Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:33 PM GMT

PDB ID	:	5A1H
Title	:	Crystal structure of human Spindlin3
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Deposited on	:	2015-04-30
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

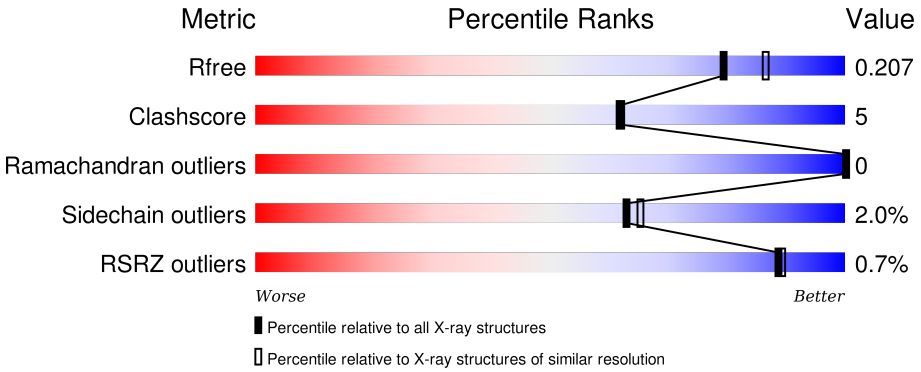
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	222	75% 12% 13%
1	B	222	% 73% 10% 16%
1	C	222	% 74% 9% 16%
1	D	222	71% 9% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6529 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 SPINDLIN-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1549	1001	252	289	7			
1	B	186	Total	C	N	O	S	0	0	0
			1474	957	240	270	7			
1	C	186	Total	C	N	O	S	0	1	0
			1479	956	244	272	7			
1	D	178	Total	C	N	O	S	0	1	0
			1428	925	235	261	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	EXPRESSION TAG	UNP Q5JUX0
A	259	ALA	-	EXPRESSION TAG	UNP Q5JUX0
A	260	GLU	-	EXPRESSION TAG	UNP Q5JUX0
A	261	ASN	-	EXPRESSION TAG	UNP Q5JUX0
A	262	LEU	-	EXPRESSION TAG	UNP Q5JUX0
A	263	TYR	-	EXPRESSION TAG	UNP Q5JUX0
A	264	PHE	-	EXPRESSION TAG	UNP Q5JUX0
A	265	GLN	-	EXPRESSION TAG	UNP Q5JUX0
B	44	MET	-	EXPRESSION TAG	UNP Q5JUX0
B	259	ALA	-	EXPRESSION TAG	UNP Q5JUX0
B	260	GLU	-	EXPRESSION TAG	UNP Q5JUX0
B	261	ASN	-	EXPRESSION TAG	UNP Q5JUX0
B	262	LEU	-	EXPRESSION TAG	UNP Q5JUX0
B	263	TYR	-	EXPRESSION TAG	UNP Q5JUX0
B	264	PHE	-	EXPRESSION TAG	UNP Q5JUX0
B	265	GLN	-	EXPRESSION TAG	UNP Q5JUX0
C	44	MET	-	EXPRESSION TAG	UNP Q5JUX0
C	259	ALA	-	EXPRESSION TAG	UNP Q5JUX0
C	260	GLU	-	EXPRESSION TAG	UNP Q5JUX0
C	261	ASN	-	EXPRESSION TAG	UNP Q5JUX0
C	262	LEU	-	EXPRESSION TAG	UNP Q5JUX0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	263	TYR	-	EXPRESSION TAG	UNP Q5JUX0
C	264	PHE	-	EXPRESSION TAG	UNP Q5JUX0
C	265	GLN	-	EXPRESSION TAG	UNP Q5JUX0
D	44	MET	-	EXPRESSION TAG	UNP Q5JUX0
D	259	ALA	-	EXPRESSION TAG	UNP Q5JUX0
D	260	GLU	-	EXPRESSION TAG	UNP Q5JUX0
D	261	ASN	-	EXPRESSION TAG	UNP Q5JUX0
D	262	LEU	-	EXPRESSION TAG	UNP Q5JUX0
D	263	TYR	-	EXPRESSION TAG	UNP Q5JUX0
D	264	PHE	-	EXPRESSION TAG	UNP Q5JUX0
D	265	GLN	-	EXPRESSION TAG	UNP Q5JUX0

- Molecule 2 is water.

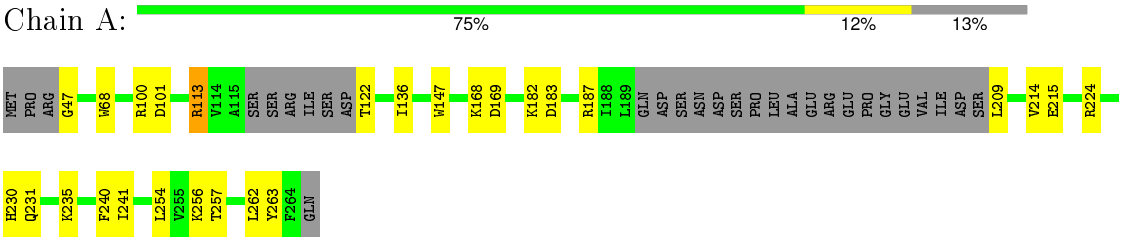
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	149	Total O 149 149	0	0
2	B	139	Total O 139 139	0	0
2	C	165	Total O 165 165	0	0
2	D	146	Total O 146 146	0	0

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.

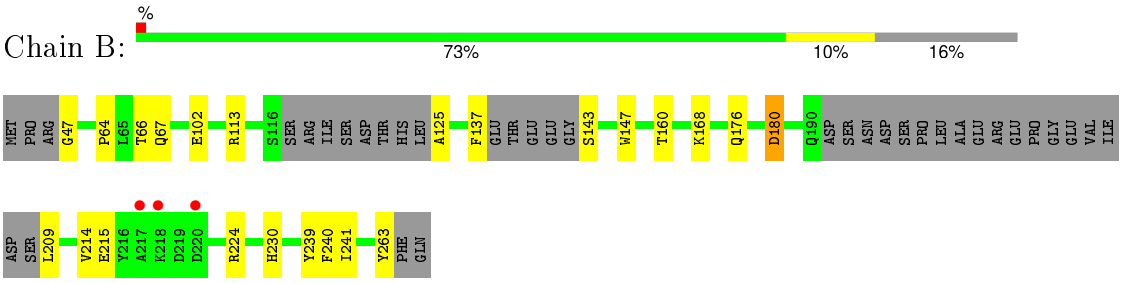
- Molecule 1: SPINDLIN-3

Chain A:



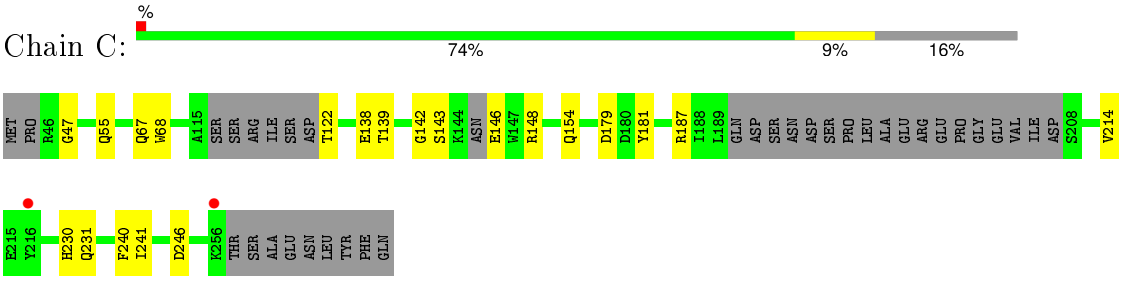
- Molecule 1: SPINDLIN-3

Chain B:



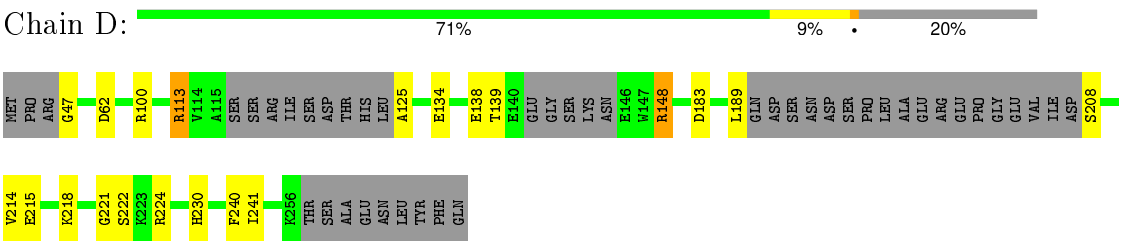
- Molecule 1: SPINDLIN-3

Chain C:



- Molecule 1: SPINDLIN-3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.58Å 129.40Å 129.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.14 – 2.00 26.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (26.14-2.00) 99.5 (26.14-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.172 , 0.212 0.165 , 0.207	Depositor DCC
R_{free} test set	3267 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.6	EDS
Estimated twinning fraction	0.502 for H, K, L 0.498 for -H, L, K 0.479 for -h,l,k	Xtriage
Reported twinning fraction	0.502 for H, K, L 0.498 for -H, L, K	Depositor
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 67086 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6529	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.76% 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, 0.375 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	0.71	0/1587	0.79	2/2153 (0.1%)
1	B	0.65	0/1508	0.77	2/2044 (0.1%)
1	C	0.72	0/1514	0.77	1/2050 (0.0%)
1	D	0.73	0/1461	0.83	4/1978 (0.2%)
All	All	0.70	0/6070	0.79	9/8225 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	113	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	113	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	D	183	ASP	CB-CG-OD1	7.61	125.15	118.30
1	D	113	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	113	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	100	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	113	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	180	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	C	47	GLY	N-CA-C	-5.20	100.11	113.10

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	1549	0	1482	21	1
1	B	1474	0	1393	17	0
1	C	1479	0	1389	13	1
1	D	1428	0	1365	16	0
2	A	149	0	0	10	0
2	B	139	0	0	9	1
2	C	165	0	0	8	2
2	D	146	0	0	7	1
All	All	6529	0	5629	62	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 5.

All (62) 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:47:GLY:N	2:A:2001:HOH:O	1.88	1.05
1:B:64:PRO:O	2:B:2023:HOH:O	1.84	0.96
1:A:122:THR:N	2:A:2079:HOH:O	2.10	0.82
1:C:246:ASP:OD1	2:C:2158:HOH:O	1.96	0.82
1:B:180:ASP:OD2	2:B:2122:HOH:O	2.00	0.79
1:C:122:THR:N	2:C:2091:HOH:O	2.17	0.78
1:B:160:THR:OG1	2:B:2117:HOH:O	2.02	0.77
1:B:214:VAL:HA	1:B:263:TYR:HB3	1.69	0.74
1:A:187:ARG:NH1	2:A:2095:HOH:O	2.21	0.72
1:D:47:GLY:N	2:D:2002:HOH:O	2.22	0.72
1:A:113:ARG:HD3	1:C:68:TRP:CZ2	2.25	0.71
1:A:169:ASP:O	2:A:2103:HOH:O	2.09	0.71
1:B:176:GLN:HG2	2:B:2117:HOH:O	1.90	0.70
1:D:125:ALA:N	2:D:2066:HOH:O	2.26	0.69
1:B:125:ALA:N	2:B:2099:HOH:O	2.34	0.60
1:C:146:GLU:N	2:C:2101:HOH:O	2.34	0.59
1:B:67:GLN:OE1	2:B:2010:HOH:O	2.15	0.59
1:A:68:TRP:CZ2	1:D:113:ARG:HD3	2.38	0.59
1:B:47:GLY:N	2:B:2001:HOH:O	2.36	0.57
1:D:218:LYS:HD2	1:D:224:ARG:HB2	1.88	0.55
1:C:231:GLN:O	2:C:2146:HOH:O	2.18	0.55
1:B:66:THR:HG23	2:B:2023:HOH:O	2.07	0.55
1:A:101:ASP:N	2:A:2054:HOH:O	2.40	0.53
1:C:142:GLY:N	2:C:2103:HOH:O	2.42	0.52
1:A:214:VAL:HG21	1:A:241:ILE:HD13	1.91	0.52
1:A:47:GLY:N	1:B:263:TYR:HH	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HD3	1:C:68:TRP:HZ2	1.70	0.52
1:D:214:VAL:HG21	1:D:241:ILE:HD13	1.92	0.52
1:D:62:ASP:N	1:D:62:ASP:OD1	2.41	0.51
1:A:254:LEU:HD21	1:A:263:TYR:OH	2.11	0.51
1:D:221:GLY:N	2:D:2122:HOH:O	2.44	0.51
1:C:214:VAL:HG21	1:C:241:ILE:HD13	1.92	0.50
1:A:231:GLN:HG3	2:A:2138:HOH:O	2.11	0.50
1:C:154:GLN:HG3	2:C:2114:HOH:O	2.12	0.49
1:B:214:VAL:HG21	1:B:241:ILE:HD13	1.94	0.49
1:A:230:HIS:HB3	1:A:240:PHE:HB2	1.96	0.48
1:D:134:GLU:HG3	1:D:148:ARG:HH11	1.80	0.47
1:A:100:ARG:NH1	2:A:2061:HOH:O	2.48	0.47
1:B:209:LEU:HD12	1:B:239:TYR:CZ	2.50	0.46
1:A:68:TRP:HZ2	1:D:113:ARG:HD3	1.80	0.45
1:B:230:HIS:HB3	1:B:240:PHE:HB2	1.99	0.45
1:B:209:LEU:N	2:B:2127:HOH:O	2.49	0.45
1:A:147:TRP:CD1	1:A:168:LYS:HD2	2.51	0.45
1:A:182:LYS:NZ	2:A:2119:HOH:O	2.48	0.45
1:D:208:SER:O	2:D:2112:HOH:O	2.21	0.44
1:C:230:HIS:HB3	1:C:240:PHE:HB2	1.99	0.43
1:D:222:SER:N	2:D:2122:HOH:O	2.34	0.43
1:C:138:GLU:HA	1:C:143:SER:O	2.19	0.43
1:A:215:GLU:HA	1:A:224:ARG:O	2.20	0.42
1:B:147:TRP:CD1	1:B:168:LYS:HD2	2.55	0.42
1:A:209:LEU:N	2:A:2123:HOH:O	2.53	0.42
1:B:215:GLU:HA	1:B:224:ARG:O	2.20	0.42
1:D:139:THR:HG22	2:D:2078:HOH:O	2.20	0.41
1:D:230[B]:HIS:HB3	1:D:240:PHE:HB2	2.02	0.41
1:C:55:GLN:NE2	2:C:2014:HOH:O	2.49	0.41
1:B:137:PHE:CD2	1:B:143:SER:O	2.74	0.41
1:D:113:ARG:N	1:D:113:ARG:HD2	2.36	0.41
1:D:215:GLU:HA	1:D:224:ARG:O	2.21	0.41
1:A:256:LYS:HG2	1:A:257:THR:N	2.36	0.41
1:A:183:ASP:HA	2:A:2117:HOH:O	2.21	0.41
1:C:122:THR:N	2:C:2090:HOH:O	2.53	0.40
1:D:214:VAL:CG1	2:D:2115:HOH:O	2.69	0.40

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)
2:B:2064:HOH:O	2:C:2085:HOH:O[3_644]	2.08	0.12
1:A:215:GLU:OE2	1:C:181:TYR:OH[3_544]	2.19	0.01
2:C:2106:HOH:O	2:D:2144:HOH:O[2_455]	2.19	0.01

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	187/222 (84%)	183 (98%)	4 (2%)	0	100	100
1	B	178/222 (80%)	174 (98%)	4 (2%)	0	100	100
1	C	179/222 (81%)	177 (99%)	2 (1%)	0	100	100
1	D	171/222 (77%)	168 (98%)	3 (2%)	0	100	100
All	All	715/888 (80%)	702 (98%)	13 (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	164/198 (83%)	161 (98%)	3 (2%)	66	69
1	B	151/198 (76%)	150 (99%)	1 (1%)	88	91
1	C	151/198 (76%)	145 (96%)	6 (4%)	38	33
1	D	149/198 (75%)	146 (98%)	3 (2%)	63	65
All	All	615/792 (78%)	602 (98%)	13 (2%)	63	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ILE
1	A	235	LYS
1	A	262	LEU
1	B	102	GLU
1	C	67[A]	GLN
1	C	67[B]	GLN
1	C	139	THR
1	C	148	ARG
1	C	179	ASP
1	C	187	ARG
1	D	138	GLU
1	D	148	ARG
1	D	189	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	67	GLN

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 (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	193/222 (86%)	-0.65	0 100 100	10, 19, 36, 45	0
1	B	186/222 (83%)	-0.36	3 (1%) 74 75	13, 24, 52, 89	0
1	C	186/222 (83%)	-0.51	2 (1%) 82 83	11, 20, 54, 76	0
1	D	178/222 (80%)	-0.56	0 100 100	11, 20, 46, 63	0
All	All	743/888 (83%)	-0.52	5 (0%) 89 89	10, 20, 48, 89	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	216	TYR	3.9
1	B	217	ALA	3.5
1	B	218	LYS	3.1
1	C	256	LYS	3.0
1	B	220	ASP	2.1

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 (i)

There are no such residues in this entry.