



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 06:29 AM EDT

PDB ID : 4YE5
Title : The crystal structure of a peptidoglycan synthetase from *Bifidobacterium adolescentis* ATCC 15703
Authors : Cuff, M.; Tan, K.; Joachimiak, G.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : unknown
Resolution : 2.05 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

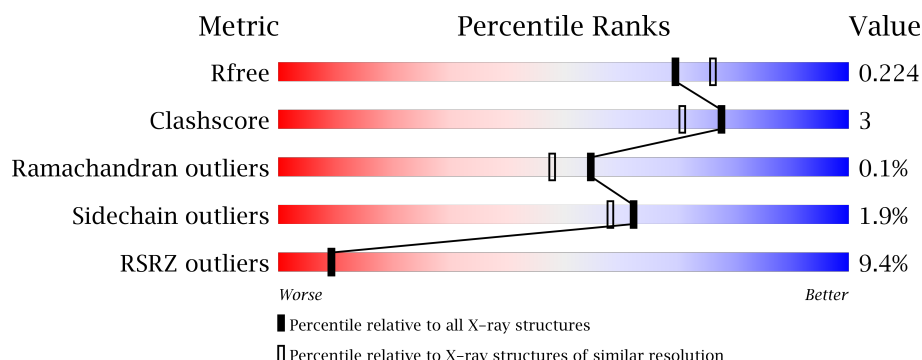
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)

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	566	<div> <div style="width: 90%;"></div> <div style="width: 6%;"></div> <div style="width: 4%;"></div> </div>
1	B	566	<div> <div style="width: 17%;"></div> <div style="width: 82%;"></div> <div style="width: 12%;"></div> <div style="width: 6%;"></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	701	-	-	-	X
2	GOL	A	703	-	-	-	X
2	GOL	A	704	-	-	-	X
2	GOL	A	705	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8565 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 Peptidoglycan synthetase penicillin-binding protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	546	4090	2535	708	829	2	16	0	3	0
1	B	534	3886	2412	673	783	2	16	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

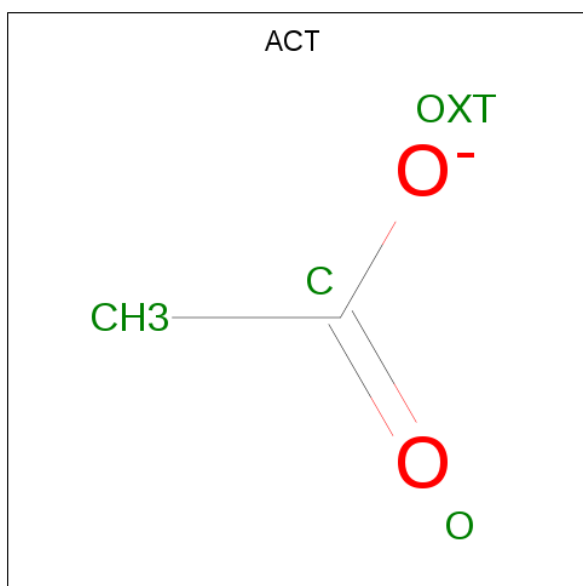
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	-	expression tag	UNP A1A2F5
A	36	ASN	-	expression tag	UNP A1A2F5
A	37	ALA	-	expression tag	UNP A1A2F5
B	35	SER	-	expression tag	UNP A1A2F5
B	36	ASN	-	expression tag	UNP A1A2F5
B	37	ALA	-	expression tag	UNP A1A2F5

- Molecule 2 is GLYCEROL (three-letter code: 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	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	473	Total	O	0	0
			473	473		
4	B	82	Total	O	0	0
			82	82		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.96Å 85.71Å 227.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.39 – 2.05 47.39 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.39-2.05) 97.2 (47.39-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.93 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.224 0.187 , 0.224	Depositor DCC
R_{free} test set	5101 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.067 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8565	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: GOL, ACT

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	0.45	0/4134	0.56	0/5576
1	B	0.30	0/3933	0.48	0/5316
All	All	0.39	0/8067	0.53	0/10892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	4090	0	4045	22	0
1	B	3886	0	3729	33	0
2	A	30	0	40	3	0
3	B	4	0	3	0	0
4	A	473	0	0	4	0
4	B	82	0	0	1	0
All	All	8565	0	7817	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 3.

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)
1:B:393:ARG:NH1	1:B:429:ARG:O	2.21	0.74
1:B:431:THR:HB	1:B:436:GLN:HB2	1.68	0.73
1:B:504:GLU:OE2	1:B:592:ARG:NH1	2.25	0.69
1:A:348:THR:HG22	1:A:357:LYS:HG2	1.80	0.64
1:A:516:ARG:HH22	2:A:705:GOL:H12	1.62	0.64
1:B:346:PRO:HA	1:B:379:VAL:HG11	1.83	0.60
1:B:69:ILE:HB	1:B:78:ALA:HB3	1.83	0.59
1:A:218:ARG:NH2	4:A:948:HOH:O	2.31	0.58
1:A:516:ARG:NH2	2:A:705:GOL:H12	2.19	0.57
1:B:337:HIS:ND1	4:B:861:HOH:O	2.32	0.57
1:B:70:MSE:HE3	1:B:74:GLY:HA2	1.87	0.56
1:B:82:GLU:HG2	1:B:159:PRO:HG3	1.86	0.56
1:A:111:GLN:NE2	4:A:1254:HOH:O	2.38	0.55
1:B:334:LEU:HD13	1:B:392:GLN:HE21	1.72	0.55
1:B:283:ASP:HB2	1:B:290:LEU:HD11	1.90	0.54
1:B:466:SER:HA	1:B:477:GLN:HG2	1.90	0.54
1:A:259:TRP:CD1	1:B:582[B]:GLN:HG3	2.45	0.52
1:A:111:GLN:HG3	4:A:1129:HOH:O	2.10	0.51
1:B:569:ALA:O	1:B:573:THR:HG23	2.10	0.51
1:A:352:GLU:OE1	1:A:426:ARG:NE	2.42	0.50
1:B:299:GLU:HB2	1:B:302:SER:HB3	1.94	0.50
1:A:582:GLN:OE1	4:A:973:HOH:O	2.20	0.50
1:A:280:MSE:SE	1:A:443:MSE:HA	2.63	0.49
1:B:135:MSE:HE1	1:B:154:LYS:HB2	1.95	0.48
1:B:205:ALA:N	1:B:209:GLN:HB2	2.28	0.48
1:B:326:LEU:HD22	1:B:400:PHE:CG	2.48	0.48
1:A:347:ASN:HB3	1:A:362:HIS:O	2.14	0.48
1:A:398:SER:O	1:A:404:GLN:NE2	2.47	0.47
1:A:397:ILE:HD13	1:A:432:VAL:HG22	1.96	0.47
1:B:388:MSE:HG2	1:B:393:ARG:HG3	1.97	0.47
1:A:81:VAL:HG12	1:A:83:ARG:HG2	1.98	0.46
1:A:320:GLY:O	1:A:435:GLY:HA3	2.15	0.46
1:A:63:LYS:HG2	1:A:178:LEU:HD23	1.97	0.46
1:B:63:LYS:HA	1:B:219:ASP:OD1	2.16	0.46
1:B:193:LEU:O	1:B:207:ILE:HD12	2.16	0.46
1:A:426:ARG:HA	1:A:426:ARG:HD2	1.72	0.45
1:B:193:LEU:HG	1:B:207:ILE:HD11	1.99	0.45
1:A:290:LEU:HD21	2:A:701:GOL:H2	1.99	0.45
1:B:420:PRO:HG2	1:B:423:SER:HB3	1.99	0.45
1:B:133:LEU:HD21	1:B:165:ILE:HD11	1.99	0.44
1:B:345:VAL:O	1:B:364:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:HG23	1:B:155:LYS:HA	2.00	0.43
1:B:280:MSE:SE	1:B:443:MSE:HA	2.68	0.43
1:B:212:ASN:O	1:B:216:THR:N	2.42	0.43
1:B:332:LEU:HD21	1:B:339:ILE:HB	2.01	0.43
1:A:431:THR:HB	1:A:436:GLN:HB2	2.01	0.42
1:A:466:SER:HA	1:A:477:GLN:HG2	2.01	0.42
1:A:569:ALA:O	1:A:573:THR:HG23	2.20	0.41
1:B:334:LEU:HD11	1:B:392:GLN:HB3	2.02	0.41
1:B:516:ARG:NH1	1:B:547:ASP:HB3	2.36	0.41
1:A:396:PHE:O	1:A:400:PHE:HD2	2.03	0.41
1:B:372:ILE:HG23	1:B:377:SER:HB3	2.03	0.40
1:B:381:MSE:O	1:B:385:GLY:N	2.55	0.40
1:B:396:PHE:O	1:B:400:PHE:HD1	2.04	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	547/566 (97%)	540 (99%)	7 (1%)	0	100	100
1	B	530/566 (94%)	505 (95%)	24 (4%)	1 (0%)	51	42
All	All	1077/1132 (95%)	1045 (97%)	31 (3%)	1 (0%)	55	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	595	ALA

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	442/437 (101%)	436 (99%)	6 (1%)	71	69
1	B	397/437 (91%)	387 (98%)	10 (2%)	53	47
All	All	839/874 (96%)	823 (98%)	16 (2%)	62	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	71	ASP
1	A	179	SER
1	A	228	ASN
1	A	290	LEU
1	A	347	ASN
1	B	70	MSE
1	B	71	ASP
1	B	138	THR
1	B	240	SER
1	B	241	LYS
1	B	242	ASP
1	B	285	GLN
1	B	428	THR
1	B	523	THR
1	B	534	THR

Some 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 [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](#)

6 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	GOL	A	701	-	5,5,5	0.22	0	5,5,5	0.66	0
2	GOL	A	702	-	5,5,5	0.32	0	5,5,5	0.22	0
2	GOL	A	703	-	5,5,5	0.41	0	5,5,5	0.05	0
2	GOL	A	704	-	5,5,5	0.38	0	5,5,5	0.33	0
2	GOL	A	705	-	5,5,5	0.31	0	5,5,5	0.34	0
3	ACT	B	701	-	1,3,3	1.43	0	0,3,3	0.00	-

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	701	-	-	0/4/4/4	0/0/0/0
2	GOL	A	702	-	-	0/4/4/4	0/0/0/0
2	GOL	A	703	-	-	0/4/4/4	0/0/0/0
2	GOL	A	704	-	-	0/4/4/4	0/0/0/0
2	GOL	A	705	-	-	0/4/4/4	0/0/0/0
3	ACT	B	701	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GOL	1	0
2	A	705	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	530/566 (93%)	-0.10	1 (0%) 94 95	12, 28, 52, 71	0
1	B	518/566 (91%)	1.01	98 (18%) 1 1	25, 69, 101, 119	0
All	All	1048/1132 (92%)	0.45	99 (9%) 9 9	12, 43, 94, 119	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	LEU	8.2
1	B	360	VAL	6.8
1	B	359	ALA	6.6
1	B	228	ASN	6.4
1	B	364	ASN	5.7
1	B	221	TYR	5.6
1	B	217	GLY	5.5
1	B	244	VAL	5.4
1	B	55	SER	5.3
1	B	332	LEU	4.9
1	B	339	ILE	4.8
1	B	474	VAL	4.6
1	B	229	SER	4.4
1	B	600	TRP	4.4
1	B	223	VAL	4.2
1	B	146	ILE	4.2
1	B	344	THR	4.1
1	B	335	GLY	4.0
1	B	598	VAL	4.0
1	B	216	THR	3.9
1	B	246	GLY	3.9
1	B	370	ALA	3.9
1	B	422	ASP	3.8
1	B	243	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	249	VAL	3.7
1	B	363	GLY	3.7
1	B	227	GLY	3.7
1	B	343	PHE	3.7
1	B	379	VAL	3.5
1	B	433	LEU	3.5
1	B	424	TRP	3.5
1	B	56	ARG	3.4
1	B	63	LYS	3.4
1	B	202	LYS	3.4
1	B	69	ILE	3.4
1	B	533	LEU	3.4
1	B	207	ILE	3.4
1	B	362	HIS	3.4
1	B	57	THR	3.2
1	B	201	GLY	3.2
1	B	369	LEU	3.2
1	B	225	GLN	3.2
1	B	68	LYS	3.2
1	B	347	ASN	3.1
1	B	432	VAL	3.1
1	B	231	VAL	3.0
1	B	214	THR	3.0
1	B	60	VAL	3.0
1	B	59	THR	3.0
1	B	160	ALA	3.0
1	B	468	THR	2.9
1	B	383	ILE	2.9
1	B	526	VAL	2.9
1	B	152	VAL	2.8
1	B	338	LYS	2.8
1	B	66	ARG	2.8
1	B	218	ARG	2.7
1	B	178	LEU	2.7
1	B	78	ALA	2.7
1	B	472	GLY	2.6
1	B	428	THR	2.6
1	B	196	GLY	2.6
1	B	245	ASN	2.6
1	B	365	GLU	2.6
1	B	65	ARG	2.5
1	B	238	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	184	TYR	2.5
1	B	385	GLY	2.5
1	B	366	HIS	2.4
1	B	80	SER	2.4
1	A	360	VAL	2.4
1	B	490	SER	2.4
1	B	478	GLN	2.4
1	B	204	VAL	2.4
1	B	230	GLY	2.3
1	B	203	GLY	2.3
1	B	224	TYR	2.3
1	B	377	SER	2.3
1	B	367	TRP	2.2
1	B	208	GLU	2.2
1	B	156	ASP	2.2
1	B	429	ARG	2.2
1	B	372	ILE	2.2
1	B	64	ALA	2.2
1	B	166	SER	2.1
1	B	308	GLY	2.1
1	B	467	ILE	2.1
1	B	393	ARG	2.1
1	B	213	LYS	2.1
1	B	140	LEU	2.1
1	B	396	PHE	2.1
1	B	305	ALA	2.1
1	B	83	ARG	2.0
1	B	183	LEU	2.0
1	B	181	GLU	2.0
1	B	147	SER	2.0
1	B	226	GLN	2.0
1	B	325	VAL	2.0
1	B	222	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 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	703	6/6	0.90	0.21	9.84	59,60,61,61	0
2	GOL	A	705	6/6	0.90	0.19	3.78	34,53,59,65	0
2	GOL	A	704	6/6	0.86	0.15	3.09	47,65,67,68	0
2	GOL	A	701	6/6	0.87	0.16	2.96	37,40,43,46	0
3	ACT	B	701	4/4	0.93	0.12	-0.88	68,70,71,72	0
2	GOL	A	702	6/6	0.77	0.18	-	81,85,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.