



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2017 – 02:21 PM EDT

PDB ID : 5IHR
Title : STRUCTURE OF E298Q-BETA-GALACTOSIDASE FROM AS-
PERGILLUS NIGER IN COMPLEX WITH ALLOLACTOSE
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cerra, M.; Sanz-Aparicio, J.
Deposited on : 2016-02-29
Resolution : 2.40 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
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) : rb-20029077

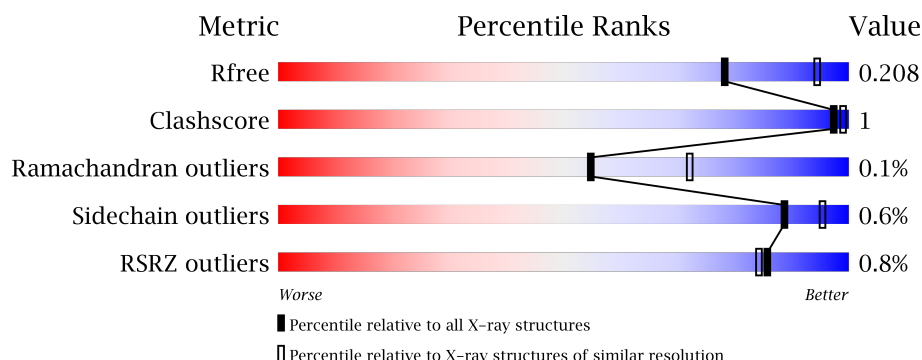
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

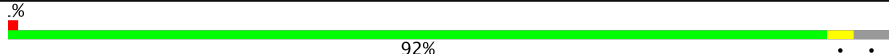
The reported resolution of this entry is 2.40 Å.

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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	1013	

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
2	NAG	A	1522	-	-	-	X
2	NAG	A	1739	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	1917	-	-	-	X
5	SO4	A	2001	-	-	-	X
7	DMS	A	3002	-	-	-	X
7	DMS	A	3003	-	-	-	X
7	DMS	A	3006	-	-	-	X
7	DMS	A	3009	-	-	-	X
9	GLC	A	4002	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 8157 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.

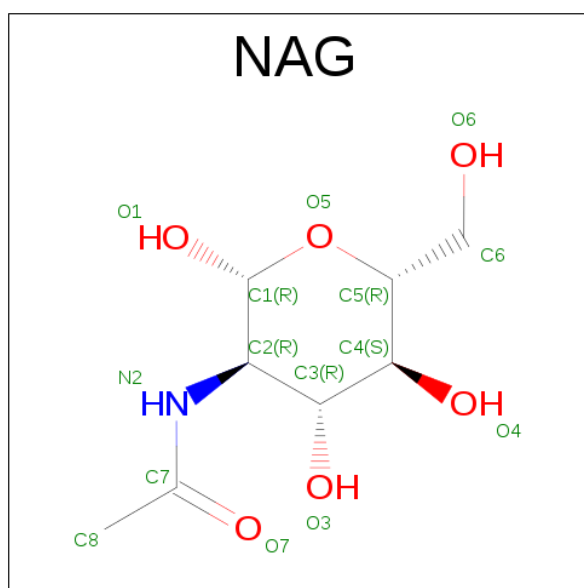
- Molecule 1 is a protein called Probable beta-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	968	7482	4780	1220	1471	11	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

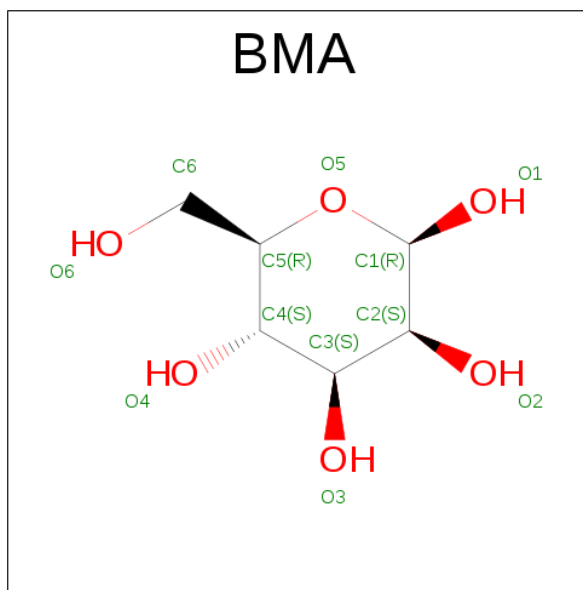
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLN	GLU	engineered mutation	UNP A2QAN3
A	1008	HIS	-	expression tag	UNP A2QAN3
A	1009	HIS	-	expression tag	UNP A2QAN3
A	1010	HIS	-	expression tag	UNP A2QAN3
A	1011	HIS	-	expression tag	UNP A2QAN3
A	1012	HIS	-	expression tag	UNP A2QAN3
A	1013	HIS	-	expression tag	UNP A2QAN3

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



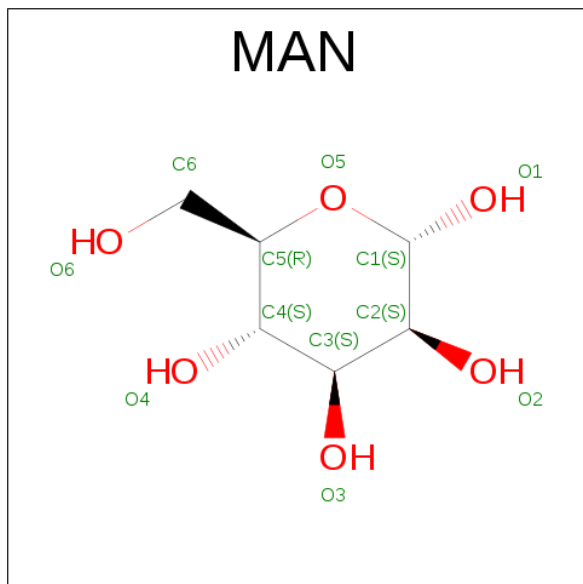
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



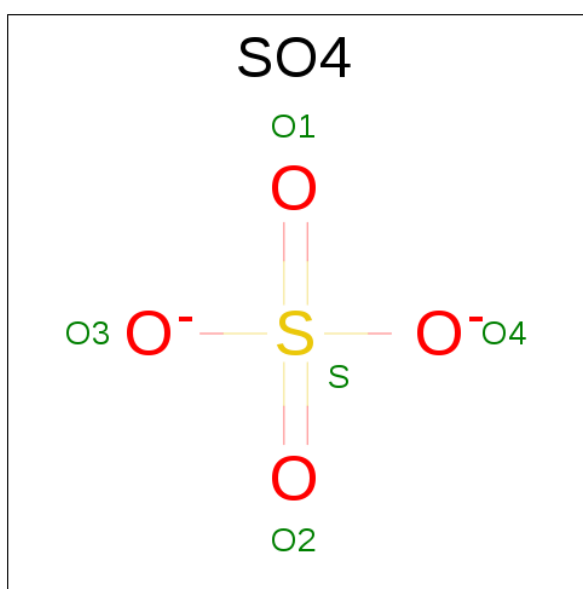
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

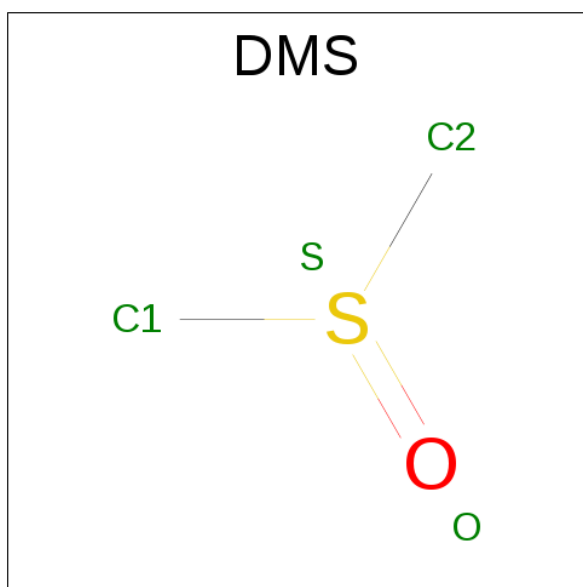


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

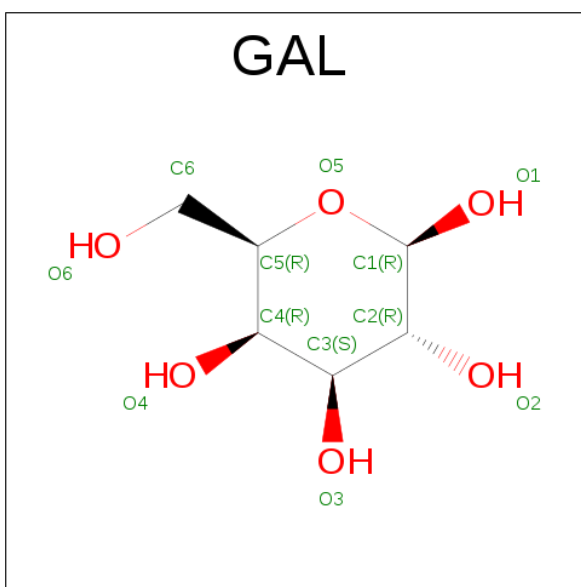
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



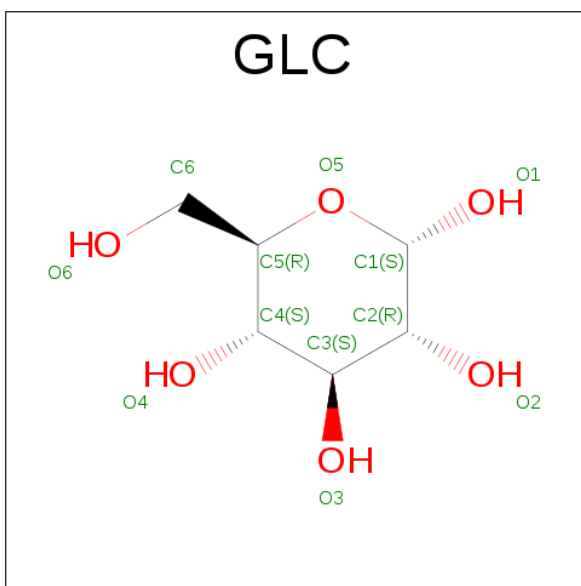
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

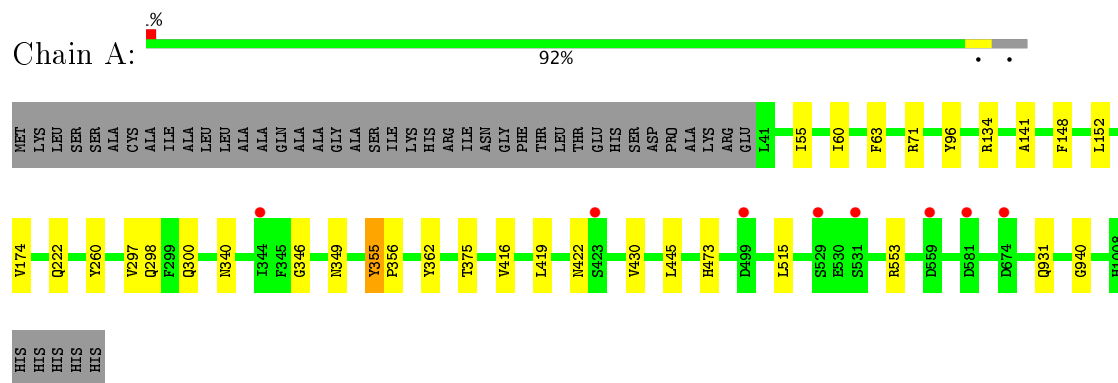
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	266	Total 266	O 266	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: Probable beta-galactosidase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.14Å 111.41Å 125.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.42 – 2.40 46.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (83.42-2.40) 99.2 (46.61-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.162 , 0.200 0.170 , 0.208	Depositor DCC
R_{free} test set	2364 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8157	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, DMS, NAG, CL, GLC, GAL, 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	0.37	0/7685	0.56	0/10488

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	7482	0	7180	16	0
2	A	168	0	150	2	0
3	A	33	0	25	0	0
4	A	143	0	122	0	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	A	36	0	54	0	0
8	A	12	0	11	0	0
9	A	11	0	9	0	0
10	A	266	0	0	0	0
All	All	8157	0	7551	16	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 1.

All (16) 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:134:ARG:HH12	1:A:298:GLN:HE21	1.38	0.69
1:A:96:TYR:CE2	1:A:141:ALA:HB2	2.43	0.53
1:A:71:ARG:HE	1:A:349:ASN:ND2	2.08	0.52
1:A:355:TYR:HB2	1:A:356:PRO:HD2	1.94	0.50
1:A:174:VAL:HG11	1:A:222:GLN:HB3	1.94	0.49
1:A:55:ILE:HD12	1:A:60:ILE:HG21	1.95	0.48
1:A:148:PHE:CG	1:A:152:LEU:HD12	2.51	0.46
1:A:260:TYR:HA	1:A:300:GLN:HB2	1.98	0.46
1:A:445:LEU:HD11	1:A:473:HIS:CD2	2.51	0.45
1:A:96:TYR:CD2	1:A:141:ALA:HB2	2.52	0.45
1:A:375:THR:HG21	2:A:1373:NAG:H82	1.99	0.45
1:A:416:VAL:HG22	1:A:430:VAL:HG22	1.99	0.44
1:A:346:GLY:HA3	1:A:362:TYR:O	2.18	0.44
1:A:419:LEU:HD12	1:A:419:LEU:N	2.33	0.42
1:A:940:GLY:HA2	2:A:1914:NAG:H83	2.02	0.42
1:A:297:VAL:O	1:A:340:ASN:HB3	2.21	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	966/1013 (95%)	936 (97%)	29 (3%)	1 (0%)	55 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	ASN

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	808/842 (96%)	803 (99%)	5 (1%)	89 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	355	TYR
1	A	515	LEU
1	A	553	ARG
1	A	931	GLN

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	242	ASN
1	A	298	GLN
1	A	349	ASN
1	A	458	GLN
1	A	466	ASN
1	A	577	GLN
1	A	663	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 1 is monoatomic - leaving 40 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	$\# Z > 2$
2	NAG	A	1156	1	14,14,15	0.65	0	15,19,21	1.39	1 (6%)
2	NAG	A	1373	1,2	14,14,15	0.46	0	15,19,21	1.36	2 (13%)
2	NAG	A	1374	3,2	14,14,15	0.78	0	15,19,21	0.85	0
3	BMA	A	1375	2,4	11,11,12	0.34	0	13,15,17	1.01	1 (7%)
4	MAN	A	1376	3,4	11,11,12	0.74	0	13,15,17	1.95	3 (23%)
4	MAN	A	1377	4	11,11,12	0.51	0	13,15,17	2.05	1 (7%)
4	MAN	A	1378	4	11,11,12	0.57	0	13,15,17	0.77	0
4	MAN	A	1379	3,4	11,11,12	0.60	0	13,15,17	1.21	2 (15%)
4	MAN	A	1380	4	11,11,12	0.63	0	13,15,17	0.95	1 (7%)
2	NAG	A	1478	1	14,14,15	0.48	0	15,19,21	0.85	0
2	NAG	A	1522	1	14,14,15	0.54	0	15,19,21	1.06	0
2	NAG	A	1622	1,2	14,14,15	0.64	0	15,19,21	1.00	0
2	NAG	A	1623	3,2	14,14,15	0.68	0	15,19,21	0.93	0
3	BMA	A	1624	2,4	11,11,12	0.34	0	13,15,17	0.69	0
4	MAN	A	1625	3,4	11,11,12	0.60	0	13,15,17	0.70	0
4	MAN	A	1626	4	11,11,12	0.60	0	13,15,17	0.83	0
4	MAN	A	1627	3,4	11,11,12	0.59	0	13,15,17	0.98	1 (7%)
4	MAN	A	1628	4	11,11,12	0.60	0	13,15,17	0.99	1 (7%)
4	MAN	A	1629	4	11,11,12	0.58	0	13,15,17	0.68	0
2	NAG	A	1739	1	14,14,15	0.69	0	15,19,21	1.12	2 (13%)
2	NAG	A	1760	1	14,14,15	0.47	0	15,19,21	1.56	1 (6%)
2	NAG	A	1777	1	14,14,15	0.49	0	15,19,21	0.99	1 (6%)
2	NAG	A	1914	1,2	14,14,15	0.78	1 (7%)	15,19,21	0.97	0
2	NAG	A	1915	3,2	14,14,15	0.57	0	15,19,21	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	1916	2,4	11,11,12	0.62	0	13,15,17	1.41	3 (23%)
4	MAN	A	1917	3,4	11,11,12	0.49	0	13,15,17	1.31	1 (7%)
4	MAN	A	1918	4	11,11,12	0.54	0	13,15,17	1.16	1 (7%)
4	MAN	A	1919	4	11,11,12	0.61	0	13,15,17	0.98	1 (7%)
5	SO4	A	2001	-	4,4,4	0.42	0	6,6,6	0.27	0
7	DMS	A	3001	-	3,3,3	0.48	0	3,3,3	0.64	0
7	DMS	A	3002	-	3,3,3	0.49	0	3,3,3	0.54	0
7	DMS	A	3003	-	3,3,3	0.47	0	3,3,3	0.67	0
7	DMS	A	3004	-	3,3,3	0.59	0	3,3,3	0.44	0
7	DMS	A	3005	-	3,3,3	0.47	0	3,3,3	0.67	0
7	DMS	A	3006	-	3,3,3	0.55	0	3,3,3	0.50	0
7	DMS	A	3007	-	3,3,3	0.54	0	3,3,3	0.47	0
7	DMS	A	3008	-	3,3,3	0.52	0	3,3,3	0.52	0
7	DMS	A	3009	-	3,3,3	0.49	0	3,3,3	0.67	0
8	GAL	A	4001	9	12,12,12	0.84	0	17,17,17	1.46	3 (17%)
9	GLC	A	4002	8	11,11,12	0.66	0	15,16,17	1.40	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	1156	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1373	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1374	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1375	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1376	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1377	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1378	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1379	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1380	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1478	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1522	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1622	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1623	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1624	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1625	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1626	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1627	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1628	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	1629	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1739	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1777	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1914	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1915	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1916	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1917	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1918	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1919	4	-	0/2/19/22	0/1/1/1
5	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3001	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3002	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3003	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3004	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3005	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3006	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3007	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3008	-	-	0/0/0/0	0/0/0/0
7	DMS	A	3009	-	-	0/0/0/0	0/0/0/0
8	GAL	A	4001	9	-	0/2/22/22	0/1/1/1
9	GLC	A	4002	8	-	0/0/20/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1914	NAG	O5-C1	-2.22	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1373	NAG	O5-C1-C2	-3.31	106.87	111.47
8	A	4001	GAL	O1-C1-O5	-2.57	102.61	110.20
8	A	4001	GAL	O5-C5-C4	-2.54	104.98	109.66
2	A	1739	NAG	C1-C2-N2	-2.46	106.29	110.49
2	A	1777	NAG	C1-C2-N2	-2.43	106.33	110.49
4	A	1376	MAN	C6-C5-C4	-2.39	107.41	113.00
9	A	4002	GLC	C6-C5-C4	-2.18	109.19	113.07
3	A	1916	BMA	O5-C1-C2	-2.02	107.63	110.79
4	A	1376	MAN	O2-C2-C1	-2.01	105.08	109.18
4	A	1628	MAN	O2-C2-C3	-2.01	106.24	110.17
4	A	1919	MAN	C1-O5-C5	2.00	114.93	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1375	BMA	C1-O5-C5	2.01	114.94	112.17
3	A	1916	BMA	C1-O5-C5	2.07	115.02	112.17
3	A	1916	BMA	C3-C4-C5	2.07	113.87	110.22
4	A	1379	MAN	C1-O5-C5	2.09	115.04	112.17
2	A	1739	NAG	C1-O5-C5	2.10	115.06	112.17
4	A	1380	MAN	C1-C2-C3	2.41	112.71	109.65
4	A	1627	MAN	C1-O5-C5	2.43	115.52	112.17
4	A	1379	MAN	C1-C2-C3	2.51	112.83	109.65
2	A	1373	NAG	C1-C2-N2	2.62	114.96	110.49
8	A	4001	GAL	C1-O5-C5	2.83	118.49	113.39
4	A	1918	MAN	C1-O5-C5	2.99	116.29	112.17
4	A	1917	MAN	C1-O5-C5	3.11	116.45	112.17
9	A	4002	GLC	O5-C5-C4	3.61	115.57	109.62
2	A	1156	NAG	C1-O5-C5	3.85	117.48	112.17
2	A	1760	NAG	C1-O5-C5	4.37	118.19	112.17
4	A	1376	MAN	C1-O5-C5	5.88	120.27	112.17
4	A	1377	MAN	C1-O5-C5	6.32	120.88	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1373	NAG	1	0
2	A	1914	NAG	1	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, 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	968/1013 (95%)	-0.27	8 (0%) 86 84	11, 20, 34, 53	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ASP	3.3
1	A	529	SER	2.4
1	A	581	ASP	2.4
1	A	531	SER	2.3
1	A	559	ASP	2.2
1	A	423	SER	2.1
1	A	674	ASP	2.1
1	A	344	ILE	2.1

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](#)

There are no carbohydrates in this entry.

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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	DMS	A	3006	4/4	0.91	0.22	6.40	67,68,68,68	0
7	DMS	A	3003	4/4	0.81	0.27	6.16	52,53,53,54	0
9	GLC	A	4002	11/12	0.65	0.31	6.07	62,69,73,75	0
2	NAG	A	1739	14/15	0.89	0.25	4.32	44,46,49,53	0
7	DMS	A	3009	4/4	0.79	0.28	3.82	66,67,70,70	0
2	NAG	A	1522	14/15	0.87	0.33	3.07	44,47,50,51	0
5	SO4	A	2001	5/5	0.98	0.21	2.71	40,40,41,43	0
4	MAN	A	1917	11/12	0.92	0.15	2.58	37,39,42,45	0
7	DMS	A	3002	4/4	0.82	0.28	2.53	63,67,68,68	0
7	DMS	A	3001	4/4	0.94	0.15	1.83	58,59,61,62	0
8	GAL	A	4001	12/12	0.85	0.23	1.21	34,41,43,49	0
2	NAG	A	1623	14/15	0.94	0.13	0.43	19,21,23,26	0
2	NAG	A	1914	14/15	0.95	0.14	0.13	20,21,24,25	0
2	NAG	A	1760	14/15	0.91	0.17	-0.06	27,31,33,33	0
2	NAG	A	1777	14/15	0.93	0.14	-0.24	26,28,31,31	0
2	NAG	A	1622	14/15	0.97	0.12	-0.40	19,19,21,21	0
2	NAG	A	1373	14/15	0.95	0.12	-0.46	19,20,21,21	0
2	NAG	A	1374	14/15	0.96	0.11	-0.57	20,22,23,25	0
6	CL	A	2002	1/1	0.99	0.07	-1.43	21,21,21,21	0
4	MAN	A	1378	11/12	0.87	0.40	-	55,57,58,58	0
4	MAN	A	1628	11/12	0.94	0.10	-	38,39,42,47	0
4	MAN	A	1379	11/12	0.81	0.37	-	55,63,66,66	0
4	MAN	A	1626	11/12	0.95	0.11	-	27,28,29,29	0
4	MAN	A	1376	11/12	0.94	0.14	-	33,34,39,41	0
7	DMS	A	3007	4/4	0.87	0.41	-	71,71,71,75	0
3	BMA	A	1375	11/12	0.94	0.13	-	27,31,37,47	0
7	DMS	A	3005	4/4	0.90	0.16	-	49,50,53,53	0
7	DMS	A	3008	4/4	0.95	0.17	-	66,67,68,70	0
4	MAN	A	1625	11/12	0.95	0.11	-	25,26,28,30	0
4	MAN	A	1919	11/12	0.88	0.39	-	60,63,65,66	0
4	MAN	A	1629	11/12	0.81	0.28	-	54,58,60,62	0
3	BMA	A	1916	11/12	0.88	0.17	-	37,39,40,40	0
4	MAN	A	1380	11/12	0.81	0.22	-	68,70,71,71	0
2	NAG	A	1156	14/15	0.79	0.39	-	44,48,52,53	0
7	DMS	A	3004	4/4	0.93	0.15	-	44,44,45,47	0
4	MAN	A	1377	11/12	0.96	0.24	-	46,48,49,52	0
4	MAN	A	1918	11/12	0.91	0.16	-	48,49,53,55	0
4	MAN	A	1627	11/12	0.94	0.10	-	29,30,31,34	0
2	NAG	A	1478	14/15	0.81	0.31	-	48,53,55,58	0
2	NAG	A	1915	14/15	0.95	0.14	-	28,30,31,33	0
3	BMA	A	1624	11/12	0.97	0.09	-	23,24,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.