



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:09 pm BST

PDB ID : 5YMR
Title : The Crystal Structure of IseG
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Deposited on : 2017-10-22
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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

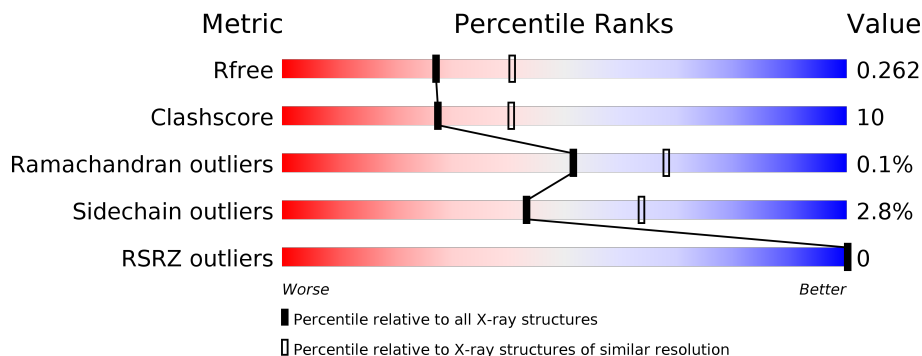
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	808	 78% 20% ..
1	B	808	 76% 21% ..
1	C	808	 78% 20% ..
1	D	808	 79% 19% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25800 atoms, of which 68 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 Formate acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	798	Total 6251	C 3980	N 1062	O 1177	S 32	0	0	0
1	D	798	Total 6232	C 3970	N 1059	O 1171	S 32	0	0	0
1	C	797	Total 6229	C 3961	N 1061	O 1175	S 32	0	0	0
1	A	798	Total 6219	C 3962	N 1052	O 1173	S 32	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

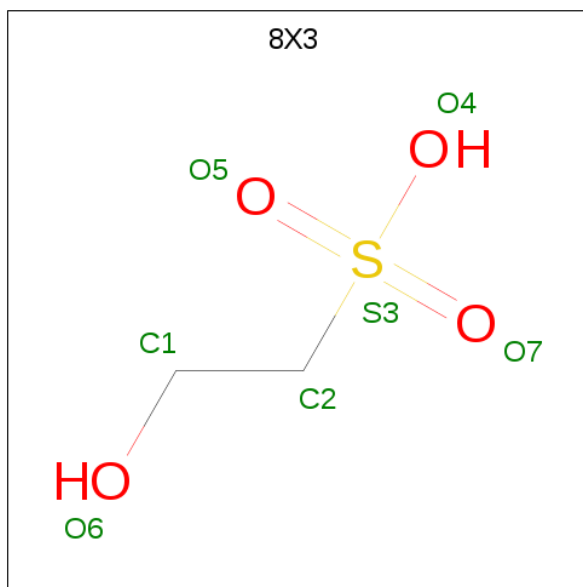
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	SER	-	expression tag	UNP Q727N1
B	22	ASN	-	expression tag	UNP Q727N1
B	23	ALA	-	expression tag	UNP Q727N1
B	133	ALA	GLU	engineered mutation	UNP Q727N1
B	134	ALA	ASP	engineered mutation	UNP Q727N1
B	136	ALA	ARG	engineered mutation	UNP Q727N1
D	21	SER	-	expression tag	UNP Q727N1
D	22	ASN	-	expression tag	UNP Q727N1
D	23	ALA	-	expression tag	UNP Q727N1
D	133	ALA	GLU	engineered mutation	UNP Q727N1
D	134	ALA	ASP	engineered mutation	UNP Q727N1
D	136	ALA	ARG	engineered mutation	UNP Q727N1
C	21	SER	-	expression tag	UNP Q727N1
C	22	ASN	-	expression tag	UNP Q727N1
C	23	ALA	-	expression tag	UNP Q727N1
C	133	ALA	GLU	engineered mutation	UNP Q727N1
C	134	ALA	ASP	engineered mutation	UNP Q727N1
C	136	ALA	ARG	engineered mutation	UNP Q727N1
A	21	SER	-	expression tag	UNP Q727N1
A	22	ASN	-	expression tag	UNP Q727N1
A	23	ALA	-	expression tag	UNP Q727N1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ALA	GLU	engineered mutation	UNP Q727N1
A	134	ALA	ASP	engineered mutation	UNP Q727N1
A	136	ALA	ARG	engineered mutation	UNP Q727N1

- Molecule 2 is 2-hydroxyethylsulfonic acid (three-letter code: 8X3) (formula: C₂H₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
2	B	1	12	2	5	4	1	0	0
2	D	1	12	2	5	4	1	0	0
2	C	1	12	2	5	4	1	0	0
2	A	1	12	2	5	4	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

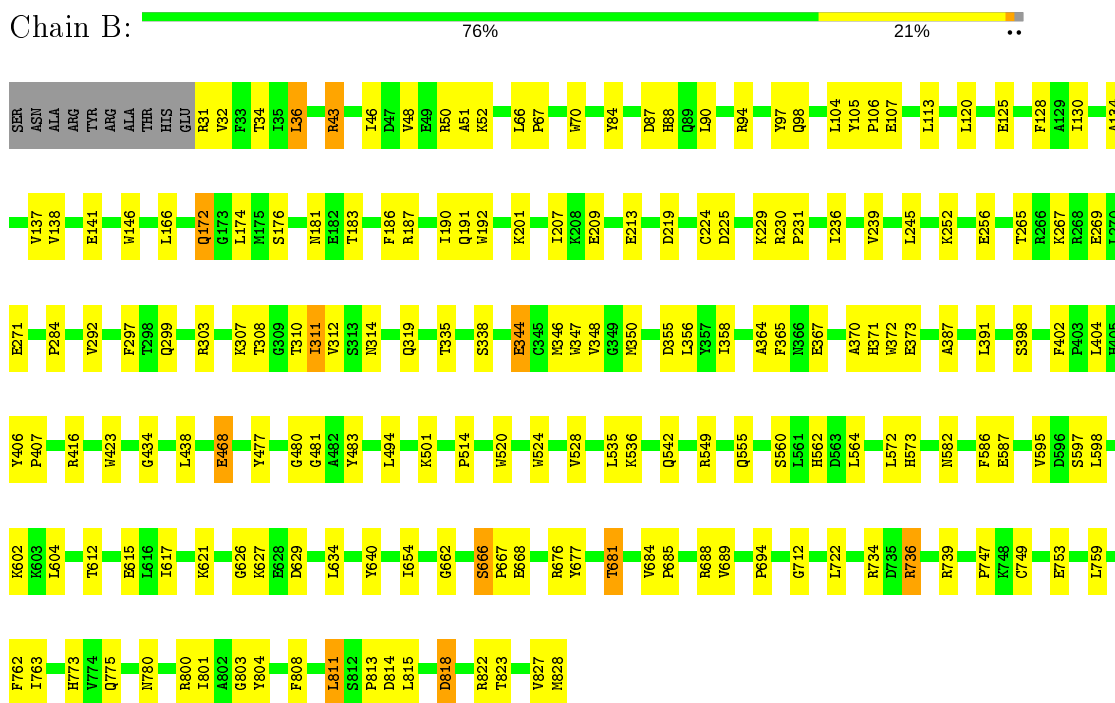
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	204	Total	O	0	0
			204	204		
4	D	154	Total	O	0	0
			154	154		
4	C	161	Total	O	0	0
			161	161		
4	A	218	Total	O	0	0
			218	218		

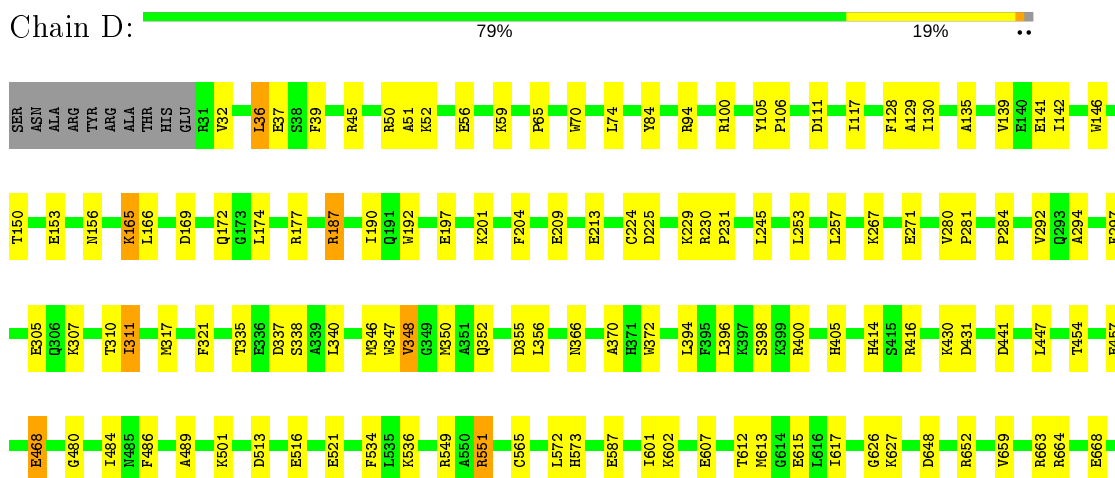
3 Residue-property plots

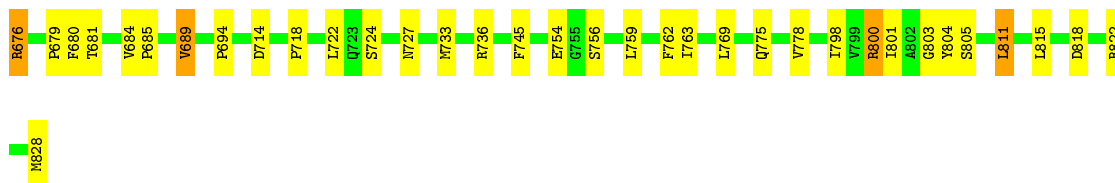
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Formate acetyltransferase

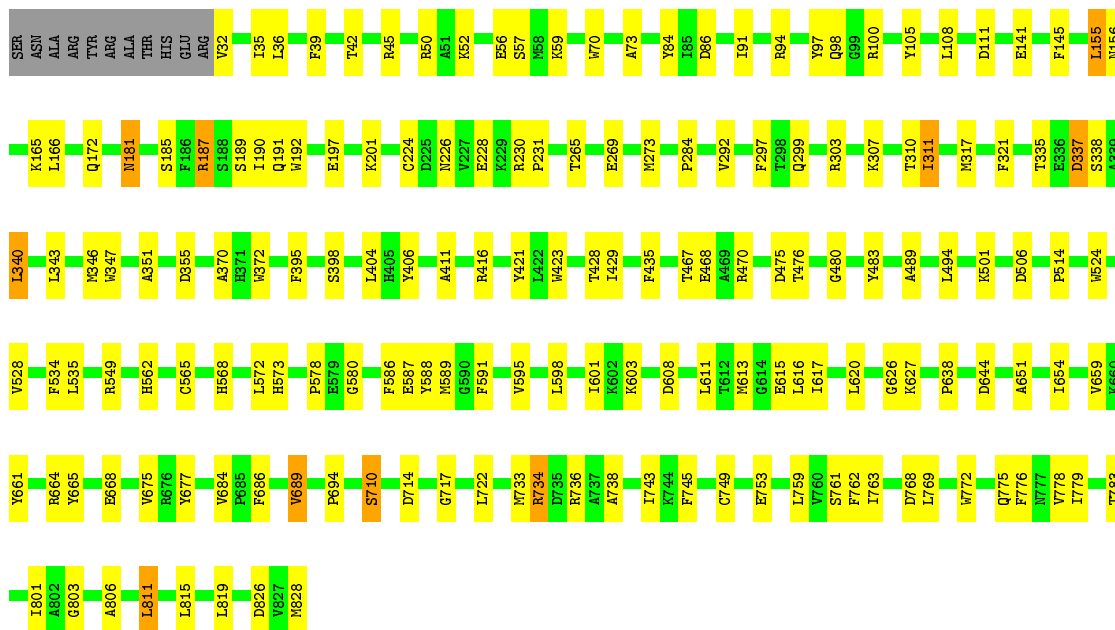


- Molecule 1: Formate acetyltransferase

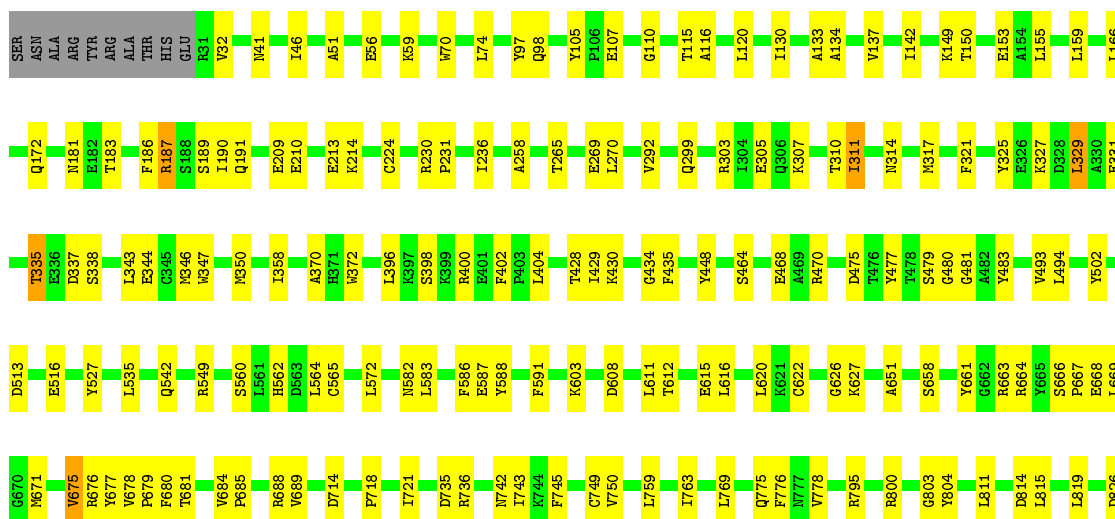




• Molecule 1: Formate acetyltransferase



• Molecule 1: Formate acetyltransferase



1827
1828

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.11Å 159.44Å 115.38Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	48.27 – 2.40 48.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.27-2.40) 87.5 (48.27-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.212 , 0.262 0.212 , 0.262	Depositor DCC
R_{free} test set	15307 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for l,k,-h 0.087 for h,-k,-l 0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25800	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: 8X3, 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	0.44	0/6377	0.58	0/8673
1	B	0.43	0/6409	0.58	2/8713 (0.0%)
1	C	0.40	0/6387	0.56	0/8683
1	D	0.41	0/6390	0.57	0/8685
All	All	0.42	0/25563	0.57	2/34754 (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	736	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	736	ARG	NE-CZ-NH2	-5.04	117.78	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	6219	0	5936	131	0
1	B	6251	0	5992	128	0
1	C	6229	0	5937	119	0
1	D	6232	0	5965	120	0
2	A	7	5	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	5	0	0	0
2	C	7	5	0	0	0
2	D	7	5	0	1	0
3	A	12	16	16	1	0
3	B	12	16	16	1	0
3	C	6	8	8	0	0
3	D	6	8	8	2	0
4	A	218	0	0	9	0
4	B	204	0	0	2	0
4	C	161	0	0	6	0
4	D	154	0	0	10	0
All	All	25732	68	23878	489	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 10.

The worst 5 of 489 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:48:VAL:HG21	1:B:137:VAL:HG21	1.28	1.07
1:C:36:LEU:HD11	1:C:404:LEU:HD11	1.36	1.07
1:A:775:GLN:HE22	1:A:803:GLY:H	1.03	1.01
1:D:347:TRP:HZ3	1:D:398:SER:HG	1.04	0.97
1:D:659:VAL:HG12	1:D:733:MET:HE1	1.41	0.97

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	796/808 (98%)	775 (97%)	20 (2%)	1 (0%)	51 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	796/808 (98%)	771 (97%)	24 (3%)	1 (0%)	51 68
1	C	795/808 (98%)	771 (97%)	23 (3%)	1 (0%)	51 68
1	D	796/808 (98%)	773 (97%)	22 (3%)	1 (0%)	51 68
All	All	3183/3232 (98%)	3090 (97%)	89 (3%)	4 (0%)	51 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	ILE
1	D	311	ILE
1	C	311	ILE
1	A	311	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	642/680 (94%)	630 (98%)	12 (2%)	57 75
1	B	649/680 (95%)	630 (97%)	19 (3%)	42 62
1	C	642/680 (94%)	621 (97%)	21 (3%)	38 57
1	D	643/680 (95%)	624 (97%)	19 (3%)	41 61
All	All	2576/2720 (95%)	2505 (97%)	71 (3%)	43 63

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	664	ARG
1	C	70	TRP
1	A	468	GLU
1	D	676	ARG
1	D	800	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	8X3	A	901	-	6,6,6	3.84	1 (16%)	7,8,8	1.20	1 (14%)
2	8X3	B	901	-	6,6,6	2.03	1 (16%)	7,8,8	2.39	2 (28%)
2	8X3	C	901	-	6,6,6	3.04	1 (16%)	7,8,8	1.63	1 (14%)
3	GOL	B	903	-	5,5,5	0.49	0	5,5,5	0.77	0
3	GOL	C	902	-	5,5,5	0.33	0	5,5,5	0.50	0
3	GOL	D	902	-	5,5,5	0.43	0	5,5,5	0.76	0
3	GOL	A	902	-	5,5,5	0.50	0	5,5,5	0.64	0
3	GOL	B	902	-	5,5,5	0.49	0	5,5,5	0.49	0
3	GOL	A	903	-	5,5,5	0.32	0	5,5,5	0.56	0
2	8X3	D	901	-	6,6,6	2.03	1 (16%)	7,8,8	1.67	1 (14%)

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	8X3	A	901	-	-	4/4/4/4	-
2	8X3	B	901	-	-	4/4/4/4	-
2	8X3	C	901	-	-	4/4/4/4	-
3	GOL	B	903	-	-	0/4/4/4	-
3	GOL	C	902	-	-	2/4/4/4	-
3	GOL	D	902	-	-	4/4/4/4	-
3	GOL	A	902	-	-	2/4/4/4	-
3	GOL	B	902	-	-	3/4/4/4	-
3	GOL	A	903	-	-	2/4/4/4	-
2	8X3	D	901	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	8X3	C2-S3	9.22	1.90	1.77
2	C	901	8X3	C2-S3	7.28	1.87	1.77
2	B	901	8X3	C2-S3	4.74	1.84	1.77
2	D	901	8X3	C2-S3	4.63	1.84	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	8X3	O7-S3-C2	-5.20	100.66	106.92
2	D	901	8X3	O7-S3-C2	-3.37	102.86	106.92
2	C	901	8X3	O6-C1-C2	-2.79	104.77	110.38
2	A	901	8X3	O7-S3-C2	-2.16	104.31	106.92
2	B	901	8X3	O5-S3-C2	-2.15	104.32	106.92

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	8X3	C1-C2-S3-O5
2	A	901	8X3	C1-C2-S3-O7
2	B	901	8X3	C1-C2-S3-O4
2	B	901	8X3	C1-C2-S3-O5

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Mol	Chain	Res	Type	Atoms
2	C	901	8X3	C1-C2-S3-O5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	GOL	2	0
3	B	902	GOL	1	0
3	A	903	GOL	1	0
2	D	901	8X3	1	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 [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	798/808 (98%)	-0.83	0 100 100	14, 22, 34, 52	0
1	B	798/808 (98%)	-0.80	0 100 100	15, 24, 40, 54	0
1	C	797/808 (98%)	-0.68	0 100 100	18, 29, 45, 57	0
1	D	798/808 (98%)	-0.71	0 100 100	19, 28, 43, 56	0
All	All	3191/3232 (98%)	-0.76	0 100 100	14, 25, 42, 57	0

There are no RSRZ outliers to report.

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 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. 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
3	GOL	B	902	6/6	0.93	0.12	29,35,43,46	0
3	GOL	A	903	6/6	0.93	0.27	32,41,48,49	0
3	GOL	B	903	6/6	0.95	0.10	30,39,47,52	0
3	GOL	A	902	6/6	0.95	0.14	23,33,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	D	902	6/6	0.96	0.08	28,35,42,45	0
3	GOL	C	902	6/6	0.97	0.09	37,45,51,62	0
2	8X3	A	901	7/7	0.99	0.09	13,19,24,24	0
2	8X3	B	901	7/7	0.99	0.12	15,19,23,23	0
2	8X3	C	901	7/7	0.99	0.08	17,25,30,30	0
2	8X3	D	901	7/7	0.99	0.08	17,25,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.