wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 11:56 pm BST

PDB ID	:	5NGO
Title	:	Crystal structure of the PARP domain of Arabidopsis RADICAL-INDUCED CELL DEATH1
Authors	:	Wirthmueller, L.; Banfield, M.J.
Deposited on	:	2017-03-18
Resolution	:	2.50 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:

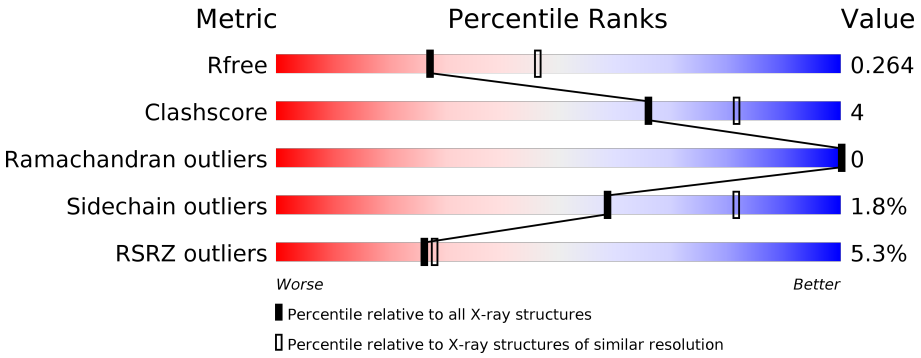
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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.



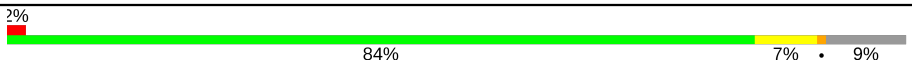
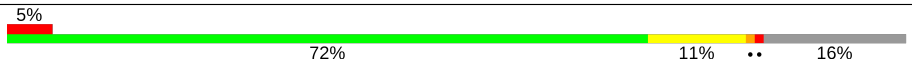
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	194	2% 81% 10% • 8%
1	B	194	7% 78% 7% • 14%
1	C	194	5% 73% 10% •• 16%
1	D	194	4% 83% 8% • 9%
1	E	194	9% 81% 8% • 10%
1	F	194	4% 76% 8% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	194	
1	H	194	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10837 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 Inactive poly [ADP-ribose] polymerase RCD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1407	899	245	253	10			
1	B	167	Total	C	N	O	S	0	0	0
			1311	838	227	236	10			
1	E	174	Total	C	N	O	S	0	0	0
			1384	886	240	248	10			
1	G	177	Total	C	N	O	S	0	0	0
			1399	895	243	251	10			
1	D	177	Total	C	N	O	S	0	0	0
			1399	895	243	251	10			
1	F	163	Total	C	N	O	S	0	0	0
			1276	815	220	231	10			
1	H	162	Total	C	N	O	S	0	0	0
			1275	816	219	230	10			
1	C	163	Total	C	N	O	S	0	0	0
			1279	818	220	231	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLY	-	expression tag	UNP Q8RY59
A	268	PRO	-	expression tag	UNP Q8RY59
B	267	GLY	-	expression tag	UNP Q8RY59
B	268	PRO	-	expression tag	UNP Q8RY59
E	267	GLY	-	expression tag	UNP Q8RY59
E	268	PRO	-	expression tag	UNP Q8RY59
G	267	GLY	-	expression tag	UNP Q8RY59
G	268	PRO	-	expression tag	UNP Q8RY59
D	267	GLY	-	expression tag	UNP Q8RY59
D	268	PRO	-	expression tag	UNP Q8RY59
F	267	GLY	-	expression tag	UNP Q8RY59
F	268	PRO	-	expression tag	UNP Q8RY59
H	267	GLY	-	expression tag	UNP Q8RY59

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	268	PRO	-	expression tag	UNP Q8RY59
C	267	GLY	-	expression tag	UNP Q8RY59
C	268	PRO	-	expression tag	UNP Q8RY59

- Molecule 2 is water.

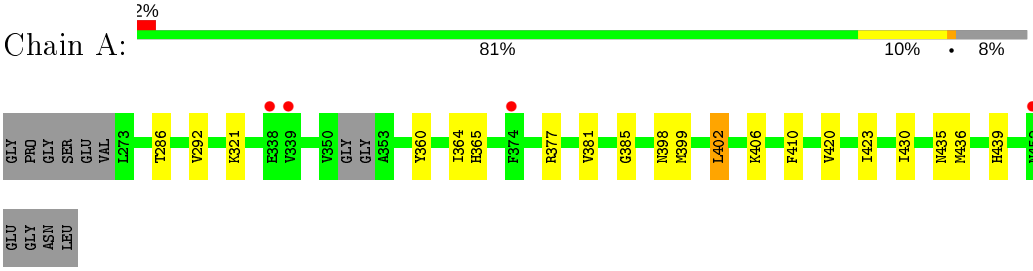
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	21	Total O 21 21	0	0
2	B	11	Total O 11 11	0	0
2	E	7	Total O 7 7	0	0
2	G	24	Total O 24 24	0	0
2	D	12	Total O 12 12	0	0
2	F	9	Total O 9 9	0	0
2	H	12	Total O 12 12	0	0
2	C	11	Total O 11 11	0	0

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 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.

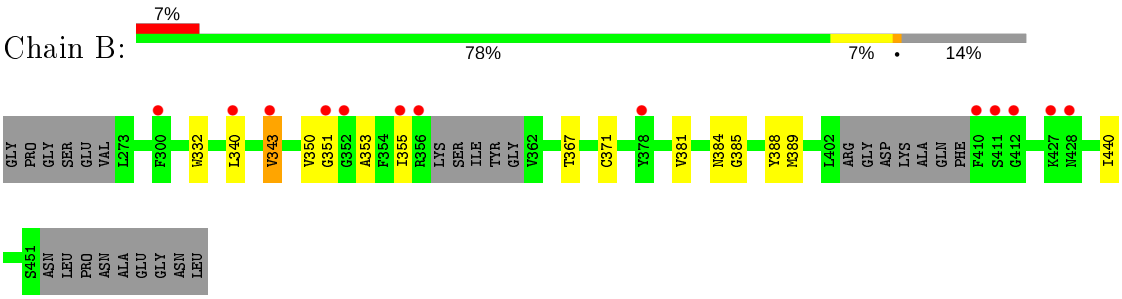
- Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain A:



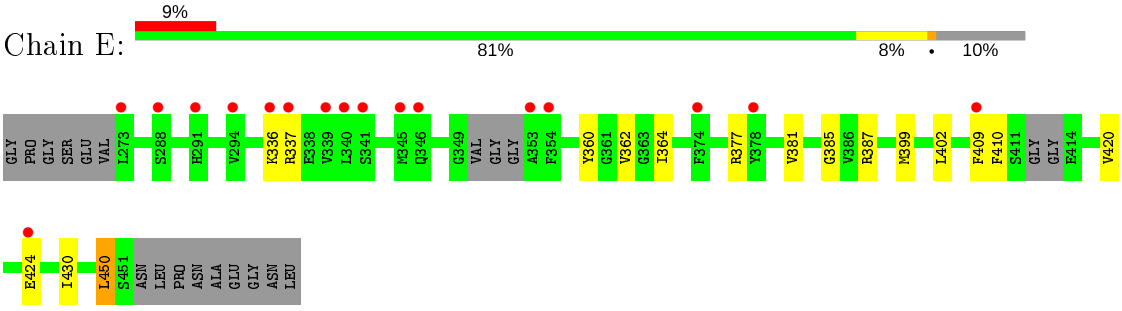
- Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain B:



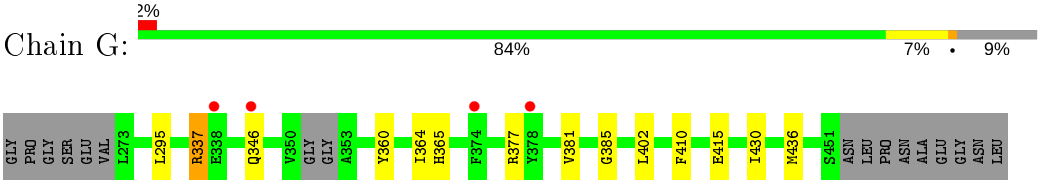
- Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain E:



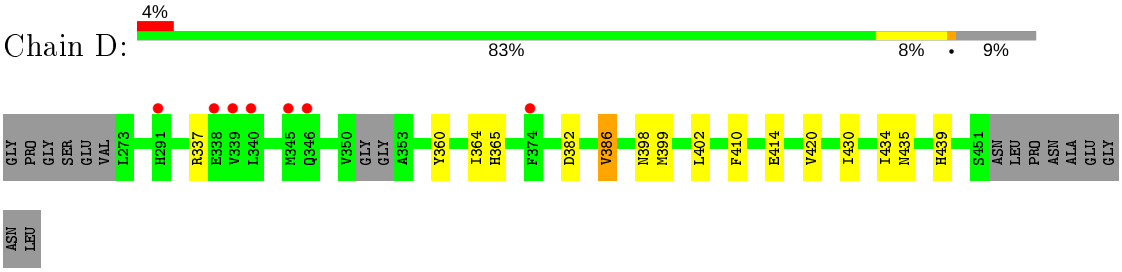
- Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain G:



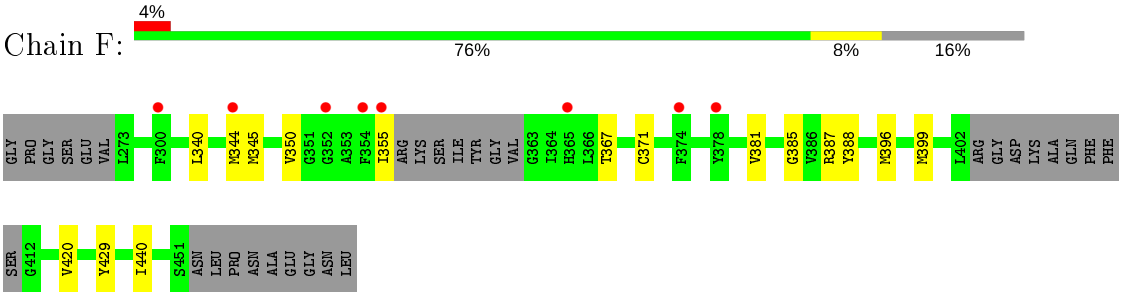
• Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain D:



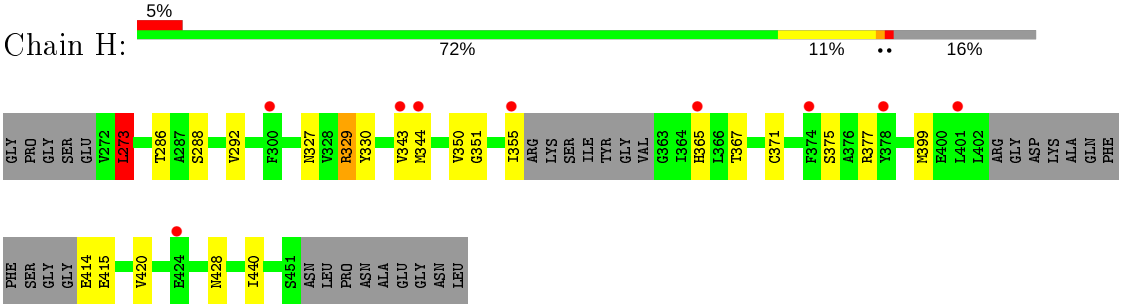
• Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain F:



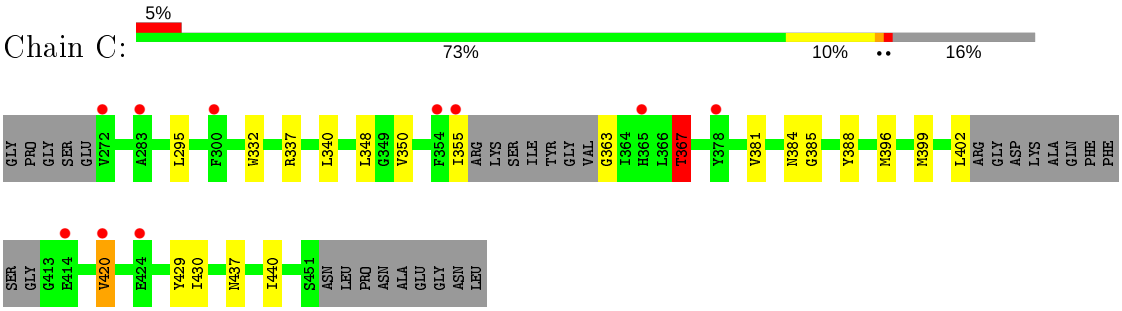
• Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain H:



• Molecule 1: Inactive poly [ADP-ribose] polymerase RCD1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	129.95Å 129.95Å 468.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	156.13 – 2.50 55.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (156.13-2.50) 99.4 (55.87-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.05 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.236 , 0.263 0.237 , 0.264	Depositor DCC
R_{free} test set	2684 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10837	wwPDB-VP
Average B, all atoms (Å^2)	62.0	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 64.03 % 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 8.8298e-06. 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, 0.333 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	0.56	0/1435	0.78	0/1933
1	B	0.61	0/1336	0.79	1/1800 (0.1%)
1	C	0.59	0/1303	0.82	2/1757 (0.1%)
1	D	0.58	1/1427 (0.1%)	0.75	0/1922
1	E	0.60	0/1411	0.79	0/1899
1	F	0.59	0/1300	0.81	3/1752 (0.2%)
1	G	0.60	0/1427	0.80	2/1922 (0.1%)
1	H	0.64	1/1299 (0.1%)	0.84	2/1752 (0.1%)
All	All	0.60	2/10938 (0.0%)	0.80	10/14737 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	288	SER	CB-OG	-6.42	1.33	1.42
1	D	386	VAL	CB-CG1	-5.77	1.40	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	367	THR	CA-CB-CG2	7.87	123.42	112.40
1	F	387	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	G	337	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	H	329	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	G	295	LEU	CB-CG-CD1	6.03	121.25	111.00

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	1407	0	1402	14	0
1	B	1311	0	1305	10	0
1	C	1279	0	1275	19	0
1	D	1399	0	1396	16	0
1	E	1384	0	1380	12	0
1	F	1276	0	1269	8	0
1	G	1399	0	1396	7	0
1	H	1275	0	1272	11	0
2	A	21	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	D	12	0	0	0	0
2	E	7	0	0	0	0
2	F	9	0	0	0	0
2	G	24	0	0	0	0
2	H	12	0	0	0	0
All	All	10837	0	10695	85	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 4.

The worst 5 of 85 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:332:TRP:HB2	1:C:367:THR:HG23	1.28	1.14
1:C:402:LEU:HD11	1:C:430:ILE:HG21	1.64	0.80
1:A:321:LYS:HG2	1:C:295:LEU:O	1.84	0.78
1:D:382:ASP:OD1	1:D:386:VAL:HG12	1.86	0.76
1:C:363:GLY:HA3	1:C:430:ILE:HD11	1.71	0.73

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	174/194 (90%)	170 (98%)	4 (2%)	0	100	100
1	B	161/194 (83%)	159 (99%)	2 (1%)	0	100	100
1	C	157/194 (81%)	153 (98%)	4 (2%)	0	100	100
1	D	173/194 (89%)	170 (98%)	3 (2%)	0	100	100
1	E	168/194 (87%)	165 (98%)	3 (2%)	0	100	100
1	F	157/194 (81%)	154 (98%)	3 (2%)	0	100	100
1	G	173/194 (89%)	170 (98%)	3 (2%)	0	100	100
1	H	156/194 (80%)	152 (97%)	4 (3%)	0	100	100
All	All	1319/1552 (85%)	1293 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	149/159 (94%)	145 (97%)	4 (3%)	44	71
1	B	139/159 (87%)	139 (100%)	0	100	100
1	C	136/159 (86%)	134 (98%)	2 (2%)	65	85
1	D	148/159 (93%)	147 (99%)	1 (1%)	84	94
1	E	147/159 (92%)	142 (97%)	5 (3%)	37	63
1	F	135/159 (85%)	134 (99%)	1 (1%)	84	94
1	G	148/159 (93%)	145 (98%)	3 (2%)	55	79
1	H	136/159 (86%)	132 (97%)	4 (3%)	42	69
All	All	1138/1272 (90%)	1118 (98%)	20 (2%)	59	81

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	337	ARG
1	G	377	ARG
1	H	377	ARG
1	E	424	GLU
1	E	450	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	346	GLN
1	G	433	ASN
1	H	428	ASN
1	E	428	ASN
1	D	439	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	178/194 (91%)	0.15	4 (2%) 62 65	36, 56, 88, 99	0
1	B	167/194 (86%)	0.37	13 (7%) 13 13	37, 57, 83, 115	0
1	C	163/194 (84%)	0.51	10 (6%) 21 22	45, 65, 91, 104	0
1	D	177/194 (91%)	0.36	7 (3%) 38 41	41, 65, 96, 112	0
1	E	174/194 (89%)	0.48	17 (9%) 7 7	41, 64, 109, 127	0
1	F	163/194 (84%)	0.36	8 (4%) 29 31	39, 61, 85, 107	0
1	G	177/194 (91%)	0.11	4 (2%) 60 63	35, 52, 82, 94	0
1	H	162/194 (83%)	0.34	9 (5%) 24 25	39, 58, 83, 93	0
All	All	1361/1552 (87%)	0.33	72 (5%) 26 28	35, 60, 91, 127	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	339	VAL	7.1
1	C	378	TYR	5.5
1	D	339	VAL	5.1
1	F	300	PHE	4.5
1	H	424	GLU	4.4

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.