



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:16 AM UTC

PDB ID : 3APN / pdb_00003apn
Title : Crystal structure of the human wild-type PAD4 protein
Authors : Horikoshi, N.; Tachiwana, H.; Saito, K.; Osakabe, A.; Sato, M.; Yamada, M.; Akashi, S.; Nishimura, Y.; Kagawa, W.; Kurumizaka, H.
Deposited on : 2010-10-19
Resolution : 2.70 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

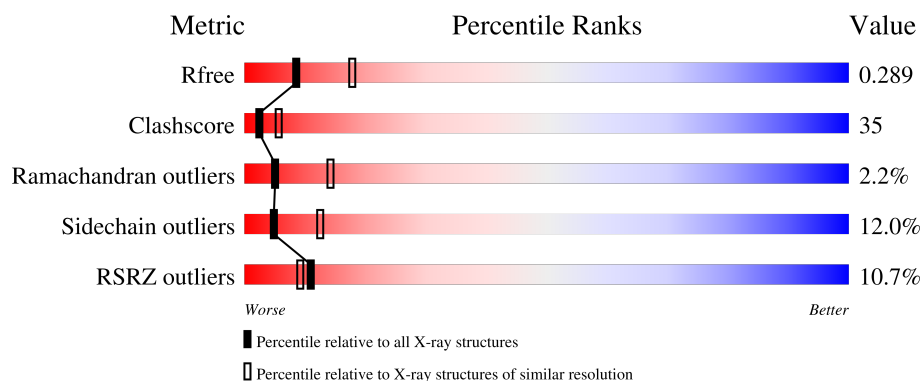
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	666	9% 38% 39% 6% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4407 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 Protein-arginine deiminase type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	4407	2820	742	814	31	0	0	0

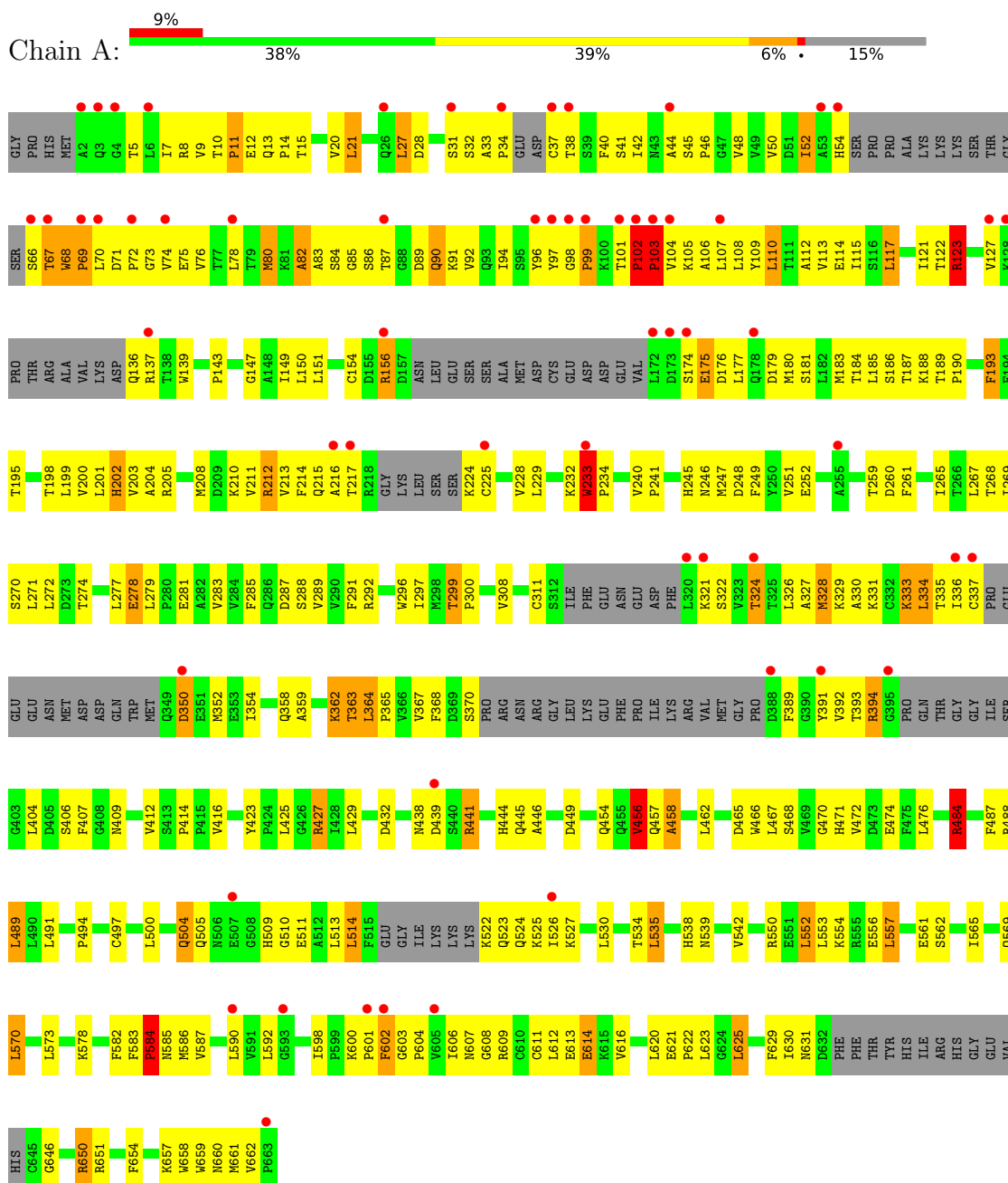
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9UM07
A	-1	PRO	-	expression tag	UNP Q9UM07
A	0	HIS	-	expression tag	UNP Q9UM07
A	55	SER	GLY	engineered mutation	UNP Q9UM07
A	82	ALA	VAL	engineered mutation	UNP Q9UM07
A	112	ALA	GLY	engineered mutation	UNP Q9UM07

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein-arginine deiminase type-4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.25Å 61.06Å 113.57Å 90.00° 123.74° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.70) 99.5 (30.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.72Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.246 , 0.293 0.246 , 0.289	Depositor DCC
R_{free} test set	1179 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4407	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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	0.55	1/4504 (0.0%)	1.04	27/6105 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	PRO	CA-C	5.09	1.56	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	GLN	N-CA-C	-14.09	87.36	109.76
1	A	195	THR	N-CA-C	-7.23	104.60	113.50
1	A	102	PRO	CA-C-N	7.02	128.62	119.84
1	A	102	PRO	C-N-CA	7.02	128.62	119.84
1	A	322	SER	N-CA-C	-6.61	103.90	112.23
1	A	193	PHE	N-CA-C	6.34	118.19	111.28
1	A	299	THR	CA-C-N	5.87	125.84	120.03
1	A	299	THR	C-N-CA	5.87	125.84	120.03
1	A	82	ALA	N-CA-C	5.81	117.37	108.42
1	A	363	THR	N-CA-C	-5.81	100.71	109.95
1	A	414	PRO	N-CA-C	-5.55	103.93	110.70
1	A	98	GLY	CA-C-N	5.45	126.65	119.84
1	A	98	GLY	C-N-CA	5.45	126.65	119.84
1	A	202	HIS	N-CA-C	5.41	117.20	109.14
1	A	438	ASN	N-CA-C	-5.30	106.07	112.54
1	A	296	TRP	N-CA-C	-5.29	100.67	109.46
1	A	11	PRO	N-CA-C	-5.26	106.87	114.18
1	A	103	PRO	N-CA-C	5.24	123.27	112.47
1	A	441	ARG	N-CA-C	-5.24	102.44	110.14
1	A	556	GLU	N-CA-C	5.08	117.71	111.82
1	A	5	THR	N-CA-C	5.07	117.00	109.69
1	A	650	ARG	N-CA-C	-5.07	101.69	109.76
1	A	233	TRP	CA-C-N	5.07	124.76	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	TRP	C-N-CA	5.07	124.76	119.64
1	A	456	VAL	N-CA-C	5.06	119.86	109.34
1	A	414	PRO	CA-C-N	-5.03	114.58	119.76
1	A	414	PRO	C-N-CA	-5.03	114.58	119.76

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	4407	0	4412	309	0
All	All	4407	0	4412	309	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 35.

All (309) 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:362:LYS:HE3	1:A:364:LEU:HB2	1.35	1.02
1:A:80:MET:HG2	1:A:112:ALA:HB2	1.51	0.90
1:A:590:LEU:HD21	1:A:592:LEU:HD13	1.57	0.86
1:A:180:MET:HE2	1:A:252:GLU:OE1	1.77	0.84
1:A:505:GLN:NE2	1:A:527:LYS:HD2	1.92	0.84
1:A:404:LEU:HD13	1:A:432:ASP:HA	1.59	0.83
1:A:462:LEU:HD23	1:A:552:LEU:HD23	1.62	0.81
1:A:504:GLN:OE1	1:A:606:ILE:HG13	1.80	0.81
1:A:514:LEU:HG	1:A:604:PRO:HD3	1.63	0.81
1:A:113:VAL:HB	1:A:189:THR:HG22	1.63	0.80
1:A:358:GLN:HG3	1:A:363:THR:HG22	1.64	0.79
1:A:67:THR:C	1:A:68:TRP:HE3	1.91	0.78
1:A:484:ARG:HH11	1:A:484:ARG:CG	1.97	0.78
1:A:42:ILE:HD11	1:A:94:ILE:HG23	1.64	0.78
1:A:484:ARG:HH11	1:A:484:ARG:HG2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ARG:HG3	1:A:650:ARG:HH11	1.50	0.75
1:A:354:ILE:HG21	1:A:650:ARG:HG2	1.66	0.75
1:A:54:HIS:CD2	1:A:67:THR:HG21	2.22	0.75
1:A:208:MET:HE1	1:A:234:PRO:HD3	1.69	0.75
1:A:52:ILE:HG23	1:A:66:SER:HA	1.70	0.74
1:A:362:LYS:CE	1:A:364:LEU:HB2	2.15	0.73
1:A:80:MET:HE1	1:A:110:LEU:HB3	1.68	0.73
1:A:42:ILE:HG21	1:A:50:VAL:HG11	1.70	0.72
1:A:71:ASP:O	1:A:74:VAL:HG12	1.89	0.72
1:A:456:VAL:HG21	1:A:658:TRP:HB2	1.71	0.72
1:A:333:LYS:HG3	1:A:334:LEU:N	2.05	0.72
1:A:38:THR:O	1:A:70:LEU:HB2	1.90	0.71
1:A:601:PRO:O	1:A:603:GLY:N	2.24	0.71
1:A:70:LEU:HD13	1:A:70:LEU:O	1.91	0.71
1:A:45:SER:HB2	1:A:90:GLN:HG3	1.73	0.70
1:A:96:TYR:O	1:A:103:PRO:HB2	1.91	0.70
1:A:42:ILE:CD1	1:A:94:ILE:HG23	2.23	0.69
1:A:394:ARG:CA	1:A:394:ARG:HH11	2.05	0.69
1:A:538:HIS:HD2	1:A:573:LEU:H	1.40	0.69
1:A:630:ILE:HG22	1:A:631:ASN:N	2.08	0.68
1:A:488:ARG:HG2	1:A:565:ILE:HD12	1.74	0.68
1:A:104:VAL:HG12	1:A:105:LYS:N	2.09	0.68
1:A:308:VAL:HB	1:A:334:LEU:HD22	1.77	0.67
1:A:268:THR:HA	1:A:288:SER:HB3	1.76	0.66
1:A:350:ASP:OD2	1:A:646:GLY:HA2	1.94	0.66
1:A:67:THR:HB	1:A:69:PRO:HD2	1.78	0.66
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.59	0.66
1:A:466:TRP:CZ3	1:A:542:VAL:HG13	2.31	0.66
1:A:68:TRP:H	1:A:69:PRO:HD3	1.60	0.66
1:A:215:GLN:HB2	1:A:228:VAL:HG11	1.78	0.66
1:A:333:LYS:HG3	1:A:334:LEU:H	1.59	0.66
1:A:367:VAL:HG23	1:A:389:PHE:HD2	1.61	0.65
1:A:91:LYS:HE2	1:A:109:TYR:HE2	1.62	0.65
1:A:362:LYS:NZ	1:A:364:LEU:HD12	2.13	0.64
1:A:364:LEU:HD23	1:A:365:PRO:O	1.97	0.64
1:A:609:ARG:HD2	1:A:614:GLU:HG3	1.79	0.64
1:A:11:PRO:HB3	1:A:104:VAL:HG11	1.79	0.64
1:A:48:VAL:HG23	1:A:90:GLN:CG	2.27	0.64
1:A:175:GLU:OE1	1:A:176:ASP:HB2	1.98	0.63
1:A:102:PRO:N	1:A:103:PRO:HD3	2.14	0.62
1:A:38:THR:HG23	1:A:99:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HB	1:A:106:ALA:HB3	1.82	0.62
1:A:85:GLY:N	1:A:89:ASP:OD1	2.31	0.62
1:A:425:LEU:HD12	1:A:456:VAL:HG13	1.81	0.62
1:A:203:VAL:HG22	1:A:267:LEU:HD23	1.81	0.61
1:A:484:ARG:HH11	1:A:484:ARG:CB	2.12	0.61
1:A:444:HIS:CD2	1:A:446:ALA:HB3	2.34	0.61
1:A:137:ARG:HG2	1:A:137:ARG:NH1	2.16	0.60
1:A:80:MET:HE1	1:A:110:LEU:CB	2.31	0.60
1:A:40:PHE:HE1	1:A:42:ILE:HG12	1.65	0.60
1:A:101:THR:HB	1:A:103:PRO:HD3	1.84	0.59
1:A:444:HIS:HD2	1:A:446:ALA:HB3	1.67	0.59
1:A:27:LEU:HD13	1:A:78:LEU:HD13	1.84	0.59
1:A:513:LEU:HD13	1:A:523:GLN:OE1	2.02	0.59
1:A:11:PRO:HB3	1:A:104:VAL:CG1	2.32	0.59
1:A:44:ALA:HB1	1:A:91:LYS:O	2.02	0.59
1:A:203:VAL:HG22	1:A:267:LEU:CD2	2.31	0.59
1:A:590:LEU:CD2	1:A:592:LEU:HD13	2.30	0.59
1:A:33:ALA:HB1	1:A:34:PRO:HD2	1.84	0.59
1:A:102:PRO:N	1:A:103:PRO:CD	2.66	0.59
1:A:299:THR:HG21	1:A:651:ARG:HB2	1.84	0.59
1:A:10:THR:HG22	1:A:32:SER:HB2	1.85	0.58
1:A:154:CYS:HB3	1:A:391:TYR:H	1.68	0.58
1:A:604:PRO:HB2	1:A:611:CYS:SG	2.43	0.58
1:A:583:PHE:O	1:A:584:PRO:C	2.46	0.58
1:A:68:TRP:N	1:A:69:PRO:CD	2.67	0.58
1:A:9:VAL:HG21	1:A:94:ILE:HG13	1.86	0.58
1:A:48:VAL:HG23	1:A:90:GLN:HG2	1.86	0.58
1:A:308:VAL:CG2	1:A:592:LEU:HD11	2.34	0.58
1:A:156:ARG:HG3	1:A:156:ARG:HH11	1.69	0.57
1:A:11:PRO:HB3	1:A:104:VAL:CB	2.34	0.57
1:A:538:HIS:CD2	1:A:573:LEU:H	2.21	0.57
1:A:527:LYS:HG3	1:A:527:LYS:O	2.03	0.57
1:A:394:ARG:NH1	1:A:394:ARG:HB2	2.19	0.57
1:A:117:LEU:HD13	1:A:289:VAL:HG13	1.86	0.57
1:A:13:GLN:HB2	1:A:14:PRO:HD2	1.86	0.57
1:A:104:VAL:CG1	1:A:105:LYS:N	2.67	0.56
1:A:183:MET:HE1	1:A:267:LEU:HD13	1.87	0.56
1:A:327:ALA:HB2	1:A:334:LEU:HD23	1.87	0.56
1:A:367:VAL:HG23	1:A:389:PHE:CD2	2.39	0.56
1:A:394:ARG:HH11	1:A:394:ARG:CB	2.18	0.56
1:A:27:LEU:HD22	1:A:78:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PRO:HG3	1:A:37:CYS:SG	2.46	0.56
1:A:86:SER:O	1:A:89:ASP:OD2	2.24	0.55
1:A:216:ALA:HB3	1:A:248:ASP:HB2	1.89	0.55
1:A:240:VAL:HG22	1:A:247:MET:HE3	1.87	0.55
1:A:327:ALA:CB	1:A:334:LEU:HD23	2.37	0.55
1:A:44:ALA:HB2	1:A:92:VAL:HA	1.89	0.55
1:A:441:ARG:HG3	1:A:441:ARG:HH11	1.72	0.55
1:A:20:VAL:HG21	1:A:285:PHE:CG	2.41	0.55
1:A:211:VAL:HG22	1:A:212:ARG:N	2.21	0.55
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.42	0.54
1:A:404:LEU:CD2	1:A:470:GLY:O	2.56	0.54
1:A:68:TRP:N	1:A:69:PRO:HD3	2.22	0.54
1:A:28:ASP:OD2	1:A:31:SER:OG	2.20	0.54
1:A:123:ARG:HG2	1:A:659:TRP:CD1	2.43	0.54
1:A:205:ARG:O	1:A:208:MET:HG2	2.07	0.54
1:A:308:VAL:HG22	1:A:592:LEU:HD11	1.88	0.54
1:A:333:LYS:CG	1:A:334:LEU:N	2.71	0.54
1:A:156:ARG:C	1:A:156:ARG:HD2	2.33	0.54
1:A:625:LEU:N	1:A:625:LEU:HD22	2.22	0.54
1:A:52:ILE:CG2	1:A:66:SER:HA	2.37	0.53
1:A:269:ILE:HG22	1:A:287:ASP:O	2.08	0.53
1:A:11:PRO:HB3	1:A:104:VAL:HB	1.90	0.53
1:A:139:TRP:CH2	1:A:292:ARG:HD2	2.43	0.53
1:A:394:ARG:HH11	1:A:394:ARG:HA	1.73	0.53
1:A:40:PHE:CE1	1:A:42:ILE:HG12	2.42	0.53
1:A:606:ILE:O	1:A:607:ASN:C	2.51	0.53
1:A:80:MET:HG2	1:A:112:ALA:CB	2.33	0.53
1:A:214:PHE:O	1:A:249:PHE:HA	2.08	0.53
1:A:370:SER:HA	1:A:393:THR:HG23	1.91	0.53
1:A:484:ARG:NH1	1:A:484:ARG:HB3	2.24	0.53
1:A:650:ARG:HG3	1:A:650:ARG:NH1	2.22	0.53
1:A:362:LYS:HZ2	1:A:364:LEU:HD12	1.73	0.53
1:A:27:LEU:HD13	1:A:78:LEU:CD1	2.39	0.52
1:A:416:VAL:HG21	1:A:557:LEU:O	2.09	0.52
1:A:84:SER:HB3	1:A:89:ASP:CG	2.35	0.52
1:A:84:SER:HB3	1:A:89:ASP:OD1	2.09	0.52
1:A:509:HIS:CD2	1:A:606:ILE:HD12	2.45	0.52
1:A:404:LEU:HD23	1:A:470:GLY:O	2.08	0.52
1:A:123:ARG:HD3	1:A:123:ARG:N	2.25	0.52
1:A:468:SER:HA	1:A:578:LYS:HB3	1.92	0.52
1:A:52:ILE:HG23	1:A:66:SER:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:HG2	1:A:565:ILE:CD1	2.40	0.51
1:A:232:LYS:HB3	1:A:233:TRP:CD1	2.44	0.51
1:A:14:PRO:HB3	1:A:107:LEU:HB2	1.92	0.51
1:A:42:ILE:CG2	1:A:50:VAL:HG11	2.39	0.51
1:A:149:ILE:HD13	1:A:659:TRP:CE3	2.45	0.51
1:A:299:THR:HG23	1:A:299:THR:O	2.08	0.51
1:A:630:ILE:CG2	1:A:631:ASN:N	2.72	0.51
1:A:186:SER:HA	1:A:246:ASN:HB3	1.92	0.51
1:A:71:ASP:C	1:A:73:GLY:H	2.18	0.51
1:A:278:GLU:OE1	1:A:278:GLU:HA	2.08	0.51
1:A:299:THR:CG2	1:A:651:ARG:HB2	2.40	0.51
1:A:358:GLN:HG3	1:A:363:THR:CG2	2.37	0.51
1:A:368:PHE:HE1	1:A:394:ARG:H	1.59	0.51
1:A:484:ARG:HH11	1:A:484:ARG:HB3	1.75	0.51
1:A:554:LYS:HE3	1:A:561:GLU:OE2	2.11	0.51
1:A:609:ARG:HD2	1:A:614:GLU:CG	2.40	0.51
1:A:156:ARG:HG3	1:A:156:ARG:NH1	2.26	0.51
1:A:613:GLU:HG3	1:A:629:PHE:CE1	2.46	0.51
1:A:336:ILE:N	1:A:336:ILE:HD12	2.26	0.50
1:A:585:ASN:HD21	1:A:587:VAL:HG12	1.75	0.50
1:A:179:ASP:OD2	1:A:362:LYS:NZ	2.44	0.50
1:A:553:LEU:O	1:A:557:LEU:HB2	2.11	0.50
1:A:202:HIS:HE1	1:A:270:SER:OG	1.94	0.50
1:A:336:ILE:HG22	1:A:337:CYS:N	2.26	0.50
1:A:48:VAL:HG23	1:A:90:GLN:HG3	1.94	0.49
1:A:113:VAL:CB	1:A:189:THR:HG22	2.38	0.49
1:A:354:ILE:CG2	1:A:650:ARG:HG2	2.40	0.49
1:A:368:PHE:CD2	1:A:407:PHE:HE1	2.30	0.49
1:A:34:PRO:HG2	1:A:37:CYS:HB3	1.94	0.49
1:A:174:SER:C	1:A:176:ASP:N	2.70	0.49
1:A:488:ARG:HH21	1:A:623:LEU:HD21	1.77	0.49
1:A:151:LEU:HD21	1:A:359:ALA:HB2	1.95	0.49
1:A:427:ARG:O	1:A:429:LEU:HD13	2.12	0.49
1:A:630:ILE:HG22	1:A:631:ASN:H	1.76	0.49
1:A:11:PRO:CB	1:A:104:VAL:HG11	2.43	0.49
1:A:233:TRP:CD1	1:A:233:TRP:N	2.80	0.49
1:A:535:LEU:HD22	1:A:539:ASN:ND2	2.27	0.49
1:A:68:TRP:CD1	1:A:97:TYR:OH	2.66	0.49
1:A:150:LEU:HG	1:A:291:PHE:CD2	2.48	0.49
1:A:211:VAL:HB	1:A:265:ILE:HD13	1.94	0.48
1:A:7:ILE:HB	1:A:27:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD23	1:A:181:SER:OG	2.14	0.48
1:A:190:PRO:HG2	1:A:193:PHE:HB2	1.95	0.48
1:A:358:GLN:OE1	1:A:657:LYS:CD	2.61	0.48
1:A:484:ARG:HG2	1:A:484:ARG:NH1	2.21	0.48
1:A:328:MET:HE2	1:A:328:MET:O	2.13	0.48
1:A:334:LEU:HD13	1:A:335:THR:N	2.29	0.48
1:A:174:SER:C	1:A:176:ASP:H	2.20	0.48
1:A:409:ASN:OD1	1:A:471:HIS:HA	2.13	0.48
1:A:606:ILE:O	1:A:609:ARG:N	2.46	0.48
1:A:115:ILE:CD1	1:A:271:LEU:HD22	2.44	0.48
1:A:45:SER:HB3	1:A:46:PRO:HD2	1.95	0.47
1:A:54:HIS:NE2	1:A:67:THR:HG21	2.29	0.47
1:A:136:GLN:O	1:A:137:ARG:CB	2.62	0.47
1:A:156:ARG:HD2	1:A:156:ARG:O	2.14	0.47
1:A:661:MET:HG2	1:A:662:VAL:H	1.78	0.47
1:A:101:THR:CB	1:A:103:PRO:HD3	2.44	0.47
1:A:52:ILE:HD12	1:A:76:VAL:HG22	1.96	0.47
1:A:83:ALA:CB	1:A:188:LYS:HG2	2.45	0.47
1:A:586:MET:HE1	1:A:612:LEU:HB3	1.96	0.47
1:A:52:ILE:HA	1:A:75:GLU:O	2.15	0.47
1:A:175:GLU:CD	1:A:176:ASP:HB2	2.40	0.47
1:A:510:GLY:HA2	1:A:526:ILE:HG23	1.96	0.47
1:A:297:ILE:HD13	1:A:425:LEU:HD13	1.97	0.47
1:A:104:VAL:CG1	1:A:105:LYS:H	2.28	0.46
1:A:240:VAL:HG22	1:A:247:MET:CE	2.45	0.46
1:A:358:GLN:OE1	1:A:657:LYS:HD3	2.15	0.46
1:A:554:LYS:CE	1:A:561:GLU:OE2	2.64	0.46
1:A:489:LEU:HD22	1:A:491:LEU:HG	1.97	0.46
1:A:444:HIS:CD2	1:A:446:ALA:H	2.33	0.46
1:A:586:MET:SD	1:A:601:PRO:HG3	2.55	0.46
1:A:42:ILE:HD12	1:A:94:ILE:HD12	1.98	0.46
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.81	0.46
1:A:423:TYR:CD1	1:A:427:ARG:HD2	2.50	0.46
1:A:488:ARG:HH21	1:A:623:LEU:CD2	2.29	0.46
1:A:509:HIS:C	1:A:511:GLU:H	2.24	0.46
1:A:101:THR:C	1:A:103:PRO:HD3	2.40	0.46
1:A:240:VAL:HG13	1:A:245:HIS:HD2	1.81	0.46
1:A:427:ARG:HH11	1:A:427:ARG:CG	2.29	0.46
1:A:484:ARG:HE	1:A:562:SER:HB2	1.81	0.46
1:A:484:ARG:HD3	1:A:488:ARG:HH12	1.81	0.45
1:A:321:LYS:O	1:A:324:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:CG	1:A:246:ASN:N	2.84	0.45
1:A:260:ASP:OD2	1:A:260:ASP:N	2.49	0.45
1:A:423:TYR:CG	1:A:427:ARG:HD2	2.51	0.45
1:A:630:ILE:CG2	1:A:631:ASN:H	2.30	0.45
1:A:393:THR:O	1:A:393:THR:HG22	2.15	0.45
1:A:114:GLU:HB3	1:A:188:LYS:HB3	1.98	0.45
1:A:620:LEU:O	1:A:623:LEU:HB2	2.16	0.45
1:A:585:ASN:ND2	1:A:587:VAL:HG12	2.31	0.45
1:A:71:ASP:OD2	1:A:72:PRO:HD2	2.17	0.45
1:A:311:CYS:HA	1:A:337:CYS:SG	2.57	0.45
1:A:570:LEU:HB3	1:A:582:PHE:HB3	1.97	0.45
1:A:15:THR:HB	1:A:108:LEU:HD13	1.99	0.45
1:A:67:THR:C	1:A:68:TRP:CE3	2.82	0.44
1:A:42:ILE:HD12	1:A:94:ILE:CD1	2.48	0.44
1:A:211:VAL:HG22	1:A:212:ARG:H	1.81	0.44
1:A:467:LEU:HD13	1:A:474:GLU:HB2	1.99	0.44
1:A:623:LEU:HB2	1:A:625:LEU:HD23	2.00	0.44
1:A:215:GLN:HB2	1:A:228:VAL:CG1	2.48	0.44
1:A:216:ALA:HA	1:A:225:CYS:SG	2.57	0.44
1:A:127:VAL:HG23	1:A:127:VAL:O	2.17	0.44
1:A:394:ARG:NH1	1:A:394:ARG:CB	2.79	0.44
1:A:457:GLN:O	1:A:458:ALA:C	2.59	0.44
1:A:476:LEU:C	1:A:476:LEU:HD12	2.42	0.44
1:A:607:ASN:O	1:A:608:GLY:C	2.61	0.44
1:A:143:PRO:HA	1:A:660:ASN:ND2	2.33	0.44
1:A:466:TRP:CD1	1:A:466:TRP:H	2.35	0.44
1:A:199:LEU:HD12	1:A:240:VAL:HG21	1.99	0.44
1:A:176:ASP:O	1:A:177:LEU:HD23	2.18	0.43
1:A:330:ALA:O	1:A:331:LYS:CG	2.66	0.43
1:A:299:THR:O	1:A:299:THR:CG2	2.66	0.43
1:A:21:LEU:HD21	1:A:82:ALA:HA	1.99	0.43
1:A:511:GLU:OE1	1:A:525:LYS:HE3	2.18	0.43
1:A:625:LEU:HD22	1:A:625:LEU:H	1.84	0.43
1:A:630:ILE:N	1:A:630:ILE:HD12	2.33	0.43
1:A:8:ARG:HG2	1:A:8:ARG:NH1	2.33	0.43
1:A:200:VAL:HG13	1:A:270:SER:HB2	2.00	0.43
1:A:336:ILE:CG2	1:A:337:CYS:N	2.80	0.43
1:A:441:ARG:HG3	1:A:441:ARG:NH1	2.31	0.43
1:A:505:GLN:HE21	1:A:527:LYS:HB2	1.83	0.43
1:A:94:ILE:O	1:A:105:LYS:HA	2.19	0.43
1:A:586:MET:SD	1:A:616:VAL:HG21	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LYS:HD2	1:A:602:PHE:CZ	2.54	0.43
1:A:394:ARG:HA	1:A:394:ARG:HD3	1.88	0.43
1:A:456:VAL:CG1	1:A:457:GLN:HG3	2.49	0.42
1:A:203:VAL:HG12	1:A:204:ALA:N	2.33	0.42
1:A:102:PRO:O	1:A:103:PRO:O	2.37	0.42
1:A:217:THR:HG21	1:A:224:LYS:NZ	2.35	0.42
1:A:272:LEU:HD13	1:A:281:GLU:CD	2.45	0.42
1:A:510:GLY:C	1:A:526:ILE:HG23	2.44	0.42
1:A:660:ASN:HD22	1:A:660:ASN:HA	1.71	0.42
1:A:487:PHE:CD1	1:A:487:PHE:C	2.96	0.42
1:A:494:PRO:HA	1:A:569:GLN:O	2.19	0.42
1:A:114:GLU:O	1:A:187:THR:HA	2.19	0.42
1:A:208:MET:CE	1:A:234:PRO:HD3	2.45	0.42
1:A:609:ARG:NH1	1:A:613:GLU:HG2	2.35	0.42
1:A:241:PRO:HD2	1:A:245:HIS:CD2	2.55	0.42
1:A:42:ILE:CD1	1:A:94:ILE:HD12	2.50	0.42
1:A:538:HIS:CD2	1:A:573:LEU:HB2	2.54	0.42
1:A:70:LEU:O	1:A:70:LEU:CD1	2.65	0.42
1:A:308:VAL:HB	1:A:334:LEU:CD2	2.48	0.42
1:A:407:PHE:H	1:A:407:PHE:HD2	1.67	0.41
1:A:272:LEU:CD2	1:A:283:VAL:HG22	2.50	0.41
1:A:621:GLU:N	1:A:622:PRO:HD2	2.35	0.41
1:A:139:TRP:CZ2	1:A:292:ARG:HD2	2.55	0.41
1:A:210:LYS:HD2	1:A:261:PHE:CE1	2.55	0.41
1:A:488:ARG:NH2	1:A:623:LEU:HD21	2.35	0.41
1:A:524:GLN:HE21	1:A:524:GLN:HB2	1.58	0.41
1:A:213:VAL:HB	1:A:229:LEU:HB2	2.02	0.41
1:A:425:LEU:HD12	1:A:456:VAL:CG1	2.47	0.41
1:A:445:GLN:HG3	1:A:449:ASP:OD2	2.21	0.41
1:A:268:THR:CA	1:A:288:SER:HB3	2.48	0.41
1:A:625:LEU:N	1:A:625:LEU:CD2	2.84	0.41
1:A:91:LYS:HE2	1:A:109:TYR:CE2	2.48	0.41
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.85	0.41
1:A:354:ILE:HG21	1:A:650:ARG:CG	2.44	0.41
1:A:416:VAL:CG2	1:A:557:LEU:O	2.68	0.41
1:A:657:LYS:HB3	1:A:659:TRP:CE2	2.55	0.41
1:A:213:VAL:HG22	1:A:251:VAL:HG22	2.03	0.41
1:A:268:THR:HG22	1:A:269:ILE:N	2.36	0.41
1:A:504:GLN:HB3	1:A:526:ILE:HD11	2.03	0.41
1:A:122:THR:O	1:A:123:ARG:C	2.64	0.40
1:A:491:LEU:CD1	1:A:550:ARG:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:TRP:NE1	1:A:659:TRP:HE3	2.20	0.40
1:A:625:LEU:H	1:A:625:LEU:CD2	2.34	0.40
1:A:497:CYS:HB3	1:A:570:LEU:HD13	2.02	0.40
1:A:598:ILE:O	1:A:629:PHE:HA	2.22	0.40
1:A:123:ARG:NH1	1:A:139:TRP:CZ2	2.90	0.40
1:A:200:VAL:CG1	1:A:270:SER:HB2	2.51	0.40
1:A:300:PRO:HG3	1:A:654:PHE:HZ	1.87	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	539/666 (81%)	475 (88%)	52 (10%)	12 (2%)	5	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	A	103	PRO
1	A	484	ARG
1	A	12	GLU
1	A	69	PRO
1	A	456	VAL
1	A	584	PRO
1	A	602	PHE
1	A	102	PRO
1	A	123	ARG
1	A	458	ALA
1	A	465	ASP

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	499/590 (85%)	439 (88%)	60 (12%)	5 12

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	27	LEU
1	A	41	SER
1	A	52	ILE
1	A	67	THR
1	A	68	TRP
1	A	80	MET
1	A	87	THR
1	A	90	GLN
1	A	103	PRO
1	A	110	LEU
1	A	117	LEU
1	A	121	ILE
1	A	123	ARG
1	A	156	ARG
1	A	175	GLU
1	A	184	THR
1	A	185	LEU
1	A	198	THR
1	A	201	LEU
1	A	212	ARG
1	A	233	TRP
1	A	259	THR
1	A	274	THR
1	A	277	LEU
1	A	278	GLU
1	A	279	LEU
1	A	324	THR
1	A	326	LEU
1	A	328	MET

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Mol	Chain	Res	Type
1	A	329	LYS
1	A	333	LYS
1	A	334	LEU
1	A	350	ASP
1	A	352	MET
1	A	362	LYS
1	A	364	LEU
1	A	392	VAL
1	A	394	ARG
1	A	406	SER
1	A	412	VAL
1	A	427	ARG
1	A	439	ASP
1	A	456	VAL
1	A	472	VAL
1	A	484	ARG
1	A	489	LEU
1	A	500	LEU
1	A	504	GLN
1	A	514	LEU
1	A	522	LYS
1	A	530	LEU
1	A	534	THR
1	A	535	LEU
1	A	552	LEU
1	A	557	LEU
1	A	570	LEU
1	A	584	PRO
1	A	614	GLU
1	A	625	LEU

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

Mol	Chain	Res	Type
1	A	13	GLN
1	A	43	ASN
1	A	90	GLN
1	A	93	GLN
1	A	178	GLN
1	A	202	HIS
1	A	215	GLN
1	A	245	HIS

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	303	GLN
1	A	306	GLN
1	A	444	HIS
1	A	445	GLN
1	A	502	GLN
1	A	505	GLN
1	A	506	ASN
1	A	524	GLN
1	A	538	HIS
1	A	585	ASN
1	A	588	ASN
1	A	607	ASN
1	A	626	GLN
1	A	660	ASN

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 ⓘ

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	A	563/666 (84%)	0.81	60 (10%) 11 9	46, 75, 110, 121	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	LEU	5.6
1	A	53	ALA	3.9
1	A	172	LEU	3.9
1	A	103	PRO	3.6
1	A	99	PRO	3.6
1	A	2	ALA	3.4
1	A	178	GLN	3.3
1	A	216	ALA	3.2
1	A	74	VAL	3.2
1	A	225	CYS	3.1
1	A	601	PRO	3.1
1	A	127	VAL	3.1
1	A	87	THR	3.1
1	A	128	LYS	3.0
1	A	102	PRO	3.0
1	A	321	LYS	3.0
1	A	4	GLY	2.9
1	A	34	PRO	2.9
1	A	97	TYR	2.9
1	A	605	VAL	2.9
1	A	101	THR	2.9
1	A	107	LEU	2.9
1	A	54	HIS	2.9
1	A	137	ARG	2.8
1	A	350	ASP	2.8
1	A	98	GLY	2.7
1	A	526	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	593	GLY	2.7
1	A	590	LEU	2.6
1	A	67	THR	2.6
1	A	26	GLN	2.6
1	A	217	THR	2.5
1	A	391	TYR	2.5
1	A	69	PRO	2.5
1	A	663	PRO	2.5
1	A	3	GLN	2.5
1	A	38	THR	2.4
1	A	156	ARG	2.4
1	A	395	GLY	2.4
1	A	104	VAL	2.4
1	A	336	ILE	2.4
1	A	439	ASP	2.4
1	A	233	TRP	2.3
1	A	388	ASP	2.3
1	A	31	SER	2.3
1	A	173	ASP	2.3
1	A	337	CYS	2.3
1	A	66	SER	2.3
1	A	507	GLU	2.2
1	A	6	LEU	2.2
1	A	255	ALA	2.2
1	A	72	PRO	2.1
1	A	324	THR	2.1
1	A	174	SER	2.1
1	A	70	LEU	2.1
1	A	602	PHE	2.1
1	A	44	ALA	2.1
1	A	37	CYS	2.1
1	A	78	LEU	2.0
1	A	96	TYR	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 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.