



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:33 am GMT

PDB ID : 2RHU  
Title : Crystal structure of the 3-MBT repeats from human L3MBTL1 bound to dimethyl-lysine and in chimera with histone H3.3(28-34)  
Authors : Li, H.; Patel, D.J.  
Deposited on : 2007-10-09  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

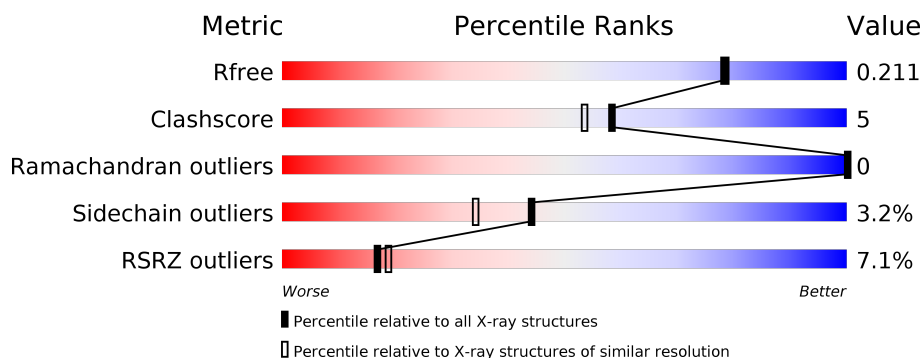
# 1 Overall quality at a glance

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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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  $\geq 3$ , 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	329	

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	MLY	A	530	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3182 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.

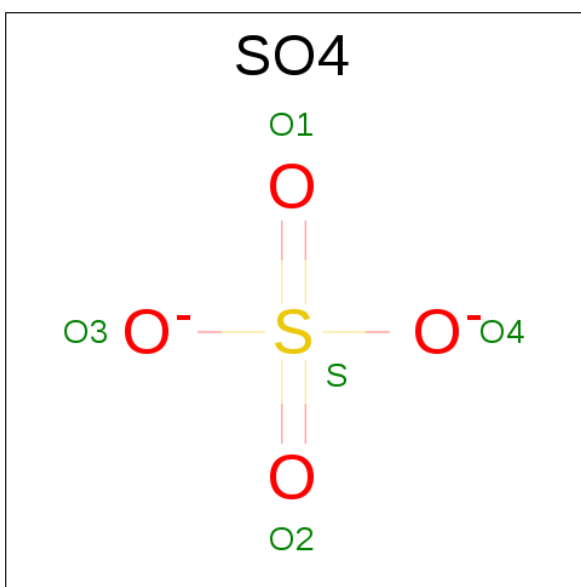
- Molecule 1 is a protein called Lethal(3)malignant brain tumor-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2623	1679	444	488	12			

There are 15 discrepancies between the modelled and reference sequences:

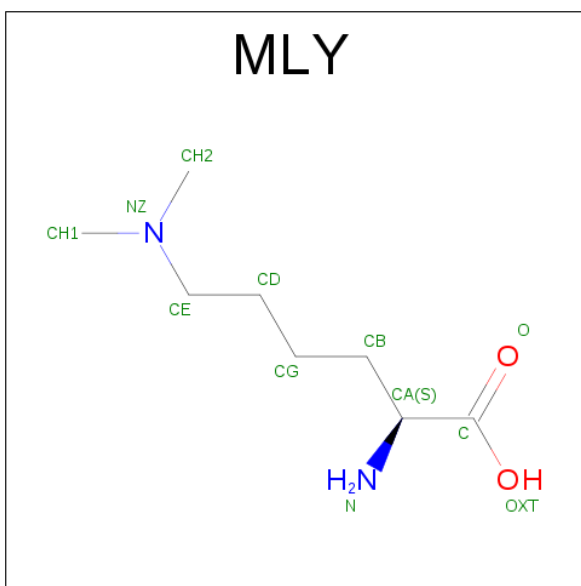
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLY	-	EXPRESSION TAG	UNP Q9Y468
A	202	PRO	-	EXPRESSION TAG	UNP Q9Y468
A	203	LEU	-	EXPRESSION TAG	UNP Q9Y468
A	204	GLY	-	EXPRESSION TAG	UNP Q9Y468
A	205	SER	-	EXPRESSION TAG	UNP Q9Y468
A	520	GLY	-	LINKER	UNP Q9Y468
A	521	GLY	-	LINKER	UNP Q9Y468
A	522	GLY	-	LINKER	UNP Q9Y468
A	523	SER	-	SEE REMARK 999	UNP Q9Y468
A	524	ALA	-	SEE REMARK 999	UNP Q9Y468
A	525	PRO	-	SEE REMARK 999	UNP Q9Y468
A	526	SER	-	SEE REMARK 999	UNP Q9Y468
A	527	THR	-	SEE REMARK 999	UNP Q9Y468
A	528	GLY	-	SEE REMARK 999	UNP Q9Y468
A	529	GLY	-	SEE REMARK 999	UNP Q9Y468

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



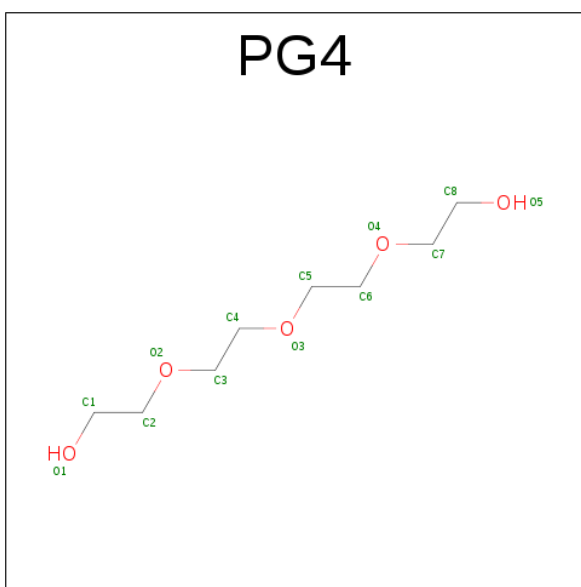
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is N-DIMETHYL-LYSINE (three-letter code: MLY) (formula:  $C_8H_{18}N_2O_2$ ).



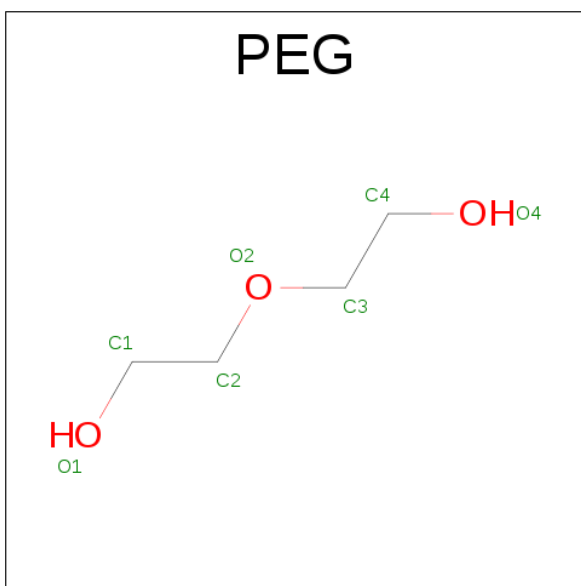
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

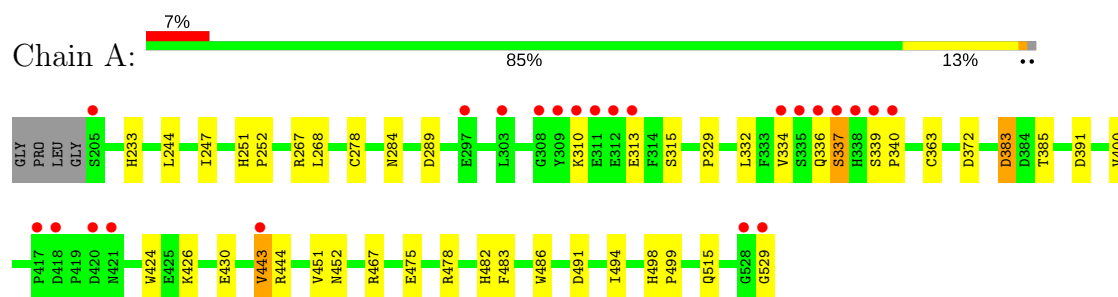
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	522	Total 522	O 522	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 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: Lethal(3)malignant brain tumor-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.17Å 94.02Å 59.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-1.90) 97.3 (19.82-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.61 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.194 , 0.215 0.192 , 0.211	Depositor DCC
$R_{free}$ test set	2232 reflections (6.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, PG4, MLY, CML, SO4

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	0.38	0/2693	0.67	2/3675 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	337	SER	N-CA-CB	-5.35	102.48	110.50
1	A	444	ARG	N-CA-CB	-5.01	101.59	110.60

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	2623	0	2435	28	0
2	A	5	0	0	0	0
3	A	12	0	17	0	0
4	A	13	0	18	2	0
5	A	7	0	10	0	0
6	A	522	0	0	4	0
All	All	3182	0	2480	28	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 (28) 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:443:VAL:HB	6:A:709:HOH:O	1.71	0.91
1:A:337:SER:HA	1:A:372:ASP:OD1	1.77	0.84
1:A:339:SER:OG	1:A:340:PRO:CD	2.28	0.82
1:A:339:SER:OG	1:A:340:PRO:HD3	1.87	0.75
1:A:310:LYS:O	1:A:313:GLU:HB2	1.93	0.68
1:A:339:SER:OG	1:A:340:PRO:HD2	1.94	0.67
1:A:329:PRO:HD2	1:A:332:LEU:HD22	1.80	0.64
1:A:426:LYS:O	1:A:430:GLU:HG3	1.99	0.63
1:A:337:SER:HA	1:A:372:ASP:CG	2.18	0.63
1:A:475:GLU:OE1	1:A:478:ARG:HD3	2.06	0.55
1:A:486:TRP:CZ3	4:A:531:PG4:H72	2.44	0.52
1:A:451:VAL:O	1:A:452:ASN:HB2	2.10	0.52
1:A:400:VAL:HG13	1:A:424:TRP:CG	2.48	0.49
1:A:251:HIS:N	1:A:252:PRO:HD3	2.29	0.48
1:A:267:ARG:HG2	1:A:284:ASN:HD22	1.78	0.48
1:A:482:HIS:HD2	1:A:491:ASP:OD1	1.96	0.48
1:A:247:ILE:HG12	1:A:289:ASP:HB3	1.97	0.47
1:A:467:ARG:HG2	1:A:515:GLN:HB2	1.97	0.45
1:A:426:LYS:HD2	6:A:923:HOH:O	2.16	0.45
1:A:383:ASP:OD2	1:A:385:THR:HG22	2.17	0.44
1:A:334:VAL:HB	6:A:650:HOH:O	2.18	0.43
1:A:494:ILE:HD11	1:A:498:HIS:CG	2.53	0.43
1:A:482:HIS:HE1	1:A:529:GLY:O	2.01	0.42
1:A:486:TRP:CE3	4:A:531:PG4:H72	2.55	0.42
1:A:278:CML:C1	1:A:278:CML:O5	2.68	0.41
1:A:467:ARG:HB2	1:A:483:PHE:CD1	2.56	0.41
1:A:498:HIS:HA	1:A:499:PRO:HD3	1.90	0.41
1:A:385:THR:HG21	6:A:986:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	321/329 (98%)	313 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	280/282 (99%)	271 (97%)	9 (3%)	44	34

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

Mol	Chain	Res	Type
1	A	233	HIS
1	A	244	LEU
1	A	268	LEU
1	A	315	SER
1	A	336	GLN
1	A	363	CYS
1	A	383	ASP
1	A	391	ASP
1	A	443	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	250	GLN
1	A	284	ASN
1	A	414	GLN
1	A	482	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	CML	A	278	1	5,13,14	0.96	0	3,16,18	1.61	1 (33%)
1	CML	A	423	1	5,13,14	1.10	1 (20%)	3,16,18	1.65	1 (33%)

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	CML	A	278	1	-	0/7/15/17	0/0/0/0
1	CML	A	423	1	-	0/7/15/17	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	CML	CA-C	2.24	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	CML	C3-C2-C1	-2.26	108.50	112.84
1	A	278	CML	C3-C2-C1	-2.09	108.84	112.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	278	CML	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	SO4	A	1	-	4,4,4	0.27	0	6,6,6	0.08	0
5	PEG	A	2	-	6,6,6	0.53	0	5,5,5	0.37	0
3	MLY	A	530	-	6,11,11	0.34	0	6,13,13	0.60	0
4	PG4	A	531	-	12,12,12	0.54	0	11,11,11	0.49	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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
5	PEG	A	2	-	-	0/4/4/4	0/0/0/0
3	MLY	A	530	-	-	0/7/11/11	0/0/0/0
4	PG4	A	531	-	-	0/10/10/10	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	531	PG4	2	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/329 (98%)	0.29	23 (7%) <b>17</b> <b>19</b>	15, 23, 48, 59	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	SER	14.0
1	A	338	HIS	9.0
1	A	336	GLN	7.2
1	A	339	SER	5.9
1	A	312	GLU	5.0
1	A	421	ASN	4.8
1	A	334	VAL	4.7
1	A	335	SER	4.4
1	A	308	GLY	4.4
1	A	340	PRO	4.3
1	A	309	TYR	4.2
1	A	529	GLY	4.2
1	A	311	GLU	3.7
1	A	205	SER	3.7
1	A	310	LYS	3.6
1	A	420	ASP	3.5
1	A	313	GLU	3.4
1	A	297	GLU	2.8
1	A	443	VAL	2.8
1	A	528	GLY	2.3
1	A	418	ASP	2.1
1	A	417	PRO	2.1
1	A	303	LEU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CML	A	278	14/15	0.89	0.16	-	23,39,46,47	0
1	CML	A	423	14/15	0.90	0.15	-	25,37,45,46	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MLY	A	530	12/12	0.76	0.20	5.04	30,39,45,45	0
2	SO4	A	1	5/5	0.97	0.18	1.84	54,54,54,56	0
4	PG4	A	531	13/13	0.85	0.15	1.23	29,38,49,50	0
5	PEG	A	2	7/7	0.77	0.20	1.15	55,56,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.