Full wwPDB X-ray Structure Validation Report (i)

Mar 28, 2023 – 04:51 pm BST

PDB ID	:	8C9T
Title	:	Catechol O-methyltransferase from Streptomyces avermitilis
Authors	:	Zhang, L.; Groves, M.R.
Deposited on	:	2023-01-23
Resolution	:	1.50 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 (1)) were used in the production of this report:

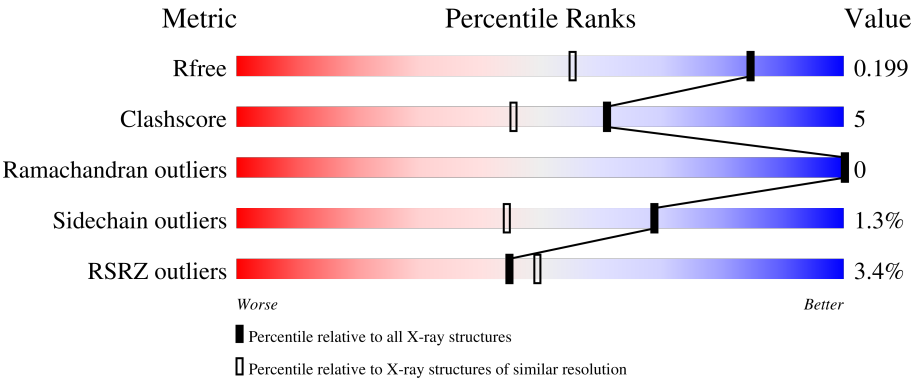
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	232	3% 91% 5% ·
1	B	232	% 87% 8% 5%
1	C	232	7% 88% 10% ·
1	D	232	% 83% 9% · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14429 atoms, of which 6872 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 Putative O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	H	N	O	41	5	0
			3443	1081	1723	304	335			
1	B	221	Total	C	H	N	O	37	3	0
			3407	1071	1709	301	326			
1	C	228	Total	C	H	N	O	48	4	0
			3527	1111	1766	316	334			
1	D	216	Total	C	H	N	O	35	3	0
			3312	1041	1658	292	321			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	LEU	-	expression tag	UNP Q82B68
A	226	GLU	-	expression tag	UNP Q82B68
A	227	HIS	-	expression tag	UNP Q82B68
A	228	HIS	-	expression tag	UNP Q82B68
A	229	HIS	-	expression tag	UNP Q82B68
A	230	HIS	-	expression tag	UNP Q82B68
A	231	HIS	-	expression tag	UNP Q82B68
A	232	HIS	-	expression tag	UNP Q82B68
B	225	LEU	-	expression tag	UNP Q82B68
B	226	GLU	-	expression tag	UNP Q82B68
B	227	HIS	-	expression tag	UNP Q82B68
B	228	HIS	-	expression tag	UNP Q82B68
B	229	HIS	-	expression tag	UNP Q82B68
B	230	HIS	-	expression tag	UNP Q82B68
B	231	HIS	-	expression tag	UNP Q82B68
B	232	HIS	-	expression tag	UNP Q82B68
C	225	LEU	-	expression tag	UNP Q82B68
C	226	GLU	-	expression tag	UNP Q82B68
C	227	HIS	-	expression tag	UNP Q82B68
C	228	HIS	-	expression tag	UNP Q82B68
C	229	HIS	-	expression tag	UNP Q82B68

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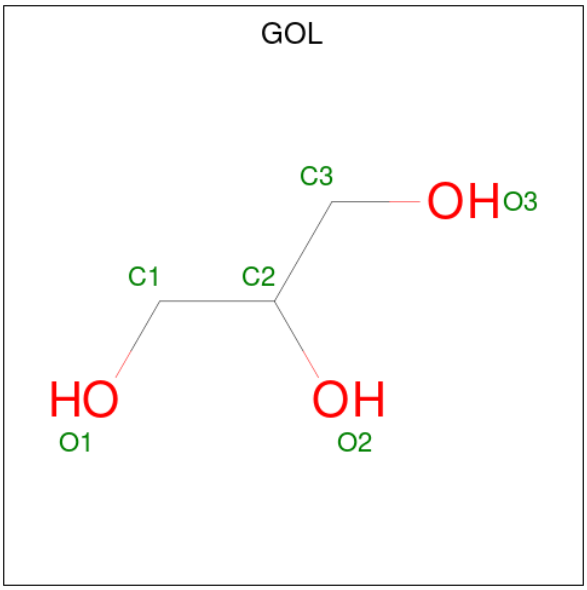
Chain	Residue	Modelled	Actual	Comment	Reference
C	230	HIS	-	expression tag	UNP Q82B68
C	231	HIS	-	expression tag	UNP Q82B68
C	232	HIS	-	expression tag	UNP Q82B68
D	225	LEU	-	expression tag	UNP Q82B68
D	226	GLU	-	expression tag	UNP Q82B68
D	227	HIS	-	expression tag	UNP Q82B68
D	228	HIS	-	expression tag	UNP Q82B68
D	229	HIS	-	expression tag	UNP Q82B68
D	230	HIS	-	expression tag	UNP Q82B68
D	231	HIS	-	expression tag	UNP Q82B68
D	232	HIS	-	expression tag	UNP Q82B68

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C H O 14 3 8 3	2	0
2	D	1	Total C H O 14 3 8 3	2	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	171	Total O 171 171	0	0
3	B	179	Total O 179 179	0	0

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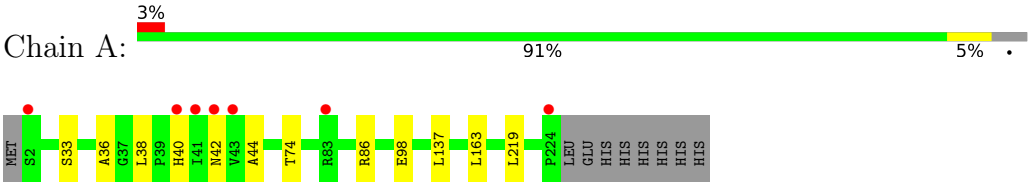
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	193	Total O 193 193	0	0
3	D	169	Total O 169 169	0	0

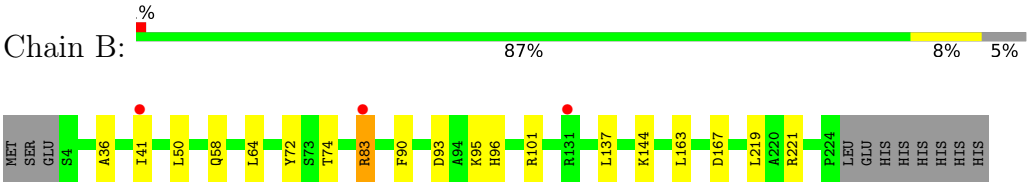
3 Residue-property plots (i)

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.

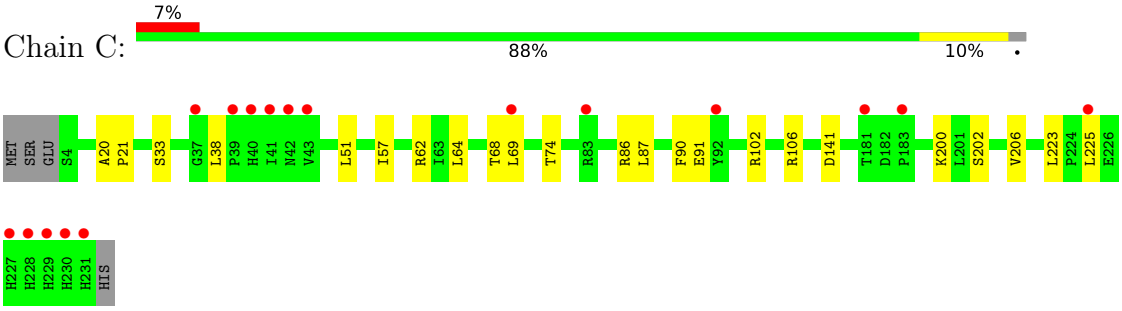
• Molecule 1: Putative O-methyltransferase



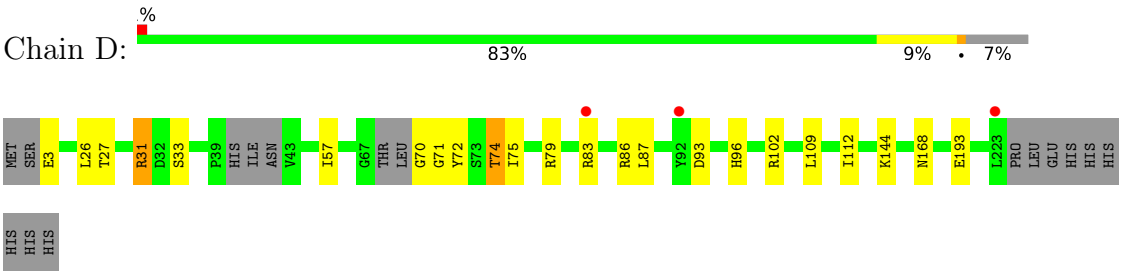
• Molecule 1: Putative O-methyltransferase



• Molecule 1: Putative O-methyltransferase



• Molecule 1: Putative O-methyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.46Å 168.74Å 57.24Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	46.71 – 1.50 46.71 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.71-1.50) 96.1 (46.71-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.194 0.174 , 0.199	Depositor DCC
R_{free} test set	6583 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	13.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14429	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

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	0.83	2/1758 (0.1%)	0.92	1/2393 (0.0%)
1	B	0.78	0/1733	0.95	3/2360 (0.1%)
1	C	0.78	0/1810	0.89	1/2465 (0.0%)
1	D	0.80	0/1688	0.96	4/2294 (0.2%)
All	All	0.80	2/6989 (0.0%)	0.93	9/9512 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CD-OE2	6.48	1.32	1.25
1	A	98	GLU	CD-OE1	6.03	1.32	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	102	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	102	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	79	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	221	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	31	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	106	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	101	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	72	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	86	ARG	NE-CZ-NH2	-5.27	117.66	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	1720	1723	1717	15	0
1	B	1698	1709	1703	22	0
1	C	1761	1766	1760	17	0
1	D	1654	1658	1653	11	0
2	C	6	8	8	0	0
2	D	6	8	8	0	0
3	A	171	0	0	1	0
3	B	179	0	0	3	0
3	C	193	0	0	5	0
3	D	169	0	0	1	0
All	All	7557	6872	6849	62	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 5.

All (62) 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:163[B]:LEU:HD11	1:B:219:LEU:CD1	1.79	1.13
1:A:163[A]:LEU:HD11	1:A:219:LEU:CD1	1.81	1.10
1:A:163[A]:LEU:HD11	1:A:219:LEU:HD11	1.10	1.10
1:B:64:LEU:HD11	1:B:90:PHE:HE2	1.21	1.06
1:B:163[B]:LEU:CD1	1:B:219:LEU:HD11	1.85	1.05
1:B:163[B]:LEU:HD11	1:B:219:LEU:HD11	1.07	1.03
1:A:163[A]:LEU:CD1	1:A:219:LEU:HD11	1.91	0.99
1:B:64:LEU:HD11	1:B:90:PHE:CE2	2.08	0.86
1:A:44:ALA:HA	3:A:376:HOH:O	1.77	0.83
1:B:41:ILE:HG22	3:B:424:HOH:O	1.92	0.70
1:B:93:ASP:OD2	1:B:96:HIS:HD2	1.77	0.68
1:C:62:ARG:HH22	1:C:86:ARG:HH11	1.42	0.66
1:D:33:SER:HG	1:D:70:GLY:N	1.94	0.65
1:B:163[B]:LEU:CG	1:B:219:LEU:HD11	2.27	0.65
1:B:163[B]:LEU:CD1	1:B:219:LEU:CD1	2.62	0.64
1:B:58:GLN:HG3	1:B:163[A]:LEU:HG	1.82	0.61
1:A:163[A]:LEU:HD21	1:A:219:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163[B]:LEU:HD21	1:B:219:LEU:HD11	1.84	0.59
1:D:93:ASP:OD1	1:D:96:HIS:HD2	1.85	0.59
1:A:163[A]:LEU:CG	1:A:219:LEU:HD11	2.33	0.59
1:A:163[A]:LEU:CD1	1:A:219:LEU:CD1	2.65	0.58
1:D:71:GLY:O	1:D:75:ILE:HG13	2.04	0.58
1:C:62:ARG:HH12	1:C:86:ARG:HD2	1.68	0.58
1:A:40:HIS:HE1	1:A:42:ASN:OD1	1.89	0.56
1:D:74:THR:HG22	1:D:87:LEU:HD21	1.89	0.55
1:A:163[B]:LEU:HD21	1:D:57:ILE:HG12	1.87	0.55
1:B:163[B]:LEU:CD2	1:B:219:LEU:HD11	2.37	0.54
1:C:64:LEU:HD11	1:C:90:PHE:HE2	1.73	0.52
1:C:200:LYS:HD3	3:C:424:HOH:O	2.09	0.52
1:B:96:HIS:HE1	3:B:307:HOH:O	1.94	0.51
1:C:141:ASP:OD1	3:C:401:HOH:O	2.18	0.50
1:A:163[A]:LEU:CD2	1:A:219:LEU:HD11	2.40	0.50
1:A:163[A]:LEU:HD21	1:A:219:LEU:CD1	2.41	0.49
1:B:163[A]:LEU:HD21	1:C:57:ILE:HG12	1.94	0.49
1:A:36:ALA:HB3	1:A:38:LEU:HD13	1.95	0.49
1:C:64:LEU:HD11	1:C:90:PHE:CE2	2.48	0.49
1:B:163[B]:LEU:HD21	1:B:219:LEU:CD1	2.42	0.48
1:C:200:LYS:HZ1	1:C:225:LEU:HD13	1.77	0.48
1:A:137:LEU:HA	1:A:163[A]:LEU:O	2.16	0.46
1:B:36:ALA:O	1:B:95:LYS:HE2	2.14	0.46
1:B:93:ASP:OD2	1:B:96:HIS:CD2	2.65	0.46
1:D:93:ASP:OD1	1:D:96:HIS:CD2	2.67	0.45
1:D:144:LYS:HE2	1:D:168:ASN:O	2.16	0.45
1:D:26:LEU:HD22	1:D:72:TYR:CE2	2.52	0.44
1:D:27[B]:THR:HG22	1:D:31:ARG:NH1	2.33	0.44
1:C:20:ALA:N	1:C:21:PRO:CD	2.81	0.43
1:B:137:LEU:HA	1:B:163[B]:LEU:O	2.18	0.43
1:B:163[B]:LEU:CG	1:B:219:LEU:CD1	2.95	0.43
1:D:109:LEU:O	1:D:112:ILE:HG13	2.19	0.42
1:D:193:GLU:HG3	3:D:404:HOH:O	2.19	0.42
1:C:68:THR:HB	1:C:91:GLU:HB2	2.00	0.42
1:B:50:LEU:HD22	1:C:206[B]:VAL:HG21	2.02	0.42
1:C:87:LEU:HD23	1:C:87:LEU:C	2.40	0.42
1:C:202:SER:HB2	1:C:223:LEU:HD11	2.02	0.42
1:C:141:ASP:CG	3:C:401:HOH:O	2.56	0.41
1:B:83:ARG:HD3	3:B:407:HOH:O	2.19	0.41
1:B:144:LYS:NZ	1:B:167:ASP:O	2.54	0.41
1:A:163[A]:LEU:CG	1:A:219:LEU:CD1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33[B]:SER:OG	1:A:38:LEU:HD22	2.21	0.40
1:C:102:ARG:HD3	3:C:423:HOH:O	2.20	0.40
1:C:69:LEU:HD12	3:C:403:HOH:O	2.21	0.40
1:C:33[B]:SER:OG	1:C:38:LEU:HD12	2.22	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	226/232 (97%)	217 (96%)	9 (4%)	0	100	100
1	B	222/232 (96%)	218 (98%)	4 (2%)	0	100	100
1	C	230/232 (99%)	224 (97%)	6 (3%)	0	100	100
1	D	213/232 (92%)	206 (97%)	7 (3%)	0	100	100
All	All	891/928 (96%)	865 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	182/186 (98%)	181 (100%)	1 (0%)	88	78
1	B	178/186 (96%)	176 (99%)	2 (1%)	73	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	186/186 (100%)	184 (99%)	2 (1%)	73 53
1	D	173/186 (93%)	169 (98%)	4 (2%)	50 20
All	All	719/744 (97%)	710 (99%)	9 (1%)	69 44

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

Mol	Chain	Res	Type
1	A	74	THR
1	B	74	THR
1	B	83	ARG
1	C	51	LEU
1	C	74	THR
1	D	3	GLU
1	D	74	THR
1	D	83	ARG
1	D	86	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	146	ASN
1	A	147	ASN
1	B	96	HIS
1	B	146	ASN
1	B	147	ASN
1	C	146	ASN
1	D	96	HIS
1	D	147	ASN
1	D	168	ASN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	C	301	-	5,5,5	0.08	0	5,5,5	0.37	0
2	GOL	D	301	-	5,5,5	0.22	0	5,5,5	0.70	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
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	GOL	C1-C2-C3-O3
2	D	301	GOL	O2-C2-C3-O3

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

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	223/232 (96%)	-0.08	7 (3%) 49 54	8, 12, 24, 41	0
1	B	221/232 (95%)	-0.18	3 (1%) 75 79	8, 13, 25, 45	0
1	C	228/232 (98%)	0.07	17 (7%) 14 14	8, 13, 28, 49	0
1	D	216/232 (93%)	-0.05	3 (1%) 75 79	8, 14, 27, 46	0
All	All	888/928 (95%)	-0.06	30 (3%) 45 49	8, 13, 27, 49	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	7.0
1	A	42	ASN	4.9
1	B	83	ARG	4.7
1	A	41	ILE	4.2
1	C	39	PRO	4.2
1	A	2	SER	3.8
1	C	41	ILE	3.7
1	A	40	HIS	3.6
1	C	42	ASN	3.4
1	C	228	HIS	3.4
1	D	83	ARG	3.2
1	C	225	LEU	3.1
1	C	43	VAL	3.1
1	D	92	TYR	2.9
1	C	40	HIS	2.9
1	A	83	ARG	2.9
1	A	224	PRO	2.9
1	C	69	LEU	2.9
1	B	131	ARG	2.8
1	C	92	TYR	2.6
1	C	183	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	227	HIS	2.4
1	D	223	LEU	2.3
1	B	41	ILE	2.2
1	C	37	GLY	2.2
1	C	231	HIS	2.2
1	C	83	ARG	2.2
1	C	230	HIS	2.2
1	C	229	HIS	2.1
1	C	181	THR	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
2	GOL	C	301	6/6	0.83	0.16	28,32,33,33	2
2	GOL	D	301	6/6	0.88	0.13	17,26,30,30	2

6.5 Other polymers (i)

There are no such residues in this entry.