wwPDB X-ray Structure Validation Summary Report (i)

Apr 11, 2016 – 01:33 PM EDT

PDB ID	:	5CXT
Title	:	Crystal structure of a RNA-binding protein 39 (RBM39) in complex with fragment of splicing factor (U2AF) from Unknown at 2.20 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG); Partnership for T-Cell Biology (TCELL)
Deposited on	:	2015-07-29
Resolution	:	2.20 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 (i) symbol.

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

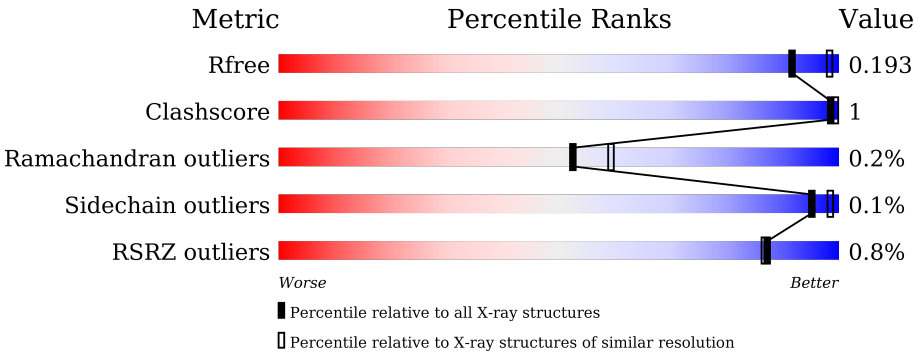
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	114	96%
1	C	114	96%
1	E	114	90% 8%
1	G	114	96%
1	I	114	97%
1	K	114	2% 93% 5%

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Mol	Chain	Length	Quality of chain
1	M	114	97%
1	O	114	96%
1	Q	114	91% 6%
2	B	29	31% 69%
2	D	29	38% 62%
2	F	29	34% 66%
2	H	29	38% 62%
2	J	29	38% 62%
2	L	29	10% 38% 62%
2	N	29	38% 62%
2	P	29	34% 66%
2	R	29	34% 66%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9144 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 RNA-binding protein 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	2	0
			865	555	143	161	6			
1	C	112	Total	C	N	O	S	0	3	0
			884	566	147	164	7			
1	E	112	Total	C	N	O	S	0	0	0
			862	552	145	159	6			
1	G	112	Total	C	N	O	S	0	1	0
			873	558	147	161	7			
1	I	111	Total	C	N	O	S	0	2	0
			868	556	143	162	7			
1	K	113	Total	C	N	O	S	0	0	0
			866	555	145	160	6			
1	M	111	Total	C	N	O	S	0	3	0
			882	564	147	164	7			
1	O	110	Total	C	N	O	S	0	2	0
			859	551	142	159	7			
1	Q	112	Total	C	N	O	S	0	2	0
			876	563	145	162	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	-	expression tag	UNP Q8VH51
A	468	TYR	ASN	engineered mutation	UNP Q8VH51
C	417	GLY	-	expression tag	UNP Q8VH51
C	468	TYR	ASN	engineered mutation	UNP Q8VH51
E	417	GLY	-	expression tag	UNP Q8VH51
E	468	TYR	ASN	engineered mutation	UNP Q8VH51
G	417	GLY	-	expression tag	UNP Q8VH51
G	468	TYR	ASN	engineered mutation	UNP Q8VH51
I	417	GLY	-	expression tag	UNP Q8VH51
I	468	TYR	ASN	engineered mutation	UNP Q8VH51
K	0	GLY	-	expression tag	UNP Q8VH51

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Chain	Residue	Modelled	Actual	Comment	Reference
K	468	TYR	ASN	engineered mutation	UNP Q8VH51
M	417	GLY	-	expression tag	UNP Q8VH51
M	468	TYR	ASN	engineered mutation	UNP Q8VH51
O	417	GLY	-	expression tag	UNP Q8VH51
O	468	TYR	ASN	engineered mutation	UNP Q8VH51
Q	417	GLY	-	expression tag	UNP Q8VH51
Q	468	TYR	ASN	engineered mutation	UNP Q8VH51

- Molecule 2 is a protein called Splicing factor U2AF 65 kDa subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			82	56	14	12			
2	D	11	Total	C	N	O	0	0	0
			91	61	16	14			
2	F	10	Total	C	N	O	0	0	0
			86	58	15	13			
2	H	11	Total	C	N	O	0	0	0
			87	58	15	14			
2	J	11	Total	C	N	O	0	0	0
			87	58	15	14			
2	L	11	Total	C	N	O	0	0	0
			91	61	16	14			
2	N	11	Total	C	N	O	0	0	0
			91	61	16	14			
2	P	10	Total	C	N	O	0	0	0
			86	58	15	13			
2	R	10	Total	C	N	O	0	0	0
			82	55	14	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	84	GLY	-	expression tag	UNP P26369
D	84	GLY	-	expression tag	UNP P26369
F	84	GLY	-	expression tag	UNP P26369
H	84	GLY	-	expression tag	UNP P26369
J	84	GLY	-	expression tag	UNP P26369
L	84	GLY	-	expression tag	UNP P26369
N	84	GLY	-	expression tag	UNP P26369
P	84	GLY	-	expression tag	UNP P26369
R	84	GLY	-	expression tag	UNP P26369

- Molecule 3 is water.

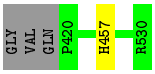
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 58 58	0	1
3	B	2	Total O 2 2	0	0
3	C	56	Total O 57 57	0	1
3	D	5	Total O 5 5	0	0
3	E	41	Total O 42 42	0	1
3	F	2	Total O 2 2	0	0
3	G	59	Total O 59 59	0	0
3	H	2	Total O 2 2	0	0
3	I	64	Total O 65 65	0	1
3	J	4	Total O 4 4	0	0
3	K	59	Total O 59 59	0	0
3	L	5	Total O 5 5	0	0
3	M	58	Total O 60 60	0	2
3	N	3	Total O 3 3	0	0
3	O	58	Total O 59 59	0	1
3	P	2	Total O 2 2	0	0
3	Q	40	Total O 41 41	0	1
3	R	1	Total O 1 1	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.

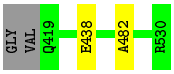
- Molecule 1: RNA-binding protein 39

Chain A:



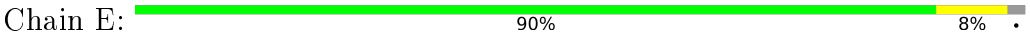
- Molecule 1: RNA-binding protein 39

Chain C:



- Molecule 1: RNA-binding protein 39

Chain E:

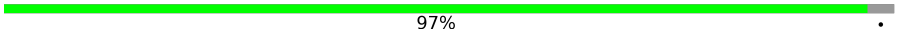


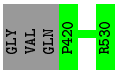
- Molecule 1: RNA-binding protein 39

Chain G:

- Molecule 1: RNA-binding protein 39

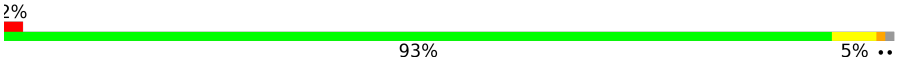
Chain I:

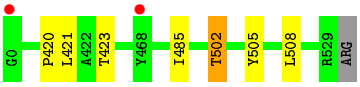




- Molecule 1: RNA-binding protein 39

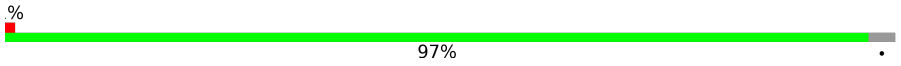
Chain K:

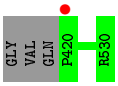




• Molecule 1: RNA-binding protein 39

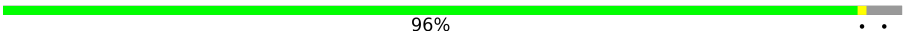
Chain M:

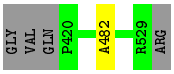




• Molecule 1: RNA-binding protein 39

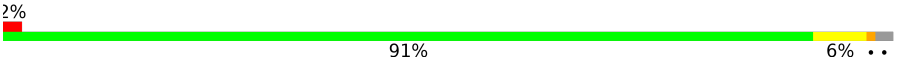
Chain O:

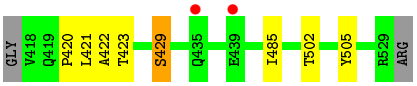




• Molecule 1: RNA-binding protein 39

Chain Q:





• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain B:

• Molecule 2: Splicing factor U2AF 65 kDa subunit

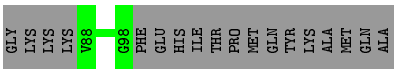
Chain D:

• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain F:

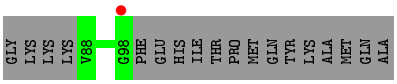
• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain H:



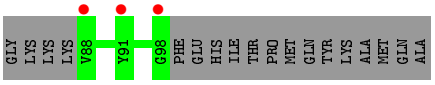
• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain J:



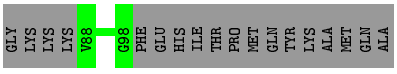
• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain L:



• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain N:



• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain P:

• Molecule 2: Splicing factor U2AF 65 kDa subunit

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	127.28Å 127.28Å 78.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.43 – 2.20 37.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.43-2.20) 99.6 (37.13-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.174 , 0.190 0.177 , 0.193	Depositor DCC
R_{free} test set	3638 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 18.7	EDS
Estimated twinning fraction	0.806 for H, K, L 0.194 for -K, -H, -L 0.023 for -h,-k,l 0.029 for h,-h-k,-l 0.287 for -k,-h,-l	Xtriage
Reported twinning fraction	0.806 for H, K, L 0.194 for -K, -H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 72348 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9144	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.24 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5712e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.92	0/894	0.84	2/1219 (0.2%)
1	C	0.94	1/916 (0.1%)	0.83	0/1248
1	E	0.85	0/885	0.84	2/1209 (0.2%)
1	G	0.89	0/899	0.82	0/1225
1	I	0.88	0/896	0.78	0/1221
1	K	0.89	1/889 (0.1%)	0.86	2/1215 (0.2%)
1	M	0.92	0/911	0.80	0/1240
1	O	0.90	0/888	0.78	0/1211
1	Q	0.86	0/905	0.77	0/1238
2	B	1.37	0/87	0.82	0/120
2	D	0.80	0/96	0.70	0/132
2	F	0.97	0/91	0.77	0/125
2	H	0.90	0/92	0.73	0/128
2	J	0.90	0/92	0.73	0/128
2	L	0.73	0/96	0.65	0/132
2	N	0.91	0/96	0.73	0/132
2	P	1.03	0/90	0.96	0/124
2	R	0.86	0/87	0.88	0/121
All	All	0.90	2/8910 (0.0%)	0.81	6/12168 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	438	GLU	CB-CG	7.47	1.66	1.52
1	K	502	THR	CA-CB	5.39	1.67	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	HIS	CB-CA-C	9.87	130.15	110.40
1	K	508	LEU	CB-CG-CD1	9.80	127.65	111.00
1	E	508	LEU	CB-CG-CD1	9.75	127.57	111.00
1	E	508	LEU	CB-CG-CD2	-6.82	99.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	508	LEU	CB-CG-CD2	-6.73	99.56	111.00

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	865	0	844	0	0
1	C	884	0	867	1	0
1	E	862	0	833	4	0
1	G	873	0	849	2	0
1	I	868	0	844	0	0
1	K	866	0	839	5	0
1	M	882	0	865	0	0
1	O	859	0	840	1	0
1	Q	876	0	860	5	0
2	B	82	0	78	0	0
2	D	91	0	83	0	0
2	F	86	0	81	0	0
2	H	87	0	72	0	0
2	J	87	0	72	0	0
2	L	91	0	83	0	0
2	N	91	0	83	0	0
2	P	86	0	74	0	0
2	R	82	0	70	0	0
3	A	58	0	0	0	0
3	B	2	0	0	0	0
3	C	57	0	0	0	0
3	D	5	0	0	0	0
3	E	42	0	0	0	0
3	F	2	0	0	0	0
3	G	59	0	0	0	0
3	H	2	0	0	0	0
3	I	65	0	0	0	0
3	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	59	0	0	1	0
3	L	5	0	0	0	0
3	M	60	0	0	0	0
3	N	3	0	0	0	0
3	O	59	0	0	0	0
3	P	2	0	0	0	0
3	Q	41	0	0	1	0
3	R	1	0	0	0	0
All	All	9144	0	8337	15	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 1.

The worst 5 of 15 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:Q:420:PRO:HA	1:Q:505:TYR:CE2	2.38	0.57
1:C:482:ALA:HB2	1:E:485:ILE:HD12	1.87	0.55
1:E:496:PHE:HB3	1:E:501:ILE:HD11	1.89	0.55
1:K:420:PRO:HA	1:K:505:TYR:CE2	2.41	0.55
1:G:496:PHE:HB3	1:G:501:ILE:HD11	1.91	0.52

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	111/114 (97%)	108 (97%)	3 (3%)	0	100 100
1	C	113/114 (99%)	110 (97%)	3 (3%)	0	100 100
1	E	110/114 (96%)	107 (97%)	2 (2%)	1 (1%)	21 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
1	I	111/114 (97%)	109 (98%)	2 (2%)	0	100	100
1	K	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
1	M	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	O	110/114 (96%)	107 (97%)	3 (3%)	0	100	100
1	Q	112/114 (98%)	109 (97%)	2 (2%)	1 (1%)	21	19
2	B	7/29 (24%)	6 (86%)	1 (14%)	0	100	100
2	D	9/29 (31%)	9 (100%)	0	0	100	100
2	F	8/29 (28%)	7 (88%)	1 (12%)	0	100	100
2	H	9/29 (31%)	9 (100%)	0	0	100	100
2	J	9/29 (31%)	9 (100%)	0	0	100	100
2	L	9/29 (31%)	9 (100%)	0	0	100	100
2	N	9/29 (31%)	9 (100%)	0	0	100	100
2	P	8/29 (28%)	7 (88%)	1 (12%)	0	100	100
2	R	8/29 (28%)	5 (62%)	3 (38%)	0	100	100
All	All	1077/1287 (84%)	1045 (97%)	30 (3%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	422	ALA
1	Q	422	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	93/95 (98%)	93 (100%)	0	100	100
1	C	96/95 (101%)	96 (100%)	0	100	100
1	E	91/95 (96%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	93/95 (98%)	93 (100%)	0	100 100
1	I	93/95 (98%)	93 (100%)	0	100 100
1	K	91/95 (96%)	91 (100%)	0	100 100
1	M	96/95 (101%)	96 (100%)	0	100 100
1	O	93/95 (98%)	93 (100%)	0	100 100
1	Q	95/95 (100%)	94 (99%)	1 (1%)	80 89
2	B	9/25 (36%)	9 (100%)	0	100 100
2	D	9/25 (36%)	9 (100%)	0	100 100
2	F	9/25 (36%)	9 (100%)	0	100 100
2	H	8/25 (32%)	8 (100%)	0	100 100
2	J	8/25 (32%)	8 (100%)	0	100 100
2	L	9/25 (36%)	9 (100%)	0	100 100
2	N	9/25 (36%)	9 (100%)	0	100 100
2	P	8/25 (32%)	8 (100%)	0	100 100
2	R	8/25 (32%)	8 (100%)	0	100 100
All	All	918/1080 (85%)	917 (100%)	1 (0%)	95 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	429	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

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	111/114 (97%)	-0.42	0 100 100	21, 30, 64, 88	0
1	C	112/114 (98%)	-0.39	0 100 100	22, 32, 66, 96	0
1	E	112/114 (98%)	-0.35	0 100 100	23, 36, 76, 93	0
1	G	112/114 (98%)	-0.44	0 100 100	22, 32, 67, 85	0
1	I	111/114 (97%)	-0.42	0 100 100	21, 30, 68, 86	0
1	K	113/114 (99%)	-0.32	2 (1%) 71 70	25, 37, 75, 106	0
1	M	111/114 (97%)	-0.47	1 (0%) 85 85	23, 32, 71, 94	0
1	O	110/114 (96%)	-0.50	0 100 100	21, 33, 64, 85	0
1	Q	112/114 (98%)	-0.36	2 (1%) 71 70	26, 37, 76, 105	0
2	B	9/29 (31%)	-0.48	0 100 100	30, 34, 50, 54	0
2	D	11/29 (37%)	-0.07	0 100 100	30, 43, 68, 76	0
2	F	10/29 (34%)	0.23	0 100 100	38, 44, 71, 75	0
2	H	11/29 (37%)	-0.06	0 100 100	30, 39, 68, 69	0
2	J	11/29 (37%)	-0.14	1 (9%) 11 11	27, 41, 65, 73	0
2	L	11/29 (37%)	0.79	3 (27%) 1 1	44, 50, 86, 91	0
2	N	11/29 (37%)	-0.05	0 100 100	34, 39, 61, 64	0
2	P	10/29 (34%)	-0.32	0 100 100	33, 40, 58, 69	0
2	R	10/29 (34%)	-0.06	0 100 100	43, 46, 73, 75	0
All	All	1098/1287 (85%)	-0.37	9 (0%) 87 87	21, 34, 73, 106	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	0	GLY	4.4
2	L	88	VAL	3.1
2	J	98	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	468	TYR	2.6
2	L	98	GLY	2.6

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.