



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:32 AM BST

PDB ID : 4Q1Q
Title : Crystal structure of TibC-catalyzed hyper-glycosylated TibA55-350 fragment
Authors : Yao, Q.; Lu, Q.; Shao, F.
Deposited on : 2014-04-04
Resolution : 2.11 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

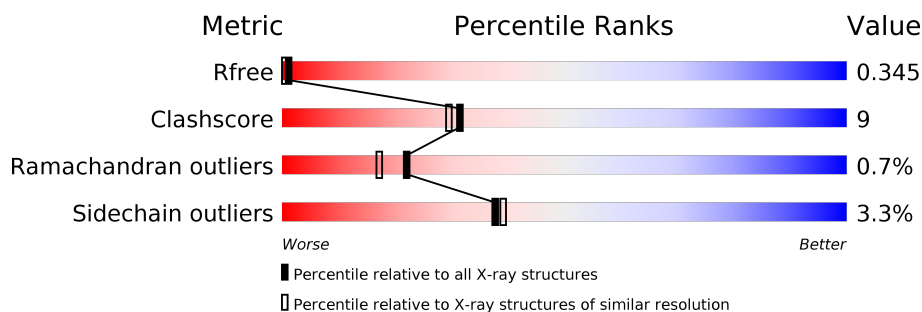
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	

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	289	A	402	X	-	-	-
2	289	A	406	X	-	-	-
2	289	A	413	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	289	A	421	X	-	-	-
2	289	A	433	X	-	-	-
2	289	A	435	X	-	-	-
2	289	B	408	X	-	-	-
2	289	B	433	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4712 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.

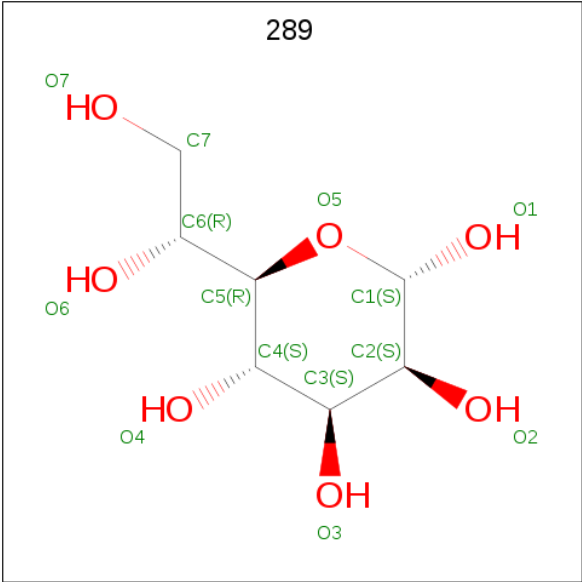
- Molecule 1 is a protein called Adhesin/invasin TibA autotransporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	Se	0	0	0
			1864	1102	345	413	4			
1	B	274	Total	C	N	O	Se	0	0	0
			1864	1102	345	413	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MSE	-	expression tag	UNP Q9XD84
A	47	ASP	-	expression tag	UNP Q9XD84
A	48	TYR	-	expression tag	UNP Q9XD84
A	49	LYS	-	expression tag	UNP Q9XD84
A	50	ASP	-	expression tag	UNP Q9XD84
A	51	ASP	-	expression tag	UNP Q9XD84
A	52	ASP	-	expression tag	UNP Q9XD84
A	53	ASP	-	expression tag	UNP Q9XD84
A	54	LYS	-	expression tag	UNP Q9XD84
B	46	MSE	-	expression tag	UNP Q9XD84
B	47	ASP	-	expression tag	UNP Q9XD84
B	48	TYR	-	expression tag	UNP Q9XD84
B	49	LYS	-	expression tag	UNP Q9XD84
B	50	ASP	-	expression tag	UNP Q9XD84
B	51	ASP	-	expression tag	UNP Q9XD84
B	52	ASP	-	expression tag	UNP Q9XD84
B	53	ASP	-	expression tag	UNP Q9XD84
B	54	LYS	-	expression tag	UNP Q9XD84

- Molecule 2 is D-glycero-alpha-D-manno-heptopyranose (three-letter code: 289) (formula: $C_7H_{14}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		

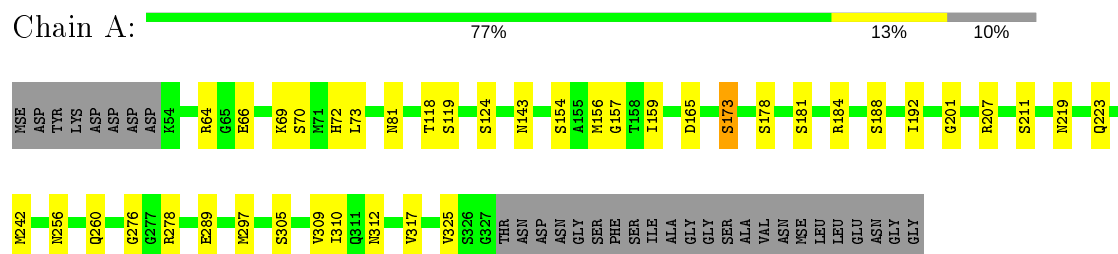
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	52	Total	O	0	0
			52	52		

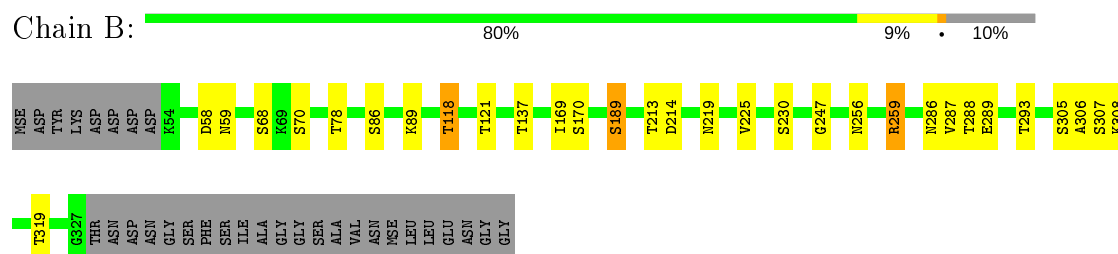
3 Residue-property plots [i](#)

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. 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. 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: Adhesin/invasin TibA autotransporter



- Molecule 1: Adhesin/invasin TibA autotransporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.81Å 62.17Å 97.29Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	19.87 – 2.11 19.86 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.87-2.11) 98.0 (19.86-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.205 , 0.248 0.335 , 0.345	Depositor DCC
R_{free} test set	1598 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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:
289

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	0.32	0/1877	0.83	0/2530
1	B	0.35	0/1877	0.86	1/2530 (0.0%)
All	All	0.34	0/3754	0.84	1/5060 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH1	7.26	123.93	120.30

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	1864	0	1737	26	4
1	B	1864	0	1737	19	2
2	A	455	0	419	32	6
2	B	455	0	407	24	9
3	A	22	0	0	0	0
3	B	52	0	0	1	1
All	All	4712	0	4300	80	11

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 9.

All (80) 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)
2:B:435:289:C2	2:B:435:289:C3	1.79	1.58
2:B:433:289:C3	2:B:433:289:C2	1.85	1.51
2:A:413:289:C5	2:A:413:289:O5	1.64	1.44
2:B:433:289:C5	2:B:433:289:O5	1.64	1.42
2:B:406:289:O2	2:B:408:289:O6	1.55	1.24
2:A:413:289:C4	2:A:413:289:O5	2.06	1.02
2:B:433:289:C5	2:B:433:289:C1	2.50	0.89
2:B:435:289:C3	2:B:435:289:H2	2.04	0.88
2:B:433:289:C4	2:B:433:289:C2	2.53	0.86
2:A:413:289:C5	2:A:413:289:C1	2.51	0.83
2:A:410:289:H3	2:A:434:289:O3	1.79	0.81
2:B:404:289:H2	2:B:406:289:O4	1.81	0.81
1:B:286:ASN:HA	1:B:305:SER:O	1.80	0.80
1:B:286:ASN:OD1	1:B:305:SER:HB3	1.83	0.78
2:A:412:289:O7	2:A:412:289:O4	2.04	0.75
2:B:433:289:C4	2:B:433:289:O5	2.35	0.75
2:B:435:289:C2	2:B:435:289:C4	2.62	0.75
1:A:154:SER:OG	2:A:434:289:O3	2.05	0.74
2:B:428:289:O6	3:B:549:HOH:O	2.05	0.74
2:A:406:289:HO3	2:A:406:289:HO6	1.29	0.73
1:B:287:VAL:O	1:B:306:ALA:HA	1.93	0.69
2:A:432:289:O4	2:A:433:289:H6	1.92	0.69
2:A:413:289:H4	2:A:413:289:O5	1.96	0.65
1:B:230:SER:HB2	2:B:416:289:O2	1.98	0.63
2:B:406:289:C2	2:B:408:289:O6	2.47	0.62
1:B:286:ASN:OD1	1:B:305:SER:CB	2.47	0.61
1:B:70:SER:HA	1:B:89:LYS:O	2.00	0.60
1:A:188:SER:HB3	2:A:412:289:H5	1.83	0.60
2:B:433:289:O5	2:B:433:289:H4	2.03	0.59
1:A:156:MSE:HB3	2:A:434:289:O2	2.03	0.59
1:A:81:ASN:OD1	2:A:430:289:H6	2.02	0.58
2:B:433:289:O5	2:B:433:289:C6	2.47	0.57
2:A:432:289:HO4	2:A:433:289:C7	2.17	0.57
2:B:404:289:H2	2:B:406:289:HO4	1.70	0.56
1:A:223:GLN:OE1	1:A:242:MSE:HG3	2.05	0.56
1:B:169:ILE:HD12	2:B:411:289:H2	1.88	0.55
1:B:287:VAL:HG22	1:B:306:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:289:C4	2:B:433:289:C1	2.85	0.55
1:A:154:SER:HB2	2:A:410:289:C5	2.37	0.54
1:B:256:ASN:HB2	2:B:425:289:H7A	1.90	0.53
1:A:188:SER:CB	2:A:412:289:H5	2.38	0.53
2:B:433:289:C5	2:B:433:289:C2	2.86	0.53
1:A:256:ASN:OD1	1:A:276:GLY:HA3	2.10	0.52
2:B:433:289:O4	2:B:433:289:H7	2.10	0.52
1:B:306:ALA:O	1:B:307:SER:HB3	2.10	0.52
2:A:406:289:C3	2:A:406:289:HO6	2.23	0.52
2:B:433:289:C2	2:B:433:289:O3	2.39	0.51
1:B:58:ASP:OD1	1:B:59:ASN:ND2	2.42	0.50
1:A:156:MSE:CB	2:A:434:289:O2	2.61	0.48
1:A:119:SER:HB3	2:A:431:289:H7	1.96	0.48
1:A:72:HIS:C	1:A:73:LEU:HD12	2.35	0.47
1:B:213:THR:HG22	1:B:214:ASP:OD2	2.14	0.47
1:A:154:SER:HB2	2:A:410:289:H5	1.97	0.46
2:A:413:289:O4	2:A:413:289:H7	2.15	0.46
1:A:278:ARG:HA	1:A:297:MSE:O	2.16	0.46
1:A:173:SER:HB2	2:A:410:289:O5	2.16	0.45
1:B:225:VAL:HG12	1:B:247:GLY:HA3	1.99	0.45
1:A:154:SER:CB	2:A:410:289:C5	2.94	0.45
2:A:412:289:C4	2:A:412:289:O7	2.63	0.44
2:A:413:289:C6	2:A:413:289:O5	2.55	0.43
1:A:188:SER:CB	2:A:412:289:C5	2.97	0.43
1:B:289:GLU:HA	1:B:308:LYS:O	2.18	0.43
1:A:165:ASP:OD1	1:A:184:ARG:HB2	2.19	0.43
1:B:219:ASN:CG	2:B:424:289:H7	2.39	0.43
2:A:425:289:C4	2:A:425:289:HO7	2.31	0.42
1:B:118:THR:CG2	2:B:432:289:O2	2.67	0.42
1:A:181:SER:HA	1:A:201:GLY:HA3	2.00	0.42
1:A:157:GLY:O	1:A:159:ILE:HD12	2.20	0.42
1:A:211:SER:OG	2:A:416:289:H7	2.19	0.42
1:A:309:VAL:HG21	1:A:325:VAL:HG13	2.00	0.42
1:A:207:ARG:NE	2:A:414:289:O2	2.45	0.42
1:A:219:ASN:ND2	2:A:424:289:O6	2.53	0.42
1:A:143:ASN:ND2	2:A:420:289:O3	2.53	0.41
1:A:173:SER:HA	1:A:192:ILE:O	2.21	0.41
1:A:242:MSE:SE	1:A:260:GLN:HE21	2.54	0.41
2:A:420:289:H7	2:A:420:289:H4	1.84	0.41
2:A:425:289:C4	2:A:425:289:O7	2.69	0.41
1:B:286:ASN:OD1	1:B:305:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:SER:HA	1:B:189:SER:O	2.22	0.40
1:B:288:THR:HA	1:B:307:SER:O	2.21	0.40

All (11) 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)
1:A:312:ASN:OD1	3:B:549:HOH:O[2_656]	1.57	0.63
2:A:420:289:C7	2:B:416:289:O7[1_665]	1.59	0.61
2:A:403:289:O4	2:B:409:289:O7[1_665]	1.76	0.44
2:A:403:289:O3	2:B:409:289:O4[1_665]	1.81	0.39
2:A:408:289:O6	2:B:430:289:O3[1_655]	2.06	0.14
1:B:293:THR:OG1	2:B:420:289:O3[1_455]	2.06	0.14
2:A:420:289:C7	2:B:416:289:C7[1_665]	2.12	0.08
1:A:310:ILE:CG2	2:B:428:289:O7[2_656]	2.12	0.08
2:A:420:289:C4	2:B:416:289:O7[1_665]	2.14	0.06
1:A:289:GLU:OE1	2:B:424:289:O3[1_655]	2.18	0.02
1:A:317:VAL:N	1:B:319:THR:O[2_656]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	272/305 (89%)	257 (94%)	13 (5%)	2 (1%)	22	17
1	B	272/305 (89%)	260 (96%)	10 (4%)	2 (1%)	22	17
All	All	544/610 (89%)	517 (95%)	23 (4%)	4 (1%)	22	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG

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Mol	Chain	Res	Type
1	A	124	SER
1	B	86	SER
1	B	189	SER

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	197/216 (91%)	190 (96%)	7 (4%)	35	35
1	B	197/216 (91%)	191 (97%)	6 (3%)	41	43
All	All	394/432 (91%)	381 (97%)	13 (3%)	38	39

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	69	LYS
1	A	70	SER
1	A	118	THR
1	A	173	SER
1	A	178	SER
1	A	305	SER
1	B	68	SER
1	B	78	THR
1	B	118	THR
1	B	121	THR
1	B	137	THR
1	B	259	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	320	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

70 ligands 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	289	B	423	1	13,13,14	0.23	0	17,18,20	1.23	2 (11%)
2	289	A	409	1	13,13,14	0.43	0	17,18,20	1.76	5 (29%)
2	289	A	419	1	13,13,14	0.21	0	17,18,20	2.48	7 (41%)
2	289	B	409	1	13,13,14	0.29	0	17,18,20	1.54	3 (17%)
2	289	B	422	1	13,13,14	0.26	0	17,18,20	1.22	2 (11%)
2	289	B	416	1	13,13,14	5.28	5 (38%)	17,18,20	3.64	8 (47%)
2	289	B	431	1	13,13,14	0.30	0	17,18,20	1.53	4 (23%)
2	289	A	433	1	13,13,14	0.31	0	17,18,20	1.44	3 (17%)
2	289	A	404	1	13,13,14	0.24	0	17,18,20	1.72	5 (29%)
2	289	B	417	1	13,13,14	0.36	0	17,18,20	1.08	2 (11%)
2	289	A	427	1	13,13,14	0.26	0	17,18,20	1.58	3 (17%)
2	289	A	425	1	13,13,14	0.39	0	17,18,20	2.25	7 (41%)
2	289	A	405	1	13,13,14	0.24	0	17,18,20	1.43	2 (11%)
2	289	B	407	1	13,13,14	0.26	0	17,18,20	2.07	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	289	B	428	1	13,13,14	0.25	0	17,18,20	1.72	4 (23%)
2	289	B	424	1	13,13,14	0.31	0	17,18,20	2.40	8 (47%)
2	289	B	410	1	13,13,14	0.32	0	17,18,20	1.44	2 (11%)
2	289	B	415	1	13,13,14	0.33	0	17,18,20	1.51	4 (23%)
2	289	A	406	1	13,13,14	0.38	0	17,18,20	1.28	2 (11%)
2	289	B	411	1	13,13,14	0.37	0	17,18,20	1.61	2 (11%)
2	289	B	427	1	13,13,14	0.27	0	17,18,20	1.63	4 (23%)
2	289	A	402	1	13,13,14	0.33	0	17,18,20	1.39	2 (11%)
2	289	A	429	1	13,13,14	0.24	0	17,18,20	1.78	4 (23%)
2	289	A	410	1	13,13,14	0.24	0	17,18,20	0.67	0
2	289	B	401	1	13,13,14	0.38	0	17,18,20	1.67	5 (29%)
2	289	A	432	1	13,13,14	0.22	0	17,18,20	0.64	0
2	289	B	418	1	13,13,14	0.28	0	17,18,20	1.54	2 (11%)
2	289	B	413	1	13,13,14	0.49	0	17,18,20	1.78	5 (29%)
2	289	A	422	1	13,13,14	0.21	0	17,18,20	1.35	1 (5%)
2	289	B	432	1	13,13,14	0.39	0	17,18,20	1.70	5 (29%)
2	289	A	401	1	13,13,14	0.37	0	17,18,20	2.29	7 (41%)
2	289	A	431	1	13,13,14	0.21	0	17,18,20	1.17	2 (11%)
2	289	B	429	1	13,13,14	0.31	0	17,18,20	2.10	7 (41%)
2	289	A	434	1	13,13,14	2.95	6 (46%)	17,18,20	4.50	10 (58%)
2	289	B	434	1	13,13,14	6.99	7 (53%)	17,18,20	3.91	14 (82%)
2	289	A	430	1	13,13,14	0.29	0	17,18,20	1.16	1 (5%)
2	289	B	430	1	13,13,14	0.32	0	17,18,20	1.76	5 (29%)
2	289	A	415	1	13,13,14	0.31	0	17,18,20	1.63	4 (23%)
2	289	B	435	1	13,13,14	8.52	5 (38%)	17,18,20	7.09	11 (64%)
2	289	B	405	1	13,13,14	0.21	0	17,18,20	1.78	4 (23%)
2	289	B	420	1	13,13,14	0.43	0	17,18,20	2.57	5 (29%)
2	289	B	426	1	13,13,14	0.25	0	17,18,20	3.28	8 (47%)
2	289	A	424	1	13,13,14	0.25	0	17,18,20	1.27	2 (11%)
2	289	B	408	1	13,13,14	0.34	0	17,18,20	1.72	4 (23%)
2	289	A	417	1	13,13,14	0.33	0	17,18,20	2.46	4 (23%)
2	289	B	404	1	13,13,14	0.33	0	17,18,20	2.12	4 (23%)
2	289	A	426	1	13,13,14	0.27	0	17,18,20	0.96	1 (5%)
2	289	B	402	1	13,13,14	0.16	0	17,18,20	1.75	3 (17%)
2	289	A	413	1	13,13,14	4.64	1 (7%)	17,18,20	4.31	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	289	A	418	1	13,13,14	0.42	0	17,18,20	1.51	2 (11%)
2	289	A	416	1	13,13,14	0.45	0	17,18,20	1.73	3 (17%)
2	289	B	414	1	13,13,14	0.30	0	17,18,20	2.18	4 (23%)
2	289	B	433	1	13,13,14	9.40	6 (46%)	17,18,20	3.78	7 (41%)
2	289	B	403	1	13,13,14	0.33	0	17,18,20	1.51	1 (5%)
2	289	B	406	1	13,13,14	0.20	0	17,18,20	0.64	0
2	289	B	419	1	13,13,14	0.25	0	17,18,20	2.22	4 (23%)
2	289	A	412	1	13,13,14	0.46	0	17,18,20	2.22	7 (41%)
2	289	A	411	1	13,13,14	0.33	0	17,18,20	2.24	6 (35%)
2	289	A	414	1	13,13,14	0.28	0	17,18,20	1.81	4 (23%)
2	289	A	420	1	13,13,14	0.21	0	17,18,20	0.66	0
2	289	A	403	1	13,13,14	0.39	0	17,18,20	1.13	1 (5%)
2	289	B	412	1	13,13,14	0.36	0	17,18,20	2.84	9 (52%)
2	289	B	421	1	13,13,14	0.46	0	17,18,20	1.67	2 (11%)
2	289	A	421	1	13,13,14	0.22	0	17,18,20	1.37	2 (11%)
2	289	B	425	1	13,13,14	0.34	0	17,18,20	2.26	8 (47%)
2	289	A	407	1	13,13,14	0.27	0	17,18,20	1.65	4 (23%)
2	289	A	435	1	13,13,14	0.34	0	17,18,20	1.38	2 (11%)
2	289	A	428	1	13,13,14	0.20	0	17,18,20	2.07	3 (17%)
2	289	A	408	1	13,13,14	0.24	0	17,18,20	1.51	1 (5%)
2	289	A	423	1	13,13,14	0.28	0	17,18,20	1.47	2 (11%)

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	289	B	423	1	-	4/6/23/26	0/1/1/1
2	289	A	409	1	-	4/6/23/26	0/1/1/1
2	289	A	419	1	-	4/6/23/26	0/1/1/1
2	289	B	409	1	-	0/6/23/26	0/1/1/1
2	289	B	422	1	-	0/6/23/26	0/1/1/1
2	289	B	416	1	-	0/6/23/26	0/1/1/1
2	289	B	431	1	-	6/6/23/26	0/1/1/1
2	289	A	433	1	1/1/5/6	4/6/23/26	0/1/1/1
2	289	A	404	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	289	B	417	1	-	1/6/23/26	0/1/1/1
2	289	A	427	1	-	4/6/23/26	0/1/1/1
2	289	A	425	1	-	6/6/23/26	0/1/1/1
2	289	A	405	1	-	2/6/23/26	0/1/1/1
2	289	B	407	1	-	6/6/23/26	0/1/1/1
2	289	B	428	1	-	4/6/23/26	0/1/1/1
2	289	B	424	1	-	5/6/23/26	0/1/1/1
2	289	B	410	1	-	6/6/23/26	0/1/1/1
2	289	B	415	1	-	2/6/23/26	0/1/1/1
2	289	A	406	1	1/1/5/6	6/6/23/26	0/1/1/1
2	289	B	411	1	-	2/6/23/26	1/1/1/1
2	289	B	427	1	-	0/6/23/26	0/1/1/1
2	289	A	402	1	1/1/5/6	2/6/23/26	0/1/1/1
2	289	A	429	1	-	4/6/23/26	0/1/1/1
2	289	A	410	1	-	0/6/23/26	0/1/1/1
2	289	B	401	1	-	1/6/23/26	0/1/1/1
2	289	A	432	1	-	1/6/23/26	0/1/1/1
2	289	B	418	1	-	6/6/23/26	0/1/1/1
2	289	B	413	1	-	4/6/23/26	0/1/1/1
2	289	A	422	1	-	1/6/23/26	0/1/1/1
2	289	B	432	1	-	4/6/23/26	0/1/1/1
2	289	A	401	1	-	2/6/23/26	0/1/1/1
2	289	A	431	1	-	0/6/23/26	0/1/1/1
2	289	B	429	1	-	2/6/23/26	0/1/1/1
2	289	A	434	1	-	0/6/23/26	0/1/1/1
2	289	B	434	1	-	0/6/23/26	0/1/1/1
2	289	A	430	1	-	3/6/23/26	0/1/1/1
2	289	B	430	1	-	3/6/23/26	0/1/1/1
2	289	A	415	1	-	2/6/23/26	0/1/1/1
2	289	B	435	1	-	0/6/23/26	0/1/1/1
2	289	B	405	1	-	2/6/23/26	0/1/1/1
2	289	B	420	1	-	4/6/23/26	0/1/1/1
2	289	B	408	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	A	424	1	-	4/6/23/26	0/1/1/1
2	289	B	426	1	-	2/6/23/26	0/1/1/1
2	289	A	417	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	289	B	404	1	-	3/6/23/26	0/1/1/1
2	289	A	426	1	-	4/6/23/26	0/1/1/1
2	289	B	402	1	-	4/6/23/26	0/1/1/1
2	289	A	413	1	-	1/6/23/26	0/1/1/1
2	289	A	418	1	-	6/6/23/26	0/1/1/1
2	289	A	416	1	-	2/6/23/26	0/1/1/1
2	289	B	414	1	-	6/6/23/26	0/1/1/1
2	289	B	433	1	-	0/6/23/26	0/1/1/1
2	289	B	403	1	-	3/6/23/26	0/1/1/1
2	289	B	406	1	-	0/6/23/26	0/1/1/1
2	289	B	419	1	-	4/6/23/26	0/1/1/1
2	289	A	412	1	-	3/6/23/26	0/1/1/1
2	289	A	411	1	-	4/6/23/26	0/1/1/1
2	289	A	414	1	-	1/6/23/26	0/1/1/1
2	289	A	420	1	-	1/6/23/26	0/1/1/1
2	289	A	403	1	-	4/6/23/26	0/1/1/1
2	289	B	412	1	-	4/6/23/26	0/1/1/1
2	289	B	421	1	-	4/6/23/26	0/1/1/1
2	289	A	421	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	B	425	1	-	6/6/23/26	0/1/1/1
2	289	A	407	1	-	4/6/23/26	0/1/1/1
2	289	A	435	1	1/1/5/6	4/6/23/26	0/1/1/1
2	289	A	428	1	-	4/6/23/26	0/1/1/1
2	289	A	408	1	-	4/6/23/26	0/1/1/1
2	289	A	423	1	-	2/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	435	289	O3-C3	-22.95	0.88	1.43
2	B	433	289	C2-C3	22.48	1.85	1.52
2	B	434	289	C7-C6	-20.75	0.96	1.52
2	B	435	289	C2-C3	18.44	1.79	1.52
2	B	433	289	O3-C3	-17.29	1.02	1.43
2	B	433	289	O5-C5	16.68	1.64	1.43
2	A	413	289	O5-C5	16.63	1.64	1.43
2	B	416	289	C2-C3	-15.49	1.29	1.52
2	B	434	289	O5-C1	-9.68	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	416	289	O2-C2	8.97	1.62	1.43
2	B	435	289	O2-C2	-7.78	1.26	1.43
2	B	434	289	C6-C5	-6.50	1.39	1.52
2	A	434	289	O3-C3	6.01	1.57	1.43
2	A	434	289	O5-C1	5.84	1.53	1.43
2	B	433	289	C4-C3	-5.65	1.38	1.52
2	B	434	289	O5-C5	5.18	1.49	1.43
2	B	433	289	O2-C2	5.10	1.54	1.43
2	B	416	289	C1-C2	4.63	1.62	1.52
2	A	434	289	O2-C2	4.18	1.52	1.43
2	B	434	289	C2-C3	3.53	1.57	1.52
2	B	434	289	C4-C5	-3.33	1.43	1.52
2	A	434	289	O5-C5	3.20	1.47	1.43
2	B	435	289	C4-C3	3.06	1.60	1.52
2	B	433	289	O5-C1	3.04	1.48	1.43
2	B	416	289	C4-C3	3.03	1.60	1.52
2	B	416	289	O4-C4	2.86	1.49	1.43
2	A	434	289	C4-C3	-2.72	1.45	1.52
2	B	434	289	O6-C6	2.37	1.48	1.43
2	A	434	289	C7-C6	2.34	1.58	1.52
2	B	435	289	C4-C5	2.13	1.58	1.52

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	289	O3-C3-C2	23.68	155.34	109.99
2	A	413	289	O5-C5-C4	-17.05	80.78	110.73
2	A	434	289	C1-C2-C3	-11.60	95.41	109.67
2	B	416	289	O2-C2-C1	-10.52	87.63	109.15
2	A	434	289	C2-C3-C4	9.44	127.23	110.89
2	B	433	289	C3-C4-C5	8.74	129.63	109.68
2	B	433	289	O5-C5-C4	-8.58	95.67	110.73
2	B	434	289	C1-O5-C5	7.72	124.14	111.48
2	B	435	289	C1-C2-C3	7.05	118.33	109.67
2	B	435	289	O4-C4-C3	-6.65	94.98	110.35
2	A	417	289	C1-C2-C3	-6.60	101.55	109.67
2	B	435	289	O3-C3-C4	-6.57	95.17	110.35
2	B	414	289	C6-C5-C4	-6.26	103.65	114.03
2	B	420	289	C1-O5-C5	6.15	121.56	111.48
2	B	416	289	C1-C2-C3	6.15	117.22	109.67
2	B	426	289	O7-C7-C6	-6.12	97.74	111.07
2	B	419	289	C6-C5-C4	-6.11	103.91	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	420	289	C6-C5-C4	6.02	124.01	114.03
2	B	426	289	C1-C2-C3	-5.98	102.32	109.67
2	B	435	289	O5-C1-C2	5.80	119.72	110.77
2	A	419	289	C6-C5-C4	-5.75	104.50	114.03
2	B	425	289	C1-C2-C3	-5.69	102.67	109.67
2	B	426	289	O6-C6-C5	5.65	122.68	109.14
2	B	435	289	O2-C2-C3	5.64	121.44	110.14
2	B	435	289	C2-C3-C4	-5.53	101.33	110.89
2	B	434	289	O7-C7-C6	-5.49	99.11	111.07
2	A	434	289	O3-C3-C2	5.44	120.42	109.99
2	B	434	289	O3-C3-C2	5.34	120.22	109.99
2	B	404	289	C1-C2-C3	-5.30	103.15	109.67
2	A	417	289	O5-C1-C2	-5.26	102.66	110.77
2	B	412	289	C1-C2-C3	-5.26	103.20	109.67
2	B	404	289	O5-C1-C2	-5.25	102.67	110.77
2	B	426	289	C6-C5-C4	5.23	122.70	114.03
2	B	428	289	C6-C5-C4	-5.21	105.39	114.03
2	A	428	289	C1-C2-C3	-5.10	103.40	109.67
2	B	412	289	C3-C4-C5	5.07	121.27	109.68
2	B	435	289	C3-C4-C5	5.05	121.22	109.68
2	B	411	289	C1-O5-C5	5.04	119.74	111.48
2	B	424	289	C1-C2-C3	-5.01	103.51	109.67
2	B	412	289	O5-C1-C2	-4.93	103.15	110.77
2	B	421	289	O5-C1-C2	-4.91	103.19	110.77
2	A	419	289	C1-C2-C3	-4.84	103.71	109.67
2	B	433	289	C2-C3-C4	-4.83	102.53	110.89
2	A	412	289	C6-C5-C4	4.71	121.84	114.03
2	B	434	289	O2-C2-C3	-4.71	100.71	110.14
2	A	411	289	O5-C1-C2	4.67	117.98	110.77
2	B	416	289	O3-C3-C2	4.58	118.76	109.99
2	B	405	289	C6-C5-C4	-4.55	106.48	114.03
2	A	411	289	C1-O5-C5	4.55	118.93	111.48
2	A	425	289	C6-C5-C4	4.54	121.56	114.03
2	A	434	289	O5-C1-C2	4.52	117.75	110.77
2	B	424	289	O5-C1-C2	-4.52	103.80	110.77
2	A	401	289	C1-O5-C5	4.52	118.88	111.48
2	B	433	289	O5-C1-C2	4.48	117.69	110.77
2	B	416	289	O2-C2-C3	4.41	118.97	110.14
2	B	402	289	C1-C2-C3	-4.39	104.27	109.67
2	A	425	289	C7-C6-C5	4.38	121.03	112.17
2	A	408	289	C1-O5-C5	4.37	118.64	111.48
2	A	434	289	O3-C3-C4	-4.36	100.27	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	289	C1-O5-C5	4.35	118.60	111.48
2	B	434	289	O3-C3-C4	4.33	120.35	110.35
2	B	419	289	C2-C3-C4	-4.32	103.43	110.89
2	A	421	289	O5-C1-C2	-4.31	104.12	110.77
2	B	407	289	O6-C6-C5	4.25	119.32	109.14
2	B	434	289	C3-C4-C5	4.24	119.37	109.68
2	B	435	289	O5-C5-C4	4.17	118.07	110.73
2	B	412	289	C1-O5-C5	-4.10	104.75	111.48
2	B	434	289	O6-C6-C7	-4.07	99.59	109.14
2	B	408	289	C1-C2-C3	4.07	114.67	109.67
2	A	427	289	C1-C2-C3	-4.01	104.74	109.67
2	B	433	289	C1-C2-C3	3.99	114.58	109.67
2	B	434	289	O4-C4-C3	-3.97	101.17	110.35
2	A	414	289	O4-C4-C3	-3.95	101.23	110.35
2	A	405	289	C1-C2-C3	-3.93	104.84	109.67
2	B	413	289	O5-C5-C4	-3.89	103.90	110.73
2	B	426	289	O4-C4-C3	-3.87	101.41	110.35
2	A	401	289	C6-C5-C4	3.83	120.38	114.03
2	A	429	289	C1-C2-C3	-3.81	104.98	109.67
2	A	433	289	O5-C1-C2	-3.79	104.92	110.77
2	B	409	289	O5-C1-C2	-3.79	104.93	110.77
2	B	430	289	C6-C5-C4	3.77	120.29	114.03
2	A	412	289	O2-C2-C3	3.77	117.68	110.14
2	B	427	289	C1-C2-C3	-3.75	105.05	109.67
2	B	413	289	O2-C2-C3	3.74	117.64	110.14
2	A	428	289	C1-O5-C5	3.70	117.55	111.48
2	B	407	289	O7-C7-C6	-3.68	103.06	111.07
2	A	416	289	O5-C5-C4	-3.66	104.31	110.73
2	A	434	289	O2-C2-C3	-3.65	102.82	110.14
2	A	404	289	O4-C4-C3	-3.65	101.91	110.35
2	B	401	289	C1-C2-C3	-3.61	105.22	109.67
2	B	410	289	C1-C2-C3	-3.59	105.26	109.67
2	B	403	289	C6-C5-C4	-3.55	108.14	114.03
2	B	433	289	O4-C4-C3	-3.54	102.18	110.35
2	B	420	289	O5-C5-C4	-3.51	104.57	110.73
2	A	401	289	O4-C4-C3	-3.50	102.27	110.35
2	A	429	289	C6-C5-C4	3.49	119.82	114.03
2	B	434	289	O6-C6-C5	3.48	117.48	109.14
2	B	426	289	C1-O5-C5	3.46	117.15	111.48
2	A	409	289	C6-C5-C4	3.46	119.76	114.03
2	B	416	289	O4-C4-C5	-3.44	100.82	109.94
2	A	428	289	O5-C1-C2	-3.38	105.55	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	289	C1-C2-C3	3.36	113.80	109.67
2	A	411	289	C3-C4-C5	3.36	117.36	109.68
2	B	429	289	C1-O5-C5	3.35	116.97	111.48
2	B	412	289	O2-C2-C1	3.34	115.98	109.15
2	B	429	289	O2-C2-C1	3.32	115.94	109.15
2	B	414	289	O2-C2-C1	3.31	115.92	109.15
2	B	427	289	O5-C1-C2	-3.30	105.67	110.77
2	A	416	289	C6-C5-C4	3.30	119.50	114.03
2	B	405	289	O7-C7-C6	-3.27	103.94	111.07
2	A	425	289	O5-C5-C4	-3.25	105.02	110.73
2	A	431	289	O5-C1-C2	-3.23	105.78	110.77
2	B	408	289	O2-C2-C3	-3.22	103.69	110.14
2	B	432	289	C6-C5-C4	3.22	119.36	114.03
2	B	420	289	O4-C4-C3	-3.20	102.95	110.35
2	A	418	289	O5-C1-C2	-3.16	105.89	110.77
2	A	419	289	O3-C3-C2	3.16	116.04	109.99
2	B	418	289	O7-C7-C6	-3.16	104.19	111.07
2	B	432	289	C1-C2-C3	-3.15	105.79	109.67
2	A	418	289	C6-C5-C4	3.14	119.24	114.03
2	B	429	289	C6-C5-C4	3.14	119.23	114.03
2	B	424	289	C1-O5-C5	3.12	116.59	111.48
2	A	423	289	C1-C2-C3	-3.10	105.85	109.67
2	B	433	289	C1-O5-C5	-3.09	106.41	111.48
2	B	425	289	O2-C2-C3	3.09	116.33	110.14
2	B	423	289	O7-C7-C6	-3.07	104.38	111.07
2	B	416	289	O4-C4-C3	3.06	117.43	110.35
2	A	415	289	O5-C1-C2	-3.04	106.07	110.77
2	A	412	289	C2-C3-C4	3.03	116.14	110.89
2	A	409	289	O4-C4-C3	-3.03	103.35	110.35
2	A	412	289	C3-C4-C5	3.02	116.58	109.68
2	A	434	289	O5-C5-C4	-3.00	105.45	110.73
2	B	434	289	C6-C5-C4	3.00	119.00	114.03
2	B	407	289	C6-C5-C4	3.00	119.00	114.03
2	B	409	289	C1-C2-C3	-2.99	105.98	109.67
2	A	403	289	C6-C5-C4	2.99	118.99	114.03
2	A	422	289	O5-C1-C2	-2.98	106.18	110.77
2	A	407	289	C6-C5-C4	2.95	118.93	114.03
2	B	414	289	O5-C1-C2	2.94	115.31	110.77
2	B	415	289	O4-C4-C3	-2.94	103.56	110.35
2	A	401	289	O7-C7-C6	2.92	117.44	111.07
2	A	414	289	O5-C1-C2	-2.92	106.27	110.77
2	A	404	289	C3-C4-C5	2.92	116.34	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	289	O5-C1-C2	-2.91	106.28	110.77
2	A	424	289	C1-C2-C3	-2.91	106.09	109.67
2	A	414	289	C1-C2-C3	-2.87	106.14	109.67
2	A	434	289	C6-C5-C4	-2.87	109.27	114.03
2	A	425	289	O7-C7-C6	2.87	117.32	111.07
2	A	404	289	C1-C2-C3	-2.86	106.15	109.67
2	A	407	289	O6-C6-C5	2.86	115.99	109.14
2	A	419	289	O5-C5-C4	2.86	115.76	110.73
2	B	412	289	C6-C5-C4	-2.85	109.30	114.03
2	A	426	289	C1-C2-C3	-2.85	106.17	109.67
2	B	424	289	C7-C6-C5	-2.81	106.49	112.17
2	A	416	289	C1-C2-C3	-2.81	106.22	109.67
2	B	434	289	C1-C2-C3	2.80	113.11	109.67
2	B	425	289	O5-C5-C4	-2.80	105.82	110.73
2	A	401	289	O5-C5-C4	-2.80	105.82	110.73
2	A	412	289	C1-C2-C3	-2.78	106.25	109.67
2	A	435	289	O5-C1-C2	-2.78	106.48	110.77
2	B	434	289	O5-C5-C4	-2.78	105.86	110.73
2	A	434	289	C3-C4-C5	-2.77	103.36	109.68
2	A	401	289	C3-C4-C5	2.76	115.98	109.68
2	A	409	289	O7-C7-C6	2.76	117.08	111.07
2	B	431	289	O5-C5-C4	-2.75	105.90	110.73
2	A	413	289	C2-C3-C4	2.73	115.62	110.89
2	B	419	289	O2-C2-C1	2.73	114.73	109.15
2	B	401	289	C3-C4-C5	2.72	115.90	109.68
2	B	435	289	O4-C4-C5	2.72	117.15	109.94
2	A	427	289	C1-O5-C5	2.71	115.92	111.48
2	B	431	289	O4-C4-C3	-2.71	104.09	110.35
2	B	425	289	O4-C4-C3	-2.71	104.09	110.35
2	A	411	289	O4-C4-C3	-2.70	104.10	110.35
2	B	413	289	O3-C3-C2	2.70	115.17	109.99
2	A	407	289	C1-C2-C3	-2.70	106.35	109.67
2	B	435	289	O2-C2-C1	-2.70	103.64	109.15
2	B	414	289	C1-O5-C5	2.67	115.86	111.48
2	B	415	289	C1-O5-C5	2.67	115.85	111.48
2	B	424	289	C6-C5-C4	2.66	118.44	114.03
2	B	405	289	O5-C1-C2	-2.66	106.66	110.77
2	B	426	289	C7-C6-C5	-2.66	106.79	112.17
2	A	429	289	O5-C5-C4	-2.66	106.07	110.73
2	A	402	289	C6-C5-C4	2.66	118.43	114.03
2	B	424	289	O7-C7-C6	-2.65	105.29	111.07
2	A	427	289	O2-C2-C1	2.65	114.58	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	414	289	C6-C5-C4	2.65	118.42	114.03
2	A	425	289	O4-C4-C3	-2.61	104.32	110.35
2	B	423	289	C1-O5-C5	2.61	115.75	111.48
2	B	426	289	O5-C1-C2	-2.58	106.78	110.77
2	B	425	289	C6-C5-C4	2.57	118.30	114.03
2	B	430	289	O7-C7-C6	-2.57	105.47	111.07
2	B	408	289	C1-O5-C5	2.57	115.69	111.48
2	B	419	289	O7-C7-C6	-2.56	105.50	111.07
2	B	432	289	O5-C5-C4	-2.54	106.27	110.73
2	A	425	289	O2-C2-C1	2.54	114.35	109.15
2	B	424	289	O6-C6-C5	2.54	115.23	109.14
2	A	407	289	O4-C4-C3	-2.53	104.50	110.35
2	B	429	289	O4-C4-C5	2.53	116.64	109.94
2	B	412	289	O4-C4-C3	-2.53	104.51	110.35
2	B	427	289	O5-C5-C4	-2.51	106.32	110.73
2	B	429	289	O5-C5-C4	-2.50	106.33	110.73
2	B	402	289	C1-O5-C5	2.50	115.57	111.48
2	B	409	289	O5-C5-C4	-2.49	106.36	110.73
2	A	417	289	C6-C5-C4	2.48	118.14	114.03
2	B	429	289	O3-C3-C2	-2.47	105.26	109.99
2	A	435	289	O2-C2-C1	2.47	114.20	109.15
2	B	415	289	O5-C5-C4	-2.46	106.42	110.73
2	B	407	289	C1-O5-C5	2.44	115.48	111.48
2	B	404	289	O2-C2-C1	2.43	114.13	109.15
2	B	425	289	O2-C2-C1	-2.42	104.20	109.15
2	A	402	289	C1-C2-C3	-2.42	106.69	109.67
2	A	419	289	O6-C6-C5	-2.41	103.35	109.14
2	B	418	289	C6-C5-C4	2.41	118.03	114.03
2	A	412	289	O5-C1-C2	-2.40	107.06	110.77
2	B	401	289	O5-C1-C2	-2.40	107.07	110.77
2	A	423	289	O7-C7-C6	-2.40	105.85	111.07
2	A	429	289	O5-C1-C2	-2.40	107.07	110.77
2	A	409	289	O5-C5-C4	-2.39	106.53	110.73
2	A	404	289	O5-C1-C2	-2.39	107.09	110.77
2	A	409	289	C7-C6-C5	2.38	116.99	112.17
2	A	421	289	C1-C2-C3	-2.37	106.75	109.67
2	B	432	289	O2-C2-C3	2.36	114.88	110.14
2	B	428	289	O5-C1-C2	-2.36	107.13	110.77
2	A	433	289	O5-C5-C4	-2.35	106.60	110.73
2	B	434	289	O5-C1-C2	2.34	114.38	110.77
2	A	433	289	O3-C3-C2	2.33	114.46	109.99
2	B	404	289	C3-C4-C5	2.33	115.00	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	431	289	C1-C2-C3	-2.33	106.81	109.67
2	B	413	289	O5-C1-C2	2.32	114.36	110.77
2	B	401	289	O3-C3-C2	-2.32	105.55	109.99
2	B	416	289	O5-C5-C4	2.32	114.81	110.73
2	A	406	289	O5-C1-C2	-2.32	107.20	110.77
2	B	430	289	O2-C2-C3	2.31	114.77	110.14
2	B	412	289	O5-C5-C4	2.31	114.80	110.73
2	B	407	289	C1-C2-C3	-2.31	106.83	109.67
2	B	412	289	O4-C4-C5	-2.31	103.83	109.94
2	B	421	289	O5-C5-C4	2.30	114.77	110.73
2	B	422	289	C6-C5-C4	-2.29	110.24	114.03
2	A	415	289	O4-C4-C5	2.28	115.99	109.94
2	B	434	289	O4-C4-C5	2.27	115.96	109.94
2	B	416	289	C6-C5-C4	-2.24	110.32	114.03
2	B	401	289	O2-C2-C1	2.23	113.72	109.15
2	B	411	289	O6-C6-C5	2.22	114.47	109.14
2	B	405	289	C1-C2-C3	-2.21	106.95	109.67
2	B	429	289	C2-C3-C4	2.20	114.71	110.89
2	B	430	289	O5-C1-C2	-2.20	107.38	110.77
2	B	428	289	O2-C2-C1	2.19	113.64	109.15
2	B	417	289	O5-C1-C2	2.19	114.15	110.77
2	B	413	289	C1-C2-C3	-2.19	106.98	109.67
2	A	424	289	O4-C4-C3	-2.18	105.30	110.35
2	A	434	289	C7-C6-C5	-2.18	107.75	112.17
2	B	431	289	O5-C1-C2	2.18	114.14	110.77
2	B	425	289	C1-O5-C5	2.18	115.05	111.48
2	A	401	289	O2-C2-C1	2.17	113.60	109.15
2	B	432	289	O5-C1-C2	-2.17	107.42	110.77
2	A	413	289	C1-C2-C3	2.16	112.33	109.67
2	B	420	289	O5-C1-C2	2.16	114.11	110.77
2	B	410	289	O2-C2-C1	2.15	113.56	109.15
2	A	430	289	O5-C1-C2	2.14	114.08	110.77
2	B	408	289	C3-C4-C5	2.14	114.57	109.68
2	B	431	289	C2-C3-C4	2.12	114.57	110.89
2	A	419	289	O2-C2-C3	2.12	114.38	110.14
2	B	415	289	C3-C4-C5	2.11	114.51	109.68
2	B	428	289	O7-C7-C6	-2.07	106.56	111.07
2	A	417	289	O4-C4-C3	-2.06	105.58	110.35
2	A	405	289	C2-C3-C4	-2.06	107.33	110.89
2	B	417	289	C1-O5-C5	2.05	114.84	111.48
2	A	415	289	O2-C2-C3	2.04	114.22	110.14
2	A	404	289	O5-C5-C4	-2.04	107.16	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	289	O3-C3-C2	2.02	113.87	109.99
2	B	427	289	O3-C3-C4	-2.02	105.67	110.35
2	B	425	289	O6-C6-C5	2.02	113.98	109.14
2	A	411	289	O2-C2-C3	-2.02	106.09	110.14
2	A	425	289	C2-C3-C4	2.02	114.39	110.89
2	B	424	289	O3-C3-C4	2.02	115.01	110.35
2	A	412	289	O4-C4-C3	-2.01	105.70	110.35
2	A	419	289	O5-C1-C2	-2.01	107.67	110.77
2	A	406	289	C3-C4-C5	2.00	114.26	109.68
2	B	422	289	O2-C2-C1	2.00	113.25	109.15

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	433	289	C1
2	A	406	289	C1
2	A	402	289	C1
2	B	408	289	C1
2	A	421	289	C1
2	A	435	289	C1

All (195) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	423	289	O5-C5-C6-C7
2	B	423	289	C4-C5-C6-C7
2	B	423	289	O5-C5-C6-O6
2	B	423	289	C4-C5-C6-O6
2	A	409	289	O5-C5-C6-C7
2	A	409	289	C4-C5-C6-C7
2	A	409	289	O5-C5-C6-O6
2	A	409	289	C4-C5-C6-O6
2	A	433	289	O5-C5-C6-C7
2	A	433	289	C4-C5-C6-C7
2	A	433	289	O5-C5-C6-O6
2	A	433	289	C4-C5-C6-O6
2	B	431	289	O5-C5-C6-C7
2	B	431	289	C4-C5-C6-C7
2	B	431	289	O5-C5-C6-O6
2	B	431	289	C4-C5-C6-O6
2	A	419	289	O5-C5-C6-C7
2	A	419	289	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	419	289	O5-C5-C6-O6
2	A	419	289	C4-C5-C6-O6
2	A	427	289	O5-C5-C6-C7
2	A	427	289	C4-C5-C6-C7
2	A	427	289	O5-C5-C6-O6
2	A	427	289	C4-C5-C6-O6
2	A	425	289	O6-C6-C7-O7
2	A	425	289	C5-C6-C7-O7
2	A	425	289	O5-C5-C6-C7
2	A	425	289	C4-C5-C6-C7
2	A	425	289	O5-C5-C6-O6
2	A	425	289	C4-C5-C6-O6
2	A	405	289	O5-C5-C6-O6
2	B	407	289	C5-C6-C7-O7
2	B	407	289	O5-C5-C6-C7
2	B	407	289	C4-C5-C6-C7
2	B	407	289	O5-C5-C6-O6
2	B	407	289	C4-C5-C6-O6
2	B	424	289	O5-C5-C6-C7
2	B	424	289	C4-C5-C6-C7
2	B	424	289	O5-C5-C6-O6
2	B	424	289	C4-C5-C6-O6
2	B	410	289	O5-C5-C6-O6
2	B	410	289	C4-C5-C6-O6
2	B	415	289	O5-C5-C6-O6
2	A	406	289	O6-C6-C7-O7
2	A	406	289	C5-C6-C7-O7
2	A	406	289	O5-C5-C6-C7
2	A	406	289	C4-C5-C6-C7
2	A	406	289	O5-C5-C6-O6
2	A	406	289	C4-C5-C6-O6
2	B	411	289	O6-C6-C7-O7
2	B	411	289	C5-C6-C7-O7
2	A	426	289	O5-C5-C6-O6
2	A	402	289	O6-C6-C7-O7
2	B	430	289	C4-C5-C6-C7
2	B	430	289	O5-C5-C6-O6
2	A	407	289	O5-C5-C6-C7
2	A	407	289	C4-C5-C6-C7
2	A	407	289	O5-C5-C6-O6
2	A	407	289	C4-C5-C6-O6
2	B	428	289	O5-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	B	428	289	C4-C5-C6-C7
2	B	428	289	O5-C5-C6-O6
2	B	428	289	C4-C5-C6-O6
2	B	401	289	O5-C5-C6-O6
2	B	418	289	O5-C5-C6-C7
2	B	418	289	C4-C5-C6-C7
2	B	418	289	O5-C5-C6-O6
2	B	418	289	C4-C5-C6-O6
2	B	413	289	O5-C5-C6-O6
2	B	413	289	C4-C5-C6-O6
2	B	432	289	O5-C5-C6-C7
2	B	432	289	C4-C5-C6-C7
2	B	432	289	O5-C5-C6-O6
2	B	432	289	C4-C5-C6-O6
2	B	429	289	C5-C6-C7-O7
2	B	426	289	O6-C6-C7-O7
2	B	426	289	C5-C6-C7-O7
2	B	405	289	O6-C6-C7-O7
2	B	405	289	C5-C6-C7-O7
2	B	420	289	O5-C5-C6-C7
2	B	420	289	C4-C5-C6-C7
2	B	420	289	O5-C5-C6-O6
2	B	420	289	C4-C5-C6-O6
2	A	428	289	O5-C5-C6-C7
2	A	428	289	C4-C5-C6-C7
2	A	428	289	O5-C5-C6-O6
2	A	428	289	C4-C5-C6-O6
2	A	424	289	O5-C5-C6-C7
2	A	424	289	C4-C5-C6-C7
2	A	424	289	O5-C5-C6-O6
2	A	417	289	O5-C5-C6-C7
2	A	417	289	C4-C5-C6-C7
2	A	417	289	O5-C5-C6-O6
2	A	417	289	C4-C5-C6-O6
2	B	404	289	C4-C5-C6-C7
2	B	404	289	O5-C5-C6-O6
2	B	404	289	C4-C5-C6-O6
2	A	413	289	O5-C5-C6-O6
2	A	418	289	O6-C6-C7-O7
2	A	418	289	C5-C6-C7-O7
2	A	418	289	O5-C5-C6-C7
2	A	418	289	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	418	289	O5-C5-C6-O6
2	A	418	289	C4-C5-C6-O6
2	A	416	289	O6-C6-C7-O7
2	B	414	289	C4-C5-C6-C7
2	B	414	289	O5-C5-C6-O6
2	B	414	289	C4-C5-C6-O6
2	B	419	289	C4-C5-C6-O6
2	B	403	289	O6-C6-C7-O7
2	A	415	289	O6-C6-C7-O7
2	A	415	289	C5-C6-C7-O7
2	B	402	289	O6-C6-C7-O7
2	B	402	289	C5-C6-C7-O7
2	B	402	289	O5-C5-C6-O6
2	A	411	289	O5-C5-C6-C7
2	A	411	289	C4-C5-C6-C7
2	A	411	289	O5-C5-C6-O6
2	A	411	289	C4-C5-C6-O6
2	A	403	289	C4-C5-C6-C7
2	A	403	289	O5-C5-C6-O6
2	A	403	289	C4-C5-C6-O6
2	B	412	289	O5-C5-C6-C7
2	B	412	289	C4-C5-C6-C7
2	B	412	289	O5-C5-C6-O6
2	B	412	289	C4-C5-C6-O6
2	B	421	289	O5-C5-C6-C7
2	B	421	289	C4-C5-C6-C7
2	B	421	289	O5-C5-C6-O6
2	B	421	289	C4-C5-C6-O6
2	B	425	289	O6-C6-C7-O7
2	B	425	289	O5-C5-C6-C7
2	B	425	289	C4-C5-C6-C7
2	B	425	289	O5-C5-C6-O6
2	B	425	289	C4-C5-C6-O6
2	A	429	289	O5-C5-C6-C7
2	A	429	289	C4-C5-C6-C7
2	A	429	289	O5-C5-C6-O6
2	A	429	289	C4-C5-C6-O6
2	A	435	289	C4-C5-C6-C7
2	A	412	289	O6-C6-C7-O7
2	A	412	289	C5-C6-C7-O7
2	A	408	289	O5-C5-C6-C7
2	A	408	289	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	408	289	O5-C5-C6-O6
2	A	408	289	C4-C5-C6-O6
2	B	431	289	O6-C6-C7-O7
2	B	407	289	O6-C6-C7-O7
2	B	410	289	O6-C6-C7-O7
2	A	426	289	O6-C6-C7-O7
2	A	401	289	O6-C6-C7-O7
2	B	429	289	O6-C6-C7-O7
2	B	414	289	O6-C6-C7-O7
2	A	435	289	O6-C6-C7-O7
2	A	402	289	C5-C6-C7-O7
2	A	416	289	C5-C6-C7-O7
2	B	414	289	C5-C6-C7-O7
2	B	403	289	C5-C6-C7-O7
2	A	435	289	C5-C6-C7-O7
2	B	410	289	C5-C6-C7-O7
2	A	401	289	C5-C6-C7-O7
2	B	424	289	O6-C6-C7-O7
2	A	423	289	O6-C6-C7-O7
2	A	426	289	C5-C6-C7-O7
2	A	414	289	C5-C6-C7-O7
2	B	425	289	C5-C6-C7-O7
2	A	430	289	O6-C6-C7-O7
2	B	419	289	O6-C6-C7-O7
2	B	410	289	O5-C5-C6-C7
2	A	426	289	O5-C5-C6-C7
2	B	413	289	O5-C5-C6-C7
2	A	430	289	O5-C5-C6-C7
2	B	414	289	O5-C5-C6-C7
2	B	419	289	O5-C5-C6-C7
2	A	403	289	O5-C5-C6-C7
2	B	418	289	O6-C6-C7-O7
2	A	424	289	C4-C5-C6-O6
2	A	432	289	C4-C5-C6-C7
2	B	413	289	C4-C5-C6-C7
2	A	420	289	C4-C5-C6-C7
2	A	412	289	C4-C5-C6-C7
2	A	435	289	O5-C5-C6-O6
2	B	431	289	C5-C6-C7-O7
2	A	422	289	O6-C6-C7-O7
2	A	423	289	C5-C6-C7-O7
2	A	405	289	O5-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	B	415	289	O5-C5-C6-C7
2	B	402	289	O5-C5-C6-C7
2	B	417	289	C4-C5-C6-O6
2	B	430	289	C4-C5-C6-O6
2	B	410	289	C4-C5-C6-C7
2	A	430	289	C4-C5-C6-C7
2	B	419	289	C4-C5-C6-C7
2	B	403	289	C4-C5-C6-C7
2	B	418	289	C5-C6-C7-O7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	411	289	C1-C2-C3-C4-C5-O5

30 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	409	289	0	2
2	B	416	289	1	3
2	A	433	289	2	0
2	A	425	289	2	0
2	B	428	289	1	1
2	B	424	289	1	1
2	A	406	289	2	0
2	B	411	289	1	0
2	A	410	289	5	0
2	A	432	289	2	0
2	B	432	289	1	0
2	A	431	289	1	0
2	A	434	289	4	0
2	A	430	289	1	0
2	B	430	289	0	1
2	B	435	289	3	0
2	B	420	289	0	1
2	A	424	289	1	0
2	B	408	289	2	0
2	B	404	289	2	0
2	A	413	289	6	0
2	A	416	289	1	0
2	B	433	289	11	0
2	B	406	289	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	412	289	5	0
2	A	414	289	1	0
2	A	420	289	2	3
2	A	403	289	0	2
2	B	425	289	1	0
2	A	408	289	0	1

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.