



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 4F0I / pdb_00004f0i
Title : Crystal structure of apo TrkA
Authors : Liu, J.
Deposited on : 2012-05-04
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

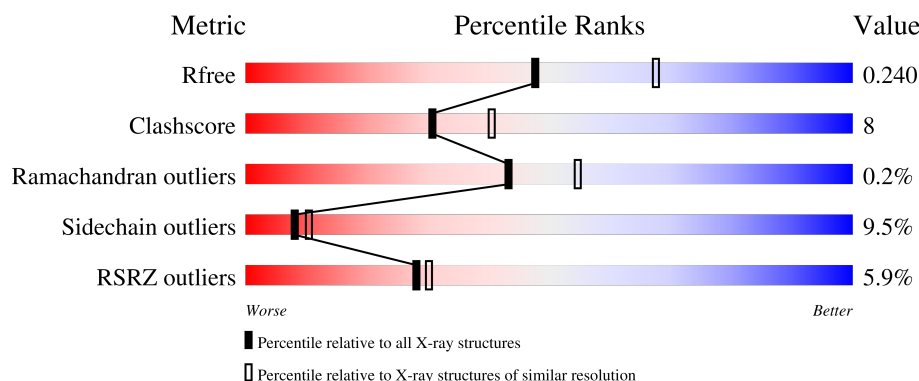
1 Overall quality at a glance

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	300	
1	B	300	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4932 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 High affinity nerve growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2269	1452	411	390	16			
1	B	294	Total	C	N	O	S	0	0	0
			2351	1502	422	411	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	GLY	-	expression tag	UNP P04629
B	496	GLY	-	expression tag	UNP P04629

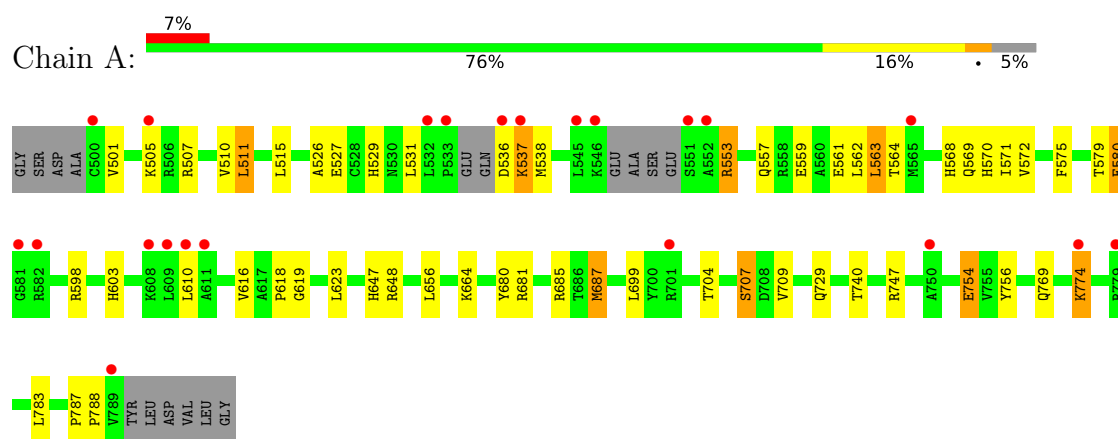
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total	O	0	0
			113	113		
2	B	199	Total	O	0	0
			199	199		

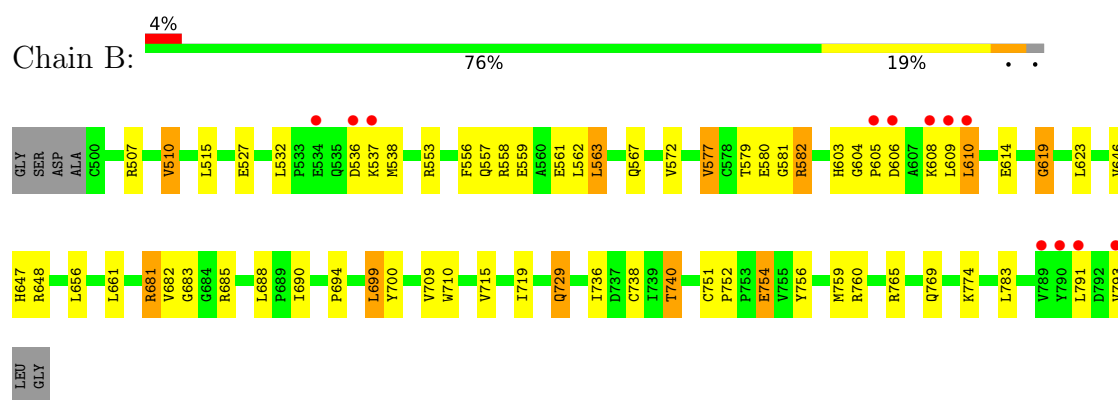
3 Residue-property plots [i](#)

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: High affinity nerve growth factor receptor



- Molecule 1: High affinity nerve growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.59Å 92.59Å 181.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.43 – 2.30 44.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.43-2.30) 99.3 (44.43-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.182 , 0.241 0.183 , 0.240	Depositor DCC
R_{free} test set	1789 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4932	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.45	0/2325	0.81	3/3144 (0.1%)
1	B	0.54	0/2410	0.85	6/3263 (0.2%)
All	All	0.50	0/4735	0.83	9/6407 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	752	PRO	CA-C-N	5.40	125.48	119.32
1	B	752	PRO	C-N-CA	5.40	125.48	119.32
1	B	532	LEU	CA-C-N	5.34	126.51	119.84
1	B	532	LEU	C-N-CA	5.34	126.51	119.84
1	B	619	GLY	CA-C-N	5.16	125.17	119.90
1	B	619	GLY	C-N-CA	5.16	125.17	119.90
1	A	501	VAL	N-CA-C	5.13	115.71	109.30
1	A	564	THR	N-CA-C	-5.08	107.26	113.50
1	A	685	ARG	N-CA-C	5.04	112.91	108.78

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	2269	0	2271	40	0
1	B	2351	0	2342	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	113	0	0	1	0
2	B	199	0	0	3	0
All	All	4932	0	4613	77	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 (77) 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:553:ARG:NH2	1:A:579:THR:HB	1.97	0.78
1:B:729:GLN:H	1:B:729:GLN:HE21	1.29	0.78
1:A:553:ARG:HH11	1:A:553:ARG:HG2	1.51	0.76
1:B:603:HIS:HD2	1:B:619:GLY:O	1.70	0.74
1:B:736:ILE:O	1:B:740:THR:HB	1.88	0.74
1:A:557:GLN:O	1:A:561:GLU:HG3	1.89	0.73
1:A:553:ARG:HH11	1:A:553:ARG:CG	2.02	0.71
1:A:572:VAL:HG21	1:A:656:LEU:HD12	1.73	0.71
1:B:559:GLU:HG2	1:B:563:LEU:HD22	1.74	0.69
1:A:529:HIS:NE2	1:A:537:LYS:HE3	2.09	0.68
1:A:707:SER:HB3	2:A:849:HOH:O	1.93	0.68
1:A:704:THR:H	1:A:707:SER:HB2	1.59	0.67
1:A:774:LYS:HA	1:A:774:LYS:HE2	1.77	0.66
1:A:647:HIS:O	1:A:648:ARG:HB2	1.96	0.64
1:B:572:VAL:HG21	1:B:656:LEU:HD12	1.79	0.64
1:B:553:ARG:HH21	1:B:582:ARG:HH11	1.46	0.64
1:B:603:HIS:CD2	1:B:619:GLY:O	2.51	0.64
1:B:577:VAL:HG13	1:B:579:THR:HG23	1.82	0.62
1:A:603:HIS:HD2	1:A:619:GLY:O	1.82	0.62
1:B:581:GLY:C	1:B:582:ARG:HE	2.11	0.59
1:B:507:ARG:HD2	2:B:919:HOH:O	2.03	0.58
1:A:553:ARG:HH22	1:A:579:THR:HB	1.69	0.57
1:A:569:GLN:HG3	1:A:570:HIS:CD2	2.40	0.57
1:B:604:GLY:C	1:B:606:ASP:H	2.12	0.57
1:A:559:GLU:O	1:A:563:LEU:HD22	2.06	0.54
1:A:527:GLU:HA	1:A:538:MET:O	2.08	0.54
1:B:510:VAL:HG13	1:B:527:GLU:HB2	1.90	0.53
1:B:567:GLN:HG2	2:B:859:HOH:O	2.09	0.53
1:B:715:VAL:O	1:B:719:ILE:HG13	2.09	0.53
1:A:529:HIS:CE1	1:A:537:LYS:HE3	2.44	0.52
1:B:556:PHE:CZ	1:B:577:VAL:HG22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLU:HB3	1:A:537:LYS:HE2	1.92	0.52
1:A:580:GLU:O	1:A:580:GLU:HG2	2.10	0.51
1:A:553:ARG:CG	1:A:553:ARG:NH1	2.68	0.50
1:B:694:PRO:HB3	1:B:710:TRP:CD2	2.46	0.50
1:B:751:CYS:SG	1:B:759:MET:HE3	2.52	0.50
1:A:603:HIS:CD2	1:A:619:GLY:O	2.63	0.50
1:B:558:ARG:NE	2:B:900:HOH:O	2.43	0.50
1:A:536:ASP:O	1:A:537:LYS:C	2.55	0.49
1:A:531:LEU:HD21	1:A:575:PHE:CG	2.48	0.49
1:A:527:GLU:CB	1:A:537:LYS:HE2	2.43	0.49
1:A:747:ARG:HG3	1:A:756:TYR:HB2	1.95	0.48
1:B:740:THR:O	1:B:765:ARG:NH2	2.45	0.48
1:A:505:LYS:HD3	1:A:507:ARG:NH1	2.29	0.48
1:B:610:LEU:HD12	1:B:610:LEU:C	2.39	0.48
1:A:687:MET:HA	1:A:687:MET:HE3	1.96	0.48
1:A:511:LEU:HA	1:A:526:ALA:HB2	1.97	0.47
1:A:536:ASP:O	1:A:538:MET:HB2	2.14	0.47
1:B:682:VAL:HG21	1:B:688:LEU:HD12	1.96	0.47
1:B:729:GLN:H	1:B:729:GLN:NE2	2.04	0.47
1:A:510:VAL:HG13	1:A:527:GLU:HB2	1.97	0.47
1:A:754:GLU:H	1:A:754:GLU:CD	2.23	0.46
1:B:681:ARG:HD2	1:B:683:GLY:O	2.16	0.46
1:B:690:ILE:HD13	1:B:736:ILE:HG13	1.95	0.46
1:B:699:LEU:HB3	1:B:700:TYR:CD2	2.50	0.46
1:B:756:TYR:O	1:B:760:ARG:HG3	2.16	0.46
1:B:553:ARG:HE	1:B:582:ARG:NH1	2.12	0.46
1:A:610:LEU:HG	1:A:618:PRO:HB3	1.98	0.45
1:A:527:GLU:OE2	1:A:537:LYS:HE2	2.17	0.44
1:A:568:HIS:HB3	1:A:571:ILE:HG12	1.98	0.44
1:B:537:LYS:O	1:B:537:LYS:HE3	2.17	0.44
1:B:557:GLN:O	1:B:561:GLU:HG2	2.19	0.43
1:B:608:LYS:H	1:B:608:LYS:HG2	1.63	0.43
1:A:680:TYR:CA	1:A:687:MET:HE1	2.49	0.43
1:A:680:TYR:HA	1:A:687:MET:HE1	2.01	0.42
1:A:680:TYR:C	1:A:687:MET:HE3	2.44	0.42
1:B:699:LEU:HB3	1:B:700:TYR:CE2	2.54	0.42
1:A:681:ARG:N	1:A:687:MET:HE3	2.35	0.42
1:B:604:GLY:C	1:B:606:ASP:N	2.77	0.41
1:A:687:MET:HA	1:A:687:MET:CE	2.51	0.41
1:A:787:PRO:HA	1:A:788:PRO:HD2	1.85	0.41
1:B:754:GLU:CD	1:B:754:GLU:H	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:GLN:O	1:A:664:LYS:HE2	2.20	0.41
1:B:646:VAL:HG12	1:B:648:ARG:HG3	2.02	0.41
1:B:580:GLU:O	1:B:580:GLU:HG3	2.20	0.41
1:B:553:ARG:NH2	1:B:582:ARG:HH11	2.16	0.40
1:B:647:HIS:O	1:B:648:ARG:HB2	2.20	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	278/300 (93%)	270 (97%)	8 (3%)	0	100	100
1	B	292/300 (97%)	284 (97%)	7 (2%)	1 (0%)	36	46
All	All	570/600 (95%)	554 (97%)	15 (3%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	605	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/250 (95%)	218 (92%)	20 (8%)	10	14
1	B	247/250 (99%)	221 (90%)	26 (10%)	6	8
All	All	485/500 (97%)	439 (90%)	46 (10%)	8	10

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	LEU
1	A	515	LEU
1	A	537	LYS
1	A	553	ARG
1	A	562	LEU
1	A	563	LEU
1	A	580	GLU
1	A	598	ARG
1	A	616	VAL
1	A	623	LEU
1	A	687	MET
1	A	699	LEU
1	A	707	SER
1	A	709	VAL
1	A	729	GLN
1	A	740	THR
1	A	754	GLU
1	A	769	GLN
1	A	774	LYS
1	A	783	LEU
1	B	510	VAL
1	B	515	LEU
1	B	536	ASP
1	B	538	MET
1	B	562	LEU
1	B	563	LEU
1	B	577	VAL
1	B	582	ARG
1	B	609	LEU
1	B	610	LEU
1	B	614	GLU
1	B	623	LEU

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Mol	Chain	Res	Type
1	B	661	LEU
1	B	681	ARG
1	B	685	ARG
1	B	699	LEU
1	B	709	VAL
1	B	729	GLN
1	B	738	CYS
1	B	740	THR
1	B	754	GLU
1	B	769	GLN
1	B	774	LYS
1	B	783	LEU
1	B	791	LEU
1	B	793	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	502	HIS
1	A	530	ASN
1	A	557	GLN
1	A	567	GLN
1	A	570	HIS
1	A	603	HIS
1	A	768	GLN
1	A	771	HIS
1	A	785	GLN
1	B	529	HIS
1	B	530	ASN
1	B	557	GLN
1	B	567	GLN
1	B	603	HIS
1	B	644	HIS
1	B	725	GLN
1	B	729	GLN
1	B	768	GLN
1	B	769	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](#)

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	284/300 (94%)	0.30	22 (7%) 19 21	22, 44, 86, 133	0
1	B	294/300 (98%)	-0.16	12 (4%) 41 43	17, 30, 71, 108	0
All	All	578/600 (96%)	0.06	34 (5%) 28 30	17, 37, 84, 133	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	609	LEU	6.5
1	A	789	VAL	5.6
1	B	610	LEU	4.9
1	A	500	CYS	4.5
1	A	551	SER	4.0
1	A	552	ALA	3.9
1	A	533	PRO	3.9
1	A	750	ALA	3.9
1	B	793	VAL	3.5
1	A	582	ARG	3.5
1	A	537	LYS	3.4
1	A	536	ASP	3.4
1	B	608	LYS	3.1
1	A	774	LYS	3.0
1	A	546	LYS	3.0
1	B	605	PRO	2.9
1	A	565	MET	2.9
1	B	537	LYS	2.8
1	B	606	ASP	2.8
1	A	610	LEU	2.7
1	A	532	LEU	2.6
1	A	581	GLY	2.5
1	B	791	LEU	2.5
1	A	609	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	536	ASP	2.5
1	A	611	ALA	2.4
1	B	534	GLU	2.4
1	A	779	ARG	2.3
1	A	545	LEU	2.1
1	A	701	ARG	2.1
1	B	790	TYR	2.1
1	A	505	LYS	2.1
1	A	608	LYS	2.1
1	B	789	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.