



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:30 am GMT

PDB ID : 3KL8
Title : CaMKIINtide Inhibitor Complex
Authors : Kuriyan, J.; Chao, L.H.; Pellicena, P.; Deindl, S.; Barclay, L.A.; Schulman, H.
Deposited on : 2009-11-06
Resolution : 3.37 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

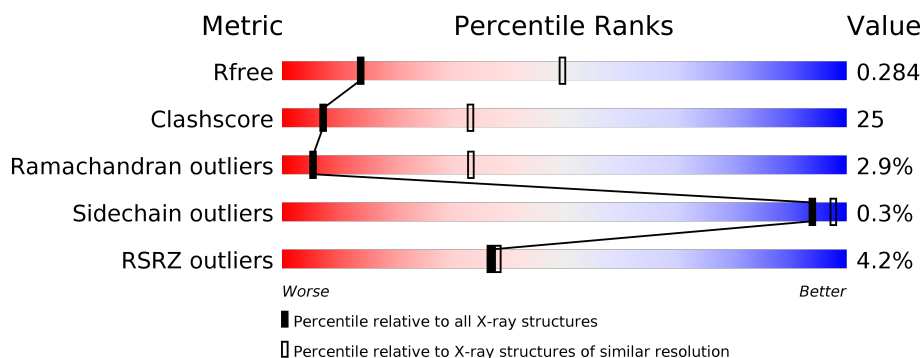
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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}	100719	1241 (3.46-3.30)
Clashscore	112137	1319 (3.46-3.30)
Ramachandran outliers	110173	1298 (3.46-3.30)
Sidechain outliers	110143	1297 (3.46-3.30)
RSRZ outliers	101464	1251 (3.46-3.30)

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 $\leq 5\%$. 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	269	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>39%</div> <div>• 5%</div> </div> </div>
1	C	269	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>38%</div> <div>5%</div> </div> </div>
1	E	269	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>38%</div> <div>5%</div> </div> </div>
1	G	269	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>• •</div> </div> </div>
1	I	269	<div> <div>6%</div> <div> <div></div> <div>51%</div> <div>43%</div> <div>6%</div> </div> </div>
2	B	18	<div> <div></div> <div> <div>28%</div> <div>50%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	18	<div><div></div><div></div><div></div><div></div></div> <div>39%28%22%11%</div>
2	F	18	<div><div></div><div></div><div></div><div></div></div> <div>22%56%17%6%</div>
2	H	18	<div><div></div><div></div><div></div><div></div><div></div></div> <div>11%28%44%17%6%6%</div>
2	J	18	<div><div></div><div></div><div></div><div></div><div></div></div> <div>6%28%61%6%6%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12188 atoms, of which 1227 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 Calcium/calmodulin dependent protein kinase II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	256	Total	C	H	N	O	S	0	0	0
			2263	1310	219	348	379	7			
1	C	256	Total	C	H	N	O	S	0	0	0
			2268	1312	225	344	380	7			
1	E	256	Total	C	H	N	O	S	0	0	0
			2266	1311	222	347	379	7			
1	G	259	Total	C	H	N	O	S	0	0	0
			2292	1322	228	350	385	7			
1	I	254	Total	C	H	N	O	S	0	0	0
			2249	1296	228	343	375	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ASN	ASP	ENGINEERED	UNP Q9U6Q0
C	135	ASN	ASP	ENGINEERED	UNP Q9U6Q0
E	135	ASN	ASP	ENGINEERED	UNP Q9U6Q0
G	135	ASN	ASP	ENGINEERED	UNP Q9U6Q0
I	135	ASN	ASP	ENGINEERED	UNP Q9U6Q0

- Molecule 2 is a protein called Calcium/calmodulin-dependent protein kinase II inhibitor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	18	Total	C	H	N	O		0	0	0
			162	89	22	31	20				
2	D	16	Total	C	H	N	O		0	0	0
			144	80	17	29	18				
2	F	17	Total	C	H	N	O		0	0	0
			157	86	22	30	19				
2	H	17	Total	C	H	N	O		0	0	0
			157	86	22	30	19				
2	J	17	Total	C	H	N	O		0	0	0
			153	83	22	29	19				

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	ALA	-	INSERTION	UNP Q9JI15
D	298	ALA	-	INSERTION	UNP Q9JI15
F	298	ALA	-	INSERTION	UNP Q9JI15
H	298	ALA	-	INSERTION	UNP Q9JI15
J	298	ALA	-	INSERTION	UNP Q9JI15

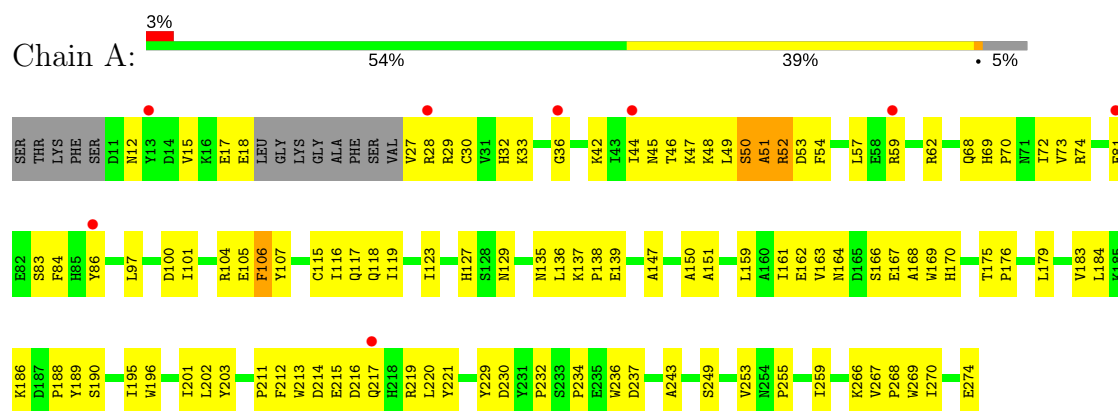
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	C	10	Total O 10 10	0	0
3	D	1	Total O 1 1	0	0
3	E	11	Total O 11 11	0	0
3	F	1	Total O 1 1	0	0
3	G	17	Total O 17 17	0	0
3	I	19	Total O 19 19	0	0
3	J	1	Total O 1 1	0	0

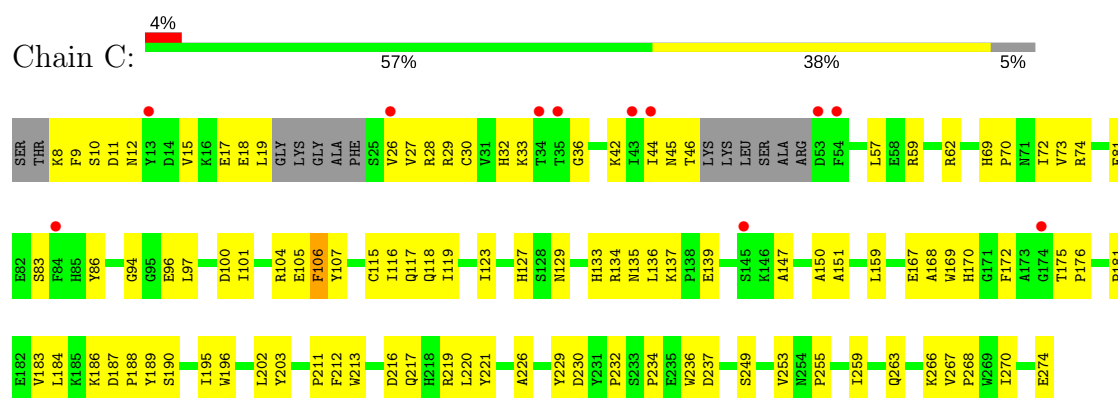
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

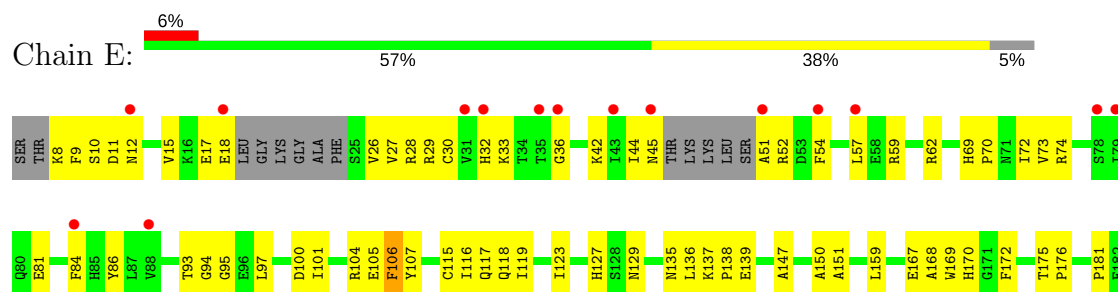
- Molecule 1: Calcium/calmodulin dependent protein kinase II



- Molecule 1: Calcium/calmodulin dependent protein kinase II

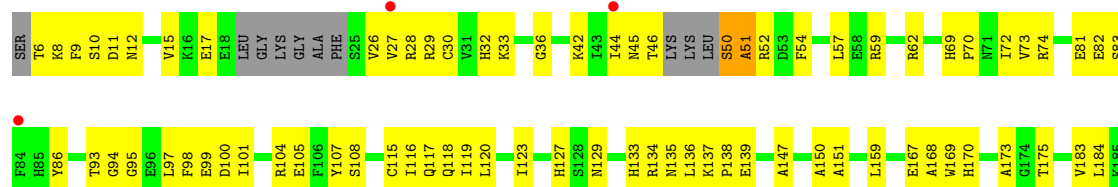


- Molecule 1: Calcium/calmodulin dependent protein kinase II

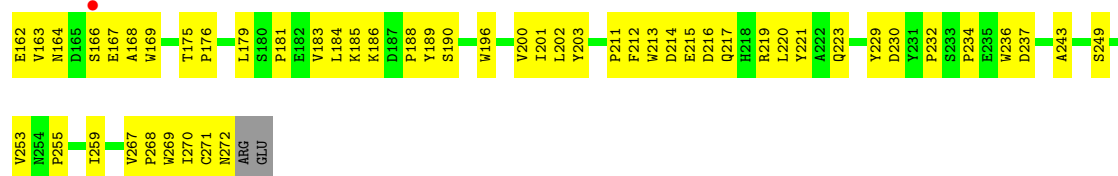
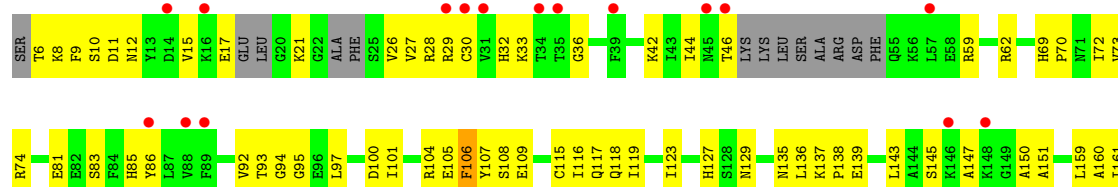




- Molecule 1: Calcium/calmodulin dependent protein kinase II



- Molecule 1: Calcium/calmodulin dependent protein kinase II



- Molecule 2: Calcium/calmodulin-dependent protein kinase II inhibitor 1

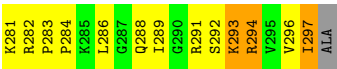


- Molecule 2: Calcium/calmodulin-dependent protein kinase II inhibitor 1



- Molecule 2: Calcium/calmodulin-dependent protein kinase II inhibitor 1





● Molecule 2: Calcium/calmodulin-dependent protein kinase II inhibitor 1



● Molecule 2: Calcium/calmodulin-dependent protein kinase II inhibitor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.41Å 83.08Å 145.13Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	71.71 – 3.37 71.71 – 3.37	Depositor EDS
% Data completeness (in resolution range)	89.5 (71.71-3.37) 89.6 (71.71-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.230 , 0.281 0.229 , 0.284	Depositor DCC
R_{free} test set	1823 reflections (8.41%)	DCC
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12188	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.52	0/2094	0.73	3/2842 (0.1%)
1	C	0.49	0/2093	0.57	0/2841
1	E	0.47	0/2094	0.60	2/2841 (0.1%)
1	G	0.50	0/2114	0.63	2/2869 (0.1%)
1	I	0.50	0/2069	0.58	0/2805
2	B	0.46	0/141	1.78	2/186 (1.1%)
2	D	0.46	0/128	1.84	3/168 (1.8%)
2	F	0.47	0/136	0.82	0/179
2	H	1.08	1/136 (0.7%)	1.76	7/179 (3.9%)
2	J	0.40	0/132	1.29	2/175 (1.1%)
All	All	0.51	1/11137 (0.0%)	0.71	21/15085 (0.1%)

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	1
2	B	0	1
2	D	0	1
2	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	283	PRO	N-CD	11.61	1.64	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	ARG	C-N-CD	-18.36	80.21	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	282	ARG	C-N-CD	-16.08	85.23	120.60
1	A	52	ARG	NE-CZ-NH1	-14.96	112.82	120.30
1	A	52	ARG	NE-CZ-NH2	13.99	127.30	120.30
2	D	282	ARG	CB-CA-C	12.26	134.91	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	SER	Peptide
2	B	281	LYS	Peptide
2	D	281	LYS	Peptide
2	H	281	LYS	Peptide

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	2044	219	2014	107	3
1	C	2043	225	2005	101	0
1	E	2044	222	2005	89	0
1	G	2064	228	2024	108	3
1	I	2021	228	1996	101	0
2	B	140	22	166	12	0
2	D	127	17	150	8	0
2	F	135	22	161	30	0
2	H	135	22	161	12	0
2	J	131	22	153	10	0
3	A	17	0	0	0	0
3	C	10	0	0	0	0
3	D	1	0	0	0	0
3	E	11	0	0	0	0
3	F	1	0	0	0	0
3	G	17	0	0	1	0
3	I	19	0	0	5	0
3	J	1	0	0	2	0
All	All	10961	1227	10835	542	3

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 25.

The worst 5 of 542 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:164:ASN:HB3	1:C:263:GLN:HE21	1.02	1.16
2:F:281:LYS:NZ	1:G:211:PRO:O	1.77	1.15
1:A:164:ASN:HB3	1:C:263:GLN:NE2	1.64	1.13
2:F:281:LYS:HB2	2:F:283:PRO:HD3	1.14	1.12
1:I:44:ILE:CG1	1:I:85:HIS:HB3	1.99	0.92

All (3) 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:52:ARG:NE	1:G:82:GLU:O[1_455]	1.60	0.60
1:A:52:ARG:CD	1:G:82:GLU:O[1_455]	1.71	0.49
1:A:52:ARG:CZ	1:G:82:GLU:O[1_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	252/269 (94%)	210 (83%)	38 (15%)	4 (2%)	11	45
1	C	250/269 (93%)	211 (84%)	34 (14%)	5 (2%)	9	41
1	E	250/269 (93%)	210 (84%)	35 (14%)	5 (2%)	9	41
1	G	253/269 (94%)	210 (83%)	38 (15%)	5 (2%)	9	41
1	I	246/269 (91%)	206 (84%)	34 (14%)	6 (2%)	7	37
2	B	16/18 (89%)	10 (62%)	2 (12%)	4 (25%)	0	0
2	D	14/18 (78%)	9 (64%)	1 (7%)	4 (29%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	15/18 (83%)	11 (73%)	2 (13%)	2 (13%)	0	2
2	H	15/18 (83%)	11 (73%)	2 (13%)	2 (13%)	0	2
2	J	15/18 (83%)	12 (80%)	2 (13%)	1 (7%)	1	12
All	All	1326/1435 (92%)	1100 (83%)	188 (14%)	38 (3%)	5	33

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
2	B	283	PRO
1	C	73	VAL
2	D	283	PRO
1	E	73	VAL

5.3.2 Protein sidechains ⓘ

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	219/231 (95%)	219 (100%)	0	100	100
1	C	220/231 (95%)	220 (100%)	0	100	100
1	E	219/231 (95%)	218 (100%)	1 (0%)	91	95
1	G	222/231 (96%)	221 (100%)	1 (0%)	91	95
1	I	218/231 (94%)	218 (100%)	0	100	100
2	B	15/15 (100%)	15 (100%)	0	100	100
2	D	14/15 (93%)	14 (100%)	0	100	100
2	F	15/15 (100%)	14 (93%)	1 (7%)	19	56
2	H	15/15 (100%)	15 (100%)	0	100	100
2	J	14/15 (93%)	14 (100%)	0	100	100
All	All	1171/1230 (95%)	1168 (100%)	3 (0%)	94	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	245	SER
2	F	297	ILE
1	G	50	SER

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	256/269 (95%)	0.23	8 (3%) 49 51	39, 66, 126, 145	0
1	C	256/269 (95%)	0.26	11 (4%) 36 37	37, 67, 127, 145	0
1	E	256/269 (95%)	0.36	15 (5%) 23 25	39, 68, 129, 143	0
1	G	259/269 (96%)	0.10	3 (1%) 79 81	34, 67, 125, 143	0
1	I	254/269 (94%)	0.34	17 (6%) 19 21	39, 68, 127, 143	0
2	B	18/18 (100%)	-0.06	0 100 100	51, 72, 104, 111	0
2	D	16/18 (88%)	0.04	0 100 100	53, 71, 99, 112	0
2	F	17/18 (94%)	0.00	0 100 100	50, 63, 96, 110	0
2	H	17/18 (94%)	0.50	2 (11%) 5 5	51, 70, 103, 114	0
2	J	17/18 (94%)	0.23	1 (5%) 23 25	50, 68, 99, 109	0
All	All	1366/1435 (95%)	0.25	57 (4%) 37 38	34, 68, 127, 145	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	PHE	5.8
1	I	46	THR	5.8
1	C	35	THR	5.5
1	A	13	TYR	5.5
1	E	54	PHE	4.7

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.