



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 07:54 PM EST

PDB ID : 1RWH  
Title : Crystal structure of *Arthrobacter aurescens* chondroitin AC lyase in complex with chondroitin tetrasaccharide  
Authors : Lunin, V.V.; Li, Y.; Miyazono, H.; Kyogashima, M.; Bell, A.W.; Cygler, M.  
Deposited on : 2003-12-16  
Resolution : 1.25 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

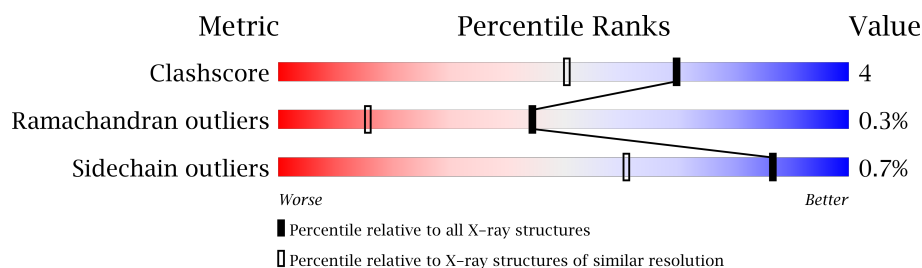
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.25 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))
Clashscore	112137	1781 (1.30-1.22)
Ramachandran outliers	110173	1716 (1.30-1.22)
Sidechain outliers	110143	1714 (1.30-1.22)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	757	 92% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GCT	A	811	-	-	X	-
6	PO4	A	850	-	-	X	-

## 2 Entry composition [i](#)

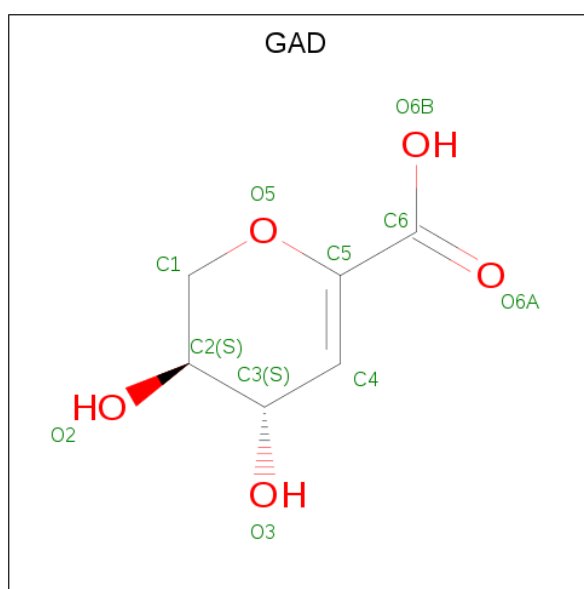
There are 8 unique types of molecules in this entry. The entry contains 6837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 chondroitin AC lyase.

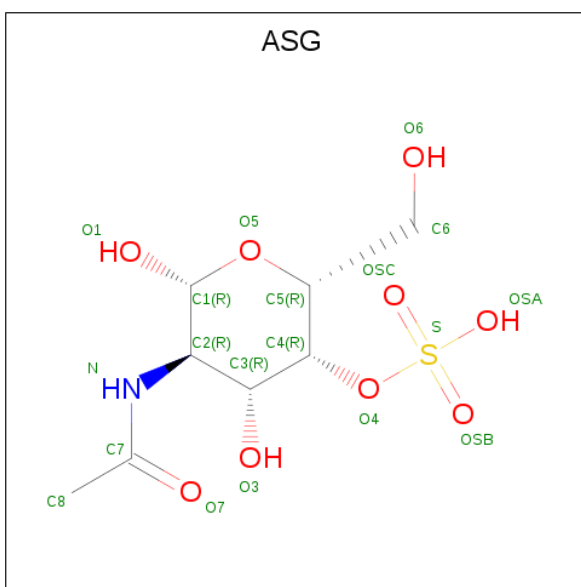
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	754	5646	3544	989	1095	18	0	15	0

- Molecule 2 is 2,6-ANHYDRO-3-DEOXY-D-ERYTHRO-HEX-2-ENONIC ACID (three-letter code: GAD) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>5</sub>).



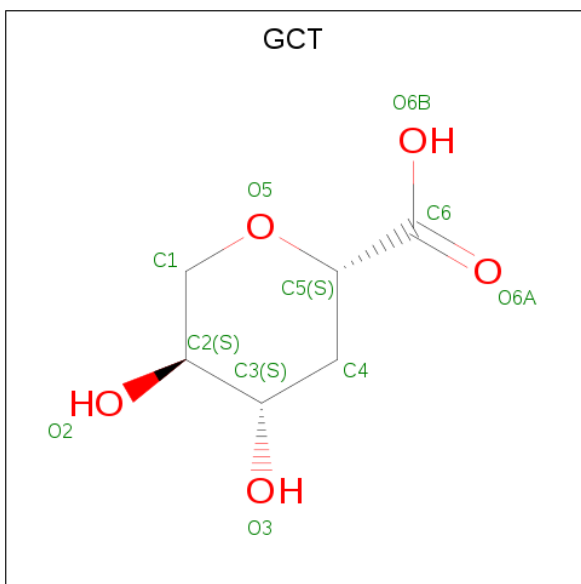
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	11	6	5	0	0

- Molecule 3 is 2-DEOXY-2-ACETAMIDO-BETA-D-GALACTOSE-4-SULFATE (three-letter code: ASG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>9</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	8	1	9	1		
3	A	1	Total	C	N	O	S	0	0
			19	8	1	9	1		

- Molecule 4 is 4,5-DIHYDROXY-TETRAHYDRO-PYRAN-2-CARBOXYLIC ACID (three-letter code: GCT) (formula:  $C_6H_{10}O_5$ ).

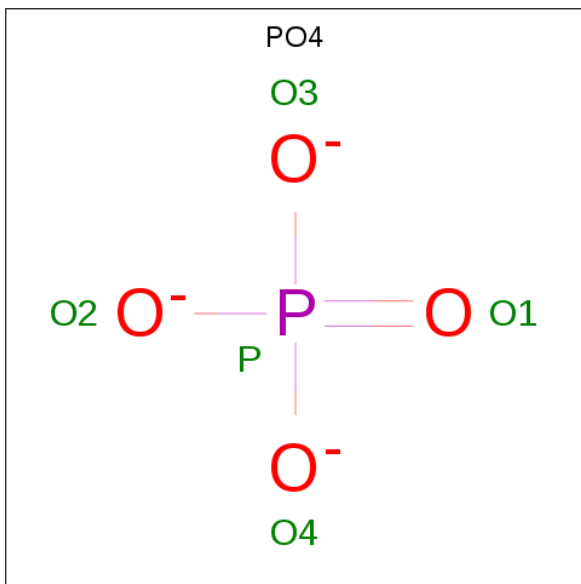


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

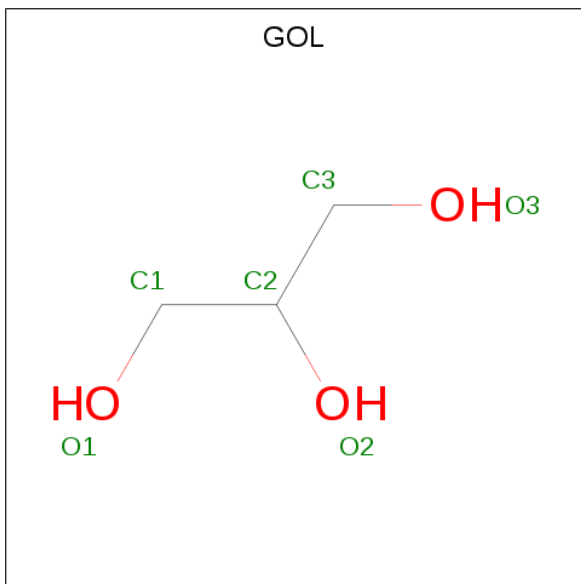
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is water.

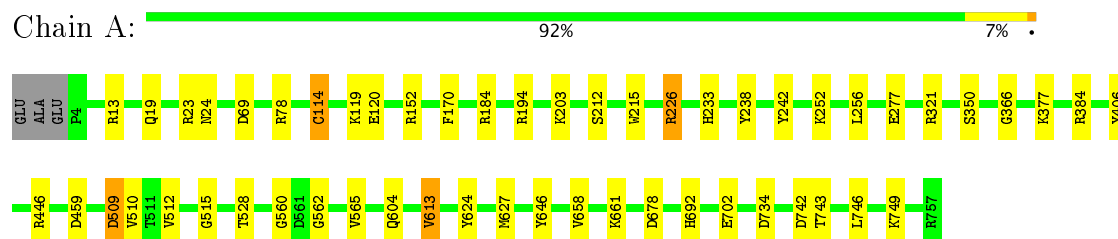
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1107	Total 1107	O 1107	0	0

### 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 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.

Note EDS was not executed.

- Molecule 1: chondroitin AC lyase



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.62Å 86.31Å 80.51Å 90.00° 106.95° 90.00°	Depositor
Resolution (Å)	25.24 – 1.25	Depositor
% Data completeness (in resolution range)	100.0 (25.24-1.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	REFMAC 5.1.08	Depositor
R, $R_{free}$	0.113 , 0.142	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, PO4, ASG, GCT, GAD

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	1.00	12/5844 (0.2%)	1.00	15/7965 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509[A]	ASP	CB-CG	-7.87	1.35	1.51
1	A	509[B]	ASP	CB-CG	-7.87	1.35	1.51
1	A	661	LYS	CE-NZ	7.14	1.67	1.49
1	A	24	ASN	CG-OD1	6.79	1.38	1.24
1	A	24	ASN	CB-CG	6.51	1.66	1.51
1	A	565	VAL	CB-CG1	-6.43	1.39	1.52
1	A	613[A]	VAL	CB-CG2	-6.32	1.39	1.52
1	A	613[B]	VAL	CB-CG2	-6.32	1.39	1.52
1	A	604	GLN	CG-CD	5.79	1.64	1.51
1	A	277[A]	GLU	CD-OE2	5.48	1.31	1.25
1	A	277[B]	GLU	CD-OE2	5.48	1.31	1.25
1	A	114	CYS	CB-SG	-5.01	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	A	459	ASP	CB-CG-OD2	9.53	126.88	118.30
1	A	152	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	A	184	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	78	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	69	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	226	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	13	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	384	ARG	NE-CZ-NH2	-5.75	117.43	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	23	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	742	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	678	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	734	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	446	ARG	NE-CZ-NH2	-5.12	117.74	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	5646	0	5522	38	0
2	A	11	0	6	0	0
3	A	38	0	25	9	0
4	A	11	0	7	11	0
5	A	1	0	0	0	0
6	A	5	0	0	3	0
7	A	18	0	24	0	0
8	A	1107	0	0	16	2
All	All	6837	0	5584	47	2

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 4.

All (47) 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:510[A]:VAL:HG11	1:A:627[A]:MET:CE	1.45	1.41
3:A:810:ASG:O1	4:A:811:GCT:HC42	1.17	1.35
3:A:810:ASG:C1	4:A:811:GCT:HC42	1.73	1.18
1:A:114:CYS:HB3	8:A:1677:HOH:O	1.47	1.15
1:A:510[A]:VAL:CG1	1:A:627[A]:MET:CE	2.23	1.14
1:A:510[A]:VAL:CG1	1:A:627[A]:MET:HE3	1.79	1.11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:SG	8:A:1677:HOH:O	2.10	1.08
1:A:510[A]:VAL:HG11	1:A:627[A]:MET:HE3	1.05	1.03
1:A:114:CYS:CB	8:A:1677:HOH:O	2.02	0.91
1:A:366:GLY:HA2	8:A:2101:HOH:O	1.73	0.89
1:A:510[A]:VAL:CG1	1:A:627[A]:MET:HE2	2.05	0.85
1:A:203:LYS:NZ	8:A:1662:HOH:O	2.10	0.82
1:A:242:TYR:HH	4:A:811:GCT:HC5	1.43	0.82
1:A:242:TYR:OH	4:A:811:GCT:HC5	1.85	0.75
1:A:510[A]:VAL:HG11	1:A:627[A]:MET:HE1	1.68	0.71
1:A:510[A]:VAL:HG13	1:A:627[A]:MET:HE2	1.74	0.69
4:A:811:GCT:HC2	6:A:850:PO4:O4	1.95	0.67
1:A:509[B]:ASP:OD1	8:A:1398:HOH:O	2.12	0.66
4:A:811:GCT:C2	6:A:850:PO4:O4	2.45	0.63
1:A:692:HIS:HD2	8:A:1544:HOH:O	1.85	0.58
3:A:810:ASG:O1	4:A:811:GCT:C5	2.50	0.57
1:A:226:ARG:NH2	8:A:1345:HOH:O	2.22	0.57
1:A:233:HIS:CD2	3:A:812:ASG:OSA	2.58	0.57
1:A:562:GLY:O	8:A:2034:HOH:O	2.18	0.55
1:A:510[B]:VAL:HG21	1:A:646:TYR:CE2	2.43	0.53
3:A:810:ASG:H1	4:A:811:GCT:HC42	1.83	0.52
1:A:512:VAL:HG11	1:A:658[A]:VAL:HG11	1.92	0.51
1:A:743:THR:HA	1:A:746:LEU:HD12	1.93	0.49
3:A:810:ASG:O1	4:A:811:GCT:HC5	2.12	0.48
1:A:515:GLY:HA3	1:A:624:TYR:CE2	2.48	0.48
3:A:812:ASG:H6A	8:A:2051:HOH:O	2.12	0.48
1:A:119:LYS:HE3	1:A:120:GLU:O	2.15	0.47
1:A:528:THR:HB	1:A:613[A]:VAL:HG22	1.98	0.46
1:A:226:ARG:NE	8:A:1345:HOH:O	2.40	0.46
1:A:377:LYS:HD2	8:A:1682:HOH:O	2.15	0.46
1:A:692:HIS:CD2	8:A:1544:HOH:O	2.66	0.45
1:A:212:SER:HA	1:A:215:TRP:CZ2	2.52	0.44
1:A:242:TYR:CD2	3:A:810:ASG:H8B	2.53	0.44
1:A:749:LYS:HE2	8:A:1308:HOH:O	2.17	0.44
1:A:350:SER:C	8:A:1560:HOH:O	2.57	0.43
1:A:377:LYS:HB3	8:A:1682:HOH:O	2.18	0.43
1:A:19[B]:GLN:HE22	1:A:256:LEU:N	2.17	0.42
1:A:528:THR:HB	1:A:613[A]:VAL:CG2	2.50	0.42
1:A:19[A]:GLN:HE22	1:A:252:LYS:HB3	1.85	0.42
4:A:811:GCT:C1	6:A:850:PO4:O4	2.67	0.41
1:A:242:TYR:HH	4:A:811:GCT:C5	2.23	0.41
1:A:233:HIS:NE2	3:A:812:ASG:H4	2.36	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1486:HOH:O	8:A:2077:HOH:O[1_556]	1.79	0.41
8:A:1955:HOH:O	8:A:2074:HOH:O[1_655]	2.18	0.02

## 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	767/757 (101%)	752 (98%)	13 (2%)	2 (0%)	44 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	560	GLY
1	A	170	PHE

### 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	583/570 (102%)	579 (99%)	4 (1%)	87 61

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	238	TYR
1	A	406	TYR
1	A	702	GLU

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	189	GLN
1	A	216	GLN

### 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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	GOL	A	801	-	5,5,5	0.66	0	5,5,5	0.51	0
7	GOL	A	802	-	5,5,5	0.33	0	5,5,5	0.69	0
7	GOL	A	803	-	5,5,5	0.50	0	5,5,5	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GAD	A	809	3	7,11,11	1.73	3 (42%)	6,15,15	2.84	2 (33%)
3	ASG	A	810	2,4	19,19,19	1.12	1 (5%)	23,28,28	1.43	3 (13%)
4	GCT	A	811	3	8,11,11	1.53	1 (12%)	9,15,15	3.16	4 (44%)
3	ASG	A	812	4	19,19,19	1.22	1 (5%)	23,28,28	1.63	7 (30%)
6	PO4	A	850	-	4,4,4	1.60	1 (25%)	6,6,6	1.34	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	801	-	-	0/4/4/4	0/0/0/0
7	GOL	A	802	-	-	0/4/4/4	0/0/0/0
7	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	GAD	A	809	3	-	0/0/17/17	0/1/1/1
3	ASG	A	810	2,4	-	0/11/31/31	0/1/1/1
4	GCT	A	811	3	-	0/0/17/17	0/1/1/1
3	ASG	A	812	4	-	0/11/31/31	0/1/1/1
6	PO4	A	850	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	811	GCT	O3-C3	-3.92	1.34	1.43
2	A	809	GAD	O5-C1	-2.82	1.40	1.45
6	A	850	PO4	P-O2	-2.56	1.45	1.54
2	A	809	GAD	O5-C5	2.01	1.40	1.37
3	A	810	ASG	O4-S	2.07	1.62	1.56
2	A	809	GAD	C3-C4	2.85	1.54	1.50
3	A	812	ASG	OSC-S	4.00	1.60	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	809	GAD	O5-C5-C4	-6.42	119.16	124.84
4	A	811	GCT	O2-C2-C3	-3.47	102.51	110.17
3	A	812	ASG	O3-C3-C2	-3.12	103.28	109.61
4	A	811	GCT	C4-C3-C2	-3.05	106.43	110.34
3	A	812	ASG	C3-C4-C5	-2.48	105.61	110.88
3	A	810	ASG	C3-C2-N	-2.24	106.33	110.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	812	ASG	O5-C1-C2	-2.13	107.37	109.52
6	A	850	PO4	O4-P-O1	-2.09	102.09	110.97
3	A	812	ASG	C8-C7-N	-2.01	112.47	116.11
6	A	850	PO4	O3-P-O2	2.18	115.92	107.90
3	A	810	ASG	OSA-S-OSC	2.27	116.84	108.79
2	A	809	GAD	C3-C4-C5	2.48	125.79	121.60
3	A	812	ASG	C1-C2-C3	2.65	114.16	110.54
3	A	812	ASG	C1-C2-N	2.85	114.03	110.73
3	A	812	ASG	O5-C5-C6	3.20	114.08	106.41
4	A	811	GCT	O5-C1-C2	3.24	115.87	110.79
3	A	810	ASG	C1-C2-N	3.97	115.33	110.73
4	A	811	GCT	C1-O5-C5	6.97	124.94	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	810	ASG	6	0
4	A	811	GCT	11	0
3	A	812	ASG	3	0
6	A	850	PO4	3	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.