



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5Z06 / pdb_00005z06
Title : Crystal structure of beta-1,2-glucanase from Parabacteroides distasonis
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Deposited on : 2017-12-18
Resolution : 2.10 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

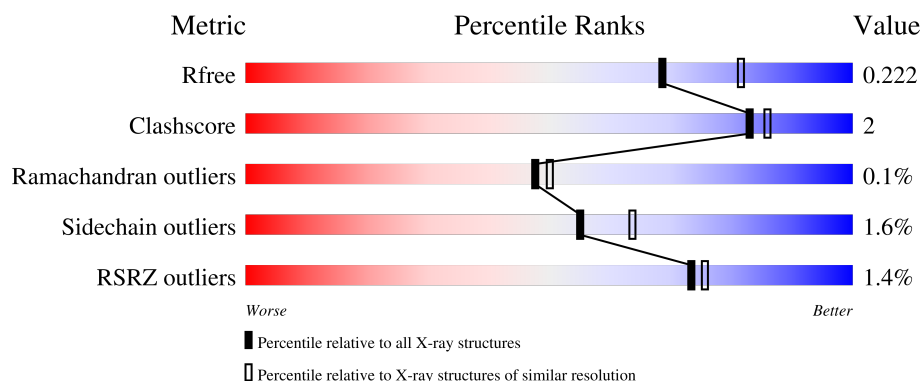
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	712	90% 7% 90% 7%
1	B	712	90% 8% 90% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11921 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 BDI_3064 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	1	0
			5666	3641	945	1056	24			
1	B	698	Total	C	N	O	S	0	0	0
			5667	3642	946	1056	23			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP A6LGF6
A	722	LEU	-	expression tag	UNP A6LGF6
A	723	GLU	-	expression tag	UNP A6LGF6
A	724	HIS	-	expression tag	UNP A6LGF6
A	725	HIS	-	expression tag	UNP A6LGF6
A	726	HIS	-	expression tag	UNP A6LGF6
A	727	HIS	-	expression tag	UNP A6LGF6
A	728	HIS	-	expression tag	UNP A6LGF6
A	729	HIS	-	expression tag	UNP A6LGF6
B	18	MET	-	initiating methionine	UNP A6LGF6
B	722	LEU	-	expression tag	UNP A6LGF6
B	723	GLU	-	expression tag	UNP A6LGF6
B	724	HIS	-	expression tag	UNP A6LGF6
B	725	HIS	-	expression tag	UNP A6LGF6
B	726	HIS	-	expression tag	UNP A6LGF6
B	727	HIS	-	expression tag	UNP A6LGF6
B	728	HIS	-	expression tag	UNP A6LGF6
B	729	HIS	-	expression tag	UNP A6LGF6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

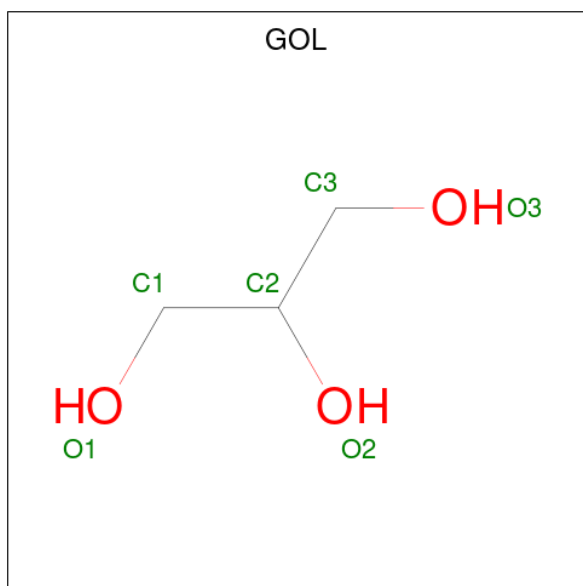
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total 249	O 249	0	0
4	B	277	Total 277	O 277	0	0

- Molecule 1: BDI 3064 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.08Å 123.34Å 101.38Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	46.73 – 2.10 46.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.73-2.10) 97.9 (46.73-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.219 0.185 , 0.222	Depositor DCC
R_{free} test set	4328 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11921	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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

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	0.76	0/5838	0.85	1/7936 (0.0%)
1	B	0.77	0/5839	0.84	1/7937 (0.0%)
All	All	0.77	0/11677	0.85	2/15873 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	GLY	N-CA-C	-6.45	97.89	113.18
1	A	68	GLY	N-CA-C	-5.60	99.91	113.18

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	5666	0	5384	23	0
1	B	5667	0	5389	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	48	1	0
3	B	24	0	32	2	0
4	A	249	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	277	0	0	0	0
All	All	11921	0	10853	53	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 (53) 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:449:TRP:CG	1:A:490:ALA:HA	2.36	0.59
1:B:449:TRP:CG	1:B:490:ALA:HA	2.42	0.55
1:A:488:MET:HE1	1:A:566:PHE:CZ	2.43	0.54
1:B:119:LEU:HD23	1:B:189:ILE:HD11	1.90	0.53
1:B:409:LEU:HD13	1:B:452:TYR:CG	2.46	0.51
1:B:258:MET:HE1	1:B:663:TYR:CE2	2.49	0.47
1:B:326:LEU:HD22	1:B:343:SER:HB3	1.97	0.47
1:A:316:TYR:OH	1:A:682:GLY:O	2.29	0.47
1:B:326:LEU:HD21	1:B:371:ILE:HG23	1.96	0.47
1:A:481:ASN:HA	1:A:553:PHE:CE2	2.50	0.46
1:A:328:ARG:NH2	4:A:910:HOH:O	2.47	0.46
1:A:366:GLN:OE1	1:A:432:LYS:HE2	2.16	0.46
1:A:326:LEU:HD22	1:A:343:SER:HB3	1.98	0.46
1:B:316:TYR:OH	1:B:682:GLY:O	2.24	0.46
1:A:316:TYR:CZ	1:A:686:ALA:HB2	2.52	0.45
1:A:126:TYR:HA	1:A:171:LYS:O	2.17	0.45
1:B:341:GLY:HA3	1:B:411:GLU:OE1	2.17	0.45
1:B:83:TRP:O	1:B:179:PRO:HD3	2.16	0.45
1:A:264:PHE:CE2	1:A:656:GLY:HA3	2.52	0.45
1:A:148:VAL:HG23	1:A:150:HIS:CE1	2.52	0.45
1:B:316:TYR:CZ	1:B:686:ALA:HB2	2.51	0.44
1:A:216:LYS:HG3	1:A:218:TYR:CE1	2.51	0.44
1:A:641:PRO:HB3	1:A:695:TYR:CE1	2.52	0.44
1:B:488:MET:CE	1:B:714:ILE:HD13	2.48	0.43
1:A:552:PHE:CD1	1:A:556:TYR:CE2	3.06	0.43
1:B:400:PHE:CZ	3:B:802:GOL:H12	2.52	0.43
1:B:487:TYR:CD2	1:B:507:TRP:HB2	2.53	0.43
1:B:552:PHE:CD2	1:B:556:TYR:CE2	3.07	0.43
1:A:37:TYR:CE2	1:A:39:TYR:HB2	2.53	0.43
1:A:601:ASP:O	1:A:647:ALA:HA	2.19	0.43
1:A:235:LYS:HA	1:A:281:TYR:CE1	2.54	0.42
1:B:235:LYS:HA	1:B:281:TYR:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:SER:O	1:B:561:LEU:HB3	2.20	0.42
1:B:264:PHE:CE1	1:B:656:GLY:HA3	2.55	0.42
1:B:400:PHE:CZ	3:B:802:GOL:C1	3.03	0.42
1:B:513:TYR:CD1	1:B:513:TYR:C	2.97	0.42
1:A:500:PRO:HB2	1:A:720:ILE:HD11	2.01	0.42
1:B:41:GLN:HA	1:B:55:HIS:O	2.20	0.42
1:B:488:MET:HG3	1:B:561:LEU:HD22	2.01	0.41
1:A:341:GLY:HA3	1:A:411:GLU:OE1	2.20	0.41
1:B:341:GLY:HA2	1:B:414:PHE:HB2	2.01	0.41
1:A:477:LEU:HB3	1:A:487:TYR:HE1	1.86	0.41
1:B:601:ASP:O	1:B:647:ALA:HA	2.21	0.41
1:A:487:TYR:CD1	1:A:507:TRP:HB2	2.56	0.41
1:B:526:ASP:OD1	1:B:526:ASP:N	2.53	0.41
1:B:488:MET:HE3	1:B:492:MET:HE3	2.03	0.41
1:B:604:GLY:O	1:B:632:GLY:HA3	2.21	0.41
1:B:641:PRO:HB3	1:B:695:TYR:CE1	2.56	0.41
1:B:217:ALA:HB2	1:B:294:ALA:HB1	2.02	0.41
1:B:74:THR:HA	1:B:187:TYR:O	2.20	0.40
1:B:344:GLY:HA3	1:B:415:LEU:HA	2.03	0.40
1:A:554:ILE:HD12	1:A:639:TYR:CD2	2.57	0.40
1:A:614:TYR:CD1	3:A:806:GOL:H31	2.56	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	694/712 (98%)	670 (96%)	24 (4%)	0	100	100
1	B	694/712 (98%)	667 (96%)	26 (4%)	1 (0%)	48	50
All	All	1388/1424 (98%)	1337 (96%)	50 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	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	593/607 (98%)	582 (98%)	11 (2%)	50	58
1	B	593/607 (98%)	585 (99%)	8 (1%)	61	69
All	All	1186/1214 (98%)	1167 (98%)	19 (2%)	55	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	141	LEU
1	A	142	LYS
1	A	145	ARG
1	A	214	GLU
1	A	438	LYS
1	A	477	LEU
1	A	512	GLU
1	A	637	PHE
1	A	687	PRO
1	A	712	LYS
1	B	95	ASN
1	B	142	LYS
1	B	162	ASN
1	B	213	GLN
1	B	395	LYS
1	B	456	LYS
1	B	526	ASP
1	B	637	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	55	HIS
1	A	249	GLN
1	A	323	ASN
1	A	454	GLN
1	A	534	ASN
1	A	540	ASN
1	A	613	ASN
1	A	698	ASN
1	B	162	ASN
1	B	208	ASN
1	B	213	GLN
1	B	442	ASN
1	B	454	GLN
1	B	534	ASN
1	B	540	ASN
1	B	698	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
3	GOL	A	803	-	5,5,5	0.29	0	5,5,5	1.08	0
3	GOL	A	805	-	5,5,5	0.37	0	5,5,5	0.44	0
3	GOL	A	806	-	5,5,5	0.18	0	5,5,5	1.01	0
3	GOL	B	802	-	5,5,5	0.30	0	5,5,5	0.89	0
3	GOL	A	802	-	5,5,5	0.40	0	5,5,5	0.47	0
3	GOL	A	807	-	5,5,5	0.52	0	5,5,5	1.24	1 (20%)
3	GOL	B	805	-	5,5,5	0.48	0	5,5,5	1.21	0
3	GOL	B	803	-	5,5,5	0.40	0	5,5,5	0.71	0
3	GOL	A	804	-	5,5,5	0.40	0	5,5,5	0.74	0
3	GOL	B	804	-	5,5,5	0.28	0	5,5,5	0.28	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
3	GOL	A	803	-	-	1/4/4/4	-
3	GOL	A	805	-	-	0/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	B	802	-	-	0/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	A	807	-	-	0/4/4/4	-
3	GOL	B	805	-	-	4/4/4/4	-
3	GOL	B	803	-	-	2/4/4/4	-
3	GOL	A	804	-	-	1/4/4/4	-
3	GOL	B	804	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	807	GOL	O3-C3-C2	2.13	119.98	110.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	GOL	O1-C1-C2-C3
3	B	805	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	805	GOL	O1-C1-C2-O2
3	A	802	GOL	O1-C1-C2-C3
3	A	806	GOL	C1-C2-C3-O3
3	B	805	GOL	O1-C1-C2-C3
3	A	802	GOL	O1-C1-C2-O2
3	A	806	GOL	O2-C2-C3-O3
3	B	803	GOL	O1-C1-C2-O2
3	B	805	GOL	O2-C2-C3-O3
3	A	803	GOL	C1-C2-C3-O3
3	A	804	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	806	GOL	1	0
3	B	802	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	697/712 (97%)	-0.06	8 (1%) 78 80	17, 32, 50, 71	1 (0%)
1	B	698/712 (98%)	-0.09	12 (1%) 69 71	22, 31, 49, 76	0
All	All	1395/1424 (97%)	-0.08	20 (1%) 73 75	17, 31, 50, 76	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ILE	3.4
1	B	246	ILE	3.3
1	A	720	ILE	3.2
1	B	231	LYS	3.0
1	B	720	ILE	2.8
1	A	142	LYS	2.7
1	B	335	ASN	2.6
1	B	455	PHE	2.5
1	A	715	GLN	2.4
1	B	206	ALA	2.4
1	A	204	VAL	2.4
1	B	204	VAL	2.3
1	B	162	ASN	2.2
1	B	228	PRO	2.2
1	B	719	SER	2.2
1	A	206	ALA	2.1
1	A	228	PRO	2.1
1	A	203	SER	2.0
1	B	205	SER	2.0
1	B	145	ARG	2.0

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
3	GOL	A	806	6/6	0.85	0.16	45,49,51,59	0
3	GOL	A	804	6/6	0.87	0.14	54,55,56,58	0
3	GOL	A	807	6/6	0.87	0.15	39,43,44,47	0
3	GOL	B	803	6/6	0.87	0.14	40,44,45,51	0
3	GOL	A	802	6/6	0.89	0.13	38,46,48,54	0
3	GOL	A	803	6/6	0.89	0.11	35,38,39,44	0
3	GOL	B	802	6/6	0.90	0.14	45,49,50,53	0
3	GOL	B	804	6/6	0.90	0.11	37,42,42,46	0
3	GOL	B	805	6/6	0.90	0.14	54,55,57,57	0
3	GOL	A	805	6/6	0.91	0.10	35,40,42,45	0
2	CA	A	801	1/1	0.99	0.03	31,31,31,31	0
2	CA	B	801	1/1	0.99	0.02	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.