



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:11 PM GMT

PDB ID : 4BRO
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
<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

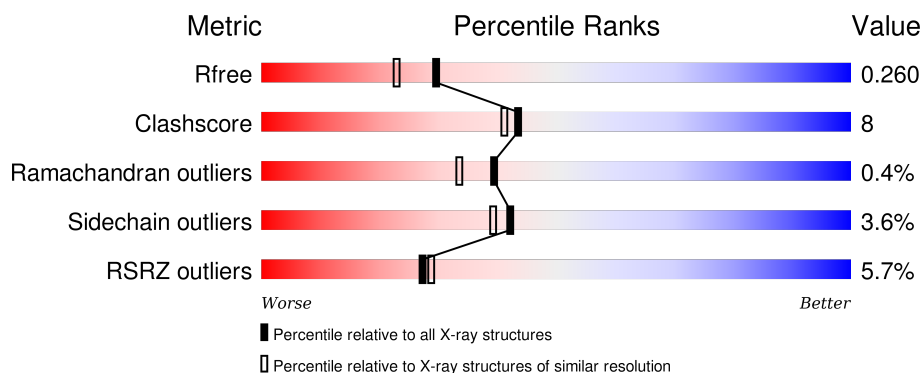
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	A	368	<div> <div>2%</div> <div>81% 14% • 5%</div> </div>
1	B	368	<div> <div>8%</div> <div>73% 20% • 5%</div> </div>

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			

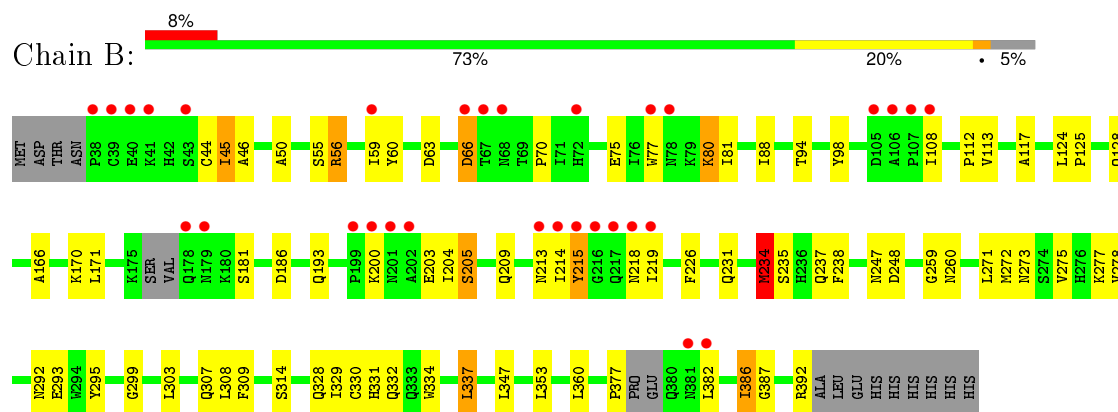
There are 22 discrepancies between the modelled and reference sequences:

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

- Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	155.99 Å 155.99 Å 79.22 Å 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) 99.4 (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 2.00 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.215 , 0.241 0.236 , 0.260	Depositor DCC
R_{free} test set	1446 reflections (1.98%)	DCC
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 , 50.2	EDS
Estimated twinning fraction	0.837 for H, K, L 0.163 for K, H, -L 0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.837 for H, K, L 0.163 for K, H, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.66	0/2916	0.80	5/3975 (0.1%)
1	B	0.53	0/2879	0.69	2/3924 (0.1%)
All	All	0.60	0/5795	0.75	7/7899 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	MET	CG-SD-CE	7.70	112.51	100.20
1	B	337	LEU	CA-CB-CG	7.48	132.51	115.30
1	A	234	MET	CG-SD-CE	6.82	111.11	100.20
1	A	134	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	122	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	134	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	308	LEU	CA-CB-CG	-5.14	103.48	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2825	0	2692	24	0
1	B	2796	0	2643	66	0
2	A	73	0	0	2	0
2	B	32	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5726	0	5335	89	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 8.

All (89) 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:272:MET:HE1	1:B:360:LEU:HD12	1.48	0.95
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:234:MET:CE	1:B:238:PHE:CD2	2.61	0.82
1:B:234:MET:HE3	1:B:238:PHE:HD2	1.47	0.79
1:B:88:ILE:HD12	1:B:94:THR:HG22	1.64	0.78
1:B:234:MET:HE1	1:B:238:PHE:CD2	2.22	0.75
1:B:234:MET:HE3	1:B:238:PHE:CD2	2.24	0.73
1:B:181:SER:H	1:B:292:ASN:HB2	1.54	0.72
1:A:307:GLN:CD	1:A:307:GLN:H	1.94	0.70
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:234:MET:O	1:B:234:MET:HE3	1.96	0.66
1:B:81:ILE:HD12	1:B:81:ILE:O	1.95	0.65
1:B:337:LEU:HG	1:B:347:LEU:HD21	1.80	0.64
1:B:231:GLN:HG3	1:B:353:LEU:CD2	2.28	0.63
1:B:234:MET:HE2	1:B:235:SER:HA	1.79	0.63
1:B:272:MET:HE1	1:B:360:LEU:CD1	2.27	0.63
1:B:272:MET:HE2	1:B:360:LEU:HA	1.82	0.61
1:B:272:MET:CE	1:B:360:LEU:HA	2.32	0.59
1:B:81:ILE:HD12	1:B:81:ILE:C	2.24	0.58
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:213:ASN:HA	1:B:218:ASN:HA	1.87	0.56
1:B:334:TRP:HZ3	1:B:347:LEU:HD23	1.70	0.56
1:B:247:ASN:O	1:B:248:ASP:HB2	2.04	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:HE2	1:A:154:ILE:HG22	1.90	0.54
1:B:303:LEU:HD11	1:B:309:PHE:CE2	2.44	0.52
1:B:307:GLN:H	1:B:307:GLN:CD	2.13	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: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:234:MET:HG3	1:B:235:SER:N	2.26	0.51
1:A:216:GLY:O	1:A:217:GLN:HB3	2.11	0.50
1:A:307:GLN:CD	1:A:307:GLN:N	2.65	0.50
1:B:66:ASP:N	1:B:66:ASP:OD1	2.36	0.50
1:B:50:ALA:HB3	1:B:117:ALA:HA	1.92	0.50
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:234:MET:HE3	1:B:234:MET:C	2.34	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:276:HIS:HE2	1:B:237[B]:GLN:HG3	1.80	0.47
1:A:270:SER:O	1:A:274:SER:HB2	2.15	0.47
1:B:214:ILE:O	1:B:215:TYR:C	2.54	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:HG3	1:B:392:ARG:H	1.58	0.46
1:B:307:GLN:CD	1:B:307:GLN:N	2.69	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
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:58:HIS:NE2	2:A:2003:HOH:O	2.37	0.43
1:A:50:ALA:HB3	1:A:117:ALA:HA	2.01	0.43
1:B:386:ILE:HG13	1:B:387:GLY:N	2.34	0.43
1:B:226:PHE:CE2	1:B:278:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:TYR:CE1	1:B:386:ILE:HG22	2.53	0.43
1:A:261:ALA:HB3	1:A:262:PRO:HD3	2.00	0.43
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.82	0.42
1:A:286:LEU:HA	1:A:286:LEU:HD23	1.77	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:B:292:ASN:O	1:B:293:GLU:HG3	2.20	0.41
1:A:187:MET:HA	1:A:192:VAL:HG12	2.02	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: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

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%)	46	41
1	B	349/368 (95%)	330 (95%)	17 (5%)	2 (1%)	30	22
All	All	700/736 (95%)	659 (94%)	38 (5%)	3 (0%)	39	33

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%)	303 (96%)	12 (4%)	40	36
1	B	309/328 (94%)	299 (97%)	10 (3%)	46	44
All	All	624/656 (95%)	602 (96%)	22 (4%)	42	40

All (22) 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	214	ILE
1	A	241	SER
1	A	270	SER
1	A	288	LEU
1	A	300	ILE
1	A	301	SER
1	A	383	ASP
1	A	394	LEU
1	B	45	ILE
1	B	56	ARG
1	B	66	ASP
1	B	75	GLU
1	B	80	LYS
1	B	108	ILE
1	B	203	GLU
1	B	205	SER
1	B	234	MET
1	B	386	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	B	289	ASN
1	B	292	ASN
1	B	331	HIS
1	B	349	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 ⓘ

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%)	0.34	9 (2%) 59 60	18, 28, 46, 64	0
1	B	351/368 (95%)	0.58	31 (8%) 12 13	22, 36, 61, 76	0
All	All	702/736 (95%)	0.46	40 (5%) 27 29	18, 32, 55, 76	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	GLY	4.9
1	B	77	TRP	4.9
1	B	43	SER	4.7
1	B	202	ALA	4.3
1	A	202	ALA	4.0
1	B	214	ILE	3.6
1	B	108	ILE	3.6
1	A	68	ASN	3.5
1	B	66	ASP	3.4
1	B	67	THR	3.4
1	B	178	GLN	3.1
1	B	218	ASN	3.1
1	B	68	ASN	3.1
1	A	203	GLU	2.9
1	B	38	PRO	2.9
1	B	213	ASN	2.9
1	A	218	ASN	2.8
1	B	106	ALA	2.7
1	B	199	PRO	2.7
1	B	179	ASN	2.6
1	B	215	TYR	2.6
1	B	382	LEU	2.5
1	A	200	LYS	2.5
1	B	40	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASN	2.4
1	B	217	GLN	2.4
1	B	39	CYS	2.4
1	A	342	PRO	2.4
1	B	105	ASP	2.3
1	B	41	LYS	2.3
1	B	381	ASN	2.3
1	A	175	LYS	2.3
1	B	107	PRO	2.2
1	A	343	ASP	2.2
1	B	219	ILE	2.1
1	A	206	LYS	2.1
1	B	201	ASN	2.0
1	B	59	ILE	2.0
1	B	72	HIS	2.0
1	B	200	LYS	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 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.