wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2023 – 11:38 PM EDT

PDB ID	:	7RXZ
Title	:	human Hsp90_MC domain structure
Authors	:	Peng, S.; Deng, J.; Matts, R.
Deposited on	:	2021-08-24
Resolution	:	3.15 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:

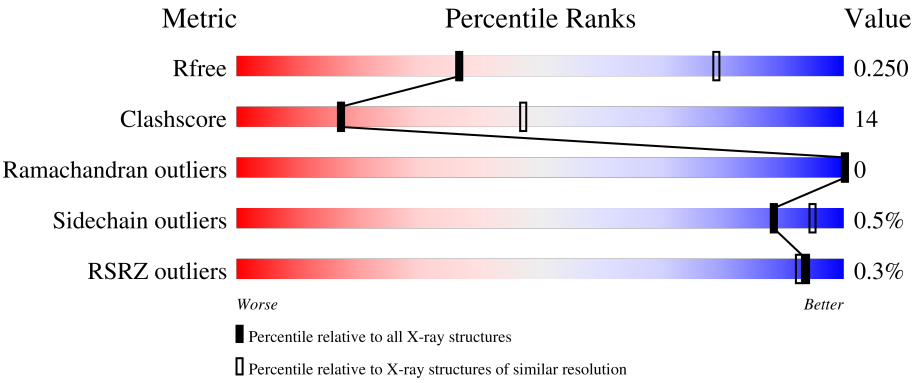
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	425	65% 27% 8%
1	B	425	64% 29% 6%
1	C	425	68% 25% 6%
1	D	425	65% 26% 9%
1	E	425	66% 27% 7%

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Mol	Chain	Length	Quality of chain
1	F	425	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19425 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3232	2055	546	613	18			
1	B	399	Total	C	N	O	S	0	0	0
			3280	2082	556	624	18			
1	C	398	Total	C	N	O	S	0	0	0
			3272	2078	555	621	18			
1	D	386	Total	C	N	O	S	0	0	0
			3177	2020	537	604	16			
1	E	397	Total	C	N	O	S	0	0	0
			3263	2072	553	620	18			
1	F	389	Total	C	N	O	S	0	0	0
			3201	2036	543	606	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	-	expression tag	UNP P07900
A	291	HIS	-	expression tag	UNP P07900
A	292	MET	-	expression tag	UNP P07900
B	290	GLY	-	expression tag	UNP P07900
B	291	HIS	-	expression tag	UNP P07900
B	292	MET	-	expression tag	UNP P07900
C	290	GLY	-	expression tag	UNP P07900
C	291	HIS	-	expression tag	UNP P07900
C	292	MET	-	expression tag	UNP P07900
D	290	GLY	-	expression tag	UNP P07900
D	291	HIS	-	expression tag	UNP P07900
D	292	MET	-	expression tag	UNP P07900
E	290	GLY	-	expression tag	UNP P07900
E	291	HIS	-	expression tag	UNP P07900
E	292	MET	-	expression tag	UNP P07900
F	290	GLY	-	expression tag	UNP P07900
F	291	HIS	-	expression tag	UNP P07900

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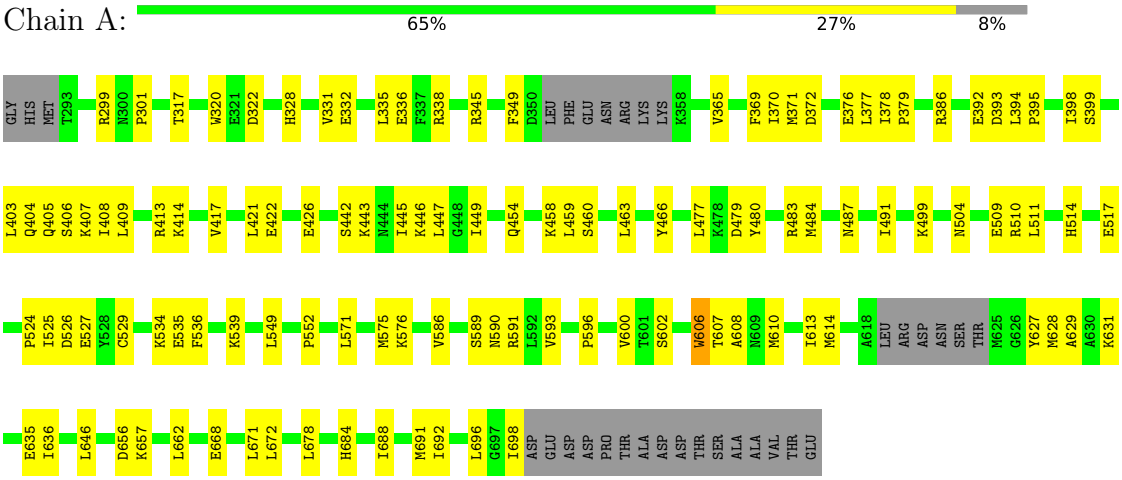
Chain	Residue	Modelled	Actual	Comment	Reference
F	292	MET	-	expression tag	UNP P07900

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.

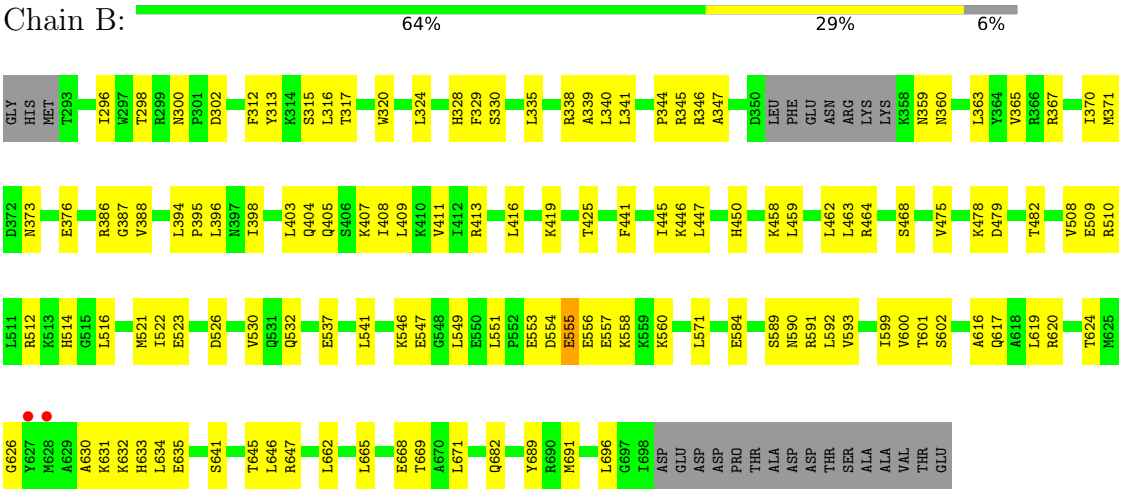
• Molecule 1: Heat shock protein HSP 90-alpha

Chain A:



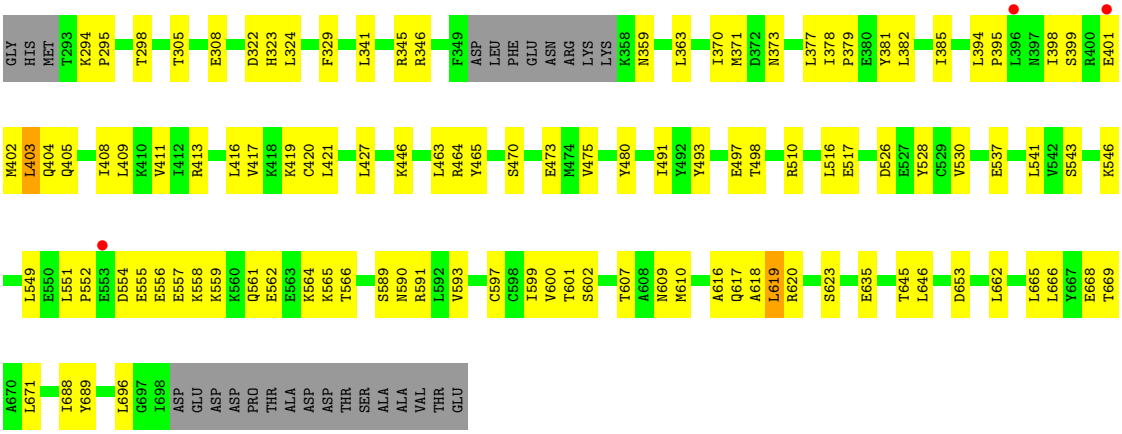
• Molecule 1: Heat shock protein HSP 90-alpha

Chain B:



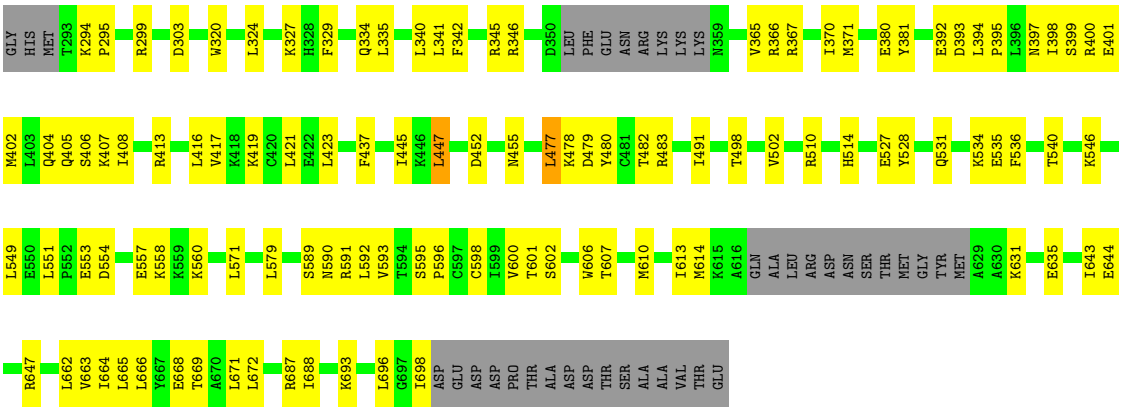
• Molecule 1: Heat shock protein HSP 90-alpha

Chain C:



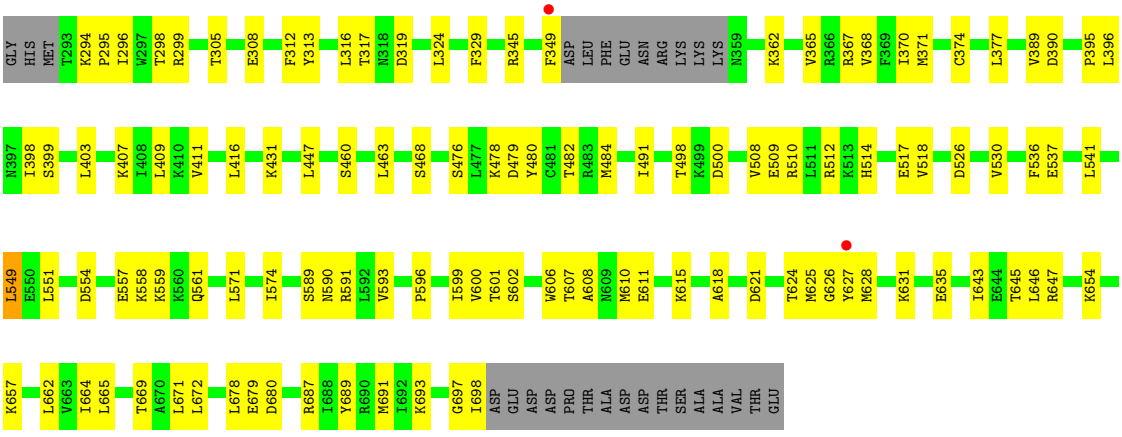
• Molecule 1: Heat shock protein HSP 90-alpha

Chain D:



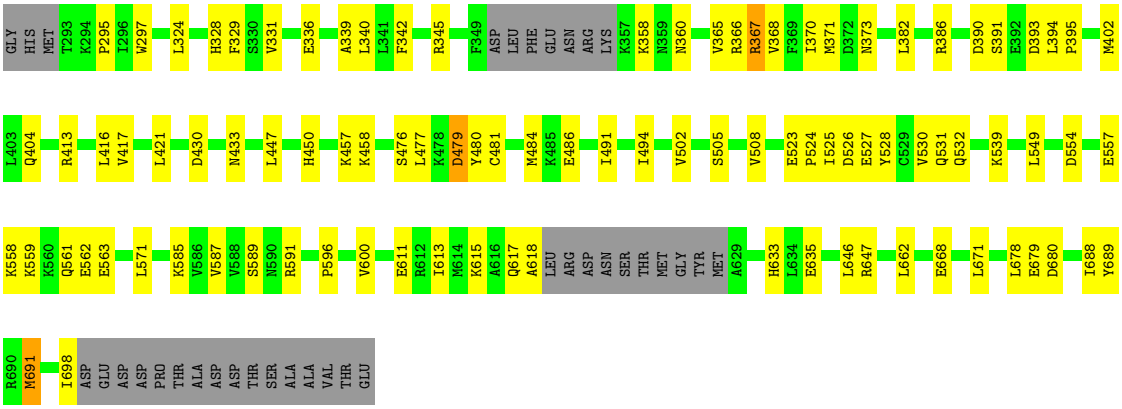
• Molecule 1: Heat shock protein HSP 90-alpha

Chain E:



• Molecule 1: Heat shock protein HSP 90-alpha

Chain F:


GLY HIS MET T293 K294 P295 I296 W297 L324 H328 F329 S330 V331 E336 A339 L340 L341 F342 R345 F349 ASP LEU PHE GLU ASN ARG LYS K357 K358 N359 N360 V365 R366 R367 V368 F369 I370 M371 D372 N373 L382 R386 D390 S391 E392 D393 L394 P395 M402
L403 Q404 R413 L416 V417 L421 D430 N433 L447 H450 K457 K458 S476 L477 K478 D479 Y480 C481 M484 K485 E486 I491 I494 V502 S505 V508 E523 P524 I525 D526 E527 Y528 C529 V530 Q531 Q532 K539 L549 D554 E557
K558 K559 K560 Q561 E562 E563 L571 K585 V586 V587 V588 S589 N590 R591 P596 V600 E611 R612 I613 M614 K615 A616 Q617 A618 LEU ARG ASP ASN SER THR MET GLY TYR MET A629 H633 L634 E635 L646 R647 L662 E668 L671 L678 E679 D680 I688 Y689
R690 M691 I698 ASP GLU ASP ASP PRO THR ALA ASP ASP THR SER ALA ALA VAL THR GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	153.83Å 87.99Å 166.18Å 90.00° 114.36° 90.00°	Depositor
Resolution (Å)	48.09 – 3.15 48.09 – 3.15	Depositor EDS
% Data completeness (in resolution range)	91.8 (48.09-3.15) 91.1 (48.09-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.191 , 0.248 0.195 , 0.250	Depositor DCC
R_{free} test set	1997 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å^2)	76.9	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19425	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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	0.56	0/3285	0.76	1/4410 (0.0%)
1	B	0.55	1/3334 (0.0%)	0.75	2/4478 (0.0%)
1	C	0.55	1/3326 (0.0%)	0.75	2/4467 (0.0%)
1	D	0.53	0/3229	0.72	2/4337 (0.0%)
1	E	0.54	0/3317	0.74	1/4456 (0.0%)
1	F	0.55	0/3253	0.76	0/4367
All	All	0.55	2/19744 (0.0%)	0.75	8/26515 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	522	ILE	C-N	5.58	1.46	1.34
1	C	597	CYS	CB-SG	-5.09	1.73	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	463	LEU	CB-CG-CD2	-6.99	99.11	111.00
1	C	427	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	B	555	GLU	N-CA-C	5.58	126.07	111.00
1	A	299	ARG	C-N-CA	-5.58	107.76	121.70
1	C	619	LEU	CA-CB-CG	5.40	127.71	115.30

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	3232	0	3277	127	1
1	B	3280	0	3324	99	0
1	C	3272	0	3320	95	1
1	D	3177	0	3221	84	0
1	E	3263	0	3307	109	0
1	F	3201	0	3256	78	0
All	All	19425	0	19705	543	1

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 14.

The worst 5 of 543 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:335:LEU:CD1	1:A:393:ASP:HB2	1.44	1.47
1:A:395:PRO:HB2	1:A:398:ILE:CD1	1.57	1.32
1:F:365:VAL:O	1:F:368:VAL:HG22	1.31	1.28
1:E:697:GLY:O	1:E:698:ILE:HG13	1.32	1.24
1:A:395:PRO:CB	1:A:398:ILE:HD12	1.73	1.17

All (1) 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:A:338:ARG:NH2	1:C:653:ASP:OD2[2_647]	2.16	0.04

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	387/425 (91%)	368 (95%)	19 (5%)	0	100	100
1	B	395/425 (93%)	380 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	394/425 (93%)	368 (93%)	26 (7%)	0	100	100
1	D	380/425 (89%)	362 (95%)	18 (5%)	0	100	100
1	E	393/425 (92%)	373 (95%)	20 (5%)	0	100	100
1	F	383/425 (90%)	367 (96%)	16 (4%)	0	100	100
All	All	2332/2550 (92%)	2218 (95%)	114 (5%)	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	363/391 (93%)	362 (100%)	1 (0%)	92	97
1	B	369/391 (94%)	368 (100%)	1 (0%)	92	97
1	C	368/391 (94%)	366 (100%)	2 (0%)	88	95
1	D	358/391 (92%)	358 (100%)	0	100	100
1	E	367/391 (94%)	364 (99%)	3 (1%)	81	92
1	F	360/391 (92%)	357 (99%)	3 (1%)	81	92
All	All	2185/2346 (93%)	2175 (100%)	10 (0%)	88	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	367	ARG
1	F	479	ASP
1	F	691	MET
1	C	403	LEU
1	E	349	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	633	HIS
1	C	306	ASN
1	F	404	GLN
1	A	684	HIS
1	A	454	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 monosaccharides 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	393/425 (92%)	-0.22	0 100 100	46, 82, 130, 164	0
1	B	399/425 (93%)	-0.21	2 (0%) 91 86	49, 81, 133, 191	0
1	C	398/425 (93%)	-0.20	3 (0%) 86 78	48, 89, 139, 187	0
1	D	386/425 (90%)	-0.22	0 100 100	45, 86, 127, 166	0
1	E	397/425 (93%)	-0.24	2 (0%) 91 86	49, 84, 136, 186	0
1	F	389/425 (91%)	-0.25	0 100 100	48, 84, 133, 168	0
All	All	2362/2550 (92%)	-0.22	7 (0%) 94 92	45, 84, 134, 191	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	627	TYR	4.4
1	B	627	TYR	3.6
1	C	396	LEU	2.9
1	C	401	GLU	2.6
1	B	628	MET	2.6

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.