



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2Z43 / pdb_00002z43
Title : Structure of a twinned crystal of RadA
Authors : Chen, L.T.; Ko, T.P.; Wang, A.H.J.; Wang, T.F.
Deposited on : 2007-06-12
Resolution : 1.93 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

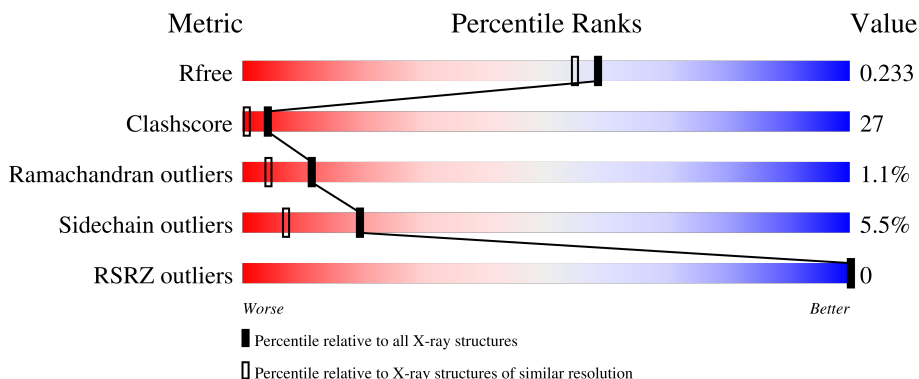
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	324	
1	B	324	
1	C	324	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7397 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 DNA repair and recombination protein radA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1799	1130	326	338	5			
1	B	290	Total	C	N	O	S	0	0	0
			2254	1417	400	432	5			
1	C	289	Total	C	N	O	S	0	0	0
			2245	1412	399	429	5			

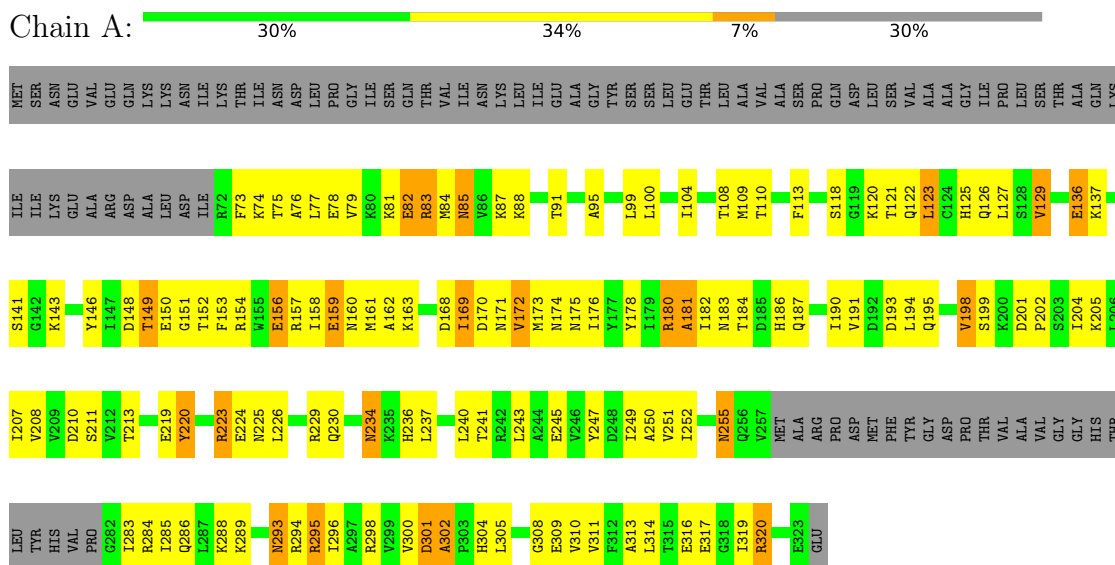
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	347	Total	O	0	0
			347	347		
2	B	379	Total	O	0	0
			379	379		
2	C	373	Total	O	0	0
			373	373		

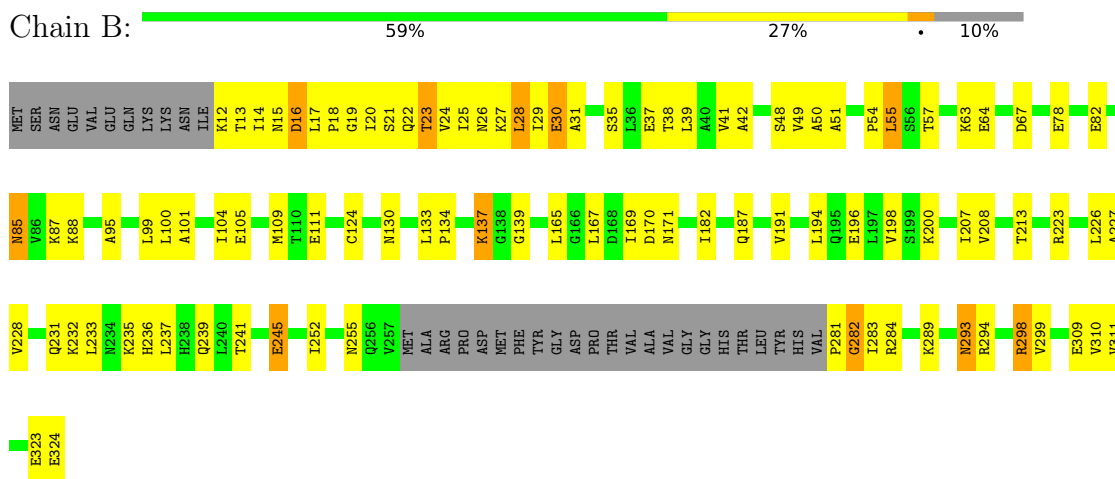
3 Residue-property plots

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: DNA repair and recombination protein radA



- Molecule 1: DNA repair and recombination protein radA



- Molecule 1: DNA repair and recombination protein radA



MET	SER	ASN	GLU	VAL	GLU	GLN	LYS	LYS	ASN	ILE	K12	T13	I14	N15	D16	L17	P18	G19	I20	S21	Q22	T23		N26	K27	L28	I29	E30	A31	G32	Y33		E37	T38	L39	A40	V41	A42		Q45		V49	A50	A51		A58	Q59	K60	I61	I62	K63	E64		D67		E78		E82	R83	
M84	N85		Q94		L99		I104	M109		C124		E136		R154		I158		I169		R180	A181	I182		Q187		L194		S199	K200		I207	V208		T213	S214		R217		Y220	P221	G222	R223	E224	N225	L226		R229		K235	H236		Q239		E245	V246	Y247	D248	I249		
A250	V251	I252		N255	G256	V257	MET	ALA	ARG	PRO	ASP	MET	PHE	TYR	GLY	ASP	PRO	THR	VAL	ALA	ALA	VAL	GLY	GLY	HIS	THR	LEU	TYR	HIS	VAL	P281	G282	I283	R284	I285		K288	K289	S290	R291	G292	N293	R294	R295	I296	A297	R298		P303	H304	L305	P306	E307		V310		D321	A322	E323	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	99.55Å 99.55Å 99.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.93 30.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-1.93) 94.2 (30.00-1.93)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.93Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.241 0.191 , 0.233	Depositor DCC
R_{free} test set	3645 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.487 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7397	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	0.95	1/1823 (0.1%)	1.23	12/2456 (0.5%)
1	B	0.98	1/2283 (0.0%)	1.10	4/3083 (0.1%)
1	C	1.03	2/2274 (0.1%)	1.14	11/3071 (0.4%)
All	All	0.99	4/6380 (0.1%)	1.15	27/8610 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	MET	SD-CE	-11.40	1.51	1.79
1	C	84	MET	SD-CE	-7.46	1.60	1.79
1	A	84	MET	SD-CE	7.23	1.97	1.79
1	C	109	MET	SD-CE	-6.99	1.62	1.79

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ALA	CA-C-N	7.66	127.38	119.56
1	A	302	ALA	C-N-CA	7.66	127.38	119.56
1	C	245	GLU	N-CA-C	7.52	119.56	111.36
1	A	181	ALA	N-CA-C	-7.16	97.57	108.96
1	A	169	ILE	N-CA-C	6.94	117.45	110.23

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	1799	0	1837	176	0
1	B	2254	0	2315	105	0
1	C	2245	0	2309	71	0
2	A	347	0	0	41	0
2	B	379	0	0	18	0
2	C	373	0	0	16	0
All	All	7397	0	6461	349	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 27.

The worst 5 of 349 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:181:ALA:HB3	2:A:441:HOH:O	1.47	1.12
1:B:85:ASN:HD21	1:B:87:LYS:HE2	1.23	1.00
1:A:85:ASN:HB3	2:A:357:HOH:O	1.59	1.00
1:A:129:VAL:HG23	2:A:518:HOH:O	1.62	0.99
1:A:123:LEU:HA	1:A:319:ILE:HD11	1.47	0.94

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	224/324 (69%)	216 (96%)	7 (3%)	1 (0%)	30	22
1	B	286/324 (88%)	271 (95%)	11 (4%)	4 (1%)	9	2
1	C	285/324 (88%)	270 (95%)	11 (4%)	4 (1%)	9	2
All	All	795/972 (82%)	757 (95%)	29 (4%)	9 (1%)	11	4

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	GLU
1	C	20	ILE
1	C	30	GLU
1	B	19	GLY
1	B	28	LEU

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	195/275 (71%)	176 (90%)	19 (10%)	8	1
1	B	246/275 (90%)	239 (97%)	7 (3%)	38	25
1	C	245/275 (89%)	233 (95%)	12 (5%)	22	9
All	All	686/825 (83%)	648 (94%)	38 (6%)	19	7

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	180	ARG
1	C	293	ASN
1	C	199	SER
1	C	239	GLN
1	C	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	293	ASN
1	C	85	ASN
1	C	293	ASN
1	C	160	ASN
1	C	59	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	228/324 (70%)	-1.28	0 100 100	29, 46, 73, 88	0
1	B	290/324 (89%)	-1.38	0 100 100	16, 32, 82, 87	0
1	C	289/324 (89%)	-1.37	0 100 100	15, 31, 82, 85	0
All	All	807/972 (83%)	-1.35	0 100 100	15, 37, 82, 88	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 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.