Full wwPDB X-ray Structure Validation Report

Aug 6, 2020 – 04:34 PM BST

PDB ID	:	2WZE
Title	:	High resolution crystallographic structure of the Clostridium thermocellum N-terminal endo-1,4-beta-D-xylanase 10B (Xyn10B) CBM22-1- GH10 modules complexed with xylohexaose
Authors	:	Najmudin, S.; Pinheiro, B.A.; Romao, M.J.; Prates, J.A.M.; Fontes, C.M.G.A.
Deposited on	:	2009-11-27
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

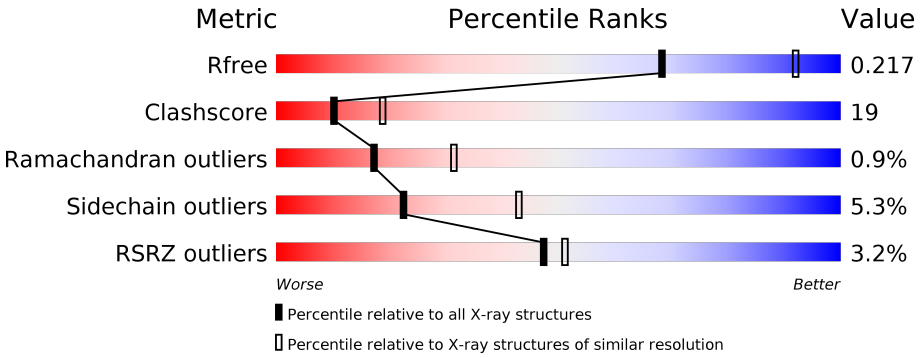
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	540	2% 71% 20% • • 5%
1	B	540	4% 76% 17% • •
2	C	3	100%
2	D	3	33% 67%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1556	-	-	X	-
4	GOL	A	1557	-	X	-	-
4	GOL	A	1561	-	-	-	X
4	GOL	B	1557	-	X	X	-
4	GOL	B	1558	-	-	X	-
4	GOL	B	1559	-	-	X	-
4	GOL	B	1561	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9212 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 ENDO-1,4-BETA-XYLANASE Y.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	Se	0	4	0
			4055	2546	689	802	8	10			
1	B	516	Total	C	N	O	S	Se	0	6	0
			4083	2562	694	809	8	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	-	expression tag	UNP P51584
A	13	GLY	-	expression tag	UNP P51584
A	14	SER	-	expression tag	UNP P51584
A	15	SER	-	expression tag	UNP P51584
A	16	HIS	-	expression tag	UNP P51584
A	17	HIS	-	expression tag	UNP P51584
A	18	HIS	-	expression tag	UNP P51584
A	19	HIS	-	expression tag	UNP P51584
A	20	HIS	-	expression tag	UNP P51584
A	21	HIS	-	expression tag	UNP P51584
A	22	SER	-	expression tag	UNP P51584
A	23	SER	-	expression tag	UNP P51584
A	24	GLY	-	expression tag	UNP P51584
A	25	LEU	-	expression tag	UNP P51584
A	26	VAL	-	expression tag	UNP P51584
A	27	PRO	-	expression tag	UNP P51584
A	28	ARG	-	expression tag	UNP P51584
A	29	GLY	-	expression tag	UNP P51584
A	30	SER	-	expression tag	UNP P51584
A	31	HIS	-	expression tag	UNP P51584
A	32	MSE	-	expression tag	UNP P51584
B	12	MSE	-	expression tag	UNP P51584
B	13	GLY	-	expression tag	UNP P51584
B	14	SER	-	expression tag	UNP P51584
B	15	SER	-	expression tag	UNP P51584

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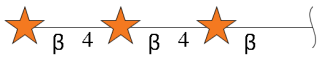
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	HIS	-	expression tag	UNP P51584
B	17	HIS	-	expression tag	UNP P51584
B	18	HIS	-	expression tag	UNP P51584
B	19	HIS	-	expression tag	UNP P51584
B	20	HIS	-	expression tag	UNP P51584
B	21	HIS	-	expression tag	UNP P51584
B	22	SER	-	expression tag	UNP P51584
B	23	SER	-	expression tag	UNP P51584
B	24	GLY	-	expression tag	UNP P51584
B	25	LEU	-	expression tag	UNP P51584
B	26	VAL	-	expression tag	UNP P51584
B	27	PRO	-	expression tag	UNP P51584
B	28	ARG	-	expression tag	UNP P51584
B	29	GLY	-	expression tag	UNP P51584
B	30	SER	-	expression tag	UNP P51584
B	31	HIS	-	expression tag	UNP P51584
B	32	MSE	-	expression tag	UNP P51584
A	337	ALA	GLU	engineered mutation	UNP P51584
B	337	ALA	GLU	engineered mutation	UNP P51584

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.

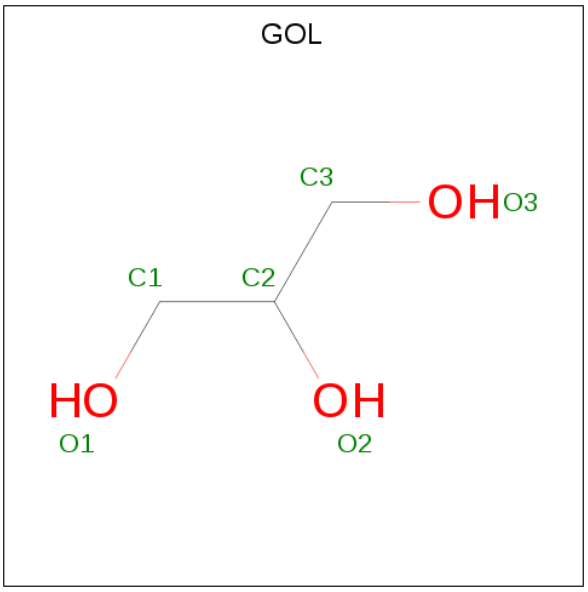


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	3	Total C O 28 15 13	0	0	0
2	D	3	Total C O 28 15 13	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

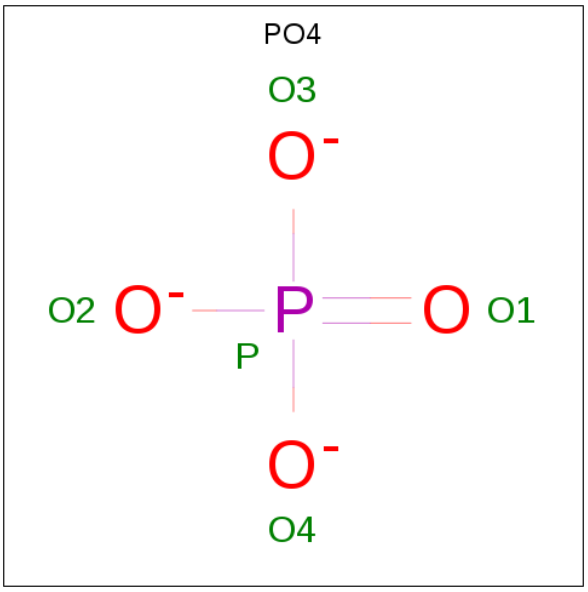
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

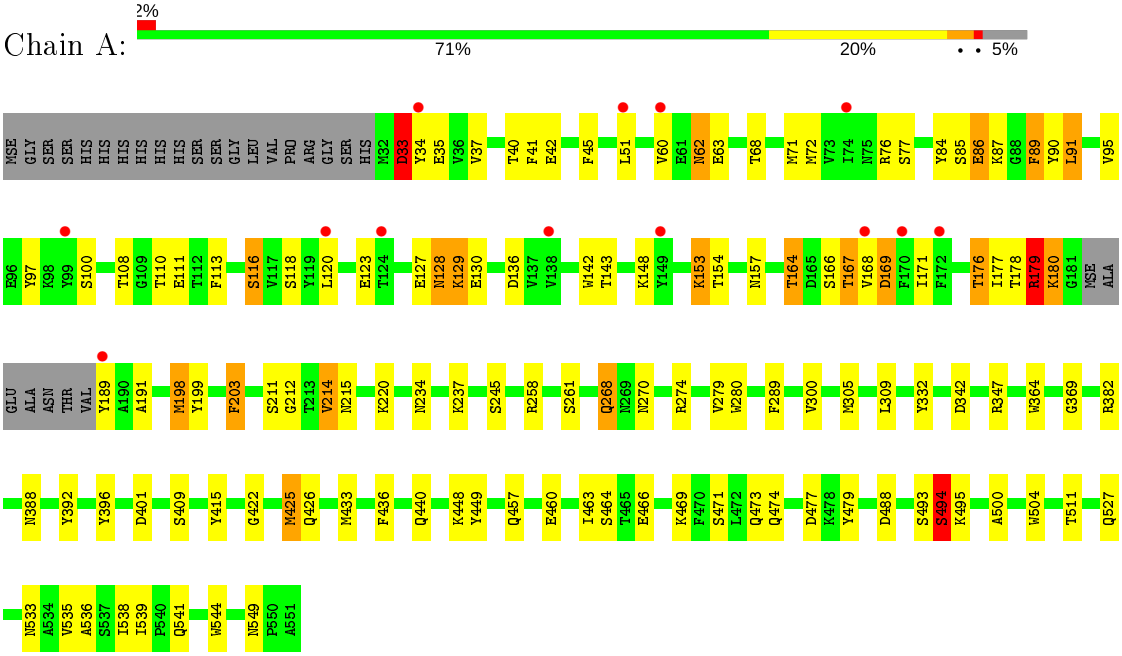
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	422	Total O 422 422	0	0
6	B	512	Total O 512 512	0	0

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.

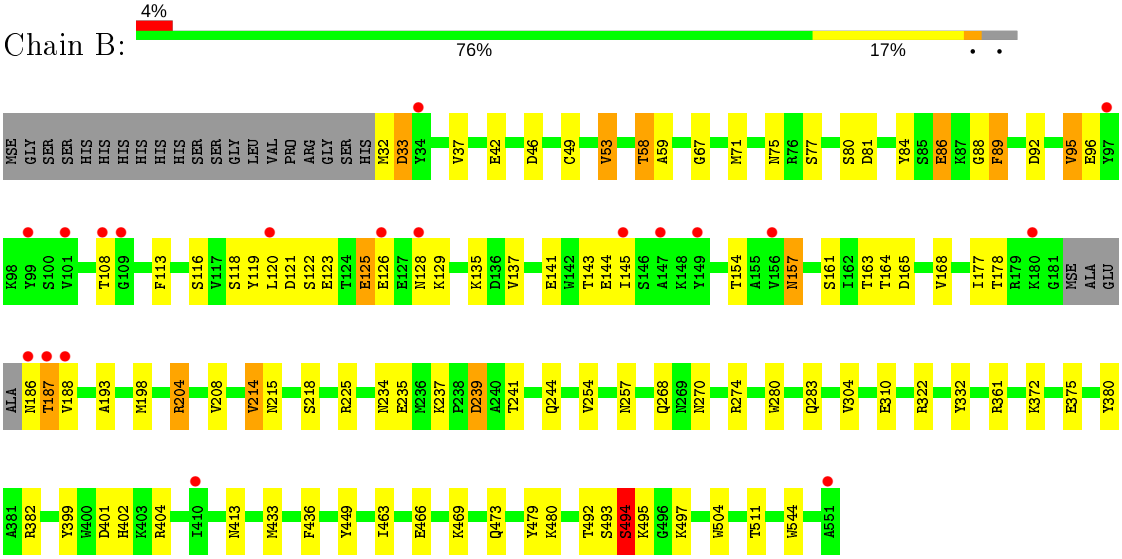
- Molecule 1: ENDO-1,4-BETA-XYLANASE Y

Chain A:



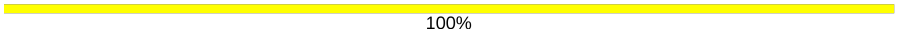
- Molecule 1: ENDO-1,4-BETA-XYLANASE Y

Chain B:



• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain C:



• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.04Å 173.04Å 136.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.02 – 2.50 100.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.02-2.50) 100.0 (100.77-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.147 , 0.189 0.176 , 0.217	Depositor DCC
R_{free} test set	4129 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9212	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, CA, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.07	4/4146 (0.1%)	0.94	8/5615 (0.1%)
1	B	1.19	7/4180 (0.2%)	0.98	6/5663 (0.1%)
All	All	1.14	11/8326 (0.1%)	0.96	14/11278 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86[A]	GLU	CG-CD	6.27	1.61	1.51
1	A	86[B]	GLU	CG-CD	6.27	1.61	1.51
1	B	42	GLU	CB-CG	6.21	1.64	1.52
1	A	203	PHE	CE1-CZ	6.14	1.49	1.37
1	B	42	GLU	CG-CD	5.69	1.60	1.51
1	B	84	TYR	CE2-CZ	5.63	1.45	1.38
1	B	235	GLU	CG-CD	5.39	1.60	1.51
1	B	399	TYR	CD1-CE1	5.12	1.47	1.39
1	B	304	VAL	CB-CG2	5.05	1.63	1.52
1	B	449	TYR	CD1-CE1	-5.03	1.31	1.39
1	A	533	ASN	CB-CG	5.01	1.62	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	361	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	B	361	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	204	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	46	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	169	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	169	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	274	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	179	ARG	N-CA-C	-5.67	95.69	111.00
1	A	198[B]	MSE	CB-CG-SE	5.31	128.63	112.70
1	A	198[C]	MSE	CB-CG-SE	5.31	128.63	112.70
1	A	342	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	425	MSE	CG-SE-CE	-5.14	87.60	98.90
1	A	258	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	239	ASP	CB-CG-OD1	-5.04	113.77	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	GLY	Peptide
1	A	494	SER	Peptide
1	B	494	SER	Peptide

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	4055	0	3865	180	0
1	B	4083	0	3893	102	0
2	C	28	0	0	0	0
2	D	28	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	48	13	0
4	B	36	0	47	21	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	422	0	0	76	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	512	0	0	58	1
All	All	9212	0	7853	302	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 19.

All (302) 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:B:493:SER:HA	1:B:494:SER:OG	1.30	1.21
1:A:169:ASP:HB3	6:A:2107:HOH:O	1.36	1.19
1:A:425:MSE:HE3	1:A:449:TYR:CD2	1.76	1.18
1:A:77:SER:HB3	6:A:2034:HOH:O	1.45	1.16
4:B:1556:GOL:H31	6:B:2497:HOH:O	1.46	1.11
1:A:527[B]:GLN:OE1	6:A:2389:HOH:O	1.66	1.11
1:A:136:ASP:HB2	6:A:2077:HOH:O	1.49	1.10
1:A:448:LYS:HE2	6:A:2332:HOH:O	1.51	1.10
1:A:539:ILE:HD13	6:A:2398:HOH:O	1.51	1.10
1:A:493:SER:HA	1:A:494:SER:HB2	1.19	1.09
1:A:425:MSE:HE3	1:A:449:TYR:HD2	1.10	1.09
1:A:493:SER:HA	1:A:494:SER:CB	1.83	1.08
1:A:300:VAL:HG21	1:A:305:MSE:HE2	1.17	1.08
1:A:198[B]:MSE:HE3	1:A:539:ILE:H	1.14	1.07
1:A:300:VAL:HG21	1:A:305:MSE:CE	1.84	1.05
1:A:179:ARG:HD2	6:A:2111:HOH:O	1.57	1.04
1:B:493:SER:OG	1:B:494:SER:HB2	1.59	1.03
1:A:108:THR:HG22	6:A:2061:HOH:O	1.59	1.02
4:B:1561:GOL:H11	6:B:2510:HOH:O	1.60	1.01
1:A:436:PHE:H	4:A:1556:GOL:H11	1.22	1.01
1:A:527[B]:GLN:NE2	6:A:2390:HOH:O	1.93	1.01
1:A:179:ARG:HB2	1:A:180:LYS:HB3	1.39	1.00
1:B:413:ASN:HB2	6:B:2362:HOH:O	1.59	1.00
1:A:466:GLU:HG2	6:A:2340:HOH:O	1.62	1.00
4:B:1561:GOL:H12	6:B:2509:HOH:O	1.60	1.00
1:B:244:GLN:HG2	6:B:2206:HOH:O	1.60	0.99
1:A:493:SER:OG	1:A:494:SER:HB3	1.62	0.99
1:A:300:VAL:CG2	1:A:305:MSE:CE	2.43	0.95
1:A:89:PHE:CE1	6:A:2138:HOH:O	2.19	0.94
1:A:179:ARG:CB	1:A:180:LYS:HB3	1.99	0.91
1:B:493:SER:HA	1:B:494:SER:CB	2.01	0.91
1:A:493:SER:HB2	6:A:2369:HOH:O	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198[B]:MSE:HE3	1:A:539:ILE:N	1.86	0.89
4:B:1558:GOL:H12	6:B:2502:HOH:O	1.72	0.89
1:A:300:VAL:CG2	1:A:305:MSE:HE2	2.02	0.88
1:A:436:PHE:N	4:A:1556:GOL:H11	1.89	0.88
1:A:448:LYS:CE	6:A:2332:HOH:O	2.12	0.88
1:A:198[B]:MSE:CE	1:A:539:ILE:H	1.87	0.86
1:A:270:ASN:HB2	6:A:2199:HOH:O	1.75	0.86
1:A:76:ARG:NH2	1:A:166:SER:O	2.09	0.86
1:B:493:SER:CB	1:B:494:SER:HB2	2.04	0.85
1:A:425:MSE:SE	6:A:2291:HOH:O	2.44	0.85
1:A:527[B]:GLN:HG2	6:A:2391:HOH:O	1.76	0.85
1:B:32:MSE:HE2	6:B:2006:HOH:O	1.76	0.84
1:A:89:PHE:CE2	1:A:214:VAL:HG22	2.12	0.84
1:B:404:ARG:HH12	4:B:1561:GOL:H2	1.41	0.84
1:A:211:SER:HB2	6:A:2136:HOH:O	1.78	0.83
1:A:493:SER:CA	1:A:494:SER:CB	2.55	0.83
1:B:204:ARG:HH21	4:B:1559:GOL:H32	1.42	0.83
1:B:234:ASN:HA	1:B:237:LYS:HD2	1.58	0.83
1:B:237:LYS:HE2	1:B:280:TRP:CZ3	2.13	0.82
1:A:539:ILE:HA	6:A:2398:HOH:O	1.79	0.82
4:A:1558:GOL:H31	6:A:2416:HOH:O	1.80	0.82
1:B:493:SER:CA	1:B:494:SER:OG	2.23	0.81
1:B:495:LYS:HE2	6:B:2364:HOH:O	1.80	0.81
1:A:300:VAL:HG22	1:A:305:MSE:HE3	1.62	0.81
1:B:154:THR:HB	6:B:2084:HOH:O	1.80	0.81
1:A:300:VAL:CG2	1:A:305:MSE:HE3	2.09	0.80
1:B:75:ASN:HB2	6:B:2034:HOH:O	1.80	0.79
4:B:1559:GOL:H31	6:B:2506:HOH:O	1.82	0.78
1:A:110:THR:HG21	1:A:136:ASP:HB3	1.64	0.78
1:B:237:LYS:HE2	1:B:280:TRP:HZ3	1.48	0.78
1:B:493:SER:CA	1:B:494:SER:CB	2.61	0.78
1:A:113:PHE:HA	6:A:2066:HOH:O	1.84	0.77
2:D:2:XYP:O4	2:D:3:XYP:C2	2.32	0.77
1:A:527[A]:GLN:HG2	6:A:2391:HOH:O	1.85	0.77
1:A:116:SER:HB2	6:A:2067:HOH:O	1.83	0.77
1:A:237:LYS:HE2	1:A:280:TRP:CZ3	2.19	0.77
1:A:425:MSE:CE	1:A:449:TYR:CD2	2.65	0.76
1:A:198[B]:MSE:HE1	1:A:538:ILE:H	1.48	0.76
1:A:180:LYS:HE2	1:A:180:LYS:HA	1.66	0.75
1:B:493:SER:HA	1:B:494:SER:HG	1.50	0.75
1:A:153:LYS:HG3	6:A:2094:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1557:GOL:C3	6:B:2500:HOH:O	2.35	0.75
1:A:425:MSE:HE3	1:A:449:TYR:CE2	2.21	0.74
1:A:535:VAL:HG13	6:A:2122:HOH:O	1.88	0.73
1:B:67:GLY:HA2	6:B:2022:HOH:O	1.87	0.73
4:A:1558:GOL:O1	6:A:2417:HOH:O	2.07	0.73
1:A:488:ASP:HB3	6:A:2357:HOH:O	1.88	0.73
2:D:2:XYP:C4	2:D:3:XYP:C1	2.66	0.73
1:A:34:TYR:CE1	6:A:2113:HOH:O	2.40	0.73
1:B:494:SER:CB	6:B:2445:HOH:O	2.36	0.73
1:A:493:SER:CA	1:A:494:SER:HB2	2.10	0.73
1:B:466:GLU:HG2	6:B:2409:HOH:O	1.89	0.73
1:A:469:LYS:HZ1	4:B:1558:GOL:H31	1.55	0.72
1:A:274:ARG:HE	1:A:457:GLN:NE2	1.87	0.72
4:B:1561:GOL:H31	6:B:2356:HOH:O	1.90	0.72
4:A:1560:GOL:C1	6:A:2400:HOH:O	2.37	0.72
1:A:473[A]:GLN:HG2	6:A:2348:HOH:O	1.90	0.71
1:B:80:SER:HA	6:B:2041:HOH:O	1.89	0.71
1:A:469:LYS:NZ	4:B:1558:GOL:H31	2.06	0.71
1:A:179:ARG:CA	1:A:180:LYS:HB3	2.21	0.71
4:B:1557:GOL:C2	6:B:2500:HOH:O	2.37	0.70
1:B:144:GLU:HG3	6:B:2064:HOH:O	1.91	0.70
1:B:494:SER:HB2	6:B:2445:HOH:O	1.91	0.70
1:A:179:ARG:CA	1:A:180:LYS:CB	2.71	0.69
1:A:76:ARG:HH12	1:A:164:THR:H	1.41	0.69
1:B:493:SER:OG	1:B:494:SER:CB	2.39	0.69
1:A:471:SER:HB2	1:A:473[A]:GLN:OE1	1.93	0.68
1:A:153:LYS:HE2	1:A:154:THR:HG23	1.75	0.68
1:A:34:TYR:CD2	6:A:2005:HOH:O	2.46	0.68
1:A:180:LYS:CG	6:A:2052:HOH:O	2.41	0.68
1:B:86:GLU:OE1	1:B:157[B]:ASN:OD1	2.12	0.68
1:A:110:THR:CG2	1:A:136:ASP:HB3	2.23	0.67
1:A:415:TYR:OH	1:A:495:LYS:HE2	1.94	0.67
1:A:433:MSE:HE1	1:A:477:ASP:O	1.93	0.67
1:B:204:ARG:HH21	4:B:1559:GOL:C3	2.07	0.67
1:A:440:GLN:HG3	6:A:2322:HOH:O	1.95	0.67
1:A:198[C]:MSE:HE3	1:A:544:TRP:CZ2	2.29	0.67
1:A:234:ASN:HA	1:A:237:LYS:HD2	1.76	0.66
1:A:176:THR:HG22	6:A:2110:HOH:O	1.95	0.65
1:A:237:LYS:HE2	1:A:280:TRP:HZ3	1.61	0.65
1:A:425:MSE:CE	1:A:449:TYR:HD2	1.97	0.65
1:A:180:LYS:HG2	6:A:2052:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:HA	6:B:2051:HOH:O	1.96	0.65
1:A:268:GLN:HG2	6:A:2192:HOH:O	1.96	0.65
1:A:179:ARG:HA	1:A:180:LYS:CB	2.28	0.64
1:B:141:GLU:HA	6:B:2109:HOH:O	1.97	0.64
4:B:1561:GOL:C1	6:B:2509:HOH:O	2.30	0.64
4:A:1558:GOL:C3	6:A:2416:HOH:O	2.42	0.64
1:B:88:GLY:HA3	1:B:215:ASN:OD1	1.98	0.64
1:A:35:GLU:HA	1:A:178:THR:HG22	1.79	0.64
1:B:225:ARG:HD3	6:B:2193:HOH:O	1.96	0.64
4:B:1557:GOL:C1	6:B:2500:HOH:O	2.47	0.64
1:B:58:THR:HG22	6:B:2018:HOH:O	1.97	0.64
1:A:433:MSE:HE3	1:A:477:ASP:HB3	1.79	0.63
1:B:120:LEU:HG	6:B:2089:HOH:O	1.98	0.63
1:B:493:SER:CB	1:B:494:SER:CB	2.76	0.62
1:A:118:SER:OG	1:A:129:LYS:HB3	2.00	0.61
4:A:1556:GOL:H2	6:A:2412:HOH:O	1.99	0.61
1:B:58:THR:HG23	1:B:322:ARG:NH1	2.15	0.61
1:A:473[A]:GLN:H	1:A:473[A]:GLN:CD	2.04	0.61
1:A:463:ILE:HD12	1:A:479:TYR:CD1	2.36	0.61
1:A:549:ASN:HB3	6:A:2406:HOH:O	2.00	0.61
1:B:198[B]:MSE:HG2	1:B:544:TRP:CE2	2.35	0.61
1:A:167:THR:HG23	6:A:2106:HOH:O	1.99	0.60
1:A:87:LYS:HB2	1:A:91:LEU:HD22	1.82	0.60
1:A:130:GLU:HB2	6:A:2091:HOH:O	2.02	0.60
1:A:130:GLU:HB3	6:A:2074:HOH:O	2.02	0.60
4:B:1557:GOL:H31	6:B:2500:HOH:O	1.96	0.60
1:A:198[B]:MSE:HE1	1:A:538:ILE:N	2.17	0.59
1:A:493:SER:CB	1:A:494:SER:HB3	2.31	0.59
1:A:440:GLN:CG	6:A:2322:HOH:O	2.48	0.59
1:A:289:PHE:HA	1:A:305:MSE:HE1	1.84	0.59
1:B:495:LYS:CE	6:B:2364:HOH:O	2.42	0.59
1:A:180:LYS:HA	1:A:180:LYS:CE	2.32	0.59
1:A:473[A]:GLN:CG	6:A:2348:HOH:O	2.51	0.58
1:B:186:ASN:O	1:B:187:THR:HB	2.02	0.58
1:A:198[B]:MSE:HG3	1:A:539:ILE:HB	1.84	0.58
1:A:198[B]:MSE:HE2	1:A:199:TYR:OH	2.03	0.58
1:A:179:ARG:HA	1:A:180:LYS:HB2	1.85	0.58
1:A:211:SER:CB	6:A:2136:HOH:O	2.45	0.58
1:A:469:LYS:NZ	4:B:1558:GOL:C3	2.67	0.58
1:A:457:GLN:HG2	1:A:500:ALA:HB3	1.86	0.58
1:B:33:ASP:HB3	6:B:2005:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198[B]:MSE:HE3	1:A:539:ILE:HG12	1.85	0.57
1:A:220:LYS:HE3	6:A:2148:HOH:O	2.04	0.57
1:B:239:ASP:HB3	6:B:2203:HOH:O	2.03	0.57
1:A:40:THR:O	1:A:42:GLU:HG2	2.05	0.57
1:A:34:TYR:HE1	6:A:2113:HOH:O	1.84	0.57
1:B:135:LYS:HB2	6:B:2097:HOH:O	2.04	0.57
1:B:493:SER:HB2	6:B:2442:HOH:O	2.04	0.57
1:A:463:ILE:HD12	1:A:479:TYR:CG	2.40	0.57
1:B:198[A]:MSE:HG2	1:B:544:TRP:CE2	2.39	0.57
4:A:1556:GOL:H12	1:B:469:LYS:NZ	2.19	0.57
4:A:1556:GOL:C2	6:A:2412:HOH:O	2.50	0.56
1:A:464:SER:HB2	4:A:1559:GOL:H31	1.87	0.56
1:A:541:GLN:HA	1:A:544:TRP:CE2	2.40	0.56
1:B:204:ARG:NH2	4:B:1559:GOL:H32	2.15	0.56
1:A:86[B]:GLU:HG3	1:A:157:ASN:OD1	2.05	0.55
1:A:388:ASN:HB3	6:A:2283:HOH:O	2.05	0.55
1:B:113:PHE:HA	6:B:2077:HOH:O	2.05	0.55
1:B:463:ILE:HD12	1:B:479:TYR:CD1	2.42	0.55
1:A:128:ASN:CB	6:A:2073:HOH:O	2.55	0.55
1:A:164:THR:HG22	6:A:2066:HOH:O	2.06	0.55
1:B:125:GLU:OE2	1:B:125:GLU:HA	2.07	0.54
1:A:494:SER:HB2	6:A:2371:HOH:O	2.08	0.54
1:B:116:SER:HB2	1:B:161[B]:SER:OG	2.07	0.54
1:B:214:VAL:O	1:B:214:VAL:HG13	2.07	0.54
1:A:425:MSE:CE	1:A:449:TYR:CE2	2.87	0.54
1:A:214:VAL:HG12	1:A:215:ASN:ND2	2.23	0.54
1:B:53:VAL:HB	6:B:2014:HOH:O	2.08	0.53
1:B:135:LYS:HB3	1:B:145:ILE:HD12	1.89	0.53
1:A:198[B]:MSE:HE2	1:A:199:TYR:CZ	2.44	0.53
1:A:60:VAL:HG23	1:A:63:GLU:HB2	1.91	0.53
1:A:433:MSE:CE	1:A:477:ASP:C	2.77	0.53
1:A:90:TYR:HA	6:A:2149:HOH:O	2.08	0.53
1:B:436:PHE:HB2	4:B:1558:GOL:H32	1.91	0.52
1:B:497:LYS:HE3	6:B:2436:HOH:O	2.09	0.52
1:B:32:MSE:HG3	1:B:33:ASP:N	2.25	0.52
1:A:180:LYS:HG3	6:A:2052:HOH:O	2.06	0.52
1:B:375:GLU:HG2	6:B:2329:HOH:O	2.10	0.52
1:A:33:ASP:HA	6:A:2002:HOH:O	2.08	0.51
1:A:198[B]:MSE:SE	1:A:536:ALA:HA	2.61	0.51
1:B:86:GLU:HG2	6:B:2021:HOH:O	2.09	0.51
1:A:535:VAL:HG22	6:A:2122:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:O	1:A:179:ARG:O	2.27	0.51
1:A:108:THR:HA	6:A:2059:HOH:O	2.10	0.51
1:A:95:VAL:HG11	6:A:2111:HOH:O	2.10	0.51
1:A:128:ASN:HB2	6:A:2073:HOH:O	2.10	0.51
1:A:34:TYR:HD2	6:A:2005:HOH:O	1.87	0.50
1:B:208:VAL:HG21	1:B:504:TRP:CE3	2.47	0.50
1:B:401[A]:ASP:OD1	1:B:402:HIS:N	2.44	0.50
1:A:189:TYR:CE2	1:A:191:ALA:HA	2.47	0.50
1:A:76:ARG:HH12	1:A:164:THR:N	2.09	0.50
1:A:40:THR:O	1:A:42:GLU:N	2.44	0.50
1:A:198[B]:MSE:CE	1:A:535:VAL:O	2.60	0.49
1:B:118:SER:HB2	6:B:2082:HOH:O	2.11	0.49
1:A:63:GLU:O	1:A:142:TRP:HZ2	1.96	0.49
1:A:215:ASN:HB3	6:A:2099:HOH:O	2.12	0.48
1:A:45:PHE:CD1	1:A:71:MSE:HE1	2.49	0.48
1:B:372:LYS:HE2	6:B:2260:HOH:O	2.14	0.48
1:A:34:TYR:CD1	6:A:2113:HOH:O	2.63	0.48
1:A:309:LEU:HD13	1:A:364:TRP:CH2	2.49	0.48
1:A:84:TYR:HE1	6:A:2042:HOH:O	1.97	0.48
1:A:212:GLY:N	6:A:2136:HOH:O	2.47	0.48
1:A:198[B]:MSE:CG	1:A:539:ILE:HB	2.44	0.47
1:A:268:GLN:OE1	4:A:1561:GOL:H11	2.14	0.47
1:A:289:PHE:HA	1:A:305:MSE:CE	2.44	0.47
1:B:92:ASP:HB2	1:B:95:VAL:CG2	2.44	0.47
4:A:1560:GOL:H12	6:A:2400:HOH:O	2.08	0.47
1:B:37:VAL:HB	1:B:177:ILE:HG13	1.97	0.47
1:B:270:ASN:HB2	6:B:2234:HOH:O	2.14	0.47
1:A:111:GLU:OE1	1:A:111:GLU:HA	2.15	0.47
2:D:2:XYP:O4	2:D:3:XYP:O5	2.30	0.47
1:A:164:THR:HG21	1:A:168:VAL:CG1	2.45	0.47
1:B:81:ASP:O	1:B:163:THR:HG22	2.15	0.47
1:B:137:VAL:HG22	1:B:143:THR:HG21	1.97	0.46
1:A:433:MSE:CE	1:A:477:ASP:HB3	2.43	0.46
1:A:425:MSE:CE	6:A:2291:HOH:O	2.62	0.46
1:A:128:ASN:HB3	6:A:2073:HOH:O	2.15	0.46
1:B:494:SER:HA	1:B:497:LYS:NZ	2.30	0.46
1:B:58:THR:HG23	1:B:322:ARG:HH12	1.80	0.46
1:A:129:LYS:NZ	1:A:129:LYS:HB2	2.31	0.46
1:A:215:ASN:HB2	6:A:2137:HOH:O	2.15	0.46
1:A:388:ASN:H	1:A:388:ASN:HD22	1.63	0.45
1:A:189:TYR:N	6:A:2114:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:HA	6:B:2070:HOH:O	2.16	0.45
1:B:75:ASN:N	6:B:2034:HOH:O	2.50	0.45
1:B:95:VAL:HG11	6:B:2140:HOH:O	2.16	0.45
1:B:121:ASP:C	6:B:2084:HOH:O	2.56	0.44
1:B:32:MSE:N	6:B:2001:HOH:O	2.50	0.44
1:A:527[A]:GLN:CG	6:A:2391:HOH:O	2.56	0.44
1:B:126:GLU:HG3	6:B:2088:HOH:O	2.17	0.44
1:B:494:SER:HB3	6:B:2445:HOH:O	2.10	0.44
1:A:549:ASN:HA	6:A:2405:HOH:O	2.17	0.44
1:B:32:MSE:HG3	1:B:33:ASP:H	1.82	0.44
1:A:129:LYS:NZ	6:A:2071:HOH:O	2.50	0.44
1:A:392:TYR:CE2	1:A:422:GLY:HA3	2.53	0.44
1:B:283:GLN:H	4:B:1557:GOL:C2	2.30	0.44
1:B:92:ASP:HB2	1:B:95:VAL:HG21	2.00	0.44
4:A:1556:GOL:H12	1:B:469:LYS:HZ2	1.82	0.44
1:A:189:TYR:HE2	1:A:191:ALA:HA	1.82	0.44
1:A:198[C]:MSE:HG2	1:A:544:TRP:CE2	2.53	0.44
1:B:129:LYS:HE3	6:B:2093:HOH:O	2.17	0.43
1:A:274:ARG:HE	1:A:457:GLN:HE22	1.60	0.43
1:A:471:SER:CB	1:A:473[A]:GLN:OE1	2.65	0.43
1:B:59:ALA:HB2	1:B:71:MSE:HE1	1.99	0.43
1:A:127:GLU:HB2	1:B:126:GLU:OE1	2.18	0.43
1:A:153:LYS:CG	6:A:2094:HOH:O	2.56	0.43
1:B:193:ALA:HB1	1:B:198[A]:MSE:HE3	2.00	0.43
1:A:388:ASN:ND2	1:A:388:ASN:H	2.16	0.43
1:B:96:GLU:O	6:B:2056:HOH:O	2.21	0.43
1:B:161[A]:SER:HB2	6:B:2129:HOH:O	2.18	0.43
1:A:279:VAL:HG13	1:A:364:TRP:CE2	2.53	0.43
1:A:85:SER:OG	1:A:87:LYS:HE2	2.19	0.43
1:A:37:VAL:HB	1:A:177:ILE:HG13	2.01	0.43
1:B:270:ASN:CB	6:B:2234:HOH:O	2.66	0.43
1:A:493:SER:CA	1:A:494:SER:HB3	2.38	0.43
1:A:97:TYR:O	1:A:148:LYS:HA	2.19	0.43
1:A:469:LYS:HZ2	4:B:1558:GOL:C3	2.31	0.43
1:A:433:MSE:HE1	1:A:477:ASP:C	2.40	0.42
1:A:466:GLU:CG	6:A:2340:HOH:O	2.41	0.42
1:A:471:SER:OG	1:A:474:GLN:HG3	2.18	0.42
1:B:49:CYS:HB3	1:B:257:ASN:CG	2.39	0.42
1:B:119:TYR:N	6:B:2082:HOH:O	2.47	0.42
1:B:186:ASN:O	1:B:187:THR:CB	2.65	0.42
1:B:433:MSE:HE2	6:B:2373:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:MSE:HB2	1:B:433:MSE:HE2	1.92	0.42
1:A:153:LYS:HE2	1:A:154:THR:CG2	2.45	0.42
1:A:396:TYR:HB3	1:A:426:GLN:OE1	2.20	0.42
1:A:460:GLU:HG2	1:A:504:TRP:CE3	2.55	0.42
1:B:122:SER:N	6:B:2084:HOH:O	2.52	0.42
1:B:215:ASN:HB3	6:B:2179:HOH:O	2.20	0.42
1:A:72:MSE:HG3	1:A:171:ILE:HG12	2.01	0.42
1:B:164:THR:HG21	1:B:168:VAL:HG12	2.01	0.42
1:B:123:GLU:HB3	6:B:2123:HOH:O	2.19	0.42
1:A:169:ASP:CB	6:A:2107:HOH:O	2.20	0.41
1:A:68:THR:HA	6:A:2007:HOH:O	2.20	0.41
1:A:179:ARG:HA	1:A:180:LYS:HB3	1.94	0.41
1:B:310:GLU:HG3	1:B:380:TYR:CD1	2.55	0.41
1:B:241:THR:O	1:B:254:VAL:HA	2.21	0.41
1:B:492:THR:HG22	1:B:493:SER:N	2.36	0.41
1:A:97:TYR:HA	1:A:178:THR:O	2.21	0.41
1:B:493:SER:OG	1:B:494:SER:CA	2.69	0.41
1:B:544:TRP:N	1:B:544:TRP:CD1	2.86	0.41
1:A:45:PHE:CG	1:A:71:MSE:HE1	2.56	0.40
1:B:67:GLY:CA	6:B:2022:HOH:O	2.59	0.40
1:A:401:ASP:HB2	6:A:2296:HOH:O	2.21	0.40
1:A:198[B]:MSE:SE	1:A:536:ALA:C	3.10	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)
6:A:2364:HOH:O	6:B:2255:HOH:O[6_765]	2.13	0.07

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	513/540 (95%)	485 (94%)	23 (4%)	5 (1%)	15	28
1	B	518/540 (96%)	488 (94%)	26 (5%)	4 (1%)	19	35
All	All	1031/1080 (96%)	973 (94%)	49 (5%)	9 (1%)	17	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PHE
1	A	180	LYS
1	B	187	THR
1	B	494	SER
1	A	33	ASP
1	A	494	SER
1	A	62	ASN
1	B	188	VAL
1	B	214	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	436/443 (98%)	409 (94%)	27 (6%)	18	35
1	B	441/443 (100%)	421 (96%)	20 (4%)	27	51
All	All	877/886 (99%)	830 (95%)	47 (5%)	22	42

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	51	LEU
1	A	62	ASN
1	A	89	PHE
1	A	91	LEU
1	A	100	SER
1	A	116	SER

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Mol	Chain	Res	Type
1	A	120	LEU
1	A	123	GLU
1	A	128	ASN
1	A	129	LYS
1	A	143	THR
1	A	153	LYS
1	A	164	THR
1	A	167	THR
1	A	176	THR
1	A	179	ARG
1	A	203	PHE
1	A	214	VAL
1	A	245	SER
1	A	261	SER
1	A	268	GLN
1	A	332	TYR
1	A	347	ARG
1	A	382	ARG
1	A	409	SER
1	A	511	THR
1	B	33	ASP
1	B	53	VAL
1	B	58	THR
1	B	77	SER
1	B	86	GLU
1	B	89	PHE
1	B	95	VAL
1	B	125	GLU
1	B	128	ASN
1	B	157[A]	ASN
1	B	157[B]	ASN
1	B	165	ASP
1	B	178	THR
1	B	218	SER
1	B	268	GLN
1	B	332	TYR
1	B	382	ARG
1	B	473	GLN
1	B	480	LYS
1	B	511	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	283	GLN
1	A	388	ASN
1	A	457	GLN
1	A	484	GLN
1	B	328	ASN
1	B	366	GLN
1	B	541	GLN

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

6 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	XYP	C	1	2	10,10,10	1.04	0	14,14,14	2.11	3 (21%)
2	XYP	C	2	2	9,9,10	1.45	2 (22%)	10,12,14	1.56	2 (20%)
2	XYP	C	3	2	9,9,10	1.20	1 (11%)	10,12,14	2.87	6 (60%)
2	XYP	D	1	2	10,10,10	1.45	0	14,14,14	1.99	6 (42%)
2	XYP	D	2	2	9,9,10	1.40	1 (11%)	10,12,14	2.22	6 (60%)
2	XYP	D	3	2	9,9,10	1.01	0	10,12,14	2.23	3 (30%)

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	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3	2	-	-	0/1/1/1
2	XYP	D	1	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1
2	XYP	D	3	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	XYP	O5-C5	3.86	1.50	1.42
2	C	2	XYP	C4-C3	-3.37	1.47	1.52
2	C	2	XYP	O4-C4	2.42	1.48	1.43
2	C	3	XYP	O4-C4	2.36	1.48	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	XYP	C5-O5-C1	5.38	119.80	111.52
2	C	1	XYP	C5-O5-C1	5.31	121.64	112.71
2	D	1	XYP	C5-O5-C1	4.63	120.50	112.71
2	D	3	XYP	C5-C4-C3	4.46	115.15	109.67
2	D	2	XYP	O4-C4-C5	4.44	118.25	109.15
2	C	3	XYP	C1-C2-C3	-4.36	104.30	109.67
2	C	2	XYP	O4-C4-C5	3.59	116.49	109.15
2	D	3	XYP	C5-O5-C1	3.55	116.98	111.52
2	C	3	XYP	O3-C3-C2	-3.37	103.54	109.99
2	D	1	XYP	O5-C5-C4	-3.33	105.63	110.77
2	C	1	XYP	O3-C3-C4	-3.27	103.74	109.99
2	D	2	XYP	C5-O5-C1	3.15	116.37	111.52
2	C	3	XYP	O4-C4-C5	2.96	115.20	109.15
2	D	3	XYP	C4-C3-C2	-2.78	107.62	110.92
2	C	3	XYP	O4-C4-C3	2.60	115.34	110.14
2	C	1	XYP	O1-C1-O5	-2.51	103.17	109.72
2	D	2	XYP	C4-C3-C2	2.24	113.58	110.92
2	C	2	XYP	C5-C4-C3	-2.24	106.91	109.67
2	D	2	XYP	C1-C2-C3	-2.21	106.95	109.67
2	D	2	XYP	C5-C4-C3	2.16	112.33	109.67
2	D	1	XYP	O4-C4-C5	-2.15	104.75	109.15
2	C	3	XYP	O3-C3-C4	-2.14	105.89	109.99
2	D	1	XYP	C5-C4-C3	-2.08	107.11	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	XYP	O2-C2-C3	2.07	115.13	110.35
2	D	2	XYP	O2-C2-C1	-2.06	104.93	109.15
2	D	1	XYP	O3-C3-C4	-2.01	106.15	109.99

There are no chirality outliers.

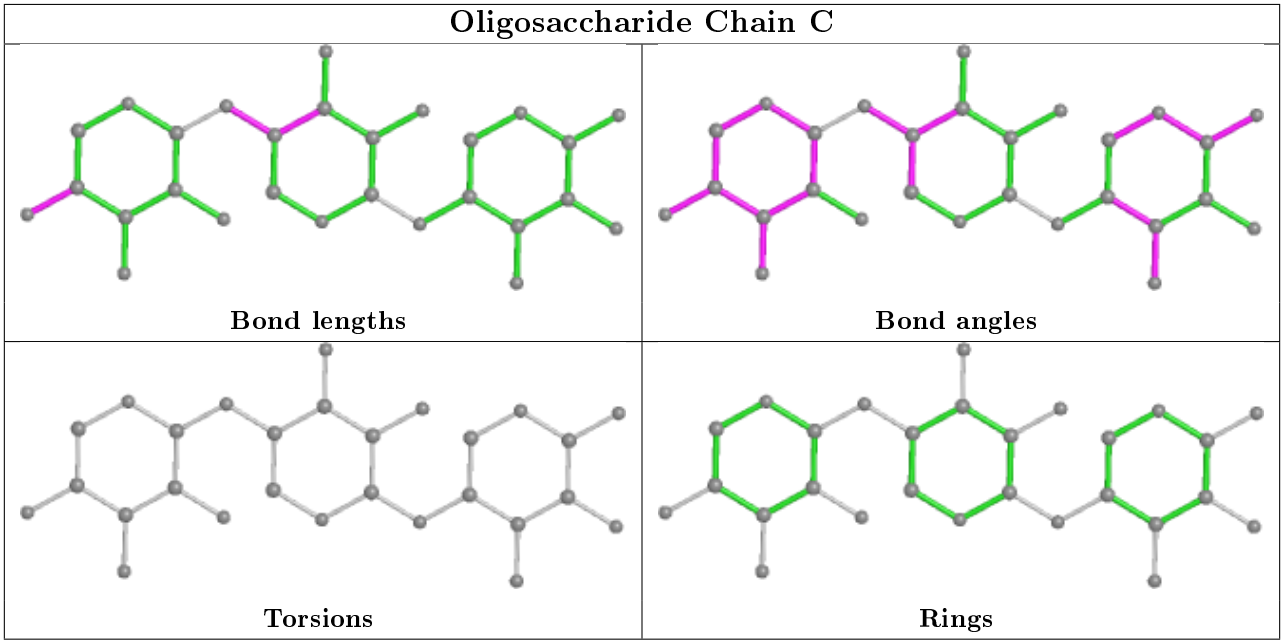
There are no torsion outliers.

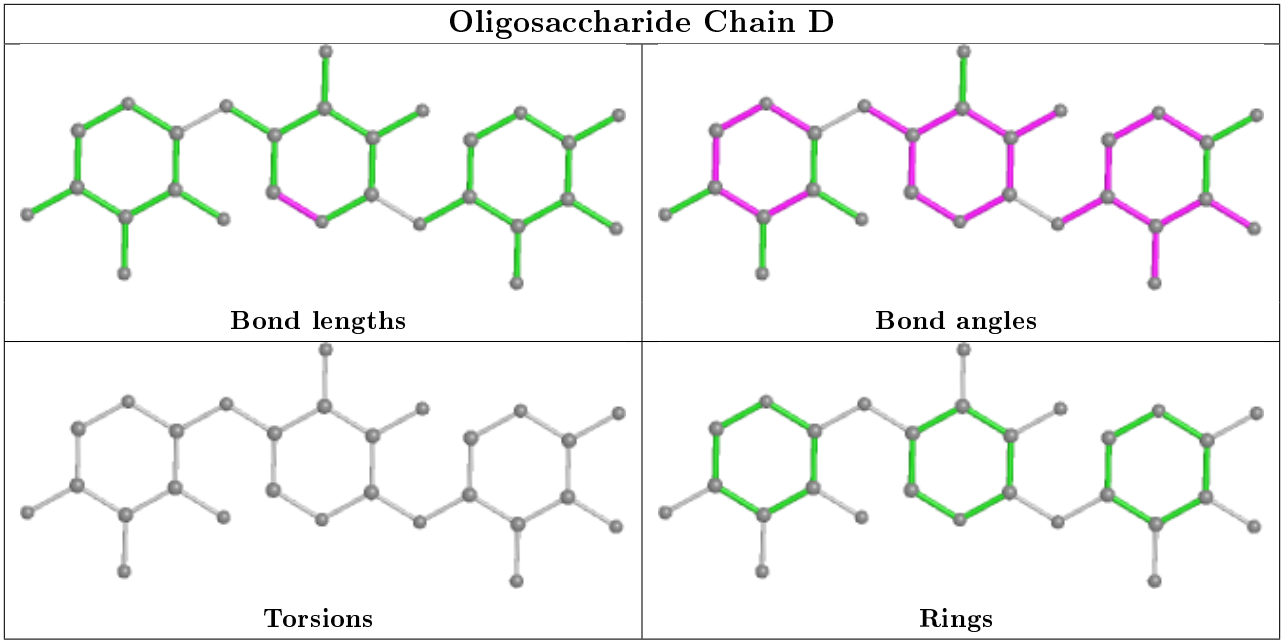
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	XYP	3	0
2	D	3	XYP	3	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
4	GOL	A	1561	-	5,5,5	0.47	0	5,5,5	1.36	0
4	GOL	B	1561	-	5,5,5	0.65	0	5,5,5	1.22	0
5	PO4	A	1562	-	4,4,4	1.35	1 (25%)	6,6,6	1.58	1 (16%)
4	GOL	B	1559	-	5,5,5	0.48	0	5,5,5	1.20	0
4	GOL	A	1556	-	5,5,5	0.80	0	5,5,5	0.94	0
4	GOL	A	1560	-	5,5,5	0.44	0	5,5,5	0.80	0
4	GOL	A	1558	-	5,5,5	0.94	0	5,5,5	1.31	1 (20%)
4	GOL	B	1558	-	5,5,5	0.57	0	5,5,5	0.77	0
4	GOL	B	1557	-	5,5,5	1.72	1 (20%)	5,5,5	2.55	3 (60%)
4	GOL	A	1557	-	5,5,5	1.30	1 (20%)	5,5,5	2.37	2 (40%)
4	GOL	B	1560	-	5,5,5	0.40	0	5,5,5	0.87	0
5	PO4	B	1562	-	4,4,4	1.01	0	6,6,6	1.19	1 (16%)
4	GOL	A	1559	-	5,5,5	1.24	0	5,5,5	1.87	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	B	1556	-	5,5,5	0.70	0	5,5,5	0.61	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
4	GOL	A	1561	-	-	0/4/4/4	-
4	GOL	B	1561	-	-	4/4/4/4	-
4	GOL	B	1559	-	-	4/4/4/4	-
4	GOL	A	1556	-	-	1/4/4/4	-
4	GOL	A	1560	-	-	2/4/4/4	-
4	GOL	A	1558	-	-	4/4/4/4	-
4	GOL	B	1558	-	-	2/4/4/4	-
4	GOL	B	1557	-	-	3/4/4/4	-
4	GOL	A	1557	-	-	4/4/4/4	-
4	GOL	B	1560	-	-	2/4/4/4	-
4	GOL	A	1559	-	-	4/4/4/4	-
4	GOL	B	1556	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1557	GOL	C1-C2	2.68	1.62	1.51
5	A	1562	PO4	P-O1	2.42	1.56	1.50
4	A	1557	GOL	C3-C2	2.13	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1559	GOL	O3-C3-C2	3.88	128.82	110.20
4	A	1557	GOL	O3-C3-C2	3.67	127.81	110.20
4	B	1557	GOL	O1-C1-C2	3.52	127.08	110.20
4	B	1557	GOL	O2-C2-C1	3.48	124.46	109.12
4	A	1557	GOL	O2-C2-C1	-3.28	94.69	109.12
5	A	1562	PO4	O4-P-O2	-2.37	100.36	107.97
4	A	1558	GOL	O3-C3-C2	2.19	120.68	110.20
4	B	1557	GOL	C3-C2-C1	2.17	120.14	111.70
5	B	1562	PO4	O4-P-O3	2.06	114.60	107.97

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1561	GOL	O1-C1-C2-C3
4	B	1559	GOL	O1-C1-C2-O2
4	B	1559	GOL	O1-C1-C2-C3
4	B	1559	GOL	C1-C2-C3-O3
4	A	1560	GOL	C1-C2-C3-O3
4	A	1558	GOL	O1-C1-C2-C3
4	A	1558	GOL	C1-C2-C3-O3
4	B	1557	GOL	O1-C1-C2-C3
4	B	1557	GOL	C1-C2-C3-O3
4	A	1557	GOL	O1-C1-C2-O2
4	A	1557	GOL	O1-C1-C2-C3
4	A	1559	GOL	O1-C1-C2-O2
4	A	1559	GOL	O1-C1-C2-C3
4	A	1559	GOL	C1-C2-C3-O3
4	B	1561	GOL	C1-C2-C3-O3
4	A	1556	GOL	C1-C2-C3-O3
4	B	1558	GOL	C1-C2-C3-O3
4	A	1557	GOL	C1-C2-C3-O3
4	B	1560	GOL	O1-C1-C2-C3
4	B	1556	GOL	O1-C1-C2-C3
4	B	1556	GOL	C1-C2-C3-O3
4	B	1559	GOL	O2-C2-C3-O3
4	A	1558	GOL	O2-C2-C3-O3
4	B	1560	GOL	O1-C1-C2-O2
4	B	1556	GOL	O1-C1-C2-O2
4	A	1560	GOL	O2-C2-C3-O3
4	A	1557	GOL	O2-C2-C3-O3
4	B	1561	GOL	O1-C1-C2-O2
4	A	1558	GOL	O1-C1-C2-O2
4	B	1558	GOL	O2-C2-C3-O3
4	A	1559	GOL	O2-C2-C3-O3
4	B	1557	GOL	O2-C2-C3-O3
4	B	1556	GOL	O2-C2-C3-O3
4	B	1561	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1561	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1561	GOL	5	0
4	B	1559	GOL	4	0
4	A	1556	GOL	6	0
4	A	1560	GOL	2	0
4	A	1558	GOL	3	0
4	B	1558	GOL	6	0
4	B	1557	GOL	5	0
4	A	1559	GOL	1	0
4	B	1556	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	504/540 (93%)	0.81	13 (2%) 56 59	33, 57, 113, 139	0
1	B	507/540 (93%)	0.90	19 (3%) 41 45	28, 46, 102, 145	0
All	All	1011/1080 (93%)	0.85	32 (3%) 47 51	28, 52, 109, 145	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	THR	6.2
1	B	126	GLU	5.5
1	B	120	LEU	4.5
1	B	108	THR	4.1
1	A	170	PHE	3.5
1	A	34	TYR	3.4
1	A	138	VAL	3.1
1	A	124	THR	3.1
1	B	99	TYR	3.1
1	A	51	LEU	2.7
1	B	551	ALA	2.7
1	A	99	TYR	2.6
1	B	180	LYS	2.5
1	B	128	ASN	2.5
1	A	60	VAL	2.5
1	B	188	VAL	2.4
1	A	168	VAL	2.4
1	B	149	TYR	2.3
1	B	34	TYR	2.3
1	A	149	TYR	2.3
1	B	101	VAL	2.2
1	A	189	TYR	2.2
1	A	74	ILE	2.2
1	B	145	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	2.1
1	A	172	PHE	2.1
1	B	147	ALA	2.1
1	B	186	ASN	2.1
1	B	109	GLY	2.1
1	B	156	VAL	2.1
1	B	97	TYR	2.1
1	B	410	ILE	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)

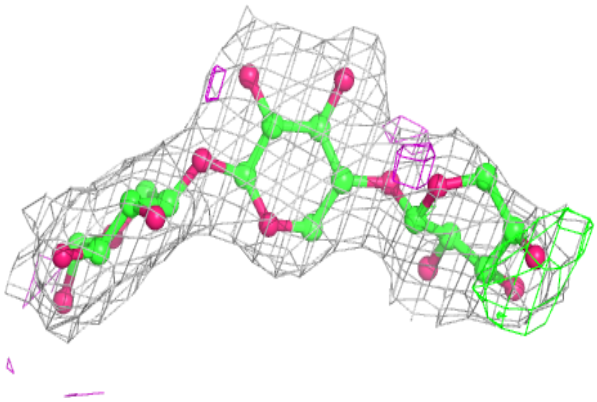
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

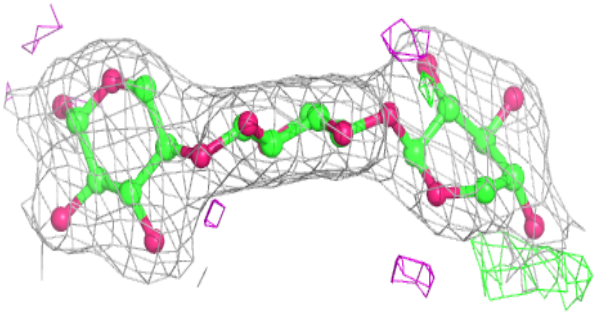
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYP	C	3	9/10	0.91	0.18	56,65,74,78	0
2	XYP	D	3	9/10	0.93	0.17	61,66,70,77	0
2	XYP	C	2	9/10	0.98	0.22	30,33,39,40	0
2	XYP	D	2	9/10	0.99	0.20	30,34,41,43	0
2	XYP	C	1	10/10	0.99	0.23	35,36,38,40	0
2	XYP	D	1	10/10	0.99	0.23	29,33,36,38	0

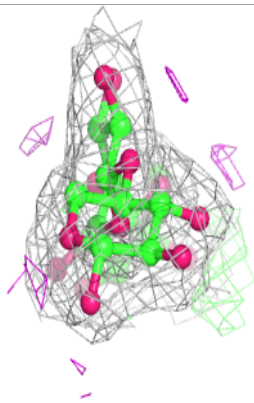
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

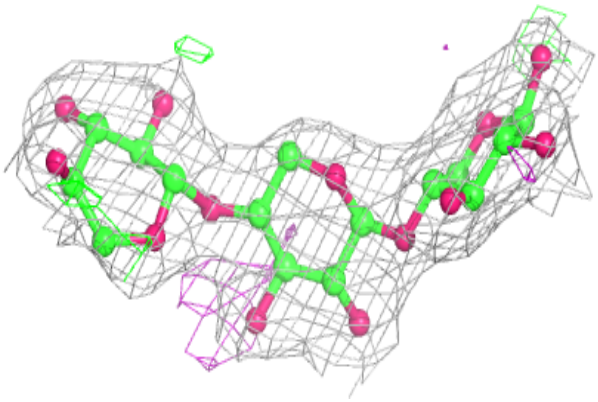


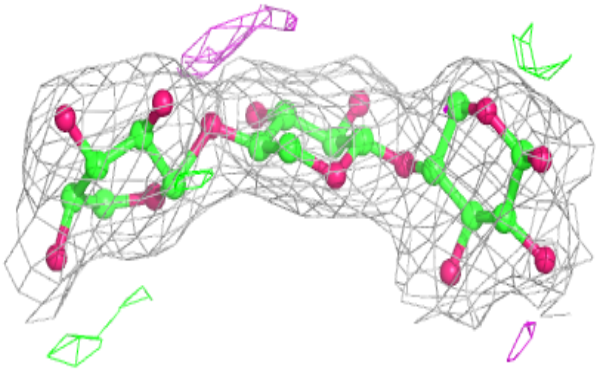


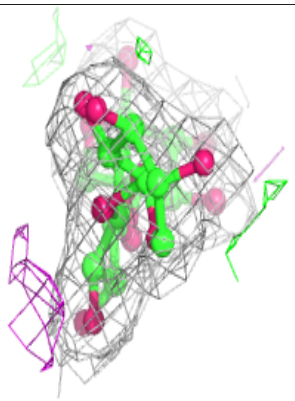


Electron density around Chain D:

$2mF_o$-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, 95^{th} 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	GOL	B	1561	6/6	0.73	0.24	81,82,84,84	0
4	GOL	A	1558	6/6	0.73	0.27	81,87,89,91	0
4	GOL	B	1557	6/6	0.74	0.32	51,62,67,67	0
4	GOL	B	1558	6/6	0.79	0.23	64,75,78,78	0
4	GOL	A	1561	6/6	0.79	0.51	91,99,100,103	0
4	GOL	A	1560	6/6	0.84	0.21	73,74,77,80	0
4	GOL	A	1556	6/6	0.84	0.24	67,74,75,77	0
4	GOL	B	1559	6/6	0.85	0.28	74,78,81,81	0
4	GOL	A	1559	6/6	0.85	0.27	51,66,67,67	0
4	GOL	A	1557	6/6	0.89	0.31	56,65,69,70	0
4	GOL	B	1556	6/6	0.89	0.28	51,62,69,78	0
5	PO4	B	1562	5/5	0.90	0.31	97,98,102,103	0
4	GOL	B	1560	6/6	0.94	0.33	66,72,75,79	0
3	CA	A	1552	1/1	0.96	0.20	76,76,76,76	0
5	PO4	A	1562	5/5	0.97	0.23	72,73,77,78	0
3	CA	B	1552	1/1	0.98	0.22	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.