wwPDB X-ray Structure Validation Summary Report (i)

Jul 7, 2016 – 02:55 PM EDT

The following versions of software and data (see references (i)) were used in the production of this report:
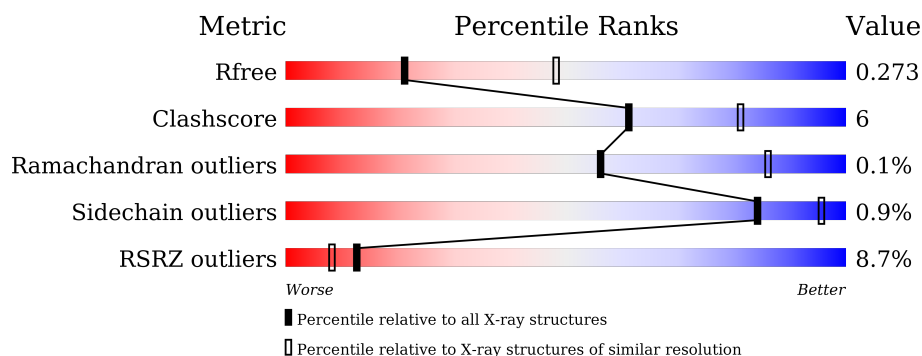
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	153	5% / 82% / 11% · 6%
1	B	153	3% / 72% / 11% / 17%
1	C	153	7% / 70% / 16% · 14%
1	D	153	8% / 72% / 10% · 17%
1	E	153	12% / 67% / 14% / 18%
1	F	153	9% / 69% / 12% / 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6312 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total 1168	C 738	N 212	O 212	S 6	0	0	0
1	B	127	Total 1031	C 655	N 182	O 188	S 6	0	0	0
1	C	132	Total 1066	C 673	N 191	O 196	S 6	0	0	0
1	D	127	Total 1024	C 647	N 182	O 189	S 6	0	0	0
1	E	125	Total 1012	C 641	N 180	O 185	S 6	0	0	0
1	F	123	Total 996	C 630	N 177	O 183	S 6	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	GLY	-	expression tag	UNP Q9UQM7
A	324	SER	-	expression tag	UNP Q9UQM7
A	325	SER	-	expression tag	UNP Q9UQM7
A	326	HIS	-	expression tag	UNP Q9UQM7
A	327	HIS	-	expression tag	UNP Q9UQM7
A	328	HIS	-	expression tag	UNP Q9UQM7
A	329	HIS	-	expression tag	UNP Q9UQM7
A	330	HIS	-	expression tag	UNP Q9UQM7
A	331	HIS	-	expression tag	UNP Q9UQM7
A	332	SER	-	expression tag	UNP Q9UQM7
A	333	SER	-	expression tag	UNP Q9UQM7
A	334	GLY	-	expression tag	UNP Q9UQM7
A	335	LEU	-	expression tag	UNP Q9UQM7
A	336	GLU	-	expression tag	UNP Q9UQM7
A	337	VAL	-	expression tag	UNP Q9UQM7
A	338	LEU	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	339	PHE	-	expression tag	UNP Q9UQM7
A	340	GLN	-	expression tag	UNP Q9UQM7
A	341	GLY	-	expression tag	UNP Q9UQM7
A	342	PRO	-	expression tag	UNP Q9UQM7
A	343	HIS	-	expression tag	UNP Q9UQM7
A	344	MET	-	expression tag	UNP Q9UQM7
B	323	GLY	-	expression tag	UNP Q9UQM7
B	324	SER	-	expression tag	UNP Q9UQM7
B	325	SER	-	expression tag	UNP Q9UQM7
B	326	HIS	-	expression tag	UNP Q9UQM7
B	327	HIS	-	expression tag	UNP Q9UQM7
B	328	HIS	-	expression tag	UNP Q9UQM7
B	329	HIS	-	expression tag	UNP Q9UQM7
B	330	HIS	-	expression tag	UNP Q9UQM7
B	331	HIS	-	expression tag	UNP Q9UQM7
B	332	SER	-	expression tag	UNP Q9UQM7
B	333	SER	-	expression tag	UNP Q9UQM7
B	334	GLY	-	expression tag	UNP Q9UQM7
B	335	LEU	-	expression tag	UNP Q9UQM7
B	336	GLU	-	expression tag	UNP Q9UQM7
B	337	VAL	-	expression tag	UNP Q9UQM7
B	338	LEU	-	expression tag	UNP Q9UQM7
B	339	PHE	-	expression tag	UNP Q9UQM7
B	340	GLN	-	expression tag	UNP Q9UQM7
B	341	GLY	-	expression tag	UNP Q9UQM7
B	342	PRO	-	expression tag	UNP Q9UQM7
B	343	HIS	-	expression tag	UNP Q9UQM7
B	344	MET	-	expression tag	UNP Q9UQM7
C	323	GLY	-	expression tag	UNP Q9UQM7
C	324	SER	-	expression tag	UNP Q9UQM7
C	325	SER	-	expression tag	UNP Q9UQM7
C	326	HIS	-	expression tag	UNP Q9UQM7
C	327	HIS	-	expression tag	UNP Q9UQM7
C	328	HIS	-	expression tag	UNP Q9UQM7
C	329	HIS	-	expression tag	UNP Q9UQM7
C	330	HIS	-	expression tag	UNP Q9UQM7
C	331	HIS	-	expression tag	UNP Q9UQM7
C	332	SER	-	expression tag	UNP Q9UQM7
C	333	SER	-	expression tag	UNP Q9UQM7
C	334	GLY	-	expression tag	UNP Q9UQM7
C	335	LEU	-	expression tag	UNP Q9UQM7
C	336	GLU	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	337	VAL	-	expression tag	UNP Q9UQM7
C	338	LEU	-	expression tag	UNP Q9UQM7
C	339	PHE	-	expression tag	UNP Q9UQM7
C	340	GLN	-	expression tag	UNP Q9UQM7
C	341	GLY	-	expression tag	UNP Q9UQM7
C	342	PRO	-	expression tag	UNP Q9UQM7
C	343	HIS	-	expression tag	UNP Q9UQM7
C	344	MET	-	expression tag	UNP Q9UQM7
D	323	GLY	-	expression tag	UNP Q9UQM7
D	324	SER	-	expression tag	UNP Q9UQM7
D	325	SER	-	expression tag	UNP Q9UQM7
D	326	HIS	-	expression tag	UNP Q9UQM7
D	327	HIS	-	expression tag	UNP Q9UQM7
D	328	HIS	-	expression tag	UNP Q9UQM7
D	329	HIS	-	expression tag	UNP Q9UQM7
D	330	HIS	-	expression tag	UNP Q9UQM7
D	331	HIS	-	expression tag	UNP Q9UQM7
D	332	SER	-	expression tag	UNP Q9UQM7
D	333	SER	-	expression tag	UNP Q9UQM7
D	334	GLY	-	expression tag	UNP Q9UQM7
D	335	LEU	-	expression tag	UNP Q9UQM7
D	336	GLU	-	expression tag	UNP Q9UQM7
D	337	VAL	-	expression tag	UNP Q9UQM7
D	338	LEU	-	expression tag	UNP Q9UQM7
D	339	PHE	-	expression tag	UNP Q9UQM7
D	340	GLN	-	expression tag	UNP Q9UQM7
D	341	GLY	-	expression tag	UNP Q9UQM7
D	342	PRO	-	expression tag	UNP Q9UQM7
D	343	HIS	-	expression tag	UNP Q9UQM7
D	344	MET	-	expression tag	UNP Q9UQM7
E	323	GLY	-	expression tag	UNP Q9UQM7
E	324	SER	-	expression tag	UNP Q9UQM7
E	325	SER	-	expression tag	UNP Q9UQM7
E	326	HIS	-	expression tag	UNP Q9UQM7
E	327	HIS	-	expression tag	UNP Q9UQM7
E	328	HIS	-	expression tag	UNP Q9UQM7
E	329	HIS	-	expression tag	UNP Q9UQM7
E	330	HIS	-	expression tag	UNP Q9UQM7
E	331	HIS	-	expression tag	UNP Q9UQM7
E	332	SER	-	expression tag	UNP Q9UQM7
E	333	SER	-	expression tag	UNP Q9UQM7
E	334	GLY	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	335	LEU	-	expression tag	UNP Q9UQM7
E	336	GLU	-	expression tag	UNP Q9UQM7
E	337	VAL	-	expression tag	UNP Q9UQM7
E	338	LEU	-	expression tag	UNP Q9UQM7
E	339	PHE	-	expression tag	UNP Q9UQM7
E	340	GLN	-	expression tag	UNP Q9UQM7
E	341	GLY	-	expression tag	UNP Q9UQM7
E	342	PRO	-	expression tag	UNP Q9UQM7
E	343	HIS	-	expression tag	UNP Q9UQM7
E	344	MET	-	expression tag	UNP Q9UQM7
F	323	GLY	-	expression tag	UNP Q9UQM7
F	324	SER	-	expression tag	UNP Q9UQM7
F	325	SER	-	expression tag	UNP Q9UQM7
F	326	HIS	-	expression tag	UNP Q9UQM7
F	327	HIS	-	expression tag	UNP Q9UQM7
F	328	HIS	-	expression tag	UNP Q9UQM7
F	329	HIS	-	expression tag	UNP Q9UQM7
F	330	HIS	-	expression tag	UNP Q9UQM7
F	331	HIS	-	expression tag	UNP Q9UQM7
F	332	SER	-	expression tag	UNP Q9UQM7
F	333	SER	-	expression tag	UNP Q9UQM7
F	334	GLY	-	expression tag	UNP Q9UQM7
F	335	LEU	-	expression tag	UNP Q9UQM7
F	336	GLU	-	expression tag	UNP Q9UQM7
F	337	VAL	-	expression tag	UNP Q9UQM7
F	338	LEU	-	expression tag	UNP Q9UQM7
F	339	PHE	-	expression tag	UNP Q9UQM7
F	340	GLN	-	expression tag	UNP Q9UQM7
F	341	GLY	-	expression tag	UNP Q9UQM7
F	342	PRO	-	expression tag	UNP Q9UQM7
F	343	HIS	-	expression tag	UNP Q9UQM7
F	344	MET	-	expression tag	UNP Q9UQM7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	O 3	0	0
2	B	6	Total 6	O 6	0	0
2	C	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	O 2	0	0
2	E	1	Total 1	O 1	0	0
2	F	1	Total 1	O 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 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.
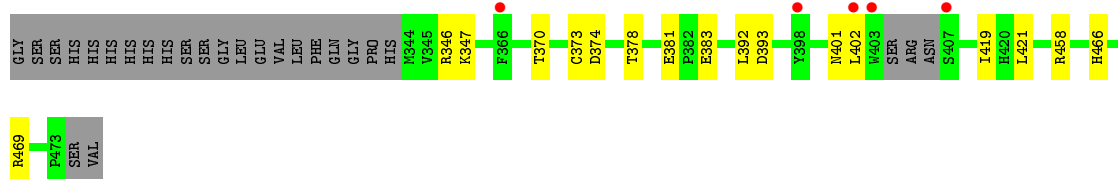
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha
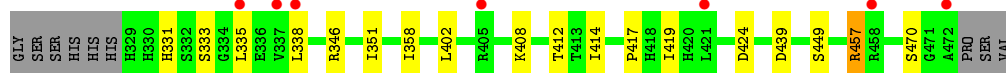
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

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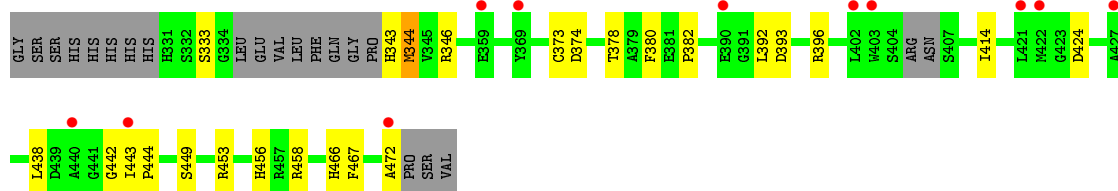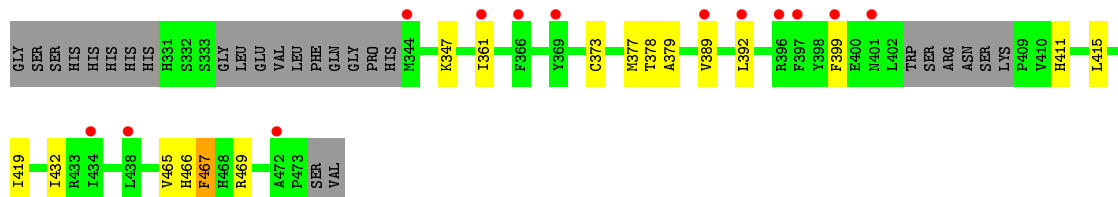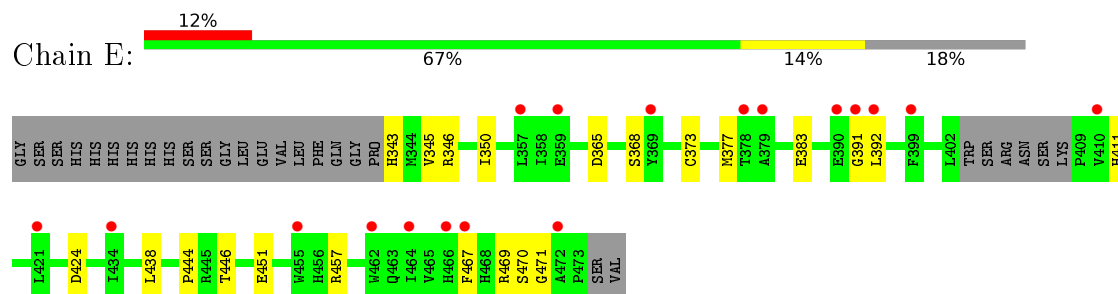- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain E:

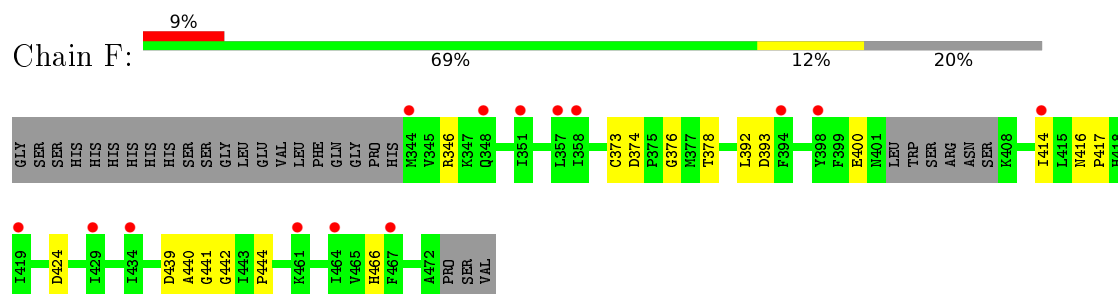• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.89Å 89.89Å 226.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.75 48.63 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-2.75) 99.9 (48.63-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$<I/\sigma(I)>$ [1]	1.77 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.220 , 0.268 0.225 , 0.273	Depositor DCC
R_{free} test set	1184 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.6	EDS
L-test for twinning [2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6312	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.25	0/1201	0.41	0/1625
1	B	0.25	0/1058	0.41	0/1431
1	C	0.25	0/1093	0.42	0/1475
1	D	0.24	0/1049	0.41	0/1416
1	E	0.26	0/1038	0.42	0/1403
1	F	0.24	0/1020	0.41	0/1377
All	All	0.25	0/6459	0.41	0/8727

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	1168	0	1117	14	0
1	B	1031	0	994	12	0
1	C	1066	0	1018	14	0
1	D	1024	0	983	9	0
1	E	1012	0	974	15	0
1	F	996	0	961	11	0
2	A	3	0	0	0	0
2	B	6	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	6312	0	6047	68	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 6.

The worst 5 of 68 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:C:374:ASP:OD2	1:C:458:ARG:NH1	1.90	1.03
1:B:374:ASP:OD1	1:B:458:ARG:NH1	1.93	1.01
1:A:331:HIS:HA	1:A:412:THR:O	1.73	0.88
1:B:393:ASP:OD2	1:E:411:HIS:NE2	2.20	0.74
1:C:346:ARG:NH1	1:C:424:ASP:O	2.24	0.70

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	142/153 (93%)	136 (96%)	6 (4%)	0	100	100
1	B	123/153 (80%)	120 (98%)	3 (2%)	0	100	100
1	C	126/153 (82%)	120 (95%)	6 (5%)	0	100	100
1	D	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
1	E	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
1	F	119/153 (78%)	118 (99%)	0	1 (1%)	24	55
All	All	752/918 (82%)	730 (97%)	21 (3%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	440	ALA

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	125/133 (94%)	124 (99%)	1 (1%)	86	96
1	B	110/133 (83%)	110 (100%)	0	100	100
1	C	114/133 (86%)	111 (97%)	3 (3%)	54	84
1	D	110/133 (83%)	109 (99%)	1 (1%)	84	95
1	E	108/133 (81%)	107 (99%)	1 (1%)	84	95
1	F	106/133 (80%)	106 (100%)	0	100	100
All	All	673/798 (84%)	667 (99%)	6 (1%)	84	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	344	MET
1	E	424	ASP
1	C	380	PHE
1	C	343	HIS
1	D	467	PHE

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	401	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 (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	144/153 (94%)	0.36	7 (4%)	33	26	52, 78, 140, 186	0
1	B	127/153 (83%)	0.38	5 (3%)	43	36	52, 76, 134, 150	0
1	C	132/153 (86%)	0.62	11 (8%)	14	9	50, 91, 144, 173	0
1	D	127/153 (83%)	0.58	13 (10%)	9	5	53, 94, 136, 164	0
1	E	125/153 (81%)	0.79	18 (14%)	3	2	57, 101, 164, 214	0
1	F	123/153 (80%)	0.82	14 (11%)	7	4	58, 100, 155, 193	0
All	All	778/918 (84%)	0.59	68 (8%)	13	8	50, 91, 149, 214	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	390	GLU	7.6
1	E	369	TYR	6.5
1	A	335	LEU	4.3
1	F	394	PHE	4.3
1	E	379	ALA	4.2

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.