



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:44 AM UTC

PDB ID : 1BXX / pdb_00001bxx
Title : MU2 ADAPTIN SUBUNIT (AP50) OF AP2 ADAPTOR (SECOND DOMAIN), COMPLEXED WITH TGN38 INTERNALIZATION PEPTIDE DYQRLN
Authors : Owen, D.J.; Evans, P.R.
Deposited on : 1998-10-08
Resolution : 2.70 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

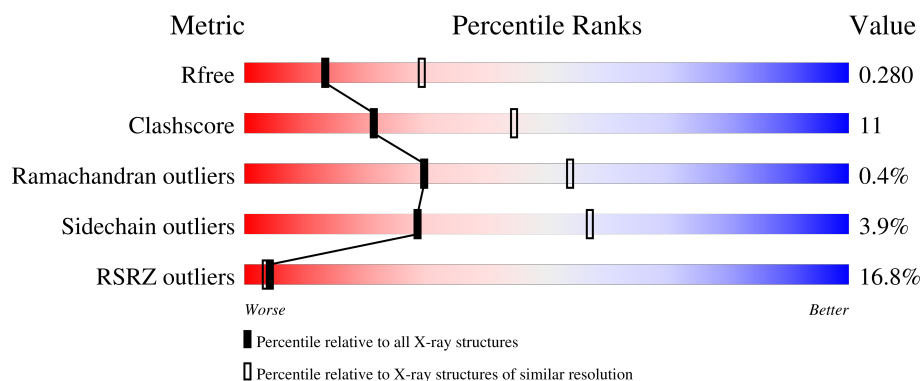
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	285	15% 55% 28% 6% 10%
2	P	6	50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2142 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 PROTEIN (AP50).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2036	1312	349	361	14			

- Molecule 2 is a protein called PROTEIN (TGN38 PEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			57	34	11	12			

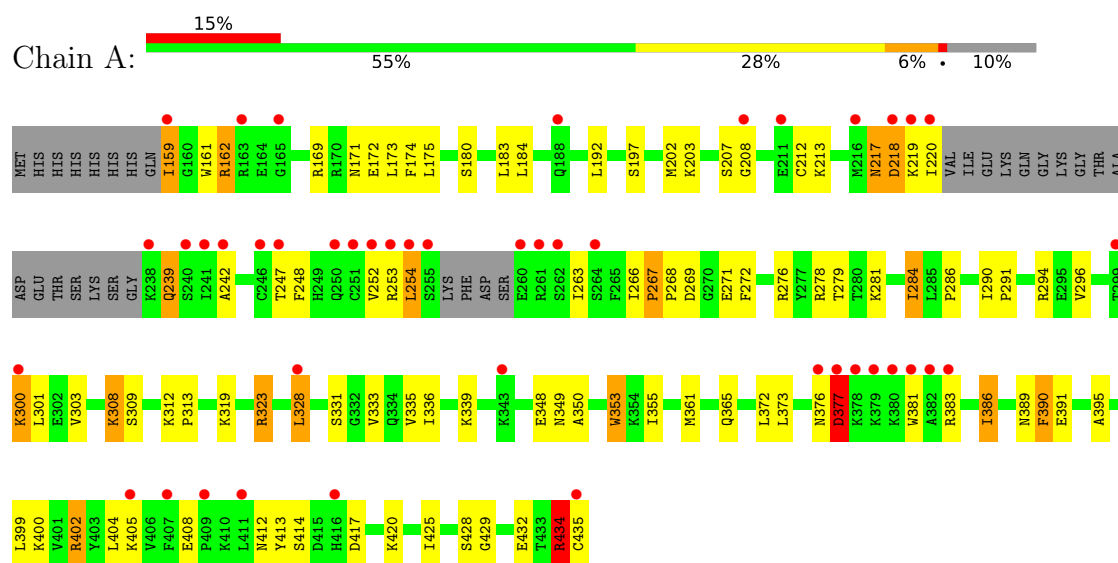
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	P	2	Total	O	0	0
			2	2		

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: PROTEIN (AP50)



- Molecule 2: PROTEIN (TGN38 PEPTIDE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	125.26Å 125.26Å 73.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.00 – 2.70 22.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (22.00-2.70) 98.2 (22.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.67Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.263 , 0.325 0.234 , 0.280	Depositor DCC
R_{free} test set	932 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2142	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.79	0/2077	2.04	68/2797 (2.4%)
2	P	0.71	0/57	2.10	2/74 (2.7%)
All	All	0.79	0/2134	2.04	70/2871 (2.4%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ARG	CD-NE-CZ	11.43	140.40	124.40
1	A	336	ILE	N-CA-CB	8.42	123.81	111.52
1	A	192	LEU	CA-C-O	8.01	129.24	119.79
1	A	425	ILE	CA-C-N	-7.79	114.81	122.36
1	A	425	ILE	C-N-CA	-7.79	114.81	122.36
1	A	169	ARG	CA-C-O	7.75	128.93	119.79
1	A	372	LEU	N-CA-C	7.72	122.02	109.59
1	A	417	ASP	N-CA-C	-7.65	103.75	113.23
1	A	434	ARG	NE-CZ-NH1	7.62	129.12	121.50
1	A	217	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	278	ARG	CA-C-O	7.35	129.42	121.11
1	A	323	ARG	CB-CA-C	7.30	122.69	110.79
1	A	239	GLN	CB-CG-CD	7.29	124.99	112.60
1	A	395	ALA	CA-C-O	7.17	123.95	119.29
1	A	429	GLY	N-CA-C	-7.09	96.37	113.18
1	A	402	ARG	NE-CZ-NH2	7.06	125.55	119.20
1	A	434	ARG	NE-CZ-NH2	-7.03	112.88	119.20
1	A	162	ARG	CD-NE-CZ	6.96	134.14	124.40
1	A	267	PRO	N-CA-C	6.96	119.19	110.70
1	A	365	GLN	OE1-CD-NE2	6.89	129.49	122.60
2	P	3	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	A	412	ASN	N-CA-C	6.69	121.81	112.72
1	A	432	GLU	N-CA-C	6.67	120.55	109.95
1	A	218	ASP	N-CA-C	6.60	120.98	112.26
1	A	172	GLU	N-CA-CB	-6.55	99.45	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	269	ASP	CA-C-O	-6.41	113.66	121.36
1	A	323	ARG	N-CA-CB	-6.33	99.95	110.47
1	A	414	SER	O-C-N	-6.12	114.47	122.97
1	A	183	LEU	N-CA-C	6.04	119.08	108.75
2	P	3	GLN	CB-CG-CD	6.03	122.86	112.60
1	A	266	ILE	N-CA-C	-5.96	96.00	108.88
1	A	414	SER	CA-C-O	5.96	129.40	121.78
1	A	301	LEU	N-CA-CB	5.90	120.59	110.68
1	A	333	VAL	N-CA-C	5.89	116.77	108.17
1	A	323	ARG	NH1-CZ-NH2	5.88	126.95	119.30
1	A	386	ILE	N-CA-C	-5.88	101.21	109.21
1	A	197	SER	CA-C-N	-5.86	116.90	121.82
1	A	197	SER	C-N-CA	-5.86	116.90	121.82
1	A	389	ASN	N-CA-C	-5.80	99.56	109.24
1	A	309	SER	O-C-N	-5.79	116.47	123.13
1	A	300	LYS	N-CA-C	5.71	118.08	109.23
1	A	390	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	335	VAL	CB-CA-C	-5.66	101.63	110.69
1	A	247	THR	CA-C-O	5.66	127.73	121.11
1	A	278	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	A	353	TRP	O-C-N	5.60	129.88	123.27
1	A	432	GLU	CA-CB-CG	-5.56	102.98	114.10
1	A	420	LYS	N-CA-C	5.50	117.93	109.07
1	A	408	GLU	CB-CA-C	5.50	119.67	110.55
1	A	389	ASN	N-CA-CB	5.47	120.90	111.00
1	A	432	GLU	N-CA-CB	-5.43	102.17	110.85
1	A	350	ALA	N-CA-C	5.42	117.08	108.79
1	A	281	LYS	CA-C-N	5.41	131.87	121.54
1	A	281	LYS	C-N-CA	5.41	131.87	121.54
1	A	365	GLN	O-C-N	5.39	129.69	123.17
1	A	308	LYS	CA-C-O	-5.39	114.54	120.36
1	A	276	ARG	N-CA-CB	-5.39	101.25	111.00
1	A	323	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	A	171	ASN	CA-C-O	5.33	126.63	120.60
1	A	377	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	284	ILE	CB-CA-C	-5.27	105.54	111.23
1	A	171	ASN	OD1-CG-ND2	5.27	127.87	122.60
1	A	349	ASN	OD1-CG-ND2	5.19	127.79	122.60
1	A	208	GLY	CA-C-N	5.17	127.18	122.37
1	A	208	GLY	C-N-CA	5.17	127.18	122.37
1	A	395	ALA	O-C-N	-5.16	117.05	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLU	N-CA-C	5.15	117.63	109.50
1	A	353	TRP	CA-C-O	-5.13	114.68	120.32
1	A	303	VAL	CA-C-O	5.09	125.73	120.39

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	2036	0	2094	45	0
2	P	57	0	53	1	0
3	A	47	0	0	1	0
3	P	2	0	0	0	0
All	All	2142	0	2147	46	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 11.

All (46) 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:A:220:ILE:HG12	1:A:242:ALA:HA	1.54	0.89
1:A:328:LEU:HD12	1:A:328:LEU:H	1.45	0.82
1:A:434:ARG:HD3	3:A:16:HOH:O	1.85	0.77
1:A:239:GLN:HB2	1:A:402:ARG:NH2	2.06	0.71
1:A:239:GLN:HB2	1:A:402:ARG:HH22	1.55	0.69
1:A:175:LEU:HD11	1:A:404:LEU:HD22	1.79	0.64
1:A:328:LEU:H	1:A:328:LEU:CD1	2.11	0.62
1:A:173:LEU:CD1	1:A:404:LEU:HD23	2.30	0.62
1:A:252:VAL:HG13	1:A:263:ILE:HG23	1.82	0.61
1:A:328:LEU:HD12	1:A:328:LEU:N	2.16	0.61
1:A:217:ASN:HB3	1:A:402:ARG:HH21	1.67	0.59
1:A:331:SER:HB3	1:A:373:LEU:HG	1.85	0.58
1:A:399:LEU:HD23	1:A:400:LYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:CE1	1:A:263:ILE:HG12	2.40	0.57
1:A:323:ARG:HH22	1:A:348:GLU:HB3	1.69	0.56
1:A:254:LEU:H	1:A:254:LEU:HD22	1.70	0.56
1:A:284:ILE:O	1:A:286:PRO:HD3	2.06	0.55
1:A:248:PHE:HE1	1:A:263:ILE:HG12	1.72	0.54
1:A:361:MET:HE3	1:A:361:MET:HA	1.89	0.53
1:A:376:ASN:HD22	1:A:376:ASN:C	2.17	0.53
1:A:161:TRP:HH2	1:A:253:ARG:HH21	1.56	0.53
1:A:173:LEU:HD13	1:A:404:LEU:HD23	1.90	0.52
1:A:376:ASN:HD22	1:A:377:ASP:N	2.07	0.52
1:A:212:CYS:HA	1:A:405:LYS:O	2.09	0.51
1:A:174:PHE:HB2	1:A:203:LYS:HB2	1.93	0.49
1:A:207:SER:HB2	1:A:413:TYR:CE1	2.48	0.48
1:A:159:ILE:HG22	1:A:162:ARG:H	1.79	0.48
1:A:213:LYS:HB2	1:A:405:LYS:HB2	1.96	0.47
2:P:5:LEU:O	2:P:6:ASN:C	2.58	0.47
1:A:252:VAL:CG1	1:A:263:ILE:HG23	2.44	0.46
1:A:290:ILE:HD13	1:A:308:LYS:HE2	1.98	0.46
1:A:390:PHE:CE2	1:A:428:SER:HB3	2.52	0.45
1:A:219:LYS:O	1:A:220:ILE:HB	2.16	0.45
1:A:399:LEU:HD23	1:A:399:LEU:C	2.41	0.45
1:A:296:VAL:HB	1:A:300:LYS:HB2	1.99	0.44
1:A:202:MET:HE3	1:A:404:LEU:HD21	2.00	0.44
1:A:312:LYS:HA	1:A:313:PRO:HD3	1.86	0.43
1:A:268:PRO:HD2	1:A:272:PHE:CE1	2.54	0.43
1:A:319:LYS:NZ	1:A:391:GLU:CD	2.78	0.42
1:A:353:TRP:CE2	1:A:355:ILE:HD11	2.54	0.42
1:A:381:TRP:CE3	1:A:383:ARG:HG2	2.54	0.42
1:A:203:LYS:HG2	1:A:271:GLU:HB2	2.02	0.41
1:A:267:PRO:HA	1:A:268:PRO:HD3	1.92	0.41
1:A:268:PRO:HD2	1:A:272:PHE:CD1	2.56	0.41
1:A:218:ASP:O	1:A:219:LYS:C	2.65	0.40
1:A:291:PRO:HB3	1:A:386:ILE:HD12	2.03	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	250/285 (88%)	230 (92%)	19 (8%)	1 (0%)	30	54
2	P	4/6 (67%)	4 (100%)	0	0	100	100
All	All	254/291 (87%)	234 (92%)	19 (8%)	1 (0%)	30	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU

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	225/257 (88%)	216 (96%)	9 (4%)	28	56
2	P	6/6 (100%)	6 (100%)	0	100	100
All	All	231/263 (88%)	222 (96%)	9 (4%)	28	57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	180	SER
1	A	184	LEU
1	A	279	THR
1	A	328	LEU

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Mol	Chain	Res	Type
1	A	339	LYS
1	A	377	ASP
1	A	434	ARG
1	A	435	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	365	GLN
1	A	376	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 [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	256/285 (89%)	1.00	44 (17%) 4 3	48, 72, 119, 140	0
2	P	6/6 (100%)	0.70	0 100 100	58, 79, 80, 102	0
All	All	262/291 (90%)	1.00	44 (16%) 4 3	48, 72, 117, 140	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	9.5
1	A	261	ARG	7.4
1	A	254	LEU	6.9
1	A	255	SER	5.3
1	A	299	THR	4.8
1	A	379	LYS	4.5
1	A	238	LYS	4.4
1	A	219	LYS	4.4
1	A	260	GLU	4.2
1	A	377	ASP	3.9
1	A	382	ALA	3.8
1	A	376	ASN	3.8
1	A	208	GLY	3.7
1	A	409	PRO	3.7
1	A	380	LYS	3.6
1	A	407	PHE	3.6
1	A	262	SER	3.4
1	A	383	ARG	3.4
1	A	159	ILE	3.4
1	A	328	LEU	3.3
1	A	188	GLN	3.2
1	A	218	ASP	3.1
1	A	378	LYS	2.9
1	A	253	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	381	TRP	2.8
1	A	165	GLY	2.7
1	A	250	GLN	2.7
1	A	246	CYS	2.6
1	A	163	ARG	2.6
1	A	240	SER	2.6
1	A	242	ALA	2.6
1	A	241	ILE	2.6
1	A	405	LYS	2.4
1	A	247	THR	2.3
1	A	251	CYS	2.3
1	A	300	LYS	2.3
1	A	416	HIS	2.2
1	A	264	SER	2.2
1	A	435	CYS	2.2
1	A	411	LEU	2.2
1	A	211	GLU	2.1
1	A	343	LYS	2.1
1	A	216	MET	2.1
1	A	252	VAL	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.