



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:30 AM GMT

PDB ID : 2XD5  
Title : STRUCTURAL INSIGHTS INTO THE CATALYTIC MECHANISM AND  
THE ROLE OF STREPTOCOCCUS PNEUMONIAE PBP1B  
Authors : Macheboeuf, P.; Lemaire, D.; Jamin, M.; Dideberg, O.; Dessen, A.  
Deposited on : 2010-04-29  
Resolution : 2.50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

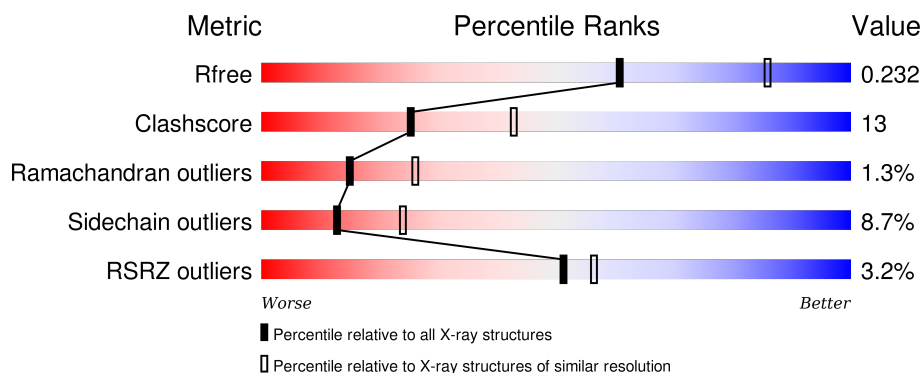
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


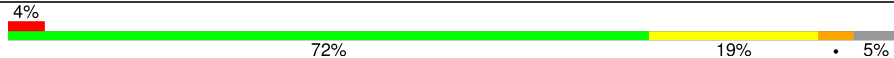
The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 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	494	
1	B	494	

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
3	S2D	A	1792	-	-	-	X
3	S2D	B	1791	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7547 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 PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	4	5	0
			3657	2285	621	736	15			
1	B	468	Total	C	N	O	S	2	2	0
			3610	2256	609	729	16			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ASP	-	EXPRESSION TAG	UNP Q7CRA4
A	102	ILE	-	EXPRESSION TAG	UNP Q7CRA4
A	103	SER	-	EXPRESSION TAG	UNP Q7CRA4
A	104	SER	-	EXPRESSION TAG	UNP Q7CRA4
A	105	ILE	-	EXPRESSION TAG	UNP Q7CRA4
A	106	SER	-	EXPRESSION TAG	UNP Q7CRA4
A	107	GLU	-	EXPRESSION TAG	UNP Q7CRA4
A	108	ILE	-	EXPRESSION TAG	UNP Q7CRA4
A	109	THR	-	EXPRESSION TAG	UNP Q7CRA4
A	110	TYR	-	EXPRESSION TAG	UNP Q7CRA4
A	111	SER	-	EXPRESSION TAG	UNP Q7CRA4
A	112	ASP	-	EXPRESSION TAG	UNP Q7CRA4
A	113	GLY	-	EXPRESSION TAG	UNP Q7CRA4
A	114	THR	-	EXPRESSION TAG	UNP Q7CRA4
A	115	VAL	-	EXPRESSION TAG	UNP Q7CRA4
A	116	ILE	-	EXPRESSION TAG	UNP Q7CRA4
A	117	ALA	-	EXPRESSION TAG	UNP Q7CRA4
A	118	SER	-	EXPRESSION TAG	UNP Q7CRA4
A	119	ILE	-	EXPRESSION TAG	UNP Q7CRA4
A	120	GLU	-	EXPRESSION TAG	UNP Q7CRA4
A	121	SER	-	EXPRESSION TAG	UNP Q7CRA4
A	122	ASP	-	EXPRESSION TAG	UNP Q7CRA4
A	123	MET	-	EXPRESSION TAG	UNP Q7CRA4
A	124	LEU	-	EXPRESSION TAG	UNP Q7CRA4
A	125	ARG	-	EXPRESSION TAG	UNP Q7CRA4

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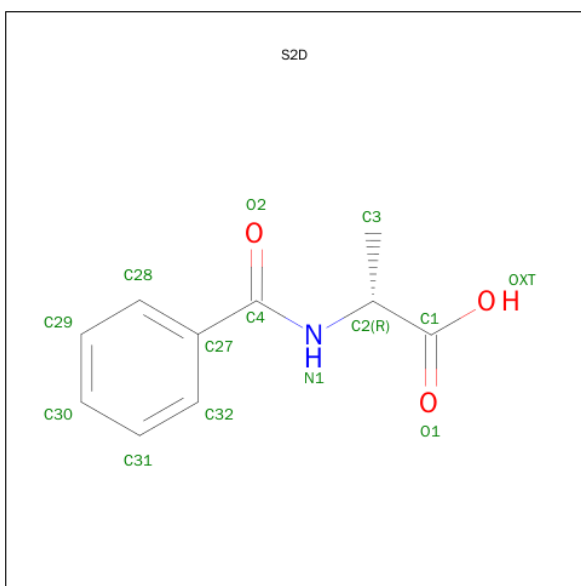
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
A	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
A	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	101	ASP	-	EXPRESSION TAG	UNP Q7CRA4
B	102	ILE	-	EXPRESSION TAG	UNP Q7CRA4
B	103	SER	-	EXPRESSION TAG	UNP Q7CRA4
B	104	SER	-	EXPRESSION TAG	UNP Q7CRA4
B	105	ILE	-	EXPRESSION TAG	UNP Q7CRA4
B	106	SER	-	EXPRESSION TAG	UNP Q7CRA4
B	107	GLU	-	EXPRESSION TAG	UNP Q7CRA4
B	108	ILE	-	EXPRESSION TAG	UNP Q7CRA4
B	109	THR	-	EXPRESSION TAG	UNP Q7CRA4
B	110	TYR	-	EXPRESSION TAG	UNP Q7CRA4
B	111	SER	-	EXPRESSION TAG	UNP Q7CRA4
B	112	ASP	-	EXPRESSION TAG	UNP Q7CRA4
B	113	GLY	-	EXPRESSION TAG	UNP Q7CRA4
B	114	THR	-	EXPRESSION TAG	UNP Q7CRA4
B	115	VAL	-	EXPRESSION TAG	UNP Q7CRA4
B	116	ILE	-	EXPRESSION TAG	UNP Q7CRA4
B	117	ALA	-	EXPRESSION TAG	UNP Q7CRA4
B	118	SER	-	EXPRESSION TAG	UNP Q7CRA4
B	119	ILE	-	EXPRESSION TAG	UNP Q7CRA4
B	120	GLU	-	EXPRESSION TAG	UNP Q7CRA4
B	121	SER	-	EXPRESSION TAG	UNP Q7CRA4
B	122	ASP	-	EXPRESSION TAG	UNP Q7CRA4
B	123	MET	-	EXPRESSION TAG	UNP Q7CRA4
B	124	LEU	-	EXPRESSION TAG	UNP Q7CRA4
B	125	ARG	-	EXPRESSION TAG	UNP Q7CRA4
B	336	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4

- Molecule 2 is SULFATE ION (three-letter code: 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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is N-BENZOYL-D-ALANINE (three-letter code: S2D) (formula:  $C_{10}H_{11}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total 116	O 116	0	0
5	B	134	Total 134	O 134	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.80 Å 101.10 Å 145.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.05 – 2.50 45.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.05-2.50) 99.9 (45.91-2.50)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.24 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.181 , 0.233 0.181 , 0.232	Depositor DCC
$R_{free}$ test set	2481 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.5	EDS
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 49863 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, S2D, 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	1.36	8/3730 (0.2%)	1.09	14/5063 (0.3%)
1	B	1.62	12/3682 (0.3%)	1.80	14/5001 (0.3%)
All	All	1.49	20/7412 (0.3%)	1.49	28/10064 (0.3%)

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	1	3
1	B	1	5
All	All	2	8

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	445	GLU	CD-OE1	62.91	1.94	1.25
1	A	742	GLU	CD-OE2	38.34	1.67	1.25
1	A	397	LYS	CD-CE	-14.72	1.14	1.51
1	A	460	SER	C-O	10.62	1.43	1.23
1	A	346	GLU	CB-CG	10.50	1.72	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	GLU	OE1-CD-OE2	-100.70	2.46	123.30
1	A	742	GLU	CG-CD-OE2	-18.20	81.89	118.30
1	B	460	SER	O-C-N	-11.67	104.03	122.70
1	A	460	SER	O-C-N	-10.02	106.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	SER	CB-CA-C	10.00	129.10	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	460	SER	CA
1	B	460	SER	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	SER	Peptide
1	A	460	SER	Mainchain
1	A	742	GLU	Sidechain
1	B	361	VAL	Peptide
1	B	372	GLN	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	3657	0	3505	92	0
1	B	3610	0	3448	86	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	5	0	4	2	0
3	B	13	0	10	1	0
4	A	2	0	0	0	0
5	A	116	0	0	2	0
5	B	134	0	0	3	0
All	All	7547	0	6967	178	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 13.

The worst 5 of 178 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:461:THR:CG2	1:A:567:HIS:HE1	1.41	1.32
1:B:460:SER:CB	1:B:463:LYS:HE3	1.78	1.13
1:A:461:THR:CG2	1:A:567:HIS:CE1	2.32	1.12
1:A:461:THR:HG23	1:A:567:HIS:HE1	1.16	1.04
1:B:373[A]:LYS:HD3	1:B:376:ARG:HH11	1.25	1.01

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	470/494 (95%)	438 (93%)	25 (5%)	7 (2%)	13	22
1	B	464/494 (94%)	433 (93%)	26 (6%)	5 (1%)	17	31
All	All	934/988 (94%)	871 (93%)	51 (6%)	12 (1%)	15	26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	THR
1	B	121	SER
1	B	372	GLN
1	B	788	GLY
1	A	363	ALA

### 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	389/409 (95%)	353 (91%)	36 (9%)	11	21
1	B	384/409 (94%)	353 (92%)	31 (8%)	15	27
All	All	773/818 (94%)	706 (91%)	67 (9%)	13	24

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	745	GLU
1	B	119	ILE
1	B	746	VAL
1	A	746	VAL
1	A	769	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	686	GLN
1	B	348	GLN
1	B	682	HIS
1	A	695	ASN
1	A	706	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	SO4	A	1791	-	4,4,4	0.86	0	6,6,6	0.24	0
3	S2D	A	1792	1	3,4,14	1.61	0	0,4,18	0.00	-
2	SO4	B	1790	-	4,4,4	0.88	0	6,6,6	0.75	0
3	S2D	B	1791	1	12,13,14	2.33	4 (33%)	15,16,18	3.98	5 (33%)

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	SO4	A	1791	-	-	0/0/0/0	0/0/0/0
3	S2D	A	1792	1	-	0/0/2/12	0/0/0/1
2	SO4	B	1790	-	-	0/0/0/0	0/0/0/0
3	S2D	B	1791	1	-	0/8/10/12	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1791	S2D	C27-C4	2.34	1.55	1.50
3	B	1791	S2D	C32-C27	2.49	1.43	1.39
3	B	1791	S2D	C4-N1	3.03	1.41	1.34
3	B	1791	S2D	C2-N1	5.40	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1791	S2D	O2-C4-C27	-4.07	114.01	120.97
3	B	1791	S2D	C27-C4-N1	2.06	120.60	116.93
3	B	1791	S2D	C1-C2-N1	3.44	117.87	110.64
3	B	1791	S2D	C3-C2-N1	8.94	120.01	109.61
3	B	1791	S2D	C2-N1-C4	10.82	141.60	122.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1792	S2D	2	0
3	B	1791	S2D	1	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	469/494 (94%)	-0.03	12 (2%) 59 63	15, 30, 59, 74	4 (0%)
1	B	468/494 (94%)	-0.01	18 (3%) 44 49	14, 27, 62, 79	3 (0%)
All	All	937/988 (94%)	-0.02	30 (3%) 51 56	14, 29, 61, 79	7 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	GLY	4.9
1	B	741	VAL	4.7
1	B	363	ALA	3.5
1	B	124	LEU	3.4
1	B	362	SER	3.2

### 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
3	S2D	A	1792	5/14	0.72	0.32	6.31	33,39,45,47	0
3	S2D	B	1791	13/14	0.85	0.27	5.26	33,43,46,47	6
2	SO4	A	1791	5/5	0.99	0.13	0.33	26,28,31,31	0
4	CL	A	1793	1/1	1.00	0.16	-0.44	21,21,21,21	0
2	SO4	B	1790	5/5	1.00	0.10	-2.22	18,20,20,22	0
4	CL	A	1794	1/1	0.97	0.28	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.