



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 PM GMT

PDB ID : 3TV8  
Title : Pharmacological Chaperoning in Human alpha-Galactosidase  
Authors : Rogich, J.J.; Guce, A.I.; Clark, N.E.; Garman, S.C.  
Deposited on : 2011-09-19  
Resolution : 2.64 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 (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

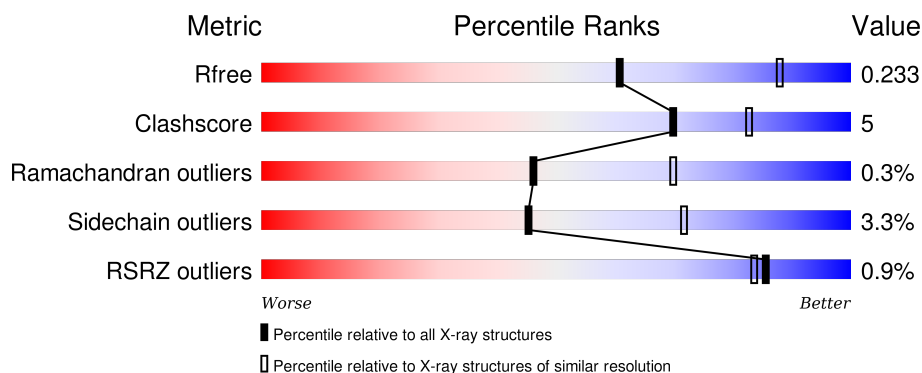
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>9%</span> <span>• •</span> </div> </div>
1	B	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 85%, yellow 11%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>85%</span> <span>11%</span> <span>• •</span> </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	2PE	A	11	-	-	-	X
5	2PE	A	9	-	-	-	X
6	DGJ	A	801	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6516 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-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3119	1987	534	572	26			
1	B	391	Total	C	N	O	S	0	1	0
			3136	1997	537	575	27			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	ASP	ENGINEERED MUTATION	UNP P06280
A	430	HIS	-	EXPRESSION TAG	UNP P06280
A	431	HIS	-	EXPRESSION TAG	UNP P06280
A	432	HIS	-	EXPRESSION TAG	UNP P06280
A	433	HIS	-	EXPRESSION TAG	UNP P06280
A	434	HIS	-	EXPRESSION TAG	UNP P06280
A	435	HIS	-	EXPRESSION TAG	UNP P06280
B	170	ALA	ASP	ENGINEERED MUTATION	UNP P06280
B	430	HIS	-	EXPRESSION TAG	UNP P06280
B	431	HIS	-	EXPRESSION TAG	UNP P06280
B	432	HIS	-	EXPRESSION TAG	UNP P06280
B	433	HIS	-	EXPRESSION TAG	UNP P06280
B	434	HIS	-	EXPRESSION TAG	UNP P06280
B	435	HIS	-	EXPRESSION TAG	UNP P06280

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

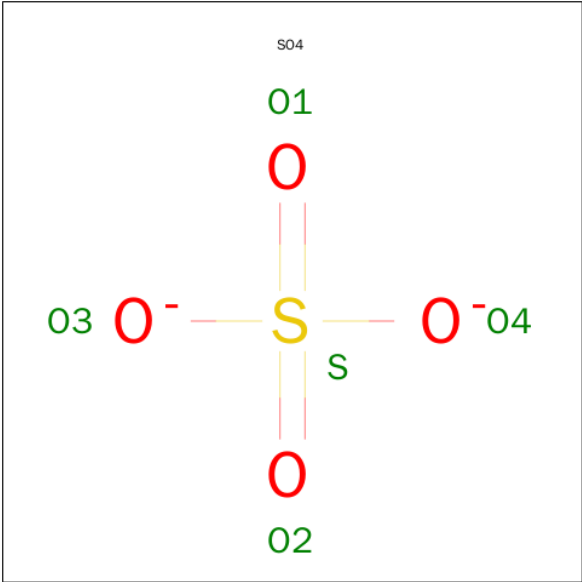


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

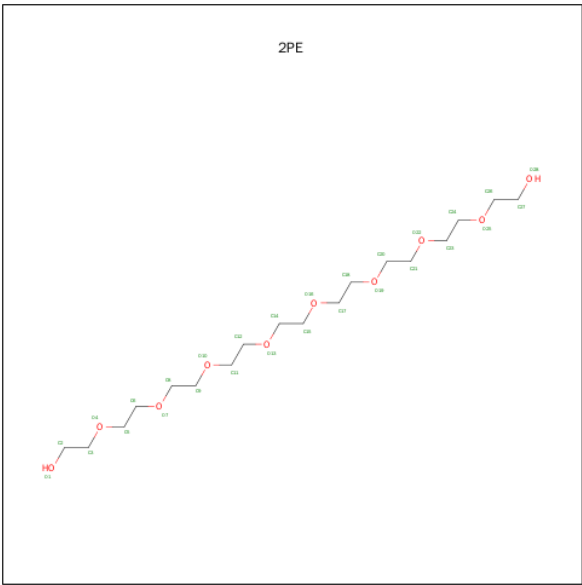
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



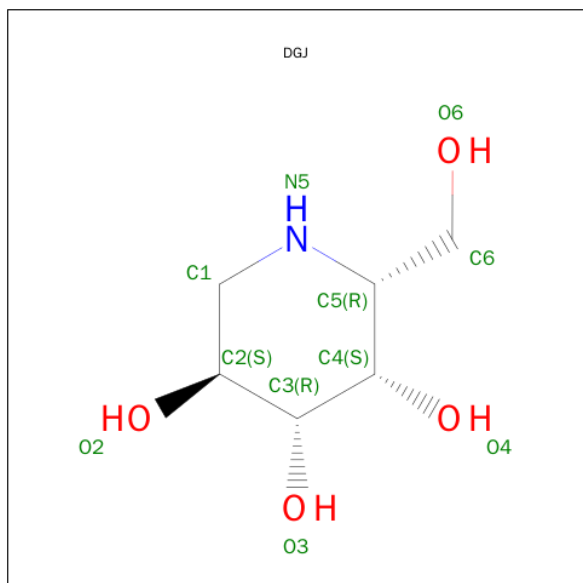
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (2R,3S,4R,5S)-2-(HYDROXYMETHYL)PIPERIDINE-3,4,5-TRIOL (three-letter code: DGJ) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>).



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

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	28	Total	O	0	0
			28	28		





- Molecule 1: Alpha-galactosidase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.47Å 90.47Å 216.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.54 – 2.64 44.54 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.54-2.64) 99.7 (44.54-2.64)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.201 , 0.239 0.199 , 0.233	Depositor DCC
$R_{free}$ test set	1582 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.2	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30933 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: BMA, NAG, DGJ, 2PE, SO4, 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	0.43	4/3206 (0.1%)	0.59	3/4354 (0.1%)
1	B	0.47	5/3223 (0.2%)	0.58	3/4376 (0.1%)
All	All	0.45	9/6429 (0.1%)	0.58	6/8730 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	418	GLU	CD-OE1	9.23	1.35	1.25
1	B	241	SER	CB-OG	8.22	1.52	1.42
1	B	418	GLU	CD-OE2	6.58	1.32	1.25
1	B	218	GLU	CD-OE1	-5.77	1.19	1.25
1	A	218	GLU	CD-OE1	-5.58	1.19	1.25
1	A	218	GLU	CD-OE2	-5.50	1.19	1.25
1	A	341	GLU	CD-OE1	-5.30	1.19	1.25
1	B	218	GLU	CD-OE2	-5.22	1.20	1.25
1	A	241	SER	CB-OG	5.17	1.49	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLU	OE1-CD-OE2	-7.09	114.80	123.30
1	B	218	GLU	OE1-CD-OE2	-7.04	114.85	123.30
1	A	341	GLU	OE1-CD-OE2	-6.81	115.13	123.30
1	B	341	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	A	136	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	136	ASP	CB-CG-OD1	5.24	123.01	118.30

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	3119	0	2982	26	0
1	B	3136	0	2998	31	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	39	0	34	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	11	0	12	0	0
5	B	4	0	4	0	0
6	A	11	0	13	0	0
6	B	11	0	13	0	0
7	B	50	0	43	0	0
8	A	36	0	0	0	0
8	B	28	0	0	0	0
All	All	6516	0	6151	57	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 5.

All (57) 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:105:ARG:HH11	1:A:158:THR:HG23	1.10	1.14
1:A:403:LEU:HD11	1:A:415:LEU:HD13	1.57	0.86
1:A:105:ARG:NH1	1:A:158:THR:HG23	1.90	0.86
1:A:99:GLN:HE21	1:A:99:GLN:HA	1.41	0.86
1:B:99:GLN:HA	1:B:99:GLN:HE21	1.42	0.82
1:A:105:ARG:HH11	1:A:158:THR:CG2	1.92	0.81
1:A:369:VAL:HA	1:A:372:LEU:HD12	1.65	0.76
1:A:351:VAL:HG21	1:A:372:LEU:HD22	1.68	0.75
1:A:366:THR:HG22	1:A:404:ARG:HD3	1.71	0.72
1:B:403:LEU:HD21	1:B:415:LEU:HD13	1.75	0.68
1:A:403:LEU:HD11	1:A:415:LEU:CD1	2.25	0.67
1:A:99:GLN:HE21	1:A:99:GLN:CA	2.07	0.67
1:B:99:GLN:HE21	1:B:99:GLN:CA	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:CG2	1:A:404:ARG:HD3	2.27	0.65
1:B:351:VAL:HG21	1:B:372:LEU:CD2	2.26	0.65
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.32	0.64
1:B:351:VAL:HG21	1:B:372:LEU:HD23	1.80	0.64
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.33	0.63
1:B:236:TRP:CE2	1:B:240:LYS:HD2	2.39	0.57
1:B:177:LEU:HD12	1:B:211:PHE:HB3	1.89	0.55
1:B:369:VAL:HA	1:B:372:LEU:HD13	1.89	0.55
1:B:236:TRP:NE1	1:B:240:LYS:HD2	2.23	0.54
1:A:420:THR:O	1:A:421:MET:HG2	2.07	0.53
1:B:369:VAL:HA	1:B:372:LEU:CD1	2.39	0.53
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.90	0.52
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.93	0.50
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.93	0.50
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.94	0.48
1:A:101:ASP:HB3	1:A:107:GLN:OE1	2.13	0.48
1:B:177:LEU:HD11	1:B:212:GLN:HG2	1.96	0.47
1:B:418:GLU:HA	1:B:418:GLU:OE2	2.15	0.47
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.97	0.47
1:B:99:GLN:NE2	1:B:99:GLN:CA	2.78	0.46
1:A:99:GLN:CA	1:A:99:GLN:NE2	2.77	0.46
1:B:351:VAL:CG2	1:B:372:LEU:HD23	2.45	0.45
1:B:75:LEU:HD11	1:B:301:ARG:HG2	1.97	0.45
1:B:101:ASP:HB3	1:B:107:GLN:OE1	2.16	0.45
1:A:418:GLU:HA	1:A:418:GLU:OE2	2.18	0.44
1:A:69:PHE:CZ	1:A:91:ILE:HG23	2.53	0.43
1:B:180:LEU:HD23	1:B:208:MET:HG3	1.98	0.43
1:B:335:ASP:OD1	1:B:335:ASP:O	2.37	0.43
1:B:324:LEU:HD13	1:B:326:LYS:HG3	2.01	0.43
1:A:75:LEU:HD11	1:A:301:ARG:HG2	2.00	0.42
1:B:351:VAL:HG21	1:B:372:LEU:HD22	2.00	0.42
1:A:214:PRO:O	1:A:252:ARG:NH2	2.53	0.42
1:A:124:VAL:HG13	1:A:129:LEU:HB2	2.02	0.42
1:B:369:VAL:HG22	1:B:401:SER:O	2.19	0.42
1:B:366:THR:CG2	1:B:404:ARG:HG2	2.49	0.42
1:B:124:VAL:HG13	1:B:129:LEU:HB2	2.02	0.42
1:B:69:PHE:CZ	1:B:91:ILE:HG23	2.54	0.42
1:B:403:LEU:HD21	1:B:415:LEU:CD1	2.48	0.42
1:B:89:LEU:O	1:B:131:LEU:HD12	2.21	0.41
1:B:366:THR:HG22	1:B:404:ARG:HG2	2.03	0.40
1:B:386:GLN:HA	1:B:415:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TRP:HB3	1:A:205:PRO:HD3	2.03	0.40
1:A:335:ASP:OD1	1:A:363:ARG:NH1	2.48	0.40
1:A:89:LEU:O	1:A:131:LEU:HD12	2.22	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	388/404 (96%)	379 (98%)	8 (2%)	1 (0%)	46	70
1	B	390/404 (96%)	379 (97%)	10 (3%)	1 (0%)	46	70
All	All	778/808 (96%)	758 (97%)	18 (2%)	2 (0%)	46	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	266	ASP

### 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	330/344 (96%)	318 (96%)	12 (4%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	332/344 (96%)	322 (97%)	10 (3%)	48	75
All	All	662/688 (96%)	640 (97%)	22 (3%)	45	72

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	107	GLN
1	A	154	ILE
1	A	158	THR
1	A	241	SER
1	A	256	VAL
1	A	336	ASN
1	A	345	SER
1	A	403	LEU
1	A	404	ARG
1	A	418	GLU
1	A	421	MET
1	B	99	GLN
1	B	107	GLN
1	B	154	ILE
1	B	158	THR
1	B	196	ARG
1	B	213	LYS
1	B	256	VAL
1	B	324	LEU
1	B	345	SER
1	B	418	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	228	ASN
1	A	336	ASN
1	B	99	GLN
1	B	179	ASN
1	B	212	GLN
1	B	228	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

7 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$
3	NAG	A	692	1,3	14,14,15	0.46	0	15,19,21	0.75	0
3	NAG	A	693	3	14,14,15	0.45	0	15,19,21	1.26	2 (13%)
3	BMA	A	694	3	11,11,12	0.41	0	14,15,17	0.84	0
7	NAG	B	692	1,7	14,14,15	0.50	0	15,19,21	1.16	1 (6%)
7	NAG	B	693	7	14,14,15	0.48	0	15,19,21	0.84	1 (6%)
7	BMA	B	694	7	11,11,12	0.47	0	14,15,17	1.38	1 (7%)
7	MAN	B	695	7	11,11,12	0.57	0	14,15,17	0.83	1 (7%)

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	692	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	693	3	-	0/6/23/26	0/1/1/1
3	BMA	A	694	3	-	0/2/19/22	0/1/1/1
7	NAG	B	692	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	693	7	-	0/6/23/26	0/1/1/1
7	BMA	B	694	7	-	0/2/19/22	0/1/1/1
7	MAN	B	695	7	-	0/2/19/22	0/1/1/1



There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	692	NAG	C4-C3-C2	-3.05	106.49	111.23
3	A	693	NAG	C3-C4-C5	-2.11	106.51	110.20
7	B	695	MAN	C1-O5-C5	2.04	114.84	112.25
3	A	693	NAG	C1-O5-C5	2.18	115.02	112.25
7	B	693	NAG	C1-O5-C5	2.25	115.10	112.25
7	B	694	BMA	O3-C3-C2	3.61	116.52	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

12 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	$\# Z  > 2$
5	2PE	A	11	-	3,3,27	0.47	0	2,2,26	0.29	0
2	NAG	A	639	1	14,14,15	0.48	0	15,19,21	0.92	1 (6%)
2	NAG	A	715	1	14,14,15	0.57	0	15,19,21	1.11	1 (6%)
4	SO4	A	8	-	4,4,4	0.28	0	6,6,6	0.07	0
6	DGJ	A	801	-	11,11,11	0.82	1 (9%)	11,15,15	0.61	0
5	2PE	A	9	-	6,6,27	0.48	0	5,5,26	0.19	0
5	2PE	B	12	-	3,3,27	0.46	0	2,2,26	0.23	0
4	SO4	B	6	-	4,4,4	0.29	0	6,6,6	0.11	0
2	NAG	B	639	1	14,14,15	0.49	0	15,19,21	0.84	0
4	SO4	B	7	-	4,4,4	0.20	0	6,6,6	0.06	0
2	NAG	B	715	1	14,14,15	0.54	0	15,19,21	0.92	1 (6%)
6	DGJ	B	802	-	11,11,11	0.74	0	11,15,15	0.71	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
5	2PE	A	11	-	-	0/1/1/25	0/0/0/0
2	NAG	A	639	1	-	0/6/23/26	0/1/1/1
2	NAG	A	715	1	-	0/6/23/26	0/1/1/1
4	SO4	A	8	-	-	0/0/0/0	0/0/0/0
6	DGJ	A	801	-	-	0/2/19/19	0/1/1/1
5	2PE	A	9	-	-	0/4/4/25	0/0/0/0
5	2PE	B	12	-	-	0/1/1/25	0/0/0/0
4	SO4	B	6	-	-	0/0/0/0	0/0/0/0
2	NAG	B	639	1	-	0/6/23/26	0/1/1/1
4	SO4	B	7	-	-	0/0/0/0	0/0/0/0
2	NAG	B	715	1	-	0/6/23/26	0/1/1/1
6	DGJ	B	802	-	-	0/2/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	DGJ	C5-N5	-2.32	1.45	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	639	NAG	C1-O5-C5	2.20	115.04	112.25
2	B	715	NAG	C1-O5-C5	2.28	115.14	112.25
2	A	715	NAG	C1-O5-C5	2.60	115.55	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	390/404 (96%)	-0.10	5 (1%) 79 76	17, 31, 55, 73	0
1	B	391/404 (96%)	-0.01	2 (0%) 91 90	18, 36, 60, 79	0
All	All	781/808 (96%)	-0.05	7 (0%) 85 83	17, 33, 58, 79	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	SER	3.7
1	A	175	ASP	3.2
1	A	182	ASP	2.5
1	A	211	PHE	2.3
1	B	161	ASP	2.3
1	A	183	GLY	2.1
1	A	178	GLU	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
7	NAG	B	692	14/15	0.90	0.26	1.17	39,53,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	692	14/15	0.95	0.15	-0.27	8,31,36,38	0
3	NAG	A	693	14/15	0.94	0.14	-1.01	43,51,64,65	0
7	NAG	B	693	14/15	0.91	0.30	-	42,62,66,68	0
3	BMA	A	694	11/12	0.66	0.27	-	62,73,80,83	0
7	BMA	B	694	11/12	0.80	0.34	-	67,73,80,84	0
7	MAN	B	695	11/12	0.76	0.24	-	84,87,89,91	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	2PE	A	9	7/28	0.78	0.31	5.32	49,59,64,66	0
5	2PE	A	11	4/28	0.90	0.26	2.68	53,54,61,63	0
6	DGJ	A	801	11/11	0.94	0.25	2.52	22,33,40,43	0
2	NAG	A	639	14/15	0.83	0.37	1.80	77,81,82,82	0
2	NAG	B	639	14/15	0.63	0.28	1.26	83,89,91,92	0
4	SO4	B	6	5/5	0.98	0.23	0.26	53,56,63,66	0
6	DGJ	B	802	11/11	0.96	0.15	0.20	23,33,36,37	0
4	SO4	A	8	5/5	0.98	0.15	-0.16	38,40,44,46	0
2	NAG	A	715	14/15	0.90	0.19	-	42,53,57,58	0
5	2PE	B	12	4/28	0.77	0.30	-	75,76,78,80	0
4	SO4	B	7	5/5	0.92	0.36	-	88,89,92,93	0
2	NAG	B	715	14/15	0.78	0.25	-	81,87,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.