Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:41 pm BST

PDB ID	:	5CLR
Title	:	Crystal structure of LegK4_APO Kinase
Authors	:	Flayhan, A.; Terradot, L.
Deposited on	:	2015-07-16
Resolution	:	3.71 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 following versions of software and data (see references ⓘ) were used in the production of this report:

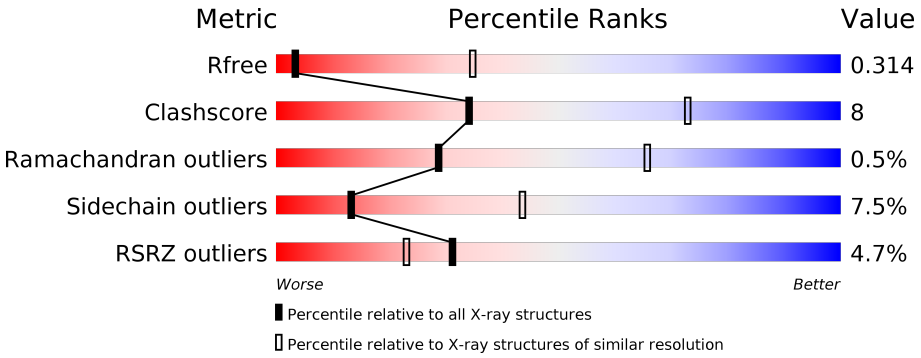
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.71 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	451	2% 64% 18% • 17%
1	B	451	5% 51% 16% • 29%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5596 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 LegK4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	0	0
			3017	1955	496	553	5	8			
1	B	321	Total	C	N	O	S	Se	0	0	0
			2579	1685	424	460	3	7			

There are 14 discrepancies between the modelled and reference sequences:

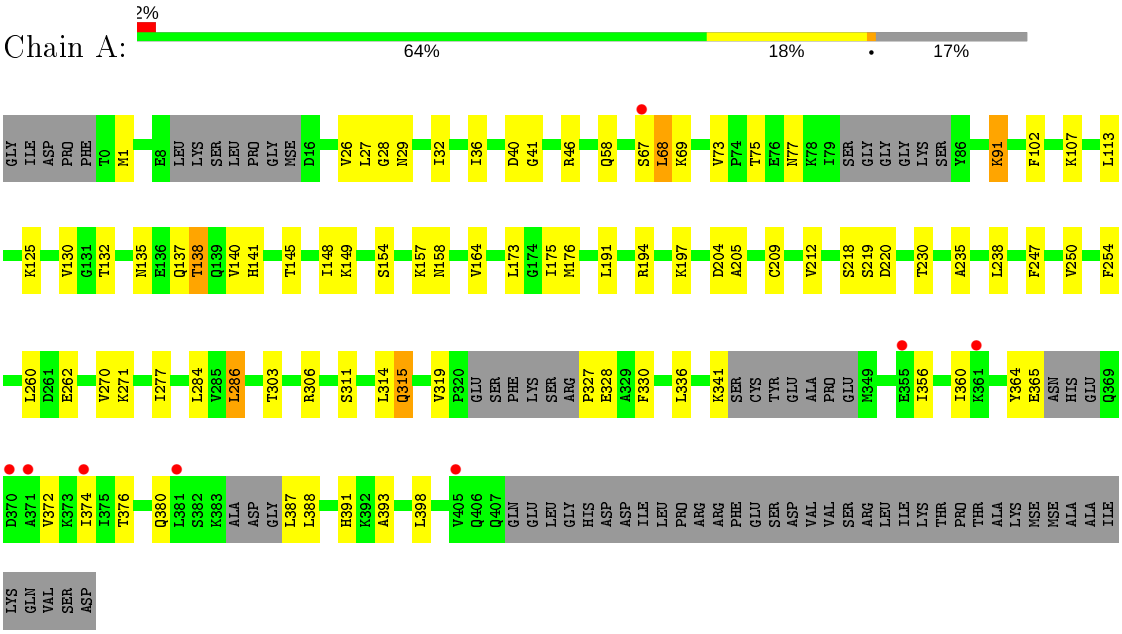
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q5WZW9
A	-4	ILE	-	expression tag	UNP Q5WZW9
A	-3	ASP	-	expression tag	UNP Q5WZW9
A	-2	PRO	-	expression tag	UNP Q5WZW9
A	-1	PHE	-	expression tag	UNP Q5WZW9
A	0	THR	-	expression tag	UNP Q5WZW9
A	1	MSE	-	expression tag	UNP Q5WZW9
B	-5	GLY	-	expression tag	UNP Q5WZW9
B	-4	ILE	-	expression tag	UNP Q5WZW9
B	-3	ASP	-	expression tag	UNP Q5WZW9
B	-2	PRO	-	expression tag	UNP Q5WZW9
B	-1	PHE	-	expression tag	UNP Q5WZW9
B	0	THR	-	expression tag	UNP Q5WZW9
B	1	MSE	-	expression tag	UNP Q5WZW9

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 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.

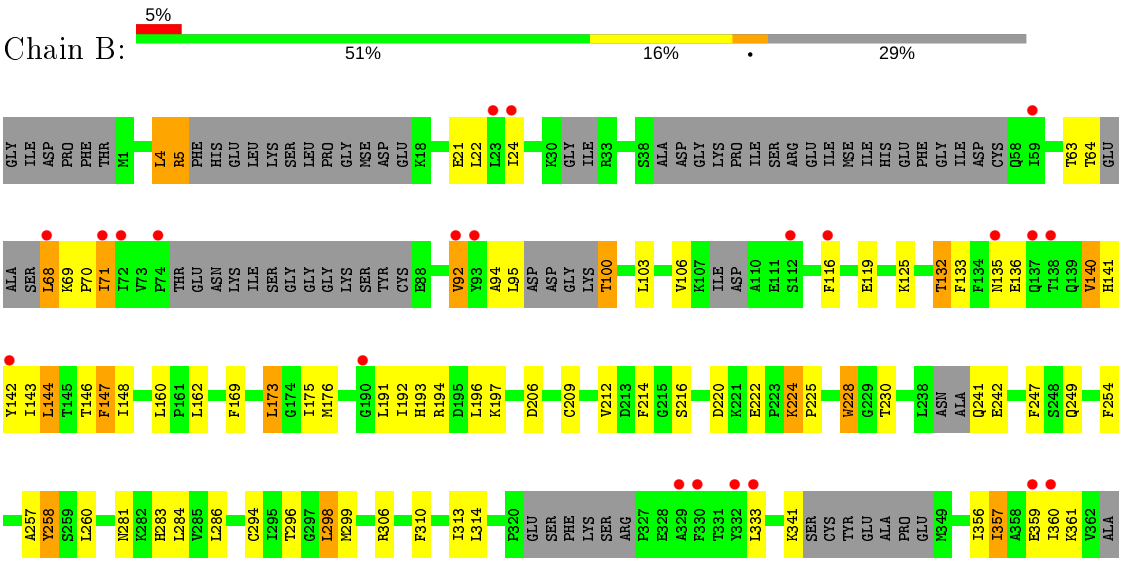
- Molecule 1: LegK4

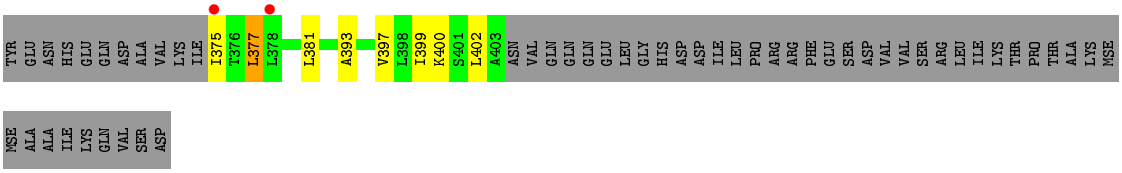
Chain A:



- Molecule 1: LegK4

Chain B:




TYR GLU ASN HIS GLU GLN ASP ALA VAL LYS ILE I375 T376 L377 L378 L381 A393 V397 L398 I399 K400 S401 L402 A403 ASN VAL GLN GLN GLN GLU LEU GLY HIS ASP ASP ILE LEU PRO ARG ARG PHE GLU SER ASP VAL VAL SER ARG LEU ILE LYS THR PRO THR ALA LYS MSE
MSE ALA ALA ILE LYS GLN VAL SER ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.82Å 154.82Å 87.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.69 – 3.71 44.69 – 3.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.69-3.71) 96.1 (44.69-3.71)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.282 , 0.311 0.293 , 0.314	Depositor DCC
R_{free} test set	651 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	104.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5596	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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	0.21	0/3061	0.38	0/4111
1	B	0.21	0/2613	0.36	0/3502
All	All	0.21	0/5674	0.37	0/7613

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	3017	0	3108	52	0
1	B	2579	0	2695	47	0
All	All	5596	0	5803	96	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 8.

All (96) 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:194:ARG:NH1	1:A:218:SER:HB3	2.04	0.72
1:A:311:SER:O	1:A:315:GLN:NE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG12	1:A:306:ARG:HD2	1.75	0.68
1:B:136:GLU:OE2	1:B:136:GLU:N	2.29	0.65
1:A:135:ASN:ND2	1:A:137:GLN:O	2.31	0.63
1:B:228:TRP:HA	1:B:228:TRP:CE3	2.32	0.63
1:B:228:TRP:HA	1:B:228:TRP:HE3	1.65	0.61
1:B:135:ASN:HB2	1:B:140:VAL:HG23	1.83	0.59
1:B:257:ALA:HB2	1:B:298:LEU:HB3	1.84	0.58
1:A:197:LYS:HE3	1:A:230:THR:HG21	1.86	0.57
1:A:286:LEU:HD12	1:A:393:ALA:HB2	1.87	0.57
1:A:271:LYS:HA	1:B:299:MSE:HE1	1.87	0.57
1:B:132:THR:OG1	1:B:141:HIS:NE2	2.39	0.56
1:B:360:ILE:HD13	1:B:377:LEU:HD22	1.88	0.55
1:B:103:LEU:HD11	1:B:142:TYR:HB3	1.89	0.54
1:A:69:LYS:HB3	1:A:69:LYS:NZ	2.21	0.54
1:B:106:VAL:HG11	1:B:116:PHE:HB2	1.89	0.54
1:B:71:ILE:HG12	1:B:92:VAL:HB	1.89	0.54
1:A:250:VAL:HG11	1:A:303:THR:HG23	1.90	0.53
1:A:154:SER:O	1:A:158:ASN:ND2	2.40	0.53
1:A:235:ALA:HB3	1:A:238:LEU:HG	1.91	0.53
1:B:375:ILE:HG23	1:B:399:ILE:HG23	1.90	0.53
1:A:29:ASN:HB2	1:A:32:ILE:HG13	1.90	0.52
1:A:27:LEU:N	1:A:28:GLY:HA3	2.23	0.52
1:B:356:ILE:HD13	1:B:381:LEU:HB2	1.90	0.52
1:B:254:PHE:HB2	1:B:306:ARG:HH11	1.74	0.51
1:A:204:ASP:OD1	1:A:205:ALA:N	2.41	0.51
1:A:270:VAL:HG11	1:B:296:THR:HA	1.92	0.51
1:B:220:ASP:HB3	1:B:222:GLU:HG2	1.92	0.51
1:A:107:LYS:NZ	1:A:138:THR:HG22	2.25	0.50
1:B:125:LYS:NZ	1:B:191:LEU:HD11	2.27	0.50
1:A:270:VAL:HG12	1:B:299:MSE:HE2	1.93	0.50
1:A:26:VAL:C	1:A:28:GLY:HA3	2.33	0.49
1:B:284:LEU:HD23	1:B:397:VAL:HG22	1.94	0.49
1:A:77:ASN:ND2	1:A:91:LYS:O	2.46	0.49
1:B:281:ASN:HB3	1:B:283:HIS:CE1	2.48	0.48
1:B:341:LYS:NZ	1:B:341:LYS:HB3	2.28	0.48
1:A:194:ARG:NH2	1:A:220:ASP:O	2.41	0.48
1:A:1:MSE:HE1	1:A:36:ILE:HG22	1.96	0.48
1:A:376:THR:O	1:A:380:GLN:HG2	2.14	0.47
1:B:21:GLU:O	1:B:24:ILE:HG12	2.15	0.47
1:A:67:SER:HB2	1:A:68:LEU:HB3	1.97	0.47
1:B:169:PHE:O	1:B:173:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:HIS:CE1	1:B:400:LYS:HG2	2.49	0.47
1:A:132:THR:OG1	1:A:141:HIS:NE2	2.39	0.47
1:A:125:LYS:HD2	1:A:191:LEU:HD11	1.96	0.46
1:A:356:ILE:O	1:A:360:ILE:HG12	2.15	0.46
1:A:176:MSE:HE3	1:A:260:LEU:HG	1.97	0.46
1:A:336:LEU:HD23	1:A:398:LEU:HD11	1.98	0.46
1:A:138:THR:HB	1:A:140:VAL:HG23	1.98	0.46
1:A:40:ASP:HA	1:A:41:GLY:HA2	1.51	0.46
1:B:294:CYS:HB3	1:B:313:ILE:HB	1.97	0.45
1:B:359:GLU:HG3	1:B:377:LEU:HD23	1.98	0.45
1:B:119:GLU:HG3	1:B:214:PHE:HB2	1.98	0.45
1:A:102:PHE:HD2	1:A:145:THR:HB	1.81	0.45
1:A:77:ASN:OD1	1:A:77:ASN:N	2.48	0.45
1:B:175:ILE:HG23	1:B:209:CYS:SG	2.57	0.45
1:A:135:ASN:HD21	1:A:137:GLN:HB2	1.82	0.44
1:A:107:LYS:HZ2	1:A:138:THR:HG22	1.83	0.44
1:B:103:LEU:HD13	1:B:144:LEU:HD12	1.99	0.44
1:B:258:TYR:HD1	1:B:258:TYR:HA	1.73	0.44
1:A:67:SER:HA	1:A:68:LEU:HA	1.69	0.44
1:A:77:ASN:HD22	1:A:91:LYS:HG3	1.82	0.44
1:B:64:THR:HG21	1:B:69:LYS:HE3	2.00	0.44
1:B:63:THR:HA	1:B:68:LEU:HD22	2.00	0.44
1:A:327:PRO:HB2	1:A:328:GLU:H	1.64	0.44
1:A:58:GLN:HB2	1:A:73:VAL:HG13	2.00	0.44
1:B:94:ALA:H	1:B:100:THR:N	2.16	0.44
1:B:298:LEU:HD21	1:B:310:PHE:HB2	2.00	0.44
1:A:330:PHE:HE1	1:A:374:ILE:HG13	1.83	0.43
1:B:4:LEU:HB2	1:B:5:ARG:H	1.59	0.43
1:A:69:LYS:HB3	1:A:69:LYS:HZ3	1.83	0.42
1:A:194:ARG:HH12	1:A:218:SER:HB3	1.82	0.42
1:B:357:ILE:O	1:B:361:LYS:HG3	2.19	0.42
1:A:254:PHE:HB2	1:A:306:ARG:NH1	2.34	0.42
1:B:356:ILE:O	1:B:360:ILE:HG12	2.19	0.42
1:A:194:ARG:HG2	1:A:247:PHE:HB3	2.02	0.41
1:B:176:MSE:HE3	1:B:260:LEU:HG	2.02	0.41
1:A:330:PHE:HA	1:A:330:PHE:HD1	1.76	0.41
1:A:341:LYS:NZ	1:A:341:LYS:HB3	2.36	0.41
1:B:70:PRO:HG2	1:B:95:LEU:HB2	2.01	0.41
1:A:388:LEU:HD12	1:A:391:HIS:HE1	1.85	0.41
1:B:194:ARG:HG3	1:B:247:PHE:CG	2.56	0.41
1:B:393:ALA:O	1:B:397:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:OG	1:A:219:SER:N	2.54	0.41
1:A:387:LEU:HD11	1:A:391:HIS:HB2	2.01	0.41
1:A:175:ILE:HG23	1:A:209:CYS:SG	2.61	0.41
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.91	0.41
1:B:192:ILE:HG23	1:B:249:GLN:HA	2.03	0.40
1:A:46:ARG:HD2	1:A:75:THR:HG21	2.03	0.40
1:B:286:LEU:HD12	1:B:286:LEU:H	1.86	0.40
1:B:146:THR:HB	1:B:147:PHE:HD1	1.86	0.40
1:B:194:ARG:HB2	1:B:216:SER:HB3	2.04	0.40
1:B:224:LYS:HG2	1:B:225:PRO:HD2	2.02	0.40
1:A:157:LYS:HE2	1:A:262:GLU:O	2.21	0.40
1:A:277:ILE:HD12	1:A:284:LEU:HB2	2.04	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	362/451 (80%)	344 (95%)	17 (5%)	1 (0%)	41 74
1	B	297/451 (66%)	284 (96%)	11 (4%)	2 (1%)	22 59
All	All	659/902 (73%)	628 (95%)	28 (4%)	3 (0%)	29 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	PHE
1	B	148	ILE
1	A	130	VAL

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	338/390 (87%)	322 (95%)	16 (5%)	26 56
1	B	290/390 (74%)	259 (89%)	31 (11%)	6 30
All	All	628/780 (80%)	581 (92%)	47 (8%)	13 43

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	91	LYS
1	A	113	LEU
1	A	138	THR
1	A	148	ILE
1	A	149	LYS
1	A	164	VAL
1	A	173	LEU
1	A	212	VAL
1	A	286	LEU
1	A	314	LEU
1	A	315	GLN
1	A	319	VAL
1	A	364	TYR
1	A	365	GLU
1	A	372	VAL
1	B	4	LEU
1	B	5	ARG
1	B	22	LEU
1	B	68	LEU
1	B	71	ILE
1	B	92	VAL
1	B	100	THR
1	B	132	THR
1	B	133	PHE
1	B	140	VAL
1	B	143	ILE

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	160	LEU
1	B	162	LEU
1	B	173	LEU
1	B	193	HIS
1	B	197	LYS
1	B	206	ASP
1	B	212	VAL
1	B	224	LYS
1	B	228	TRP
1	B	230	THR
1	B	241	GLN
1	B	242	GLU
1	B	258	TYR
1	B	298	LEU
1	B	314	LEU
1	B	333	LEU
1	B	357	ILE
1	B	377	LEU
1	B	402	LEU

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

Mol	Chain	Res	Type
1	A	135	ASN

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

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	368/451 (81%)	0.17	8 (2%) 62 50	76, 96, 154, 184	0
1	B	314/451 (69%)	0.48	24 (7%) 13 10	77, 116, 186, 233	0
All	All	682/902 (75%)	0.31	32 (4%) 31 23	76, 100, 176, 233	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	TYR	4.5
1	B	59	ILE	4.4
1	B	360	ILE	4.0
1	B	92	VAL	3.9
1	B	332	TYR	3.9
1	B	330	PHE	3.9
1	B	23	LEU	3.7
1	B	24	ILE	3.5
1	B	375	ILE	3.5
1	A	374	ILE	3.2
1	B	329	ALA	3.2
1	B	142	TYR	3.1
1	A	67	SER	2.8
1	B	359	GLU	2.8
1	B	74	PRO	2.7
1	B	112	SER	2.6
1	B	138	THR	2.5
1	B	378	LEU	2.5
1	B	71	ILE	2.5
1	B	72	ILE	2.4
1	A	381	LEU	2.3
1	B	135	ASN	2.3
1	A	371	ALA	2.3
1	B	137	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	361	LYS	2.2
1	B	116	PHE	2.2
1	A	370	ASP	2.1
1	B	190	GLY	2.1
1	A	405	VAL	2.0
1	A	355	GLU	2.0
1	B	68	LEU	2.0
1	B	333	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.