



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:59 AM UTC

PDB ID : 1AA7 / pdb_00001aa7
Title : INFLUENZA VIRUS MATRIX PROTEIN CRYSTAL STRUCTURE AT PH 4.0
Authors : Sha, B.; Luo, M.
Deposited on : 1997-01-24
Resolution : 2.08 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

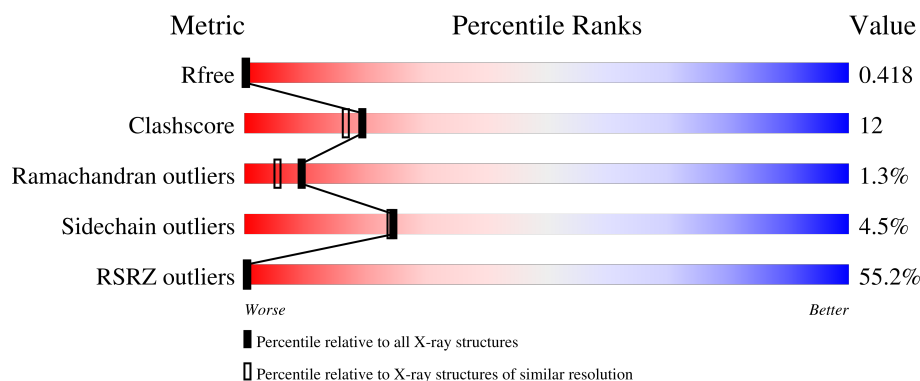
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	158	45% 77%18%6%
1	B	158	65% 72%24%. .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3238 atoms, of which 724 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 INFLUENZA VIRUS MATRIX PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	H	N	O	S	0	0	0
			1496	773	278	209	228	8			
1	B	157	Total	C	H	N	O	S	0	0	0
			1484	768	274	208	227	7			

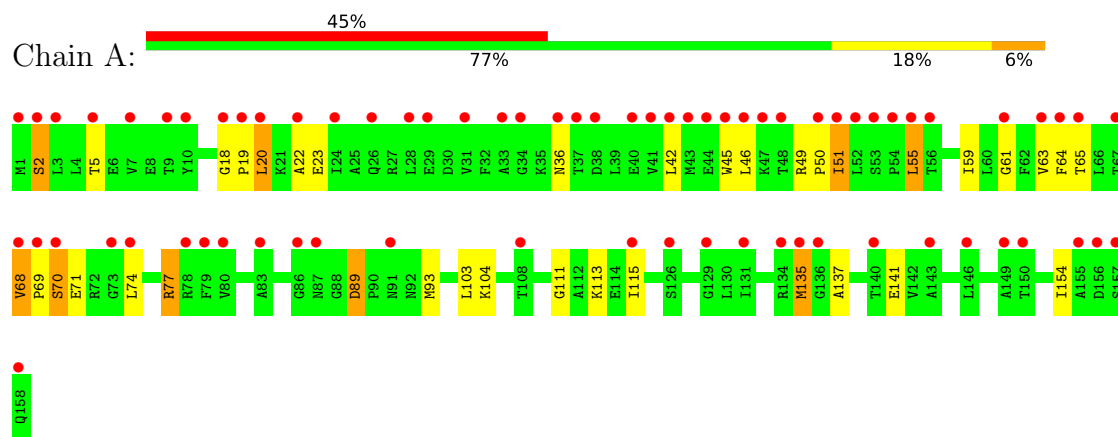
- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	49	Total	H	O	0	0
			147	98	49		
2	B	37	Total	H	O	0	0
			111	74	37		

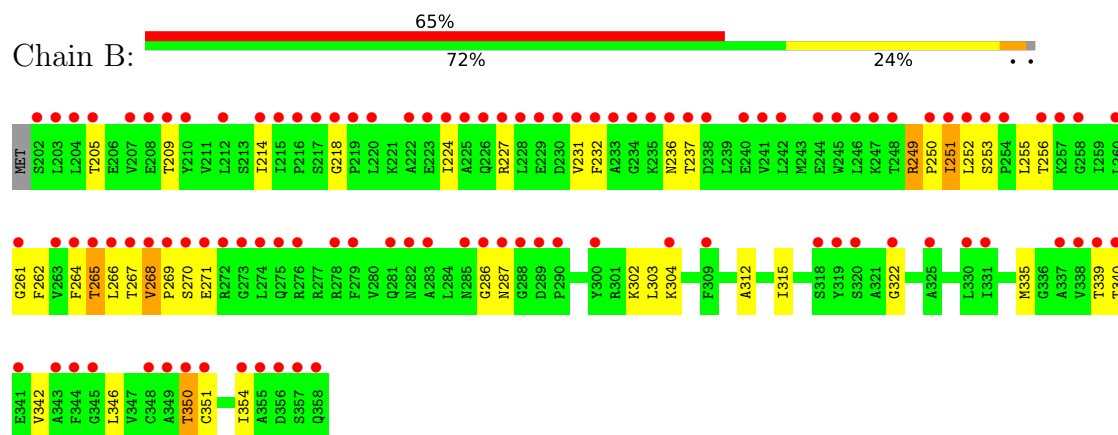
3 Residue-property plots

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: INFLUENZA VIRUS MATRIX PROTEIN



• Molecule 1: INFLUENZA VIRUS MATRIX PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.17Å 66.17Å 135.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.08 8.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.7 (8.00-2.08) 91.0 (8.00-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.06Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , 0.280 0.387 , 0.418	Depositor DCC
R_{free} test set	1904 reflections (9.51%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	3238	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [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	0.65	0/1236	1.00	5/1668 (0.3%)
1	B	0.66	0/1228	1.06	5/1658 (0.3%)
All	All	0.65	0/2464	1.03	10/3326 (0.3%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLY	CA-C-N	6.08	125.96	119.28
1	A	18	GLY	C-N-CA	6.08	125.96	119.28
1	B	271	GLU	N-CA-C	-5.79	104.93	112.23
1	B	249	ARG	CA-C-N	-5.43	115.15	120.52
1	B	249	ARG	C-N-CA	-5.43	115.15	120.52
1	A	135	MET	N-CA-C	-5.31	106.76	113.18
1	B	218	GLY	CA-C-N	5.06	124.67	119.05
1	B	218	GLY	C-N-CA	5.06	124.67	119.05
1	A	89	ASP	CA-C-N	5.02	124.80	119.28
1	A	89	ASP	C-N-CA	5.02	124.80	119.28

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	1218	278	1259	30	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1210	274	1247	28	2
2	A	49	98	0	5	2
2	B	37	74	0	1	2
All	All	2514	724	2506	57	4

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 12.

All (57) 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:303:LEU:HD23	1:B:315:ILE:HD11	1.56	0.86
1:A:103:LEU:HD23	1:A:115:ILE:HD11	1.59	0.83
1:B:261:GLY:O	1:B:265:THR:HG23	1.80	0.81
1:B:253:SER:HB3	1:B:256:THR:HG23	1.63	0.79
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.50	0.75
1:A:61:GLY:O	1:A:65:THR:HG23	1.89	0.72
1:A:74:LEU:HD13	2:A:506:HOH:O	1.91	0.69
1:B:250:PRO:O	1:B:251:ILE:HG12	1.94	0.68
1:B:214:ILE:HD11	1:B:354:ILE:HB	1.76	0.65
1:B:232:PHE:HE1	1:B:267:THR:HG21	1.60	0.65
1:A:36:ASN:HA	1:A:69:PRO:HG2	1.80	0.64
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.12	0.63
1:A:69:PRO:HG3	2:A:567:HOH:O	2.00	0.62
1:A:50:PRO:O	1:A:51:ILE:HG12	1.99	0.61
1:A:65:THR:HG21	2:A:508:HOH:O	2.02	0.59
1:A:2:SER:OG	1:A:5:THR:HG23	2.03	0.58
1:A:103:LEU:CD2	1:A:115:ILE:HD11	2.33	0.57
1:B:232:PHE:CE1	1:B:267:THR:HG21	2.39	0.56
1:B:339:THR:OG1	1:B:342:VAL:HG23	2.04	0.56
1:B:231:VAL:HG22	1:B:236:ASN:HB3	1.90	0.54
1:A:59:ILE:O	1:A:63:VAL:HG23	2.08	0.54
1:B:214:ILE:CD1	1:B:354:ILE:HB	2.38	0.54
1:B:346:LEU:O	1:B:350:THR:HG23	2.09	0.53
1:B:339:THR:HG1	1:B:342:VAL:HG23	1.74	0.52
1:A:135:MET:SD	1:B:335:MET:SD	3.07	0.52
1:A:5:THR:HG22	2:A:505:HOH:O	2.10	0.52
1:B:227:ARG:O	1:B:231:VAL:HG23	2.11	0.51
1:A:77:ARG:NH1	2:A:506:HOH:O	2.43	0.51
1:B:224:ILE:HD11	1:B:252:LEU:HD11	1.92	0.50
1:B:205:THR:O	1:B:209:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:HB2	1:B:342:VAL:HG13	1.94	0.49
1:B:266:LEU:HG	1:B:340:THR:HG23	1.95	0.48
1:A:71:GLU:O	1:A:74:LEU:HG	2.14	0.48
1:A:20:LEU:HA	1:A:23:GLU:OE1	2.13	0.48
1:B:302:LYS:NZ	2:B:548:HOH:O	2.43	0.47
1:B:264:PHE:O	1:B:268:VAL:HB	2.16	0.46
1:B:249:ARG:NE	1:B:249:ARG:HA	2.29	0.46
1:B:214:ILE:HD11	1:B:351:CYS:O	2.16	0.46
1:A:46:LEU:HD11	1:A:64:PHE:HD2	1.81	0.45
1:A:111:GLY:O	1:A:115:ILE:HG23	2.16	0.45
1:B:253:SER:HB3	1:B:256:THR:CG2	2.42	0.45
1:B:214:ILE:HA	1:B:214:ILE:HD13	1.75	0.45
1:B:269:PRO:HG2	1:B:270:SER:H	1.82	0.44
1:B:346:LEU:O	1:B:350:THR:CG2	2.65	0.44
1:A:77:ARG:HH11	1:A:77:ARG:CG	2.22	0.43
1:A:46:LEU:HD11	1:A:64:PHE:CD2	2.54	0.42
1:A:45:TRP:O	1:A:49:ARG:HG2	2.20	0.42
1:A:19:PRO:O	1:A:22:ALA:HB3	2.19	0.42
1:B:262:PHE:CD1	1:B:262:PHE:C	2.97	0.42
1:A:36:ASN:CA	1:A:69:PRO:HG2	2.46	0.42
1:B:286:GLY:O	1:B:287:ASN:OD1	2.38	0.42
1:A:89:ASP:O	1:A:93:MET:HG3	2.20	0.41
1:A:55:LEU:HD13	1:A:154:ILE:HD13	2.02	0.41
1:A:36:ASN:HA	1:A:69:PRO:CG	2.49	0.41
1:A:64:PHE:O	1:A:68:VAL:HB	2.20	0.41
1:A:104:LYS:NZ	1:A:137:ALA:O	2.53	0.41
1:A:141:GLU:H	1:A:141:GLU:CD	2.29	0.40

All (4) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:OG	2:A:529:HOH:O[5_665]	2.01	0.19
1:B:322:GLY:H	2:B:580:HOH:O[4_546]	1.46	0.14
1:B:322:GLY:N	2:B:580:HOH:O[4_546]	2.13	0.07
1:A:70:SER:CB	2:A:529:HOH:O[5_665]	2.16	0.04

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	156/158 (99%)	152 (97%)	2 (1%)	2 (1%)	9	5
1	B	155/158 (98%)	149 (96%)	4 (3%)	2 (1%)	9	5
All	All	311/316 (98%)	301 (97%)	6 (2%)	4 (1%)	9	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	ILE
1	A	2	SER
1	B	237	THR
1	A	51	ILE

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	133/133 (100%)	126 (95%)	7 (5%)	20	18
1	B	132/133 (99%)	127 (96%)	5 (4%)	29	30
All	All	265/266 (100%)	253 (96%)	12 (4%)	24	24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	42	LEU

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Mol	Chain	Res	Type
1	A	55	LEU
1	A	68	VAL
1	A	70	SER
1	A	77	ARG
1	A	113	LYS
1	B	255	LEU
1	B	265	THR
1	B	268	VAL
1	B	304	LYS
1	B	350	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	B	292	ASN

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 ⓘ

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	158/158 (100%)	2.15	71 (44%) 0 1	6, 14, 33, 43	0
1	B	157/158 (99%)	2.68	103 (65%) 0 0	4, 15, 40, 53	0
All	All	315/316 (99%)	2.41	174 (55%) 0 0	4, 14, 38, 53	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ALA	7.0
1	B	270	SER	6.3
1	A	20	LEU	5.8
1	B	203	LEU	5.8
1	B	251	ILE	5.7
1	B	287	ASN	5.4
1	B	273	GLY	5.3
1	A	51	ILE	5.2
1	A	36	ASN	5.2
1	B	202	SER	5.2
1	A	22	ALA	5.0
1	A	155	ALA	5.0
1	B	233	ALA	5.0
1	B	286	GLY	5.0
1	B	220	LEU	5.0
1	B	248	THR	5.0
1	B	256	THR	4.8
1	B	351	CYS	4.7
1	B	241	VAL	4.6
1	B	219	PRO	4.6
1	A	73	GLY	4.5
1	B	234	GLY	4.5
1	A	70	SER	4.5
1	B	355	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.4
1	A	34	GLY	4.4
1	B	252	LEU	4.4
1	B	236	ASN	4.4
1	A	31	VAL	4.3
1	B	204	LEU	4.3
1	B	285	ASN	4.3
1	B	235	LYS	4.3
1	B	229	GLU	4.3
1	B	238	ASP	4.2
1	B	228	LEU	4.2
1	B	279	PHE	4.1
1	A	67	THR	4.1
1	B	265	THR	4.1
1	A	74	LEU	4.0
1	B	240	GLU	4.0
1	A	48	THR	4.0
1	A	47	LYS	3.9
1	B	274	LEU	3.9
1	B	250	PRO	3.9
1	B	254	PRO	3.9
1	A	78	ARG	3.9
1	B	343	ALA	3.9
1	B	231	VAL	3.8
1	A	26	GLN	3.8
1	A	157	SER	3.8
1	A	9	THR	3.8
1	B	237	THR	3.7
1	A	41	VAL	3.7
1	B	209	THR	3.6
1	B	266	LEU	3.6
1	B	230	ASP	3.6
1	B	267	THR	3.6
1	A	37	THR	3.5
1	B	242	LEU	3.5
1	A	65	THR	3.5
1	B	283	ALA	3.4
1	A	158	GLN	3.4
1	B	232	PHE	3.4
1	B	322	GLY	3.4
1	B	208	GLU	3.3
1	B	350	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	269	PRO	3.3
1	B	212	LEU	3.3
1	B	245	TRP	3.3
1	A	33	ALA	3.2
1	B	349	ALA	3.2
1	B	271	GLU	3.2
1	B	225	ALA	3.1
1	B	325	ALA	3.1
1	A	29	GLU	3.1
1	B	227	ARG	3.1
1	B	272	ARG	3.1
1	B	224	ILE	3.1
1	B	318	SER	3.1
1	A	56	THR	3.1
1	A	50	PRO	3.0
1	B	216	PRO	3.0
1	A	19	PRO	3.0
1	B	264	PHE	3.0
1	A	156	ASP	3.0
1	B	247	LYS	3.0
1	A	83	ALA	3.0
1	A	143	ALA	3.0
1	B	258	GLY	3.0
1	A	126	SER	2.9
1	B	268	VAL	2.9
1	A	86	GLY	2.9
1	B	288	GLY	2.9
1	B	320	SER	2.9
1	A	136	GLY	2.9
1	B	338	VAL	2.9
1	B	218	GLY	2.9
1	A	80	VAL	2.8
1	A	52	LEU	2.8
1	A	115	ILE	2.8
1	A	18	GLY	2.8
1	A	42	LEU	2.8
1	A	54	PRO	2.8
1	B	358	GLN	2.8
1	B	330	LEU	2.8
1	A	63	VAL	2.8
1	A	68	VAL	2.8
1	B	282	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	38	ASP	2.7
1	B	341	GLU	2.7
1	B	260	LEU	2.7
1	B	226	GLN	2.7
1	B	357	SER	2.7
1	B	339	THR	2.7
1	B	205	THR	2.7
1	A	53	SER	2.7
1	B	354	ILE	2.7
1	B	223	GLU	2.6
1	A	87	ASN	2.6
1	B	281	GLN	2.6
1	B	263	VAL	2.6
1	B	331	ILE	2.6
1	A	40	GLU	2.6
1	A	150	THR	2.6
1	A	3	LEU	2.6
1	A	45	TRP	2.6
1	A	46	LEU	2.6
1	B	309	PHE	2.5
1	A	24	ILE	2.5
1	B	215	ILE	2.5
1	A	140	THR	2.5
1	A	2	SER	2.5
1	B	344	PHE	2.5
1	B	207	VAL	2.5
1	A	91	ASN	2.5
1	B	319	TYR	2.4
1	A	69	PRO	2.4
1	B	244	GLU	2.4
1	B	275	GLN	2.4
1	A	5	THR	2.4
1	B	290	PRO	2.4
1	A	146	LEU	2.4
1	A	108	THR	2.3
1	A	10	TYR	2.3
1	A	129	GLY	2.3
1	A	64	PHE	2.3
1	A	79	PHE	2.3
1	B	210	TYR	2.3
1	B	261	GLY	2.3
1	B	278	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	257	LYS	2.3
1	B	304	LYS	2.3
1	B	300	TYR	2.3
1	B	214	ILE	2.2
1	B	253	SER	2.2
1	A	28	LEU	2.2
1	B	246	LEU	2.2
1	A	43	MET	2.2
1	A	44	GLU	2.2
1	B	276	ARG	2.2
1	B	289	ASP	2.2
1	A	149	ALA	2.1
1	A	61	GLY	2.1
1	B	217	SER	2.1
1	B	348	CYS	2.1
1	A	131	ILE	2.1
1	A	55	LEU	2.1
1	A	134	ARG	2.1
1	A	7	VAL	2.1
1	B	337	ALA	2.1
1	A	135	MET	2.0
1	B	356	ASP	2.0
1	B	340	THR	2.0
1	B	345	GLY	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.