



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:50 AM GMT

PDB ID : 2BVW
Title : CELLOBIOHYDROLASE II (CEL6A) FROM HUMICOLA INSOLENS IN
COMPLEX WITH GLUCOSE AND CELLOTETRAOSE
Authors : Varrot, A.; Davies, G.J.; Schulein, M.
Deposited on : 1999-02-18
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

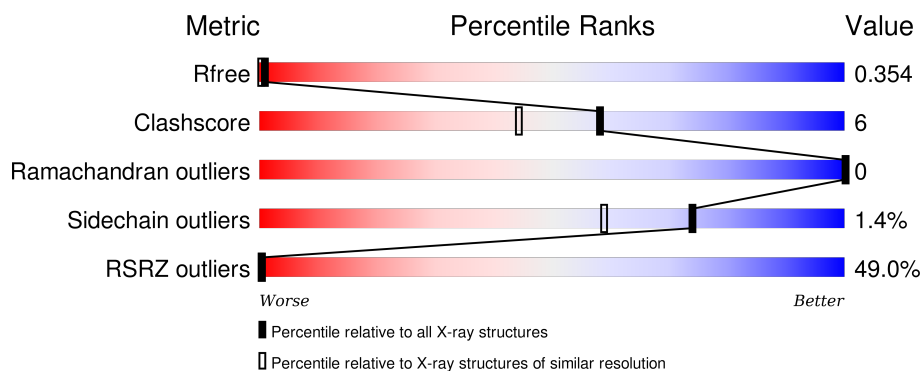
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	362	<div> <div>30%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	362	<div> <div>68%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

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
5	GOL	A	604	-	-	-	X
5	GOL	A	610	-	-	-	X
6	CTR	B	601	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6474 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 CELLOBIOHYDROLASE II.

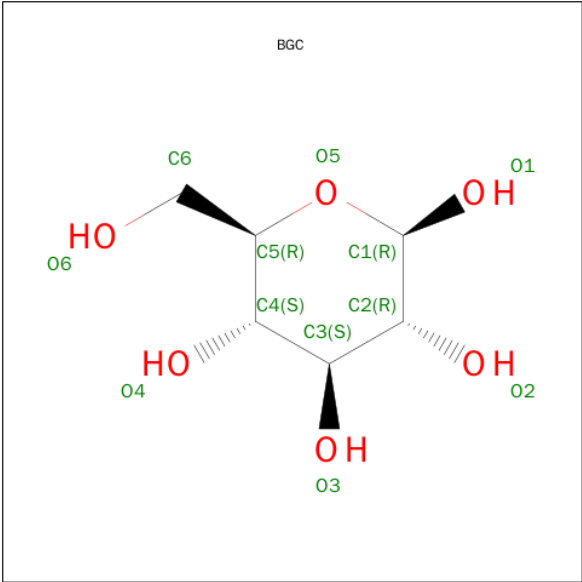
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	8	0
			2850	1803	502	535	10			
1	B	360	Total	C	N	O	S	0	7	0
			2834	1795	493	536	10			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



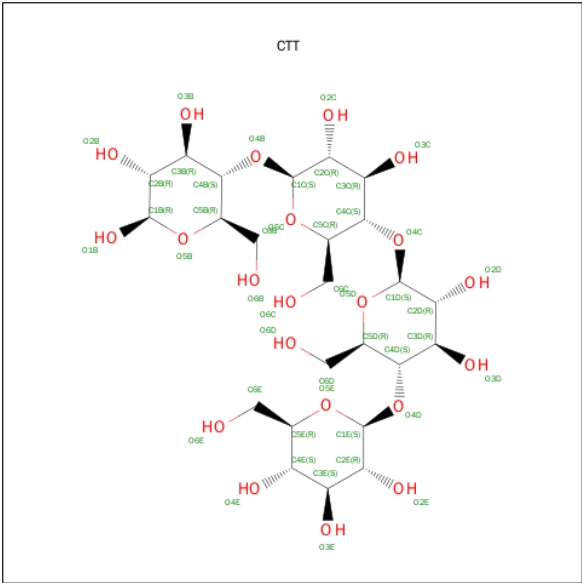
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is CELLOTETRAOSE (three-letter code: CTT) (formula: C₂₄H₄₂O₂₁).



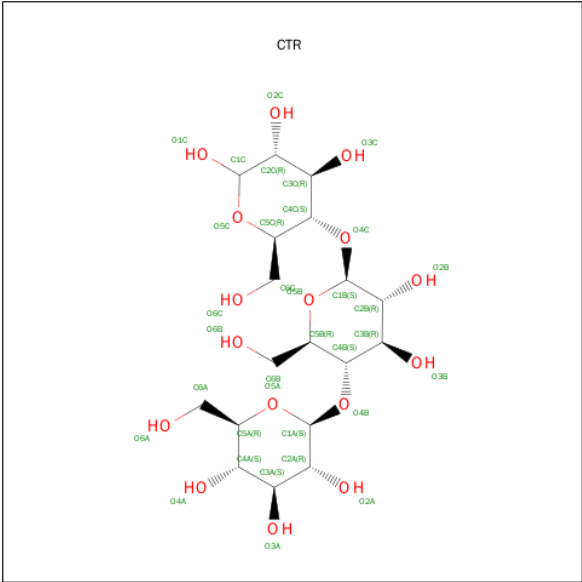
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			45	24	21		

- 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	A	1	Total	C	O	0	0
			6	3	3		
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		

- Molecule 6 is SUGAR (CELLOTRIOSE) (three-letter code: CTR) (formula: C₁₈H₃₂O₁₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			34	18	16		

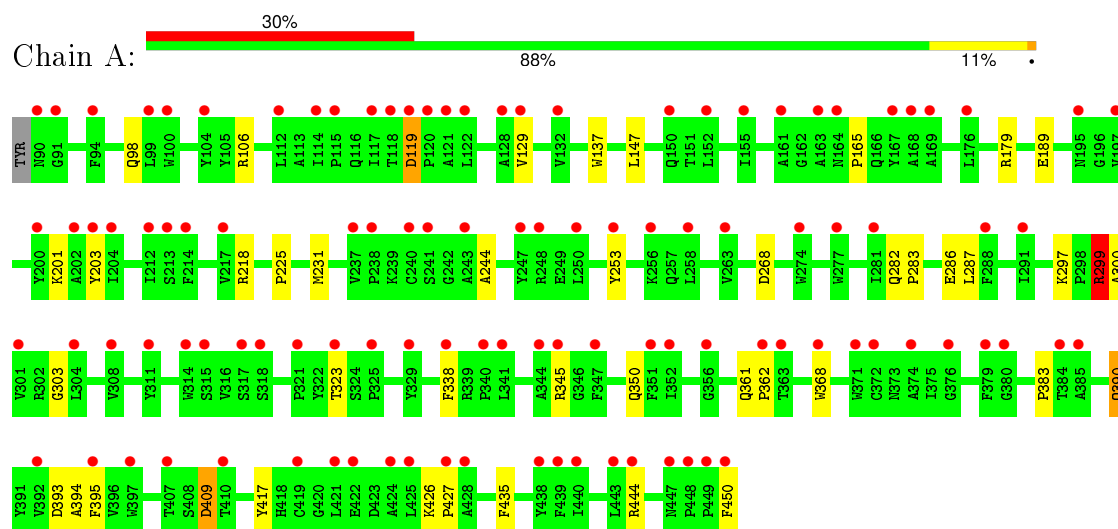
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	355	Total	O	0	0
			355	355		
7	B	262	Total	O	0	0
			262	262		

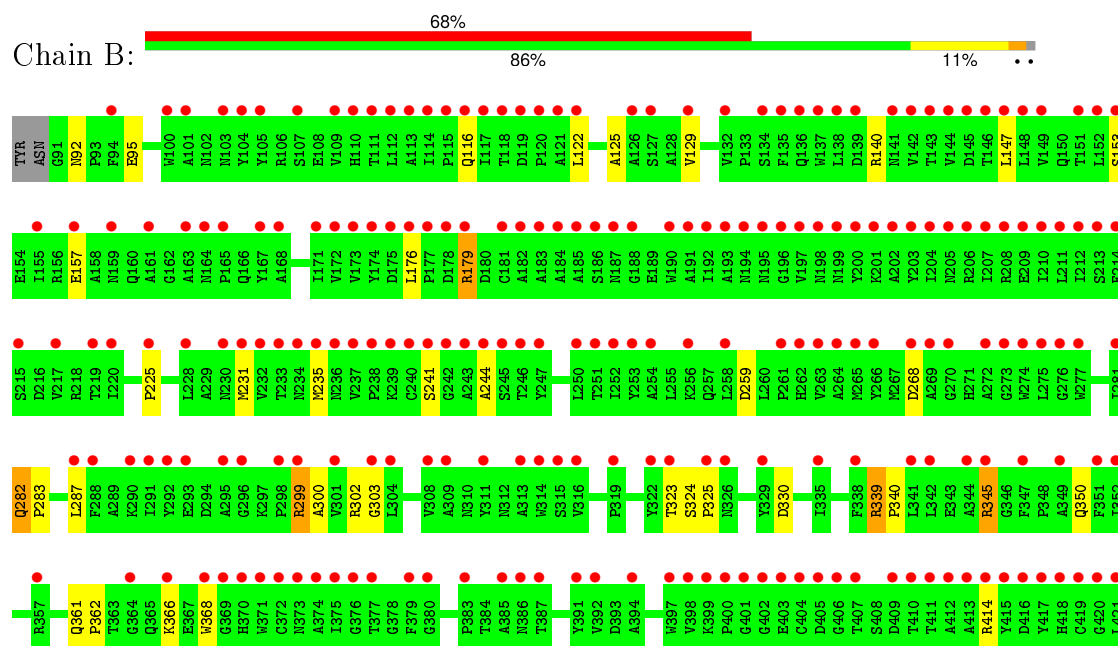
3 Residue-property plots [i](#)

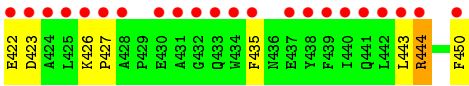
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: CELLOBIOHYDROLASE II



• Molecule 1: CELLOBIOHYDROLASE II





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.56Å 154.43Å 51.04Å 90.00° 119.31° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.80 – 1.67	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.00-1.70) 86.3 (19.80-1.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.67Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.175 , 0.226 0.336 , 0.354	Depositor DCC
R_{free} test set	3281 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.4	EDS
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 65198 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CTT, GOL, BGC, NAG, CTR

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	0.44	0/2972	1.03	8/4063 (0.2%)
1	B	0.44	0/2951	1.02	11/4035 (0.3%)
All	All	0.44	0/5923	1.03	19/8098 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ASP	CB-CG-OD1	8.05	125.55	118.30
1	A	299[A]	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	299[B]	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	330	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	345	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	414	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	345	ARG	CD-NE-CZ	5.80	131.72	123.60
1	B	259	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	189	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	203	TYR	CA-CB-CG	5.66	124.16	113.40
1	A	409	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	444[A]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	444[B]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	179	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	140	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	302	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	339	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	338	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	B	179	ARG	NE-CZ-NH1	5.30	122.95	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2850	0	2721	35	4
1	B	2834	0	2697	32	3
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	12	0	12	1	0
3	B	12	0	12	0	0
4	A	45	0	42	0	0
5	A	36	0	48	3	0
5	B	6	0	8	0	0
6	B	34	0	32	1	0
7	A	355	0	0	3	7
7	B	262	0	0	7	1
All	All	6474	0	5598	68	8

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 6.

All (68) 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:444[B]:ARG:NH1	7:A:722:HOH:O	1.81	1.14
1:A:129[A]:VAL:HG22	1:A:450:PHE:CZ	1.95	0.99
1:A:129[A]:VAL:HG22	1:A:450:PHE:CE2	2.10	0.87
1:B:299[B]:ARG:NH2	7:B:798:HOH:O	2.10	0.83
1:B:299[A]:ARG:NH2	7:B:858:HOH:O	2.12	0.83
1:B:299[B]:ARG:NH1	7:B:858:HOH:O	2.15	0.79
1:A:286:GLU:HG2	1:A:345[B]:ARG:HE	1.50	0.77
1:A:390:GLN:H	1:A:390:GLN:HE21	1.34	0.76
1:B:444[A]:ARG:HH11	1:B:444[A]:ARG:HG3	1.51	0.75
1:B:129[A]:VAL:HG13	1:B:450:PHE:CZ	2.24	0.73
1:A:444[B]:ARG:HH11	1:A:444[B]:ARG:HG2	1.55	0.71
1:A:299[A]:ARG:HG2	1:A:299[A]:ARG:HH11	1.56	0.71
1:A:390:GLN:NE2	1:A:390:GLN:H	1.90	0.68
1:A:129[A]:VAL:HG22	1:A:450:PHE:CE1	2.30	0.66
1:B:92:ASN:O	1:B:95[B]:GLU:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD12	7:A:835:HOH:O	1.98	0.63
1:B:235:MET:O	1:B:241:SER:HB3	1.99	0.63
1:B:129[A]:VAL:HG21	1:B:443:LEU:HD21	1.83	0.60
1:A:426:LYS:HB3	1:A:427:PRO:HA	1.84	0.59
1:B:129[A]:VAL:CG2	1:B:443:LEU:HD21	2.34	0.58
1:B:444[A]:ARG:HG3	1:B:444[A]:ARG:NH1	2.15	0.58
1:B:225:PRO:HA	1:B:268:ASP:CB	2.35	0.57
1:A:106:ARG:HH22	5:A:605:GOL:H12	1.70	0.56
1:B:426:LYS:HB3	1:B:427:PRO:HA	1.86	0.56
6:B:601:CTR:H6C1	7:B:610:HOH:O	2.05	0.55
1:B:129[A]:VAL:HG21	1:B:443:LEU:CD2	2.38	0.53
1:A:129[A]:VAL:CG2	1:A:450:PHE:CE2	2.88	0.52
1:A:282:GLN:O	1:A:286:GLU:HG3	2.10	0.52
1:B:125:ALA:O	1:B:129[A]:VAL:HG23	2.11	0.51
1:A:282:GLN:HB2	1:A:283:PRO:HD3	1.94	0.49
1:A:361:GLN:HA	1:A:362:PRO:C	2.32	0.49
1:B:231:MET:SD	1:B:244:ALA:HA	2.53	0.49
1:A:299[A]:ARG:HG2	1:A:299[A]:ARG:NH1	2.27	0.48
1:A:303:GLY:HA3	1:A:350:GLN:O	2.13	0.48
1:B:366:LYS:HE3	1:B:423:ASP:HB3	1.96	0.47
1:A:225:PRO:HA	1:A:268:ASP:CB	2.44	0.47
1:B:366:LYS:HB3	7:B:609:HOH:O	2.14	0.47
1:B:176:LEU:O	1:B:179:ARG:HB2	2.15	0.46
1:A:299[A]:ARG:HG3	7:A:698:HOH:O	2.15	0.46
1:A:444[B]:ARG:NH1	1:A:444[B]:ARG:HG2	2.24	0.46
1:B:122:LEU:HD22	1:B:444[B]:ARG:NH2	2.30	0.46
1:B:282:GLN:N	1:B:283:PRO:HD2	2.30	0.46
1:A:129[A]:VAL:HG22	1:A:450:PHE:CD2	2.51	0.45
1:A:286:GLU:HG2	1:A:345[A]:ARG:CZ	2.46	0.45
1:B:339:ARG:HB3	1:B:340:PRO:HD3	1.98	0.45
1:B:303:GLY:HA3	1:B:350:GLN:O	2.17	0.45
1:A:137:TRP:CE3	3:A:602:BGC:H5	2.52	0.45
1:B:299[A]:ARG:HG2	7:B:773:HOH:O	2.17	0.44
1:A:323:THR:HA	1:A:368:TRP:CE3	2.52	0.44
1:B:345:ARG:HG3	1:B:345:ARG:HH11	1.83	0.43
1:B:323:THR:HA	1:B:368:TRP:CE3	2.53	0.43
1:A:98:GLN:HG3	1:A:165:PRO:HG2	1.99	0.43
1:A:225:PRO:HA	1:A:268:ASP:CG	2.39	0.43
1:A:299[A]:ARG:HD2	1:A:300:ALA:N	2.33	0.43
1:A:383:PRO:HA	1:A:395:PHE:O	2.19	0.43
1:A:231:MET:SD	1:A:244:ALA:HA	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:SER:HA	1:B:325:PRO:HA	1.79	0.42
1:A:417:TYR:HD1	5:A:610:GOL:HO3	1.66	0.42
1:B:366:LYS:NZ	1:B:422:GLU:HB2	2.33	0.42
1:B:361:GLN:HA	1:B:362:PRO:C	2.40	0.42
1:B:225:PRO:HA	1:B:268:ASP:CG	2.40	0.42
1:B:299[A]:ARG:HG3	1:B:300:ALA:N	2.34	0.42
1:A:393:ASP:O	1:A:394:ALA:HB2	2.20	0.42
1:A:218:ARG:CZ	5:A:609:GOL:H12	2.50	0.41
1:B:147:LEU:HD23	7:B:676:HOH:O	2.21	0.41
1:B:116:GLN:HE21	1:B:116:GLN:HB3	1.68	0.41
1:A:129[A]:VAL:CG2	1:A:450:PHE:CD2	3.05	0.40

All (8) 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:253:TYR:OH	7:A:824:HOH:O[1_454]	1.62	0.58
1:B:116:GLN:OE1	7:A:920:HOH:O[1_454]	1.97	0.23
7:A:860:HOH:O	7:B:711:HOH:O[1_656]	2.02	0.18
1:B:157[B]:GLU:CG	7:A:753:HOH:O[1_454]	2.04	0.16
1:A:119:ASP:OD1	7:A:694:HOH:O[1_656]	2.07	0.13
1:A:201:LYS:NZ	7:A:850:HOH:O[1_454]	2.14	0.06
1:B:153:SER:O	7:A:753:HOH:O[1_454]	2.18	0.02
1:A:297:LYS:NZ	1:A:409:ASP:OD1[1_554]	2.19	0.01

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	367/362 (101%)	356 (97%)	11 (3%)	0	100	100
1	B	365/362 (101%)	353 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	732/724 (101%)	709 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	296/289 (102%)	291 (98%)	5 (2%)	68	51
1	B	294/289 (102%)	289 (98%)	5 (2%)	68	51
All	All	590/578 (102%)	580 (98%)	10 (2%)	74	51

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	390	GLN
1	A	435	PHE
1	B	282	GLN
1	B	287	LEU
1	B	299[A]	ARG
1	B	299[B]	ARG
1	B	435	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	166	GLN
1	A	390	GLN
1	A	445	ASN
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	166	GLN
1	B	230	ASN
1	B	234	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	NAG	A	500	1	14,14,15	1.08	1 (7%)	15,19,21	0.90	0
4	CTT	A	600	-	48,48,48	0.63	0	71,71,71	1.14	3 (4%)
3	BGC	A	602	-	12,12,12	0.67	0	17,17,17	1.11	1 (5%)
5	GOL	A	604	-	5,5,5	0.63	0	5,5,5	0.47	0
5	GOL	A	605	-	5,5,5	0.39	0	5,5,5	0.78	0
5	GOL	A	606	-	5,5,5	0.61	0	5,5,5	0.49	0
5	GOL	A	607	-	5,5,5	0.53	0	5,5,5	0.37	0
5	GOL	A	609	-	5,5,5	0.72	0	5,5,5	0.63	0
5	GOL	A	610	-	5,5,5	0.53	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	500	1	14,14,15	1.35	1 (7%)	15,19,21	1.08	0
6	CTR	B	601	-	36,36,36	0.48	0	53,53,53	0.97	2 (3%)
3	BGC	B	603	-	12,12,12	0.77	0	17,17,17	0.89	0
5	GOL	B	608	-	5,5,5	0.46	0	5,5,5	0.43	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
2	NAG	A	500	1	-	0/6/23/26	0/1/1/1
4	CTT	A	600	-	-	0/20/100/100	0/4/4/4
3	BGC	A	602	-	-	0/2/22/22	0/1/1/1
5	GOL	A	604	-	-	0/4/4/4	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
5	GOL	A	606	-	-	0/4/4/4	0/0/0/0
5	GOL	A	607	-	-	0/4/4/4	0/0/0/0
5	GOL	A	609	-	-	0/4/4/4	0/0/0/0
5	GOL	A	610	-	-	0/4/4/4	0/0/0/0
2	NAG	B	500	1	-	0/6/23/26	0/1/1/1
6	CTR	B	601	-	1/1/15/15	0/14/74/74	0/3/3/3
3	BGC	B	603	-	-	0/2/22/22	0/1/1/1
5	GOL	B	608	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NAG	O7-C7	-3.51	1.15	1.23
2	A	500	NAG	O7-C7	-3.38	1.15	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	CTT	O3C-C3C-C2C	-2.91	103.79	110.34
6	B	601	CTR	O4B-C1A-O5A	-2.34	104.76	110.68
4	A	600	CTT	O3D-C3D-C2D	-2.16	105.48	110.34
6	B	601	CTR	O5A-C5A-C4A	-2.07	105.79	109.68
4	A	600	CTT	O4D-C4D-C3D	2.08	112.53	107.17
3	A	602	BGC	O5-C1-C2	2.22	113.34	109.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	601	CTR	C1C

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	BGC	1	0
5	A	605	GOL	1	0
5	A	609	GOL	1	0
5	A	610	GOL	1	0
6	B	601	CTR	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	361/362 (99%)	1.54	108 (29%) 1 0	8, 16, 27, 36	0
1	B	360/362 (99%)	3.01	245 (68%) 0 0	9, 17, 28, 35	0
All	All	721/724 (99%)	2.27	353 (48%) 0 0	8, 17, 27, 36	0

All (353) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	ASN	11.7
1	B	412	ALA	11.4
1	B	190	TRP	9.9
1	B	413	ALA	8.6
1	B	191	ALA	8.5
1	B	404	CYS	7.4
1	B	238	PRO	7.1
1	B	163	ALA	6.9
1	B	434	TRP	6.8
1	B	411	THR	6.8
1	B	420	GLY	6.5
1	B	193	ALA	6.3
1	B	192	ILE	6.2
1	B	118	THR	6.2
1	B	371	TRP	6.2
1	B	253	TYR	6.2
1	B	235	MET	6.1
1	B	291	ILE	5.9
1	B	184	ALA	5.9
1	B	115	PRO	5.8
1	B	231	MET	5.8
1	B	410	THR	5.7
1	B	142	VAL	5.7
1	B	207	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	5.6
1	B	245	SER	5.6
1	B	147	LEU	5.5
1	B	177	PRO	5.5
1	A	450	PHE	5.4
1	B	112	LEU	5.3
1	B	236	ASN	5.3
1	B	181	CYS	5.3
1	B	414	ARG	5.2
1	B	287	LEU	5.2
1	B	104	TYR	5.1
1	B	204	ILE	5.1
1	B	149	VAL	5.1
1	B	275	LEU	5.1
1	B	187	ASN	5.1
1	B	148	LEU	5.0
1	B	254	ALA	4.9
1	B	175	ASP	4.9
1	B	424	ALA	4.9
1	B	213[A]	SER	4.8
1	B	199	ASN	4.8
1	B	385	ALA	4.8
1	B	440	ILE	4.8
1	B	247	TYR	4.8
1	B	421	LEU	4.7
1	B	435	PHE	4.7
1	B	174	TYR	4.7
1	B	309	ALA	4.7
1	B	195	ASN	4.7
1	B	242	GLY	4.7
1	B	198	ASN	4.7
1	B	428	ALA	4.6
1	B	419	CYS	4.6
1	B	417	TYR	4.5
1	B	127	SER	4.5
1	B	228	LEU	4.5
1	B	212	ILE	4.5
1	B	214	PHE	4.5
1	B	182	ALA	4.4
1	B	432	GLY	4.4
1	B	144	VAL	4.4
1	A	443	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	311	TYR	4.3
1	B	202	ALA	4.3
1	B	203	TYR	4.3
1	B	415	TYR	4.3
1	B	402	GLY	4.3
1	A	204	ILE	4.3
1	B	335	ILE	4.3
1	B	137	TRP	4.3
1	B	197	VAL	4.3
1	B	246	THR	4.2
1	B	126	ALA	4.2
1	B	138	LEU	4.2
1	B	120	PRO	4.2
1	B	196	GLY	4.2
1	A	161	ALA	4.2
1	B	400	PRO	4.1
1	B	425	LEU	4.1
1	A	121	ALA	4.1
1	B	230	ASN	4.1
1	B	338	PHE	4.1
1	B	352	ILE	4.1
1	B	368	TRP	4.1
1	B	450	PHE	4.0
1	B	299[A]	ARG	4.0
1	B	200	TYR	4.0
1	B	438	TYR	4.0
1	B	252	ILE	4.0
1	B	100	TRP	4.0
1	B	292	TYR	4.0
1	B	272	ALA	3.9
1	B	377	THR	3.9
1	B	316	VAL	3.8
1	A	374	ALA	3.8
1	A	176	LEU	3.8
1	B	173	VAL	3.8
1	B	277	TRP	3.8
1	B	430	GLU	3.8
1	B	407	THR	3.8
1	B	351	PHE	3.8
1	B	397	TRP	3.8
1	B	269	ALA	3.7
1	B	209	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	234	ASN	3.7
1	B	439	PHE	3.7
1	B	418	HIS	3.7
1	B	172	VAL	3.7
1	B	210	ILE	3.7
1	B	122	LEU	3.7
1	A	444[A]	ARG	3.6
1	B	431	ALA	3.6
1	B	109	VAL	3.6
1	B	152	LEU	3.6
1	A	344	ALA	3.6
1	B	341	LEU	3.6
1	B	111	THR	3.5
1	B	132	VAL	3.5
1	B	250	LEU	3.5
1	B	117	ILE	3.5
1	A	195	ASN	3.5
1	B	369	GLY	3.5
1	B	129[A]	VAL	3.5
1	B	232	VAL	3.5
1	B	329	TYR	3.5
1	B	444[A]	ARG	3.5
1	A	281	ILE	3.4
1	B	178	ASP	3.4
1	B	301	VAL	3.4
1	A	164	ASN	3.4
1	A	314	TRP	3.4
1	B	256	LYS	3.4
1	B	183	ALA	3.4
1	B	243	ALA	3.4
1	A	424	ALA	3.4
1	B	442	LEU	3.3
1	B	105	TYR	3.3
1	B	322	TYR	3.3
1	B	441	GLN	3.3
1	B	185	ALA	3.3
1	B	394	ALA	3.3
1	A	115	PRO	3.3
1	B	208	ARG	3.3
1	B	263	VAL	3.3
1	B	113	ALA	3.3
1	B	241	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	239	LYS	3.2
1	A	114	ILE	3.2
1	B	288	PHE	3.2
1	B	374	ALA	3.2
1	A	152	LEU	3.2
1	A	425	LEU	3.2
1	B	206	ARG	3.2
1	B	201	LYS	3.2
1	B	274	TRP	3.2
1	B	409	ASP	3.2
1	B	94	PHE	3.2
1	B	146	THR	3.2
1	B	296	GLY	3.1
1	B	392	VAL	3.1
1	B	211	LEU	3.1
1	A	247	TYR	3.1
1	B	114	ILE	3.1
1	B	171	ILE	3.1
1	A	163	ALA	3.1
1	B	136	GLN	3.1
1	B	240	CYS	3.1
1	B	391	TYR	3.1
1	B	426	LYS	3.1
1	B	375	ILE	3.0
1	B	347	PHE	3.0
1	B	176	LEU	3.0
1	A	91	GLY	3.0
1	B	372	CYS	3.0
1	B	153	SER	3.0
1	A	345[A]	ARG	3.0
1	A	392	VAL	3.0
1	B	437	GLU	3.0
1	A	129[A]	VAL	3.0
1	B	237	VAL	3.0
1	A	99	LEU	3.0
1	A	122	LEU	3.0
1	A	169	ALA	3.0
1	B	101	ALA	3.0
1	B	303	GLY	2.9
1	B	103	ASN	2.9
1	B	370	HIS	2.9
1	B	119	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	214	PHE	2.9
1	A	438	TYR	2.9
1	A	351	PHE	2.9
1	B	205	ASN	2.9
1	A	197	VAL	2.9
1	B	308	VAL	2.9
1	B	379	PHE	2.9
1	B	268	ASP	2.9
1	B	349	ALA	2.9
1	A	321	PRO	2.8
1	B	323	THR	2.8
1	B	270	GLY	2.8
1	B	273	GLY	2.8
1	B	143	THR	2.8
1	B	110	HIS	2.8
1	B	398	VAL	2.8
1	A	304	LEU	2.8
1	B	366	LYS	2.8
1	A	363	THR	2.8
1	B	233	THR	2.8
1	A	379	PHE	2.8
1	B	159	ASN	2.8
1	A	440	ILE	2.8
1	B	217	VAL	2.8
1	B	167	TYR	2.7
1	B	293	GLU	2.7
1	B	251	THR	2.7
1	B	141	ASN	2.7
1	A	119	ASP	2.7
1	A	371	TRP	2.7
1	A	428	ALA	2.7
1	A	447	ASN	2.7
1	B	225	PRO	2.7
1	A	243	ALA	2.7
1	A	238	PRO	2.6
1	A	258	LEU	2.6
1	B	427	PRO	2.6
1	B	161	ALA	2.6
1	B	399	LYS	2.6
1	A	449	PRO	2.6
1	A	291	ILE	2.6
1	A	421	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	107	SER	2.6
1	B	357	ARG	2.6
1	A	202	ALA	2.6
1	A	352	ILE	2.6
1	B	220	ILE	2.6
1	B	342	LEU	2.6
1	B	179	ARG	2.6
1	B	151	THR	2.6
1	B	262	HIS	2.6
1	A	200	TYR	2.6
1	A	253	TYR	2.6
1	B	325	PRO	2.6
1	A	380	GLY	2.6
1	B	406	GLY	2.6
1	B	314	TRP	2.5
1	B	168	ALA	2.5
1	B	295	ALA	2.5
1	A	167	TYR	2.5
1	B	188	GLY	2.5
1	B	258	LEU	2.5
1	B	266	TYR	2.5
1	A	315	SER	2.5
1	B	290	LYS	2.5
1	B	364	GLY	2.5
1	A	341	LEU	2.5
1	B	116	GLN	2.5
1	B	145	ASP	2.5
1	A	368	TRP	2.5
1	A	237	VAL	2.5
1	A	419	CYS	2.5
1	B	276	GLY	2.5
1	B	304	LEU	2.5
1	A	407	THR	2.4
1	A	256	LYS	2.4
1	A	240	CYS	2.4
1	A	117	ILE	2.4
1	A	395	PHE	2.4
1	B	319	PRO	2.4
1	B	264	ALA	2.4
1	A	112	LEU	2.4
1	B	281	ILE	2.4
1	A	104	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	329	TYR	2.4
1	B	135	PHE	2.4
1	A	427	PRO	2.4
1	A	274	TRP	2.4
1	A	132	VAL	2.4
1	A	155	ILE	2.4
1	A	318	SER	2.4
1	B	387	THR	2.4
1	B	401	GLY	2.4
1	A	448	PRO	2.4
1	B	155	ILE	2.4
1	B	261	PRO	2.4
1	A	347	PHE	2.4
1	A	150[A]	GLN	2.4
1	B	345	ARG	2.4
1	B	326	ASN	2.4
1	B	433	GLN	2.4
1	B	422	GLU	2.3
1	A	263	VAL	2.3
1	B	186	SER	2.3
1	A	128	ALA	2.3
1	B	313	ALA	2.3
1	B	344	ALA	2.3
1	A	439	PHE	2.3
1	A	308	VAL	2.3
1	B	215	SER	2.3
1	A	325	PRO	2.3
1	A	397	TRP	2.3
1	B	443	LEU	2.3
1	A	212	ILE	2.3
1	B	403	GLU	2.3
1	A	340	PRO	2.3
1	A	376	GLY	2.2
1	B	416	ASP	2.2
1	A	338	PHE	2.2
1	B	121	ALA	2.2
1	A	362	PRO	2.2
1	A	422	GLU	2.2
1	B	139	ASP	2.2
1	B	134	SER	2.2
1	A	168	ALA	2.2
1	A	248	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	94	PHE	2.2
1	B	164	ASN	2.2
1	B	298	PRO	2.2
1	A	384	THR	2.2
1	B	244	ALA	2.2
1	B	423	ASP	2.2
1	A	90	ASN	2.2
1	A	301	VAL	2.2
1	A	213	SER	2.1
1	A	241	SER	2.1
1	A	317	SER	2.1
1	A	118	THR	2.1
1	A	372	CYS	2.1
1	B	219	THR	2.1
1	A	277	TRP	2.1
1	A	356	GLY	2.1
1	B	376	GLY	2.1
1	A	323	THR	2.1
1	B	380	GLY	2.1
1	A	410	THR	2.1
1	B	383	PRO	2.1
1	A	250	LEU	2.1
1	A	311	TYR	2.1
1	A	385	ALA	2.1
1	B	373	ASN	2.1
1	B	386	ASN	2.1
1	B	265	MET	2.0
1	B	405	ASP	2.0
1	A	100	TRP	2.0
1	B	315	SER	2.0
1	A	217	VAL	2.0
1	A	203	TYR	2.0
1	B	157[A]	GLU	2.0
1	A	288	PHE	2.0
1	B	165	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	610	6/6	0.63	0.29	4.57	33,36,38,40	0
5	GOL	A	604	6/6	0.70	0.28	3.11	24,27,28,31	0
5	GOL	A	606	6/6	0.77	0.21	0.46	19,21,22,24	0
3	BGC	A	602	12/12	0.82	0.14	0.31	8,11,13,13	0
5	GOL	A	605	6/6	0.67	0.22	0.28	20,26,26,26	0
3	BGC	B	603	12/12	0.60	0.29	0.25	11,13,14,15	0
5	GOL	B	608	6/6	0.28	0.32	0.20	44,44,45,45	0
2	NAG	A	500	14/15	0.78	0.15	0.13	15,20,22,24	0
6	CTR	B	601	34/34	0.65	0.23	-0.21	11,18,30,32	0
5	GOL	A	609	6/6	0.65	0.19	-0.34	30,31,33,35	0
4	CTT	A	600	45/45	0.83	0.15	-0.34	10,19,33,35	1
2	NAG	B	500	14/15	0.49	0.28	-0.50	24,26,28,29	0
5	GOL	A	607	6/6	0.56	0.27	-	27,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.