



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6B2Y / pdb_00006b2y
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Deposited on : 2017-09-20
Resolution : 1.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

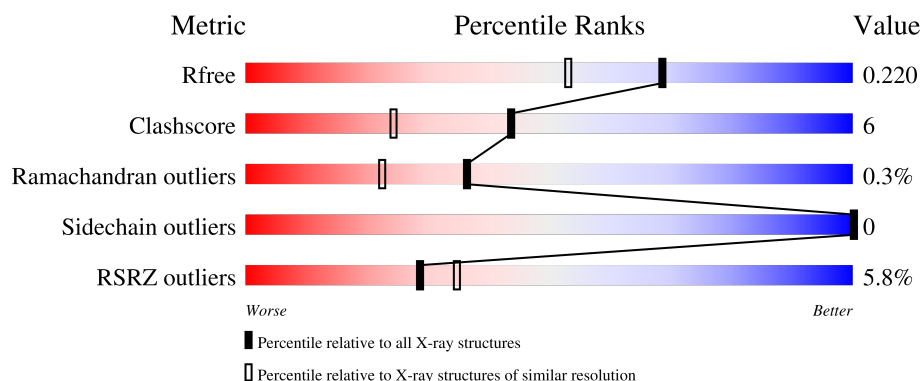
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	401	6% 74% 9% 16%
1	B	401	4% 77% 6% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5791 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 Solute-binding periplasmic protein of iron/siderophore ABC transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2606	1666	437	497	6			
1	B	331	Total	C	N	O	S	0	0	0
			2563	1645	430	482	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	LEU	-	expression tag	UNP Q8D027
A	353	GLU	-	expression tag	UNP Q8D027
A	354	HIS	-	expression tag	UNP Q8D027
A	355	HIS	-	expression tag	UNP Q8D027
A	356	HIS	-	expression tag	UNP Q8D027
A	357	HIS	-	expression tag	UNP Q8D027
A	358	HIS	-	expression tag	UNP Q8D027
A	359	HIS	-	expression tag	UNP Q8D027
A	360	HIS	-	expression tag	UNP Q8D027
A	361	HIS	-	expression tag	UNP Q8D027
A	362	HIS	-	expression tag	UNP Q8D027
A	363	HIS	-	expression tag	UNP Q8D027
B	352	LEU	-	expression tag	UNP Q8D027
B	353	GLU	-	expression tag	UNP Q8D027
B	354	HIS	-	expression tag	UNP Q8D027
B	355	HIS	-	expression tag	UNP Q8D027
B	356	HIS	-	expression tag	UNP Q8D027
B	357	HIS	-	expression tag	UNP Q8D027
B	358	HIS	-	expression tag	UNP Q8D027
B	359	HIS	-	expression tag	UNP Q8D027
B	360	HIS	-	expression tag	UNP Q8D027
B	361	HIS	-	expression tag	UNP Q8D027
B	362	HIS	-	expression tag	UNP Q8D027
B	363	HIS	-	expression tag	UNP Q8D027

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Na 2	0	0
2	B	1	Total 1	Na 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	320	Total 320	O 320	0	0
3	B	299	Total 299	O 299	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.37Å 97.01Å 74.28Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	45.57 – 1.77 45.57 – 1.77	Depositor EDS
% Data completeness (in resolution range)	90.9 (45.57-1.77) 90.9 (45.57-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.186 , 0.219 0.187 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5791	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.31	0/2661	0.53	0/3612
1	B	0.30	0/2618	0.50	0/3552
All	All	0.30	0/5279	0.52	0/7164

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2606	0	2610	47	0
1	B	2563	0	2582	16	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	320	0	0	21	1
3	B	299	0	0	6	1
All	All	5791	0	5192	63	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 6.

All (63) 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:110:LEU:O	3:A:501:HOH:O	1.83	0.97
1:B:19:ARG:NH1	3:B:501:HOH:O	1.73	0.95
1:A:190:GLU:HA	3:A:507:HOH:O	1.66	0.94
1:B:74:ILE:O	3:B:502:HOH:O	1.98	0.82
1:A:114:LEU:N	3:A:501:HOH:O	2.18	0.76
1:A:38:LYS:NZ	1:A:41:ASP:OD1	2.20	0.74
1:A:169:THR:O	3:A:502:HOH:O	2.07	0.73
1:A:192:CYS:SG	1:A:193:CYS:N	2.64	0.70
1:A:114:LEU:HG	3:A:501:HOH:O	1.93	0.69
1:A:249:ASP:N	3:A:505:HOH:O	2.22	0.66
1:A:76:ASN:H	1:A:82:ILE:HG21	1.61	0.66
1:A:85:GLU:OE2	1:A:85:GLU:N	2.29	0.65
1:A:73:LEU:HB3	1:A:82:ILE:HD13	1.79	0.65
1:A:191:GLU:N	3:A:510:HOH:O	2.31	0.63
1:B:246:PRO:HG3	1:B:259:VAL:HG22	1.81	0.63
1:B:2:THR:HG22	1:B:12:THR:HG22	1.80	0.61
1:B:128:ASN:O	3:B:503:HOH:O	2.15	0.61
1:A:326:MET:HE1	1:A:342:TYR:CD1	2.36	0.61
1:A:193:CYS:HB2	1:A:225:VAL:O	2.03	0.59
1:A:175:ASP:OD2	3:A:503:HOH:O	2.16	0.58
1:A:246:PRO:O	3:A:504:HOH:O	2.17	0.58
1:A:80:ASP:C	1:A:82:ILE:H	2.12	0.57
1:A:84:PRO:C	1:A:85:GLU:OE2	2.48	0.55
1:B:62:LYS:NZ	3:B:509:HOH:O	2.38	0.55
1:A:88:LEU:HD12	1:A:90:LEU:HD23	1.89	0.55
1:A:113:GLN:HB3	3:A:501:HOH:O	2.07	0.55
1:A:83:SER:OG	1:A:84:PRO:HD3	2.06	0.55
1:A:88:LEU:HD23	1:A:113:GLN:NE2	2.21	0.54
1:A:83:SER:O	1:A:85:GLU:OE2	2.26	0.54
1:A:310:LYS:HB3	3:A:661:HOH:O	2.08	0.53
1:A:84:PRO:HB3	1:A:88:LEU:HD13	1.91	0.52
1:B:135:LEU:HD21	1:B:158:TYR:CD2	2.45	0.52
1:A:244:LYS:NZ	3:A:518:HOH:O	2.42	0.51
1:A:73:LEU:O	1:A:84:PRO:HD2	2.10	0.51
1:A:76:ASN:N	1:A:82:ILE:HG21	2.24	0.51
1:A:227:LEU:HD21	1:A:276:GLY:HA3	1.93	0.51
1:A:332:GLN:NE2	3:A:511:HOH:O	2.31	0.51
1:A:88:LEU:HA	1:A:90:LEU:CD2	2.41	0.50
1:A:108:SER:N	3:A:522:HOH:O	2.44	0.50
1:A:226:ASN:ND2	3:A:513:HOH:O	2.35	0.50
1:B:19:ARG:NE	1:B:91:ASN:O	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLY:N	1:B:49:ASP:OD2	2.46	0.48
1:A:80:ASP:O	1:A:82:ILE:N	2.42	0.47
1:B:200:ASN:HA	3:B:520:HOH:O	2.14	0.47
1:B:290:ALA:HB3	1:B:344:ILE:HG22	1.97	0.46
1:A:110:LEU:HD12	3:A:501:HOH:O	2.16	0.45
1:B:244:LYS:NZ	1:B:251:PRO:O	2.49	0.45
1:A:76:ASN:H	1:A:82:ILE:HD12	1.82	0.45
1:A:81:SER:O	1:A:83:SER:N	2.50	0.44
1:B:184:LEU:HD11	1:B:196:ALA:HB2	2.00	0.44
1:B:226:ASN:OD1	1:B:226:ASN:N	2.51	0.43
1:A:190:GLU:N	3:A:510:HOH:O	2.51	0.43
1:A:84:PRO:HA	1:A:87:VAL:HB	2.00	0.43
1:A:1:ALA:HB1	3:A:534:HOH:O	2.19	0.43
1:A:52:LYS:CE	3:A:538:HOH:O	2.67	0.42
1:A:73:LEU:O	1:A:82:ILE:HA	2.18	0.42
1:A:185:ARG:NH2	3:A:529:HOH:O	2.48	0.42
1:A:47:GLN:HA	1:A:74:ILE:O	2.20	0.41
1:A:249:ASP:HB2	3:A:505:HOH:O	2.21	0.41
1:A:80:ASP:C	1:A:82:ILE:N	2.74	0.41
1:B:21:LEU:HD12	1:B:22:LEU:N	2.36	0.41
1:A:183:GLU:HG3	1:A:193:CYS:HA	2.02	0.40
1:B:203:ASP:OD1	3:B:504:HOH:O	2.22	0.40

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)
3:A:655:HOH:O	3:B:675:HOH:O[2_656]	2.17	0.03

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	332/401 (83%)	318 (96%)	12 (4%)	2 (1%)	21	9
1	B	325/401 (81%)	320 (98%)	5 (2%)	0	100	100
All	All	657/802 (82%)	638 (97%)	17 (3%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	82	ILE

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	281/327 (86%)	281 (100%)	0	100	100
1	B	275/327 (84%)	275 (100%)	0	100	100
All	All	556/654 (85%)	556 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	338/401 (84%)	0.34	24 (7%) 22 26	16, 28, 54, 76	0
1	B	331/401 (82%)	0.20	15 (4%) 38 44	15, 27, 51, 71	0
All	All	669/802 (83%)	0.27	39 (5%) 29 35	15, 28, 53, 76	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	VAL	4.6
1	A	88	LEU	4.2
1	A	83	SER	4.0
1	B	84	PRO	3.4
1	A	296	TYR	3.3
1	A	84	PRO	3.3
1	A	81	SER	3.1
1	B	83	SER	3.1
1	A	89	THR	2.9
1	B	224	THR	2.9
1	B	114	LEU	2.8
1	B	249	ASP	2.7
1	B	199	GLY	2.6
1	B	88	LEU	2.6
1	A	1	ALA	2.6
1	A	86	LYS	2.5
1	A	192	CYS	2.5
1	A	76	ASN	2.5
1	B	117	ALA	2.5
1	A	193	CYS	2.5
1	A	247	GLY	2.4
1	B	217	LEU	2.4
1	B	74	ILE	2.3
1	B	225	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASN	2.3
1	A	108	SER	2.3
1	A	300	TYR	2.3
1	B	192	CYS	2.2
1	A	78	THR	2.2
1	A	117	ALA	2.2
1	A	112	LYS	2.2
1	A	90	LEU	2.2
1	A	82	ILE	2.2
1	A	73	LEU	2.1
1	B	82	ILE	2.1
1	B	87	VAL	2.1
1	A	80	ASP	2.1
1	A	250	ALA	2.0
1	B	111	VAL	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 oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
2	NA	A	402	1/1	0.96	0.11	35,35,35,35	1
2	NA	A	401	1/1	0.97	0.12	33,33,33,33	0
2	NA	B	401	1/1	0.97	0.14	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.