WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 09:16 PM JST

PDB ID	:	4ZOB
Title	:	Crystal Structure of beta-glucosidase from Listeria innocua in complex with gluconolactone
Authors	:	Nakajima, M.; Yoshida, R.; Miyanaga, A.; Abe, K.; Takahashi, Y.; Sugimoto, N.; Toyoizumi, H.; Nakai, H.; Kitaoka, M.; Taguchi, H.
Deposited on	:	2015-05-06
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references (i)) 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.7%
RSRZ outliers		4.5%

Worse — Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
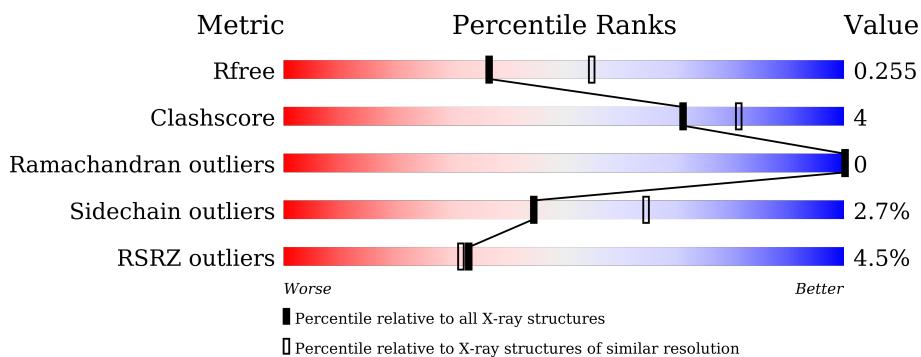
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	731	3% · 89% · 9% ··
1	B	731	5% · 88% · 10% ··

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 11648 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 Lin1840 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	2	0
			5595	3540	926	1104	25			
1	B	721	Total	C	N	O	S	0	0	0
			5570	3526	922	1098	24			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP Q92AS9
A	724	LEU	-	expression tag	UNP Q92AS9
A	725	GLU	-	expression tag	UNP Q92AS9
A	726	HIS	-	expression tag	UNP Q92AS9
A	727	HIS	-	expression tag	UNP Q92AS9
A	728	HIS	-	expression tag	UNP Q92AS9
A	729	HIS	-	expression tag	UNP Q92AS9
A	730	HIS	-	expression tag	UNP Q92AS9
A	731	HIS	-	expression tag	UNP Q92AS9
B	2	GLU	LYS	engineered mutation	UNP Q92AS9
B	724	LEU	-	expression tag	UNP Q92AS9
B	725	GLU	-	expression tag	UNP Q92AS9
B	726	HIS	-	expression tag	UNP Q92AS9
B	727	HIS	-	expression tag	UNP Q92AS9
B	728	HIS	-	expression tag	UNP Q92AS9
B	729	HIS	-	expression tag	UNP Q92AS9
B	730	HIS	-	expression tag	UNP Q92AS9
B	731	HIS	-	expression tag	UNP Q92AS9

- Molecule 2 is D-glucono-1,5-lactone (three-letter code: LGC) (formula: $C_6H_{10}O_6$).
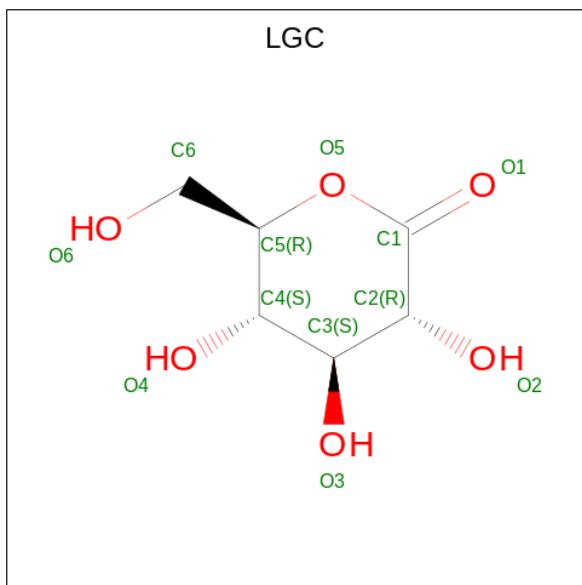
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 6	O 6	0	0
2	A	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
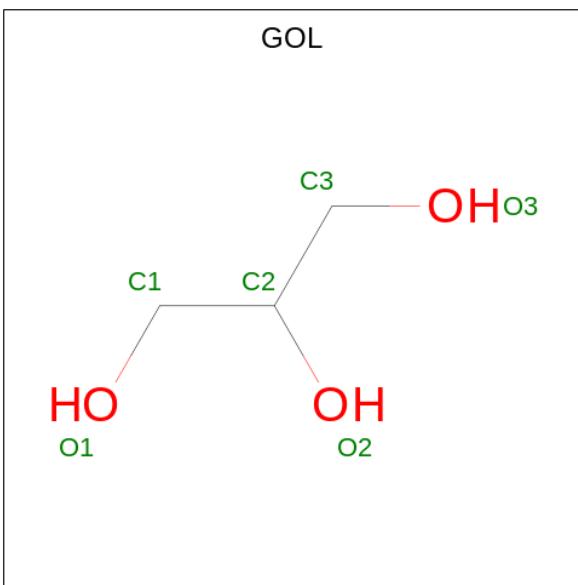
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 12	C 6	O 6	0	1
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 12	C 6	O 6	0	1
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

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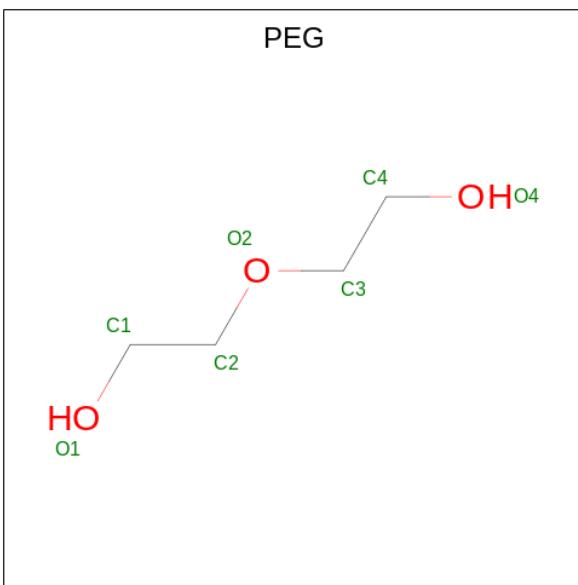
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 7	C 4	O 3	0	0

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
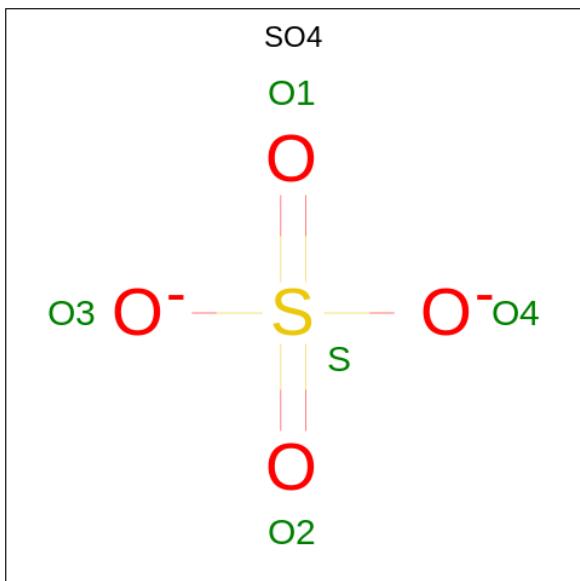
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 5	O 4	S 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	190	Total 190	O 190	0	0
7	B	177	Total 177	O 177	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: Lin1840 protein

Chain A:

• Molecule 1: Lin1840 protein

Chain B:
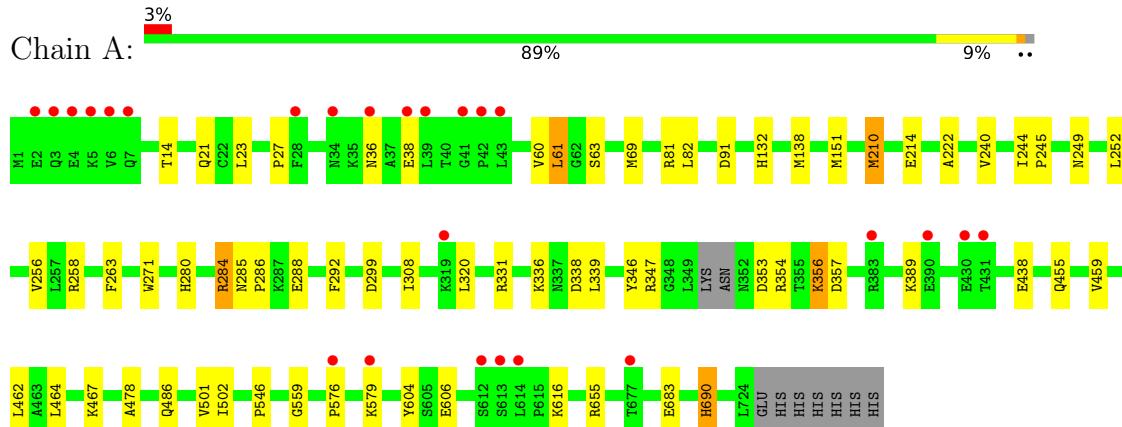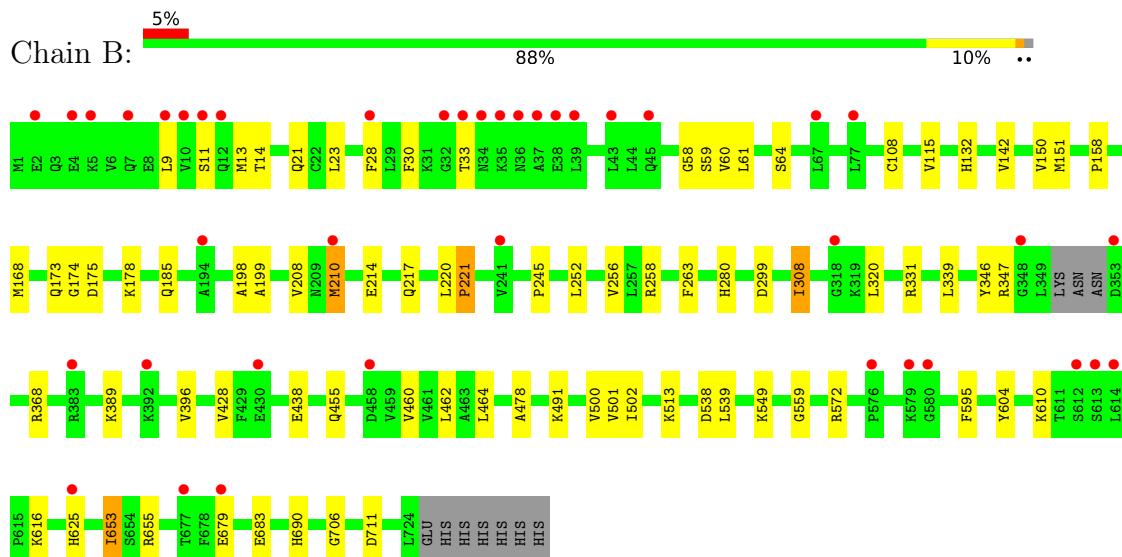
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.36Å 95.81Å 213.31Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	41.91 – 2.40 41.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.91-2.40) 99.9 (41.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.170 , 0.250 0.178 , 0.255	Depositor DCC
R_{free} test set	3569 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11648	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, PEG, SO4, LGC

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	0.64	0/5696	0.82	3/7718 (0.0%)
1	B	0.62	0/5671	0.80	3/7685 (0.0%)
All	All	0.63	0/11367	0.81	6/15403 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	B	655	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	210	MET	CG-SD-CE	5.63	109.21	100.20
1	A	338	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	501	VAL	CB-CA-C	-5.24	101.44	111.40
1	B	501	VAL	CB-CA-C	-5.12	101.68	111.40

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	5595	0	5538	41	0
1	B	5570	0	5519	41	0
2	A	24	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	36	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	40	2	0
4	B	12	0	16	2	0
5	B	7	0	10	1	0
6	B	5	0	0	0	0
7	A	190	0	0	5	0
7	B	177	0	0	0	0
All	All	11648	0	11173	79	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 4.

All (79) 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:353:ASP:OD2	1:A:356:LYS:HE3	1.29	1.25
1:A:353:ASP:OD2	1:A:356:LYS:CE	2.06	1.03
1:A:210[B]:MET:CE	1:A:214:GLU:HB3	2.19	0.72
1:A:210[B]:MET:HE2	1:A:214:GLU:HB3	1.75	0.69
1:A:299:ASP:OD1	1:A:331:ARG:NH1	2.26	0.68
1:A:353:ASP:OD2	1:A:356:LYS:CD	2.44	0.66
1:B:23:LEU:HD22	1:B:308:ILE:HG13	1.79	0.64
1:B:438:GLU:OE2	1:B:438:GLU:HA	1.96	0.64
1:A:252:LEU:O	1:A:256:VAL:HB	1.98	0.63
1:A:210[B]:MET:HE2	1:A:214:GLU:CB	2.30	0.61
1:A:353:ASP:OD2	1:A:356:LYS:HD2	2.01	0.61
1:B:30:PHE:CE2	1:B:60:VAL:HG22	2.37	0.60
1:B:625:HIS:CE1	1:B:679:GLU:HG3	2.39	0.57
1:B:217:GLN:O	4:B:807:GOL:H11	2.05	0.57
7:A:1061:HOH:O	1:B:690:HIS:HA	2.06	0.56
1:A:389:LYS:NZ	7:A:902:HOH:O	2.37	0.56
1:B:438:GLU:OE2	1:B:438:GLU:CA	2.51	0.56
1:A:576:PRO:O	1:A:579:LYS:HG2	2.07	0.55
1:A:91:ASP:OD2	2:A:801:LGC:O6	2.24	0.54
1:A:655:ARG:NH1	7:A:901:HOH:O	2.29	0.54
1:B:389:LYS:HE3	1:B:428:VAL:O	2.08	0.54
1:A:354:ARG:O	1:A:357:ASP:HB2	2.09	0.53
1:A:36:ASN:O	1:A:38:GLU:O	2.27	0.52
1:A:23:LEU:HD22	1:A:308:ILE:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ALA:O	1:B:559:GLY:HA3	2.11	0.50
1:B:462:LEU:O	1:B:502:ILE:HA	2.12	0.50
1:A:690:HIS:CD2	1:A:690:HIS:H	2.29	0.49
1:B:539:LEU:O	1:B:604:TYR:OH	2.25	0.49
1:B:299:ASP:OD1	1:B:331:ARG:NH1	2.46	0.49
1:B:513:LYS:HG3	1:B:595:PHE:CE1	2.48	0.49
1:A:299:ASP:CG	1:A:331:ARG:HH11	2.15	0.48
1:B:690:HIS:CD2	1:B:690:HIS:H	2.32	0.47
1:A:132:HIS:HB3	1:A:339:LEU:HD13	1.97	0.46
1:B:175:ASP:OD2	1:B:178:LYS:CE	2.64	0.46
1:A:438[B]:GLU:HG2	4:A:805:GOL:C1	2.45	0.46
1:B:108:CYS:HA	1:B:549:LYS:O	2.17	0.45
1:B:115:VAL:CG1	1:B:168:MET:HG2	2.46	0.45
1:B:142:VAL:HB	1:B:150:VAL:HG12	1.98	0.45
1:A:467:LYS:HB3	7:A:994:HOH:O	2.15	0.45
1:B:9:LEU:O	1:B:13:MET:HG3	2.17	0.45
1:B:214:GLU:OE1	5:B:801:PEG:H41	2.16	0.45
1:B:132:HIS:HB3	1:B:339:LEU:HD13	1.98	0.45
1:B:198:ALA:O	1:B:199:ALA:C	2.56	0.45
1:A:61:LEU:HD21	1:A:271:TRP:CZ3	2.52	0.44
1:B:175:ASP:OD2	1:B:178:LYS:HE2	2.17	0.44
1:A:346:TYR:O	1:A:347:ARG:C	2.56	0.44
1:B:245:PRO:HG3	1:B:280:HIS:CG	2.52	0.44
1:B:198:ALA:HB3	1:B:208:VAL:HG13	1.99	0.44
1:B:220:LEU:N	1:B:221:PRO:CD	2.81	0.44
1:B:460:VAL:HB	1:B:500:VAL:HG22	2.00	0.44
1:B:462:LEU:HD11	1:B:464:LEU:HD21	2.00	0.44
1:A:258:ARG:HG2	1:A:263:PHE:O	2.17	0.43
1:A:462:LEU:O	1:A:502:ILE:HA	2.17	0.43
1:A:81:ARG:NH2	1:A:82:LEU:HD21	2.32	0.43
1:A:285:ASN:HB2	1:A:286:PRO:HD2	2.00	0.43
1:B:368:ARG:NH2	1:B:538:ASP:OD2	2.51	0.43
1:A:245:PRO:HG3	1:A:280:HIS:CG	2.53	0.43
1:B:258:ARG:HG2	1:B:263:PHE:O	2.19	0.43
1:A:244:ILE:HD13	1:B:653:ILE:HD12	1.99	0.42
1:A:60:VAL:HG12	1:A:61:LEU:N	2.33	0.42
1:B:28:PHE:HA	1:B:33:THR:HG21	2.02	0.42
1:B:252:LEU:O	1:B:256:VAL:HB	2.19	0.42
1:B:706:GLY:HA3	1:B:711:ASP:O	2.19	0.42
1:A:288:GLU:HB3	1:A:292:PHE:CE2	2.55	0.42
1:A:244:ILE:HB	1:A:249:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:GLY:HA3	1:B:478:ALA:O	2.19	0.42
1:A:21:GLN:OE1	1:A:336:LYS:NZ	2.33	0.42
1:A:222:ALA:HB3	7:A:990:HOH:O	2.20	0.42
1:A:271:TRP:O	1:B:572:ARG:NH2	2.53	0.42
1:A:464:LEU:HB3	1:A:486:GLN:OE1	2.20	0.42
1:B:158:PRO:HG2	4:B:807:GOL:H12	2.01	0.42
1:A:546:PRO:HD2	1:A:604:TYR:CE2	2.56	0.41
1:B:21:GLN:O	1:B:58:GLY:HA3	2.20	0.41
1:B:346:TYR:O	1:B:347:ARG:C	2.58	0.41
1:B:59:SER:OG	1:B:60:VAL:N	2.54	0.40
1:A:27:PRO:HD3	1:A:61:LEU:O	2.21	0.40
1:A:240:VAL:HA	1:A:245:PRO:HA	2.03	0.40
1:B:173:GLN:O	1:B:174:GLY:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	720/731 (98%)	688 (96%)	32 (4%)	0	100	100
1	B	717/731 (98%)	693 (97%)	24 (3%)	0	100	100
All	All	1437/1462 (98%)	1381 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	605/612 (99%)	588 (97%)	17 (3%)	43	63
1	B	602/612 (98%)	585 (97%)	17 (3%)	43	63
All	All	1207/1224 (99%)	1173 (97%)	34 (3%)	44	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	61	LEU
1	A	63	SER
1	A	69	MET
1	A	138	MET
1	A	151	MET
1	A	210[A]	MET
1	A	210[B]	MET
1	A	284	ARG
1	A	320	LEU
1	A	356	LYS
1	A	455	GLN
1	A	459	VAL
1	A	606	GLU
1	A	616	LYS
1	A	683	GLU
1	A	690	HIS
1	B	11	SER
1	B	14	THR
1	B	61	LEU
1	B	64	SER
1	B	151	MET
1	B	185	GLN
1	B	210	MET
1	B	221	PRO
1	B	308	ILE
1	B	320	LEU
1	B	396	VAL
1	B	455	GLN
1	B	491	LYS
1	B	610	LYS
1	B	616	LYS
1	B	653	ILE

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Mol	Chain	Res	Type
1	B	683	GLU

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	690	HIS
1	B	12	GLN
1	B	625	HIS
1	B	690	HIS

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 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	#$\|Z\| > 2$
4	GOL	A	804[A]	-	5,5,5	0.46	0	5,5,5	0.34	0
4	GOL	B	807	-	5,5,5	0.54	0	5,5,5	0.48	0
2	LGC	B	803	-	12,12,12	2.50	1 (8%)	15,17,17	1.33	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	A	805	-	5,5,5	0.33	0	5,5,5	0.70	0
2	LGC	B	804	-	12,12,12	2.51	1 (8%)	15,17,17	1.40	3 (20%)
4	GOL	B	806	-	5,5,5	0.32	0	5,5,5	0.42	0
2	LGC	A	802	-	12,12,12	2.60	1 (8%)	15,17,17	1.24	2 (13%)
2	LGC	A	801	-	12,12,12	2.37	2 (16%)	15,17,17	1.14	2 (13%)
2	LGC	B	802	-	12,12,12	2.43	1 (8%)	15,17,17	0.78	1 (6%)
6	SO4	B	808	-	4,4,4	0.34	0	6,6,6	0.41	0
4	GOL	A	804[B]	-	5,5,5	0.25	0	5,5,5	0.52	0
5	PEG	B	801	-	6,6,6	0.99	0	5,5,5	1.08	0
4	GOL	A	806[B]	-	5,5,5	0.38	0	5,5,5	0.25	0
4	GOL	A	806[A]	-	5,5,5	0.45	0	5,5,5	0.38	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
4	GOL	A	804[A]	-	-	4/4/4/4	-
4	GOL	B	807	-	-	2/4/4/4	-
2	LGC	B	803	-	-	0/2/22/22	0/1/1/1
4	GOL	A	805	-	-	2/4/4/4	-
2	LGC	B	804	-	-	2/2/22/22	0/1/1/1
4	GOL	B	806	-	-	2/4/4/4	-
2	LGC	A	802	-	-	1/2/22/22	0/1/1/1
2	LGC	A	801	-	-	0/2/22/22	0/1/1/1
2	LGC	B	802	-	-	0/2/22/22	0/1/1/1
4	GOL	A	804[B]	-	-	4/4/4/4	-
5	PEG	B	801	-	-	2/4/4/4	-
4	GOL	A	806[B]	-	-	2/4/4/4	-
4	GOL	A	806[A]	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	LGC	O5-C1	8.81	1.47	1.34
2	B	804	LGC	O5-C1	8.33	1.47	1.34
2	B	803	LGC	O5-C1	8.30	1.47	1.34
2	B	802	LGC	O5-C1	7.99	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	LGC	O5-C1	7.05	1.45	1.34
2	A	801	LGC	O5-C5	-3.25	1.42	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	804	LGC	O4-C4-C5	2.99	116.72	109.30
2	A	801	LGC	O2-C2-C3	-2.91	104.52	110.53
2	A	802	LGC	O5-C5-C4	2.84	114.78	109.73
2	B	803	LGC	C4-C3-C2	2.79	114.61	110.18
2	A	801	LGC	O3-C3-C4	2.63	116.42	110.35
2	B	803	LGC	O5-C1-C2	2.46	122.88	119.20
2	B	803	LGC	O3-C3-C2	-2.30	105.29	109.68
2	B	804	LGC	O4-C4-C3	-2.17	105.34	110.35
2	B	802	LGC	O5-C1-C2	2.15	122.41	119.20
2	B	804	LGC	C3-C4-C5	-2.05	106.58	110.24
2	A	802	LGC	C4-C3-C2	-2.01	106.99	110.18

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804[A]	GOL	O1-C1-C2-O2
4	A	804[A]	GOL	O1-C1-C2-C3
4	A	804[A]	GOL	C1-C2-C3-O3
4	A	804[B]	GOL	O1-C1-C2-C3
4	A	804[B]	GOL	O2-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	A	806[A]	GOL	C1-C2-C3-O3
4	A	806[B]	GOL	C1-C2-C3-O3
4	B	806	GOL	O1-C1-C2-C3
4	B	807	GOL	C1-C2-C3-O3
4	B	807	GOL	O2-C2-C3-O3
2	B	804	LGC	O5-C5-C6-O6
2	B	804	LGC	C4-C5-C6-O6
5	B	801	PEG	O2-C3-C4-O4
4	A	804[B]	GOL	C1-C2-C3-O3
4	A	804[A]	GOL	O2-C2-C3-O3
4	A	804[B]	GOL	O1-C1-C2-O2
4	A	806[A]	GOL	O2-C2-C3-O3
4	A	806[B]	GOL	O2-C2-C3-O3
4	B	806	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	805	GOL	O1-C1-C2-O2
4	A	806[A]	GOL	O1-C1-C2-C3
2	A	802	LGC	C4-C5-C6-O6
5	B	801	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	807	GOL	2	0
4	A	805	GOL	2	0
2	A	801	LGC	1	0
5	B	801	PEG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	722/731 (98%)	-0.03	25 (3%)	44	43	13, 28, 54, 78	0
1	B	721/731 (98%)	0.09	40 (5%)	25	24	14, 31, 57, 80	0
All	All	1443/1462 (98%)	0.03	65 (4%)	33	31	13, 30, 56, 80	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	LEU	5.1
1	B	579	LYS	5.0
1	A	38	GLU	4.5
1	A	42	PRO	4.3
1	A	4	GLU	4.1
1	A	43	LEU	4.1
1	B	38	GLU	3.9
1	B	39	LEU	3.7
1	A	5	LYS	3.7
1	A	41	GLY	3.7
1	B	34	ASN	3.7
1	B	37	ALA	3.5
1	B	2	GLU	3.4
1	A	2	GLU	3.2
1	B	614	LEU	3.0
1	B	353	ASP	3.0
1	B	36	ASN	3.0
1	A	28	PHE	3.0
1	B	580	GLY	3.0
1	B	12	GLN	3.0
1	A	677	THR	2.9
1	A	34	ASN	2.9
1	B	613	SER	2.9
1	B	677	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	579	LYS	2.9
1	B	383	ARG	2.8
1	B	5	LYS	2.8
1	A	383	ARG	2.7
1	A	430	GLU	2.7
1	B	45	GLN	2.6
1	B	32	GLY	2.6
1	B	4	GLU	2.5
1	B	43	LEU	2.5
1	B	194	ALA	2.5
1	B	10	VAL	2.5
1	B	35	LYS	2.5
1	A	390	GLU	2.5
1	A	319	LYS	2.4
1	B	28	PHE	2.4
1	B	392	LYS	2.4
1	A	614	LEU	2.4
1	B	576	PRO	2.4
1	A	3	GLN	2.4
1	B	348	GLY	2.3
1	B	430	GLU	2.3
1	A	576	PRO	2.3
1	A	613	SER	2.3
1	B	77	LEU	2.3
1	B	612	SER	2.2
1	B	625	HIS	2.2
1	A	431	THR	2.2
1	B	241	VAL	2.2
1	B	33	THR	2.2
1	B	67	LEU	2.2
1	B	679	GLU	2.2
1	B	318	GLY	2.1
1	A	6	VAL	2.1
1	A	36	ASN	2.1
1	B	210	MET	2.1
1	B	458	ASP	2.0
1	B	11	SER	2.0
1	A	612	SER	2.0
1	B	9	LEU	2.0
1	A	7	GLN	2.0
1	B	7	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

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
2	LGC	B	804	12/12	0.82	0.23	49,58,64,67	0
5	PEG	B	801	7/7	0.86	0.35	27,34,36,40	0
4	GOL	B	806	6/6	0.89	0.18	44,49,55,59	0
4	GOL	A	806[B]	6/6	0.91	0.17	37,44,45,47	6
2	LGC	B	803	12/12	0.91	0.17	37,50,58,60	0
4	GOL	A	806[A]	6/6	0.91	0.17	21,26,27,29	6
4	GOL	B	807	6/6	0.92	0.23	31,38,42,44	0
2	LGC	A	802	12/12	0.92	0.14	35,46,52,60	0
4	GOL	A	804[B]	6/6	0.93	0.17	28,29,31,31	6
4	GOL	A	804[A]	6/6	0.93	0.17	9,20,23,26	6
4	GOL	A	805	6/6	0.94	0.15	34,38,42,45	0
2	LGC	A	801	12/12	0.97	0.13	12,22,25,25	0
2	LGC	B	802	12/12	0.97	0.13	22,26,28,31	0
3	MG	A	803	1/1	0.98	0.07	28,28,28,28	0
6	SO4	B	808	5/5	0.98	0.12	36,40,45,58	0
3	MG	B	805	1/1	0.99	0.03	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.