Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:15 pm BST

PDB ID	:	6EHR
Title	:	The crystal structure of the human LAMTOR-RagA CTD-RagC CTD complex
Authors	:	Scheffzek, K.; Naschberger, A.
Deposited on	:	2017-09-14
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

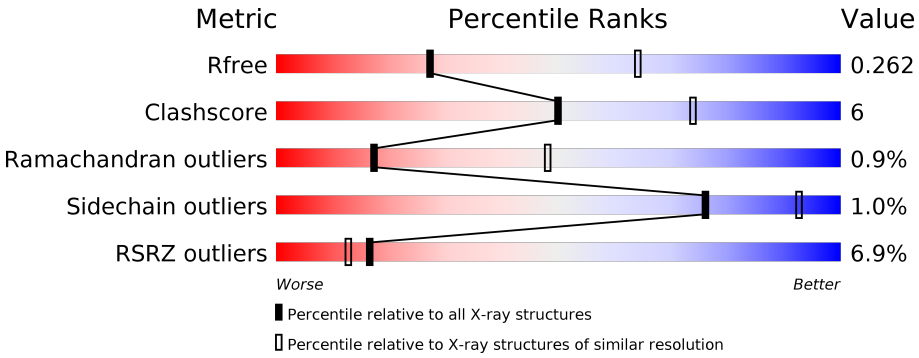
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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.



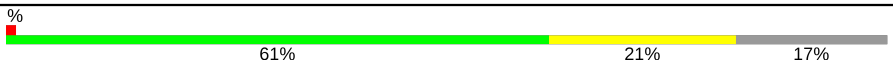
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	127	8% 83% 12% 6%
2	B	126	5% 83% 16% •
3	C	91	% 90% 10%
4	D	99	3% 84% 14% •
5	E	145	16% 65% 14% • 21%
6	F	132	8% 72% 11% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	163	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6126 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 Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			934	601	157	175	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9UHA4
A	-1	ALA	-	expression tag	UNP Q9UHA4
A	0	HIS	-	expression tag	UNP Q9UHA4

- Molecule 2 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			948	595	163	183	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP Q9Y2Q5
B	1	GLY	-	expression tag	UNP Q9Y2Q5

- Molecule 3 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			666	406	115	138	7			

- Molecule 4 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	S	0	0	0
			738	460	135	140	3			

- Molecule 5 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	115	Total	C	N	O	S	0	0	0
			892	560	155	175	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	17	SER	-	expression tag	UNP Q6IAA8
E	18	LEU	-	expression tag	UNP Q6IAA8
E	19	MET	-	expression tag	UNP Q6IAA8
E	20	THR	-	expression tag	UNP Q6IAA8

- Molecule 6 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	110	Total	C	N	O	S	0	0	0
			883	565	150	162	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	182	GLY	-	expression tag	UNP Q7L523

- Molecule 7 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	135	Total	C	N	O	S	0	0	0
			1065	686	165	206	8			

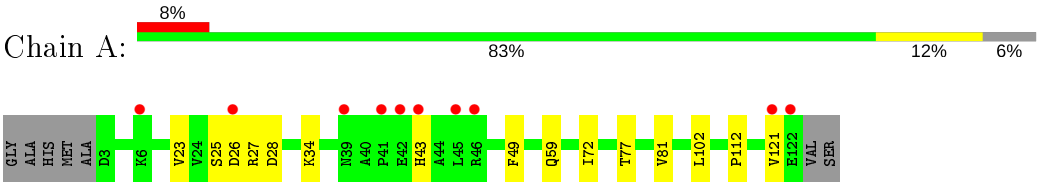
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	237	MET	-	initiating methionine	UNP Q9HB90
G	238	GLY	-	expression tag	UNP Q9HB90

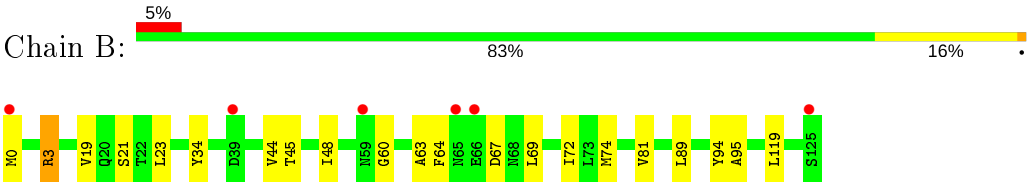
3 Residue-property plots (i)

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.

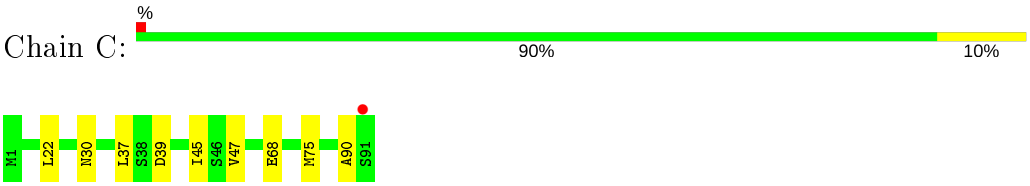
- Molecule 1: Ragulator complex protein LAMTOR3



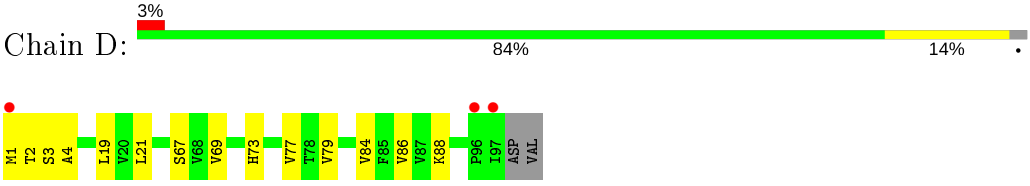
- Molecule 2: Ragulator complex protein LAMTOR2



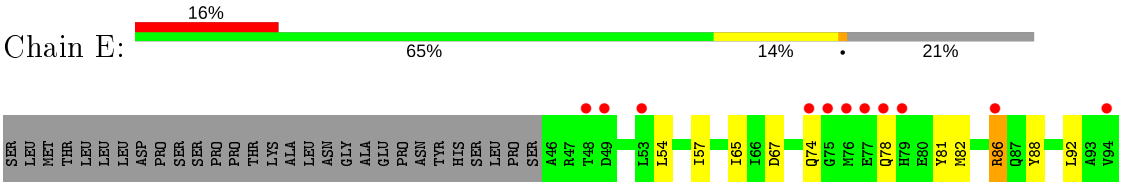
- Molecule 3: Ragulator complex protein LAMTOR5

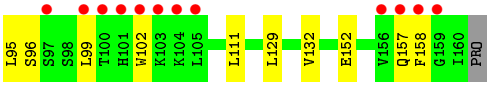


- Molecule 4: Ragulator complex protein LAMTOR4



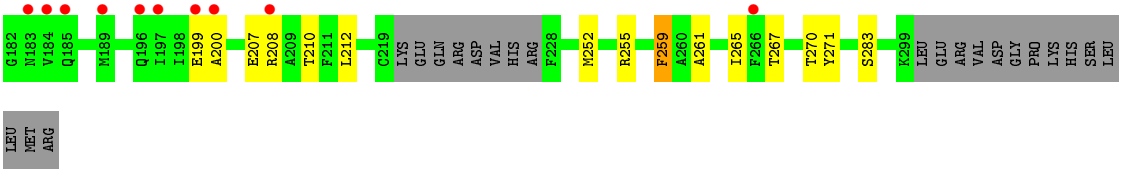
- Molecule 5: Ragulator complex protein LAMTOR1





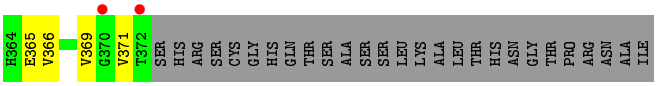
- Molecule 6: Ras-related GTP-binding protein A

Chain F:



- Molecule 7: Ras-related GTP-binding protein C

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.09Å 92.45Å 127.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.22 – 2.90 46.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (46.22-2.90) 93.8 (46.22-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.216 , 0.263 0.216 , 0.262	Depositor DCC
R_{free} test set	1109 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.4	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	0.93	EDS
Total number of atoms	6126	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.24	0/951	0.40	0/1290
2	B	0.24	0/959	0.44	0/1298
3	C	0.23	0/672	0.43	0/911
4	D	0.24	0/747	0.43	0/1008
5	E	0.23	0/908	0.36	0/1234
6	F	0.25	0/897	0.38	0/1206
7	G	0.24	0/1082	0.42	0/1461
All	All	0.24	0/6216	0.41	0/8408

There are no bond length outliers.

There are no bond angle outliers.

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	934	0	958	12	0
2	B	948	0	958	13	0
3	C	666	0	666	6	0
4	D	738	0	753	9	0
5	E	892	0	894	16	0
6	F	883	0	887	9	0
7	G	1065	0	1068	24	0
All	All	6126	0	6184	71	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 6.

All (71) 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)
5:E:67:ASP:HA	7:G:253:ASN:HB2	1.67	0.75
7:G:251:ILE:HD11	7:G:259:ALA:HB2	1.76	0.67
2:B:3:ARG:NH2	5:E:152:GLU:OE1	2.30	0.64
1:A:102:LEU:HD22	3:C:47:VAL:HG21	1.78	0.63
4:D:21:LEU:HB2	4:D:84:VAL:HB	1.83	0.61
5:E:92:LEU:O	5:E:96:SER:N	2.30	0.60
3:C:68:GLU:OE2	4:D:67:SER:OG	2.16	0.59
3:C:30:ASN:ND2	3:C:39:ASP:OD1	2.34	0.59
1:A:23:VAL:HG22	1:A:34:LYS:HG3	1.85	0.59
2:B:44:VAL:HG23	2:B:45:THR:HG23	1.85	0.58
4:D:1:MET:HG2	4:D:2:THR:HG23	1.87	0.56
7:G:288:MET:HG3	7:G:318:ILE:HD12	1.87	0.55
4:D:69:VAL:HG11	5:E:129:LEU:HD13	1.88	0.54
7:G:302:LYS:O	7:G:304:ASP:N	2.40	0.54
1:A:26:ASP:O	1:A:28:ASP:N	2.41	0.53
7:G:258:LYS:NZ	7:G:275:SER:O	2.40	0.53
6:F:252:MET:HB2	7:G:318:ILE:HG12	1.91	0.53
6:F:255:ARG:NH2	6:F:283:SER:OG	2.41	0.51
4:D:79:VAL:HB	5:E:111:LEU:HG	1.93	0.51
3:C:22:LEU:HD13	3:C:45:ILE:HD12	1.93	0.51
6:F:207:GLU:HG2	6:F:212:LEU:H	1.75	0.50
4:D:19:LEU:HB3	4:D:86:VAL:HB	1.94	0.50
1:A:25:SER:OG	1:A:26:ASP:N	2.44	0.50
2:B:0:MET:N	5:E:157:GLN:HA	2.28	0.49
2:B:74:MET:HB2	2:B:81:VAL:HB	1.95	0.48
7:G:329:LYS:HG2	7:G:356:PHE:CE2	2.48	0.48
1:A:43:HIS:HB2	2:B:63:ALA:HB2	1.97	0.47
5:E:78:GLN:HG3	5:E:81:TYR:H	1.80	0.47
6:F:208:ARG:HG3	6:F:271:TYR:HE1	1.80	0.47
7:G:256:ILE:HG21	7:G:339:CYS:HB3	1.96	0.47
5:E:95:LEU:O	5:E:99:LEU:HB2	2.16	0.46
2:B:21:SER:HB3	2:B:94:TYR:HB2	1.97	0.46
3:C:22:LEU:HD12	3:C:37:LEU:HB3	1.98	0.46
2:B:69:LEU:HD21	2:B:72:ILE:HD11	1.98	0.46
2:B:89:LEU:HD12	2:B:119:LEU:HD13	1.98	0.45
7:G:365:GLU:O	7:G:369:VAL:HG13	2.17	0.45
7:G:308:SER:O	7:G:308:SER:OG	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:366:VAL:O	7:G:369:VAL:HG22	2.17	0.45
7:G:332:THR:HG22	7:G:335:LEU:HB2	1.99	0.44
5:E:54:LEU:HD23	5:E:57:ILE:HD12	1.99	0.44
5:E:65:ILE:HD12	7:G:249:ILE:HG22	1.99	0.44
1:A:77:THR:OG1	2:B:67:ASP:OD2	2.21	0.44
7:G:278:ASP:C	7:G:280:GLN:H	2.21	0.44
5:E:82:MET:O	5:E:86:ARG:HD2	2.18	0.43
1:A:112:PRO:HB2	5:E:102:TRP:CZ2	2.53	0.43
7:G:278:ASP:O	7:G:280:GLN:N	2.52	0.43
3:C:75:MET:HB2	5:E:132:VAL:HG21	2.00	0.43
7:G:359:PHE:CZ	7:G:363:ILE:HD11	2.54	0.43
6:F:259:PHE:CD2	7:G:300:GLY:HA2	2.54	0.43
7:G:315:MET:HG3	7:G:329:LYS:HD2	2.01	0.43
1:A:72:ILE:HG23	1:A:81:VAL:HG22	2.00	0.43
1:A:121:VAL:HG12	5:E:88:TYR:CZ	2.54	0.43
7:G:264:VAL:HG21	7:G:310:TYR:CE2	2.54	0.42
4:D:77:VAL:HG13	4:D:86:VAL:HG22	2.02	0.42
7:G:251:ILE:HA	7:G:251:ILE:HD13	1.80	0.42
2:B:19:VAL:HG22	2:B:95:ALA:HB2	2.01	0.42
6:F:267:THR:OG1	6:F:270:THR:OG1	2.24	0.42
7:G:288:MET:O	7:G:292:VAL:HG23	2.19	0.41
1:A:112:PRO:HB2	5:E:102:TRP:HZ2	1.84	0.41
6:F:207:GLU:OE2	6:F:210:THR:OG1	2.30	0.41
7:G:273:ASP:OD2	7:G:275:SER:OG	2.29	0.41
1:A:59:GLN:HB3	2:B:48:ILE:HG23	2.01	0.41
6:F:259:PHE:HE1	6:F:261:ALA:HB2	1.86	0.41
2:B:23:LEU:HG	2:B:34:TYR:HD1	1.85	0.41
4:D:2:THR:O	4:D:4:ALA:N	2.54	0.41
7:G:302:LYS:HD2	7:G:306:SER:HB3	2.02	0.41
7:G:256:ILE:HG23	7:G:341:LEU:HB3	2.02	0.41
1:A:49:PHE:CE1	2:B:60:GLY:HA2	2.56	0.41
6:F:265:ILE:HG12	6:F:271:TYR:CZ	2.56	0.41
4:D:73:HIS:CG	4:D:88:LYS:HE3	2.56	0.40
5:E:95:LEU:HB3	5:E:99:LEU:HD13	2.03	0.40

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	118/127 (93%)	111 (94%)	6 (5%)	1 (1%)	19 51
2	B	124/126 (98%)	121 (98%)	3 (2%)	0	100 100
3	C	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	14 42
4	D	95/99 (96%)	89 (94%)	5 (5%)	1 (1%)	14 42
5	E	113/145 (78%)	102 (90%)	11 (10%)	0	100 100
6	F	106/132 (80%)	94 (89%)	10 (9%)	2 (2%)	8 28
7	G	133/163 (82%)	116 (87%)	15 (11%)	2 (2%)	10 34
All	All	778/883 (88%)	720 (92%)	51 (7%)	7 (1%)	17 48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
7	G	303	GLU
3	C	90	ALA
6	F	199	GLU
4	D	3	SER
6	F	200	ALA
7	G	371	VAL

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	105/109 (96%)	105 (100%)	0	100 100
2	B	98/98 (100%)	96 (98%)	2 (2%)	55 82
3	C	77/77 (100%)	77 (100%)	0	100 100
4	D	81/83 (98%)	81 (100%)	0	100 100
5	E	99/126 (79%)	96 (97%)	3 (3%)	41 75
6	F	99/120 (82%)	98 (99%)	1 (1%)	76 92
7	G	122/145 (84%)	121 (99%)	1 (1%)	81 94
All	All	681/758 (90%)	674 (99%)	7 (1%)	76 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3	ARG
2	B	64	PHE
5	E	74	GLN
5	E	86	ARG
5	E	158	PHE
6	F	259	PHE
7	G	330	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	120/127 (94%)	0.39	10 (8%) 11 8	45, 84, 137, 147	0
2	B	126/126 (100%)	0.09	6 (4%) 30 27	39, 58, 125, 162	0
3	C	91/91 (100%)	-0.18	1 (1%) 80 80	31, 48, 94, 115	0
4	D	97/99 (97%)	0.05	3 (3%) 49 44	41, 70, 114, 159	0
5	E	115/145 (79%)	0.77	23 (20%) 1 0	33, 74, 157, 200	0
6	F	110/132 (83%)	0.44	10 (9%) 9 6	43, 84, 136, 174	0
7	G	135/163 (82%)	0.06	2 (1%) 73 73	34, 55, 125, 150	0
All	All	794/883 (89%)	0.24	55 (6%) 16 13	31, 67, 137, 200	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	65	ASN	7.8
4	D	1	MET	6.3
5	E	76	MET	5.8
2	B	0	MET	5.6
5	E	79	HIS	5.5
2	B	66	GLU	4.3
1	A	42	GLU	3.8
5	E	75	GLY	3.4
2	B	125	SER	3.4
5	E	49	ASP	3.4
5	E	157	GLN	3.3
1	A	41	PRO	3.2
4	D	96	PRO	3.2
5	E	77	GLU	3.2
5	E	105	LEU	3.1
5	E	100	THR	3.1
1	A	46	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	39	ASN	3.0
5	E	102	TRP	3.0
5	E	159	GLY	2.9
6	F	197	ILE	2.9
1	A	43	HIS	2.8
5	E	48	THR	2.8
6	F	184	VAL	2.8
5	E	97	SER	2.7
5	E	94	VAL	2.7
6	F	196	GLN	2.7
6	F	189	MET	2.7
5	E	86	ARG	2.7
6	F	199	GLU	2.6
5	E	158	PHE	2.5
7	G	372	THR	2.5
3	C	91	SER	2.5
5	E	53	LEU	2.5
5	E	103	LYS	2.5
5	E	104	LYS	2.5
4	D	97	ILE	2.4
5	E	74	GLN	2.3
1	A	45	LEU	2.3
5	E	101	HIS	2.3
7	G	370	GLY	2.2
5	E	78	GLN	2.2
5	E	99	LEU	2.2
1	A	122	GLU	2.2
2	B	59	ASN	2.2
1	A	6	LYS	2.2
1	A	121	VAL	2.2
2	B	39	ASP	2.1
6	F	185	GLN	2.1
6	F	266	PHE	2.1
1	A	26	ASP	2.0
6	F	200	ALA	2.0
5	E	156	VAL	2.0
6	F	208	ARG	2.0
6	F	183	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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.