Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 04:21 pm GMT

PDB ID	:	7ANK
Title	:	Crystal structure of sarcomeric protein FATZ-1 (d91-FATZ-1 construct) in complex with half dimer of alpha-actinin-2
Authors	:	Sponga, A.; Arolas, J.L.; Rodriguez Chamorro, A.; Mlynek, G.; Hollerl, E.; Schreiner, C.; Pedron, M.; Kostan, J.; Ribeiro, E.A.; Djinovic-Carugo, K.
Deposited on	:	2020-10-12
Resolution	:	3.20 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 ⓘ 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:

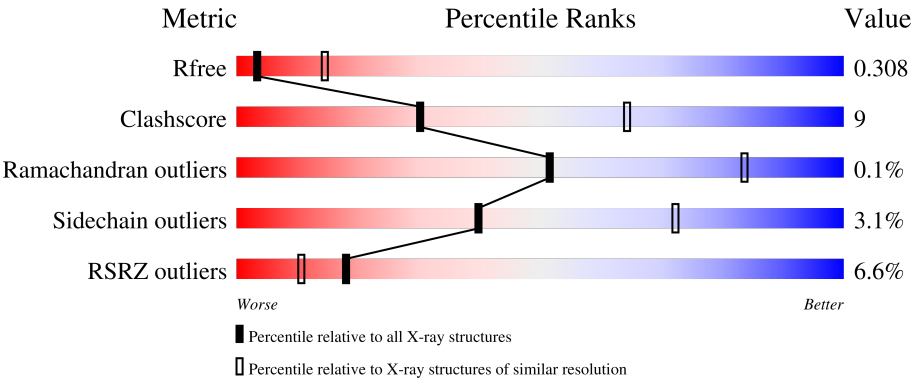
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	535	8% 66% 22% 10%
2	B	389	4% 80% 18%
3	C	209	% 16% 82%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7319 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 Alpha-actinin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3928	2463	716	728	21	71	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	SER	-	expression tag	UNP P35609
A	509	GLU	-	expression tag	UNP P35609
A	510	ARG	-	expression tag	UNP P35609
A	511	VAL	-	expression tag	UNP P35609
A	512	ARG	-	expression tag	UNP P35609
A	513	ASN	-	expression tag	UNP P35609
A	514	PHE	-	expression tag	UNP P35609
A	515	GLU	-	expression tag	UNP P35609
A	516	ASP	-	expression tag	UNP P35609
A	517	PRO	-	expression tag	UNP P35609
A	518	ALA	-	expression tag	UNP P35609
A	519	ALA	-	expression tag	UNP P35609
A	520	ASN	-	expression tag	UNP P35609
A	521	LYS	-	expression tag	UNP P35609
A	522	ALA	-	expression tag	UNP P35609
A	523	ARG	-	expression tag	UNP P35609
A	524	LYS	-	expression tag	UNP P35609
A	525	GLU	-	expression tag	UNP P35609
A	526	ALA	-	expression tag	UNP P35609
A	527	GLU	-	expression tag	UNP P35609
A	528	LEU	-	expression tag	UNP P35609
A	529	ALA	-	expression tag	UNP P35609
A	530	ALA	-	expression tag	UNP P35609
A	531	ALA	-	expression tag	UNP P35609
A	532	THR	-	expression tag	UNP P35609
A	533	ALA	-	expression tag	UNP P35609
A	534	GLU	-	expression tag	UNP P35609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLN	-	expression tag	UNP P35609

- Molecule 2 is a protein called Alpha-actinin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	382	Total	C	N	O	S	36	0	0
			3079	1926	538	599	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	GLY	-	expression tag	UNP P35609
B	507	SER	-	expression tag	UNP P35609
B	508	SER	-	expression tag	UNP P35609

- Molecule 3 is a protein called Myozenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	38	Total	C	N	O	S	0	0	0
			312	201	52	57	2			

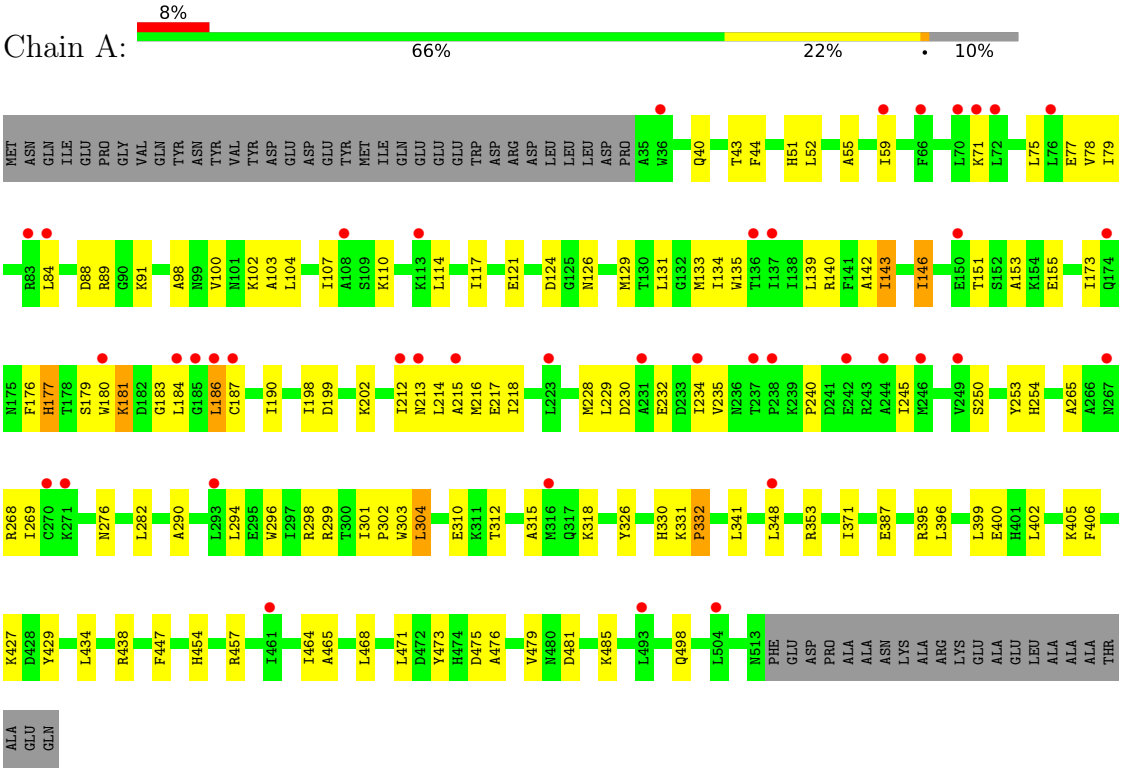
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	91	GLY	-	expression tag	UNP Q9NP98

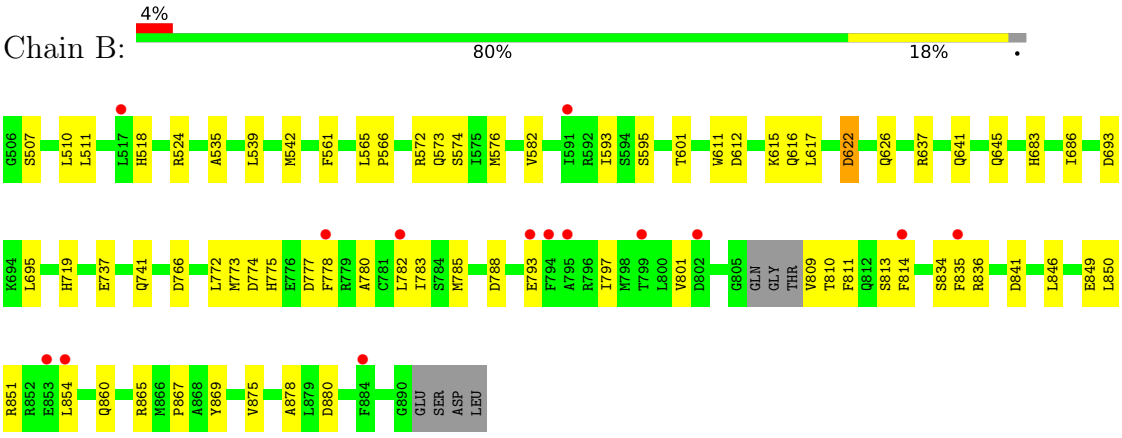
3 Residue-property plots (i)

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: Alpha-actinin-2

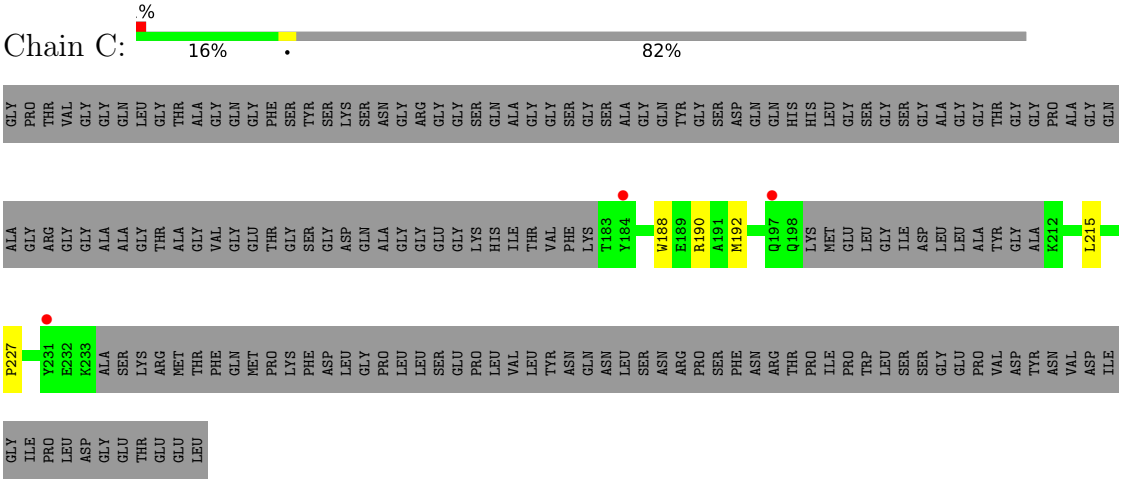


• Molecule 2: Alpha-actinin-2



• Molecule 3: Myozenin-1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.60Å 56.92Å 209.38Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	46.94 – 3.20 46.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.94-3.20) 98.9 (46.94-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.255 , 0.284 0.282 , 0.308	Depositor DCC
R_{free} test set	1288 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	127.5	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 154.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å^2)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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	0.35	0/3999	0.52	0/5386
2	B	0.33	0/3134	0.49	0/4232
3	C	0.27	0/321	0.47	0/431
All	All	0.34	0/7454	0.51	0/10049

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3928	0	3937	85	0
2	B	3079	0	3001	54	0
3	C	312	0	300	4	0
All	All	7319	0	7238	134	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 9.

All (134) 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)
2:B:611:TRP:HE1	2:B:615:LYS:HE2	1.22	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:772:LEU:HB2	2:B:811:PHE:HA	1.42	0.99
1:A:139:LEU:HA	1:A:143:ILE:HG13	1.53	0.88
1:A:282:LEU:HB3	1:A:348:LEU:HD21	1.54	0.87
2:B:810:THR:HB	2:B:813:SER:HB3	1.57	0.86
1:A:146:ILE:HD11	1:A:254:HIS:CE1	2.11	0.85
2:B:810:THR:HB	2:B:813:SER:CB	2.07	0.84
2:B:611:TRP:NE1	2:B:615:LYS:HE2	1.93	0.84
1:A:405:LYS:HZ2	2:B:542:MET:HB2	1.44	0.81
1:A:399:LEU:HD21	1:A:471:LEU:HB3	1.66	0.77
1:A:176:PHE:HA	1:A:180:TRP:CD1	2.21	0.76
1:A:282:LEU:CB	1:A:348:LEU:HD21	2.17	0.74
1:A:110:LYS:HB3	1:A:140:ARG:HE	1.53	0.73
2:B:683:HIS:ND1	2:B:686:ILE:HD11	2.04	0.72
1:A:454:HIS:HA	1:A:457:ARG:HG2	1.71	0.71
1:A:341:LEU:HD21	1:A:371:ILE:HD13	1.73	0.71
2:B:780:ALA:HA	2:B:783:ILE:CD1	2.20	0.71
1:A:190:ILE:HB	1:A:198:ILE:HD12	1.75	0.69
1:A:405:LYS:NZ	2:B:542:MET:HB2	2.08	0.69
1:A:186:LEU:N	1:A:186:LEU:HD23	2.08	0.68
2:B:851:ARG:HH21	2:B:860:GLN:HE22	1.43	0.66
2:B:524:ARG:NH2	2:B:574:SER:OG	2.31	0.64
2:B:573:GLN:HA	2:B:576:MET:HG2	1.80	0.64
1:A:183:GLY:HA3	1:A:212:ILE:HG12	1.80	0.64
2:B:611:TRP:HE1	2:B:615:LYS:CE	2.06	0.63
1:A:139:LEU:HD11	1:A:153:ALA:HB1	1.81	0.62
2:B:875:VAL:HG13	2:B:878:ALA:HB2	1.83	0.61
1:A:146:ILE:HD11	1:A:254:HIS:NE2	2.15	0.61
2:B:772:LEU:HD12	2:B:809:VAL:HG22	1.81	0.61
1:A:396:LEU:O	1:A:400:GLU:HG2	2.01	0.60
2:B:810:THR:HB	2:B:813:SER:HB2	1.81	0.60
1:A:402:LEU:HB3	1:A:468:LEU:HD21	1.82	0.60
1:A:43:THR:HA	1:A:228:MET:HB3	1.84	0.59
1:A:199:ASP:HB3	1:A:202:LYS:HZ3	1.68	0.59
1:A:353:ARG:HH12	3:C:190:ARG:HH12	1.52	0.58
1:A:173:ILE:HA	1:A:179:SER:HB3	1.86	0.57
1:A:399:LEU:HD21	1:A:471:LEU:CB	2.33	0.57
1:A:40:GLN:HB3	1:A:131:LEU:HD22	1.87	0.56
1:A:139:LEU:HA	1:A:143:ILE:CG1	2.32	0.56
1:A:183:GLY:HA2	1:A:186:LEU:HD21	1.87	0.56
1:A:199:ASP:HB3	1:A:202:LYS:NZ	2.21	0.56
2:B:535:ALA:O	2:B:539:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD23	1:A:186:LEU:H	1.68	0.55
2:B:683:HIS:HA	2:B:686:ILE:HG12	1.89	0.54
2:B:572:ARG:HH12	2:B:573:GLN:HE21	1.54	0.54
1:A:59:ILE:HG22	1:A:71:LYS:HD2	1.89	0.53
1:A:121:GLU:HA	1:A:124:ASP:HB3	1.89	0.53
1:A:181:LYS:HG3	1:A:240:PRO:HG3	1.90	0.53
1:A:240:PRO:HB2	1:A:245:ILE:HD11	1.91	0.53
1:A:230:ASP:O	1:A:234:ILE:HG12	2.09	0.52
1:A:121:GLU:HB2	1:A:129:MET:SD	2.49	0.52
1:A:476:ALA:HA	1:A:479:VAL:HG22	1.92	0.52
2:B:737:GLU:O	2:B:741:GLN:HG2	2.10	0.52
1:A:190:ILE:HB	1:A:198:ILE:CD1	2.40	0.52
1:A:265:ALA:O	1:A:269:ILE:HG12	2.10	0.52
1:A:151:THR:HB	1:A:155:GLU:HB2	1.92	0.51
1:A:353:ARG:NH1	3:C:190:ARG:HH12	2.09	0.51
1:A:434:LEU:O	1:A:438:ARG:HG2	2.11	0.51
1:A:114:LEU:HB2	1:A:117:ILE:CG2	2.41	0.50
1:A:142:ALA:O	1:A:250:SER:HB2	2.10	0.50
1:A:98:ALA:O	1:A:102:LYS:HG3	2.12	0.50
1:A:110:LYS:HB3	1:A:140:ARG:NE	2.25	0.50
1:A:117:ILE:HD12	1:A:129:MET:CG	2.42	0.50
2:B:869:TYR:HA	2:B:880:ASP:HB2	1.94	0.49
2:B:518:HIS:NE2	2:B:582:VAL:HG11	2.26	0.49
1:A:296:TRP:HD1	1:A:299:ARG:NH2	2.10	0.49
1:A:276:ASN:ND2	2:B:865:ARG:HH12	2.10	0.48
2:B:850:LEU:O	2:B:854:LEU:HB2	2.13	0.48
1:A:126:ASN:HB3	1:A:129:MET:HB3	1.95	0.48
2:B:780:ALA:HA	2:B:783:ILE:HD11	1.96	0.48
1:A:214:LEU:O	1:A:218:ILE:HG12	2.14	0.48
2:B:793:GLU:O	2:B:797:ILE:HG12	2.14	0.48
1:A:117:ILE:HD12	1:A:129:MET:HG3	1.95	0.48
2:B:778:PHE:HE2	2:B:797:ILE:HG13	1.79	0.48
1:A:40:GLN:OE1	1:A:131:LEU:HB3	2.14	0.48
1:A:296:TRP:CD1	1:A:299:ARG:NH2	2.82	0.48
2:B:565:LEU:N	2:B:566:PRO:HD2	2.29	0.48
1:A:44:PHE:HB3	1:A:134:ILE:HG21	1.95	0.47
1:A:55:ALA:HB2	1:A:78:VAL:HG21	1.96	0.47
1:A:454:HIS:HA	1:A:457:ARG:CG	2.42	0.47
1:A:51:HIS:ND1	1:A:79:ILE:HG22	2.29	0.47
1:A:303:TRP:CZ3	1:A:304:LEU:HD13	2.49	0.47
1:A:326:TYR:HA	1:A:330:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:CYS:SG	1:A:215:ALA:HB2	2.55	0.46
1:A:100:VAL:O	1:A:104:LEU:HG	2.16	0.46
1:A:103:ALA:O	1:A:107:ILE:HG12	2.16	0.46
1:A:331:LYS:N	1:A:332:PRO:HD2	2.31	0.46
2:B:867:PRO:HG2	2:B:880:ASP:HB3	1.96	0.46
1:A:177:HIS:HB2	1:A:240:PRO:HD2	1.97	0.46
1:A:117:ILE:HD13	1:A:133:MET:HB2	1.98	0.46
2:B:612:ASP:O	2:B:616:GLN:HG2	2.16	0.46
2:B:774:ASP:OD1	2:B:775:HIS:NE2	2.49	0.46
2:B:772:LEU:HD12	2:B:809:VAL:CG2	2.46	0.45
1:A:427:LYS:HG3	1:A:429:TYR:HE1	1.81	0.45
2:B:782:LEU:O	2:B:785:MET:O	2.34	0.45
1:A:447:PHE:HE1	2:B:601:THR:HG21	1.82	0.45
2:B:778:PHE:CD1	2:B:814:PHE:HE1	2.34	0.45
1:A:481:ASP:O	1:A:485:LYS:HG2	2.16	0.45
1:A:77:GLU:HG2	1:A:84:LEU:HB2	1.99	0.45
1:A:406:PHE:HA	1:A:464:ILE:HD11	1.99	0.45
2:B:573:GLN:HA	2:B:576:MET:CG	2.45	0.45
2:B:572:ARG:HH12	2:B:573:GLN:NE2	2.16	0.44
1:A:181:LYS:NZ	1:A:235:VAL:HA	2.32	0.44
2:B:645:GLN:HB2	2:B:695:LEU:HD13	1.99	0.44
2:B:836:ARG:HG2	2:B:841:ASP:HA	1.98	0.44
3:C:188:TRP:CD1	3:C:192:MET:CE	3.00	0.44
1:A:216:MET:SD	1:A:229:LEU:O	2.76	0.44
2:B:772:LEU:HB2	2:B:811:PHE:CA	2.30	0.44
2:B:507:SER:HA	2:B:510:LEU:HD12	1.98	0.44
2:B:637:ARG:O	2:B:641:GLN:HG2	2.17	0.44
1:A:176:PHE:HA	1:A:180:TRP:HD1	1.80	0.44
1:A:406:PHE:CE2	1:A:465:ALA:HB2	2.52	0.44
1:A:135:TRP:CZ2	1:A:139:LEU:HD13	2.53	0.43
2:B:846:LEU:HB2	2:B:849:GLU:HG3	2.00	0.43
2:B:778:PHE:CE2	2:B:797:ILE:HG13	2.53	0.43
2:B:801:VAL:HG22	2:B:809:VAL:HG12	1.99	0.43
2:B:539:LEU:HD23	2:B:617:LEU:HB2	2.00	0.43
2:B:766:ASP:HA	2:B:773:MET:HB3	2.00	0.43
1:A:405:LYS:NZ	2:B:542:MET:H	2.16	0.43
1:A:143:ILE:HD13	1:A:250:SER:HB3	2.00	0.43
1:A:52:LEU:HG	1:A:75:LEU:HD13	2.01	0.42
1:A:265:ALA:HA	2:B:834:SER:OG	2.18	0.42
1:A:473:TYR:CE2	1:A:475:ASP:HB3	2.54	0.42
2:B:622:ASP:O	2:B:626:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:ALA:HA	2:B:783:ILE:HG12	2.01	0.42
1:A:294:LEU:O	1:A:298:ARG:HG3	2.20	0.42
1:A:301:ILE:N	1:A:302:PRO:HD2	2.34	0.42
1:A:312:THR:HG23	1:A:315:ALA:H	1.84	0.42
1:A:213:ASN:O	1:A:217:GLU:HG2	2.19	0.41
2:B:593:ILE:HG23	2:B:595:SER:H	1.84	0.41
2:B:561:PHE:HA	3:C:227:PRO:HB3	2.03	0.41
1:A:290:ALA:O	1:A:294:LEU:HB2	2.21	0.41
1:A:146:ILE:HG13	1:A:253:TYR:CE1	2.55	0.40
2:B:773:MET:HG3	2:B:777:ASP:CB	2.52	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	477/535 (89%)	467 (98%)	10 (2%)	0	100 100
2	B	378/389 (97%)	359 (95%)	18 (5%)	1 (0%)	41 74
3	C	34/209 (16%)	32 (94%)	2 (6%)	0	100 100
All	All	889/1133 (78%)	858 (96%)	30 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	788	ASP

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	420/467 (90%)	402 (96%)	18 (4%)	29	64
2	B	332/338 (98%)	327 (98%)	5 (2%)	65	85
3	C	32/151 (21%)	31 (97%)	1 (3%)	40	72
All	All	784/956 (82%)	760 (97%)	24 (3%)	40	72

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASP
1	A	89	ARG
1	A	91	LYS
1	A	143	ILE
1	A	146	ILE
1	A	177	HIS
1	A	181	LYS
1	A	184	LEU
1	A	186	LEU
1	A	232	GLU
1	A	268	ARG
1	A	304	LEU
1	A	310	GLU
1	A	318	LYS
1	A	332	PRO
1	A	387	GLU
1	A	395	ARG
1	A	498	GLN
2	B	511	LEU
2	B	622	ASP
2	B	693	ASP
2	B	719	HIS
2	B	835	PHE
3	C	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	444	HIS
2	B	573	GLN
2	B	632	GLN
2	B	684	ASN
2	B	860	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 monosaccharides 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	470/535 (87%)	0.54	41 (8%)	10	5	134, 206, 270, 286	0
2	B	377/389 (96%)	0.24	14 (3%)	41	26	145, 191, 288, 295	0
3	C	38/209 (18%)	0.21	3 (7%)	12	6	186, 222, 241, 246	0
All	All	885/1133 (78%)	0.40	58 (6%)	18	11	134, 196, 277, 295	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	TRP	5.8
2	B	778	PHE	5.6
1	A	185	GLY	5.2
1	A	212	ILE	5.0
1	A	66	PHE	4.6
2	B	799	THR	4.6
1	A	36	TRP	4.6
1	A	108	ALA	4.6
1	A	246	MET	4.4
1	A	238	PRO	4.2
2	B	795	ALA	3.8
1	A	150	GLU	3.7
2	B	793	GLU	3.6
1	A	72	LEU	3.5
1	A	113	LYS	3.5
1	A	187	CYS	3.4
1	A	249	VAL	3.4
2	B	854	LEU	3.3
1	A	174	GLN	3.2
1	A	71	LYS	3.2
3	C	197	GLN	3.2
1	A	184	LEU	3.1
1	A	76	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	853	GLU	3.0
3	C	184	TYR	3.0
1	A	59	ILE	2.9
1	A	231	ALA	2.9
3	C	231	TYR	2.8
2	B	517	LEU	2.8
1	A	234	ILE	2.8
2	B	794	PHE	2.8
1	A	186	LEU	2.7
1	A	136	THR	2.7
1	A	237	THR	2.6
1	A	270	CYS	2.6
2	B	591	ILE	2.6
1	A	493	LEU	2.5
1	A	242	GLU	2.5
2	B	814	PHE	2.4
1	A	267	ASN	2.4
1	A	137	ILE	2.4
2	B	835	PHE	2.4
1	A	215	ALA	2.3
2	B	884	PHE	2.3
1	A	348	LEU	2.3
1	A	293	LEU	2.3
1	A	504	LEU	2.2
1	A	223	LEU	2.2
1	A	84	LEU	2.2
2	B	782	LEU	2.1
2	B	802	ASP	2.1
1	A	213	ASN	2.1
1	A	271	LYS	2.1
1	A	244	ALA	2.0
1	A	461	ILE	2.0
1	A	83	ARG	2.0
1	A	316	MET	2.0
1	A	70	LEU	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.