



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2018 – 05:23 AM EST

PDB ID : 1K25
Title : PBP2x from a Highly Penicillin-resistant *Streptococcus pneumoniae* Clinical Isolate
Authors : Dessen, A.; Mouz, N.; Hopkins, J.; Dideberg, O.
Deposited on : 2001-09-26
Resolution : 3.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

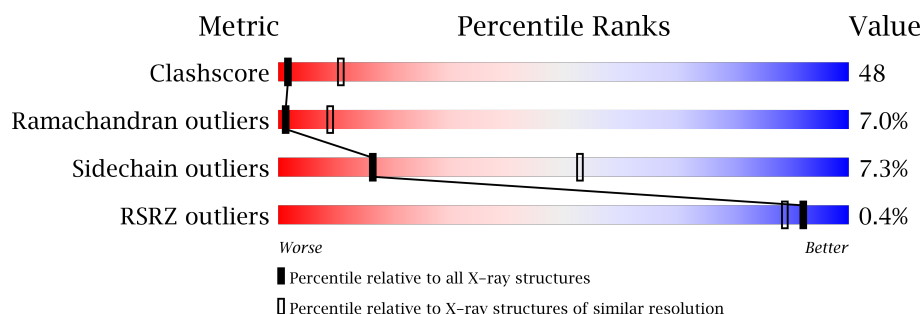
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 ≥ 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	685	
1	B	685	
1	C	685	
1	D	685	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16786 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 low-affinity PENICILLIN-BINDING PROTEIN 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4161	2606	691	849	15			
1	B	575	Total	C	N	O	S	0	0	0
			4311	2710	716	868	17			
1	C	550	Total	C	N	O	S	0	0	0
			4114	2580	685	834	15			
1	D	556	Total	C	N	O	S	0	0	0
			4179	2627	692	844	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LEU	PHE	ENGINEERED	UNP O34006
B	1364	LEU	PHE	ENGINEERED	UNP O34006
C	2364	LEU	PHE	ENGINEERED	UNP O34006
D	3364	LEU	PHE	ENGINEERED	UNP O34006

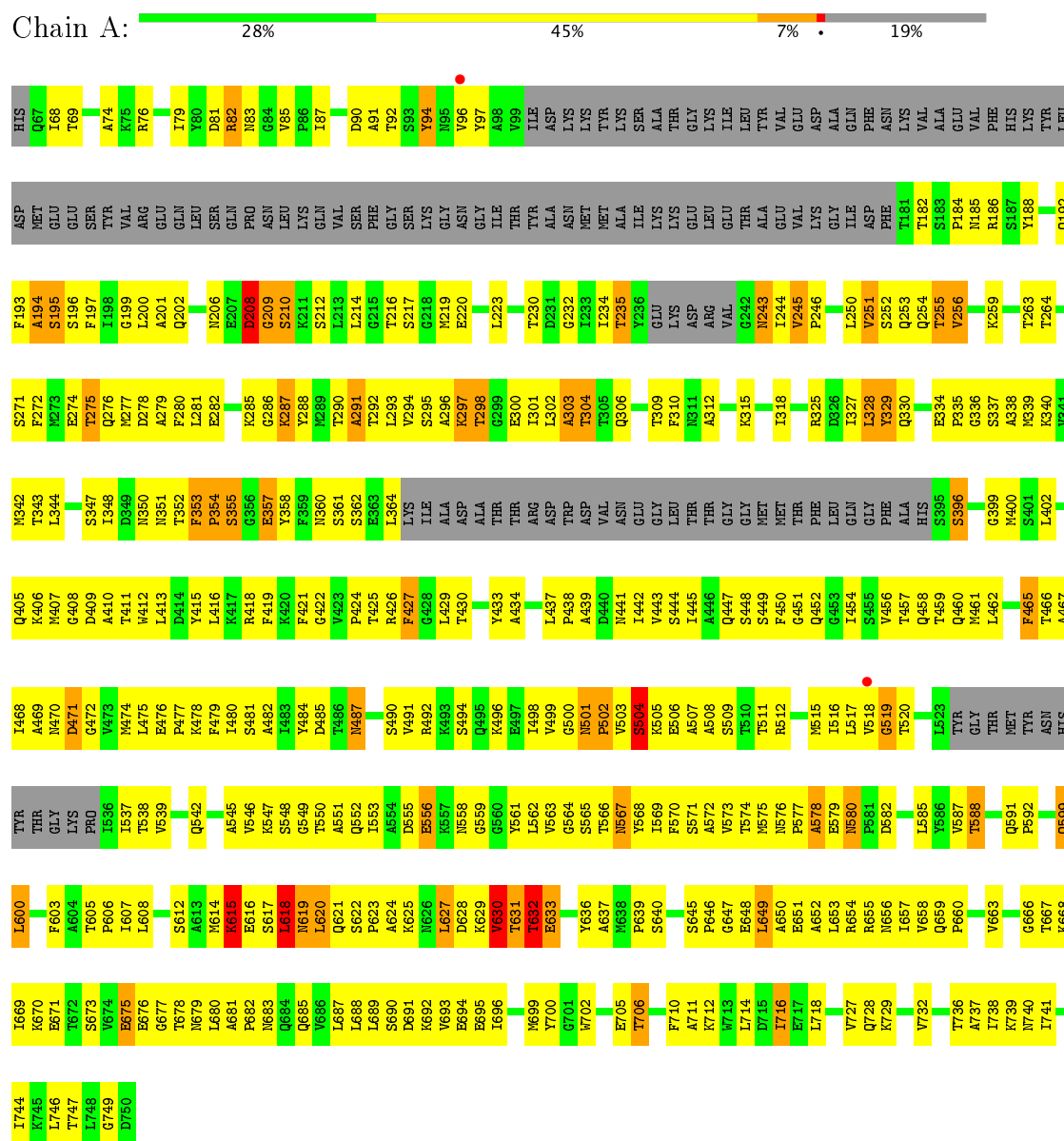
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	10	Total	O	0	0
			10	10		
2	C	2	Total	O	0	0
			2	2		
2	D	1	Total	O	0	0
			1	1		

3 Residue-property plots

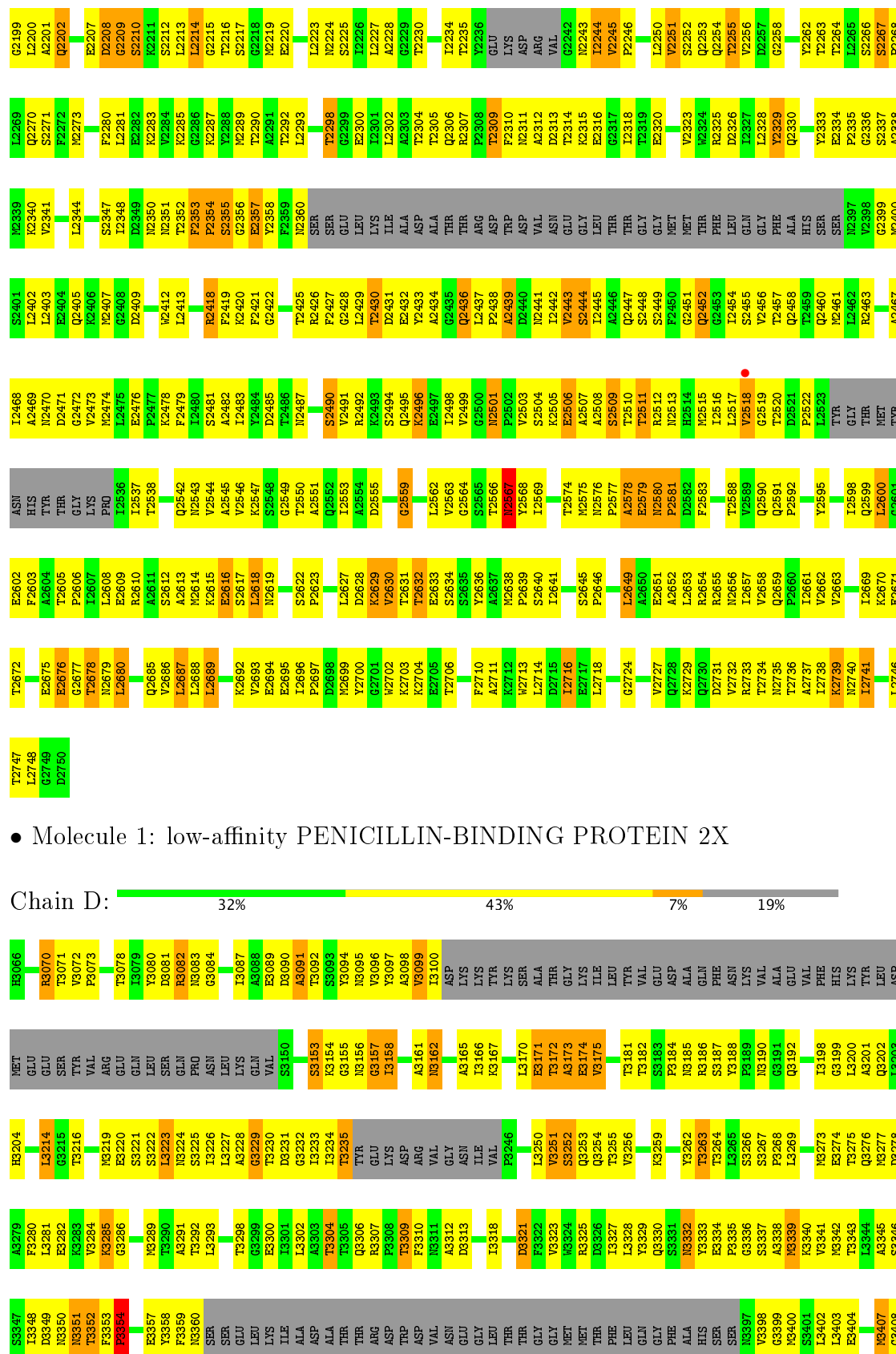
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: low-affinity PENICILLIN-BINDING PROTEIN 2X



- Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X





K3699	M3700	G3701	W3702	K3703	K3704	E3705	T3706	A3707	F3710	A3711	K3712	W3713	L3714	D3715	I3716	E3717	L3718	E3719	F3720	V3727	Q3728	K3729	V3732	R3733	T3734	N3735	T3736	A3737	I3738	K3739	N3740	I3741	K3742	K3743	I3744	R3745	L3746	T3747	L3748	G3749	ASP													
ASN	LEU	GLN	SER	PRO	ALA	LYS	ASN	LEU	ASP	LYS	VAL	THR	T3632	E3633	S3634	A3637	M3638	P3639	S3640	I3641	I3644	S3645	P3646	L3649	L3653	R3654	P3660	V3663	G3666	I3669	T3672	S3673	V3674	E3675	E3676	G3677	L3680	Q3684	V3685	L3686	L3687	L3688	L3689	S3690	V3693	D3698								
D3409	A3410	T3411	W3412	L3413	D3414	Y3415	L3416	K3417	R3418	F3419	K3420	P3424	T3425	R3426	F3427	G3428	I3429	T3430	D3431	E3432	Y3433	A3434	G3435	Q3436	L3437	N3441	I3442	V3443	Q3447	S3448	S3449	F3450	G3451	S3455	V3456	T3457	Q3458	M3461	L3462	R3463	A3464	F3465	T3466	A3467	I3468	A3469	N3470	D3471	G3472	V3473	M3474	L3475	E3476	P3477
K3478	F3479	I3480	S3481	Y3484	M3488	Q3489	S3490	V3491	R3492	Q3495	R3496	E3497	I3498	V3499	G3500	N3501	P3502	V3503	E3506	S3509	T3510	T3511	R3512	N3513	H3514	N3515	I3516	L3517	V3518	G3519	T3520	ASP	PRO	LEU	TYR	GLY	THR	MET	TYR	ASN	HIS	TYR	THR	GLY	LYS	F3535	I3536	I3537	T3538	V3539	P3540	G3541	Q3542	N3543
V3544	A3545	G3549	T3550	A3551	Q3552	I3553	A3554	D3555	E3556	L3562	V3563	G3564	S3565	T3566	N3567	V3568	I3569	F3570	S3571	A3572	V3573	T3574	M3575	N3576	P3577	A3578	I3584	T3588	V3589	Q3590	Q3591	P3592	E3593	E3594	Q3599	L3600	G3601	E3602	F3603	A3604	T3605	P3606	I3607	L3608	E3609	R3610	A3611	S3612	ALA	MET	LYS	GLU	SER	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.56Å 146.56Å 132.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.20 24.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (19.90-3.20) 89.0 (24.94-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.23Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.312 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 4.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.148 for h,-h-k,-l 0.147 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16786	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

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	0.46	0/4229	0.77	4/5747 (0.1%)
1	B	0.44	0/4383	0.74	0/5951
1	C	0.47	0/4182	0.75	1/5684 (0.0%)
1	D	0.45	0/4248	0.75	1/5766 (0.0%)
All	All	0.46	0/17042	0.75	6/23148 (0.0%)

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	C	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	630	VAL	N-CA-C	10.02	138.05	111.00
1	A	630	VAL	CB-CA-C	-9.35	93.64	111.40
1	A	630	VAL	CA-C-N	-5.79	104.46	117.20
1	A	632	THR	N-CA-C	-5.13	97.16	111.00
1	D	3437	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2329	TYR	Sidechain

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	4161	0	4017	420	0
1	B	4311	0	4182	430	0
1	C	4114	0	3962	380	0
1	D	4179	0	4052	362	0
2	A	8	0	0	1	0
2	B	10	0	0	5	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	16786	0	16213	1581	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 48.

The worst 5 of 1581 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:629:LYS:O	1:A:630:VAL:HG13	1.43	1.18
1:A:618:LEU:H	1:A:618:LEU:HD23	1.04	1.11
1:D:3672:THR:HG22	1:D:3674:VAL:H	1.07	1.09
1:D:3590:GLN:HG2	1:D:3591:GLN:HG3	1.35	1.08
1:C:2714:LEU:HD13	1:C:2738:ILE:HD11	1.34	1.04

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	546/685 (80%)	401 (73%)	105 (19%)	40 (7%)	1	8
1	B	565/685 (82%)	431 (76%)	99 (18%)	35 (6%)	2	13
1	C	540/685 (79%)	390 (72%)	106 (20%)	44 (8%)	1	6
1	D	544/685 (79%)	430 (79%)	80 (15%)	34 (6%)	1	12
All	All	2195/2740 (80%)	1652 (75%)	390 (18%)	153 (7%)	1	9

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	194	ALA
1	A	209	GLY
1	A	251	VAL
1	A	252	SER

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	449/583 (77%)	413 (92%)	36 (8%)	14	49
1	B	461/583 (79%)	429 (93%)	32 (7%)	18	55
1	C	439/583 (75%)	403 (92%)	36 (8%)	13	47
1	D	448/583 (77%)	421 (94%)	27 (6%)	22	61
All	All	1797/2332 (77%)	1666 (93%)	131 (7%)	16	53

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1501	ASN
1	C	2214	LEU
1	D	3488	ASN
1	B	1556	GLU
1	B	1620	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1728	GLN
1	C	2470	ASN
1	D	3543	ASN
1	C	2202	GLN
1	C	2501	ASN

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](#)

There are no ligands in this entry.

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, 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	556/685 (81%)	-0.26	2 (0%) 92 89	3, 26, 59, 100	0
1	B	575/685 (83%)	-0.23	4 (0%) 87 80	7, 29, 62, 81	0
1	C	550/685 (80%)	-0.26	2 (0%) 92 89	4, 27, 58, 99	0
1	D	556/685 (81%)	-0.25	1 (0%) 94 93	7, 30, 56, 88	0
All	All	2237/2740 (81%)	-0.25	9 (0%) 92 89	3, 28, 59, 100	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3520	THR	3.6
1	B	1520	THR	3.4
1	A	518	VAL	3.0
1	B	1179	ASP	2.7
1	C	2518	VAL	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.