



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:06 AM GMT

PDB ID : 2XWE
Title : X-RAY STRUCTURE OF ACID-BETA-GLUCOSIDASE WITH 5N,6S-(N'-(N-OCTYL)IMINO)-6-THIONOJIRIMYCININ THE ACTIVE SITE
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Deposited on : 2010-11-02
Resolution : 2.31 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

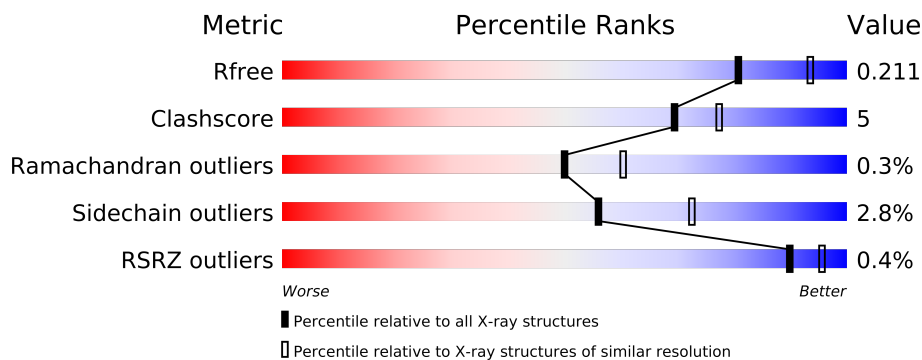
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.31 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	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (2.34-2.30)

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	505	
1	B	505	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8426 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 GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3892	2509	662	705	16			
1	B	498	Total	C	N	O	S	0	0	0
			3911	2518	667	710	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	EXPRESSION TAG	UNP P04062
A	0	PHE	-	EXPRESSION TAG	UNP P04062
A	495	HIS	ARG	VARIANT	UNP P04062
A	498	LEU	-	EXPRESSION TAG	UNP P04062
A	499	LEU	-	EXPRESSION TAG	UNP P04062
A	500	VAL	-	EXPRESSION TAG	UNP P04062
A	501	ASP	-	EXPRESSION TAG	UNP P04062
A	502	THR	-	EXPRESSION TAG	UNP P04062
A	503	MET	-	EXPRESSION TAG	UNP P04062
B	-1	GLU	-	EXPRESSION TAG	UNP P04062
B	0	PHE	-	EXPRESSION TAG	UNP P04062
B	495	HIS	ARG	VARIANT	UNP P04062
B	498	LEU	-	EXPRESSION TAG	UNP P04062
B	499	LEU	-	EXPRESSION TAG	UNP P04062
B	500	VAL	-	EXPRESSION TAG	UNP P04062
B	501	ASP	-	EXPRESSION TAG	UNP P04062
B	502	THR	-	EXPRESSION TAG	UNP P04062
B	503	MET	-	EXPRESSION TAG	UNP P04062

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

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

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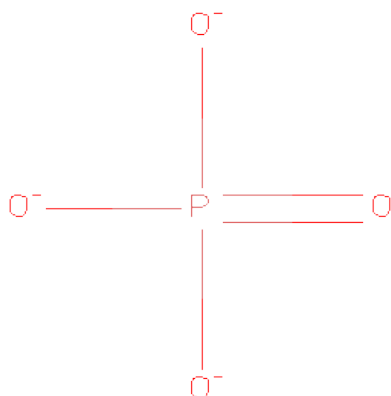
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	4	Total	C	N	O	0	0
			49	28	2	19		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	EXPRESSION TAG	UNP P04062
A	0	PHE	-	EXPRESSION TAG	UNP P04062
A	495	HIS	ARG	VARIANT	UNP P04062
A	498	LEU	-	EXPRESSION TAG	UNP P04062
A	499	LEU	-	EXPRESSION TAG	UNP P04062
A	500	VAL	-	EXPRESSION TAG	UNP P04062
A	501	ASP	-	EXPRESSION TAG	UNP P04062
A	502	THR	-	EXPRESSION TAG	UNP P04062
A	503	MET	-	EXPRESSION TAG	UNP P04062
B	-1	GLU	-	EXPRESSION TAG	UNP P04062
B	0	PHE	-	EXPRESSION TAG	UNP P04062
B	495	HIS	ARG	VARIANT	UNP P04062
B	498	LEU	-	EXPRESSION TAG	UNP P04062
B	499	LEU	-	EXPRESSION TAG	UNP P04062
B	500	VAL	-	EXPRESSION TAG	UNP P04062
B	501	ASP	-	EXPRESSION TAG	UNP P04062
B	502	THR	-	EXPRESSION TAG	UNP P04062
B	503	MET	-	EXPRESSION TAG	UNP P04062

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

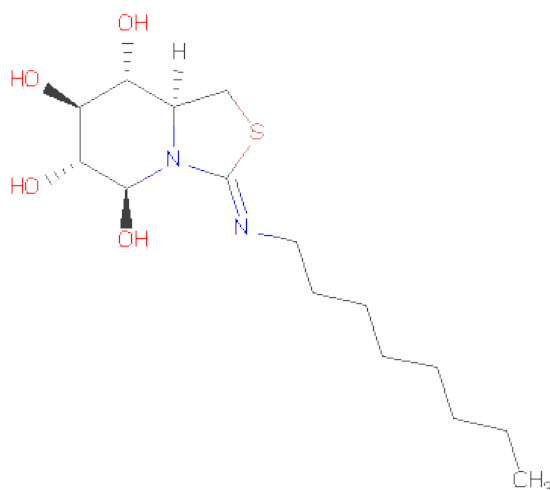


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is (3Z,5S,6R,7S,8R,8AS)-3-(OCTYLIMINO)HEXAHYDRO[1,3]THIAZOLO[3,4-A]PYRIDINE-5,6,7,8-TETROL (three-letter code: AMF) (formula: C₁₅H₂₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			22	15	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			17	10	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	256	Total	O	0	0
			256	256		

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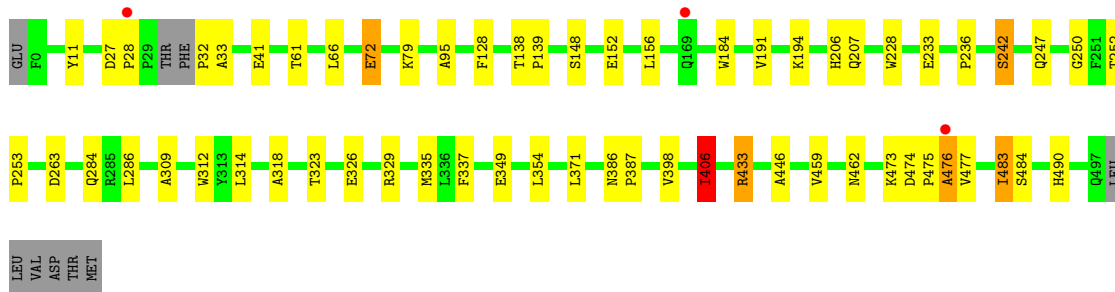
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	218	Total 218	O 218	0	0

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 ($RSRZ > 2$). 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.

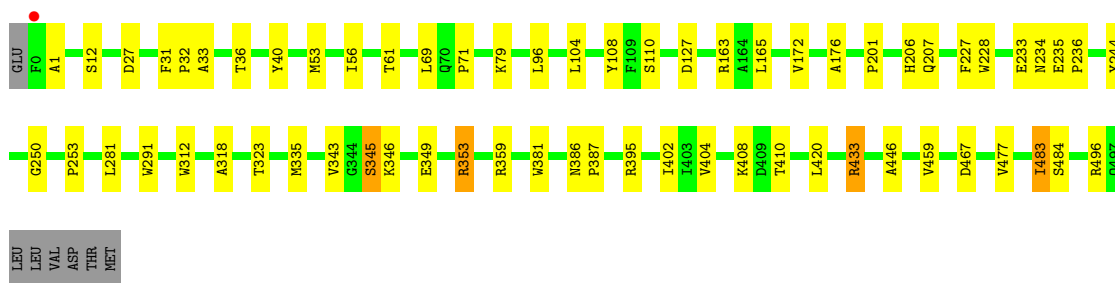
• Molecule 1: GLUCOSYLCERAMIDASE

Chain A: 



• Molecule 1: GLUCOSYLCERAMIDASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.14Å 96.69Å 82.97Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	19.82 – 2.31 19.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.82-2.31) 96.5 (19.82-2.31)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.51 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.150 , 0.213 0.150 , 0.211	Depositor DCC
R_{free} test set	2234 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 44406 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8426	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: BMA, NAG, PO4, AMF, FUC, K

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	1.05	2/4011 (0.0%)	0.88	2/5472 (0.0%)
1	B	1.01	2/4031 (0.0%)	0.88	6/5502 (0.1%)
All	All	1.03	4/8042 (0.0%)	0.88	8/10974 (0.1%)

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
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	ALA	CA-CB	6.21	1.65	1.52
1	A	72	GLU	CG-CD	5.36	1.59	1.51
1	B	244	TYR	CD2-CE2	5.20	1.47	1.39
1	B	40	TYR	CD2-CE2	5.02	1.46	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	B	433	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	420	LEU	CB-CG-CD1	-6.20	100.46	111.00
1	B	163	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	395	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	353	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	406	ILE	CB-CA-C	-5.13	101.34	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	ALA	Peptide

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	3892	0	3769	29	0
1	B	3911	0	3791	31	0
2	A	49	0	43	0	0
2	B	49	0	43	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	22	0	28	8	0
5	B	17	0	15	5	0
6	A	256	0	0	1	0
6	B	218	0	0	0	0
All	All	8426	0	7689	73	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 5.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:1510:AMF:H82C	5:B:1510:AMF:O1	1.45	1.12
5:A:1510:AMF:O1	5:A:1510:AMF:H82C	1.53	1.06
5:B:1510:AMF:C8	5:B:1510:AMF:O1	2.11	0.99
5:A:1510:AMF:O1	5:A:1510:AMF:C8	2.10	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1510:AMF:H81C	5:A:1510:AMF:C1	2.08	0.83
1:A:406:ILE:HG13	6:A:2224:HOH:O	1.87	0.75
1:B:1:ALA:N	1:B:27:ASP:OD1	2.23	0.72
5:A:1510:AMF:C1	5:A:1510:AMF:C8	2.68	0.72
1:B:346:LYS:HE2	1:B:349:GLU:CD	2.14	0.68
1:B:236:PRO:O	1:B:250:GLY:HA2	1.97	0.65
1:B:343:VAL:HG21	1:B:359:ARG:HG2	1.77	0.65
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.79	0.64
1:B:33:ALA:O	1:B:36:THR:HB	1.99	0.62
1:B:467:ASP:HB3	1:B:483:ILE:HD11	1.83	0.60
1:A:27:ASP:HB3	1:A:28:PRO:HD2	1.84	0.60
1:B:346:LYS:HG2	1:B:349:GLU:OE1	2.03	0.58
1:B:345:SER:HB3	5:B:1510:AMF:S1	2.43	0.57
1:A:446:ALA:HA	1:A:459:VAL:O	2.06	0.55
1:B:104:LEU:HD23	1:B:104:LEU:C	2.26	0.55
1:B:79:LYS:HE2	1:B:228:TRP:CE2	2.42	0.55
1:A:95:ALA:HB1	1:A:406:ILE:HG23	1.90	0.54
1:B:408:LYS:O	1:B:410:THR:HG23	2.10	0.52
5:A:1510:AMF:H154	5:A:1510:AMF:H82C	1.71	0.51
1:A:66:LEU:HD11	1:A:473:LYS:HB2	1.91	0.51
5:B:1510:AMF:H82C	5:B:1510:AMF:H154	1.67	0.51
1:B:346:LYS:HE2	1:B:349:GLU:OE2	2.10	0.51
1:A:318:ALA:HB1	1:A:323:THR:HG21	1.94	0.50
5:A:1510:AMF:H81C	5:A:1510:AMF:O1	1.94	0.50
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.42	0.49
1:A:284:GLN:HG3	1:A:314:LEU:HD12	1.93	0.49
1:A:309:ALA:HA	1:A:337:PHE:O	2.13	0.49
1:B:343:VAL:HG21	1:B:359:ARG:CG	2.40	0.48
1:A:286:LEU:C	1:A:286:LEU:HD12	2.33	0.48
1:B:56:ILE:HG21	1:B:477:VAL:HG23	1.95	0.48
1:B:12:SER:OG	3:B:1502:PO4:O3	2.25	0.48
5:B:1510:AMF:C8	5:B:1510:AMF:C1	2.91	0.48
1:A:462:ASN:HB2	1:A:484:SER:OG	2.15	0.47
1:A:371:LEU:O	1:A:433:ARG:HD2	2.14	0.47
1:A:79:LYS:HE2	1:A:228:TRP:CE2	2.51	0.46
1:B:165:LEU:CD2	1:B:172:VAL:HB	2.46	0.46
1:B:108:TYR:CE2	1:B:402:ILE:HD12	2.51	0.46
5:A:1510:AMF:H154	5:A:1510:AMF:C8	2.26	0.45
1:B:201:PRO:HA	1:B:206:HIS:CG	2.51	0.45
1:A:194:LYS:HB2	1:A:242:SER:HA	1.98	0.45
1:B:253:PRO:HB3	1:B:291:TRP:CD2	2.52	0.45
1:A:138:THR:HA	1:A:139:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:483:ILE:HG12	1:A:484:SER:N	2.31	0.45
1:A:11:TYR:HD2	1:A:354:LEU:O	2.01	0.44
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.53	0.44
1:B:234:ASN:O	1:B:235:GLU:C	2.56	0.44
1:A:386:ASN:HB2	1:A:387:PRO:CD	2.48	0.44
1:B:71:PRO:HG3	1:B:496:ARG:NH2	2.33	0.44
5:A:1510:AMF:H81C	5:A:1510:AMF:H155	1.95	0.43
1:A:206:HIS:HB3	1:A:263:ASP:OD2	2.19	0.43
1:B:318:ALA:HB1	1:B:323:THR:HG21	2.00	0.43
1:A:152:GLU:O	1:A:156:LEU:HB2	2.19	0.43
1:A:27:ASP:HB3	1:A:28:PRO:CD	2.47	0.42
1:A:32:PRO:HB2	1:A:33:ALA:H	1.52	0.42
1:A:139:PRO:HA	1:A:184:TRP:CD1	2.54	0.42
1:A:474:ASP:HA	1:A:475:PRO:HD2	1.93	0.42
1:A:41:GLU:HG3	1:A:490:HIS:CD2	2.55	0.41
1:B:346:LYS:HG2	1:B:349:GLU:CD	2.41	0.41
1:B:483:ILE:HG13	1:B:484:SER:N	2.34	0.41
1:B:96:LEU:HD21	1:B:404:VAL:HG13	2.02	0.41
1:A:191:VAL:O	1:A:247:GLN:HA	2.21	0.41
1:A:128:PHE:CZ	1:A:398:VAL:HG22	2.55	0.41
1:B:446:ALA:HA	1:B:459:VAL:O	2.21	0.41
1:A:326:GLU:OE2	1:A:329:ARG:NH2	2.45	0.40
1:A:236:PRO:O	1:A:250:GLY:HA2	2.20	0.40
1:B:127:ASP:N	1:B:127:ASP:OD1	2.54	0.40
1:B:31:PHE:HA	1:B:32:PRO:HD2	1.93	0.40
1:A:252:THR:HB	1:A:253:PRO:HD2	2.04	0.40
2:B:1498:NAG:H61	2:B:1499:NAG:C1	2.52	0.40

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	492/505 (97%)	466 (95%)	25 (5%)	1 (0%)	56 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	496/505 (98%)	474 (96%)	20 (4%)	2 (0%)	43 52
All	All	988/1010 (98%)	940 (95%)	45 (5%)	3 (0%)	50 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	B	281	LEU
1	B	233	GLU

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	413/432 (96%)	402 (97%)	11 (3%)	57 74
1	B	417/432 (96%)	405 (97%)	12 (3%)	55 71
All	All	830/864 (96%)	807 (97%)	23 (3%)	56 72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	72	GLU
1	A	148	SER
1	A	207	GLN
1	A	242	SER
1	A	312	TRP
1	A	335	MET
1	A	349	GLU
1	A	406	ILE
1	A	477	VAL
1	A	483	ILE
1	B	53	MET
1	B	61	THR
1	B	69	LEU
1	B	110	SER

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Mol	Chain	Res	Type
1	B	207	GLN
1	B	312	TRP
1	B	335	MET
1	B	345	SER
1	B	353	ARG
1	B	381	TRP
1	B	433	ARG
1	B	483	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN

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 ⓘ

8 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	1498	1,2	12,14,15	0.66	0	15,19,21	2.33	3 (20%)
2	NAG	A	1499	2	12,14,15	0.83	0	15,19,21	2.16	6 (40%)
2	BMA	A	1500	2	10,11,12	0.71	0	11,15,17	1.95	4 (36%)
2	FUC	A	1501	2	9,10,11	0.79	0	10,14,16	1.26	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1498	1,2	12,14,15	0.70	0	15,19,21	1.73	2 (13%)
2	NAG	B	1499	2	12,14,15	0.95	1 (8%)	15,19,21	1.39	1 (6%)
2	BMA	B	1500	2	10,11,12	0.67	0	11,15,17	1.39	2 (18%)
2	FUC	B	1501	2	9,10,11	0.84	0	10,14,16	1.51	3 (30%)

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	1498	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1499	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1500	2	-	0/2/19/22	0/1/1/1
2	FUC	A	1501	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1498	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1499	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1500	2	-	0/2/19/22	0/1/1/1
2	FUC	B	1501	2	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1499	NAG	O5-C5	-2.39	1.41	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1498	NAG	O5-C5-C6	5.90	113.17	106.98
2	A	1499	NAG	O5-C5-C6	5.41	112.65	106.98
2	B	1498	NAG	O5-C5-C6	5.21	112.45	106.98
2	A	1498	NAG	C2-N2-C7	-5.13	114.47	123.09
2	A	1500	BMA	O3-C3-C2	3.86	117.00	109.94
2	B	1500	BMA	O5-C5-C4	3.64	115.28	110.65
2	A	1499	NAG	C3-C2-N2	-3.41	106.57	111.76
2	B	1499	NAG	O5-C5-C4	-3.39	106.35	110.65
2	A	1499	NAG	O5-C5-C4	-2.69	107.23	110.65
2	B	1498	NAG	O5-C5-C4	-2.63	107.32	110.65
2	A	1500	BMA	O5-C5-C6	2.61	109.72	106.98
2	A	1499	NAG	C3-C4-C5	-2.59	105.57	110.20
2	B	1501	FUC	O5-C5-C6	2.54	112.12	108.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	FUC	O5-C5-C6	2.54	112.11	108.03
2	A	1500	BMA	O5-C5-C4	2.46	113.77	110.65
2	A	1498	NAG	O7-C7-C8	-2.33	117.49	122.04
2	A	1499	NAG	O4-C4-C5	2.33	115.43	109.28
2	A	1501	FUC	C4-C3-C2	2.25	113.53	110.50
2	A	1500	BMA	O2-C2-C3	2.18	114.88	110.18
2	A	1499	NAG	C2-N2-C7	-2.17	119.45	123.09
2	B	1500	BMA	C3-C4-C5	2.11	113.97	110.20
2	B	1501	FUC	O2-C2-C3	2.09	114.69	110.18
2	B	1501	FUC	C6-C5-C4	2.08	116.44	113.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1502	-	4,4,4	0.68	0	6,6,6	0.37	0
5	AMF	A	1510	-	23,23,23	1.49	4 (17%)	30,31,31	2.89	15 (50%)
3	PO4	B	1502	-	4,4,4	0.50	0	6,6,6	0.37	0
5	AMF	B	1510	-	18,18,23	2.03	5 (27%)	25,26,31	3.64	14 (56%)

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	PO4	A	1502	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AMF	A	1510	-	-	1/8/42/42	0/0/2/2
3	PO4	B	1502	-	-	0/0/0/0	0/0/0/0
5	AMF	B	1510	-	-	1/3/37/42	0/0/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1510	AMF	C7-N2	4.07	1.35	1.26
5	B	1510	AMF	C7-N1	4.04	1.45	1.36
5	A	1510	AMF	C2-C1	3.95	1.57	1.53
5	B	1510	AMF	C10-C9	3.83	1.56	1.55
5	B	1510	AMF	C2-C1	3.11	1.56	1.53
5	A	1510	AMF	C7-N1	2.95	1.42	1.36
5	A	1510	AMF	C5-N1	2.47	1.50	1.47
5	B	1510	AMF	C7-S1	-2.39	1.71	1.75
5	A	1510	AMF	C6-C5	2.08	1.56	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1510	AMF	C6-C5-C4	-8.03	105.11	115.99
5	B	1510	AMF	O1-C1-N1	-7.78	95.72	111.23
5	B	1510	AMF	C6-C5-C4	-7.05	106.44	115.99
5	B	1510	AMF	C6-S1-C7	6.83	100.14	91.39
5	B	1510	AMF	N1-C7-N2	6.78	129.90	122.46
5	A	1510	AMF	C6-C5-N1	5.05	112.54	106.25
5	B	1510	AMF	C6-C5-N1	5.03	112.51	106.25
5	B	1510	AMF	C9-C8-N2	4.96	119.50	109.24
5	A	1510	AMF	C6-S1-C7	4.72	97.43	91.39
5	A	1510	AMF	O1-C1-N1	-4.54	102.18	111.23
5	A	1510	AMF	C9-C8-N2	4.37	116.91	110.75
5	A	1510	AMF	C3-C2-C1	3.86	116.03	109.11
5	B	1510	AMF	C2-C1-N1	3.78	117.81	109.30
5	A	1510	AMF	N1-C7-N2	3.69	126.51	122.46
5	B	1510	AMF	C3-C2-C1	3.55	115.47	109.11
5	A	1510	AMF	C2-C1-N1	3.53	117.24	109.30
5	A	1510	AMF	C5-C6-S1	-3.10	101.96	105.69
5	A	1510	AMF	C8-N2-C7	-2.96	112.97	117.89
5	B	1510	AMF	S1-C7-N2	-2.83	122.59	126.67
5	B	1510	AMF	C3-C4-C5	-2.78	107.20	111.62
5	B	1510	AMF	C1-N1-C5	-2.76	116.26	120.80
5	A	1510	AMF	S1-C7-N2	-2.70	122.77	126.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1510	AMF	O2-C2-C3	-2.67	104.37	110.35
5	B	1510	AMF	C5-C6-S1	-2.64	102.51	105.69
5	A	1510	AMF	C3-C4-C5	-2.54	107.58	111.62
5	A	1510	AMF	C4-C5-N1	-2.46	107.04	109.64
5	B	1510	AMF	S1-C7-N1	-2.19	107.46	111.10
5	A	1510	AMF	O3-C3-C2	-2.15	105.54	110.35
5	A	1510	AMF	C1-N1-C5	-2.03	117.46	120.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1510	AMF	S1-C7-N2-C8
5	A	1510	AMF	S1-C7-N2-C8

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	496/505 (98%)	-0.56	3 (0%) 86 93	7, 18, 34, 55	0
1	B	498/505 (98%)	-0.49	1 (0%) 93 97	10, 21, 36, 49	0
All	All	994/1010 (98%)	-0.53	4 (0%) 90 95	7, 19, 35, 55	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	PRO	3.5
1	B	0	PHE	3.0
1	A	476	ALA	2.8
1	A	169	GLN	2.5

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	NAG	A	1498	14/15	0.11	0.40	30,33,39,46	0
2	NAG	B	1498	14/15	0.09	-0.86	26,33,37,39	0
2	FUC	B	1501	10/11	0.26	-	45,47,49,51	0
2	FUC	A	1501	10/11	0.26	-	60,63,64,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1499	14/15	0.21	-	49,52,59,60	0
2	NAG	B	1499	14/15	0.15	-	46,50,53,58	0
2	BMA	B	1500	11/12	0.29	-	68,70,70,71	0
2	BMA	A	1500	11/12	0.26	-	66,70,72,72	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
5	AMF	A	1510	22/22	0.13	1.89	10,22,47,48	0
5	AMF	B	1510	17/22	0.10	0.54	16,24,33,35	0
3	PO4	B	1502	5/5	0.08	-0.58	25,28,29,31	0
3	PO4	A	1502	5/5	0.08	-1.12	26,27,28,29	0
4	K	A	1503	1/1	0.04	-1.86	29,29,29,29	0
4	K	B	1503	1/1	0.04	-2.26	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.