



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:31 AM GMT

PDB ID : 2XD1
Title : ACTIVE SITE RESTRUCTURING REGULATES LIGAND RECOGNITION IN CLASS A PENICILLIN-BINDING PROTEINS
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Deposited on : 2010-04-28
Resolution : 3.00 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
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

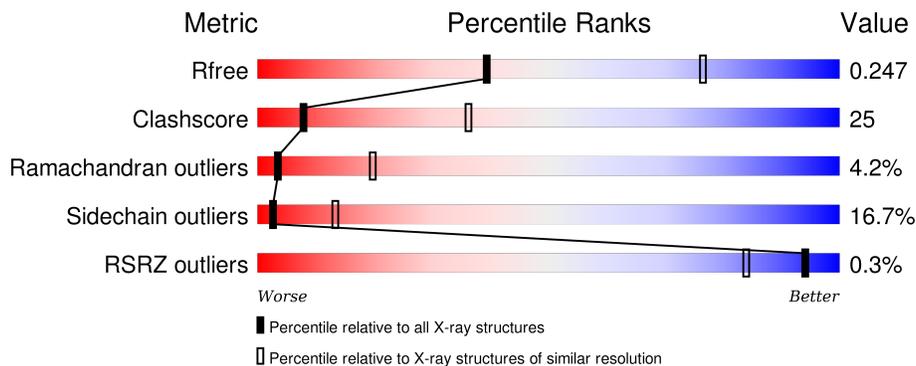
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	494	 46% 37% 11% • 5%
1	B	494	 45% 34% 11% • 8%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7278 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.

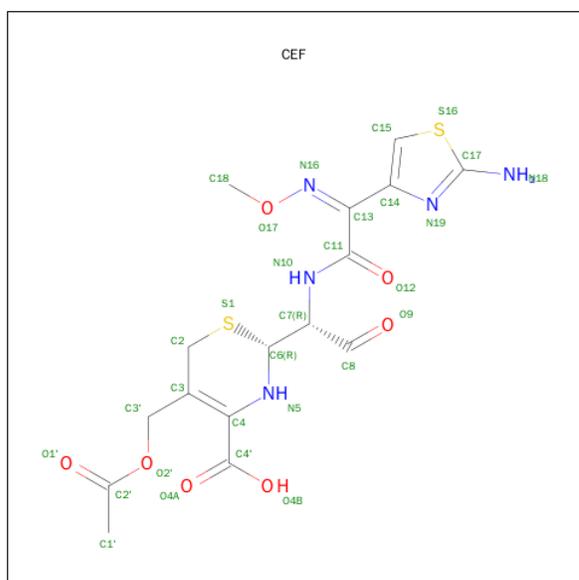
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	469	Total 3617	C 2263	N 613	O 726	S 15	0	0	0
1	B	455	Total 3508	C 2195	N 594	O 704	S 15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

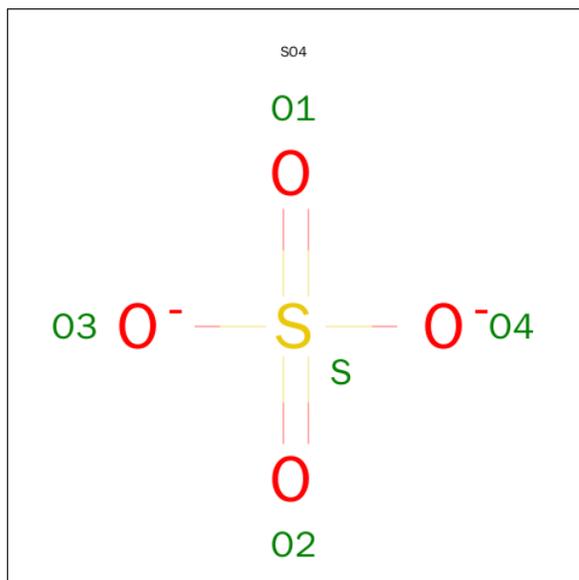
Chain	Residue	Modelled	Actual	Comment	Reference
A	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
A	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4

- Molecule 2 is CEFOTAXIME GROUP (three-letter code: CEF) (formula: $C_{16}H_{19}N_5O_7S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		
2	B	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	47	Total	O	0	0
			47	47		

Y779	Q780	N781	A782	W783	S784	S785	I786	V787	G788	S789	LEU	PRO																																									
V701	H702	A703	I704	Q705	Q706	S710	I711	R716	F717	A718	L719	E727	V728	L729	G733	Q734	K735	P736	G737	K738	V739	S740	V741	E742	G743	K744	E745	V746	E747	V748	T749	G750	S751	I752	S755	Y756	W757	A758	I759	K760	S761	G762	A763	P764	A765	T766	S767	V768	R769	F770	A771	I772	D778
S626	R627	K636	T629	T630	K633	G643	L636	N640	P641	T642	L643	A644	N645	A646	D647	K648	I649	G650	K651	T652	G653	T654	T655	M656	Q657	D658	E659	M660	M661	I664	L665	S666	T667	P668	G673	I676	D679	D680	M681	H682	S683	L684	S685	A688	M692	Y696	M697	A698	H699	L700			
R526	K536	E540	K541	H542	G543	Y544	E545	I546	E552	S553	L554	P555	I560	H567	T568	M569	Q572	Y580	K583	H584	V585	I586	I589	E590	D593	G594	M597	Y598	K603	Q606	V607	A611	T612	A613	M614	I615	M616	Q617	G618	L619	L620	R621	E622	S625									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.60Å 102.30Å 146.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 3.00 45.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.22-3.00) 99.7 (45.20-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.161 , 0.248 0.163 , 0.247	Depositor DCC
R_{free} test set	2955 reflections (11.06%)	DCC
Wilson B-factor (Å ²)	46.5	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Outliers	0 of 29671 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7278	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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, 0.375 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: CEF, SO4

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	1.62	38/3690 (1.0%)	1.48	36/5009 (0.7%)
1	B	1.64	45/3579 (1.3%)	1.44	34/4858 (0.7%)
All	All	1.63	83/7269 (1.1%)	1.46	70/9867 (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	A	0	2
1	B	0	4
All	All	0	6

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	LYS	C-N	16.50	1.62	1.33
1	A	459	ALA	C-N	15.84	1.70	1.34
1	A	727	GLU	CG-CD	10.67	1.68	1.51
1	A	460	SER	C-N	9.04	1.54	1.34
1	A	346	GLU	CG-CD	8.79	1.65	1.51

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	SER	O-C-N	-13.25	101.50	122.70
1	A	428	ASP	CB-CG-OD1	9.71	127.04	118.30
1	B	395	ASP	CB-CG-OD2	9.40	126.76	118.30
1	A	395	ASP	CB-CG-OD2	-9.39	109.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ALA	O-C-N	-9.39	107.68	122.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ASP	Peptide
1	A	460	SER	Mainchain
1	B	371	THR	Peptide
1	B	375	TYR	Peptide
1	B	459	ALA	Mainchain

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	3617	0	3484	161	1
1	B	3508	0	3363	189	0
2	A	26	0	12	2	0
2	B	26	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	44	0	0	3	0
4	B	47	0	0	6	0
All	All	7278	0	6871	350	1

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 25.

The worst 5 of 350 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:116:ILE:CD1	1:B:116:ILE:CG1	1.82	1.53
1:A:459:ALA:C	1:A:460:SER:N	1.70	1.41
1:B:376:ARG:NH1	1:B:380:ALA:HB2	1.47	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:O	1:B:376:ARG:HB3	1.49	1.10
1:B:706:GLN:NE2	1:B:706:GLN:HA	1.69	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASP:CB	1:A:411:TYR:CD2[3_645]	2.05	0.15

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	465/494 (94%)	399 (86%)	44 (10%)	22 (5%)	3	17
1	B	447/494 (90%)	388 (87%)	43 (10%)	16 (4%)	4	24
All	All	912/988 (92%)	787 (86%)	87 (10%)	38 (4%)	3	20

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	ASP
1	A	360	ASN
1	A	361	VAL
1	A	363	ALA
1	A	386	GLY

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	386/409 (94%)	322 (83%)	64 (17%)	3	13
1	B	373/409 (91%)	310 (83%)	63 (17%)	2	13
All	All	759/818 (93%)	632 (83%)	127 (17%)	3	13

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	745	GLU
1	B	357	GLN
1	B	745	GLU
1	A	754	THR
1	B	108	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	699	HIS
1	B	372	GLN
1	B	682	HIS
1	A	734	GLN
1	B	399	HIS

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

4 ligands are modelled in this entry.

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	CEF	A	1460	1	18,27,31	3.03	7 (38%)	16,37,42	6.29	8 (50%)
3	SO4	A	1790	-	4,4,4	1.55	2 (50%)	6,6,6	0.95	0
2	CEF	B	1460	1	18,27,31	3.46	8 (44%)	16,37,42	6.93	7 (43%)
3	SO4	B	1790	-	4,4,4	0.87	0	6,6,6	1.18	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	CEF	A	1460	1	-	0/10/38/43	0/1/2/2
3	SO4	A	1790	-	-	0/0/0/0	0/0/0/0
2	CEF	B	1460	1	-	0/10/38/43	0/1/2/2
3	SO4	B	1790	-	-	0/0/0/0	0/0/0/0

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1460	CEF	C2-S1	-3.47	1.74	1.82
2	B	1460	CEF	O12-C11	-3.33	1.17	1.23
2	B	1460	CEF	C2-S1	-2.99	1.75	1.82
2	A	1460	CEF	C13-C11	-2.69	1.45	1.50
2	A	1460	CEF	C4'-C4	-2.54	1.47	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1460	CEF	O12-C11-C13	-12.02	107.12	120.53
2	A	1460	CEF	C3-C2-S1	-7.25	108.25	117.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1460	CEF	O12-C11-C13	-6.30	113.50	120.53
2	B	1460	CEF	C3-C2-S1	-5.24	110.73	117.17
2	B	1460	CEF	C14-C15-S16	-3.78	107.14	111.79

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
2	A	1460	CEF	2	0
2	B	1460	CEF	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, 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%)	-0.59	2 (0%) 93 80	16, 35, 63, 85	0
1	B	455/494 (92%)	-0.56	1 (0%) 95 87	15, 31, 68, 87	0
All	All	924/988 (93%)	-0.58	3 (0%) 94 84	15, 33, 65, 87	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	2.4
1	B	743	GLY	2.1
1	A	780	GLN	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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CEF	B	1460	26/30	0.97	0.18	1.60	31,39,44,54	0
2	CEF	A	1460	26/30	0.97	0.15	0.92	28,43,50,56	0
3	SO4	A	1790	5/5	0.97	0.13	-0.06	25,26,36,37	0
3	SO4	B	1790	5/5	0.98	0.12	-0.62	37,43,48,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.