



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 04:47 AM EDT

PDB ID : 4ZOC
Title : Crystal Structure of mutant (D270A) beta-glucosidase from *Listeria innocua* in complex with sophorotriose
Authors : Nakajima, M.; Yoshida, R.; Miyanaga, A.; Abe, K.; Takahashi, Y.; Sugimoto, N.; Toyozumi, H.; Nakai, H.; Kitaoka, M.; Taguchi, H.
Deposited on : 2015-05-06
Resolution : 1.79 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

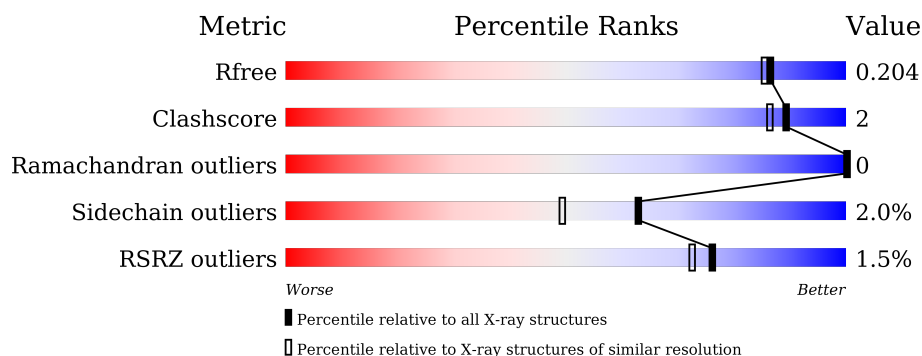
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	731	<div> <div>%</div> <div>91% 7% ..</div> </div>
1	B	731	<div> <div>2%</div> <div>91% 7% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	801[A]	-	-	X	X
2	GOL	A	801[B]	-	-	-	X
2	GOL	A	804	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12626 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	724	Total	C	N	O	S	0	7	0
			5651	3575	936	1114	26			
1	B	724	Total	C	N	O	S	0	5	0
			5632	3564	933	1108	27			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP Q92AS9
A	270	ALA	ASP	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	270	ALA	ASP	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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

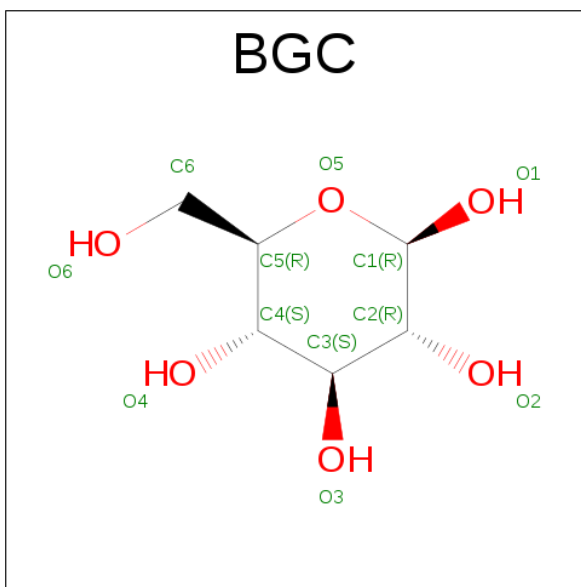


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 4 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C₆H₁₂O₆).



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

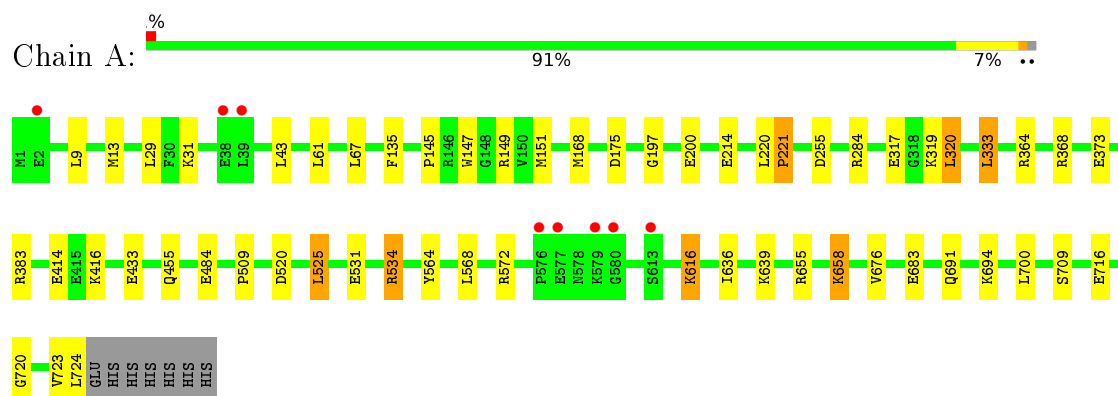
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	696	Total	O	0	0
			696	696		
5	B	603	Total	O	0	0
			603	603		

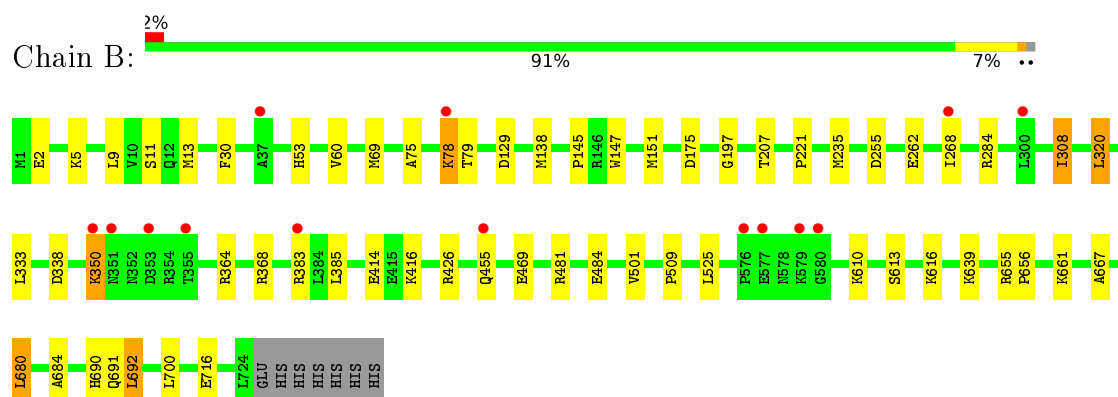
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



- Molecule 1: Lin1840 protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.62Å 94.86Å 215.06Å 90.00° 96.33° 90.00°	Depositor
Resolution (Å)	32.50 – 1.79 32.50 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (32.50-1.79) 98.9 (32.50-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.141 , 0.196 0.154 , 0.204	Depositor DCC
R_{free} test set	8390 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12626	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, BGC

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	1.02	8/5753 (0.1%)	1.02	23/7794 (0.3%)
1	B	0.98	6/5734 (0.1%)	1.05	20/7769 (0.3%)
All	All	1.00	14/11487 (0.1%)	1.03	43/15563 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	484	GLU	CD-OE1	7.64	1.34	1.25
1	B	262	GLU	CD-OE1	-7.57	1.17	1.25
1	A	200	GLU	CD-OE2	6.83	1.33	1.25
1	A	720	GLY	C-O	-6.17	1.13	1.23
1	B	11	SER	CB-OG	-5.93	1.34	1.42
1	B	484	GLU	CD-OE2	5.82	1.32	1.25
1	A	214	GLU	CD-OE1	5.61	1.31	1.25
1	A	368	ARG	CD-NE	-5.40	1.37	1.46
1	A	135	PHE	CG-CD1	5.38	1.46	1.38
1	A	484	GLU	CD-OE2	5.37	1.31	1.25
1	A	433	GLU	CD-OE1	-5.30	1.19	1.25
1	B	655	ARG	CD-NE	-5.20	1.37	1.46
1	B	469	GLU	CD-OE1	-5.09	1.20	1.25
1	A	484	GLU	CD-OE1	5.01	1.31	1.25

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	655	ARG	NE-CZ-NH2	19.63	130.12	120.30
1	B	655	ARG	NE-CZ-NH1	-15.58	112.51	120.30
1	B	284	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	A	364	ARG	NE-CZ-NH2	-11.99	114.30	120.30
1	A	655	ARG	NE-CZ-NH2	11.47	126.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	ARG	NE-CZ-NH1	-11.45	114.57	120.30
1	B	364	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	368	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	B	481	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	A	364	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	B	364	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	B	368	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	572	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	255	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	534	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	525	LEU	CA-CB-CG	-6.86	99.52	115.30
1	A	284	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	B	368	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	B	426	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	520	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	426	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	320	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	368	ARG	CB-CG-CD	-6.19	95.51	111.60
1	A	724	LEU	CA-CB-CG	6.12	129.38	115.30
1	B	320	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	255	ASP	CB-CG-OD1	5.89	123.61	118.30
1	B	692	LEU	CB-CG-CD2	5.86	120.95	111.00
1	A	572	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	333	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	692	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	525	LEU	CB-CG-CD2	5.59	120.50	111.00
1	B	284	ARG	CB-CG-CD	5.58	126.12	111.60
1	A	723	VAL	C-N-CA	5.49	135.42	121.70
1	B	338	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	484	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	A	658	LYS	CD-CE-NZ	5.22	123.72	111.70
1	A	149	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	168	MET	CG-SD-CE	-5.13	91.99	100.20
1	A	175	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	724	LEU	N-CA-CB	5.04	120.49	110.40
1	B	680	LEU	CB-CG-CD1	5.04	119.57	111.00
1	B	175	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	525	LEU	CA-CB-CG	-5.00	103.79	115.30

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	5651	0	5597	26	0
1	B	5632	0	5583	26	0
2	A	18	0	24	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
5	A	696	0	0	8	0
5	B	603	0	0	2	0
All	All	12626	0	11228	54	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 2.

All (54) 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)
2:A:801[A]:GOL:H32	1:B:207:THR:HG21	1.59	0.83
2:A:801[A]:GOL:C3	1:B:207:THR:HG21	2.12	0.78
1:B:75:ALA:HA	1:B:78:LYS:HD3	1.69	0.74
1:A:683[B]:GLU:OE2	1:A:694:LYS:NZ	2.21	0.72
1:A:658:LYS:HE2	1:A:709:SER:O	1.96	0.66
1:A:564:TYR:OH	2:A:801[A]:GOL:O2	2.14	0.63
1:B:690:HIS:CE1	1:B:691:GLN:HG3	2.36	0.61
1:B:455:GLN:HG3	5:B:1105:HOH:O	2.00	0.60
2:A:801[B]:GOL:C1	5:A:969:HOH:O	2.52	0.57
1:A:455:GLN:NE2	5:A:906:HOH:O	2.40	0.55
1:B:2:GLU:HB2	1:B:5:LYS:HE3	1.88	0.55
1:B:9:LEU:O	1:B:13:MET:HG3	2.10	0.52
2:A:801[A]:GOL:H31	1:B:207:THR:HG21	1.91	0.52
1:A:531:GLU:OE1	1:A:534:ARG:HD2	2.10	0.51
1:A:636:ILE:HD13	5:A:1307:HOH:O	2.10	0.51
1:A:616:LYS:CA	1:A:616:LYS:HE3	2.40	0.50
1:A:373:GLU:OE2	1:A:639:LYS:NZ	2.44	0.50
1:A:616:LYS:HE3	1:A:616:LYS:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:PRO:HB3	1:A:509:PRO:HD2	1.94	0.49
1:A:147:TRP:CZ3	1:A:197:GLY:HA2	2.47	0.48
1:A:317:GLU:OE1	1:A:319:LYS:NZ	2.33	0.47
1:A:29:LEU:HD21	1:A:43:LEU:HD23	1.97	0.47
1:B:2:GLU:HB2	1:B:5:LYS:CE	2.45	0.47
1:A:700:LEU:HD11	1:A:716:GLU:HB3	1.96	0.46
1:B:661:LYS:HE3	1:B:684:ALA:O	2.16	0.46
1:B:145:PRO:HB3	1:B:509:PRO:HD2	1.98	0.46
1:B:656:PRO:HG3	5:B:1384:HOH:O	2.16	0.46
1:A:636:ILE:CD1	5:A:1307:HOH:O	2.64	0.45
1:B:30:PHE:CE2	1:B:60:VAL:HG22	2.52	0.45
1:B:385:LEU:HD21	1:B:501:VAL:HG21	1.99	0.45
1:A:564:TYR:HH	2:A:801[A]:GOL:HO2	1.59	0.45
1:B:690:HIS:NE2	1:B:691:GLN:HG3	2.31	0.44
1:A:616:LYS:HE3	1:A:616:LYS:HA	1.98	0.44
1:A:383:ARG:HG2	5:A:1503:HOH:O	2.17	0.44
1:B:700:LEU:HD11	1:B:716:GLU:HB3	1.99	0.44
1:A:31:LYS:HE3	5:A:1530:HOH:O	2.17	0.43
1:A:683[B]:GLU:OE2	1:A:694:LYS:CE	2.66	0.43
1:B:414:GLU:OE1	1:B:416:LYS:HE3	2.18	0.43
2:A:801[A]:GOL:H31	1:B:207:THR:CG2	2.49	0.42
1:B:350:LYS:O	1:B:350:LYS:HD3	2.19	0.42
1:A:568:LEU:HG	2:A:801[A]:GOL:H2	2.01	0.42
1:A:9:LEU:O	1:A:13:MET:HG3	2.19	0.42
1:A:455:GLN:HG3	5:A:1133:HOH:O	2.20	0.42
1:A:220:LEU:N	1:A:221:PRO:CD	2.83	0.42
1:B:78:LYS:HG2	1:B:79:THR:HG23	2.02	0.41
1:B:53:HIS:CD2	1:B:308:ILE:HD12	2.54	0.41
1:B:639:LYS:HG2	1:B:667:ALA:HA	2.02	0.41
1:B:69[B]:MET:C	1:B:69[B]:MET:SD	2.98	0.41
2:A:801[B]:GOL:H12	5:A:969:HOH:O	2.19	0.41
1:B:235:MET:HA	1:B:268:ILE:O	2.21	0.41
1:A:414:GLU:OE1	1:A:416:LYS:HE3	2.21	0.41
1:B:147:TRP:CZ3	1:B:197:GLY:HA2	2.57	0.40
1:A:61:LEU:HD23	1:A:61:LEU:H	1.86	0.40
2:A:801[A]:GOL:C3	1:B:207:THR:CG2	2.90	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	729/731 (100%)	712 (98%)	17 (2%)	0	100	100
1	B	727/731 (100%)	709 (98%)	18 (2%)	0	100	100
All	All	1456/1462 (100%)	1421 (98%)	35 (2%)	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	611/611 (100%)	602 (98%)	9 (2%)	72	62
1	B	609/611 (100%)	594 (98%)	15 (2%)	55	39
All	All	1220/1222 (100%)	1196 (98%)	24 (2%)	63	49

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	151	MET
1	A	221	PRO
1	A	320	LEU
1	A	333	LEU
1	A	525	LEU
1	A	616	LYS
1	A	676	VAL

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Mol	Chain	Res	Type
1	A	691	GLN
1	B	78	LYS
1	B	129	ASP
1	B	138	MET
1	B	151	MET
1	B	221	PRO
1	B	308	ILE
1	B	320	LEU
1	B	333	LEU
1	B	350	LYS
1	B	383	ARG
1	B	610	LYS
1	B	613	SER
1	B	616	LYS
1	B	680	LEU
1	B	692	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	B	567	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	801[A]	-	5,5,5	0.61	0	5,5,5	1.30	0
2	GOL	A	801[B]	-	5,5,5	0.44	0	5,5,5	1.50	1 (20%)
4	BGC	A	803	-	12,12,12	0.91	0	17,17,17	1.14	3 (17%)
2	GOL	A	804	-	5,5,5	0.24	0	5,5,5	1.00	0
4	BGC	B	801	-	12,12,12	1.33	2 (16%)	17,17,17	1.45	2 (11%)

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	801[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	A	801[B]	-	-	0/4/4/4	0/0/0/0
4	BGC	A	803	-	-	0/2/22/22	0/1/1/1
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	BGC	B	801	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	BGC	C4-C3	2.03	1.57	1.52
4	B	801	BGC	O4-C4	2.22	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	BGC	C3-C4-C5	-2.18	106.35	110.23
2	A	801[B]	GOL	O2-C2-C1	-2.15	98.16	108.47
4	A	803	BGC	C1-O5-C5	2.05	117.47	113.54
4	A	803	BGC	O4-C4-C3	2.13	115.16	110.36
4	A	803	BGC	O2-C2-C3	2.18	115.27	110.36
4	B	801	BGC	O5-C5-C6	3.59	115.69	106.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801[A]	GOL	8	0
2	A	801[B]	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

6.1 Protein, DNA and RNA chains

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	724/731 (99%)	-0.17	8 (1%) 82 80	6, 11, 25, 46	0
1	B	724/731 (99%)	-0.07	14 (1%) 70 66	7, 14, 30, 51	0
All	All	1448/1462 (99%)	-0.12	22 (1%) 76 72	6, 13, 28, 51	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	ASN	5.0
1	B	576	PRO	4.4
1	A	576	PRO	4.3
1	B	350	LYS	3.6
1	B	580	GLY	3.5
1	B	579	LYS	3.5
1	A	579	LYS	3.5
1	A	580	GLY	3.3
1	B	353	ASP	3.0
1	B	355	THR	2.9
1	B	268	ILE	2.6
1	A	39	LEU	2.4
1	A	577	GLU	2.4
1	A	613	SER	2.4
1	A	2	GLU	2.4
1	B	383	ARG	2.3
1	B	37	ALA	2.2
1	A	38	GLU	2.2
1	B	455	GLN	2.2
1	B	577	GLU	2.2
1	B	78	LYS	2.1
1	B	300	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	804	6/6	0.93	0.17	12.95	29,30,34,45	0
2	GOL	A	801[B]	6/6	0.94	0.15	4.50	12,19,21,25	6
2	GOL	A	801[A]	6/6	0.94	0.15	4.33	6,8,8,9	6
4	BGC	B	801	12/12	0.95	0.09	0.38	11,15,19,21	0
4	BGC	A	803	12/12	0.96	0.07	-0.46	14,19,21,24	0
3	MG	A	802	1/1	1.00	0.05	-1.99	11,11,11,11	0
3	MG	B	802	1/1	0.99	0.05	-2.36	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.