



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:19 PM JST

PDB ID : 5ZCR
Title : DSM5389 glycosyltrehalose synthase
Authors : Tamada, T.; Okazaki, N.
Deposited on : 2018-02-20
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

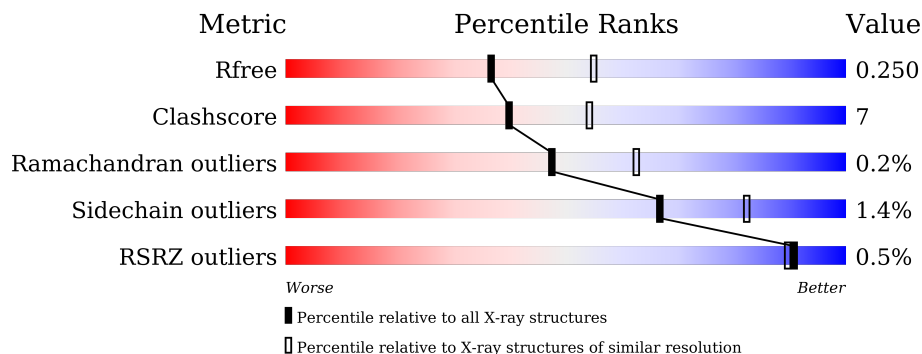
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	728	
1	B	728	

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	GOL	A	808	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12705 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 Maltooligosyl trehalose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	6060	3903	1014	1128	15	0	0	0
1	B	725	6055	3900	1014	1126	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ASN	ASP	engineered mutation	UNP Q7LYV2
A	54	ASP	HIS	engineered mutation	UNP Q7LYV2
B	22	ASN	ASP	engineered mutation	UNP Q7LYV2
B	54	ASP	HIS	engineered mutation	UNP Q7LYV2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	304	Total O 304 304	0	0

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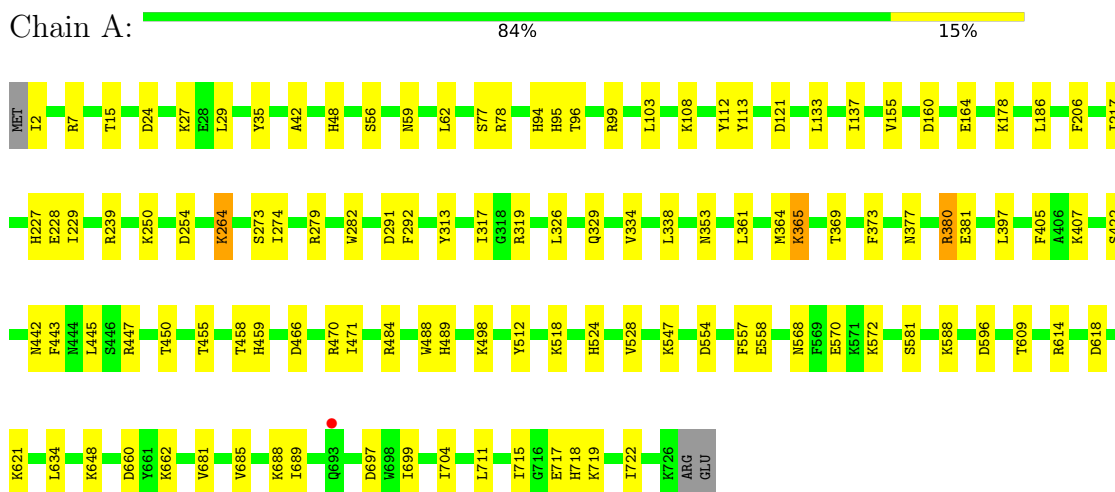
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	218	Total 218	O 218	0	0

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: Maltooligosyl trehalose synthase



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4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.13Å 84.57Å 128.66Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	70.04 – 2.40 70.04 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.9 (70.04-2.40) 92.8 (70.04-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.37Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.171 , 0.248 0.177 , 0.250	Depositor DCC
R_{free} test set	2782 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12705	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.68% 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: MG, GOL

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	0.44	0/6189	0.59	0/8346
1	B	0.43	0/6184	0.57	0/8339
All	All	0.43	0/12373	0.58	0/16685

There are no bond length outliers.

There are no bond angle outliers.

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	6060	0	6060	83	0
1	B	6055	0	6055	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	42	0	56	18	0
3	B	24	0	32	2	0
4	A	304	0	0	8	0
4	B	218	0	0	10	0
All	All	12705	0	12203	178	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 7.

All (178) 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:B:456:LEU:O	1:B:468:ARG:NH2	2.13	0.81
1:A:458:THR:HB	3:A:808:GOL:H2	1.66	0.77
1:A:94:HIS:CD2	1:A:96:THR:HG22	2.23	0.74
1:A:95:HIS:CD2	1:A:155:VAL:H	2.07	0.72
1:B:72:VAL:HG11	1:B:234:PRO:HG2	1.72	0.72
1:A:334:VAL:HG13	1:A:338:LEU:HD12	1.73	0.70
1:B:689:ILE:HD11	1:B:714:LEU:HD21	1.76	0.66
1:B:693:GLN:HG3	1:B:706:SER:HB2	1.76	0.66
1:B:25:TYR:HB2	1:B:623:ARG:HD3	1.78	0.64
1:A:685:VAL:HG11	1:A:711:LEU:HD23	1.80	0.64
1:A:717:GLU:HB3	3:A:805:GOL:H32	1.80	0.64
1:A:95:HIS:HD2	1:A:155:VAL:H	1.45	0.64
1:B:352:VAL:HG21	1:B:357:LEU:HD13	1.81	0.63
1:A:361:LEU:HD21	1:A:397:LEU:HD11	1.81	0.63
1:B:284:VAL:HG12	1:B:286:GLY:H	1.63	0.63
1:A:217:ILE:HD11	1:A:227:HIS:HE1	1.64	0.63
1:A:228:GLU:OE1	4:A:901:HOH:O	2.16	0.63
1:A:568:ASN:O	1:A:572:LYS:NZ	2.32	0.63
1:B:320:LYS:NZ	4:B:907:HOH:O	2.34	0.61
1:B:640:ARG:NH1	4:B:901:HOH:O	2.07	0.61
1:B:250:LYS:HE2	1:B:281:ASP:HB2	1.82	0.61
1:B:74:GLU:OE2	1:B:78:ARG:NH2	2.33	0.61
1:B:371:LEU:HD22	1:B:394:ILE:HG21	1.83	0.60
1:B:250:LYS:NZ	1:B:254:ASP:OD2	2.35	0.59
1:B:28:GLU:HG2	1:B:626:LEU:HD21	1.85	0.58
1:B:676:LEU:HD13	1:B:689:ILE:HD12	1.84	0.57
1:B:250:LYS:HD3	1:B:373:PHE:CZ	2.40	0.57
1:A:103:LEU:HD13	1:A:113:TYR:HA	1.86	0.57
1:A:447:ARG:HD2	4:A:961:HOH:O	2.04	0.57
1:A:94:HIS:HD2	1:A:96:THR:H	1.51	0.57
1:B:277:LYS:HE3	1:B:278:LEU:H	1.69	0.56
1:B:68:TYR:O	1:B:72:VAL:HG23	2.06	0.56
1:A:450:THR:OG1	3:A:806:GOL:H31	2.05	0.56
1:A:164:GLU:HG2	4:A:1171:HOH:O	2.06	0.56
1:A:42:ALA:H	1:A:59:ASN:ND2	2.04	0.56
1:B:468:ARG:NH1	4:B:914:HOH:O	2.38	0.56
1:A:470:ARG:HD3	4:A:1043:HOH:O	2.07	0.55
1:B:56:SER:OG	1:B:99:ARG:NH2	2.40	0.55
1:A:7:ARG:HB2	3:A:808:GOL:H31	1.89	0.54
1:A:718:HIS:NE2	3:A:805:GOL:H2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:GLN:HA	1:B:706:SER:HA	1.89	0.54
1:A:458:THR:CB	3:A:808:GOL:H2	2.36	0.54
1:B:422:SER:HB3	1:B:471:ILE:HB	1.90	0.54
1:A:662:LYS:HD2	1:B:381:GLU:OE2	2.08	0.54
1:B:12:LYS:HE2	4:B:1105:HOH:O	2.09	0.53
1:A:108:LYS:NZ	1:A:121:ASP:HB2	2.24	0.53
1:A:688:LYS:NZ	4:A:912:HOH:O	2.42	0.52
1:B:552:PHE:O	1:B:556:VAL:HG13	2.09	0.52
1:B:133:LEU:HD11	1:B:186:LEU:HD13	1.92	0.52
1:A:518:LYS:HB3	1:A:557:PHE:CE2	2.44	0.52
1:B:464:SER:HB3	1:B:607:LEU:HB2	1.90	0.52
1:B:470:ARG:HD3	4:B:988:HOH:O	2.11	0.51
1:A:24:ASP:OD1	1:A:78:ARG:NH1	2.43	0.51
1:A:699:ILE:HD13	1:A:722:ILE:HD13	1.93	0.51
1:B:369:THR:HG21	1:B:379:ILE:HG22	1.92	0.51
1:B:590:LEU:O	1:B:670:ARG:NH1	2.37	0.51
1:A:313:TYR:O	1:A:317:ILE:HG12	2.10	0.50
1:A:217:ILE:HD11	1:A:227:HIS:CE1	2.44	0.50
1:A:95:HIS:HB3	1:A:155:VAL:O	2.12	0.50
1:B:301:VAL:HG21	1:B:423:LEU:HD21	1.94	0.50
1:A:133:LEU:HD11	1:A:186:LEU:HD13	1.95	0.49
1:B:300:LEU:HD11	1:B:584:ALA:HB2	1.94	0.49
1:A:160:ASP:O	1:A:164:GLU:HG3	2.13	0.49
1:B:95:HIS:HB3	1:B:155:VAL:O	2.13	0.49
1:A:137:ILE:HD11	1:A:186:LEU:HD12	1.95	0.49
1:B:42:ALA:H	1:B:59:ASN:ND2	2.10	0.48
1:A:681:VAL:HG12	1:A:719:LYS:HG3	1.95	0.48
1:B:198:LYS:NZ	4:B:912:HOH:O	2.38	0.48
1:B:435:LEU:HD12	1:B:435:LEU:HA	1.70	0.48
1:B:51:ASP:HB2	1:B:92:ALA:HB2	1.94	0.48
1:B:491:LEU:HD21	1:B:561:SER:HB2	1.96	0.48
1:B:489:HIS:O	1:B:493:ARG:HD3	2.14	0.48
1:B:582:LEU:HD13	1:B:604:TRP:HH2	1.79	0.48
1:A:35:TYR:OH	3:A:808:GOL:H12	2.14	0.47
1:B:243:ILE:HA	1:B:246:LEU:HD13	1.96	0.47
1:A:94:HIS:HD2	1:A:96:THR:HG22	1.75	0.47
1:B:479:LYS:O	1:B:483:GLU:HG3	2.15	0.47
1:B:619:PHE:O	1:B:623:ARG:HG3	2.14	0.47
1:A:27:LYS:HD3	1:A:78:ARG:O	2.15	0.47
1:A:334:VAL:HG11	1:A:407:LYS:HB2	1.97	0.47
1:A:459:HIS:CE1	3:A:808:GOL:H11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:HG2	1:B:112:TYR:CZ	2.49	0.47
1:B:288:THR:HA	1:B:453:MET:SD	2.55	0.47
1:B:151:TYR:CZ	1:B:152:ARG:HD3	2.50	0.47
1:B:257:ARG:NH2	4:B:923:HOH:O	2.47	0.47
1:B:410:GLU:HA	1:B:414:LEU:HD12	1.96	0.46
1:B:492:LEU:O	1:B:494:PRO:HD3	2.14	0.46
1:B:667:GLY:HA3	1:B:675:VAL:O	2.15	0.46
1:B:103:LEU:HD13	1:B:113:TYR:HA	1.96	0.46
1:B:277:LYS:HD2	1:B:277:LYS:HA	1.71	0.46
1:A:206:PHE:CZ	3:A:803:GOL:H2	2.51	0.46
1:A:334:VAL:HG11	1:A:407:LYS:CB	2.46	0.46
1:A:365:LYS:NZ	1:A:381:GLU:HG2	2.31	0.46
1:A:524:HIS:O	1:A:528:VAL:HG23	2.15	0.45
1:B:590:LEU:HD11	1:B:649:LEU:HD22	1.97	0.45
1:B:25:TYR:HB2	1:B:623:ARG:CD	2.46	0.45
1:A:443:PHE:O	1:A:447:ARG:HG3	2.17	0.45
1:B:247:TYR:CZ	1:B:395:MET:HE2	2.52	0.45
1:B:83:ILE:HD13	1:B:237:GLY:HA3	1.99	0.45
1:A:250:LYS:HG2	1:A:373:PHE:CZ	2.52	0.45
1:A:512:TYR:CD2	1:A:570:GLU:HG2	2.52	0.45
1:A:377:ASN:O	1:A:380:ARG:HB3	2.16	0.45
1:B:250:LYS:HD3	1:B:373:PHE:CE1	2.52	0.45
1:A:291:ASP:OD2	4:A:902:HOH:O	2.21	0.45
1:B:545:TYR:HD1	1:B:548:LYS:HE3	1.82	0.45
1:A:56:SER:HA	1:A:229:ILE:HG12	1.98	0.44
1:A:292:PHE:CZ	1:A:588:LYS:HA	2.52	0.44
1:B:614:ARG:HH12	3:B:804:GOL:H2	1.81	0.44
1:A:554:ASP:O	1:A:558:GLU:HB2	2.17	0.44
1:A:489:HIS:CE1	1:A:498:LYS:HD3	2.52	0.44
1:B:604:TRP:CE3	1:B:642:LYS:HD2	2.53	0.44
1:A:279:ARG:HB2	1:A:282:TRP:CD1	2.52	0.44
1:B:253:LEU:HD23	1:B:253:LEU:HA	1.85	0.44
1:A:648:LYS:HD3	1:A:699:ILE:HA	1.99	0.44
1:A:264:LYS:N	1:A:264:LYS:HD3	2.31	0.44
1:A:718:HIS:CE1	3:A:805:GOL:H2	2.53	0.44
1:B:225:GLU:O	1:B:228:GLU:HG3	2.18	0.44
1:B:431:ARG:HD2	4:B:1039:HOH:O	2.18	0.44
1:A:459:HIS:CE1	3:A:808:GOL:HO2	2.29	0.44
1:A:484:ARG:HB3	1:A:488:TRP:CZ2	2.53	0.44
3:A:803:GOL:O1	3:A:804:GOL:H31	2.18	0.43
1:B:658:LEU:HD22	1:B:670:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ILE:HD13	1:A:689:ILE:HA	1.78	0.43
1:B:515:PHE:CZ	1:B:563:ARG:HA	2.54	0.43
1:A:596:ASP:OD2	3:A:808:GOL:H32	2.18	0.43
1:B:126:LEU:HB2	1:B:193:LEU:HD23	2.00	0.43
1:B:678:SER:HA	1:B:679:PRO:HD3	1.89	0.43
1:B:391:GLU:O	1:B:395:MET:HG3	2.18	0.43
1:B:609:THR:HB	4:B:938:HOH:O	2.19	0.42
1:A:547:LYS:HG3	4:A:1163:HOH:O	2.18	0.42
1:A:614:ARG:HH22	3:A:804:GOL:H32	1.84	0.42
1:A:7:ARG:CB	3:A:808:GOL:H31	2.47	0.42
1:B:545:TYR:CD1	1:B:548:LYS:HE3	2.54	0.42
1:A:99:ARG:HG2	1:A:112:TYR:CZ	2.54	0.42
1:A:422:SER:HB3	1:A:471:ILE:HB	2.01	0.42
1:B:629:LEU:HD12	1:B:629:LEU:HA	1.89	0.42
1:A:250:LYS:NZ	1:A:254:ASP:OD2	2.25	0.42
1:B:525:ILE:HD13	1:B:525:ILE:HA	1.78	0.42
1:A:27:LYS:HD2	1:A:27:LYS:HA	1.77	0.42
1:B:470:ARG:NH1	1:B:574:VAL:HG22	2.34	0.42
1:A:364:MET:HE1	1:A:369:THR:HG23	2.02	0.42
1:A:442:ASN:HA	1:A:445:LEU:HD12	2.00	0.42
1:B:68:TYR:CE2	1:B:233:LEU:HD22	2.55	0.42
1:B:589:PHE:HA	1:B:595:PRO:HB3	2.02	0.42
1:A:634:LEU:HA	1:A:634:LEU:HD23	1.75	0.42
1:B:363:CYS:O	1:B:365:LYS:NZ	2.27	0.42
1:A:108:LYS:HZ1	1:A:121:ASP:HB2	1.83	0.41
1:B:68:TYR:HE2	1:B:233:LEU:HD22	1.85	0.41
1:A:459:HIS:HE1	3:A:808:GOL:H11	1.84	0.41
1:B:125:ILE:O	1:B:127:PRO:HD3	2.20	0.41
1:B:361:LEU:HD21	1:B:397:LEU:HD11	2.01	0.41
1:A:48:HIS:HA	4:A:1035:HOH:O	2.20	0.41
1:A:273:SER:HB3	1:A:274:ILE:H	1.75	0.41
1:B:205:ARG:HA	1:B:212:LEU:O	2.20	0.41
1:B:694:LYS:N	1:B:694:LYS:HD3	2.36	0.41
1:A:326:LEU:HA	1:A:329:GLN:HG2	2.03	0.41
1:B:20:ILE:HA	1:B:23:LEU:HG	2.02	0.41
1:B:94:HIS:ND1	1:B:96:THR:HG22	2.36	0.41
1:A:609:THR:HG21	3:A:807:GOL:H11	2.02	0.41
1:A:614:ARG:HH22	3:A:804:GOL:C3	2.33	0.41
1:A:15:THR:HB	1:A:62:LEU:O	2.21	0.41
1:A:697:ASP:HB2	1:A:704:ILE:HD11	2.03	0.41
1:B:216:ARG:HH11	1:B:216:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:VAL:HG22	1:B:720:VAL:HB	2.02	0.41
1:B:589:PHE:HB2	1:B:649:LEU:HD13	2.03	0.41
1:B:7:ARG:HB3	1:B:598:TYR:HA	2.03	0.41
1:B:48:HIS:HA	4:B:1017:HOH:O	2.21	0.41
1:A:29:LEU:HD12	1:A:29:LEU:HA	1.95	0.40
1:A:715:ILE:HD12	1:A:719:LYS:HA	2.02	0.40
1:B:257:ARG:HG3	1:B:283:LYS:HB3	2.03	0.40
1:B:644:LEU:O	1:B:648:LYS:HG2	2.21	0.40
1:B:494:PRO:HB2	1:B:496:ILE:HG12	2.03	0.40
1:B:638:ASP:OD1	1:B:640:ARG:HD3	2.21	0.40
1:A:466:ASP:OD1	1:A:581:SER:OG	2.32	0.40
1:A:618:ASP:OD2	1:A:621:LYS:HB2	2.21	0.40
1:B:137:ILE:HD11	1:B:186:LEU:HD12	2.03	0.40
1:B:484:ARG:HB3	1:B:488:TRP:CZ2	2.57	0.40
1:B:614:ARG:HH22	3:B:804:GOL:H2	1.86	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	723/728 (99%)	696 (96%)	26 (4%)	1 (0%)	51 68
1	B	723/728 (99%)	692 (96%)	29 (4%)	2 (0%)	41 55
All	All	1446/1456 (99%)	1388 (96%)	55 (4%)	3 (0%)	47 62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	705	SER
1	B	390	ASP
1	A	660	ASP

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	674/677 (100%)	663 (98%)	11 (2%)	62	79
1	B	673/677 (99%)	665 (99%)	8 (1%)	71	85
All	All	1347/1354 (100%)	1328 (99%)	19 (1%)	67	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	77	SER
1	A	178	LYS
1	A	239	ARG
1	A	264	LYS
1	A	319	ARG
1	A	353	ASN
1	A	365	LYS
1	A	380	ARG
1	A	405	PHE
1	A	455	THR
1	B	31	VAL
1	B	35	TYR
1	B	131	ASP
1	B	405	PHE
1	B	455	THR
1	B	492	LEU
1	B	678	SER
1	B	693	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	95	HIS
1	A	693	GLN

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Mol	Chain	Res	Type
1	B	693	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	802	2	5,5,5	0.45	0	5,5,5	0.31	0
3	GOL	A	807	-	5,5,5	0.60	0	5,5,5	1.00	0
3	GOL	B	805	-	5,5,5	0.47	0	5,5,5	0.40	0
3	GOL	A	808	-	5,5,5	0.51	0	5,5,5	0.74	0
3	GOL	A	804	-	5,5,5	0.62	0	5,5,5	0.80	0
3	GOL	A	806	-	5,5,5	0.39	0	5,5,5	0.81	0
3	GOL	A	803	2	5,5,5	0.36	0	5,5,5	0.66	0
3	GOL	A	805	-	5,5,5	0.27	0	5,5,5	0.90	0
3	GOL	B	804	-	5,5,5	0.62	0	5,5,5	0.86	0
3	GOL	B	803	2	5,5,5	0.24	0	5,5,5	0.78	0
3	GOL	A	802	2	5,5,5	0.29	0	5,5,5	0.80	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
3	GOL	B	802	2	-	0/4/4/4	-
3	GOL	A	807	-	-	1/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	A	804	-	-	4/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	A	803	2	-	2/4/4/4	-
3	GOL	A	805	-	-	1/4/4/4	-
3	GOL	B	804	-	-	2/4/4/4	-
3	GOL	B	803	2	-	0/4/4/4	-
3	GOL	A	802	2	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
3	A	806	GOL	O1-C1-C2-C3
3	A	808	GOL	C1-C2-C3-O3
3	B	804	GOL	O1-C1-C2-O2
3	B	804	GOL	O1-C1-C2-C3
3	B	805	GOL	O1-C1-C2-O2
3	B	805	GOL	O1-C1-C2-C3
3	A	802	GOL	O1-C1-C2-C3
3	A	804	GOL	O1-C1-C2-C3
3	A	804	GOL	C1-C2-C3-O3
3	A	807	GOL	O1-C1-C2-C3
3	A	806	GOL	O1-C1-C2-O2
3	A	803	GOL	O2-C2-C3-O3
3	A	804	GOL	O2-C2-C3-O3
3	A	805	GOL	O2-C2-C3-O3
3	A	804	GOL	O1-C1-C2-O2
3	A	808	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	807	GOL	1	0
3	A	808	GOL	9	0
3	A	804	GOL	3	0
3	A	806	GOL	1	0
3	A	803	GOL	2	0
3	A	805	GOL	3	0
3	B	804	GOL	2	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	725/728 (99%)	-0.54	1 (0%) 95 95	19, 29, 48, 71	0
1	B	725/728 (99%)	-0.43	6 (0%) 86 84	19, 34, 53, 84	0
All	All	1450/1456 (99%)	-0.48	7 (0%) 91 89	19, 32, 52, 84	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	692	ARG	3.0
1	B	275	ASN	2.7
1	B	380	ARG	2.5
1	B	693	GLN	2.3
1	A	693	GLN	2.2
1	B	274	ILE	2.2
1	B	694	LYS	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](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
3	GOL	A	804	6/6	0.88	0.19	23,32,35,39	0
3	GOL	A	806	6/6	0.89	0.16	37,44,50,52	0
3	GOL	B	804	6/6	0.89	0.19	25,29,36,37	0
3	GOL	A	805	6/6	0.90	0.27	29,34,38,39	0
3	GOL	A	807	6/6	0.91	0.18	21,24,26,29	0
3	GOL	A	803	6/6	0.95	0.12	24,25,27,27	0
3	GOL	B	802	6/6	0.96	0.14	29,31,33,38	0
3	GOL	B	803	6/6	0.96	0.11	24,30,30,32	0
3	GOL	A	808	6/6	0.96	0.24	24,26,32,33	0
3	GOL	B	805	6/6	0.97	0.16	29,33,37,48	0
2	MG	B	801	1/1	0.98	0.10	24,24,24,24	0
3	GOL	A	802	6/6	0.98	0.12	21,23,24,25	0
2	MG	A	801	1/1	0.99	0.10	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.