



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4YE6 / pdb_00004ye6
Title : The crystal structure of the intact human GlnRS
Authors : Ognjenovic, J.; Wu, J.; Ling, J.; Simonovic, M.
Deposited on : 2015-02-23
Resolution : 2.40 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

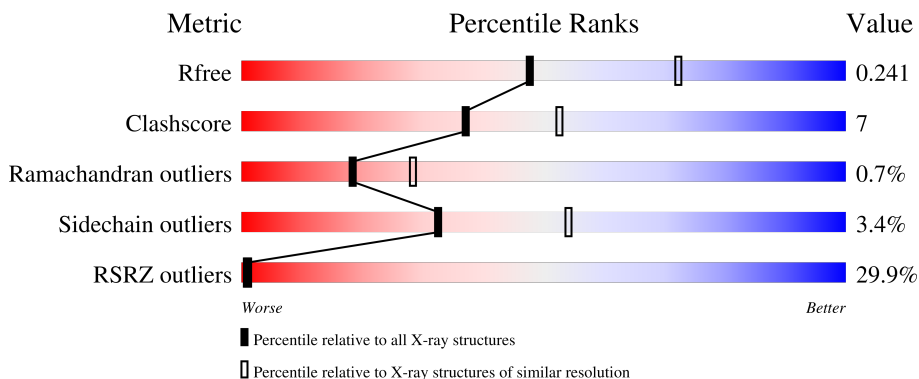
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	776	27% 74% 16% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5477 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 Glutamine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	709	5240	3330	921	961	28	0	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P47897

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	237	Total	O	0	0
			237	237		

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: Glutamine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	333.68Å 57.98Å 86.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.40 28.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.99-2.40) 90.5 (28.99-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.239 0.219 , 0.241	Depositor DCC
R_{free} test set	3358 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5477	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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	0.64	3/5384 (0.1%)	1.00	26/7336 (0.4%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	704	PRO	CG-CD	6.01	1.71	1.50
1	A	97	HIS	C-N	5.44	1.38	1.33
1	A	706	GLU	CB-CG	5.09	1.67	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	ALA	CA-C-N	9.44	130.23	120.04
1	A	609	ALA	C-N-CA	9.44	130.23	120.04
1	A	645	ILE	N-CA-C	7.78	125.52	109.34
1	A	606	VAL	CA-C-N	7.52	127.96	119.92
1	A	606	VAL	C-N-CA	7.52	127.96	119.92
1	A	582	PHE	CA-C-N	7.49	128.16	119.47
1	A	582	PHE	C-N-CA	7.49	128.16	119.47
1	A	549	GLU	CA-C-N	6.59	126.83	119.32
1	A	549	GLU	C-N-CA	6.59	126.83	119.32
1	A	97	HIS	CA-C-N	-6.42	114.28	120.83
1	A	97	HIS	C-N-CA	-6.42	114.28	120.83
1	A	658	VAL	N-CA-C	-6.31	100.52	108.84
1	A	646	GLU	N-CA-C	6.20	119.36	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	PHE	N-CA-C	6.01	118.85	110.20
1	A	595	PHE	CA-C-N	5.82	127.11	119.84
1	A	595	PHE	C-N-CA	5.82	127.11	119.84
1	A	246	THR	CA-C-N	-5.71	113.94	119.87
1	A	246	THR	C-N-CA	-5.71	113.94	119.87
1	A	269	PRO	N-CA-C	5.62	117.56	110.70
1	A	719	SER	CB-CA-C	-5.60	109.61	117.23
1	A	728	VAL	N-CA-C	5.48	116.25	108.42
1	A	401	THR	CA-C-N	-5.41	115.53	123.00
1	A	401	THR	C-N-CA	-5.41	115.53	123.00
1	A	95	ARG	N-CA-C	-5.35	103.07	110.35
1	A	178	GLY	CA-C-N	5.20	125.20	119.90
1	A	178	GLY	C-N-CA	5.20	125.20	119.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Peptide
1	A	581	ASN	Peptide
1	A	743	PHE	Peptide

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	5240	0	4741	71	0
2	A	237	0	0	3	0
All	All	5477	0	4741	71	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 7.

All (71) 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:96:SER:O	1:A:97:HIS:ND1	1.73	1.20
1:A:68:ARG:NH2	1:A:97:HIS:O	2.07	0.87
1:A:83:THR:HG22	1:A:85:PRO:HD2	1.55	0.86
1:A:96:SER:C	1:A:97:HIS:HD1	1.87	0.83
1:A:404:MET:HE3	1:A:470:LEU:HD13	1.69	0.73
1:A:651:VAL:HG12	1:A:652:LYS:H	1.63	0.63
1:A:99:LEU:O	1:A:101:PRO:HD3	2.00	0.61
1:A:743:PHE:HB3	1:A:746:LEU:HD13	1.84	0.59
1:A:217:THR:HG21	1:A:538:ARG:HG2	1.84	0.59
1:A:525:ARG:NH2	1:A:554:GLU:OE2	2.34	0.58
1:A:324:TRP:CE2	1:A:529:PRO:HG3	2.37	0.58
1:A:4:LEU:O	1:A:34[A]:ARG:NH2	2.23	0.58
1:A:706:GLU:HB3	1:A:708:PRO:HD3	1.85	0.57
1:A:704:PRO:HB2	1:A:707:VAL:HA	1.86	0.56
1:A:508:VAL:HG13	1:A:513:ASP:HB3	1.89	0.54
1:A:238:TYR:HA	1:A:243:TYR:CD2	2.43	0.53
1:A:148:LEU:O	1:A:152:GLU:HG3	2.09	0.53
1:A:68:ARG:HG3	1:A:94:VAL:HG13	1.91	0.52
1:A:179:PRO:HG3	1:A:259:ILE:HG12	1.91	0.52
1:A:653:GLY:N	1:A:657:CYS:O	2.40	0.52
1:A:490:HIS:HB3	1:A:699:LYS:O	2.10	0.52
1:A:599:GLU:C	1:A:601:LYS:H	2.18	0.51
1:A:356:TYR:CD2	1:A:376:ARG:HA	2.45	0.51
1:A:524:ARG:HE	1:A:753:PRO:HD2	1.74	0.51
1:A:343:TYR:CZ	1:A:391:ARG:HD2	2.46	0.51
1:A:419[A]:ARG:NE	2:A:887:HOH:O	2.45	0.50
1:A:745:ARG:H	1:A:746:LEU:HD12	1.76	0.50
1:A:99:LEU:C	1:A:101:PRO:CD	2.85	0.49
1:A:408:MET:HE3	1:A:412:LYS:HB3	1.94	0.49
1:A:96:SER:C	1:A:97:HIS:ND1	2.59	0.49
1:A:737:PRO:HA	1:A:751:VAL:HB	1.95	0.49
1:A:150:MET:HE3	1:A:166:LYS:HB2	1.94	0.48
1:A:122:ILE:HA	1:A:157:LEU:HD11	1.95	0.48
1:A:232:HIS:HD2	2:A:984:HOH:O	1.96	0.48
1:A:269:PRO:HA	1:A:301:ARG:O	2.13	0.48
1:A:690:ARG:HB3	1:A:720:LEU:HD21	1.96	0.48
1:A:514:PRO:HB3	1:A:525:ARG:HB2	1.95	0.48
1:A:145:ASN:HB3	1:A:148:LEU:HD13	1.97	0.47
1:A:482:TRP:CZ3	1:A:484:TYR:HB3	2.50	0.46
1:A:381[B]:GLU:H	1:A:381[B]:GLU:CD	2.23	0.46
1:A:122:ILE:HG12	1:A:157:LEU:HD13	1.98	0.46
1:A:371:LEU:HD12	1:A:372:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TYR:CE2	1:A:358:CYS:HB2	2.52	0.45
1:A:72:LEU:HD11	1:A:94:VAL:HG21	2.00	0.44
1:A:458:LYS:HG2	1:A:483:GLU:HB2	1.99	0.44
1:A:382:GLU:O	1:A:386:LEU:HG	2.18	0.44
1:A:704:PRO:HA	1:A:708:PRO:HD2	2.00	0.44
1:A:510:ASP:HB3	1:A:512[B]:ASP:OD1	2.18	0.44
1:A:180:LYS:N	2:A:1027:HOH:O	2.46	0.44
1:A:359:HIS:HB2	1:A:375:TRP:CH2	2.53	0.44
1:A:517:PHE:HA	1:A:522:LEU:HD21	2.00	0.43
1:A:646:GLU:O	1:A:663:VAL:HA	2.18	0.43
1:A:349[A]:LEU:HG	1:A:354:LEU:HB2	2.00	0.42
1:A:77:ALA:C	1:A:79:LYS:H	2.27	0.42
1:A:689:VAL:HG22	1:A:762:PHE:HB2	2.00	0.42
1:A:286:PHE:CD2	1:A:455:LEU:HD13	2.53	0.42
1:A:578:ILE:O	1:A:662:GLU:HA	2.20	0.42
1:A:704:PRO:CB	1:A:707:VAL:HA	2.50	0.42
1:A:68:ARG:NH1	1:A:100:ASP:HA	2.35	0.41
1:A:563:ASP:OD1	1:A:563:ASP:N	2.53	0.41
1:A:166:LYS:NZ	1:A:170:ASP:OD2	2.43	0.41
1:A:409:GLU:OE2	1:A:465:SER:HB2	2.20	0.41
1:A:511:TRP:CZ3	1:A:520:THR:HG21	2.55	0.41
1:A:739:ASP:O	1:A:751:VAL:HG23	2.21	0.41
1:A:489:LEU:O	1:A:492:ALA:HB3	2.21	0.41
1:A:150:MET:HG3	1:A:169:VAL:HG21	2.03	0.41
1:A:101:PRO:CD	1:A:101:PRO:O	2.69	0.40
1:A:168:GLU:OE2	1:A:172:GLN:NE2	2.34	0.40
1:A:530:GLU:H	1:A:530:GLU:CD	2.28	0.40
1:A:267:ARG:NH1	1:A:269:PRO:HG3	2.36	0.40
1:A:604:HIS:CD2	1:A:731:SER:HB2	2.57	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	704/776 (91%)	647 (92%)	52 (7%)	5 (1%)	18 28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	269	PRO
1	A	101	PRO
1	A	624	GLU
1	A	732	VAL

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	479/666 (72%)	463 (97%)	16 (3%)	33 55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	27	SER
1	A	54	ILE
1	A	96	SER
1	A	104	THR
1	A	239	LYS
1	A	401	THR
1	A	483	GLU
1	A	493	VAL
1	A	495	SER
1	A	508	VAL
1	A	563	ASP
1	A	583	PRO
1	A	651	VAL
1	A	744	GLU
1	A	756	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	709/776 (91%)	1.19	212 (29%) 1 1	21, 73, 145, 160	9 (1%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	618	ASP	7.2
1	A	650	VAL	6.9
1	A	580	THR	6.9
1	A	676	ALA	6.4
1	A	608	PHE	6.2
1	A	649	HIS	5.9
1	A	648	GLN	5.9
1	A	546	THR	5.4
1	A	619	PHE	5.4
1	A	541	VAL	5.2
1	A	641	THR	5.2
1	A	575	LEU	5.2
1	A	543	VAL	5.1
1	A	462	ALA	5.1
1	A	584	ALA	5.0
1	A	702	GLU	5.0
1	A	664	THR	5.0
1	A	699	LYS	5.0
1	A	698	HIS	4.9
1	A	711	PHE	4.9
1	A	651	VAL	4.9
1	A	647	LEU	4.8
1	A	687	CYS	4.8
1	A	658	VAL	4.8
1	A	729	ASP	4.7
1	A	674	PRO	4.7
1	A	719	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	678	ILE	4.6
1	A	613	PHE	4.6
1	A	607	PRO	4.6
1	A	643	TYR	4.6
1	A	727	LEU	4.6
1	A	695	LEU	4.5
1	A	680	TRP	4.5
1	A	182	GLU	4.5
1	A	696	PHE	4.5
1	A	764	ARG	4.4
1	A	712	LEU	4.4
1	A	571	VAL	4.4
1	A	590	ILE	4.3
1	A	667	ARG	4.3
1	A	692	TYR	4.3
1	A	574	SER	4.3
1	A	694	ARG	4.3
1	A	595	PHE	4.3
1	A	629	ARG	4.3
1	A	545	GLN	4.3
1	A	569	MET	4.3
1	A	542	THR	4.2
1	A	757	GLN	4.1
1	A	677	PHE	4.1
1	A	609	ALA	4.1
1	A	100	ASP	4.0
1	A	771	ASP	4.0
1	A	731	SER	4.0
1	A	709	GLY	4.0
1	A	640	HIS	4.0
1	A	576	ARG	4.0
1	A	583	PRO	4.0
1	A	639	ARG	4.0
1	A	665	CYS	4.0
1	A	685	LEU	3.9
1	A	705	THR	3.9
1	A	761	VAL	3.9
1	A	679	HIS	3.9
1	A	701	PRO	3.9
1	A	767	THR	3.9
1	A	657	CYS	3.8
1	A	683	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	748	TYR	3.8
1	A	708	PRO	3.7
1	A	567	ARG	3.7
1	A	43	THR	3.7
1	A	750	SER	3.7
1	A	578	ILE	3.7
1	A	579	ILE	3.7
1	A	102	ILE	3.7
1	A	605	GLN	3.7
1	A	691	LEU	3.7
1	A	768	LEU	3.7
1	A	611	ILE	3.6
1	A	544	ALA	3.6
1	A	707	VAL	3.5
1	A	625	PRO	3.5
1	A	652	LYS	3.5
1	A	573	GLU	3.5
1	A	547	THR	3.5
1	A	570	ALA	3.5
1	A	710	GLY	3.5
1	A	572	LEU	3.4
1	A	734	LEU	3.4
1	A	740	LYS	3.4
1	A	612	VAL	3.4
1	A	760	LEU	3.3
1	A	706	GLU	3.3
1	A	181	LEU	3.3
1	A	622	GLU	3.3
1	A	370	THR	3.3
1	A	749	PHE	3.3
1	A	703	ASP	3.3
1	A	645	ILE	3.2
1	A	516	LEU	3.2
1	A	564	THR	3.2
1	A	655	SER	3.1
1	A	589	ASP	3.1
1	A	715	LEU	3.1
1	A	758	GLY	3.1
1	A	582	PHE	3.1
1	A	659	GLU	3.1
1	A	741	PHE	3.1
1	A	746	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	654	PRO	3.1
1	A	660	SER	3.1
1	A	759	LYS	3.0
1	A	725	ALA	3.0
1	A	762	PHE	3.0
1	A	763	ASN	3.0
1	A	506	GLY	3.0
1	A	493	VAL	3.0
1	A	505	THR	3.0
1	A	458	LYS	3.0
1	A	693	GLU	3.0
1	A	720	LEU	3.0
1	A	627	PHE	3.0
1	A	515	ARG	2.9
1	A	593	PRO	2.9
1	A	747	GLY	2.9
1	A	690	ARG	2.9
1	A	596	PRO	2.9
1	A	606	VAL	2.9
1	A	732	VAL	2.8
1	A	733	ALA	2.8
1	A	286	PHE	2.8
1	A	615	GLU	2.8
1	A	642	GLY	2.8
1	A	98	PRO	2.8
1	A	597	ALA	2.8
1	A	730	CYS	2.8
1	A	48	ILE	2.8
1	A	217	THR	2.8
1	A	656	GLY	2.7
1	A	742	GLN	2.7
1	A	45	GLY	2.7
1	A	661	LEU	2.7
1	A	646	GLU	2.7
1	A	603	PHE	2.7
1	A	548	MET	2.7
1	A	666	ARG	2.7
1	A	686	MET	2.6
1	A	717	LEU	2.6
1	A	718	ALA	2.6
1	A	491	TYR	2.6
1	A	704	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	566	PRO	2.6
1	A	689	VAL	2.6
1	A	728	VAL	2.6
1	A	628	LYS	2.6
1	A	581	ASN	2.5
1	A	592	VAL	2.5
1	A	723	VAL	2.5
1	A	756	HIS	2.5
1	A	713	SER	2.5
1	A	744	GLU	2.5
1	A	722	VAL	2.5
1	A	599	GLU	2.5
1	A	662	GLU	2.5
1	A	688	GLU	2.5
1	A	644	VAL	2.5
1	A	621	GLU	2.4
1	A	489	LEU	2.4
1	A	697	GLN	2.4
1	A	104	THR	2.4
1	A	623	PRO	2.4
1	A	684	PRO	2.4
1	A	44	LEU	2.4
1	A	568	ALA	2.4
1	A	510	ASP	2.4
1	A	616	ARG	2.4
1	A	765	THR	2.4
1	A	488	ASN	2.4
1	A	482	TRP	2.4
1	A	83	THR	2.3
1	A	79	LYS	2.3
1	A	101	PRO	2.3
1	A	508	VAL	2.3
1	A	577	VAL	2.3
1	A	507	ALA	2.3
1	A	610	PRO	2.3
1	A	653	GLY	2.3
1	A	71	PHE	2.3
1	A	663	VAL	2.3
1	A	617	THR	2.2
1	A	514	PRO	2.2
1	A	504	ALA	2.2
1	A	99	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	675	LYS	2.2
1	A	700	ASN	2.1
1	A	770	GLU	2.1
1	A	714	ASP	2.1
1	A	85	PRO	2.1
1	A	218	LEU	2.1
1	A	486	ARG	2.1
1	A	620	LYS	2.1
1	A	604	HIS	2.1
1	A	513	ASP	2.1
1	A	755	SER	2.1
1	A	549	GLU	2.0
1	A	769	LYS	2.0
1	A	539	VAL	2.0
1	A	614	ILE	2.0
1	A	682	SER	2.0
1	A	721	HIS	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.