



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 4BRO / pdb_00004bro
Title : Legionella pneumophila NTPDase1 crystal form IV (part-open)
Authors : Zebisch, M.; Schaefer, P.; Lauble, P.; Straeter, N.
Deposited on : 2013-06-04
Resolution : 1.99 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

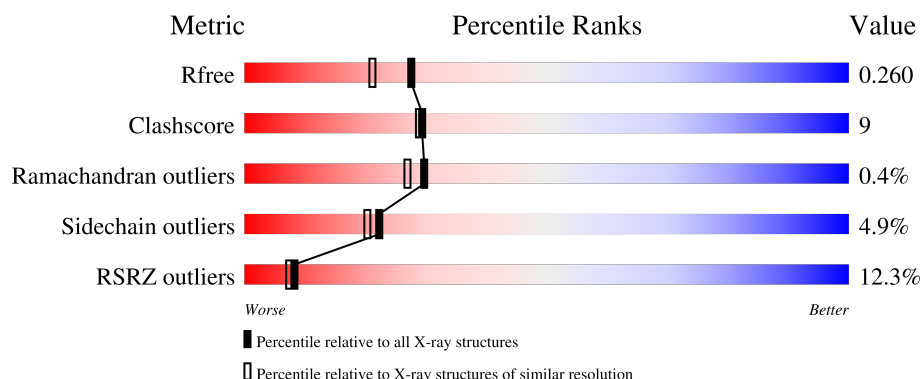
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	368	
1	B	368	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5726 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 ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	6	0
			2825	1800	464	547	14			
1	B	351	Total	C	N	O	S	0	4	0
			2796	1778	460	544	14			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	expression tag	UNP Q5ZUA2
A	394	LEU	-	expression tag	UNP Q5ZUA2
A	395	GLU	-	expression tag	UNP Q5ZUA2
A	396	HIS	-	expression tag	UNP Q5ZUA2
A	397	HIS	-	expression tag	UNP Q5ZUA2
A	398	HIS	-	expression tag	UNP Q5ZUA2
A	399	HIS	-	expression tag	UNP Q5ZUA2
A	400	HIS	-	expression tag	UNP Q5ZUA2
A	401	HIS	-	expression tag	UNP Q5ZUA2
A	137	ASP	GLU	conflict	UNP Q5ZUA2
A	149	VAL	ALA	conflict	UNP Q5ZUA2
B	34	MET	-	expression tag	UNP Q5ZUA2
B	394	LEU	-	expression tag	UNP Q5ZUA2
B	395	GLU	-	expression tag	UNP Q5ZUA2
B	396	HIS	-	expression tag	UNP Q5ZUA2
B	397	HIS	-	expression tag	UNP Q5ZUA2
B	398	HIS	-	expression tag	UNP Q5ZUA2
B	399	HIS	-	expression tag	UNP Q5ZUA2
B	400	HIS	-	expression tag	UNP Q5ZUA2
B	401	HIS	-	expression tag	UNP Q5ZUA2
B	137	ASP	GLU	conflict	UNP Q5ZUA2
B	149	VAL	ALA	conflict	UNP Q5ZUA2

- Molecule 2 is water.

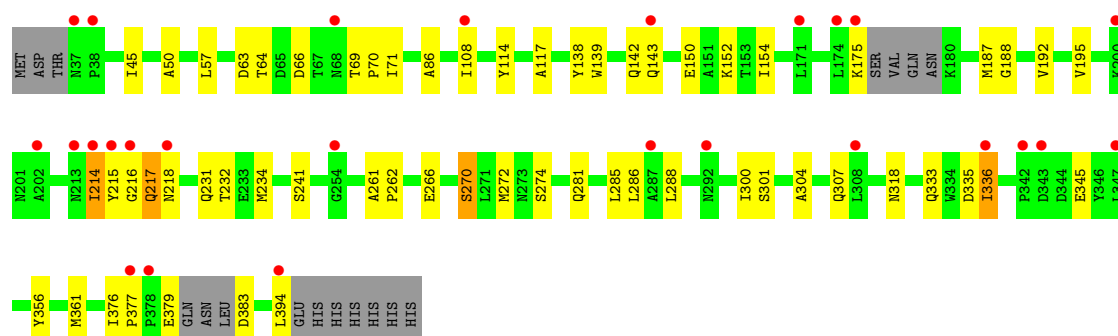
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total 73	O 73	0	2
2	B	32	Total 32	O 32	0	0

3 Residue-property plots [i](#)

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.

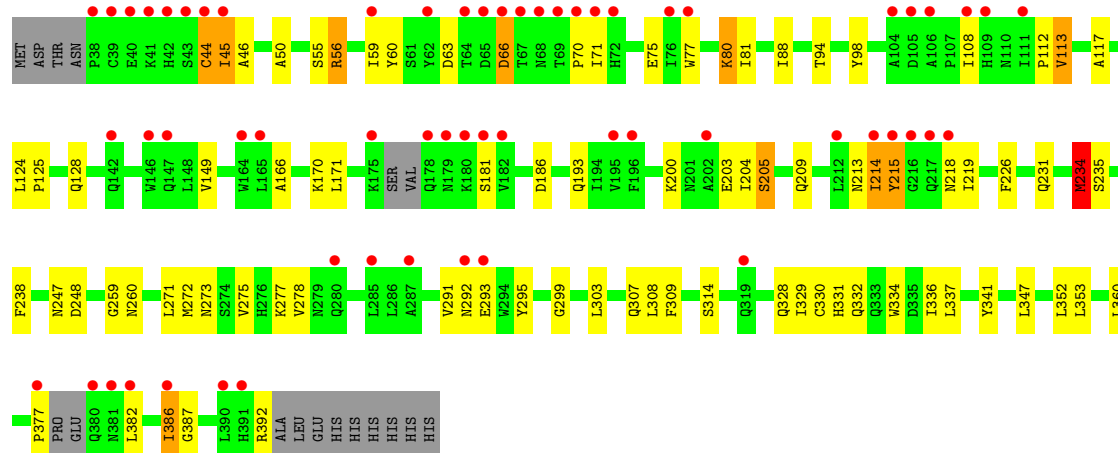
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I

Chain A: 



• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	155.99Å 155.99Å 79.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.17 – 1.99 34.17 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.17-1.99) 99.3 (34.17-1.99)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.215 , 0.241 0.235 , 0.260	Depositor DCC
R_{free} test set	1905 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.837 for H, K, L 0.163 for K, H, -L	Depositor
Outliers	0 of 74531 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5726	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	0.85	0/2916	1.07	7/3975 (0.2%)
1	B	0.70	0/2879	0.97	5/3924 (0.1%)
All	All	0.78	0/5795	1.02	12/7899 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	CYS	N-CA-C	6.39	118.66	109.14
1	B	341	TYR	CA-C-N	6.03	126.47	119.47
1	B	341	TYR	C-N-CA	6.03	126.47	119.47
1	A	272	MET	N-CA-C	5.92	117.53	111.14
1	A	86	ALA	CA-C-N	-5.81	113.35	122.65
1	A	86	ALA	C-N-CA	-5.81	113.35	122.65
1	B	234	MET	CG-SD-CE	5.28	112.51	100.90
1	A	304	ALA	N-CA-C	5.26	117.70	111.33
1	A	188	GLY	CA-C-N	5.17	125.72	119.98
1	A	188	GLY	C-N-CA	5.17	125.72	119.98
1	A	218	ASN	N-CA-C	5.16	117.02	108.20
1	B	149	VAL	N-CA-C	-5.12	105.85	110.82

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	2825	0	2692	27	0
1	B	2796	0	2643	67	0
2	A	73	0	0	1	0
2	B	32	0	0	2	0
All	All	5726	0	5335	94	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 9.

All (94) 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:234:MET:HE3	1:B:238:PHE:CD2	2.03	0.94
1:B:214:ILE:HD11	1:B:219:ILE:HD12	1.52	0.92
1:B:44:CYS:HB2	1:B:60:TYR:O	1.71	0.91
1:B:234:MET:CE	1:B:238:PHE:HD2	1.85	0.88
1:B:272:MET:HE1	1:B:360:LEU:HD12	1.57	0.87
1:B:234:MET:HE3	1:B:238:PHE:HD2	1.36	0.86
1:B:272:MET:HE2	1:B:360:LEU:HA	1.58	0.85
1:B:234:MET:CE	1:B:238:PHE:CD2	2.61	0.82
1:B:88:ILE:HD12	1:B:94:THR:HG22	1.64	0.78
1:B:234:MET:HE2	1:B:235:SER:HA	1.67	0.75
1:A:307:GLN:H	1:A:307:GLN:CD	1.94	0.75
1:B:181:SER:H	1:B:292:ASN:HB2	1.54	0.72
1:B:328:GLN:O	1:B:332:GLN:HG3	1.92	0.70
1:B:231:GLN:HG3	1:B:353:LEU:HD22	1.76	0.68
1:B:170:LYS:HD2	1:B:382:LEU:HB2	1.76	0.68
1:B:81:ILE:HD12	1:B:81:ILE:O	1.95	0.65
1:A:234:MET:HE2	1:A:356:TYR:CG	2.32	0.64
1:B:337:LEU:HG	1:B:347:LEU:HD21	1.80	0.64
1:B:234:MET:HE1	1:B:352:LEU:HD11	1.80	0.64
1:B:231:GLN:HG3	1:B:353:LEU:CD2	2.28	0.63
1:B:81:ILE:HD12	1:B:81:ILE:C	2.24	0.63
1:B:272:MET:CE	1:B:360:LEU:HA	2.32	0.59
1:B:205:SER:HB3	2:B:2019:HOH:O	2.03	0.57
1:A:335:ASP:HB2	2:A:2069:HOH:O	2.04	0.57
1:B:170:LYS:HB2	1:B:382:LEU:HD13	1.87	0.57
1:B:307:GLN:H	1:B:307:GLN:CD	2.13	0.57
1:B:234:MET:HE3	1:B:238:PHE:CE2	2.40	0.56
1:B:213:ASN:HA	1:B:218:ASN:HA	1.87	0.56
1:B:247:ASN:O	1:B:248:ASP:HB2	2.04	0.56
1:B:334:TRP:HZ3	1:B:347:LEU:HD23	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASP:O	1:B:70:PRO:HA	2.04	0.56
1:A:281:GLN:O	1:A:285:LEU:HD13	2.05	0.56
1:B:299:GLY:HA3	2:B:2016:HOH:O	2.05	0.55
1:B:186:ASP:HB3	1:B:193:GLN:HB2	1.88	0.55
1:A:307:GLN:CD	1:A:307:GLN:N	2.65	0.54
1:A:152:LYS:HE2	1:A:154:ILE:HG22	1.90	0.54
1:A:234:MET:HE2	1:A:356:TYR:CD1	2.44	0.53
1:B:303:LEU:HD11	1:B:309:PHE:CE2	2.44	0.52
1:A:63:ASP:O	1:A:70:PRO:HA	2.09	0.52
1:B:259:GLY:HA3	1:B:330:CYS:O	2.10	0.52
1:A:175:LYS:HE3	1:A:215:TYR:HB3	1.92	0.51
1:A:64:THR:HA	1:A:69:THR:O	2.09	0.51
1:B:214:ILE:O	1:B:215:TYR:C	2.54	0.51
1:B:328:GLN:HB2	1:B:329:ILE:HD12	1.91	0.51
1:A:139:TRP:O	1:A:143[B]:GLN:HG2	2.11	0.51
1:B:307:GLN:CD	1:B:307:GLN:N	2.69	0.51
1:B:272:MET:HE1	1:B:360:LEU:CD1	2.36	0.50
1:A:216:GLY:O	1:A:217:GLN:HB3	2.11	0.50
1:B:50:ALA:HB3	1:B:117:ALA:HA	1.92	0.50
1:B:66:ASP:OD1	1:B:66:ASP:N	2.36	0.50
1:B:234:MET:HG3	1:B:235:SER:N	2.26	0.50
1:B:234:MET:HE2	1:B:235:SER:CA	2.40	0.49
1:B:273:ASN:O	1:B:277:LYS:HD3	2.12	0.49
1:B:81:ILE:HD13	1:B:98:TYR:CE1	2.48	0.49
1:A:63:ASP:HB2	1:A:71:ILE:HG13	1.95	0.48
1:B:166:ALA:HA	1:B:386:ILE:HD11	1.96	0.48
1:B:204:ILE:HB	1:B:209:GLN:NE2	2.29	0.48
1:A:262:PRO:O	1:A:266:GLU:HG3	2.14	0.47
1:A:376:ILE:N	1:A:376:ILE:HD12	2.29	0.47
1:A:270:SER:O	1:A:274:SER:HB2	2.15	0.47
1:A:318:ASN:OD1	1:A:361:MET:HE3	2.14	0.46
1:B:234:MET:HE1	1:B:238:PHE:CD2	2.47	0.46
1:B:308:LEU:O	1:B:328:GLN:HG3	2.16	0.46
1:A:231:GLN:HG3	1:A:232:THR:N	2.30	0.46
1:B:392:ARG:H	1:B:392:ARG:HG3	1.58	0.46
1:B:271:LEU:HD12	1:B:275:VAL:HB	1.97	0.45
1:B:124:LEU:HD13	1:B:128:GLN:HG2	1.99	0.45
1:B:45:ILE:HG22	1:B:112:PRO:HG2	1.99	0.45
1:B:59:ILE:HD12	1:B:77:TRP:HB3	1.99	0.45
1:A:333:GLN:HB3	1:A:336:ILE:HG22	1.98	0.44
1:B:125:PRO:HG2	1:B:128:GLN:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:O	1:A:215:TYR:C	2.59	0.44
1:B:55:SER:HB2	1:B:81:ILE:HD11	2.00	0.44
1:B:231:GLN:CG	1:B:353:LEU:HD21	2.48	0.44
1:A:50:ALA:HB3	1:A:117:ALA:HA	2.01	0.43
1:B:226:PHE:CE2	1:B:278:VAL:HG22	2.53	0.43
1:B:386:ILE:HG13	1:B:387:GLY:N	2.34	0.43
1:A:261:ALA:HB3	1:A:262:PRO:HD3	2.00	0.43
1:B:60:TYR:CE1	1:B:386:ILE:HG22	2.53	0.43
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.77	0.42
1:B:308:LEU:HA	1:B:308:LEU:HD23	1.82	0.42
1:A:138:TYR:O	1:A:142:GLN:HG3	2.19	0.42
1:B:231:GLN:CG	1:B:353:LEU:CD2	2.97	0.42
1:B:46:ALA:HB3	1:B:113:VAL:HG13	2.01	0.42
1:A:45:ILE:HD11	1:A:114:TYR:CE1	2.55	0.42
1:A:187:MET:HA	1:A:192:VAL:HG12	2.02	0.41
1:B:292:ASN:O	1:B:293:GLU:HG3	2.20	0.41
1:B:260:ASN:HD22	1:B:331:HIS:CE1	2.38	0.41
1:B:171:LEU:HD11	1:B:295:TYR:CZ	2.56	0.41
1:B:56:ARG:HG3	1:B:80:LYS:HG3	2.03	0.41
1:B:81:ILE:C	1:B:81:ILE:CD1	2.93	0.41
1:B:334:TRP:HZ3	1:B:347:LEU:CD2	2.33	0.40
1:B:314:SER:OG	1:B:377:PRO:HG3	2.21	0.40
1:A:377:PRO:HB2	1:A:379:GLU:CD	2.46	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	351/368 (95%)	329 (94%)	21 (6%)	1 (0%)	36	35
1	B	349/368 (95%)	330 (95%)	17 (5%)	2 (1%)	21	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	700/736 (95%)	659 (94%)	38 (5%)	3 (0%)	30	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	B	200	LYS
1	B	215	TYR

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	315/328 (96%)	300 (95%)	15 (5%)	23	21
1	B	309/328 (94%)	294 (95%)	15 (5%)	22	20
All	All	624/656 (95%)	594 (95%)	30 (5%)	22	21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	66	ASP
1	A	108	ILE
1	A	150	GLU
1	A	195	VAL
1	A	214	ILE
1	A	241	SER
1	A	270	SER
1	A	288	LEU
1	A	300	ILE
1	A	301	SER
1	A	336	ILE
1	A	345	GLU
1	A	383	ASP
1	A	394	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	45	ILE
1	B	56	ARG
1	B	66	ASP
1	B	71	ILE
1	B	75	GLU
1	B	80	LYS
1	B	108	ILE
1	B	113	VAL
1	B	203	GLU
1	B	205	SER
1	B	214	ILE
1	B	234	MET
1	B	291	VAL
1	B	336	ILE
1	B	386	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	147	GLN
1	A	201	ASN
1	A	333	GLN
1	B	128	GLN
1	B	217	GLN
1	B	289	ASN
1	B	292	ASN
1	B	331	HIS
1	B	338	ASN
1	B	349	GLN

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 [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

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	351/368 (95%)	0.51	26 (7%)	20 19	13, 27, 46, 64	6 (1%)
1	B	351/368 (95%)	1.08	60 (17%)	4 4	15, 36, 61, 76	4 (1%)
All	All	702/736 (95%)	0.79	86 (12%)	8 7	13, 32, 55, 76	10 (1%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	TYR	5.7
1	A	175	LYS	4.5
1	B	38	PRO	4.2
1	B	105	ASP	4.0
1	B	44	CYS	4.0
1	B	214	ILE	3.9
1	A	342	PRO	3.9
1	A	68	ASN	3.8
1	B	175	LYS	3.8
1	B	68	ASN	3.7
1	B	178	GLN	3.7
1	B	381	ASN	3.7
1	B	382	LEU	3.7
1	A	292[A]	ASN	3.6
1	B	39	CYS	3.6
1	B	77	TRP	3.4
1	B	72	HIS	3.2
1	B	377	PRO	3.2
1	B	59	ILE	3.2
1	A	202	ALA	3.2
1	B	41	LYS	3.2
1	A	174	LEU	3.1
1	B	182	VAL	3.1
1	A	394	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	212	LEU	3.1
1	A	171	LEU	3.0
1	B	40	GLU	2.9
1	A	336	ILE	2.9
1	A	215	TYR	2.8
1	A	143[A]	GLN	2.8
1	B	196	PHE	2.8
1	B	109	HIS	2.8
1	B	108	ILE	2.8
1	B	43	SER	2.8
1	A	37	ASN	2.8
1	B	380	GLN	2.8
1	A	343	ASP	2.8
1	B	216	GLY	2.7
1	B	69	THR	2.7
1	B	217	GLN	2.7
1	A	200	LYS	2.7
1	B	180	LYS	2.7
1	A	378	PRO	2.7
1	B	66	ASP	2.6
1	B	181	SER	2.6
1	B	285	LEU	2.6
1	B	287	ALA	2.6
1	A	377	PRO	2.6
1	A	216	GLY	2.6
1	B	319	GLN	2.5
1	A	308	LEU	2.5
1	B	195	VAL	2.5
1	A	287	ALA	2.5
1	B	111	ILE	2.4
1	B	67	THR	2.4
1	B	390	LEU	2.3
1	B	45	ILE	2.3
1	B	202	ALA	2.3
1	B	71	ILE	2.3
1	B	76	ILE	2.3
1	B	147	GLN	2.3
1	B	179	ASN	2.3
1	B	218	ASN	2.3
1	A	213	ASN	2.2
1	B	146	TRP	2.2
1	B	42	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	164	TRP	2.2
1	B	391	HIS	2.2
1	B	142	GLN	2.2
1	B	64	THR	2.2
1	B	65	ASP	2.2
1	A	347	LEU	2.2
1	B	104	ALA	2.2
1	A	108	ILE	2.1
1	B	386	ILE	2.1
1	B	280	GLN	2.1
1	B	165	LEU	2.1
1	A	214	ILE	2.1
1	B	62	TYR	2.1
1	B	293	GLU	2.1
1	B	292	ASN	2.1
1	B	70	PRO	2.1
1	A	254	GLY	2.0
1	B	106	ALA	2.0
1	A	218	ASN	2.0
1	A	38	PRO	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.