Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2025 – 04:05 pm BST

PDB ID	:	9FN6 / pdb_00009fn6
Title	:	Full-length crystal structure of human Fascin 1
Authors	:	Quereda-Moraleda, I.; Grieco, A.; Martin-Garcia, J.M.
Deposited on	:	2024-06-09
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

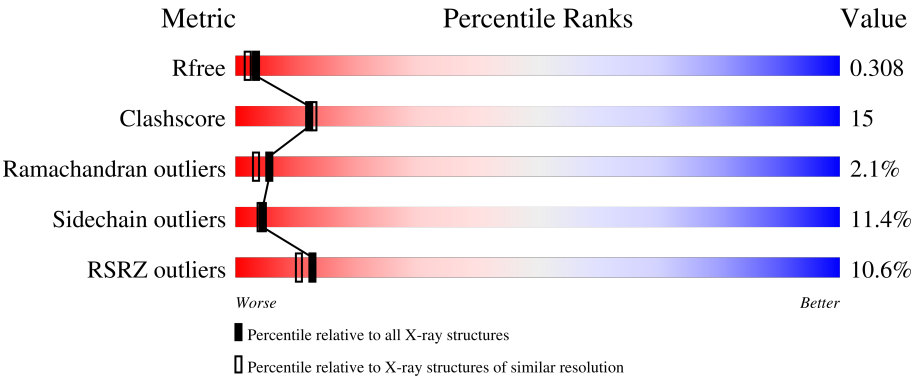
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	493	3% 69% 25%
1	B	493	18% 62% 31% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8077 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 Fascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	9	0
			3881	2423	698	745	15			
1	B	486	Total	C	N	O	S	0	11	0
			3888	2425	695	753	15			

- Molecule 2 is water.

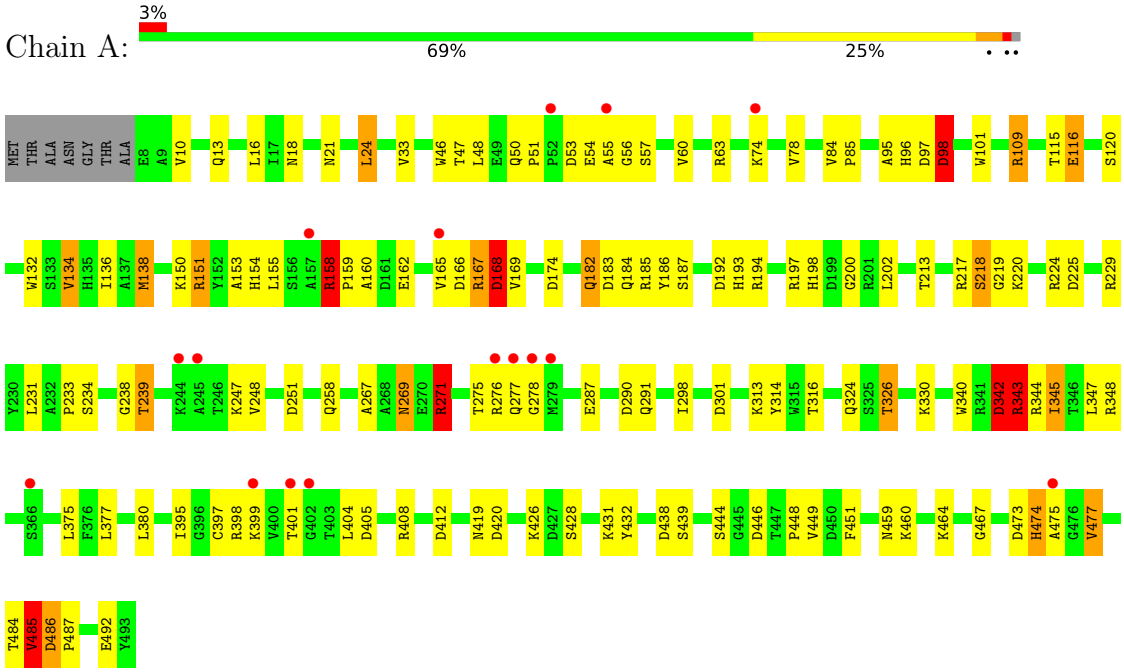
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	131	Total	O	0	0
			131	131		

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.

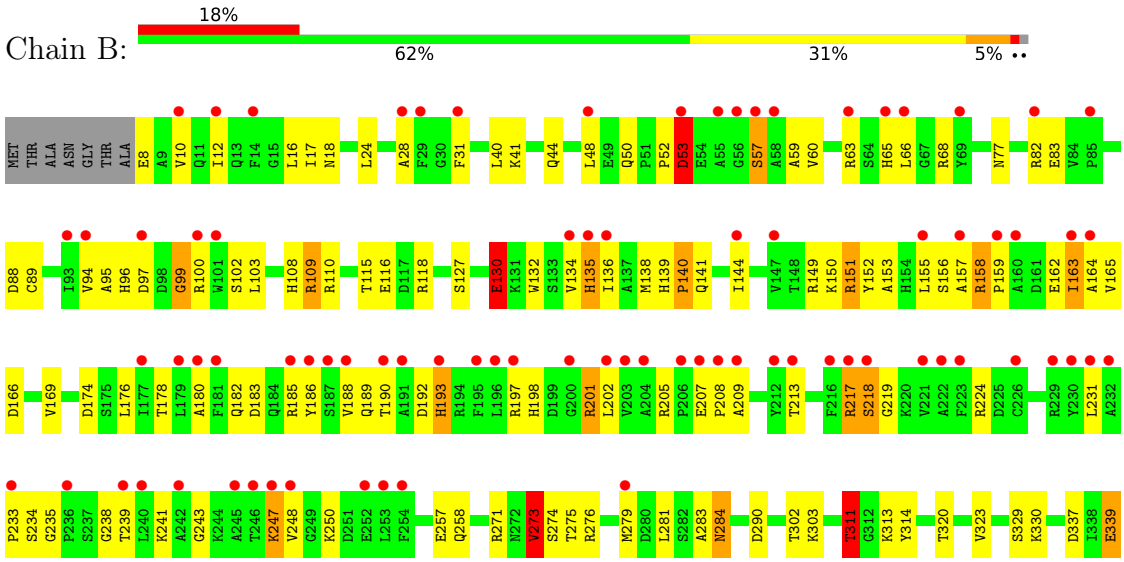
- Molecule 1: Fascin

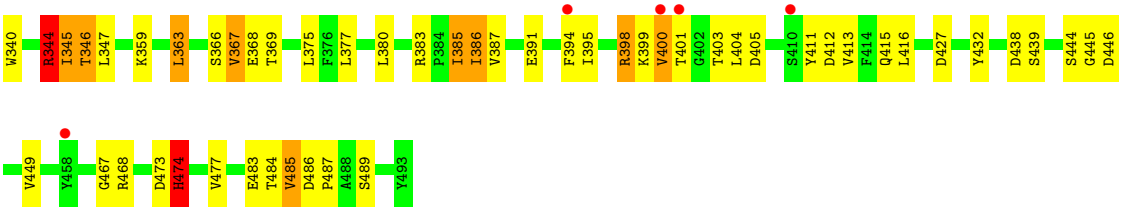
Chain A:



- Molecule 1: Fascin

Chain B:




W340
R344
I345
T346
L347
K359
L363
S366
V367
E368
T369
L375
F376
L377
L380
R383
P384
I385
I386
V387
E391
F394
I395
R398
K399
V400
T401
G402
T403
L404
D405
S410
Y411
D412
V413
F414
Q415
L416
D427
Y432
D438
S439
S444
G445
D446
V449
Y458
G467
R468
D473
H474
V477
E483
T484
V485
D486
P487
A488
S489
Y493

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.57Å 70.80Å 122.21Å 90.00° 92.78° 90.00°	Depositor
Resolution (Å)	43.42 – 2.20 43.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.42-2.20) 99.2 (43.42-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.234 , 0.304 0.237 , 0.308	Depositor DCC
R_{free} test set	2421 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8077	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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	0.61	0/3962	1.13	13/5350 (0.2%)
1	B	0.61	0/3970	1.16	14/5368 (0.3%)
All	All	0.61	0/7932	1.14	27/10718 (0.3%)

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	4
1	B	0	5
All	All	0	9

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	THR	CA-CB-OG1	-9.91	94.73	109.60
1	A	412	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	275	THR	CA-CB-OG1	-6.86	99.31	109.60
1	B	140	PRO	N-CA-C	6.55	121.49	114.68
1	B	337	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	342	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	339	GLU	CB-CG-CD	6.43	123.54	112.60
1	B	273	VAL	N-CA-CB	6.33	118.93	110.26
1	B	130	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	485	VAL	N-CA-CB	6.22	117.31	110.53
1	A	301	ASP	CB-CA-C	6.18	121.06	110.86
1	A	182	GLN	CB-CA-C	6.13	122.62	110.42
1	A	275	THR	CA-CB-OG1	-6.05	100.52	109.60
1	B	182	GLN	N-CA-CB	-5.82	106.17	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	290	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	486	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	367	VAL	N-CA-CB	5.62	119.86	110.86
1	A	116	GLU	CB-CG-CD	5.59	122.11	112.60
1	B	412	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	492	GLU	CB-CG-CD	-5.50	103.25	112.60
1	B	290	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	473	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	225	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	53	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	250	LYS	CB-CA-C	-5.14	102.81	110.88
1	A	239	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	348	ARG	Sidechain
1	A	63	ARG	Sidechain
1	B	110	ARG	Sidechain
1	B	205	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	344	ARG	Sidechain
1	B	99	GLY	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	3881	0	3764	90	1
1	B	3888	0	3747	148	1
2	A	177	0	0	15	0
2	B	131	0	0	28	0
All	All	8077	0	7511	235	1

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 (235) 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:B:140:PRO:HB2	2:B:554:HOH:O	1.55	1.07
1:B:144:ILE:HG23	1:B:153:ALA:HB3	1.42	1.01
1:A:168:ASP:HB3	2:A:567:HOH:O	1.67	0.94
1:B:180:ALA:HA	1:B:411:TYR:OH	1.67	0.94
1:B:50:GLN:HG3	1:B:219:GLY:HA2	1.53	0.88
1:B:213:THR:HG23	1:B:224:ARG:HB3	1.57	0.85
1:B:188:VAL:O	2:B:501:HOH:O	1.98	0.80
1:B:197[B]:ARG:HD2	1:B:207[B]:GLU:OE2	1.80	0.80
1:B:192:ASP:O	1:B:193:HIS:HB2	1.81	0.79
1:A:343:ARG:HH11	1:A:343:ARG:CG	1.97	0.78
1:B:144:ILE:CG2	1:B:153:ALA:HB3	2.13	0.77
1:B:217:ARG:O	1:B:218:SER:O	2.02	0.76
1:B:156:SER:O	2:B:502:HOH:O	2.02	0.76
1:A:13:GLN:HE21	1:A:47:THR:HG22	1.51	0.76
1:B:193:HIS:NE2	1:B:385:ILE:HD11	2.01	0.76
1:A:154:HIS:HE1	1:A:166:ASP:OD1	1.68	0.76
1:A:343:ARG:HH11	1:A:343:ARG:HG3	1.51	0.76
1:B:445:GLY:HA2	2:B:583:HOH:O	1.88	0.74
1:B:17:ILE:O	2:B:503:HOH:O	2.04	0.74
1:B:149:ARG:NH1	1:B:234:SER:O	2.22	0.73
1:B:134:VAL:O	2:B:504:HOH:O	2.08	0.71
1:A:460:LYS:NZ	2:A:503:HOH:O	2.24	0.70
1:A:57:SER:O	1:A:218:SER:HB2	1.90	0.70
1:B:241:LYS:NZ	2:B:508:HOH:O	2.23	0.69
1:A:158:ARG:HB2	1:A:159:PRO:CD	2.22	0.69
1:B:40:LEU:HD12	2:B:515:HOH:O	1.91	0.69
1:B:165:VAL:HG13	1:B:165:VAL:O	1.93	0.68
1:A:474:HIS:O	1:A:475:ALA:HB3	1.93	0.68
1:B:394:PHE:CG	1:B:411:TYR:HB3	2.28	0.68
1:B:65[A]:HIS:HA	2:B:582:HOH:O	1.93	0.67
1:B:394:PHE:CD2	1:B:411:TYR:HB3	2.30	0.66
1:B:198:HIS:CE1	1:B:209:ALA:HB1	2.30	0.66
1:B:383:ARG:HB3	1:B:386[A]:ILE:HG23	1.77	0.66
1:B:346:THR:HG22	2:B:527:HOH:O	1.96	0.65
1:B:180:ALA:CA	1:B:411:TYR:OH	2.43	0.64
1:B:178:THR:HG23	2:B:554:HOH:O	1.97	0.64
1:B:217:ARG:HD3	1:B:248:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:SER:O	1:B:157:ALA:C	2.40	0.64
1:A:474:HIS:O	1:A:475:ALA:CB	2.45	0.64
1:A:477:VAL:HG11	1:B:484:THR:HG21	1.80	0.64
1:B:155:LEU:HD11	1:B:190[A]:THR:HB	1.79	0.64
1:B:391:GLU:C	2:B:529:HOH:O	2.40	0.64
1:B:165:VAL:HG11	1:B:233:PRO:HB3	1.80	0.63
1:A:13:GLN:HE21	1:A:47:THR:CG2	2.10	0.63
1:A:48:LEU:HD11	1:A:60:VAL:HG21	1.80	0.63
1:B:65[C]:HIS:HA	2:B:582:HOH:O	1.98	0.63
1:B:144:ILE:HG23	1:B:153:ALA:CB	2.24	0.63
1:B:96:HIS:HB2	1:B:99:GLY:O	1.99	0.63
1:B:198:HIS:CE1	1:B:209:ALA:CB	2.82	0.63
1:B:385:ILE:HG23	1:B:413:VAL:HG13	1.80	0.62
1:A:165:VAL:HG12	1:A:238:GLY:O	2.00	0.62
1:B:102:SER:C	1:B:103:LEU:HD22	2.25	0.61
1:B:150:LYS:O	1:B:151:ARG:HD3	2.00	0.60
1:B:323:VAL:HB	1:B:363:LEU:CD1	2.31	0.60
1:A:276:ARG:HD3	1:A:291:GLN:OE1	2.02	0.60
1:B:366:SER:OG	2:B:505:HOH:O	2.16	0.60
1:B:155:LEU:HD11	1:B:190[B]:THR:HB	1.85	0.59
1:A:167:ARG:O	1:A:168:ASP:CB	2.50	0.59
1:B:82:ARG:HD2	1:B:89:CYS:SG	2.42	0.59
1:A:486:ASP:HB2	1:A:487:PRO:HD2	1.84	0.59
1:B:127:SER:OG	1:B:130:GLU:OE1	2.17	0.59
1:A:342:ASP:O	1:A:343:ARG:HB2	2.03	0.58
1:B:50:GLN:HG3	1:B:219:GLY:CA	2.29	0.58
1:A:158:ARG:HB2	1:A:159:PRO:HD3	1.84	0.58
1:A:167:ARG:NH1	1:A:174:ASP:OD1	2.36	0.58
1:A:183:ASP:HB2	2:A:513:HOH:O	2.03	0.58
1:A:343:ARG:HD3	1:A:420:ASP:O	2.04	0.58
1:B:323:VAL:HB	1:B:363:LEU:HD12	1.87	0.57
1:A:377:LEU:HD23	1:A:377:LEU:C	2.28	0.57
1:B:243:GLY:HA3	2:B:534:HOH:O	2.05	0.57
1:B:344:ARG:O	1:B:345:ILE:HD12	2.05	0.56
1:A:150:LYS:O	1:A:151:ARG:HD3	2.05	0.56
1:B:399:LYS:O	1:B:400:VAL:O	2.24	0.56
1:B:411:TYR:CD1	1:B:411:TYR:C	2.83	0.56
1:B:247:LYS:HA	1:B:247:LYS:HE2	1.87	0.56
1:B:50:GLN:CG	1:B:219:GLY:HA2	2.32	0.56
1:B:486:ASP:HB2	1:B:487:PRO:HD2	1.87	0.56
1:A:399[B]:LYS:NZ	2:A:508:HOH:O	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:HIS:HD2	1:B:141:GLN:H	1.54	0.56
1:B:198:HIS:NE2	1:B:209:ALA:HB1	2.21	0.55
1:A:324:GLN:HG3	1:A:326:THR:HB	1.88	0.55
1:B:438:ASP:O	1:B:439:SER:HB2	2.07	0.55
1:B:178:THR:CG2	2:B:554:HOH:O	2.54	0.55
1:A:340:TRP:CE3	1:A:345:ILE:HD11	2.42	0.55
1:A:438:ASP:O	1:A:439:SER:HB2	2.06	0.55
1:B:48:LEU:HD11	1:B:60:VAL:HG21	1.87	0.55
1:B:340:TRP:CE3	1:B:345:ILE:HD11	2.41	0.55
1:B:213:THR:CG2	1:B:224:ARG:HB3	2.34	0.54
1:B:136:ILE:HG23	1:B:138:MET:SD	2.48	0.54
1:B:100:ARG:HE	1:B:213:THR:CB	2.20	0.54
1:A:269:ASN:ND2	1:A:271:ARG:HB2	2.23	0.54
1:B:394:PHE:CE2	1:B:411:TYR:HD2	2.25	0.54
1:B:368:GLU:HG2	1:B:369:THR:HG23	1.90	0.54
1:B:207[B]:GLU:HB2	1:B:208:PRO:HD2	1.89	0.53
1:A:184[B]:GLN:NE2	1:A:185[B]:ARG:NH1	2.55	0.53
1:B:31:PHE:CE1	1:B:68:ARG:HD3	2.44	0.53
1:B:193:HIS:NE2	1:B:385:ILE:CD1	2.71	0.53
1:A:165:VAL:CG1	1:A:233:PRO:HB3	2.39	0.53
1:B:217:ARG:CD	1:B:248:VAL:HG11	2.39	0.53
1:A:47:THR:HG23	2:A:588:HOH:O	2.09	0.53
1:A:48:LEU:HD11	1:A:60:VAL:CG2	2.38	0.52
1:A:192:ASP:OD2	1:A:194:ARG:NE	2.40	0.52
1:B:63:ARG:HH11	1:B:63:ARG:HG2	1.75	0.52
1:B:100:ARG:NH2	1:B:185:ARG:HA	2.25	0.52
1:B:311:THR:HG22	1:B:313:LYS:HG2	1.91	0.52
1:B:139:HIS:HE1	1:B:387:VAL:O	1.92	0.52
1:A:200:GLY:O	2:A:501:HOH:O	2.18	0.52
1:B:201:ARG:HD2	1:B:202:LEU:H	1.75	0.52
1:B:183[A]:ASP:OD1	1:B:183[A]:ASP:O	2.28	0.52
1:A:217:ARG:HD3	2:A:519:HOH:O	2.09	0.51
1:B:52:PRO:O	1:B:53:ASP:HB3	2.10	0.51
1:B:103:LEU:HD22	1:B:103:LEU:N	2.25	0.51
1:B:18:ASN:HB3	1:B:132:TRP:CZ3	2.45	0.51
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.76	0.51
1:B:95:ALA:HA	1:B:100:ARG:O	2.10	0.50
1:A:342:ASP:O	1:A:343:ARG:CB	2.59	0.50
1:A:258:GLN:NE2	2:A:507:HOH:O	2.43	0.50
1:B:183[B]:ASP:C	1:B:185:ARG:H	2.19	0.50
1:B:189:GLN:O	2:B:506:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97[B]:ASP:OD1	1:B:224:ARG:NH1	2.39	0.49
1:B:44:GLN:HB2	2:B:515:HOH:O	2.12	0.49
1:B:399:LYS:O	1:B:400:VAL:C	2.55	0.49
1:B:165:VAL:HG12	1:B:238:GLY:O	2.12	0.49
1:B:284:ASN:C	1:B:284:ASN:HD22	2.20	0.49
1:B:314:TYR:CE1	1:B:330:LYS:HE2	2.48	0.49
1:A:18:ASN:HB3	1:A:132:TRP:CZ3	2.48	0.49
1:A:397:CYS:HB3	2:A:607:HOH:O	2.12	0.49
1:A:431:LYS:HD2	1:A:444:SER:O	2.12	0.49
1:B:77:ASN:ND2	2:B:526:HOH:O	2.45	0.49
1:B:207[A]:GLU:HB2	1:B:208:PRO:HD2	1.95	0.49
1:B:432:TYR:O	1:B:444:SER:O	2.30	0.49
1:B:100:ARG:N	2:B:519:HOH:O	2.41	0.49
1:B:377:LEU:C	1:B:377:LEU:HD23	2.38	0.49
1:B:136:ILE:HG12	1:B:186:TYR:CZ	2.48	0.48
1:A:397:CYS:CB	2:A:607:HOH:O	2.61	0.48
1:A:343:ARG:CG	1:A:343:ARG:NH1	2.66	0.48
1:A:96:HIS:O	1:A:98:ASP:O	2.32	0.48
1:B:8:GLU:CA	2:B:615:HOH:O	2.62	0.47
1:B:151:ARG:HH11	1:B:151:ARG:CG	2.27	0.47
1:B:190[B]:THR:HG22	2:B:501:HOH:O	2.13	0.47
1:B:398:ARG:NH1	1:B:405:ASP:OD1	2.47	0.47
1:B:95:ALA:HB1	1:B:213:THR:HG21	1.95	0.47
1:A:136:ILE:HG12	1:A:186:TYR:CZ	2.50	0.47
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.80	0.47
1:A:136:ILE:HG23	1:A:138:MET:SD	2.55	0.47
1:B:41:LYS:N	2:B:515:HOH:O	2.48	0.47
1:A:24:LEU:HD13	1:A:46:TRP:CE2	2.50	0.47
1:A:109:ARG:HD2	1:A:109:ARG:N	2.30	0.47
1:A:217:ARG:HD2	1:A:248:VAL:HG11	1.97	0.47
1:B:52:PRO:O	1:B:53:ASP:CB	2.63	0.47
1:B:180:ALA:CB	1:B:411:TYR:OH	2.63	0.47
1:A:97:ASP:C	1:A:98:ASP:O	2.56	0.47
1:A:238:GLY:O	1:A:239:THR:C	2.58	0.47
1:B:12:ILE:HD13	1:B:138:MET:HE3	1.96	0.47
1:A:167:ARG:O	1:A:168:ASP:HB2	2.14	0.46
1:A:408[B]:ARG:NH2	2:A:506:HOH:O	2.30	0.46
1:B:386[A]:ILE:HD11	1:B:416:LEU:HB2	1.97	0.46
1:A:485:VAL:HG13	2:A:647:HOH:O	2.15	0.46
1:B:158:ARG:O	1:B:159:PRO:C	2.58	0.46
1:A:51:PRO:HB2	1:A:54:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:GLY:O	1:B:468:ARG:HD2	2.15	0.46
1:A:95:ALA:HB1	1:A:213:THR:CG2	2.46	0.46
1:A:398:ARG:HB2	1:A:405:ASP:OD2	2.15	0.46
1:B:95:ALA:HB1	1:B:213:THR:CG2	2.46	0.46
1:A:344:ARG:O	1:A:345:ILE:HD12	2.16	0.45
1:B:190[B]:THR:HG21	1:B:202:LEU:HD13	1.97	0.45
1:A:98:ASP:O	1:A:185[A]:ARG:NH2	2.50	0.45
1:A:432:TYR:CD2	1:A:448:PRO:HB3	2.52	0.45
1:A:314:TYR:CE1	1:A:330:LYS:HE2	2.51	0.45
1:B:155:LEU:HD11	1:B:190[A]:THR:CG2	2.46	0.45
1:A:101:TRP:CE2	1:A:134:VAL:HG21	2.52	0.45
1:A:426:LYS:HD3	1:A:432:TYR:CZ	2.52	0.45
1:B:192:ASP:O	1:B:193:HIS:CB	2.59	0.45
1:B:344:ARG:C	1:B:345:ILE:HD12	2.41	0.45
1:A:84:VAL:HG23	1:A:85:PRO:HD2	1.98	0.44
1:B:40:LEU:HD22	1:B:135:HIS:CD2	2.52	0.44
1:A:184[B]:GLN:CD	2:A:513:HOH:O	2.60	0.44
1:A:193:HIS:HE1	2:A:556:HOH:O	2.00	0.44
1:B:57:SER:C	1:B:59:ALA:H	2.24	0.44
1:A:182:GLN:NE2	1:A:187:SER:HB3	2.32	0.44
1:B:157:ALA:O	1:B:158:ARG:CB	2.65	0.44
1:B:176:LEU:O	2:B:507:HOH:O	2.21	0.44
1:A:97:ASP:OD1	1:A:224:ARG:NH1	2.45	0.44
1:A:398:ARG:NH1	1:A:405:ASP:OD1	2.50	0.44
1:B:155:LEU:HB2	1:B:174:ASP:HB2	1.99	0.44
1:B:273:VAL:HA	1:B:283:ALA:HA	1.99	0.44
1:A:198:HIS:CE1	1:A:229:ARG:HH22	2.36	0.44
1:B:302:THR:O	1:B:303:LYS:HB2	2.18	0.44
1:B:136:ILE:HG22	2:B:547:HOH:O	2.17	0.44
1:B:238:GLY:O	1:B:239:THR:C	2.61	0.43
1:B:28:ALA:HA	1:B:66:LEU:HD11	2.01	0.43
1:B:340:TRP:HE3	1:B:345:ILE:HD11	1.82	0.43
1:B:151:ARG:HG2	1:B:151:ARG:NH1	2.33	0.43
1:B:155:LEU:N	1:B:155:LEU:HD12	2.33	0.43
1:B:158:ARG:N	1:B:159:PRO:HD2	2.33	0.43
1:B:157:ALA:O	1:B:158:ARG:HB2	2.18	0.43
1:B:108:HIS:O	1:B:109:ARG:HB2	2.19	0.43
1:A:276:ARG:NH2	1:A:287[A]:GLU:OE1	2.44	0.43
1:B:162:GLU:O	1:B:163:ILE:C	2.62	0.43
1:B:12:ILE:CD1	1:B:138:MET:HE3	2.50	0.42
1:B:48:LEU:HD11	1:B:60:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ASP:HB2	2:B:509:HOH:O	2.18	0.42
1:A:408[B]:ARG:HE	1:A:408[B]:ARG:HB3	1.59	0.42
1:B:100:ARG:HB3	2:B:519:HOH:O	2.20	0.42
1:A:459:ASN:OD1	1:A:460:LYS:HG2	2.19	0.42
1:B:103:LEU:N	1:B:103:LEU:CD2	2.83	0.42
1:A:219:GLY:O	1:A:220:LYS:HD3	2.19	0.42
1:A:399[A]:LYS:HD3	1:A:399[A]:LYS:HA	1.92	0.42
1:B:155:LEU:HD21	1:B:190[B]:THR:OG1	2.19	0.41
1:A:217:ARG:O	1:A:218:SER:C	2.62	0.41
1:A:474:HIS:CE1	1:B:483:GLU:OE2	2.73	0.41
1:B:151:ARG:HG3	1:B:166:ASP:C	2.45	0.41
1:A:344:ARG:C	1:A:345:ILE:HD12	2.45	0.41
1:A:449:VAL:CG2	1:A:451:PHE:CE1	3.04	0.41
1:B:162:GLU:O	1:B:164:ALA:N	2.53	0.41
1:A:438:ASP:O	1:A:439:SER:CB	2.66	0.41
1:B:155:LEU:HD13	1:B:174:ASP:O	2.21	0.41
1:A:267:ALA:HB3	1:A:269:ASN:ND2	2.36	0.41
1:A:153:ALA:HA	1:A:165:VAL:HA	2.03	0.41
1:A:187:SER:HB2	2:A:565:HOH:O	2.21	0.41
1:A:395:ILE:HA	1:A:405:ASP:O	2.21	0.41
1:A:464:LYS:HE3	1:A:467:GLY:HA2	2.03	0.41
1:B:40:LEU:CD1	2:B:515:HOH:O	2.59	0.41
1:A:419:ASN:O	1:A:420:ASP:C	2.64	0.41
1:B:201:ARG:NH1	1:B:201:ARG:HB3	2.36	0.41
1:B:217:ARG:C	1:B:218:SER:O	2.62	0.41
1:B:281:LEU:HB2	1:B:363:LEU:HD11	2.03	0.41
1:A:50:GLN:HB3	1:A:55:ALA:HA	2.02	0.40
1:A:97:ASP:O	1:A:185[B]:ARG:NH2	2.53	0.40
1:B:152:TYR:OH	1:B:257:GLU:OE1	2.28	0.40
1:A:217:ARG:O	1:A:218:SER:O	2.40	0.40
1:B:473:ASP:O	1:B:474:HIS:C	2.65	0.40
1:A:401:THR:HG21	1:B:485:VAL:HG22	2.03	0.40
1:B:155:LEU:N	1:B:155:LEU:CD1	2.85	0.40
1:B:395:ILE:HA	1:B:405:ASP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLY:O	1:B:415:GLN:NE2[3_444]	2.15	0.05

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	493/493 (100%)	455 (92%)	28 (6%)	10 (2%)	6	4
1	B	495/493 (100%)	447 (90%)	38 (8%)	10 (2%)	6	4
All	All	988/986 (100%)	902 (91%)	66 (7%)	20 (2%)	5	4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
1	A	218	SER
1	A	474	HIS
1	B	53	ASP
1	B	158	ARG
1	B	163	ILE
1	B	218	SER
1	B	400	VAL
1	A	168	ASP
1	A	342	ASP
1	A	343	ARG
1	B	474	HIS
1	A	160	ALA
1	B	193	HIS
1	B	57	SER
1	A	167	ARG
1	B	398	ARG
1	A	56	GLY
1	A	158	ARG
1	B	235	GLY

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	408/404 (101%)	363 (89%)	45 (11%)	5 4
1	B	410/404 (102%)	362 (88%)	48 (12%)	4 4
All	All	818/808 (101%)	725 (89%)	93 (11%)	4 4

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	16	LEU
1	A	21	ASN
1	A	24	LEU
1	A	33	VAL
1	A	53	ASP
1	A	74[A]	LYS
1	A	74[B]	LYS
1	A	78	VAL
1	A	98	ASP
1	A	109	ARG
1	A	115	THR
1	A	116	GLU
1	A	120	SER
1	A	134	VAL
1	A	138	MET
1	A	151	ARG
1	A	155	LEU
1	A	158	ARG
1	A	162	GLU
1	A	168	ASP
1	A	169	VAL
1	A	202	LEU
1	A	231	LEU
1	A	234	SER
1	A	247	LYS
1	A	251	ASP
1	A	269	ASN
1	A	271	ARG
1	A	277	GLN
1	A	298	ILE

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Mol	Chain	Res	Type
1	A	313	LYS
1	A	316	THR
1	A	326	THR
1	A	343	ARG
1	A	345	ILE
1	A	347	LEU
1	A	375	LEU
1	A	380	LEU
1	A	404	LEU
1	A	428	SER
1	A	446	ASP
1	A	477	VAL
1	A	484	THR
1	A	485	VAL
1	B	10	VAL
1	B	16	LEU
1	B	24	LEU
1	B	83	GLU
1	B	94	VAL
1	B	109	ARG
1	B	115	THR
1	B	116	GLU
1	B	118	ARG
1	B	130	GLU
1	B	135	HIS
1	B	151	ARG
1	B	169	VAL
1	B	201	ARG
1	B	231	LEU
1	B	247	LYS
1	B	258	GLN
1	B	271	ARG
1	B	273	VAL
1	B	274	SER
1	B	276	ARG
1	B	279	MET
1	B	284	ASN
1	B	311	THR
1	B	320	THR
1	B	329	SER
1	B	339	GLU
1	B	344	ARG

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Mol	Chain	Res	Type
1	B	345	ILE
1	B	346	THR
1	B	347	LEU
1	B	359	LYS
1	B	363	LEU
1	B	367	VAL
1	B	375	LEU
1	B	380	LEU
1	B	385	ILE
1	B	386[A]	ILE
1	B	386[B]	ILE
1	B	401	THR
1	B	403	THR
1	B	404	LEU
1	B	446	ASP
1	B	449	VAL
1	B	474	HIS
1	B	477	VAL
1	B	485	VAL
1	B	489	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	143	ASN
1	A	154	HIS
1	A	182	GLN
1	A	189	GLN
1	A	193	HIS
1	A	258	GLN
1	A	269	ASN
1	A	392	HIS
1	B	135	HIS
1	B	139	HIS
1	B	291	GLN

5.3.3 RNA

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, 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	486/493 (98%)	0.23	16 (3%) 49 46	16, 42, 70, 110	9 (1%)
1	B	486/493 (98%)	1.04	87 (17%) 4 4	16, 52, 88, 138	11 (2%)
All	All	972/986 (98%)	0.64	103 (10%) 13 10	16, 47, 82, 138	20 (2%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	PHE	5.3
1	A	279[A]	MET	5.2
1	B	240	LEU	5.1
1	B	202	LEU	5.0
1	B	204	ALA	4.9
1	B	196	LEU	4.8
1	B	203	VAL	4.6
1	A	278	GLY	4.6
1	B	65[A]	HIS	4.6
1	B	200	GLY	4.4
1	B	190[A]	THR	4.3
1	B	163	ILE	4.2
1	B	248	VAL	4.1
1	B	179	LEU	3.9
1	B	56	GLY	3.8
1	B	144	ILE	3.8
1	A	399[A]	LYS	3.8
1	B	209	ALA	3.7
1	B	29	PHE	3.6
1	B	157	ALA	3.6
1	B	213	THR	3.5
1	B	231	LEU	3.5
1	B	58	ALA	3.5
1	B	212	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	181	PHE	3.5
1	B	253	LEU	3.4
1	B	245	ALA	3.4
1	B	188	VAL	3.3
1	B	197[A]	ARG	3.2
1	B	246	THR	3.2
1	B	186	TYR	3.2
1	B	12	ILE	3.1
1	B	180	ALA	3.1
1	B	48	LEU	3.1
1	B	226	CYS	3.0
1	B	222	ALA	3.0
1	A	244[A]	LYS	3.0
1	B	185	ARG	3.0
1	B	230	TYR	3.0
1	B	458	TYR	3.0
1	B	69	TYR	2.9
1	B	101	TRP	2.9
1	B	400	VAL	2.9
1	B	159	PRO	2.9
1	B	191	ALA	2.8
1	B	232	ALA	2.8
1	B	187	SER	2.8
1	A	157	ALA	2.8
1	B	177	ILE	2.8
1	B	254	PHE	2.7
1	B	100	ARG	2.7
1	B	55	ALA	2.7
1	A	55	ALA	2.7
1	B	31	PHE	2.6
1	B	160	ALA	2.6
1	B	242	ALA	2.6
1	B	252	GLU	2.5
1	A	475	ALA	2.5
1	B	155	LEU	2.5
1	A	277	GLN	2.5
1	B	206	PRO	2.5
1	B	233	PRO	2.5
1	B	394	PHE	2.5
1	A	165	VAL	2.5
1	B	28	ALA	2.5
1	B	66	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	276	ARG	2.5
1	B	85	PRO	2.5
1	B	97[A]	ASP	2.4
1	B	401	THR	2.4
1	B	82	ARG	2.4
1	B	410	SER	2.4
1	B	164	ALA	2.4
1	B	218	SER	2.3
1	B	63	ARG	2.3
1	B	223	PHE	2.3
1	A	245	ALA	2.3
1	B	14	PHE	2.3
1	B	195	PHE	2.3
1	B	136	ILE	2.3
1	A	52	PRO	2.3
1	B	135	HIS	2.3
1	B	53	ASP	2.3
1	A	402	GLY	2.2
1	B	208	PRO	2.2
1	B	279	MET	2.2
1	B	10	VAL	2.2
1	B	147	VAL	2.2
1	B	229	ARG	2.2
1	B	193	HIS	2.2
1	B	134	VAL	2.2
1	B	207[A]	GLU	2.1
1	A	401	THR	2.1
1	B	221	VAL	2.1
1	B	57	SER	2.1
1	A	74[A]	LYS	2.1
1	B	239	THR	2.1
1	A	366	SER	2.1
1	B	247	LYS	2.1
1	B	236	PRO	2.1
1	B	94	VAL	2.0
1	B	93	ILE	2.0
1	B	217	ARG	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.