



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2WFF
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Deposited on : 2009-04-05
Resolution : 4.00 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

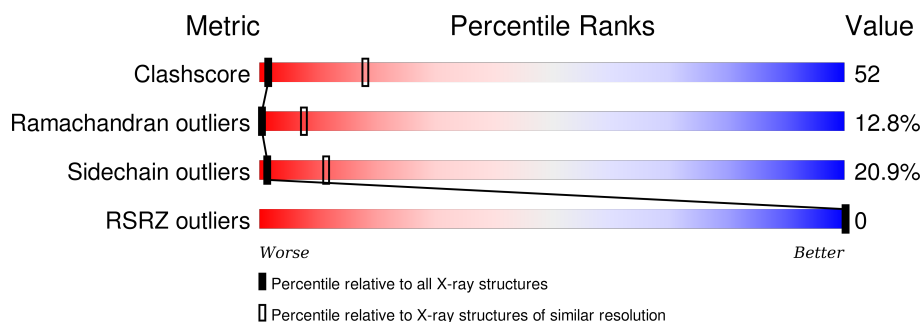
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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))
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	1	246	
2	2	230	
3	3	226	
4	4	80	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5506 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 P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	246	Total	C	N	O	S	0	0	0
			1929	1240	329	352	8			

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	219	Total	C	N	O	S	0	0	0
			1692	1081	290	314	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	21	VAL	ALA	CONFLICT	UNP B9VV85
2	85	SER	GLY	CONFLICT	UNP B9VV85

- Molecule 3 is a protein called P1.

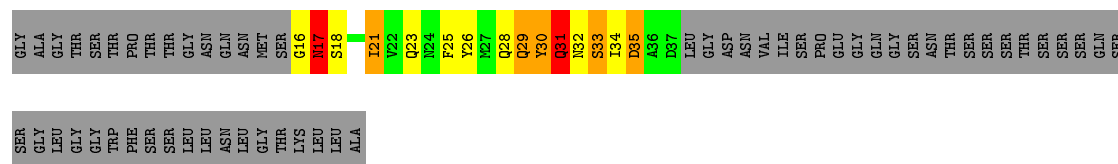
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	226	Total	C	N	O	S	0	0	0
			1719	1107	280	326	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	LYS	ARG	CONFLICT	UNP B9VV85

- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	22	Total	C	N	O	S	0	0	1
			166	101	29	35	1			



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	314.00Å 497.80Å 556.50Å 90.00° 92.35° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 49.85 – 3.49	Depositor EDS
% Data completeness (in resolution range)	35.0 (20.00-4.00) 22.9 (49.85-3.49)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.462 , (Not available) 0.448 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 104.1	EDS
Estimated twinning fraction	0.095 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 491857 reflections	Xtriage
F_o, F_c correlation	0.22	EDS
Total number of atoms	5506	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% 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

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	1	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
2	2	0.86	1/1746 (0.1%)	1.17	8/2397 (0.3%)
3	3	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
4	4	0.78	0/168	1.03	0/226
All	All	0.85	7/5676 (0.1%)	1.12	21/7764 (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
3	3	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	119	LYS	CE-NZ	7.39	1.67	1.49
3	3	120	PHE	N-CA	6.32	1.58	1.46
3	3	141	CYS	CB-SG	-5.87	1.72	1.81
3	3	12	ASP	CB-CG	5.58	1.63	1.51
2	2	35	CYS	CB-SG	-5.28	1.73	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	58	LEU	CA-CB-CG	9.43	136.99	115.30
3	3	149	GLY	N-CA-C	-9.01	90.58	113.10
3	3	120	PHE	CB-CA-C	-8.33	93.74	110.40
3	3	119	LYS	CD-CE-NZ	7.53	129.02	111.70
2	2	92	GLY	N-CA-C	7.40	131.60	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	26	TYR	Sidechain
3	3	53	PHE	Sidechain

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	1	1929	0	1864	213	0
2	2	1692	0	1666	221	0
3	3	1719	0	1677	191	0
4	4	166	0	146	17	0
All	All	5506	0	5353	560	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 560 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)
3:3:119:LYS:CE	3:3:119:LYS:NZ	1.67	1.56
1:1:13:THR:HB	3:3:157:ASN:HB2	1.27	1.11
2:2:104:VAL:HG13	2:2:222:VAL:HG22	1.15	1.09
2:2:44:PRO:HB2	2:2:47:VAL:HG22	1.36	1.06
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.73	1.02

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	1	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
2	2	217/230 (94%)	145 (67%)	49 (23%)	23 (11%)	0	11
3	3	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
4	4	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	2
All	All	705/782 (90%)	455 (64%)	160 (23%)	90 (13%)	0	7

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	10	PRO
1	1	18	ALA
1	1	22	VAL
1	1	26	VAL
1	1	63	THR

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	1	208/208 (100%)	173 (83%)	35 (17%)	2	20
2	2	193/204 (95%)	150 (78%)	43 (22%)	1	10
3	3	190/190 (100%)	146 (77%)	44 (23%)	1	8
4	4	18/65 (28%)	13 (72%)	5 (28%)	0	4
All	All	609/667 (91%)	482 (79%)	127 (21%)	1	11

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

Mol	Chain	Res	Type
2	2	159	PRO
2	2	197	LEU
3	3	195	ASP

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Mol	Chain	Res	Type
2	2	162	LEU
2	2	178	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	101	HIS
2	2	136	HIS
4	4	24	ASN
2	2	134	HIS
2	2	153	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 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	1	246/246 (100%)	-0.66	0 100 100	2, 4, 42, 72	0
2	2	219/230 (95%)	-0.65	0 100 100	2, 4, 47, 93	0
3	3	226/226 (100%)	-0.76	0 100 100	2, 3, 23, 56	0
4	4	22/80 (27%)	-0.49	0 100 100	13, 36, 45, 55	0
All	All	713/782 (91%)	-0.68	0 100 100	2, 4, 41, 93	0

There are no RSRZ outliers to report.

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.