



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:21 PM EDT

PDB ID : 7EW8 / pdb_00007ew8
Title : Legionella pneumophila effector AnkD
Authors : Chen, T.T.; Lin, Y.L.
Deposited on : 2021-05-24
Resolution : 2.59 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

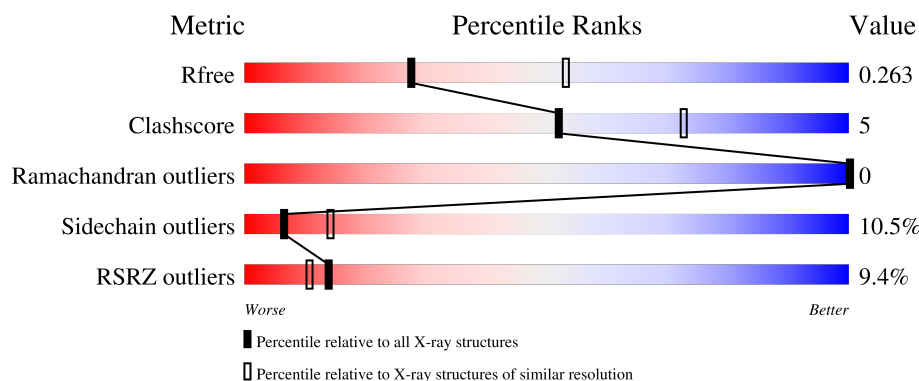
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	494	5% 71% 14% • 13%
1	B	494	11% 68% 15% • • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6826 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 ANK_REP_REGION domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	Se	0	0	0
			3348	2100	581	652	3	12			
1	B	429	Total	C	N	O	S	Se	0	0	0
			3328	2085	579	649	3	12			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	expression tag	UNP A0A2S6F2G5
A	-21	GLY	-	expression tag	UNP A0A2S6F2G5
A	-20	SER	-	expression tag	UNP A0A2S6F2G5
A	-19	SER	-	expression tag	UNP A0A2S6F2G5
A	-18	HIS	-	expression tag	UNP A0A2S6F2G5
A	-17	HIS	-	expression tag	UNP A0A2S6F2G5
A	-16	HIS	-	expression tag	UNP A0A2S6F2G5
A	-15	HIS	-	expression tag	UNP A0A2S6F2G5
A	-14	HIS	-	expression tag	UNP A0A2S6F2G5
A	-13	HIS	-	expression tag	UNP A0A2S6F2G5
A	-12	SER	-	expression tag	UNP A0A2S6F2G5
A	-11	SER	-	expression tag	UNP A0A2S6F2G5
A	-10	GLY	-	expression tag	UNP A0A2S6F2G5
A	-9	LEU	-	expression tag	UNP A0A2S6F2G5
A	-8	VAL	-	expression tag	UNP A0A2S6F2G5
A	-7	PRO	-	expression tag	UNP A0A2S6F2G5
A	-6	ARG	-	expression tag	UNP A0A2S6F2G5
A	-5	GLY	-	expression tag	UNP A0A2S6F2G5
A	-4	SER	-	expression tag	UNP A0A2S6F2G5
A	-3	HIS	-	expression tag	UNP A0A2S6F2G5
A	-2	MSE	-	expression tag	UNP A0A2S6F2G5
A	-1	ALA	-	expression tag	UNP A0A2S6F2G5
A	0	SER	-	expression tag	UNP A0A2S6F2G5
B	-22	MSE	-	expression tag	UNP A0A2S6F2G5
B	-21	GLY	-	expression tag	UNP A0A2S6F2G5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP A0A2S6F2G5
B	-19	SER	-	expression tag	UNP A0A2S6F2G5
B	-18	HIS	-	expression tag	UNP A0A2S6F2G5
B	-17	HIS	-	expression tag	UNP A0A2S6F2G5
B	-16	HIS	-	expression tag	UNP A0A2S6F2G5
B	-15	HIS	-	expression tag	UNP A0A2S6F2G5
B	-14	HIS	-	expression tag	UNP A0A2S6F2G5
B	-13	HIS	-	expression tag	UNP A0A2S6F2G5
B	-12	SER	-	expression tag	UNP A0A2S6F2G5
B	-11	SER	-	expression tag	UNP A0A2S6F2G5
B	-10	GLY	-	expression tag	UNP A0A2S6F2G5
B	-9	LEU	-	expression tag	UNP A0A2S6F2G5
B	-8	VAL	-	expression tag	UNP A0A2S6F2G5
B	-7	PRO	-	expression tag	UNP A0A2S6F2G5
B	-6	ARG	-	expression tag	UNP A0A2S6F2G5
B	-5	GLY	-	expression tag	UNP A0A2S6F2G5
B	-4	SER	-	expression tag	UNP A0A2S6F2G5
B	-3	HIS	-	expression tag	UNP A0A2S6F2G5
B	-2	MSE	-	expression tag	UNP A0A2S6F2G5
B	-1	ALA	-	expression tag	UNP A0A2S6F2G5
B	0	SER	-	expression tag	UNP A0A2S6F2G5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	35	Total	O	0	0
			35	35		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.06Å 76.00Å 104.81Å 90.00° 90.81° 90.00°	Depositor
Resolution (Å)	45.21 – 2.59 45.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.8 (45.21-2.59) 92.7 (45.21-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.201 , 0.268 0.228 , 0.263	Depositor DCC
R_{free} test set	1485 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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	0.76	1/3397 (0.0%)	1.20	29/4540 (0.6%)
1	B	0.70	2/3375 (0.1%)	1.16	29/4508 (0.6%)
All	All	0.73	3/6772 (0.0%)	1.18	58/9048 (0.6%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	SER	C-N	-7.68	1.23	1.33
1	B	376	CYS	C-N	-7.41	1.24	1.33
1	A	239	PRO	C-O	-6.34	1.16	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ASN	N-CA-C	17.33	136.64	113.77
1	B	53	ILE	N-CA-C	-10.26	101.40	110.74
1	A	433	LYS	CB-CA-C	-10.07	93.78	110.29
1	A	56	LYS	N-CA-C	-9.87	95.30	109.31
1	B	191	PHE	N-CA-C	-9.15	91.32	110.80
1	A	358	ASN	CB-CA-C	9.00	123.92	111.86
1	B	79	GLU	N-CA-C	-8.69	92.29	110.80
1	A	55	ASN	N-CA-C	8.16	128.18	110.80
1	B	241	ARG	N-CA-C	-8.01	93.32	107.73
1	B	79	GLU	CB-CA-C	7.65	125.65	110.42
1	A	421	GLU	N-CA-C	-7.07	104.74	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASN	N-CA-C	7.04	125.37	109.81
1	A	56	LYS	N-CA-CB	7.01	120.03	109.94
1	A	433	LYS	N-CA-C	6.91	119.83	109.25
1	A	344	ASN	CB-CA-C	6.78	122.31	111.66
1	B	183	SER	CB-CA-C	-6.68	98.14	109.83
1	B	242	ASN	CB-CA-C	-6.67	97.03	110.17
1	B	396	VAL	N-CA-C	-6.62	105.29	111.45
1	B	191	PHE	CB-CA-C	6.61	123.57	110.42
1	B	36	GLU	N-CA-C	-6.40	101.01	110.48
1	B	261	ILE	CA-C-O	-6.23	116.64	120.88
1	B	344	ASN	CB-CA-C	6.21	121.36	111.48
1	B	427	ASP	N-CA-C	-6.02	105.20	112.54
1	B	80	LEU	N-CA-C	-5.96	105.11	112.38
1	B	49	LEU	N-CA-C	-5.61	105.08	111.14
1	A	426	PRO	N-CA-CB	5.61	109.17	103.00
1	A	419	LEU	N-CA-C	-5.55	105.13	112.34
1	A	312	LYS	N-CA-C	-5.54	106.36	113.23
1	A	190	GLN	CA-C-N	-5.51	114.25	122.74
1	A	190	GLN	C-N-CA	-5.51	114.25	122.74
1	B	190	GLN	CA-C-O	-5.48	114.04	122.32
1	B	171	LYS	CA-C-N	-5.48	112.94	120.28
1	B	171	LYS	C-N-CA	-5.48	112.94	120.28
1	B	54	LEU	N-CA-C	-5.42	98.15	108.17
1	A	190	GLN	N-CA-C	5.41	120.54	113.30
1	A	298	SER	N-CA-C	-5.37	105.53	111.71
1	B	376	CYS	CA-C-N	5.37	127.47	120.28
1	B	376	CYS	C-N-CA	5.37	127.47	120.28
1	A	241	ARG	N-CA-C	-5.34	103.92	110.65
1	B	428	LEU	CA-C-N	-5.33	113.51	120.44
1	B	428	LEU	C-N-CA	-5.33	113.51	120.44
1	A	108	GLU	CB-CA-C	-5.31	100.53	110.36
1	B	165	GLU	N-CA-C	-5.30	106.19	113.30
1	B	344	ASN	N-CA-C	-5.30	105.90	112.47
1	A	395	SER	N-CA-C	-5.28	105.61	111.36
1	A	20	LEU	N-CA-C	-5.24	106.93	113.38
1	A	72	MSE	CG-SE-CE	5.21	110.38	98.92
1	B	266	LYS	CB-CA-C	5.16	117.23	110.06
1	B	236	PHE	N-CA-C	-5.16	99.82	110.80
1	A	164	LYS	N-CA-C	-5.15	107.17	112.93
1	A	360	ASN	CB-CA-C	5.13	120.16	109.95
1	A	447	LYS	N-CA-C	5.11	116.69	110.41
1	A	236	PHE	N-CA-C	-5.10	100.56	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	THR	CB-CA-C	5.09	117.65	109.41
1	A	142	VAL	N-CA-C	-5.03	105.94	110.82
1	B	241	ARG	CB-CA-C	-5.03	103.93	111.73
1	A	233	ALA	N-CA-C	5.03	118.33	111.39
1	A	427	ASP	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASN	Peptide

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	3348	0	3346	26	0
1	B	3328	0	3325	42	0
2	A	115	0	0	0	0
2	B	35	0	0	0	0
All	All	6826	0	6671	68	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 5.

All (68) 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:53:ILE:HG22	1:B:54:LEU:HG	1.57	0.83
1:B:53:ILE:HG22	1:B:54:LEU:H	1.48	0.77
1:B:201:MSE:O	1:B:205:VAL:HG23	1.86	0.76
1:B:265:CYS:HB3	1:B:270:MSE:HE1	1.67	0.76
1:B:53:ILE:HG22	1:B:54:LEU:N	2.01	0.75
1:B:53:ILE:CG2	1:B:54:LEU:N	2.53	0.71
1:B:177:LEU:HD11	1:B:411:LYS:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:HG11	1:B:411:LYS:HG3	1.73	0.70
1:B:172:ASN:OD1	1:B:411:LYS:HE3	1.94	0.68
1:A:242:ASN:HB2	1:A:243:PRO:HD3	1.78	0.65
1:B:205:VAL:HG11	1:B:221:ILE:HG22	1.80	0.64
1:A:55:ASN:CG	1:A:55:ASN:O	2.41	0.61
1:B:27:LEU:O	1:B:31:ASN:ND2	2.33	0.61
1:A:179:ILE:HA	1:A:434:GLU:HG2	1.84	0.59
1:B:27:LEU:O	1:B:31:ASN:CG	2.46	0.59
1:B:173:PHE:HE1	1:B:414:GLU:HG2	1.70	0.56
1:B:205:VAL:CG1	1:B:221:ILE:HG22	2.35	0.56
1:B:53:ILE:CG2	1:B:54:LEU:HG	2.31	0.55
1:B:296:LYS:HG3	1:B:299:GLU:HG3	1.89	0.54
1:A:179:ILE:HG23	1:A:434:GLU:HB3	1.90	0.54
1:A:418:ALA:C	1:A:420:LYS:N	2.66	0.52
1:B:242:ASN:CG	1:B:242:ASN:O	2.53	0.52
1:B:419:LEU:HD22	1:B:431:LEU:HD23	1.92	0.52
1:A:434:GLU:H	1:A:437:LYS:HB2	1.74	0.51
1:B:173:PHE:CE1	1:B:414:GLU:HG2	2.45	0.51
1:A:215:ASN:O	1:A:219:GLN:HG2	2.11	0.50
1:B:297:SER:HA	1:B:300:HIS:CD2	2.46	0.50
1:A:252:ARG:NH1	1:A:258:LEU:O	2.45	0.49
1:A:296:LYS:HD3	1:A:296:LYS:HA	1.69	0.48
1:B:201:MSE:HG2	1:B:363:ILE:HD13	1.94	0.48
1:B:264:SER:HB3	1:B:325:HIS:H	1.78	0.48
1:B:420:LYS:HA	1:B:420:LYS:HD3	1.67	0.48
1:B:177:LEU:CD2	1:B:412:VAL:HG13	2.44	0.47
1:B:343:GLY:C	1:B:345:LYS:N	2.71	0.47
1:B:80:LEU:O	1:B:84:GLN:HG2	2.15	0.47
1:A:166:LYS:H	1:A:166:LYS:HG2	1.58	0.46
1:B:377:GLN:HG2	1:B:380:ARG:HH21	1.80	0.46
1:A:141:ALA:O	1:A:145:ILE:HG12	2.17	0.45
1:A:278:GLY:O	1:A:281:SER:HB3	2.15	0.45
1:A:321:MSE:SE	1:A:334:ILE:HG23	2.66	0.45
1:A:141:ALA:HB2	1:A:188:PRO:HG2	1.97	0.45
1:B:141:ALA:O	1:B:145:ILE:HG12	2.16	0.45
1:B:244:GLU:HA	1:B:247:ASN:HD22	1.81	0.45
1:B:177:LEU:HD22	1:B:412:VAL:HG12	1.98	0.45
1:A:424:GLN:HE21	1:A:424:GLN:HB2	1.67	0.45
1:B:29:GLN:HA	1:B:32:GLU:HG3	1.98	0.44
1:A:286:LEU:HB2	1:A:307:ILE:HD11	1.98	0.44
1:B:296:LYS:H	1:B:296:LYS:HG2	1.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:HA	1:A:411:LYS:HD3	1.79	0.44
1:B:373:ILE:O	1:B:377:GLN:HG3	2.17	0.43
1:B:428:LEU:HD13	1:B:428:LEU:HA	1.81	0.43
1:A:264:SER:O	1:A:324:GLY:HA3	2.19	0.43
1:B:79:GLU:C	1:B:81:PHE:N	2.75	0.43
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.87	0.43
1:A:420:LYS:C	1:A:422:ASN:H	2.27	0.43
1:A:34:THR:HA	1:A:135:ALA:O	2.19	0.43
1:B:177:LEU:HD22	1:B:412:VAL:CG1	2.49	0.43
1:B:58:LYS:HA	1:B:58:LYS:HD2	1.35	0.43
1:B:398:LYS:HA	1:B:398:LYS:HD2	1.43	0.42
1:A:434:GLU:HG3	1:A:438:GLN:CB	2.50	0.42
1:B:90:LYS:HA	1:B:94:TYR:O	2.18	0.42
1:A:418:ALA:C	1:A:420:LYS:H	2.27	0.42
1:A:249:LEU:HB2	1:A:318:ILE:HG21	2.01	0.42
1:B:28:LYS:HD3	1:B:28:LYS:HA	1.92	0.42
1:A:114:GLN:HG3	1:A:142:VAL:HG21	2.02	0.41
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.85	0.41
1:A:411:LYS:NZ	1:A:414:GLU:OE1	2.50	0.41
1:B:405:LYS:HB3	1:B:405:LYS:HE3	1.46	0.40

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	425/494 (86%)	405 (95%)	20 (5%)	0	100	100
1	B	421/494 (85%)	400 (95%)	21 (5%)	0	100	100
All	All	846/988 (86%)	805 (95%)	41 (5%)	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	368/408 (90%)	335 (91%)	33 (9%)	9	20
1	B	366/408 (90%)	322 (88%)	44 (12%)	5	10
All	All	734/816 (90%)	657 (90%)	77 (10%)	6	14

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	29	GLN
1	A	39	LYS
1	A	43	LEU
1	A	54	LEU
1	A	58	LYS
1	A	71	LEU
1	A	77	GLN
1	A	79	GLU
1	A	82	LYS
1	A	129	LEU
1	A	166	LYS
1	A	169	PRO
1	A	180	LYS
1	A	190	GLN
1	A	220	GLU
1	A	242	ASN
1	A	244	GLU
1	A	258	LEU
1	A	296	LYS
1	A	298	SER
1	A	345	LYS
1	A	357	LYS
1	A	398	LYS
1	A	419	LEU
1	A	424	GLN
1	A	430	ASN

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Mol	Chain	Res	Type
1	A	431	LEU
1	A	433	LYS
1	A	434	GLU
1	A	436	LEU
1	A	441	ASN
1	A	445	LYS
1	B	28	LYS
1	B	39	LYS
1	B	47	MSE
1	B	53	ILE
1	B	54	LEU
1	B	55	ASN
1	B	56	LYS
1	B	58	LYS
1	B	70	GLU
1	B	79	GLU
1	B	80	LEU
1	B	82	LYS
1	B	86	SER
1	B	87	LYS
1	B	105	THR
1	B	108	GLU
1	B	140	LYS
1	B	170	VAL
1	B	171	LYS
1	B	184	VAL
1	B	185	ASP
1	B	244	GLU
1	B	260	THR
1	B	265	CYS
1	B	296	LYS
1	B	335	MSE
1	B	336	SER
1	B	380	ARG
1	B	381	GLU
1	B	398	LYS
1	B	405	LYS
1	B	417	LYS
1	B	420	LYS
1	B	421	GLU
1	B	428	LEU
1	B	431	LEU

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Mol	Chain	Res	Type
1	B	432	THR
1	B	433	LYS
1	B	441	ASN
1	B	445	LYS
1	B	446	LEU
1	B	447	LYS
1	B	448	GLN
1	B	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	240	GLN
1	A	300	HIS
1	A	424	GLN
1	A	448	GLN
1	B	31	ASN
1	B	120	GLN
1	B	172	ASN
1	B	190	GLN
1	B	229	ASN
1	B	240	GLN
1	B	247	ASN
1	B	327	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	419/494 (84%)	0.30	27 (6%) 25 20	17, 34, 69, 93	0
1	B	417/494 (84%)	0.94	52 (12%) 8 6	30, 60, 83, 105	0
All	All	836/988 (84%)	0.62	79 (9%) 14 11	17, 50, 80, 105	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	ILE	7.3
1	B	442	ALA	5.3
1	A	444	PRO	5.1
1	A	242	ASN	5.0
1	A	426	PRO	4.8
1	B	444	PRO	4.7
1	B	446	LEU	4.7
1	B	426	PRO	4.4
1	A	435	TYR	4.2
1	A	442	ALA	4.2
1	B	205	VAL	4.0
1	B	57	ALA	3.8
1	B	409	VAL	3.6
1	B	54	LEU	3.5
1	A	55	ASN	3.3
1	B	430	ASN	3.3
1	B	448	GLN	3.3
1	B	450	LEU	3.3
1	B	243	PRO	3.2
1	B	20	LEU	3.2
1	A	440	PRO	3.1
1	B	38	THR	3.0
1	A	424	GLN	2.9
1	B	52	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	165	GLU	2.9
1	B	307	ILE	2.9
1	B	403	PHE	2.9
1	A	445	LYS	2.8
1	B	242	ASN	2.8
1	B	280	GLY	2.8
1	A	446	LEU	2.8
1	B	424	GLN	2.7
1	A	431	LEU	2.7
1	B	55	ASN	2.6
1	B	433	LYS	2.6
1	B	19	LYS	2.6
1	B	427	ASP	2.6
1	A	179	ILE	2.6
1	A	57	ALA	2.6
1	B	182	THR	2.6
1	B	40	LEU	2.5
1	B	76	LEU	2.5
1	B	83	GLU	2.5
1	B	163	GLU	2.5
1	A	56	LYS	2.5
1	B	420	LYS	2.5
1	A	449	THR	2.5
1	B	336	SER	2.5
1	B	449	THR	2.5
1	B	77	GLN	2.4
1	B	58	LYS	2.4
1	A	163	GLU	2.4
1	B	283	SER	2.3
1	A	244	GLU	2.3
1	A	450	LEU	2.3
1	A	296	LYS	2.3
1	B	95	ASP	2.3
1	B	161	PRO	2.3
1	A	190	GLN	2.2
1	B	190	GLN	2.2
1	A	436	LEU	2.2
1	B	74	LEU	2.2
1	B	434	GLU	2.2
1	B	162	PRO	2.2
1	B	382	VAL	2.1
1	B	415	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	447	LYS	2.1
1	B	173	PHE	2.1
1	B	445	LYS	2.1
1	B	396	VAL	2.1
1	A	433	LYS	2.1
1	B	56	LYS	2.1
1	A	191	PHE	2.1
1	A	422	ASN	2.0
1	A	20	LEU	2.0
1	A	434	GLU	2.0
1	B	348	ILE	2.0
1	B	432	THR	2.0
1	A	439	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.