



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:44 PM GMT

PDB ID : 3APM
Title : Crystal structure of the human SNP 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 : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

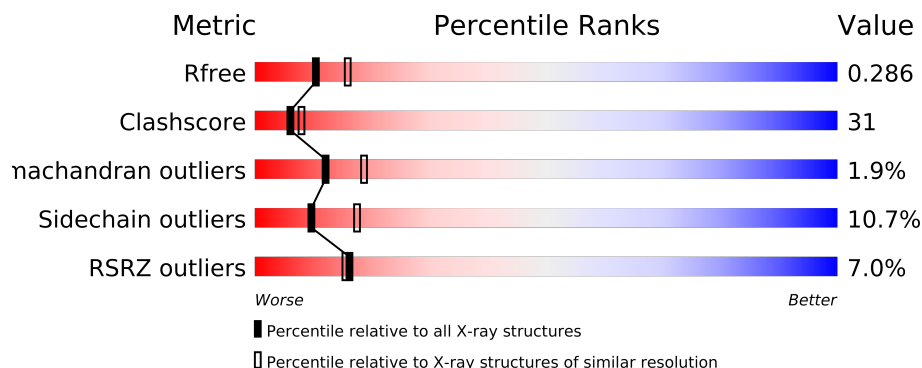
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	666	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4383 atoms, of which 0 are hydrogen and 0 are deuterium.

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	559	4383	2806	738	809	30	0	0	0

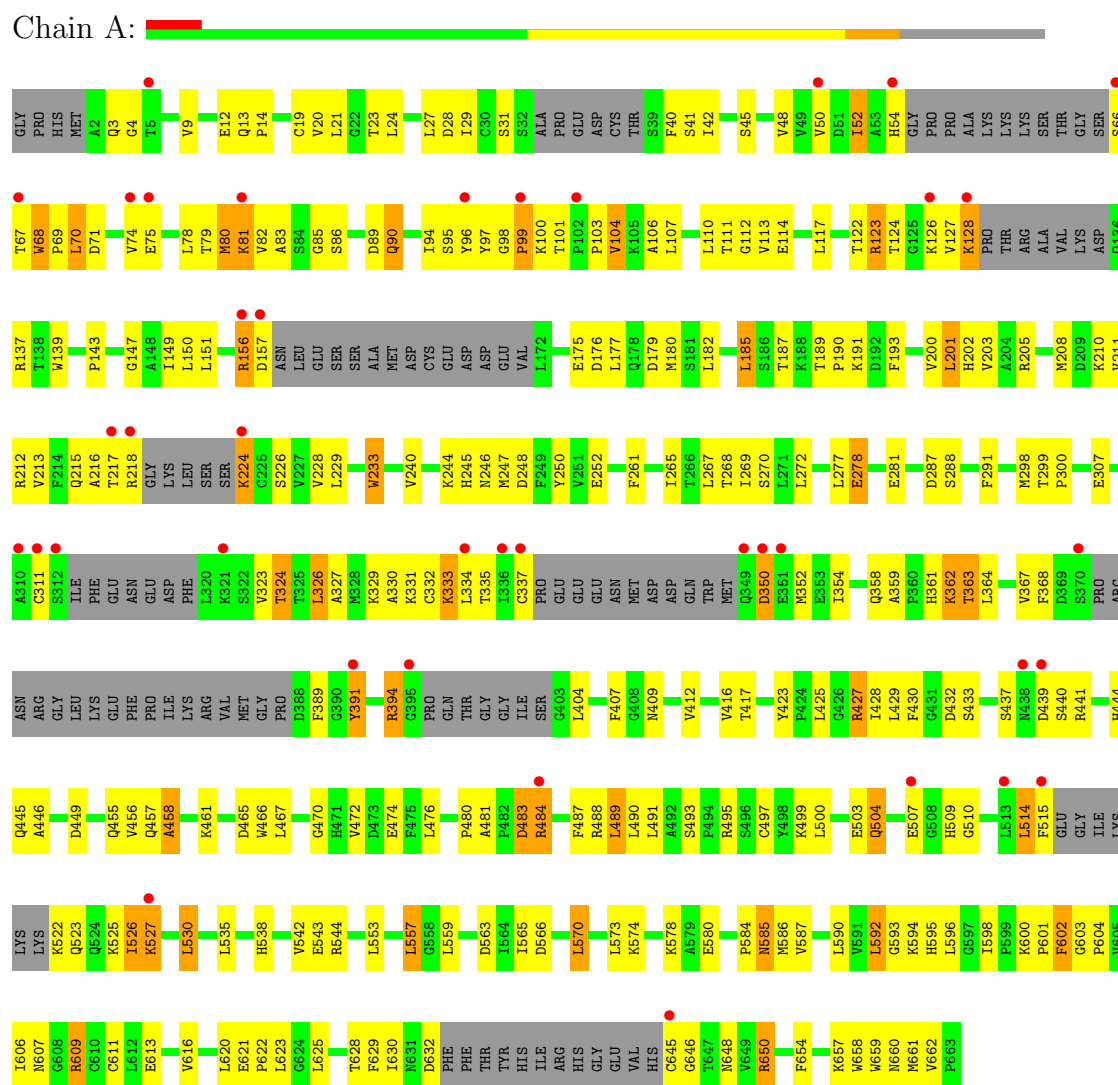
There are 3 discrepancies between the modelled and reference sequences:

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	145.56Å 61.24Å 113.47Å 90.00° 123.85° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 33.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 99.7 (33.66-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	39.55 (at 2.51Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.260 , 0.287 0.261 , 0.286	Depositor DCC
R_{free} test set	1469 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28933 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4383	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.44	0/4479	0.69	0/6069

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4383	0	4390	270	0
All	All	4383	0	4390	270	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (270) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:TYR:HB2	1:A:104:VAL:HG12	1.33	1.10
1:A:52:ILE:HG23	1:A:66:SER:HA	1.39	1.05
1:A:488:ARG:HH21	1:A:623:LEU:HD21	1.19	1.05
1:A:354:ILE:HG21	1:A:650:ARG:HG2	1.43	1.00
1:A:45:SER:HB2	1:A:90:GLN:HG3	1.44	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:609:ARG:HH11	1:A:609:ARG:HG2	1.29	0.94
1:A:650:ARG:HH11	1:A:650:ARG:HG3	1.31	0.92
1:A:81:LYS:HG3	1:A:82:VAL:HG23	1.53	0.89
1:A:333:LYS:HG3	1:A:334:LEU:N	1.87	0.88
1:A:20:VAL:O	1:A:23:THR:HG22	1.77	0.84
1:A:48:VAL:HG23	1:A:90:GLN:HG2	1.60	0.83
1:A:27:LEU:HD22	1:A:78:LEU:HD11	1.60	0.82
1:A:42:ILE:HG21	1:A:50:VAL:HG11	1.63	0.81
1:A:404:LEU:HD13	1:A:432:ASP:HA	1.62	0.81
1:A:54:HIS:CD2	1:A:67:THR:HG21	2.15	0.81
1:A:277:LEU:HD12	1:A:277:LEU:H	1.47	0.78
1:A:151:LEU:HD21	1:A:359:ALA:HB2	1.66	0.77
1:A:45:SER:CB	1:A:90:GLN:HG3	2.14	0.76
1:A:128:LYS:HE2	1:A:128:LYS:H	1.50	0.75
1:A:609:ARG:HH11	1:A:609:ARG:CG	1.99	0.74
1:A:19:CYS:HB2	1:A:80:MET:CE	2.17	0.74
1:A:445:GLN:HE21	1:A:449:ASP:CG	1.91	0.73
1:A:585:ASN:HD21	1:A:587:VAL:HG12	1.52	0.73
1:A:96:TYR:CB	1:A:104:VAL:HG12	2.16	0.72
1:A:52:ILE:HG23	1:A:66:SER:CA	2.17	0.72
1:A:590:LEU:HD21	1:A:592:LEU:HD13	1.71	0.72
1:A:298:MET:HB3	1:A:412:VAL:HG21	1.71	0.72
1:A:416:VAL:HG21	1:A:557:LEU:O	1.90	0.72
1:A:484:ARG:HB2	1:A:488:ARG:HH12	1.54	0.71
1:A:488:ARG:NH2	1:A:623:LEU:HD21	2.03	0.71
1:A:179:ASP:CG	1:A:362:LYS:HZ1	1.94	0.70
1:A:488:ARG:HH21	1:A:623:LEU:CD2	2.02	0.70
1:A:52:ILE:CG2	1:A:66:SER:HA	2.20	0.70
1:A:585:ASN:ND2	1:A:587:VAL:HG12	2.06	0.69
1:A:137:ARG:NE	1:A:137:ARG:HA	2.08	0.68
1:A:201:LEU:HD13	1:A:229:LEU:CD1	2.23	0.68
1:A:350:ASP:OD1	1:A:646:GLY:HA2	1.94	0.68
1:A:650:ARG:HH11	1:A:650:ARG:CG	2.07	0.67
1:A:216:ALA:HB3	1:A:248:ASP:HB2	1.77	0.67
1:A:361:HIS:O	1:A:362:LYS:HB2	1.96	0.66
1:A:311:CYS:HA	1:A:337:CYS:SG	2.36	0.66
1:A:298:MET:CE	1:A:428:ILE:HD12	2.25	0.66
1:A:54:HIS:HD2	1:A:67:THR:HG21	1.58	0.66
1:A:499:LYS:O	1:A:503:GLU:HG3	1.95	0.65
1:A:150:LEU:HG	1:A:291:PHE:HB3	1.79	0.65
1:A:215:GLN:HE21	1:A:228:VAL:HG11	1.61	0.65
1:A:68:TRP:HD1	1:A:97:TYR:OH	1.80	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:THR:C	1:A:68:TRP:HE3	2.00	0.65
1:A:596:LEU:HD21	1:A:625:LEU:HD12	1.78	0.65
1:A:538:HIS:HD2	1:A:573:LEU:H	1.43	0.65
1:A:211:VAL:HB	1:A:265:ILE:HD13	1.80	0.64
1:A:122:THR:OG1	1:A:124:THR:HG22	1.97	0.64
1:A:128:LYS:N	1:A:128:LYS:HE2	2.14	0.63
1:A:48:VAL:HG23	1:A:90:GLN:CG	2.28	0.63
1:A:620:LEU:O	1:A:623:LEU:HB2	2.00	0.62
1:A:13:GLN:HB2	1:A:14:PRO:HD2	1.81	0.61
1:A:68:TRP:CD1	1:A:97:TYR:OH	2.53	0.61
1:A:404:LEU:CD1	1:A:432:ASP:HA	2.29	0.61
1:A:601:PRO:O	1:A:603:GLY:N	2.34	0.61
1:A:334:LEU:HD13	1:A:335:THR:N	2.15	0.61
1:A:484:ARG:HB2	1:A:488:ARG:NH1	2.16	0.61
1:A:650:ARG:HG3	1:A:650:ARG:NH1	2.10	0.60
1:A:268:THR:HA	1:A:288:SER:HB3	1.83	0.60
1:A:590:LEU:CD2	1:A:592:LEU:HD13	2.32	0.60
1:A:298:MET:HE1	1:A:428:ILE:HD12	1.84	0.60
1:A:85:GLY:N	1:A:89:ASP:OD1	2.35	0.59
1:A:201:LEU:HD13	1:A:229:LEU:HD12	1.85	0.59
1:A:126:LYS:NZ	1:A:126:LYS:HB3	2.17	0.59
1:A:86:SER:O	1:A:89:ASP:OD2	2.20	0.59
1:A:613:GLU:HG3	1:A:629:PHE:CE1	2.37	0.59
1:A:19:CYS:HB2	1:A:80:MET:HE1	1.84	0.59
1:A:481:ALA:HB3	1:A:487:PHE:N	2.19	0.58
1:A:52:ILE:HD13	1:A:52:ILE:C	2.23	0.58
1:A:609:ARG:NH1	1:A:609:ARG:CG	2.64	0.58
1:A:493:SER:HB2	1:A:566:ASP:HB3	1.86	0.58
1:A:277:LEU:HD12	1:A:277:LEU:N	2.17	0.58
1:A:368:PHE:CD2	1:A:407:PHE:HE1	2.22	0.58
1:A:203:VAL:HG22	1:A:267:LEU:HD23	1.86	0.58
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.69	0.58
1:A:156:ARG:C	1:A:156:ARG:HD2	2.24	0.58
1:A:444:HIS:HD2	1:A:446:ALA:HB3	1.69	0.57
1:A:553:LEU:O	1:A:557:LEU:HB2	2.05	0.57
1:A:114:GLU:O	1:A:187:THR:HA	2.04	0.57
1:A:19:CYS:HB2	1:A:80:MET:HE2	1.86	0.57
1:A:137:ARG:HE	1:A:137:ARG:HA	1.68	0.57
1:A:327:ALA:O	1:A:330:ALA:HB3	2.04	0.57
1:A:466:TRP:CZ3	1:A:542:VAL:HG13	2.40	0.57
1:A:201:LEU:HD13	1:A:229:LEU:HD11	1.87	0.56
1:A:489:LEU:HD12	1:A:559:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:354:ILE:CG2	1:A:650:ARG:HG2	2.26	0.56
1:A:445:GLN:NE2	1:A:449:ASP:OD1	2.38	0.56
1:A:326:LEU:HD13	1:A:592:LEU:HD23	1.88	0.55
1:A:278:GLU:HA	1:A:278:GLU:OE1	2.06	0.55
1:A:428:ILE:HG12	1:A:457:GLN:HB3	1.88	0.55
1:A:71:ASP:O	1:A:74:VAL:HG12	2.06	0.55
1:A:661:MET:HG2	1:A:662:VAL:H	1.72	0.55
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.42	0.55
1:A:514:LEU:HD22	1:A:515:PHE:CD1	2.42	0.54
1:A:52:ILE:HD12	1:A:67:THR:N	2.23	0.54
1:A:362:LYS:HE3	1:A:364:LEU:HB2	1.89	0.54
1:A:3:GLN:HG3	1:A:4:GLY:N	2.23	0.54
1:A:594:LYS:HG2	1:A:595:HIS:HD2	1.73	0.53
1:A:467:LEU:HD13	1:A:474:GLU:HB2	1.89	0.53
1:A:68:TRP:N	1:A:69:PRO:CD	2.72	0.53
1:A:202:HIS:HE1	1:A:270:SER:OG	1.91	0.53
1:A:267:LEU:HD12	1:A:291:PHE:HE1	1.73	0.53
1:A:68:TRP:HE3	1:A:68:TRP:N	2.07	0.53
1:A:151:LEU:CD2	1:A:359:ALA:HB2	2.37	0.53
1:A:216:ALA:HB2	1:A:250:TYR:HE1	1.74	0.52
1:A:78:LEU:O	1:A:79:THR:HG23	2.09	0.52
1:A:504:GLN:OE1	1:A:606:ILE:HG12	2.09	0.52
1:A:632:ASP:OD2	1:A:645:CYS:HB2	2.09	0.52
1:A:4:GLY:HA3	1:A:24:LEU:O	2.10	0.52
1:A:42:ILE:CD1	1:A:94:ILE:HD12	2.39	0.52
1:A:29:ILE:O	1:A:96:TYR:OH	2.27	0.51
1:A:272:LEU:HD13	1:A:281:GLU:CD	2.30	0.51
1:A:40:PHE:HB3	1:A:70:LEU:HD23	1.93	0.51
1:A:358:GLN:HE21	1:A:658:TRP:HD1	1.57	0.51
1:A:510:GLY:HA2	1:A:526:ILE:HG23	1.91	0.51
1:A:497:CYS:HB3	1:A:570:LEU:HD13	1.92	0.51
1:A:600:LYS:HB2	1:A:630:ILE:O	2.11	0.51
1:A:52:ILE:HD11	1:A:67:THR:OG1	2.10	0.51
1:A:333:LYS:HG3	1:A:334:LEU:H	1.73	0.51
1:A:604:PRO:HB2	1:A:611:CYS:SG	2.51	0.51
1:A:433:SER:HB3	1:A:465:ASP:OD1	2.11	0.50
1:A:127:VAL:HG11	1:A:182:LEU:HD23	1.93	0.50
1:A:625:LEU:N	1:A:625:LEU:HD22	2.26	0.50
1:A:598:ILE:O	1:A:629:PHE:HA	2.12	0.50
1:A:657:LYS:HB3	1:A:659:TRP:CE2	2.46	0.50
1:A:299:THR:HG23	1:A:299:THR:O	2.12	0.50
1:A:493:SER:CB	1:A:566:ASP:HB3	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:ARG:HD2	1:A:147:GLY:O	2.12	0.50
1:A:467:LEU:CD1	1:A:474:GLU:HB2	2.42	0.50
1:A:156:ARG:HH11	1:A:156:ARG:HG3	1.76	0.49
1:A:28:ASP:OD2	1:A:31:SER:HB3	2.12	0.49
1:A:67:THR:C	1:A:68:TRP:CE3	2.84	0.49
1:A:354:ILE:HD12	1:A:354:ILE:N	2.27	0.49
1:A:124:THR:HG21	1:A:126:LYS:NZ	2.28	0.49
1:A:68:TRP:H	1:A:69:PRO:HD3	1.77	0.49
1:A:489:LEU:HD23	1:A:490:LEU:N	2.26	0.49
1:A:267:LEU:HD12	1:A:291:PHE:CE1	2.48	0.49
1:A:427:ARG:O	1:A:429:LEU:HD13	2.13	0.49
1:A:149:ILE:HD13	1:A:659:TRP:CE3	2.48	0.49
1:A:96:TYR:O	1:A:103:PRO:HA	2.12	0.49
1:A:412:VAL:HG13	1:A:428:ILE:HD13	1.94	0.49
1:A:323:VAL:HG13	1:A:324:THR:N	2.28	0.49
1:A:52:ILE:HA	1:A:75:GLU:O	2.12	0.48
1:A:298:MET:SD	1:A:412:VAL:HG22	2.53	0.48
1:A:362:LYS:HD2	1:A:363:THR:N	2.28	0.48
1:A:113:VAL:HB	1:A:189:THR:HG22	1.95	0.48
1:A:457:GLN:O	1:A:458:ALA:C	2.50	0.48
1:A:527:LYS:C	1:A:527:LYS:HD3	2.33	0.48
1:A:362:LYS:HE3	1:A:364:LEU:HD12	1.94	0.48
1:A:625:LEU:HD22	1:A:625:LEU:H	1.78	0.48
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.78	0.48
1:A:368:PHE:CD2	1:A:407:PHE:CE1	3.02	0.48
1:A:41:SER:HB2	1:A:95:SER:HB2	1.95	0.48
1:A:14:PRO:HB3	1:A:107:LEU:HB2	1.96	0.48
1:A:190:PRO:HG2	1:A:193:PHE:HB2	1.96	0.47
1:A:480:PRO:HG2	1:A:593:GLY:O	2.14	0.47
1:A:277:LEU:H	1:A:277:LEU:CD1	2.21	0.47
1:A:514:LEU:HD23	1:A:603:GLY:HA2	1.96	0.47
1:A:21:LEU:HD21	1:A:82:VAL:HA	1.95	0.47
1:A:487:PHE:C	1:A:487:PHE:CD1	2.88	0.47
1:A:526:ILE:O	1:A:530:LEU:HD22	2.14	0.47
1:A:621:GLU:C	1:A:623:LEU:H	2.17	0.47
1:A:489:LEU:HD22	1:A:491:LEU:HG	1.97	0.47
1:A:495:ARG:HB2	1:A:543:GLU:OE2	2.14	0.47
1:A:176:ASP:O	1:A:177:LEU:HD23	2.14	0.47
1:A:143:PRO:HA	1:A:660:ASN:ND2	2.30	0.47
1:A:156:ARG:NH1	1:A:156:ARG:HG3	2.31	0.46
1:A:212:ARG:HB3	1:A:252:GLU:HG3	1.96	0.46
1:A:594:LYS:HG3	1:A:594:LYS:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:307:GLU:OE2	1:A:333:LYS:HE2	2.15	0.46
1:A:80:MET:HG2	1:A:112:GLY:HA3	1.97	0.46
1:A:441:ARG:NH1	1:A:441:ARG:HG3	2.30	0.46
1:A:217:THR:HG21	1:A:224:LYS:NZ	2.31	0.46
1:A:423:TYR:CD2	1:A:427:ARG:HD2	2.50	0.46
1:A:13:GLN:HB2	1:A:14:PRO:CD	2.45	0.46
1:A:394:ARG:HB2	1:A:394:ARG:NH1	2.31	0.46
1:A:476:LEU:HA	1:A:490:LEU:O	2.16	0.46
1:A:661:MET:HG2	1:A:662:VAL:N	2.31	0.46
1:A:650:ARG:CG	1:A:650:ARG:NH1	2.70	0.45
1:A:80:MET:HE3	1:A:112:GLY:N	2.31	0.45
1:A:217:THR:HG21	1:A:224:LYS:HZ1	1.80	0.45
1:A:151:LEU:HD21	1:A:359:ALA:CB	2.43	0.45
1:A:203:VAL:HG23	1:A:229:LEU:HD13	1.98	0.45
1:A:82:VAL:HG12	1:A:83:ALA:N	2.31	0.45
1:A:80:MET:HE2	1:A:112:GLY:HA2	1.98	0.45
1:A:362:LYS:HD2	1:A:363:THR:C	2.37	0.45
1:A:200:VAL:CG1	1:A:270:SER:HB2	2.47	0.45
1:A:354:ILE:HG21	1:A:650:ARG:CG	2.28	0.45
1:A:68:TRP:N	1:A:69:PRO:HD3	2.32	0.45
1:A:586:MET:SD	1:A:601:PRO:HG3	2.56	0.45
1:A:216:ALA:HB2	1:A:250:TYR:CE1	2.52	0.45
1:A:300:PRO:HG3	1:A:654:PHE:HZ	1.82	0.45
1:A:409:ASN:OD1	1:A:472:VAL:HG13	2.17	0.45
1:A:98:GLY:HA3	1:A:99:PRO:HD2	1.75	0.44
1:A:368:PHE:HE1	1:A:394:ARG:H	1.65	0.44
1:A:3:GLN:HG3	1:A:4:GLY:H	1.80	0.44
1:A:185:LEU:O	1:A:246:ASN:HA	2.17	0.44
1:A:218:ARG:HA	1:A:218:ARG:NE	2.33	0.44
1:A:394:ARG:HB2	1:A:394:ARG:CZ	2.48	0.44
1:A:525:LYS:C	1:A:527:LYS:H	2.22	0.44
1:A:269:ILE:HG22	1:A:287:ASP:O	2.18	0.44
1:A:68:TRP:CE3	1:A:68:TRP:N	2.85	0.44
1:A:80:MET:HE3	1:A:111:THR:C	2.38	0.44
1:A:80:MET:HE1	1:A:110:LEU:HB3	2.00	0.43
1:A:613:GLU:HG3	1:A:629:PHE:CZ	2.53	0.43
1:A:484:ARG:HG2	1:A:563:ASP:OD1	2.18	0.43
1:A:660:ASN:HD22	1:A:660:ASN:HA	1.67	0.43
1:A:425:LEU:HD12	1:A:456:VAL:HG22	2.01	0.43
1:A:476:LEU:C	1:A:476:LEU:HD12	2.39	0.43
1:A:127:VAL:HG23	1:A:127:VAL:O	2.19	0.43
1:A:437:SER:HB2	1:A:440:SER:OG	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:245:HIS:CG	1:A:246:ASN:N	2.86	0.43
1:A:404:LEU:CD2	1:A:470:GLY:O	2.67	0.43
1:A:240:VAL:HG22	1:A:247:MET:CE	2.49	0.43
1:A:81:LYS:HE3	1:A:81:LYS:HA	1.99	0.43
1:A:538:HIS:CD2	1:A:573:LEU:HB2	2.54	0.43
1:A:394:ARG:HH11	1:A:394:ARG:HA	1.84	0.43
1:A:210:LYS:HD2	1:A:261:PHE:CE1	2.54	0.43
1:A:621:GLU:N	1:A:622:PRO:HD2	2.34	0.42
1:A:354:ILE:HG13	1:A:367:VAL:HG22	2.01	0.42
1:A:523:GLN:HG2	1:A:523:GLN:H	1.64	0.42
1:A:367:VAL:HG23	1:A:389:PHE:HD2	1.83	0.42
1:A:354:ILE:HD12	1:A:354:ILE:H	1.83	0.42
1:A:82:VAL:CG1	1:A:83:ALA:N	2.83	0.42
1:A:211:VAL:HG22	1:A:212:ARG:N	2.34	0.42
1:A:94:ILE:HB	1:A:106:ALA:HB3	2.01	0.42
1:A:427:ARG:NH1	1:A:458:ALA:O	2.52	0.42
1:A:574:LYS:HG3	1:A:580:GLU:CD	2.40	0.42
1:A:574:LYS:HG3	1:A:580:GLU:OE2	2.18	0.42
1:A:658:TRP:NE1	1:A:659:TRP:HE3	2.18	0.42
1:A:590:LEU:CD2	1:A:592:LEU:HD22	2.49	0.42
1:A:430:PHE:CZ	1:A:461:LYS:HG2	2.55	0.42
1:A:205:ARG:O	1:A:208:MET:HG2	2.20	0.42
1:A:9:VAL:HG21	1:A:94:ILE:HG13	2.02	0.41
1:A:127:VAL:CG1	1:A:182:LEU:HD23	2.50	0.41
1:A:483:ASP:OD1	1:A:488:ARG:NH2	2.53	0.41
1:A:177:LEU:HD22	1:A:180:MET:SD	2.60	0.41
1:A:427:ARG:HH11	1:A:427:ARG:CG	2.32	0.41
1:A:514:LEU:O	1:A:515:PHE:CB	2.68	0.41
1:A:224:LYS:N	1:A:224:LYS:HD3	2.34	0.41
1:A:391:TYR:CD1	1:A:391:TYR:N	2.88	0.41
1:A:416:VAL:HG22	1:A:417:THR:N	2.34	0.41
1:A:86:SER:HA	1:A:190:PRO:HB3	2.03	0.41
1:A:488:ARG:HG2	1:A:565:ILE:CG1	2.50	0.41
1:A:621:GLU:C	1:A:623:LEU:N	2.74	0.41
1:A:326:LEU:HD22	1:A:326:LEU:O	2.20	0.41
1:A:213:VAL:O	1:A:228:VAL:HG22	2.19	0.41
1:A:509:HIS:CD2	1:A:606:ILE:HG13	2.56	0.41
1:A:210:LYS:HD2	1:A:261:PHE:CD1	2.55	0.41
1:A:97:TYR:CB	1:A:103:PRO:HG3	2.51	0.41
1:A:126:LYS:HZ2	1:A:126:LYS:HB3	1.86	0.41
1:A:586:MET:SD	1:A:616:VAL:HG21	2.61	0.41
1:A:97:TYR:HB3	1:A:103:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:488:ARG:HG2	1:A:565:ILE:HG12	2.03	0.41
1:A:354:ILE:CD1	1:A:648:ASN:HB3	2.51	0.41
1:A:590:LEU:HD21	1:A:592:LEU:HD22	2.03	0.41
1:A:298:MET:HB2	1:A:298:MET:HE3	1.90	0.41
1:A:514:LEU:HD23	1:A:602:PHE:O	2.21	0.41
1:A:525:LYS:C	1:A:527:LYS:N	2.74	0.41
1:A:326:LEU:HD21	1:A:595:HIS:HB3	2.02	0.41
1:A:358:GLN:OE1	1:A:657:LYS:HD3	2.21	0.40
1:A:123:ARG:HG2	1:A:659:TRP:CD1	2.56	0.40
1:A:514:LEU:O	1:A:515:PHE:HB2	2.22	0.40
1:A:233:TRP:N	1:A:233:TRP:CD1	2.89	0.40
1:A:441:ARG:HH12	1:A:578:LYS:HE3	1.85	0.40
1:A:330:ALA:O	1:A:331:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/666 (80%)	488 (91%)	37 (7%)	10 (2%)	12	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	A	455	GLN
1	A	484	ARG
1	A	12	GLU
1	A	458	ALA
1	A	602	PHE
1	A	191	LYS
1	A	362	LYS
1	A	584	PRO
1	A	526	ILE

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	497/590 (84%)	444 (89%)	53 (11%)	10	17

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	68	TRP
1	A	70	LEU
1	A	80	MET
1	A	81	LYS
1	A	90	GLN
1	A	100	LYS
1	A	101	THR
1	A	104	VAL
1	A	117	LEU
1	A	123	ARG
1	A	128	LYS
1	A	156	ARG
1	A	157	ASP
1	A	175	GLU
1	A	185	LEU
1	A	201	LEU
1	A	224	LYS
1	A	226	SER
1	A	233	TRP
1	A	244	LYS
1	A	278	GLU
1	A	324	THR
1	A	326	LEU
1	A	329	LYS
1	A	332	CYS
1	A	333	LYS
1	A	350	ASP
1	A	352	MET
1	A	363	THR
1	A	391	TYR

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Mol	Chain	Res	Type
1	A	394	ARG
1	A	427	ARG
1	A	439	ASP
1	A	483	ASP
1	A	489	LEU
1	A	500	LEU
1	A	504	GLN
1	A	507	GLU
1	A	514	LEU
1	A	522	LYS
1	A	527	LYS
1	A	530	LEU
1	A	535	LEU
1	A	544	ARG
1	A	557	LEU
1	A	570	LEU
1	A	585	ASN
1	A	592	LEU
1	A	607	ASN
1	A	609	ARG
1	A	628	THR
1	A	650	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	54	HIS
1	A	90	GLN
1	A	197	HIS
1	A	202	HIS
1	A	215	GLN
1	A	358	GLN
1	A	444	HIS
1	A	445	GLN
1	A	448	GLN
1	A	455	GLN
1	A	471	HIS
1	A	505	GLN
1	A	506	ASN
1	A	524	GLN
1	A	538	HIS

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Mol	Chain	Res	Type
1	A	585	ASN
1	A	595	HIS
1	A	607	ASN
1	A	660	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	A	559/666 (83%)	0.33	39 (6%) 16 15	35, 63, 102, 113	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	LYS	5.2
1	A	645	CYS	5.1
1	A	350	ASP	4.6
1	A	156	ARG	4.6
1	A	439	ASP	4.4
1	A	349	GLN	4.2
1	A	102	PRO	4.2
1	A	66	SER	4.1
1	A	311	CYS	3.9
1	A	81	LYS	3.8
1	A	395	GLY	3.6
1	A	157	ASP	3.6
1	A	96	TYR	3.4
1	A	67	THR	3.2
1	A	217	THR	3.2
1	A	391	TYR	3.0
1	A	224	LYS	2.8
1	A	312	SER	2.8
1	A	50	VAL	2.8
1	A	54	HIS	2.6
1	A	438	ASN	2.6
1	A	337	CYS	2.6
1	A	99	PRO	2.6
1	A	74	VAL	2.4
1	A	321	LYS	2.4
1	A	218	ARG	2.4
1	A	370	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	336	ILE	2.3
1	A	527	LYS	2.3
1	A	507	GLU	2.2
1	A	351	GLU	2.1
1	A	5	THR	2.1
1	A	484	ARG	2.1
1	A	334	LEU	2.1
1	A	515	PHE	2.0
1	A	513	LEU	2.0
1	A	75	GLU	2.0
1	A	310	ALA	2.0
1	A	126	LYS	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.