



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VT0
Title : X-ray structure of a conjugate with conduritol-beta-epoxide of acid-beta-glucosidase overexpressed in cultured plant cells
Authors : Brumshtein, B.; Greenblatt, H.M.; Shaaltiel, Y.; Aviezer, D.; Silman, I.; Futerman, A.H.; Sussman, J.L.
Deposited on : 2008-05-03
Resolution : 2.15 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

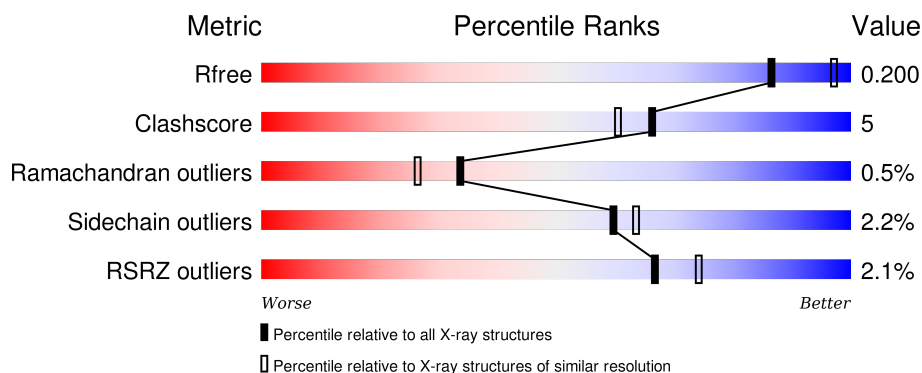
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	 2% 85% 12% ..
1	B	505	 2% 83% 13% ..

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	MAN	A	1502	X	-	-	-
4	SO4	A	1505	-	-	-	X
4	SO4	B	1502	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8346 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.

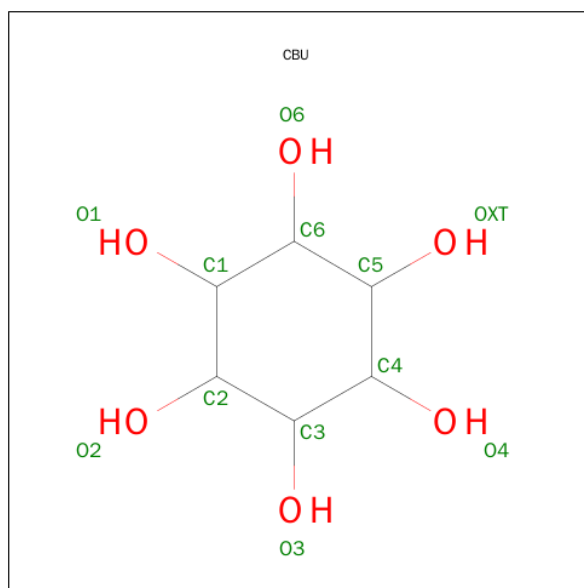
- Molecule 1 is a protein called GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	1
			3886	2504	665	701	16			
1	B	489	Total	C	N	O	S	0	0	0
			3837	2475	653	693	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	PRO	THR	CONFLICT	UNP Q9BDT0
A	495	HIS	ARG	CONFLICT	UNP Q9BDT0
B	55	PRO	THR	CONFLICT	UNP Q9BDT0
B	495	HIS	ARG	CONFLICT	UNP Q9BDT0

- Molecule 2 is (1R,2R,3S,4S,5S,6S)-CYCLOHEXANE-1,2,3,4,5,6-HEXOL (three-letter code: CBU) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	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
			49	28	2	19		

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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

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

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

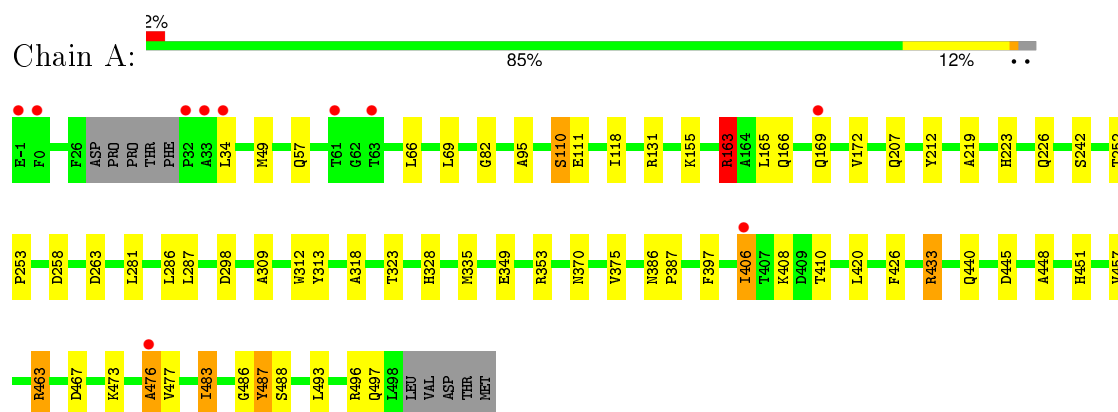
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	230	Total	O	0	0
			230	230		
6	B	234	Total	O	0	0
			234	234		

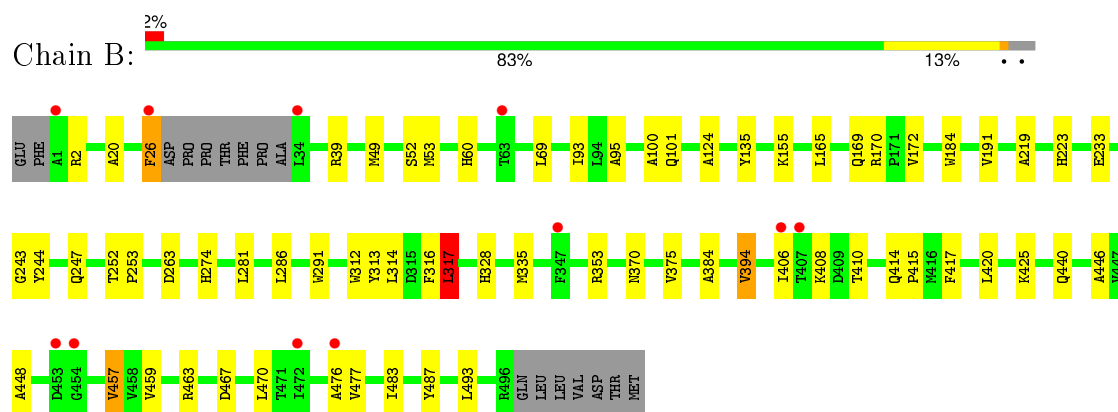
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: 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	68.18Å 96.88Å 83.17Å 90.00° 103.73° 90.00°	Depositor
Resolution (Å)	19.77 – 2.15 19.77 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.77-2.15) 98.2 (19.77-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.152 , 0.201 0.151 , 0.200	Depositor DCC
R_{free} test set	2838 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56078 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8346	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 5.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, SO4, CBU, NAG, FUC

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	1.16	8/4004 (0.2%)	1.02	11/5460 (0.2%)
1	B	1.18	9/3953 (0.2%)	0.98	10/5391 (0.2%)
All	All	1.17	17/7957 (0.2%)	1.00	21/10851 (0.2%)

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	2
3	A	1	0
All	All	1	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	TYR	C-O	7.18	1.36	1.23
1	B	184	TRP	CB-CG	6.50	1.61	1.50
1	A	212	TYR	CD1-CE1	6.40	1.49	1.39
1	B	394	VAL	CB-CG1	-6.28	1.39	1.52
1	B	384	ALA	CA-CB	6.17	1.65	1.52
1	A	353	ARG	CZ-NH2	-6.14	1.25	1.33
1	B	487	TYR	C-O	5.90	1.34	1.23
1	B	135	TYR	CE2-CZ	5.82	1.46	1.38
1	B	417	PHE	CE1-CZ	5.65	1.48	1.37
1	B	457	VAL	CB-CG2	-5.48	1.41	1.52
1	A	397	PHE	CD1-CE1	5.33	1.50	1.39
1	A	349	GLU	CB-CG	-5.32	1.42	1.52
1	B	291	TRP	CG-CD1	5.21	1.44	1.36
1	A	207	GLN	CG-CD	5.11	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	ALA	CA-CB	5.08	1.63	1.52
1	A	110	SER	CB-OG	-5.01	1.35	1.42
1	B	26	PHE	CE1-CZ	5.00	1.46	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ARG	NE-CZ-NH2	-17.88	111.36	120.30
1	A	433	ARG	NE-CZ-NH1	17.24	128.92	120.30
1	A	353	ARG	NE-CZ-NH2	8.78	124.69	120.30
1	B	457	VAL	CG1-CB-CG2	-7.63	98.69	110.90
1	B	317	LEU	CA-CB-CG	7.60	132.79	115.30
1	B	353	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	39	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	463	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	463	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	131	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	A	163	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	263	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	131	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	B	394	VAL	CA-CB-CG1	5.70	119.45	110.90
1	A	463	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	463	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	B	49	MET	CG-SD-CE	-5.35	91.65	100.20
1	A	49	MET	CG-SD-CE	-5.32	91.69	100.20
1	A	258	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	39	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	263	ASP	CB-CG-OD1	-5.21	113.61	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1502	MAN	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LEU	Peptide
1	A	476	ALA	Peptide

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	3886	0	3774	37	0
1	B	3837	0	3726	35	0
2	A	11	0	10	1	0
2	B	11	0	9	1	0
3	A	49	0	43	2	0
4	A	30	0	0	1	0
4	B	20	0	0	0	0
5	B	38	0	34	1	0
6	A	230	0	0	10	0
6	B	234	0	0	5	0
All	All	8346	0	7596	75	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 5.

All (75) 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:476:ALA:HB3	1:A:477:VAL:HG23	1.56	0.86
1:B:316:PHE:CZ	1:B:317:LEU:HD22	2.10	0.86
1:B:69:LEU:HD11	1:B:448:ALA:HB1	1.66	0.78
1:A:487:TYR:HA	6:A:2222:HOH:O	1.83	0.78
1:A:467:ASP:HB3	1:A:483:ILE:HD11	1.68	0.75
1:B:328:HIS:HD2	6:B:2157:HOH:O	1.72	0.72
1:B:169:GLN:HG3	1:B:170:ARG:HG3	1.70	0.71
1:A:286:LEU:C	1:A:286:LEU:HD12	2.11	0.71
3:A:1500:NAG:O4	3:A:1509:FUC:H5	1.91	0.70
1:B:95:ALA:HB1	1:B:406:ILE:HD12	1.74	0.70
1:A:328:HIS:HD2	6:A:2151:HOH:O	1.79	0.65
1:B:2:ARG:NE	6:B:2001:HOH:O	2.28	0.64
1:A:487:TYR:CA	6:A:2222:HOH:O	2.43	0.64
1:A:487:TYR:C	6:A:2222:HOH:O	2.36	0.63
1:B:440:GLN:NE2	6:B:2204:HOH:O	2.30	0.63
1:A:298:ASP:OD2	6:A:2128:HOH:O	2.16	0.61
1:A:487:TYR:HE1	4:A:1508:SO4:O1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLN:CG	1:B:170:ARG:HG3	2.34	0.58
1:B:457:VAL:HG22	1:B:493:LEU:CD2	2.34	0.58
1:A:386:ASN:HB2	1:A:387:PRO:CD	2.35	0.57
1:A:408:LYS:O	1:A:410:THR:HG23	2.05	0.56
1:A:69:LEU:HD11	1:A:448:ALA:HB1	1.88	0.55
1:B:457:VAL:HG22	1:B:493:LEU:HD23	1.90	0.54
1:B:408:LYS:O	1:B:410:THR:HG23	2.06	0.53
1:B:26:PHE:CG	1:B:425:LYS:HE2	2.44	0.53
1:B:69:LEU:HD11	1:B:448:ALA:CB	2.38	0.53
1:A:406:ILE:HG22	6:A:2191:HOH:O	2.10	0.52
1:A:313:TYR:CZ	2:A:1499:CBU:H4	2.45	0.52
1:A:488:SER:N	6:A:2222:HOH:O	2.42	0.51
1:B:219:ALA:O	1:B:223:HIS:HD2	1.93	0.51
1:A:111:GLU:HG2	1:A:169:GLN:CB	2.41	0.50
1:A:445:ASP:OD2	1:A:463:ARG:HD3	2.12	0.50
1:B:313:TYR:CZ	2:B:1497:CBU:H4	2.47	0.50
1:B:286:LEU:HD12	1:B:286:LEU:C	2.32	0.50
1:B:20:ALA:HA	1:B:100:ALA:HB2	1.95	0.49
1:B:476:ALA:HB3	1:B:477:VAL:HG23	1.94	0.49
1:A:476:ALA:CB	1:A:477:VAL:HG23	2.37	0.48
1:A:169:GLN:N	6:A:2075:HOH:O	2.42	0.48
1:B:316:PHE:CE2	1:B:317:LEU:HD22	2.48	0.48
1:A:426:PHE:O	1:A:451:HIS:NE2	2.47	0.47
1:B:467:ASP:HB3	1:B:483:ILE:HD11	1.97	0.47
1:A:163:ARG:HH21	1:A:166:GLN:HE21	1.62	0.46
1:A:477:VAL:HG21	1:A:496:ARG:HB3	1.97	0.45
1:A:440:GLN:NE2	6:A:2206:HOH:O	2.45	0.45
1:A:486:GLY:O	1:A:487:TYR:C	2.55	0.45
3:A:1501:NAG:C1	3:A:1509:FUC:H5	2.47	0.45
1:A:286:LEU:HD12	1:A:287:LEU:N	2.31	0.44
1:B:60:HIS:HE1	6:B:2218:HOH:O	2.00	0.44
1:A:95:ALA:HB1	1:A:406:ILE:HD12	2.00	0.44
1:A:165:LEU:CD2	1:A:172:VAL:HB	2.48	0.44
1:B:93:ILE:O	1:B:101:GLN:HG2	2.17	0.44
1:A:82:GLY:HA3	1:A:118:ILE:O	2.17	0.44
1:A:457:VAL:HG23	1:A:493:LEU:HD23	2.00	0.43
1:B:165:LEU:CD2	1:B:172:VAL:HB	2.48	0.43
1:B:446:ALA:HA	1:B:459:VAL:O	2.19	0.43
1:A:252:THR:HB	1:A:253:PRO:HD2	2.01	0.43
1:A:219:ALA:O	1:A:223:HIS:HD2	2.01	0.42
1:B:286:LEU:HD21	1:B:314:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLN:HG3	6:A:2220:HOH:O	2.19	0.42
1:B:286:LEU:HD21	1:B:314:LEU:HD12	2.02	0.42
1:A:370:ASN:HB3	1:A:375:VAL:HB	2.01	0.42
1:B:470:LEU:N	1:B:470:LEU:HD23	2.35	0.42
1:B:191:VAL:O	1:B:247:GLN:HA	2.20	0.41
5:B:1499:NAG:O4	6:B:2229:HOH:O	2.21	0.41
1:B:69:LEU:CD1	1:B:448:ALA:CB	2.98	0.41
1:A:69:LEU:HD11	1:A:448:ALA:CB	2.51	0.41
1:B:52:SER:O	1:B:53:MET:HG3	2.20	0.41
1:A:286:LEU:CD1	1:A:286:LEU:C	2.84	0.41
1:B:370:ASN:HB3	1:B:375:VAL:HB	2.02	0.41
1:B:243:GLY:O	1:B:244:TYR:C	2.58	0.41
1:B:414:GLN:O	1:B:415:PRO:C	2.58	0.41
1:A:66:LEU:HD11	1:A:473:LYS:HB2	2.03	0.41
1:A:318:ALA:HB1	1:A:323:THR:HG21	2.02	0.41
1:B:286:LEU:HD23	1:B:314:LEU:HB2	2.04	0.40
1:B:252:THR:HB	1:B:253:PRO:HD2	2.04	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	491/505 (97%)	468 (95%)	21 (4%)	2 (0%)	39	34
1	B	485/505 (96%)	464 (96%)	18 (4%)	3 (1%)	30	21
All	All	976/1010 (97%)	932 (96%)	39 (4%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLN

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Mol	Chain	Res	Type
1	B	233	GLU
1	A	281	LEU
1	B	281	LEU
1	B	124	ALA

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	414/432 (96%)	403 (97%)	11 (3%)	52	53
1	B	408/432 (94%)	401 (98%)	7 (2%)	68	74
All	All	822/864 (95%)	804 (98%)	18 (2%)	60	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	SER
1	A	155	LYS
1	A	163	ARG
1	A	226	GLN
1	A	242	SER
1	A	312	TRP
1	A	335	MET
1	A	406	ILE
1	A	420	LEU
1	A	433	ARG
1	A	483	ILE
1	B	155	LYS
1	B	274	HIS
1	B	312	TRP
1	B	317	LEU
1	B	335	MET
1	B	394	VAL
1	B	420	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	223	HIS
1	A	226	GLN
1	A	274	HIS
1	A	275	ASN
1	A	328	HIS
1	A	350	GLN
1	A	440	GLN
1	B	166	GLN
1	B	223	HIS
1	B	274	HIS
1	B	328	HIS
1	B	350	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 ⓘ

7 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	1500	1,3	14,14,15	0.85	0	15,19,21	1.90	3 (20%)
3	NAG	A	1501	3	14,14,15	0.91	0	15,19,21	2.24	5 (33%)
3	MAN	A	1502	3	11,11,12	1.16	1 (9%)	14,15,17	1.75	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	A	1509	3	10,10,11	0.88	0	14,14,16	3.58	10 (71%)
5	NAG	B	1498	1,5	14,14,15	1.13	1 (7%)	15,19,21	1.67	2 (13%)
5	NAG	B	1499	5	14,14,15	0.84	0	15,19,21	1.61	4 (26%)
5	FUC	B	1504	5	10,10,11	0.73	0	14,14,16	1.78	3 (21%)

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	1500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1501	3	-	0/6/23/26	0/1/1/1
3	MAN	A	1502	3	1/1/4/5	0/2/19/22	0/1/1/1
3	FUC	A	1509	3	-	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	FUC	B	1504	5	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	MAN	C2-C3	3.03	1.56	1.52
5	B	1498	NAG	C1-C2	3.32	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1509	FUC	O5-C1-C2	-7.98	97.91	110.86
3	A	1509	FUC	C1-C2-C3	-6.98	101.28	109.54
3	A	1500	NAG	C2-N2-C7	-5.83	115.55	123.04
3	A	1501	NAG	C1-O5-C5	-5.43	105.36	112.25
5	B	1498	NAG	C2-N2-C7	-4.49	117.28	123.04
5	B	1504	FUC	O5-C1-C2	-3.59	105.03	110.86
3	A	1501	NAG	C3-C2-N2	-3.05	103.25	110.56
3	A	1501	NAG	C2-N2-C7	-3.01	119.17	123.04
5	B	1504	FUC	O4-C4-C3	-2.88	103.86	110.34
5	B	1499	NAG	O7-C7-C8	-2.63	117.23	122.06
3	A	1509	FUC	C2-C3-C4	-2.54	106.73	111.04
3	A	1500	NAG	O4-C4-C3	-2.26	105.25	110.34
5	B	1499	NAG	C2-N2-C7	-2.22	120.19	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1499	NAG	O6-C6-C5	-2.12	104.31	111.33
3	A	1509	FUC	C3-C4-C5	2.09	113.25	109.72
3	A	1509	FUC	O5-C5-C4	2.11	113.18	109.53
5	B	1499	NAG	O5-C5-C6	2.21	112.13	107.35
3	A	1509	FUC	O3-C3-C2	2.25	114.06	110.00
5	B	1504	FUC	O5-C5-C6	2.49	110.25	106.13
3	A	1502	MAN	O3-C3-C2	2.52	114.55	110.00
3	A	1500	NAG	O3-C3-C4	2.62	116.24	110.34
3	A	1509	FUC	O5-C5-C6	2.82	110.80	106.13
3	A	1501	NAG	C4-C3-C2	2.94	115.80	111.23
3	A	1509	FUC	O3-C3-C4	3.03	117.16	110.34
3	A	1501	NAG	O7-C7-C8	3.10	127.75	122.06
3	A	1502	MAN	O2-C2-C3	3.26	116.67	110.12
3	A	1509	FUC	O2-C2-C1	3.48	116.19	109.21
3	A	1502	MAN	C2-C3-C4	3.49	116.96	111.04
5	B	1498	NAG	O3-C3-C2	3.51	116.07	109.11
3	A	1509	FUC	O2-C2-C3	3.90	117.96	110.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1502	MAN	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1500	NAG	1	0
3	A	1501	NAG	1	0
3	A	1509	FUC	2	0
5	B	1499	NAG	1	0

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
2	CBU	A	1499	1	11,11,12	2.25	6 (54%)	15,16,18	1.36	2 (13%)
4	SO4	A	1503	-	4,4,4	0.78	0	6,6,6	0.47	0
4	SO4	A	1504	-	4,4,4	0.59	0	6,6,6	0.85	0
4	SO4	A	1505	-	4,4,4	0.50	0	6,6,6	0.39	0
4	SO4	A	1506	-	4,4,4	0.12	0	6,6,6	0.69	0
4	SO4	A	1507	-	4,4,4	0.29	0	6,6,6	0.47	0
4	SO4	A	1508	-	4,4,4	0.09	0	6,6,6	0.58	0
2	CBU	B	1497	1	11,11,12	2.38	5 (45%)	15,16,18	1.58	6 (40%)
4	SO4	B	1500	-	4,4,4	0.41	0	6,6,6	0.54	0
4	SO4	B	1501	-	4,4,4	0.50	0	6,6,6	0.40	0
4	SO4	B	1502	-	4,4,4	0.57	0	6,6,6	0.19	0
4	SO4	B	1503	-	4,4,4	0.16	0	6,6,6	0.47	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	CBU	A	1499	1	-	0/0/20/24	0/1/1/1
4	SO4	A	1503	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1505	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1506	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1507	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1508	-	-	0/0/0/0	0/0/0/0
2	CBU	B	1497	1	-	0/0/20/24	0/1/1/1
4	SO4	B	1500	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1502	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1503	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1497	CBU	C6-C1	-2.98	1.48	1.52
2	B	1497	CBU	O2-C2	-2.56	1.36	1.43
2	A	1499	CBU	C3-C2	-2.36	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1499	CBU	O6-C6	-2.34	1.38	1.43
2	A	1499	CBU	C4-C3	2.22	1.55	1.52
2	B	1497	CBU	C5-C4	2.34	1.56	1.52
2	A	1499	CBU	O3-C3	2.35	1.48	1.43
2	A	1499	CBU	O2-C2	2.47	1.48	1.43
2	B	1497	CBU	O6-C6	2.48	1.48	1.43
2	A	1499	CBU	C5-C6	4.64	1.60	1.52
2	B	1497	CBU	C5-C6	5.43	1.61	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1497	CBU	C6-C1-C2	-2.39	106.98	111.04
2	B	1497	CBU	O3-C3-C4	-2.29	105.86	110.00
2	A	1499	CBU	C6-C1-C2	-2.22	107.27	111.04
2	B	1497	CBU	O2-C2-C3	-2.11	105.58	110.34
2	B	1497	CBU	C5-C6-C1	-2.11	107.69	110.56
2	B	1497	CBU	O4-C4-C3	2.03	114.21	110.12
2	A	1499	CBU	O3-C3-C4	2.47	114.46	110.00
2	B	1497	CBU	O6-C6-C1	2.88	115.90	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1499	CBU	1	0
4	A	1508	SO4	1	0
2	B	1497	CBU	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 ⓘ

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	495/505 (98%)	-0.33	10 (2%) 68 75	11, 20, 34, 54	0
1	B	489/505 (96%)	-0.42	11 (2%) 65 73	12, 20, 33, 47	0
All	All	984/1010 (97%)	-0.37	21 (2%) 67 74	11, 20, 33, 54	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	LEU	5.2
1	A	0	PHE	4.3
1	A	476	ALA	4.2
1	A	-1	GLU	3.5
1	B	454	GLY	3.4
1	B	63	THR	3.2
1	A	33	ALA	3.0
1	B	406	ILE	3.0
1	A	32	PRO	2.8
1	A	34	LEU	2.7
1	B	347	PHE	2.6
1	B	1	ALA	2.6
1	B	472	ILE	2.5
1	A	406	ILE	2.5
1	A	61	THR	2.5
1	A	169	GLN	2.5
1	A	63	THR	2.5
1	B	26	PHE	2.4
1	B	476	ALA	2.4
1	B	407	THR	2.3
1	B	453	ASP	2.0

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	1498	14/15	0.94	0.16	-	28,34,38,39	0
5	FUC	B	1504	10/11	0.95	0.23	-	37,40,41,43	0
5	NAG	B	1499	14/15	0.95	0.22	-	42,46,50,55	0
3	FUC	A	1509	10/11	0.70	0.44	-	64,67,68,70	0
3	MAN	A	1502	11/12	0.57	0.36	-	72,77,81,82	0
3	NAG	A	1501	14/15	0.78	0.28	-	57,61,67,69	0
3	NAG	A	1500	14/15	0.92	0.15	-	36,44,53,56	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	1502	5/5	0.92	0.32	9.73	58,59,61,63	0
4	SO4	A	1505	5/5	0.95	0.26	8.01	52,57,59,60	0
2	CBU	B	1497	11/12	0.98	0.10	1.04	13,16,19,20	0
2	CBU	A	1499	11/12	0.99	0.09	0.43	10,12,15,16	0
4	SO4	A	1503	5/5	0.99	0.07	-1.18	26,27,29,30	0
4	SO4	B	1500	5/5	0.99	0.06	-1.85	22,27,28,31	0
4	SO4	A	1504	5/5	0.91	0.17	-	45,52,54,54	0
4	SO4	B	1501	5/5	0.99	0.16	-	40,41,42,43	0
4	SO4	A	1506	5/5	0.81	0.38	-	95,96,98,98	0
4	SO4	B	1503	5/5	0.85	0.28	-	78,80,82,82	0
4	SO4	A	1508	5/5	0.86	0.44	-	95,97,98,98	0
4	SO4	A	1507	5/5	0.92	0.27	-	86,86,88,88	0

6.5 Other polymers

There are no such residues in this entry.