



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:55 AM GMT

PDB ID : 1L19
Title : ENHANCED PROTEIN THERMOSTABILITY FROM DESIGNED MUTATIONS THAT INTERACT WITH ALPHA-HELIX DIPOLES
Authors : Nicholson, H.; Matthews, B.W.
Deposited on : 1989-05-01
Resolution : 1.70 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

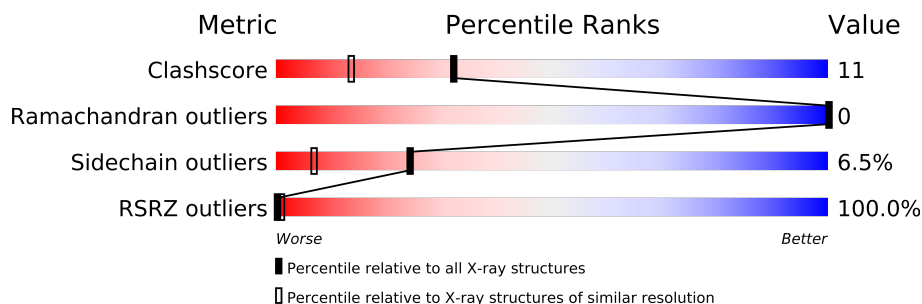
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	164	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1462 atoms, of which 0 are hydrogen and 0 are deuterium.

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 T4 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1311	824	238	242	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ASP	SER	CONFLICT	UNP P00720

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	151	Total	O	0	0
			151	151		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 61.10Å 97.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 1.70 19.59 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.70) 67.2 (19.59-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.153 , (Not available) 0.151 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 125.5	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15856 reflections	Xtriage
F_o, F_c correlation	0.48	EDS
Total number of atoms	1462	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.96	3/1331 (0.2%)	1.44	25/1791 (1.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CD-OE2	5.39	1.31	1.25
1	A	128	GLU	CD-OE2	5.34	1.31	1.25
1	A	136	SER	CB-OG	5.24	1.49	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	80	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	47	ASP	CB-CG-OD2	-9.80	109.48	118.30
1	A	163	ASN	N-CA-CB	-8.26	95.74	110.60
1	A	8	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	80	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	92	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	47	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	14	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	20	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	38	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	38	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	70	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	92	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	14	ARG	CD-NE-CZ	6.53	132.75	123.60
1	A	154	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	61	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	72	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	127	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	163	ASN	CB-CA-C	-5.54	99.32	110.40
1	A	163	ASN	C-N-CA	5.35	135.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	106	MET	CA-CB-CG	5.26	122.25	113.30
1	A	70	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	26	THR	CA-CB-CG2	5.01	119.42	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1311	0	1333	30	0
2	A	151	0	0	5	1
All	All	1462	0	1333	30	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:ASN:HB3	1:A:164:LEU:HD13	1.39	1.05
1:A:163:ASN:CB	1:A:164:LEU:HD13	2.06	0.85
1:A:16:LYS:HE3	1:A:57:VAL:HG23	1.71	0.73
1:A:38:ASP:OD1	1:A:40:ASN:HB2	1.90	0.70
1:A:14:ARG:HG3	2:A:532:HOH:O	1.97	0.65
1:A:80:ARG:NH2	2:A:277:HOH:O	2.29	0.64
1:A:151:THR:HG22	2:A:543:HOH:O	1.97	0.63
1:A:148:ARG:HD3	1:A:164:LEU:HD21	1.81	0.63
1:A:16:LYS:HE3	1:A:57:VAL:CG2	2.30	0.62
1:A:8:ARG:NH1	2:A:247:HOH:O	2.33	0.61
1:A:108:GLU:HB2	2:A:316:HOH:O	2.03	0.58
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.70	0.56
1:A:148:ARG:HD3	1:A:164:LEU:CD2	2.36	0.54
1:A:16:LYS:HE2	1:A:56:GLY:O	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:LYS:HD2	1:A:57:VAL:HG22	1.93	0.49
1:A:1:MET:HG2	1:A:158:TRP:CE3	2.48	0.49
1:A:164:LEU:N	1:A:164:LEU:HD13	2.29	0.48
1:A:164:LEU:N	1:A:164:LEU:CD1	2.77	0.47
1:A:106:MET:HE2	1:A:138:TRP:CD1	2.50	0.46
1:A:125:ARG:HD3	1:A:125:ARG:HH11	1.59	0.45
1:A:1:MET:HA	1:A:5:GLU:OE1	2.17	0.45
1:A:1:MET:HG3	1:A:2:ASN:N	2.33	0.43
1:A:163:ASN:HB3	1:A:164:LEU:CD1	2.27	0.43
1:A:85:LYS:NZ	1:A:89:ASP:OD1	2.50	0.43
1:A:16:LYS:CE	1:A:57:VAL:CG2	2.97	0.42
1:A:1:MET:HB2	1:A:1:MET:HE3	1.97	0.42
1:A:106:MET:CE	1:A:138:TRP:CD1	3.03	0.42
1:A:39:LEU:HG	1:A:43:LYS:HD2	2.01	0.42
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.35	0.40
1:A:163:ASN:HB2	1:A:164:LEU:HD13	1.98	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	Distance(Å)	Clash(Å)
2:A:168:HOH:O	2:A:525:HOH:O[4_655]	2.07	0.13

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	162/164 (99%)	159 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	138/138 (100%)	129 (94%)	9 (6%)	24 7

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	LYS
1	A	36	SER
1	A	53	ASN
1	A	83	LYS
1	A	122	GLN
1	A	127	ASP
1	A	154	ARG
1	A	164	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	123	GLN
1	A	144	ASN
1	A	163	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	154/164 (93%)	12.92	154 (100%) 0 1	12, 20, 45, 73	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ARG	52.5
1	A	78	ILE	36.5
1	A	97	CYS	34.8
1	A	111	VAL	33.6
1	A	153	PHE	33.3
1	A	126	TRP	28.0
1	A	24	TYR	27.3
1	A	110	GLY	26.8
1	A	54	CYS	26.3
1	A	98	ALA	25.9
1	A	84	LEU	25.7
1	A	86	PRO	24.5
1	A	75	VAL	24.1
1	A	131	VAL	23.9
1	A	26	THR	23.8
1	A	15	LEU	22.7
1	A	25	TYR	22.4
1	A	39	LEU	22.2
1	A	18	TYR	21.4
1	A	112	ALA	21.3
1	A	16	LYS	21.1
1	A	17	ILE	19.7
1	A	121	LEU	19.5
1	A	28	GLY	19.3
1	A	118	LEU	19.0
1	A	103	VAL	18.7
1	A	115	THR	18.7

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Mol	Chain	Res	Type	RSRZ
1	A	82	ALA	18.4
1	A	41	ALA	18.3
1	A	36	SER	17.6
1	A	31	HIS	17.5
1	A	102	MET	17.2
1	A	37	PRO	17.1
1	A	138	TRP	16.9
1	A	109	THR	16.8
1	A	130	ALA	16.5
1	A	129	ALA	16.3
1	A	59	THR	16.2
1	A	79	LEU	15.9
1	A	85	LYS	15.7
1	A	114	PHE	15.0
1	A	42	ALA	14.9
1	A	33	LEU	14.8
1	A	100	ILE	14.8
1	A	119	ARG	14.8
1	A	38	ASP	14.5
1	A	116	ASN	14.3
1	A	55	ASN	14.0
1	A	127	ASP	13.6
1	A	40	ASN	13.6
1	A	164	LEU	13.5
1	A	143	PRO	13.2
1	A	120	MET	13.2
1	A	149	VAL	13.2
1	A	83	LYS	13.2
1	A	20	ASP	13.1
1	A	91	LEU	13.1
1	A	81	ASN	13.1
1	A	150	ILE	13.0
1	A	128	GLU	13.0
1	A	108	GLU	12.9
1	A	144	ASN	12.8
1	A	12	GLY	12.8
1	A	80	ARG	12.7
1	A	117	SER	12.7
1	A	13	LEU	12.5
1	A	43	LYS	12.5
1	A	74	ALA	12.5
1	A	99	LEU	12.2

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Mol	Chain	Res	Type	RSRZ
1	A	95	ARG	12.1
1	A	87	VAL	12.1
1	A	56	GLY	12.1
1	A	45	GLU	12.0
1	A	71	VAL	11.9
1	A	122	GLN	11.8
1	A	19	LYS	11.8
1	A	34	THR	11.8
1	A	123	GLN	11.4
1	A	158	TRP	11.4
1	A	88	TYR	10.9
1	A	6	MET	10.6
1	A	44	SER	10.6
1	A	94	VAL	10.6
1	A	53	ASN	10.6
1	A	148	ARG	10.4
1	A	9	ILE	10.4
1	A	104	PHE	10.3
1	A	90	SER	10.3
1	A	154	ARG	10.2
1	A	29	ILE	10.1
1	A	134	ALA	10.1
1	A	135	LYS	10.1
1	A	132	ASN	10.0
1	A	106	MET	9.9
1	A	4	PHE	9.8
1	A	30	GLY	9.8
1	A	125	ARG	9.8
1	A	35	LYS	9.6
1	A	101	ASN	9.5
1	A	133	LEU	9.4
1	A	107	GLY	9.2
1	A	163	ASN	9.1
1	A	7	LEU	9.1
1	A	72	ASP	9.0
1	A	156	GLY	9.0
1	A	66	LEU	9.0
1	A	77	GLY	8.8
1	A	113	GLY	8.6
1	A	139	TYR	8.6
1	A	70	ASP	8.4
1	A	146	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	ILE	8.1
1	A	67	PHE	8.0
1	A	92	ASP	8.0
1	A	151	THR	8.0
1	A	76	ARG	7.9
1	A	152	THR	7.9
1	A	23	GLY	7.5
1	A	89	ASP	7.3
1	A	145	ARG	7.2
1	A	2	ASN	7.1
1	A	47	ASP	7.1
1	A	60	LYS	7.1
1	A	73	ALA	7.0
1	A	63	ALA	6.9
1	A	3	ILE	6.7
1	A	1	MET	6.7
1	A	61	ASP	6.6
1	A	155	THR	6.6
1	A	69	GLN	6.6
1	A	159	ASP	6.4
1	A	64	GLU	6.3
1	A	46	LEU	6.2
1	A	137	ARG	6.2
1	A	105	GLN	6.1
1	A	161	TYR	6.1
1	A	162	LYS	6.0
1	A	96	ARG	6.0
1	A	93	ALA	6.0
1	A	8	ARG	5.7
1	A	141	GLN	5.7
1	A	11	GLU	5.1
1	A	124	LYS	5.1
1	A	68	ASN	5.0
1	A	157	THR	4.8
1	A	65	LYS	4.5
1	A	147	LYS	4.5
1	A	160	ALA	4.5
1	A	22	GLU	4.3
1	A	49	ALA	4.1
1	A	21	THR	3.9
1	A	62	GLU	3.1
1	A	5	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	10	ASP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.