



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:33 AM UTC

PDB ID : 9FMN / pdb_00009fmn
Title : Structure of Human PADI6
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Deposited on : 2024-06-06
Resolution : 2.44 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

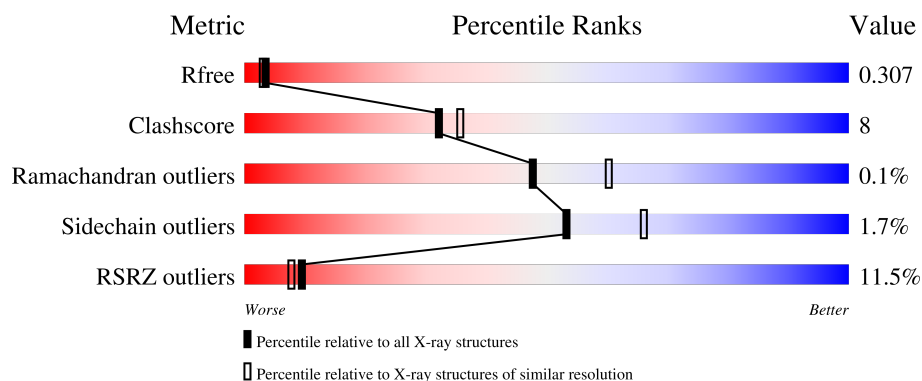
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	694	12% 80% 16% .
1	B	694	10% 79% 17% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20268 atoms, of which 10044 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.

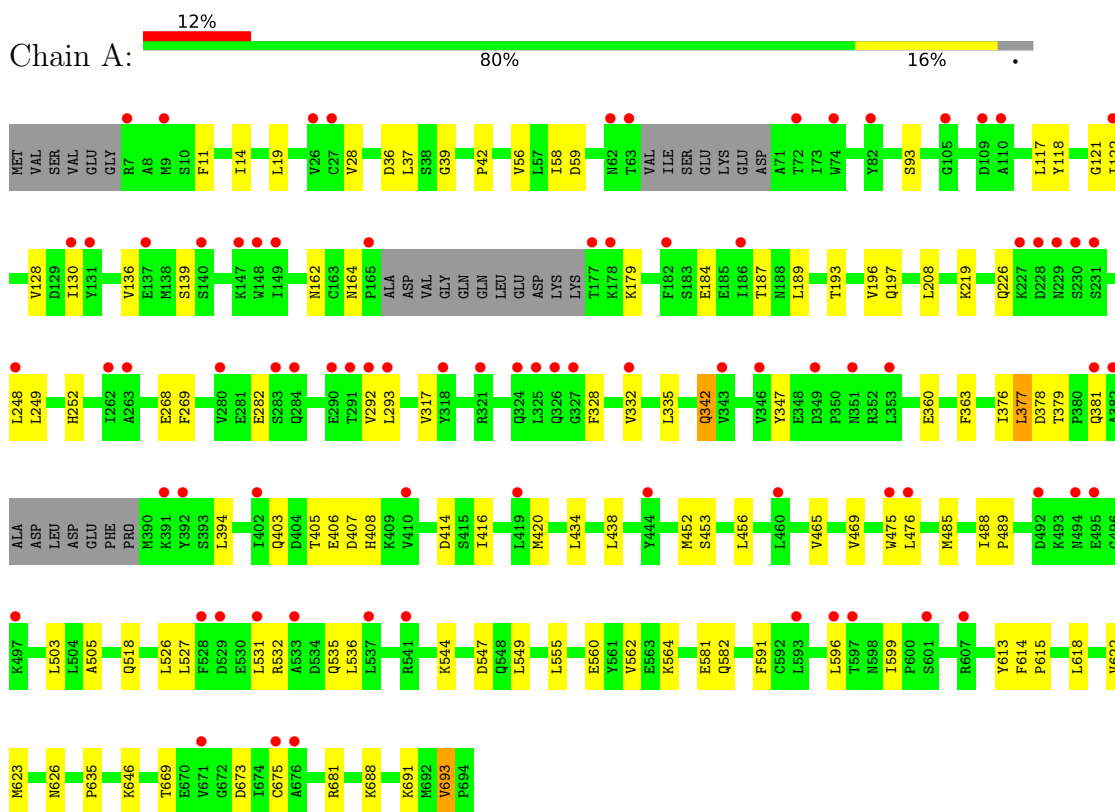
- Molecule 1 is a protein called Protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	663	Total	C	H	N	O	S	0	0	0
			10078	3261	4993	827	959	38			
1	B	666	Total	C	H	N	O	S	0	0	0
			10190	3293	5051	840	968	38			

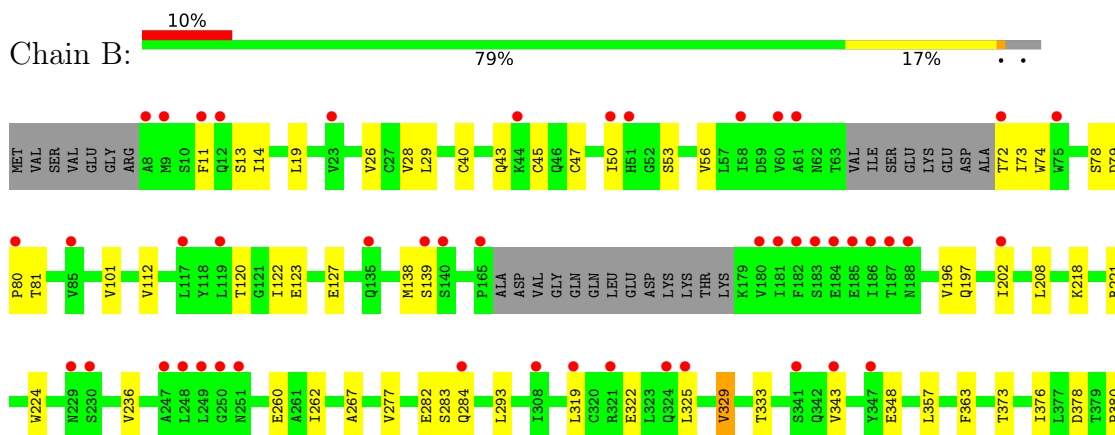
3 Residue-property plots [i](#)

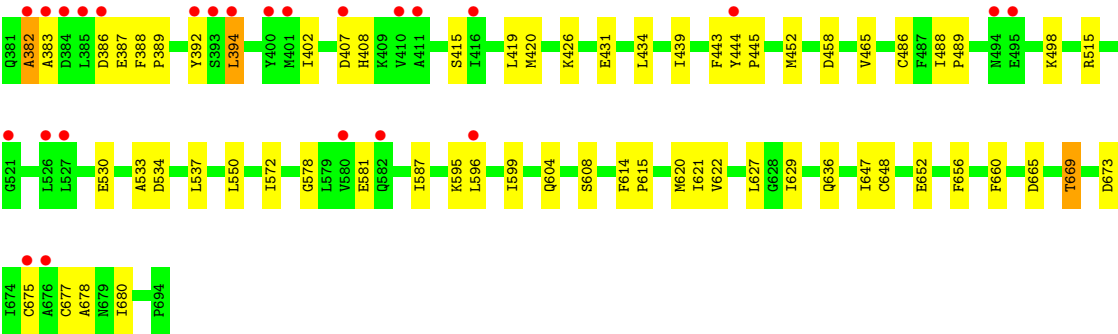
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Protein-arginine deiminase type-6



• Molecule 1: Protein-arginine deiminase type-6





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.04Å 123.33Å 126.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.06 – 2.44 54.06 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.06-2.44) 99.2 (54.06-2.44)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.258 , 0.307 0.259 , 0.307	Depositor DCC
R_{free} test set	3050 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20268	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/5199	0.33	0/7067
1	B	0.16	0/5258	0.33	0/7152
All	All	0.16	0/10457	0.33	0/14219

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	382	ALA	Peptide
1	B	386	ASP	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	5085	4993	4990	84	0
1	B	5139	5051	5050	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10224	10044	10040	163	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 8.

All (163) 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:475:TRP:CZ3	1:A:476:LEU:HG	2.07	0.89
1:B:587:ILE:HG23	1:B:647:ILE:HD11	1.58	0.86
1:A:532:ARG:O	1:A:536:LEU:HD12	1.85	0.77
1:A:582:GLN:N	1:A:582:GLN:OE1	2.18	0.76
1:A:268:GLU:N	1:A:268:GLU:OE1	2.19	0.76
1:B:196:VAL:HG21	1:B:208:LEU:HD11	1.71	0.73
1:A:282:GLU:N	1:A:282:GLU:OE1	2.23	0.71
1:A:420:MET:HE1	1:A:485:MET:HE2	1.71	0.71
1:A:196:VAL:HG21	1:A:208:LEU:HD11	1.72	0.71
1:A:363:PHE:CE1	1:A:376:ILE:HD11	2.27	0.69
1:A:452:MET:SD	1:A:456:LEU:HD23	2.32	0.69
1:A:36:ASP:OD1	1:A:39:GLY:N	2.28	0.66
1:B:669:THR:HG22	1:B:673:ASP:HB2	1.78	0.65
1:A:452:MET:CG	1:A:456:LEU:HD23	2.28	0.64
1:B:47:CYS:HG	1:B:74:TRP:CD1	2.16	0.64
1:A:179:LYS:HE3	1:A:226:GLN:OE1	1.99	0.62
1:A:184:GLU:OE2	1:A:184:GLU:N	2.31	0.61
1:A:19:LEU:HD21	1:A:42:PRO:HD3	1.81	0.61
1:B:284:GLN:N	1:B:284:GLN:OE1	2.32	0.61
1:A:184:GLU:O	1:A:187:THR:HG22	2.00	0.61
1:B:50:ILE:HG13	1:B:101:VAL:HG22	1.83	0.61
1:B:11:PHE:CE2	1:B:293:LEU:HD13	2.36	0.60
1:A:693:VAL:HG13	1:A:693:VAL:O	2.00	0.60
1:B:325:LEU:HA	1:B:329:VAL:HG22	1.84	0.59
1:A:292:VAL:HG21	1:B:444:TYR:CD1	2.37	0.59
1:A:596:LEU:HD22	1:A:599:ILE:HG12	1.84	0.59
1:A:438:LEU:HD23	1:A:469:VAL:HB	1.85	0.58
1:A:56:VAL:HG12	1:A:58:ILE:CD1	2.34	0.58
1:B:382:ALA:O	1:B:383:ALA:HB2	2.04	0.58
1:A:488:ILE:HD13	1:A:503:LEU:HD11	1.86	0.57
1:A:526:LEU:HD12	1:A:544:LYS:C	2.30	0.57
1:A:317:VAL:HG21	1:A:623:MET:HE1	1.86	0.56
1:A:56:VAL:HG12	1:A:58:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:GLN:NE2	1:A:547:ASP:OD1	2.38	0.56
1:A:693:VAL:O	1:A:693:VAL:CG1	2.52	0.56
1:A:475:TRP:CE3	1:A:476:LEU:HG	2.40	0.56
1:B:43:GLN:O	1:B:43:GLN:NE2	2.37	0.56
1:A:581:GLU:HG3	1:B:14:ILE:HD12	1.88	0.56
1:B:19:LEU:HD11	1:B:40:CYS:O	2.07	0.55
1:B:533:ALA:O	1:B:537:LEU:HD23	2.05	0.55
1:A:526:LEU:HD12	1:A:544:LYS:O	2.07	0.55
1:B:53:SER:O	1:B:56:VAL:HG12	2.09	0.53
1:A:377:LEU:HD11	1:A:403:GLN:CB	2.38	0.53
1:A:420:MET:CE	1:A:485:MET:HE2	2.36	0.53
1:B:363:PHE:CE2	1:B:376:ILE:HD11	2.44	0.53
1:B:434:LEU:HD12	1:B:465:VAL:HB	1.90	0.53
1:B:419:LEU:HD23	1:B:419:LEU:C	2.34	0.52
1:A:128:VAL:HG23	1:A:130:ILE:HG22	1.91	0.52
1:A:14:ILE:HD12	1:B:581:GLU:HG3	1.92	0.52
1:B:348:GLU:N	1:B:348:GLU:OE1	2.40	0.51
1:B:79:ASP:HB3	1:B:80:PRO:HD3	1.93	0.50
1:A:414:ASP:OD1	1:A:453:SER:OG	2.19	0.50
1:B:621:ILE:CG2	1:B:680:ILE:HD11	2.42	0.50
1:B:407:ASP:OD2	1:B:408:HIS:N	2.45	0.49
1:A:452:MET:HE2	1:A:456:LEU:CD2	2.42	0.49
1:B:407:ASP:OD2	1:B:407:ASP:C	2.55	0.49
1:B:599:ILE:HD11	1:B:604:GLN:HA	1.94	0.49
1:A:407:ASP:C	1:A:408:HIS:ND1	2.70	0.49
1:A:164:ASN:C	1:A:164:ASN:OD1	2.55	0.49
1:B:322:GLU:HG3	1:B:675:CYS:O	2.12	0.49
1:A:11:PHE:CE2	1:A:293:LEU:HD13	2.48	0.49
1:B:45:CYS:SG	1:B:112:VAL:HG21	2.52	0.49
1:A:363:PHE:CE1	1:A:681:ARG:HB2	2.47	0.49
1:B:267:ALA:HB2	1:B:458:ASP:HB3	1.94	0.49
1:A:249:LEU:N	1:A:249:LEU:HD23	2.28	0.48
1:A:219:LYS:HD2	1:A:269:PHE:CG	2.49	0.48
1:B:382:ALA:O	1:B:383:ALA:CB	2.61	0.48
1:B:420:MET:HE1	1:B:486:CYS:HA	1.96	0.48
1:A:555:LEU:HD21	1:A:613:TYR:CE1	2.48	0.48
1:A:505:ALA:HB2	1:A:618:LEU:HD13	1.96	0.48
1:B:587:ILE:HD12	1:B:647:ILE:HD13	1.96	0.48
1:A:184:GLU:H	1:A:184:GLU:CD	2.21	0.48
1:A:292:VAL:HG21	1:B:444:TYR:CE1	2.49	0.48
1:B:127:GLU:OE2	1:B:138:MET:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:OE1	1:B:283:SER:N	2.48	0.47
1:B:587:ILE:HD12	1:B:647:ILE:CD1	2.43	0.47
1:B:629:ILE:O	1:B:660:PHE:HA	2.15	0.47
1:A:405:THR:HB	1:A:414:ASP:OD2	2.14	0.47
1:B:218:LYS:O	1:B:262:ILE:HD11	2.15	0.47
1:B:363:PHE:CD2	1:B:376:ILE:HD11	2.50	0.47
1:B:392:TYR:HD2	1:B:394:LEU:HG	1.80	0.47
1:B:376:ILE:HG13	1:B:394:LEU:HD21	1.96	0.47
1:A:614:PHE:O	1:A:615:PRO:C	2.59	0.46
1:A:317:VAL:N	1:A:342:GLN:O	2.48	0.46
1:A:249:LEU:HD23	1:A:249:LEU:H	1.81	0.46
1:A:527:LEU:HD12	1:A:635:PRO:HD3	1.96	0.46
1:B:363:PHE:CZ	1:B:376:ILE:HD11	2.50	0.46
1:B:388:PHE:N	1:B:389:PRO:CD	2.79	0.46
1:A:197:GLN:HG2	1:A:252:HIS:ND1	2.30	0.46
1:A:414:ASP:OD1	1:A:453:SER:CB	2.64	0.46
1:B:443:PHE:CE1	1:B:572:ILE:HD11	2.50	0.46
1:A:162:ASN:OD1	1:A:162:ASN:C	2.58	0.46
1:B:587:ILE:CG2	1:B:647:ILE:HD11	2.38	0.46
1:A:347:TYR:N	1:A:347:TYR:CD1	2.84	0.46
1:B:439:ILE:HB	1:B:452:MET:HE3	1.97	0.46
1:B:11:PHE:CD2	1:B:293:LEU:HB3	2.51	0.45
1:B:595:LYS:HE2	1:B:608:SER:OG	2.15	0.45
1:B:614:PHE:O	1:B:615:PRO:C	2.58	0.45
1:B:221:ARG:NH1	1:B:260:GLU:OE2	2.50	0.45
1:B:319:LEU:HD23	1:B:678:ALA:HB2	1.99	0.45
1:B:419:LEU:HD23	1:B:420:MET:N	2.32	0.45
1:A:360:GLU:OE2	1:A:381:GLN:NE2	2.50	0.45
1:A:669:THR:HG22	1:A:673:ASP:HB2	1.99	0.45
1:B:378:ASP:CG	1:B:380:PRO:HD3	2.42	0.45
1:B:29:LEU:HD12	1:B:123:GLU:HB2	1.99	0.45
1:A:377:LEU:HD11	1:A:403:GLN:HB2	1.99	0.44
1:B:444:TYR:HB2	1:B:445:PRO:HD2	2.00	0.44
1:B:498:LYS:NZ	1:B:578:GLY:O	2.50	0.44
1:A:688:LYS:HB2	1:A:691:LYS:HG3	1.99	0.44
1:B:120:THR:HG21	1:B:202:ILE:CD1	2.47	0.44
1:A:527:LEU:HD22	1:A:549:LEU:HD11	2.00	0.44
1:B:357:LEU:HB3	1:B:677:CYS:SG	2.57	0.44
1:A:292:VAL:CG2	1:B:444:TYR:CE1	3.01	0.44
1:A:438:LEU:CD2	1:A:469:VAL:HB	2.48	0.44
1:B:11:PHE:HE2	1:B:293:LEU:HD13	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:HD22	1:A:535:GLN:OE1	2.18	0.43
1:B:620:MET:HE3	1:B:627:LEU:HB3	1.99	0.43
1:A:328:PHE:CE1	1:A:332:VAL:HG21	2.53	0.43
1:A:381:GLN:CD	1:A:381:GLN:C	2.86	0.43
1:A:317:VAL:CG2	1:A:623:MET:HE1	2.48	0.43
1:B:73:ILE:HD12	1:B:73:ILE:N	2.34	0.43
1:B:620:MET:HE1	1:B:627:LEU:HD13	1.99	0.43
1:B:587:ILE:HG23	1:B:647:ILE:CD1	2.40	0.43
1:A:562:VAL:HG11	1:A:591:PHE:CD1	2.54	0.43
1:A:347:TYR:N	1:A:347:TYR:HD1	2.17	0.43
1:A:376:ILE:CG1	1:A:394:LEU:HD21	2.48	0.43
1:B:11:PHE:CE1	1:B:26:VAL:HG12	2.54	0.43
1:A:377:LEU:HD11	1:A:403:GLN:HB3	2.00	0.42
1:B:26:VAL:HG22	1:B:120:THR:HB	2.01	0.42
1:A:28:VAL:HA	1:A:122:ILE:O	2.19	0.42
1:B:78:SER:O	1:B:81:THR:OG1	2.38	0.42
1:A:196:VAL:HG11	1:A:248:LEU:HD11	2.02	0.42
1:B:489:PRO:HD3	1:B:622:VAL:HG11	2.01	0.42
1:A:121:GLY:C	1:A:122:ILE:HD13	2.45	0.42
1:B:426:LYS:HG3	1:B:431:GLU:HG2	2.01	0.42
1:B:376:ILE:HG13	1:B:394:LEU:CD2	2.49	0.42
1:A:434:LEU:HD12	1:A:465:VAL:HB	2.02	0.42
1:A:560:GLU:O	1:A:564:LYS:HG3	2.20	0.42
1:B:357:LEU:CD1	1:B:392:TYR:OH	2.68	0.42
1:B:530:GLU:OE2	1:B:636:GLN:NE2	2.48	0.42
1:A:489:PRO:HD3	1:A:622:VAL:HG11	2.03	0.41
1:B:333:THR:HG23	1:B:343:VAL:HG21	2.02	0.41
1:A:376:ILE:HG12	1:A:394:LEU:CD2	2.50	0.41
1:A:376:ILE:HG13	1:A:394:LEU:HD21	2.02	0.41
1:B:28:VAL:HA	1:B:122:ILE:O	2.20	0.41
1:A:37:LEU:HD23	1:A:37:LEU:N	2.35	0.41
1:B:515:ARG:HG2	1:B:550:LEU:CD2	2.51	0.41
1:A:136:VAL:HG11	1:A:193:THR:OG1	2.20	0.41
1:A:378:ASP:OD1	1:A:379:THR:N	2.54	0.41
1:B:488:ILE:HD12	1:B:656:PHE:CZ	2.56	0.41
1:B:123:GLU:HB3	1:B:197:GLN:HB2	2.02	0.41
1:A:197:GLN:CG	1:A:252:HIS:ND1	2.84	0.41
1:B:120:THR:HG21	1:B:202:ILE:HD11	2.02	0.41
1:B:378:ASP:HB3	1:B:402:ILE:HD13	2.03	0.41
1:B:596:LEU:HD23	1:B:599:ILE:HD13	2.03	0.41
1:A:335:LEU:HD11	1:A:626:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:O	1:B:277:VAL:HG13	2.21	0.40
1:B:534:ASP:OD2	1:B:534:ASP:N	2.53	0.40
1:B:648:CYS:O	1:B:652:GLU:HG3	2.21	0.40
1:A:416:ILE:HD12	1:A:416:ILE:HA	1.96	0.40
1:B:224:TRP:HB2	1:B:236:VAL:HG11	2.04	0.40
1:A:117:LEU:HD23	1:A:118:TYR:N	2.36	0.40
1:B:378:ASP:C	1:B:380:PRO:HD3	2.46	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	655/694 (94%)	638 (97%)	17 (3%)	0	100	100
1	B	660/694 (95%)	633 (96%)	26 (4%)	1 (0%)	43	53
All	All	1315/1388 (95%)	1271 (97%)	43 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	GLU

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	555/616 (90%)	545 (98%)	10 (2%)	51	64
1	B	565/616 (92%)	556 (98%)	9 (2%)	55	68
All	All	1120/1232 (91%)	1101 (98%)	19 (2%)	53	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	93	SER
1	A	139	SER
1	A	189	LEU
1	A	342	GLN
1	A	377	LEU
1	A	406	GLU
1	A	646	LYS
1	A	675	CYS
1	A	693	VAL
1	B	13	SER
1	B	72	THR
1	B	139	SER
1	B	329	VAL
1	B	373	THR
1	B	394	LEU
1	B	415	SER
1	B	665	ASP
1	B	669	THR

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

Mol	Chain	Res	Type
1	A	51	HIS
1	A	381	GLN
1	A	418	ASN
1	A	626	ASN
1	B	241	GLN
1	B	480	HIS
1	B	567	HIS
1	B	598	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 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	663/694 (95%)	0.81	81 (12%) 8 6	57, 84, 139, 192	0
1	B	666/694 (95%)	0.77	72 (10%) 11 8	54, 78, 135, 200	0
All	All	1329/1388 (95%)	0.79	153 (11%) 9 8	54, 81, 137, 200	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	SER	5.3
1	A	671	VAL	5.2
1	A	284	GLN	4.8
1	A	410	VAL	4.8
1	A	492	ASP	4.6
1	B	382	ALA	4.5
1	B	250	GLY	4.5
1	B	187	THR	4.5
1	B	182	PHE	4.2
1	A	228	ASP	4.1
1	B	392	TYR	4.1
1	A	177	THR	4.1
1	A	148	TRP	4.0
1	A	122	ILE	3.9
1	A	230	SER	3.7
1	A	325	LEU	3.7
1	B	249	LEU	3.7
1	A	324	GLN	3.6
1	A	392	TYR	3.5
1	A	326	GLN	3.5
1	B	139	SER	3.5
1	B	676	ALA	3.4
1	B	494	ASN	3.4
1	B	12	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	119	LEU	3.4
1	B	526	LEU	3.4
1	B	325	LEU	3.3
1	B	385	LEU	3.3
1	B	140	SER	3.2
1	A	353	LEU	3.2
1	A	26	VAL	3.2
1	B	186	ILE	3.2
1	B	80	PRO	3.1
1	A	27	CYS	3.1
1	A	82	TYR	3.1
1	B	72	THR	3.1
1	A	351	ASN	3.1
1	A	227	LYS	3.0
1	A	62	ASN	3.0
1	A	263	ALA	3.0
1	A	165	PRO	3.0
1	A	528	PHE	3.0
1	B	11	PHE	3.0
1	B	384	ASP	3.0
1	B	8	ALA	2.9
1	B	50	ILE	2.9
1	B	180	VAL	2.9
1	B	165	PRO	2.9
1	A	280	VAL	2.9
1	B	248	LEU	2.9
1	A	74	TRP	2.9
1	A	130	ILE	2.8
1	A	541	ARG	2.8
1	A	291	THR	2.8
1	B	188	ASN	2.8
1	A	7	ARG	2.8
1	A	293	LEU	2.7
1	B	324	GLN	2.7
1	B	229	ASN	2.7
1	A	321	ARG	2.7
1	A	292	VAL	2.7
1	B	393	SER	2.7
1	A	137	GLU	2.7
1	A	475	TRP	2.7
1	B	675	CYS	2.6
1	A	72	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	476	LEU	2.6
1	B	495	GLU	2.6
1	A	63	THR	2.6
1	A	382	ALA	2.6
1	A	597	THR	2.6
1	A	147	LYS	2.6
1	B	321	ARG	2.6
1	A	444	TYR	2.6
1	B	308	ILE	2.5
1	B	251	ASN	2.5
1	B	341	SER	2.5
1	A	105	GLY	2.5
1	B	75	TRP	2.5
1	A	182	PHE	2.5
1	B	411	ALA	2.5
1	B	23	VAL	2.5
1	A	537	LEU	2.5
1	B	319	LEU	2.5
1	B	343	VAL	2.5
1	B	410	VAL	2.5
1	A	529	ASP	2.4
1	A	419	LEU	2.4
1	B	394	LEU	2.4
1	B	582	GLN	2.4
1	B	185	GLU	2.4
1	A	533	ALA	2.4
1	A	290	GLU	2.4
1	A	495	GLU	2.4
1	A	497	LYS	2.4
1	B	9	MET	2.4
1	B	60	VAL	2.4
1	A	381	GLN	2.4
1	A	593	LEU	2.4
1	A	596	LEU	2.4
1	B	135	GLN	2.4
1	B	383	ALA	2.4
1	B	184	GLU	2.4
1	A	262	ILE	2.3
1	B	527	LEU	2.3
1	B	347	TYR	2.3
1	A	332	VAL	2.3
1	A	346	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	110	ALA	2.3
1	B	444	TYR	2.3
1	A	186	ILE	2.3
1	A	531	LEU	2.3
1	A	676	ALA	2.2
1	A	402	ILE	2.2
1	B	596	LEU	2.2
1	A	494	ASN	2.2
1	A	283	SER	2.2
1	B	51	HIS	2.2
1	A	675	CYS	2.2
1	B	85	VAL	2.2
1	A	9	MET	2.2
1	B	400	TYR	2.2
1	B	416	ILE	2.2
1	B	386	ASP	2.2
1	A	343	VAL	2.1
1	A	229	ASN	2.1
1	B	247	ALA	2.1
1	B	580	VAL	2.1
1	B	401	MET	2.1
1	A	248	LEU	2.1
1	A	131	TYR	2.1
1	A	178	LYS	2.1
1	B	284	GLN	2.1
1	B	521	GLY	2.1
1	A	607	ARG	2.1
1	B	44	LYS	2.1
1	A	601	SER	2.1
1	B	61	ALA	2.1
1	B	117	LEU	2.1
1	B	58	ILE	2.1
1	B	181	ILE	2.1
1	B	202	ILE	2.1
1	B	230	SER	2.1
1	A	460	LEU	2.0
1	A	327	GLY	2.0
1	A	149	ILE	2.0
1	A	109	ASP	2.0
1	A	391	LYS	2.0
1	A	349	ASP	2.0
1	B	407	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	2.0
1	A	231	SER	2.0
1	A	318	TYR	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.