



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 8, 2026 – 06:10 PM EDT

PDB ID : 9P3H / pdb\_00009p3h  
Title : Crystal Structure of Conserved Hypothetical Protein from *Stenotrophomonas maltophilia* (strain K279a)  
Authors : Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Wawrzak, Z.; Kiryukhina, O.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)  
Deposited on : 2025-06-13  
Resolution : 1.85 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

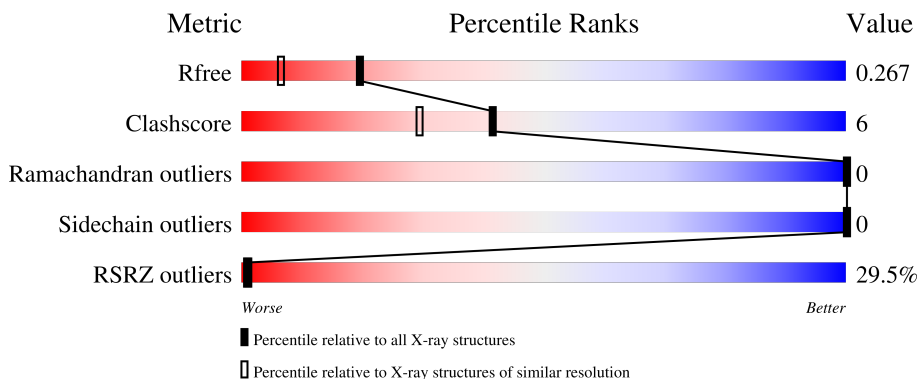
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


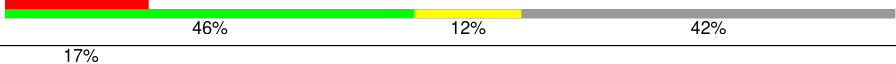
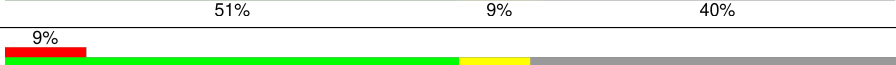

The reported resolution of this entry is 1.85 Å.

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))
$R_{free}$	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	444	
1	B	444	
1	C	444	
1	D	444	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9177 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 Conserved hyopthetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	Se	0	3	0
			2213	1379	402	428	1	3			
1	B	258	Total	C	N	O	S	Se	0	1	0
			2064	1283	375	403	1	2			
1	C	265	Total	C	N	O	S	Se	0	1	0
			2130	1329	383	415	1	2			
1	D	259	Total	C	N	O	S	Se	0	1	0
			2069	1285	375	406	1	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B2FKX1
A	-1	ASN	-	expression tag	UNP B2FKX1
A	0	ALA	-	expression tag	UNP B2FKX1
B	-2	SER	-	expression tag	UNP B2FKX1
B	-1	ASN	-	expression tag	UNP B2FKX1
B	0	ALA	-	expression tag	UNP B2FKX1
C	-2	SER	-	expression tag	UNP B2FKX1
C	-1	ASN	-	expression tag	UNP B2FKX1
C	0	ALA	-	expression tag	UNP B2FKX1
D	-2	SER	-	expression tag	UNP B2FKX1
D	-1	ASN	-	expression tag	UNP B2FKX1
D	0	ALA	-	expression tag	UNP B2FKX1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).

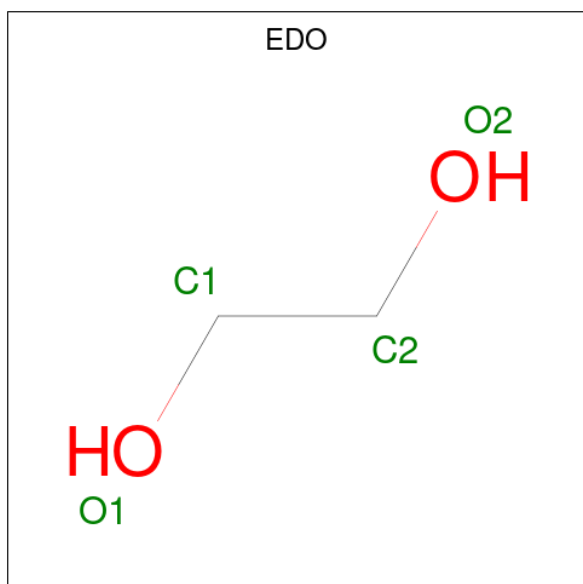


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

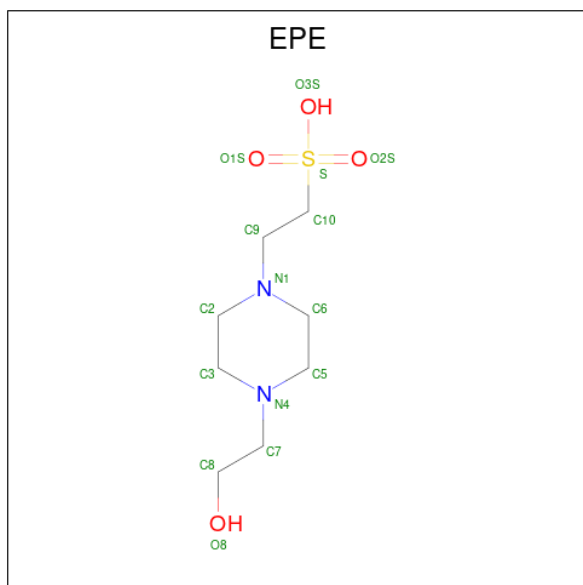
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	109	Total	O	0	1
			110	110		
7	B	147	Total	O	0	1
			148	148		
7	C	148	Total	O	0	3
			151	151		
7	D	182	Total	O	0	5
			187	187		

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- Molecule 1: Conserved hypothetical protein







GLY	MSE	PRO	THR	ALA	VAL	ALA	ALA	GLN	THR	PRO	VAL	ALA	GLU	SER	LEU	GLN	GLN	LEU	ALA	VAL	VAL	GLY	ASP	GLN	ARG	GLU	LEU	ALA	ALA	ARG	GLN	ASN	GLU	GLN	GLN	GLN	ALA	LEU	ASP	ALA	ALA	ARG	THR	GLN	GLU	GLN	GLN	SER	HIS	ALA	MSE	ARG	MSE	GLY
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.40Å 144.74Å 79.04Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.1 (30.00-1.85) 95.0 (30.00-1.85)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, $R_{free}$	0.192 , 0.215 0.244 , 0.267	Depositor DCC
$R_{free}$ test set	5173 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: CL, PGE, EPE, EDO, 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	0.44	0/2263	0.93	1/3068 (0.0%)
1	B	0.45	0/2105	0.95	1/2854 (0.0%)
1	C	0.45	0/2175	0.96	1/2950 (0.0%)
1	D	0.46	0/2110	1.00	1/2862 (0.0%)
All	All	0.45	0/8653	0.96	4/11734 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	PRO	N-CA-C	-5.41	103.29	111.41
1	D	114	PRO	N-CA-C	-5.17	103.70	111.57
1	A	114	PRO	N-CA-C	-5.08	103.84	111.57
1	C	114	PRO	N-CA-C	-5.04	103.86	111.41

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	2213	0	2133	38	0
1	B	2064	0	1999	33	0
1	C	2130	0	2048	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2069	0	1997	20	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	25	0	0	0	0
3	A	10	0	14	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
5	B	4	0	6	0	0
5	C	8	0	12	0	0
6	D	15	0	18	0	0
7	A	110	0	0	1	0
7	B	148	0	0	1	0
7	C	151	0	0	2	0
7	D	187	0	0	0	0
All	All	9177	0	8227	108	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 6.

The worst 5 of 108 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:D:13:SER:OG	1:D:99:ARG:NH2	2.21	0.74
1:C:89:ASP:OD1	1:C:92:ARG:NH2	2.27	0.68
1:A:137:THR:HB	1:A:138:PRO:HD3	1.79	0.65
1:B:204:LEU:HA	1:B:217:LYS:HE2	1.80	0.63
1:B:255:ASN:O	1:B:259:GLU:HG3	1.99	0.62

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	275/444 (62%)	264 (96%)	11 (4%)	0	100	100
1	B	255/444 (57%)	247 (97%)	8 (3%)	0	100	100
1	C	262/444 (59%)	255 (97%)	7 (3%)	0	100	100
1	D	256/444 (58%)	254 (99%)	2 (1%)	0	100	100
All	All	1048/1776 (59%)	1020 (97%)	28 (3%)	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	234/359 (65%)	234 (100%)	0	100	100
1	B	221/359 (62%)	221 (100%)	0	100	100
1	C	228/359 (64%)	228 (100%)	0	100	100
1	D	221/359 (62%)	221 (100%)	0	100	100
All	All	904/1436 (63%)	904 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	134	ASN
1	C	212	ASN
1	D	160	ASN
1	D	30	GLN
1	C	129	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\# Z  > 2$
2	SO4	D	504	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	502	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	C	501	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	D	505	-	4,4,4	0.32	0	6,6,6	0.06	0
5	EDO	C	504	-	3,3,3	0.08	0	2,2,2	0.10	0
5	EDO	B	504	-	3,3,3	0.07	0	2,2,2	0.16	0
5	EDO	C	505	-	3,3,3	0.07	0	2,2,2	0.16	0
2	SO4	C	503	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	D	506	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	C	502	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	D	503	-	4,4,4	0.33	0	6,6,6	0.08	0
3	PGE	A	504	-	9,9,9	0.17	0	8,8,8	0.09	0
2	SO4	D	507	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	503	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	503	-	4,4,4	0.34	0	6,6,6	0.07	0
6	EPE	D	508	-	15,15,15	0.59	1 (6%)	19,20,20	0.59	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
5	EDO	C	504	-	-	1/1/1/1	-
5	EDO	B	504	-	-	0/1/1/1	-
5	EDO	C	505	-	-	1/1/1/1	-
3	PGE	A	504	-	-	4/7/7/7	-
6	EPE	D	508	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	508	EPE	O3S-S	2.15	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	PGE	O1-C1-C2-O2
3	A	504	PGE	O3-C5-C6-O4
3	A	504	PGE	O2-C3-C4-O3
5	C	505	EDO	O1-C1-C2-O2
3	A	504	PGE	C6-C5-O3-C4

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 [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	273/444 (61%)	2.19	122 (44%) 0 0	11, 27, 70, 104	3 (1%)
1	B	256/444 (57%)	1.44	73 (28%) 1 1	11, 21, 43, 53	1 (0%)
1	C	263/444 (59%)	1.54	75 (28%) 1 1	7, 21, 52, 73	1 (0%)
1	D	257/444 (57%)	0.97	39 (15%) 5 5	8, 19, 38, 63	1 (0%)
All	All	1049/1776 (59%)	1.54	309 (29%) 1 1	7, 22, 53, 104	6 (0%)

The worst 5 of 309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	VAL	9.8
1	A	67	ALA	8.8
1	A	136	TRP	8.0
1	B	286	VAL	7.5
1	A	135	CYS	7.4

### 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
2	SO4	D	506	5/5	0.49	0.16	73,77,77,79	0
2	SO4	D	505	5/5	0.51	0.18	47,48,53,57	0
2	SO4	A	503	5/5	0.57	0.18	72,73,75,78	0
3	PGE	A	504	10/10	0.59	0.26	52,53,55,55	0
5	EDO	C	505	4/4	0.66	0.22	47,49,49,50	0
5	EDO	C	504	4/4	0.68	0.17	41,41,42,42	0
2	SO4	B	502	5/5	0.68	0.16	50,54,56,58	0
2	SO4	D	507	5/5	0.70	0.23	58,62,68,69	0
2	SO4	C	502	5/5	0.71	0.14	68,68,69,71	0
2	SO4	C	503	5/5	0.75	0.14	41,47,48,49	0
2	SO4	A	502	5/5	0.77	0.14	45,51,53,55	0
2	SO4	D	504	5/5	0.81	0.13	51,52,54,55	0
6	EPE	D	508	15/15	0.81	0.16	34,37,44,47	0
2	SO4	A	501	5/5	0.82	0.15	70,72,73,74	0
2	SO4	C	501	5/5	0.84	0.19	83,85,87,88	0
4	CL	D	501	1/1	0.85	0.21	65,65,65,65	0
4	CL	B	501	1/1	0.85	0.20	61,61,61,61	0
2	SO4	B	503	5/5	0.87	0.11	72,73,74,75	0
2	SO4	D	503	5/5	0.88	0.14	36,45,45,46	0
5	EDO	B	504	4/4	0.89	0.12	37,37,38,39	0
4	CL	D	502	1/1	0.93	0.14	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.