



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:26 PM UTC

PDB ID : 5H3Z / pdb_00005h3z
Title : Crystal Structure of 1,2-beta-oligoglucan phosphorylase from Lachnoclostridium phytofermentans
Authors : Nakajima, M.; Tanaka, N.; Furukawa, N.; Nihira, T.; Kodutsumi, Y.; Takahashi, Y.; Sugimoto, N.; Miyanaga, A.; Fushinobu, S.; Taguchi, H.; Nakai, H.
Deposited on : 2016-10-28
Resolution : 2.00 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

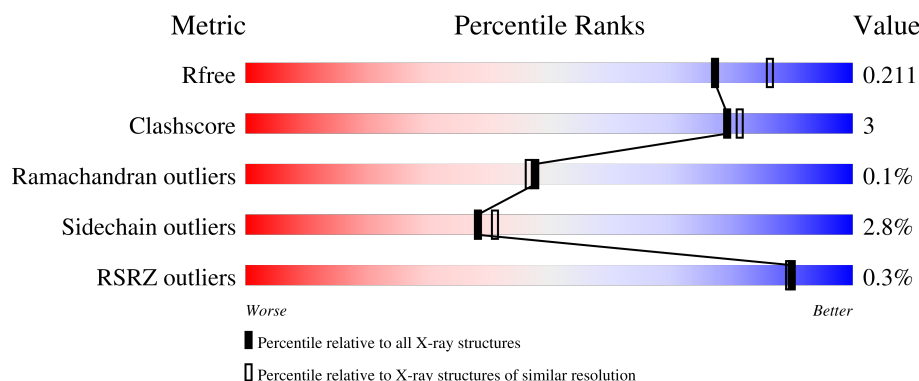
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1122	 92% 7% ..
1	B	1122	 91% 7% ..

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
2	GOL	A	1203	-	X	-	-
4	PEG	A	1207	-	-	X	-
4	PEG	B	1209	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18799 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1113	Total	C	N	O	S	Se	0	0	0
			8918	5712	1483	1691	14	18			
1	B	1113	Total	C	N	O	S	Se	0	1	0
			8926	5717	1484	1692	14	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP A9KJS6
A	1	GLY	-	expression tag	UNP A9KJS6
A	1114	LEU	-	expression tag	UNP A9KJS6
A	1115	GLU	-	expression tag	UNP A9KJS6
A	1116	HIS	-	expression tag	UNP A9KJS6
A	1117	HIS	-	expression tag	UNP A9KJS6
A	1118	HIS	-	expression tag	UNP A9KJS6
A	1119	HIS	-	expression tag	UNP A9KJS6
A	1120	HIS	-	expression tag	UNP A9KJS6
A	1121	HIS	-	expression tag	UNP A9KJS6
B	0	MSE	-	expression tag	UNP A9KJS6
B	1	GLY	-	expression tag	UNP A9KJS6
B	1114	LEU	-	expression tag	UNP A9KJS6
B	1115	GLU	-	expression tag	UNP A9KJS6
B	1116	HIS	-	expression tag	UNP A9KJS6
B	1117	HIS	-	expression tag	UNP A9KJS6
B	1118	HIS	-	expression tag	UNP A9KJS6
B	1119	HIS	-	expression tag	UNP A9KJS6
B	1120	HIS	-	expression tag	UNP A9KJS6
B	1121	HIS	-	expression tag	UNP A9KJS6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

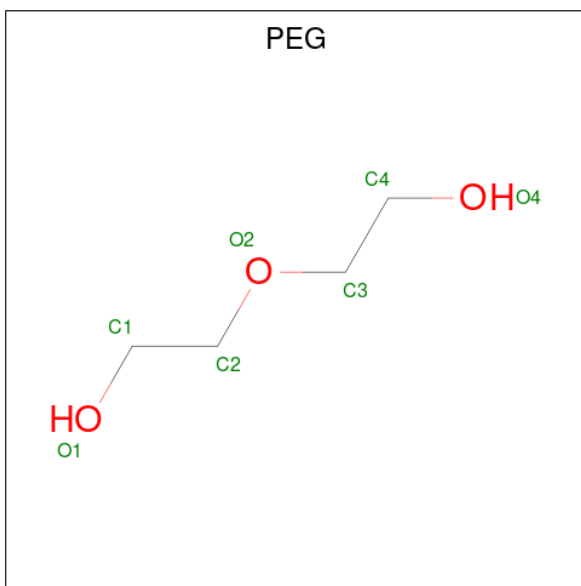


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total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

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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

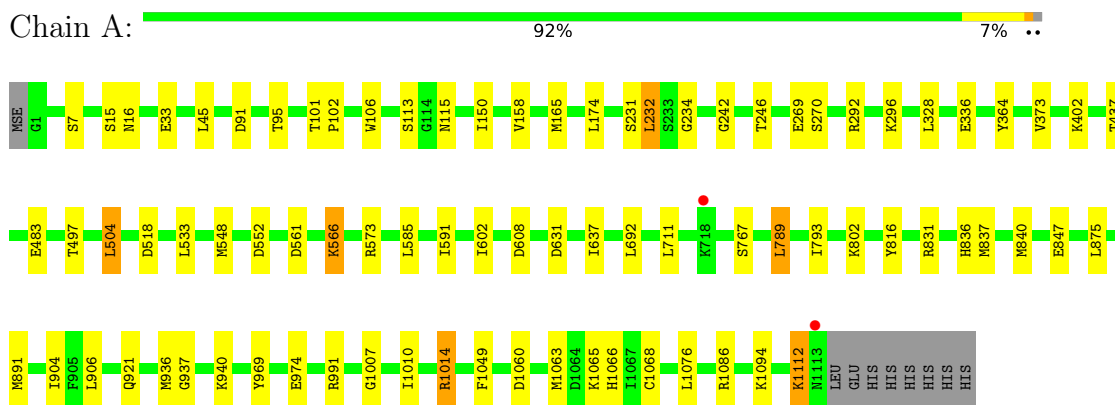
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	432	Total	O	0	0
			432	432		
5	B	439	Total	O	0	0
			439	439		

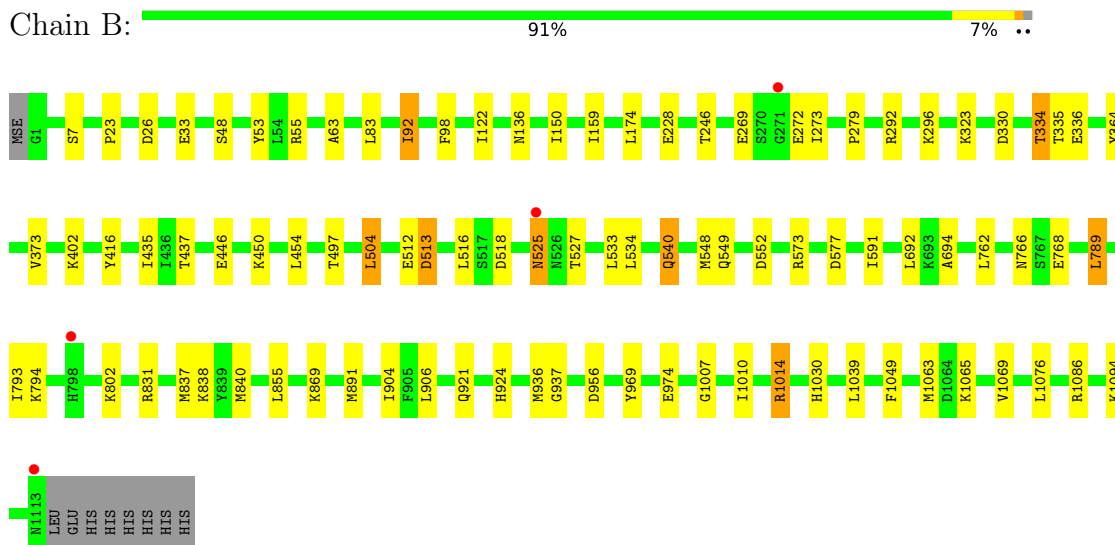
3 Residue-property plots [i](#)

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.76Å 94.78Å 157.94Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	42.72 – 2.00 42.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.72-2.00) 99.9 (42.72-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.168 , 0.204 0.177 , 0.211	Depositor DCC
R_{free} test set	8658 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.0	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	0.96	EDS
Total number of atoms	18799	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: CA, GOL, PEG

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	1.23	9/9125 (0.1%)	0.98	3/12366 (0.0%)
1	B	1.22	9/9133 (0.1%)	0.99	9/12376 (0.1%)
All	All	1.23	18/18258 (0.1%)	0.99	12/24742 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	540	GLN	CD-OE1	8.46	1.39	1.23
1	B	228	GLU	CA-C	-6.47	1.44	1.52
1	A	437	THR	N-CA	-5.93	1.38	1.46
1	A	150	ILE	C-O	-5.78	1.17	1.24
1	B	450	LYS	N-CA	-5.78	1.39	1.46
1	B	956	ASP	C-O	-5.71	1.16	1.24
1	A	591	ILE	CA-C	5.52	1.59	1.52
1	A	991	ARG	C-O	-5.27	1.18	1.24
1	A	816	TYR	N-CA	5.26	1.52	1.46
1	B	437	THR	N-CA	-5.25	1.39	1.46
1	B	416	TYR	C-O	-5.22	1.18	1.23
1	A	585	LEU	C-O	-5.21	1.17	1.23
1	A	608	ASP	N-CA	5.16	1.52	1.46
1	B	63	ALA	CA-C	-5.07	1.46	1.52
1	B	1030	HIS	CA-C	-5.07	1.46	1.52
1	B	591	ILE	C-O	-5.06	1.18	1.25
1	A	637	ILE	CA-C	5.04	1.59	1.52
1	A	561	ASP	C-O	-5.02	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	GLU	N-CA-C	-6.90	100.27	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ILE	N-CA-C	-6.61	96.78	107.28
1	A	936	MSE	CA-CB-CG	-6.12	101.85	114.10
1	A	891	MSE	CG-SE-CE	6.02	112.17	98.92
1	B	1063	MSE	CB-CA-C	5.99	121.68	109.76
1	B	891	MSE	CG-SE-CE	5.80	111.67	98.92
1	B	936	MSE	CA-CB-CG	-5.48	103.14	114.10
1	B	292	ARG	N-CA-CB	-5.33	102.50	110.17
1	B	694	ALA	N-CA-C	5.16	116.59	111.07
1	A	373	VAL	CB-CA-C	5.16	116.81	111.09
1	B	373	VAL	CB-CA-C	5.06	116.71	111.09
1	B	273	ILE	CB-CA-C	5.05	117.56	110.99

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	8918	0	8675	41	0
1	B	8926	0	8683	48	0
2	A	24	0	31	3	0
2	B	36	0	48	2	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	14	0	20	4	0
4	B	7	0	10	8	0
5	A	432	0	0	13	0
5	B	439	0	0	8	0
All	All	18799	0	17467	96	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 3.

All (96) 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:1063:MSE:HE2	1:A:1112:LYS:HB3	1.44	0.98
1:B:516:LEU:HD11	1:B:534:LEU:HD11	1.56	0.87
1:B:540:GLN:HG3	5:B:1519:HOH:O	1.78	0.83
1:A:165:MSE:HE3	5:A:1633:HOH:O	1.80	0.80
2:A:1204:GOL:H2	5:A:1307:HOH:O	1.90	0.71
1:B:435:ILE:HD12	1:B:454:LEU:HD13	1.73	0.71
1:B:573:ARG:NH2	1:B:577:ASP:OD2	2.29	0.66
1:A:1063:MSE:HE2	1:A:1112:LYS:CB	2.25	0.65
1:A:504:LEU:HD12	1:A:552:ASP:HA	1.80	0.63
1:A:518:ASP:HA	1:A:533:LEU:O	2.00	0.62
1:B:53:TYR:OH	2:B:1204:GOL:H2	2.00	0.61
1:A:483:GLU:O	1:A:483:GLU:HG3	2.00	0.61
4:A:1207:PEG:H21	5:A:1667:HOH:O	2.01	0.61
1:A:548:MSE:HE3	5:A:1694:HOH:O	2.00	0.60
1:B:548:MSE:HE3	5:B:1692:HOH:O	2.00	0.60
1:A:1063:MSE:HE3	1:A:1065:LYS:O	2.02	0.60
4:A:1207:PEG:C2	5:A:1667:HOH:O	2.51	0.59
1:B:518:ASP:HA	1:B:533:LEU:O	2.03	0.58
1:A:1065:LYS:HE2	1:A:1068:CYS:HB2	1.84	0.58
1:A:1112:LYS:O	1:A:1112:LYS:HG3	2.03	0.57
1:B:435:ILE:CD1	1:B:454:LEU:HD13	2.34	0.57
1:A:296:LYS:H	1:A:296:LYS:HE2	1.70	0.57
1:B:335:THR:HB	4:B:1209:PEG:H12	1.86	0.56
1:B:573:ARG:HH21	1:B:573:ARG:HG2	1.71	0.56
1:B:33:GLU:HB2	1:B:246:THR:HG21	1.88	0.56
1:A:497:THR:HG21	1:A:504:LEU:HD22	1.89	0.55
1:B:1049:PHE:CD1	1:B:1094:LYS:HD2	2.41	0.55
1:B:136:ASN:HB2	5:B:1591:HOH:O	2.05	0.55
1:A:1063:MSE:HE1	1:A:1066:HIS:O	2.07	0.54
1:B:336:GLU:HB3	4:B:1209:PEG:H21	1.90	0.54
1:A:831:ARG:HG3	1:A:837:MSE:HG2	1.90	0.54
1:A:1063:MSE:HE2	1:A:1112:LYS:N	2.23	0.53
1:A:402:LYS:CE	5:A:1338:HOH:O	2.55	0.53
1:B:504:LEU:HD12	1:B:552:ASP:HA	1.90	0.53
1:A:15:SER:HB3	5:A:1303:HOH:O	2.09	0.52
1:B:831:ARG:HG3	1:B:837:MSE:HG2	1.92	0.52
1:B:402:LYS:HE2	5:B:1452:HOH:O	2.10	0.52
1:A:16:ASN:N	5:A:1303:HOH:O	2.34	0.51
1:A:631:ASP:OD1	5:A:1301:HOH:O	2.19	0.51
1:A:566:LYS:O	1:A:566:LYS:HE2	2.12	0.50
1:B:766:ASN:OD1	1:B:768:GLU:HG2	2.12	0.50
1:A:402:LYS:HE3	5:A:1338:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:PHE:CD1	1:A:1094:LYS:HD2	2.47	0.48
4:B:1209:PEG:H22	5:B:1368:HOH:O	2.13	0.48
1:B:92:ILE:N	1:B:92:ILE:HD13	2.29	0.48
1:A:402:LYS:HE2	5:A:1338:HOH:O	2.14	0.48
1:A:840:MSE:HE1	1:A:904:ILE:HG21	1.96	0.47
1:A:33:GLU:HB2	1:A:246:THR:HG21	1.96	0.47
1:B:48:SER:O	2:B:1204:GOL:H12	2.15	0.47
1:A:1060:ASP:O	1:A:1063:MSE:HG3	2.15	0.47
1:B:525:ASN:HB3	1:B:527:THR:H	1.79	0.47
1:A:336:GLU:N	4:A:1207:PEG:H11	2.29	0.47
1:B:446:GLU:HG2	1:B:549:GLN:HG2	1.97	0.46
1:A:631:ASP:OD2	2:A:1202:GOL:H11	2.15	0.46
1:B:540:GLN:CG	5:B:1519:HOH:O	2.51	0.46
1:B:335:THR:CB	4:B:1209:PEG:H12	2.46	0.46
1:A:937:GLY:HA3	1:A:1086:ARG:HD3	1.97	0.45
1:B:1010:ILE:O	1:B:1014:ARG:HD2	2.16	0.45
2:A:1203:GOL:H11	5:A:1361:HOH:O	2.16	0.45
1:B:869:LYS:NZ	5:B:1308:HOH:O	2.49	0.45
1:B:454:LEU:HD12	1:B:454:LEU:HA	1.74	0.45
1:A:789:LEU:HD22	1:A:793:ILE:HD12	1.99	0.44
1:B:937:GLY:HA3	1:B:1086:ARG:HD3	1.98	0.44
1:A:969:TYR:CZ	1:A:1007:GLY:HA3	2.52	0.44
1:B:335:THR:CA	4:B:1209:PEG:H12	2.48	0.44
1:B:497:THR:HG21	1:B:504:LEU:HD22	1.99	0.44
1:A:115:ASN:HA	1:A:232:LEU:O	2.17	0.44
1:B:512:GLU:O	1:B:513:ASP:HB2	2.17	0.44
4:B:1209:PEG:H22	5:B:1610:HOH:O	2.17	0.44
1:A:789:LEU:HD22	1:A:793:ILE:CD1	2.49	0.43
1:A:1010:ILE:O	1:A:1014:ARG:HD2	2.19	0.43
1:B:323:LYS:HE2	1:B:573:ARG:CZ	2.48	0.43
1:B:548:MSE:HE3	1:B:548:MSE:HB2	1.94	0.43
1:B:330:ASP:O	1:B:334:THR:HG23	2.19	0.43
1:B:336:GLU:H	4:B:1209:PEG:C2	2.32	0.43
1:B:55:ARG:CZ	1:B:122:ILE:HD11	2.48	0.43
1:B:969:TYR:CZ	1:B:1007:GLY:HA3	2.53	0.43
1:A:548:MSE:HE3	1:A:548:MSE:HB2	1.91	0.42
1:B:92:ILE:N	1:B:92:ILE:CD1	2.82	0.42
1:B:516:LEU:CD1	1:B:534:LEU:HD11	2.40	0.42
1:A:836:HIS:CD2	1:A:836:HIS:C	2.98	0.42
1:B:840:MSE:HE1	1:B:904:ILE:HG21	2.01	0.42
1:A:497:THR:CG2	1:A:504:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:HB	1:A:102:PRO:CD	2.50	0.42
1:B:789:LEU:HD22	1:B:793:ILE:CD1	2.49	0.42
1:B:789:LEU:HD22	1:B:793:ILE:HD12	2.00	0.41
1:A:113:SER:HA	1:A:234:GLY:O	2.21	0.41
1:B:336:GLU:CB	4:B:1209:PEG:H21	2.51	0.41
1:B:23:PRO:HB2	1:B:279:PRO:HD3	2.02	0.41
1:A:1063:MSE:CE	1:A:1112:LYS:HB3	2.30	0.41
1:B:150:ILE:HD12	1:B:159:ILE:HD12	2.03	0.41
1:A:106:TRP:CZ2	1:A:242:GLY:HA3	2.56	0.41
1:B:83:LEU:HB2	1:B:98:PHE:HB3	2.03	0.40
1:B:525:ASN:HB3	1:B:527:THR:N	2.35	0.40
4:A:1207:PEG:H22	5:A:1667:HOH:O	2.20	0.40
1:B:924:HIS:CD2	1:B:924:HIS:C	2.99	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	1111/1122 (99%)	1073 (97%)	37 (3%)	1 (0%)	48	46
1	B	1112/1122 (99%)	1073 (96%)	38 (3%)	1 (0%)	48	46
All	All	2223/2244 (99%)	2146 (96%)	75 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	906	LEU
1	B	906	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	975/965 (101%)	945 (97%)	30 (3%)	35	37
1	B	976/965 (101%)	951 (97%)	25 (3%)	40	44
All	All	1951/1930 (101%)	1896 (97%)	55 (3%)	38	41

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	45	LEU
1	A	91	ASP
1	A	95	THR
1	A	158	VAL
1	A	174	LEU
1	A	231	SER
1	A	232	LEU
1	A	269	GLU
1	A	270	SER
1	A	292	ARG
1	A	328	LEU
1	A	364	TYR
1	A	504	LEU
1	A	566	LYS
1	A	573	ARG
1	A	602	ILE
1	A	692	LEU
1	A	711	LEU
1	A	767	SER
1	A	789	LEU
1	A	802	LYS
1	A	847	GLU
1	A	875	LEU
1	A	921	GLN
1	A	940	LYS
1	A	974	GLU

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Mol	Chain	Res	Type
1	A	1014	ARG
1	A	1076	LEU
1	A	1112	LYS
1	B	7	SER
1	B	26	ASP
1	B	92	ILE
1	B	174	LEU
1	B	269	GLU
1	B	296	LYS
1	B	334	THR
1	B	364	TYR
1	B	504	LEU
1	B	513	ASP
1	B	525	ASN
1	B	692	LEU
1	B	762	LEU
1	B	789	LEU
1	B	794	LYS
1	B	802	LYS
1	B	838	LYS
1	B	855	LEU
1	B	921	GLN
1	B	974	GLU
1	B	1014	ARG
1	B	1039	LEU
1	B	1065	LYS
1	B	1069	VAL
1	B	1076	LEU

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	41	GLN
1	A	176	GLN
1	A	215	ASN
1	A	397	GLN
1	A	456	HIS
1	A	472	ASN
1	A	582	ASN
1	A	621	GLN
1	A	913	ASN
1	B	215	ASN

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Mol	Chain	Res	Type
1	B	397	GLN
1	B	409	GLN
1	B	465	HIS
1	B	582	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	$\# Z > 2$
2	GOL	A	1204	-	5,5,5	1.36	1 (20%)	5,5,5	0.83	0
2	GOL	A	1201	-	5,5,5	0.99	0	5,5,5	1.24	1 (20%)
4	PEG	B	1209	-	6,6,6	1.06	0	5,5,5	0.84	0
2	GOL	B	1202	-	5,5,5	0.69	0	5,5,5	0.56	0
2	GOL	B	1201	-	5,5,5	0.66	0	5,5,5	0.56	0
2	GOL	B	1203	-	5,5,5	0.34	0	5,5,5	1.42	1 (20%)
2	GOL	A	1202	-	5,5,5	1.05	0	5,5,5	0.90	0
2	GOL	B	1205	-	5,5,5	0.28	0	5,5,5	1.44	1 (20%)
4	PEG	A	1207	-	6,6,6	0.92	0	5,5,5	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1204	-	5,5,5	0.61	0	5,5,5	1.44	1 (20%)
4	PEG	A	1206	-	6,6,6	0.62	0	5,5,5	0.48	0
2	GOL	B	1206	-	5,5,5	0.75	0	5,5,5	0.40	0
2	GOL	A	1203	-	5,5,5	0.68	0	5,5,5	1.68	2 (40%)

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	GOL	A	1204	-	-	2/4/4/4	-
2	GOL	A	1201	-	-	4/4/4/4	-
4	PEG	B	1209	-	-	1/4/4/4	-
2	GOL	B	1202	-	-	0/4/4/4	-
2	GOL	B	1201	-	-	0/4/4/4	-
2	GOL	B	1203	-	-	2/4/4/4	-
2	GOL	A	1202	-	-	3/4/4/4	-
2	GOL	B	1205	-	-	4/4/4/4	-
4	PEG	A	1207	-	-	1/4/4/4	-
2	GOL	B	1204	-	-	2/4/4/4	-
4	PEG	A	1206	-	-	2/4/4/4	-
2	GOL	B	1206	-	-	0/4/4/4	-
2	GOL	A	1203	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1204	GOL	O3-C3	2.36	1.52	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1204	GOL	O2-C2-C1	2.57	119.82	109.18
2	A	1203	GOL	C3-C2-C1	-2.51	102.58	111.80
2	B	1203	GOL	O2-C2-C1	2.28	118.60	109.18
2	A	1203	GOL	O2-C2-C1	2.20	118.28	109.18
2	B	1205	GOL	O1-C1-C2	-2.13	100.77	110.38
2	A	1201	GOL	C3-C2-C1	-2.11	104.06	111.80

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	GOL	O1-C1-C2-O2
2	A	1201	GOL	O1-C1-C2-C3
2	A	1203	GOL	O1-C1-C2-C3
2	A	1203	GOL	C1-C2-C3-O3
2	A	1204	GOL	C1-C2-C3-O3
2	B	1203	GOL	C1-C2-C3-O3
2	B	1204	GOL	O1-C1-C2-C3
2	A	1201	GOL	C1-C2-C3-O3
2	A	1202	GOL	O1-C1-C2-C3
2	B	1205	GOL	O1-C1-C2-C3
2	B	1205	GOL	C1-C2-C3-O3
4	A	1206	PEG	O2-C3-C4-O4
2	A	1203	GOL	O1-C1-C2-O2
2	A	1203	GOL	O2-C2-C3-O3
2	B	1203	GOL	O2-C2-C3-O3
2	B	1205	GOL	O1-C1-C2-O2
2	B	1205	GOL	O2-C2-C3-O3
2	B	1204	GOL	O1-C1-C2-O2
2	A	1202	GOL	O1-C1-C2-O2
2	A	1204	GOL	O2-C2-C3-O3
4	A	1206	PEG	C4-C3-O2-C2
4	A	1207	PEG	C1-C2-O2-C3
2	A	1201	GOL	O2-C2-C3-O3
4	B	1209	PEG	C4-C3-O2-C2
2	A	1202	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1204	GOL	1	0
4	B	1209	PEG	8	0
2	A	1202	GOL	1	0
4	A	1207	PEG	4	0
2	B	1204	GOL	2	0
2	A	1203	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1095/1122 (97%)	-0.20	2 (0%) 91 90	17, 29, 49, 70	0
1	B	1095/1122 (97%)	-0.21	4 (0%) 88 88	18, 29, 47, 70	0
All	All	2190/2244 (97%)	-0.21	6 (0%) 90 89	17, 29, 48, 70	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	3.2
1	A	1113	ASN	2.7
1	B	525	ASN	2.4
1	B	798	HIS	2.3
1	B	1113	ASN	2.3
1	A	718	LYS	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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1204	6/6	0.80	0.14	36,48,50,51	0
2	GOL	B	1205	6/6	0.82	0.14	46,53,59,60	0
4	PEG	B	1209	7/7	0.82	0.14	33,37,42,43	0
2	GOL	A	1203	6/6	0.86	0.12	36,43,46,48	0
4	PEG	A	1207	7/7	0.87	0.12	35,37,40,43	0
4	PEG	A	1206	7/7	0.87	0.14	38,48,55,61	0
2	GOL	A	1204	6/6	0.88	0.12	35,38,41,42	0
2	GOL	A	1202	6/6	0.88	0.13	33,39,46,53	0
2	GOL	B	1203	6/6	0.89	0.11	29,36,40,42	0
2	GOL	A	1201	6/6	0.89	0.11	27,30,33,33	0
2	GOL	B	1202	6/6	0.91	0.12	31,43,45,47	0
2	GOL	B	1206	6/6	0.92	0.11	31,33,36,39	0
3	CA	B	1207	1/1	0.93	0.12	59,59,59,59	0
2	GOL	B	1201	6/6	0.96	0.06	24,26,27,28	0
3	CA	B	1208	1/1	0.98	0.09	37,37,37,37	0
3	CA	A	1205	1/1	0.98	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.