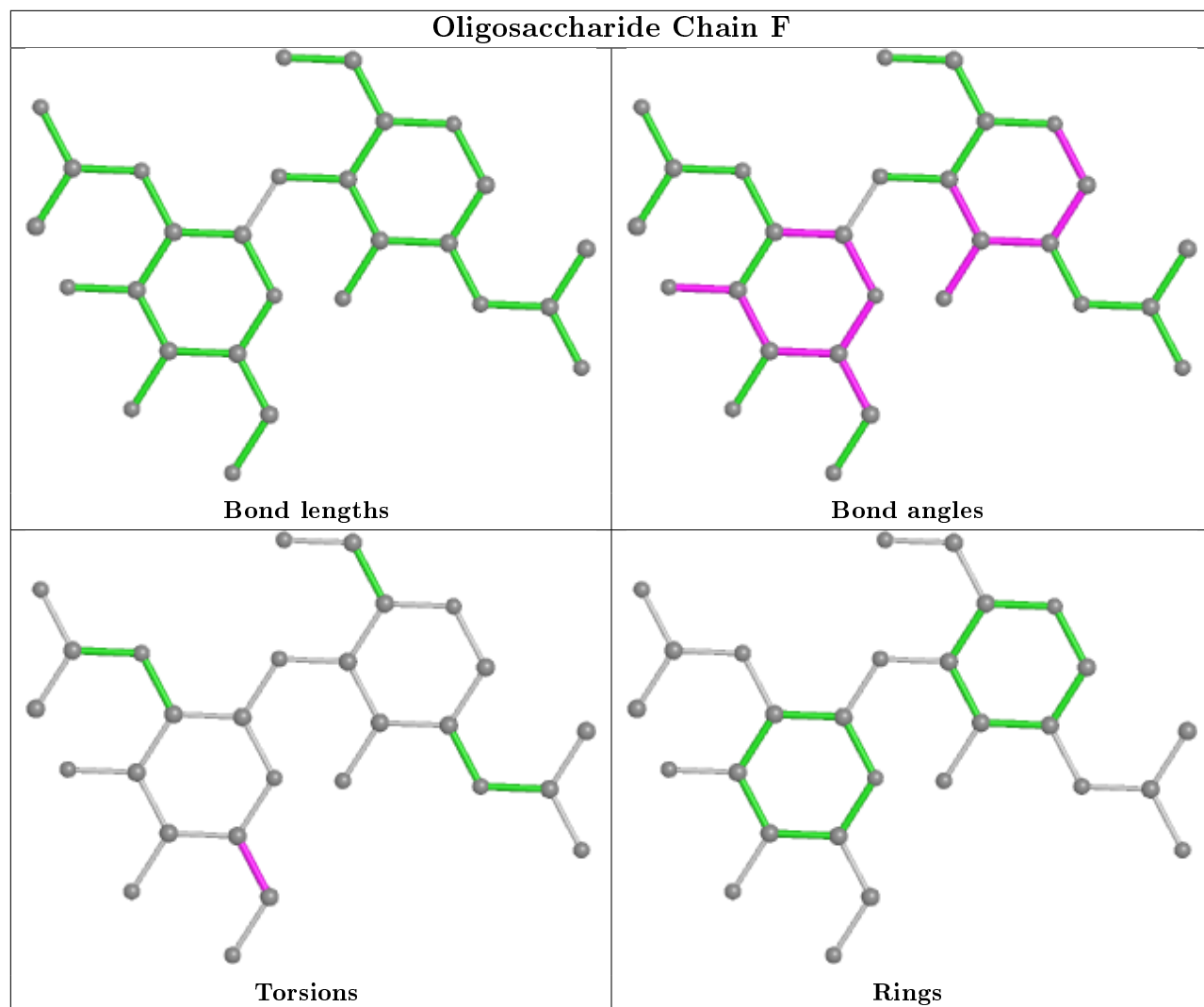
5 monomers are involved in 13 short contacts:

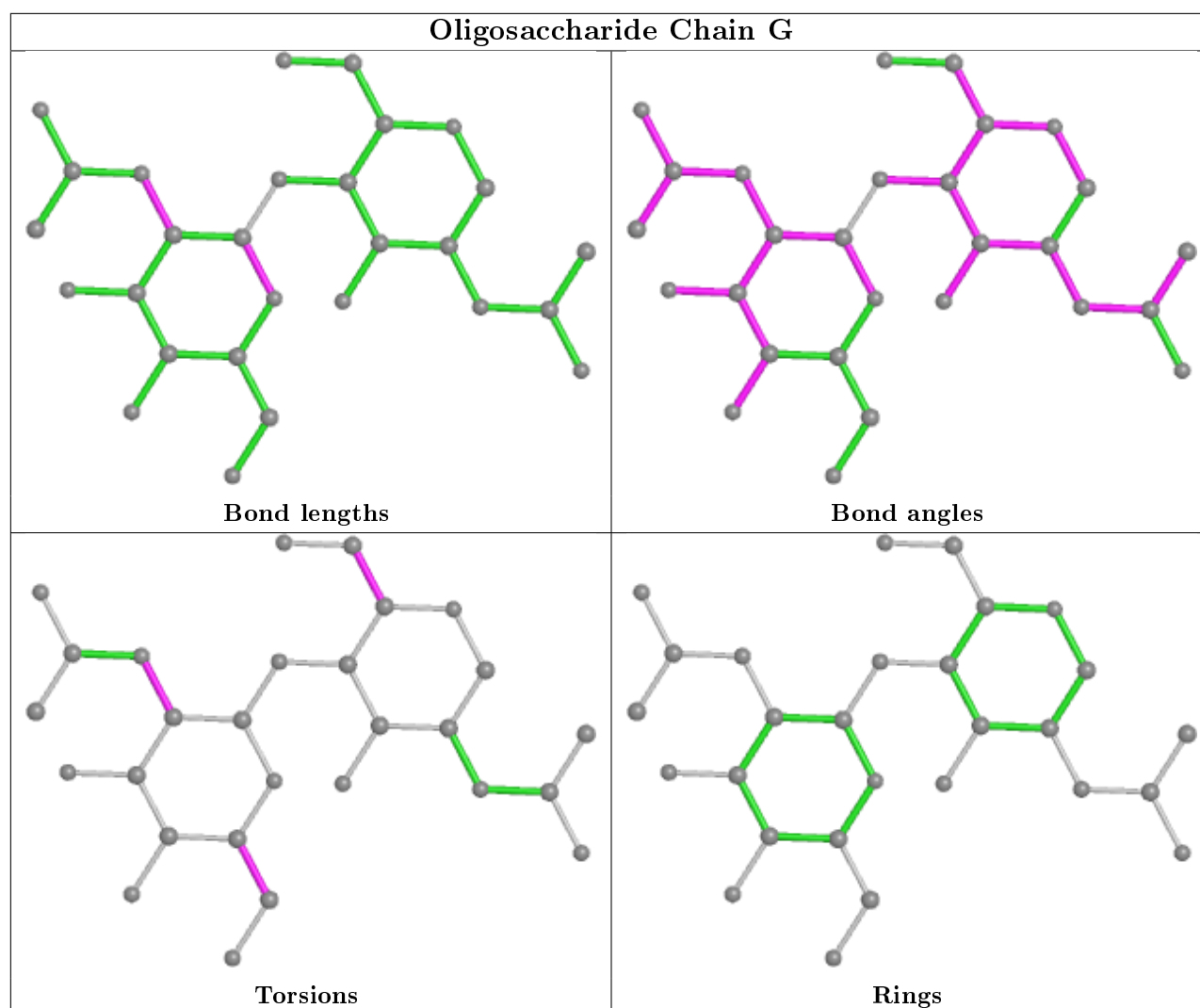
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	0
2	E	2	NAG	1	0
2	G	1	NAG	1	0
2	E	1	NAG	6	0
2	H	1	NAG	1	0

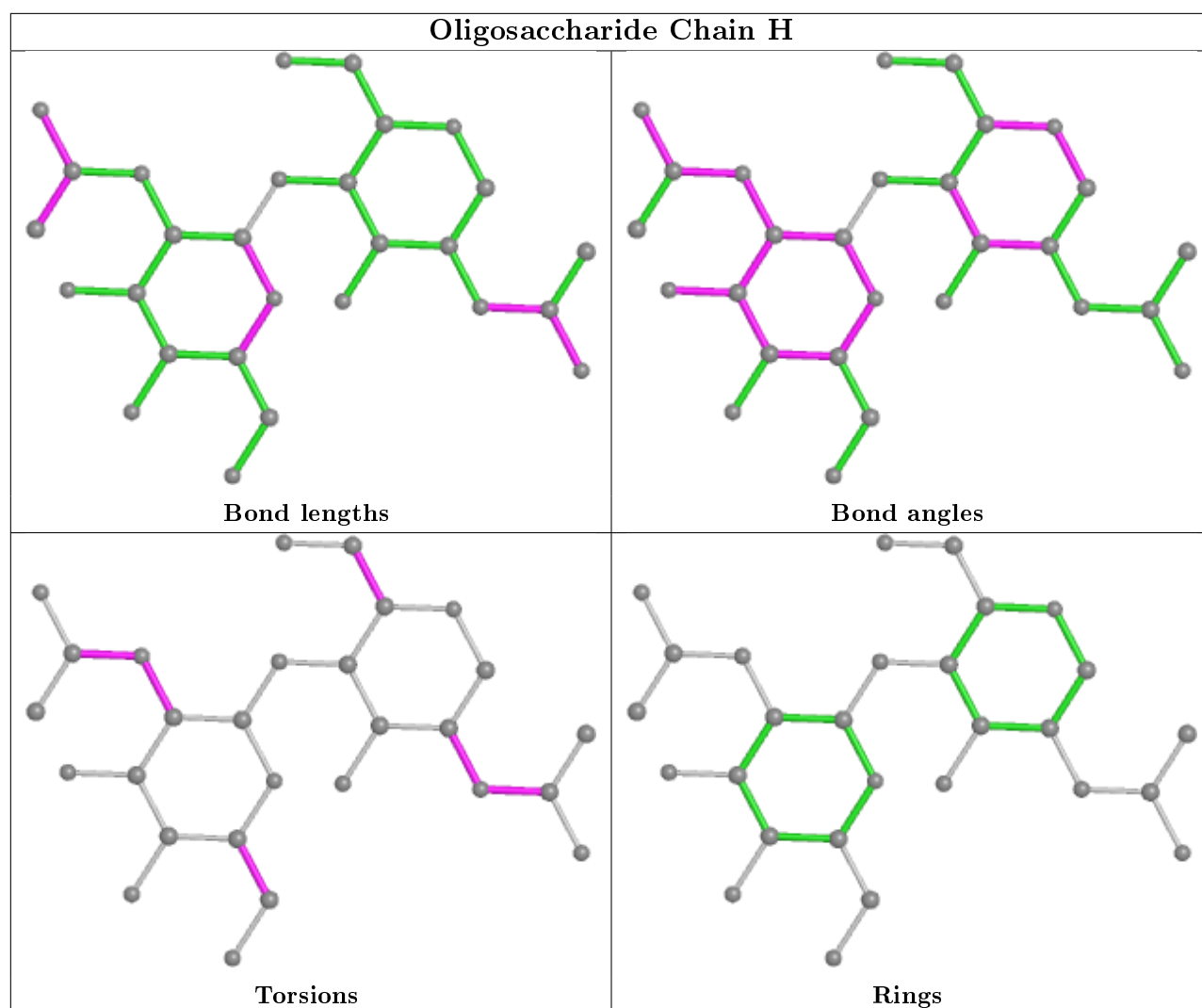
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 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	$\# Z > 2$
5	GOL	B	511	-	5,5,5	0.25	0	5,5,5	0.65	0
4	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	A	507	-	4,4,4	0.19	0	6,6,6	0.30	0
6	PER	B	514	3	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PER	C	510	3	0,1,1	0.00	-	-		
5	GOL	C	507	-	5,5,5	0.17	0	5,5,5	0.39	0
5	GOL	C	506	-	5,5,5	0.22	0	5,5,5	0.64	0
5	GOL	B	508	-	5,5,5	0.60	0	5,5,5	0.99	0
4	SO4	B	507	-	4,4,4	0.22	0	6,6,6	0.21	0
4	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.44	0
4	SO4	B	506	-	4,4,4	0.33	0	6,6,6	0.36	0
5	GOL	B	510	-	5,5,5	0.27	0	5,5,5	0.45	0
4	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.43	0
5	GOL	B	509	-	5,5,5	0.23	0	5,5,5	0.76	0
6	PER	A	512	3	0,1,1	0.00	-	-		
7	NAG	C	509	1	14,14,15	0.90	1 (7%)	17,19,21	1.66	6 (35%)
4	SO4	B	505	-	4,4,4	0.29	0	6,6,6	0.31	0
5	GOL	A	508	-	5,5,5	0.26	0	5,5,5	0.62	0
5	GOL	A	509	-	5,5,5	0.24	0	5,5,5	0.58	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
5	GOL	B	511	-	-	2/4/4/4	-
5	GOL	B	509	-	-	0/4/4/4	-
5	GOL	A	508	-	-	3/4/4/4	-
5	GOL	C	506	-	-	4/4/4/4	-
5	GOL	B	508	-	-	4/4/4/4	-
5	GOL	A	509	-	-	0/4/4/4	-
5	GOL	B	510	-	-	2/4/4/4	-
5	GOL	C	507	-	-	3/4/4/4	-
7	NAG	C	509	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	509	NAG	O7-C7	-2.02	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	509	NAG	C1-O5-C5	4.27	117.98	112.19
7	C	509	NAG	C6-C5-C4	-2.34	107.53	113.00
7	C	509	NAG	O3-C3-C2	-2.17	104.98	109.47
7	C	509	NAG	O5-C5-C6	2.16	110.59	107.20
7	C	509	NAG	O3-C3-C4	2.14	115.31	110.35
7	C	509	NAG	O5-C1-C2	2.00	114.45	111.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	506	GOL	O1-C1-C2-C3
5	C	507	GOL	C1-C2-C3-O3
5	B	508	GOL	O1-C1-C2-C3
5	B	508	GOL	C1-C2-C3-O3
5	B	510	GOL	C1-C2-C3-O3
5	B	510	GOL	O2-C2-C3-O3
5	C	506	GOL	O2-C2-C3-O3
5	C	507	GOL	O2-C2-C3-O3
5	C	506	GOL	C1-C2-C3-O3
5	B	511	GOL	O1-C1-C2-C3
5	A	508	GOL	C1-C2-C3-O3
5	B	511	GOL	O1-C1-C2-O2
5	B	508	GOL	O1-C1-C2-O2
5	B	508	GOL	O2-C2-C3-O3
5	C	506	GOL	O1-C1-C2-O2
5	A	508	GOL	O2-C2-C3-O3
5	C	507	GOL	O1-C1-C2-C3
5	A	508	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	511	GOL	2	0
6	C	510	PER	1	0
5	C	507	GOL	1	0
5	C	506	GOL	6	0
5	B	508	GOL	5	0
4	B	506	SO4	5	0
5	B	510	GOL	1	0
4	C	505	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	509	GOL	1	0
7	C	509	NAG	1	0
5	A	508	GOL	5	0
5	A	509	GOL	1	0

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	495/495 (100%)	-0.52	8 (1%) 72 77	10, 18, 32, 44	0
1	B	495/495 (100%)	-0.39	5 (1%) 82 86	11, 21, 38, 53	0
1	C	495/495 (100%)	-0.36	13 (2%) 56 64	11, 22, 38, 53	0
All	All	1485/1485 (100%)	-0.42	26 (1%) 68 75	10, 20, 36, 53	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	415	SER	3.7
1	B	320	ASN	3.6
1	C	328	CYS	3.3
1	B	415	SER	3.0
1	C	164	GLY	3.0
1	C	433	VAL	2.9
1	C	165	ALA	2.8
1	C	321	PRO	2.6
1	C	381	ASN	2.5
1	C	320	ASN	2.5
1	A	164	GLY	2.5
1	A	415	SER	2.4
1	A	320	ASN	2.4
1	A	394	GLY	2.3
1	C	393	ALA	2.3
1	B	433	VAL	2.3
1	A	161	GLY	2.2
1	B	362	GLY	2.2
1	C	161	GLY	2.2
1	A	313	SER	2.1
1	C	323	GLN	2.1
1	C	324	GLY	2.1
1	C	372	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	433	VAL	2.1
1	A	165	ALA	2.0
1	B	298	THR	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](#)

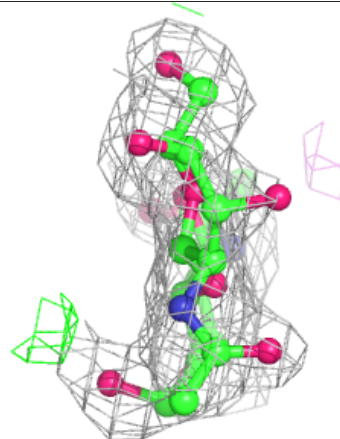
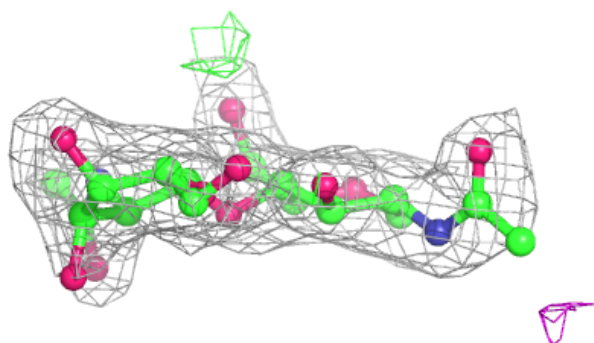
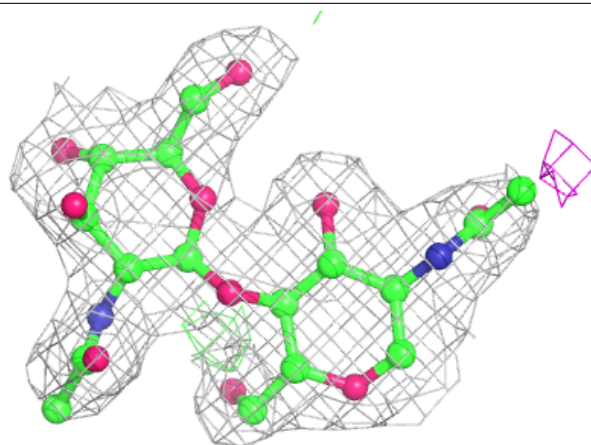
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.57	0.31	77,80,80,80	0
2	NAG	G	2	14/15	0.63	0.43	69,71,73,73	0
2	NAG	E	2	14/15	0.65	0.34	59,62,63,63	0
2	NAG	F	1	14/15	0.69	0.26	76,79,79,80	0
2	NAG	H	2	14/15	0.75	0.22	61,62,65,66	0
2	NAG	H	1	14/15	0.79	0.21	57,60,63,63	0
2	NAG	G	1	14/15	0.82	0.17	52,56,60,65	0
2	NAG	E	1	14/15	0.85	0.15	41,45,50,55	0
2	NAG	D	2	14/15	0.88	0.23	50,52,53,55	0
2	NAG	D	1	14/15	0.89	0.14	38,40,42,45	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.

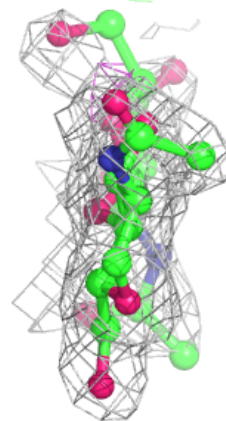
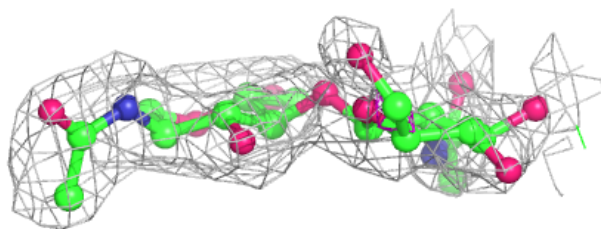
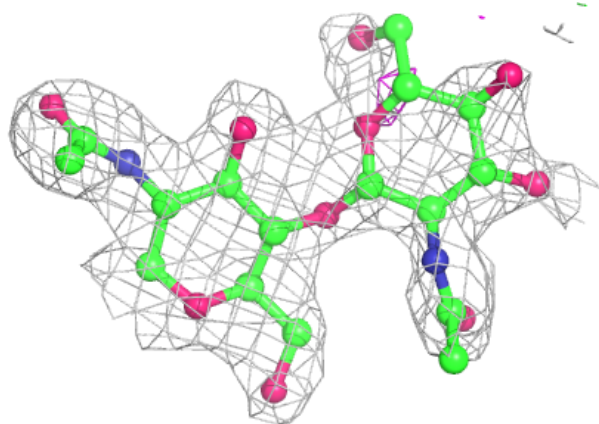
Electron density around Chain D:

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



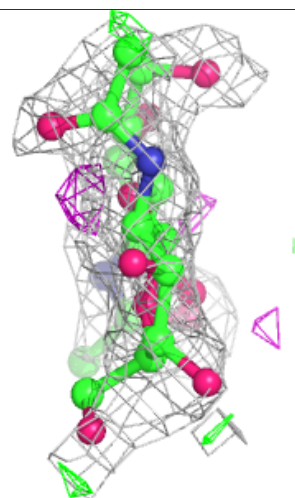
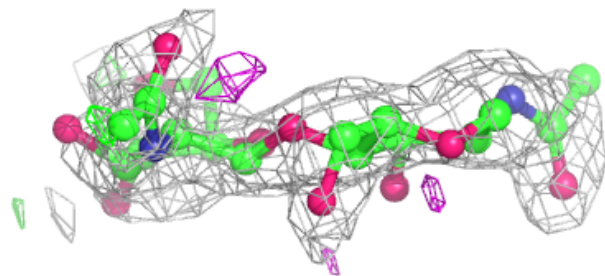
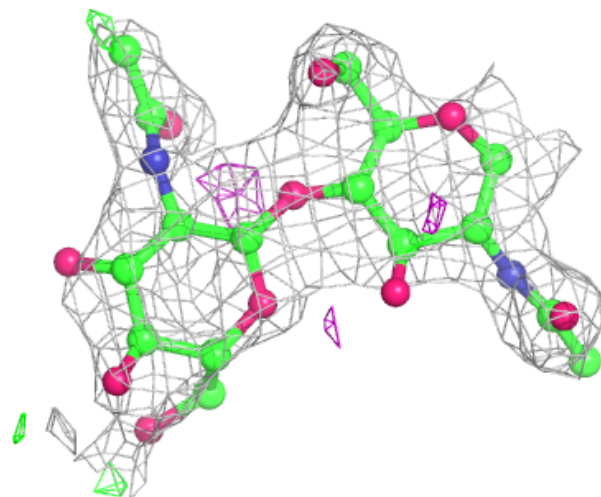
Electron density around Chain E:

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



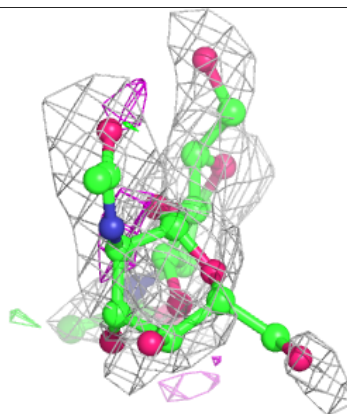
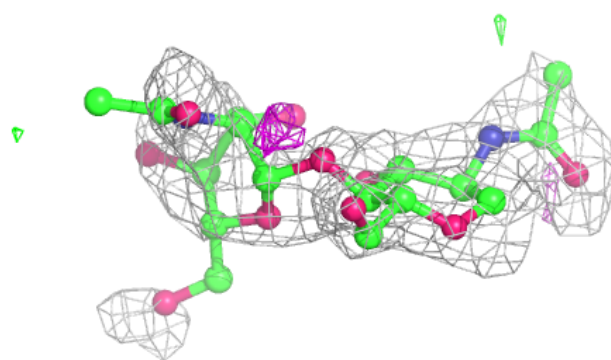
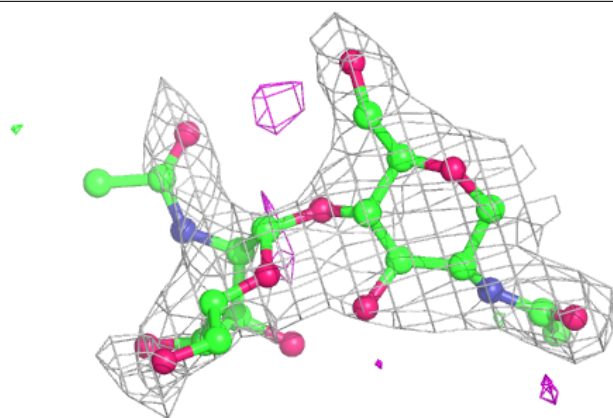
Electron density around Chain F:

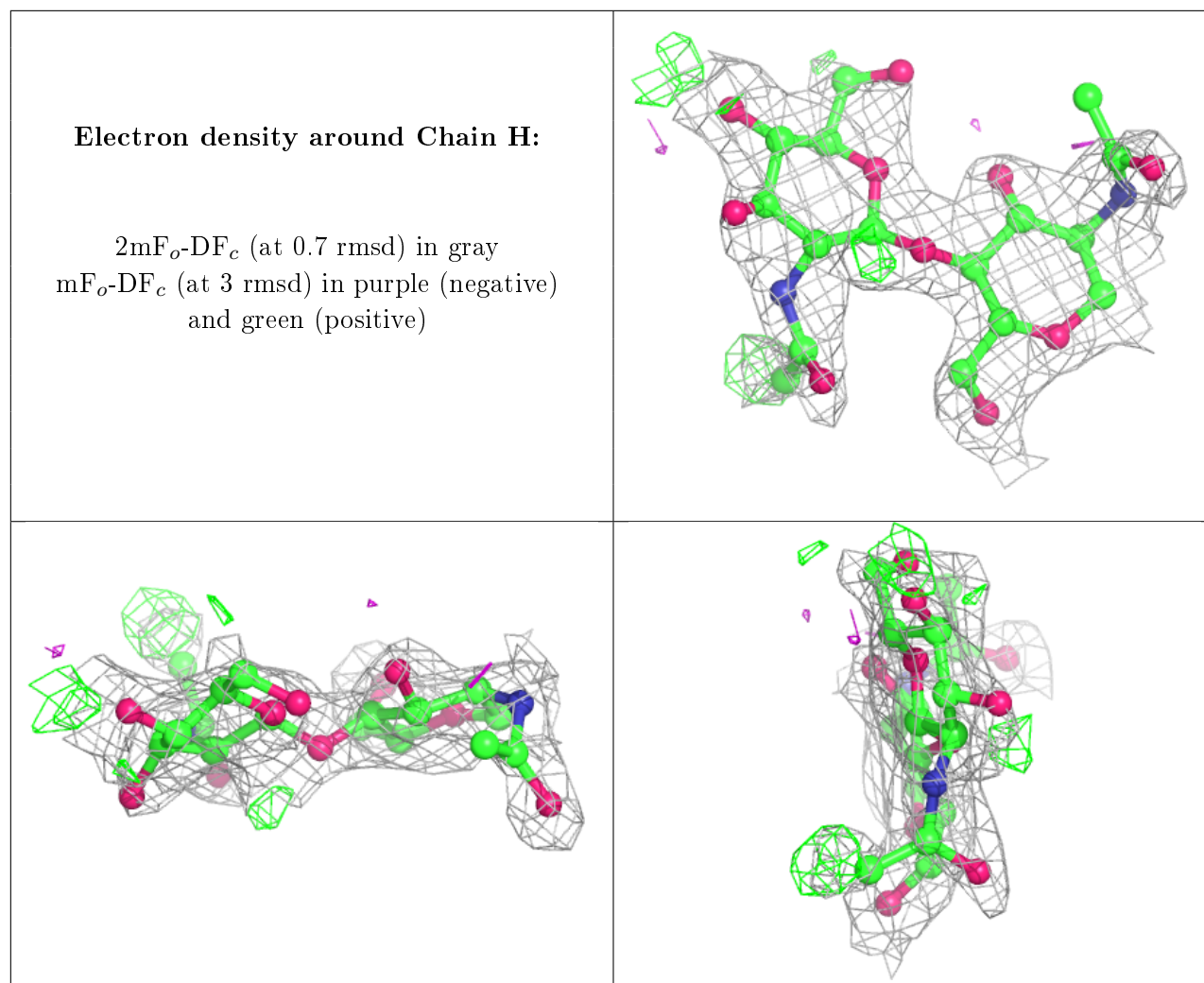
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
5	GOL	C	506	6/6	0.79	0.25	41,44,47,49	0
4	SO4	C	505	5/5	0.80	0.33	34,35,35,36	5
7	NAG	C	509	14/15	0.82	0.18	58,60,61,63	0
5	GOL	A	508	6/6	0.83	0.18	40,41,42,42	0
5	GOL	B	508	6/6	0.90	0.33	38,40,42,43	0
5	GOL	B	510	6/6	0.90	0.16	39,40,41,43	0
5	GOL	C	507	6/6	0.91	0.14	27,29,32,36	0
4	SO4	B	507	5/5	0.93	0.13	25,25,26,26	5
5	GOL	B	509	6/6	0.94	0.09	27,31,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	507	5/5	0.95	0.10	18,20,20,21	5
4	SO4	A	505	5/5	0.96	0.11	41,42,43,43	0
5	GOL	A	509	6/6	0.96	0.08	21,26,26,28	0
5	GOL	B	511	6/6	0.97	0.09	22,25,26,27	0
4	SO4	A	506	5/5	0.98	0.15	53,53,53,54	0
6	PER	C	510	2/2	0.99	0.08	18,18,18,20	0
3	CU	B	504	1/1	0.99	0.05	20,20,20,20	0
4	SO4	B	505	5/5	0.99	0.04	16,21,23,23	0
6	PER	A	512	2/2	0.99	0.12	30,30,30,33	0
4	SO4	B	506	5/5	0.99	0.06	24,25,28,28	0
6	PER	B	514	2/2	0.99	0.08	36,36,36,37	0
3	CU	C	504	1/1	0.99	0.07	19,19,19,19	0
3	CU	A	502	1/1	0.99	0.06	18,18,18,18	0
3	CU	A	504	1/1	1.00	0.04	16,16,16,16	0
3	CU	C	503	1/1	1.00	0.06	15,15,15,15	0
3	CU	C	502	1/1	1.00	0.07	20,20,20,20	0
3	CU	A	501	1/1	1.00	0.04	18,18,18,18	0
3	CU	B	503	1/1	1.00	0.05	18,18,18,18	0
3	CU	B	501	1/1	1.00	0.06	17,17,17,17	0
3	CU	B	502	1/1	1.00	0.05	21,21,21,21	0
3	CU	A	503	1/1	1.00	0.06	14,14,14,14	0
3	CU	C	501	1/1	1.00	0.04	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.