



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 PM UTC

PDB ID : 6I2M / pdb_00006i2m
Title : Crystal structure of vaccinia virus protein A55 BTB-Back domain in complex with human Cullin-3 N-terminus
Authors : Gao, G.; Graham, S.C.
Deposited on : 2018-11-01
Resolution : 2.30 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

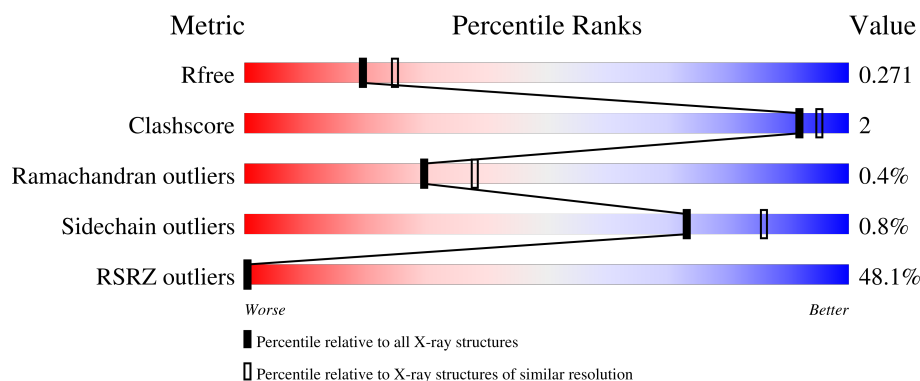
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	259	53% 71% 24%
2	B	388	32% 82% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4402 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 Kelch repeat and BTB domain-containing protein A55.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1587	1013	252	315	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLY	-	expression tag	UNP P24768
A	252	SER	-	expression tag	UNP P24768
A	253	LYS	-	expression tag	UNP P24768
A	254	HIS	-	expression tag	UNP P24768
A	255	HIS	-	expression tag	UNP P24768
A	256	HIS	-	expression tag	UNP P24768
A	257	HIS	-	expression tag	UNP P24768
A	258	HIS	-	expression tag	UNP P24768
A	259	HIS	-	expression tag	UNP P24768

- Molecule 2 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	343	Total	C	N	O	S	0	0	0
			2815	1771	491	529	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	ARG	ILE	engineered mutation	UNP Q13618
B	346	ASP	LEU	engineered mutation	UNP Q13618
B	389	ALA	-	expression tag	UNP Q13618
B	390	GLU	-	expression tag	UNP Q13618
B	391	ASN	-	expression tag	UNP Q13618
B	392	LEU	-	expression tag	UNP Q13618
B	393	TYR	-	expression tag	UNP Q13618

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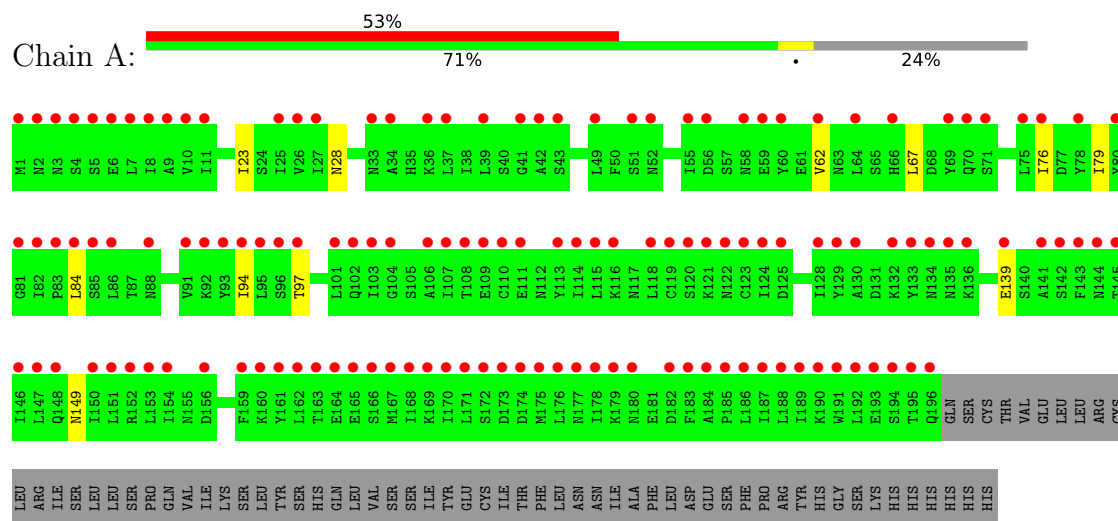
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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	PHE	-	expression tag	UNP Q13618
B	395	GLN	-	expression tag	UNP Q13618
B	396	SER	-	expression tag	UNP Q13618
B	397	HIS	-	expression tag	UNP Q13618
B	398	HIS	-	expression tag	UNP Q13618
B	399	HIS	-	expression tag	UNP Q13618
B	400	HIS	-	expression tag	UNP Q13618
B	401	HIS	-	expression tag	UNP Q13618
B	402	HIS	-	expression tag	UNP Q13618
B	403	ASP	-	expression tag	UNP Q13618
B	404	TYR	-	expression tag	UNP Q13618
B	405	LYS	-	expression tag	UNP Q13618
B	406	ASP	-	expression tag	UNP Q13618
B	407	ASP	-	expression tag	UNP Q13618
B	408	ASP	-	expression tag	UNP Q13618
B	409	ASP	-	expression tag	UNP Q13618
B	410	LYS	-	expression tag	UNP Q13618

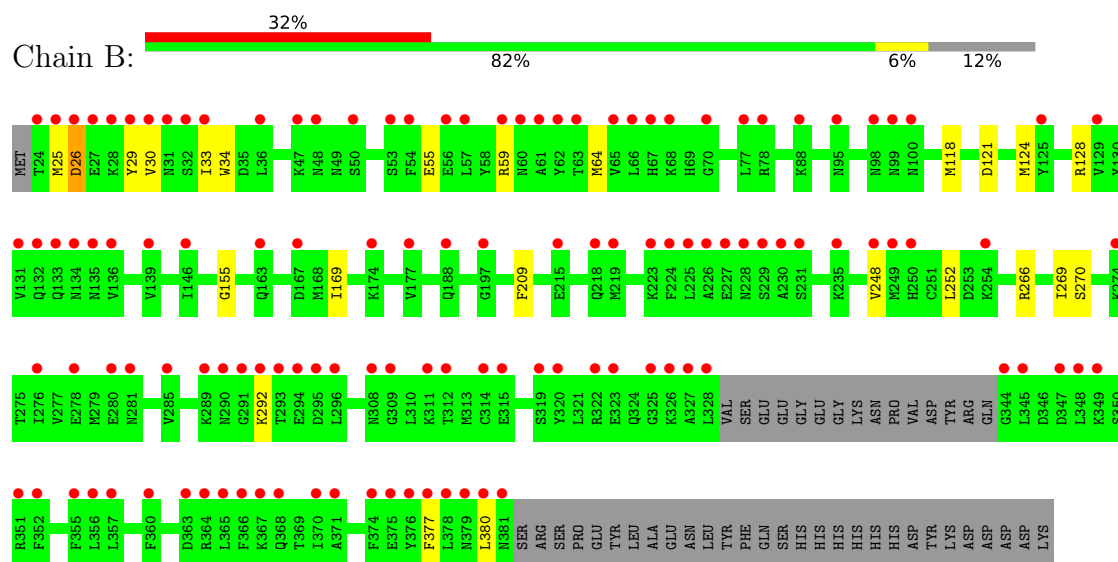
3 Residue-property plots

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: Kelch repeat and BTB domain-containing protein A55



- Molecule 2: Cullin-3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.82Å 42.52Å 148.77Å 90.00° 128.41° 90.00°	Depositor
Resolution (Å)	58.29 – 2.30 58.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	53.0 (58.29-2.30) 53.2 (58.29-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.266 , 0.282 (Not available) , 0.271	Depositor DCC
R_{free} test set	1170 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4402	wwPDB-VP
Average B, all atoms (Å ²)	73.0	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	0.78	0/1613	1.36	2/2183 (0.1%)
2	B	0.73	0/2856	1.42	2/3833 (0.1%)
All	All	0.75	0/4469	1.40	4/6016 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ASN	CA-C-N	5.29	127.43	120.60
1	A	149	ASN	C-N-CA	5.29	127.43	120.60
2	B	292	LYS	CA-C-N	5.23	128.06	120.79
2	B	292	LYS	C-N-CA	5.23	128.06	120.79

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	1587	0	1562	4	0
2	B	2815	0	2805	10	0
All	All	4402	0	4367	14	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 2.

All (14) 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)
2:B:266:ARG:HA	2:B:270:SER:HB2	1.93	0.49
2:B:26:ASP:HA	2:B:29:TYR:HB3	1.96	0.48
2:B:34:TRP:HB2	2:B:64:MET:HE1	1.97	0.47
2:B:377:PHE:HA	2:B:380:LEU:HD12	1.97	0.47
2:B:55:GLU:O	2:B:59:ARG:HG2	2.15	0.47
1:A:23:ILE:HD11	1:A:62:VAL:HG23	1.98	0.46
1:A:67:LEU:HD22	1:A:97:THR:HG23	1.99	0.45
2:B:124:MET:HE2	2:B:128:ARG:HG3	1.98	0.44
2:B:30:VAL:HA	2:B:33:ILE:HG12	2.00	0.43
2:B:169:ILE:HG21	2:B:209:PHE:HE1	1.84	0.43
1:A:84:LEU:HD21	1:A:94:ILE:HG21	2.03	0.41
2:B:248:VAL:HG22	2:B:252:LEU:HD12	2.02	0.41
2:B:118:MET:HA	2:B:121:ASP:HB2	2.03	0.40
1:A:76:ILE:HA	1:A:79:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

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	194/259 (75%)	182 (94%)	11 (6%)	1 (0%)	24	31
2	B	339/388 (87%)	330 (97%)	8 (2%)	1 (0%)	36	46
All	All	533/647 (82%)	512 (96%)	19 (4%)	2 (0%)	30	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	155	GLY
1	A	28	ASN

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	183/244 (75%)	182 (100%)	1 (0%)	81	90
2	B	313/355 (88%)	310 (99%)	3 (1%)	68	82
All	All	496/599 (83%)	492 (99%)	4 (1%)	73	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLU
2	B	25	MET
2	B	26	ASP
2	B	269	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	28	ASN
1	A	52	ASN
1	A	88	ASN
1	A	122	ASN
2	B	31	ASN
2	B	42	GLN
2	B	60	ASN
2	B	84	HIS
2	B	163	GLN
2	B	218	GLN
2	B	281	ASN
2	B	308	ASN
2	B	362	ASN

5.3.3 RNA ⓘ

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 [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	196/259 (75%)	2.74	136 (69%) 0 0	68, 85, 109, 143	0
2	B	343/388 (88%)	1.70	123 (35%) 1 1	33, 60, 104, 140	0
All	All	539/647 (83%)	2.07	259 (48%) 0 0	33, 75, 106, 143	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	345	LEU	10.3
1	A	196	GLN	7.3
1	A	175	MET	7.2
2	B	328	LEU	7.0
2	B	229	SER	6.3
1	A	171	LEU	6.2
1	A	184	ALA	6.2
1	A	60	TYR	6.2
2	B	344	GLY	6.1
2	B	24	THR	6.1
1	A	176	LEU	5.9
1	A	183	PHE	5.9
1	A	147	LEU	5.8
2	B	235	LYS	5.8
2	B	374	PHE	5.6
2	B	378	LEU	5.5
1	A	191	TRP	5.3
1	A	178	ILE	5.2
1	A	108	THR	5.2
1	A	123	CYS	5.0
1	A	153	LEU	5.0
2	B	379	ASN	4.9
1	A	81	GLY	4.7
1	A	95	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	107	ILE	4.7
1	A	169	LYS	4.6
1	A	144	ASN	4.5
1	A	160	LYS	4.5
2	B	60	ASN	4.5
2	B	59	ARG	4.4
2	B	349	LYS	4.4
1	A	151	LEU	4.3
1	A	170	ILE	4.3
1	A	55	ILE	4.3
1	A	172	SER	4.3
2	B	323	GLU	4.3
2	B	380	LEU	4.3
2	B	376	TYR	4.2
1	A	86	LEU	4.2
1	A	162	LEU	4.2
1	A	192	LEU	4.2
1	A	37	LEU	4.1
1	A	179	LYS	4.1
1	A	1	MET	4.1
1	A	188	LEU	4.1
1	A	104	GLY	4.0
1	A	8	ILE	4.0
2	B	99	ASN	4.0
2	B	50	SER	4.0
1	A	186	LEU	3.9
1	A	124	ILE	3.9
2	B	381	ASN	3.9
2	B	29	TYR	3.9
2	B	28	LYS	3.9
2	B	370	ILE	3.9
1	A	103	ILE	3.8
1	A	148	GLN	3.8
2	B	56	GLU	3.8
1	A	91	VAL	3.8
1	A	159	PHE	3.8
1	A	122	ASN	3.7
2	B	352	PHE	3.7
1	A	187	ILE	3.7
2	B	348	LEU	3.7
1	A	41	GLY	3.7
2	B	249	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	146	ILE	3.6
1	A	180	ASN	3.6
2	B	131	VAL	3.6
2	B	355	PHE	3.6
1	A	195	THR	3.5
1	A	42	ALA	3.5
2	B	322	ARG	3.5
1	A	4	SER	3.5
2	B	33	ILE	3.5
1	A	113	TYR	3.5
1	A	7	LEU	3.5
2	B	281	ASN	3.5
1	A	136	LYS	3.5
1	A	189	ILE	3.5
2	B	356	LEU	3.4
2	B	365	LEU	3.4
1	A	82	ILE	3.4
1	A	110	CYS	3.4
2	B	224	PHE	3.4
2	B	367	LYS	3.3
1	A	168	ILE	3.3
1	A	185	PRO	3.3
1	A	173	ASP	3.3
2	B	294	GLU	3.3
1	A	80	TYR	3.3
1	A	154	ILE	3.3
1	A	78	TYR	3.3
1	A	190	LYS	3.2
1	A	36	LYS	3.2
1	A	84	LEU	3.2
2	B	27	GLU	3.2
1	A	93	TYR	3.2
2	B	30	VAL	3.2
2	B	31	ASN	3.2
1	A	66	HIS	3.2
1	A	115	LEU	3.2
1	A	11	ILE	3.2
2	B	68	LYS	3.1
2	B	129	VAL	3.1
2	B	248	VAL	3.1
2	B	315	GLU	3.1
2	B	360	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	65	VAL	3.1
2	B	357	LEU	3.1
1	A	145	THR	3.1
1	A	6	GLU	3.1
1	A	166	SER	3.1
2	B	364	ARG	3.1
1	A	70	GLN	3.0
2	B	132	GLN	3.0
2	B	227	GLU	3.0
1	A	121	LYS	3.0
1	A	152	ARG	3.0
1	A	56	ASP	3.0
1	A	64	LEU	3.0
2	B	377	PHE	2.9
2	B	320	TYR	2.9
1	A	142	SER	2.9
1	A	52	ASN	2.9
2	B	167	ASP	2.9
1	A	132	LYS	2.9
1	A	150	ILE	2.9
1	A	133	TYR	2.9
1	A	125	ASP	2.9
2	B	326	LYS	2.9
2	B	254	LYS	2.9
1	A	5	SER	2.8
1	A	177	ASN	2.9
2	B	290	ASN	2.9
2	B	66	LEU	2.8
2	B	26	ASP	2.8
2	B	219	MET	2.8
1	A	43	SER	2.8
1	A	128	ILE	2.8
2	B	36	LEU	2.8
2	B	25	MET	2.8
1	A	143	PHE	2.8
1	A	39	LEU	2.7
2	B	77	LEU	2.7
2	B	225	LEU	2.7
2	B	136	VAL	2.7
2	B	218	GLN	2.7
2	B	291	GLY	2.7
1	A	193	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	174	LYS	2.7
1	A	167	MET	2.7
2	B	67	HIS	2.7
2	B	70	GLY	2.7
1	A	165	GLU	2.7
2	B	133	GLN	2.7
2	B	47	LYS	2.7
1	A	25	ILE	2.7
2	B	230	ALA	2.6
1	A	194	SER	2.6
1	A	33	ASN	2.6
1	A	58	ASN	2.6
2	B	32	SER	2.6
2	B	319	SER	2.6
2	B	226	ALA	2.6
1	A	111	GLU	2.6
2	B	215	GLU	2.6
2	B	134	ASN	2.6
1	A	27	ILE	2.6
1	A	92	LYS	2.6
2	B	292	LYS	2.6
1	A	49	LEU	2.5
1	A	118	LEU	2.5
2	B	54	PHE	2.5
2	B	125	TYR	2.5
1	A	119	CYS	2.5
1	A	134	ASN	2.5
1	A	141	ALA	2.5
2	B	289	LYS	2.5
2	B	293	THR	2.5
2	B	139	VAL	2.5
1	A	109	GLU	2.5
1	A	75	LEU	2.5
1	A	106	ALA	2.5
1	A	97	THR	2.5
2	B	228	ASN	2.4
2	B	368	GLN	2.4
2	B	375	GLU	2.4
1	A	96	SER	2.4
1	A	10	VAL	2.4
1	A	94	ILE	2.4
2	B	311	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	101	LEU	2.4
1	A	129	TYR	2.4
1	A	3	ASN	2.4
2	B	146	ILE	2.4
1	A	161	TYR	2.3
2	B	197	GLY	2.3
1	A	26	VAL	2.3
1	A	156	ASP	2.3
2	B	62	TYR	2.3
2	B	223	LYS	2.3
1	A	59	GLU	2.3
1	A	62	VAL	2.3
2	B	163	GLN	2.3
2	B	188	GLN	2.3
2	B	296	LEU	2.3
1	A	135	ASN	2.3
2	B	295	ASP	2.3
2	B	351	ARG	2.3
1	A	76	ILE	2.3
1	A	114	ILE	2.3
2	B	285	VAL	2.3
2	B	363	ASP	2.3
2	B	366	PHE	2.2
2	B	95	ASN	2.2
2	B	308	ASN	2.2
2	B	78	ARG	2.2
2	B	312	THR	2.2
1	A	88	ASN	2.2
1	A	174	ASP	2.2
2	B	325	GLY	2.2
1	A	164	GLU	2.2
2	B	250	HIS	2.2
1	A	9	ALA	2.2
2	B	61	ALA	2.2
2	B	327	ALA	2.2
2	B	177	VAL	2.2
1	A	139	GLU	2.2
1	A	102	GLN	2.2
1	A	71	SER	2.2
2	B	63	THR	2.2
2	B	278	GLU	2.2
1	A	163	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	2.1
2	B	100	ASN	2.1
1	A	130	ALA	2.1
1	A	116	LYS	2.1
2	B	48	ASN	2.1
2	B	280	GLU	2.1
2	B	347	ASP	2.1
2	B	309	GLY	2.1
1	A	120	SER	2.1
2	B	274	LYS	2.1
2	B	98	ASN	2.1
2	B	276	ILE	2.1
1	A	69	TYR	2.1
1	A	51	SER	2.0
1	A	85	SER	2.0
2	B	371	ALA	2.0
2	B	57	LEU	2.0
1	A	83	PRO	2.0
2	B	53	SER	2.0
2	B	231	SER	2.0
1	A	34	ALA	2.0
2	B	314	CYS	2.0
1	A	182	ASP	2.0
2	B	135	ASN	2.0
2	B	88	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 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.