Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 04:09 pm BST

PDB ID	:	4BK5 / pdb_00004bk5
Title	:	crystal structure of the human EphA4 ectodomain in complex with human ephrin A5 (amine-methylated sample)
Authors	:	Seiradake, E.; Schaupp, A.; del Toro Ruiz, D.; Kaufmann, R.; Mitakidis, N.; Harlos, K.; Aricescu, A.R.; Klein, R.; Jones, E.Y.
Deposited on	:	2013-04-22
Resolution	:	4.00 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:

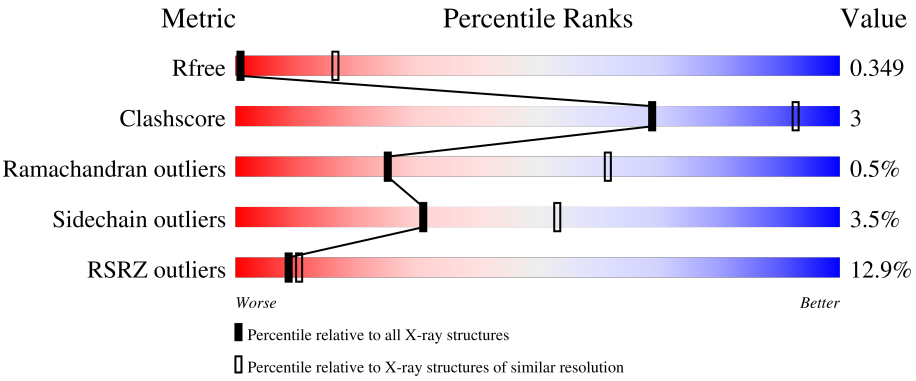
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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 <=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	568	13% 76% 12% · 11%
2	C	180	6% 69% 7% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5087 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 EPHRIN TYPE-A RECEPTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	3948	2461	682	779	26	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P54764
A	-10	GLY	-	expression tag	UNP P54764
A	-9	ILE	-	expression tag	UNP P54764
A	-8	LEU	-	expression tag	UNP P54764
A	-7	PRO	-	expression tag	UNP P54764
A	-6	SER	-	expression tag	UNP P54764
A	-5	PRO	-	expression tag	UNP P54764
A	-4	GLY	-	expression tag	UNP P54764
A	-3	MET	-	expression tag	UNP P54764
A	-2	PRO	-	expression tag	UNP P54764
A	-1	ALA	-	expression tag	UNP P54764
A	0	LEU	-	expression tag	UNP P54764
A	1	LEU	-	expression tag	UNP P54764
A	2	SER	-	expression tag	UNP P54764
A	3	LEU	-	expression tag	UNP P54764
A	4	VAL	-	expression tag	UNP P54764
A	5	SER	-	expression tag	UNP P54764
A	6	LEU	-	expression tag	UNP P54764
A	7	LEU	-	expression tag	UNP P54764
A	8	SER	-	expression tag	UNP P54764
A	9	VAL	-	expression tag	UNP P54764
A	10	LEU	-	expression tag	UNP P54764
A	11	LEU	-	expression tag	UNP P54764
A	12	MET	-	expression tag	UNP P54764
A	13	GLY	-	expression tag	UNP P54764
A	14	CYS	-	expression tag	UNP P54764
A	15	VAL	-	expression tag	UNP P54764

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Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	expression tag	UNP P54764
A	17	GLU	-	expression tag	UNP P54764
A	18	THR	-	expression tag	UNP P54764
A	19	GLY	-	expression tag	UNP P54764
A	548	GLY	-	expression tag	UNP P54764
A	549	THR	-	expression tag	UNP P54764
A	550	LYS	-	expression tag	UNP P54764
A	551	HIS	-	expression tag	UNP P54764
A	552	HIS	-	expression tag	UNP P54764
A	553	HIS	-	expression tag	UNP P54764
A	554	HIS	-	expression tag	UNP P54764
A	555	HIS	-	expression tag	UNP P54764
A	556	HIS	-	expression tag	UNP P54764

- Molecule 2 is a protein called EPHRIN-A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	1
			1139	728	197	206	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	expression tag	UNP P52803
C	1	GLY	-	expression tag	UNP P52803
C	2	ILE	-	expression tag	UNP P52803
C	3	LEU	-	expression tag	UNP P52803
C	4	PRO	-	expression tag	UNP P52803
C	5	SER	-	expression tag	UNP P52803
C	6	PRO	-	expression tag	UNP P52803
C	7	GLY	-	expression tag	UNP P52803
C	8	MET	-	expression tag	UNP P52803
C	9	PRO	-	expression tag	UNP P52803
C	10	ALA	-	expression tag	UNP P52803
C	11	LEU	-	expression tag	UNP P52803
C	12	LEU	-	expression tag	UNP P52803
C	13	SER	-	expression tag	UNP P52803
C	14	LEU	-	expression tag	UNP P52803
C	15	VAL	-	expression tag	UNP P52803
C	16	SER	-	expression tag	UNP P52803
C	17	LEU	-	expression tag	UNP P52803
C	18	LEU	-	expression tag	UNP P52803

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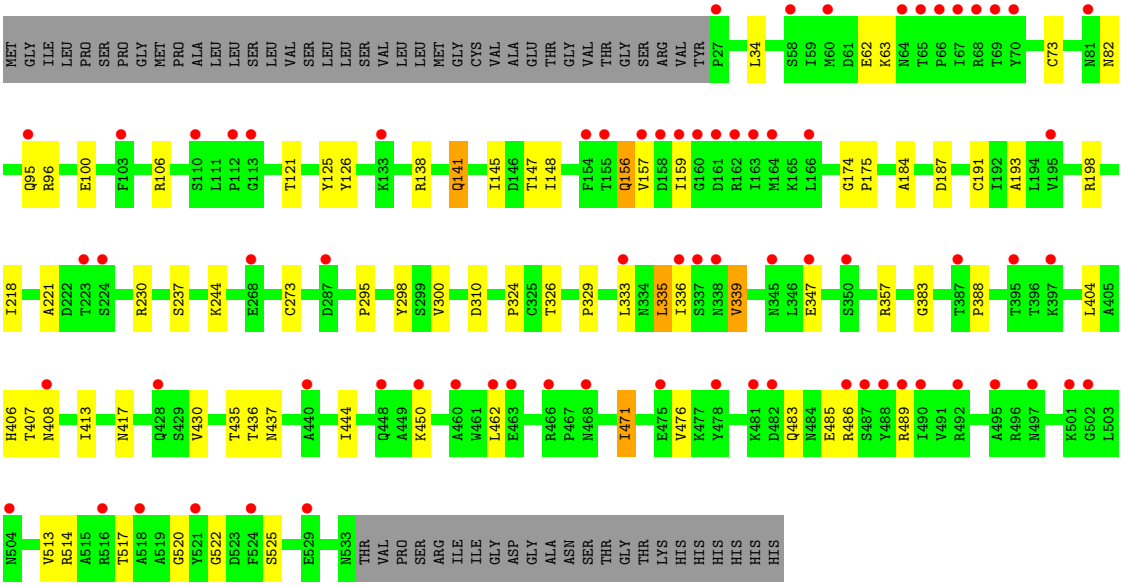
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	SER	-	expression tag	UNP P52803
C	20	VAL	-	expression tag	UNP P52803
C	21	LEU	-	expression tag	UNP P52803
C	22	LEU	-	expression tag	UNP P52803
C	23	MET	-	expression tag	UNP P52803
C	24	GLY	-	expression tag	UNP P52803
C	25	CYS	-	expression tag	UNP P52803
C	26	VAL	-	expression tag	UNP P52803
C	27	ALA	-	expression tag	UNP P52803
C	28	GLU	-	expression tag	UNP P52803
C	29	THR	-	expression tag	UNP P52803
C	30	GLY	-	expression tag	UNP P52803
C	172	GLY	-	expression tag	UNP P52803
C	173	THR	-	expression tag	UNP P52803
C	174	LYS	-	expression tag	UNP P52803
C	175	HIS	-	expression tag	UNP P52803
C	176	HIS	-	expression tag	UNP P52803
C	177	HIS	-	expression tag	UNP P52803
C	178	HIS	-	expression tag	UNP P52803
C	179	HIS	-	expression tag	UNP P52803
C	180	HIS	-	expression tag	UNP P52803

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.

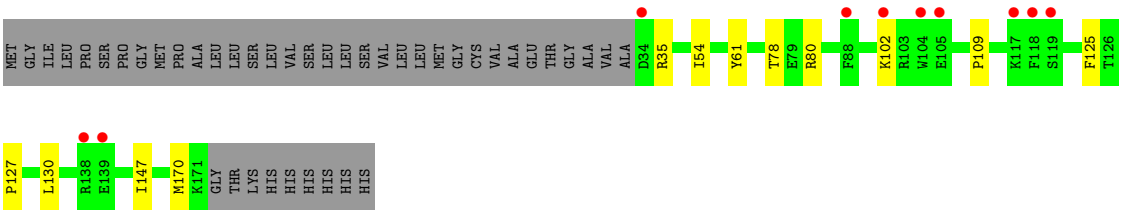
• Molecule 1: EPHRIN TYPE-A RECEPTOR 4

Chain A:



• Molecule 2: EPHRIN-A5

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	256.95Å 256.95Å 252.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.41 – 4.00 70.41 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.41-4.00) 99.9 (70.41-4.00)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 4.01Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.312 , 0.321 0.341 , 0.349	Depositor DCC
R_{free} test set	1362 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	154.9	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 215.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	5087	wwPDB-VP
Average B, all atoms (Å^2)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.72	0/4032	1.15	4/5484 (0.1%)
2	C	0.68	1/1177 (0.1%)	1.03	0/1592
All	All	0.71	1/5209 (0.0%)	1.13	4/7076 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	170	MET	C-N	-5.59	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	333	LEU	N-CA-C	7.77	119.75	111.28
1	A	159	ILE	N-CA-C	5.16	115.93	110.72
1	A	156	GLN	N-CA-C	5.12	117.99	111.69
1	A	520	GLY	N-CA-C	5.06	117.41	110.58

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	3948	0	3801	31	0
2	C	1139	0	1053	6	0
All	All	5087	0	4854	34	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 3.

All (34) 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:138:ARG:HB3	1:A:141:GLN:HB2	1.85	0.58
2:C:35:ARG:HG2	2:C:61:TYR:HB2	1.86	0.58
1:A:329:PRO:HD3	1:A:417:ASN:HB2	1.87	0.57
1:A:471:ILE:HA	1:A:517:THR:HG22	1.87	0.56
1:A:336:ILE:HB	1:A:347:GLU:HB3	1.87	0.56
1:A:100:GLU:HB3	1:A:198:ARG:HB2	1.88	0.54
1:A:106:ARG:HD3	1:A:157:VAL:HG23	1.90	0.53
2:C:80:ARG:HB3	2:C:147:ILE:HD12	1.90	0.53
1:A:73:CYS:HB2	2:C:127:PRO:HG3	1.90	0.53
1:A:125:TYR:HB2	1:A:184:ALA:HB3	1.91	0.51
1:A:513:VAL:H	1:A:525:SER:HB2	1.76	0.51
1:A:298:TYR:HB2	1:A:310:ASP:HB3	1.94	0.49
1:A:106:ARG:HH21	2:C:125:PHE:HB3	1.78	0.49
1:A:82:ASN:HB2	1:A:187:ASP:HB3	1.95	0.49
1:A:126:TYR:HB3	1:A:145:ILE:HD11	1.95	0.49
1:A:106:ARG:HB2	1:A:191:CYS:HB3	1.95	0.48
2:C:78:THR:HG21	2:C:109:PRO:HG3	1.97	0.47
1:A:193:ALA:HB2	2:C:127:PRO:HB2	1.97	0.46
1:A:406:HIS:H	1:A:437:ASN:HB2	1.80	0.46
1:A:486:ARG:HD3	1:A:489:ARG:HH12	1.81	0.46
1:A:175:PRO:HB3	1:A:221:ALA:HB1	2.00	0.44
1:A:335:LEU:HD11	1:A:413:ILE:HD12	1.99	0.44
1:A:230:ARG:HG2	1:A:244:LYS:HB3	2.00	0.44
1:A:339:VAL:HG21	1:A:436:THR:HA	1.98	0.44
1:A:295:PRO:HD2	1:A:324:PRO:HB3	1.98	0.44
1:A:514:ARG:HH11	1:A:522:GLY:H	1.65	0.43
1:A:237:SER:HB2	1:A:273:CYS:SG	2.58	0.43
1:A:121:THR:HB	1:A:147:THR:HG22	2.01	0.41
1:A:62:GLU:HA	1:A:63:LYS:HA	1.77	0.41
1:A:335:LEU:HD12	1:A:430:VAL:HG12	2.02	0.41
1:A:476:VAL:HG22	1:A:513:VAL:HG22	2.02	0.41
1:A:96:ARG:HG3	1:A:174:GLY:HA3	2.02	0.40
1:A:156:GLN:N	1:A:157:VAL:HA	2.36	0.40
1:A:326:THR:HG21	1:A:357:ARG:HG2	2.03	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	503/568 (89%)	477 (95%)	23 (5%)	3 (1%)	22 58
2	C	133/180 (74%)	124 (93%)	9 (7%)	0	100 100
All	All	636/748 (85%)	601 (94%)	32 (5%)	3 (0%)	25 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	PRO
1	A	485	GLU
1	A	383	GLY

5.3.2 Protein sidechains (i)

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	439/489 (90%)	422 (96%)	17 (4%)	27 50
2	C	126/161 (78%)	123 (98%)	3 (2%)	44 63
All	All	565/650 (87%)	545 (96%)	20 (4%)	31 53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	95	GLN
1	A	141	GLN

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	218	ILE
1	A	300	VAL
1	A	335	LEU
1	A	339	VAL
1	A	404	LEU
1	A	407	THR
1	A	408	ASN
1	A	435	THR
1	A	444	ILE
1	A	450	LYS
1	A	462	LEU
1	A	471	ILE
1	A	483	GLN
2	C	54	ILE
2	C	102	LYS
2	C	130	LEU

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	29	ASN
1	A	109	ASN
1	A	123	ASN
1	A	131	ASN
1	A	213	GLN
1	A	259	ASN
1	A	266	HIS
1	A	391	ASN
1	A	438	GLN
1	A	483	GLN
2	C	53	HIS
2	C	59	ASN
2	C	68	HIS
2	C	123	GLN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	148:PRO	C	150:ASP	N	3.28
1	A	202:LYS	C	203:LYS	N	3.25

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, 95^{th} 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	507/568 (89%)	0.92	73 (14%) 7 9	76, 162, 253, 293	0
2	C	137/180 (76%)	0.63	10 (7%) 22 20	135, 244, 285, 291	0
All	All	644/748 (86%)	0.86	83 (12%) 9 10	76, 176, 270, 293	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	TYR	8.0
1	A	287	ASP	5.5
1	A	66	PRO	4.9
1	A	478	TYR	4.9
1	A	338	ASN	4.8
1	A	159	ILE	4.7
1	A	387	THR	4.7
1	A	333	LEU	4.7
1	A	162	ARG	4.6
1	A	450	LYS	4.5
2	C	117	LYS	4.4
1	A	492	ARG	4.3
1	A	487	SER	4.2
1	A	58	SER	4.2
1	A	345	ASN	4.1
1	A	68	ARG	4.1
2	C	119	SER	4.0
1	A	482	ASP	3.9
1	A	463	GLU	3.9
1	A	488	TYR	3.8
1	A	163	ILE	3.8
1	A	486	ARG	3.7
1	A	524	PHE	3.5
1	A	489	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	164	MET	3.4
1	A	518	ALA	3.4
1	A	395	THR	3.4
2	C	139	GLU	3.4
1	A	347	GLU	3.3
1	A	448	GLN	3.3
1	A	64	ASN	3.3
1	A	60	MET	3.3
1	A	350	SER	3.3
1	A	502	GLY	3.3
1	A	475	GLU	3.1
1	A	65	THR	3.1
1	A	504	ASN	3.1
1	A	268	GLU	3.1
1	A	157	VAL	3.0
2	C	88	PHE	3.0
1	A	166	LEU	2.9
1	A	110	SER	2.9
1	A	529	GLU	2.9
1	A	112	PRO	2.9
1	A	336	ILE	2.8
1	A	67	ILE	2.8
1	A	224	SER	2.8
1	A	462	LEU	2.7
1	A	195	VAL	2.7
1	A	397	LYS	2.6
1	A	223	THR	2.6
1	A	440	ALA	2.6
1	A	516	ARG	2.6
1	A	490	ILE	2.6
2	C	104	TRP	2.5
1	A	155	THR	2.5
1	A	70	TYR	2.5
2	C	138	ARG	2.5
2	C	105	GLU	2.5
1	A	497	ASN	2.4
1	A	428	GLN	2.4
1	A	81	ASN	2.3
1	A	27	PRO	2.3
2	C	34	ASP	2.3
1	A	95	GLN	2.3
1	A	113	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	158	ASP	2.3
1	A	69	THR	2.2
1	A	133	LYS	2.2
2	C	118	PHE	2.2
1	A	161	ASP	2.2
1	A	501	LYS	2.2
1	A	460	ALA	2.2
1	A	337	SER	2.1
1	A	103	PHE	2.1
1	A	481	LYS	2.1
1	A	468	ASN	2.1
1	A	154	PHE	2.1
1	A	160	GLY	2.0
2	C	102	LYS	2.0
1	A	466	ARG	2.0
1	A	495	ALA	2.0
1	A	408	ASN	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.