



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:07 PM GMT

PDB ID : 3W81  
Title : Human alpha-l-iduronidase  
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Deposited on : 2013-03-11  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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

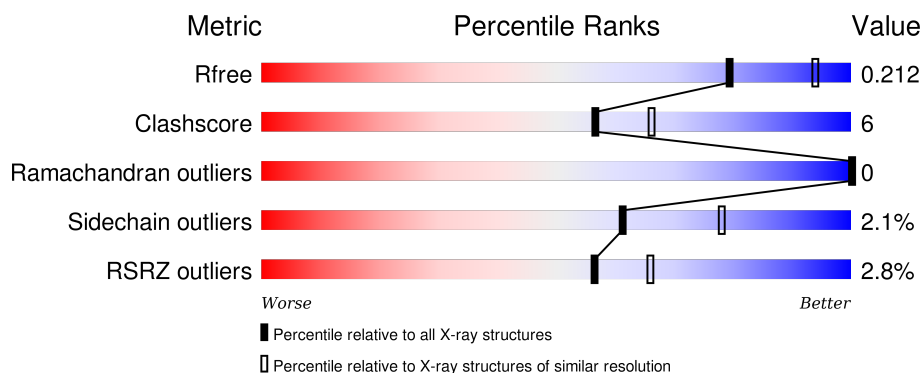
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


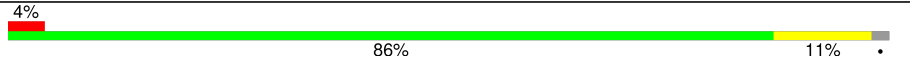
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	627	 2% 86% 12% ..
1	B	627	 4% 86% 11% .

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	TLA	A	714	-	-	-	X
5	TLA	A	716	-	-	-	X
6	GOL	B	722	-	-	X	X
7	PO4	B	724	-	-	X	X
8	CL	A	719	-	-	X	-
8	CL	B	727	-	-	X	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10862 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.

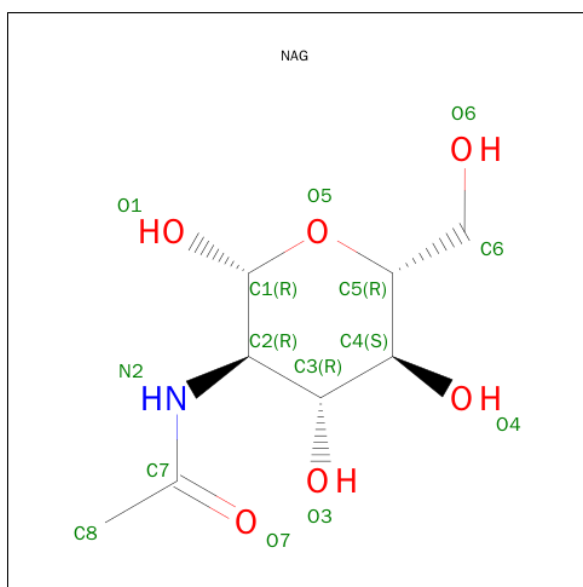
- Molecule 1 is a protein called Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4885	3119	885	869	12			
1	B	616	Total	C	N	O	S	0	0	0
			4885	3119	885	869	12			

- Molecule 2 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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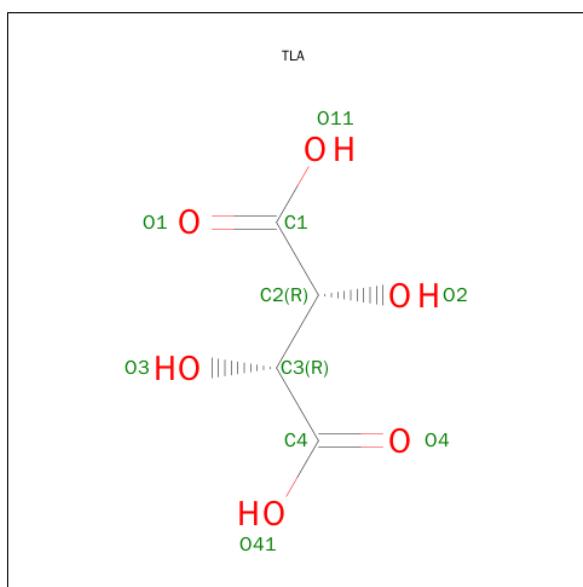
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



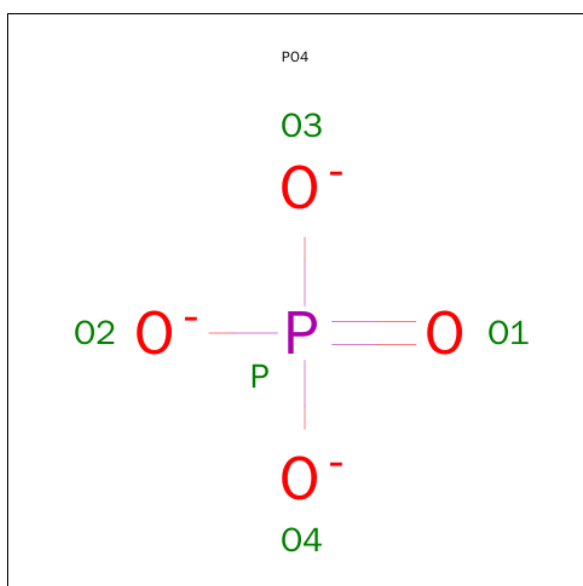
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		
5	A	1	Total	C	O	0	0
			10	4	6		
5	A	1	Total	C	O	0	0
			10	4	6		
5	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

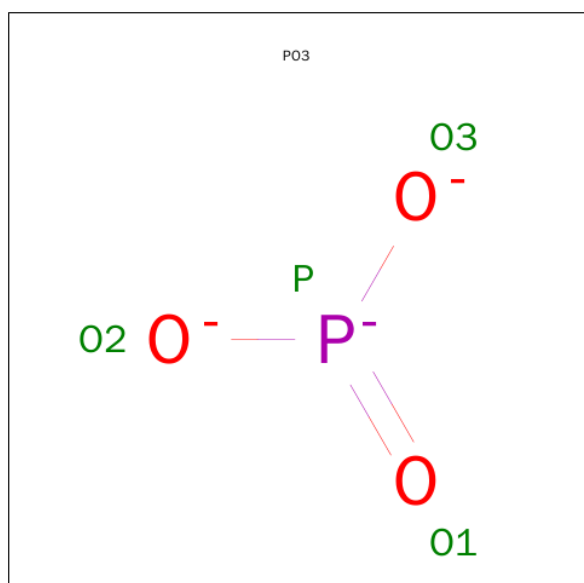
- Molecule 9 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 10 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	7	Total	C	N	O	0	0
			85	48	3	34		

- Molecule 11 is PHOSPHITE ION (three-letter code: PO3) (formula: O<sub>3</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	O	P	0	0
			4	3	1		

- Molecule 12 is water.

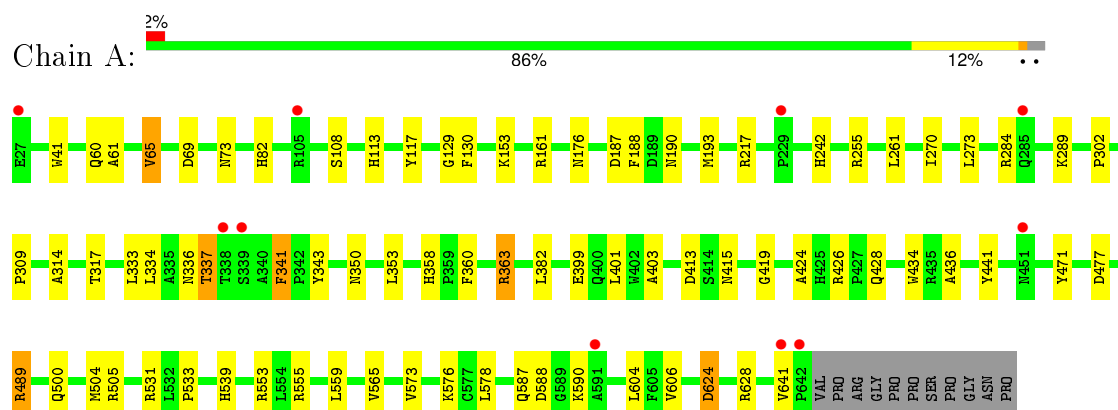
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	337	Total	O	0	0
			337	337		
12	B	273	Total	O	0	0
			273	273		



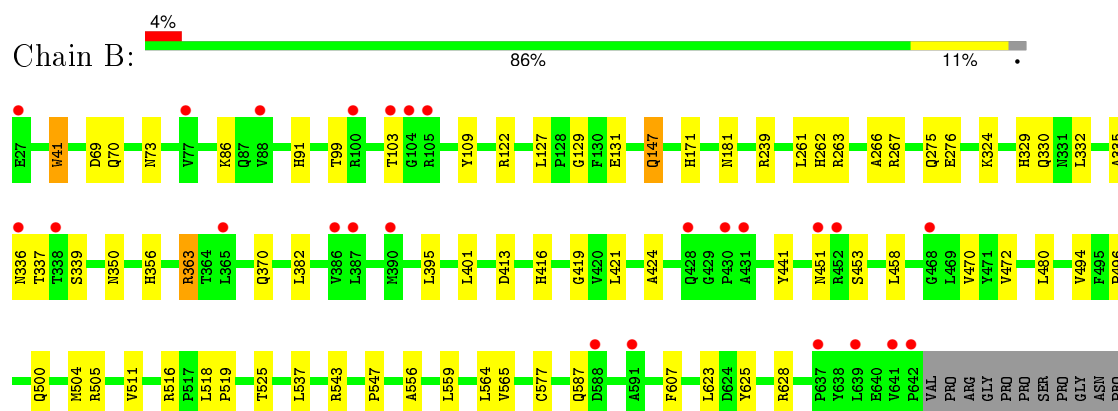
### 3 Residue-property plots

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: Alpha-L-iduronidase



#### • Molecule 1: Alpha-L-iduronidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.23 Å   259.23 Å   71.83 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	36.56 – 2.30 36.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.56-2.30) 97.3 (36.53-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.169 , 0.210 0.170 , 0.212	Depositor DCC
$R_{free}$ test set	4009 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.2	EDS
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78041 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, BMA, NAG, CL, PO4, PO3, TLA, GAL, FUC, MAN

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	0.55	0/5037	0.73	5/6884 (0.1%)
1	B	0.54	0/5037	0.70	2/6884 (0.0%)
All	All	0.55	0/10074	0.72	7/13768 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	A	363	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	363	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	161	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	129	GLY	N-CA-C	-5.23	100.03	113.10

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	4885	0	4779	60	0
1	B	4885	0	4777	61	0
2	A	116	0	97	1	0
3	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	26	2	0
4	A	28	0	25	1	0
4	B	28	0	25	0	0
5	A	30	0	12	1	0
5	B	10	0	4	0	0
6	A	6	0	8	0	0
6	B	6	0	8	5	0
7	A	5	0	0	0	0
7	B	15	0	0	2	0
8	A	1	0	0	4	0
8	B	1	0	0	2	0
9	B	105	0	88	1	0
10	B	85	0	73	0	0
11	B	4	0	0	0	0
12	A	337	0	0	12	0
12	B	273	0	0	5	0
All	All	10862	0	9935	123	0

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.

The worst 5 of 123 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:HIS:HB2	7:B:724:PO4:O3	1.60	1.01
1:B:263:ARG:HH11	1:B:275:GLN:HE21	1.11	0.94
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.35	0.89
1:B:518:LEU:HD12	1:B:519:PRO:HD2	1.60	0.84
1:B:470:VAL:HG23	1:B:516:ARG:O	1.77	0.83

There are no symmetry-related clashes.

## 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	614/627 (98%)	586 (95%)	28 (5%)	0	100	100
1	B	614/627 (98%)	584 (95%)	30 (5%)	0	100	100
All	All	1228/1254 (98%)	1170 (95%)	58 (5%)	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	518/527 (98%)	506 (98%)	12 (2%)	58	75
1	B	518/527 (98%)	508 (98%)	10 (2%)	65	81
All	All	1036/1054 (98%)	1014 (98%)	22 (2%)	61	78

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	B	41	TRP
1	B	587	GLN
1	A	489	ARG
1	A	555	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	GLN
1	B	70	GLN
1	B	275	GLN
1	A	350	ASN
1	B	186	HIS

### 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 ⓘ

30 carbohydrates 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	701	1,2	14,14,15	0.59	0	15,19,21	1.20	1 (6%)
2	NAG	A	702	2	14,14,15	0.82	0	15,19,21	1.56	4 (26%)
2	BMA	A	703	2	11,11,12	0.48	0	14,15,17	0.93	0
2	MAN	A	704	2	11,11,12	0.56	0	14,15,17	1.66	3 (21%)
2	MAN	A	705	2	11,11,12	0.81	0	14,15,17	1.41	3 (21%)
2	MAN	A	706	2	11,11,12	0.65	0	14,15,17	1.10	1 (7%)
2	MAN	A	707	2	11,11,12	0.62	0	14,15,17	1.29	2 (14%)
2	MAN	A	708	2	11,11,12	0.74	0	14,15,17	1.21	2 (14%)
2	MAN	A	709	2	11,11,12	0.66	0	14,15,17	1.57	3 (21%)
2	MAN	A	710	2	11,11,12	0.68	0	14,15,17	1.59	2 (14%)
4	NAG	A	712	1,4	14,14,15	0.77	0	15,19,21	0.90	0
4	NAG	A	713	4	14,14,15	0.54	0	15,19,21	2.55	3 (20%)
9	NAG	B	701	1,9	14,14,15	0.94	1 (7%)	15,19,21	1.29	2 (13%)
9	NAG	B	702	9	14,14,15	0.93	0	15,19,21	1.15	1 (6%)
9	BMA	B	703	9	11,11,12	0.30	0	14,15,17	1.26	1 (7%)
9	MAN	B	704	9	11,11,12	0.55	0	14,15,17	1.02	1 (7%)
9	MAN	B	705	9	11,11,12	0.66	0	14,15,17	1.63	3 (21%)
9	MAN	B	706	9	11,11,12	0.66	0	14,15,17	1.66	2 (14%)
9	MAN	B	707	9	11,11,12	0.54	0	14,15,17	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	B	708	9	11,11,12	0.81	1 (9%)	14,15,17	1.32	1 (7%)
9	MAN	B	709	9	11,11,12	0.77	0	14,15,17	1.45	1 (7%)
10	NAG	B	711	1,10	14,14,15	0.55	0	15,19,21	1.04	2 (13%)
10	NAG	B	712	10	14,14,15	0.55	0	15,19,21	0.79	0
10	BMA	B	713	10	11,11,12	0.58	0	14,15,17	0.99	2 (14%)
10	MAN	B	714	10	11,11,12	0.54	0	14,15,17	1.41	1 (7%)
10	NAG	B	715	10	14,14,15	0.55	0	15,19,21	1.45	3 (20%)
10	GAL	B	716	10	11,11,12	0.63	0	14,15,17	1.12	2 (14%)
10	FUC	B	717	10	10,10,11	0.58	0	14,14,16	2.52	4 (28%)
4	NAG	B	718	1,4	14,14,15	0.53	0	15,19,21	0.97	1 (6%)
4	NAG	B	719	4	14,14,15	0.50	0	15,19,21	1.91	2 (13%)

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	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	702	2	-	0/6/23/26	0/1/1/1
2	BMA	A	703	2	-	0/2/19/22	0/1/1/1
2	MAN	A	704	2	-	0/2/19/22	0/1/1/1
2	MAN	A	705	2	-	0/2/19/22	0/1/1/1
2	MAN	A	706	2	-	0/2/19/22	0/1/1/1
2	MAN	A	707	2	-	0/2/19/22	0/1/1/1
2	MAN	A	708	2	-	0/2/19/22	0/1/1/1
2	MAN	A	709	2	-	0/2/19/22	0/1/1/1
2	MAN	A	710	2	-	0/2/19/22	0/1/1/1
4	NAG	A	712	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	713	4	-	0/6/23/26	0/1/1/1
9	NAG	B	701	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	702	9	-	0/6/23/26	0/1/1/1
9	BMA	B	703	9	-	0/2/19/22	0/1/1/1
9	MAN	B	704	9	-	0/2/19/22	0/1/1/1
9	MAN	B	705	9	-	0/2/19/22	0/1/1/1
9	MAN	B	706	9	-	0/2/19/22	0/1/1/1
9	MAN	B	707	9	-	0/2/19/22	0/1/1/1
9	MAN	B	708	9	-	0/2/19/22	0/1/1/1
9	MAN	B	709	9	-	0/2/19/22	0/1/1/1
10	NAG	B	711	1,10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	712	10	-	0/6/23/26	0/1/1/1
10	BMA	B	713	10	-	0/2/19/22	0/1/1/1
10	MAN	B	714	10	-	0/2/19/22	0/1/1/1
10	NAG	B	715	10	-	0/6/23/26	0/1/1/1
10	GAL	B	716	10	-	0/2/19/22	0/1/1/1
10	FUC	B	717	10	-	0/0/17/20	0/1/1/1
4	NAG	B	718	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	719	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	701	NAG	O5-C1	-2.58	1.39	1.43
9	B	708	MAN	C2-C3	2.06	1.55	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	705	MAN	C1-C2-C3	-3.76	105.09	109.54
2	A	709	MAN	O2-C2-C3	-3.57	102.95	110.12
2	A	704	MAN	O5-C1-C2	-2.86	106.22	110.86
9	B	701	NAG	C3-C4-C5	-2.77	105.37	110.20
2	A	702	NAG	C6-C5-C4	-2.67	106.42	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	NAG	1	0
4	A	713	NAG	1	0
9	B	709	MAN	1	0

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	711	1	14,14,15	0.40	0	15,19,21	1.29	2 (13%)
5	TLA	A	714	-	3,9,9	0.30	0	6,12,12	2.05	2 (33%)
5	TLA	A	715	-	3,9,9	0.50	0	6,12,12	1.39	2 (33%)
5	TLA	A	716	-	3,9,9	0.65	0	6,12,12	1.94	2 (33%)
6	GOL	A	717	-	5,5,5	0.62	0	5,5,5	0.96	0
7	PO4	A	718	-	4,4,4	0.40	0	6,6,6	0.26	0
3	NAG	B	710	1	14,14,15	0.60	0	15,19,21	1.52	3 (20%)
3	NAG	B	720	1	14,14,15	0.48	0	15,19,21	1.08	1 (6%)
5	TLA	B	721	-	3,9,9	0.68	0	6,12,12	1.39	1 (16%)
6	GOL	B	722	-	5,5,5	0.34	0	5,5,5	0.41	0
11	PO3	B	723	-	0,3,3	0.00	-	0,3,3	0.00	-
7	PO4	B	724	-	4,4,4	0.45	0	6,6,6	0.28	0
7	PO4	B	725	-	4,4,4	0.42	0	6,6,6	0.27	0
7	PO4	B	726	-	4,4,4	0.31	0	6,6,6	0.27	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
3	NAG	A	711	1	-	0/6/23/26	0/1/1/1
5	TLA	A	714	-	-	0/4/12/12	0/0/0/0
5	TLA	A	715	-	-	0/4/12/12	0/0/0/0
5	TLA	A	716	-	-	0/4/12/12	0/0/0/0
6	GOL	A	717	-	-	0/4/4/4	0/0/0/0
7	PO4	A	718	-	-	0/0/0/0	0/0/0/0
3	NAG	B	710	1	-	0/6/23/26	0/1/1/1
3	NAG	B	720	1	-	0/6/23/26	0/1/1/1
5	TLA	B	721	-	-	0/4/12/12	0/0/0/0
6	GOL	B	722	-	-	0/4/4/4	0/0/0/0
11	PO3	B	723	-	-	0/0/0/0	0/0/0/0
7	PO4	B	724	-	-	0/0/0/0	0/0/0/0
7	PO4	B	725	-	-	0/0/0/0	0/0/0/0
7	PO4	B	726	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	716	TLA	C4-C3-C2	-3.83	105.50	113.35
5	A	714	TLA	C4-C3-C2	-3.12	106.95	113.35
5	A	714	TLA	C1-C2-C3	-3.05	107.10	113.35
5	B	721	TLA	C1-C2-C3	-3.02	107.15	113.35
5	A	715	TLA	C4-C3-C2	-2.28	108.68	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	714	TLA	1	0
3	B	720	NAG	2	0
6	B	722	GOL	5	0
7	B	724	PO4	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	616/627 (98%)	-0.40	10 (1%)	74 80	17, 28, 51, 91	0
1	B	616/627 (98%)	-0.19	25 (4%)	41 50	19, 31, 63, 90	0
All	All	1232/1254 (98%)	-0.30	35 (2%)	56 66	17, 29, 58, 91	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	641	VAL	4.2
1	A	338	THR	3.9
1	A	641	VAL	3.8
1	B	105	ARG	3.7
1	B	588	ASP	3.6

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MAN	A	707	11/12	0.91	0.09	-0.28	44,49,54,56	0
2	NAG	A	702	14/15	0.97	0.08	-0.79	25,31,35,41	0
2	NAG	A	701	14/15	0.98	0.07	-1.17	26,27,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	A	708	11/12	0.94	0.12	-	46,49,51,52	0
4	NAG	A	713	14/15	0.85	0.30	-	81,86,89,92	0
9	BMA	B	703	11/12	0.96	0.09	-	37,40,43,49	0
9	MAN	B	704	11/12	0.96	0.22	-	57,62,67,71	0
9	MAN	B	709	11/12	0.87	0.21	-	45,53,59,63	0
9	MAN	B	707	11/12	0.84	0.16	-	63,68,77,88	0
4	NAG	B	718	14/15	0.93	0.14	-	39,45,54,64	0
9	MAN	B	706	11/12	0.96	0.13	-	38,44,51,64	0
4	NAG	B	719	14/15	0.79	0.36	-	77,89,95,96	0
10	GAL	B	716	11/12	0.72	0.38	-	102,114,122,122	0
9	MAN	B	705	11/12	0.81	0.24	-	50,63,66,73	0
2	BMA	A	703	11/12	0.96	0.07	-	31,33,37,46	0
2	MAN	A	709	11/12	0.92	0.10	-	43,45,48,50	0
10	NAG	B	712	14/15	0.80	0.36	-	71,98,105,112	0
10	NAG	B	715	14/15	0.71	0.36	-	90,114,120,121	0
2	MAN	A	705	11/12	0.76	0.20	-	71,75,79,79	0
9	MAN	B	708	11/12	0.71	0.27	-	77,86,90,91	0
10	FUC	B	717	10/11	0.78	0.42	-	100,108,116,117	0
2	MAN	A	710	11/12	0.89	0.18	-	41,47,49,49	0
2	MAN	A	704	11/12	0.84	0.15	-	55,61,62,68	0
4	NAG	A	712	14/15	0.93	0.12	-	45,55,66,76	0
10	NAG	B	711	14/15	0.80	0.22	-	53,71,88,102	0
10	MAN	B	714	11/12	0.69	0.36	-	99,111,119,120	0
9	NAG	B	702	14/15	0.98	0.09	-	29,32,36,39	0
2	MAN	A	706	11/12	0.97	0.09	-	36,41,44,44	0
10	BMA	B	713	11/12	0.56	0.41	-	108,115,119,119	0
9	NAG	B	701	14/15	0.97	0.11	-	29,33,39,44	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	PO4	B	724	5/5	0.79	0.30	13.54	99,105,111,114	0
5	TLA	A	716	10/10	0.85	0.28	7.32	37,48,53,56	0
6	GOL	B	722	6/6	0.89	0.20	3.44	41,46,53,62	0
5	TLA	A	714	10/10	0.88	0.27	3.27	41,53,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TLA	B	721	10/10	0.92	0.10	1.25	37,42,44,44	0
6	GOL	A	717	6/6	0.95	0.11	0.57	30,34,36,41	0
8	CL	B	727	1/1	1.00	0.10	-0.45	24,24,24,24	0
5	TLA	A	715	10/10	0.94	0.10	-1.04	32,42,47,50	0
11	PO3	B	723	4/4	0.95	0.07	-1.12	46,56,61,64	0
8	CL	A	719	1/1	1.00	0.07	-1.24	24,24,24,24	0
3	NAG	A	711	14/15	0.91	0.19	-	39,46,54,54	0
3	NAG	B	720	14/15	0.84	0.49	-	85,90,100,100	0
7	PO4	A	718	5/5	0.79	0.21	-	93,95,103,105	0
7	PO4	B	726	5/5	0.88	0.23	-	85,88,95,96	0
3	NAG	B	710	14/15	0.82	0.27	-	55,68,76,78	0
7	PO4	B	725	5/5	0.82	0.22	-	106,108,109,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.