Full wwPDB X-ray Structure Validation Report

May 26, 2020 – 11:28 pm BST

PDB ID	:	5MEH
Title	:	Crystal structure of alpha-1,2-mannosidase from Caulobacter K31 strain in complex with 1-deoxymannojirimycin
Authors	:	Males, A.; Davies, G.J.
Deposited on	:	2016-11-14
Resolution	:	0.95 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 following versions of software and data (see references (1)) were used in the production of this report:

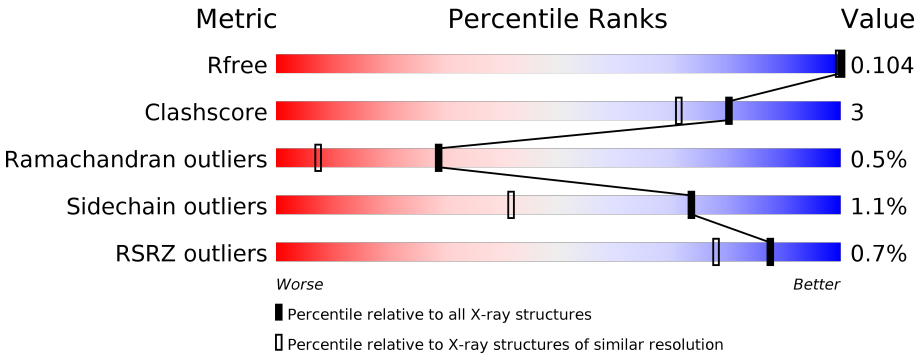
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 0.95 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	1243 (1.06-0.86)
Clashscore	141614	1321 (1.06-0.86)
Ramachandran outliers	138981	1233 (1.06-0.86)
Sidechain outliers	138945	1235 (1.06-0.86)
RSRZ outliers	127900	1209 (1.06-0.86)

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 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	447	% 89% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4229 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.

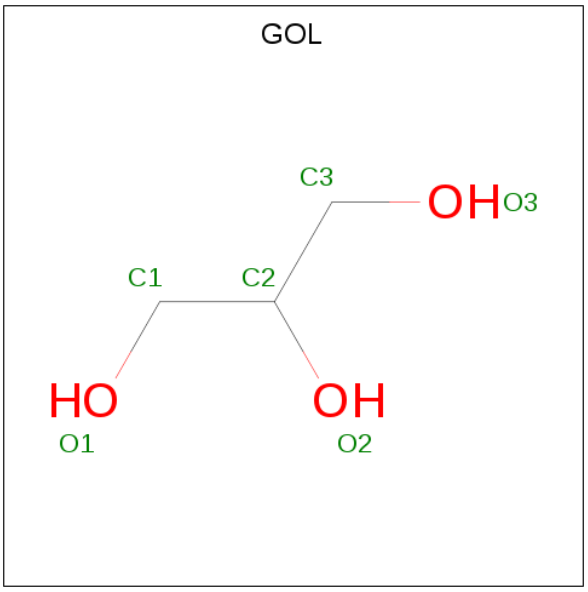
- Molecule 1 is a protein called Mannosyl-oligosaccharide 1,2-alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	34	1
			3666	2355	629	667	15			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP B0SWV2
A	25	ALA	-	expression tag	UNP B0SWV2
A	26	SER	-	expression tag	UNP B0SWV2
A	463	LEU	-	expression tag	UNP B0SWV2
A	464	GLU	-	expression tag	UNP B0SWV2
A	465	HIS	-	expression tag	UNP B0SWV2
A	466	HIS	-	expression tag	UNP B0SWV2
A	467	HIS	-	expression tag	UNP B0SWV2
A	468	HIS	-	expression tag	UNP B0SWV2
A	469	HIS	-	expression tag	UNP B0SWV2
A	470	HIS	-	expression tag	UNP B0SWV2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

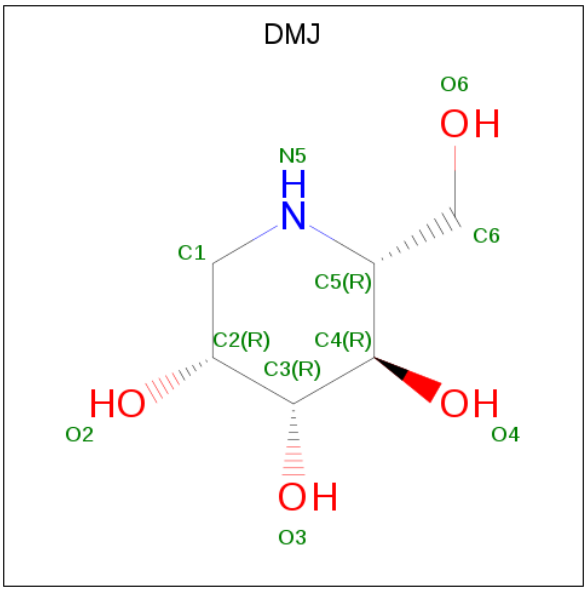
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

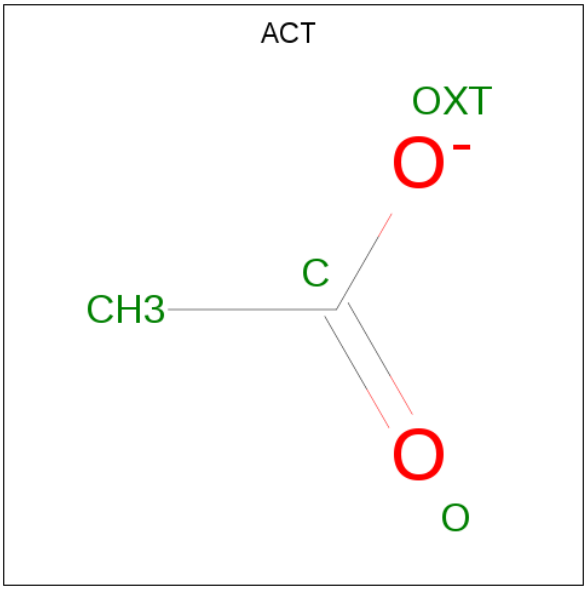
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is 1-DEOXYMANNOJIRIMYCIN (three-letter code: DMJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			22	12	2	8		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

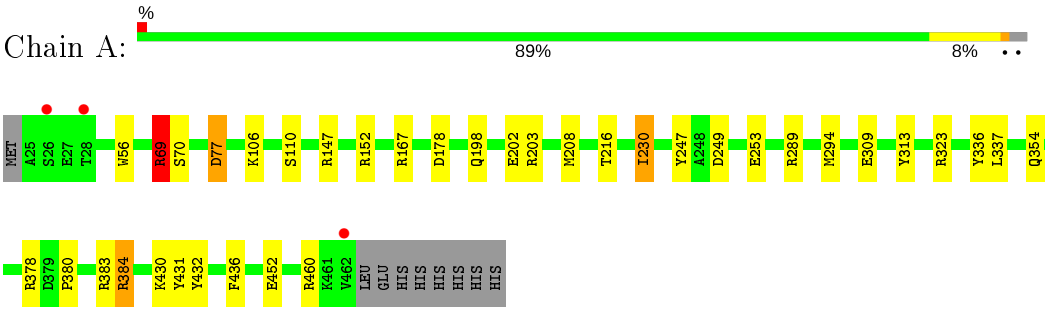
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	505	Total O 522 522	0	17

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 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: Mannosyl-oligosaccharide 1,2-alpha-mannosidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	145.37Å 145.37Å 50.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.14 – 0.95 47.14 – 0.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.14-0.95) 98.9 (47.14-0.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 0.95Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.091 , 0.103 0.092 , 0.104	Depositor DCC
R_{free} test set	12618 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	7.7	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4229	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: GOL, DMJ, ACT, CA, NA

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	1.36	18/3869 (0.5%)	1.28	34/5244 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69[A]	ARG	C-O	18.36	1.58	1.23
1	A	69[B]	ARG	C-O	18.36	1.58	1.23
1	A	354[A]	GLN	CD-OE1	11.22	1.48	1.24
1	A	354[B]	GLN	CD-OE1	11.22	1.48	1.24
1	A	384[A]	ARG	CZ-NH1	7.88	1.43	1.33
1	A	384[B]	ARG	CZ-NH1	7.88	1.43	1.33
1	A	309	GLU	CD-OE1	7.71	1.34	1.25
1	A	110	SER	CA-CB	7.22	1.63	1.52
1	A	69[A]	ARG	CZ-NH2	6.51	1.41	1.33
1	A	69[B]	ARG	CZ-NH2	6.51	1.41	1.33
1	A	253	GLU	CD-OE2	6.25	1.32	1.25
1	A	378	ARG	CZ-NH2	-6.17	1.25	1.33
1	A	202[A]	GLU	CD-OE2	6.08	1.32	1.25
1	A	202[B]	GLU	CD-OE2	6.08	1.32	1.25
1	A	378	ARG	NE-CZ	6.01	1.40	1.33
1	A	247	TYR	CG-CD1	5.73	1.46	1.39
1	A	56	TRP	CD2-CE2	5.25	1.47	1.41
1	A	452	GLU	CD-OE2	5.21	1.31	1.25

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	ARG	NE-CZ-NH1	-20.54	110.03	120.30
1	A	384[A]	ARG	NE-CZ-NH1	20.29	130.44	120.30
1	A	384[B]	ARG	NE-CZ-NH1	20.29	130.44	120.30
1	A	289[A]	ARG	NE-CZ-NH1	-16.90	111.85	120.30
1	A	289[B]	ARG	NE-CZ-NH1	-16.90	111.85	120.30
1	A	384[A]	ARG	NE-CZ-NH2	-14.51	113.05	120.30
1	A	384[B]	ARG	NE-CZ-NH2	-14.51	113.05	120.30
1	A	69[A]	ARG	O-C-N	-13.64	100.87	122.70
1	A	69[B]	ARG	O-C-N	-13.64	100.87	122.70
1	A	203[A]	ARG	NE-CZ-NH1	-10.13	115.24	120.30
1	A	203[B]	ARG	NE-CZ-NH1	-10.13	115.24	120.30
1	A	203[C]	ARG	NE-CZ-NH1	-10.13	115.24	120.30
1	A	69[A]	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	69[B]	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	384[A]	ARG	CD-NE-CZ	8.48	135.47	123.60
1	A	384[B]	ARG	CD-NE-CZ	8.48	135.47	123.60
1	A	69[A]	ARG	CA-C-O	8.46	137.87	120.10
1	A	69[B]	ARG	CA-C-O	8.46	137.87	120.10
1	A	323[A]	ARG	CB-CG-CD	6.69	129.00	111.60
1	A	323[B]	ARG	CB-CG-CD	6.69	129.00	111.60
1	A	208[A]	MET	CA-CB-CG	6.51	124.37	113.30
1	A	208[B]	MET	CA-CB-CG	6.51	124.37	113.30
1	A	289[A]	ARG	NH1-CZ-NH2	6.50	126.55	119.40
1	A	289[B]	ARG	NH1-CZ-NH2	6.50	126.55	119.40
1	A	294[A]	MET	CG-SD-CE	-5.91	90.75	100.20
1	A	294[B]	MET	CG-SD-CE	-5.91	90.75	100.20
1	A	152	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	460	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	460	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	A	147	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	167	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	436	PHE	CB-CG-CD1	5.21	124.45	120.80
1	A	431	TYR	CB-CG-CD1	5.03	124.02	121.00
1	A	432	TYR	CB-CG-CD1	5.03	124.02	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	TYR	Sidechain
1	A	383	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	69[A]	ARG	Mainchain
1	A	69[B]	ARG	Mainchain

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	3666	0	3645	17	1
2	A	12	0	15	1	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	22	0	22	1	0
6	A	4	0	3	1	0
7	A	522	0	0	15	1
All	All	4229	0	3685	20	1

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 (20) 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:359[B]:HIS:CD2	7:A:604:HOH:O	2.05	1.06
1:A:106[B]:LYS:HE2	7:A:1002[B]:HOH:O	1.71	0.88
1:A:69[B]:ARG:CZ	7:A:603:HOH:O	2.26	0.83
1:A:357:ARG:HH11	1:A:359[A]:HIS:HE1	1.27	0.82
6:A:507:ACT:H1	7:A:629:HOH:O	1.79	0.81
2:A:501:GOL:H12	7:A:901[B]:HOH:O	1.82	0.78
1:A:69[B]:ARG:NH1	7:A:603:HOH:O	2.15	0.77
1:A:70[A]:SER:OG	7:A:602:HOH:O	2.03	0.75
1:A:69[B]:ARG:NE	7:A:603:HOH:O	2.21	0.73
1:A:106[B]:LYS:CE	7:A:1002[B]:HOH:O	2.35	0.67
5:A:506[B]:DMJ:H12	7:A:621:HOH:O	1.96	0.65
1:A:198[A]:GLN:HG2	7:A:605:HOH:O	2.09	0.53
1:A:357:ARG:HH11	1:A:359[A]:HIS:CE1	2.16	0.52
1:A:359[B]:HIS:NE2	7:A:604:HOH:O	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198[A]:GLN:CG	7:A:605:HOH:O	2.62	0.47
1:A:216:THR:HG22	1:A:230:ILE:HD13	1.97	0.46
1:A:359[B]:HIS:HD2	7:A:604:HOH:O	1.65	0.46
1:A:198[A]:GLN:NE2	7:A:605:HOH:O	2.34	0.43
1:A:336[B]:TYR:CE2	1:A:337:LEU:HD23	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384[A]:ARG:NH2	7:A:924:HOH:O[5_555]	1.48	0.72

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	472/447 (106%)	458 (97%)	12 (2%)	2 (0%)	34 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASP
1	A	178	ASP

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	386/362 (107%)	382 (99%)	4 (1%)	76 46

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	230	ILE
1	A	380	PRO
1	A	430	LYS

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	372	ASN
1	A	416	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 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	$\#\|Z\|>2$
5	DMJ	A	506[A]	3	11,11,11	2.56	4 (36%)	13,15,15	1.31	2 (15%)
2	GOL	A	502	-	5,5,5	1.13	1 (20%)	5,5,5	0.54	0
6	ACT	A	507	-	1,3,3	11.39	1 (100%)	0,3,3	0.00	-
5	DMJ	A	506[B]	3	11,11,11	2.17	3 (27%)	13,15,15	2.01	5 (38%)
2	GOL	A	501	-	5,5,5	0.53	0	5,5,5	0.73	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	DMJ	A	506[A]	3	-	0/2/19/19	0/1/1/1
2	GOL	A	502	-	-	0/4/4/4	-
5	DMJ	A	506[B]	3	-	0/2/19/19	0/1/1/1
2	GOL	A	501	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	507	ACT	CH3-C	-11.39	1.34	1.48
5	A	506[A]	DMJ	C5-N5	4.79	1.54	1.47
5	A	506[A]	DMJ	C1-C2	4.55	1.56	1.52
5	A	506[B]	DMJ	C1-C2	4.40	1.56	1.52
5	A	506[B]	DMJ	C2-C3	4.07	1.58	1.52
5	A	506[A]	DMJ	C2-C3	3.16	1.57	1.52
5	A	506[A]	DMJ	C1-N5	2.96	1.51	1.47
5	A	506[B]	DMJ	C1-N5	-2.65	1.43	1.47
2	A	502	GOL	O1-C1	-2.18	1.33	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	506[B]	DMJ	C1-N5-C5	4.00	118.25	109.61
5	A	506[A]	DMJ	C1-C2-C3	3.45	114.38	110.33
5	A	506[B]	DMJ	O3-C3-C2	-3.31	103.65	109.99
5	A	506[B]	DMJ	C3-C4-C5	3.27	115.81	111.02
5	A	506[A]	DMJ	C1-N5-C5	2.75	115.56	109.61
5	A	506[B]	DMJ	O2-C2-C3	-2.37	105.39	110.14
5	A	506[B]	DMJ	C1-C2-C3	-2.23	107.71	110.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	ACT	1	0
5	A	506[B]	DMJ	1	0
2	A	501	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	438/447 (97%)	-0.87	3 (0%) 87 78	5, 8, 17, 53	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	SER	3.9
1	A	28	THR	3.2
1	A	462	VAL	2.6

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

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
6	ACT	A	507	4/4	0.90	0.10	15,19,24,35	0
2	GOL	A	502	6/6	0.96	0.09	8,12,13,15	1
5	DMJ	A	506[A]	11/11	0.99	0.03	5,6,6,7	11
5	DMJ	A	506[B]	11/11	0.99	0.03	5,6,8,9	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	501	6/6	0.99	0.05	8,10,24,350	0
3	CA	A	504	1/1	1.00	0.04	5,5,5,5	1
3	CA	A	503	1/1	1.00	0.03	5,5,5,5	0
4	NA	A	505	1/1	1.00	0.04	5,5,5,5	0

6.5 Other polymers

There are no such residues in this entry.