



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 04:27 pm BST

PDB ID : 6FRL / pdb\_00006frl  
Title : BrvH, a flavin-dependent halogenase from Brevundimonas sp. BAL3  
Authors : Widmann, C.; Neubauer, P.R.; Sewald, N.; Niemann, H.H.  
Deposited on : 2018-02-16  
Resolution : 2.50 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

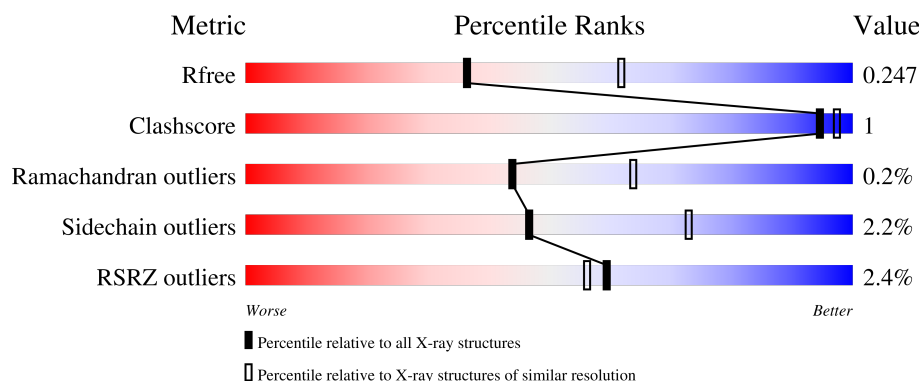
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

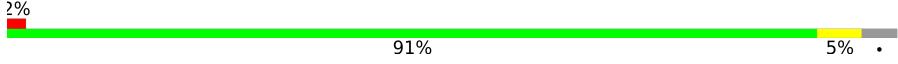
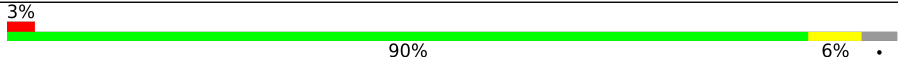
The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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  $\geq 3$ , 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	511	
1	B	511	

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
2	TLA	B	601	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8101 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.

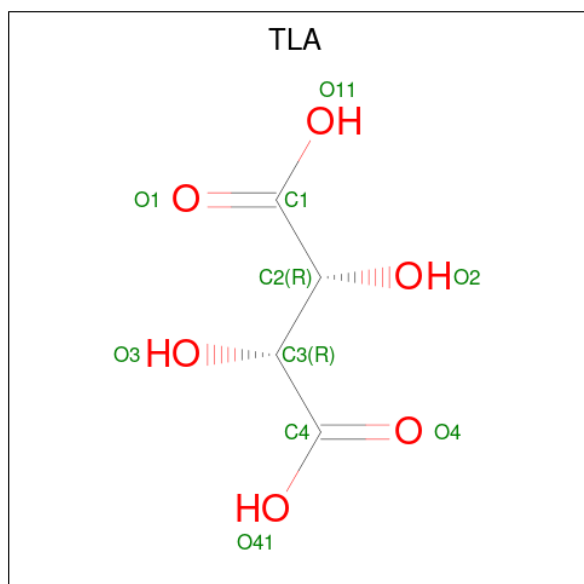
- Molecule 1 is a protein called Tryptophan halogenase superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			3866	2460	704	688	14			
1	B	492	Total	C	N	O	S	0	0	0
			3864	2460	701	689	14			

There are 4 discrepancies between the modelled and reference sequences:

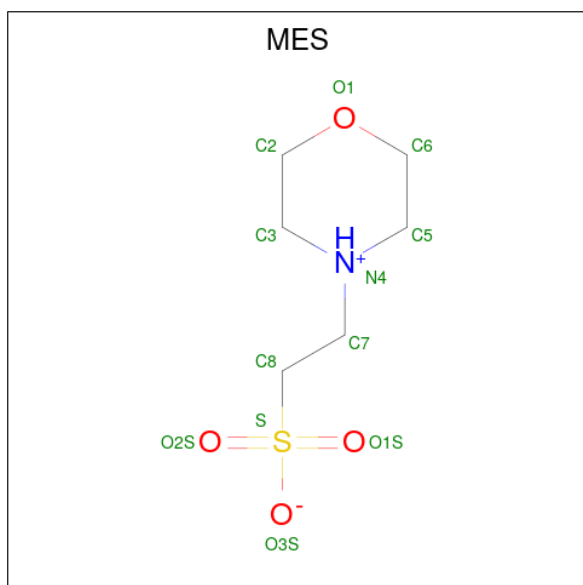
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B4WBL8
A	0	ALA	-	expression tag	UNP B4WBL8
B	-1	GLY	-	expression tag	UNP B4WBL8
B	0	ALA	-	expression tag	UNP B4WBL8

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

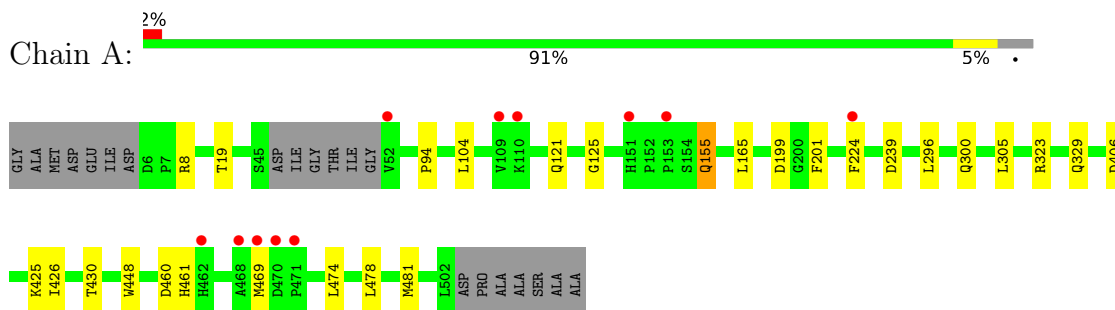
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	138	Total	O	0	0
			138	138		

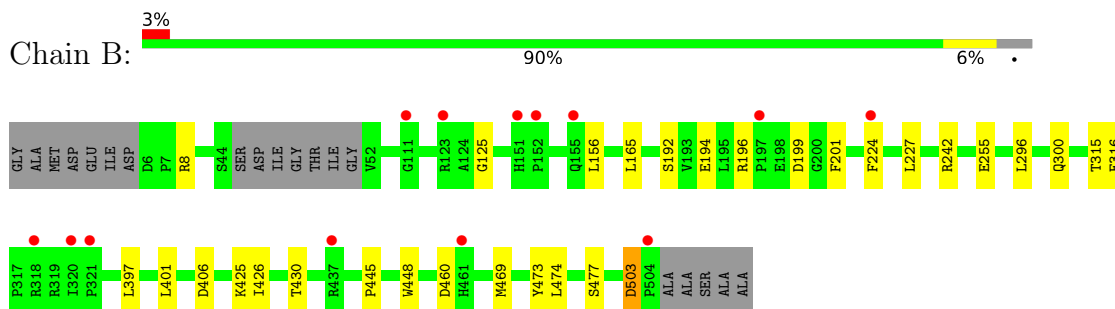
### 3 Residue-property plots [i](#)

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: Tryptophan halogenase superfamily



- Molecule 1: Tryptophan halogenase superfamily



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.62Å 88.35Å 70.11Å 90.00° 99.07° 90.00°	Depositor
Resolution (Å)	89.18 – 2.50 89.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (89.18-2.50) 96.5 (89.18-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.195 , 0.241 0.202 , 0.247	Depositor DCC
$R_{free}$ test set	1809 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GOL, TLA

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	0.90	0/3973	0.98	3/5397 (0.1%)
1	B	0.89	0/3972	0.99	3/5398 (0.1%)
All	All	0.89	0/7945	0.98	6/10795 (0.1%)

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	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	406	ASP	N-CA-C	6.32	120.25	112.54
1	B	406	ASP	N-CA-C	6.14	120.03	112.54
1	B	196	ARG	CB-CA-C	5.74	116.96	108.87
1	A	125	GLY	N-CA-C	5.14	119.08	113.58
1	B	125	GLY	N-CA-C	5.12	119.06	113.58
1	A	461	HIS	N-CA-CB	-5.09	102.02	110.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	503	ASP	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	3866	0	3775	10	0
1	B	3864	0	3769	9	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
3	A	12	0	13	0	0
3	B	12	0	13	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	177	0	0	1	0
5	B	138	0	0	0	0
All	All	8101	0	7594	19	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 1.

All (19) 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:104:LEU:HD12	1:A:155:GLN:HE22	1.57	0.67
1:B:469:MET:HE2	1:B:474:LEU:HD13	1.85	0.57
1:B:192:SER:OG	1:B:194:GLU:OE2	2.20	0.56
1:B:315:THR:OG1	1:B:316:GLU:N	2.43	0.51
1:A:469:MET:HE2	1:A:474:LEU:HD13	1.94	0.51
1:A:224:PHE:CZ	1:A:323:ARG:HB3	2.48	0.49
1:A:296:LEU:HD22	1:A:300:GLN:HB3	1.96	0.48
1:B:426:ILE:O	1:B:430:THR:HG23	2.14	0.47
1:A:426:ILE:O	1:A:430:THR:HG23	2.14	0.47
1:B:199:ASP:HB3	1:B:201:PHE:CD1	2.48	0.47
1:B:296:LEU:HD22	1:B:300:GLN:HB3	1.97	0.46
1:A:199:ASP:HB3	1:A:201:PHE:CD1	2.50	0.45
1:B:473:TYR:CD1	1:B:473:TYR:C	2.94	0.45
1:A:425:LYS:HE2	1:A:448:TRP:CZ2	2.54	0.43
1:A:121:GLN:OE1	1:A:474:LEU:HD23	2.19	0.42
1:A:478:LEU:HD12	1:A:481:MET:CE	2.50	0.42
1:B:425:LYS:HE2	1:B:448:TRP:CZ2	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:HD11	1:B:401:LEU:HD11	2.02	0.41
1:A:329:GLN:HG3	5:A:830:HOH:O	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	488/511 (96%)	469 (96%)	18 (4%)	1 (0%)	44	64
1	B	488/511 (96%)	466 (96%)	21 (4%)	1 (0%)	44	64
All	All	976/1022 (96%)	935 (96%)	39 (4%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	A	8	ARG

### 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	389/400 (97%)	382 (98%)	7 (2%)	54	78
1	B	389/400 (97%)	379 (97%)	10 (3%)	41	68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	778/800 (97%)	761 (98%)	17 (2%)	47 73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	94	PRO
1	A	155	GLN
1	A	165	LEU
1	A	239	ASP
1	A	305	LEU
1	A	460	ASP
1	B	156	LEU
1	B	165	LEU
1	B	224	PHE
1	B	227	LEU
1	B	242	ARG
1	B	255	GLU
1	B	445	PRO
1	B	460	ASP
1	B	477	SER
1	B	503	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	107	GLN
1	A	155	GLN
1	A	283	HIS
1	A	461	HIS
1	B	116	HIS
1	B	256	ASN
1	B	283	HIS

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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$
3	MES	B	602	-	12,12,12	2.03	1 (8%)	14,16,16	2.01	4 (28%)
2	TLA	B	601	-	9,9,9	2.02	1 (11%)	12,12,12	3.58	9 (75%)
2	TLA	A	601	-	9,9,9	0.99	0	12,12,12	1.28	1 (8%)
4	GOL	B	603	-	5,5,5	0.28	0	5,5,5	0.56	0
4	GOL	A	603	-	5,5,5	0.55	0	5,5,5	0.49	0
3	MES	A	602	-	12,12,12	2.00	1 (8%)	14,16,16	1.71	3 (21%)

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
3	MES	B	602	-	-	2/6/14/14	0/1/1/1
2	TLA	B	601	-	-	8/12/12/12	-
2	TLA	A	601	-	-	0/12/12/12	-
4	GOL	B	603	-	-	1/4/4/4	-
4	GOL	A	603	-	-	3/4/4/4	-
3	MES	A	602	-	-	5/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	MES	C8-S	-6.38	1.68	1.77
3	B	602	MES	C8-S	-6.32	1.68	1.77
2	B	601	TLA	C2-C1	-5.55	1.45	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TLA	O2-C2-C1	-5.19	99.78	110.66
2	B	601	TLA	O1-C1-C2	-5.15	108.08	121.63
2	B	601	TLA	C2-C3-C4	5.15	121.38	109.87
2	B	601	TLA	O2-C2-C3	5.10	120.36	110.23
3	B	602	MES	C6-C5-N4	4.05	116.24	110.10
3	A	602	MES	O1S-S-C8	4.01	111.74	106.92
2	B	601	TLA	O3-C3-C2	-4.00	102.29	110.23
3	B	602	MES	O3S-S-C8	3.52	111.46	105.77
2	B	601	TLA	O11-C1-O1	3.21	131.37	124.09
3	A	602	MES	C6-O1-C2	3.03	120.02	109.89
3	B	602	MES	C5-N4-C3	2.80	115.13	108.83
2	B	601	TLA	O41-C4-O4	-2.75	117.85	124.09
2	B	601	TLA	O11-C1-C2	2.65	120.43	113.27
3	B	602	MES	O1-C6-C5	-2.64	105.97	111.80
2	A	601	TLA	O3-C3-C4	2.62	116.16	110.66
2	B	601	TLA	O41-C4-C3	2.40	119.77	113.27
3	A	602	MES	C7-N4-C3	2.26	117.01	111.23

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	MES	C8-C7-N4-C3
3	A	602	MES	N4-C7-C8-S
3	B	602	MES	C8-C7-N4-C3
3	B	602	MES	N4-C7-C8-S
4	A	603	GOL	O1-C1-C2-C3
2	B	601	TLA	O1-C1-C2-O2
2	B	601	TLA	O11-C1-C2-O2
3	A	602	MES	C7-C8-S-O3S
4	A	603	GOL	O1-C1-C2-O2
2	B	601	TLA	O1-C1-C2-C3
2	B	601	TLA	O11-C1-C2-C3
2	B	601	TLA	C1-C2-C3-C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	603	GOL	O1-C1-C2-O2
2	B	601	TLA	C2-C3-C4-O4
2	B	601	TLA	C2-C3-C4-O41
2	B	601	TLA	O2-C2-C3-O3
3	A	602	MES	C7-C8-S-O1S
3	A	602	MES	C7-C8-S-O2S
4	A	603	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<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	491/511 (96%)	-0.14	11 (2%) 62 59	21, 34, 65, 101	1 (0%)
1	B	492/511 (96%)	-0.03	13 (2%) 57 54	23, 35, 68, 108	0
All	All	983/1022 (96%)	-0.08	24 (2%) 59 56	21, 35, 67, 108	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	PRO	4.4
1	A	153	PRO	3.2
1	B	151	HIS	3.2
1	B	321	PRO	3.1
1	A	224	PHE	2.9
1	A	462	HIS	2.8
1	B	224	PHE	2.6
1	A	109	VAL	2.6
1	B	111	GLY	2.6
1	A	468	ALA	2.5
1	A	471	PRO	2.5
1	A	469	MET	2.5
1	B	461	HIS	2.4
1	A	470	ASP	2.4
1	B	123	ARG	2.4
1	B	318	ARG	2.3
1	B	320	ILE	2.3
1	B	152	PRO	2.3
1	A	52	VAL	2.3
1	B	437	ARG	2.2
1	B	155	GLN	2.1
1	A	151	HIS	2.1
1	A	110	LYS	2.0
1	B	197	PRO	2.0



## 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 oligosaccharides 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	603	6/6	0.82	0.17	50,62,67,67	0
4	GOL	B	603	6/6	0.86	0.19	70,72,75,76	0
3	MES	A	602	12/12	0.89	0.12	41,48,60,63	0
2	TLA	B	601	10/10	0.93	0.07	31,35,37,46	0
3	MES	B	602	12/12	0.94	0.09	29,36,47,49	0
2	TLA	A	601	10/10	0.96	0.06	19,23,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.