



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 AM GMT

PDB ID : 2XWD
Title : X-RAY STRUCTURE OF ACID-BETA-GLUCOSIDASE WITH 5N,6O-(N'-(N-OCTYL)IMINO)NOJIRIMYCIN IN THE ACTIVE SITE
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Deposited on : 2010-11-01
Resolution : 2.66 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

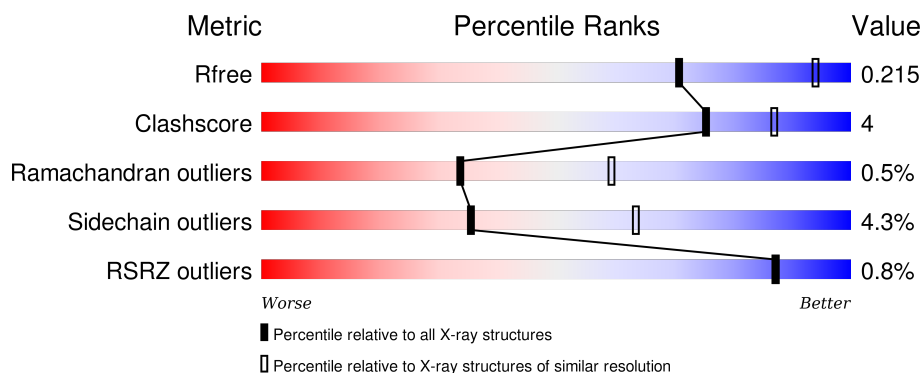
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.66 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	505	 87% 10% ..
1	B	505	 84% 12% ..

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
3	SO4	A	1503	-	-	-	X
3	SO4	B	1502	-	-	X	-
3	SO4	B	1505	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8183 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 GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3861	2492	654	699	16			
1	B	492	Total	C	N	O	S	0	0	0
			3860	2486	659	699	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).

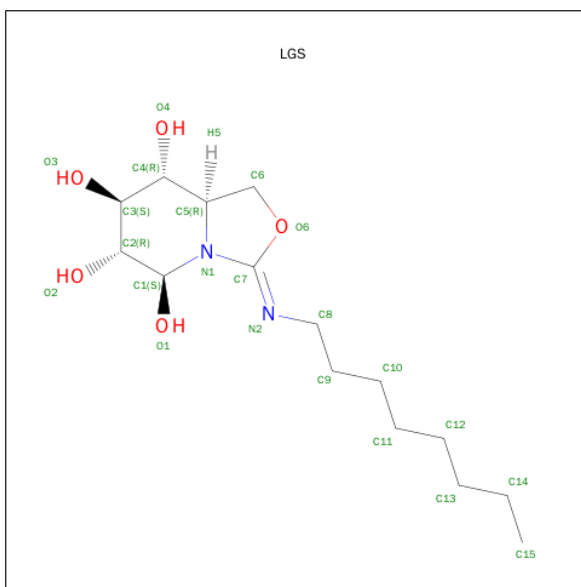
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is (3Z,5S,6R,7S,8R,8AR)-3-(OCTYLIMINO)HEXAHYDRO[1,3]OXAZOLO[3,4-A]PYRIDINE-5,6,7,8-TETROL (three-letter code: LGS) (formula: C₁₅H₂₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	9	2	5		
4	B	1	Total	C	N	O	0	1
			32	18	4	10		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

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

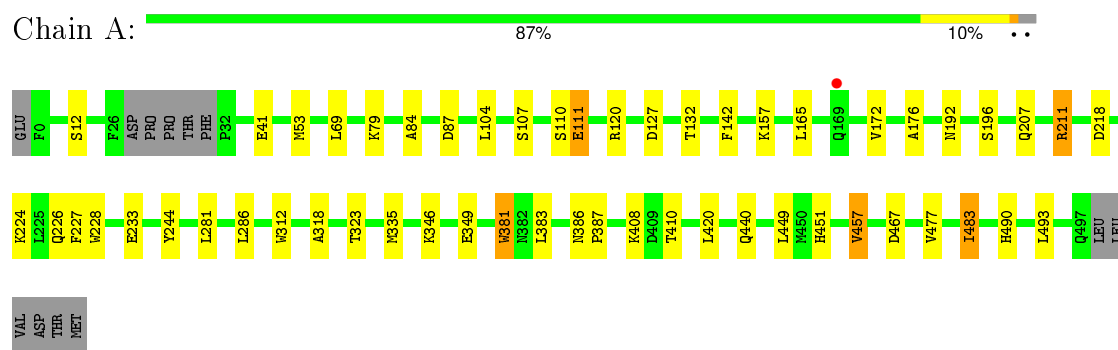
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	137	Total	O	0	0
			137	137		
6	B	129	Total	O	0	0
			129	129		

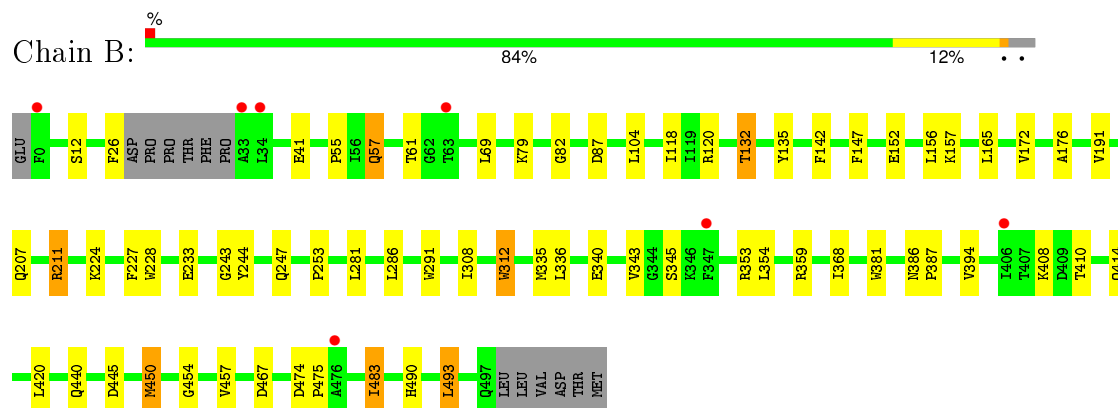
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



• Molecule 1: GLUCOSYLCERAMIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.04Å 96.62Å 83.16Å 90.00° 103.69° 90.00°	Depositor
Resolution (Å)	29.92 – 2.66 29.92 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.92-2.66) 98.8 (29.92-2.66)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.150 , 0.219 0.151 , 0.215	Depositor DCC
R_{free} test set	1526 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29888 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8183	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SO4, FUC, LGS, 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	0.80	1/3978 (0.0%)	0.73	1/5426 (0.0%)
1	B	0.77	0/3976	0.75	0/5423
All	All	0.79	1/7954 (0.0%)	0.74	1/10849 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	GLU	CB-CG	7.17	1.65	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	CB-CG-OD1	7.21	124.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3861	0	3737	23	0
1	B	3860	0	3744	32	0
2	A	49	0	43	0	0
3	A	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	3	0
4	A	16	0	13	1	0
4	B	32	0	26	5	0
5	B	49	0	43	0	0
6	A	137	0	0	3	0
6	B	129	0	0	1	0
All	All	8183	0	7606	60	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 4.

All (60) 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)
4:B:1510[A]:LGS:H82C	4:B:1510[A]:LGS:O1	1.59	1.01
4:B:1510[A]:LGS:H82C	4:B:1510[A]:LGS:C1	1.98	0.93
1:B:340:GLU:OE2	4:B:1510[B]:LGS:H154	1.89	0.71
1:B:12:SER:OG	3:B:1502:SO4:O3	2.09	0.70
1:B:467:ASP:HB3	1:B:483:ILE:HD11	1.74	0.70
1:B:353:ARG:NH1	3:B:1502:SO4:O1	2.26	0.68
4:A:1510:LGS:O1	4:A:1510:LGS:H82C	1.92	0.68
4:B:1510[A]:LGS:C1	4:B:1510[A]:LGS:C8	2.75	0.64
1:A:467:ASP:HB3	1:A:483:ILE:HD11	1.80	0.64
1:A:79:LYS:HE2	1:A:228:TRP:CE2	2.36	0.60
1:A:451:HIS:HB3	6:A:2129:HOH:O	2.04	0.56
4:B:1510[A]:LGS:H82C	4:B:1510[A]:LGS:H155	1.65	0.56
1:A:286:LEU:C	1:A:286:LEU:HD12	2.27	0.55
1:A:318:ALA:HB1	1:A:323:THR:HG21	1.89	0.54
1:B:79:LYS:HE2	1:B:228:TRP:CE2	2.42	0.54
1:B:353:ARG:NH1	3:B:1502:SO4:S	2.80	0.54
1:A:142:PHE:O	1:A:211:ARG:NH2	2.41	0.53
1:B:152:GLU:O	1:B:156:LEU:HB2	2.09	0.53
1:A:408:LYS:O	1:A:410:THR:HG23	2.10	0.52
1:B:457:VAL:HG13	1:B:493:LEU:HD23	1.92	0.51
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.45	0.51
1:A:165:LEU:CD2	1:A:172:VAL:HB	2.41	0.50
1:A:386:ASN:HB2	1:A:387:PRO:CD	2.41	0.50
1:B:243:GLY:O	1:B:244:TYR:C	2.50	0.50
1:B:408:LYS:O	1:B:410:THR:HG23	2.14	0.48
1:B:343:VAL:HG21	1:B:359:ARG:HG2	1.94	0.48
1:B:165:LEU:CD2	1:B:172:VAL:HB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	1:A:107:SER:HB2	2.13	0.48
1:A:346:LYS:HB2	1:A:349:GLU:OE1	2.13	0.47
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.50	0.47
1:B:104:LEU:HD23	1:B:104:LEU:C	2.36	0.46
1:A:84:ALA:O	1:A:383:LEU:HG	2.16	0.46
1:A:41:GLU:HG3	1:A:490:HIS:CD2	2.50	0.46
1:B:354:LEU:HA	1:B:414:GLN:OE1	2.16	0.46
1:B:120:ARG:HD3	6:B:2084:HOH:O	2.17	0.45
1:B:191:VAL:O	1:B:247:GLN:HA	2.16	0.45
1:A:457:VAL:HB	1:A:493:LEU:HD23	1.99	0.45
1:A:192:ASN:HB2	1:A:244:TYR:O	2.17	0.45
1:B:142:PHE:O	1:B:211:ARG:NH2	2.49	0.45
1:B:308:ILE:HB	1:B:336:LEU:HD23	1.99	0.45
1:B:286:LEU:HD12	1:B:286:LEU:C	2.36	0.45
1:B:132:THR:HG22	1:B:132:THR:O	2.16	0.45
1:A:41:GLU:HG3	1:A:490:HIS:NE2	2.31	0.45
1:B:82:GLY:HA3	1:B:118:ILE:O	2.18	0.44
1:A:449:LEU:N	1:A:449:LEU:HD12	2.33	0.43
1:B:368:ILE:HG21	1:B:445:ASP:HB3	2.00	0.43
1:A:196:SER:HB2	6:A:2067:HOH:O	2.18	0.43
1:B:253:PRO:HB3	1:B:291:TRP:CD2	2.54	0.43
1:A:120:ARG:HD3	6:A:2098:HOH:O	2.18	0.42
1:B:135:TYR:O	1:B:147:PHE:HA	2.18	0.42
1:A:87:ASP:OD1	1:A:157:LYS:HD2	2.19	0.42
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.49	0.42
1:B:55:PRO:HG2	1:B:57:GLN:OE1	2.19	0.42
1:B:474:ASP:HA	1:B:475:PRO:HD2	1.83	0.41
1:B:312:TRP:CD1	1:B:312:TRP:C	2.94	0.41
1:A:12:SER:OG	3:A:1505:SO4:O1	2.31	0.41
1:B:450:MET:HE3	1:B:454:GLY:HA2	2.03	0.41
1:B:41:GLU:HG3	1:B:490:HIS:CD2	2.56	0.40
1:B:87:ASP:OD1	1:B:157:LYS:HD2	2.22	0.40
1:A:127:ASP:N	1:A:127:ASP:OD1	2.55	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	489/505 (97%)	465 (95%)	21 (4%)	3 (1%)	30	54
1	B	488/505 (97%)	460 (94%)	26 (5%)	2 (0%)	39	65
All	All	977/1010 (97%)	925 (95%)	47 (5%)	5 (0%)	34	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	B	233	GLU
1	A	281	LEU
1	A	381	TRP
1	B	281	LEU

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	408/432 (94%)	391 (96%)	17 (4%)	36	64
1	B	411/432 (95%)	393 (96%)	18 (4%)	35	62
All	All	819/864 (95%)	784 (96%)	35 (4%)	35	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	MET

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	110	SER
1	A	111	GLU
1	A	132	THR
1	A	207	GLN
1	A	211	ARG
1	A	224	LYS
1	A	226	GLN
1	A	312	TRP
1	A	335	MET
1	A	381	TRP
1	A	420	LEU
1	A	440	GLN
1	A	457	VAL
1	A	477	VAL
1	A	483	ILE
1	B	26	PHE
1	B	57	GLN
1	B	61	THR
1	B	69	LEU
1	B	132	THR
1	B	207	GLN
1	B	211	ARG
1	B	224	LYS
1	B	312	TRP
1	B	335	MET
1	B	345	SER
1	B	381	TRP
1	B	394	VAL
1	B	420	LEU
1	B	440	GLN
1	B	450	MET
1	B	483	ILE
1	B	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	166	GLN
1	A	226	GLN
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	166	GLN
1	B	226	GLN
1	B	270	ASN
1	B	440	GLN

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 ⓘ

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	14,14,15	0.75	0	15,19,21	2.24	4 (26%)
2	NAG	A	1499	2	14,14,15	0.52	0	15,19,21	1.35	2 (13%)
2	MAN	A	1500	2	11,11,12	0.89	0	14,15,17	1.57	4 (28%)
2	FUC	A	1501	2	10,10,11	1.20	1 (10%)	14,14,16	2.35	8 (57%)
5	NAG	B	1498	1,5	14,14,15	0.56	0	15,19,21	1.45	2 (13%)
5	NAG	B	1499	5	14,14,15	0.56	0	15,19,21	1.48	3 (20%)
5	BMA	B	1500	5	11,11,12	0.97	0	14,15,17	2.39	5 (35%)
5	FUC	B	1501	5	10,10,11	0.80	0	14,14,16	1.71	2 (14%)

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	MAN	A	1500	2	-	0/2/19/22	0/1/1/1
2	FUC	A	1501	2	-	0/0/17/20	0/1/1/1
5	NAG	B	1498	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1499	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1500	5	-	0/2/19/22	0/1/1/1
5	FUC	B	1501	5	-	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	A	1501	FUC	C4-C5	2.17	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1498	NAG	C2-N2-C7	-6.00	115.33	123.04
2	A	1501	FUC	O5-C1-C2	-4.41	103.70	110.86
2	A	1499	NAG	C2-N2-C7	-3.35	118.74	123.04
2	A	1498	NAG	C4-C3-C2	-3.21	106.24	111.23
5	B	1499	NAG	C2-N2-C7	-3.14	119.00	123.04
5	B	1501	FUC	O5-C1-C2	-3.03	105.95	110.86
2	A	1501	FUC	C2-C3-C4	-2.88	106.16	111.04
2	A	1498	NAG	C1-O5-C5	-2.83	108.65	112.25
5	B	1498	NAG	C2-N2-C7	-2.76	119.49	123.04
2	A	1500	MAN	C3-C4-C5	-2.34	106.12	110.20
5	B	1500	BMA	C2-C3-C4	-2.15	107.39	111.04
2	A	1501	FUC	C1-C2-C3	-2.08	107.08	109.54
5	B	1500	BMA	O2-C2-C3	2.01	114.15	110.12
2	A	1499	NAG	O4-C4-C5	2.05	114.67	109.24
2	A	1501	FUC	O4-C4-C5	2.10	114.78	109.84
2	A	1500	MAN	C1-O5-C5	2.25	115.10	112.25
5	B	1499	NAG	C1-O5-C5	2.27	115.13	112.25
2	A	1500	MAN	O5-C5-C6	2.30	112.32	107.35
2	A	1500	MAN	O5-C1-C2	2.35	114.67	110.86
5	B	1499	NAG	O4-C4-C5	2.37	115.52	109.24
2	A	1501	FUC	O2-C2-C3	2.49	115.12	110.12
2	A	1498	NAG	O3-C3-C4	2.73	116.48	110.34
2	A	1501	FUC	C3-C4-C5	2.75	114.36	109.72
2	A	1501	FUC	O2-C2-C1	3.12	115.46	109.21
5	B	1498	NAG	C1-O5-C5	3.14	116.24	112.25
2	A	1501	FUC	O5-C5-C6	3.34	111.66	106.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1500	BMA	O3-C3-C2	3.46	116.25	110.00
5	B	1500	BMA	O5-C1-C2	3.92	117.21	110.86
5	B	1501	FUC	O5-C5-C6	4.70	113.90	106.13
5	B	1500	BMA	C1-O5-C5	5.59	119.34	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

13 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
3	SO4	A	1502	-	4,4,4	0.24	0	6,6,6	0.45	0
3	SO4	A	1503	-	4,4,4	0.28	0	6,6,6	0.60	0
3	SO4	A	1504	-	4,4,4	0.22	0	6,6,6	0.31	0
3	SO4	A	1505	-	4,4,4	0.36	0	6,6,6	0.58	0
3	SO4	A	1506	-	4,4,4	0.22	0	6,6,6	0.55	0
4	LGS	A	1510	-	14,17,23	1.71	2 (14%)	16,25,31	2.81	4 (25%)
3	SO4	B	1502	-	4,4,4	0.27	0	6,6,6	0.94	1 (16%)
3	SO4	B	1503	-	4,4,4	0.42	0	6,6,6	0.41	0
3	SO4	B	1504	-	4,4,4	0.11	0	6,6,6	0.27	0
3	SO4	B	1505	-	4,4,4	0.20	0	6,6,6	0.31	0
3	SO4	B	1506	-	4,4,4	0.13	0	6,6,6	0.39	0
4	LGS	B	1510[A]	-	14,17,23	1.75	3 (21%)	16,25,31	2.03	5 (31%)
4	LGS	B	1510[B]	-	14,17,23	1.20	1 (7%)	16,25,31	1.75	4 (25%)

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	SO4	A	1502	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1503	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1504	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1505	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1506	-	-	0/0/0/0	0/0/0/0
4	LGS	A	1510	-	-	0/1/36/42	0/2/2/2
3	SO4	B	1502	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1503	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1504	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1505	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1506	-	-	0/0/0/0	0/0/0/0
4	LGS	B	1510[A]	-	-	0/1/36/42	0/2/2/2
4	LGS	B	1510[B]	-	-	0/1/36/42	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1510[B]	LGS	C2-C1	2.64	1.55	1.52
4	A	1510	LGS	O6-C7	2.84	1.39	1.35
4	B	1510[A]	LGS	O6-C7	2.99	1.40	1.35
4	B	1510[A]	LGS	O1-C1	3.45	1.45	1.41
4	B	1510[A]	LGS	C2-C1	4.18	1.57	1.52
4	A	1510	LGS	C2-C1	5.06	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1510[A]	LGS	O6-C6-C5	-4.04	102.03	105.50
4	B	1510[A]	LGS	C3-C4-C5	-3.71	106.38	111.39
4	A	1510	LGS	O2-C2-C3	-2.23	105.32	110.34
3	B	1502	SO4	O2-S-O1	-2.15	102.68	109.50
4	B	1510[A]	LGS	C5-N1-C7	-2.15	105.57	110.57
4	B	1510[B]	LGS	C3-C2-C1	2.35	112.86	109.13
4	B	1510[B]	LGS	C8-N2-C7	2.66	122.52	118.15
4	B	1510[B]	LGS	O6-C6-C5	2.79	107.89	105.50
4	B	1510[A]	LGS	C6-C5-N1	3.08	102.56	100.00
4	B	1510[A]	LGS	C3-C2-C1	3.38	114.50	109.13
4	A	1510	LGS	C3-C2-C1	3.91	115.33	109.13
4	B	1510[B]	LGS	C6-C5-N1	4.11	103.42	100.00
4	A	1510	LGS	C6-C5-N1	4.98	104.14	100.00
4	A	1510	LGS	C8-N2-C7	8.12	131.50	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1505	SO4	1	0
4	A	1510	LGS	1	0
3	B	1502	SO4	3	0
4	B	1510[A]	LGS	4	0
4	B	1510[B]	LGS	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	493/505 (97%)	-0.71	1 (0%) 95 96	3, 12, 26, 46	0
1	B	492/505 (97%)	-0.68	7 (1%) 78 76	4, 13, 27, 43	0
All	All	985/1010 (97%)	-0.70	8 (0%) 87 87	3, 13, 26, 46	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	PHE	2.9
1	B	33	ALA	2.9
1	B	63	THR	2.5
1	B	347	PHE	2.4
1	A	169	GLN	2.1
1	B	34	LEU	2.1
1	B	476	ALA	2.0
1	B	406	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	NAG	B	1499	14/15	0.91	0.25	-	41,44,48,52	0
5	FUC	B	1501	10/11	0.94	0.27	-	32,34,36,36	0
2	MAN	A	1500	11/12	0.69	0.33	-	72,75,76,76	0
5	NAG	B	1498	14/15	0.95	0.19	-	19,29,33,33	0
5	BMA	B	1500	11/12	0.77	0.39	-	56,62,64,64	0
2	NAG	A	1498	14/15	0.95	0.16	-	27,36,41,46	0
2	FUC	A	1501	10/11	0.81	0.33	-	57,59,60,60	0
2	NAG	A	1499	14/15	0.87	0.24	-	50,55,59,62	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
3	SO4	B	1505	5/5	0.95	0.29	4.89	45,45,46,47	0
3	SO4	A	1503	5/5	0.95	0.25	4.14	37,38,39,40	0
4	LGS	B	1510[A]	16/22	0.95	0.15	0.86	2,6,8,9	16
4	LGS	B	1510[B]	16/22	0.95	0.15	0.52	4,8,9,10	16
4	LGS	A	1510	16/22	0.97	0.12	0.23	5,13,24,24	0
3	SO4	A	1505	5/5	0.99	0.10	-0.34	10,12,16,17	0
3	SO4	B	1502	5/5	0.99	0.07	-2.01	15,17,18,19	0
3	SO4	A	1504	5/5	0.98	0.11	-	36,37,38,39	0
3	SO4	B	1506	5/5	0.89	0.35	-	52,53,54,54	0
3	SO4	A	1502	5/5	0.92	0.26	-	52,53,54,55	0
3	SO4	B	1503	5/5	0.98	0.12	-	32,32,34,34	0
3	SO4	B	1504	5/5	0.91	0.25	-	47,49,49,50	0
3	SO4	A	1506	5/5	0.94	0.25	-	43,46,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.