



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:03 pm GMT

PDB ID : 3W82  
Title : Human alpha-L-iduronidase in complex with iduronic acid  
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Deposited on : 2013-03-11  
Resolution : 2.76 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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

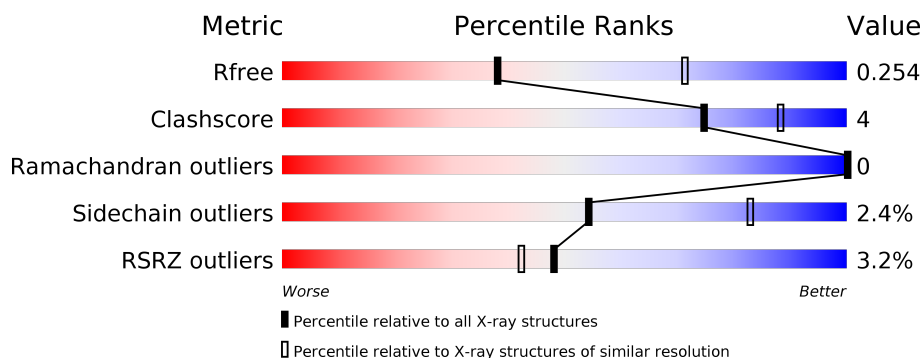
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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))
$R_{free}$	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
1	B	627	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <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
10	TLA	B	716	-	-	-	X
5	IDR	B	715	-	-	-	X
7	CL	A	716	-	-	X	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10232 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.

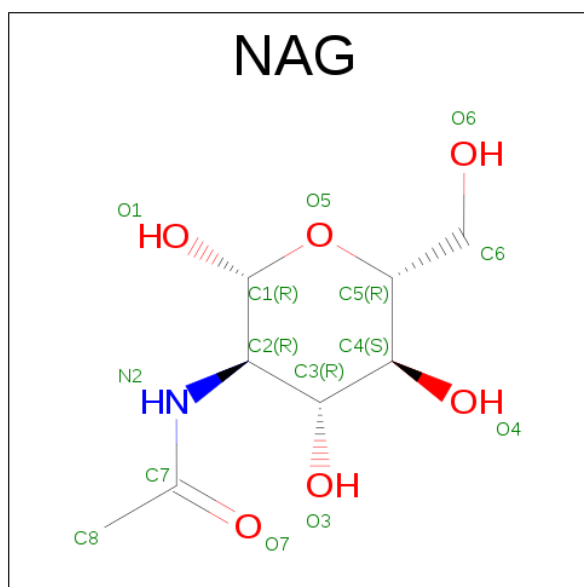
- Molecule 1 is a protein called Alpha-L-iduronidase.

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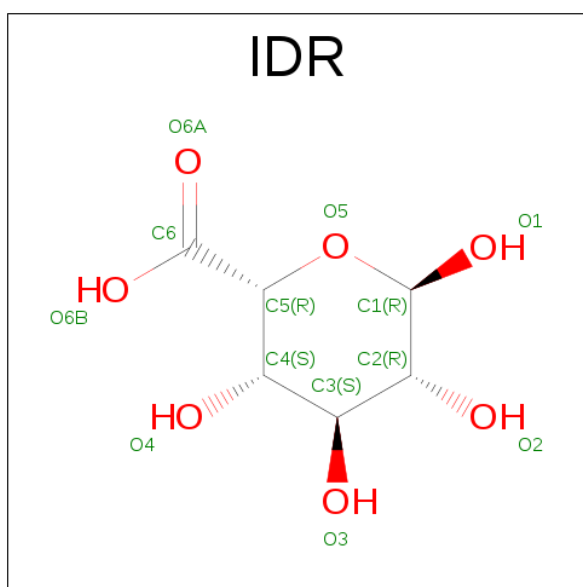
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 SUGAR (L-IDURONIC ACID) (three-letter code: IDR) (formula: C<sub>6</sub>H<sub>10</sub>O<sub>7</sub>).



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

- 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		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

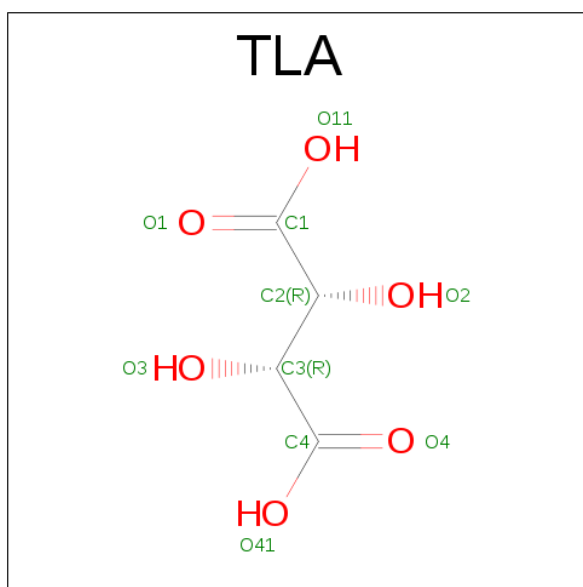
- Molecule 8 is a polymer of unknown type called SUGAR (9-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

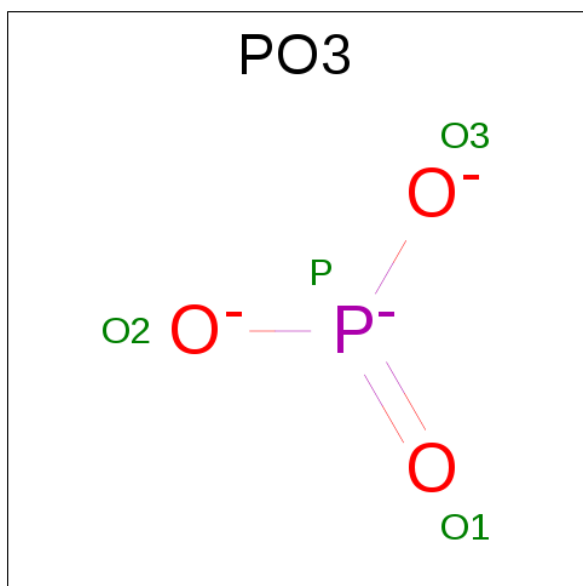
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 10 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
10	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 11 is PHOSPHITE ION (three-letter code: PO3) (formula:  $\text{O}_3\text{P}$ ).



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

- Molecule 12 is water.

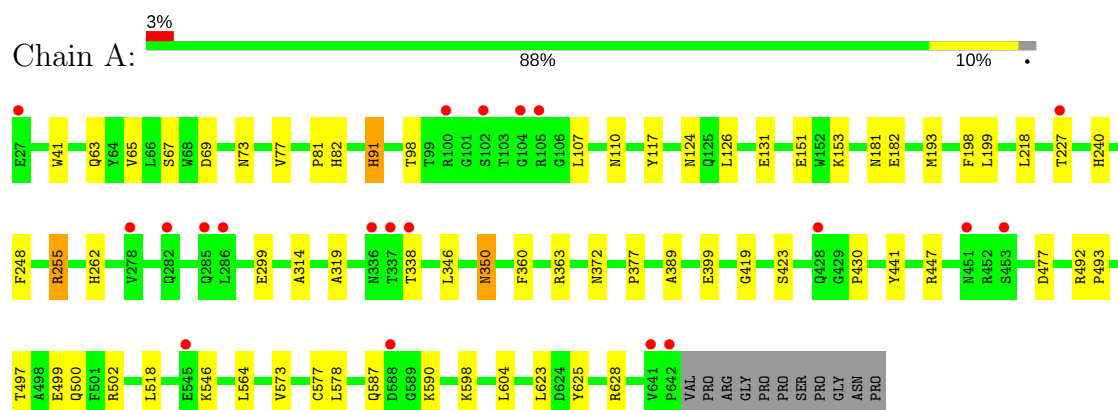
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	46	Total 46	O 46	0	0
12	B	35	Total 35	O 35	0	0



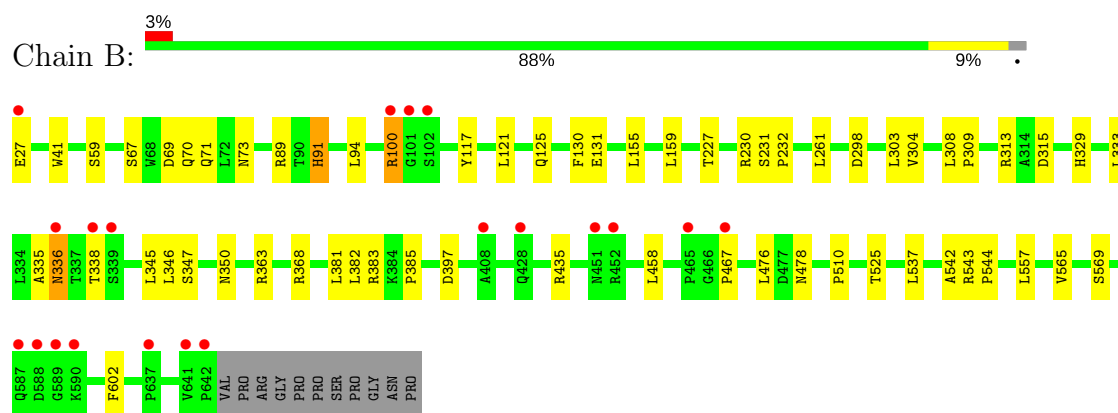
### 3 Residue-property plots [i](#)

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.

#### • 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, $\alpha$ , $\beta$ , $\gamma$	259.98Å 259.98Å 65.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.55 – 2.76 37.52 – 2.76	Depositor EDS
% Data completeness (in resolution range)	95.7 (37.55-2.76) 95.8 (37.52-2.76)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.195 , 0.254 0.199 , 0.254	Depositor DCC
$R_{free}$ test set	2042 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, PO4, IDR, PO3, TLA, 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	0.37	0/5037	0.54	0/6884
1	B	0.37	0/5037	0.54	0/6884
All	All	0.37	0/10074	0.54	0/13768

There are no bond length outliers.

There are no bond angle outliers.

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	38	0
1	B	4885	0	4778	33	0
2	A	116	0	97	0	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
4	A	28	0	25	1	0
4	B	28	0	25	0	0
5	A	13	0	9	2	0
5	B	13	0	9	2	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	2	0
7	B	1	0	0	1	0
8	B	105	0	88	1	0
9	B	24	0	22	1	0
10	B	10	0	4	0	0
11	B	4	0	0	0	0
12	A	46	0	0	1	0
12	B	35	0	0	0	0
All	All	10232	0	9862	74	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 4.

All (74) 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)
4:A:712:NAG:O3	4:A:713:NAG:H61	1.89	0.73
1:A:447:ARG:NH1	12:A:842:HOH:O	2.23	0.72
1:A:497:THR:OG1	1:A:500:GLN:HG3	1.90	0.70
1:A:363:ARG:HD3	7:A:716:CL:CL	2.28	0.70
1:B:335:ALA:O	1:B:336:ASN:C	2.34	0.65
1:A:65:VAL:HG13	1:A:117:TYR:CD2	2.32	0.64
1:B:397:ASP:OD1	1:B:435:ARG:NH1	2.33	0.62
1:B:363:ARG:HD3	7:B:719:CL:CL	2.38	0.60
1:B:298:ASP:HA	1:B:347:SER:HB3	1.84	0.60
1:B:303:LEU:HB3	1:B:313:ARG:HH21	1.68	0.58
1:B:125:GLN:NE2	1:B:569:SER:OG	2.37	0.57
1:A:363:ARG:CD	7:A:716:CL:CL	2.91	0.56
1:B:94:LEU:HD21	1:B:159:LEU:HD11	1.89	0.54
1:B:155:LEU:O	1:B:159:LEU:HB2	2.08	0.53
1:A:363:ARG:NH2	5:A:714:IDR:O4	2.41	0.53
1:A:573:VAL:HG11	1:A:578:LEU:HD11	1.91	0.53
1:B:100:ARG:NH2	3:B:710:NAG:O7	2.42	0.52
1:A:65:VAL:CG1	1:A:117:TYR:CD2	2.93	0.51
1:A:372:ASN:HA	1:A:377:PRO:HB3	1.93	0.50
1:A:181:ASN:O	1:A:182:GLU:C	2.49	0.50
9:B:711:NAG:H4	9:B:712:FUC:O5	2.12	0.50
1:B:346:LEU:C	1:B:346:LEU:HD23	2.32	0.49
1:B:117:TYR:CE1	1:B:121:LEU:HD11	2.47	0.49
1:B:91:HIS:ND1	1:B:131:GLU:OE1	2.44	0.49
1:A:218:LEU:HB3	1:A:255:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:HE22	1:B:73:ASN:HD22	1.60	0.49
1:A:430:PRO:HB2	1:A:546:LYS:HD3	1.94	0.48
1:A:350:ASN:N	1:A:350:ASN:HD22	2.11	0.48
1:A:98:THR:OG1	1:A:110:ASN:HB3	2.14	0.48
1:A:587:GLN:O	1:A:590:LYS:HG2	2.14	0.47
1:A:81:PRO:HB2	1:A:82:HIS:CD2	2.48	0.47
1:A:199:LEU:HB3	1:A:240:HIS:CD2	2.49	0.47
1:A:314:ALA:HB1	1:A:360:PHE:HB3	1.94	0.47
1:B:363:ARG:NH2	5:B:715:IDR:O4	2.47	0.47
1:A:350:ASN:HD22	1:A:350:ASN:H	1.61	0.47
1:B:345:LEU:HD13	1:B:346:LEU:N	2.29	0.46
1:B:308:LEU:HD12	1:B:309:PRO:HD2	1.98	0.46
1:A:604:LEU:C	1:A:604:LEU:HD23	2.36	0.46
1:A:73:ASN:O	1:A:77:VAL:HG23	2.16	0.46
1:B:231:SER:N	1:B:232:PRO:CD	2.80	0.45
1:A:91:HIS:ND1	1:A:131:GLU:OE1	2.49	0.45
1:B:303:LEU:O	1:B:363:ARG:NH1	2.50	0.45
1:B:557:LEU:HB2	1:B:565:VAL:HB	1.99	0.45
1:B:315:ASP:HB2	1:B:478:ASN:OD1	2.17	0.45
1:A:193:MET:SD	1:A:198:PHE:HA	2.57	0.44
1:B:368:ARG:HA	1:B:381:LEU:HD23	2.00	0.44
1:A:63:GLN:O	1:A:67:SER:HB3	2.17	0.44
1:A:153:LYS:HD3	1:A:248:PHE:CE1	2.52	0.44
1:A:299:GLU:OE1	5:A:714:IDR:H1	2.18	0.44
1:B:329:HIS:O	1:B:333:LEU:HB3	2.18	0.44
1:A:499:GLU:HA	1:A:502:ARG:NH1	2.33	0.43
1:B:130:PHE:CZ	1:B:159:LEU:HD21	2.54	0.43
1:A:564:LEU:HD12	1:A:564:LEU:C	2.39	0.43
1:B:467:PRO:HB2	1:B:543:ARG:HB3	1.99	0.43
1:B:476:LEU:HG	1:B:510:PRO:HB3	2.01	0.43
8:B:708:MAN:O3	5:B:715:IDR:H2	2.18	0.43
1:A:124:ASN:O	1:A:126:LEU:HG	2.18	0.43
1:A:107:LEU:HD22	1:A:151:GLU:OE2	2.19	0.42
1:B:383:ARG:HD3	1:B:602:PHE:CZ	2.54	0.42
1:B:315:ASP:HA	1:B:385:PRO:HG2	2.01	0.42
1:A:419:GLY:HA3	1:A:441:TYR:CZ	2.55	0.42
1:A:492:ARG:N	1:A:493:PRO:CD	2.83	0.42
1:B:261:LEU:HD12	1:B:261:LEU:C	2.40	0.42
1:A:262:HIS:CE1	1:A:299:GLU:OE2	2.73	0.42
1:A:577:CYS:HB3	1:A:625:TYR:CD2	2.56	0.41
1:B:303:LEU:HB3	1:B:313:ARG:NH2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:SER:O	1:B:71:GLN:HG3	2.20	0.41
1:A:477:ASP:C	1:A:477:ASP:OD2	2.59	0.41
1:B:542:ALA:O	1:B:544:PRO:HD3	2.20	0.41
1:A:346:LEU:C	1:A:346:LEU:HD23	2.40	0.41
1:B:89:ARG:CZ	1:B:131:GLU:OE2	2.69	0.41
1:A:399:GLU:O	1:A:423:SER:HA	2.22	0.40
1:B:458:LEU:O	1:B:525:THR:HA	2.22	0.40
1:A:319:ALA:HB1	1:A:389:ALA:HB2	2.02	0.40

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%)	584 (95%)	30 (5%)	0	100	100
1	B	614/627 (98%)	585 (95%)	29 (5%)	0	100	100
All	All	1228/1254 (98%)	1169 (95%)	59 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	518/527 (98%)	507 (98%)	11 (2%)	59	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	518/527 (98%)	504 (97%)	14 (3%)	50 80
All	All	1036/1054 (98%)	1011 (98%)	25 (2%)	54 83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	69	ASP
1	A	91	HIS
1	A	227	THR
1	A	255	ARG
1	A	338	THR
1	A	350	ASN
1	A	518	LEU
1	A	598	LYS
1	A	623	LEU
1	A	628	ARG
1	B	27	GLU
1	B	41	TRP
1	B	59	SER
1	B	69	ASP
1	B	91	HIS
1	B	100	ARG
1	B	227	THR
1	B	230	ARG
1	B	304	VAL
1	B	336	ASN
1	B	338	THR
1	B	350	ASN
1	B	382	LEU
1	B	537	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	176	ASN
1	A	240	HIS
1	A	336	ASN
1	A	350	ASN
1	A	356	HIS

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	82	HIS
1	B	125	GLN
1	B	147	GLN
1	B	196	GLN
1	B	350	ASN
1	B	358	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 ⓘ

25 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	0.69	0	15,19,21	1.39	3 (20%)
2	NAG	A	702	2	14,14,15	0.63	0	15,19,21	1.10	2 (13%)
2	BMA	A	703	2	11,11,12	0.28	0	13,15,17	1.21	1 (7%)
2	MAN	A	704	2	11,11,12	0.55	0	13,15,17	1.41	2 (15%)
2	MAN	A	705	2	11,11,12	0.65	0	13,15,17	0.86	0
2	MAN	A	706	2	11,11,12	0.94	0	13,15,17	1.10	1 (7%)
2	MAN	A	707	2	11,11,12	0.59	0	13,15,17	1.29	1 (7%)
2	MAN	A	708	2	11,11,12	0.65	0	13,15,17	1.13	1 (7%)
2	MAN	A	709	2	11,11,12	0.71	0	13,15,17	0.92	0
2	MAN	A	710	2	11,11,12	0.60	0	13,15,17	0.60	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	712	1,4	14,14,15	0.63	0	15,19,21	0.82	0
4	NAG	A	713	4	14,14,15	0.46	0	15,19,21	2.00	2 (13%)
8	NAG	B	701	1,8	14,14,15	0.72	0	15,19,21	1.30	1 (6%)
8	NAG	B	702	8	14,14,15	0.58	0	15,19,21	0.92	1 (6%)
8	BMA	B	703	8	11,11,12	0.26	0	13,15,17	0.71	0
8	MAN	B	704	8	11,11,12	0.63	0	13,15,17	1.07	1 (7%)
8	MAN	B	705	8	11,11,12	0.70	0	13,15,17	0.94	1 (7%)
8	MAN	B	706	8	11,11,12	0.89	1 (9%)	13,15,17	1.15	0
8	MAN	B	707	8	11,11,12	0.58	0	13,15,17	0.93	1 (7%)
8	MAN	B	708	8	11,11,12	0.65	0	13,15,17	0.69	0
8	MAN	B	709	8	11,11,12	0.65	0	13,15,17	0.79	0
9	NAG	B	711	1,9	14,14,15	0.51	0	15,19,21	1.46	1 (6%)
9	FUC	B	712	9	9,10,11	0.53	0	13,14,16	1.69	2 (15%)
4	NAG	B	713	1,4	14,14,15	0.69	0	15,19,21	1.74	3 (20%)
4	NAG	B	714	4	14,14,15	0.38	0	15,19,21	1.24	1 (6%)

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
8	NAG	B	701	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	702	8	-	0/6/23/26	0/1/1/1
8	BMA	B	703	8	-	0/2/19/22	0/1/1/1
8	MAN	B	704	8	-	0/2/19/22	0/1/1/1
8	MAN	B	705	8	-	0/2/19/22	0/1/1/1
8	MAN	B	706	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	B	707	8	-	0/2/19/22	0/1/1/1
8	MAN	B	708	8	-	0/2/19/22	0/1/1/1
8	MAN	B	709	8	-	0/2/19/22	0/1/1/1
9	NAG	B	711	1,9	-	0/6/23/26	0/1/1/1
9	FUC	B	712	9	-	0/0/17/20	0/1/1/1
4	NAG	B	713	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	714	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	706	MAN	O5-C1	-2.05	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	701	NAG	O5-C1-C2	-3.26	106.94	111.47
4	B	713	NAG	O5-C1-C2	-3.11	107.15	111.47
2	A	707	MAN	O2-C2-C3	-2.77	104.73	110.17
2	A	703	BMA	O3-C3-C2	-2.49	105.50	110.02
8	B	702	NAG	O5-C1-C2	-2.44	108.08	111.47
4	B	713	NAG	O4-C4-C3	-2.32	105.31	110.36
2	A	706	MAN	O5-C1-C2	-2.28	107.21	110.79
8	B	707	MAN	O2-C2-C3	-2.28	105.70	110.17
4	A	713	NAG	C1-C2-N2	-2.23	106.67	110.49
2	A	701	NAG	C6-C5-C4	-2.22	107.80	113.00
2	A	702	NAG	C6-C5-C4	-2.14	108.00	113.00
2	A	701	NAG	O3-C3-C2	-2.09	104.92	109.39
2	A	702	NAG	O3-C3-C4	-2.06	105.87	110.36
8	B	705	MAN	C2-C3-C4	2.02	114.39	110.88
2	A	704	MAN	C3-C4-C5	2.20	114.09	110.22
8	B	704	MAN	C1-C2-C3	2.31	112.58	109.65
2	A	701	NAG	C1-O5-C5	2.63	115.79	112.17
2	A	708	MAN	C1-O5-C5	2.98	116.27	112.17
2	A	704	MAN	O2-C2-C1	3.33	115.95	109.18
4	B	713	NAG	C1-O5-C5	3.73	117.31	112.17
9	B	712	FUC	C1-C2-C3	3.74	114.39	109.65
9	B	712	FUC	C1-O5-C5	3.90	121.02	112.39
4	B	714	NAG	C1-O5-C5	3.96	117.62	112.17
9	B	711	NAG	C1-O5-C5	4.51	118.38	112.17
4	A	713	NAG	C1-O5-C5	6.70	121.41	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	712	NAG	1	0
4	A	713	NAG	1	0
8	B	708	MAN	1	0
9	B	711	NAG	1	0
9	B	712	FUC	1	0

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
3	NAG	A	711	1	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
5	IDR	A	714	-	10,13,13	1.10	0	15,19,19	0.83	0
6	PO4	A	715	-	4,4,4	0.71	0	6,6,6	0.36	0
3	NAG	B	710	1	14,14,15	0.52	0	15,19,21	1.44	2 (13%)
5	IDR	B	715	-	10,13,13	0.80	0	15,19,19	0.53	0
10	TLA	B	716	-	3,9,9	0.55	0	6,12,12	1.10	1 (16%)
11	PO3	B	717	-	0,3,3	0.00	-	0,3,3	0.00	-
6	PO4	B	718	-	4,4,4	0.73	0	6,6,6	0.38	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	IDR	A	714	-	-	0/0/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PO4	A	715	-	-	0/0/0/0	0/0/0/0
3	NAG	B	710	1	-	0/6/23/26	0/1/1/1
5	IDR	B	715	-	-	0/0/24/24	0/1/1/1
10	TLA	B	716	-	-	0/4/12/12	0/0/0/0
11	PO3	B	717	-	-	0/0/0/0	0/0/0/0
6	PO4	B	718	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	710	NAG	O7-C7-C8	-2.24	117.99	122.06
10	B	716	TLA	O2-C2-C1	-2.12	105.97	111.13
3	A	711	NAG	C1-O5-C5	2.14	115.11	112.17
3	B	710	NAG	C1-O5-C5	3.86	117.49	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	714	IDR	2	0
3	B	710	NAG	1	0
5	B	715	IDR	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.08	20 (3%)	48 42	15, 24, 48, 75	0
1	B	616/627 (98%)	-0.11	20 (3%)	48 42	15, 26, 51, 76	0
All	All	1232/1254 (98%)	-0.09	40 (3%)	48 42	15, 25, 48, 76	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	THR	4.7
1	B	27	GLU	4.5
1	B	451	ASN	4.1
1	A	100	ARG	3.8
1	B	588	ASP	3.5
1	A	641	VAL	3.5
1	B	465	PRO	3.4
1	B	642	PRO	3.4
1	A	642	PRO	3.3
1	B	467	PRO	3.2
1	A	27	GLU	3.2
1	A	588	ASP	3.1
1	A	428	GLN	2.9
1	B	336	ASN	2.8
1	A	337	THR	2.8
1	B	589	GLY	2.8
1	A	451	ASN	2.7
1	A	338	THR	2.7
1	B	339	SER	2.6
1	A	285	GLN	2.5
1	B	101	GLY	2.5
1	A	453	SER	2.5
1	B	637	PRO	2.4
1	A	336	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	2.4
1	B	452	ARG	2.3
1	A	282	GLN	2.3
1	B	100	ARG	2.3
1	B	428	GLN	2.3
1	A	102	SER	2.2
1	B	408	ALA	2.2
1	B	102	SER	2.1
1	A	227	THR	2.1
1	A	278	VAL	2.1
1	A	545	GLU	2.0
1	B	590	LYS	2.0
1	B	587	GLN	2.0
1	A	286	LEU	2.0
1	A	105	ARG	2.0
1	B	641	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	NAG	A	712	14/15	0.91	0.21	1.92	41,44,51,62	0
2	MAN	A	707	11/12	0.94	0.14	0.53	26,27,27,28	0
2	NAG	A	701	14/15	0.97	0.13	-0.20	16,17,18,19	0
2	NAG	A	702	14/15	0.97	0.12	-0.56	19,20,21,22	0
2	MAN	A	710	11/12	0.91	0.24	-	26,28,29,30	0
8	MAN	B	705	11/12	0.81	0.41	-	61,65,69,69	0
2	MAN	A	706	11/12	0.95	0.14	-	23,25,27,27	0
4	NAG	A	713	14/15	0.79	0.38	-	69,74,83,85	0
2	MAN	A	704	11/12	0.92	0.15	-	38,41,43,46	0
8	MAN	B	706	11/12	0.93	0.22	-	44,49,52,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	B	711	14/15	0.69	0.42	-	60,72,83,84	0
2	MAN	A	708	11/12	0.94	0.16	-	24,25,26,27	0
8	MAN	B	707	11/12	0.79	0.29	-	52,58,61,63	0
2	MAN	A	705	11/12	0.84	0.24	-	50,55,58,59	0
8	MAN	B	704	11/12	0.81	0.35	-	54,55,61,62	0
8	MAN	B	708	11/12	0.85	0.31	-	62,66,67,68	0
4	NAG	B	713	14/15	0.94	0.20	-	35,41,46,53	0
2	MAN	A	709	11/12	0.93	0.19	-	25,26,28,28	0
9	FUC	B	712	10/11	0.82	0.49	-	83,87,91,91	0
8	MAN	B	709	11/12	0.86	0.29	-	50,53,56,57	0
4	NAG	B	714	14/15	0.89	0.39	-	61,65,67,68	0
2	BMA	A	703	11/12	0.95	0.12	-	24,26,27,33	0
8	BMA	B	703	11/12	0.92	0.21	-	39,40,43,49	0
8	NAG	B	702	14/15	0.94	0.20	-	31,33,35,38	0
8	NAG	B	701	14/15	0.94	0.17	-	28,30,32,34	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
5	IDR	B	715	13/13	0.90	0.21	3.78	30,35,37,38	0
10	TLA	B	716	10/10	0.92	0.19	2.98	36,38,38,39	0
11	PO3	B	717	4/4	0.89	0.19	0.93	45,45,49,50	0
5	IDR	A	714	13/13	0.95	0.14	-0.56	21,22,23,23	0
7	CL	A	716	1/1	0.99	0.12	-2.26	18,18,18,18	0
7	CL	B	719	1/1	0.99	0.08	-6.47	15,15,15,15	0
6	PO4	B	718	5/5	0.92	0.29	-	54,55,57,58	0
3	NAG	B	710	14/15	0.87	0.31	-	30,34,39,39	0
3	NAG	A	711	14/15	0.90	0.24	-	38,40,44,45	0
6	PO4	A	715	5/5	0.70	0.45	-	95,95,99,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.