



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:26 AM UTC

PDB ID : 1K25 / pdb_00001k25
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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

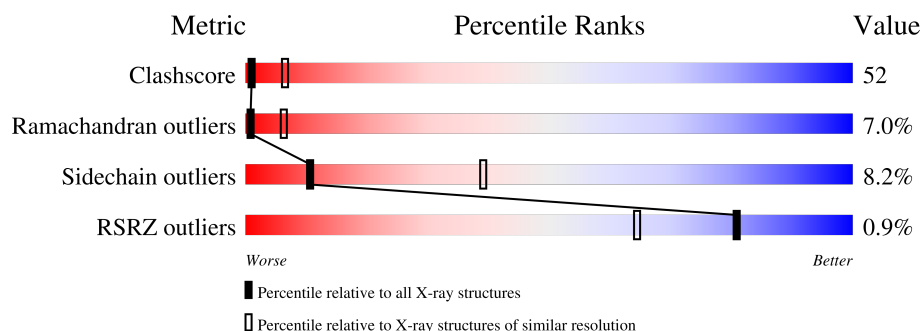
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	% 25% 45% 10% • 19%
1	B	685	% 25% 50% 9% 16%
1	C	685	28% 41% 11% • 20%
1	D	685	% 27% 42% 11% • 19%

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 mutation	UNP O34006
B	1364	LEU	PHE	engineered mutation	UNP O34006
C	2364	LEU	PHE	engineered mutation	UNP O34006
D	3364	LEU	PHE	engineered mutation	UNP O34006

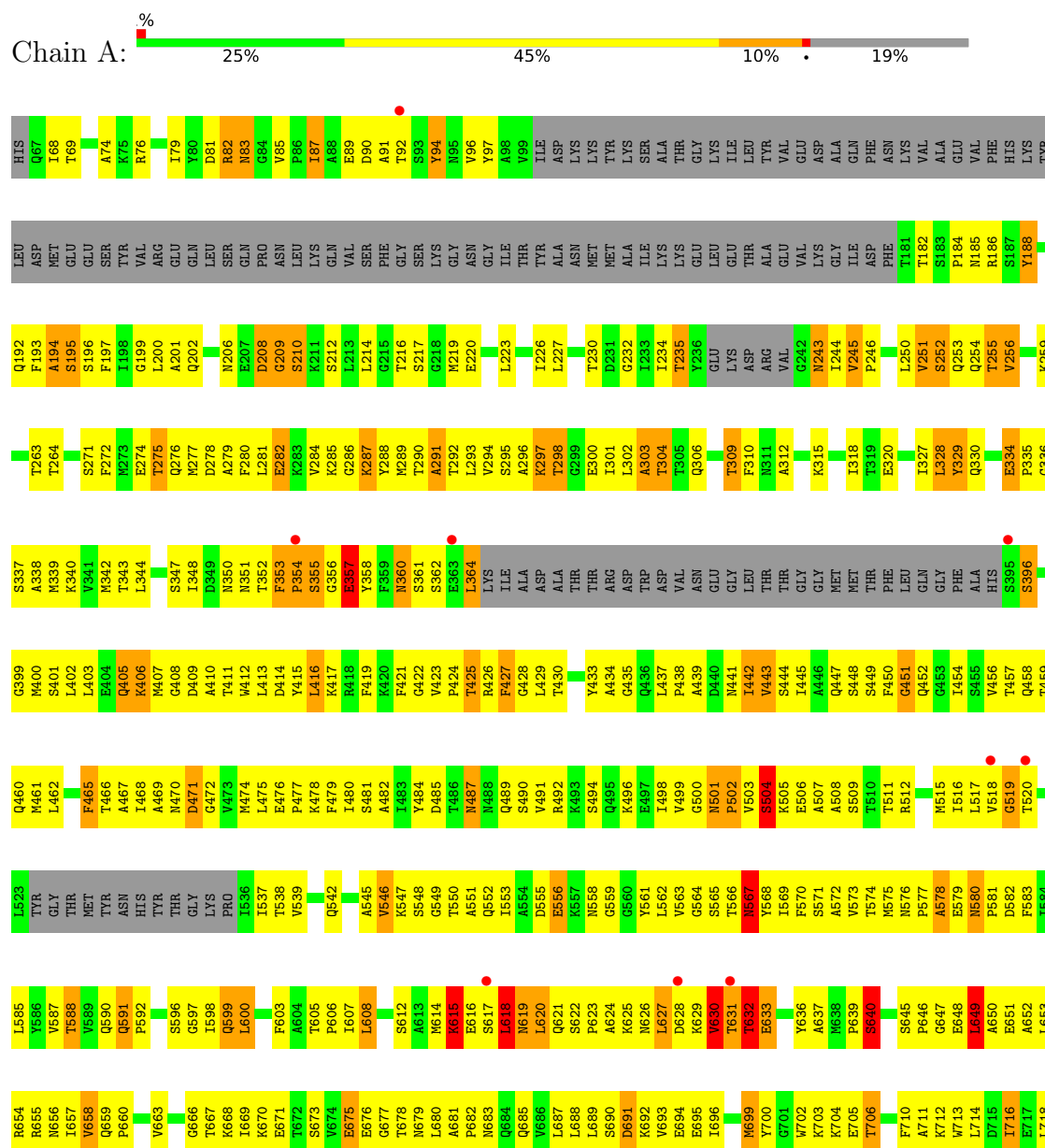
- Molecule 2 is water.

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

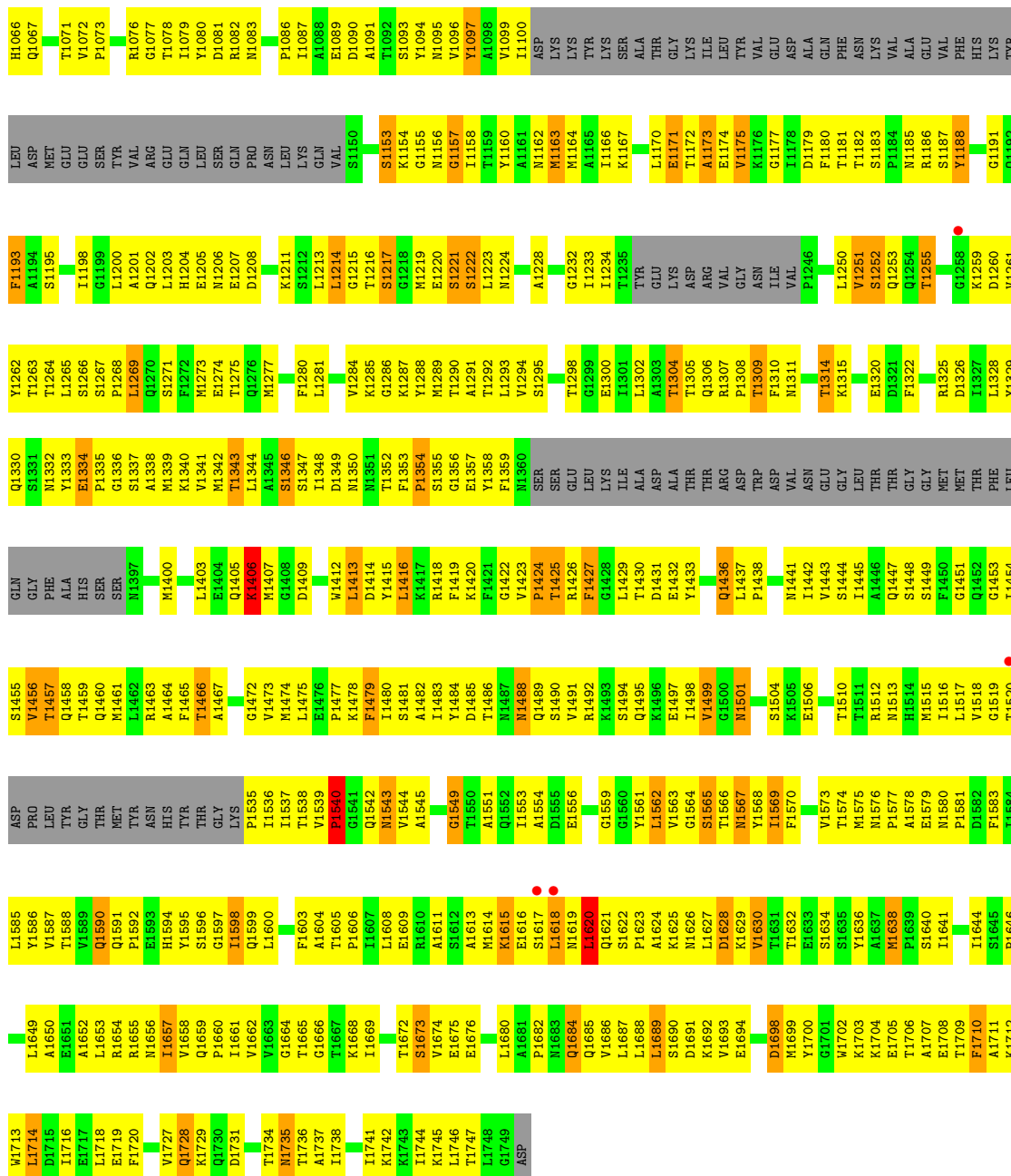
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





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



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





N3740	T3665	S3596	HIS	F3465	M3400	K3340	E3274	L3200
K3742	G3666	G3597	TYR	T3466	S3401	V3341	T3275	A3201
K3743	I3669	I3598	THR	A3467	L3402	M3342	Q3276	Q3202
I3744	L3600	Q3599	GLY	I3468	L3403	T3343	M3277	L3203
K3745	L3601	L3600	LYS	A3469	E3404	E3344	K3278	K3204
L3746	T3672	E3602	P3535	N3470	Q3405	A3345	A3279	E3205
T3747	S3673	F3603	I3536	D3471	K3406	S3346	F3280	
E3675	F3674	A3604	I3537	Q3472	M3407	S3347	L3281	L3214
E3676	E3675	T3605	T3538	F3473	G3408	S3348	E3282	G3215
G3749	E3677	P3606	P3540	L3475	D3409	K3349	K3283	T3216
ASP	G3677	I3607	G3541	E3476	A3410	N3350	V3284	
	L3680	L3608	Q3542	P3477	T3411	N3351	K3285	K3219
	Q3684	R3610	Q3543	K3478	M3412	T3352	F3220	E3220
Q3685	A3611	A3544	N3543	F3479	L3413	F3353	S3221	S3221
L3686	S3612	A3545	V3544	S3481	D3414	P3354	S3222	S3222
L3687	ALA	Q3549	G3549	Y3484	Y3415	S3355	N3290	L3223
L3688	MET	T3550	T3550		L3416	G3356	A3291	N3224
L3689	LYS	A3551	A3551		K3417	E3357	T3292	S3225
S3690	GLU	Q3552	K3557		R3418	V3358	L3293	I3226
V3693	LYS	GLN			F3419	F3359	L3227	L3227
	GLU	PRU			K3420	N3360	A3228	A3228
	LEU	LEU			F3421	SER	K3297	G3229
	ASN	ASN			G3422	GLU	T3298	T3230
	LEU	GLN			V3423	THR	G3299	D3231
	GLN				P3424	LEU	E3300	G3232
					T3425	LYS	I3301	T3233
					R3426	ILE	L3302	I3234
					F3427	ALA	T3235	T3235
					G3428	ASP	A3303	T3235
					L3429	ALA	T3305	GLU
					T3430	THR	Q3306	LYS
					D3431	THR	R3307	ASP
					E3432	ARG	P3308	ARG
					Y3433	ASP	T3309	VAL
					A3434	TRP	F3310	GLY
					G3435	ASP	N3311	ASN
					Q3436	VAL	A3312	ILE
						ASN	D3313	VAL
					M3441	GLU		F3246
					I3442	GLY	I3318	
					V3443	LEU		L3250
					S3444	THR	D3321	V3251
					I3445	THR	F3322	S3252
					N3513	GLY	V3323	Q3253
					H3514	GLY	M3324	Q3254
					M3515	MET	R3325	T3255
					I3516	MET	D3326	V3256
					L3517	THR	I3327	
					V3518	PHE	L3328	K3259
					G3519	LEU	Y3329	
					T3520	GLN	Q3330	
					ASP	GLY	S3331	Y3262
					PRO	PHE	N3332	T3263
					LEU	ALA	T3264	T3264
					TYR	HIS	Y3333	L3265
					GLY	SER	E3334	S3266
					THR	THR	P3335	S3267
					MET	SER	G3336	P3268
					TYR	TYR	S3337	L3269
					ASN	N3397	A3338	
						V3398		M3273
						G3399		

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 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (19.90-3.20) 88.6 (19.90-3.20)	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 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.1	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	0.85	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.61	0/4229	1.18	46/5747 (0.8%)
1	B	0.57	0/4383	1.12	29/5951 (0.5%)
1	C	0.61	0/4182	1.15	42/5684 (0.7%)
1	D	0.59	1/4248 (0.0%)	1.16	43/5766 (0.7%)
All	All	0.60	1/17042 (0.0%)	1.15	160/23148 (0.7%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3219	MET	SD-CE	-5.74	1.65	1.79

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	630	VAL	N-CA-C	13.80	138.05	109.34
1	A	630	VAL	CB-CA-C	-10.76	93.64	111.29
1	D	3434	ALA	N-CA-C	10.64	122.57	110.97
1	B	1580	ASN	CA-C-N	10.47	132.93	119.84
1	B	1580	ASN	C-N-CA	10.47	132.93	119.84

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	452	0
1	B	4311	0	4182	469	0
1	C	4114	0	3962	409	0
1	D	4179	0	4052	396	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	1715	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 52.

The worst 5 of 1715 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:HD23	1:A:618:LEU:H	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	6
1	B	565/685 (82%)	431 (76%)	99 (18%)	35 (6%)	1	9
1	C	540/685 (79%)	390 (72%)	106 (20%)	44 (8%)	1	4
1	D	544/685 (79%)	430 (79%)	80 (15%)	34 (6%)	1	8
All	All	2195/2740 (80%)	1652 (75%)	390 (18%)	153 (7%)	1	6

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 [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	449/583 (77%)	409 (91%)	40 (9%)	9	34
1	B	461/583 (79%)	427 (93%)	34 (7%)	13	43
1	C	439/583 (75%)	401 (91%)	38 (9%)	9	36
1	D	448/583 (77%)	412 (92%)	36 (8%)	11	40
All	All	1797/2332 (77%)	1649 (92%)	148 (8%)	10	39

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3162	ASN
1	D	3649	LEU
1	D	3205	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3427	PHE
1	B	1269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2350	ASN
1	C	2599	GLN
1	D	3567	ASN
1	C	2470	ASN
1	C	2542	GLN

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 oligosaccharides 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%)	0.01	9 (1%) 70 51	3, 26, 59, 100	0
1	B	575/685 (83%)	0.01	4 (0%) 84 69	7, 29, 62, 81	0
1	C	550/685 (80%)	-0.03	3 (0%) 87 76	4, 27, 58, 99	0
1	D	556/685 (81%)	-0.02	4 (0%) 84 69	7, 30, 56, 88	0
All	All	2237/2740 (81%)	-0.01	20 (0%) 81 64	3, 28, 59, 100	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1617	SER	3.6
1	A	520	THR	3.4
1	D	3520	THR	3.1
1	A	518	VAL	3.0
1	D	3675	GLU	3.0

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 oligosaccharides 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.