wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 07:13 AM EDT

PDB ID	:	2DG0
Title	:	Crystal structure of Drp35, a 35kDa drug responsive protein from Staphylococcus aureus
Authors	:	Tanaka, Y.; Ohki, Y.; Morikawa, K.; Yao, M.; Watanabe, N.; Ohta, T.; Tanaka, I.
Deposited on	:	2006-03-07
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

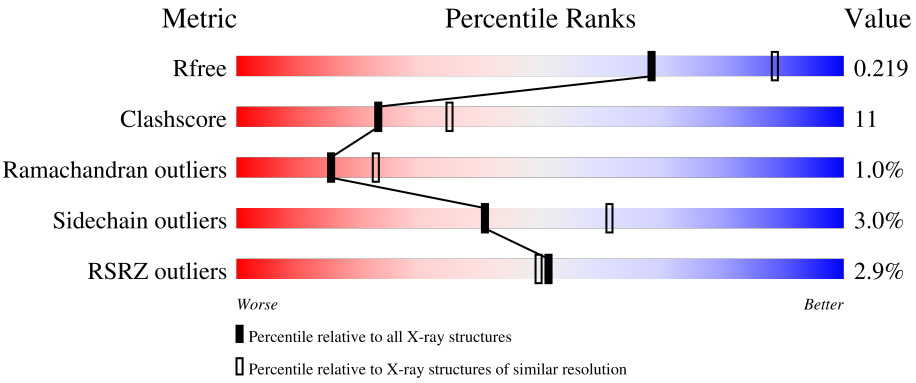
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	333	5% 73% 23%
1	B	333	2% 74% 20%
1	C	333	2% 73% 21%
1	D	333	3% 74% 20%
1	E	333	2% 74% 20%

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Mol	Chain	Length	Quality of chain
1	F	333	2% 74% 20%
1	G	333	% 72% 22%
1	H	333	% 74% 22%
1	I	333	2% 73% 21%
1	J	333	5% 74% 21%
1	K	333	2% 74% 21%
1	L	333	5% 71% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31391 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 DrP35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	Se	0	0	0
			2520	1609	417	484	5	5			
1	B	320	Total	C	N	O	S	Se	0	0	0
			2503	1598	414	481	5	5			
1	C	320	Total	C	N	O	S	Se	0	0	0
			2503	1598	414	481	5	5			
1	D	320	Total	C	N	O	S	Se	0	0	0
			2503	1598	414	481	5	5			
1	E	321	Total	C	N	O	S	Se	0	0	0
			2511	1604	415	482	5	5			
1	F	321	Total	C	N	O	S	Se	0	0	0
			2512	1603	416	483	5	5			
1	G	320	Total	C	N	O	S	Se	0	0	0
			2503	1598	414	481	5	5			
1	H	321	Total	C	N	O	S	Se	0	0	0
			2512	1603	416	483	5	5			
1	I	319	Total	C	N	O	S	Se	0	0	0
			2494	1593	412	479	5	5			
1	J	321	Total	C	N	O	S	Se	0	0	0
			2511	1604	415	482	5	5			
1	K	321	Total	C	N	O	S	Se	0	0	0
			2512	1603	416	483	5	5			
1	L	321	Total	C	N	O	S	Se	0	0	0
			2512	1603	416	483	5	5			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
A	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
A	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
A	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
A	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
A	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
A	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
A	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
A	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
A	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
A	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
A	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
A	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
A	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
B	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
B	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
B	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
B	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
B	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
B	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
B	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
B	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
B	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
B	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
B	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
B	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
B	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
B	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
B	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
C	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
C	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
C	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
C	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
C	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
C	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
C	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
C	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
C	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
C	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
C	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
C	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
C	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
C	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
C	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
D	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
D	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
D	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
D	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
D	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
D	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
D	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
D	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
D	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
D	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
D	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
D	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
D	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
D	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
D	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
D	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
E	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
E	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
E	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
E	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
E	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
E	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
E	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
E	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
E	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
E	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
E	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
E	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
E	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
E	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
E	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
E	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
F	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
F	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
F	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
F	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
F	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
F	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
F	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
F	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
F	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
F	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
F	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
F	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
F	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
F	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
F	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
G	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
G	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
G	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
G	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
G	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
G	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
G	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
G	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
G	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
G	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
G	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
G	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
G	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
G	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
G	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
G	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
H	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
H	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
H	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
H	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
H	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
H	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
H	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
H	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
H	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
H	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
H	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
H	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
H	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
H	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
H	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
H	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
I	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
I	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
I	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
I	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
I	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
I	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
I	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
I	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
I	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
I	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
I	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
I	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
I	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
I	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
I	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
J	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
J	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
J	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
J	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
J	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
J	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
J	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
J	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
J	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
J	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
J	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
J	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
J	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
J	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
J	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
J	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
K	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
K	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
K	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
K	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
K	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
K	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
K	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
K	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
K	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
K	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
K	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
K	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
K	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
K	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
K	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3
L	1	MSE	-	CLONING ARTIFACT	UNP Q9S0S3
L	2	ALA	-	CLONING ARTIFACT	UNP Q9S0S3
L	3	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
L	140	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
L	250	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
L	279	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
L	303	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
L	308	MSE	MET	MODIFIED RESIDUE	UNP Q9S0S3
L	326	LEU	-	EXPRESSION TAG	UNP Q9S0S3
L	327	GLU	-	EXPRESSION TAG	UNP Q9S0S3
L	328	HIS	-	EXPRESSION TAG	UNP Q9S0S3
L	329	HIS	-	EXPRESSION TAG	UNP Q9S0S3
L	330	HIS	-	EXPRESSION TAG	UNP Q9S0S3
L	331	HIS	-	EXPRESSION TAG	UNP Q9S0S3
L	332	HIS	-	EXPRESSION TAG	UNP Q9S0S3
L	333	HIS	-	EXPRESSION TAG	UNP Q9S0S3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	96	Total O 96 96	0	0
2	B	159	Total O 159 159	0	0
2	C	79	Total O 79 79	0	0
2	D	74	Total O 74 74	0	0
2	E	121	Total O 121 121	0	0
2	F	109	Total O 109 109	0	0
2	G	122	Total O 122 122	0	0
2	H	161	Total O 161 161	0	0
2	I	92	Total O 92 92	0	0
2	J	61	Total O 61 61	0	0

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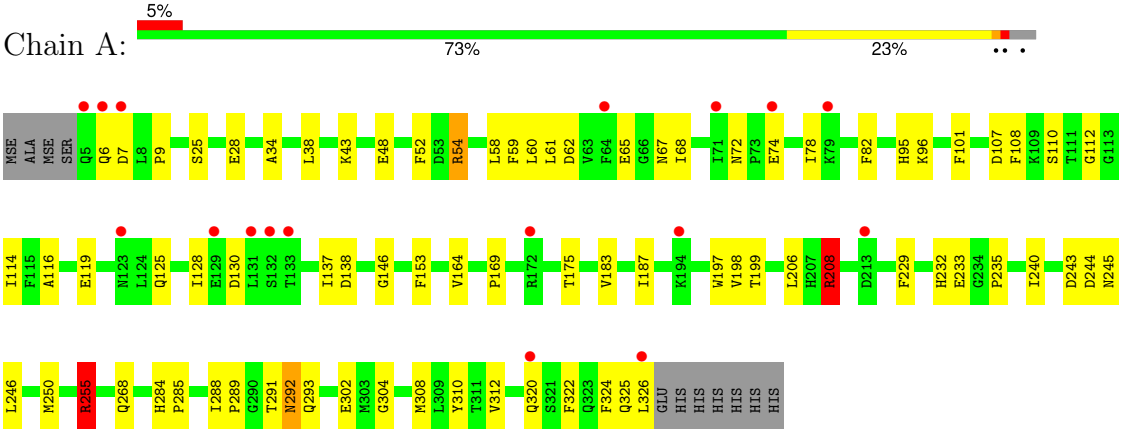
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	142	Total O 142 142	0	0
2	L	79	Total O 79 79	0	0

3 Residue-property plots (i)

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.

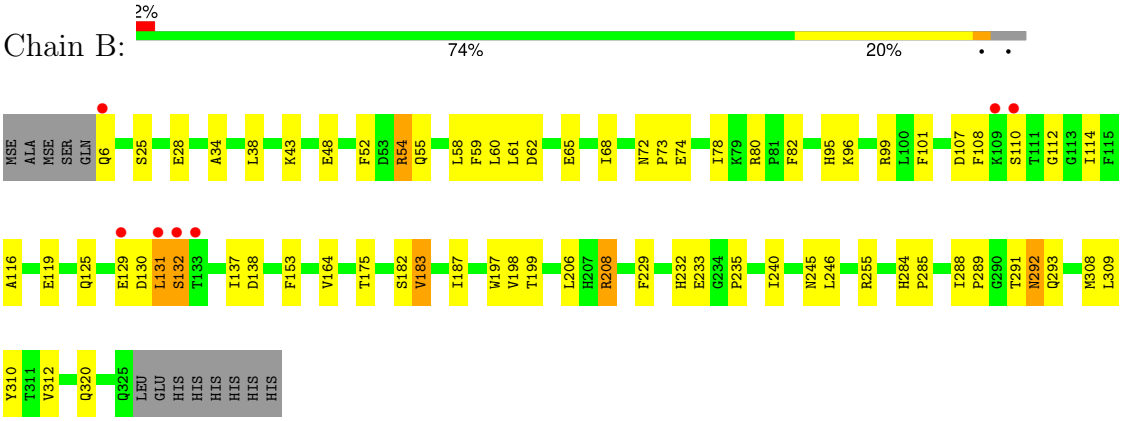
• Molecule 1: DrP35

Chain A:



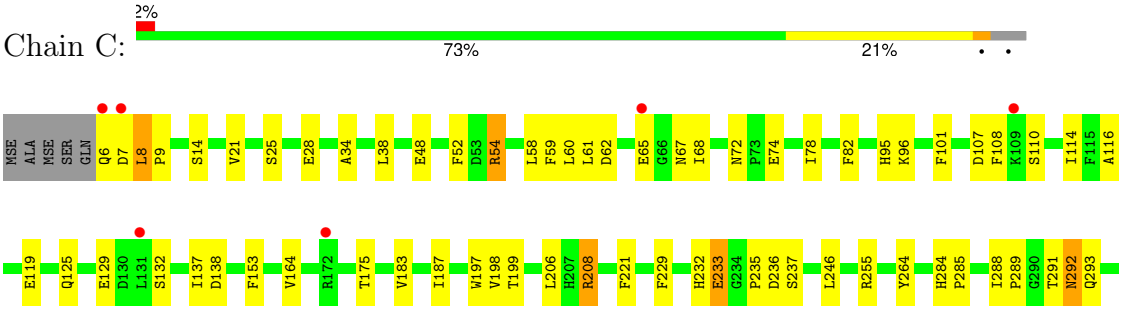
• Molecule 1: DrP35

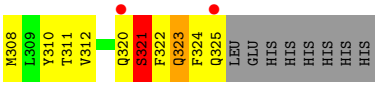
Chain B:



• Molecule 1: DrP35

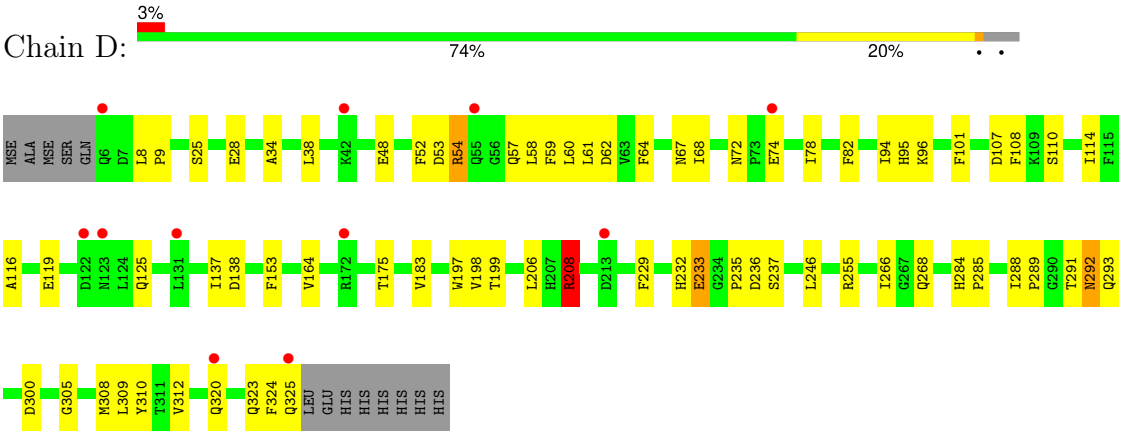
Chain C:





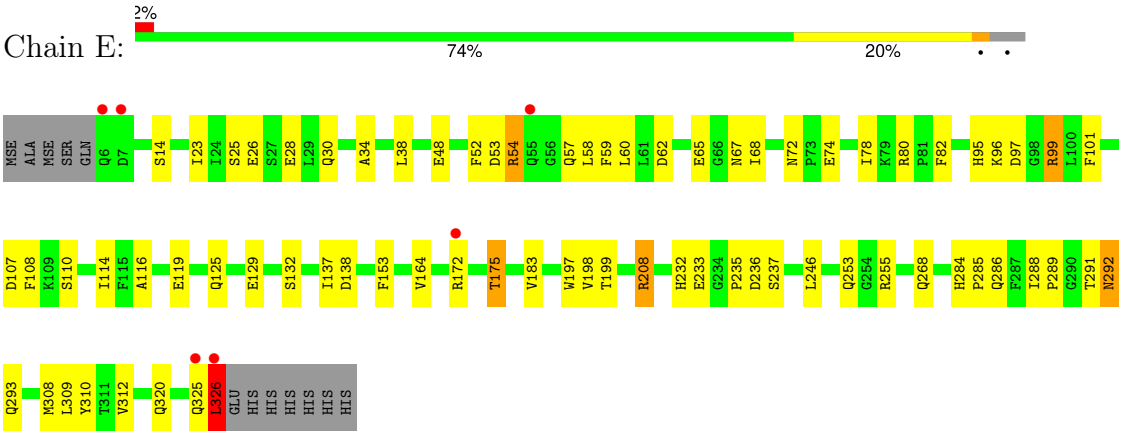
• Molecule 1: DrP35

Chain D:



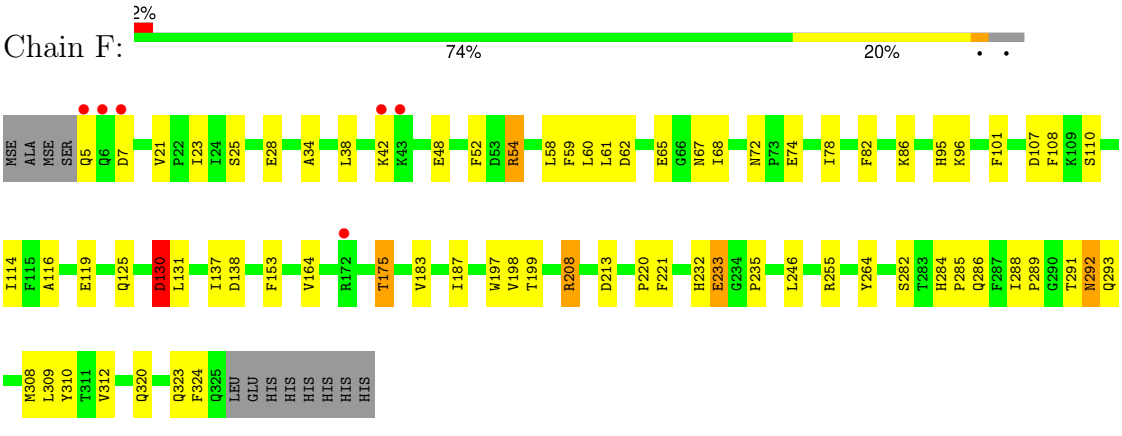
• Molecule 1: DrP35

Chain E:



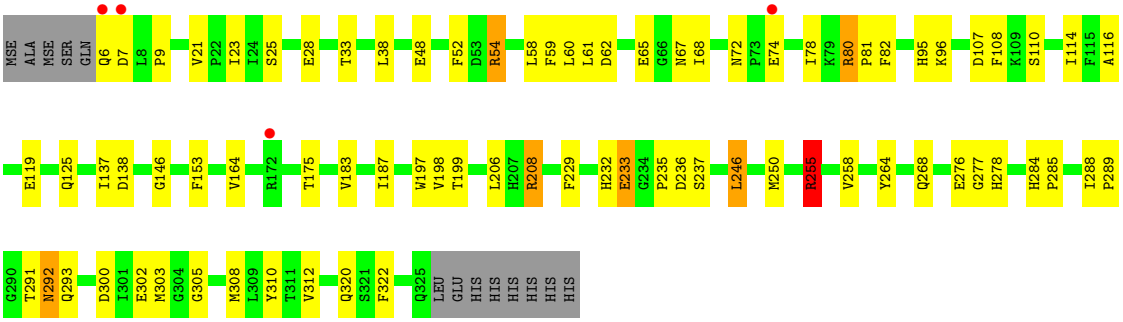
• Molecule 1: DrP35

Chain F:



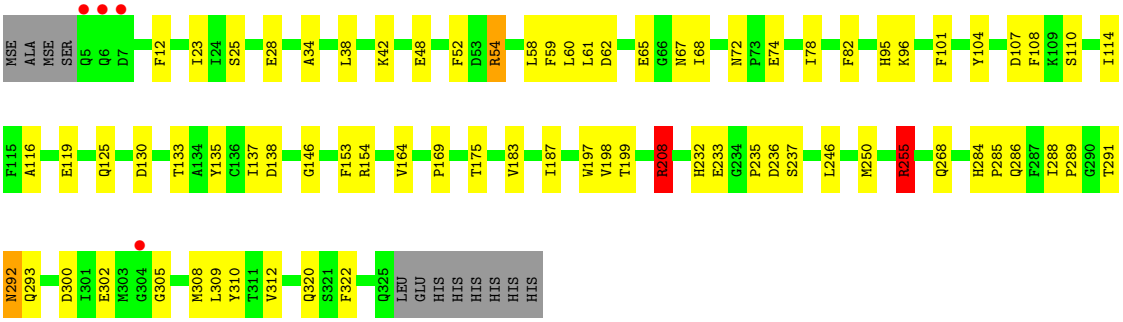
• Molecule 1: DrP35

Chain G:



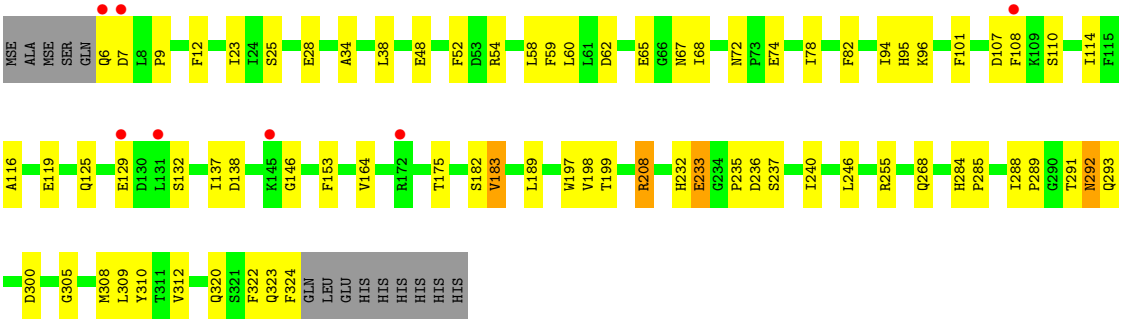
• Molecule 1: DrP35

Chain H:



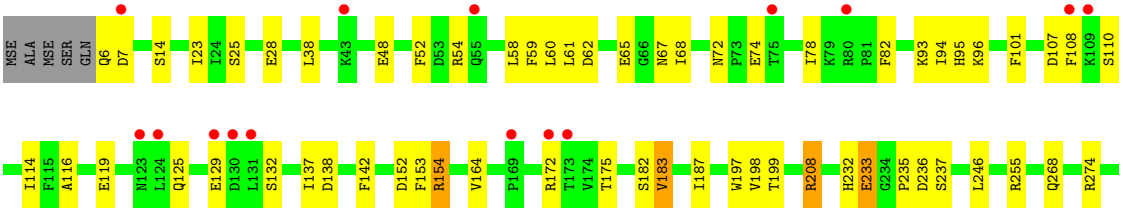
• Molecule 1: DrP35

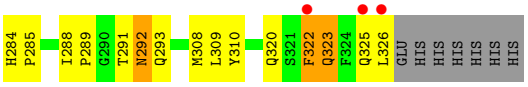
Chain I:



• Molecule 1: DrP35

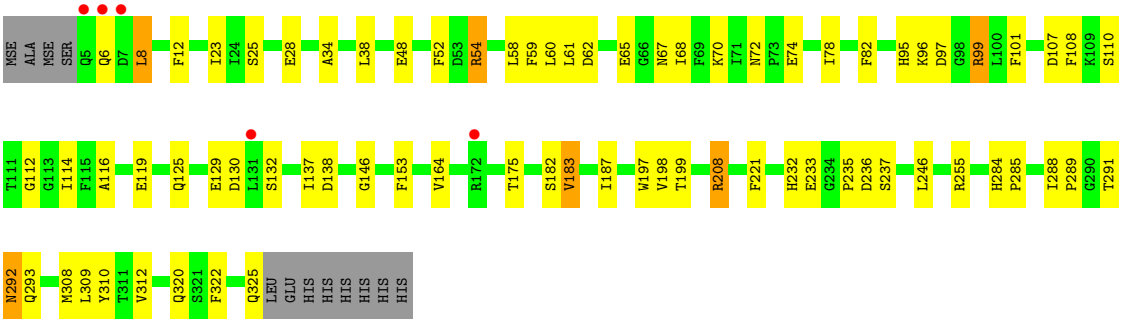
Chain J:





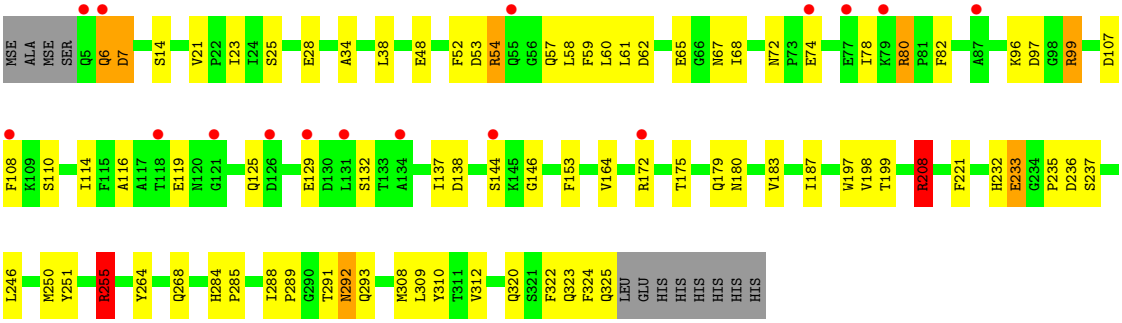
• Molecule 1: DrP35

Chain K:



• Molecule 1: DrP35

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.09Å 146.06Å 151.95Å 90.00° 93.39° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (15.00-2.40) 95.0 (15.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.60 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.222 0.194 , 0.219	Depositor DCC
R_{free} test set	13838 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31391	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.37	0/2575	0.87	8/3484 (0.2%)
1	B	0.37	0/2558	0.76	7/3461 (0.2%)
1	C	0.36	0/2558	0.78	7/3461 (0.2%)
1	D	0.36	0/2558	0.74	6/3461 (0.2%)
1	E	0.38	0/2566	0.93	14/3472 (0.4%)
1	F	0.36	0/2567	0.76	6/3473 (0.2%)
1	G	0.37	0/2558	0.81	8/3461 (0.2%)
1	H	0.37	0/2567	0.89	10/3473 (0.3%)
1	I	0.37	0/2549	0.89	10/3449 (0.3%)
1	J	0.39	0/2566	0.95	13/3472 (0.4%)
1	K	0.38	0/2567	0.90	10/3473 (0.3%)
1	L	0.37	0/2567	0.92	13/3473 (0.4%)
All	All	0.37	0/30756	0.85	112/41613 (0.3%)

There are no bond length outliers.

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	154	ARG	NE-CZ-NH2	-17.10	111.75	120.30
1	A	54	ARG	NE-CZ-NH2	-16.59	112.01	120.30
1	J	154	ARG	NE-CZ-NH1	16.53	128.56	120.30
1	H	154	ARG	NE-CZ-NH1	16.51	128.55	120.30
1	J	54	ARG	NE-CZ-NH2	-16.40	112.10	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	2520	0	2445	59	0
1	B	2503	0	2426	54	0
1	C	2503	0	2426	61	0
1	D	2503	0	2426	56	0
1	E	2511	0	2437	58	0
1	F	2512	0	2434	53	0
1	G	2503	0	2426	57	0
1	H	2512	0	2434	56	0
1	I	2494	0	2418	57	0
1	J	2511	0	2437	62	0
1	K	2512	0	2434	55	0
1	L	2512	0	2434	65	0
2	A	96	0	0	5	0
2	B	159	0	0	3	0
2	C	79	0	0	1	0
2	D	74	0	0	2	0
2	E	121	0	0	5	0
2	F	109	0	0	4	0
2	G	122	0	0	4	0
2	H	161	0	0	6	0
2	I	92	0	0	1	0
2	J	61	0	0	1	0
2	K	142	0	0	1	0
2	L	79	0	0	1	0
All	All	31391	0	29177	670	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 11.

The worst 5 of 670 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:F:5:GLN:NE2	1:F:293:GLN:HB2	1.72	1.04
1:C:8:LEU:HD12	1:C:8:LEU:H	1.25	1.01
1:L:80:ARG:HG3	1:L:80:ARG:HH11	1.32	0.94
1:F:130:ASP:HB3	1:F:131:LEU:HD22	1.48	0.94
1:C:323:GLN:H	1:C:323:GLN:HE21	0.98	0.92

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	320/333 (96%)	296 (92%)	21 (7%)	3 (1%)	17	25
1	B	318/333 (96%)	300 (94%)	14 (4%)	4 (1%)	12	17
1	C	318/333 (96%)	296 (93%)	18 (6%)	4 (1%)	12	17
1	D	318/333 (96%)	298 (94%)	17 (5%)	3 (1%)	17	25
1	E	319/333 (96%)	301 (94%)	15 (5%)	3 (1%)	17	25
1	F	319/333 (96%)	294 (92%)	21 (7%)	4 (1%)	12	17
1	G	318/333 (96%)	303 (95%)	12 (4%)	3 (1%)	17	25
1	H	319/333 (96%)	301 (94%)	15 (5%)	3 (1%)	17	25
1	I	317/333 (95%)	299 (94%)	15 (5%)	3 (1%)	17	25
1	J	319/333 (96%)	298 (93%)	18 (6%)	3 (1%)	17	25
1	K	319/333 (96%)	302 (95%)	14 (4%)	3 (1%)	17	25
1	L	319/333 (96%)	298 (93%)	18 (6%)	3 (1%)	17	25
All	All	3823/3996 (96%)	3586 (94%)	198 (5%)	39 (1%)	15	23

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	SER
1	C	321	SER
1	F	130	ASP
1	A	110	SER
1	B	110	SER

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	275/278 (99%)	268 (98%)	7 (2%)	47	67
1	B	273/278 (98%)	265 (97%)	8 (3%)	42	62
1	C	273/278 (98%)	262 (96%)	11 (4%)	31	49
1	D	273/278 (98%)	266 (97%)	7 (3%)	46	66
1	E	274/278 (99%)	268 (98%)	6 (2%)	52	71
1	F	274/278 (99%)	264 (96%)	10 (4%)	35	54
1	G	273/278 (98%)	265 (97%)	8 (3%)	42	62
1	H	274/278 (99%)	267 (97%)	7 (3%)	46	66
1	I	272/278 (98%)	266 (98%)	6 (2%)	52	71
1	J	274/278 (99%)	266 (97%)	8 (3%)	42	62
1	K	274/278 (99%)	266 (97%)	8 (3%)	42	62
1	L	274/278 (99%)	262 (96%)	12 (4%)	28	45
All	All	3283/3336 (98%)	3185 (97%)	98 (3%)	41	61

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	48	GLU
1	J	175	THR
1	H	208	ARG
1	I	175	THR
1	J	292	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	18	ASN
1	L	123	ASN
1	J	159	ASN
1	K	123	ASN
1	L	320	GLN

5.3.3 RNA

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	317/333 (95%)	-0.06	17 (5%)	25	24	21, 39, 64, 87	0
1	B	315/333 (94%)	-0.24	7 (2%)	62	60	16, 32, 58, 74	0
1	C	315/333 (94%)	-0.18	8 (2%)	57	55	22, 38, 63, 76	0
1	D	315/333 (94%)	-0.11	11 (3%)	44	43	24, 41, 65, 79	0
1	E	316/333 (94%)	-0.27	6 (1%)	66	64	20, 36, 59, 72	0
1	F	316/333 (94%)	-0.26	6 (1%)	66	64	22, 36, 61, 81	0
1	G	315/333 (94%)	-0.29	4 (1%)	77	75	19, 36, 58, 74	0
1	H	316/333 (94%)	-0.33	4 (1%)	77	75	19, 33, 56, 81	0
1	I	314/333 (94%)	-0.18	7 (2%)	62	60	24, 40, 62, 71	0
1	J	316/333 (94%)	0.02	18 (5%)	23	22	23, 43, 67, 85	0
1	K	316/333 (94%)	-0.28	5 (1%)	72	70	18, 34, 58, 82	0
1	L	316/333 (94%)	0.12	16 (5%)	28	26	23, 41, 65, 88	0
All	All	3787/3996 (94%)	-0.17	109 (2%)	51	50	16, 37, 62, 88	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLN	10.4
1	J	326	LEU	8.0
1	B	6	GLN	7.3
1	L	6	GLN	6.8
1	J	322	PHE	6.3

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 (i)

There are no monosaccharides 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.