



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 AM GMT

PDB ID : 2QJV
Title : Crystal structure of an iolb-like protein (stm4420) from salmonella typhimurium lt2 at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-07-09
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

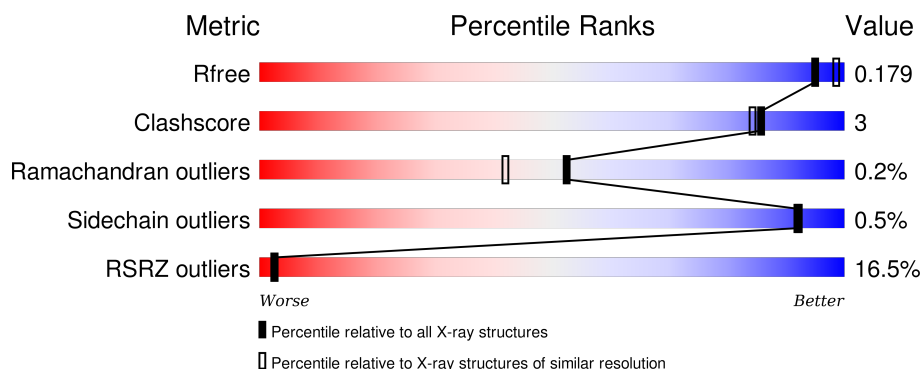
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	270	<div> <div>16%</div> <div>90%</div> <div>8%</div> </div>
1	B	270	<div> <div>15%</div> <div>90%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	275	-	-	-	X
3	CL	B	274	-	-	-	X
5	GOL	B	277	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5072 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 Uncharacterized IolB-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	Se	0	9	0
			2170	1375	381	403	7	4			
1	B	263	Total	C	N	O	S	Se	0	6	0
			2138	1357	370	400	7	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q8ZK62
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
A	36	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	62	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
A	95	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	132	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	161	ALA	GLU	ENGINEERED	UNP Q8ZK62
A	163	ALA	ASP	ENGINEERED	UNP Q8ZK62
A	171	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	213	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
A	222	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	225	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
A	244	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
A	250	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	0	GLY	-	LEADER SEQUENCE	UNP Q8ZK62
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
B	36	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	62	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
B	95	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	132	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	161	ALA	GLU	ENGINEERED	UNP Q8ZK62
B	163	ALA	ASP	ENGINEERED	UNP Q8ZK62
B	171	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	213	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
B	222	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	225	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62
B	244	MSE	MET	MODIFIED RESIDUE	UNP Q8ZK62
B	250	MLY	LYS	MODIFIED RESIDUE	UNP Q8ZK62

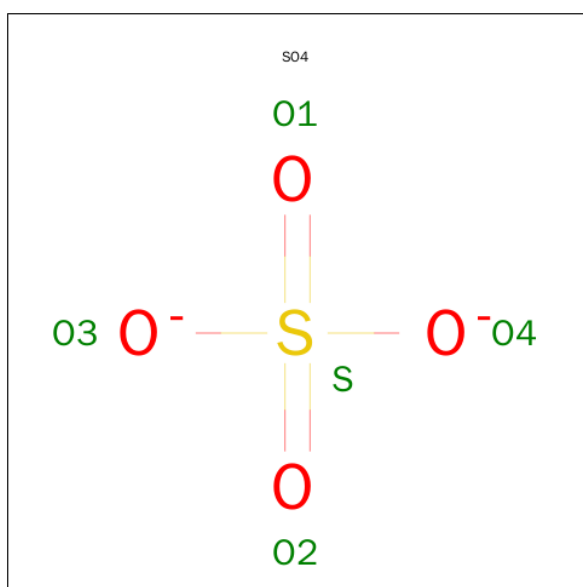
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ni 2 2	0	0
2	A	2	Total Ni 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

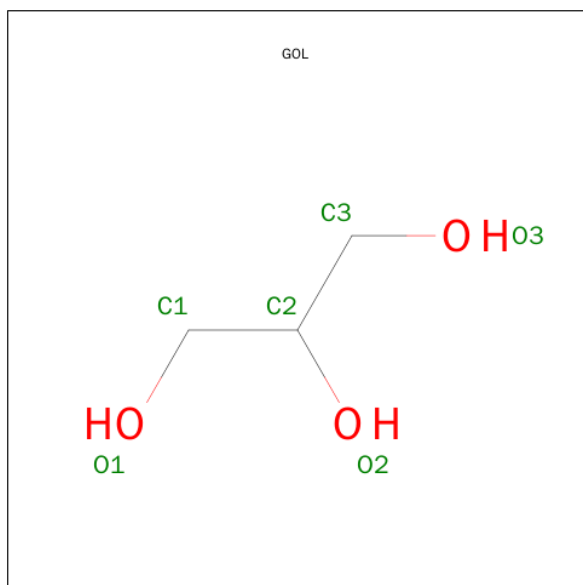
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Cl 3 3	0	0
3	A	4	Total Cl 4 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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



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

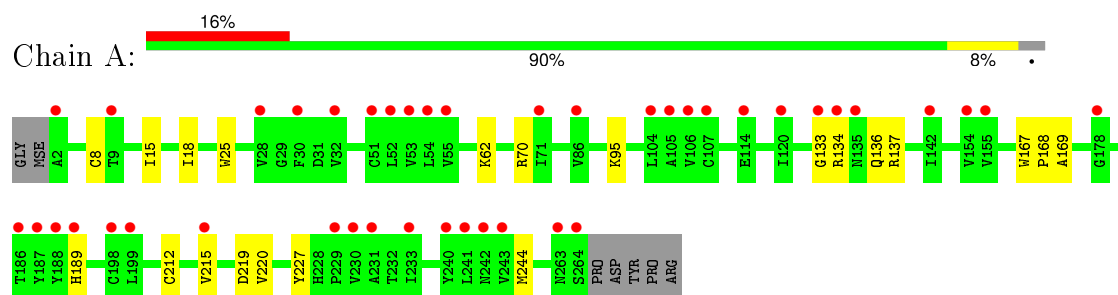
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	366	Total O 366 366	0	0
6	B	355	Total O 355 355	0	0

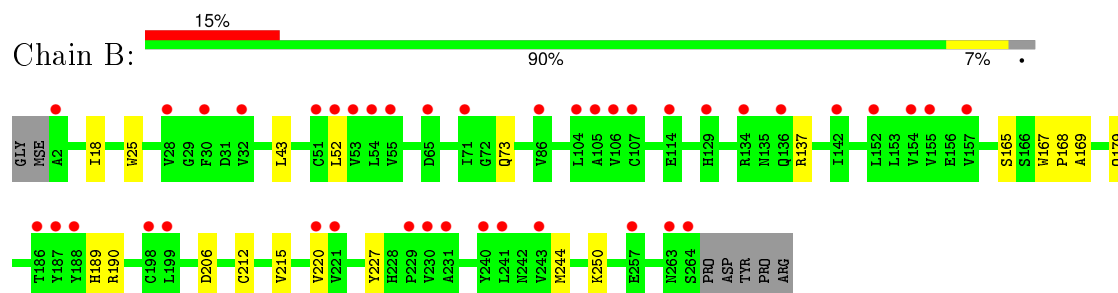
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Uncharacterized IolB-like protein



• Molecule 1: Uncharacterized IolB-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	200.14Å 200.14Å 200.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 1.90 29.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.51-1.90) 99.9 (29.51-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.160 , 0.181 0.160 , 0.179	Depositor DCC
R_{free} test set	5190 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.3	EDS
Estimated twinning fraction	0.025 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 104011 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5072	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CL, SO4, MLY, NI

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	0.82	1/2140 (0.0%)	0.94	4/2918 (0.1%)
1	B	0.82	0/2109	0.92	2/2878 (0.1%)
All	All	0.82	1/4249 (0.0%)	0.93	6/5796 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	GLN	CB-CG	5.07	1.66	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70[A]	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	70[B]	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	206	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	190	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	219	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	134	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2170	0	2071	13	0
1	B	2138	0	2031	13	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	1	0
3	B	3	0	0	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	366	0	0	5	0
6	B	355	0	0	4	0
All	All	5072	0	4118	24	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 3.

All (24) 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:244:MSE:HE2	6:B:428:HOH:O	1.74	0.86
1:A:244:MSE:HE2	6:A:423:HOH:O	1.86	0.74
1:A:8[B]:CYS:SG	6:A:525:HOH:O	2.54	0.64
1:A:212[B]:CYS:HB2	1:B:212[B]:CYS:HB2	1.80	0.63
1:A:62:MLY:HH12	6:A:425:HOH:O	2.01	0.60
1:B:244:MSE:CE	6:B:428:HOH:O	2.43	0.59
1:A:95:MLY:HH22	6:A:572:HOH:O	2.03	0.59
1:B:179[A]:GLN:HG3	6:B:589:HOH:O	2.08	0.52
1:A:137:ARG:NH1	3:A:274:CL:CL	2.81	0.51
1:A:167:TRP:HA	1:A:168:PRO:C	2.32	0.50
1:B:169:ALA:HB1	1:B:227:TYR:HB3	1.92	0.50
1:B:189:HIS:CD2	1:B:215:VAL:HG11	2.47	0.49
1:A:212[B]:CYS:HB2	1:B:212[B]:CYS:CB	2.42	0.49
1:A:189:HIS:CD2	1:A:215:VAL:HG11	2.52	0.45
1:B:18:ILE:HG13	1:B:220:VAL:HG11	1.99	0.45
1:B:250:MLY:HH23	6:B:630:HOH:O	2.16	0.44
1:B:167:TRP:HA	1:B:168:PRO:C	2.37	0.44
1:A:133:GLY:N	6:A:546:HOH:O	2.51	0.43
1:B:43:LEU:CD1	1:B:52:LEU:HD21	2.48	0.43
1:B:137:ARG:HD3	1:B:165:SER:CB	2.49	0.42
1:A:169:ALA:HB1	1:A:227:TYR:HB3	2.01	0.42
1:A:8[A]:CYS:SG	1:A:15:ILE:HD12	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18[A]:ILE:HG13	1:A:220:VAL:HG11	2.03	0.40
1:B:137:ARG:NH1	3:B:273:CL:CL	2.92	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	262/270 (97%)	251 (96%)	11 (4%)	0	100	100
1	B	259/270 (96%)	245 (95%)	12 (5%)	2 (1%)	24	11
All	All	521/540 (96%)	496 (95%)	23 (4%)	2 (0%)	52	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73[A]	GLN
1	B	73[B]	GLN

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	223/218 (102%)	222 (100%)	1 (0%)	93	94
1	B	219/218 (100%)	218 (100%)	1 (0%)	92	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	442/436 (101%)	440 (100%)	2 (0%)	92	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	TRP
1	B	25	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MLY	A	132	1	5,6,11	0.96	0	4,6,13	1.41	1 (25%)
1	MLY	A	171	1	9,10,11	0.90	0	9,11,13	0.94	1 (11%)
1	MLY	A	222	1	9,10,11	1.12	1 (11%)	9,11,13	0.91	1 (11%)
1	MLY	A	225	1	9,10,11	1.10	1 (11%)	9,11,13	0.73	0
1	MLY	A	250	1	9,10,11	1.12	0	9,11,13	0.93	1 (11%)
1	MLY	A	36	1	9,10,11	0.96	0	9,11,13	0.82	1 (11%)
1	MLY	A	62	1	9,10,11	0.83	0	9,11,13	1.06	0
1	MLY	A	95	1	9,10,11	0.89	0	9,11,13	0.78	0
1	MLY	B	132	1	4,5,11	0.62	0	3,5,13	1.41	1 (33%)
1	MLY	B	171	1	9,10,11	0.78	0	9,11,13	0.89	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	222	1	9,10,11	1.07	1 (11%)	9,11,13	0.79	0
1	MLY	B	225	1	9,10,11	1.00	0	9,11,13	1.01	1 (11%)
1	MLY	B	250	1	9,10,11	0.92	0	9,11,13	0.84	0
1	MLY	B	36	1	9,10,11	0.85	0	9,11,13	0.82	1 (11%)
1	MLY	B	62	1	9,10,11	0.96	0	9,11,13	0.85	1 (11%)
1	MLY	B	95	1	9,10,11	0.65	0	9,11,13	0.79	1 (11%)

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
1	MLY	A	132	1	-	0/3/5/11	0/0/0/0
1	MLY	A	171	1	-	0/7/9/11	0/0/0/0
1	MLY	A	222	1	-	0/7/9/11	0/0/0/0
1	MLY	A	225	1	-	0/7/9/11	0/0/0/0
1	MLY	A	250	1	-	0/7/9/11	0/0/0/0
1	MLY	A	36	1	-	0/7/9/11	0/0/0/0
1	MLY	A	62	1	-	0/7/9/11	0/0/0/0
1	MLY	A	95	1	-	0/7/9/11	0/0/0/0
1	MLY	B	132	1	-	0/2/4/11	0/0/0/0
1	MLY	B	171	1	-	0/7/9/11	0/0/0/0
1	MLY	B	222	1	-	0/7/9/11	0/0/0/0
1	MLY	B	225	1	-	0/7/9/11	0/0/0/0
1	MLY	B	250	1	-	0/7/9/11	0/0/0/0
1	MLY	B	36	1	-	0/7/9/11	0/0/0/0
1	MLY	B	62	1	-	0/7/9/11	0/0/0/0
1	MLY	B	95	1	-	0/7/9/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	MLY	CB-CA	-2.28	1.51	1.53
1	B	222	MLY	CH2-NZ	2.08	1.52	1.46
1	A	225	MLY	CB-CA	2.10	1.55	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	MLY	O-C-CA	-2.77	118.28	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	MLY	O-C-CA	-2.43	119.16	125.49
1	A	222	MLY	O-C-CA	-2.41	119.21	125.49
1	B	62	MLY	O-C-CA	-2.41	119.22	125.49
1	B	36	MLY	O-C-CA	-2.24	119.67	125.49
1	B	225	MLY	O-C-CA	-2.17	119.83	125.49
1	B	95	MLY	O-C-CA	-2.11	119.99	125.49
1	A	36	MLY	O-C-CA	-2.09	120.05	125.49
1	A	250	MLY	O-C-CA	-2.04	120.18	125.49
1	A	171	MLY	CD-CE-NZ	2.11	119.37	113.92
1	B	171	MLY	CD-CE-NZ	2.15	119.46	113.92

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
1	A	62	MLY	1	0
1	A	95	MLY	1	0
1	B	250	MLY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	$\# Z > 2$
4	SO4	A	276	-	4,4,4	0.19	0	6,6,6	0.74	0
4	SO4	A	277	-	4,4,4	0.24	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	278	-	5,5,5	0.26	0	5,5,5	0.79	0
4	SO4	B	275	-	4,4,4	0.13	0	6,6,6	0.62	0
4	SO4	B	276	-	4,4,4	0.26	0	6,6,6	0.90	1 (16%)
5	GOL	B	277	-	5,5,5	0.46	0	5,5,5	0.87	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
4	SO4	A	276	-	-	0/0/0/0	0/0/0/0
4	SO4	A	277	-	-	0/0/0/0	0/0/0/0
5	GOL	A	278	-	-	0/4/4/4	0/0/0/0
4	SO4	B	275	-	-	0/0/0/0	0/0/0/0
4	SO4	B	276	-	-	0/0/0/0	0/0/0/0
5	GOL	B	277	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	276	SO4	O2-S-O1	-2.15	102.69	109.50

There are no chirality outliers.

There are no torsion outliers.

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, 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	252/270 (93%)	0.77	42 (16%) 2 2	33, 38, 52, 72	0
1	B	252/270 (93%)	0.73	41 (16%) 2 3	33, 38, 52, 72	0
All	All	504/540 (93%)	0.75	83 (16%) 2 2	33, 38, 52, 72	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	6.2
1	A	241	LEU	5.6
1	B	2	ALA	5.6
1	B	241	LEU	5.5
1	A	264	SER	5.5
1	A	134	ARG	5.5
1	B	264	SER	5.0
1	A	230	VAL	4.9
1	B	243	VAL	4.8
1	B	230	VAL	3.9
1	B	65	ASP	3.8
1	B	53	VAL	3.8
1	A	243	VAL	3.8
1	A	105	ALA	3.7
1	A	53	VAL	3.6
1	A	154	VAL	3.4
1	B	106	VAL	3.4
1	B	105	ALA	3.4
1	A	106	VAL	3.4
1	A	155	VAL	3.4
1	A	199	LEU	3.3
1	A	240	TYR	3.3
1	B	54	LEU	3.2
1	B	134	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	199	LEU	3.0
1	A	104	LEU	3.0
1	B	155	VAL	3.0
1	B	86	VAL	2.9
1	A	30	PHE	2.9
1	A	135	ASN	2.9
1	A	188	TYR	2.9
1	B	107	CYS	2.9
1	B	240	TYR	2.9
1	A	55	VAL	2.8
1	B	229	PRO	2.8
1	A	187	TYR	2.8
1	A	51	CYS	2.8
1	A	133	GLY	2.8
1	A	32	VAL	2.7
1	B	52	LEU	2.7
1	B	30	PHE	2.7
1	A	231	ALA	2.7
1	B	221	VAL	2.6
1	B	231	ALA	2.6
1	A	71	ILE	2.6
1	B	257	GLU	2.6
1	A	186	THR	2.6
1	B	71	ILE	2.6
1	B	198	CYS	2.6
1	A	107	CYS	2.5
1	A	229	PRO	2.5
1	A	263	ASN	2.5
1	B	51	CYS	2.5
1	B	104	LEU	2.5
1	A	215	VAL	2.5
1	B	154	VAL	2.5
1	A	52	LEU	2.5
1	B	187	TYR	2.4
1	A	142	ILE	2.4
1	A	114	GLU	2.4
1	B	129	HIS	2.4
1	A	178	GLY	2.4
1	A	242	ASN	2.4
1	B	55	VAL	2.4
1	B	28	VAL	2.4
1	B	188	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	189	HIS	2.3
1	B	186	THR	2.3
1	B	136	GLN	2.3
1	B	220	VAL	2.2
1	A	198	CYS	2.2
1	B	142	ILE	2.2
1	A	9	THR	2.1
1	B	263	ASN	2.1
1	B	152	LEU	2.1
1	B	157	VAL	2.1
1	B	114	GLU	2.1
1	A	28	VAL	2.1
1	A	86	VAL	2.1
1	B	32	VAL	2.1
1	A	233	ILE	2.0
1	A	54	LEU	2.0
1	A	120	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	MLY	A	62	11/12	0.95	0.10	-	36,39,45,46	0
1	MLY	B	171	11/12	0.95	0.14	-	33,37,40,42	0
1	MLY	B	36	11/12	0.95	0.20	-	35,39,73,80	0
1	MLY	A	250	11/12	0.92	0.20	-	37,42,75,75	0
1	MLY	A	36	11/12	0.95	0.20	-	34,37,67,71	0
1	MLY	A	171	11/12	0.96	0.11	-	33,34,42,44	0
1	MLY	B	225	11/12	0.96	0.11	-	36,38,58,67	0
1	MLY	B	250	11/12	0.93	0.18	-	36,39,74,84	0
1	MLY	A	225	11/12	0.95	0.13	-	36,38,58,65	0
1	MLY	B	222	11/12	0.95	0.13	-	37,39,46,46	0
1	MLY	B	62	11/12	0.93	0.17	-	36,39,66,70	0
1	MLY	B	132	6/12	0.94	0.20	-	50,54,55,58	0
1	MLY	A	222	11/12	0.94	0.12	-	36,38,46,48	0
1	MLY	A	95	11/12	0.95	0.09	-	37,39,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MLY	B	95	11/12	0.96	0.10	-	36,38,48,55	0
1	MLY	A	132	7/12	0.86	0.28	-	54,56,57,59	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	275	1/1	0.98	0.24	5.99	41,41,41,41	0
3	CL	B	274	1/1	0.93	0.34	4.14	60,60,60,60	0
5	GOL	B	277	6/6	0.91	0.24	3.14	42,64,68,68	0
3	CL	A	272	1/1	0.96	0.28	1.76	62,62,62,62	0
3	CL	A	273	1/1	0.90	0.12	-0.84	69,69,69,69	0
2	NI	A	271	1/1	1.00	0.09	-1.44	22,22,22,22	0
3	CL	A	274	1/1	0.96	0.13	-1.64	50,50,50,50	0
2	NI	B	271	1/1	1.00	0.08	-1.91	22,22,22,22	0
3	CL	B	273	1/1	0.93	0.07	-2.49	54,54,54,54	0
4	SO4	A	276	5/5	0.93	0.37	-	58,68,79,84	0
3	CL	B	272	1/1	0.89	0.22	-	65,65,65,65	0
2	NI	A	270	1/1	0.95	0.21	-	59,59,59,59	0
2	NI	B	270	1/1	0.89	0.19	-	58,58,58,58	0
4	SO4	B	276	5/5	0.94	0.32	-	59,59,64,73	0
4	SO4	A	277	5/5	0.97	0.23	-	49,51,56,58	0
5	GOL	A	278	6/6	0.81	0.37	-	61,67,74,76	0
4	SO4	B	275	5/5	0.87	0.43	-	70,85,93,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.