



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2016 – 01:59 PM EDT

PDB ID : 5AE6
Title : The structure of Hypocrea jecorina beta-xylosidase Xyl3A (Bxl1) in complex with 4-thioxylobiose
Authors : Mikkelsen, N.E.; Gudmundsson, M.; Karkehabadi, S.; Hansson, H.; Sandgren, M.; Larenas, E.; Mitchinson, C.; Keleman, B.; Kaper, T.
Deposited on : 2015-08-26
Resolution : 2.10 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

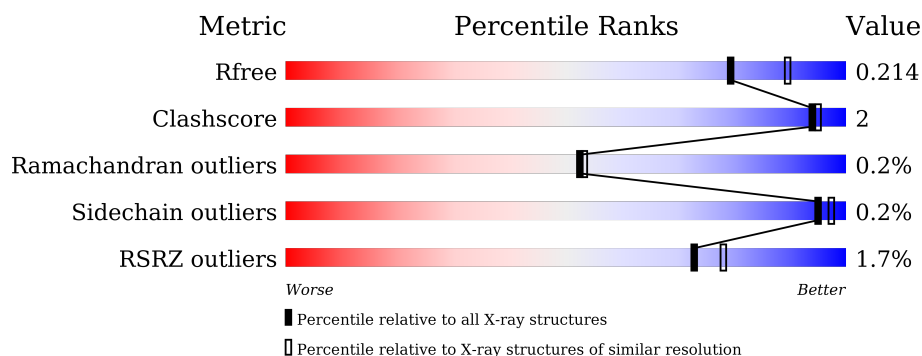
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

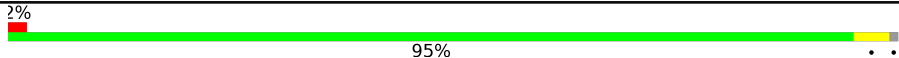
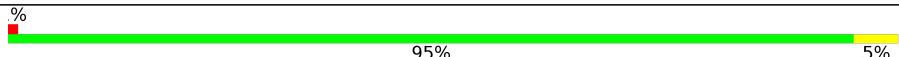
The reported resolution of this entry is 2.10 Å.

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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	767	
1	B	767	

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	1301	-	-	-	X
2	NAG	B	1301	-	-	-	X
3	NAG	A	1101	-	-	-	X
4	NAG	A	1401	-	-	-	X
5	NAG	A	1501	-	-	-	X
7	TXB	A	1769	-	-	-	X
7	TXB	B	1769	-	-	-	X

2 Entry composition [i](#)

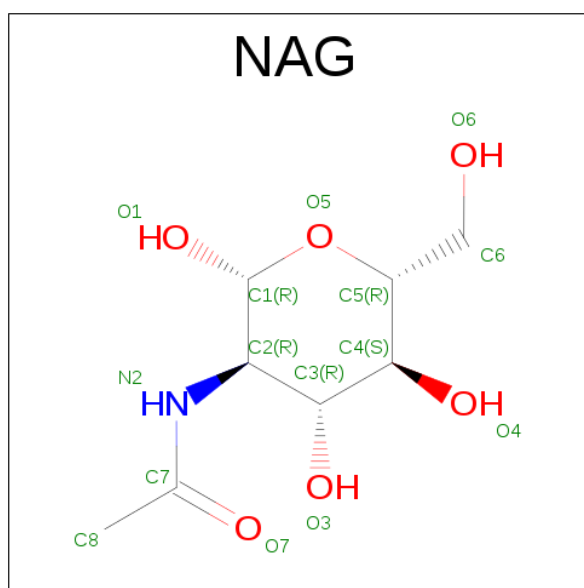
There are 10 unique types of molecules in this entry. The entry contains 13404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	6	0
			5947	3790	1000	1145	12			
1	B	767	Total	C	N	O	S	0	13	0
			6024	3840	1013	1159	12			

- Molecule 2 is SUGAR (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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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 (4-MER).

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

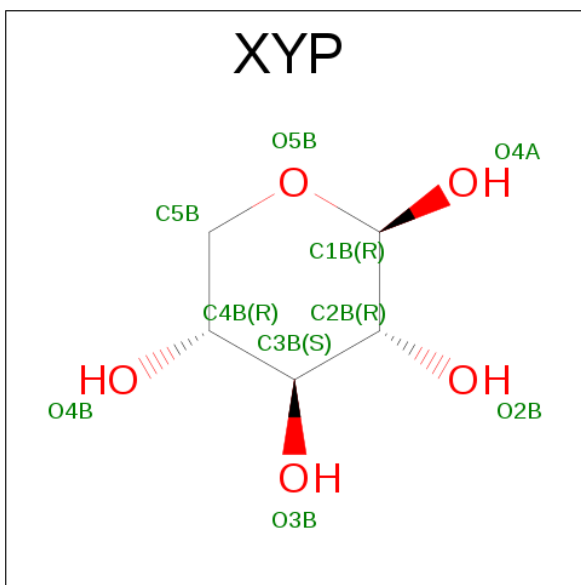
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	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		
4	B	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 a polymer of unknown type called SUGAR (3-MER).

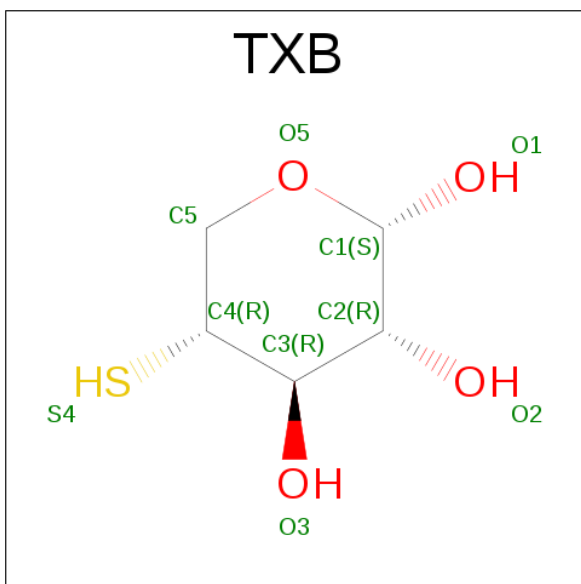
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	5	4		
6	B	1	Total	C	O	0	0
			9	5	4		

- Molecule 7 is (2S,3R,4R,5R)-5-SULFANYLOXANE-2,3,4-TRIOL (three-letter code: TXB) (formula: C₅H₁₀O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			10	5	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			10	5	4	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	7	Total	Zn	0	1
			8	8		
8	A	5	Total	Zn	0	1
			6	6		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	5	Total	C	N	O	0	0
			61	34	2	25		

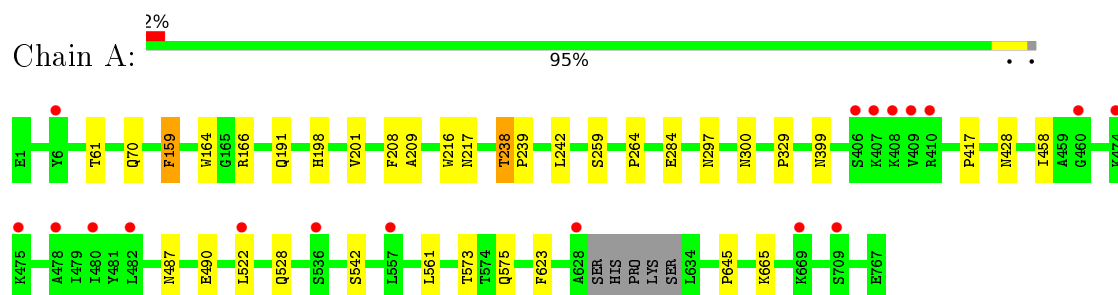
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	508	Total	O	0	5
			509	509		
10	B	442	Total	O	0	10
			442	442		

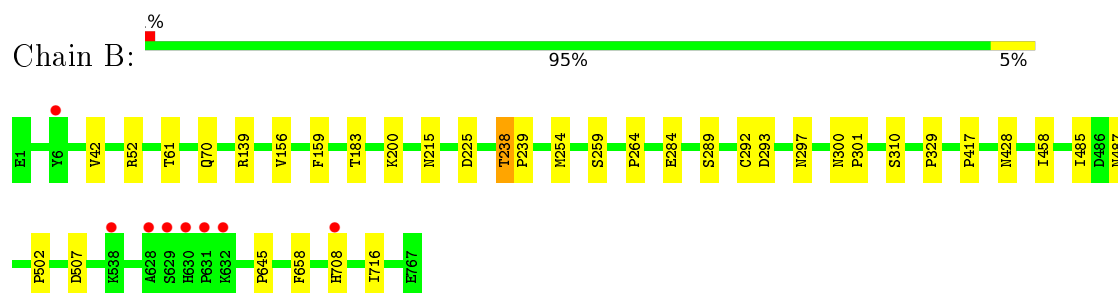
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: BETA-XYLOSIDASE



• Molecule 1: BETA-XYLOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.24Å 202.44Å 82.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	202.44 – 2.10 29.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (202.44-2.10) 99.9 (29.81-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.178 , 0.214 0.178 , 0.214	Depositor DCC
R_{free} test set	4912 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13404	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 2.97% 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: XYP, ZN, BMA, NAG, TXB, PCA, 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	0.38	0/6113	0.54	0/8331
1	B	0.38	0/6214	0.54	0/8469
All	All	0.38	0/12327	0.54	0/16800

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	5947	0	5734	25	0
1	B	6024	0	5828	23	1
2	A	70	0	65	1	0
2	B	70	0	65	0	0
3	A	50	0	43	0	0
4	A	56	0	50	0	0
4	B	84	0	75	0	0
5	A	39	0	34	0	0
6	A	9	0	8	0	0
6	B	9	0	8	0	0
7	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	0	0	0
8	A	6	0	0	0	0
8	B	8	0	0	0	0
9	B	61	0	52	1	0
10	A	509	0	0	1	0
10	B	442	0	0	4	1
All	All	13404	0	11962	45	1

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 2.

All (45) 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:198[A]:HIS:NE2	10:A:2191[A]:HOH:O	2.20	0.74
1:B:708:HIS:NE2	10:B:2419:HOH:O	2.27	0.67
1:A:216:TRP:CE3	1:A:217:ASN:HB2	2.41	0.56
1:A:284:GLU:HB2	1:B:284[B]:GLU:CD	2.25	0.56
1:A:428:ASN:HB3	1:A:487:ASN:HD21	1.71	0.56
1:B:70:GLN:HB3	1:B:329:PRO:HG3	1.90	0.52
1:B:417:PRO:HB2	1:B:458:ILE:HG12	1.92	0.51
1:A:428:ASN:HB3	1:A:487:ASN:ND2	2.26	0.51
1:B:254:MET:HA	1:B:289:SER:O	2.10	0.51
1:A:284:GLU:CD	1:B:284[B]:GLU:HB2	2.32	0.50
1:B:428:ASN:HB3	1:B:487:ASN:ND2	2.27	0.50
1:A:645:PRO:HD3	1:B:61:THR:HG22	1.93	0.50
1:A:70:GLN:HB3	1:A:329:PRO:HG3	1.93	0.49
1:A:297:ASN:HA	1:A:300:ASN:O	2.13	0.49
1:A:528:GLN:HB3	1:A:575:GLN:HG3	1.94	0.48
1:A:242:LEU:C	1:A:242:LEU:HD23	2.35	0.47
1:A:159:PHE:CD2	1:A:573:THR:HG21	2.50	0.47
1:B:156:VAL:HG11	1:B:183:THR:OG1	2.15	0.47
1:B:300:ASN:HA	1:B:301:PRO:HA	1.78	0.47
1:B:225[A]:ASP:HB3	10:B:2197[A]:HOH:O	2.14	0.46
1:B:485:ILE:HG22	1:B:502:PRO:HG3	1.97	0.46
1:A:238:THR:N	1:A:239:PRO:CD	2.79	0.46
1:A:522:LEU:HD11	1:A:561:LEU:HD21	1.98	0.46
1:B:139:ARG:HD3	1:B:200:LYS:O	2.16	0.46
1:A:61:THR:HG22	1:B:645:PRO:HD3	1.98	0.46
1:A:238:THR:N	1:A:239:PRO:HD2	2.30	0.46
1:B:297:ASN:HA	1:B:300:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:HG2	1:A:201:VAL:O	2.17	0.44
1:A:216:TRP:CZ3	1:A:217:ASN:HB2	2.53	0.44
1:A:417:PRO:HB2	1:A:458:ILE:HG12	2.00	0.44
9:B:1504:MAN:H61	10:B:2312:HOH:O	2.18	0.43
2:A:1301:NAG:H5	1:B:310[B]:SER:OG	2.19	0.43
1:B:658:PHE:CZ	1:B:716[A]:ILE:HD12	2.54	0.43
1:B:428:ASN:HB3	1:B:487:ASN:HD21	1.85	0.42
1:A:399:ASN:OD1	1:A:542:SER:OG	2.36	0.42
1:A:487:ASN:HA	1:A:490:GLU:O	2.20	0.42
1:B:238:THR:N	1:B:239:PRO:CD	2.82	0.41
1:A:208:PHE:CD1	1:A:209:ALA:HB2	2.56	0.41
1:B:259:SER:HA	1:B:264:PRO:HA	2.02	0.41
1:B:292:CYS:HA	1:B:293:ASP:HA	1.85	0.41
1:A:259:SER:HA	1:A:264:PRO:HA	2.02	0.41
1:B:225[B]:ASP:HB2	10:B:2189[B]:HOH:O	2.21	0.41
1:A:623:PHE:HA	1:A:665:LYS:O	2.21	0.41
1:A:164:TRP:CE2	1:A:166:ARG:HB2	2.55	0.40
1:B:42:VAL:HA	1:B:52:ARG:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ASP:OD2	10:B:2366:HOH:O[2_645]	2.17	0.03

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	764/767 (100%)	738 (97%)	25 (3%)	1 (0%)	56	58
1	B	778/767 (101%)	752 (97%)	24 (3%)	2 (0%)	46	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1542/1534 (100%)	1490 (97%)	49 (3%)	3 (0%)	52 53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	ASN
1	A	238	THR
1	B	238	THR

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	632/631 (100%)	631 (100%)	1 (0%)	95 97
1	B	644/631 (102%)	643 (100%)	1 (0%)	95 97
All	All	1276/1262 (101%)	1274 (100%)	2 (0%)	95 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	PHE
1	B	159	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	487	ASN
1	A	523	GLN
1	B	168	GLN
1	B	326	GLN
1	B	487	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	0.50	0	9,10,12	1.02	1 (11%)
1	PCA	B	1	1	7,8,9	0.38	0	9,10,12	0.99	1 (11%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	O-C-CA	-2.14	119.83	125.69
1	B	1	PCA	O-C-CA	-2.09	119.99	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

22 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	1101	1,3	14,14,15	0.55	0	15,19,21	1.10	0
3	NAG	A	1102	3	14,14,15	0.68	0	15,19,21	0.68	0
3	BMA	A	1103	3	11,11,12	0.31	0	15,15,17	1.46	2 (13%)
3	MAN	A	1104	3	11,11,12	0.56	0	15,15,17	1.12	1 (6%)
4	NAG	A	1401	1,4	14,14,15	0.47	0	15,19,21	1.05	1 (6%)
4	NAG	A	1402	4	14,14,15	0.55	0	15,19,21	1.06	1 (6%)
5	NAG	A	1501	1,5	14,14,15	0.60	0	15,19,21	0.72	0
5	NAG	A	1502	5	14,14,15	0.54	0	15,19,21	0.74	0
5	BMA	A	1503	5	11,11,12	0.37	0	15,15,17	0.87	1 (6%)
4	NAG	A	1601	1,4	14,14,15	0.58	0	15,19,21	0.79	0
4	NAG	A	1602	4	14,14,15	0.52	0	15,19,21	1.15	1 (6%)
4	NAG	B	1101	1,4	14,14,15	0.64	0	15,19,21	1.24	1 (6%)
4	NAG	B	1102	4	14,14,15	0.53	0	15,19,21	0.66	0
4	NAG	B	1401	1,4	14,14,15	0.57	0	15,19,21	0.92	1 (6%)
4	NAG	B	1402	4	14,14,15	0.53	0	15,19,21	1.20	1 (6%)
9	NAG	B	1501	1,9	14,14,15	0.56	0	15,19,21	0.60	0
9	NAG	B	1502	9	14,14,15	0.42	0	15,19,21	0.90	0
9	BMA	B	1503	9	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
9	MAN	B	1504	9	11,11,12	0.61	0	15,15,17	1.48	2 (13%)
9	MAN	B	1505	9	11,11,12	0.75	0	15,15,17	0.64	0
4	NAG	B	1601	1,4	14,14,15	0.57	0	15,19,21	0.79	0
4	NAG	B	1602	4	14,14,15	0.45	0	15,19,21	1.30	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
3	NAG	A	1101	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1102	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1103	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1104	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1502	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1503	5	-	0/2/19/22	0/1/1/1
4	NAG	A	1601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1602	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1101	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1102	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	4	-	0/6/23/26	0/1/1/1
9	NAG	B	1501	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	1502	9	-	0/6/23/26	0/1/1/1
9	BMA	B	1503	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1504	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1505	9	-	0/2/19/22	0/1/1/1
4	NAG	B	1601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1602	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1101	NAG	O5-C5-C4	-2.21	106.48	110.13
4	A	1402	NAG	O5-C5-C6	2.04	111.70	107.34
5	A	1503	BMA	C1-C2-C3	2.09	112.08	109.55
3	A	1103	BMA	C1-C2-C3	2.11	112.11	109.55
9	B	1504	MAN	O5-C5-C6	2.46	112.61	107.34
4	B	1401	NAG	C1-O5-C5	2.52	115.84	112.14
4	A	1401	NAG	C1-O5-C5	2.60	115.97	112.14
3	A	1104	MAN	C1-O5-C5	2.95	116.48	112.14
4	B	1402	NAG	C4-C3-C2	3.00	116.00	111.34
9	B	1503	BMA	C1-C2-C3	3.44	113.72	109.55
4	A	1602	NAG	C1-O5-C5	3.88	117.84	112.14
4	B	1602	NAG	C1-O5-C5	3.98	118.00	112.14
9	B	1504	MAN	C1-C2-C3	4.12	114.54	109.55
3	A	1103	BMA	C1-O5-C5	4.27	118.42	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1504	MAN	1	0

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1001	1	14,14,15	0.56	0	15,19,21	0.62	0
2	NAG	A	1201	1	14,14,15	0.43	0	15,19,21	1.31	1 (6%)
2	NAG	A	1301	1	14,14,15	0.50	0	15,19,21	1.11	1 (6%)
6	XYP	A	1768	7	9,9,10	0.91	0	12,12,14	1.14	1 (8%)
7	TXB	A	1769	6	9,10,10	1.25	0	9,14,14	0.82	1 (11%)
2	NAG	A	1801	1	14,14,15	0.53	0	15,19,21	0.92	0
2	NAG	A	901	1	14,14,15	0.57	0	15,19,21	1.00	1 (6%)
2	NAG	B	1001	1	14,14,15	0.58	0	15,19,21	0.69	0
2	NAG	B	1301	1	14,14,15	0.43	0	15,19,21	1.33	1 (6%)
2	NAG	B	1701	1	14,14,15	0.59	0	15,19,21	0.69	0
6	XYP	B	1768	7	9,9,10	1.28	1 (11%)	12,12,14	1.14	1 (8%)
7	TXB	B	1769	6	9,10,10	1.39	2 (22%)	9,14,14	0.54	0
2	NAG	B	1801	1	14,14,15	0.57	0	15,19,21	0.75	1 (6%)
2	NAG	B	901	1	14,14,15	0.50	0	15,19,21	0.96	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	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
6	XYP	A	1768	7	-	0/0/14/17	0/1/1/1
7	TXB	A	1769	6	-	0/0/17/17	0/1/1/1
2	NAG	A	1801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1701	1	-	0/6/23/26	0/1/1/1
6	XYP	B	1768	7	-	0/0/14/17	0/1/1/1
7	TXB	B	1769	6	-	0/0/17/17	0/1/1/1
2	NAG	B	1801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1769	TXB	O5-C5	2.14	1.47	1.43
7	B	1769	TXB	O5-C1	2.47	1.45	1.43
6	B	1768	XYP	C2B-C3B	3.12	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAG	C2-N2-C7	-2.00	120.50	123.11
7	A	1769	TXB	C3-C4-S4	2.00	115.00	111.23
2	B	1801	NAG	C1-O5-C5	2.21	115.39	112.14
6	B	1768	XYP	C1B-C2B-C3B	2.65	112.77	109.55
6	A	1768	XYP	C1B-C2B-C3B	3.02	113.21	109.55
2	A	1301	NAG	C1-O5-C5	3.78	117.70	112.14
2	A	1201	NAG	C1-O5-C5	4.17	118.27	112.14
2	B	1301	NAG	C1-O5-C5	4.54	118.82	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0

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	761/767 (99%)	-0.14	18 (2%) 62 68	12, 21, 43, 60	0
1	B	766/767 (99%)	-0.39	8 (1%) 84 87	12, 19, 32, 67	0
All	All	1527/1534 (99%)	-0.27	26 (1%) 73 78	12, 20, 40, 67	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	630	HIS	4.6
1	A	407	LYS	3.9
1	A	409	VAL	3.9
1	A	475	LYS	3.3
1	A	410	ARG	3.2
1	B	629	SER	3.2
1	A	6	TYR	3.0
1	A	522	LEU	3.0
1	B	632	LYS	2.8
1	B	631	PRO	2.7
1	A	669	LYS	2.7
1	A	709	SER	2.5
1	A	460	GLY	2.5
1	A	557	LEU	2.5
1	A	628	ALA	2.3
1	B	628	ALA	2.3
1	A	408	LYS	2.3
1	B	6	TYR	2.2
1	A	406	SER	2.2
1	B	708	HIS	2.1
1	A	536	SER	2.1
1	A	474	LYS	2.1
1	A	478	ALA	2.1
1	A	482	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	538	LYS	2.0
1	A	480	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PCA	A	1	8/9	0.92	0.11	-	21,22,23,23	0
1	PCA	B	1	8/9	0.95	0.09	-	22,22,23,24	0

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, 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(Å ²)	Q<0.9
5	NAG	A	1501	14/15	0.89	0.17	3.31	29,32,34,34	0
4	NAG	A	1401	14/15	0.90	0.18	3.22	29,33,37,40	0
3	NAG	A	1101	14/15	0.87	0.13	2.04	25,27,30,32	0
4	NAG	B	1101	14/15	0.90	0.11	0.76	24,27,31,32	0
9	NAG	B	1501	14/15	0.96	0.11	0.69	25,26,28,29	0
9	NAG	B	1502	14/15	0.92	0.15	-	32,35,36,39	0
9	BMA	B	1503	11/12	0.80	0.34	-	43,44,51,51	0
4	NAG	A	1601	14/15	0.79	0.32	-	48,55,56,59	0
9	MAN	B	1505	11/12	0.70	0.19	-	33,34,35,35	11
4	NAG	B	1401	14/15	0.93	0.14	-	27,29,30,35	0
5	BMA	A	1503	11/12	0.73	0.33	-	44,46,48,49	11
3	NAG	A	1102	14/15	0.96	0.15	-	27,29,32,32	0
3	BMA	A	1103	11/12	0.85	0.15	-	34,36,37,39	0
5	NAG	A	1502	14/15	0.93	0.26	-	37,39,42,44	0
4	NAG	A	1602	14/15	0.79	0.47	-	62,65,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	1601	14/15	0.91	0.17	-	29,31,34,39	0
9	MAN	B	1504	11/12	0.65	0.38	-	36,39,40,40	11
3	MAN	A	1104	11/12	0.88	0.18	-	39,40,42,43	0
4	NAG	A	1402	14/15	0.63	0.39	-	42,49,53,54	0
4	NAG	B	1102	14/15	0.88	0.22	-	34,37,41,42	0
4	NAG	B	1402	14/15	0.86	0.28	-	39,41,42,45	0
4	NAG	B	1602	14/15	0.88	0.36	-	43,48,50,51	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, 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
2	NAG	B	1301	14/15	0.82	0.35	11.98	36,45,50,51	0
2	NAG	A	1301	14/15	0.84	0.21	8.61	31,35,39,40	0
7	TXB	B	1769	10/10	0.89	0.18	4.13	30,40,43,43	0
7	TXB	A	1769	10/10	0.94	0.13	2.29	27,36,38,38	0
2	NAG	A	1801	14/15	0.93	0.18	1.81	40,43,45,45	0
2	NAG	A	1001	14/15	0.92	0.20	1.33	31,34,37,38	0
6	XYP	B	1768	9/10	0.94	0.12	1.32	20,24,27,27	0
2	NAG	B	901	14/15	0.83	0.19	0.77	29,35,36,36	0
2	NAG	B	1801	14/15	0.94	0.13	0.46	30,32,34,34	0
2	NAG	B	1001	14/15	0.89	0.18	0.23	37,41,43,44	0
6	XYP	A	1768	9/10	0.97	0.10	0.12	19,20,22,23	0
8	ZN	B	1907	1/1	1.00	0.10	-0.11	19,19,19,19	1
2	NAG	A	901	14/15	0.91	0.14	-0.15	29,31,33,34	0
8	ZN	A	1911	1/1	0.97	0.06	-1.59	31,31,31,31	1
8	ZN	A	1901	1/1	0.99	0.03	-1.75	25,25,25,25	0
8	ZN	B	1911	1/1	0.98	0.05	-2.77	34,34,34,34	1
2	NAG	A	1201	14/15	0.82	0.29	-	40,44,47,52	0
2	NAG	B	1701	14/15	0.81	0.24	-	32,34,36,36	0
8	ZN	A	1906[B]	1/1	0.97	0.09	-	47,47,47,47	1
8	ZN	A	1904	1/1	1.00	0.02	-	21,21,21,21	0
8	ZN	B	1906[A]	1/1	0.92	0.12	-	39,39,39,39	1
8	ZN	B	1914	1/1	0.98	0.03	-	37,37,37,37	0
8	ZN	B	1901	1/1	0.99	0.02	-	23,23,23,23	0
8	ZN	A	1906[A]	1/1	0.97	0.09	-	46,46,46,46	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	ZN	A	1902	1/1	0.84	0.09	-	62,62,62,62	1
8	ZN	B	1906[B]	1/1	0.92	0.12	-	51,51,51,51	1
8	ZN	B	1904	1/1	1.00	0.01	-	22,22,22,22	0
8	ZN	B	1910	1/1	0.94	0.07	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.