



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 12:07 PM JST

PDB ID : 7E6F  
Title : Crystal structure of PMP-bound form of cysteine desulfurase SufS R376A from *Bacillus subtilis* in L-cycloserine-inhibition  
Authors : Nakamura, R.; Takahashi, Y.; Fujishiro, T.  
Deposited on : 2021-02-22  
Resolution : 2.74 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 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	:	2.26
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)	:	2.26

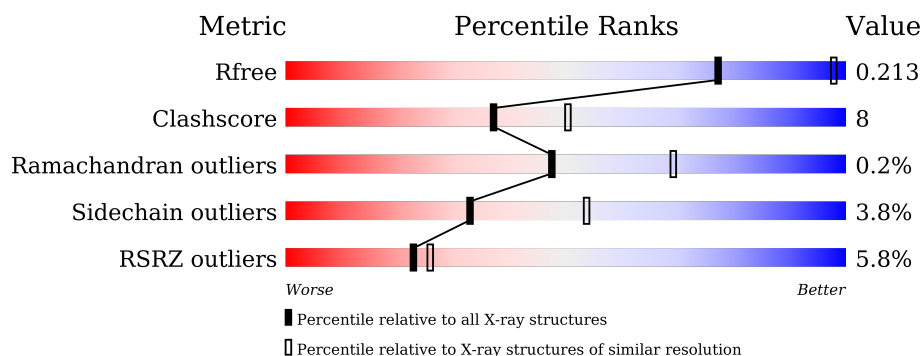
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	419	<div> <div>6%</div> <div>82%</div> <div>15%</div> <div>..</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
2	PEG	A	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3234 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.

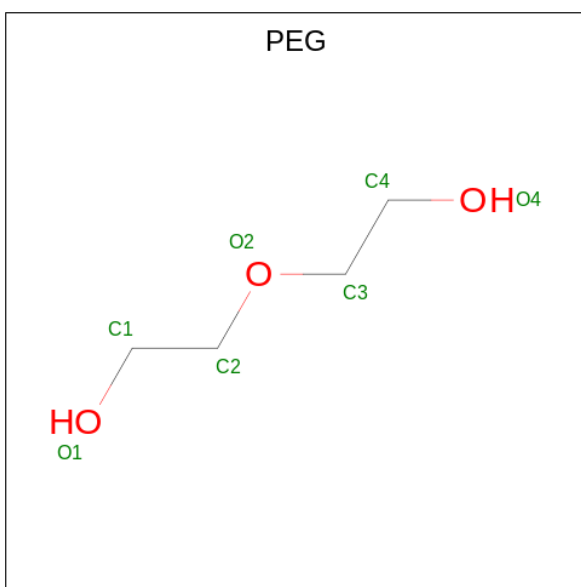
- Molecule 1 is a protein called Cysteine desulfurase SufS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3199	2029	541	616	13			

There are 14 discrepancies between the modelled and reference sequences:

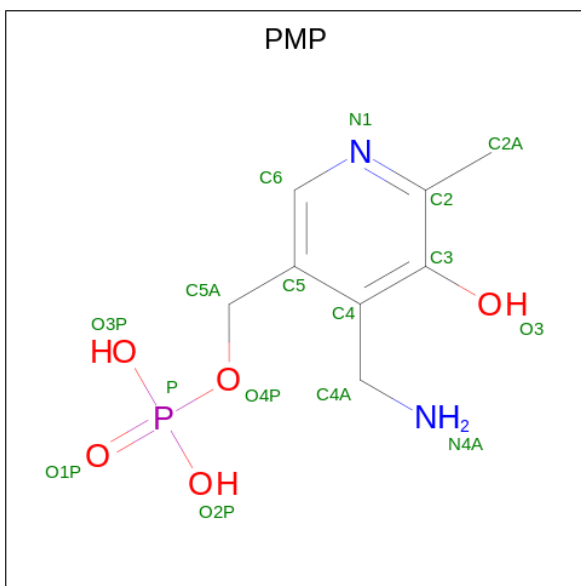
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP O32164
A	-1	GLY	-	expression tag	UNP O32164
A	0	HIS	-	expression tag	UNP O32164
A	376	ALA	ARG	engineered mutation	UNP O32164
A	407	VAL	-	expression tag	UNP O32164
A	408	ASP	-	expression tag	UNP O32164
A	409	LEU	-	expression tag	UNP O32164
A	410	GLU	-	expression tag	UNP O32164
A	411	HIS	-	expression tag	UNP O32164
A	412	HIS	-	expression tag	UNP O32164
A	413	HIS	-	expression tag	UNP O32164
A	414	HIS	-	expression tag	UNP O32164
A	415	HIS	-	expression tag	UNP O32164
A	416	HIS	-	expression tag	UNP O32164

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

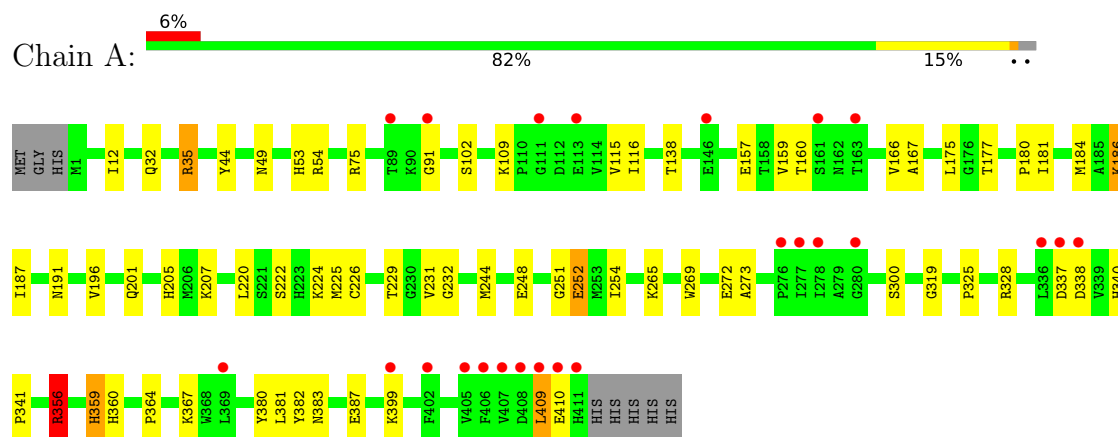
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		

### 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: Cysteine desulfurase SufS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.80Å 92.80Å 129.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 2.74 46.40 – 2.74	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.44-2.74) 100.0 (46.40-2.74)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.165 , 0.212 0.165 , 0.213	Depositor DCC
$R_{free}$ test set	874 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: PEG, EDO, PMP

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	0.61	1/3266 (0.0%)	1.04	6/4437 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	GLU	CD-OE2	6.13	1.32	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	A	356	ARG	CG-CD-NE	8.79	130.26	111.80
1	A	75	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	328	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	54	ARG	CG-CD-NE	-6.04	99.11	111.80
1	A	35	ARG	CB-CG-CD	5.61	126.19	111.60

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	3199	0	3148	50	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	10	6	0
3	A	16	0	11	0	0
4	A	4	0	6	0	0
5	A	8	0	0	0	0
All	All	3234	0	3175	50	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 8.

All (50) 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:356:ARG:HH22	1:A:360:HIS:H	1.23	0.86
1:A:319:GLY:HA3	1:A:399:LYS:NZ	1.98	0.77
1:A:356:ARG:NH2	1:A:360:HIS:H	1.86	0.72
1:A:364:PRO:HA	1:A:367:LYS:HD2	1.70	0.72
1:A:265:LYS:NZ	2:A:501:PEG:H21	2.12	0.65
1:A:319:GLY:HA3	1:A:399:LYS:HZ2	1.65	0.61
1:A:201:GLN:NE2	1:A:224:LYS:NZ	2.50	0.60
1:A:381:LEU:H	1:A:381:LEU:HD23	1.67	0.58
1:A:225:MET:O	1:A:226:CYS:HB2	2.04	0.58
1:A:248:GLU:HG3	1:A:273:ALA:HB3	1.86	0.57
1:A:35:ARG:HH21	1:A:35:ARG:HG2	1.70	0.56
1:A:53:HIS:HB3	2:A:501:PEG:H12	1.88	0.55
1:A:269:TRP:CD2	2:A:501:PEG:H32	2.42	0.54
1:A:180:PRO:O	1:A:184:MET:HG3	2.07	0.54
1:A:175:LEU:HB2	1:A:177:THR:HG23	1.90	0.53
1:A:159:VAL:HG21	1:A:187:ILE:HG22	1.91	0.51
1:A:116:ILE:HG22	1:A:167:ALA:HB3	1.93	0.51
1:A:201:GLN:HE22	1:A:224:LYS:HZ1	1.59	0.51
1:A:222:SER:HB3	1:A:231:VAL:HG13	1.92	0.51
1:A:254:ILE:O	1:A:254:ILE:HD12	2.10	0.51
1:A:265:LYS:HZ2	2:A:501:PEG:H31	1.77	0.50
1:A:265:LYS:HZ1	2:A:501:PEG:H21	1.77	0.49
1:A:319:GLY:HA3	1:A:399:LYS:HZ1	1.76	0.49
1:A:167:ALA:HA	1:A:196:VAL:HG23	1.95	0.49
1:A:91:GLY:HA2	1:A:232:GLY:HA3	1.94	0.49
1:A:201:GLN:HE22	1:A:224:LYS:NZ	2.10	0.48
1:A:337:ASP:O	1:A:338:ASP:HB3	2.12	0.48
1:A:319:GLY:CA	1:A:399:LYS:NZ	2.75	0.47
1:A:115:VAL:HG22	1:A:166:VAL:HG22	1.95	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HD2	2:A:501:PEG:H31	1.96	0.47
1:A:160:THR:C	1:A:191:ASN:HD22	2.19	0.46
1:A:201:GLN:O	1:A:205:HIS:HD2	2.00	0.45
1:A:32:GLN:NE2	1:A:32:GLN:HA	2.32	0.45
1:A:175:LEU:CB	1:A:177:THR:HG23	2.47	0.44
1:A:12:ILE:HG21	1:A:32:GLN:NE2	2.33	0.44
1:A:251:GLY:O	1:A:252:GLU:HB2	2.18	0.44
1:A:340:HIS:CG	1:A:341:PRO:HD2	2.53	0.44
1:A:177:THR:HG22	1:A:325:PRO:CD	2.48	0.43
1:A:383:ASN:HA	1:A:387:GLU:OE2	2.19	0.43
1:A:220:LEU:HD12	1:A:220:LEU:C	2.38	0.43
1:A:222:SER:CB	1:A:231:VAL:HG13	2.49	0.43
1:A:359:HIS:H	1:A:359:HIS:CD2	2.37	0.42
1:A:44:TYR:CZ	1:A:49:ASN:HA	2.55	0.42
1:A:186:LYS:HE3	1:A:187:ILE:HG13	2.03	0.41
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.92	0.41
1:A:201:GLN:NE2	1:A:224:LYS:HZ2	2.18	0.41
1:A:115:VAL:HG21	1:A:159:VAL:HG12	2.03	0.40
1:A:254:ILE:HD12	1:A:254:ILE:C	2.41	0.40
1:A:102:SER:OG	1:A:244:MET:HB3	2.21	0.40
1:A:181:ILE:HD13	1:A:181:ILE:HA	1.84	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	409/419 (98%)	392 (96%)	16 (4%)	1 (0%)	47 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLU

### 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	341/348 (98%)	328 (96%)	13 (4%)	33 54

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	138	THR
1	A	157	GLU
1	A	186	LYS
1	A	207	LYS
1	A	229	THR
1	A	300	SER
1	A	356	ARG
1	A	359	HIS
1	A	380	TYR
1	A	382	TYR
1	A	409	LEU
1	A	410	GLU

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	191	ASN
1	A	201	GLN
1	A	243	ASN
1	A	359	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

3 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	$\# Z  > 2$
4	EDO	A	503	-	3,3,3	0.15	0	2,2,2	0.34	0
2	PEG	A	501	-	6,6,6	0.47	0	5,5,5	0.40	0
3	PMP	A	502	-	16,16,16	0.54	0	21,23,23	0.81	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	EDO	A	503	-	-	0/1/1/1	-
2	PEG	A	501	-	-	3/4/4/4	-
3	PMP	A	502	-	-	2/8/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PMP	C3-C4-C4A-N4A
2	A	501	PEG	O1-C1-C2-O2
2	A	501	PEG	O2-C3-C4-O4
3	A	502	PMP	C5-C4-C4A-N4A
2	A	501	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PEG	6	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	411/419 (98%)	0.19	24 (5%)	23 26	49, 72, 105, 159	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	HIS	5.4
1	A	410	GLU	4.7
1	A	407	VAL	4.1
1	A	406	PHE	4.0
1	A	409	LEU	3.8
1	A	337	ASP	3.3
1	A	405	VAL	3.2
1	A	408	ASP	3.2
1	A	277	ILE	3.1
1	A	402	PHE	2.8
1	A	336	LEU	2.7
1	A	163	THR	2.7
1	A	146	GLU	2.7
1	A	111	GLY	2.6
1	A	91	GLY	2.6
1	A	338	ASP	2.4
1	A	369	LEU	2.2
1	A	278	ILE	2.2
1	A	161	SER	2.2
1	A	89	THR	2.1
1	A	399	LYS	2.1
1	A	113	GLU	2.1
1	A	280	GLY	2.1
1	A	276	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 monosaccharides 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	EDO	A	503	4/4	0.73	0.29	91,93,93,95	0
2	PEG	A	501	7/7	0.91	0.23	59,67,73,74	0
3	PMP	A	502	16/16	0.97	0.19	64,73,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.