



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:36 AM UTC

PDB ID : 5DXF / pdb_00005dx
Title : Structure of Candida albicans trehalose-6-phosphate phosphatase N-terminal domain
Authors : Miao, Y.; Brennan, R.G.
Deposited on : 2015-09-23
Resolution : 2.56 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

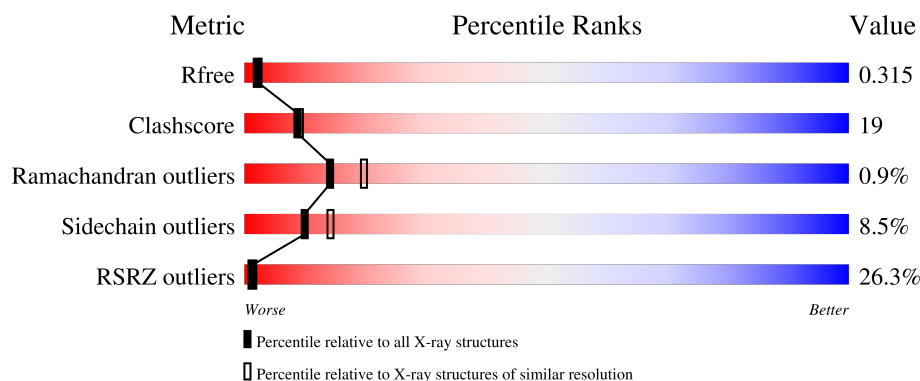
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	534	
1	B	534	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7549 atoms, of which 0 are hydrogens and 0 are deuteriums.

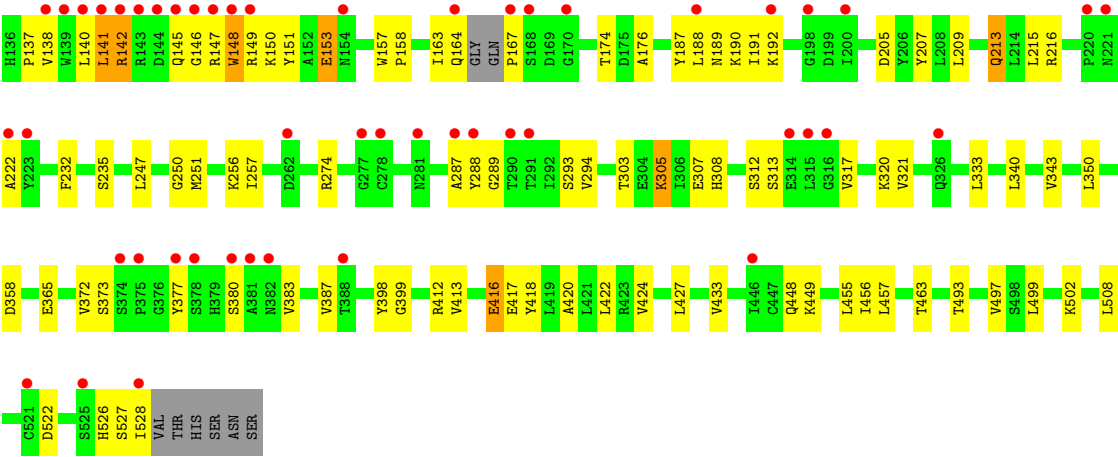
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called trehalose-6-phosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3687	2366	620	686	15			
1	B	468	Total	C	N	O	S	0	0	0
			3764	2414	636	699	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		
2	B	71	Total	O	0	0
			71	71		



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.31Å 98.31Å 452.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 2.56 48.87 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.87-2.56) 93.8 (48.87-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.298 0.292 , 0.315	Depositor DCC
R_{free} test set	2000 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7549	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.57	6/3766 (0.2%)	0.94	13/5102 (0.3%)
1	B	0.37	0/3847	0.85	9/5204 (0.2%)
All	All	0.48	6/7613 (0.1%)	0.89	22/10306 (0.2%)

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	2
1	B	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	LEU	C-N	6.19	1.40	1.34
1	A	232	PHE	C-N	6.13	1.40	1.33
1	A	297	LEU	C-N	5.44	1.40	1.33
1	A	233	PRO	N-CD	5.40	1.55	1.47
1	A	41	PRO	N-CD	5.20	1.55	1.47
1	A	298	PRO	N-CD	5.16	1.54	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-CB	8.37	110.31	103.36
1	A	128	ASP	N-CA-C	-8.29	103.27	112.72
1	B	24	LYS	N-CA-C	8.03	121.60	108.99
1	B	134	ASN	N-CA-C	7.95	121.42	108.55
1	A	142	ARG	N-CA-C	7.24	120.71	110.50
1	A	232	PHE	CA-C-N	-7.12	113.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	PHE	C-N-CA	-7.12	113.33	120.31
1	A	297	LEU	CA-C-N	-6.48	113.09	119.76
1	A	297	LEU	C-N-CA	-6.48	113.09	119.76
1	B	123	GLU	N-CA-C	-6.32	104.32	111.14
1	B	25	GLY	N-CA-C	6.25	127.99	113.18
1	A	40	LEU	CA-C-N	-6.22	113.73	119.82
1	A	40	LEU	C-N-CA	-6.22	113.73	119.82
1	A	141	LEU	N-CA-C	6.12	118.03	111.36
1	A	404	THR	CA-C-N	5.99	125.20	118.97
1	A	404	THR	C-N-CA	5.99	125.20	118.97
1	B	129	ALA	N-CA-C	-5.59	106.31	113.02
1	B	66	SER	N-CA-C	5.26	117.09	111.36
1	B	131	GLY	N-CA-C	-5.20	107.94	115.27
1	B	29	LEU	N-CA-C	5.17	119.55	112.68
1	A	137	PRO	CA-N-CD	-5.08	104.89	112.00
1	B	289	GLY	N-CA-C	-5.04	107.13	114.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	CYS	Peptide
1	A	63	ARG	Peptide
1	B	24	LYS	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	3687	0	3675	188	0
1	B	3764	0	3770	92	0
2	A	27	0	0	3	0
2	B	71	0	0	1	0
All	All	7549	0	7445	279	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 19.

All (279) 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:256:LYS:NZ	1:A:295:GLU:OE2	1.74	1.21
1:A:147:ARG:CG	1:A:179:ASP:OD2	1.88	1.20
1:B:122:ILE:O	1:B:126:LEU:HD21	1.40	1.19
1:A:62:VAL:O	1:A:64:GLY:N	1.82	1.12
1:A:44:ILE:HB	1:A:91:GLU:HG3	1.24	1.07
1:A:40:LEU:HD12	1:A:87:ALA:HB3	1.26	1.07
1:B:126:LEU:HD23	1:B:126:LEU:H	1.19	1.06
1:A:61:THR:CG2	1:A:63:ARG:HB2	1.88	1.04
1:A:147:ARG:HG3	1:A:179:ASP:OD2	1.55	1.02
1:A:134:ASN:O	1:A:136:HIS:CD2	2.15	0.98
1:A:415:LYS:H	1:A:415:LYS:HD2	1.28	0.97
1:B:118:ASP:HA	1:B:121:LYS:HG2	1.48	0.95
1:A:213:GLN:HE21	1:A:217:MET:HG2	1.32	0.94
1:A:142:ARG:HH22	1:A:143:ARG:HH21	1.15	0.93
1:A:85:LEU:HB3	1:A:135:ILE:HG23	1.52	0.92
1:A:40:LEU:HD12	1:A:87:ALA:CB	1.98	0.92
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.35	0.90
1:A:44:ILE:CB	1:A:91:GLU:HG3	2.02	0.90
1:B:40:LEU:HD13	1:B:87:ALA:HB3	1.55	0.89
1:A:40:LEU:CD1	1:A:87:ALA:HB3	2.02	0.89
1:B:122:ILE:O	1:B:126:LEU:CD2	2.22	0.88
1:B:42:LEU:HD12	1:B:62:VAL:HG11	1.54	0.88
1:B:116:GLU:HA	1:B:121:LYS:HE2	1.56	0.85
1:A:246:GLN:N	1:A:246:GLN:OE1	2.08	0.85
1:A:62:VAL:C	1:A:64:GLY:H	1.86	0.84
1:B:21:PHE:HD1	1:B:81:TRP:CD1	1.94	0.84
1:A:86:ILE:HD13	1:A:191:ILE:HG12	1.59	0.83
1:B:120:SER:HA	1:B:123:GLU:HG2	1.60	0.83
1:B:85:LEU:HB3	1:B:135:ILE:HG22	1.61	0.83
1:A:142:ARG:HG2	1:A:143:ARG:N	1.95	0.81
1:A:149:ARG:HH11	1:A:149:ARG:HG3	1.44	0.81
1:A:147:ARG:CD	1:A:179:ASP:OD2	2.28	0.81
1:A:44:ILE:HB	1:A:91:GLU:CG	2.07	0.80
1:A:125:LYS:NZ	1:A:125:LYS:HB2	1.98	0.79
1:A:415:LYS:H	1:A:415:LYS:CD	1.94	0.79
1:A:147:ARG:HG2	1:A:179:ASP:OD2	1.83	0.78
1:A:235:SER:OG	1:A:274:ARG:NH1	2.15	0.78
1:A:120:SER:HA	1:A:123:GLU:HG3	1.66	0.78
1:A:136:HIS:HD1	1:A:194:VAL:HG21	1.49	0.78
1:A:147:ARG:HG3	1:A:179:ASP:CG	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:HG22	1:A:63:ARG:HB2	1.65	0.77
1:A:187:TYR:O	1:A:191:ILE:HG13	1.86	0.76
1:A:512:VAL:O	1:A:516:THR:HG22	1.85	0.76
1:B:146:GLY:O	1:B:150:LYS:N	2.16	0.75
1:A:452:ASN:HA	1:A:500:GLU:HG3	1.67	0.75
1:A:33:ILE:C	1:A:34:LEU:HD23	2.12	0.74
1:A:41:PRO:O	1:A:61:THR:HB	1.88	0.74
1:B:21:PHE:CD1	1:B:81:TRP:CD1	2.75	0.74
1:A:141:LEU:N	1:A:141:LEU:HD23	2.03	0.73
1:B:358:ASP:OD1	1:B:398:TYR:OH	2.08	0.72
1:A:169:ASP:OD1	1:A:169:ASP:N	2.23	0.71
1:A:141:LEU:HD23	1:A:141:LEU:H	1.53	0.71
1:A:142:ARG:HG3	1:A:142:ARG:NH1	1.97	0.71
1:B:149:ARG:NH1	1:B:377:TYR:OH	2.24	0.71
1:A:145:GLN:O	1:A:147:ARG:N	2.26	0.69
1:A:218:GLU:C	1:A:219:PHE:HD1	2.01	0.69
1:A:142:ARG:HH12	1:A:143:ARG:NH2	1.91	0.68
1:A:40:LEU:HB2	1:A:89:THR:HG22	1.73	0.68
1:A:122:ILE:HA	1:A:125:LYS:HG2	1.74	0.68
1:A:136:HIS:ND1	1:A:194:VAL:HG21	2.09	0.68
1:A:36:VAL:HG23	1:A:202:TRP:O	1.96	0.66
1:B:158:PRO:HB3	1:B:163:ILE:HB	1.78	0.65
1:B:126:LEU:H	1:B:126:LEU:CD2	1.93	0.65
1:A:415:LYS:HD2	1:A:415:LYS:N	2.09	0.65
1:A:339:ARG:HG2	1:A:374:SER:HB2	1.79	0.64
1:A:134:ASN:O	1:A:136:HIS:HD2	1.75	0.64
1:A:65:ASN:HB2	1:A:69:TYR:CE2	2.33	0.63
1:A:84:HIS:HD2	1:A:136:HIS:NE2	1.97	0.63
1:B:321:VAL:HG13	1:B:424:VAL:HG22	1.81	0.62
1:A:61:THR:HG23	1:A:63:ARG:HB2	1.75	0.62
1:A:147:ARG:HD2	1:A:179:ASP:OD2	1.99	0.62
1:A:303:THR:HG23	1:A:446:ILE:HD11	1.82	0.62
1:B:118:ASP:O	1:B:121:LYS:HB2	1.98	0.62
1:A:40:LEU:HB2	1:A:89:THR:CG2	2.28	0.62
1:A:134:ASN:O	1:A:136:HIS:NE2	2.33	0.62
1:A:512:VAL:O	1:A:516:THR:CG2	2.49	0.61
1:A:195:TYR:CE1	1:A:199:ASP:HB2	2.36	0.61
1:A:303:THR:HG23	1:A:446:ILE:CD1	2.31	0.61
1:A:142:ARG:HH22	1:A:143:ARG:NH2	1.91	0.60
1:A:331:LYS:NZ	1:A:365:GLU:O	2.33	0.60
1:B:118:ASP:HA	1:B:121:LYS:CG	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD22	1:A:428:ALA:N	2.16	0.60
1:A:117:GLU:O	1:A:120:SER:HB2	2.02	0.60
1:A:45:ILE:HG22	1:A:45:ILE:O	2.02	0.59
1:A:92:LEU:HD23	1:A:92:LEU:C	2.26	0.59
1:A:122:ILE:HG23	1:A:125:LYS:HG2	1.84	0.59
1:A:243:LYS:HB3	1:A:246:GLN:HG2	1.84	0.59
1:B:320:LYS:HE2	1:B:417:GLU:HG3	1.84	0.59
1:A:145:GLN:C	1:A:147:ARG:H	2.09	0.59
1:A:44:ILE:HG22	1:A:44:ILE:O	2.02	0.59
1:A:142:ARG:NH2	1:A:143:ARG:HH21	1.94	0.59
1:A:321:VAL:HG13	1:A:424:VAL:HG22	1.85	0.58
1:A:451:ASN:ND2	2:A:607:HOH:O	2.35	0.58
1:A:61:THR:HG22	1:A:63:ARG:H	1.68	0.58
1:A:243:LYS:O	1:A:246:GLN:HG2	2.03	0.58
1:B:65:ASN:OD1	1:B:65:ASN:N	2.37	0.58
1:A:88:TRP:CZ2	1:A:90:GLY:HA3	2.39	0.58
1:B:164:GLN:HG2	1:B:167:PRO:HG3	1.84	0.58
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.15	0.58
1:A:87:ALA:O	1:A:138:VAL:HG23	2.04	0.58
1:A:180:TYR:OH	1:A:206:TYR:O	2.20	0.58
1:A:136:HIS:CD2	1:A:136:HIS:N	2.72	0.58
1:A:34:LEU:HD22	1:A:84:HIS:HB2	1.85	0.57
1:A:39:SER:HA	1:A:88:TRP:O	2.04	0.57
1:A:147:ARG:CG	1:A:179:ASP:CG	2.72	0.57
1:B:151:TYR:HB2	1:B:176:ALA:HB1	1.87	0.56
1:A:68:LEU:HD13	1:A:229:HIS:CE1	2.40	0.56
1:B:232:PHE:HE1	1:B:251:MET:HE1	1.70	0.56
1:B:26:LYS:HG2	1:B:27:LEU:HG	1.86	0.56
1:B:380:SER:O	1:B:383:VAL:HB	2.06	0.56
1:A:255:ASP:OD2	1:A:255:ASP:N	2.38	0.56
1:A:140:LEU:HD23	1:A:148:TRP:CD2	2.41	0.56
1:A:147:ARG:HA	1:A:150:LYS:HG3	1.88	0.56
1:B:21:PHE:HD1	1:B:81:TRP:HD1	1.51	0.56
1:A:145:GLN:C	1:A:147:ARG:N	2.62	0.56
1:B:132:THR:HG21	1:B:135:ILE:HG23	1.87	0.56
1:A:132:THR:N	1:A:133:PRO:HA	2.21	0.55
1:A:332:LYS:HG3	1:A:363:TRP:HZ3	1.71	0.55
1:B:141:LEU:O	1:B:142:ARG:CB	2.54	0.55
1:A:142:ARG:NH2	1:A:143:ARG:HE	2.04	0.55
1:A:216:ARG:O	1:A:219:PHE:O	2.25	0.55
1:A:125:LYS:HB2	1:A:125:LYS:HZ2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:CG2	1:A:91:GLU:HG3	2.37	0.54
1:A:354:GLU:OE1	1:A:393:ARG:NH1	2.41	0.54
1:A:218:GLU:C	1:A:219:PHE:CD1	2.85	0.54
1:B:502:LYS:NZ	2:B:605:HOH:O	2.41	0.54
1:B:120:SER:HA	1:B:123:GLU:CG	2.36	0.54
1:A:117:GLU:O	1:A:120:SER:N	2.37	0.54
1:B:40:LEU:CD1	1:B:87:ALA:HB3	2.34	0.54
1:A:44:ILE:HA	1:A:45:ILE:HD12	1.89	0.54
1:A:149:ARG:HG3	1:A:149:ARG:NH1	2.19	0.54
1:B:457:LEU:HD21	1:B:463:THR:HG23	1.89	0.54
1:B:153:GLU:OE2	1:B:207:TYR:OH	2.24	0.53
1:B:412:ARG:NH1	1:B:413:VAL:O	2.42	0.53
1:A:218:GLU:HG3	1:A:219:PHE:CE1	2.43	0.53
1:B:256:LYS:HE2	1:B:522:ASP:HB3	1.90	0.53
1:B:118:ASP:O	1:B:122:ILE:HD12	2.07	0.53
1:A:140:LEU:HB3	1:A:148:TRP:CZ2	2.44	0.53
1:B:21:PHE:CD1	1:B:81:TRP:HD1	2.24	0.52
1:B:216:ARG:NH2	1:B:222:ALA:O	2.43	0.52
1:B:141:LEU:O	1:B:142:ARG:HB3	2.10	0.52
1:A:427:LEU:CD2	1:A:428:ALA:N	2.73	0.52
1:A:219:PHE:CD1	1:A:219:PHE:N	2.77	0.52
1:A:139:TRP:C	1:A:140:LEU:HD13	2.35	0.52
1:B:213:GLN:HB2	1:B:250:GLY:HA2	1.91	0.51
1:A:75:LEU:HB3	1:A:83:THR:OG1	2.11	0.51
1:A:141:LEU:H	1:A:141:LEU:CD2	2.16	0.51
1:B:188:LEU:HD12	1:B:215:LEU:HD23	1.92	0.51
1:A:343:VAL:O	1:A:433:VAL:N	2.42	0.51
1:A:430:ILE:HB	1:A:457:LEU:HD12	1.93	0.51
1:B:140:LEU:HB3	1:B:148:TRP:CZ2	2.45	0.51
1:A:37:MET:HE2	1:A:68:LEU:HG	1.93	0.51
1:A:33:ILE:O	1:A:34:LEU:HD23	2.11	0.50
1:A:123:GLU:O	1:A:126:LEU:HB3	2.11	0.50
1:A:427:LEU:CD2	1:A:428:ALA:H	2.25	0.50
1:A:149:ARG:CG	1:A:149:ARG:NH1	2.74	0.50
1:B:129:ALA:HB1	1:B:134:ASN:OD1	2.11	0.50
1:B:209:LEU:HD13	1:B:251:MET:HE2	1.93	0.50
1:B:125:LYS:HD3	1:B:137:PRO:HD2	1.94	0.50
1:B:153:GLU:O	1:B:157:TRP:HB3	2.12	0.49
1:B:416:GLU:CD	1:B:416:GLU:H	2.20	0.49
1:B:493:THR:O	1:B:497:VAL:HG12	2.12	0.49
1:A:88:TRP:CZ2	1:A:90:GLY:CA	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:C	1:A:92:LEU:CD2	2.86	0.49
1:A:34:LEU:HD23	1:A:34:LEU:N	2.26	0.49
1:A:218:GLU:O	1:A:219:PHE:HD1	1.94	0.49
1:A:256:LYS:HZ2	1:A:295:GLU:CD	1.99	0.49
1:A:411:MET:HE2	1:B:399:GLY:C	2.37	0.49
1:B:21:PHE:CD2	1:B:21:PHE:N	2.73	0.49
1:A:307:GLU:OE1	1:A:449:LYS:NZ	2.35	0.49
1:B:117:GLU:N	1:B:117:GLU:OE1	2.46	0.48
1:A:246:GLN:H	1:A:246:GLN:CD	2.06	0.48
1:B:420:ALA:O	1:B:424:VAL:HG23	2.13	0.48
1:B:116:GLU:HG2	1:B:141:LEU:HD11	1.95	0.48
1:A:120:SER:HA	1:A:123:GLU:CG	2.40	0.48
1:A:337:ARG:NH2	2:A:610:HOH:O	2.47	0.48
1:A:119:LYS:HD3	1:A:122:ILE:HD12	1.94	0.48
1:A:142:ARG:NH1	1:A:143:ARG:NH2	2.60	0.48
1:A:256:LYS:HD3	1:A:293:SER:HB3	1.96	0.48
1:A:427:LEU:HD22	1:A:428:ALA:O	2.13	0.48
1:B:307:GLU:OE1	1:B:449:LYS:NZ	2.42	0.48
1:A:65:ASN:HB2	1:A:69:TYR:CZ	2.49	0.48
1:A:309:ASP:HA	1:A:315:LEU:HD12	1.96	0.48
1:A:416:GLU:CD	1:A:416:GLU:H	2.22	0.48
1:B:427:LEU:HD11	1:B:456:ILE:HG13	1.96	0.48
1:A:125:LYS:NZ	1:A:125:LYS:CB	2.73	0.47
1:A:218:GLU:OE2	1:A:218:GLU:HA	2.13	0.47
1:B:189:ASN:HA	1:B:192:LYS:HE2	1.96	0.47
1:B:209:LEU:HD12	1:B:247:LEU:HD22	1.96	0.47
1:B:138:VAL:HG22	1:B:190:LYS:HG3	1.97	0.47
1:B:422:LEU:O	1:B:448:GLN:NE2	2.48	0.47
1:A:229:HIS:HA	1:A:260:GLN:HE21	1.80	0.47
1:B:257:ILE:HB	1:B:294:VAL:HG12	1.96	0.47
1:A:62:VAL:C	1:A:64:GLY:N	2.51	0.47
1:B:122:ILE:O	1:B:122:ILE:HG22	2.16	0.46
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.15	0.46
1:A:184:ASN:OD1	1:A:210:LEU:HB2	2.15	0.46
1:A:142:ARG:CG	1:A:143:ARG:N	2.73	0.46
1:A:256:LYS:NZ	1:A:295:GLU:CD	2.63	0.46
1:B:118:ASP:CA	1:B:121:LYS:HG2	2.32	0.46
1:A:119:LYS:O	1:A:122:ILE:HB	2.16	0.46
1:B:119:LYS:HA	1:B:119:LYS:HD3	1.56	0.46
1:B:343:VAL:O	1:B:433:VAL:N	2.42	0.46
1:B:365:GLU:OE1	1:B:365:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:CG	1:A:89:THR:N	2.84	0.46
1:A:139:TRP:CD1	1:A:139:TRP:N	2.85	0.46
1:A:188:LEU:HD22	1:A:214:LEU:HB3	1.98	0.45
1:A:61:THR:HG22	1:A:63:ARG:CB	2.41	0.45
1:A:145:GLN:H	1:A:145:GLN:HG2	1.46	0.45
1:B:340:LEU:HG	1:B:373:SER:HB3	1.97	0.45
1:A:139:TRP:C	1:A:140:LEU:CD1	2.89	0.45
1:A:411:MET:HE3	1:A:411:MET:HB3	1.77	0.45
1:A:428:ALA:HB2	1:A:444:PHE:CE1	2.50	0.45
1:A:235:SER:O	1:A:239:ARG:HG3	2.17	0.45
1:A:340:LEU:HG	1:A:373:SER:HB2	1.98	0.45
1:A:44:ILE:O	1:A:45:ILE:C	2.59	0.45
1:A:142:ARG:NH2	1:A:143:ARG:NH2	2.60	0.45
1:B:146:GLY:O	1:B:149:ARG:HB2	2.17	0.45
1:A:125:LYS:HB2	1:A:125:LYS:HZ3	1.75	0.45
1:A:140:LEU:HD13	1:A:140:LEU:N	2.33	0.45
1:A:269:ILE:HD11	1:A:294:VAL:HG21	1.99	0.44
1:B:412:ARG:CZ	1:B:413:VAL:O	2.65	0.44
1:A:458:SER:O	1:A:461:THR:HG22	2.16	0.44
1:B:418:TYR:CZ	1:B:422:LEU:HD11	2.52	0.44
1:A:195:TYR:CE2	1:A:197:PRO:HA	2.52	0.44
1:B:126:LEU:HG	1:B:127:CYS:H	1.82	0.44
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.53	0.44
1:B:235:SER:OG	1:B:274:ARG:NH1	2.49	0.44
1:A:299:ILE:HA	1:A:515:TRP:CD1	2.53	0.44
1:B:287:ALA:O	1:B:288:TYR:HB2	2.18	0.44
1:B:455:LEU:HD21	1:B:457:LEU:HD13	1.99	0.44
1:A:37:MET:HE2	1:A:68:LEU:CG	2.48	0.44
1:A:323:ALA:O	1:A:327:VAL:HG23	2.18	0.43
1:A:118:ASP:O	1:A:121:LYS:HE2	2.18	0.43
1:A:140:LEU:CD1	1:A:140:LEU:N	2.82	0.43
1:A:120:SER:O	1:A:123:GLU:HB2	2.18	0.43
1:B:527:SER:O	1:B:528:ILE:HG13	2.18	0.43
1:A:409:TYR:OH	2:A:601:HOH:O	2.20	0.43
1:A:125:LYS:HG3	1:A:126:LEU:N	2.32	0.43
1:A:190:LYS:O	1:A:193:SER:HB3	2.19	0.43
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.77	0.42
1:B:157:TRP:HB3	1:B:158:PRO:HD3	2.00	0.42
1:B:29:LEU:HD12	1:B:29:LEU:HA	1.83	0.42
1:B:308:HIS:O	1:B:312:SER:HB2	2.19	0.42
1:A:216:ARG:NE	1:A:253:GLY:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HD3	1:B:122:ILE:HD13	2.02	0.42
1:B:187:TYR:O	1:B:191:ILE:HG12	2.20	0.42
1:A:65:ASN:O	1:A:69:TYR:N	2.43	0.42
1:B:350:LEU:HD11	1:B:387:VAL:HG13	2.02	0.42
1:A:145:GLN:O	1:A:146:GLY:C	2.63	0.42
1:A:61:THR:HG22	1:A:63:ARG:N	2.34	0.42
1:A:139:TRP:O	1:A:140:LEU:HD12	2.20	0.41
1:A:206:TYR:HA	1:A:209:LEU:HG	2.01	0.41
1:A:216:ARG:HA	1:A:219:PHE:O	2.20	0.41
1:B:33:ILE:HG13	1:B:81:TRP:HB3	2.02	0.41
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.80	0.41
1:A:378:SER:C	1:A:380:SER:H	2.27	0.41
1:B:293:SER:HB2	1:B:526:HIS:CD2	2.56	0.41
1:A:448:GLN:OE1	1:A:451:ASN:HB3	2.20	0.41
1:B:116:GLU:HA	1:B:121:LYS:CE	2.39	0.41
1:B:150:LYS:HA	1:B:150:LYS:HD3	1.84	0.41
1:A:35:ASN:O	1:A:85:LEU:HD12	2.20	0.41
1:B:22:GLU:OE1	1:B:24:LYS:NZ	2.51	0.41
1:B:115:ASP:O	1:B:116:GLU:HB2	2.21	0.41
1:B:303:THR:HG21	1:B:508:LEU:HG	2.02	0.41
1:A:270:SER:O	1:A:274:ARG:HG3	2.21	0.41
1:A:86:ILE:HA	1:A:136:HIS:O	2.21	0.41
1:A:88:TRP:CH2	1:A:90:GLY:HA3	2.55	0.41
1:B:118:ASP:O	1:B:121:LYS:CB	2.68	0.41
1:A:142:ARG:NH1	1:A:143:ARG:CZ	2.83	0.40
1:A:142:ARG:NH2	1:A:143:ARG:NE	2.69	0.40
1:A:124:LYS:HD3	1:A:124:LYS:HA	1.73	0.40
1:A:415:LYS:CD	1:A:415:LYS:N	2.73	0.40
1:A:460:PHE:HE2	1:A:474:ASN:OD1	2.04	0.40
1:A:149:ARG:O	1:A:153:GLU:HG2	2.21	0.40
1:A:149:ARG:HD3	1:A:377:TYR:HE2	1.86	0.40
1:B:499:LEU:HA	1:B:502:LYS:HE2	2.02	0.40
1:B:163:ILE:HD11	1:B:343:VAL:HG13	2.03	0.40
1:B:305:LYS:HB3	1:B:305:LYS:HE3	1.63	0.40

There are no symmetry-related clashes.

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	450/534 (84%)	427 (95%)	19 (4%)	4 (1%)	14	20
1	B	460/534 (86%)	434 (94%)	22 (5%)	4 (1%)	14	20
All	All	910/1068 (85%)	861 (95%)	41 (4%)	8 (1%)	14	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	133	PRO
1	B	147	ARG
1	A	146	GLY
1	B	142	ARG
1	B	153	GLU
1	A	131	GLY
1	B	25	GLY

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	409/478 (86%)	364 (89%)	45 (11%)	6	7
1	B	419/478 (88%)	394 (94%)	25 (6%)	17	25
All	All	828/956 (87%)	758 (92%)	70 (8%)	10	14

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	42	LEU
1	A	59	VAL
1	A	63	ARG
1	A	79	LYS
1	A	80	GLU
1	A	91	GLU
1	A	92	LEU
1	A	125	LYS
1	A	136	HIS
1	A	138	VAL
1	A	140	LEU
1	A	141	LEU
1	A	142	ARG
1	A	143	ARG
1	A	145	GLN
1	A	169	ASP
1	A	171	LYS
1	A	174	THR
1	A	197	PRO
1	A	234	SER
1	A	236	GLU
1	A	242	SER
1	A	246	GLN
1	A	255	ASP
1	A	270	SER
1	A	284	SER
1	A	293	SER
1	A	319	GLU
1	A	320	LYS
1	A	322	GLN
1	A	333	LEU
1	A	341	ASP
1	A	358	ASP
1	A	372	VAL
1	A	379	HIS
1	A	411	MET
1	A	415	LYS
1	A	416	GLU
1	A	427	LEU
1	A	473	VAL
1	A	479	VAL
1	A	500	GLU

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Mol	Chain	Res	Type
1	A	509	SER
1	A	516	THR
1	B	21	PHE
1	B	22	GLU
1	B	26	LYS
1	B	28	LYS
1	B	29	LEU
1	B	40	LEU
1	B	62	VAL
1	B	65	ASN
1	B	79	LYS
1	B	117	GLU
1	B	119	LYS
1	B	126	LEU
1	B	135	ILE
1	B	141	LEU
1	B	145	GLN
1	B	148	TRP
1	B	174	THR
1	B	205	ASP
1	B	213	GLN
1	B	305	LYS
1	B	313	SER
1	B	317	VAL
1	B	333	LEU
1	B	372	VAL
1	B	416	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	451	ASN
1	A	526	HIS
1	B	84	HIS
1	B	178	HIS
1	B	213	GLN
1	B	379	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	460/534 (86%)	1.64	153 (33%) ⓘ ⓘ	33, 63, 108, 134	0
1	B	468/534 (87%)	0.98	91 (19%) ⓘ ⓘ	24, 43, 98, 130	0
All	All	928/1068 (86%)	1.31	244 (26%) ⓘ ⓘ	24, 56, 105, 134	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	ILE	6.9
1	B	21	PHE	6.4
1	A	288	TYR	6.3
1	A	132	THR	6.1
1	A	147	ARG	5.4
1	A	81	TRP	5.1
1	B	144	ASP	5.1
1	B	81	TRP	4.9
1	B	134	ASN	4.8
1	A	59	VAL	4.7
1	A	89	THR	4.7
1	B	170	GLY	4.7
1	A	128	ASP	4.6
1	A	169	ASP	4.5
1	B	121	LYS	4.5
1	B	28	LYS	4.5
1	B	42	LEU	4.4
1	B	148	TRP	4.4
1	B	146	GLY	4.3
1	B	23	GLY	4.2
1	A	61	THR	4.2
1	A	315	LEU	4.2
1	B	126	LEU	4.0
1	A	168	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	4.0
1	A	316	GLY	4.0
1	A	2	ALA	3.9
1	B	221	ASN	3.9
1	A	90	GLY	3.9
1	A	91	GLU	3.9
1	A	291	THR	3.9
1	A	80	GLU	3.8
1	A	3	PRO	3.8
1	B	192	LYS	3.8
1	A	465	THR	3.8
1	B	29	LEU	3.8
1	A	6	VAL	3.8
1	A	117	GLU	3.7
1	B	167	PRO	3.7
1	B	133	PRO	3.7
1	A	188	LEU	3.6
1	A	200	ILE	3.6
1	A	377	TYR	3.6
1	A	130	SER	3.6
1	A	284	SER	3.6
1	A	71	SER	3.5
1	A	92	LEU	3.5
1	B	131	GLY	3.5
1	B	18	PRO	3.5
1	A	127	CYS	3.5
1	A	62	VAL	3.5
1	A	275	VAL	3.5
1	B	164	GLN	3.5
1	A	289	GLY	3.5
1	A	215	LEU	3.4
1	A	285	VAL	3.4
1	B	141	LEU	3.4
1	B	25	GLY	3.4
1	A	287	ALA	3.4
1	B	140	LEU	3.3
1	A	173	GLU	3.3
1	B	116	GLU	3.3
1	B	198	GLY	3.3
1	A	42	LEU	3.3
1	B	315	LEU	3.3
1	B	89	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	187	TYR	3.3
1	A	131	GLY	3.3
1	A	219	PHE	3.2
1	A	191	ILE	3.2
1	A	255	ASP	3.2
1	A	430	ILE	3.2
1	B	381	ALA	3.2
1	A	75	LEU	3.2
1	B	90	GLY	3.2
1	A	44	ILE	3.2
1	B	145	GLN	3.1
1	A	183	PHE	3.1
1	B	82	GLU	3.1
1	A	223	TYR	3.1
1	A	135	ILE	3.1
1	A	185	GLU	3.1
1	A	139	TRP	3.1
1	A	86	ILE	3.1
1	A	133	PRO	3.1
1	B	143	ARG	3.1
1	A	33	ILE	3.1
1	A	174	THR	3.0
1	B	291	THR	3.0
1	A	34	LEU	3.0
1	B	316	GLY	3.0
1	B	288	TYR	3.0
1	B	65	ASN	3.0
1	A	253	GLY	3.0
1	B	129	ALA	3.0
1	A	214	LEU	3.0
1	A	172	ALA	2.9
1	A	4	GLN	2.9
1	A	271	CYS	2.9
1	A	278	CYS	2.9
1	A	528	ILE	2.9
1	A	83	THR	2.9
1	B	287	ALA	2.9
1	A	179	ASP	2.9
1	A	376	GLY	2.9
1	A	45	ILE	2.9
1	B	138	VAL	2.9
1	A	122	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	117	GLU	2.9
1	A	209	LEU	2.8
1	A	283	ASP	2.8
1	B	123	GLU	2.8
1	A	525	SER	2.8
1	B	135	ILE	2.8
1	B	278	CYS	2.8
1	A	129	ALA	2.8
1	B	83	THR	2.8
1	B	128	ASP	2.8
1	B	142	ARG	2.8
1	A	126	LEU	2.8
1	B	521	CYS	2.8
1	B	80	GLU	2.8
1	B	33	ILE	2.7
1	A	222	ALA	2.7
1	A	523	ILE	2.7
1	A	148	TRP	2.7
1	A	124	LYS	2.7
1	A	470	ALA	2.7
1	B	262	ASP	2.7
1	A	138	VAL	2.7
1	A	269	ILE	2.6
1	B	22	GLU	2.6
1	A	290	THR	2.6
1	B	277	GLY	2.6
1	A	220	PRO	2.6
1	A	524	LEU	2.6
1	B	314	GLU	2.6
1	A	176	ALA	2.6
1	A	257	ILE	2.6
1	B	147	ARG	2.6
1	A	358	ASP	2.6
1	B	44	ILE	2.6
1	A	280	VAL	2.6
1	A	261	SER	2.6
1	B	378	SER	2.6
1	B	132	THR	2.6
1	A	202	TRP	2.5
1	A	319	GLU	2.5
1	B	281	ASN	2.5
1	A	76	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	217	MET	2.5
1	A	137	PRO	2.5
1	B	64	GLY	2.5
1	B	375	PRO	2.5
1	B	122	ILE	2.5
1	A	145	GLN	2.5
1	B	62	VAL	2.5
1	B	120	SER	2.5
1	A	63	ARG	2.5
1	B	127	CYS	2.5
1	A	121	LYS	2.5
1	A	186	ALA	2.5
1	A	292	ILE	2.5
1	A	171	LYS	2.5
1	A	211	LEU	2.5
1	A	412	ARG	2.5
1	A	279	GLU	2.4
1	A	68	LEU	2.4
1	A	286	SER	2.4
1	B	446	ILE	2.4
1	A	40	LEU	2.4
1	A	379	HIS	2.4
1	B	388	THR	2.4
1	A	197	PRO	2.4
1	A	449	LYS	2.4
1	A	213	GLN	2.4
1	B	34	LEU	2.4
1	A	310	ALA	2.4
1	A	70	SER	2.4
1	B	32	ARG	2.4
1	A	37	MET	2.4
1	A	294	VAL	2.4
1	A	270	SER	2.3
1	A	312	SER	2.3
1	A	252	LEU	2.3
1	B	223	TYR	2.3
1	B	30	SER	2.3
1	B	188	LEU	2.3
1	A	490	MET	2.3
1	A	207	TYR	2.3
1	B	377	TYR	2.3
1	A	300	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	168	SER	2.3
1	A	282	ARG	2.3
1	A	306	ILE	2.3
1	B	220	PRO	2.3
1	A	442	LEU	2.2
1	A	457	LEU	2.2
1	B	380	SER	2.2
1	B	525	SER	2.2
1	B	139	TRP	2.2
1	A	77	GLU	2.2
1	B	78	ASN	2.2
1	B	222	ALA	2.2
1	B	382	ASN	2.2
1	A	526	HIS	2.2
1	A	329	LYS	2.2
1	A	203	ILE	2.2
1	A	64	GLY	2.2
1	A	199	ASP	2.2
1	A	146	GLY	2.2
1	A	225	GLY	2.2
1	B	27	LEU	2.2
1	A	79	LYS	2.2
1	B	326	GLN	2.1
1	A	170	GLY	2.1
1	A	527	SER	2.1
1	B	63	ARG	2.1
1	B	24	LYS	2.1
1	A	73	HIS	2.1
1	A	194	VAL	2.1
1	A	5	GLN	2.1
1	A	254	ALA	2.1
1	A	85	LEU	2.1
1	A	224	ILE	2.1
1	A	212	PRO	2.1
1	A	88	TRP	2.1
1	A	177	TRP	2.1
1	B	154	ASN	2.1
1	A	142	ARG	2.1
1	A	242	SER	2.1
1	A	431	THR	2.1
1	B	290	THR	2.1
1	A	118	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	2.0
1	A	491	LEU	2.0
1	A	120	SER	2.0
1	A	259	PHE	2.0
1	B	149	ARG	2.0
1	A	463	THR	2.0
1	B	200	ILE	2.0
1	A	293	SER	2.0
1	B	84	HIS	2.0
1	B	374	SER	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.