Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 11:44 am GMT

PDB ID	:	4UCF
Title	:	Crystal structure of Bifidobacterium bifidum beta-galactosidase in complex with alpha-galactose
Authors	:	Godoy, A.S.; Murakami, M.T.; Camilo, C.M.; Bernardes, A.; Polikarpov, I.
Deposited on	:	2014-12-03
Resolution	:	1.94 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:

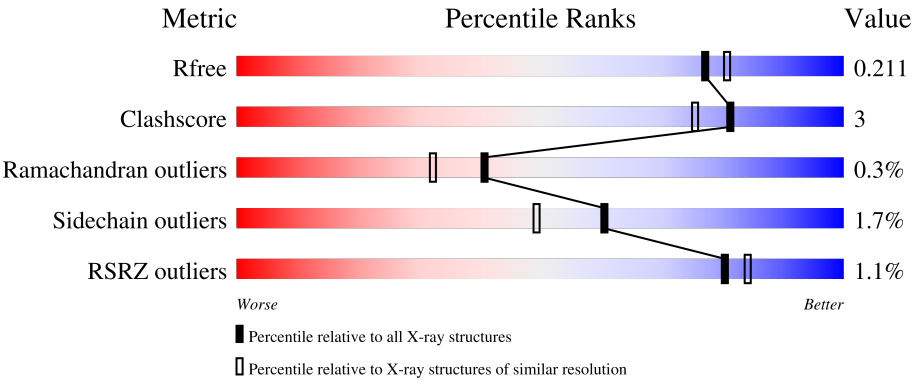
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	689	92% 7%
1	B	689	2% 91% 8%
1	C	689	90% 9%

2 Entry composition

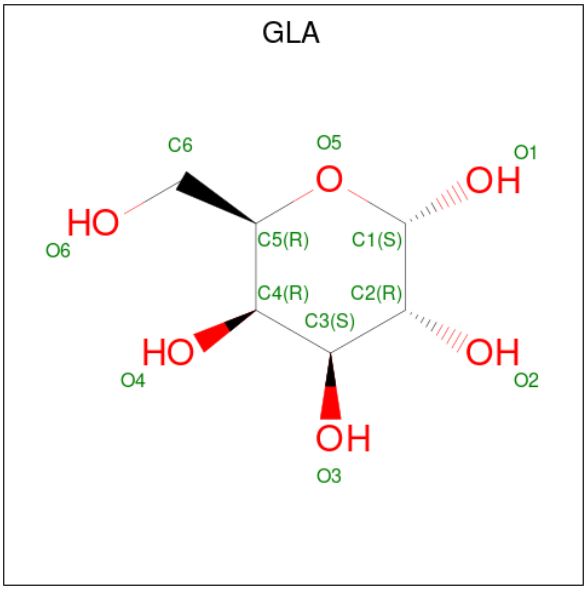
There are 5 unique types of molecules in this entry. The entry contains 18271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	3	0
			5383	3407	926	1025	25			
1	B	686	Total	C	N	O	S	0	1	0
			5391	3413	932	1021	25			
1	C	684	Total	C	N	O	S	0	0	0
			5381	3407	930	1019	25			

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



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

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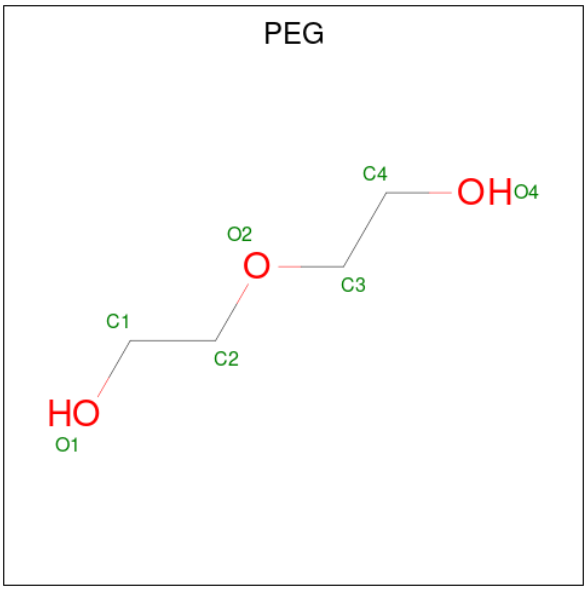
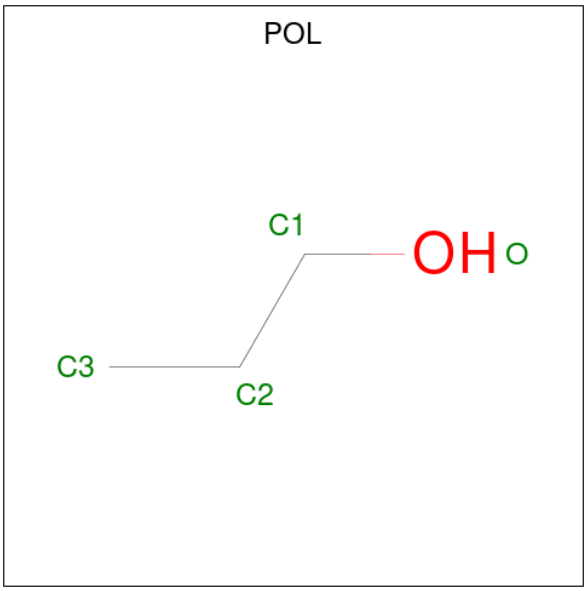
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



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

- Molecule 5 is water.

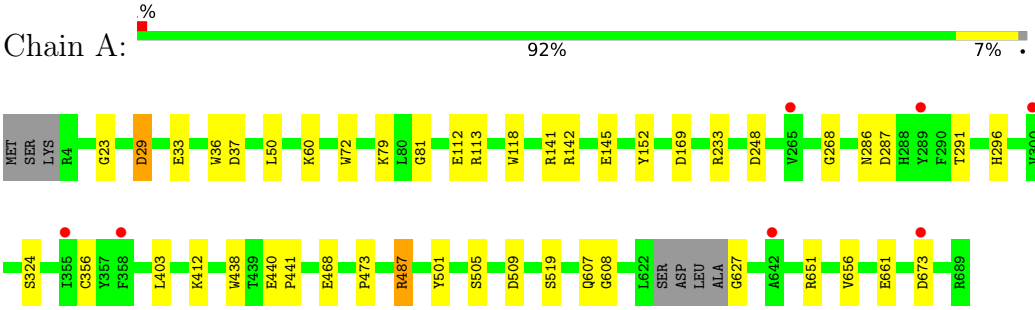
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	657	Total O 657 657	0	0
5	B	676	Total O 676 676	0	0
5	C	688	Total O 688 688	0	0

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.

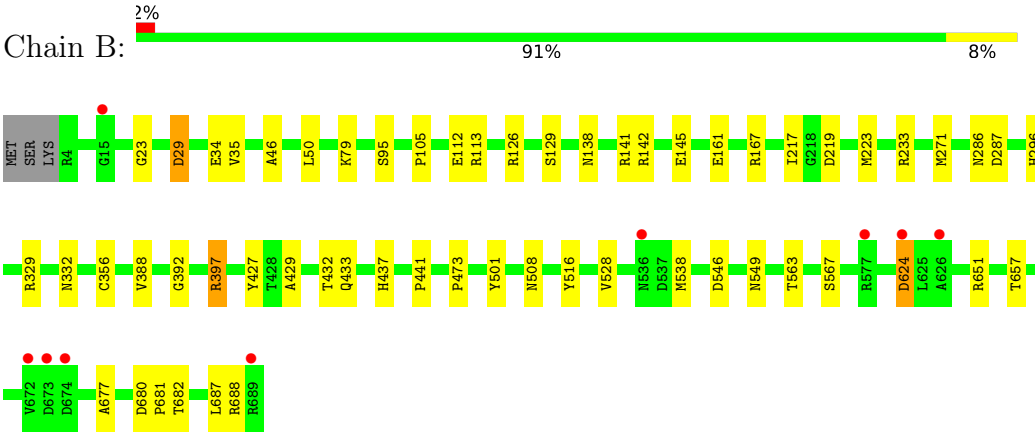
• Molecule 1: BETA-GALACTOSIDASE

Chain A:



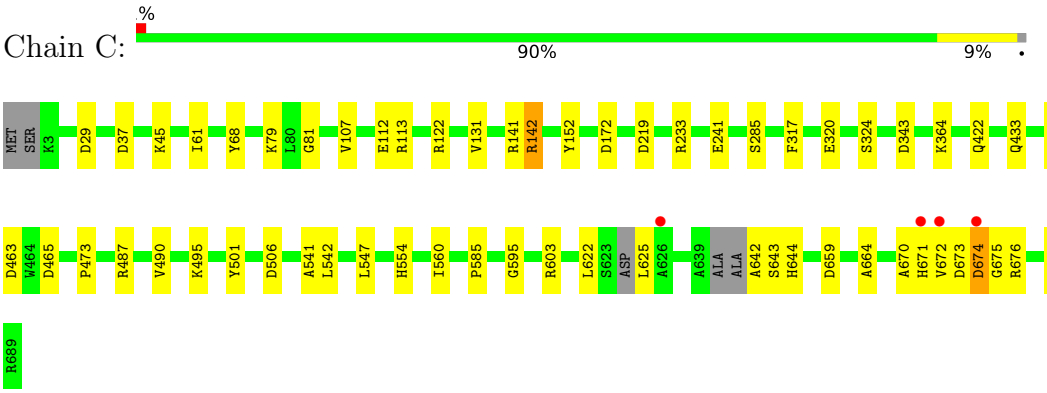
• Molecule 1: BETA-GALACTOSIDASE

Chain B:



• Molecule 1: BETA-GALACTOSIDASE

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.72Å 101.59Å 114.62Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	110.51 – 1.94 42.81 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.0 (110.51-1.94) 97.0 (42.81-1.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.007	Depositor
R, R_{free}	0.155 , 0.206 0.165 , 0.211	Depositor DCC
R_{free} test set	7688 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.2	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	0.96	EDS
Total number of atoms	18271	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: POL, GLA, 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	0.82	0/5544	0.90	11/7551 (0.1%)
1	B	0.85	0/5547	0.90	8/7558 (0.1%)
1	C	0.90	0/5532	0.93	13/7533 (0.2%)
All	All	0.86	0/16623	0.91	32/22642 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	113	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	B	287	ASP	CB-CG-OD1	6.66	124.29	118.30
1	C	343	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	461	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	248	ASP	CB-CG-OD1	6.34	124.00	118.30
1	B	219	ASP	CB-CG-OD1	6.31	123.97	118.30
1	A	29	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	287	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	113	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	113	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	487	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	651	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	141	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	C	233	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	29	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	487	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	506	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	29	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	233	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	546	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	169	ASP	CB-CG-OD1	5.37	123.14	118.30
1	C	463	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	172	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	113	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	29	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	233	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	233	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	122	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	219	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	651	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5383	0	5067	24	0
1	B	5391	0	5074	28	0
1	C	5381	0	5064	28	0
2	A	36	0	36	2	0
2	B	24	0	24	2	0
2	C	24	0	24	3	0
3	C	7	0	10	0	0
4	C	4	0	8	0	0
5	A	657	0	0	6	0
5	B	676	0	0	7	0
5	C	688	0	0	10	0
All	All	18271	0	15307	83	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 (83) 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:C:659:ASP:CB	5:C:939:HOH:O	1.84	1.22
1:B:112[B]:GLU:OE2	5:B:801:HOH:O	1.74	1.03
1:C:320:GLU:OE1	2:C:701:GLA:O1	1.76	1.01
1:C:112:GLU:OE1	5:C:801:HOH:O	1.77	1.00
2:A:702:GLA:H5	5:A:1343:HOH:O	1.65	0.94
1:A:627:GLY:N	5:A:801:HOH:O	2.14	0.80
1:A:320:GLU:OE1	2:A:701:GLA:O1	2.03	0.77
1:C:37:ASP:OD1	1:C:79:LYS:NZ	2.18	0.76
1:B:508:ASN:ND2	5:B:802:HOH:O	2.06	0.73
1:C:642:ALA:N	5:C:804:HOH:O	2.24	0.70
2:C:702:GLA:H5	5:C:838:HOH:O	1.93	0.68
2:B:702:GLA:H5	5:B:1382:HOH:O	1.93	0.67
1:A:142:ARG:HD3	5:A:1272:HOH:O	1.98	0.63
1:B:320:GLU:OE1	2:B:701:GLA:O1	2.08	0.63
1:C:541:ALA:O	5:C:802:HOH:O	2.16	0.63
1:B:23:GLY:HA3	1:B:50:LEU:O	2.02	0.59
1:C:241:GLU:OE2	5:C:803:HOH:O	2.17	0.59
1:A:112:GLU:OE1	5:A:802:HOH:O	2.17	0.59
2:C:702:GLA:H1	5:C:1292:HOH:O	2.05	0.57
1:A:145:GLU:OE2	5:A:803:HOH:O	2.18	0.57
1:B:167:ARG:HD2	1:B:271:MET:CE	2.35	0.56
5:A:1395:HOH:O	1:C:364:LYS:CD	2.54	0.55
1:A:412:LYS:HD3	1:A:468:GLU:OE1	2.07	0.54
1:A:23:GLY:HA3	1:A:50:LEU:O	2.08	0.53
1:C:465:ASP:OD1	1:C:465:ASP:N	2.35	0.52
1:A:60:LYS:HG2	1:A:72:TRP:CZ2	2.45	0.52
1:B:549:ASN:HB3	5:B:895:HOH:O	2.10	0.52
1:B:138:ASN:O	1:B:142:ARG:HG2	2.11	0.51
1:B:624:ASP:OD1	1:B:624:ASP:N	2.43	0.51
1:B:657:THR:HA	1:B:677:ALA:O	2.11	0.51
1:B:296:HIS:C	1:B:296:HIS:CD2	2.84	0.51
1:B:112[B]:GLU:CD	5:B:801:HOH:O	2.36	0.50
1:C:670:ALA:HB1	1:C:685:VAL:CG1	2.42	0.50
1:B:217:ILE:HD13	1:B:223:MET:HE2	1.94	0.50
1:B:142:ARG:HD2	5:B:1258:HOH:O	2.12	0.50
1:B:167:ARG:HD2	1:B:271:MET:HE1	1.93	0.50
1:C:560:ILE:HD12	1:C:585:PRO:O	2.12	0.49
1:A:286:ASN:HB2	1:A:307:MET:SD	2.51	0.49
1:B:141:ARG:O	1:B:145:GLU:HG3	2.13	0.48
1:A:505:SER:HB3	1:A:509:ASP:HA	1.96	0.48
1:C:487:ARG:HD2	5:C:1180:HOH:O	2.14	0.48
1:C:107:VAL:HG12	1:C:131:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:GLN:HA	1:C:437:HIS:HB3	1.96	0.47
1:B:680:ASP:HB3	1:B:681:PRO:CD	2.45	0.47
1:B:46:ALA:O	1:B:392:GLY:HA3	2.14	0.46
1:C:495:LYS:HD3	1:C:622:LEU:HD11	1.98	0.46
1:C:673:ASP:O	1:C:674:ASP:C	2.51	0.46
1:A:37:ASP:OD1	1:A:79:LYS:NZ	2.46	0.46
1:A:118:TRP:CZ3	5:B:1082:HOH:O	2.67	0.46
1:C:81:GLY:HA3	1:C:152:TYR:CG	2.51	0.46
1:B:563:THR:HB	1:B:567:SER:OG	2.15	0.46
1:B:397:ARG:O	1:B:397:ARG:HD3	2.16	0.45
1:C:45:LYS:HE3	5:C:1115:HOH:O	2.17	0.45
1:B:286:ASN:HB2	1:B:307:MET:SD	2.56	0.45
1:A:81:GLY:HA3	1:A:152:TYR:CG	2.51	0.44
1:B:427:TYR:CE2	1:B:429:ALA:HB3	2.52	0.44
1:A:440:GLU:N	1:A:441:PRO:HD2	2.33	0.44
1:B:329:ARG:HB2	1:B:332:ASN:OD1	2.18	0.44
1:C:542:LEU:HD12	1:C:542:LEU:HA	1.84	0.44
1:A:60:LYS:HG2	1:A:72:TRP:CE2	2.53	0.43
1:B:23:GLY:O	1:B:356:CYS:HA	2.18	0.43
1:C:547:LEU:HD12	1:C:547:LEU:N	2.34	0.43
1:C:490:VAL:O	1:C:595:GLY:HA3	2.19	0.43
1:C:675:GLY:O	1:C:676:ARG:HD2	2.19	0.42
1:B:664:ALA:HA	1:B:687:LEU:HD23	2.02	0.42
1:A:33:GLU:HG2	1:A:36:TRP:CH2	2.53	0.42
1:C:642:ALA:CA	5:C:804:HOH:O	2.67	0.42
1:B:516:TYR:HB2	1:B:528:VAL:HB	2.02	0.42
1:A:23:GLY:O	1:A:356:CYS:HA	2.19	0.42
1:B:437:HIS:O	1:B:441:PRO:HD2	2.20	0.41
1:A:33:GLU:HG2	1:A:36:TRP:CZ2	2.56	0.41
1:C:554:HIS:O	1:C:603:ARG:HB3	2.20	0.41
1:A:291:THR:HG23	1:B:538:MET:HE1	2.02	0.41
1:C:285:SER:HA	1:C:317:PHE:O	2.21	0.41
1:A:50:LEU:C	1:A:50:LEU:HD23	2.41	0.41
1:A:296:HIS:CD2	1:A:296:HIS:C	2.94	0.41
1:B:126:ARG:HB2	1:B:129:SER:HB2	2.02	0.41
1:C:61:ILE:O	1:C:68:TYR:HA	2.21	0.41
1:A:268:GLY:HA2	1:A:438:TRP:CD2	2.56	0.40
1:A:487:ARG:NH2	1:A:519:SER:O	2.55	0.40
1:A:607[B]:GLN:HG2	1:A:608:GLY:H	1.86	0.40
1:C:142:ARG:HD2	1:C:142:ARG:HA	1.72	0.40
1:C:664:ALA:HB2	1:C:672:VAL:HG21	2.03	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	681/689 (99%)	661 (97%)	18 (3%)	2 (0%)	41	32
1	B	685/689 (99%)	661 (96%)	22 (3%)	2 (0%)	41	32
1	C	678/689 (98%)	653 (96%)	22 (3%)	3 (0%)	34	24
All	All	2044/2067 (99%)	1975 (97%)	62 (3%)	7 (0%)	41	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	GLU
1	A	473	PRO
1	A	324	SER
1	C	324	SER
1	C	674	ASP
1	B	473	PRO
1	C	473	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	557/566 (98%)	551 (99%)	6 (1%)	73	67
1	B	554/566 (98%)	540 (98%)	14 (2%)	47	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	554/566 (98%)	545 (98%)	9 (2%)	62 52
All	All	1665/1698 (98%)	1636 (98%)	29 (2%)	60 49

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	403	LEU
1	A	501	TYR
1	A	656	VAL
1	A	661	GLU
1	A	673	ASP
1	B	29	ASP
1	B	34	GLU
1	B	35	VAL
1	B	79	LYS
1	B	95	SER
1	B	105	PRO
1	B	388	VAL
1	B	397	ARG
1	B	432	THR
1	B	433	GLN
1	B	501	TYR
1	B	624	ASP
1	B	682	THR
1	B	688	ARG
1	C	29	ASP
1	C	142	ARG
1	C	433	GLN
1	C	501	TYR
1	C	625	LEU
1	C	643	SER
1	C	644	HIS
1	C	671	HIS
1	C	687	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

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	GLA	B	701	-	12,12,12	0.88	0	17,17,17	1.14	1 (5%)
2	GLA	A	702	-	12,12,12	1.92	2 (16%)	17,17,17	2.57	7 (41%)
2	GLA	A	701	-	12,12,12	1.08	0	17,17,17	1.42	3 (17%)
2	GLA	B	702	-	12,12,12	1.96	3 (25%)	17,17,17	1.80	5 (29%)
2	GLA	A	703	-	12,12,12	1.75	4 (33%)	17,17,17	1.83	4 (23%)
3	PEG	C	703	-	6,6,6	0.24	0	5,5,5	0.91	0
4	POL	C	704	-	3,3,3	0.44	0	2,2,2	0.12	0
2	GLA	C	701	-	12,12,12	0.98	0	17,17,17	0.83	0
2	GLA	C	702	-	12,12,12	1.37	1 (8%)	17,17,17	1.36	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	GLA	B	701	-	-	0/2/22/22	0/1/1/1
2	GLA	A	702	-	-	2/2/22/22	0/1/1/1
2	GLA	A	701	-	-	0/2/22/22	0/1/1/1
2	GLA	B	702	-	-	2/2/22/22	0/1/1/1
2	GLA	A	703	-	-	0/2/22/22	0/1/1/1
3	PEG	C	703	-	-	3/4/4/4	-
4	POL	C	704	-	-	0/1/1/1	-
2	GLA	C	701	-	-	0/2/22/22	0/1/1/1
2	GLA	C	702	-	-	1/2/22/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	GLA	O3-C3	5.44	1.55	1.43
2	B	702	GLA	O3-C3	5.08	1.54	1.43
2	A	703	GLA	O5-C1	3.17	1.50	1.42
2	C	702	GLA	O3-C3	3.10	1.50	1.43
2	A	703	GLA	O2-C2	2.84	1.49	1.43
2	B	702	GLA	O5-C1	2.72	1.49	1.42
2	A	702	GLA	O5-C1	2.56	1.49	1.42
2	B	702	GLA	C3-C2	-2.47	1.46	1.52
2	A	703	GLA	C3-C2	-2.23	1.46	1.52
2	A	703	GLA	O3-C3	2.07	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	702	GLA	O2-C2-C1	-7.37	92.06	109.16
2	A	703	GLA	C1-O5-C5	4.21	121.61	113.66
2	A	703	GLA	O5-C1-C2	3.58	116.68	110.28
2	B	702	GLA	O4-C4-C5	3.34	117.58	109.30
2	A	701	GLA	O1-C1-C2	3.24	118.15	109.03
2	A	702	GLA	C1-O5-C5	-3.17	107.68	113.66
2	B	701	GLA	O1-C1-C2	3.12	117.82	109.03
2	A	702	GLA	C1-C2-C3	3.06	116.66	110.31
2	B	702	GLA	O1-C1-C2	3.04	117.58	109.03
2	B	702	GLA	O5-C5-C4	3.01	115.15	109.69
2	A	701	GLA	C1-C2-C3	2.96	116.45	110.31
2	A	703	GLA	O3-C3-C2	-2.85	103.76	110.35
2	A	702	GLA	O2-C2-C3	-2.72	104.07	110.35
2	A	702	GLA	O5-C5-C6	-2.68	99.78	106.44
2	B	702	GLA	C1-C2-C3	2.63	115.77	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	702	GLA	O3-C3-C2	2.55	116.24	110.35
2	C	702	GLA	O5-C1-C2	-2.53	105.78	110.28
2	A	701	GLA	O2-C2-C3	2.43	115.96	110.35
2	B	702	GLA	O5-C5-C6	-2.28	100.77	106.44
2	A	703	GLA	C1-C2-C3	2.20	114.87	110.31
2	C	702	GLA	O5-C5-C4	2.11	113.53	109.69
2	A	702	GLA	O1-C1-O5	-2.10	104.07	110.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	702	GLA	O5-C5-C6-O6
2	A	702	GLA	O5-C5-C6-O6
2	A	702	GLA	C4-C5-C6-O6
2	B	702	GLA	C4-C5-C6-O6
2	C	702	GLA	O5-C5-C6-O6
3	C	703	PEG	O2-C3-C4-O4
3	C	703	PEG	C4-C3-O2-C2
3	C	703	PEG	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	GLA	1	0
2	A	702	GLA	1	0
2	A	701	GLA	1	0
2	B	702	GLA	1	0
2	C	701	GLA	1	0
2	C	702	GLA	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, 95^{th} 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	682/689 (98%)	-0.31	7 (1%) 82 86	15, 24, 41, 67	0
1	B	686/689 (99%)	-0.36	11 (1%) 72 77	15, 23, 39, 80	0
1	C	684/689 (99%)	-0.44	4 (0%) 89 92	14, 22, 39, 63	0
All	All	2052/2067 (99%)	-0.37	22 (1%) 80 84	14, 23, 40, 80	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	673	ASP	3.2
1	B	674	ASP	3.1
1	A	355	ILE	2.8
1	C	671	HIS	2.7
1	B	673	ASP	2.6
1	A	289	TYR	2.5
1	B	626	ALA	2.5
1	B	624	ASP	2.4
1	A	642	ALA	2.4
1	A	265	VAL	2.4
1	B	577	ARG	2.3
1	A	300	VAL	2.3
1	B	15	GLY	2.3
1	B	672	VAL	2.2
1	B	536	ASN	2.2
1	C	672	VAL	2.2
1	B	689	ARG	2.1
1	C	674	ASP	2.1
1	C	626	ALA	2.1
1	A	358	PHE	2.1
1	B	665	ILE	2.1
1	B	660	VAL	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 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, 95^{th} 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
4	POL	C	704	4/4	0.76	0.13	42,44,44,47	0
2	GLA	A	702	12/12	0.77	0.18	24,27,27,27	0
2	GLA	C	702	12/12	0.79	0.23	26,28,29,29	0
2	GLA	B	702	12/12	0.84	0.18	25,27,28,29	0
3	PEG	C	703	7/7	0.90	0.09	44,45,48,48	0
2	GLA	A	703	12/12	0.92	0.31	24,26,28,30	0
2	GLA	C	701	12/12	0.95	0.16	18,19,22,23	0
2	GLA	B	701	12/12	0.97	0.12	18,21,22,23	0
2	GLA	A	701	12/12	0.97	0.17	19,20,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.