WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 25, 2024 – 04:12 PM EST

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PDB ID	:	5KZF
Title	:	Crystal structure of near full-length hexameric Mycobacterium tuberculosis proteasomal ATPase Mpa in apo form
Authors	:	Li, H.; Hu, K.; Yang, S.; Bai, L.
Deposited on	:	2016-07-25
Resolution	:	3.49 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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.
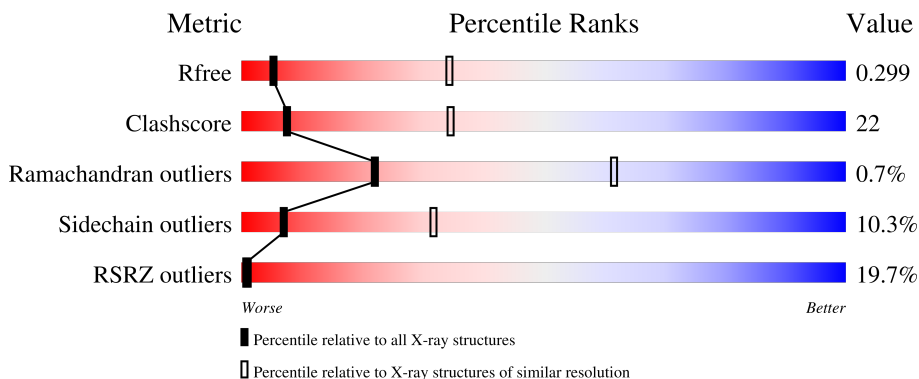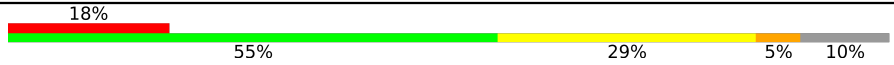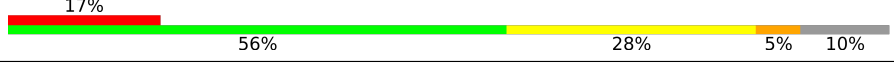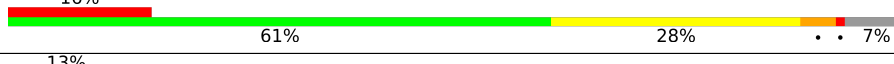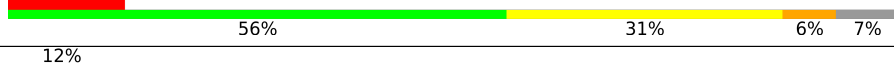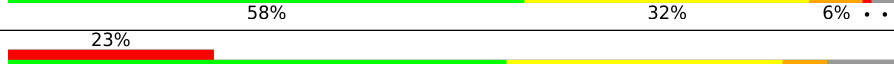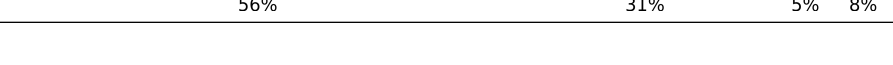
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	513	21% / 57% 31% · · 6%
1	B	513	19% / 60% 29% · 7%
1	C	513	19% / 60% 27% · 8%
1	D	513	22% / 56% 29% 5% 10%
1	E	513	27% / 59% 26% 5% 10%

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Mol	Chain	Length	Quality of chain
1	F	513	18% 55% 29% 5% 10%
1	G	513	17% 56% 28% 5% 10%
1	H	513	16% 61% 28% · · 7%
1	I	513	13% 56% 31% 6% 7%
1	J	513	12% 59% 30% · · 6%
1	K	513	10% 58% 32% 6% · ·
1	L	513	23% 56% 31% 5% 8%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 44298 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 Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3747	2360	647	729	11			
1	B	475	Total	C	N	O	S	0	0	0
			3707	2337	637	722	11			
1	C	472	Total	C	N	O	S	0	0	0
			3649	2300	632	706	11			
1	D	460	Total	C	N	O	S	0	0	0
			3593	2266	621	695	11			
1	E	461	Total	C	N	O	S	0	0	0
			3597	2268	622	696	11			
1	F	460	Total	C	N	O	S	0	0	0
			3589	2267	615	696	11			
1	G	461	Total	C	N	O	S	0	0	0
			3595	2270	615	698	12			
1	H	478	Total	C	N	O	S	0	0	0
			3729	2351	639	727	12			
1	I	478	Total	C	N	O	S	0	0	0
			3735	2352	645	726	12			
1	J	484	Total	C	N	O	S	0	0	0
			3775	2377	646	740	12			
1	K	498	Total	C	N	O	S	0	0	0
			3887	2442	672	761	12			
1	L	473	Total	C	N	O	S	0	0	0
			3695	2329	635	720	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A5U4E1
B	1	MET	-	initiating methionine	UNP A5U4E1
C	1	MET	-	initiating methionine	UNP A5U4E1
D	1	MET	-	initiating methionine	UNP A5U4E1
E	1	MET	-	initiating methionine	UNP A5U4E1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP A5U4E1
G	1	MET	-	initiating methionine	UNP A5U4E1
H	1	MET	-	initiating methionine	UNP A5U4E1
I	1	MET	-	initiating methionine	UNP A5U4E1
J	1	MET	-	initiating methionine	UNP A5U4E1
K	1	MET	-	initiating methionine	UNP A5U4E1
L	1	MET	-	initiating methionine	UNP A5U4E1

3 Residue-property plots ⓘ

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: Proteasome-associated ATPase

Chain A:

• Molecule 1: Proteasome-associated ATPase

Chain B:

• Molecule 1: Proteasome-associated ATPase

Chain C:

• Molecule 1: Proteasome-associated ATPase

Chain D:

• Molecule 1: Proteasome-associated ATPase

R484 Y487 I488 R489 T493 G494 K495 D504 T505 GLU SER ASN LEU GLY GLN TYR LEU

• Molecule 1: Proteasome-associated ATPase

Chain F:

18%

55% 29% 5% 10%

MET P2 S3 G4 Y5 G6 V7 L8 L9 A10 T11 H12 D13 D14 D15 T16 V17 D18 V19 F20 T21 S22 M26 R27 L28 A36 L39 K40 K41 G42 V45 R46 L47 L51 T52 V53 V54 E55 A56 G57 T58 F59 E60 A61 V62 I65 S66 T67 L68 R69 E70 I71 L72 A73

D74 G75 H76 R77 A78 L79 V80 V81 E87 R88 V89 L92 A93 D94 P95 L96 I97 ALA GLU ASP LEU PRO ASP GLY LEU PRO GLU ALA LEU ASN ASP ASP THR ARG PRO ARG LYS L118 L124 L125 V126 A130 G131 Y132 A133 F134 E135 R136 I137 P138 K139 A140 E141 L145 V146

L147 E148 E149 V150 P151 D152 V153 S154 Y155 I158 L161 S162 R163 Q164 I165 E166 Q167 I168 V172 E173 L174 P175 F176 L177 L187 R188 P189 P190 K191 G192 V193 L194 L195 G200 C201 K202 K203 T204 L205 I206 A207 K208 A209 V210 L214 A215 K216 K217 M218 A219 GLU VAL ARG GLY

ASP ASP ALA HIS GLU ALA K230 S231 Y232 F233 L234 N235 I236 K237 G238 P239 E240 L241 L242 N243 K244 F245 V246 G247 E248 T249 E250 R251 H252 I253 R254 L255 I256 A260 A264 T268 P269 V270 I271 V272 F273 F274 D275 E276 M277 D278 F281 ARG THR ARG GLY THR GLY VAL SER SER

ASP VAL GLU THR THR V296 V297 P298 Q299 I304 D305 E308 G309 L310 E311 N312 V313 I314 E322 D323 P327 A328 R331 P332 G333 R334 L335 D336 V337 K338 I339 K340 I341 E342 R343 D351 K355 Y356 L357 T358 E359 F360 L361 P362 V363 H364 R375 C378 I379 K380 A381

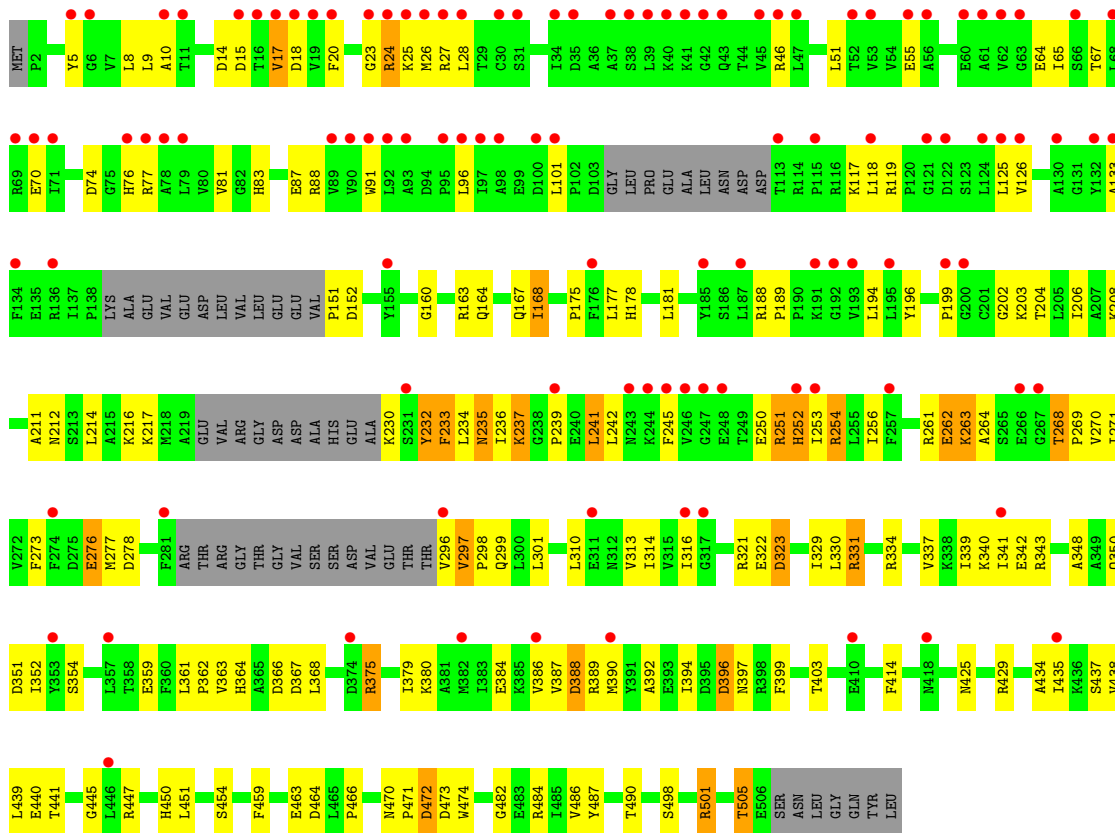M382 I383 E384 K385 V386 V387 D388 R389 E393 I394 D395 D396 N397 R398 F399 T403 F414 K415 D416 F417 N418 S419 N425 V426 V427 D428 R429 A430 K431 A434 I435 K436 S437 V438 L439 E440 T441 G442 Q443 P444 G445 L446 H450 S454 E458 F459 N462 E463 D464 T468

P471 D472 D473 W474 A475 R476 R484 Y487 I488 R489 V492 K495 S500 T505 GLU SER ASN LEU GLY GLN TYR LEU

• Molecule 1: Proteasome-associated ATPase

Chain G:

17%

56% 28% 5% 10%

M1 P2 S3 V7 L8 L9 A10 T11 H12 D13 D14 D15 T16 V17 D18 V19 L28 T29 C30 S31 A36 A37 S38 L39 K40 K41 G42 Q43 T44 V45 R46 L47 L51 T52 V53 V54 E55 A56 G57 E60 A61 L68 R69 E70 A78 L79 V80 V81 E87 R88 V89 V90

W91 L92 A93 D94 P95 L96 I97 ALA GLU ASP LEU PRO ASP GLY LEU PRO GLU ALA LEU ASN ASP ASP THR ARG PRO ARG LYS L118 R119 P120 L124 A130 G131 Y132 A133 F134 E135 K139 A140 E141 V142 E143 D144 L145 V146 L147 E148 E149 V150 P151 D152 V153 A156 D157 I158

L161 S162 R163 Q164 I165 E166 Q167 I168 R169 D170 A171 V172 E173 L174 P175 F176 L177 H178 K179 E180 L181 L194 L195 Y196 G197 P198 P199 G200 C201 G202 K203 T204 L205 I206 A207 K208 A209 V210 A211 N212 S213 L214 A215 K216 K217 M218 A219 GLU VAL ARG GLY ASP ASP ALA HIS GLU ALA LYS S231

Y232 F233 L234 N235 I236 K237 G238 P239 E240 L241 L242 N243 K244 F245 V246 G247 E248 T249 E250 R251 H252 I253 R254 L255 Q258 R259 A260 K263 A264 S265 T268 P269 V270 I271 F274 M277 D278 F281 ARG THR ARG GLY THR GLY VAL SER SER ASP VAL GLU THR T295 V296 V297
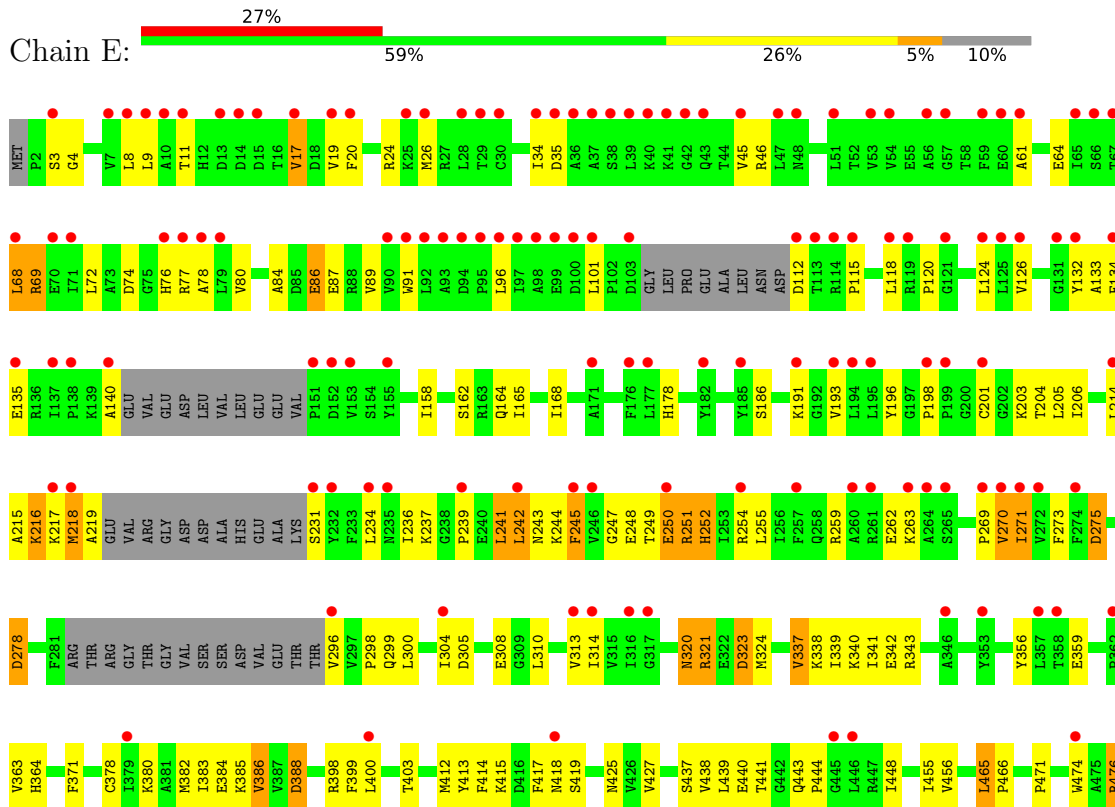
• Molecule 1: Proteasome-associated ATPase

Chain H:

• Molecule 1: Proteasome-associated ATPase

Chain I:

G247 E248 T249 E250 R251 H252 I253 R254 L255 I256 F257 Q258 R259 A260 R261 E262 K263 A264 T268 P269 V270 I271 V272 F273 F274 D275 E276 M277 D278 S279 I280 F281 R282 T283 R284 GLY THR GLY VAL SER SER ASP VAL GLU THR V296 V297 P298 Q299 L300 L301 S302 E303 L310 E311 N312 V313

I314 V315 I316 G317 A318 S319 N320 D323 D326 P327 A328 I329 L330 R331 R334 R335 L335 D336 V337 K338 I339 K340 I341 E342 R343 P344 D351 I352 Y353 F360 L361 P362 V363 D367 R375 K380 E384 K385 V386 R389 I394 N397 R398 F399 L400 E401 V402 T403

N406 G407 D408 M412 D416 F417 N418 S419 M422 V426 R429 K432 S437 V438 T441 G442 Q443 P444 R447 I448 Q449 H450 L451 I455 E458 D464 P471 W474 A475 R476 I485 V486 Y487 T490 T493 G494 K495 S498 R501 A502 I503
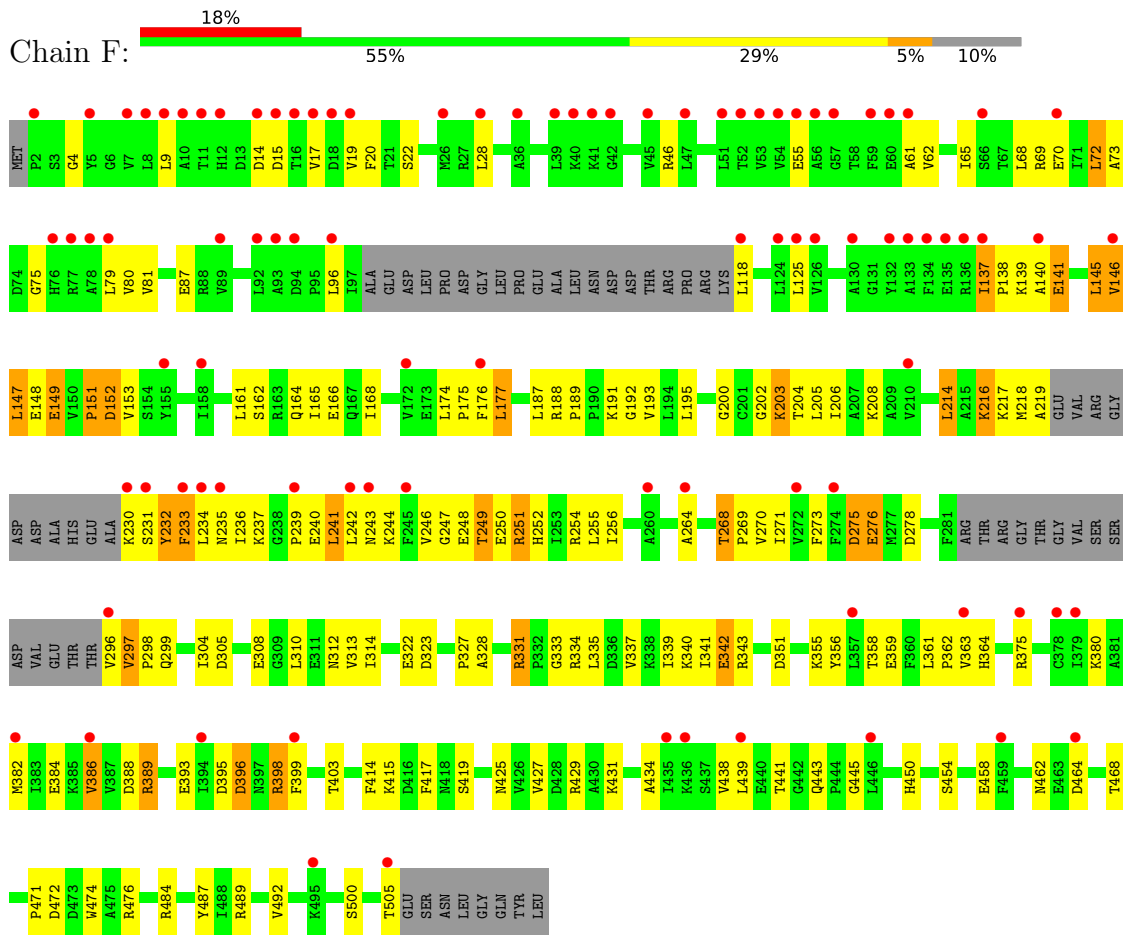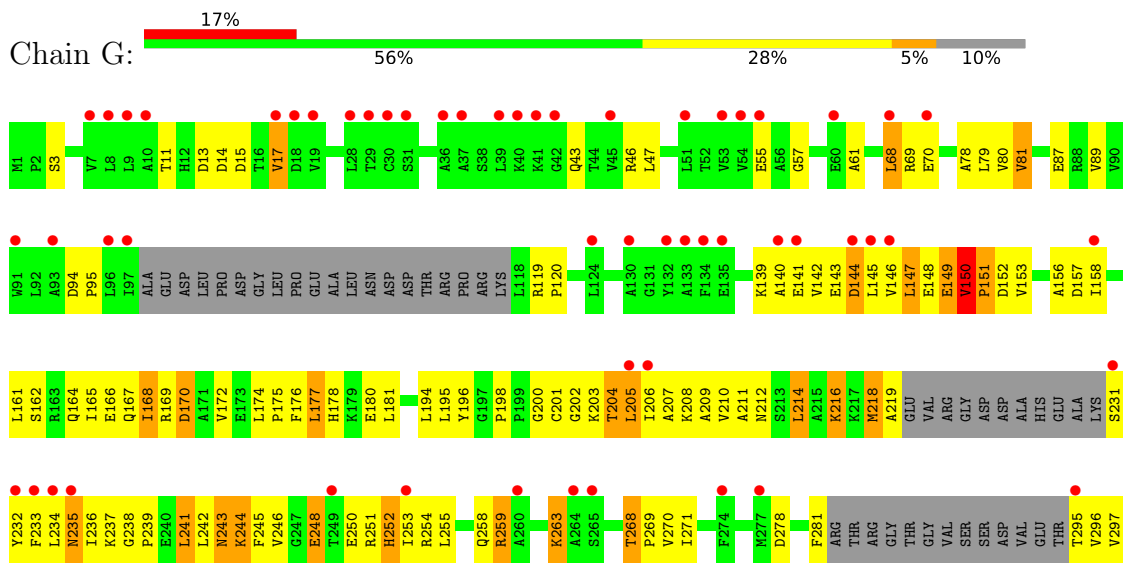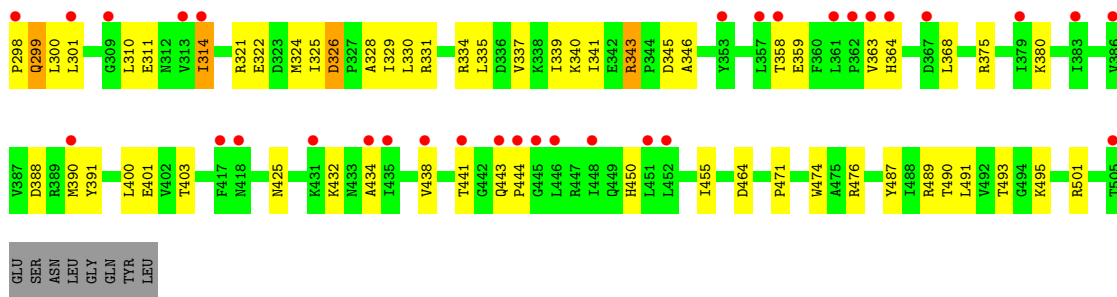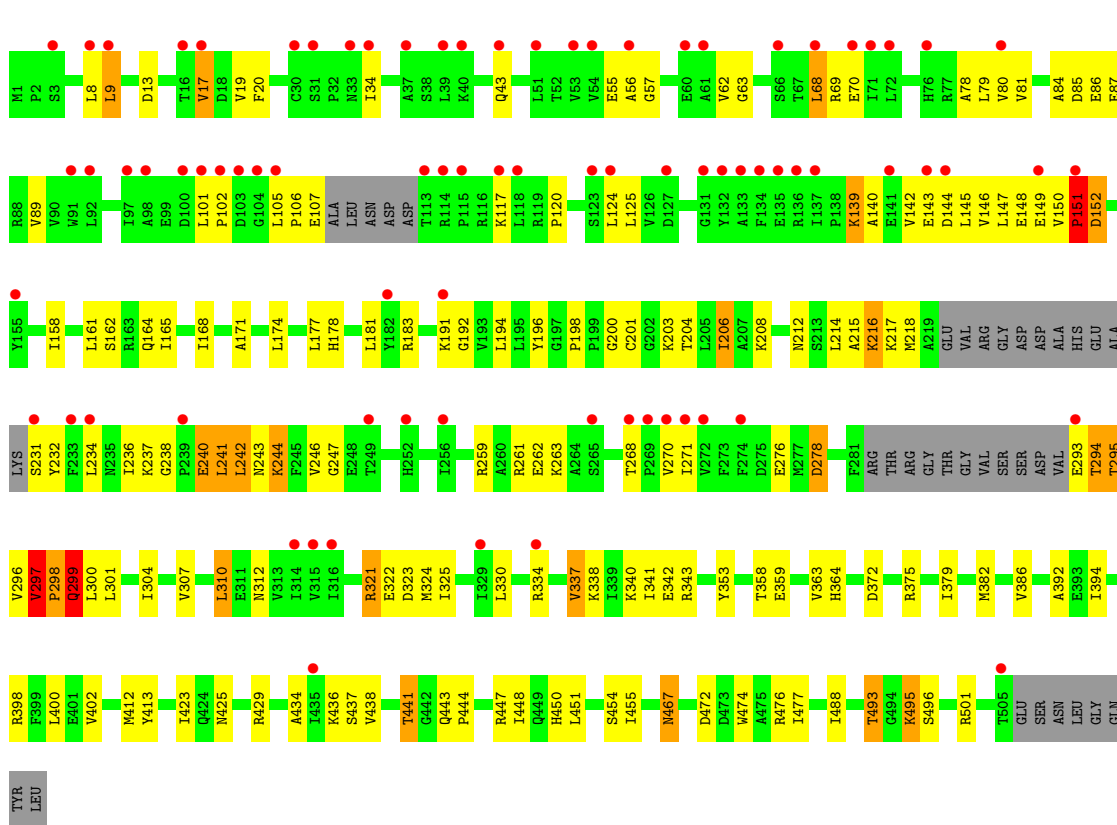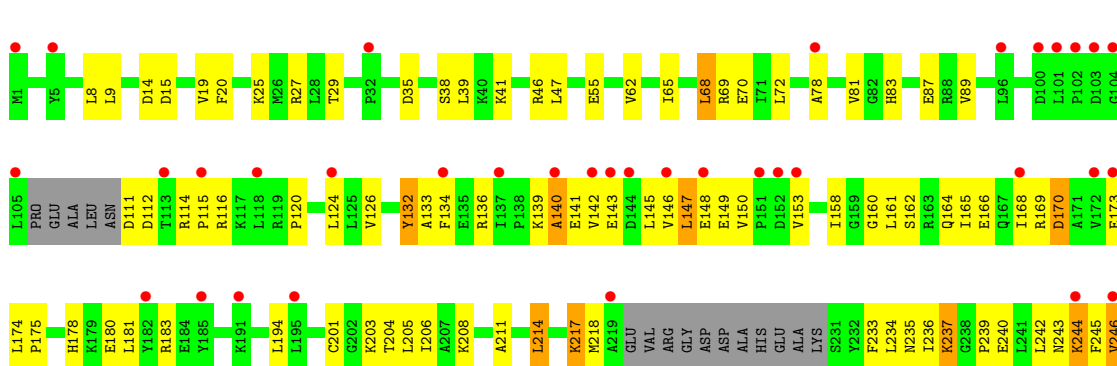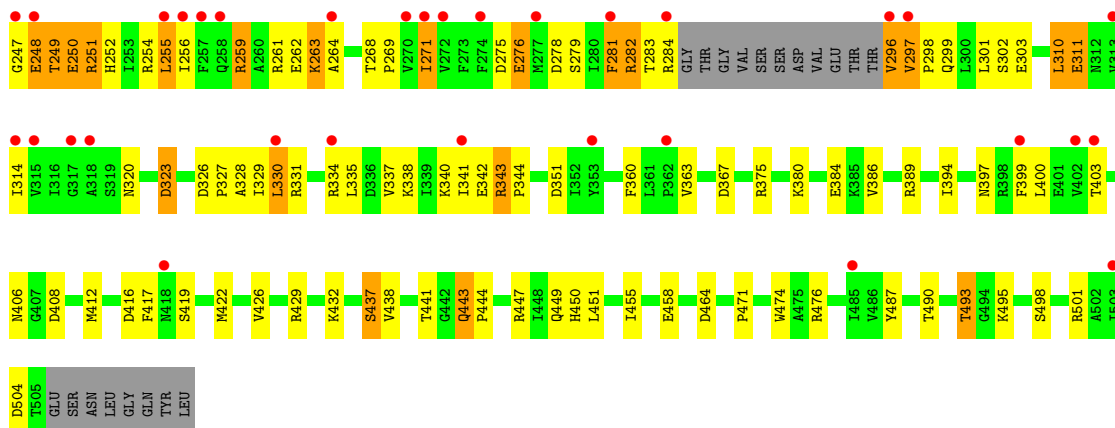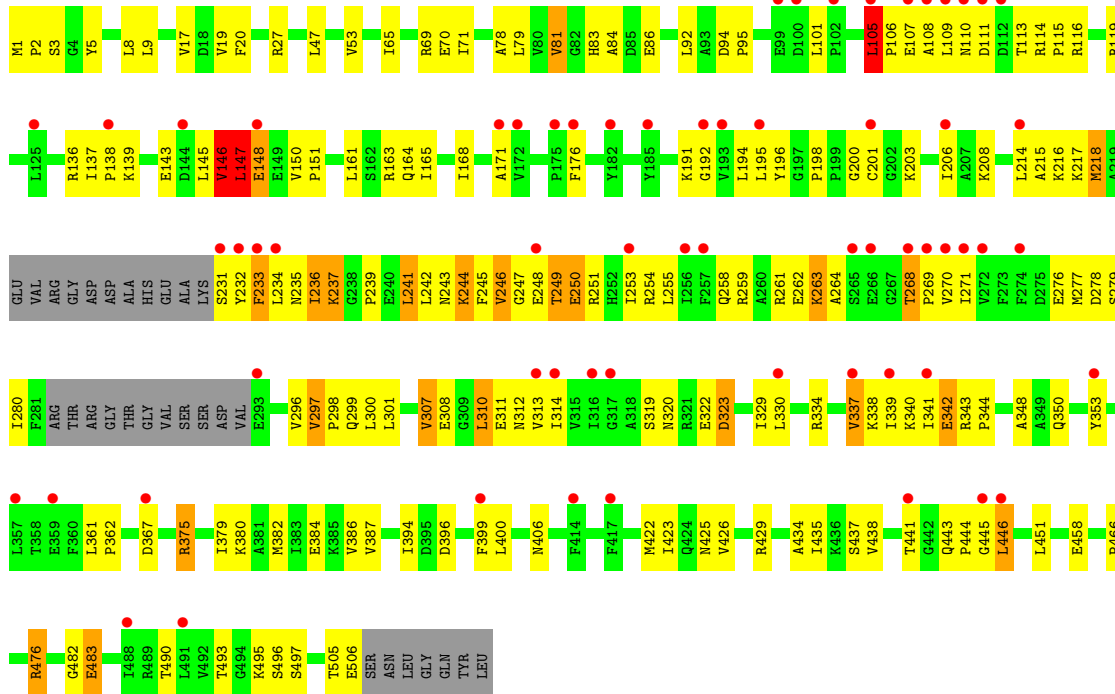
D504 T505 GLU ASN LEU GLY GLN TYR LEU

• Molecule 1: Proteasome-associated ATPase

Chain J:

M1 P2 S3 G4 Y5 L8 L9 V17 D18 V19 F20 R27 L47 V53 I65 R69 E70 I71 A78 L79 V80 V81 G82 H83 A84 D85 E86 L92 A93 D94 P95 E99 D100 L101 P102 L105 P106 E107 A108 L109 N110 D111 D112 T113 R114 P115 L116 R119

L125 R136 I137 P138 K139 E143 D144 L145 V146 L147 E148 E149 V150 P151 L161 S162 R163 Q164 I165 I168 A171 V172 P175 F176 Y182 Y185 K191 G192 V193 L194 L195 Y196 G197 P198 P199 G200 C201 G202 K203 I206 A207 K208 L214 A215 K216 K217 M218 A219

GLU VAL ARG GLY ASP ASP ALA HIS GLU ALA LYS S231 Y232 F233 L234 N235 I236 K237 G238 P239 E240 L241 L242 N243 K244 F245 V246 G247 E248 T249 E250 R251 H252 I253 R254 L255 I256 F257 Q258 R259 A260 R261 E262 K263 A264 S265 E266 G267 T268 P269 V270 I271 V272 F273 F274 D275 E276 M277 D278 S279

I280 F281 ARG THR ARG GLY THR GLY VAL SER SER ASP VAL E293 V296 V297 P298 Q299 L300 L301 V307 E308 G309 L310 E311 N312 V313 I314 V315 I316 G317 A318 S319 N320 R321 E322 D323 I329 L330 R334 V337 K338 I339 K340 I341 E342 R343 P344 A348 A349 Q350 Y353

L357 T358 E359 F360 L361 P362 D367 R375 I379 K380 A381 M382 I383 E384 K385 V386 V387 I394 D395 D396 F399 L400 N406 F414 F417 M422 I423 Q424 N425 V426 R429 A434 I435 K436 S437 V438 T441 G442 Q443 P444 G445 L446 L451 E458 P466

R476 G482 E483 T488 R489 T490 L491 V492 T493 G494 K495 S496 S497 T505 E506 SER ASN LEU GLY GLN TYR LEU

• Molecule 1: Proteasome-associated ATPase

Chain K:

M1 P2 S3 L8 L9 H12 D13 D14 D15 T16 V17 D18 V19 F20 L28 L39 K40 K41 G42 Q43 R46 L47 L51 A56 F59 H76 R77 H83 A84 D85 E86 L92 D103 G104 L105 P106 E107 A108 L109 N110 D111 D112 T113 R114 P115 R116 R119

R136 K139 A140 E141 V142 E143 D144 L145 V146 L147 E148 E149 V150 P151 D152 V153 I158 S162 I165 E166 Q167 I168 R169 D170 A171 V172 E173 L174 P175 F176 L177 H178 Y182 R183 E184 Y185 S186 L187 K191 G192 V193 L194 L195 P198 C201 G202 K203 I206 A207

• Molecule 1: Proteasome-associated ATPase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.27Å 202.59Å 303.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.13 – 3.49 71.13 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (71.13-3.49) 99.4 (71.13-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.268 , 0.306 0.262 , 0.299	Depositor DCC
R_{free} test set	1996 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å^2)	119.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 92.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	44298	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.35	1/3808 (0.0%)	0.60	1/5150 (0.0%)
1	B	0.32	0/3766	0.56	3/5092 (0.1%)
1	C	0.31	0/3706	0.56	1/5011 (0.0%)
1	D	0.30	0/3651	0.53	1/4933 (0.0%)
1	E	0.31	1/3655 (0.0%)	0.55	3/4939 (0.1%)
1	F	0.32	0/3646	0.57	2/4929 (0.0%)
1	G	0.35	1/3652 (0.0%)	0.56	1/4939 (0.0%)
1	H	0.35	1/3789 (0.0%)	0.58	2/5126 (0.0%)
1	I	0.34	0/3794	0.60	1/5130 (0.0%)
1	J	0.32	0/3836	0.58	2/5192 (0.0%)
1	K	0.37	0/3950	0.62	3/5346 (0.1%)
1	L	0.31	0/3754	0.56	0/5076
All	All	0.33	4/45007 (0.0%)	0.57	20/60863 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	G	0	2
1	H	0	3
1	I	0	2
1	J	0	1
1	K	0	4
1	L	0	2
All	All	0	21

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	466	PRO	N-CD	5.37	1.55	1.47
1	A	151	PRO	N-CD	5.20	1.55	1.47
1	H	298	PRO	N-CD	5.18	1.55	1.47
1	G	151	PRO	N-CD	5.08	1.54	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	148	GLU	N-CA-C	7.45	131.12	111.00
1	E	251	ARG	N-CA-C	7.28	130.66	111.00
1	H	150	VAL	C-N-CD	-6.30	106.75	120.60
1	K	251	ARG	N-CA-C	-5.73	95.53	111.00
1	G	150	VAL	C-N-CD	5.69	140.36	128.40

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLY	Peptide
1	A	215	ALA	Peptide
1	A	222	ARG	Peptide
1	B	297	VAL	Peptide
1	C	24	ARG	Peptide

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	3747	0	3755	190	0
1	B	3707	0	3718	145	0
1	C	3649	0	3644	136	3
1	D	3593	0	3607	120	0
1	E	3597	0	3610	131	0
1	F	3589	0	3606	137	0
1	G	3595	0	3611	219	0
1	H	3729	0	3741	180	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3735	0	3749	205	0
1	J	3775	0	3778	206	0
1	K	3887	0	3888	270	3
1	L	3695	0	3704	166	0
All	All	44298	0	44411	1957	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 22.

The worst 5 of 1957 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:K:229:ALA:CA	1:K:230:LYS:HB2	1.46	1.45
1:A:150:VAL:CG2	1:A:231:SER:HA	1.52	1.38
1:H:296:VAL:CG2	1:I:242:LEU:HD21	1.51	1.38
1:K:153:VAL:O	1:K:212:ASN:ND2	1.57	1.38
1:G:148:GLU:CG	1:G:150:VAL:HG13	1.54	1.34

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)
1:C:180:GLU:CG	1:K:230:LYS:CD[3_444]	1.97	0.23
1:C:180:GLU:CG	1:K:230:LYS:CE[3_444]	2.05	0.15
1:C:180:GLU:CG	1:K:230:LYS:NZ[3_444]	2.11	0.09

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	474/513 (92%)	440 (93%)	29 (6%)	5 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	467/513 (91%)	441 (94%)	23 (5%)	3 (1%)	25	64
1	C	462/513 (90%)	429 (93%)	30 (6%)	3 (1%)	25	64
1	D	450/513 (88%)	433 (96%)	17 (4%)	0	100	100
1	E	451/513 (88%)	431 (96%)	19 (4%)	1 (0%)	47	81
1	F	452/513 (88%)	424 (94%)	24 (5%)	4 (1%)	17	56
1	G	453/513 (88%)	428 (94%)	21 (5%)	4 (1%)	17	56
1	H	470/513 (92%)	442 (94%)	24 (5%)	4 (1%)	17	56
1	I	470/513 (92%)	446 (95%)	23 (5%)	1 (0%)	47	81
1	J	478/513 (93%)	442 (92%)	33 (7%)	3 (1%)	25	64
1	K	494/513 (96%)	457 (92%)	29 (6%)	8 (2%)	9	43
1	L	465/513 (91%)	434 (93%)	27 (6%)	4 (1%)	17	56
All	All	5586/6156 (91%)	5247 (94%)	299 (5%)	40 (1%)	22	61

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	PRO
1	E	250	GLU
1	H	151	PRO
1	H	152	ASP
1	K	222	ARG

5.3.2 Protein sidechains ⓘ

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	405/433 (94%)	371 (92%)	34 (8%)	11	40
1	B	402/433 (93%)	362 (90%)	40 (10%)	7	32
1	C	389/433 (90%)	351 (90%)	38 (10%)	8	33
1	D	389/433 (90%)	346 (89%)	43 (11%)	6	28
1	E	389/433 (90%)	351 (90%)	38 (10%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	389/433 (90%)	345 (89%)	44 (11%)	6	27
1	G	390/433 (90%)	347 (89%)	43 (11%)	6	29
1	H	405/433 (94%)	362 (89%)	43 (11%)	6	30
1	I	405/433 (94%)	362 (89%)	43 (11%)	6	30
1	J	410/433 (95%)	376 (92%)	34 (8%)	11	40
1	K	421/433 (97%)	371 (88%)	50 (12%)	5	25
1	L	401/433 (93%)	356 (89%)	45 (11%)	6	27
All	All	4795/5196 (92%)	4300 (90%)	495 (10%)	7	32

5 of 495 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	468	THR
1	K	380	LYS
1	H	201	CYS
1	K	325	ILE
1	L	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	243	ASN
1	L	443	GLN
1	K	252	HIS
1	L	212	ASN
1	G	243	ASN

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, 95th 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(Å²)	Q<0.9
1	A	480/513 (93%)	1.17	107 (22%)	0	0	56, 117, 190, 215	0
1	B	475/513 (92%)	1.19	100 (21%)	1	1	57, 133, 189, 213	0
1	C	472/513 (92%)	1.13	100 (21%)	0	1	55, 134, 193, 231	0
1	D	460/513 (89%)	1.33	111 (24%)	0	0	66, 127, 215, 230	0
1	E	461/513 (89%)	1.61	136 (29%)	0	0	71, 149, 212, 231	0
1	F	460/513 (89%)	1.14	93 (20%)	1	1	66, 136, 191, 226	0
1	G	461/513 (89%)	1.11	88 (19%)	1	1	69, 128, 195, 223	0
1	H	478/513 (93%)	1.10	81 (16%)	1	2	61, 107, 191, 209	0
1	I	478/513 (93%)	0.93	68 (14%)	2	3	62, 107, 176, 217	0
1	J	484/513 (94%)	0.88	63 (13%)	3	4	70, 120, 191, 215	0
1	K	498/513 (97%)	0.78	51 (10%)	6	7	67, 114, 164, 191	0
1	L	473/513 (92%)	1.36	119 (25%)	0	0	64, 146, 205, 219	0
All	All	5680/6156 (92%)	1.14	1117 (19%)	1	1	55, 125, 200, 231	0

The worst 5 of 1117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	231	SER	11.2
1	D	78	ALA	11.2
1	C	231	SER	10.9
1	L	146	VAL	10.4
1	L	232	TYR	10.1

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 monosaccharides 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.