



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:54 AM UTC

PDB ID : 1R5B / pdb_00001r5b
Title : Crystal structure analysis of sup35
Authors : Kong, C.; Song, H.
Deposited on : 2003-10-10
Resolution : 2.35 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

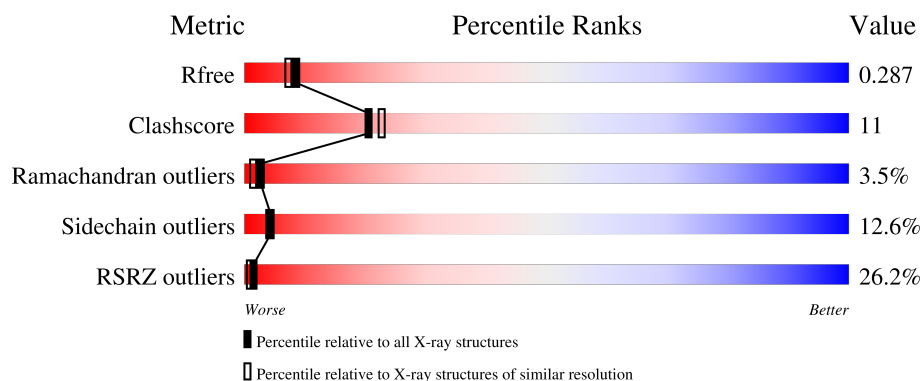
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	467	23% 63% 18% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3381 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 Eukaryotic peptide chain release factor GTP-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3222	2024	557	622	19			

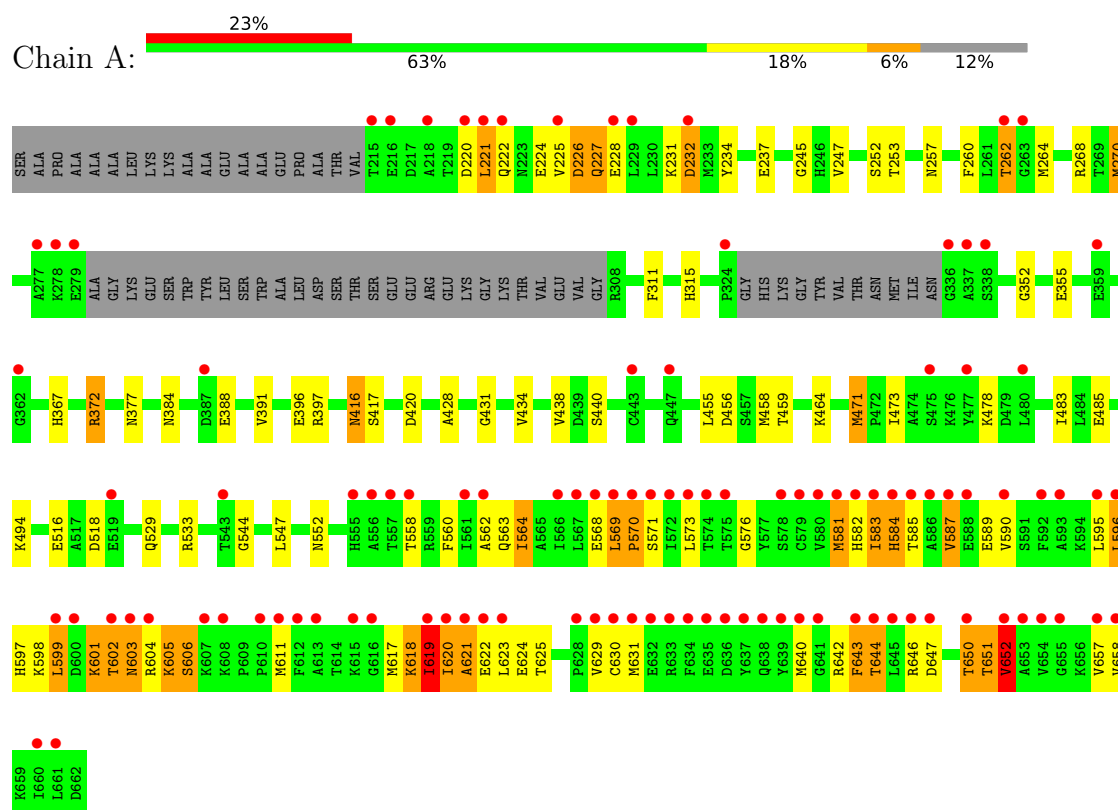
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	159	Total	O	0	0
			159	159		

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: Eukaryotic peptide chain release factor GTP-binding subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.80Å 83.80Å 165.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.35) 99.1 (20.00-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.255 , 0.284 0.258 , 0.287	Depositor DCC
R_{free} test set	1284 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.7	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	0.89	EDS
Total number of atoms	3381	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.77	4/3273 (0.1%)	0.92	5/4412 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ARG	NE-CZ	8.78	1.42	1.33
1	A	471	MET	SD-CE	-6.80	1.62	1.79
1	A	581	MET	SD-CE	-6.30	1.63	1.79
1	A	640	MET	SD-CE	-5.08	1.66	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	619	ILE	N-CA-C	7.53	116.89	107.70
1	A	643	PHE	N-CA-C	5.75	118.14	109.23
1	A	621	ALA	N-CA-C	5.50	116.62	108.60
1	A	583	ILE	CB-CA-C	-5.38	106.13	111.30
1	A	226	ASP	N-CA-C	5.22	116.46	108.52

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	3222	0	3234	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	159	0	0	6	0
All	All	3381	0	3234	72	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 (72) 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:597:HIS:HB2	1:A:620:ILE:HG23	1.65	0.77
1:A:388:GLU:O	1:A:391:VAL:O	2.05	0.74
1:A:590:VAL:HG21	1:A:623:LEU:HD23	1.70	0.74
1:A:262:THR:HG21	1:A:311:PHE:HB2	1.71	0.72
1:A:384:ASN:HD21	1:A:428:ALA:H	1.34	0.71
1:A:584:HIS:HE1	1:A:630:CYS:O	1.78	0.66
1:A:262:THR:HG23	1:A:264:MET:HE2	1.78	0.65
1:A:431:GLY:O	1:A:434:VAL:HG12	1.96	0.65
1:A:599:LEU:HD11	1:A:620:ILE:HG22	1.80	0.64
1:A:222:GLN:O	1:A:225:VAL:HG22	2.00	0.61
1:A:560:PHE:CZ	1:A:581:MET:HE1	2.35	0.61
1:A:416:ASN:C	1:A:416:ASN:HD22	2.10	0.60
1:A:352:GLY:C	2:A:57:HOH:O	2.45	0.59
1:A:651:THR:O	1:A:652:VAL:HG13	2.02	0.58
1:A:257:ASN:HA	1:A:270:MET:HE2	1.83	0.58
1:A:598:LYS:HD3	1:A:617:MET:HE3	1.87	0.57
1:A:620:ILE:O	1:A:620:ILE:HG13	2.05	0.56
1:A:355:GLU:OE1	2:A:57:HOH:O	2.18	0.56
1:A:596:LEU:HD22	1:A:597:HIS:CE1	2.42	0.55
1:A:619:ILE:HD11	1:A:621:ALA:HB3	1.88	0.54
1:A:560:PHE:CE1	1:A:631:MET:HE1	2.43	0.54
1:A:264:MET:HE3	1:A:311:PHE:HA	1.87	0.54
1:A:544:GLY:HA2	1:A:585:THR:HG23	1.90	0.53
1:A:562:ALA:HB1	1:A:643:PHE:HZ	1.73	0.53
1:A:552:ASN:HB3	2:A:99:HOH:O	2.10	0.52
1:A:372:ARG:HH11	1:A:377:ASN:HD22	1.58	0.52
1:A:221:LEU:HD23	1:A:644:THR:HG23	1.92	0.51
1:A:558:THR:O	1:A:624:GLU:HA	2.10	0.51
1:A:619:ILE:CD1	1:A:621:ALA:HB3	2.40	0.51
1:A:582:HIS:O	1:A:643:PHE:HB2	2.10	0.51
1:A:563:GLN:HA	1:A:619:ILE:O	2.11	0.51
1:A:597:HIS:CB	1:A:620:ILE:HG23	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:C	1:A:416:ASN:ND2	2.69	0.50
1:A:596:LEU:HB3	1:A:597:HIS:ND1	2.26	0.50
1:A:605:LYS:O	1:A:606:SER:CB	2.60	0.50
1:A:234:TYR:CE2	1:A:642:ARG:HG3	2.47	0.49
1:A:221:LEU:HD12	1:A:584:HIS:HA	1.95	0.49
1:A:262:THR:HG23	1:A:264:MET:CE	2.43	0.48
1:A:473:ILE:O	1:A:585:THR:HG21	2.14	0.48
1:A:582:HIS:ND1	1:A:587:VAL:HG22	2.29	0.48
1:A:658:VAL:HB	2:A:117:HOH:O	2.13	0.48
1:A:260:PHE:CD2	1:A:270:MET:HE3	2.49	0.47
1:A:596:LEU:H	1:A:621:ALA:HB2	1.79	0.47
1:A:221:LEU:HD13	1:A:222:GLN:HG2	1.96	0.47
1:A:471:MET:HE2	1:A:547:LEU:HD12	1.95	0.47
1:A:231:LYS:O	1:A:232:ASP:CB	2.62	0.47
1:A:352:GLY:N	2:A:57:HOH:O	2.50	0.46
1:A:315:HIS:HD2	1:A:456:ASP:OD2	1.97	0.45
1:A:569:LEU:N	1:A:570:PRO:CD	2.79	0.45
1:A:622:GLU:O	1:A:623:LEU:HD12	2.17	0.45
1:A:602:THR:O	1:A:604:ARG:N	2.50	0.45
1:A:245:GLY:C	1:A:367:HIS:CE1	2.95	0.44
1:A:237:GLU:OE2	1:A:464:LYS:NZ	2.46	0.44
1:A:483:ILE:HD13	1:A:533:ARG:HA	2.00	0.44
1:A:581:MET:HE2	1:A:643:PHE:CG	2.52	0.44
1:A:226:ASP:O	1:A:227:GLN:HB2	2.18	0.43
1:A:231:LYS:O	1:A:232:ASP:HB3	2.19	0.43
1:A:564:ILE:O	1:A:618:LYS:HA	2.19	0.43
1:A:603:ASN:ND2	2:A:138:HOH:O	2.53	0.42
1:A:225:VAL:HG21	1:A:642:ARG:HH21	1.85	0.42
1:A:596:LEU:HD22	1:A:597:HIS:HE1	1.82	0.42
1:A:582:HIS:O	1:A:643:PHE:CB	2.67	0.42
1:A:589:GLU:O	1:A:625:THR:HG22	2.20	0.42
1:A:598:LYS:CD	1:A:617:MET:HE3	2.50	0.42
1:A:221:LEU:HD22	1:A:221:LEU:C	2.45	0.42
1:A:560:PHE:HZ	1:A:581:MET:HE1	1.84	0.42
1:A:650:THR:O	1:A:651:THR:HG22	2.19	0.42
1:A:416:ASN:O	1:A:420:ASP:HB2	2.19	0.41
1:A:564:ILE:N	1:A:619:ILE:HG22	2.34	0.41
1:A:563:GLN:HE21	1:A:563:GLN:HB3	1.74	0.41
1:A:582:HIS:CE1	1:A:587:VAL:HG22	2.56	0.41
1:A:597:HIS:O	1:A:619:ILE:HA	2.21	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	403/467 (86%)	359 (89%)	30 (7%)	14 (4%)	3 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	PRO
1	A	603	ASN
1	A	606	SER
1	A	220	ASP
1	A	227	GLN
1	A	518	ASP
1	A	605	LYS
1	A	652	VAL
1	A	576	GLY
1	A	228	GLU
1	A	232	ASP
1	A	601	LYS
1	A	573	LEU
1	A	587	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	356/398 (89%)	311 (87%)	45 (13%)	4 4

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	224	GLU
1	A	247	VAL
1	A	252	SER
1	A	253	THR
1	A	262	THR
1	A	270	MET
1	A	372	ARG
1	A	396	GLU
1	A	397	ARG
1	A	416	ASN
1	A	417	SER
1	A	438	VAL
1	A	440	SER
1	A	455	LEU
1	A	458	MET
1	A	459	THR
1	A	478	LYS
1	A	485	GLU
1	A	494	LYS
1	A	516	GLU
1	A	529	GLN
1	A	564	ILE
1	A	568	GLU
1	A	569	LEU
1	A	571	SER
1	A	583	ILE
1	A	584	HIS
1	A	595	LEU
1	A	596	LEU
1	A	599	LEU
1	A	601	LYS
1	A	602	THR
1	A	611	MET
1	A	618	LYS
1	A	619	ILE
1	A	620	ILE
1	A	629	VAL
1	A	644	THR
1	A	646	ARG
1	A	647	ASP
1	A	650	THR
1	A	651	THR

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Mol	Chain	Res	Type
1	A	652	VAL
1	A	657	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	227	GLN
1	A	240	ASN
1	A	257	ASN
1	A	315	HIS
1	A	363	GLN
1	A	377	ASN
1	A	378	HIS
1	A	384	ASN
1	A	416	ASN
1	A	460	HIS
1	A	466	ASN
1	A	506	GLN
1	A	542	GLN
1	A	563	GLN
1	A	584	HIS
1	A	648	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	409/467 (87%)	1.30	107 (26%) 1 1	25, 36, 42, 52	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	596	LEU	8.3
1	A	585	THR	8.2
1	A	583	ILE	7.8
1	A	337	ALA	6.9
1	A	215	THR	6.6
1	A	221	LEU	6.6
1	A	556	ALA	6.4
1	A	570	PRO	6.1
1	A	637	TYR	6.0
1	A	639	TYR	5.6
1	A	630	CYS	5.6
1	A	640	MET	5.5
1	A	621	ALA	5.4
1	A	584	HIS	5.2
1	A	586	ALA	5.2
1	A	218	ALA	5.1
1	A	641	GLY	4.7
1	A	588	GLU	4.6
1	A	603	ASN	4.5
1	A	611	MET	4.5
1	A	636	ASP	4.3
1	A	645	LEU	4.3
1	A	638	GLN	4.2
1	A	572	ILE	4.1
1	A	587	VAL	4.1
1	A	568	GLU	4.1
1	A	653	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	579	CYS	4.1
1	A	338	SER	4.0
1	A	647	ASP	4.0
1	A	571	SER	3.8
1	A	578	SER	3.8
1	A	600	ASP	3.8
1	A	222	GLN	3.8
1	A	555	HIS	3.8
1	A	616	GLY	3.7
1	A	613	ALA	3.7
1	A	604	ARG	3.6
1	A	567	LEU	3.5
1	A	580	VAL	3.5
1	A	612	PHE	3.5
1	A	225	VAL	3.4
1	A	634	PHE	3.4
1	A	661	LEU	3.3
1	A	562	ALA	3.3
1	A	232	ASP	3.2
1	A	228	GLU	3.2
1	A	362	GLY	3.2
1	A	573	LEU	3.2
1	A	607	LYS	3.2
1	A	629	VAL	3.1
1	A	654	VAL	3.1
1	A	229	LEU	3.0
1	A	566	ILE	3.0
1	A	646	ARG	3.0
1	A	278	LYS	3.0
1	A	620	ILE	2.9
1	A	595	LEU	2.9
1	A	599	LEU	2.9
1	A	574	THR	2.9
1	A	652	VAL	2.8
1	A	359	GLU	2.8
1	A	631	MET	2.8
1	A	582	HIS	2.8
1	A	643	PHE	2.7
1	A	657	VAL	2.7
1	A	447	GLN	2.6
1	A	216	GLU	2.6
1	A	581	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	558	THR	2.6
1	A	644	THR	2.6
1	A	557	THR	2.5
1	A	569	LEU	2.5
1	A	650	THR	2.5
1	A	279	GLU	2.4
1	A	635	GLU	2.4
1	A	615	LYS	2.4
1	A	519	GLU	2.4
1	A	475	SER	2.4
1	A	655	GLY	2.3
1	A	619	ILE	2.3
1	A	387	ASP	2.3
1	A	324	PRO	2.3
1	A	633	ARG	2.3
1	A	632	GLU	2.3
1	A	610	PRO	2.2
1	A	263	GLY	2.2
1	A	593	ALA	2.2
1	A	628	PRO	2.2
1	A	608	LYS	2.2
1	A	277	ALA	2.2
1	A	575	THR	2.2
1	A	477	TYR	2.2
1	A	220	ASP	2.2
1	A	443	CYS	2.2
1	A	561	ILE	2.1
1	A	590	VAL	2.1
1	A	543	THR	2.1
1	A	602	THR	2.1
1	A	622	GLU	2.1
1	A	623	LEU	2.1
1	A	658	VAL	2.1
1	A	336	GLY	2.1
1	A	480	LEU	2.0
1	A	592	PHE	2.0
1	A	262	THR	2.0
1	A	660	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.