Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:16 PM GMT

PDB ID	:	4RED
Title	:	Crystal structure of human AMPK alpha1 KD-AID with K43A mutation
Authors	:	Zhou, X.E.; Ke, J.; Li, X.; Wang, L.; Gu, X.; de Waal, P.W.; Tan, M.H.E.; Wang, D.; Wu, D.; Xu, H.E.; Melcher, K.
Deposited on	:	2014-09-22
Resolution	:	2.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

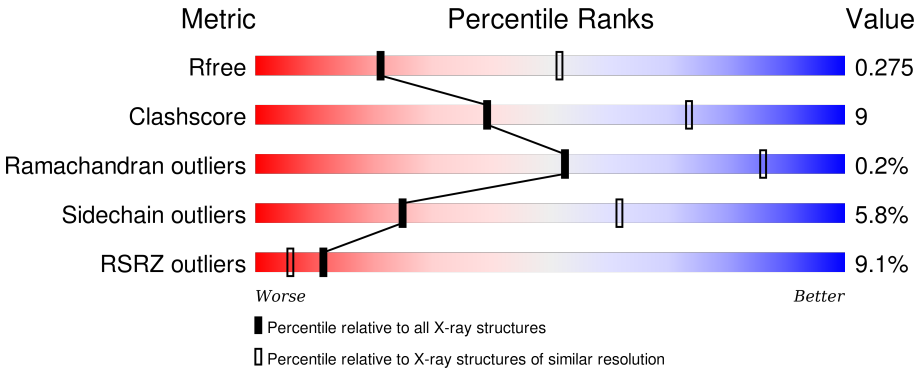
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	351	11% 72% 19% • 7%
1	B	351	6% 75% 17% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5323 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2628	1683	448	481	16			
1	B	332	Total	C	N	O	S	0	0	0
			2665	1704	454	490	17			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	EXPRESSION TAG	UNP Q13131
A	4	GLY	-	EXPRESSION TAG	UNP Q13131
A	5	HIS	-	EXPRESSION TAG	UNP Q13131
A	6	HIS	-	EXPRESSION TAG	UNP Q13131
A	7	HIS	-	EXPRESSION TAG	UNP Q13131
A	8	HIS	-	EXPRESSION TAG	UNP Q13131
A	9	HIS	-	EXPRESSION TAG	UNP Q13131
A	10	HIS	-	EXPRESSION TAG	UNP Q13131
A	11	GLY	-	EXPRESSION TAG	UNP Q13131
A	12	SER	-	EXPRESSION TAG	UNP Q13131
A	43	ALA	LYS	ENGINEERED MUTATION	UNP Q13131
A	260	SER	THR	CONFLICT	UNP Q13131
A	287	THR	SER	CONFLICT	UNP Q13131
B	3	MET	-	EXPRESSION TAG	UNP Q13131
B	4	GLY	-	EXPRESSION TAG	UNP Q13131
B	5	HIS	-	EXPRESSION TAG	UNP Q13131
B	6	HIS	-	EXPRESSION TAG	UNP Q13131
B	7	HIS	-	EXPRESSION TAG	UNP Q13131
B	8	HIS	-	EXPRESSION TAG	UNP Q13131
B	9	HIS	-	EXPRESSION TAG	UNP Q13131
B	10	HIS	-	EXPRESSION TAG	UNP Q13131
B	11	GLY	-	EXPRESSION TAG	UNP Q13131
B	12	SER	-	EXPRESSION TAG	UNP Q13131
B	43	ALA	LYS	ENGINEERED MUTATION	UNP Q13131
B	260	SER	THR	CONFLICT	UNP Q13131

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Chain	Residue	Modelled	Actual	Comment	Reference
B	287	THR	SER	CONFLICT	UNP Q13131

- Molecule 2 is water.

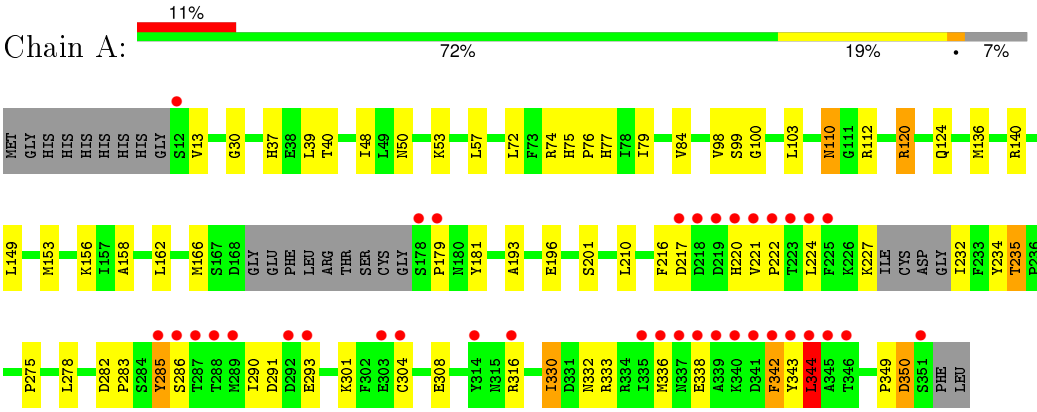
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	15	Total O 15 15	0	0

3 Residue-property plots (i)

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.

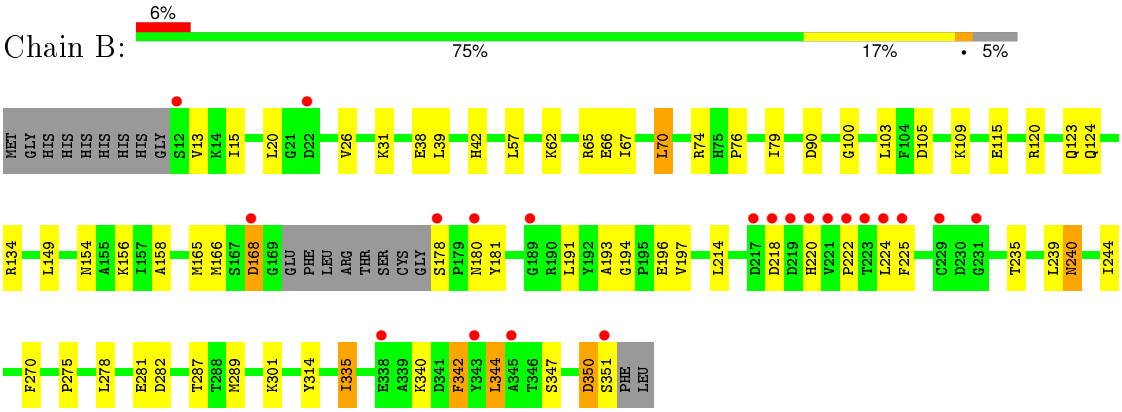
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1

Chain A:



- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.53Å 119.53Å 215.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.95 29.88 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.90-2.95) 99.9 (29.88-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.42 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.230 , 0.277 0.228 , 0.275	Depositor DCC
R_{free} test set	1222 reflections (7.82%)	DCC
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 16852 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5323	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/2688	0.72	1/3634 (0.0%)
1	B	0.44	0/2726	0.63	0/3685
All	All	0.45	0/5414	0.67	1/7319 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	MET	CA-CB-CG	5.15	122.06	113.30

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	2628	0	2620	51	0
1	B	2665	0	2660	49	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
All	All	5323	0	5280	94	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 (94) 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:335:ILE:H	1:B:335:ILE:HD13	1.31	0.94
1:A:344:LEU:HD11	1:B:74:ARG:HB3	1.62	0.82
1:B:168:ASP:OD1	1:B:168:ASP:N	2.15	0.77
1:A:285:TYR:HD1	1:A:286:SER:H	1.36	0.72
1:A:285:TYR:CD1	1:A:286:SER:N	2.59	0.71
1:A:120:ARG:NH2	1:A:153:MET:O	2.25	0.69
1:B:13:VAL:HG12	1:B:20:LEU:HD23	1.74	0.69
1:B:350:ASP:OD1	1:B:350:ASP:N	2.26	0.68
1:A:301:LYS:HB3	1:B:39:LEU:HD23	1.75	0.68
1:A:110:ASN:OD1	1:A:110:ASN:N	2.27	0.68
1:B:240:ASN:HD22	1:B:240:ASN:H	1.39	0.68
1:A:148:LEU:HD21	1:A:158:ALA:HB2	1.76	0.68
1:B:79:ILE:HD13	1:B:158:ALA:HA	1.75	0.67
1:A:343:TYR:O	1:A:344:LEU:HD13	1.97	0.64
1:B:134:ARG:NH1	1:B:282:ASP:OD2	2.30	0.63
1:A:350:ASP:OD1	1:A:350:ASP:N	2.32	0.63
1:B:287:THR:HG22	1:B:314:TYR:OH	1.99	0.63
1:A:343:TYR:O	1:A:344:LEU:HD22	1.98	0.63
1:A:76:PRO:O	1:A:156:LYS:NZ	2.31	0.62
1:A:338:GLU:HA	1:A:342:PHE:CD2	2.36	0.61
1:B:218:ASP:HB2	1:B:224:LEU:HA	1.82	0.60
1:B:180:ASN:HB2	1:B:214:LEU:HD13	1.82	0.60
1:A:220:HIS:CE1	1:A:222:PRO:HD2	2.37	0.60
1:A:338:GLU:HA	1:A:342:PHE:HD2	1.68	0.58
1:B:193:ALA:N	1:B:196:GLU:OE2	2.31	0.58
1:B:38:GLU:HG3	1:B:39:LEU:HD12	1.85	0.58
1:B:289:MET:HE1	1:B:342:PHE:HB3	1.86	0.57
1:A:99:SER:N	2:A:404:HOH:O	2.29	0.57
1:B:15:ILE:HG22	1:B:20:LEU:HD21	1.86	0.56
1:B:62:LYS:O	1:B:65:ARG:HB3	2.05	0.56
1:B:100:GLY:HA3	1:B:149:LEU:O	2.06	0.56
1:A:75:HIS:HD2	1:B:344:LEU:HD12	1.70	0.56
1:A:220:HIS:ND1	1:A:222:PRO:HD2	2.21	0.55
1:B:194:GLY:HA2	1:B:197:VAL:HG22	1.88	0.55
1:A:112:ARG:HD2	1:A:210:LEU:O	2.06	0.54
1:B:103:LEU:HA	1:B:149:LEU:HD22	1.90	0.54
1:B:76:PRO:O	1:B:156:LYS:NZ	2.34	0.54
1:A:316:ARG:HB3	1:A:349:PRO:HB3	1.91	0.53
1:B:335:ILE:N	1:B:335:ILE:HD13	2.11	0.53
1:A:193:ALA:N	1:A:196:GLU:OE2	2.34	0.53
1:B:335:ILE:H	1:B:335:ILE:CD1	2.03	0.53
1:A:275:PRO:HB2	1:A:278:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ASN:HB2	1:B:214:LEU:CD1	2.39	0.52
1:A:39:LEU:HD23	1:B:301:LYS:HB3	1.93	0.51
1:B:115:GLU:OE1	1:B:240:ASN:ND2	2.44	0.51
1:B:105:ASP:O	1:B:109:LYS:HG2	2.11	0.51
1:A:30:GLY:HA3	1:A:48:ILE:O	2.11	0.50
1:B:240:ASN:HD22	1:B:240:ASN:N	2.10	0.50
1:A:179:PRO:HB2	1:A:217:ASP:OD2	2.13	0.49
1:A:216:PHE:HB3	1:A:227:LYS:HB3	1.95	0.49
1:A:50:ASN:OD1	1:A:53:LYS:HG3	2.13	0.49
1:A:37:HIS:HB3	1:A:40:THR:O	2.12	0.48
1:A:332:ASN:OD1	1:B:42:HIS:CD2	2.67	0.48
1:A:120:ARG:O	1:A:124:GLN:HG3	2.13	0.48
1:A:136:MET:HE1	1:A:140:ARG:HD3	1.97	0.47
1:A:136:MET:CE	1:A:140:ARG:HD3	2.45	0.47
1:B:342:PHE:HD1	1:B:342:PHE:H	1.62	0.46
1:B:344:LEU:O	1:B:344:LEU:HG	2.16	0.46
1:A:221:VAL:HA	1:A:224:LEU:HD12	1.98	0.46
1:A:57:LEU:HA	1:A:57:LEU:HD12	1.72	0.46
1:A:77:HIS:O	1:A:156:LYS:HA	2.16	0.45
1:A:100:GLY:HA3	1:A:149:LEU:O	2.17	0.45
1:B:26:VAL:HG12	1:B:31:LYS:HG2	1.99	0.45
1:A:282:ASP:N	1:A:283:PRO:HD3	2.31	0.45
1:A:75:HIS:CD2	1:B:344:LEU:HD12	2.51	0.44
1:B:120:ARG:O	1:B:124:GLN:HG3	2.18	0.44
1:A:234:TYR:CD1	1:A:235:THR:N	2.85	0.44
1:B:67:ILE:HA	1:B:70:LEU:HD22	1.98	0.44
1:A:144:PRO:HB2	1:A:181:TYR:OH	2.18	0.44
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.88	0.44
1:B:38:GLU:HG3	1:B:39:LEU:CD1	2.46	0.44
1:A:316:ARG:HD2	1:A:349:PRO:HB3	2.01	0.43
1:B:149:LEU:HA	1:B:154:ASN:O	2.18	0.43
1:A:221:VAL:HB	1:A:222:PRO:HD3	2.00	0.43
1:B:123:GLN:NE2	1:B:270:PHE:O	2.51	0.43
1:A:304:CYS:HB2	1:A:308:GLU:OE1	2.19	0.43
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.71	0.42
1:B:239:LEU:HB3	1:B:244:ILE:HD11	2.02	0.42
1:A:79:ILE:HD12	1:A:158:ALA:HA	2.01	0.42
1:A:293:GLU:HB2	1:A:333:ARG:HH11	1.84	0.42
1:B:340:LYS:HB2	1:B:340:LYS:HE2	1.63	0.41
1:A:330:ILE:HA	1:A:330:ILE:HD13	1.88	0.41
1:B:178:SER:O	1:B:180:ASN:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:SER:O	1:A:290:ILE:N	2.49	0.41
1:B:180:ASN:CG	1:B:181:TYR:H	2.24	0.41
1:A:238:TYR:O	1:A:238:TYR:CG	2.73	0.41
1:B:220:HIS:ND1	1:B:222:PRO:HD2	2.36	0.41
1:A:286:SER:O	1:A:290:ILE:HG13	2.21	0.41
1:B:66:GLU:O	1:B:70:LEU:HD13	2.20	0.41
1:A:148:LEU:CD2	1:A:158:ALA:HB2	2.49	0.41
1:B:196:GLU:HG3	1:B:197:VAL:H	1.86	0.41
1:B:224:LEU:HG	1:B:225:PHE:CD1	2.56	0.40
1:B:275:PRO:HB2	1:B:278:LEU:HG	2.03	0.40
1:A:291:ASP:OD2	1:A:330:ILE:HD11	2.21	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	321/351 (92%)	305 (95%)	15 (5%)	1 (0%)	46 81
1	B	328/351 (93%)	315 (96%)	13 (4%)	0	100 100
All	All	649/702 (92%)	620 (96%)	28 (4%)	1 (0%)	52 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	LEU

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	293/314 (93%)	274 (94%)	19 (6%)	21 56
1	B	298/314 (95%)	283 (95%)	15 (5%)	30 68
All	All	591/628 (94%)	557 (94%)	34 (6%)	25 62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	72	LEU
1	A	74	ARG
1	A	84	VAL
1	A	98	VAL
1	A	103	LEU
1	A	110	ASN
1	A	120	ARG
1	A	145	GLU
1	A	148	LEU
1	A	166	MET
1	A	201	SER
1	A	232	ILE
1	A	235	THR
1	A	285	TYR
1	A	330	ILE
1	A	342	PHE
1	A	344	LEU
1	A	350	ASP
1	B	70	LEU
1	B	90	ASP
1	B	165	MET
1	B	166	MET
1	B	168	ASP
1	B	191	LEU
1	B	235	THR
1	B	240	ASN
1	B	281	GLU
1	B	335	ILE
1	B	342	PHE
1	B	344	LEU
1	B	347	SER
1	B	350	ASP

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Mol	Chain	Res	Type
1	B	351	SER

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

Mol	Chain	Res	Type
1	B	240	ASN

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 carbohydrates 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	327/351 (93%)	0.39	39 (11%) 6 3	41, 68, 135, 177	0
1	B	332/351 (94%)	0.11	21 (6%) 23 12	45, 63, 124, 156	0
All	All	659/702 (93%)	0.25	60 (9%) 11 6	41, 65, 128, 177	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	ASP	6.9
1	A	339	ALA	6.8
1	A	343	TYR	6.6
1	B	224	LEU	6.5
1	A	222	PRO	6.4
1	B	220	HIS	6.2
1	A	221	VAL	6.1
1	A	225	PHE	6.0
1	B	12	SER	5.4
1	A	220	HIS	5.2
1	A	336	MET	5.1
1	A	287	THR	4.7
1	B	223	THR	4.6
1	A	223	THR	4.6
1	B	225	PHE	4.5
1	B	219	ASP	4.5
1	A	292	ASP	4.2
1	A	237	GLN	4.2
1	A	178	SER	4.1
1	A	342	PHE	4.1
1	A	238	TYR	3.9
1	A	337	ASN	3.8
1	A	285	TYR	3.8
1	A	289	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	3.7
1	B	221	VAL	3.4
1	B	168	ASP	3.3
1	A	217	ASP	3.2
1	B	218	ASP	3.2
1	A	338	GLU	3.1
1	B	229	CYS	3.1
1	A	303	GLU	3.0
1	B	338	GLU	3.0
1	B	217	ASP	3.0
1	A	340	LYS	2.9
1	A	288	THR	2.8
1	B	345	ALA	2.7
1	A	224	LEU	2.6
1	B	180	ASN	2.6
1	A	286	SER	2.5
1	B	351	SER	2.5
1	A	316	ARG	2.5
1	B	231	GLY	2.5
1	A	12	SER	2.5
1	B	189	GLY	2.4
1	A	179	PRO	2.4
1	A	351	SER	2.4
1	A	304	CYS	2.4
1	A	341	ASP	2.3
1	A	335	ILE	2.3
1	B	178	SER	2.2
1	A	293	GLU	2.2
1	A	345	ALA	2.2
1	A	344	LEU	2.1
1	A	346	THR	2.1
1	B	22	ASP	2.1
1	B	222	PRO	2.1
1	A	257	LYS	2.1
1	B	343	TYR	2.1
1	A	314	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.