W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 10:06 am GMT

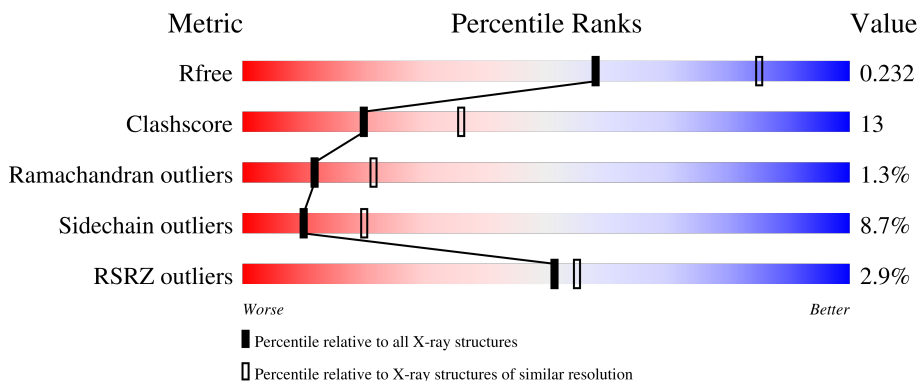|		
PDB ID	:	2XD5
Title	:	Structural insights into the catalytic mechanism and the role of Streptococcus pneumoniae PBP1b
Authors	:	Macheboeuf, P.; Lemaire, D.; Jamin, M.; Dideberg, O.; Dessen, A.
Deposited on	:	2010-04-29
Resolution	:	2.50 Å(reported)

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	Percentile Ranks	Value
Rfree		0.232
Clashscore		13
Ramachandran outliers		1.3%
Sidechain outliers		8.7%
RSRZ outliers		2.9%

Worse ... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 >=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 <=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	2% / 70% / 20% / • 5%
1	B	494	3% / 72% / 19% / • 5%

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 3657	C 2285	N 621	O 736	S 15	4	5	0
1	B	468	Total 3610	C 2256	N 609	O 729	S 16	2	2	0

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_4S).

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

• Molecule 3 is N-BENZOYL-D-ALANINE (three-letter code: S2D) (formula: $C_{10}H_{11}NO_3$).
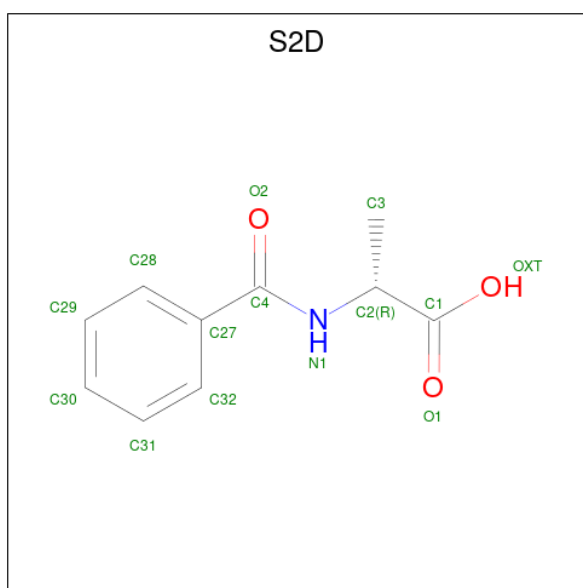
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	C 3	N 1 O 1	0	0
3	B	1	Total 13	C 10	N 1 O 2	0	0

- 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

3 Residue-property plots ⓘ

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: PENICILLIN-BINDING PROTEIN 1B

Chain A:
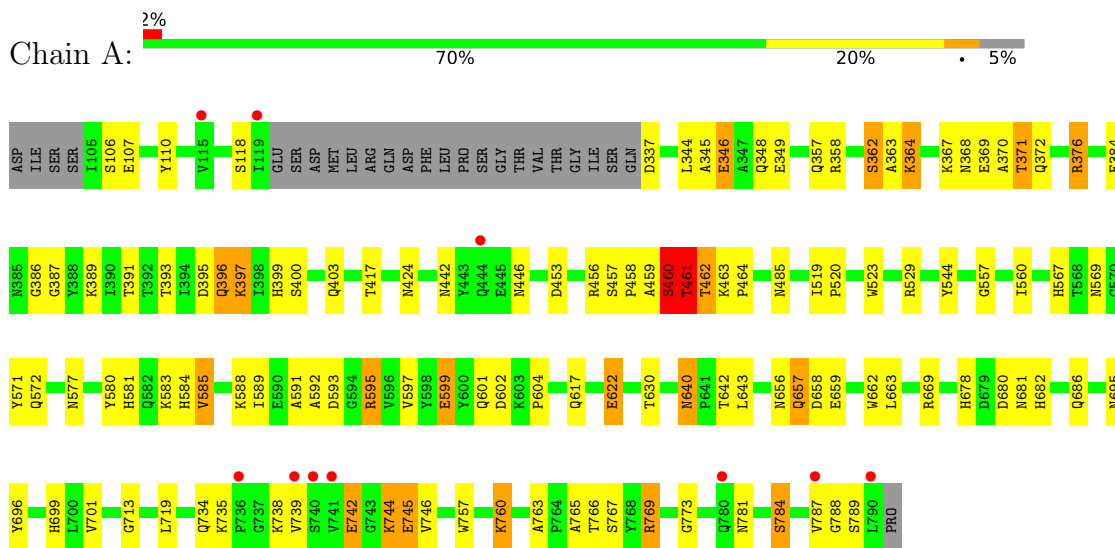
• Molecule 1: PENICILLIN-BINDING PROTEIN 1B

Chain B:
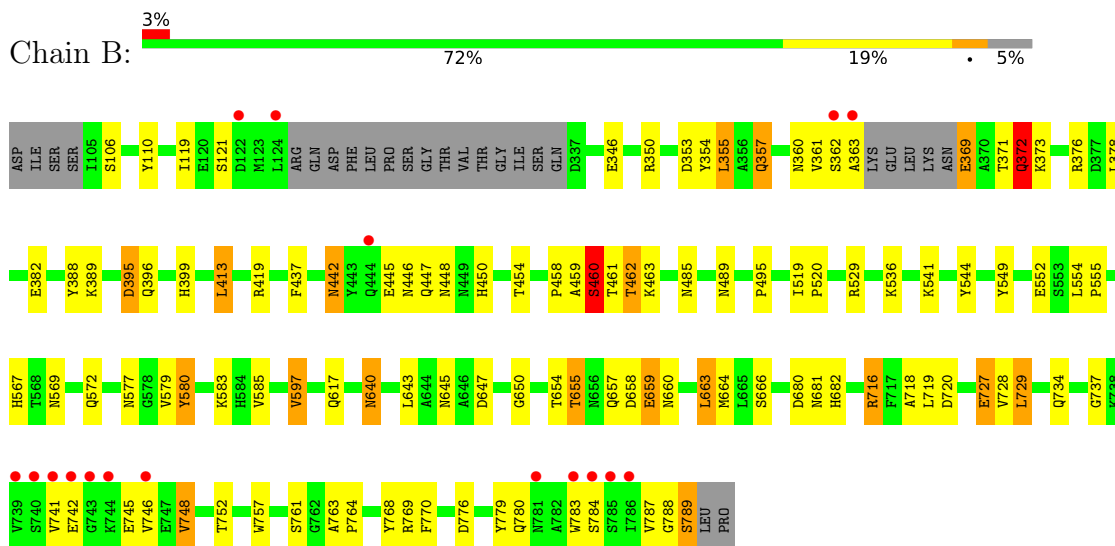
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.80Å 101.10Å 145.00Å 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
$< I/\sigma(I) >$ [1]	7.24 (at 2.51Å)	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 (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.5	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7547	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 ⓘ

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	470/494 (95%)	438 (93%)	25 (5%)	7 (2%)	10	18
1	B	464/494 (94%)	433 (93%)	26 (6%)	5 (1%)	14	26
All	All	934/988 (94%)	871 (93%)	51 (6%)	12 (1%)	12	21

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 ⓘ

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%)	9	17
1	B	384/409 (94%)	353 (92%)	31 (8%)	11	23
All	All	773/818 (94%)	706 (91%)	67 (9%)	10	20

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

Mol	Chain	Res	Type
1	B	716	ARG
1	B	727	GLU
1	B	784	SER
1	A	663	LEU
1	A	640	ASN

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

Mol	Chain	Res	Type
1	B	357	GLN
1	B	485	ASN
1	B	780	GLN
1	B	360	ASN
1	B	424	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 monosaccharides 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	B	1790	-	4,4,4	0.42	0	6,6,6	1.15	0
3	S2D	B	1791	1	12,13,14	2.41	6 (50%)	13,16,18	3.84	3 (23%)
2	SO4	A	1791	-	4,4,4	0.41	0	6,6,6	0.40	0
3	S2D	A	1792	1	3,4,14	1.73	1 (33%)	2,4,18	2.36	1 (50%)

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1791	S2D	C2-N1	5.40	1.52	1.46
3	B	1791	S2D	C4-N1	3.16	1.41	1.34
3	B	1791	S2D	C32-C27	2.49	1.43	1.39
3	B	1791	S2D	C3-C2	2.34	1.58	1.51
3	B	1791	S2D	C27-C4	2.34	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1791	S2D	C3-C2-N1	9.36	120.01	109.61
3	B	1791	S2D	C2-N1-C4	8.86	141.60	122.55
3	B	1791	S2D	O2-C4-C27	-3.88	114.01	120.94
3	A	1792	S2D	C3-C2-N1	3.21	120.02	109.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1791	S2D	O2-C4-N1-C2
3	B	1791	S2D	C27-C4-N1-C2
3	B	1791	S2D	C1-C2-N1-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1791	S2D	1	0
3	A	1792	S2D	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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^2)	Q<0.9
1	A	469/494 (94%)	-0.09	10 (2%)	63	66	15, 30, 59, 74	4 (0%)
1	B	468/494 (94%)	-0.07	17 (3%)	42	46	14, 27, 62, 79	3 (0%)
All	All	937/988 (94%)	-0.08	27 (2%)	51	55	14, 29, 61, 79	7 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	GLY	4.7
1	B	741	VAL	4.5
1	B	363	ALA	3.3
1	B	124	LEU	3.2
1	B	362	SER	3.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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(Å²)	Q<0.9
3	S2D	A	1792	5/14	0.73	0.32	33,39,45,47	0
3	S2D	B	1791	13/14	0.85	0.27	33,43,46,47	6
4	CL	A	1794	1/1	0.97	0.28	46,46,46,46	0
2	SO4	A	1791	5/5	0.99	0.13	26,28,31,31	0
4	CL	A	1793	1/1	1.00	0.16	21,21,21,21	0
2	SO4	B	1790	5/5	1.00	0.10	18,20,20,22	0

6.5   Other polymers ⓘ

There are no such residues in this entry.