



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:39 pm BST

PDB ID : 1WD8
Title : Calcium free form of human peptidylarginine deiminase type4 (PAD4)
Authors : Arita, K.; Hashimoto, H.; Shimizu, T.; Nakashima, K.; Yamada, M.; Sato, M.
Deposited on : 2004-05-12
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

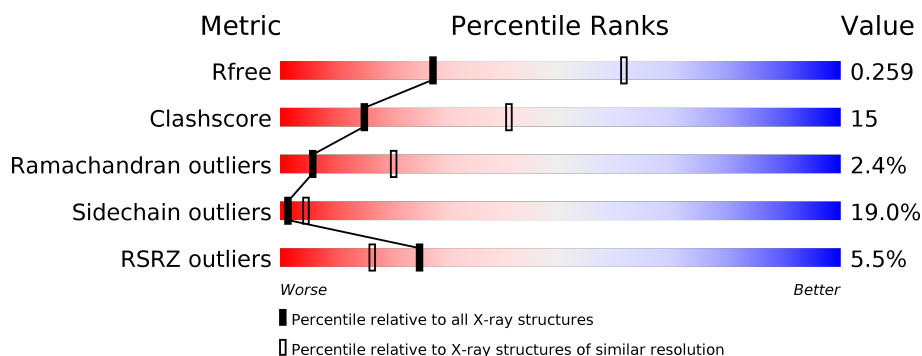
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	670	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4382 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4382	2805	738	809	30	79	0	0

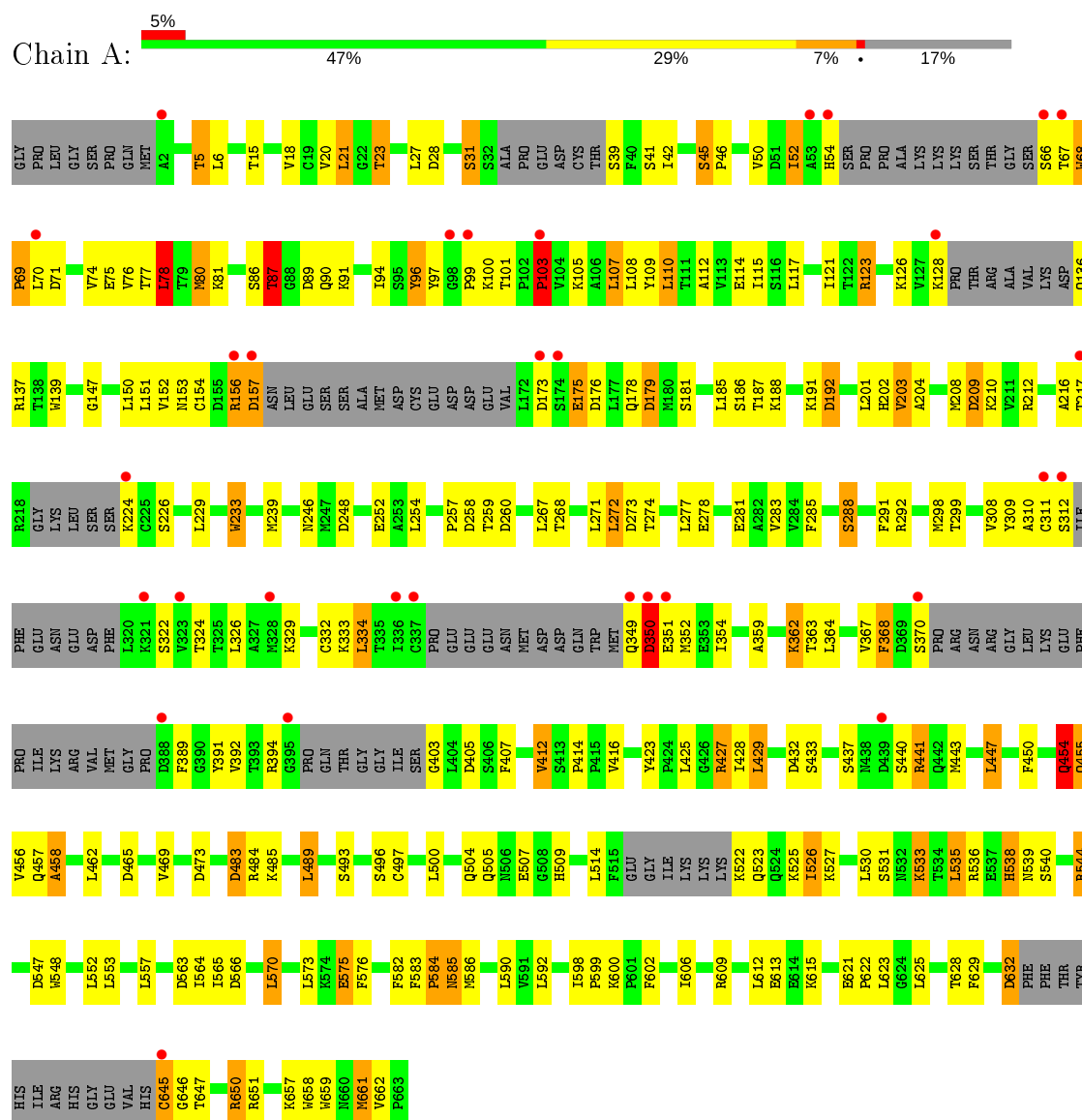
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q9UM07
A	-5	PRO	-	EXPRESSION TAG	UNP Q9UM07
A	-4	LEU	-	EXPRESSION TAG	UNP Q9UM07
A	-3	GLY	-	EXPRESSION TAG	UNP Q9UM07
A	-2	SER	-	EXPRESSION TAG	UNP Q9UM07
A	-1	PRO	-	EXPRESSION TAG	UNP Q9UM07
A	0	GLN	-	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 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 IV



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.61Å 60.44Å 113.49Å 90.00° 123.61° 90.00°	Depositor
Resolution (Å)	33.44 – 2.80 33.44 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (33.44-2.80) 96.0 (33.44-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.20 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.231 , 0.264 0.234 , 0.259	Depositor DCC
R_{free} test set	1961 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4382	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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	1.07	11/4478 (0.2%)	1.19	42/6068 (0.7%)

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	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	483	ASP	CB-CG	-25.65	0.97	1.51
1	A	96	TYR	CB-CG	16.55	1.76	1.51
1	A	75	GLU	CB-CG	-15.64	1.22	1.52
1	A	191	LYS	CB-CG	-10.94	1.23	1.52
1	A	128	LYS	CB-CG	-10.85	1.23	1.52
1	A	105	LYS	CB-CG	10.25	1.80	1.52
1	A	188	LYS	CB-CG	-9.67	1.26	1.52
1	A	81	LYS	CB-CG	9.62	1.78	1.52
1	A	126	LYS	CB-CG	-7.98	1.30	1.52
1	A	107	LEU	CB-CG	-7.67	1.30	1.52
1	A	600	LYS	CB-CG	-6.92	1.33	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	TYR	CB-CG-CD1	-19.45	109.33	121.00
1	A	483	ASP	CB-CG-OD2	19.08	135.47	118.30
1	A	483	ASP	CB-CG-OD1	-18.52	101.63	118.30
1	A	96	TYR	CB-CG-CD2	13.92	129.35	121.00
1	A	188	LYS	CA-CB-CG	12.67	141.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LEU	CA-CB-CG	10.15	138.65	115.30
1	A	96	TYR	CA-CB-CG	-9.97	94.46	113.40
1	A	105	LYS	CA-CB-CG	-8.97	93.66	113.40
1	A	192	ASP	CB-CG-OD2	8.67	126.10	118.30
1	A	483	ASP	CA-CB-CG	8.47	132.03	113.40
1	A	209	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	191	LYS	CA-CB-CG	7.88	130.75	113.40
1	A	100	LYS	CA-CB-CG	7.83	130.62	113.40
1	A	105	LYS	CB-CG-CD	-7.11	93.12	111.60
1	A	441	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	107	LEU	CB-CG-CD2	6.61	122.24	111.00
1	A	273	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	260	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	137	ARG	CA-CB-CG	6.36	127.38	113.40
1	A	173	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	632	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	566	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	78	LEU	CA-CB-CG	5.84	128.72	115.30
1	A	179	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	188	LYS	CB-CG-CD	5.64	126.28	111.60
1	A	405	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	455	GLN	N-CA-C	5.59	126.10	111.00
1	A	651	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	87	THR	N-CA-CB	5.52	120.79	110.30
1	A	465	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	441	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	602	PHE	N-CA-C	-5.39	96.45	111.00
1	A	91	LYS	CA-CB-CG	5.37	125.21	113.40
1	A	176	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	473	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	432	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	203	VAL	CB-CA-C	-5.18	101.56	111.40
1	A	178	GLN	CA-CB-CG	-5.17	102.02	113.40
1	A	547	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	126	LYS	CB-CG-CD	5.07	124.79	111.60
1	A	544	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	414	PRO	N-CD-CG	-5.02	95.67	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	GLN	Mainchain,Peptide
1	A	96	TYR	Sidechain

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	4382	0	4388	129	0
All	All	4382	0	4388	129	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 15.

All (129) 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:101:THR:HB	1:A:103:PRO:HD3	1.54	0.88
1:A:42:ILE:HG21	1:A:50:VAL:HG11	1.55	0.87
1:A:456:VAL:HG23	1:A:661:MET:SD	2.16	0.84
1:A:20:VAL:O	1:A:23:THR:HG23	1.80	0.82
1:A:179:ASP:OD2	1:A:362:LYS:NZ	2.15	0.78
1:A:590:LEU:HD21	1:A:592:LEU:HD13	1.70	0.74
1:A:86:SER:O	1:A:87:THR:CG2	2.36	0.73
1:A:416:VAL:HG21	1:A:557:LEU:O	1.89	0.73
1:A:526:ILE:O	1:A:530:LEU:HD22	1.90	0.71
1:A:151:LEU:HD21	1:A:359:ALA:HB2	1.73	0.71
1:A:535:LEU:HD22	1:A:539:ASN:ND2	2.09	0.67
1:A:450:PHE:O	1:A:454:GLN:HG2	1.94	0.67
1:A:150:LEU:HG	1:A:291:PHE:HB3	1.76	0.66
1:A:52:ILE:HG23	1:A:66:SER:HA	1.78	0.66
1:A:456:VAL:CG2	1:A:661:MET:SD	2.85	0.64
1:A:154:CYS:HB3	1:A:391:TYR:H	1.63	0.64
1:A:86:SER:O	1:A:87:THR:HG22	1.98	0.62
1:A:272:LEU:HD23	1:A:283:VAL:HG22	1.82	0.62
1:A:613:GLU:HG3	1:A:629:PHE:CE1	2.36	0.61
1:A:27:LEU:HD22	1:A:78:LEU:HD11	1.82	0.60
1:A:553:LEU:HD23	1:A:557:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:HB	1:A:103:PRO:CD	2.29	0.59
1:A:257:PRO:HD2	1:A:454:GLN:HE22	1.68	0.58
1:A:535:LEU:HD22	1:A:539:ASN:HD21	1.68	0.58
1:A:443:MET:HE2	1:A:447:LEU:HD13	1.86	0.57
1:A:71:ASP:O	1:A:74:VAL:HG12	2.05	0.57
1:A:86:SER:O	1:A:87:THR:HG23	2.04	0.57
1:A:42:ILE:CD1	1:A:94:ILE:HG23	2.36	0.56
1:A:564:ILE:HG22	1:A:565:ILE:N	2.21	0.56
1:A:202:HIS:HA	1:A:229:LEU:HD21	1.88	0.56
1:A:403:GLY:N	1:A:469:VAL:O	2.39	0.56
1:A:216:ALA:HB3	1:A:248:ASP:HB2	1.87	0.56
1:A:621:GLU:N	1:A:622:PRO:HD2	2.22	0.55
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.41	0.55
1:A:45:SER:HB3	1:A:46:PRO:HD2	1.90	0.54
1:A:527:LYS:HA	1:A:530:LEU:HD23	1.88	0.54
1:A:299:THR:O	1:A:299:THR:CG2	2.56	0.54
1:A:349:GLN:HE21	1:A:351:GLU:HG3	1.73	0.53
1:A:523:GLN:O	1:A:523:GLN:HG3	2.09	0.53
1:A:80:MET:HE2	1:A:112:ALA:HB2	1.91	0.53
1:A:416:VAL:CG2	1:A:557:LEU:O	2.57	0.53
1:A:115:ILE:CD1	1:A:271:LEU:HD22	2.38	0.53
1:A:526:ILE:O	1:A:530:LEU:CD2	2.56	0.52
1:A:590:LEU:CD2	1:A:592:LEU:HD13	2.38	0.52
1:A:152:VAL:HG12	1:A:153:ASN:N	2.24	0.52
1:A:299:THR:O	1:A:299:THR:HG23	2.10	0.52
1:A:362:LYS:NZ	1:A:364:LEU:HD12	2.25	0.51
1:A:650:ARG:HH11	1:A:650:ARG:HG3	1.76	0.50
1:A:5:THR:OG1	1:A:6:LEU:N	2.45	0.50
1:A:154:CYS:HB3	1:A:391:TYR:N	2.26	0.50
1:A:52:ILE:CG2	1:A:66:SER:HA	2.41	0.49
1:A:151:LEU:HD21	1:A:359:ALA:CB	2.42	0.49
1:A:362:LYS:HZ1	1:A:364:LEU:HD12	1.78	0.48
1:A:583:PHE:O	1:A:584:PRO:C	2.49	0.48
1:A:570:LEU:HB3	1:A:582:PHE:HB3	1.95	0.48
1:A:585:ASN:O	1:A:599:PRO:HG2	2.12	0.48
1:A:489:LEU:HD22	1:A:489:LEU:C	2.33	0.48
1:A:443:MET:CE	1:A:447:LEU:HD22	2.44	0.48
1:A:457:GLN:O	1:A:458:ALA:C	2.51	0.48
1:A:42:ILE:HD13	1:A:94:ILE:HG23	1.96	0.48
1:A:114:GLU:O	1:A:187:THR:HA	2.13	0.47
1:A:553:LEU:HD23	1:A:557:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:HG13	1:A:457:GLN:HB3	1.97	0.47
1:A:139:TRP:CZ2	1:A:292:ARG:HD2	2.50	0.47
1:A:310:ALA:HA	1:A:646:GLY:O	2.15	0.47
1:A:42:ILE:HD11	1:A:94:ILE:HG23	1.97	0.47
1:A:80:MET:CE	1:A:112:ALA:HB2	2.44	0.47
1:A:657:LYS:HB3	1:A:659:TRP:CE2	2.49	0.46
1:A:233:TRP:CD1	1:A:233:TRP:N	2.83	0.46
1:A:443:MET:HE1	1:A:447:LEU:HD22	1.97	0.46
1:A:15:THR:HB	1:A:108:LEU:HD13	1.98	0.46
1:A:484:ARG:O	1:A:485:LYS:HB2	2.16	0.46
1:A:493:SER:HB3	1:A:496:SER:HB3	1.96	0.46
1:A:658:TRP:O	1:A:661:MET:HB2	2.16	0.46
1:A:209:ASP:O	1:A:254:LEU:HD12	2.15	0.46
1:A:80:MET:HE1	1:A:110:LEU:HB3	1.98	0.46
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.71	0.46
1:A:429:LEU:HG	1:A:462:LEU:HD11	1.98	0.46
1:A:52:ILE:HD12	1:A:76:VAL:HG22	1.96	0.45
1:A:272:LEU:CD2	1:A:283:VAL:HG22	2.46	0.45
1:A:484:ARG:NH1	1:A:563:ASP:OD1	2.49	0.45
1:A:368:PHE:CD2	1:A:407:PHE:HE1	2.35	0.45
1:A:632:ASP:OD2	1:A:645:CYS:HB2	2.17	0.45
1:A:203:VAL:HG12	1:A:204:ALA:N	2.32	0.45
1:A:186:SER:HA	1:A:246:ASN:HB3	1.98	0.44
1:A:423:TYR:CD2	1:A:427:ARG:HD2	2.53	0.44
1:A:565:ILE:HG22	1:A:565:ILE:O	2.16	0.44
1:A:212:ARG:NH1	1:A:252:GLU:OE2	2.51	0.44
1:A:308:VAL:CG2	1:A:592:LEU:HD11	2.47	0.44
1:A:598:ILE:O	1:A:629:PHE:HA	2.16	0.44
1:A:497:CYS:HB3	1:A:570:LEU:HD13	1.99	0.44
1:A:586:MET:HA	1:A:599:PRO:HD2	2.00	0.44
1:A:437:SER:HB2	1:A:440:SER:OG	2.18	0.44
1:A:425:LEU:HD12	1:A:456:VAL:HG22	2.00	0.44
1:A:613:GLU:HG3	1:A:629:PHE:CZ	2.52	0.44
1:A:203:VAL:HG23	1:A:229:LEU:HD22	1.99	0.43
1:A:153:ASN:ND2	1:A:252:GLU:OE1	2.44	0.43
1:A:74:VAL:O	1:A:74:VAL:HG13	2.18	0.43
1:A:298:MET:SD	1:A:412:VAL:HG22	2.59	0.43
1:A:309:TYR:O	1:A:647:THR:HA	2.18	0.43
1:A:68:TRP:CD1	1:A:97:TYR:OH	2.71	0.43
1:A:612:LEU:O	1:A:613:GLU:C	2.56	0.43
1:A:268:THR:HG23	1:A:288:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ILE:HG22	1:A:565:ILE:H	1.83	0.42
1:A:209:ASP:OD1	1:A:210:LYS:NZ	2.46	0.42
1:A:509:HIS:CD2	1:A:606:ILE:HD12	2.53	0.42
1:A:662:VAL:HG23	1:A:662:VAL:O	2.19	0.42
1:A:156:ARG:O	1:A:157:ASP:OD1	2.37	0.42
1:A:20:VAL:HG21	1:A:285:PHE:CG	2.55	0.42
1:A:538:HIS:CD2	1:A:573:LEU:H	2.37	0.42
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.90	0.42
1:A:28:ASP:OD2	1:A:31:SER:HB2	2.19	0.42
1:A:613:GLU:CG	1:A:629:PHE:CE1	3.02	0.42
1:A:101:THR:C	1:A:103:PRO:HD2	2.40	0.42
1:A:623:LEU:HB2	1:A:625:LEU:HD23	2.01	0.42
1:A:423:TYR:CE2	1:A:427:ARG:HD2	2.55	0.41
1:A:505:GLN:HE21	1:A:527:LYS:HB2	1.84	0.41
1:A:308:VAL:HB	1:A:334:LEU:HD22	2.02	0.41
1:A:52:ILE:HG12	1:A:66:SER:HA	2.01	0.41
1:A:139:TRP:CH2	1:A:292:ARG:HD2	2.56	0.41
1:A:354:ILE:HG12	1:A:367:VAL:HG22	2.02	0.41
1:A:368:PHE:CG	1:A:407:PHE:HE1	2.38	0.41
1:A:575:GLU:O	1:A:576:PHE:HB2	2.21	0.41
1:A:548:TRP:O	1:A:552:LEU:HD13	2.21	0.41
1:A:68:TRP:N	1:A:69:PRO:HD2	2.36	0.41
1:A:350:ASP:OD2	1:A:646:GLY:HA2	2.21	0.40
1:A:531:SER:O	1:A:533:LYS:HG2	2.20	0.40
1:A:203:VAL:HG22	1:A:267:LEU:HD23	2.02	0.40
1:A:427:ARG:O	1:A:429:LEU:HD13	2.21	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	535/670 (80%)	469 (88%)	53 (10%)	13 (2%)	6	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
1	A	455	GLN
1	A	69	PRO
1	A	87	THR
1	A	99	PRO
1	A	175	GLU
1	A	575	GLU
1	A	350	ASP
1	A	123	ARG
1	A	454	GLN
1	A	458	ALA
1	A	507	GLU
1	A	584	PRO

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	496/593 (84%)	402 (81%)	94 (19%)	1	4

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	18	VAL
1	A	21	LEU
1	A	23	THR
1	A	31	SER
1	A	39	SER
1	A	41	SER
1	A	45	SER

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Mol	Chain	Res	Type
1	A	52	ILE
1	A	54	HIS
1	A	67	THR
1	A	68	TRP
1	A	70	LEU
1	A	77	THR
1	A	78	LEU
1	A	80	MET
1	A	87	THR
1	A	89	ASP
1	A	90	GLN
1	A	103	PRO
1	A	107	LEU
1	A	109	TYR
1	A	110	LEU
1	A	117	LEU
1	A	121	ILE
1	A	123	ARG
1	A	136	GLN
1	A	156	ARG
1	A	157	ASP
1	A	175	GLU
1	A	181	SER
1	A	185	LEU
1	A	192	ASP
1	A	201	LEU
1	A	208	MET
1	A	217	THR
1	A	224	LYS
1	A	226	SER
1	A	233	TRP
1	A	239	MET
1	A	258	ASP
1	A	259	THR
1	A	272	LEU
1	A	274	THR
1	A	277	LEU
1	A	278	GLU
1	A	281	GLU
1	A	288	SER
1	A	311	CYS
1	A	312	SER

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Mol	Chain	Res	Type
1	A	322	SER
1	A	324	THR
1	A	326	LEU
1	A	329	LYS
1	A	332	CYS
1	A	333	LYS
1	A	334	LEU
1	A	350	ASP
1	A	352	MET
1	A	362	LYS
1	A	363	THR
1	A	368	PHE
1	A	370	SER
1	A	389	PHE
1	A	392	VAL
1	A	394	ARG
1	A	412	VAL
1	A	427	ARG
1	A	429	LEU
1	A	433	SER
1	A	441	ARG
1	A	447	LEU
1	A	483	ASP
1	A	489	LEU
1	A	500	LEU
1	A	504	GLN
1	A	514	LEU
1	A	522	LYS
1	A	525	LYS
1	A	526	ILE
1	A	533	LYS
1	A	535	LEU
1	A	536	ARG
1	A	538	HIS
1	A	540	SER
1	A	544	ARG
1	A	570	LEU
1	A	585	ASN
1	A	609	ARG
1	A	615	LYS
1	A	628	THR
1	A	645	CYS

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Mol	Chain	Res	Type
1	A	650	ARG
1	A	661	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	54	HIS
1	A	202	HIS
1	A	215	GLN
1	A	245	HIS
1	A	349	GLN
1	A	444	HIS
1	A	448	GLN
1	A	455	GLN
1	A	505	GLN
1	A	506	ASN
1	A	538	HIS
1	A	585	ASN
1	A	660	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	559/670 (83%)	0.03	31 (5%) 25 16	43, 65, 98, 109	19 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	PRO	4.7
1	A	645	CYS	4.7
1	A	349	GLN	4.4
1	A	395	GLY	4.1
1	A	53	ALA	3.9
1	A	67	THR	3.8
1	A	311	CYS	3.4
1	A	99	PRO	3.3
1	A	174	SER	3.3
1	A	70	LEU	3.3
1	A	312	SER	3.2
1	A	224	LYS	3.2
1	A	128	LYS	3.1
1	A	54	HIS	3.0
1	A	321	LYS	3.0
1	A	388	ASP	2.9
1	A	173	ASP	2.8
1	A	66	SER	2.8
1	A	337	CYS	2.7
1	A	439	ASP	2.7
1	A	351	GLU	2.6
1	A	217	THR	2.4
1	A	156	ARG	2.4
1	A	157	ASP	2.3
1	A	370	SER	2.3
1	A	323	VAL	2.3
1	A	350	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	328	MET	2.2
1	A	98	GLY	2.2
1	A	2	ALA	2.0
1	A	336	ILE	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 carbohydrates 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.