



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:17 pm BST

PDB ID : 4CGK  
Title : Crystal structure of the essential protein PcsB from *Streptococcus pneumoniae*  
Authors : Bartual, S.G.; Straume, D.; Stamsas, G.A.; Alfonso, C.; Martinez-Ripoll, M.; Havarstein, L.S.; Hermoso, J.A.  
Deposited on : 2013-11-25  
Resolution : 2.55 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

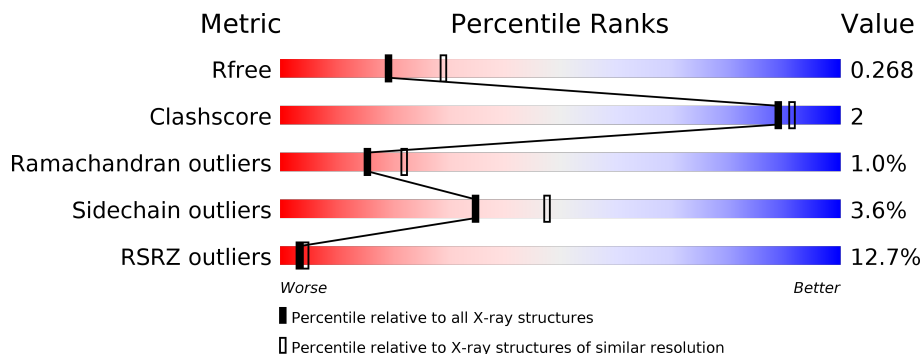
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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	392	
1	B	392	

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	EDO	A	1394	-	-	-	X

## 2 Entry composition [i](#)

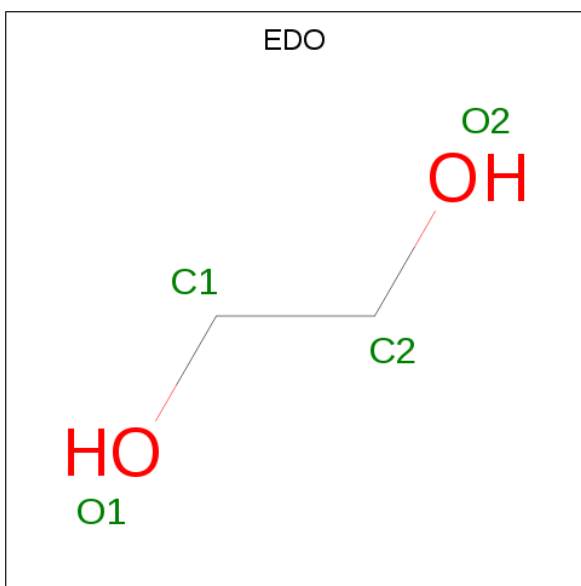
There are 6 unique types of molecules in this entry. The entry contains 5709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SECRETED 45 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	Total 2624	C 1601	N 472	O 547	S 4	0	0	0
1	B	348	Total 2607	C 1591	N 469	O 543	S 4	0	1	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

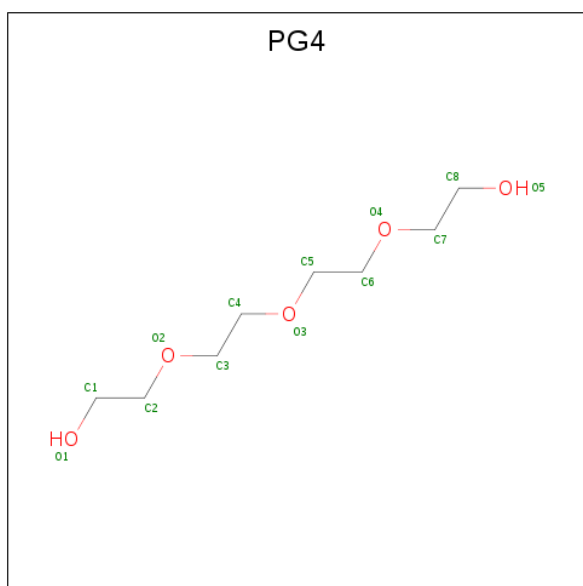
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	7	Total Cl 7 7	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

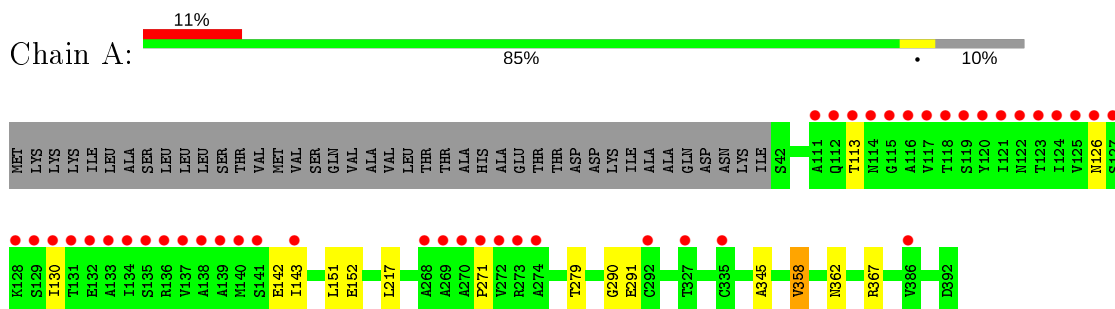
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	256	Total O 256 256	0	0
6	B	192	Total O 192 192	0	0

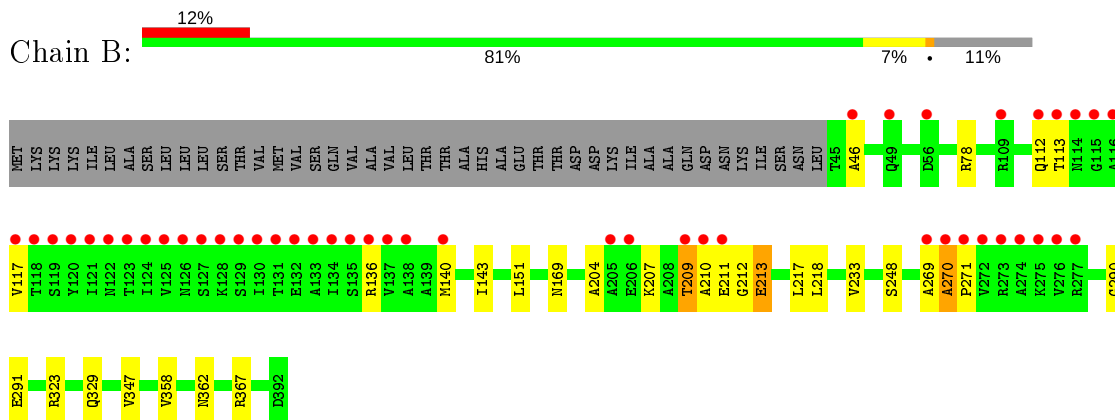
### 3 Residue-property plots [i](#)

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: SECRETED 45 KDA PROTEIN



- Molecule 1: SECRETED 45 KDA PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.81Å 125.81Å 126.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.63 – 2.55 44.63 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.63-2.55) 99.9 (44.63-2.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.238 , 0.272 0.238 , 0.268	Depositor DCC
$R_{free}$ test set	1907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtrriage
Anisotropy	1.009	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5709	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: MG, PG4, EDO, CL

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	0.33	0/2655	0.48	0/3602
1	B	0.28	0/2638	0.47	0/3579
All	All	0.30	0/5293	0.48	0/7181

There are no bond length outliers.

There are no bond angle outliers.

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	2624	0	2569	3	0
1	B	2607	0	2548	17	0
2	A	8	0	12	0	0
3	A	7	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	B	13	0	18	0	0
6	A	256	0	0	2	0
6	B	192	0	0	1	0
All	All	5709	0	5147	20	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 2.

All (20) 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:B:269:ALA:HA	1:B:270:ALA:HB3	1.65	0.78
1:B:211:GLU:HB3	1:B:213:GLU:N	2.16	0.61
6:A:2207:HOH:O	1:B:323:ARG:NH1	2.42	0.53
1:B:211:GLU:CG	1:B:212:GLY:HA3	2.39	0.52
6:A:2205:HOH:O	1:B:329[A]:GLN:NE2	2.41	0.52
1:B:112:GLN:HA	1:B:117:VAL:HG22	1.92	0.52
1:B:211:GLU:HB3	1:B:212:GLY:CA	2.40	0.51
1:A:345:ALA:HB1	1:A:358:VAL:HG13	1.94	0.50
1:B:211:GLU:CB	1:B:212:GLY:HA3	2.42	0.49
1:B:112:GLN:HA	1:B:117:VAL:CG2	2.43	0.48
1:B:347:VAL:HA	1:B:358:VAL:HG12	1.95	0.48
1:A:291:GLU:OE2	1:A:367:ARG:NH2	2.50	0.43
1:B:290:GLY:O	1:B:362:ASN:HB2	2.19	0.43
1:A:290:GLY:O	1:A:362:ASN:HB2	2.19	0.42
1:B:169:ASN:ND2	6:B:2059:HOH:O	2.52	0.42
1:B:291:GLU:OE2	1:B:367:ARG:NH2	2.51	0.42
1:B:209:THR:N	1:B:210:ALA:HA	2.35	0.42
1:B:204:ALA:O	1:B:207:LYS:HG2	2.19	0.42
1:B:211:GLU:HB3	1:B:212:GLY:C	2.39	0.41
1:B:211:GLU:CB	1:B:212:GLY:CA	2.98	0.41

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	349/392 (89%)	334 (96%)	12 (3%)	3 (1%)	17 24
1	B	347/392 (88%)	331 (95%)	12 (4%)	4 (1%)	13 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	696/784 (89%)	665 (96%)	24 (3%)	7 (1%)	15	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	THR
1	A	126	ASN
1	B	270	ALA
1	B	46	ALA
1	A	130	ILE
1	A	271	PRO
1	B	271	PRO

### 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	269/304 (88%)	261 (97%)	8 (3%)	41	55
1	B	266/304 (88%)	255 (96%)	11 (4%)	30	41
All	All	535/608 (88%)	516 (96%)	19 (4%)	35	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	142	GLU
1	A	143	ILE
1	A	151	LEU
1	A	152	GLU
1	A	217	LEU
1	A	279	THR
1	A	358	VAL
1	B	78	ARG
1	B	113	THR
1	B	136	ARG

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Mol	Chain	Res	Type
1	B	140	MET
1	B	143	ILE
1	B	151	LEU
1	B	213	GLU
1	B	217	LEU
1	B	218	LEU
1	B	233	VAL
1	B	248	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	EDO	A	1393	-	3,3,3	0.49	0	2,2,2	0.23	0
2	EDO	A	1394	-	3,3,3	0.45	0	2,2,2	0.28	0
5	PG4	B	1394	-	12,12,12	0.47	0	11,11,11	0.21	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	EDO	A	1393	-	-	1/1/1/1	-
2	EDO	A	1394	-	-	1/1/1/1	-
5	PG4	B	1394	-	-	7/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1394	PG4	O1-C1-C2-O2
5	B	1394	PG4	O4-C7-C8-O5
5	B	1394	PG4	O3-C5-C6-O4
2	A	1394	EDO	O1-C1-C2-O2
5	B	1394	PG4	O2-C3-C4-O3
2	A	1393	EDO	O1-C1-C2-O2
5	B	1394	PG4	C1-C2-O2-C3
5	B	1394	PG4	C8-C7-O4-C6
5	B	1394	PG4	C4-C3-O2-C2

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	351/392 (89%)	0.82	43 (12%) <b>4</b> <b>5</b>	40, 58, 186, 212	1 (0%)
1	B	348/392 (88%)	0.94	46 (13%) <b>3</b> <b>4</b>	38, 63, 193, 225	0
All	All	699/784 (89%)	0.88	89 (12%) <b>3</b> <b>4</b>	38, 60, 190, 225	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	ASN	14.8
1	B	115	GLY	13.1
1	B	120	TYR	10.8
1	B	270	ALA	10.1
1	B	274	ALA	9.5
1	B	128	LYS	9.2
1	A	135	SER	9.2
1	A	138	ALA	8.9
1	B	130	ILE	8.7
1	A	129	SER	8.7
1	A	120	TYR	8.3
1	A	117	VAL	8.3
1	B	117	VAL	8.0
1	A	134	ILE	8.0
1	B	121	ILE	7.9
1	A	124	ILE	7.9
1	B	118	THR	7.8
1	A	130	ILE	7.8
1	B	113	THR	7.4
1	B	271	PRO	7.3
1	B	119	SER	7.1
1	A	116	ALA	7.1
1	B	272	VAL	7.0
1	B	122	ASN	6.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	127	SER	6.9
1	B	137	VAL	6.8
1	A	131	THR	6.7
1	B	273	ARG	6.6
1	A	137	VAL	6.6
1	A	133	ALA	6.3
1	B	269	ALA	6.2
1	A	111	ALA	6.1
1	A	119	SER	6.0
1	B	135	SER	5.8
1	A	139	ALA	5.7
1	B	116	ALA	5.6
1	A	113	THR	5.5
1	A	125	VAL	5.4
1	A	122	ASN	5.4
1	A	132	GLU	5.4
1	A	114	ASN	5.3
1	A	123	THR	5.2
1	A	136	ARG	5.1
1	B	136	ARG	5.0
1	B	275	LYS	4.9
1	B	126	ASN	4.8
1	B	124	ILE	4.7
1	A	118	THR	4.7
1	B	131	THR	4.6
1	A	270	ALA	4.6
1	B	276	VAL	4.3
1	A	126	ASN	4.3
1	B	138	ALA	4.2
1	B	132	GLU	4.2
1	B	123	THR	4.0
1	B	129	SER	3.9
1	B	112	GLN	3.9
1	A	115	GLY	3.7
1	B	205	ALA	3.6
1	A	272	VAL	3.6
1	A	121	ILE	3.5
1	B	46	ALA	3.4
1	A	269	ALA	3.2
1	B	210	ALA	3.2
1	B	134	ILE	3.2
1	B	133	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	112	GLN	3.2
1	A	274	ALA	2.8
1	B	127	SER	2.8
1	A	273	ARG	2.6
1	A	128	LYS	2.6
1	B	125	VAL	2.6
1	B	209	THR	2.6
1	B	109	ARG	2.5
1	B	49	GLN	2.5
1	A	292	CYS	2.4
1	B	211	GLU	2.4
1	A	271	PRO	2.4
1	A	268	ALA	2.4
1	A	335	CYS	2.3
1	B	206	GLU	2.3
1	A	141	SER	2.2
1	B	277	ARG	2.2
1	A	327	THR	2.2
1	A	143	ILE	2.1
1	A	386	VAL	2.1
1	A	140	MET	2.1
1	B	56	ASP	2.1
1	B	140	MET	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 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	1393	4/4	0.62	0.31	82,83,83,84	0
2	EDO	A	1394	4/4	0.77	0.45	82,83,83,86	0
5	PG4	B	1394	13/13	0.78	0.33	76,82,85,85	0
3	CL	A	1399	1/1	0.81	0.47	128,128,128,128	0
3	CL	B	1395	1/1	0.82	0.11	89,89,89,89	0
3	CL	A	1400	1/1	0.85	0.10	76,76,76,76	0
3	CL	A	1401	1/1	0.88	0.14	105,105,105,105	0
3	CL	A	1398	1/1	0.90	0.10	80,80,80,80	0
3	CL	A	1395	1/1	0.90	0.09	85,85,85,85	0
3	CL	A	1396	1/1	0.94	0.10	85,85,85,85	0
3	CL	A	1397	1/1	0.95	0.14	81,81,81,81	0
4	MG	B	1393	1/1	0.96	0.15	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.