



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2017 – 11:45 AM EDT

PDB ID : 2RDB  
Title : X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase I100W Mutant  
Authors : Murray, L.J.; Garcia-Serres, R.; McCormick, M.S.; Davydov, R.; Naik, S.; Hoffman, B.M.; Huynh, B.H.; Lippard, S.J.  
Deposited on : unknown  
Resolution : 2.10 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](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 : rb-20030345  
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) : rb-20030345

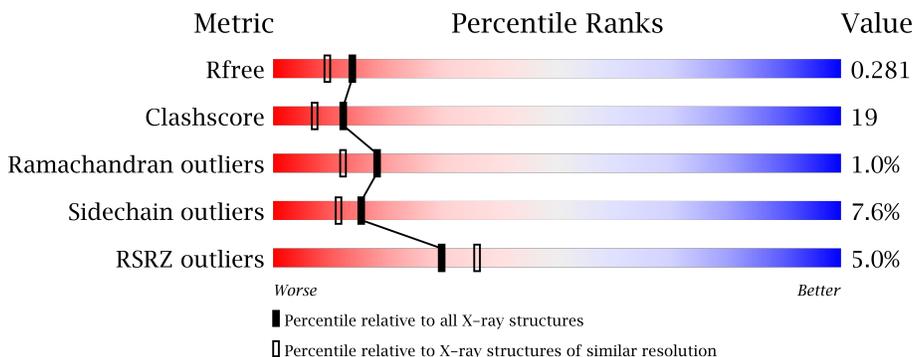
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	498	 5% 57% 35% 6% ..
2	B	330	 5% 61% 30% 7% .
3	C	86	 3% 35% 47% 12% ..

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	GOL	A	3287	-	-	-	X
5	P6G	A	4974	-	-	X	X
7	MPO	B	4401	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7556 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 Toluene, o-xylene monooxygenase oxygenase subunit;alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	4035	2580	676	753	26	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	TRP	ILE	ENGINEERED	UNP O87798

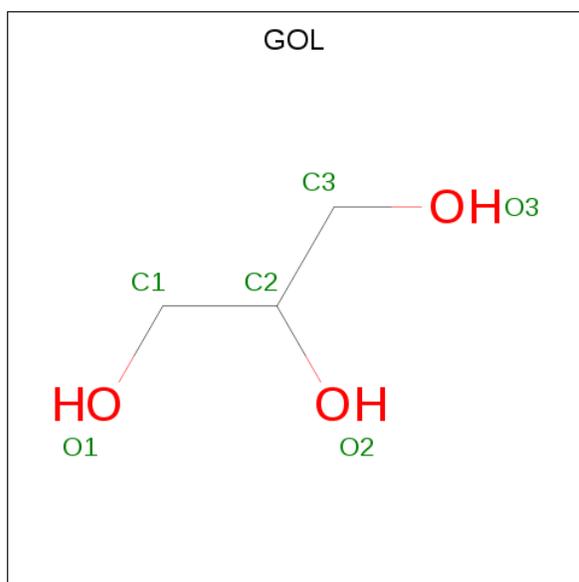
- Molecule 2 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	322	2641	1674	467	490	10	0	0	0

- Molecule 3 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;gamma.

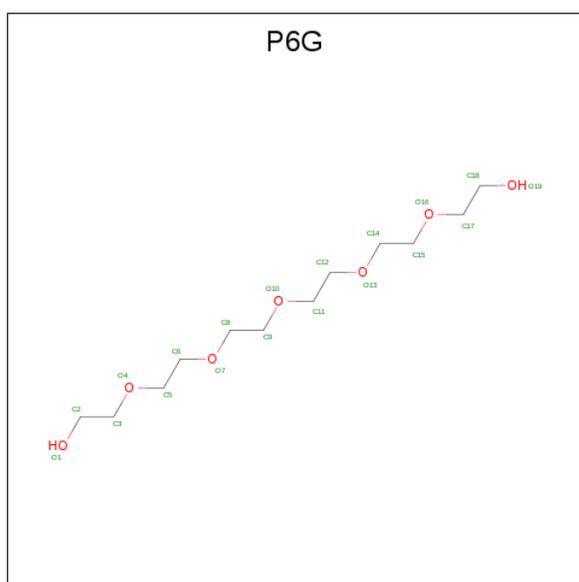
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	83	676	425	120	126	5	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).

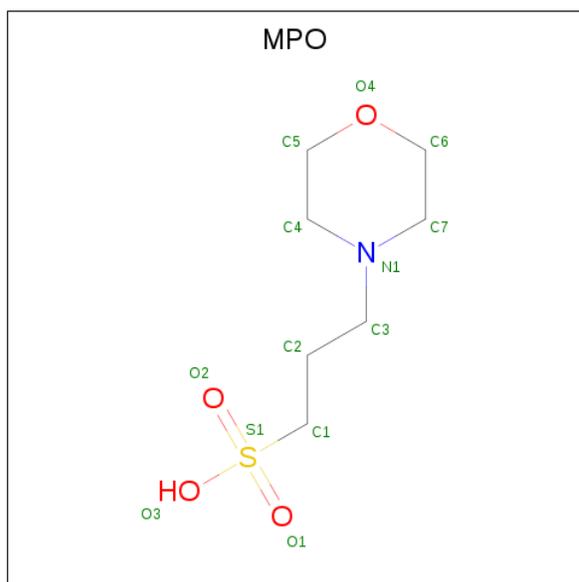


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Fe 2 2	0	0

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	B	1	13	7	1	4	1	0	0

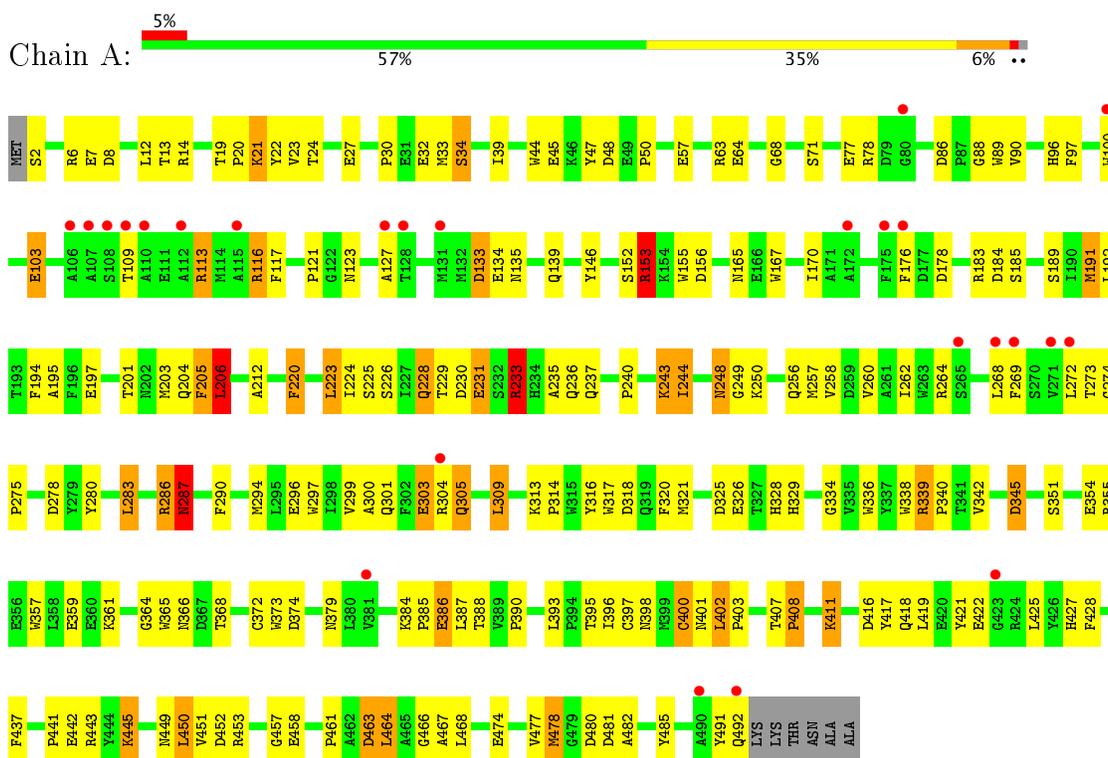
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	82	Total O 82 82	0	0
8	B	72	Total O 72 72	0	0
8	C	4	Total O 4 4	0	0

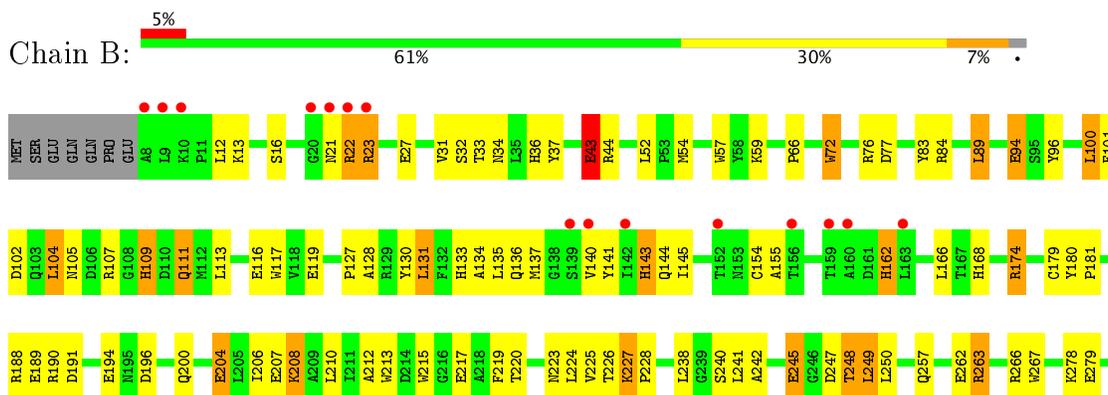
### 3 Residue-property plots [i](#)

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: Toluene, o-xylene monooxygenase oxygenase subunit;alpha

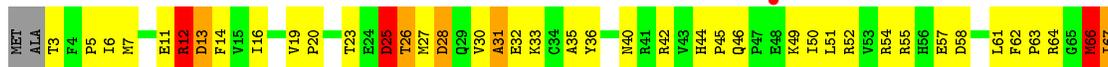


- Molecule 2: Toluene, o-xylene monooxygenase oxygenase subunit;beta





- Molecule 3: Toluene, o-xylene monooxygenase oxygenase subunit;gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.42Å 182.42Å 67.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.84 – 2.10 36.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.7 (36.84-2.10) 84.4 (36.83-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217 , 0.284 0.218 , 0.281	Depositor DCC
$R_{free}$ test set	3226 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtrriage
Anisotropy	0.952	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage'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.*

<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: GOL, FE, P6G, MPO

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	1.61	29/4166 (0.7%)	1.34	32/5664 (0.6%)
2	B	1.69	27/2713 (1.0%)	1.43	27/3688 (0.7%)
3	C	1.45	2/690 (0.3%)	1.42	7/934 (0.7%)
All	All	1.63	58/7569 (0.8%)	1.38	66/10286 (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	1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	TYR	CD1-CE1	13.31	1.59	1.39
1	A	64	GLU	CB-CG	10.37	1.71	1.52
2	B	43	GLU	CG-CD	10.24	1.67	1.51
2	B	283	GLU	CG-CD	10.23	1.67	1.51
1	A	146	TYR	CD1-CE1	-9.87	1.24	1.39

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASN	N-CA-C	8.92	135.08	111.00
1	A	233	ARG	NE-CZ-NH1	8.24	124.42	120.30
3	C	25	ASP	CB-CG-OD2	-8.13	110.99	118.30
2	B	191	ASP	CB-CG-OD1	-8.11	111.00	118.30
2	B	238	LEU	CB-CG-CD2	-7.67	97.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ARG	Peptide

## 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	4035	0	3782	163	0
2	B	2641	0	2537	92	0
3	C	676	0	667	50	0
4	A	12	0	15	4	0
5	A	19	0	25	20	0
6	A	2	0	0	0	0
7	B	13	0	15	2	0
8	A	82	0	0	7	0
8	B	72	0	0	2	0
8	C	4	0	0	0	0
All	All	7556	0	7041	273	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 19.

The worst 5 of 273 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)
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.33	1.23
1:A:372:CYS:HB3	3:C:42:ARG:HG2	1.25	1.11
2:B:162:HIS:CE1	2:B:227:LYS:NZ	2.20	1.10
2:B:72:TRP:H	7:B:4401:MPO:H71	1.19	1.05
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.19	1.02

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	490/498 (98%)	442 (90%)	44 (9%)	4 (1%)	22	17
2	B	320/330 (97%)	292 (91%)	25 (8%)	3 (1%)	20	14
3	C	81/86 (94%)	70 (86%)	9 (11%)	2 (2%)	6	2
All	All	891/914 (98%)	804 (90%)	78 (9%)	9 (1%)	18	12

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	A	287	ASN
2	B	310	GLY
1	A	408	PRO
1	A	445	LYS

### 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	418/422 (99%)	393 (94%)	25 (6%)	22	19
2	B	274/282 (97%)	252 (92%)	22 (8%)	14	10
3	C	77/79 (98%)	66 (86%)	11 (14%)	4	2
All	All	769/783 (98%)	711 (92%)	58 (8%)	15	12

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	22	ARG
2	B	111	GLN
3	C	67	ILE
2	B	23	ARG
2	B	89	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	HIS
2	B	36	HIS
2	B	153	ASN
1	A	418	GLN
2	B	162	HIS

### 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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	GOL	A	3287	-	5,5,5	0.39	0	5,5,5	0.87	0
5	P6G	A	4974	-	18,18,18	1.47	3 (16%)	17,17,17	1.26	3 (17%)
4	GOL	A	4975	6	5,5,5	1.02	0	5,5,5	1.67	2 (40%)
7	MPO	B	4401	-	13,13,13	3.04	7 (53%)	16,17,17	4.96	9 (56%)

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	GOL	A	3287	-	-	0/4/4/4	0/0/0/0
5	P6G	A	4974	-	-	0/16/16/16	0/0/0/0
4	GOL	A	4975	6	-	0/4/4/4	0/0/0/0
7	MPO	B	4401	-	-	0/7/15/15	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4401	MPO	C4-N1	-5.43	1.32	1.47
7	B	4401	MPO	C4-C5	-3.88	1.34	1.50
5	A	4974	P6G	O19-C18	-3.66	1.22	1.42
7	B	4401	MPO	C1-S1	-2.68	1.73	1.77
7	B	4401	MPO	C2-C3	2.11	1.60	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4401	MPO	O3-S1-O2	-6.81	95.76	111.37
7	B	4401	MPO	O4-C6-C7	-2.71	105.77	111.83
4	A	4975	GOL	O2-C2-C1	2.16	119.04	108.84
5	A	4974	P6G	O16-C17-C18	2.29	120.71	110.15
5	A	4974	P6G	O19-C18-C17	2.29	125.06	111.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3287	GOL	2	0
5	A	4974	P6G	20	0
4	A	4975	GOL	2	0
7	B	4401	MPO	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 [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, 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	491/498 (98%)	0.07	25 (5%) 29 35	33, 50, 65, 81	0
2	B	322/330 (97%)	-0.09	17 (5%) 27 33	33, 45, 65, 92	0
3	C	83/86 (96%)	0.05	3 (3%) 43 50	48, 63, 78, 85	0
All	All	896/914 (98%)	0.01	45 (5%) 30 36	33, 49, 69, 92	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100[A]	TRP	6.1
2	B	8	ALA	5.7
2	B	23	ARG	5.0
2	B	22	ARG	4.9
1	A	268	LEU	4.3

### 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. 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( $\text{\AA}^2$ )	Q<0.9
5	P6G	A	4974	19/19	0.88	0.19	4.17	47,56,72,76	0
4	GOL	A	3287	6/6	0.87	0.41	2.10	83,87,88,89	0
7	MPO	B	4401	13/13	0.86	0.17	2.08	60,66,72,77	0
4	GOL	A	4975	6/6	0.97	0.27	0.95	43,57,61,65	0
6	FE	A	500	1/1	0.99	0.13	-0.70	45,45,45,45	0
6	FE	A	499	1/1	1.00	0.12	-0.90	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.