



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 09:02 AM GMT

PDB ID : 3S5Y
Title : Pharmacological Chaperoning in Human alpha-Galactosidase
Authors : Guce, A.I.; Clark, N.E.; Garman, S.C.
Deposited on : 2011-05-23
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

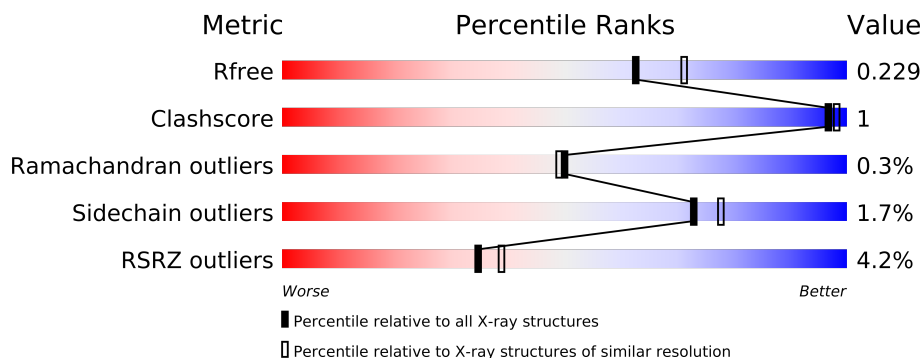
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	EDO	B	814	-	X
11	ACY	B	842	-	X
11	ACY	B	843	-	X
6	2PE	B	810	-	X
6	2PE	B	811	-	X
6	2PE	B	812	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	2PE	B	815	-	X
7	NAG	B	639	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7134 atoms, of which 0 are hydrogen and 0 are deuterium.

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	4	0
			3141	1999	538	575	29			
1	B	391	Total	C	N	O	S	0	4	0
			3150	2004	540	577	29			

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			80	45	2	33		

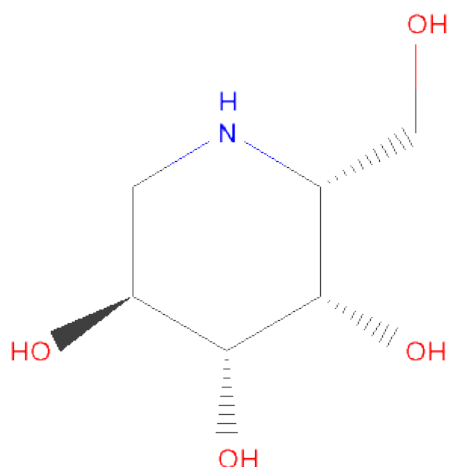
- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			58	33	2	23		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

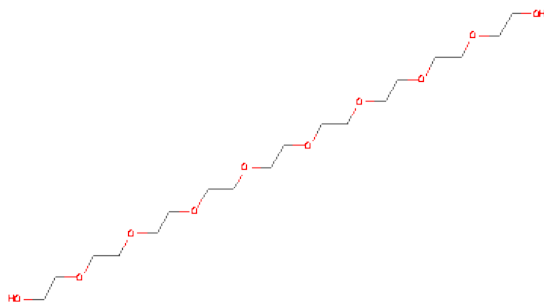
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is (2R,3S,4R,5S)-2-(HYDROXYMETHYL)PIPERIDINE-3,4,5-TRIOL (three-letter code: DGJ) (formula: C₆H₁₃NO₄).



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

- Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



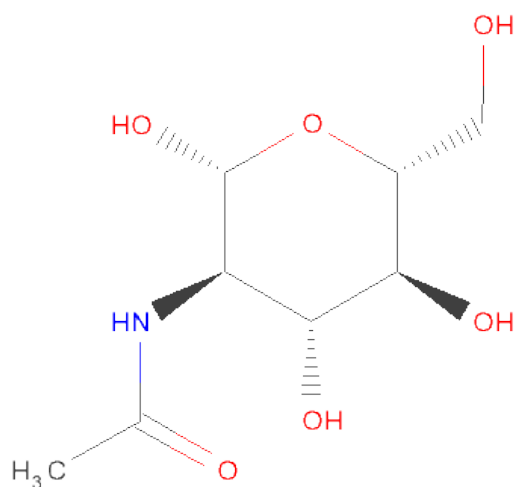
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			28	18	10		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

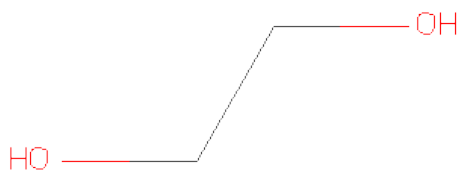
- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	5	Total	C	N	O	0	0
			59	33	2	24		

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

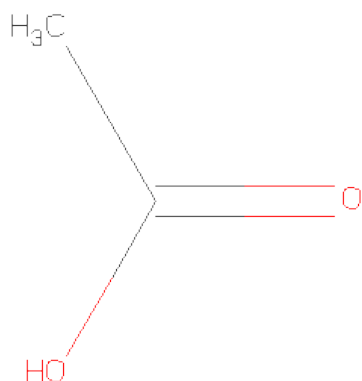
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	235	Total 235	O 235	0	0
12	B	205	Total 205	O 205	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	136.81Å 182.63Å 47.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.44 – 2.10 30.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.44-2.10) 94.5 (30.44-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.230 0.193 , 0.229	Depositor DCC
R_{free} test set	3360 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 66564 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7134	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, BMA, NAG, DGJ, EDO, 2PE, FUC, ACY, 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	0.36	0/3238	0.54	0/4396
1	B	0.37	0/3247	0.55	0/4408
All	All	0.36	0/6485	0.54	0/8804

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	3	0
3	A	3	0
8	B	3	0
All	All	9	0

There are no bond length outliers.

There are no bond angle outliers.

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	645	XYP	C4B,C2B,C3B
3	A	698	XYP	C4B,C2B,C3B
8	B	698	XYP	C4B,C2B,C3B

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3141	0	0	4	0
1	B	3150	0	0	3	0
2	A	80	0	67	0	0
3	A	58	0	49	0	0
4	A	38	0	34	0	0
5	A	11	0	13	0	0
5	B	11	0	13	0	0
6	A	10	0	13	0	0
6	B	61	0	81	0	0
7	B	14	0	13	0	0
8	B	59	0	49	0	0
9	B	49	0	43	0	0
10	B	4	0	6	0	0
11	B	8	0	6	0	0
12	A	235	0	0	2	0
12	B	205	0	0	0	0
All	All	7134	0	387	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

The worst 5 of 7 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:ASN:ND2	12:A:1183:HOH:O	2.37	0.57
1:B:202[B]:CYS:SG	1:B:223:CYS:SG	3.03	0.57
1:B:338:GLU:OE2	1:B:356:ARG:NH1	2.39	0.56
1:A:202[B]:CYS:SG	1:A:223:CYS:SG	3.08	0.52
1:A:105:ARG:NH2	12:A:1444:HOH:O	2.45	0.49

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	392/398 (98%)	383 (98%)	8 (2%)	1 (0%)	50	49
1	B	393/398 (99%)	381 (97%)	11 (3%)	1 (0%)	50	49
All	All	785/796 (99%)	764 (97%)	19 (2%)	2 (0%)	50	49

All (2) Ramachandran outliers are listed below:

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

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	335/339 (99%)	331 (99%)	4 (1%)	82	87
1	B	336/339 (99%)	329 (98%)	7 (2%)	66	70
All	All	671/678 (99%)	660 (98%)	11 (2%)	73	79

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	HIS
1	B	169	PHE
1	B	324	LEU
1	A	287	TRP
1	B	287	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

24 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	639	1,2	12,14,15	0.79	1 (8%)	15,19,21	0.99	1 (6%)
2	NAG	A	640	2	12,14,15	0.71	1 (8%)	15,19,21	1.26	2 (13%)
2	BMA	A	641	2	10,11,12	0.57	0	11,15,17	1.20	1 (9%)
2	MAN	A	642	2	10,11,12	0.74	0	11,15,17	0.66	0
2	MAN	A	643	2	10,11,12	0.71	0	11,15,17	1.23	1 (9%)
2	FUC	A	644	2	9,10,11	0.81	0	10,14,16	0.45	0
2	XYP	A	645	2	8,9,10	1.32	1 (12%)	8,12,14	0.83	0
3	NAG	A	692	1,3	12,14,15	0.61	0	15,19,21	0.74	0
3	NAG	A	693	3	12,14,15	0.60	0	15,19,21	0.93	0
3	BMA	A	694	3	10,11,12	0.47	0	11,15,17	1.36	2 (18%)
3	FUC	A	697	3	9,10,11	0.84	0	10,14,16	0.62	0
3	XYP	A	698	3	8,9,10	1.38	1 (12%)	8,12,14	0.92	0
4	NAG	A	715	1,4	12,14,15	0.68	1 (8%)	15,19,21	0.70	0
4	NAG	A	716	4	12,14,15	0.64	0	15,19,21	0.81	0
4	FUC	A	720	4	9,10,11	0.80	0	10,14,16	0.55	0
8	NAG	B	692	1,8	12,14,15	0.74	1 (8%)	15,19,21	0.78	0
8	NAG	B	693	8	12,14,15	0.63	0	15,19,21	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	B	694	8	10,11,12	0.47	0	11,15,17	0.88	0
8	MAN	B	695	8	10,11,12	0.72	0	11,15,17	0.69	0
8	XYP	B	698	8	8,9,10	1.39	1 (12%)	8,12,14	0.79	0
9	NAG	B	715	9,1	12,14,15	0.71	1 (8%)	15,19,21	0.62	0
9	NAG	B	716	9	12,14,15	0.63	0	15,19,21	1.05	1 (6%)
9	BMA	B	717	9	10,11,12	0.46	0	11,15,17	0.96	1 (9%)
9	FUC	B	720	9	9,10,11	0.79	0	10,14,16	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	639	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	640	2	-	0/6/23/26	0/1/1/1
2	BMA	A	641	2	-	0/2/19/22	0/1/1/1
2	MAN	A	642	2	-	0/2/19/22	0/1/1/1
2	MAN	A	643	2	-	0/2/19/22	0/1/1/1
2	FUC	A	644	2	-	0/0/17/20	0/1/1/1
2	XYP	A	645	2	3/3/3/4	0/0/14/17	0/1/1/1
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
3	FUC	A	697	3	-	0/0/17/20	0/1/1/1
3	XYP	A	698	3	3/3/3/4	0/0/14/17	0/1/1/1
4	NAG	A	715	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	716	4	-	0/6/23/26	0/1/1/1
4	FUC	A	720	4	-	0/0/17/20	0/1/1/1
8	NAG	B	692	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	693	8	-	0/6/23/26	0/1/1/1
8	BMA	B	694	8	-	0/2/19/22	0/1/1/1
8	MAN	B	695	8	-	0/2/19/22	0/1/1/1
8	XYP	B	698	8	3/3/3/4	0/0/14/17	0/1/1/1
9	NAG	B	715	9,1	-	0/6/23/26	0/1/1/1
9	NAG	B	716	9	-	0/6/23/26	0/1/1/1
9	BMA	B	717	9	-	0/2/19/22	0/1/1/1
9	FUC	B	720	9	-	0/0/17/20	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	698	XYP	O5B-C5B	-3.51	1.35	1.43
3	A	698	XYP	O5B-C5B	-3.49	1.35	1.43
2	A	645	XYP	O5B-C5B	-3.26	1.36	1.43
2	A	639	NAG	O5-C5	-2.49	1.40	1.45
2	A	640	NAG	O5-C5	-2.23	1.41	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	641	BMA	O5-C5-C6	3.66	110.82	106.98
2	A	643	MAN	O5-C5-C6	3.50	110.66	106.98
2	A	639	NAG	O5-C5-C4	-3.01	106.84	110.65
9	B	716	NAG	O5-C5-C6	2.90	110.03	106.98
9	B	717	BMA	O5-C5-C6	2.85	109.97	106.98

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	645	XYP	C4B
2	A	645	XYP	C2B
2	A	645	XYP	C3B
3	A	698	XYP	C4B
3	A	698	XYP	C2B

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

11 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	DGJ	A	801	-	11,11,11	0.75	0	15,15,15	1.75	2 (13%)
6	2PE	A	813	-	9,9,27	0.64	0	8,8,26	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	639	1	12,14,15	0.66	0	15,19,21	0.99	2 (13%)
5	DGJ	B	802	-	11,11,11	0.68	0	15,15,15	1.65	1 (6%)
6	2PE	B	810	-	15,15,27	0.58	0	14,14,26	0.42	0
6	2PE	B	811	-	27,27,27	0.51	0	26,26,26	0.18	0
6	2PE	B	812	-	6,6,27	0.83	0	5,5,26	0.44	0
10	EDO	B	814	-	3,3,3	0.53	0	2,2,2	0.30	0
6	2PE	B	815	-	9,9,27	0.64	0	8,8,26	0.59	0
11	ACY	B	842	-	3,3,3	0.68	0	3,3,3	0.66	0
11	ACY	B	843	-	3,3,3	0.64	0	3,3,3	0.69	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	DGJ	A	801	-	-	0/2/19/19	0/1/1/1
6	2PE	A	813	-	-	0/7/7/25	0/0/0/0
7	NAG	B	639	1	-	0/6/23/26	0/1/1/1
5	DGJ	B	802	-	-	0/2/19/19	0/1/1/1
6	2PE	B	810	-	-	0/13/13/25	0/0/0/0
6	2PE	B	811	-	-	0/25/25/25	0/0/0/0
6	2PE	B	812	-	-	0/4/4/25	0/0/0/0
10	EDO	B	814	-	-	0/1/1/1	0/0/0/0
6	2PE	B	815	-	-	0/7/7/25	0/0/0/0
11	ACY	B	842	-	-	0/0/0/0	0/0/0/0
11	ACY	B	843	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	DGJ	C1-N5-C5	5.71	120.56	110.79
5	A	801	DGJ	C1-N5-C5	5.60	120.39	110.79
5	A	801	DGJ	C2-C1-N5	-2.41	106.11	111.18
7	B	639	NAG	O5-C5-C4	-2.38	107.63	110.65
7	B	639	NAG	O5-C5-C6	2.33	109.42	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/398 (97%)	0.14	17 (4%) 33 37	18, 33, 59, 101	0
1	B	391/398 (98%)	0.17	14 (3%) 41 45	18, 30, 59, 120	0
All	All	781/796 (98%)	0.15	31 (3%) 35 41	18, 31, 59, 120	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	MET	8.5
1	B	422	GLN	7.5
1	A	421	MET	6.4
1	A	420	THR	6.0
1	B	175	ASP	4.8

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MAN	A	643	11/12	0.33	34.08	89,96,98,101	0
3	FUC	A	697	10/11	0.45	25.00	80,87,92,92	0
9	NAG	B	716	14/15	0.25	20.98	44,68,85,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	XYP	A	645	9/10	0.38	16.38	97,105,109,111	0
2	MAN	A	642	11/12	0.41	16.36	112,116,118,119	0
4	NAG	A	716	14/15	0.33	12.94	95,99,104,106	0
4	NAG	A	715	14/15	0.29	7.47	69,80,88,93	0
8	XYP	B	698	9/10	0.23	3.43	79,82,84,85	0
8	NAG	B	693	14/15	0.22	3.18	54,64,74,77	0
2	FUC	A	644	10/11	0.48	2.79	94,96,98,99	0
9	FUC	B	720	10/11	0.23	2.79	51,60,65,70	0
3	XYP	A	698	9/10	0.30	2.43	79,84,85,88	0
2	NAG	A	639	14/15	0.35	2.08	72,80,91,93	0
3	NAG	A	693	14/15	0.22	1.21	46,64,71,72	0
8	MAN	B	695	11/12	0.21	1.08	70,78,80,81	0
8	NAG	B	692	14/15	0.13	0.66	32,43,49,56	0
3	NAG	A	692	14/15	0.12	0.28	31,41,57,65	0
9	NAG	B	715	14/15	0.12	0.06	37,44,52,60	0
9	BMA	B	717	11/12	0.33	-	104,110,112,112	0
3	BMA	A	694	11/12	0.31	-	83,88,96,98	0
8	BMA	B	694	11/12	0.19	-	75,81,86,91	0
4	FUC	A	720	10/11	0.44	-	91,93,94,95	0
2	BMA	A	641	11/12	0.34	-	99,105,108,111	0
2	NAG	A	640	14/15	0.47	-	97,103,105,106	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	ACY	B	843	4/4	0.44	26.89	71,72,73,74	0
11	ACY	B	842	4/4	0.54	17.81	67,72,73,73	0
6	2PE	B	815	10/28	0.36	9.65	77,87,96,97	0
6	2PE	B	811	28/28	0.26	7.89	58,72,95,95	0
6	2PE	B	810	16/28	0.31	7.27	59,78,97,97	0
10	EDO	B	814	4/4	0.24	4.02	60,64,68,72	0
6	2PE	B	812	7/28	0.22	3.66	50,53,57,59	0
7	NAG	B	639	14/15	0.45	2.22	85,96,101,101	0
5	DGJ	A	801	11/11	0.14	0.23	24,27,30,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	2PE	A	813	10/28	0.16	0.02	65,75,76,77	0
5	DGJ	B	802	11/11	0.14	-0.07	18,21,23,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.