Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 02:17 am GMT

PDB ID	:	5JBD
Title	:	4,6-alpha-glucanotransferase GTFB from Lactobacillus reuteri 121
Authors	:	Pijning, T.; Dijkstra, B.W.; Bai, Y.; Gangoiti-Munecas, J.; Dijkhuizen, L.
Deposited on	:	2016-04-13
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

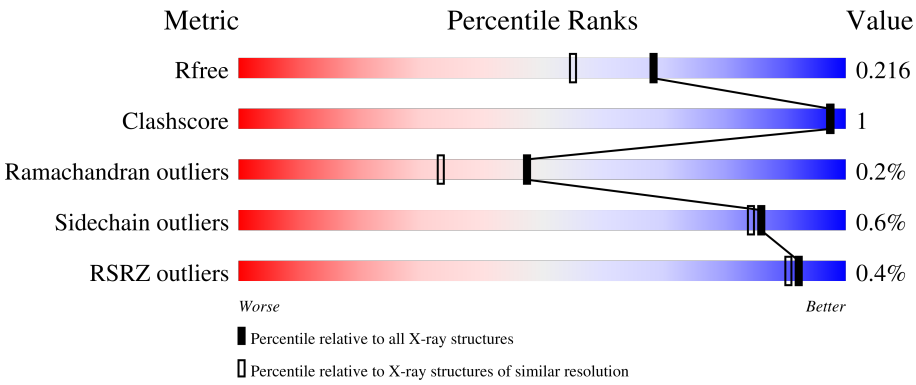
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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	893	94%
1	B	893	92%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14804 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 Inactive glucansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	854	6711	4170	1152	1363	26	0	5	0
1	B	855	6704	4169	1149	1360	26	0	4	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	733	MET	-	initiating methionine	UNP Q5SBM0
A	734	GLY	-	expression tag	UNP Q5SBM0
A	761	MET	LEU	conflict	UNP Q5SBM0
A	1620	HIS	-	expression tag	UNP Q5SBM0
A	1621	HIS	-	expression tag	UNP Q5SBM0
A	1622	HIS	-	expression tag	UNP Q5SBM0
A	1623	HIS	-	expression tag	UNP Q5SBM0
A	1624	HIS	-	expression tag	UNP Q5SBM0
A	1625	HIS	-	expression tag	UNP Q5SBM0
B	733	MET	-	initiating methionine	UNP Q5SBM0
B	734	GLY	-	expression tag	UNP Q5SBM0
B	761	MET	LEU	conflict	UNP Q5SBM0
B	1620	HIS	-	expression tag	UNP Q5SBM0
B	1621	HIS	-	expression tag	UNP Q5SBM0
B	1622	HIS	-	expression tag	UNP Q5SBM0
B	1623	HIS	-	expression tag	UNP Q5SBM0
B	1624	HIS	-	expression tag	UNP Q5SBM0
B	1625	HIS	-	expression tag	UNP Q5SBM0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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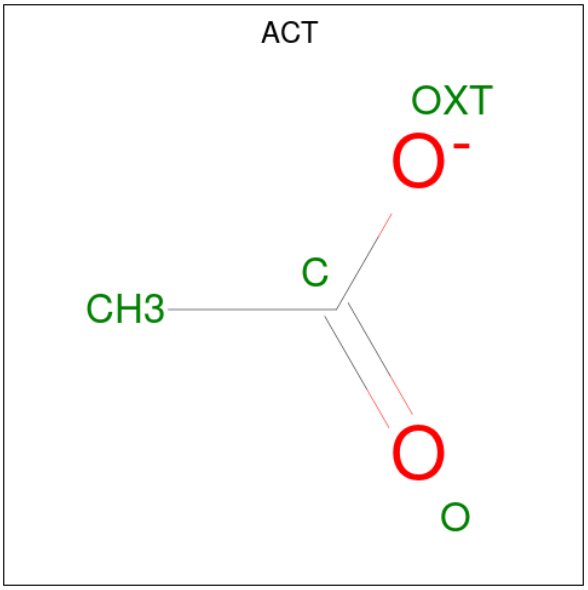
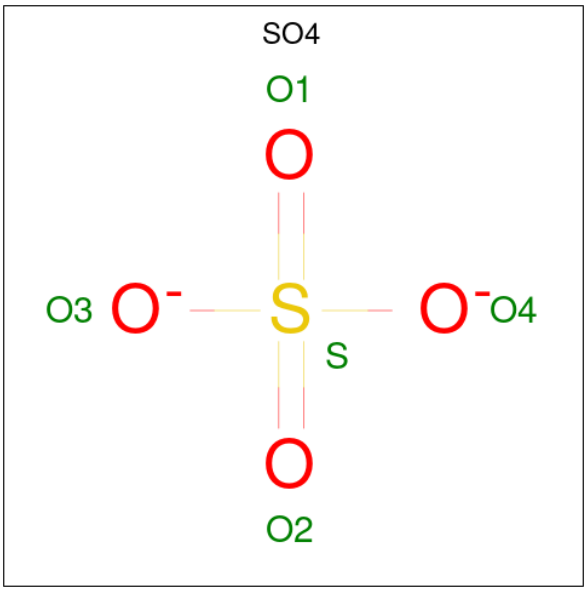
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	B	1	1	1	0	0

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



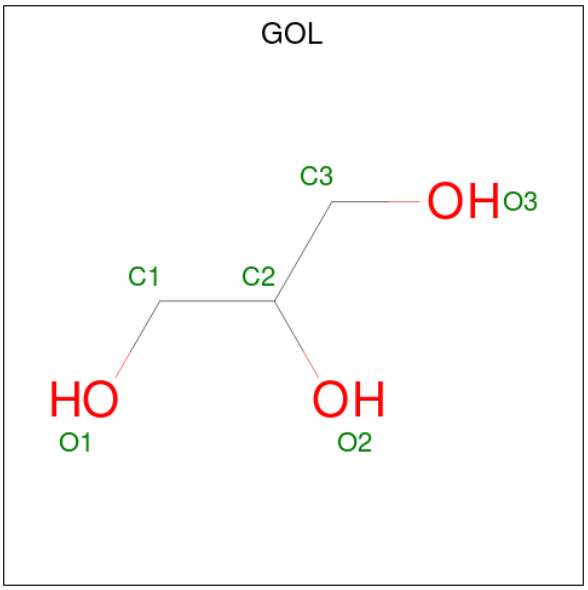
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



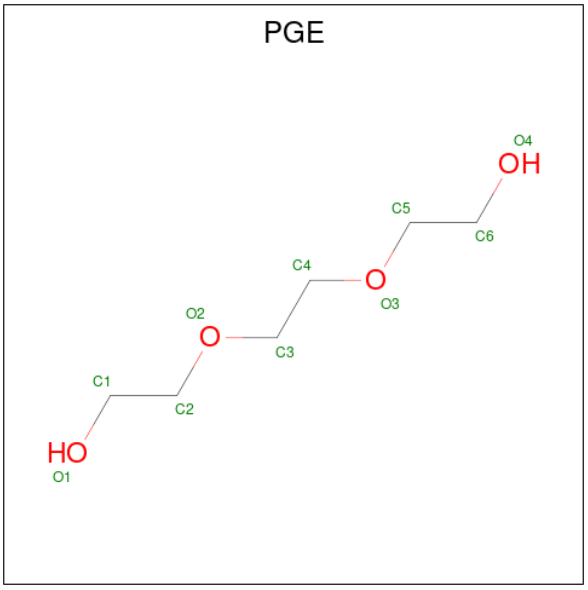
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	10	6	4	0	0

- Molecule 7 is water.

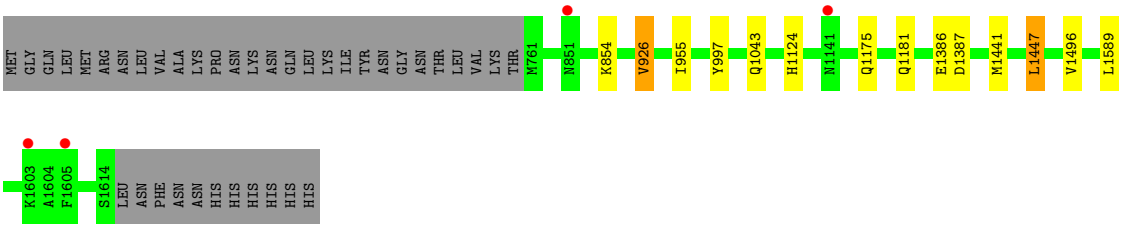
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	574	574	574	0	0
			Total	O		
7	B	709	709	709	0	0

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.

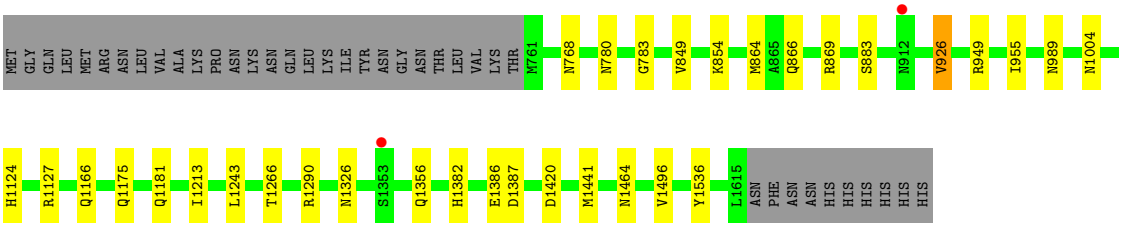
• Molecule 1: Inactive glucansucrase

Chain A: 94%



• Molecule 1: Inactive glucansucrase

Chain B: 92%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.24Å 57.85Å 150.70Å 90.00° 114.75° 90.00°	Depositor
Resolution (Å)	45.83 – 1.80 45.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.83-1.80) 99.3 (45.83-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.177 , 0.208 0.187 , 0.216	Depositor DCC
R_{free} test set	7949 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.4	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	14804	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, CA, PGE, 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	0.47	0/6854	0.63	0/9323
1	B	0.49	0/6853	0.65	3/9321 (0.0%)
All	All	0.48	0/13707	0.64	3/18644 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1127	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	949	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	1127	ARG	NE-CZ-NH2	-5.24	117.68	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	6711	0	6358	5	0
1	B	6704	0	6363	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	6	0	0
3	B	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	24	0	32	0	0
5	B	30	0	40	0	0
6	A	10	0	14	0	0
7	A	574	0	0	1	0
7	B	709	0	0	1	0
All	All	14804	0	12822	21	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 1.

All (21) 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:989:ASN:HD21	1:B:1536:TYR:H	1.42	0.66
1:B:1004:ASN:HD22	1:B:1464:ASN:HD22	1.52	0.57
1:B:1290:ARG:HH12	1:B:1326:ASN:HD22	1.55	0.54
1:A:997:TYR:CE1	1:A:1447:LEU:HD22	2.43	0.53
1:B:1166:GLN:HG2	1:B:1213:ILE:HD11	1.93	0.51
1:B:768:ASN:HD21	1:B:866:GLN:HE22	1.59	0.50
1:A:1175:GLN:HE21	1:A:1181:GLN:HE22	1.60	0.49
1:B:1175:GLN:HE21	1:B:1181:GLN:HE22	1.62	0.48
1:B:1382:HIS:HD2	1:B:1420:ASP:OD2	1.96	0.48
1:B:1382:HIS:HE1	7:B:2297:HOH:O	1.98	0.46
1:B:780:ASN:HD22	1:B:783:GLY:H	1.66	0.44
1:B:849:VAL:HG12	1:B:864:MET:CE	2.48	0.44
1:B:866:GLN:NE2	1:B:869:ARG:HH21	2.16	0.44
1:B:1124:HIS:ND1	1:B:1386:GLU:OE2	2.43	0.43
1:B:926:VAL:HG13	1:B:1496:VAL:HB	2.02	0.41
1:A:926:VAL:HG13	1:A:1496:VAL:HB	2.03	0.41
1:A:1043:GLN:NE2	7:A:1806:HOH:O	2.54	0.41
1:B:1266:THR:OG1	1:B:1356:GLN:NE2	2.51	0.40
1:B:1290:ARG:HH12	1:B:1326:ASN:ND2	2.19	0.40
1:A:1124:HIS:ND1	1:A:1386:GLU:OE2	2.44	0.40
1:B:1243:LEU:C	1:B:1243:LEU:HD12	2.42	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	857/893 (96%)	836 (98%)	19 (2%)	2 (0%)	47	33
1	B	857/893 (96%)	839 (98%)	16 (2%)	2 (0%)	47	33
All	All	1714/1786 (96%)	1675 (98%)	35 (2%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	854	LYS
1	A	955	ILE
1	B	854	LYS
1	B	955	ILE

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	725/756 (96%)	720 (99%)	5 (1%)	84	81
1	B	725/756 (96%)	721 (99%)	4 (1%)	86	84
All	All	1450/1512 (96%)	1441 (99%)	9 (1%)	86	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	926	VAL
1	A	1387	ASP

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Mol	Chain	Res	Type
1	A	1441	MET
1	A	1447	LEU
1	A	1589	LEU
1	B	883	SER
1	B	926	VAL
1	B	1387	ASP
1	B	1441	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1089	ASN
1	A	1139	HIS
1	A	1141	ASN
1	A	1175	GLN
1	A	1361	ASN
1	A	1574	ASN
1	A	1580	ASN
1	B	780	ASN
1	B	851	ASN
1	B	866	GLN
1	B	867	ASN
1	B	952	ASN
1	B	978	ASN
1	B	989	ASN
1	B	1019	ASN
1	B	1068	ASN
1	B	1106	GLN
1	B	1117	ASN
1	B	1139	HIS
1	B	1170	ASN
1	B	1175	GLN
1	B	1177	ASN
1	B	1326	ASN
1	B	1356	GLN
1	B	1382	HIS
1	B	1464	ASN
1	B	1515	ASN
1	B	1580	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	ACT	B	1704	-	3,3,3	0.74	0	3,3,3	0.84	0
5	GOL	B	1709	-	5,5,5	0.31	0	5,5,5	0.29	0
3	ACT	A	1703	-	3,3,3	0.77	0	3,3,3	0.78	0
5	GOL	A	1707	-	5,5,5	0.33	0	5,5,5	0.20	0
4	SO4	A	1704	-	4,4,4	0.33	0	6,6,6	0.14	0
3	ACT	A	1702	-	3,3,3	0.78	0	3,3,3	0.67	0
5	GOL	A	1706	-	5,5,5	0.42	0	5,5,5	0.21	0
4	SO4	B	1705	-	4,4,4	0.22	0	6,6,6	0.22	0
6	PGE	A	1710	-	9,9,9	0.49	0	8,8,8	0.34	0
5	GOL	B	1707	-	5,5,5	0.32	0	5,5,5	0.63	0
3	ACT	B	1702	-	3,3,3	0.84	0	3,3,3	0.39	0
5	GOL	A	1709	-	5,5,5	0.27	0	5,5,5	0.21	0
5	GOL	B	1711	-	5,5,5	0.29	0	5,5,5	0.32	0
5	GOL	A	1708	-	5,5,5	0.33	0	5,5,5	0.19	0
3	ACT	B	1703	-	3,3,3	0.74	0	3,3,3	0.93	0
5	GOL	B	1708	-	5,5,5	0.37	0	5,5,5	0.30	0
4	SO4	A	1705	-	4,4,4	0.34	0	6,6,6	0.26	0
4	SO4	B	1706	-	4,4,4	0.34	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	1710	-	5,5,5	0.29	0	5,5,5	0.17	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
5	GOL	A	1709	-	-	4/4/4/4	-
5	GOL	A	1706	-	-	3/4/4/4	-
5	GOL	B	1709	-	-	3/4/4/4	-
5	GOL	B	1711	-	-	0/4/4/4	-
5	GOL	A	1708	-	-	2/4/4/4	-
5	GOL	B	1710	-	-	2/4/4/4	-
5	GOL	A	1707	-	-	2/4/4/4	-
5	GOL	B	1708	-	-	2/4/4/4	-
6	PGE	A	1710	-	-	3/7/7/7	-
5	GOL	B	1707	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1708	GOL	O1-C1-C2-C3
5	B	1708	GOL	O1-C1-C2-O2
5	B	1708	GOL	O1-C1-C2-C3
5	B	1709	GOL	C1-C2-C3-O3
5	B	1710	GOL	C1-C2-C3-O3
5	B	1709	GOL	O2-C2-C3-O3
5	A	1706	GOL	O1-C1-C2-C3
5	A	1706	GOL	C1-C2-C3-O3
5	A	1707	GOL	O1-C1-C2-C3
5	A	1709	GOL	O1-C1-C2-C3
5	B	1707	GOL	O1-C1-C2-C3
5	B	1707	GOL	C1-C2-C3-O3
5	A	1708	GOL	O1-C1-C2-O2
5	B	1707	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	1710	GOL	O2-C2-C3-O3
6	A	1710	PGE	O2-C3-C4-O3
6	A	1710	PGE	O3-C5-C6-O4
5	A	1707	GOL	O1-C1-C2-O2
5	A	1706	GOL	O2-C2-C3-O3
5	A	1709	GOL	O1-C1-C2-O2
5	A	1709	GOL	O2-C2-C3-O3
5	B	1707	GOL	O2-C2-C3-O3
6	A	1710	PGE	C3-C4-O3-C5
5	A	1709	GOL	C1-C2-C3-O3
5	B	1709	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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 (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(Å^2)	Q<0.9
1	A	854/893 (95%)	-0.33	4 (0%)	91	89	19, 31, 55, 90	0
1	B	855/893 (95%)	-0.52	2 (0%)	95	93	17, 26, 42, 62	0
All	All	1709/1786 (95%)	-0.43	6 (0%)	92	90	17, 28, 48, 90	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	851	ASN	2.8
1	B	1353	SER	2.6
1	A	1141	ASN	2.4
1	A	1603	LYS	2.1
1	A	1605	PHE	2.1
1	B	912	ASN	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 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, 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
5	GOL	A	1707	6/6	0.68	0.16	61,67,68,68	0
5	GOL	B	1708	6/6	0.76	0.17	64,68,73,75	0
6	PGE	A	1710	10/10	0.76	0.18	61,73,75,78	0
5	GOL	B	1711	6/6	0.85	0.14	63,65,67,71	0
5	GOL	A	1709	6/6	0.85	0.17	47,51,53,55	0
5	GOL	A	1706	6/6	0.86	0.15	40,48,50,52	0
5	GOL	B	1709	6/6	0.86	0.28	49,59,60,60	0
5	GOL	A	1708	6/6	0.87	0.15	38,45,49,51	0
5	GOL	B	1707	6/6	0.87	0.20	35,45,50,53	0
3	ACT	B	1702	4/4	0.88	0.16	33,43,44,55	0
5	GOL	B	1710	6/6	0.88	0.13	29,47,50,54	0
3	ACT	A	1703	4/4	0.89	0.15	52,58,59,61	0
3	ACT	B	1703	4/4	0.90	0.11	48,48,50,55	0
4	SO4	A	1705	5/5	0.90	0.10	55,66,74,76	0
3	ACT	B	1704	4/4	0.91	0.16	48,56,58,58	0
3	ACT	A	1702	4/4	0.91	0.15	47,49,51,54	0
4	SO4	B	1706	5/5	0.94	0.14	79,81,85,87	0
4	SO4	A	1704	5/5	0.96	0.12	65,65,70,73	0
4	SO4	B	1705	5/5	0.98	0.10	43,46,51,54	0
2	CA	A	1701	1/1	0.99	0.07	22,22,22,22	0
2	CA	B	1701	1/1	1.00	0.07	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.