Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:25 PM GMT

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PDB ID	:	4U7N
Title	:	Inactive structure of histidine kinase
Authors	:	Cai, Y.; Hu, X.; Sang, J.
Deposited on	:	2014-07-31
Resolution	:	3.20 Å(reported)

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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.
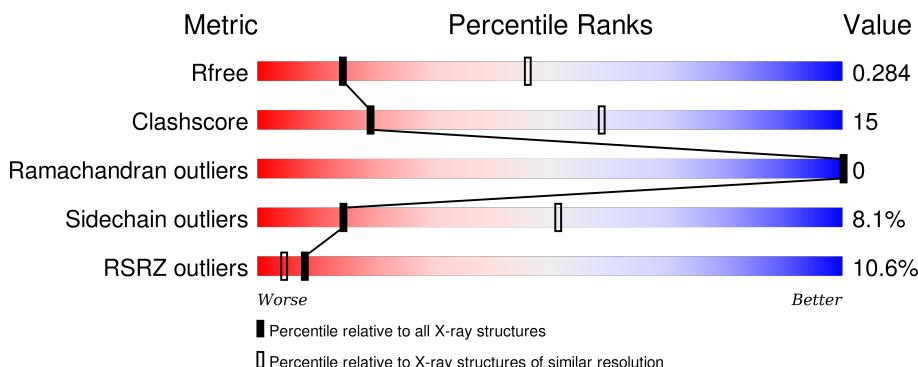
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	277	10% 47% 26% • 24%
1	B	277	6% 50% 24% • 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3394 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 Histidine protein kinase sensor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total 1695	C 1073	N 287	O 326	S 9	0	0	0
1	B	212	Total 1699	C 1075	N 288	O 327	S 9	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	MET	-	expression tag	UNP C6VIM1
A	349	GLY	-	expression tag	UNP C6VIM1
A	350	SER	-	expression tag	UNP C6VIM1
A	351	SER	-	expression tag	UNP C6VIM1
A	352	HIS	-	expression tag	UNP C6VIM1
A	353	HIS	-	expression tag	UNP C6VIM1
A	354	HIS	-	expression tag	UNP C6VIM1
A	355	HIS	-	expression tag	UNP C6VIM1
A	356	HIS	-	expression tag	UNP C6VIM1
A	357	HIS	-	expression tag	UNP C6VIM1
A	358	SER	-	expression tag	UNP C6VIM1
A	359	SER	-	expression tag	UNP C6VIM1
A	360	GLY	-	expression tag	UNP C6VIM1
A	361	LEU	-	expression tag	UNP C6VIM1
A	362	VAL	-	expression tag	UNP C6VIM1
A	363	PRO	-	expression tag	UNP C6VIM1
A	364	ARG	-	expression tag	UNP C6VIM1
A	365	GLY	-	expression tag	UNP C6VIM1
A	366	SER	-	expression tag	UNP C6VIM1
A	367	ALA	-	expression tag	UNP C6VIM1
A	368	GLU	-	expression tag	UNP C6VIM1
A	369	PHE	-	expression tag	UNP C6VIM1
B	348	MET	-	expression tag	UNP C6VIM1
B	349	GLY	-	expression tag	UNP C6VIM1
B	350	SER	-	expression tag	UNP C6VIM1

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| Chain	Residue	Modelled	Actual	Comment	Reference
B	351	SER	-	expression tag	UNP C6VIM1
B	352	HIS	-	expression tag	UNP C6VIM1
B	353	HIS	-	expression tag	UNP C6VIM1
B	354	HIS	-	expression tag	UNP C6VIM1
B	355	HIS	-	expression tag	UNP C6VIM1
B	356	HIS	-	expression tag	UNP C6VIM1
B	357	HIS	-	expression tag	UNP C6VIM1
B	358	SER	-	expression tag	UNP C6VIM1
B	359	SER	-	expression tag	UNP C6VIM1
B	360	GLY	-	expression tag	UNP C6VIM1
B	361	LEU	-	expression tag	UNP C6VIM1
B	362	VAL	-	expression tag	UNP C6VIM1
B	363	PRO	-	expression tag	UNP C6VIM1
B	364	ARG	-	expression tag	UNP C6VIM1
B	365	GLY	-	expression tag	UNP C6VIM1
B	366	SER	-	expression tag	UNP C6VIM1
B	367	ALA	-	expression tag	UNP C6VIM1
B	368	GLU	-	expression tag	UNP C6VIM1
B	369	PHE	-	expression tag	UNP C6VIM1

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Histidine protein kinase sensor protein
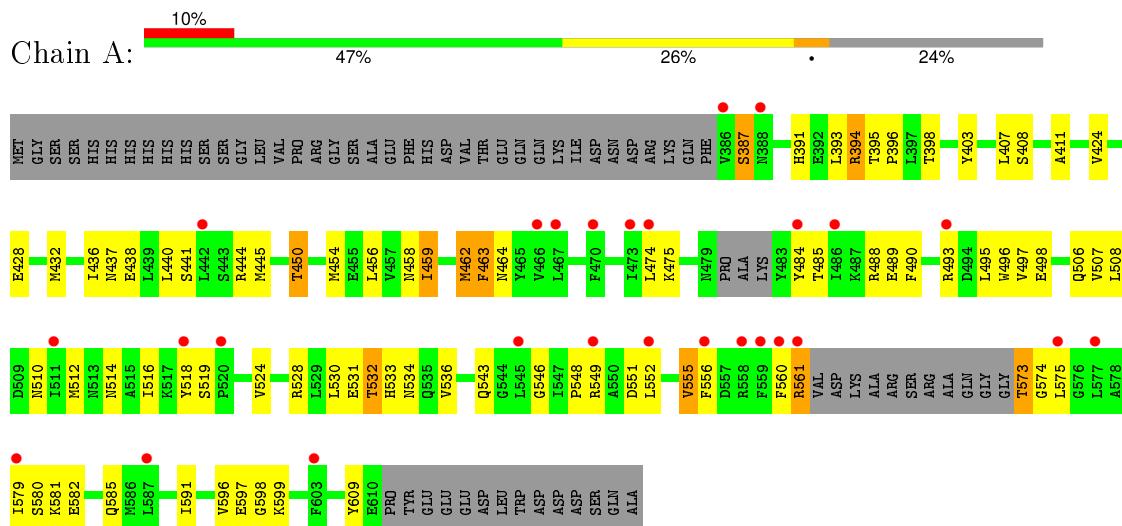
• Molecule 1: Histidine protein kinase sensor protein
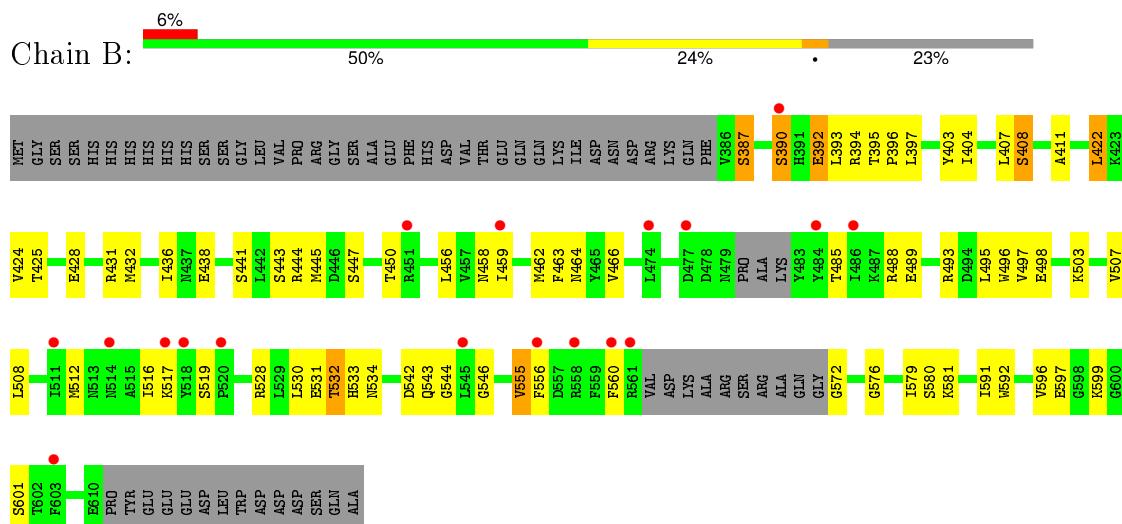
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	91.60Å 91.60Å 97.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.39 – 3.20 23.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (23.39-3.20) 90.5 (23.39-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.251 , 0.285 0.252 , 0.284	Depositor DCC
R_{free} test set	3161 reflections (10.57%)	DCC
Wilson B-factor (Å^2)	101.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 154.3	EDS
Estimated twinning fraction	0.019 for -h,-k,l 0.447 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 18166 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3394	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/1723	0.58	0/2326
1	B	0.40	0/1727	0.65	0/2331
All	All	0.39	0/3450	0.62	0/4657

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 (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	1695	0	1684	56	0
1	B	1699	0	1687	51	0
All	All	3394	0	3371	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (102) 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:407:LEU:HA	1:B:411:ALA:HB3	1.56	0.88
1:A:407:LEU:HA	1:A:411:ALA:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:HG2	1:A:579:ILE:HD11	1.57	0.84
1:B:581:LYS:HA	1:B:591:ILE:HG21	1.71	0.72
1:A:581:LYS:HA	1:A:591:ILE:HG21	1.75	0.68
1:A:403:TYR:CZ	1:A:424:VAL:HG11	2.29	0.68
1:B:489:GLU:OE1	1:B:528:ARG:NH1	2.26	0.68
1:B:403:TYR:CZ	1:B:424:VAL:HG11	2.29	0.67
1:B:493:ARG:NH2	1:B:531:GLU:HB3	2.10	0.66
1:B:493:ARG:CZ	1:B:531:GLU:HB3	2.26	0.65
1:A:445:MET:HG2	1:A:450:THR:HG21	1.78	0.65
1:A:493:ARG:CZ	1:A:531:GLU:HB3	2.27	0.65
1:B:438:GLU:HG2	1:B:579:ILE:HD11	1.79	0.64
1:A:437:ASN:HD21	1:B:394:ARG:HH12	1.47	0.63
1:A:546:GLY:HA3	1:A:597:GLU:HA	1.80	0.62
1:A:454:MET:HG2	1:A:498:GLU:HG2	1.81	0.62
1:A:493:ARG:NH2	1:A:531:GLU:HB3	2.15	0.61
1:B:519:SER:HA	1:B:544:GLY:HA3	1.81	0.61
1:B:596:VAL:O	1:B:599:LYS:N	2.34	0.61
1:A:440:LEU:HD13	1:B:390:SER:HB2	1.83	0.60
1:A:561:ARG:HH12	1:A:574:GLY:HA2	1.66	0.59
1:B:532:THR:O	1:B:532:THR:OG1	2.16	0.59
1:B:445:MET:HG2	1:B:450:THR:HG21	1.85	0.59
1:B:556:PHE:HB3	1:B:581:LYS:HD2	1.83	0.58
1:B:546:GLY:HA3	1:B:597:GLU:HA	1.86	0.57
1:B:464:ASN:OD1	1:B:488:ARG:NH1	2.37	0.57
1:A:489:GLU:OE1	1:A:528:ARG:NH1	2.38	0.56
1:A:458:ASN:HB2	1:A:496:TRP:CZ3	2.41	0.55
1:A:596:VAL:O	1:A:599:LYS:N	2.40	0.55
1:A:387:SER:O	1:A:391:HIS:ND1	2.36	0.55
1:A:403:TYR:CE1	1:A:424:VAL:HG11	2.42	0.54
1:B:493:ARG:HD2	1:B:495:LEU:HD21	1.89	0.54
1:A:507:VAL:HG22	1:A:580:SER:HA	1.91	0.54
1:A:437:ASN:OD1	1:B:394:ARG:NH1	2.41	0.53
1:B:447:SER:OG	1:B:447:SER:O	2.27	0.53
1:A:549:ARG:HA	1:A:552:LEU:HB2	1.90	0.52
1:A:393:LEU:O	1:A:396:PRO:HD2	2.10	0.51
1:A:507:VAL:HG13	1:A:580:SER:HB3	1.92	0.51
1:A:459:ILE:HD11	1:A:497:VAL:HB	1.93	0.51
1:B:445:MET:HA	1:B:450:THR:CG2	2.41	0.50
1:A:458:ASN:HB2	1:A:496:TRP:CH2	2.46	0.50
1:B:533:HIS:O	1:B:534:ASN:HB2	2.12	0.50
1:A:474:LEU:HD21	1:A:516:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:PHE:HB3	1:A:581:LYS:HD2	1.93	0.50
1:A:463:PHE:HB3	1:A:490:PHE:CE2	2.47	0.49
1:A:532:THR:O	1:A:532:THR:OG1	2.16	0.49
1:A:441:SER:HA	1:A:444:ARG:HG2	1.95	0.48
1:B:493:ARG:HH12	1:B:531:GLU:H	1.61	0.48
1:B:393:LEU:O	1:B:396:PRO:HD2	2.14	0.48
1:B:443:SER:O	1:B:447:SER:HB3	2.13	0.48
1:A:438:GLU:OE1	1:A:575:LEU:HB2	2.13	0.48
1:A:493:ARG:HH12	1:A:531:GLU:H	1.61	0.48
1:A:495:LEU:HD13	1:A:536:VAL:HG22	1.96	0.48
1:A:533:HIS:O	1:A:534:ASN:HB2	2.14	0.48
1:B:556:PHE:HE2	1:B:592:TRP:HA	1.78	0.47
1:B:542:ASP:OD1	1:B:601:SER:HB2	2.15	0.47
1:B:517:LYS:HZ3	1:B:572:GLY:N	2.12	0.47
1:A:394:ARG:HH11	1:A:398:THR:HG21	1.80	0.47
1:B:403:TYR:CE1	1:B:424:VAL:HG11	2.50	0.46
1:A:459:ILE:HA	1:A:462:MET:HB3	1.97	0.46
1:B:392:GLU:HG3	1:B:392:GLU:O	2.15	0.46
1:A:512:MET:O	1:A:516:ILE:HG13	2.16	0.46
1:B:458:ASN:HB2	1:B:496:TRP:CH2	2.51	0.46
1:B:459:ILE:HD11	1:B:497:VAL:HB	1.98	0.45
1:A:436:ILE:HA	1:A:436:ILE:HD13	1.79	0.45
1:A:438:GLU:OE1	1:A:573:THR:OG1	2.34	0.45
1:A:534:ASN:HA	1:A:609:TYR:HB3	1.99	0.45
1:B:441:SER:HA	1:B:444:ARG:HG2	1.99	0.45
1:B:576:GLY:HA2	1:B:579:ILE:HD12	1.99	0.45
1:A:394:ARG:HG2	1:B:436:ILE:HG21	1.99	0.44
1:A:548:PRO:HB2	1:A:551:ASP:OD1	2.17	0.44
1:B:428:GLU:OE2	1:B:431:ARG:NH1	2.50	0.43
1:B:458:ASN:HB2	1:B:496:TRP:CZ3	2.53	0.43
1:A:493:ARG:HD2	1:A:495:LEU:HD21	1.99	0.43
1:A:532:THR:O	1:A:533:HIS:HB2	2.18	0.43
1:A:395:THR:HB	1:A:396:PRO:HD3	2.01	0.43
1:B:555:VAL:HA	1:B:560:PHE:CD2	2.54	0.43
1:A:474:LEU:HD22	1:A:484:TYR:HB2	2.01	0.42
1:B:395:THR:HB	1:B:396:PRO:HD3	2.01	0.42
1:B:512:MET:O	1:B:516:ILE:HG13	2.19	0.42
1:B:459:ILE:HA	1:B:462:MET:HB3	2.01	0.42
1:B:438:GLU:CG	1:B:579:ILE:HD11	2.47	0.41
1:B:503:LYS:O	1:B:507:VAL:HG23	2.20	0.41
1:B:507:VAL:HG22	1:B:580:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:HB	1:A:524:VAL:HG22	2.03	0.41
1:A:597:GLU:HA	1:A:598:GLY:HA2	1.44	0.41
1:A:506:GLN:O	1:A:510:ASN:ND2	2.53	0.41
1:B:422:LEU:O	1:B:425:THR:OG1	2.29	0.41
1:A:440:LEU:HD11	1:B:387:SER:HA	2.01	0.41
1:A:555:VAL:HA	1:A:560:PHE:CD2	2.55	0.41
1:A:514:ASN:O	1:A:518:TYR:HB2	2.21	0.41
1:B:404:ILE:O	1:B:408:SER:OG	2.37	0.41
1:A:428:GLU:O	1:A:432:MET:HG3	2.21	0.41
1:A:464:ASN:OD1	1:A:488:ARG:NH1	2.53	0.41
1:B:493:ARG:HH11	1:B:495:LEU:HD21	1.85	0.41
1:B:532:THR:O	1:B:533:HIS:HB2	2.20	0.41
1:B:397:LEU:HD23	1:B:432:MET:CE	2.50	0.41
1:B:508:LEU:HD23	1:B:508:LEU:HA	1.81	0.41
1:B:462:MET:O	1:B:466:VAL:HG23	2.21	0.40
1:A:508:LEU:HA	1:A:508:LEU:HD23	1.83	0.40
1:A:531:GLU:HG3	1:A:609:TYR:CD2	2.57	0.40
1:A:534:ASN:CA	1:A:609:TYR:HB3	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	205/277 (74%)	196 (96%)	9 (4%)	0	100	100
1	B	206/277 (74%)	194 (94%)	12 (6%)	0	100	100
All	All	411/554 (74%)	390 (95%)	21 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	191/247 (77%)	173 (91%)	18 (9%)	11	41
1	B	191/247 (77%)	178 (93%)	13 (7%)	20	59
All	All	382/494 (77%)	351 (92%)	31 (8%)	15	51

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	387	SER
1	A	394	ARG
1	A	408	SER
1	A	450	THR
1	A	456	LEU
1	A	459	ILE
1	A	462	MET
1	A	463	PHE
1	A	475	LYS
1	A	519	SER
1	A	530	LEU
1	A	532	THR
1	A	543	GLN
1	A	555	VAL
1	A	561	ARG
1	A	573	THR
1	A	582	GLU
1	A	585	GLN
1	B	387	SER
1	B	390	SER
1	B	392	GLU
1	B	408	SER
1	B	422	LEU
1	B	456	LEU
1	B	463	PHE
1	B	485	THR
1	B	498	GLU

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Mol	Chain	Res	Type
1	B	530	LEU
1	B	532	THR
1	B	543	GLN
1	B	555	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	211/277 (76%)	0.68	27 (12%)	5	3	77, 146, 279, 466	0
1	B	212/277 (76%)	0.68	18 (8%)	13	7	69, 145, 260, 532	0
All	All	423/554 (76%)	0.68	45 (10%)	8	4	69, 145, 266, 532	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	TYR	12.9
1	B	558	ARG	11.0
1	B	520	PRO	10.3
1	B	560	PHE	7.8
1	A	386	VAL	7.3
1	B	561	ARG	6.4
1	A	561	ARG	5.5
1	A	484	TYR	5.3
1	A	559	PHE	5.0
1	A	545	LEU	4.7
1	A	560	PHE	4.3
1	A	552	LEU	4.2
1	A	520	PRO	4.1
1	A	558	ARG	3.8
1	A	473	ILE	3.7
1	B	486	ILE	3.6
1	B	477	ASP	3.6
1	A	474	LEU	3.6
1	A	511	ILE	3.3
1	B	474	LEU	3.2
1	A	388	ASN	3.0
1	A	603	PHE	2.9
1	A	467	LEU	2.9
1	B	603	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	486	ILE	2.8
1	B	517	LYS	2.8
1	A	556	PHE	2.7
1	B	545	LEU	2.6
1	A	579	ILE	2.6
1	B	556	PHE	2.6
1	B	511	ILE	2.6
1	A	466	VAL	2.4
1	B	518	TYR	2.4
1	A	575	LEU	2.4
1	B	514	ASN	2.3
1	A	587	LEU	2.1
1	B	390	SER	2.1
1	A	549	ARG	2.1
1	A	493	ARG	2.1
1	A	470	PHE	2.1
1	B	459	ILE	2.1
1	A	577	LEU	2.1
1	A	518	TYR	2.1
1	A	442	LEU	2.0
1	B	451	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.