Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2024 – 01:34 am BST

PDB ID	:	9FMN
Title	:	Structure of Human PADI6
Authors	:	Mouilleron, S.; Walport, L.; Williams, J.; Marsh, A.J.; Hernandez Trapero, R.
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:

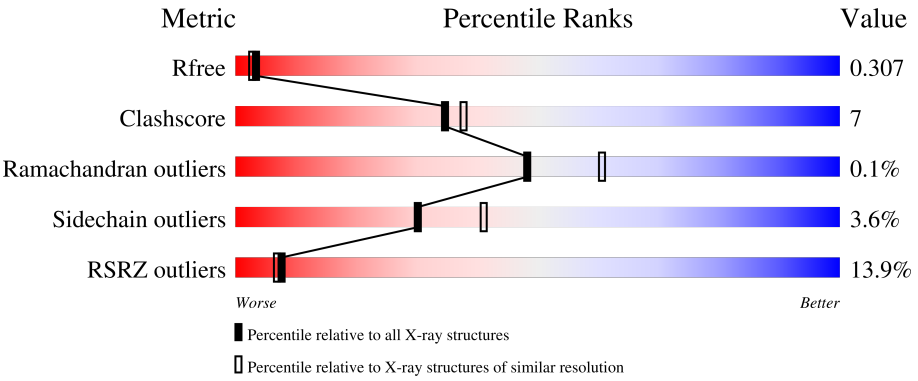
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (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 <=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	14% 78% 17% .
1	B	694	12% 78% 17% . .

2 Entry composition (i)

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.

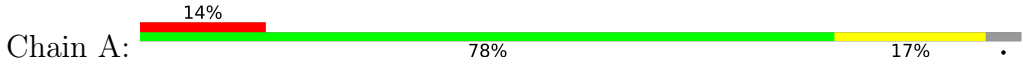
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	663	Total	C	H	N	O	S	0	0	0
			10078	3261	4993	827	959	38			
1	B	666	Total	C	H	N	O	S	0	0	0
			10190	3293	5051	840	968	38			

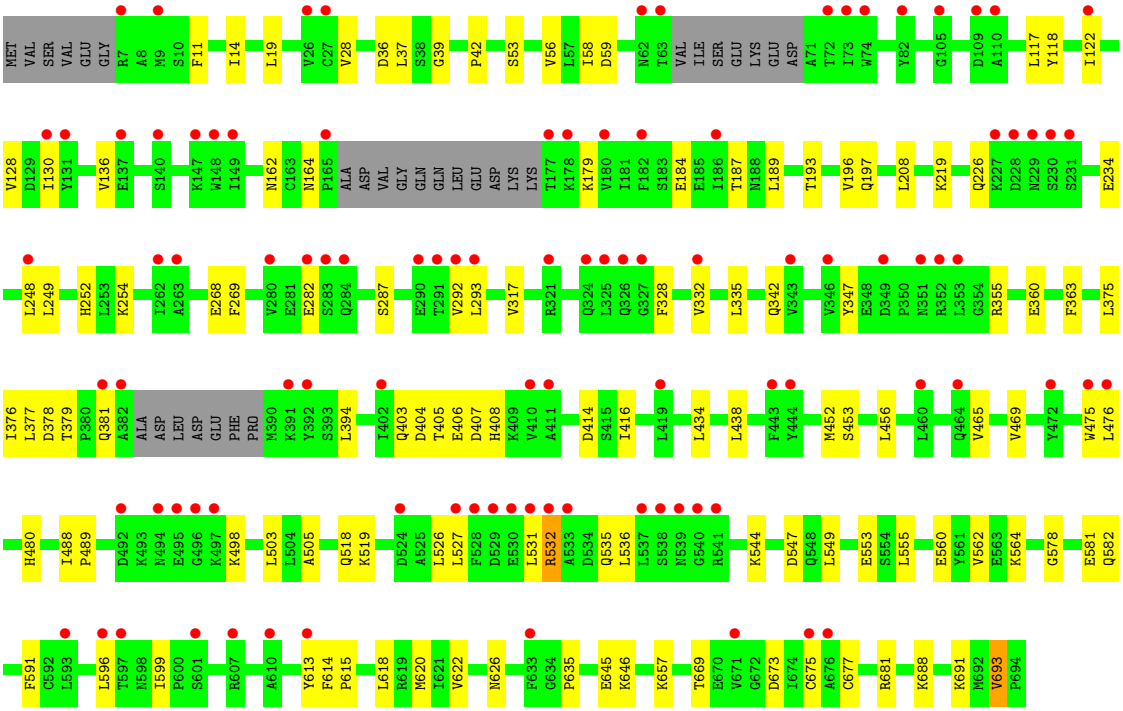
3 Residue-property plots (i)

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

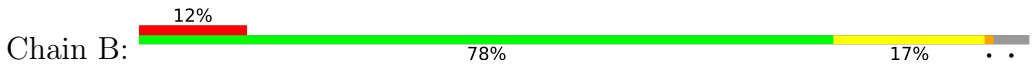
Chain A:

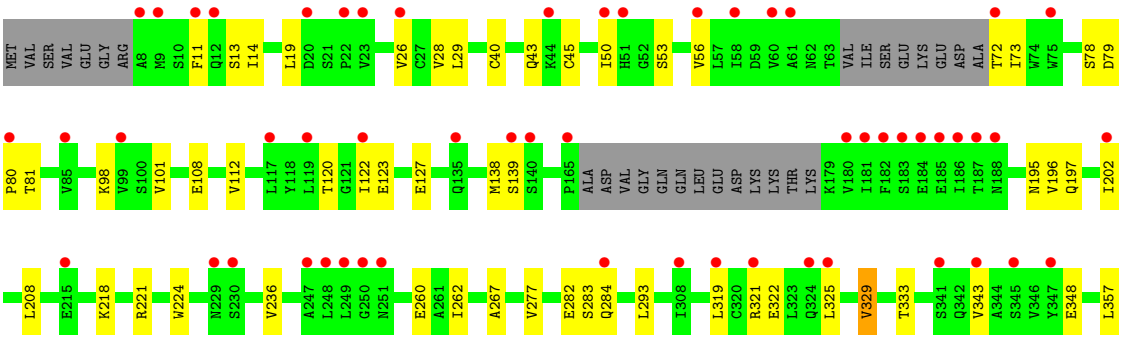


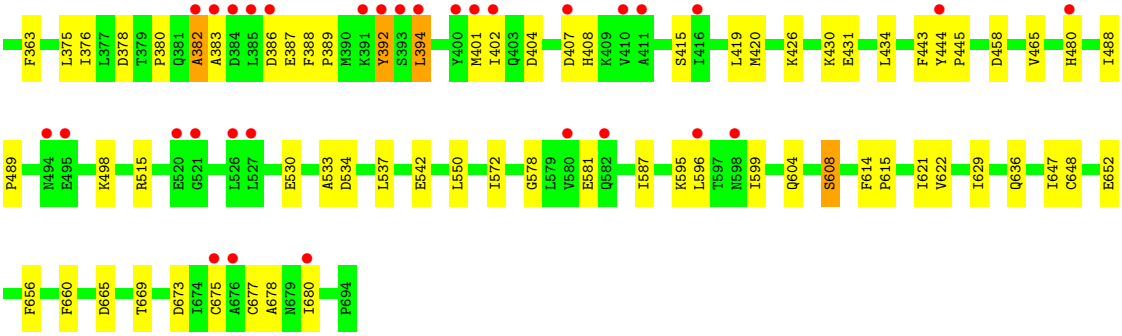


• Molecule 1: Protein-arginine deiminase type-6

Chain B:






F363
L375
I376
L377
D378
T379
P380
Q381
A382
A383
D384
L385
D386
E387
F388
P389
M390
K391
Y392
S393
L394
Y400
M401
I402
Q403
D404
D407
H408
K409
V410
A411
S415
I416
L419
M420
K426
K430
E431
L434
F443
Y444
P445
D458
V465
H480
I488
P489
N494
E495
K498
R515
E520
G521
L526
L527
E530
A533
D534
L537
E542
L550
I572
G578
L579
V580
E581
Q582
I587
K595
L596
T597
N598
I599
Q604
S608
F614
P615
I621
V622
I629
Q636
I647
C648
E652
F656
F660
D665
T669
D673
I674
C675
A676
C677
A678
N679
I680
P694

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	3051 reflections (4.98%)	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)	0.32 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/5199	0.49	0/7067
1	B	0.28	0/5258	0.49	0/7152
All	All	0.28	0/10457	0.49	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

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	77	0
1	B	5139	5051	5050	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10224	10044	10040	150	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 7.

All (150) 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: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: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:56:VAL:HG12	1:A:58:ILE:HD12	1.87	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:526:LEU:HD12	1:A:544:LYS:C	2.30	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:B:599:ILE:HD11	1:B:604:GLN:HA	1.94	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: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:292:VAL:HG21	1:B:444:TYR:CE1	2.49	0.48
1:B:419:LEU:HD23	1:B:419:LEU:C	2.34	0.48
1:B:127:GLU:OE2	1:B:138:MET:HA	2.14	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:164:ASN:C	1:A:164:ASN:OD1	2.55	0.45
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:A:407:ASP:C	1:A:408:HIS:ND1	2.70	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:407:ASP:OD2	1:B:407:ASP:C	2.55	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
1:A:531:LEU:HD22	1:A:535:GLN:OE1	2.18	0.43
1:A:328:PHE:CE1	1:A:332:VAL:HG21	2.53	0.43
1:B:73:ILE:HD12	1:B:73:ILE:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:426:LYS:HG3	1:B:431:GLU:HG2	2.01	0.42
1:A:614:PHE:O	1:A:615:PRO:C	2.59	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:A:498:LYS:NZ	1:A:578:GLY:O	2.52	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:162:ASN:OD1	1:A:162:ASN:C	2.58	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:614:PHE:O	1:B:615:PRO:C	2.58	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
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:B:378:ASP:CG	1:B:380:PRO:HD3	2.42	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

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%)	44	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%)	534 (96%)	21 (4%)	28	39
1	B	565/616 (92%)	546 (97%)	19 (3%)	32	43
All	All	1120/1232 (91%)	1080 (96%)	40 (4%)	30	41

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	59	ASP
1	A	189	LEU
1	A	234	GLU
1	A	254	LYS

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Mol	Chain	Res	Type
1	A	287	SER
1	A	355	ARG
1	A	375	LEU
1	A	404	ASP
1	A	406	GLU
1	A	480	HIS
1	A	519	LYS
1	A	532	ARG
1	A	553	GLU
1	A	620	MET
1	A	645	GLU
1	A	646	LYS
1	A	657	LYS
1	A	675	CYS
1	A	677	CYS
1	A	693	VAL
1	B	13	SER
1	B	72	THR
1	B	98	LYS
1	B	108	GLU
1	B	139	SER
1	B	195	ASN
1	B	321	ARG
1	B	329	VAL
1	B	375	LEU
1	B	392	TYR
1	B	394	LEU
1	B	401	MET
1	B	404	ASP
1	B	415	SER
1	B	430	LYS
1	B	480	HIS
1	B	542	GLU
1	B	608	SER
1	B	665	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN

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, 95^{th} 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%)	0.98	99 (14%)	7 6	57, 84, 139, 192	0
1	B	666/694 (95%)	0.88	86 (12%)	9 8	54, 78, 135, 200	0
All	All	1329/1388 (95%)	0.93	185 (13%)	7 7	54, 81, 137, 200	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	VAL	5.7
1	A	284	GLN	5.6
1	B	183	SER	5.4
1	B	250	GLY	5.1
1	A	492	ASP	5.0
1	B	382	ALA	4.9
1	A	410	VAL	4.8
1	B	187	THR	4.4
1	B	182	PHE	4.3
1	A	228	ASP	4.3
1	A	148	TRP	4.3
1	B	249	LEU	4.3
1	A	177	THR	4.2
1	B	392	TYR	4.2
1	A	325	LEU	4.2
1	A	230	SER	4.0
1	A	122	ILE	4.0
1	A	324	GLN	4.0
1	B	119	LEU	3.8
1	A	326	GLN	3.8
1	A	392	TYR	3.8
1	A	227	LYS	3.7
1	A	351	ASN	3.7
1	B	676	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	27	CYS	3.6
1	B	385	LEU	3.6
1	A	353	LEU	3.6
1	B	139	SER	3.6
1	B	325	LEU	3.5
1	B	494	ASN	3.5
1	A	528	PHE	3.5
1	B	72	THR	3.5
1	B	526	LEU	3.5
1	B	80	PRO	3.5
1	A	26	VAL	3.5
1	B	12	GLN	3.4
1	B	140	SER	3.4
1	B	384	ASP	3.4
1	A	82	TYR	3.3
1	B	186	ILE	3.3
1	A	7	ARG	3.3
1	A	476	LEU	3.3
1	B	180	VAL	3.3
1	B	248	LEU	3.2
1	A	541	ARG	3.2
1	A	165	PRO	3.2
1	A	280	VAL	3.2
1	A	444	TYR	3.1
1	A	475	TRP	3.1
1	B	11	PHE	3.1
1	A	263	ALA	3.1
1	B	165	PRO	3.1
1	A	291	THR	3.1
1	B	324	GLN	3.1
1	B	50	ILE	3.0
1	A	292	VAL	3.0
1	B	8	ALA	3.0
1	A	147	LYS	3.0
1	A	607	ARG	3.0
1	B	321	ARG	3.0
1	B	251	ASN	3.0
1	B	675	CYS	2.9
1	A	62	ASN	2.9
1	A	293	LEU	2.9
1	B	188	ASN	2.9
1	A	531	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	130	ILE	2.9
1	A	137	GLU	2.9
1	B	185	GLU	2.8
1	B	495	GLU	2.8
1	A	382	ALA	2.8
1	A	321	ARG	2.8
1	B	229	ASN	2.8
1	A	283	SER	2.8
1	B	527	LEU	2.8
1	A	63	THR	2.8
1	A	419	LEU	2.7
1	A	72	THR	2.7
1	B	75	TRP	2.7
1	A	290	GLU	2.7
1	B	521	GLY	2.7
1	B	394	LEU	2.7
1	B	9	MET	2.7
1	A	332	VAL	2.7
1	A	596	LEU	2.7
1	B	411	ALA	2.7
1	A	497	LYS	2.7
1	A	74	TRP	2.7
1	B	341	SER	2.7
1	A	597	THR	2.7
1	B	308	ILE	2.7
1	B	184	GLU	2.7
1	A	346	VAL	2.6
1	A	537	LEU	2.6
1	A	495	GLU	2.6
1	A	529	ASP	2.6
1	B	319	LEU	2.6
1	B	60	VAL	2.6
1	A	182	PHE	2.6
1	B	393	SER	2.6
1	A	533	ALA	2.6
1	A	381	GLN	2.6
1	B	582	GLN	2.6
1	A	460	LEU	2.5
1	B	596	LEU	2.5
1	B	23	VAL	2.5
1	B	343	VAL	2.5
1	B	135	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	410	VAL	2.5
1	A	110	ALA	2.5
1	A	186	ILE	2.5
1	A	105	GLY	2.5
1	A	9	MET	2.5
1	A	593	LEU	2.5
1	B	58	ILE	2.5
1	A	229	ASN	2.5
1	A	675	CYS	2.5
1	A	402	ILE	2.5
1	B	347	TYR	2.4
1	A	676	ALA	2.4
1	B	386	ASP	2.4
1	A	464	GLN	2.4
1	B	284	GLN	2.4
1	B	416	ILE	2.4
1	B	20	ASP	2.4
1	B	117	LEU	2.4
1	B	400	TYR	2.4
1	B	247	ALA	2.4
1	B	383	ALA	2.4
1	A	540	GLY	2.4
1	B	444	TYR	2.3
1	B	401	MET	2.3
1	A	601	SER	2.3
1	B	51	HIS	2.3
1	A	472	TYR	2.3
1	A	262	ILE	2.3
1	B	181	ILE	2.3
1	A	539	ASN	2.3
1	A	613	TYR	2.3
1	B	26	VAL	2.3
1	A	443	PHE	2.3
1	A	109	ASP	2.3
1	B	520	GLU	2.3
1	A	131	TYR	2.3
1	A	343	VAL	2.3
1	B	230	SER	2.2
1	A	496	GLY	2.2
1	A	527	LEU	2.2
1	A	349	ASP	2.2
1	A	73	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	149	ILE	2.2
1	A	248	LEU	2.2
1	A	494	ASN	2.2
1	A	530	GLU	2.2
1	B	85	VAL	2.2
1	B	122	ILE	2.2
1	B	402	ILE	2.2
1	A	610	ALA	2.2
1	B	44	LYS	2.2
1	A	178	LYS	2.2
1	B	99	VAL	2.2
1	B	391	LYS	2.2
1	A	411	ALA	2.2
1	A	140	SER	2.1
1	A	391	LYS	2.1
1	B	580	VAL	2.1
1	A	327	GLY	2.1
1	B	345	SER	2.1
1	B	407	ASP	2.1
1	A	180	VAL	2.1
1	A	633	PHE	2.1
1	A	231	SER	2.1
1	A	282	GLU	2.1
1	A	538	SER	2.1
1	B	215	GLU	2.1
1	A	524	ASP	2.1
1	B	202	ILE	2.1
1	B	598	ASN	2.1
1	B	56	VAL	2.0
1	A	352	ARG	2.0
1	A	532	ARG	2.0
1	B	61	ALA	2.0
1	B	480	HIS	2.0
1	B	22	PRO	2.0
1	B	680	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 monosaccharides 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.