



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2019 – 08:19 PM EDT

PDB ID : 1H2V
Title : Structure of the human nuclear cap-binding-complex (CBC)
Authors : Mazza, C.; Segref, A.; Mattaj, I.W.; Cusack, S.
Deposited on : 2002-08-16
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

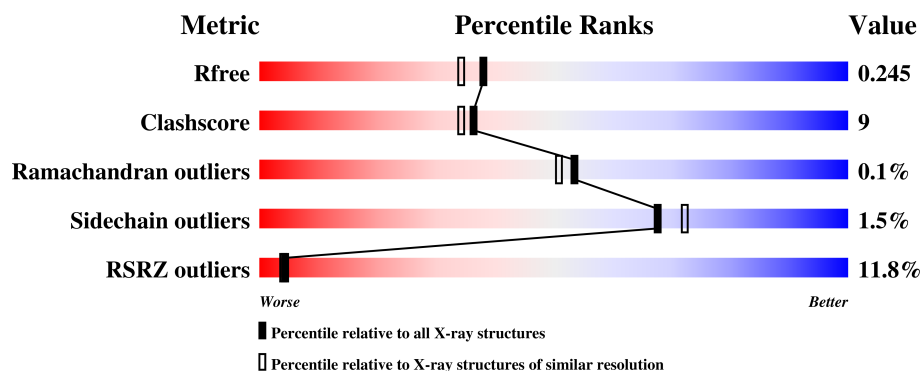
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	C	771	
2	Z	156	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6961 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 80 KDA NUCLEAR CAP BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	722	Total	C	N	O	S	0	0	0
			5905	3812	996	1059	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	479	SER	ALA	engineered mutation	UNP Q09161

- Molecule 2 is a protein called 20 KDA NUCLEAR CAP BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	93	Total	C	N	O	S	0	0	0
			762	486	127	143	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	250	Total	O	0	0
			250	250		
3	Z	44	Total	O	0	0
			44	44		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.14Å 59.60Å 75.43Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	19.67 – 2.00 19.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.4 (19.67-2.00) 79.5 (19.67-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.247 0.211 , 0.245	Depositor DCC
R_{free} test set	3112 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6961	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	C	0.33	0/6057	0.52	0/8220
2	Z	0.37	0/775	0.61	0/1035
All	All	0.34	0/6832	0.53	0/9255

There are no bond length outliers.

There are no bond angle outliers.

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	C	5905	0	5898	97	0
2	Z	762	0	756	17	0
3	C	250	0	0	9	0
3	Z	44	0	0	3	0
All	All	6961	0	6654	114	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 9.

All (114) 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:C:699:VAL:HG12	1:C:703:GLN:HE21	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:ILE:HG22	1:C:699:VAL:HG22	1.63	0.77
1:C:780:ALA:O	1:C:784:GLN:HG3	1.90	0.72
1:C:513:THR:HG22	1:C:516:GLU:HG3	1.72	0.71
1:C:557:LYS:HB3	1:C:561:HIS:HD2	1.58	0.68
2:Z:34:LYS:HD2	2:Z:38:LYS:HZ3	1.57	0.67
1:C:35:ILE:O	1:C:38:VAL:HG12	1.94	0.67
1:C:44:CYS:HB2	1:C:49:ASN:HD21	1.60	0.66
1:C:61:LEU:N	1:C:62:PRO:HD2	2.11	0.65
1:C:588:ARG:NH1	1:C:588:ARG:HB2	2.13	0.64
1:C:182:LYS:O	1:C:186:GLU:HG3	1.98	0.64
1:C:200:GLU:HG2	1:C:204:LYS:HE3	1.79	0.64
1:C:83:LEU:HD11	1:C:130:PHE:HA	1.79	0.63
1:C:588:ARG:O	1:C:592:GLU:HG3	1.99	0.63
2:Z:34:LYS:HD2	2:Z:38:LYS:NZ	2.14	0.62
1:C:557:LYS:HB3	1:C:561:HIS:CD2	2.38	0.59
1:C:262:GLU:O	1:C:265:GLN:HG3	2.04	0.58
1:C:582:GLY:O	1:C:586:VAL:HG23	2.03	0.58
2:Z:44:VAL:HG22	2:Z:113:THR:HG22	1.86	0.58
1:C:146:VAL:O	1:C:150:GLU:HG3	2.04	0.57
1:C:67:LYS:HG2	1:C:70:ARG:HH21	1.68	0.57
2:Z:112:ARG:HG2	3:Z:2029:HOH:O	2.04	0.57
1:C:588:ARG:HB2	1:C:588:ARG:HH11	1.67	0.57
1:C:135:VAL:HG12	1:C:183:GLU:HG2	1.86	0.56
1:C:493:ASN:HD22	1:C:493:ASN:N	2.02	0.56
2:Z:77:LYS:O	2:Z:78:LYS:HB2	2.06	0.56
2:Z:56:ILE:HG22	2:Z:69:ILE:HD13	1.88	0.55
1:C:586:VAL:HG11	1:C:608:MET:HE3	1.89	0.54
1:C:67:LYS:HZ3	1:C:71:LEU:HD11	1.73	0.54
1:C:699:VAL:HG12	1:C:703:GLN:NE2	2.13	0.54
1:C:247:ARG:HB3	1:C:343:ASN:ND2	2.23	0.54
1:C:105:VAL:CG1	1:C:268:LEU:HD23	2.39	0.53
1:C:425:GLN:HG3	3:C:2160:HOH:O	2.08	0.53
1:C:753:GLN:HG2	1:C:754:HIS:CE1	2.44	0.53
1:C:716:ARG:HA	1:C:716:ARG:HH11	1.73	0.52
2:Z:102:ASN:HB2	2:Z:113:THR:OG1	2.10	0.52
1:C:382:LEU:C	1:C:384:PRO:HD3	2.29	0.52
1:C:247:ARG:HB3	1:C:343:ASN:HD22	1.75	0.52
1:C:383:GLN:N	1:C:384:PRO:HD3	2.25	0.51
1:C:480:ASN:ND2	1:C:482:THR:HG23	2.25	0.51
1:C:573:PHE:HB3	1:C:613:ILE:HG23	1.90	0.51
1:C:524:VAL:HG13	1:C:542:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:LYS:HD3	1:C:561:HIS:NE2	2.26	0.50
2:Z:67:LYS:HD3	2:Z:87:GLU:OE2	2.11	0.50
1:C:52:GLY:O	1:C:56:VAL:HG23	2.11	0.50
1:C:41:LYS:HD2	3:C:2002:HOH:O	2.13	0.49
1:C:431:GLU:CD	1:C:431:GLU:H	2.16	0.49
1:C:500:VAL:HG11	1:C:524:VAL:HG22	1.94	0.49
1:C:572:VAL:O	1:C:576:LEU:HD13	2.12	0.49
1:C:712:VAL:O	1:C:716:ARG:HG2	2.12	0.49
1:C:592:GLU:HG2	3:C:2206:HOH:O	2.13	0.48
1:C:724:HIS:ND1	1:C:727:ARG:NH2	2.61	0.48
1:C:129:ARG:HD2	3:C:2019:HOH:O	2.12	0.48
1:C:499:SER:HA	1:C:502:LEU:HD12	1.94	0.48
1:C:31:LEU:H	1:C:31:LEU:HD12	1.79	0.47
1:C:74:THR:HA	1:C:77:ARG:NH1	2.29	0.47
2:Z:38:LYS:HD2	2:Z:38:LYS:N	2.30	0.47
1:C:492:SER:C	1:C:494:SER:H	2.18	0.47
1:C:498:HIS:O	1:C:502:LEU:HG	2.15	0.47
1:C:513:THR:CG2	1:C:516:GLU:HG3	2.43	0.47
2:Z:57:TYR:CD2	2:Z:69:ILE:HD12	2.49	0.46
1:C:251:ARG:HB3	1:C:253:TYR:CE1	2.50	0.46
1:C:493:ASN:HA	1:C:498:HIS:CG	2.50	0.46
1:C:35:ILE:HD12	1:C:71:LEU:HD13	1.97	0.46
1:C:480:ASN:HD22	1:C:482:THR:HG23	1.81	0.46
1:C:493:ASN:N	1:C:493:ASN:ND2	2.64	0.46
2:Z:56:ILE:HD13	2:Z:84:CYS:SG	2.56	0.46
1:C:472:THR:HG23	3:C:2187:HOH:O	2.15	0.46
1:C:738:PRO:HG2	3:C:2168:HOH:O	2.15	0.46
1:C:47:GLU:H	1:C:47:GLU:CD	2.18	0.45
1:C:200:GLU:CG	1:C:204:LYS:HE3	2.46	0.45
1:C:493:ASN:HA	1:C:498:HIS:CD2	2.52	0.45
1:C:514:ASN:OD1	1:C:571:GLU:HB2	2.17	0.45
1:C:70:ARG:HE	1:C:70:ARG:HB3	1.56	0.45
1:C:31:LEU:HD12	1:C:31:LEU:N	2.32	0.45
2:Z:78:LYS:HE3	3:Z:2022:HOH:O	2.16	0.44
2:Z:78:LYS:HG2	3:Z:2022:HOH:O	2.17	0.44
2:Z:91:ARG:O	2:Z:95:GLU:HG3	2.16	0.44
1:C:500:VAL:HG11	1:C:524:VAL:CG2	2.47	0.44
1:C:190:ALA:O	1:C:194:ARG:HG3	2.18	0.44
1:C:505:ALA:O	1:C:509:LYS:HG3	2.16	0.44
1:C:483:CYS:HB2	1:C:594:TRP:CH2	2.52	0.43
1:C:742:ASN:O	1:C:746:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:SER:C	1:C:494:SER:N	2.72	0.43
1:C:493:ASN:HD22	1:C:494:SER:N	2.17	0.43
1:C:655:ILE:HD13	1:C:698:LYS:HG2	2.01	0.43
2:Z:37:LYS:C	2:Z:38:LYS:HD2	2.38	0.43
2:Z:72:GLY:HA2	2:Z:124:GLN:O	2.19	0.43
1:C:221:LYS:HB2	1:C:221:LYS:HE3	1.89	0.43
1:C:129:ARG:HD3	1:C:179:TRP:CZ3	2.53	0.43
1:C:61:LEU:N	1:C:62:PRO:CD	2.81	0.43
1:C:348:ASN:HB2	3:C:2125:HOH:O	2.19	0.43
1:C:566:LEU:HD11	1:C:604:LEU:HD22	2.00	0.43
1:C:273:PRO:HA	1:C:274:PRO:HD3	1.92	0.43
1:C:144:SER:HB3	1:C:268:LEU:HD12	2.01	0.42
1:C:619:VAL:O	1:C:623:ILE:HG12	2.20	0.42
1:C:50:LEU:HD13	1:C:88:THR:HG21	2.00	0.42
2:Z:51:THR:HA	2:Z:55:GLN:OE1	2.20	0.42
1:C:185:TYR:O	1:C:189:ASP:HB3	2.20	0.42
1:C:513:THR:O	1:C:517:ILE:HD13	2.20	0.42
1:C:525:PRO:HG3	3:C:2198:HOH:O	2.19	0.42
1:C:588:ARG:HD3	1:C:627:GLU:CD	2.40	0.42
1:C:662:ALA:O	1:C:692:ILE:HD13	2.20	0.42
1:C:211:VAL:HB	1:C:212:PRO:HD3	2.02	0.42
1:C:476:LEU:HD12	1:C:476:LEU:N	2.35	0.41
1:C:659:LEU:HD21	1:C:696:GLN:HG2	2.02	0.41
1:C:585:HIS:O	1:C:589:VAL:HG23	2.20	0.41
1:C:692:ILE:HG23	1:C:693:GLU:N	2.35	0.41
1:C:399:TYR:OH	1:C:436:CYS:HB3	2.21	0.41
1:C:563:PHE:HZ	1:C:603:VAL:HB	1.86	0.40
1:C:112:LEU:O	1:C:116:LEU:HG	2.21	0.40
1:C:275:PRO:HD2	3:C:2081:HOH:O	2.21	0.40
1:C:206:ARG:CZ	1:C:229:LEU:HD12	2.51	0.40
1:C:64:TYR:O	1:C:68:ILE:HG13	2.22	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	C	716/771 (93%)	691 (96%)	24 (3%)	1 (0%)	53	51
2	Z	91/156 (58%)	89 (98%)	2 (2%)	0	100	100
All	All	807/927 (87%)	780 (97%)	26 (3%)	1 (0%)	53	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	490	GLU

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	C	663/708 (94%)	655 (99%)	8 (1%)	74	78
2	Z	81/130 (62%)	78 (96%)	3 (4%)	37	35
All	All	744/838 (89%)	733 (98%)	11 (2%)	67	72

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	ARG
1	C	114	GLU
1	C	247	ARG
1	C	299	GLU
1	C	464	ARG
1	C	493	ASN
1	C	711	LEU
1	C	773	GLU
2	Z	57	TYR
2	Z	76	MET
2	Z	81	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	49	ASN
1	C	63	ASN
1	C	157	GLN
1	C	198	ASN
1	C	325	HIS
1	C	343	ASN
1	C	480	ASN
1	C	493	ASN
1	C	514	ASN
1	C	553	HIS
1	C	561	HIS
1	C	585	HIS
1	C	596	ASN
1	C	649	ASN
1	C	656	GLN
1	C	696	GLN
1	C	703	GLN
1	C	706	GLN
1	C	715	GLN
1	C	753	GLN
1	C	754	HIS
1	C	756	GLN
1	C	760	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	C	722/771 (93%)	0.46	81 (11%)	5 5	27, 47, 90, 110	0
2	Z	93/156 (59%)	0.73	15 (16%)	1 1	30, 46, 84, 92	0
All	All	815/927 (87%)	0.49	96 (11%)	4 4	27, 47, 89, 110	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	CYS	7.0
1	C	43	ALA	7.0
1	C	41	LYS	5.7
1	C	511	LYS	5.6
1	C	694	ARG	5.3
2	Z	76	MET	5.3
2	Z	33	GLU	5.2
2	Z	75	LYS	4.9
1	C	29	ASP	4.9
1	C	489	ASP	4.8
1	C	525	PRO	4.7
1	C	63	ASN	4.4
2	Z	49	PHE	4.3
2	Z	35	LEU	4.3
1	C	548	VAL	4.2
1	C	539	PHE	4.1
1	C	661	GLU	4.1
1	C	510	SER	4.0
1	C	89	LEU	3.9
1	C	526	ASN	3.7
1	C	693	GLU	3.7
2	Z	50	TYR	3.7
1	C	278	GLU	3.7
2	Z	77	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	662	ALA	3.5
1	C	262	GLU	3.5
1	C	547	PHE	3.4
2	Z	80	ALA	3.4
1	C	488	GLY	3.4
1	C	491	SER	3.3
1	C	64	TYR	3.3
1	C	523	ASP	3.3
2	Z	78	LYS	3.3
2	Z	34	LYS	3.3
1	C	747	LEU	3.3
1	C	663	LYS	3.2
1	C	697	GLU	3.2
1	C	490	GLU	3.2
1	C	692	ILE	3.1
1	C	159	GLU	3.1
1	C	524	VAL	3.1
1	C	42	SER	3.1
1	C	660	GLU	3.1
1	C	493	ASN	3.0
2	Z	37	LYS	3.0
1	C	506	VAL	3.0
2	Z	36	LEU	3.0
1	C	134	LEU	3.0
1	C	504	LEU	2.9
2	Z	79	THR	2.9
1	C	45	SER	2.9
1	C	773	GLU	2.9
1	C	568	LYS	2.8
2	Z	74	ASP	2.8
1	C	772	ALA	2.7
1	C	90	VAL	2.7
1	C	270	PRO	2.7
1	C	177	LEU	2.7
1	C	540	ASN	2.7
1	C	279	ASP	2.6
1	C	522	LYS	2.6
1	C	587	LEU	2.6
1	C	160	ASP	2.6
1	C	630	ARG	2.6
1	C	557	LYS	2.6
1	C	30	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	501	ALA	2.5
1	C	492	SER	2.5
1	C	605	VAL	2.5
1	C	590	MET	2.4
1	C	40	GLU	2.4
1	C	494	SER	2.4
1	C	139	VAL	2.4
1	C	551	LEU	2.3
1	C	696	GLN	2.3
1	C	700	GLU	2.3
1	C	186	GLU	2.3
1	C	46	LEU	2.3
1	C	257	ASP	2.2
1	C	62	PRO	2.2
1	C	461	TYR	2.2
1	C	578	GLU	2.2
1	C	581	GLU	2.1
1	C	546	VAL	2.1
1	C	556	ALA	2.1
1	C	517	ILE	2.1
1	C	51	GLU	2.1
1	C	91	GLY	2.1
1	C	355	ILE	2.0
1	C	512	ALA	2.0
2	Z	122	GLY	2.0
1	C	87	THR	2.0
1	C	194	ARG	2.0
1	C	508	PHE	2.0
1	C	751	PHE	2.0
1	C	174	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.