



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:05 AM BST

PDB ID : 6TN1
Title : Unliganded Crystal Structure of Recombinant GBA
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2019-12-05
Resolution : 0.98 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

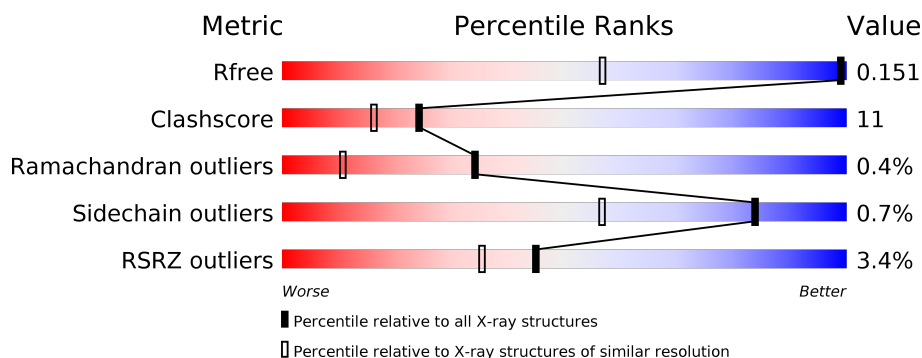
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.98 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}	130704	1166 (1.06-0.90)
Clashscore	141614	1241 (1.06-0.90)
Ramachandran outliers	138981	1159 (1.06-0.90)
Sidechain outliers	138945	1161 (1.06-0.90)
RSRZ outliers	127900	1132 (1.06-0.90)

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 respectively. 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	AAA	497	<div> <div>3%</div> <div>88%</div> <div>11%</div> </div>
2	A	3	<div> <div>67%</div> <div>33%</div> </div>

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
6	FMT	AAA	514	-	-	X	-
6	FMT	AAA	517	-	-	X	-
6	FMT	AAA	524	-	-	X	-

2 Entry composition [i](#)

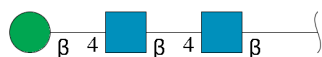
There are 8 unique types of molecules in this entry. The entry contains 9980 atoms, of which 4610 are hydrogens and 0 are deuteriums.

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 Lysosomal acid glucosylceramidase.

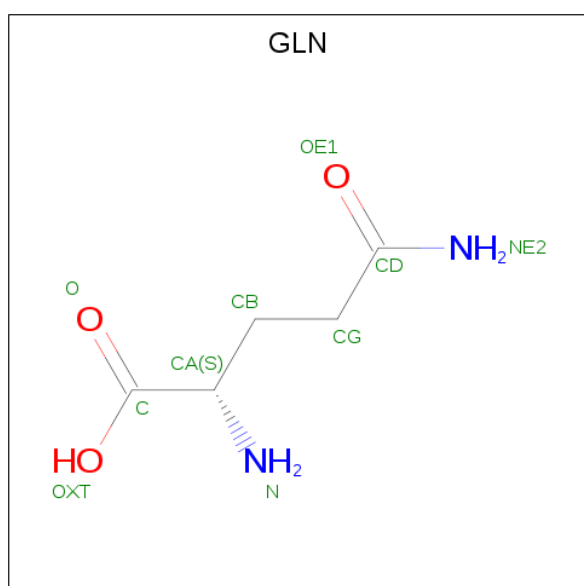
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	496	8910	2869	4433	773	813	22	230	68	0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O				
2	A	3	106	30	53	3	20		13	1	0

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



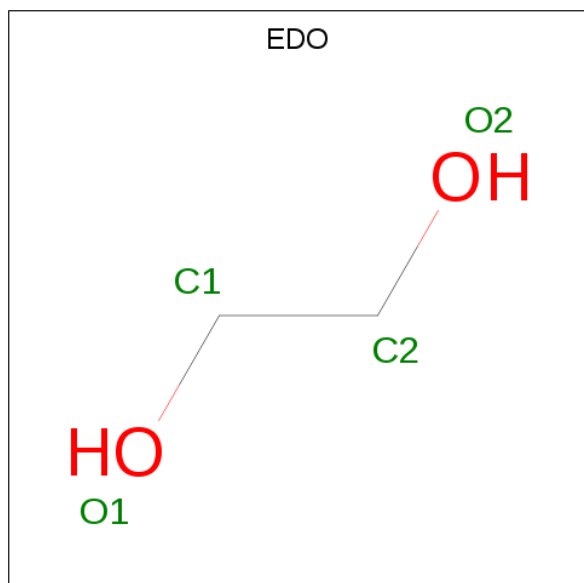
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	2	1
			19	5	10	2	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



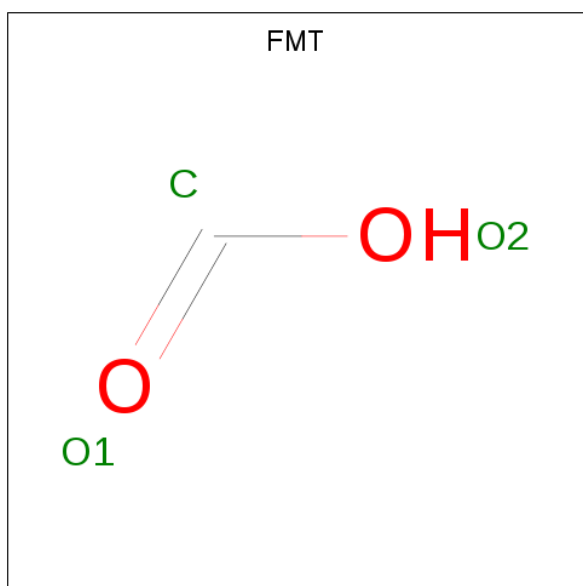
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	3	1
			30	6	18	6		
5	AAA	1	Total	C	H	O	2	1
			20	4	12	4		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	2	1
			10	2	4	4		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	2	1
			10	2	4	4		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	2	1
			10	2	4	4		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	8	Total	Mg	0	0
			8	8		

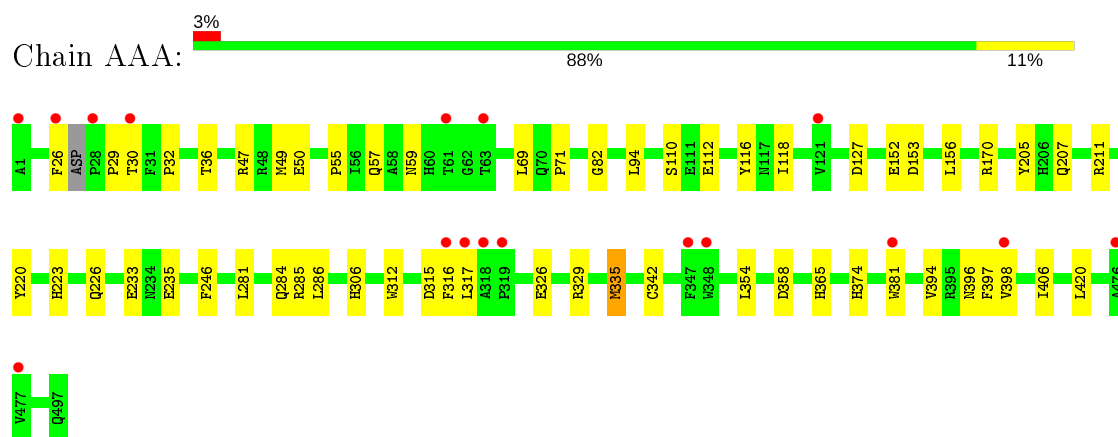
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	693	Total	O	0	16
			709	709		

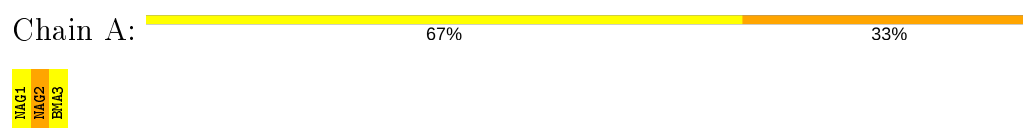
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysosomal acid glucosylceramidase



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.45Å 46.18Å 64.21Å 86.04° 75.19° 82.78°	Depositor
Resolution (Å)	31.68 – 0.98 31.68 – 0.98	Depositor EDS
% Data completeness (in resolution range)	74.2 (31.68-0.98) 74.2 (31.68-0.98)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 0.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.112 , 0.128 0.139 , 0.151	Depositor DCC
R_{free} test set	9829 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	8.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9980	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, FMT, NAG, EDO

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	AAA	0.55	0/4607	0.73	1/6260 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	116	TYR	CB-CG-CD1	5.95	124.57	121.00

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	AAA	4477	4433	4342	94	1
2	A	53	53	46	1	0
3	AAA	9	10	7	0	0
4	AAA	14	14	13	0	0
5	AAA	40	60	60	2	1
6	AAA	60	40	20	11	0
7	AAA	8	0	0	0	0
8	AAA	709	0	0	64	0
All	All	5370	4610	4488	102	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 11.

All (102) 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:AAA:285[B]:ARG:HD3	1:AAA:312:TRP:CH2	1.51	1.45
1:AAA:286[B]:LEU:CG	8:AAA:1177:HOH:O	1.66	1.28
1:AAA:335[B]:MET:SD	6:AAA:514:FMT:O2	1.94	1.25
1:AAA:285[B]:ARG:CD	1:AAA:312:TRP:CH2	2.28	1.17
1:AAA:112[B]:GLU:HG3	8:AAA:617:HOH:O	1.53	1.09
1:AAA:284:GLN:OE1	1:AAA:286[A]:LEU:CG	2.03	1.07
1:AAA:156[A]:LEU:HD23	8:AAA:854:HOH:O	0.85	1.02
1:AAA:211[C]:ARG:HG3	8:AAA:725:HOH:O	1.60	0.99
1:AAA:326[B]:GLU:OE2	1:AAA:329:ARG:NH2	1.94	0.98
1:AAA:284:GLN:NE2	1:AAA:286[A]:LEU:CG	2.26	0.98
1:AAA:397:PHE:HD1	8:AAA:631:HOH:O	1.47	0.98
1:AAA:284:GLN:HE22	1:AAA:286[A]:LEU:CG	1.76	0.97
1:AAA:156[A]:LEU:CD2	8:AAA:1066:HOH:O	2.11	0.96
1:AAA:396:ASN:N	8:AAA:607:HOH:O	1.99	0.95
1:AAA:36[B]:THR:HG23	8:AAA:816:HOH:O	1.66	0.94
6:AAA:524:FMT:O2	8:AAA:606[A]:HOH:O	1.86	0.93
1:AAA:398[C]:VAL:CG2	8:AAA:1019:HOH:O	2.18	0.92
1:AAA:246[A]:PHE:HD2	1:AAA:394:VAL:HG21	1.35	0.91
1:AAA:396:ASN:CA	8:AAA:607:HOH:O	2.16	0.91
1:AAA:284:GLN:CD	1:AAA:286[A]:LEU:CG	2.39	0.89
1:AAA:335[B]:MET:SD	8:AAA:613:HOH:O	2.32	0.87
5:AAA:525:EDO:H11	8:AAA:937:HOH:O	1.74	0.86
1:AAA:316:PHE:HB3	8:AAA:608:HOH:O	1.73	0.85
1:AAA:156[A]:LEU:HD21	8:AAA:1066:HOH:O	1.69	0.85
1:AAA:285[B]:ARG:CD	1:AAA:312:TRP:HH2	1.89	0.84
1:AAA:397:PHE:HA	8:AAA:631:HOH:O	1.78	0.84
1:AAA:285[B]:ARG:HD3	1:AAA:312:TRP:CZ3	2.12	0.83
1:AAA:397:PHE:CD1	8:AAA:631:HOH:O	2.25	0.82
1:AAA:246[A]:PHE:CD2	1:AAA:394:VAL:HG21	2.14	0.82
1:AAA:326[B]:GLU:CD	1:AAA:329:ARG:HH21	1.83	0.81
1:AAA:286[A]:LEU:HB3	8:AAA:1177:HOH:O	1.82	0.80
1:AAA:396:ASN:HB2	8:AAA:607:HOH:O	1.82	0.79
1:AAA:285[B]:ARG:CD	1:AAA:312:TRP:CZ3	2.66	0.79
1:AAA:29:PRO:HD3	8:AAA:682:HOH:O	1.85	0.76
1:AAA:26:PHE:HZ	1:AAA:49[A]:MET:SD	2.10	0.75
1:AAA:94:LEU:HD12	1:AAA:156[A]:LEU:HD12	1.70	0.74
1:AAA:26:PHE:CZ	1:AAA:49[A]:MET:SD	2.81	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:284:GLN:OE1	1:AAA:286[B]:LEU:HB2	1.88	0.73
1:AAA:316:PHE:O	8:AAA:608:HOH:O	2.06	0.71
1:AAA:397:PHE:N	8:AAA:612:HOH:O	2.21	0.71
1:AAA:211[A]:ARG:HD2	8:AAA:618:HOH:O	1.93	0.69
1:AAA:315:ASP:N	8:AAA:605:HOH:O	1.97	0.68
1:AAA:358[B]:ASP:OD1	8:AAA:609:HOH:O	2.13	0.66
6:AAA:517:FMT:C	8:AAA:774:HOH:O	2.43	0.66
1:AAA:36[B]:THR:CG2	8:AAA:816:HOH:O	2.34	0.66
1:AAA:316:PHE:C	8:AAA:608:HOH:O	2.34	0.65
1:AAA:285[A]:ARG:HD3	1:AAA:312:TRP:CZ3	2.31	0.65
1:AAA:32:PRO:HB2	1:AAA:36[B]:THR:OG1	1.98	0.63
1:AAA:235[A]:GLU:OE2	8:AAA:611:HOH:O	2.16	0.62
1:AAA:374[B]:HIS:HD2	8:AAA:603:HOH:O	1.83	0.61
1:AAA:156[A]:LEU:CD2	8:AAA:854:HOH:O	1.68	0.61
1:AAA:57[B]:GLN:OE1	8:AAA:610:HOH:O	2.16	0.61
1:AAA:398[C]:VAL:HG21	8:AAA:1019:HOH:O	1.90	0.61
1:AAA:55:PRO:HG2	1:AAA:57[A]:GLN:HE22	1.65	0.60
1:AAA:396:ASN:CB	8:AAA:607:HOH:O	2.35	0.59
1:AAA:152:GLU:O	1:AAA:156[A]:LEU:HB3	2.03	0.58
1:AAA:94:LEU:CD1	1:AAA:156[A]:LEU:HD12	2.33	0.58
6:AAA:524:FMT:C	8:AAA:606[A]:HOH:O	2.48	0.58
1:AAA:207[C]:GLN:HG2	8:AAA:618:HOH:O	2.03	0.58
1:AAA:398[A]:VAL:CG1	8:AAA:1019:HOH:O	2.53	0.55
1:AAA:286[A]:LEU:CB	8:AAA:1177:HOH:O	2.48	0.54
1:AAA:398[C]:VAL:HG22	8:AAA:1019:HOH:O	1.94	0.54
1:AAA:398[A]:VAL:HG13	8:AAA:1019:HOH:O	2.08	0.53
1:AAA:223:HIS:HE1	8:AAA:1131:HOH:O	1.92	0.53
1:AAA:153[B]:ASP:OD1	1:AAA:220:TYR:OH	2.25	0.52
1:AAA:335[B]:MET:CE	6:AAA:514:FMT:O2	2.57	0.52
1:AAA:156[A]:LEU:HD22	8:AAA:1066:HOH:O	1.94	0.52
1:AAA:94:LEU:HD12	1:AAA:156[A]:LEU:CD1	2.38	0.52
1:AAA:36[B]:THR:HG22	8:AAA:658:HOH:O	2.08	0.52
1:AAA:306:HIS:HE2	6:AAA:514:FMT:C	2.23	0.52
5:AAA:525:EDO:C1	8:AAA:937:HOH:O	2.45	0.52
1:AAA:285[A]:ARG:HD3	1:AAA:312:TRP:HZ3	1.72	0.51
1:AAA:112[A]:GLU:HG2	8:AAA:617:HOH:O	2.11	0.51
6:AAA:528:FMT:C	8:AAA:658:HOH:O	2.58	0.50
1:AAA:205:TYR:OH	6:AAA:515:FMT:O1	2.30	0.50
1:AAA:69[B]:LEU:HD23	1:AAA:71[B]:PRO:HG3	1.92	0.50
1:AAA:47:ARG:NE	8:AAA:627:HOH:O	2.44	0.49
1:AAA:30:THR:HA	8:AAA:1076:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:127[B]:ASP:OD1	8:AAA:932[B]:HOH:O	2.18	0.49
1:AAA:365:HIS:HE1	8:AAA:1122:HOH:O	1.98	0.47
1:AAA:69[B]:LEU:CD2	1:AAA:71[B]:PRO:HG3	2.45	0.47
1:AAA:246[A]:PHE:HE2	8:AAA:1137[A]:HOH:O	1.96	0.47
1:AAA:170[B]:ARG:NH2	8:AAA:630:HOH:O	2.48	0.47
1:AAA:406[A]:ILE:CG2	8:AAA:735:HOH:O	2.63	0.47
6:AAA:517:FMT:H	8:AAA:654:HOH:O	2.15	0.46
1:AAA:398[C]:VAL:HA	8:AAA:680:HOH:O	2.16	0.45
1:AAA:398[A]:VAL:HA	8:AAA:680:HOH:O	2.15	0.45
1:AAA:286[B]:LEU:CG	8:AAA:1098[B]:HOH:O	2.66	0.44
1:AAA:326[B]:GLU:HG2	8:AAA:916:HOH:O	2.17	0.44
1:AAA:398[A]:VAL:HG11	8:AAA:1019:HOH:O	2.17	0.44
8:AAA:826:HOH:O	2:A:2[A]:NAG:H81	2.18	0.44
1:AAA:285[B]:ARG:HD3	1:AAA:312:TRP:CZ2	2.34	0.44
1:AAA:226[B]:GLN:NE2	8:AAA:619:HOH:O	2.38	0.43
1:AAA:226[A]:GLN:CD	8:AAA:808:HOH:O	2.57	0.43
1:AAA:317[A]:LEU:HD23	8:AAA:608:HOH:O	2.19	0.43
1:AAA:342:CYS:SG	1:AAA:398[C]:VAL:HG11	2.58	0.42
1:AAA:59[B]:ASN:ND2	8:AAA:636:HOH:O	2.52	0.42
1:AAA:326[B]:GLU:CD	1:AAA:329:ARG:NH2	2.57	0.42
1:AAA:110[A]:SER:OG	1:AAA:112[A]:GLU:HG2	2.20	0.42
1:AAA:335[B]:MET:CE	6:AAA:514:FMT:C	2.98	0.41
1:AAA:50[A]:GLU:OE2	6:AAA:524:FMT:O1	2.38	0.41
1:AAA:82:GLY:HA3	1:AAA:118[A]:ILE:O	2.20	0.41

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:AAA:354:LEU:H	5:AAA:513[B]:EDO:HO1[1_545]	1.15	0.45

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	AAA	561/497 (113%)	538 (96%)	21 (4%)	2 (0%)	34 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	GLU
1	AAA	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	AAA	483/424 (114%)	478 (99%)	5 (1%)	76 46

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

Mol	Chain	Res	Type
1	AAA	335[A]	MET
1	AAA	335[B]	MET
1	AAA	381	TRP
1	AAA	420[A]	LEU
1	AAA	420[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 monosaccharides 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	1	1,2	14,14,15	0.53	0	17,19,21	1.18	2 (11%)
2	NAG	A	2[A]	2	14,14,15	0.44	0	17,19,21	1.26	2 (11%)
2	NAG	A	2[B]	2	14,14,15	0.35	0	17,19,21	1.06	1 (5%)
2	BMA	A	3	2	11,11,12	0.22	0	15,15,17	0.99	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
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2[A]	2	-	2/6/23/26	0/1/1/1
2	NAG	A	2[B]	2	-	1/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O5-C1-C2	-3.15	106.31	111.29
2	A	2[A]	NAG	O5-C1-C2	-3.07	106.44	111.29
2	A	2[A]	NAG	C1-O5-C5	2.45	115.52	112.19
2	A	1	NAG	C1-C2-N2	2.27	114.37	110.49
2	A	2[B]	NAG	O5-C1-C2	-2.26	107.72	111.29
2	A	3	BMA	O5-C1-C2	-2.19	107.39	110.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2[A]	NAG	O5-C5-C6-O6
2	A	2[A]	NAG	C4-C5-C6-O6
2	A	2[B]	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	$\# Z > 2$
6	FMT	AAA	516	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	527[A]	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	527[B]	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	525	-	3,3,3	0.14	0	2,2,2	0.11	0
5	EDO	AAA	510[C]	-	3,3,3	0.17	0	2,2,2	0.33	0
5	EDO	AAA	510[B]	-	3,3,3	0.21	0	2,2,2	0.04	0
5	EDO	AAA	510[A]	-	3,3,3	0.12	0	2,2,2	0.07	0
6	FMT	AAA	528	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	524	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	529	-	3,3,3	0.06	0	2,2,2	0.17	0
6	FMT	AAA	517	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	507	-	3,3,3	0.37	0	2,2,2	0.30	0
6	FMT	AAA	526	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	514	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	508	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	518	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	522	-	3,3,3	0.11	0	2,2,2	0.23	0
6	FMT	AAA	521	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	520	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	AAA	523[A]	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	523[B]	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	513[A]	-	3,3,3	0.16	0	2,2,2	0.36	0
5	EDO	AAA	513[B]	-	3,3,3	0.33	0	2,2,2	0.42	0
6	FMT	AAA	515	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAG	AAA	505	1	14,14,15	0.39	0	17,19,21	0.73	0
6	FMT	AAA	509	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	519	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	506	-	3,3,3	0.29	0	2,2,2	0.24	0
6	FMT	AAA	512[A]	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	511	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	512[B]	-	0,2,2	0.00	-	0,1,1	0.00	-

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
5	EDO	AAA	525	-	-	0/1/1/1	-
5	EDO	AAA	510[C]	-	-	0/1/1/1	-
5	EDO	AAA	522	-	-	0/1/1/1	-
5	EDO	AAA	510[B]	-	-	1/1/1/1	-
5	EDO	AAA	510[A]	-	-	0/1/1/1	-
4	NAG	AAA	505	1	-	0/6/23/26	0/1/1/1
5	EDO	AAA	513[B]	-	-	0/1/1/1	-
5	EDO	AAA	506	-	-	0/1/1/1	-
5	EDO	AAA	529	-	-	1/1/1/1	-
5	EDO	AAA	507	-	-	0/1/1/1	-
5	EDO	AAA	513[A]	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	510[B]	EDO	O1-C1-C2-O2
5	AAA	529	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	525	EDO	2	0
6	AAA	528	FMT	1	0
6	AAA	524	FMT	3	0
6	AAA	517	FMT	2	0
6	AAA	514	FMT	4	0
5	AAA	513[B]	EDO	0	1
6	AAA	515	FMT	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	AAA	496/497 (99%)	0.11	17 (3%) 45 35	5, 7, 13, 21	43 (8%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	30	THR	5.9
1	AAA	348	TRP	4.3
1	AAA	316	PHE	4.0
1	AAA	319	PRO	3.9
1	AAA	1[A]	ALA	3.8
1	AAA	347	PHE	3.6
1	AAA	317[A]	LEU	3.3
1	AAA	318	ALA	3.0
1	AAA	63	THR	2.8
1	AAA	477[A]	VAL	2.6
1	AAA	476	ALA	2.6
1	AAA	28	PRO	2.6
1	AAA	26	PHE	2.6
1	AAA	61	THR	2.3
1	AAA	398[A]	VAL	2.3
1	AAA	121	VAL	2.1
1	AAA	381	TRP	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. 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	B-factors(Å ²)	Q<0.9
2	BMA	A	3	11/12	0.94	0.23	4,5,7,7	22
2	NAG	A	2[A]	14/15	0.95	0.13	3,4,8,8	28
2	NAG	A	2[B]	14/15	0.95	0.13	4,5,8,8	28
2	NAG	A	1	14/15	0.96	0.10	7,10,13,14	3

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. 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	B-factors(Å ²)	Q<0.9
6	FMT	AAA	519	3/3	0.69	0.22	7,14,15,18	5
6	FMT	AAA	516	3/3	0.79	0.16	7,23,24,28	5
5	EDO	AAA	522	4/4	0.80	0.16	7,18,20,21	10
4	NAG	AAA	505	14/15	0.80	0.17	7,19,21,22	28
6	FMT	AAA	517	3/3	0.82	0.14	7,15,15,20	5
6	FMT	AAA	528	3/3	0.85	0.16	7,16,19,21	5
6	FMT	AAA	514	3/3	0.85	0.21	7,14,15,17	5
5	EDO	AAA	529	4/4	0.86	0.20	11,47,53,53	1
6	FMT	AAA	523[B]	3/3	0.88	0.20	7,25,28,28	5
6	FMT	AAA	523[A]	3/3	0.88	0.20	7,13,15,16	5
6	FMT	AAA	526	3/3	0.89	0.12	7,19,20,21	5
6	FMT	AAA	508	3/3	0.89	0.12	7,22,24,24	5
6	FMT	AAA	511	3/3	0.89	0.12	7,16,17,17	5
5	EDO	AAA	525	4/4	0.90	0.19	7,12,13,14	10
6	FMT	AAA	520	3/3	0.90	0.17	7,15,22,26	5
6	FMT	AAA	512[A]	3/3	0.91	0.16	7,14,15,15	5
6	FMT	AAA	512[B]	3/3	0.91	0.16	7,16,18,18	5
6	FMT	AAA	509	3/3	0.92	0.05	7,38,42,43	1
5	EDO	AAA	506	4/4	0.92	0.12	7,11,12,12	10
6	FMT	AAA	527[A]	3/3	0.92	0.14	7,11,13,14	5
6	FMT	AAA	524	3/3	0.92	0.13	7,15,20,25	5
6	FMT	AAA	527[B]	3/3	0.92	0.14	7,9,10,13	5
5	EDO	AAA	507	4/4	0.93	0.10	7,9,11,11	10
6	FMT	AAA	518	3/3	0.94	0.08	7,27,31,31	1
3	GLN	AAA	501[B]	9/10	0.95	0.10	6,7,8,9	19
5	EDO	AAA	513[B]	4/4	0.95	0.10	6,8,8,8	10
5	EDO	AAA	513[A]	4/4	0.95	0.10	7,7,9,9	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	FMT	AAA	515	3/3	0.96	0.13	7,15,17,19	5
5	EDO	AAA	510[C]	4/4	0.96	0.13	6,8,11,12	10
5	EDO	AAA	510[B]	4/4	0.96	0.13	7,9,10,14	10
5	EDO	AAA	510[A]	4/4	0.96	0.13	7,8,9,10	10
7	MG	AAA	532	1/1	0.97	0.07	22,22,22,22	1
6	FMT	AAA	521	3/3	0.98	0.12	7,12,13,17	1
7	MG	AAA	534	1/1	0.99	0.06	14,14,14,14	0
7	MG	AAA	536	1/1	1.00	0.05	15,15,15,15	0
7	MG	AAA	530	1/1	1.00	0.14	8,8,8,8	1
7	MG	AAA	535	1/1	1.00	0.04	19,19,19,19	0
7	MG	AAA	533	1/1	1.00	0.06	17,17,17,17	0
7	MG	AAA	537	1/1	1.00	0.08	14,14,14,14	0
7	MG	AAA	531	1/1	1.00	0.06	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.