



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:03 PM UTC

PDB ID : 8G5T / pdb_00008g5t
Title : Crystal structure of apo TnmK2
Authors : Liu, Y.-C.; Gui, C.; Shen, B.
Deposited on : 2023-02-14
Resolution : 1.85 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

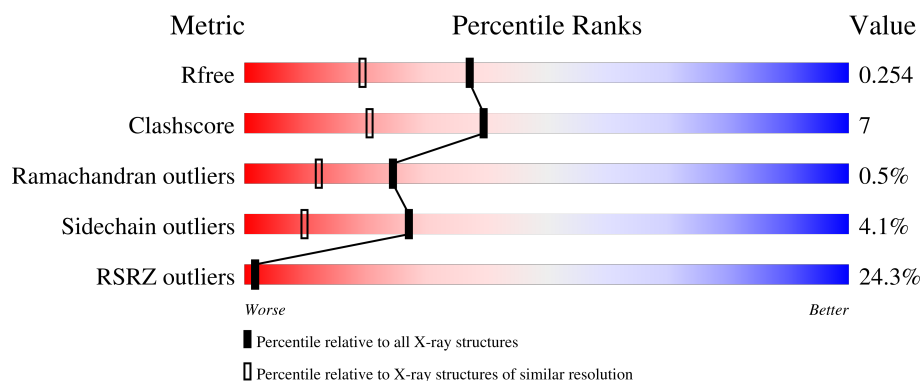
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	489	15% 86% 11% ..
1	B	489	15% 86% 11% ..
1	C	489	31% 83% 14% ..
1	D	489	34% 82% 15% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30803 atoms, of which 14506 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 TnmK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	H	N	O	S	0	0	0
			7342	2346	3627	673	684	12			
1	B	481	Total	C	H	N	O	S	0	0	0
			7342	2346	3627	673	684	12			
1	C	481	Total	C	H	N	O	S	0	0	0
			7341	2346	3626	673	684	12			
1	D	481	Total	C	H	N	O	S	0	0	0
			7341	2346	3626	673	684	12			

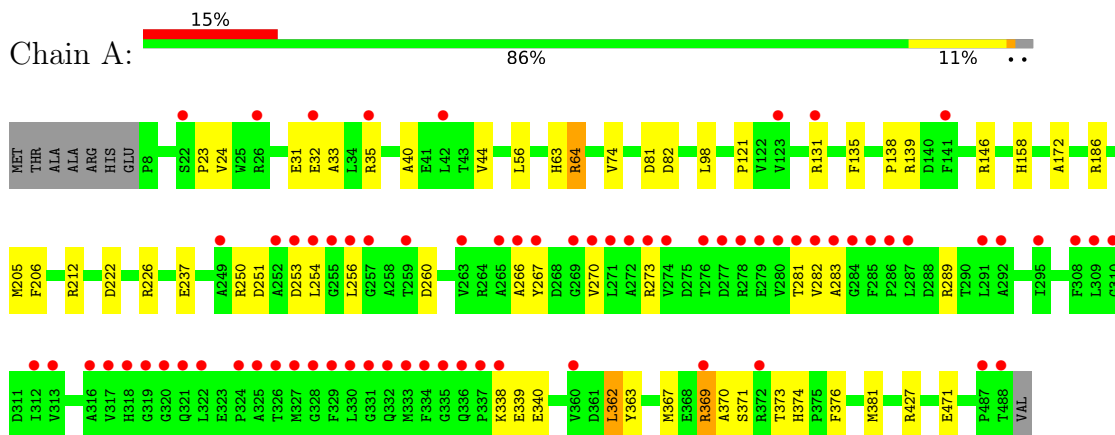
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	475	Total	O	0	0
			475	475		
2	B	459	Total	O	0	0
			459	459		
2	C	261	Total	O	0	0
			261	261		
2	D	242	Total	O	0	0
			242	242		

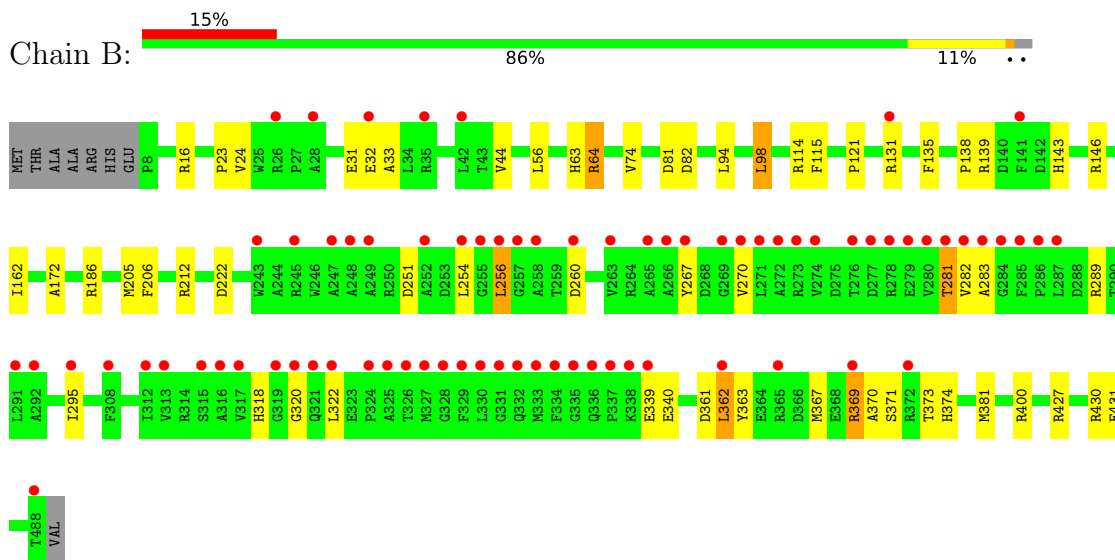
3 Residue-property plots [i](#)

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.

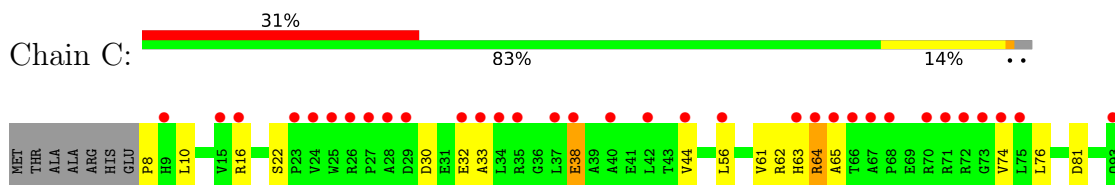
• Molecule 1: TnmK2

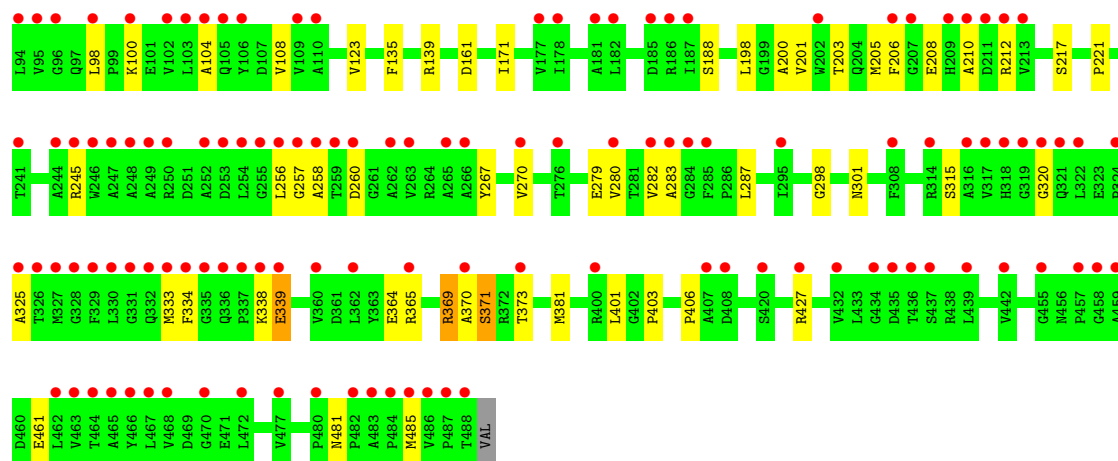


• Molecule 1: TnmK2

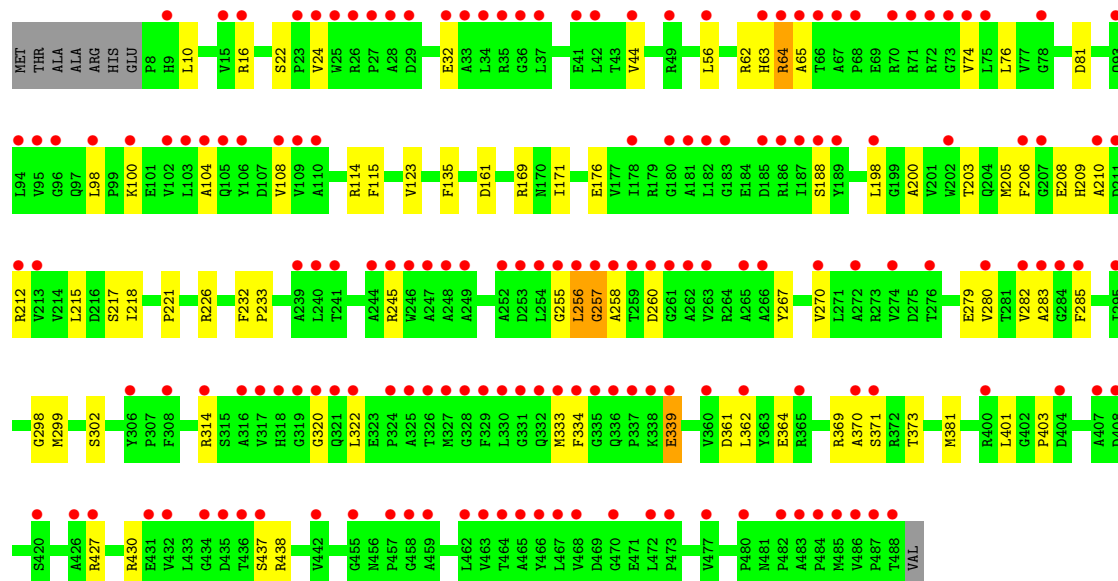
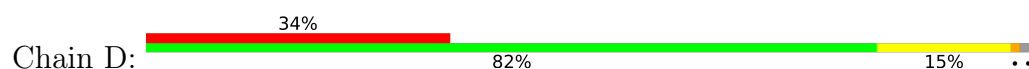


• Molecule 1: TnmK2





• Molecule 1: TnmK2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	134.12Å 134.12Å 356.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.68 – 1.85 29.68 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.68-1.85) 96.4 (29.68-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.84Å)	Xtriage
Refinement program	PHENIX (dev_2689: ???)	Depositor
R, R_{free}	0.226 , 0.253 0.226 , 0.254	Depositor DCC
R_{free} test set	10153 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30803	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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	0.25	0/3812	0.50	0/5205
1	B	0.23	0/3812	0.49	0/5205
1	C	0.20	0/3812	0.46	0/5205
1	D	0.21	0/3812	0.46	0/5205
All	All	0.22	0/15248	0.48	0/20820

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	SER	Peptide
1	D	217	SER	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	3715	3627	3626	39	1
1	B	3715	3627	3626	42	1
1	C	3715	3626	3626	53	1
1	D	3715	3626	3626	65	2
2	A	475	0	0	20	5
2	B	459	0	0	20	6
2	C	261	0	0	28	6
2	D	242	0	0	34	3
All	All	16297	14506	14504	196	13

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 (196) 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:D:205:MET:SD	2:D:514:HOH:O	2.03	1.13
1:A:205:MET:SD	2:A:873:HOH:O	2.07	1.11
1:D:203:THR:N	2:D:502:HOH:O	1.83	1.11
1:C:333:MET:SD	2:C:705:HOH:O	2.11	1.06
1:B:400:ARG:NH2	2:B:503:HOH:O	1.95	0.99
1:D:63:HIS:O	2:D:501:HOH:O	1.81	0.97
1:C:365:ARG:NE	2:C:504:HOH:O	1.98	0.96
1:C:325:ALA:O	2:C:501:HOH:O	1.83	0.95
1:B:139:ARG:NH1	2:B:507:HOH:O	2.01	0.94
1:C:258:ALA:O	2:C:502:HOH:O	1.85	0.93
1:D:437:SER:O	2:D:503:HOH:O	1.84	0.93
1:C:203:THR:N	2:C:506:HOH:O	2.02	0.92
1:C:427:ARG:NH1	2:C:507:HOH:O	2.01	0.92
1:A:266:ALA:O	2:A:501:HOH:O	1.88	0.92
1:D:333:MET:SD	2:D:680:HOH:O	2.26	0.92
1:A:471:GLU:OE1	2:A:502:HOH:O	1.91	0.88
1:D:427:ARG:NH1	2:D:509:HOH:O	2.07	0.88
1:C:200:ALA:C	2:C:506:HOH:O	2.18	0.87
1:C:481:ASN:OD1	2:C:503:HOH:O	1.92	0.86
1:C:485:MET:SD	2:C:691:HOH:O	2.32	0.86
1:B:121:PRO:O	2:B:501:HOH:O	1.93	0.85
1:C:76:LEU:N	2:C:508:HOH:O	2.09	0.84
1:A:35:ARG:O	2:A:503:HOH:O	1.96	0.84
1:A:253:ASP:O	2:A:504:HOH:O	1.96	0.83
1:A:40:ALA:O	2:A:505:HOH:O	1.97	0.82
1:D:403:PRO:O	2:D:504:HOH:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:GLU:OE2	2:C:505:HOH:O	1.98	0.81
1:C:200:ALA:O	2:C:506:HOH:O	1.98	0.81
1:A:186:ARG:NH2	2:A:510:HOH:O	2.09	0.80
1:B:295:ILE:O	2:B:505:HOH:O	1.99	0.80
1:B:361:ASP:OD2	2:B:506:HOH:O	2.00	0.80
1:A:139:ARG:O	2:A:506:HOH:O	1.99	0.79
1:B:64:ARG:NH1	2:B:513:HOH:O	2.15	0.78
1:B:172:ALA:HB3	1:B:205:MET:HE1	1.66	0.78
1:D:188:SER:O	2:D:506:HOH:O	2.02	0.77
1:D:258:ALA:O	2:D:505:HOH:O	2.00	0.77
1:B:186:ARG:NH2	2:B:512:HOH:O	2.14	0.77
1:D:76:LEU:N	2:D:506:HOH:O	2.19	0.76
1:A:23:PRO:O	2:A:507:HOH:O	2.03	0.76
1:D:267:TYR:O	1:D:270:VAL:HG12	1.86	0.76
1:B:31:GLU:OE2	2:B:508:HOH:O	2.04	0.75
1:D:339:GLU:OE1	2:D:508:HOH:O	2.05	0.75
1:A:121:PRO:O	2:A:508:HOH:O	2.06	0.74
1:B:16:ARG:NH2	2:B:510:HOH:O	2.07	0.74
1:D:210:ALA:O	2:D:507:HOH:O	2.05	0.74
1:C:267:TYR:O	1:C:270:VAL:HG12	1.88	0.73
1:B:143:HIS:O	2:B:509:HOH:O	2.06	0.73
1:C:188:SER:O	2:C:508:HOH:O	2.05	0.73
1:C:210:ALA:O	2:C:509:HOH:O	2.06	0.73
1:A:172:ALA:HB3	1:A:205:MET:HE1	1.71	0.73
1:D:169:ARG:CZ	2:D:514:HOH:O	2.37	0.72
1:A:158:HIS:O	2:A:509:HOH:O	2.07	0.72
1:A:205:MET:HE3	1:A:206:PHE:CE2	2.25	0.71
1:B:281:THR:OG1	2:B:511:HOH:O	2.07	0.70
1:B:146:ARG:NH2	2:B:502:HOH:O	1.94	0.70
1:B:318:HIS:NE2	2:B:504:HOH:O	1.98	0.69
1:C:301:ASN:OD1	2:C:511:HOH:O	2.10	0.69
1:D:32:GLU:HG2	2:D:652:HOH:O	1.92	0.69
1:C:338:LYS:HE2	2:C:543:HOH:O	1.92	0.69
1:C:403:PRO:O	2:C:510:HOH:O	2.10	0.68
1:A:64:ARG:NH1	2:A:516:HOH:O	2.27	0.67
1:C:8:PRO:N	2:C:518:HOH:O	2.27	0.67
1:A:82:ASP:HB3	2:A:804:HOH:O	1.94	0.67
1:B:267:TYR:O	1:B:270:VAL:HG12	1.95	0.67
1:D:200:ALA:C	2:D:502:HOH:O	2.39	0.66
1:D:430:ARG:NE	2:D:503:HOH:O	2.27	0.66
1:B:205:MET:HE3	1:B:206:PHE:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TYR:O	1:A:270:VAL:HG12	1.96	0.66
1:D:438:ARG:HA	2:D:503:HOH:O	1.96	0.66
1:A:63:HIS:O	1:A:64:ARG:HB2	1.96	0.65
1:B:63:HIS:O	1:B:64:ARG:HB2	1.97	0.64
1:C:279:GLU:OE2	2:C:512:HOH:O	2.14	0.64
1:D:200:ALA:O	2:D:502:HOH:O	2.14	0.64
1:D:169:ARG:NH1	2:D:514:HOH:O	2.30	0.63
1:D:298:GLY:HA3	1:D:333:MET:HE1	1.80	0.63
1:D:438:ARG:HD3	2:D:503:HOH:O	1.99	0.62
1:B:222:ASP:OD2	2:B:514:HOH:O	2.16	0.62
1:C:298:GLY:HA3	1:C:333:MET:HE1	1.83	0.61
1:A:273:ARG:NH2	2:A:519:HOH:O	2.32	0.59
1:D:161:ASP:OD1	2:D:511:HOH:O	2.17	0.58
1:C:198:LEU:C	2:C:524:HOH:O	2.45	0.58
1:D:63:HIS:O	1:D:64:ARG:HB2	2.02	0.58
1:A:32:GLU:HG2	2:A:757:HOH:O	2.05	0.57
1:B:82:ASP:HB3	2:B:801:HOH:O	2.04	0.57
1:D:430:ARG:CZ	2:D:503:HOH:O	2.53	0.57
1:C:63:HIS:O	1:C:64:ARG:HB2	2.05	0.56
1:D:279:GLU:HG2	2:D:516:HOH:O	2.06	0.56
1:B:172:ALA:CB	1:B:205:MET:HE1	2.34	0.55
1:A:282:VAL:HG23	1:A:283:ALA:H	1.71	0.55
1:A:172:ALA:CB	1:A:205:MET:HE1	2.36	0.55
1:B:282:VAL:HG23	1:B:283:ALA:H	1.71	0.55
1:B:23:PRO:O	2:B:515:HOH:O	2.18	0.54
1:A:31:GLU:OE2	2:A:511:HOH:O	2.18	0.54
1:C:139:ARG:NH1	2:C:521:HOH:O	2.40	0.54
1:D:282:VAL:HG23	1:D:283:ALA:H	1.72	0.54
1:C:201:VAL:C	2:C:506:HOH:O	2.50	0.53
1:D:205:MET:HG2	2:D:514:HOH:O	2.09	0.53
1:C:64:ARG:NE	2:C:515:HOH:O	2.24	0.52
1:C:279:GLU:HG2	2:C:512:HOH:O	2.09	0.52
1:C:16:ARG:HE	1:D:10:LEU:HD12	1.74	0.52
1:C:282:VAL:HG23	1:C:283:ALA:H	1.74	0.52
1:A:370:ALA:HA	1:A:373:THR:HG22	1.92	0.51
1:B:251:ASP:O	1:B:254:LEU:O	2.28	0.51
1:A:222:ASP:OD2	2:A:512:HOH:O	2.19	0.50
1:D:362:LEU:C	1:D:362:LEU:HD23	2.36	0.50
1:B:400:ARG:CZ	2:B:503:HOH:O	2.49	0.49
1:C:270:VAL:CG2	1:C:280:VAL:HG11	2.42	0.49
1:D:270:VAL:CG2	1:D:280:VAL:HG11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:NH1	2:B:526:HOH:O	2.45	0.49
1:A:251:ASP:O	1:A:254:LEU:O	2.31	0.49
1:B:370:ALA:HA	1:B:373:THR:HG22	1.95	0.49
1:C:334:PHE:HE2	2:C:705:HOH:O	1.95	0.49
1:D:171:ILE:HG21	1:D:198:LEU:HD11	1.93	0.49
1:D:205:MET:CG	2:D:514:HOH:O	2.49	0.49
1:C:62:ARG:HA	1:C:108:VAL:O	2.13	0.48
1:B:427:ARG:NH1	2:B:527:HOH:O	2.46	0.48
1:D:205:MET:HE3	1:D:206:PHE:CE2	2.48	0.48
1:D:226:ARG:NH2	1:D:362:LEU:HD21	2.29	0.47
1:A:362:LEU:C	1:A:362:LEU:HD23	2.40	0.47
1:B:131:ARG:NH2	1:B:340:GLU:HB2	2.30	0.47
1:C:63:HIS:O	1:C:64:ARG:CB	2.62	0.47
1:D:63:HIS:O	1:D:64:ARG:CB	2.62	0.47
1:A:138:PRO:HG3	1:A:367:MET:HE2	1.97	0.46
1:B:362:LEU:HD23	1:B:363:TYR:N	2.31	0.46
1:A:131:ARG:NH2	1:A:340:GLU:HB2	2.30	0.46
1:A:135:PHE:CD1	1:A:381:MET:HE3	2.51	0.46
1:D:64:ARG:NE	2:D:520:HOH:O	2.41	0.46
1:D:161:ASP:OD1	1:D:161:ASP:N	2.49	0.46
1:D:430:ARG:NH2	2:D:503:HOH:O	2.49	0.45
1:C:208:GLU:HG3	1:D:208:GLU:HG3	1.97	0.45
1:A:362:LEU:HD23	1:A:363:TYR:N	2.32	0.45
1:B:362:LEU:HD23	1:B:362:LEU:C	2.42	0.45
1:D:169:ARG:NH2	2:D:514:HOH:O	2.49	0.45
1:A:250:ARG:NH1	2:A:523:HOH:O	2.40	0.45
1:C:205:MET:CE	1:C:206:PHE:CE2	3.00	0.45
1:C:245:ARG:HG2	1:C:260:ASP:OD1	2.17	0.45
1:B:94:LEU:HB3	1:B:98:LEU:HD22	1.99	0.44
1:B:172:ALA:CB	1:B:205:MET:CE	2.95	0.44
1:C:135:PHE:CD1	1:C:381:MET:HE3	2.53	0.44
1:C:171:ILE:HG21	1:C:198:LEU:HD11	2.00	0.44
1:D:135:PHE:CD1	1:D:381:MET:HE3	2.52	0.44
1:B:427:ARG:O	1:B:431:GLU:HG3	2.17	0.44
1:C:161:ASP:OD1	1:C:161:ASP:N	2.47	0.44
1:C:221:PRO:HB3	1:C:401:LEU:HD12	2.00	0.44
1:A:226:ARG:NH2	1:A:362:LEU:HD21	2.33	0.44
1:C:371:SER:OG	2:C:514:HOH:O	2.21	0.44
1:D:245:ARG:HG2	1:D:260:ASP:OD1	2.18	0.44
1:D:205:MET:CE	1:D:206:PHE:CE2	3.00	0.44
1:C:10:LEU:HD12	1:D:16:ARG:HE	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ARG:HA	1:D:108:VAL:O	2.17	0.43
1:C:461:GLU:HB3	2:C:591:HOH:O	2.18	0.43
1:D:302:SER:OG	2:D:510:HOH:O	2.16	0.43
1:D:65:ALA:HB1	1:D:104:ALA:O	2.19	0.43
1:B:318:HIS:CE1	2:B:504:HOH:O	2.60	0.43
1:B:373:THR:HG23	1:B:374:HIS:ND1	2.33	0.43
1:B:369:ARG:O	1:B:373:THR:HG22	2.18	0.43
1:C:65:ALA:HB1	1:C:104:ALA:O	2.19	0.43
1:C:32:GLU:HG3	1:C:33:ALA:N	2.32	0.43
1:C:161:ASP:OD2	2:C:513:HOH:O	2.21	0.43
1:C:370:ALA:HA	1:C:373:THR:CG2	2.49	0.43
1:D:255:GLY:H	1:D:314:ARG:HD3	1.85	0.42
1:D:370:ALA:HA	1:D:373:THR:HG22	2.01	0.42
1:C:205:MET:HE3	1:C:206:PHE:CE2	2.55	0.42
1:D:314:ARG:NH1	2:D:533:HOH:O	2.53	0.42
1:A:32:GLU:HG2	1:A:33:ALA:N	2.35	0.42
1:A:172:ALA:CB	1:A:205:MET:CE	2.97	0.42
1:D:215:LEU:O	1:D:218:ILE:HD11	2.20	0.42
1:D:299:MET:HE3	2:D:680:HOH:O	2.20	0.42
1:D:161:ASP:CG	2:D:511:HOH:O	2.60	0.42
1:D:256:LEU:O	1:D:257:GLY:O	2.38	0.41
1:D:270:VAL:HG23	1:D:280:VAL:HG11	2.01	0.41
1:B:256:LEU:HD22	1:B:256:LEU:H	1.86	0.41
1:C:203:THR:O	1:C:406:PRO:HD2	2.19	0.41
1:D:334:PHE:HE2	2:D:680:HOH:O	2.02	0.41
1:D:114:ARG:O	1:D:115:PHE:HB2	2.21	0.41
1:D:283:ALA:HB3	1:D:285:PHE:HD2	1.85	0.41
1:A:237:GLU:OE2	1:A:376:PHE:HB3	2.21	0.41
1:A:338:LYS:NZ	2:A:539:HOH:O	2.53	0.41
1:B:32:GLU:CG	1:B:33:ALA:N	2.83	0.41
1:C:282:VAL:O	1:C:315:SER:OG	2.38	0.41
1:A:373:THR:HG23	1:A:374:HIS:ND1	2.35	0.41
1:B:135:PHE:CD1	1:B:381:MET:HE3	2.55	0.41
1:B:138:PRO:HG3	1:B:367:MET:HE2	2.03	0.41
1:D:203:THR:CA	2:D:502:HOH:O	2.54	0.41
1:A:369:ARG:O	1:A:373:THR:HG22	2.21	0.40
1:B:114:ARG:O	1:B:115:PHE:HB2	2.20	0.40
1:C:38:GLU:O	1:C:61:VAL:HA	2.21	0.40
1:D:176:GLU:HG3	1:D:206:PHE:CD2	2.57	0.40
1:D:221:PRO:HB3	1:D:401:LEU:HD12	2.02	0.40
1:C:369:ARG:O	1:C:373:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ALA:HA	1:C:373:THR:HG22	2.02	0.40
1:D:208:GLU:HG2	1:D:209:HIS:CD2	2.56	0.40
1:D:232:PHE:N	1:D:233:PRO:CD	2.84	0.40
1:A:427:ARG:NH1	2:A:542:HOH:O	2.55	0.40
1:B:162:ILE:C	1:B:162:ILE:HD12	2.47	0.40
1:D:370:ALA:HA	1:D:373:THR:CG2	2.51	0.40

All (13) 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)
2:B:712:HOH:O	2:D:628:HOH:O[3_655]	1.52	0.68
2:B:708:HOH:O	2:D:681:HOH:O[3_655]	1.77	0.43
2:A:679:HOH:O	2:C:651:HOH:O[3_655]	1.87	0.33
2:A:576:HOH:O	2:C:687:HOH:O[3_655]	1.94	0.26
1:D:361:ASP:OD1	2:B:502:HOH:O[2_545]	1.96	0.24
2:B:803:HOH:O	2:C:622:HOH:O[5_445]	1.98	0.22
2:B:835:HOH:O	2:C:699:HOH:O[5_445]	1.99	0.21
2:A:916:HOH:O	2:A:916:HOH:O[3_555]	2.12	0.08
1:A:146:ARG:HH22	1:C:364:GLU:OE1[3_655]	1.53	0.07
2:A:521:HOH:O	2:C:666:HOH:O[3_655]	2.17	0.03
2:A:739:HOH:O	2:C:533:HOH:O[3_655]	2.17	0.03
2:B:576:HOH:O	2:D:529:HOH:O[3_655]	2.17	0.03
1:B:146:ARG:HH22	1:D:364:GLU:OE1[3_655]	1.58	0.02

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	479/489 (98%)	456 (95%)	22 (5%)	1 (0%)	43 34
1	B	479/489 (98%)	459 (96%)	18 (4%)	2 (0%)	30 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	479/489 (98%)	456 (95%)	20 (4%)	3 (1%)	21	9
1	D	479/489 (98%)	457 (95%)	19 (4%)	3 (1%)	21	9
All	All	1916/1956 (98%)	1828 (95%)	79 (4%)	9 (0%)	24	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	64	ARG
1	D	64	ARG
1	A	64	ARG
1	B	64	ARG
1	C	257	GLY
1	D	257	GLY
1	D	320	GLY
1	B	320	GLY
1	C	320	GLY

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	378/384 (98%)	363 (96%)	15 (4%)	28	11
1	B	378/384 (98%)	362 (96%)	16 (4%)	26	8
1	C	378/384 (98%)	362 (96%)	16 (4%)	26	8
1	D	378/384 (98%)	363 (96%)	15 (4%)	28	11
All	All	1512/1536 (98%)	1450 (96%)	62 (4%)	27	10

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	44	VAL
1	A	56	LEU

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Mol	Chain	Res	Type
1	A	74	VAL
1	A	81	ASP
1	A	98	LEU
1	A	212	ARG
1	A	256	LEU
1	A	260	ASP
1	A	281	THR
1	A	289	ARG
1	A	339	GLU
1	A	362	LEU
1	A	369	ARG
1	A	371	SER
1	B	24	VAL
1	B	44	VAL
1	B	56	LEU
1	B	74	VAL
1	B	81	ASP
1	B	98	LEU
1	B	212	ARG
1	B	256	LEU
1	B	260	ASP
1	B	281	THR
1	B	289	ARG
1	B	322	LEU
1	B	339	GLU
1	B	362	LEU
1	B	369	ARG
1	B	371	SER
1	C	22	SER
1	C	30	ASP
1	C	38	GLU
1	C	44	VAL
1	C	56	LEU
1	C	74	VAL
1	C	81	ASP
1	C	98	LEU
1	C	100	LYS
1	C	123	VAL
1	C	212	ARG
1	C	256	LEU
1	C	287	LEU
1	C	339	GLU

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Mol	Chain	Res	Type
1	C	369	ARG
1	C	371	SER
1	D	22	SER
1	D	24	VAL
1	D	44	VAL
1	D	56	LEU
1	D	74	VAL
1	D	81	ASP
1	D	98	LEU
1	D	100	LYS
1	D	123	VAL
1	D	212	ARG
1	D	256	LEU
1	D	322	LEU
1	D	339	GLU
1	D	369	ARG
1	D	371	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	HIS
1	A	374	HIS
1	B	158	HIS
1	B	374	HIS
1	C	301	ASN
1	C	305	ASN
1	C	336	GLN
1	D	374	HIS

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 [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	481/489 (98%)	0.56	73 (15%) 5 6	5, 22, 67, 125	0
1	B	481/489 (98%)	0.57	75 (15%) 5 5	5, 22, 67, 127	0
1	C	481/489 (98%)	1.62	153 (31%) 1 1	15, 36, 71, 131	0
1	D	481/489 (98%)	1.65	167 (34%) 1 1	15, 37, 70, 131	0
All	All	1924/1956 (98%)	1.10	468 (24%) 2 2	5, 31, 70, 131	0

All (468) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	LEU	9.3
1	C	337	PRO	8.9
1	D	337	PRO	8.8
1	D	330	LEU	8.6
1	D	334	PHE	7.7
1	C	334	PHE	7.0
1	D	329	PHE	7.0
1	B	337	PRO	6.8
1	D	285	PHE	6.8
1	C	338	LYS	6.8
1	D	338	LYS	6.6
1	D	335	GLY	6.6
1	A	337	PRO	6.5
1	A	338	LYS	6.5
1	B	334	PHE	6.4
1	B	338	LYS	6.4
1	C	285	PHE	6.3
1	C	328	GLY	6.3
1	A	284	GLY	6.3
1	D	328	GLY	6.2
1	C	329	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	6.1
1	B	283	ALA	6.0
1	C	335	GLY	6.0
1	B	330	LEU	6.0
1	A	334	PHE	5.9
1	A	328	GLY	5.9
1	C	256	LEU	5.8
1	D	256	LEU	5.8
1	B	256	LEU	5.7
1	B	282	VAL	5.6
1	A	285	PHE	5.6
1	B	335	GLY	5.4
1	A	283	ALA	5.4
1	C	322	LEU	5.4
1	C	487	PRO	5.3
1	B	274	VAL	5.3
1	A	335	GLY	5.3
1	C	333	MET	5.3
1	A	256	LEU	5.3
1	B	327	MET	5.2
1	A	329	PHE	5.2
1	D	331	GLY	5.2
1	D	488	THR	5.2
1	A	282	VAL	5.2
1	B	284	GLY	5.1
1	B	336	GLN	5.1
1	D	487	PRO	5.1
1	B	328	GLY	5.0
1	C	283	ALA	5.0
1	B	285	PHE	5.0
1	A	274	VAL	5.0
1	D	255	GLY	5.0
1	A	327	MET	5.0
1	A	333	MET	4.9
1	D	333	MET	4.9
1	D	325	ALA	4.8
1	B	329	PHE	4.7
1	C	488	THR	4.7
1	A	270	VAL	4.6
1	D	283	ALA	4.6
1	D	254	LEU	4.5
1	D	320	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	488	THR	4.5
1	C	325	ALA	4.5
1	C	336	GLN	4.5
1	A	320	GLY	4.5
1	C	255	GLY	4.4
1	A	336	GLN	4.4
1	B	320	GLY	4.4
1	C	254	LEU	4.3
1	D	35	ARG	4.3
1	D	322	LEU	4.3
1	D	486	VAL	4.3
1	C	246	TRP	4.3
1	A	255	GLY	4.3
1	A	488	THR	4.2
1	B	255	GLY	4.2
1	C	331	GLY	4.2
1	C	35	ARG	4.2
1	B	270	VAL	4.1
1	A	319	GLY	4.1
1	B	333	MET	4.0
1	B	331	GLY	4.0
1	B	322	LEU	4.0
1	D	435	ASP	4.0
1	A	331	GLY	4.0
1	D	246	TRP	4.0
1	C	486	VAL	4.0
1	C	257	GLY	3.9
1	A	280	VAL	3.9
1	B	32	GLU	3.9
1	B	316	ALA	3.9
1	C	73	GLY	3.9
1	D	319	GLY	3.9
1	B	280	VAL	3.9
1	C	263	VAL	3.9
1	A	254	LEU	3.8
1	A	322	LEU	3.8
1	C	319	GLY	3.8
1	C	472	LEU	3.8
1	A	32	GLU	3.8
1	D	327	MET	3.7
1	C	320	GLY	3.7
1	C	435	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	472	LEU	3.6
1	B	319	GLY	3.6
1	C	65	ALA	3.6
1	D	28	ALA	3.6
1	D	16	ARG	3.6
1	B	324	PRO	3.6
1	B	317	VAL	3.6
1	A	316	ALA	3.5
1	C	28	ALA	3.5
1	D	317	VAL	3.5
1	A	332	GLN	3.5
1	C	327	MET	3.5
1	D	26	ARG	3.5
1	B	281	THR	3.4
1	D	326	THR	3.4
1	D	102	VAL	3.4
1	A	257	GLY	3.4
1	D	248	ALA	3.4
1	B	254	LEU	3.4
1	D	336	GLN	3.4
1	B	273	ARG	3.4
1	C	16	ARG	3.4
1	A	263	VAL	3.4
1	A	317	VAL	3.4
1	C	24	VAL	3.4
1	C	360	VAL	3.4
1	C	96	GLY	3.4
1	D	257	GLY	3.4
1	D	67	ALA	3.4
1	A	273	ARG	3.4
1	C	260	ASP	3.4
1	C	186	ARG	3.4
1	C	477	VAL	3.3
1	C	317	VAL	3.3
1	D	263	VAL	3.3
1	D	316	ALA	3.3
1	D	432	VAL	3.3
1	D	477	VAL	3.3
1	D	34	LEU	3.3
1	D	182	LEU	3.3
1	A	281	THR	3.3
1	A	324	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	26	ARG	3.3
1	D	73	GLY	3.3
1	D	258	ALA	3.3
1	D	468	VAL	3.3
1	C	94	LEU	3.3
1	C	253	ASP	3.3
1	D	206	PHE	3.3
1	D	74	VAL	3.2
1	B	276	THR	3.2
1	C	103	LEU	3.2
1	C	326	THR	3.2
1	D	436	THR	3.2
1	B	257	GLY	3.2
1	D	25	TRP	3.2
1	B	35	ARG	3.2
1	D	253	ASP	3.2
1	C	259	THR	3.2
1	D	65	ALA	3.2
1	D	427	ARG	3.1
1	A	312	ILE	3.1
1	C	95	VAL	3.1
1	C	104	ALA	3.1
1	D	252	ALA	3.1
1	B	295	ILE	3.1
1	C	339	GLU	3.1
1	C	34	LEU	3.1
1	C	74	VAL	3.1
1	D	24	VAL	3.1
1	B	332	GLN	3.1
1	C	64	ARG	3.1
1	A	276	THR	3.1
1	A	279	GLU	3.1
1	C	284	GLY	3.1
1	B	312	ILE	3.0
1	C	98	LEU	3.0
1	C	432	VAL	3.0
1	C	206	PHE	3.0
1	D	9	HIS	3.0
1	C	482	PRO	3.0
1	B	266	ALA	3.0
1	D	98	LEU	3.0
1	D	103	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	3.0
1	C	25	TRP	3.0
1	B	272	ALA	3.0
1	D	186	ARG	3.0
1	C	102	VAL	3.0
1	C	468	VAL	3.0
1	D	282	VAL	3.0
1	D	459	ALA	3.0
1	A	295	ILE	3.0
1	A	291	LEU	2.9
1	C	9	HIS	2.9
1	D	56	LEU	2.9
1	D	466	TYR	2.9
1	D	260	ASP	2.9
1	B	326	THR	2.9
1	D	259	THR	2.9
1	B	308	PHE	2.9
1	D	339	GLU	2.9
1	C	462	LEU	2.9
1	D	42	LEU	2.9
1	C	27	PRO	2.9
1	D	244	ALA	2.9
1	D	483	ALA	2.9
1	C	56	LEU	2.9
1	C	282	VAL	2.9
1	D	360	VAL	2.9
1	A	326	THR	2.9
1	C	436	THR	2.9
1	C	23	PRO	2.9
1	D	94	LEU	2.9
1	D	463	VAL	2.8
1	A	266	ALA	2.8
1	C	244	ALA	2.8
1	C	483	ALA	2.8
1	A	35	ARG	2.8
1	B	249	ALA	2.8
1	C	459	ALA	2.8
1	C	470	GLY	2.8
1	D	207	GLY	2.8
1	D	324	PRO	2.8
1	D	104	ALA	2.8
1	C	365	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	324	PRO	2.8
1	D	68	PRO	2.8
1	D	482	PRO	2.8
1	A	278	ARG	2.7
1	C	258	ALA	2.7
1	D	265	ALA	2.7
1	B	42	LEU	2.7
1	A	321	GLN	2.7
1	C	400	ARG	2.7
1	D	280	VAL	2.7
1	C	106	TYR	2.7
1	C	110	ALA	2.7
1	C	316	ALA	2.7
1	D	434	GLY	2.7
1	D	276	THR	2.7
1	D	187	ILE	2.7
1	A	42	LEU	2.7
1	B	291	LEU	2.7
1	C	100	LYS	2.7
1	D	63	HIS	2.7
1	D	95	VAL	2.7
1	A	252	ALA	2.6
1	C	248	ALA	2.6
1	C	249	ALA	2.6
1	D	96	GLY	2.6
1	C	427	ARG	2.6
1	A	308	PHE	2.6
1	C	362	LEU	2.6
1	C	280	VAL	2.6
1	A	272	ALA	2.6
1	C	29	ASP	2.6
1	C	210	ALA	2.6
1	D	110	ALA	2.6
1	C	466	TYR	2.6
1	A	286	PRO	2.6
1	C	37	LEU	2.6
1	C	182	LEU	2.6
1	C	187	ILE	2.6
1	C	321	GLN	2.6
1	D	29	ASP	2.6
1	D	36	GLY	2.6
1	D	284	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	321	GLN	2.6
1	B	28	ALA	2.6
1	C	15	VAL	2.6
1	D	247	ALA	2.6
1	C	457	PRO	2.6
1	A	271	LEU	2.6
1	B	321	GLN	2.6
1	B	313	VAL	2.6
1	C	265	ALA	2.6
1	C	63	HIS	2.5
1	A	267	TYR	2.5
1	D	27	PRO	2.5
1	D	308	PHE	2.5
1	B	271	LEU	2.5
1	C	42	LEU	2.5
1	D	470	GLY	2.5
1	C	67	ALA	2.5
1	C	252	ALA	2.5
1	C	262	ALA	2.5
1	D	249	ALA	2.5
1	C	66	THR	2.5
1	C	464	THR	2.5
1	B	372	ARG	2.5
1	D	64	ARG	2.5
1	D	314	ARG	2.5
1	D	332	GLN	2.5
1	C	295	ILE	2.5
1	C	270	VAL	2.5
1	D	100	LYS	2.5
1	C	207	GLY	2.5
1	C	434	GLY	2.5
1	D	105	GLN	2.5
1	A	249	ALA	2.5
1	B	252	ALA	2.5
1	C	463	VAL	2.5
1	D	270	VAL	2.5
1	C	68	PRO	2.5
1	B	278	ARG	2.4
1	D	365	ARG	2.4
1	D	400	ARG	2.4
1	C	75	LEU	2.4
1	D	37	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	75	LEU	2.4
1	D	32	GLU	2.4
1	A	292	ALA	2.4
1	C	276	THR	2.4
1	C	480	PRO	2.4
1	D	23	PRO	2.4
1	D	108	VAL	2.4
1	A	287	LEU	2.4
1	B	141	PHE	2.4
1	A	325	ALA	2.4
1	C	33	ALA	2.4
1	C	465	ALA	2.4
1	C	72	ARG	2.4
1	D	245	ARG	2.4
1	C	109	VAL	2.4
1	D	202	TRP	2.4
1	C	105	GLN	2.4
1	D	462	LEU	2.4
1	D	72	ARG	2.4
1	D	457	PRO	2.4
1	D	15	VAL	2.4
1	D	458	GLY	2.4
1	A	277	ASP	2.3
1	A	26	ARG	2.3
1	A	369	ARG	2.3
1	C	467	LEU	2.3
1	B	267	TYR	2.3
1	D	93	GLN	2.3
1	D	178	ILE	2.3
1	A	310	GLY	2.3
1	A	22	SER	2.3
1	D	185	ASP	2.3
1	C	439	LEU	2.3
1	D	66	THR	2.3
1	D	106	TYR	2.3
1	D	33	ALA	2.3
1	B	286	PRO	2.3
1	B	369	ARG	2.3
1	C	212	ARG	2.3
1	C	177	VAL	2.3
1	C	32	GLU	2.3
1	D	198	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	259	THR	2.3
1	D	318	HIS	2.3
1	D	464	THR	2.3
1	B	247	ALA	2.3
1	B	325	ALA	2.3
1	C	266	ALA	2.3
1	C	407	ALA	2.3
1	D	407	ALA	2.3
1	D	484	PRO	2.3
1	C	70	ARG	2.3
1	C	458	GLY	2.3
1	D	261	GLY	2.3
1	B	279	GLU	2.3
1	C	408	ASP	2.3
1	D	408	ASP	2.3
1	C	332	GLN	2.3
1	A	123	VAL	2.3
1	C	318	HIS	2.3
1	D	240	LEU	2.3
1	D	49	ARG	2.2
1	D	70	ARG	2.2
1	A	265	ALA	2.2
1	C	40	ALA	2.2
1	C	308	PHE	2.2
1	D	189	TYR	2.2
1	D	210	ALA	2.2
1	D	272	ALA	2.2
1	D	465	ALA	2.2
1	D	473	PRO	2.2
1	B	260	ASP	2.2
1	B	277	ASP	2.2
1	D	44	VAL	2.2
1	B	26	ARG	2.2
1	B	365	ARG	2.2
1	C	71	ARG	2.2
1	D	362	LEU	2.2
1	C	211	ASP	2.2
1	D	404	ASP	2.2
1	A	372	ARG	2.2
1	B	245	ARG	2.2
1	D	274	VAL	2.2
1	B	362	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	315	SER	2.2
1	D	180	GLY	2.2
1	D	183	GLY	2.2
1	A	487	PRO	2.2
1	D	480	PRO	2.2
1	B	265	ALA	2.2
1	D	239	ALA	2.2
1	D	266	ALA	2.2
1	A	141	PHE	2.2
1	D	71	ARG	2.2
1	D	212	ARG	2.2
1	D	485	MET	2.2
1	C	213	VAL	2.2
1	A	269	GLY	2.2
1	B	269	GLY	2.2
1	D	455	GLY	2.2
1	C	484	PRO	2.2
1	D	262	ALA	2.2
1	D	370	ALA	2.2
1	C	314	ARG	2.2
1	B	339	GLU	2.1
1	D	431	GLU	2.1
1	C	178	ILE	2.1
1	A	253	ASP	2.1
1	A	313	VAL	2.1
1	D	371	SER	2.1
1	D	437	SER	2.1
1	C	455	GLY	2.1
1	C	245	ARG	2.1
1	D	467	LEU	2.1
1	B	292	ALA	2.1
1	C	370	ALA	2.1
1	D	426	ALA	2.1
1	D	306	TYR	2.1
1	C	241	THR	2.1
1	C	420	SER	2.1
1	C	44	VAL	2.1
1	B	287	LEU	2.1
1	C	93	GLN	2.1
1	C	181	ALA	2.1
1	C	247	ALA	2.1
1	D	211	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	437	SER	2.1
1	D	188	SER	2.1
1	C	373	THR	2.1
1	D	41	GLU	2.1
1	C	485	MET	2.1
1	A	360	VAL	2.1
1	B	243	TRP	2.1
1	A	309	LEU	2.1
1	B	248	ALA	2.1
1	D	181	ALA	2.1
1	A	131	ARG	2.1
1	D	295	ILE	2.0
1	D	420	SER	2.0
1	A	318	HIS	2.0
1	C	209	HIS	2.0
1	D	78	GLY	2.0
1	C	442	VAL	2.0
1	D	109	VAL	2.0
1	D	213	VAL	2.0
1	D	442	VAL	2.0
1	C	202	TRP	2.0
1	B	131	ARG	2.0
1	B	258	ALA	2.0
1	C	185	ASP	2.0
1	C	250	ARG	2.0
1	C	38	GLU	2.0
1	D	241	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.