



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 2WQ8 / pdb_00002wq8
Title : Glycan labelling using engineered variants of galactose oxidase obtained by directed evolution
Authors : Rannes, J.G.; Ioannou, A.; Willies, S.C.; Behrens, C.; Grogan, G.J.; Flitsch, S.L.; Turner, N.J.
Deposited on : 2009-08-14
Resolution : 2.19 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

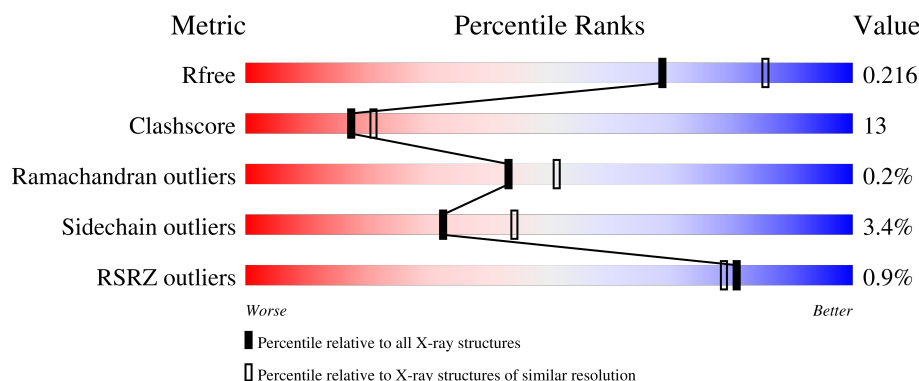
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

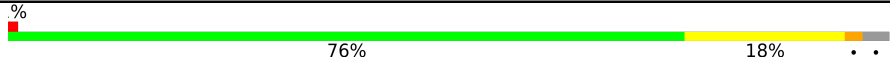
The reported resolution of this entry is 2.19 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of 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	A	661	

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
4	ACY	A	1643	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1644	-	-	X	-
5	EDO	A	1645	-	-	X	-
5	EDO	A	1646	-	-	X	-
5	EDO	A	1647	-	-	X	-
5	EDO	A	1649	-	-	X	-
5	EDO	A	1651	-	-	X	-
6	GOL	A	1653	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5278 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 GALACTOSE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	1	0
			4832	3022	836	956	18			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q01745
A	-20	GLY	-	expression tag	UNP Q01745
A	-19	HIS	-	expression tag	UNP Q01745
A	-18	HIS	-	expression tag	UNP Q01745
A	-17	HIS	-	expression tag	UNP Q01745
A	-16	HIS	-	expression tag	UNP Q01745
A	-15	HIS	-	expression tag	UNP Q01745
A	-14	HIS	-	expression tag	UNP Q01745
A	-13	HIS	-	expression tag	UNP Q01745
A	-12	HIS	-	expression tag	UNP Q01745
A	-11	HIS	-	expression tag	UNP Q01745
A	-10	HIS	-	expression tag	UNP Q01745
A	-9	SER	-	expression tag	UNP Q01745
A	-8	SER	-	expression tag	UNP Q01745
A	-7	GLY	-	expression tag	UNP Q01745
A	-6	HIS	-	expression tag	UNP Q01745
A	-5	ILE	-	expression tag	UNP Q01745
A	-4	GLU	-	expression tag	UNP Q01745
A	-3	GLY	-	expression tag	UNP Q01745
A	-2	ARG	-	expression tag	UNP Q01745
A	-1	HIS	-	expression tag	UNP Q01745
A	0	MET	-	expression tag	UNP Q01745
A	10	PRO	SER	engineered mutation	UNP Q01745
A	70	VAL	MET	engineered mutation	UNP Q01745
A	195	GLU	GLY	engineered mutation	UNP Q01745
A	290	PHE	TRP	engineered mutation	UNP Q01745
A	330	LYS	ARG	engineered mutation	UNP Q01745

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Chain	Residue	Modelled	Actual	Comment	Reference
A	406	THR	GLN	engineered mutation	UNP Q01745
A	463	ILE	PRO	engineered mutation	UNP Q01745
A	494	ALA	VAL	engineered mutation	UNP Q01745
A	535	ASP	ASN	engineered mutation	UNP Q01745

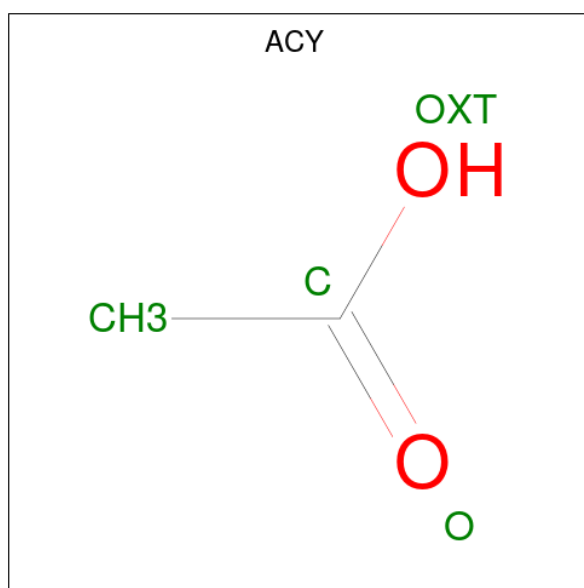
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	382	Total	O	0	0
			382	382		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	88.46Å 88.46Å 410.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.70 – 2.19 76.61 – 2.19	Depositor EDS
% Data completeness (in resolution range)	85.3 (76.70-2.19) 85.3 (76.61-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.182 , 0.242 0.166 , 0.216	Depositor DCC
R_{free} test set	2174 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5278	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 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, GOL, CU, ACY

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	1.34	11/4963 (0.2%)	1.30	29/6773 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	ASN	C-O	-6.36	1.18	1.24
1	A	352	THR	CA-CB	6.27	1.63	1.53
1	A	65	VAL	CA-CB	5.81	1.60	1.54
1	A	359	THR	C-O	-5.74	1.16	1.24
1	A	437	PHE	N-CA	5.51	1.52	1.46
1	A	57	ILE	CA-CB	-5.51	1.47	1.54
1	A	167	LEU	C-N	5.42	1.38	1.33
1	A	5	ILE	CA-CB	5.32	1.61	1.54
1	A	5	ILE	CA-C	5.09	1.58	1.52
1	A	6	GLY	N-CA	5.04	1.52	1.45
1	A	156	PRO	CA-C	-5.01	1.46	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	SER	N-CA-C	-8.19	102.85	113.17
1	A	197	SER	CA-C-N	-7.95	112.72	120.83
1	A	197	SER	C-N-CA	-7.95	112.72	120.83
1	A	256	SER	N-CA-C	6.67	119.40	111.33
1	A	518	CYS	N-CA-C	-6.60	102.30	110.41
1	A	33	GLY	N-CA-C	-6.34	106.49	115.43
1	A	3	ALA	CA-C-N	6.22	128.35	120.51
1	A	3	ALA	C-N-CA	6.22	128.35	120.51
1	A	323	ALA	N-CA-C	-6.21	105.56	112.57
1	A	472	THR	CA-C-N	6.04	126.01	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	THR	C-N-CA	6.04	126.01	120.03
1	A	155	GLN	CA-C-N	5.98	126.00	119.90
1	A	155	GLN	C-N-CA	5.98	126.00	119.90
1	A	235	GLY	N-CA-C	-5.82	107.11	114.16
1	A	242	THR	N-CA-C	5.79	118.84	109.40
1	A	425	SER	CA-C-N	-5.75	114.04	119.85
1	A	425	SER	C-N-CA	-5.75	114.04	119.85
1	A	307	LYS	CB-CA-C	-5.68	104.24	111.86
1	A	222	THR	N-CA-C	-5.52	106.13	112.92
1	A	466	ASP	N-CA-C	-5.48	105.27	112.72
1	A	84	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	A	349	GLY	N-CA-C	-5.47	101.18	112.34
1	A	384	GLY	N-CA-C	-5.39	105.03	112.25
1	A	490	SER	CB-CA-C	-5.26	100.84	109.99
1	A	339	GLY	N-CA-C	-5.23	104.43	111.54
1	A	293	GLY	CA-C-O	-5.18	118.85	122.22
1	A	611	GLY	N-CA-C	-5.16	108.26	114.66
1	A	593	THR	CB-CA-C	5.13	118.51	110.19
1	A	82	ILE	N-CA-C	5.02	115.91	108.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4832	0	4611	109	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	6	7	0
5	A	36	0	54	50	0
6	A	18	0	24	7	0
7	A	382	0	0	10	0
All	All	5278	0	4695	120	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 13.

All (120) 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)
5:A:1645:EDO:H22	7:A:2333:HOH:O	1.40	1.18
1:A:579:ALA:HB1	5:A:1646:EDO:H11	1.20	1.16
1:A:413:ASN:ND2	7:A:2240:HOH:O	1.80	1.12
1:A:81:TRP:HB3	5:A:1648:EDO:H21	1.21	1.11
1:A:530:PRO:HB3	5:A:1647:EDO:H12	1.42	1.01
1:A:157:GLY:H	5:A:1651:EDO:H12	1.28	0.98
1:A:157:GLY:H	5:A:1651:EDO:C1	1.80	0.93
5:A:1648:EDO:H12	7:A:2378:HOH:O	1.70	0.92
1:A:298:ASN:H	6:A:1653:GOL:H12	1.35	0.90
1:A:583:VAL:HG22	5:A:1649:EDO:H21	1.52	0.88
1:A:583:VAL:HG22	5:A:1649:EDO:C2	2.05	0.85
1:A:81:TRP:HB3	5:A:1648:EDO:C2	2.06	0.85
1:A:579:ALA:HB1	5:A:1646:EDO:C1	2.08	0.84
1:A:530:PRO:CB	5:A:1647:EDO:H12	2.10	0.81
1:A:475:ILE:HD12	5:A:1647:EDO:H22	1.62	0.81
1:A:77:ASN:HD22	1:A:79:ASN:H	1.30	0.79
4:A:1643:ACY:H2	5:A:1644:EDO:H11	1.66	0.78
4:A:1643:ACY:H2	5:A:1644:EDO:C1	2.14	0.78
1:A:498:ILE:HA	5:A:1646:EDO:H12	1.67	0.77
1:A:68:LEU:C	1:A:68:LEU:HD12	2.10	0.76
1:A:579:ALA:CB	5:A:1646:EDO:H11	2.11	0.76
1:A:135[A]:GLN:NE2	7:A:2086:HOH:O	2.20	0.75
1:A:77:ASN:ND2	1:A:79:ASN:H	1.89	0.71
1:A:216:ASP:OD2	7:A:2125:HOH:O	2.11	0.69
1:A:156:PRO:HA	5:A:1651:EDO:H11	1.76	0.68
1:A:530:PRO:HB3	5:A:1647:EDO:C1	2.22	0.68
1:A:381:ALA:HB2	5:A:1644:EDO:H12	1.75	0.66
1:A:413:ASN:HB2	5:A:1644:EDO:H11	1.76	0.66
1:A:381:ALA:CB	5:A:1644:EDO:H12	2.26	0.65
1:A:443:THR:HG22	5:A:1646:EDO:H21	1.76	0.65
1:A:583:VAL:HA	5:A:1649:EDO:H21	1.79	0.64
1:A:84:ARG:HH11	1:A:84:ARG:HB3	1.62	0.64
1:A:298:ASN:N	6:A:1653:GOL:H12	2.10	0.64
4:A:1643:ACY:O	5:A:1644:EDO:O2	2.17	0.62
1:A:119:ARG:HH11	1:A:119:ARG:HG3	1.64	0.61
1:A:336:TRP:CD1	5:A:1649:EDO:H11	2.35	0.61
1:A:583:VAL:CG2	5:A:1649:EDO:H21	2.26	0.61
1:A:318:ASN:HB3	1:A:319:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:VAL:HG22	5:A:1649:EDO:H22	1.83	0.60
1:A:379:PRO:HG2	5:A:1644:EDO:H22	1.84	0.60
1:A:22:GLN:HE22	1:A:43:TYR:H	1.50	0.59
1:A:416:ILE:HD11	1:A:476:TYR:OH	2.02	0.59
1:A:444:SER:H	5:A:1645:EDO:H12	1.66	0.59
1:A:147:GLN:NE2	7:A:2094:HOH:O	2.32	0.59
1:A:298:ASN:HD22	1:A:317:VAL:H	1.50	0.59
1:A:84:ARG:HB3	1:A:84:ARG:NH1	2.18	0.59
4:A:1643:ACY:H2	5:A:1644:EDO:H12	1.84	0.58
1:A:227:PHE:CE2	1:A:228:CYS:SG	2.97	0.58
1:A:215:SER:HB2	7:A:2124:HOH:O	2.03	0.58
1:A:444:SER:H	5:A:1645:EDO:C1	2.16	0.58
1:A:228:CYS:N	1:A:229:PRO:HD3	2.19	0.57
1:A:448:PRO:HA	1:A:574:ILE:HD11	1.87	0.56
1:A:495:TYR:O	1:A:496:HIS:HB2	2.04	0.56
1:A:445:VAL:HA	1:A:587:GLN:HE22	1.71	0.55
5:A:1647:EDO:H21	6:A:1655:GOL:H11	1.88	0.55
1:A:157:GLY:N	5:A:1651:EDO:H12	2.10	0.54
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.42	0.54
4:A:1643:ACY:CH3	5:A:1644:EDO:H12	2.38	0.54
1:A:615:PRO:HG3	1:A:639:GLN:HG2	1.90	0.54
1:A:68:LEU:C	1:A:68:LEU:CD1	2.80	0.53
1:A:119:ARG:HG3	1:A:119:ARG:NH1	2.22	0.53
1:A:22:GLN:NE2	1:A:43:TYR:H	2.06	0.53
1:A:498:ILE:C	1:A:498:ILE:HD12	2.33	0.53
1:A:517:ASP:OD2	1:A:517:ASP:C	2.51	0.53
1:A:582:THR:H	5:A:1646:EDO:C2	2.22	0.53
1:A:3:ALA:HB1	1:A:4:PRO:HD2	1.91	0.52
1:A:298:ASN:ND2	1:A:317:VAL:H	2.08	0.52
1:A:582:THR:HA	5:A:1646:EDO:H21	1.92	0.51
1:A:381:ALA:HB2	5:A:1644:EDO:C1	2.41	0.51
1:A:135[A]:GLN:CD	7:A:2086:HOH:O	2.50	0.51
1:A:298:ASN:H	6:A:1653:GOL:C1	2.16	0.51
1:A:323:ALA:O	1:A:324:ASP:C	2.55	0.49
1:A:350:PRO:HD2	7:A:2185:HOH:O	2.12	0.49
1:A:298:ASN:HB2	6:A:1653:GOL:H12	1.94	0.49
1:A:22:GLN:NE2	1:A:42:PHE:HA	2.28	0.48
1:A:77:ASN:HD22	1:A:78:GLN:N	2.11	0.48
1:A:583:VAL:CA	5:A:1649:EDO:H21	2.43	0.48
1:A:39:TRP:O	1:A:139:SER:HA	2.14	0.48
1:A:68:LEU:HD12	1:A:68:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HB2	1:A:399:PHE:CE2	2.49	0.47
1:A:272:TYR:OH	4:A:1642:ACY:O	2.33	0.47
1:A:332:ASP:OD1	1:A:332:ASP:C	2.58	0.47
1:A:381:ALA:HB2	5:A:1644:EDO:C2	2.46	0.46
1:A:16:VAL:HA	1:A:56:THR:O	2.15	0.46
1:A:568:ILE:HD13	1:A:622:VAL:HB	1.97	0.46
5:A:1647:EDO:C2	6:A:1655:GOL:H11	2.45	0.46
4:A:1643:ACY:CH3	5:A:1644:EDO:C1	2.91	0.46
1:A:354:MET:HE1	1:A:428:THR:HG21	1.98	0.45
1:A:157:GLY:N	5:A:1651:EDO:C1	2.63	0.45
1:A:385:ASN:OD1	5:A:1645:EDO:H11	2.17	0.45
1:A:302:TYR:HB2	1:A:309:TRP:CH2	2.52	0.45
1:A:26:GLU:OE1	1:A:29:LYS:NZ	2.50	0.45
1:A:67:GLY:HA2	1:A:114:SER:O	2.16	0.44
1:A:559:ARG:NH1	7:A:2317:HOH:O	2.50	0.44
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.53	0.44
1:A:2:SER:OG	1:A:3:ALA:N	2.50	0.44
1:A:330:LYS:HD2	1:A:405:TYR:CD2	2.53	0.44
1:A:575:ARG:HD2	1:A:618:TRP:CZ2	2.53	0.43
1:A:65:VAL:O	1:A:118:THR:HA	2.18	0.43
1:A:135[A]:GLN:HB3	1:A:136:PRO:CD	2.49	0.43
5:A:1647:EDO:H21	6:A:1655:GOL:C1	2.49	0.43
1:A:84:ARG:NH1	1:A:84:ARG:CB	2.81	0.43
1:A:475:ILE:CD1	5:A:1647:EDO:H22	2.39	0.43
1:A:222:THR:O	1:A:223:LYS:C	2.62	0.43
1:A:77:ASN:HD22	1:A:77:ASN:C	2.27	0.43
1:A:531:ASN:HB3	5:A:1647:EDO:H21	2.02	0.42
1:A:249:LYS:HB3	1:A:249:LYS:HE3	1.83	0.42
1:A:317:VAL:O	1:A:318:ASN:C	2.62	0.41
1:A:316:LYS:O	1:A:319:PRO:HD2	2.21	0.41
1:A:583:VAL:CB	5:A:1649:EDO:H21	2.49	0.41
1:A:105:TRP:CE2	1:A:112:LYS:HB3	2.55	0.41
1:A:381:ALA:HB2	5:A:1644:EDO:H21	2.02	0.41
1:A:463:ILE:O	1:A:464:PHE:HB2	2.20	0.41
1:A:465:GLU:C	1:A:467:SER:H	2.28	0.41
1:A:11:ARG:HG2	1:A:14:TRP:CZ3	2.56	0.41
1:A:330:LYS:HD3	1:A:330:LYS:HA	1.90	0.41
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.84	0.40
1:A:328:LEU:HA	1:A:331:SER:OG	2.22	0.40
1:A:77:ASN:HD21	1:A:79:ASN:CG	2.28	0.40
1:A:381:ALA:HB1	5:A:1644:EDO:H12	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	638/661 (96%)	609 (96%)	28 (4%)	1 (0%)	43 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	PRO

5.3.2 Protein sidechains [i](#)

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	527/545 (97%)	509 (97%)	18 (3%)	32 44

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

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	SER
1	A	77	ASN
1	A	84	ARG
1	A	94	THR
1	A	119	ARG
1	A	150	SER

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Mol	Chain	Res	Type
1	A	156	PRO
1	A	160	ARG
1	A	201	ILE
1	A	248	LYS
1	A	307	LYS
1	A	325	LYS
1	A	374	ASN
1	A	393	LYS
1	A	439	ARG
1	A	514	LEU
1	A	593	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	46	ASN
1	A	63	GLN
1	A	77	ASN
1	A	79	ASN
1	A	267	GLN
1	A	298	ASN
1	A	326	GLN
1	A	333	ASN
1	A	374	ASN
1	A	537	ASN
1	A	587	GLN
1	A	597	ASN
1	A	600	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	A	1652	-	3,3,3	0.51	0	2,2,2	0.67	0
6	GOL	A	1653	-	5,5,5	0.90	0	5,5,5	2.31	1 (20%)
5	EDO	A	1650	-	3,3,3	0.48	0	2,2,2	1.04	0
6	GOL	A	1654	-	5,5,5	0.60	0	5,5,5	0.55	0
5	EDO	A	1646	-	3,3,3	0.55	0	2,2,2	0.87	0
5	EDO	A	1651	-	3,3,3	0.85	0	2,2,2	1.40	0
6	GOL	A	1655	-	5,5,5	0.33	0	5,5,5	0.75	0
5	EDO	A	1645	-	3,3,3	0.45	0	2,2,2	1.09	0
5	EDO	A	1648	-	3,3,3	0.44	0	2,2,2	1.26	0
4	ACY	A	1643	-	3,3,3	1.13	0	3,3,3	0.94	0
5	EDO	A	1644	-	3,3,3	0.46	0	2,2,2	1.23	0
5	EDO	A	1649	-	3,3,3	0.58	0	2,2,2	1.39	0
4	ACY	A	1642	-	3,3,3	0.62	0	3,3,3	1.36	0
5	EDO	A	1647	-	3,3,3	0.56	0	2,2,2	0.68	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
5	EDO	A	1652	-	-	0/1/1/1	-
6	GOL	A	1653	-	-	2/4/4/4	-
5	EDO	A	1650	-	-	1/1/1/1	-
6	GOL	A	1654	-	-	2/4/4/4	-
5	EDO	A	1646	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1651	-	-	1/1/1/1	-
6	GOL	A	1655	-	-	3/4/4/4	-
5	EDO	A	1645	-	-	0/1/1/1	-
5	EDO	A	1648	-	-	1/1/1/1	-
5	EDO	A	1644	-	-	1/1/1/1	-
5	EDO	A	1649	-	-	1/1/1/1	-
5	EDO	A	1647	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1653	GOL	C3-C2-C1	-4.77	94.28	111.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1653	GOL	C1-C2-C3-O3
6	A	1654	GOL	O1-C1-C2-C3
6	A	1655	GOL	C1-C2-C3-O3
6	A	1653	GOL	O2-C2-C3-O3
6	A	1654	GOL	O1-C1-C2-O2
6	A	1655	GOL	O2-C2-C3-O3
6	A	1655	GOL	O1-C1-C2-O2
5	A	1647	EDO	O1-C1-C2-O2
5	A	1648	EDO	O1-C1-C2-O2
5	A	1649	EDO	O1-C1-C2-O2
5	A	1650	EDO	O1-C1-C2-O2
5	A	1651	EDO	O1-C1-C2-O2
5	A	1644	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1653	GOL	4	0
5	A	1646	EDO	7	0
5	A	1651	EDO	5	0
6	A	1655	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1645	EDO	4	0
5	A	1648	EDO	3	0
4	A	1643	ACY	6	0
5	A	1644	EDO	14	0
5	A	1649	EDO	8	0
4	A	1642	ACY	1	0
5	A	1647	EDO	9	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	639/661 (96%)	-0.73	6 (0%) 81 79	4, 12, 26, 49	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	7.2
1	A	3	ALA	3.6
1	A	2	SER	3.1
1	A	4	PRO	2.6
1	A	6	GLY	2.1
1	A	5	ILE	2.1

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](#)

There are no oligosaccharides in this entry.

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. 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
5	EDO	A	1652	4/4	0.77	0.21	36,41,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	1655	6/6	0.84	0.13	28,33,35,39	0
6	GOL	A	1653	6/6	0.85	0.13	22,28,30,35	0
5	EDO	A	1651	4/4	0.85	0.13	13,20,21,24	0
4	ACY	A	1642	4/4	0.86	0.14	31,32,32,33	0
6	GOL	A	1654	6/6	0.93	0.10	24,28,32,34	0
5	EDO	A	1650	4/4	0.93	0.07	14,19,20,22	0
5	EDO	A	1647	4/4	0.94	0.25	9,18,19,19	0
5	EDO	A	1649	4/4	0.94	0.22	8,15,18,19	0
5	EDO	A	1644	4/4	0.95	0.21	11,17,17,21	0
5	EDO	A	1648	4/4	0.95	0.22	10,11,14,15	0
5	EDO	A	1646	4/4	0.95	0.20	8,10,11,12	0
5	EDO	A	1645	4/4	0.96	0.16	13,13,16,17	0
4	ACY	A	1643	4/4	0.98	0.06	7,9,9,9	0
2	CU	A	1640	1/1	1.00	0.01	15,15,15,15	0
3	CA	A	1641	1/1	1.00	0.03	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.