wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2021 – 10:14 AM EDT

PDB ID	:	7L7V
Title	:	Crystal structure of Arabidopsis NRG1.1 CC-R domain K94E/K96E/R99E/ K100E/R103E/K106E/K110E mutant
Authors	:	Walton, W.G.; Wan, L.; Lietzan, A.D.; Redinbo, M.R.; Dangl, J.L.
Deposited on	:	2020-12-30
Resolution	:	2.95 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
https://www.wwpdb.org/validation/2017/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:

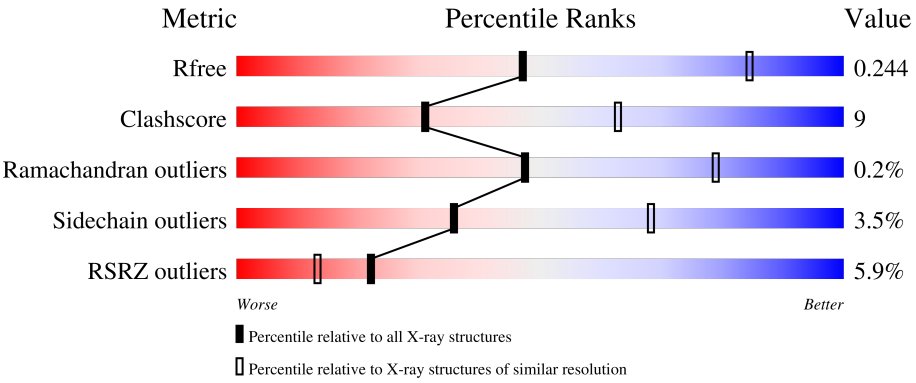
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (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 of 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	135	70% 19% • 10%
1	B	135	3% 63% 16% • 19%
1	C	135	10% 64% 17% 19%
1	D	135	% 54% 20% • 24%
1	E	135	6% 61% 17% • 20%

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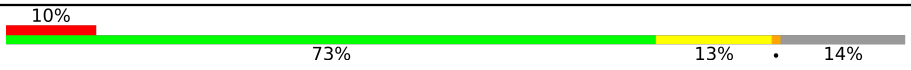
Mol	Chain	Length	Quality of chain
1	F	135	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5239 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 Probable disease resistance protein At5g66900.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			948	611	143	189	5			
1	B	109	Total	C	N	O	S	0	0	0
			867	558	136	169	4			
1	C	109	Total	C	N	O	S	0	0	0
			861	557	133	167	4			
1	D	102	Total	C	N	O	S	0	0	0
			825	532	127	162	4			
1	E	108	Total	C	N	O	S	0	0	0
			842	543	126	169	4			
1	F	116	Total	C	N	O	S	0	0	0
			896	576	141	175	4			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9FKZ1
A	2	ASN	-	expression tag	UNP Q9FKZ1
A	3	ALA	-	expression tag	UNP Q9FKZ1
A	97	GLU	LYS	engineered mutation	UNP Q9FKZ1
A	99	GLU	LYS	engineered mutation	UNP Q9FKZ1
A	102	GLU	ARG	engineered mutation	UNP Q9FKZ1
A	103	GLU	LYS	engineered mutation	UNP Q9FKZ1
A	106	GLU	ARG	engineered mutation	UNP Q9FKZ1
A	109	GLU	LYS	engineered mutation	UNP Q9FKZ1
A	113	GLU	LYS	engineered mutation	UNP Q9FKZ1
A	128	TRP	-	expression tag	UNP Q9FKZ1
A	129	SER	-	expression tag	UNP Q9FKZ1
A	130	HIS	-	expression tag	UNP Q9FKZ1
A	131	PRO	-	expression tag	UNP Q9FKZ1
A	132	GLN	-	expression tag	UNP Q9FKZ1
A	133	PHE	-	expression tag	UNP Q9FKZ1
A	134	GLU	-	expression tag	UNP Q9FKZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	135	LYS	-	expression tag	UNP Q9FKZ1
B	1	SER	-	expression tag	UNP Q9FKZ1
B	2	ASN	-	expression tag	UNP Q9FKZ1
B	3	ALA	-	expression tag	UNP Q9FKZ1
B	97	GLU	LYS	engineered mutation	UNP Q9FKZ1
B	99	GLU	LYS	engineered mutation	UNP Q9FKZ1
B	102	GLU	ARG	engineered mutation	UNP Q9FKZ1
B	103	GLU	LYS	engineered mutation	UNP Q9FKZ1
B	106	GLU	ARG	engineered mutation	UNP Q9FKZ1
B	109	GLU	LYS	engineered mutation	UNP Q9FKZ1
B	113	GLU	LYS	engineered mutation	UNP Q9FKZ1
B	128	TRP	-	expression tag	UNP Q9FKZ1
B	129	SER	-	expression tag	UNP Q9FKZ1
B	130	HIS	-	expression tag	UNP Q9FKZ1
B	131	PRO	-	expression tag	UNP Q9FKZ1
B	132	GLN	-	expression tag	UNP Q9FKZ1
B	133	PHE	-	expression tag	UNP Q9FKZ1
B	134	GLU	-	expression tag	UNP Q9FKZ1
B	135	LYS	-	expression tag	UNP Q9FKZ1
C	1	SER	-	expression tag	UNP Q9FKZ1
C	2	ASN	-	expression tag	UNP Q9FKZ1
C	3	ALA	-	expression tag	UNP Q9FKZ1
C	97	GLU	LYS	engineered mutation	UNP Q9FKZ1
C	99	GLU	LYS	engineered mutation	UNP Q9FKZ1
C	102	GLU	ARG	engineered mutation	UNP Q9FKZ1
C	103	GLU	LYS	engineered mutation	UNP Q9FKZ1
C	106	GLU	ARG	engineered mutation	UNP Q9FKZ1
C	109	GLU	LYS	engineered mutation	UNP Q9FKZ1
C	113	GLU	LYS	engineered mutation	UNP Q9FKZ1
C	128	TRP	-	expression tag	UNP Q9FKZ1
C	129	SER	-	expression tag	UNP Q9FKZ1
C	130	HIS	-	expression tag	UNP Q9FKZ1
C	131	PRO	-	expression tag	UNP Q9FKZ1
C	132	GLN	-	expression tag	UNP Q9FKZ1
C	133	PHE	-	expression tag	UNP Q9FKZ1
C	134	GLU	-	expression tag	UNP Q9FKZ1
C	135	LYS	-	expression tag	UNP Q9FKZ1
D	1	SER	-	expression tag	UNP Q9FKZ1
D	2	ASN	-	expression tag	UNP Q9FKZ1
D	3	ALA	-	expression tag	UNP Q9FKZ1
D	97	GLU	LYS	engineered mutation	UNP Q9FKZ1
D	99	GLU	LYS	engineered mutation	UNP Q9FKZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	102	GLU	ARG	engineered mutation	UNP Q9FKZ1
D	103	GLU	LYS	engineered mutation	UNP Q9FKZ1
D	106	GLU	ARG	engineered mutation	UNP Q9FKZ1
D	109	GLU	LYS	engineered mutation	UNP Q9FKZ1
D	113	GLU	LYS	engineered mutation	UNP Q9FKZ1
D	128	TRP	-	expression tag	UNP Q9FKZ1
D	129	SER	-	expression tag	UNP Q9FKZ1
D	130	HIS	-	expression tag	UNP Q9FKZ1
D	131	PRO	-	expression tag	UNP Q9FKZ1
D	132	GLN	-	expression tag	UNP Q9FKZ1
D	133	PHE	-	expression tag	UNP Q9FKZ1
D	134	GLU	-	expression tag	UNP Q9FKZ1
D	135	LYS	-	expression tag	UNP Q9FKZ1
E	1	SER	-	expression tag	UNP Q9FKZ1
E	2	ASN	-	expression tag	UNP Q9FKZ1
E	3	ALA	-	expression tag	UNP Q9FKZ1
E	97	GLU	LYS	engineered mutation	UNP Q9FKZ1
E	99	GLU	LYS	engineered mutation	UNP Q9FKZ1
E	102	GLU	ARG	engineered mutation	UNP Q9FKZ1
E	103	GLU	LYS	engineered mutation	UNP Q9FKZ1
E	106	GLU	ARG	engineered mutation	UNP Q9FKZ1
E	109	GLU	LYS	engineered mutation	UNP Q9FKZ1
E	113	GLU	LYS	engineered mutation	UNP Q9FKZ1
E	128	TRP	-	expression tag	UNP Q9FKZ1
E	129	SER	-	expression tag	UNP Q9FKZ1
E	130	HIS	-	expression tag	UNP Q9FKZ1
E	131	PRO	-	expression tag	UNP Q9FKZ1
E	132	GLN	-	expression tag	UNP Q9FKZ1
E	133	PHE	-	expression tag	UNP Q9FKZ1
E	134	GLU	-	expression tag	UNP Q9FKZ1
E	135	LYS	-	expression tag	UNP Q9FKZ1
F	1	SER	-	expression tag	UNP Q9FKZ1
F	2	ASN	-	expression tag	UNP Q9FKZ1
F	3	ALA	-	expression tag	UNP Q9FKZ1
F	97	GLU	LYS	engineered mutation	UNP Q9FKZ1
F	99	GLU	LYS	engineered mutation	UNP Q9FKZ1
F	102	GLU	ARG	engineered mutation	UNP Q9FKZ1
F	103	GLU	LYS	engineered mutation	UNP Q9FKZ1
F	106	GLU	ARG	engineered mutation	UNP Q9FKZ1
F	109	GLU	LYS	engineered mutation	UNP Q9FKZ1
F	113	GLU	LYS	engineered mutation	UNP Q9FKZ1
F	128	TRP	-	expression tag	UNP Q9FKZ1

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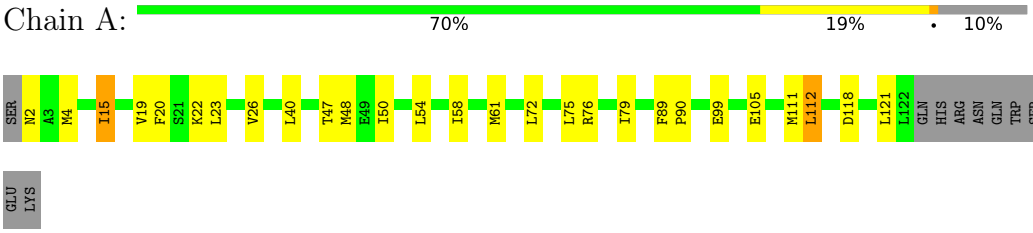
Chain	Residue	Modelled	Actual	Comment	Reference
F	129	SER	-	expression tag	UNP Q9FKZ1
F	130	HIS	-	expression tag	UNP Q9FKZ1
F	131	PRO	-	expression tag	UNP Q9FKZ1
F	132	GLN	-	expression tag	UNP Q9FKZ1
F	133	PHE	-	expression tag	UNP Q9FKZ1
F	134	GLU	-	expression tag	UNP Q9FKZ1
F	135	LYS	-	expression tag	UNP Q9FKZ1

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

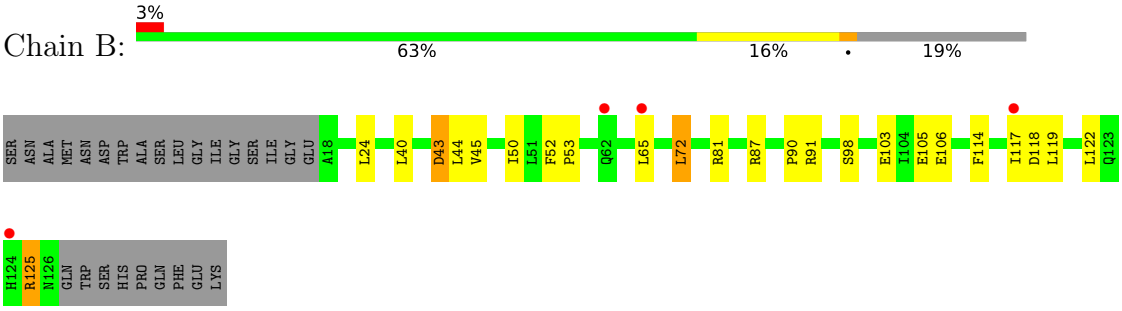
• Molecule 1: Probable disease resistance protein At5g66900

Chain A:



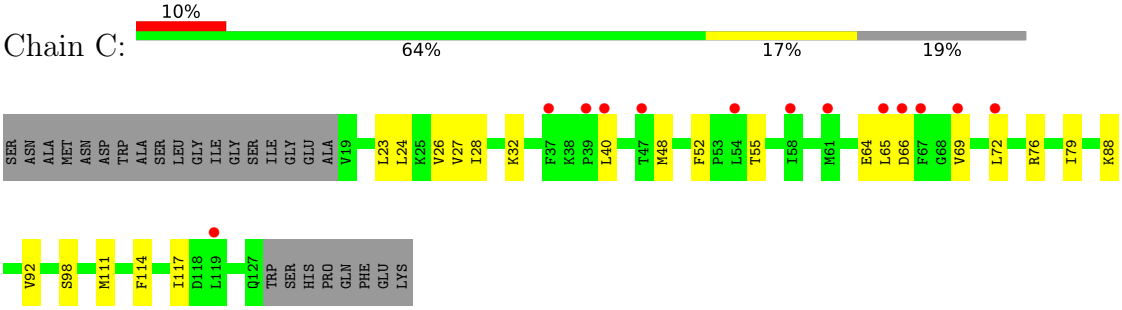
• Molecule 1: Probable disease resistance protein At5g66900

Chain B:



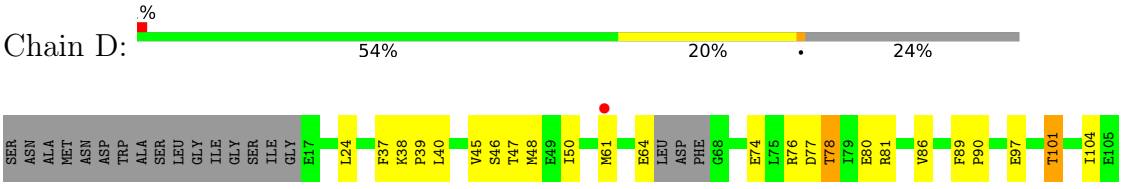
• Molecule 1: Probable disease resistance protein At5g66900

Chain C:

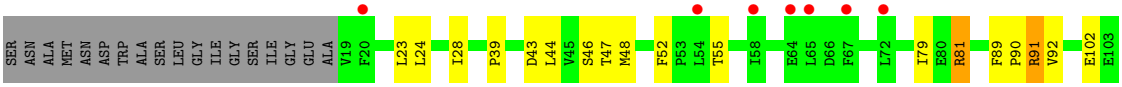


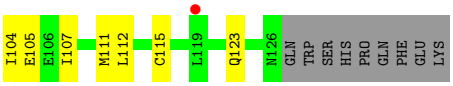
• Molecule 1: Probable disease resistance protein At5g66900

Chain D:



• Molecule 1: Probable disease resistance protein At5g66900





• Molecule 1: Probable disease resistance protein At5g66900

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.33Å 89.66Å 149.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.61 – 2.95 39.58 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.61-2.95) 99.7 (39.58-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.240 0.220 , 0.244	Depositor DCC
R_{free} test set	1285 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	83.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5239	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.39% 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	0.94	4/963 (0.4%)	0.92	0/1302
1	B	0.82	1/880 (0.1%)	0.83	2/1189 (0.2%)
1	C	0.77	0/875	0.81	0/1185
1	D	0.90	1/836 (0.1%)	0.95	0/1125
1	E	0.78	0/856	0.91	2/1163 (0.2%)
1	F	0.80	1/911 (0.1%)	0.84	0/1234
All	All	0.84	7/5321 (0.1%)	0.88	4/7198 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CD-OE1	6.76	1.33	1.25
1	D	113	GLU	CD-OE1	6.52	1.32	1.25
1	F	103	GLU	CD-OE1	6.16	1.32	1.25
1	A	99	GLU	CD-OE2	5.58	1.31	1.25
1	A	105	GLU	CD-OE2	5.54	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	91	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	B	91	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	81	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	81	ARG	NE-CZ-NH1	5.27	122.93	120.30

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	948	0	905	15	1
1	B	867	0	832	13	0
1	C	861	0	805	18	0
1	D	825	0	809	17	2
1	E	842	0	774	13	1
1	F	896	0	845	17	0
All	All	5239	0	4970	93	2

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.

The worst 5 of 93 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:D:81:ARG:NH2	1:D:106:GLU:OE1	1.87	1.08
1:E:48:MET:HG2	1:E:111:MET:HE1	1.51	0.90
1:F:75:LEU:CD2	1:F:114:PHE:HB3	2.12	0.80
1:F:75:LEU:CD2	1:F:114:PHE:CG	2.73	0.72
1:F:75:LEU:HD21	1:F:114:PHE:HB3	1.72	0.70

All (2) 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:D:110:ASP:OD2	1:E:91:ARG:NH1[1_655]	1.83	0.37
1:A:15:ILE:O	1:D:80:GLU:OE2[2_655]	1.96	0.24

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	119/135 (88%)	113 (95%)	5 (4%)	1 (1%)	19 53
1	B	107/135 (79%)	101 (94%)	6 (6%)	0	100 100
1	C	107/135 (79%)	97 (91%)	10 (9%)	0	100 100
1	D	98/135 (73%)	93 (95%)	5 (5%)	0	100 100
1	E	106/135 (78%)	100 (94%)	6 (6%)	0	100 100
1	F	114/135 (84%)	106 (93%)	8 (7%)	0	100 100
All	All	651/810 (80%)	610 (94%)	40 (6%)	1 (0%)	47 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ILE

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	99/124 (80%)	97 (98%)	2 (2%)	55 80
1	B	91/124 (73%)	87 (96%)	4 (4%)	28 62
1	C	87/124 (70%)	86 (99%)	1 (1%)	73 89
1	D	89/124 (72%)	86 (97%)	3 (3%)	37 69
1	E	87/124 (70%)	82 (94%)	5 (6%)	20 52
1	F	91/124 (73%)	87 (96%)	4 (4%)	28 62
All	All	544/744 (73%)	525 (96%)	19 (4%)	36 68

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	123	GLN
1	F	79	ILE
1	F	99	GLU
1	F	50	ILE

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Mol	Chain	Res	Type
1	D	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	B	62	GLN

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 monosaccharides 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

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	121/135 (89%)	0.12	0 100 100	51, 72, 108, 141	0
1	B	109/135 (80%)	0.29	4 (3%) 41 27	53, 77, 135, 153	0
1	C	109/135 (80%)	0.63	13 (11%) 4 2	58, 109, 158, 173	0
1	D	102/135 (75%)	0.18	1 (0%) 82 68	51, 72, 120, 145	0
1	E	108/135 (80%)	0.47	8 (7%) 14 8	54, 104, 149, 163	0
1	F	116/135 (85%)	0.61	13 (11%) 5 3	47, 104, 184, 217	0
All	All	665/810 (82%)	0.38	39 (5%) 22 13	47, 87, 152, 217	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	18	ALA	6.6
1	F	19	VAL	6.3
1	C	67	PHE	5.8
1	E	65	LEU	3.9
1	E	119	LEU	3.5

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.