



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:15 PM UTC

PDB ID : 7WWQ / pdb_00007wwq
Title : Crystal structure of human Ufd1-Npl4 complex
Authors : Nguyen, T.Q.; Le, L.T.M.; Kim, D.H.; Ko, K.S.; Lee, H.T.; Nguyen, Y.T.K.;
Kim, H.S.; Han, B.W.; Kang, W.; Yang, J.K.
Deposited on : 2022-02-14
Resolution : 2.72 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

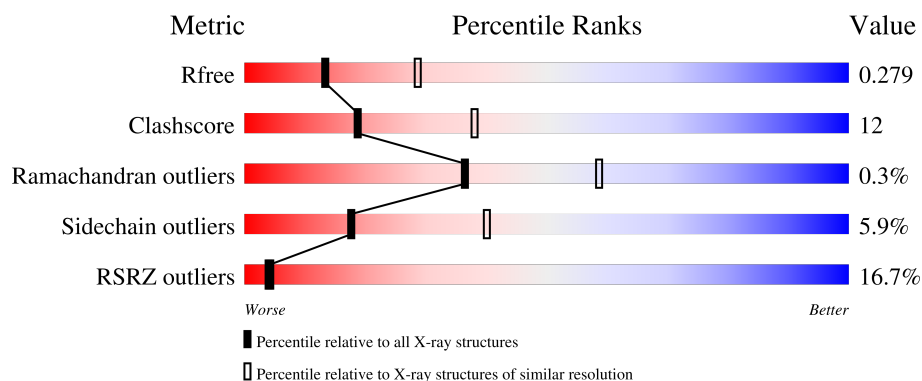
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	465	
2	B	16	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3273 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 Nuclear protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3084	1958	520	594	12			

- Molecule 2 is a protein called Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	0	0	0
			138	93	23	22			

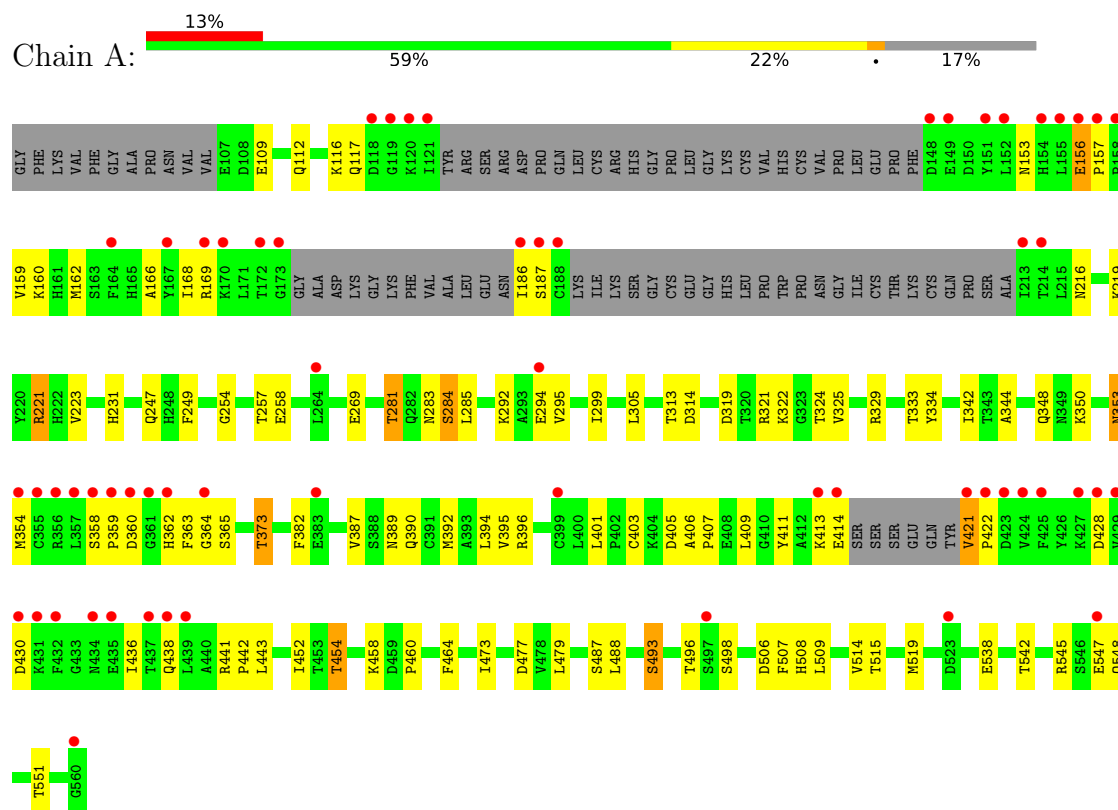
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		

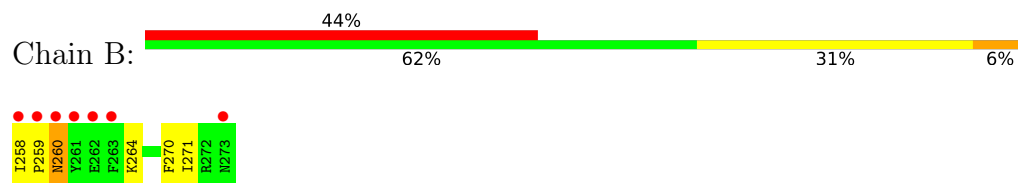
3 Residue-property plots [i](#)

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: Nuclear protein localization protein 4 homolog



- Molecule 2: Ubiquitin recognition factor in ER-associated degradation protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.96Å 165.42Å 192.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.24 – 2.72 30.24 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.24-2.72) 99.0 (30.24-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.71 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.241 , 0.277 0.242 , 0.279	Depositor DCC
R_{free} test set	1703 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3273	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	0.37	0/3153	0.61	3/4276 (0.1%)
2	B	0.41	0/141	0.93	0/188
All	All	0.38	0/3294	0.63	3/4464 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	156	GLU	CA-C-N	5.17	139.41	127.00
1	A	156	GLU	C-N-CA	5.17	139.41	127.00
1	A	156	GLU	C-N-CD	-5.01	109.57	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	VAL	Peptide

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	3084	0	2964	72	1
2	B	138	0	144	7	0
3	A	51	0	0	5	0
All	All	3273	0	3108	75	1

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 (75) 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:364:GLY:HA2	1:A:392:MET:HE1	1.56	0.87
1:A:294:GLU:H	1:A:294:GLU:CD	1.93	0.76
2:B:260:ASN:OD1	2:B:260:ASN:N	2.19	0.75
2:B:258:ILE:HB	2:B:259:PRO:HD3	1.69	0.74
1:A:548:GLN:OE1	3:A:602:HOH:O	2.09	0.69
1:A:403:CYS:HA	2:B:260:ASN:HA	1.76	0.68
1:A:254:GLY:HA2	1:A:305:LEU:HD22	1.79	0.64
1:A:409:LEU:HD13	1:A:442:PRO:HG3	1.80	0.64
1:A:407:PRO:HG3	2:B:271:ILE:HB	1.82	0.61
1:A:329:ARG:HD2	1:A:373:THR:HG21	1.83	0.61
1:A:321:ARG:HD2	3:A:639:HOH:O	2.02	0.60
1:A:405:ASP:CG	2:B:259:PRO:HD2	2.26	0.59
1:A:473:ILE:HD12	1:A:508:HIS:CD2	2.38	0.59
1:A:545:ARG:HH11	1:A:545:ARG:HG2	1.67	0.59
1:A:321:ARG:NH2	3:A:601:HOH:O	2.07	0.59
1:A:314:ASP:O	1:A:373:THR:HG22	2.04	0.57
1:A:319:ASP:OD1	1:A:322:LYS:HG2	2.06	0.56
1:A:112:GLN:O	1:A:116:LYS:HE3	2.06	0.56
1:A:389:ASN:HA	1:A:392:MET:HE3	1.86	0.55
1:A:411:TYR:CZ	1:A:441:ARG:HG3	2.41	0.55
1:A:414:GLU:C	1:A:421:VAL:HG22	2.32	0.54
2:B:258:ILE:HB	2:B:259:PRO:CD	2.37	0.53
1:A:314:ASP:HB3	1:A:373:THR:HG23	1.90	0.53
1:A:257:THR:HG21	1:A:269:GLU:OE2	2.09	0.53
1:A:409:LEU:HB3	1:A:442:PRO:HB2	1.91	0.53
1:A:344:ALA:O	1:A:348:GLN:HG3	2.09	0.52
1:A:160:LYS:HZ1	1:A:221:ARG:HH12	1.56	0.52
1:A:292:LYS:NZ	1:A:515:THR:OG1	2.42	0.52
1:A:354:MET:HE2	1:A:362:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HA	1:A:395:VAL:HG11	1.92	0.50
1:A:477:ASP:N	1:A:477:ASP:OD1	2.46	0.49
1:A:382:PHE:O	1:A:454:THR:HG21	2.13	0.48
1:A:390:GLN:O	1:A:394:LEU:HD12	2.13	0.48
1:A:358:SER:O	1:A:360:ASP:N	2.44	0.47
1:A:117:GLN:O	1:A:169:ARG:NH1	2.45	0.47
1:A:353:ASN:ND2	1:A:363:PHE:O	2.38	0.47
1:A:538:GLU:O	1:A:542:THR:HG23	2.16	0.46
1:A:258:GLU:HG2	3:A:610:HOH:O	2.16	0.46
1:A:223:VAL:O	1:A:452:ILE:HG12	2.16	0.46
1:A:348:GLN:HB3	1:A:365:SER:HB3	1.98	0.46
1:A:299:ILE:HD11	1:A:514:VAL:HG11	1.97	0.46
1:A:160:LYS:N	1:A:160:LYS:HD3	2.30	0.46
1:A:156:GLU:HA	1:A:157:PRO:O	2.17	0.45
1:A:322:LYS:HB3	1:A:324:THR:HG23	1.97	0.45
1:A:430:ASP:OD2	1:A:430:ASP:N	2.50	0.45
1:A:411:TYR:CE1	1:A:441:ARG:HG3	2.52	0.45
1:A:428:ASP:C	1:A:436:ILE:HG22	2.41	0.45
1:A:506:ASP:OD1	1:A:508:HIS:N	2.50	0.45
1:A:187:SER:HA	1:A:396:ARG:HH22	1.83	0.44
1:A:162:MET:HE2	1:A:166:ALA:HB1	1.99	0.44
1:A:401:LEU:HD22	1:A:413:LYS:HD3	2.00	0.43
1:A:216:ASN:O	1:A:390:GLN:NE2	2.51	0.43
1:A:436:ILE:HD12	1:A:436:ILE:HA	1.80	0.43
1:A:519:MET:HE2	1:A:551:THR:OG1	2.18	0.43
1:A:109:GLU:H	1:A:109:GLU:CD	2.24	0.43
1:A:409:LEU:HB3	1:A:442:PRO:CB	2.49	0.42
1:A:219:LYS:O	1:A:219:LYS:HE3	2.19	0.42
1:A:493:SER:O	1:A:496:THR:HG23	2.20	0.42
1:A:406:ALA:HA	1:A:407:PRO:HD3	1.96	0.42
1:A:488:LEU:HD13	1:A:509:LEU:HD11	2.02	0.42
1:A:519:MET:O	1:A:519:MET:HG3	2.20	0.42
1:A:249:PHE:HB3	1:A:285:LEU:HD21	2.01	0.42
1:A:292:LYS:O	1:A:295:VAL:HG12	2.20	0.41
1:A:231:HIS:HD2	3:A:649:HOH:O	2.03	0.41
1:A:409:LEU:HD22	1:A:442:PRO:HG2	2.03	0.41
1:A:333:THR:OG1	1:A:334:TYR:N	2.48	0.41
1:A:413:LYS:HD2	1:A:413:LYS:HA	1.92	0.41
1:A:458:LYS:O	1:A:460:PRO:HD3	2.21	0.41
1:A:281:THR:HG22	1:A:283:ASN:H	1.86	0.41
1:A:405:ASP:OD1	1:A:405:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:HG22	1:A:284:SER:N	2.36	0.40
1:A:421:VAL:HB	1:A:422:PRO:HD3	2.03	0.40
1:A:247:GLN:HG3	2:B:270:PHE:CE2	2.56	0.40
1:A:464:PHE:CE2	1:A:507:PHE:HB2	2.56	0.40
1:A:547:GLU:O	1:A:551:THR:HG23	2.22	0.40

All (1) 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:430:ASP:OD1	1:A:438:GLN:NE2[2_655]	2.05	0.15

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	376/465 (81%)	352 (94%)	23 (6%)	1 (0%)	36	59
2	B	14/16 (88%)	11 (79%)	3 (21%)	0	100	100
All	All	390/481 (81%)	363 (93%)	26 (7%)	1 (0%)	36	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/413 (82%)	319 (94%)	19 (6%)	19	42
2	B	15/15 (100%)	13 (87%)	2 (13%)	4	9
All	All	353/428 (82%)	332 (94%)	21 (6%)	18	40

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	159	VAL
1	A	168	ILE
1	A	186	ILE
1	A	221	ARG
1	A	281	THR
1	A	284	SER
1	A	313	THR
1	A	325	VAL
1	A	350	LYS
1	A	353	ASN
1	A	373	THR
1	A	387	VAL
1	A	443	LEU
1	A	454	THR
1	A	479	LEU
1	A	487	SER
1	A	493	SER
1	A	498	SER
2	B	260	ASN
2	B	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	225	ASN
1	A	351	HIS
1	A	438	GLN
1	A	486	HIS

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	386/465 (83%)	0.79	60 (15%) 5 4	33, 61, 132, 158	0
2	B	16/16 (100%)	2.49	7 (43%) 0 0	61, 77, 128, 144	0
All	All	402/481 (83%)	0.85	67 (16%) 4 4	33, 63, 132, 158	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	ILE	10.5
2	B	258	ILE	10.0
1	A	148	ASP	8.3
2	B	262	GLU	7.8
1	A	213	ILE	7.4
1	A	121	ILE	7.2
2	B	261	TYR	6.5
1	A	431	LYS	6.2
1	A	421	VAL	5.9
1	A	173	GLY	5.8
1	A	151	TYR	5.6
1	A	152	LEU	5.2
1	A	357	LEU	5.2
1	A	170	LYS	5.2
1	A	154	HIS	5.0
1	A	155	LEU	4.7
1	A	120	LYS	4.3
1	A	359	PRO	4.3
1	A	429	VAL	4.2
1	A	172	THR	4.1
1	A	432	PHE	4.1
1	A	414	GLU	3.9
1	A	355	CYS	3.9
1	A	158	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	3.8
1	A	422	PRO	3.8
1	A	188	CYS	3.6
2	B	260	ASN	3.5
1	A	157	PRO	3.5
1	A	187	SER	3.4
1	A	434	ASN	3.4
1	A	156	GLU	3.3
1	A	399	CYS	3.3
1	A	497	SER	3.3
2	B	273	ASN	3.3
1	A	435	GLU	3.2
1	A	430	ASP	3.2
1	A	547	GLU	3.2
1	A	413	LYS	3.1
1	A	439	LEU	3.1
1	A	167	TYR	2.9
1	A	428	ASP	2.9
1	A	424	VAL	2.9
1	A	423	ASP	2.9
1	A	294	GLU	2.8
1	A	356	ARG	2.8
1	A	358	SER	2.7
1	A	354	MET	2.7
2	B	263	PHE	2.6
1	A	438	GLN	2.6
1	A	119	GLY	2.5
1	A	427	LYS	2.5
1	A	361	GLY	2.4
1	A	560	GLY	2.3
1	A	169	ARG	2.3
1	A	437	THR	2.3
1	A	383	GLU	2.3
1	A	362	HIS	2.3
1	A	523	ASP	2.3
1	A	364	GLY	2.2
1	A	164	PHE	2.2
1	A	425	PHE	2.2
1	A	118	ASP	2.1
1	A	360	ASP	2.1
1	A	264	LEU	2.1
2	B	259	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	214	THR	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.