wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2024 – 11:41 am BST

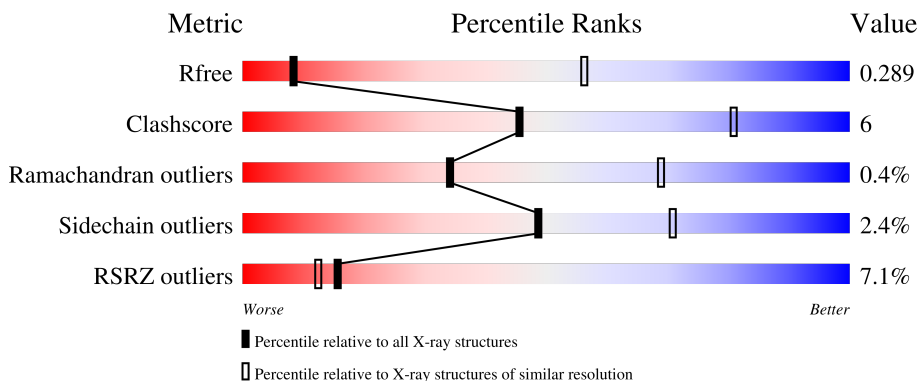|		
PDB ID	:	6TJP
Title	:	Crystal structure of T7 bacteriophage portal protein, 13mer, closed valve - P212121
Authors	:	Fabrega-Ferrer, M.; Cuervo, A.; Fernandez, F.J.; Machon, C.; Perez-Luque, R.; Pous, J.; Vega, M.C.; Carrascosa, J.L.; Coll, M.
Deposited on	:	2019-11-26
Resolution	:	3.74 Å(reported)

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 3.74 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	Percentile Ranks	Value
Rfree		0.289
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		2.4%
RSRZ outliers		7.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)

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	536	6% / 75% 12% · 12%
1	B	536	5% / 74% 14% 12%
1	C	536	9% / 72% 16% · 12%
1	D	536	7% / 73% 15% 12%
1	E	536	9% / 73% 15% · 12%

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Mol	Chain	Length	Quality of chain
1	F	536	6% / 70% / 18% / 12%
1	G	536	5% / 72% / 16% / 12%
1	H	536	4% / 71% / 17% / 12%
1	I	536	5% / 71% / 17% / 12%
1	J	536	8% / 70% / 18% / 12%
1	K	536	6% / 75% / 13% / 12%
1	L	536	6% / 73% / 15% / 12%
1	M	536	5% / 73% / 15% / 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 48126 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 Portal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			
1	B	473	Total	C	N	O	S	1	0	0
			3702	2331	627	727	17			
1	C	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			
1	D	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			
1	E	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			
1	F	473	Total	C	N	O	S	1	0	0
			3702	2331	627	727	17			
1	G	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			
1	H	473	Total	C	N	O	S	3	0	0
			3702	2331	627	727	17			
1	I	473	Total	C	N	O	S	1	0	0
			3702	2331	627	727	17			
1	J	473	Total	C	N	O	S	3	0	0
			3702	2331	627	727	17			
1	K	473	Total	C	N	O	S	1	0	0
			3702	2331	627	727	17			
1	L	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			
1	M	473	Total	C	N	O	S	2	0	0
			3702	2331	627	727	17			

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: Portal protein

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MET ALA E3 T6 G7 L8 A9 E10 N22 I39 K45 D48 ASN SER THR ASP TYR Q55 Q59 L73 M74 P79 W83 I88 S89 L96 D99 G102 V106 D107 Y120 F131 L137 N142 V143 L144 L147 E151

N156 Y161 R162 L163 Y166 D171 N175 Q178 M179 R182 F187 P191 I194 A197 V198 Q201 G202 G203 K206 H216 I217 Y218 R228 Y229 E230 V232 E233 G234 M235 E236 V237 Y244 P250 R255 G265 E280 S293 T306

R309 Q315 F319 D326 I327 L332 E333 K334 F338 T339 V340 V344 M357 L358 N359 V362 Q363 R364 T365 G366 E367 T370 A371 E372 E373 I374 V388 L398 R402 Q407 L417 P418 K419 E420 A421 V422 E423 P424 S427 Q437 E443

A451 L452 A453 P454 M455 R456 D457 D458 P459 D460 I461 N462 L463 I466 K467 L468 R469 I470 I476 D477 T478 S479 G480 I481 LEU LEU THR GLU GLU GLN LYS GLN GLN LYS MET ALA GLN GLN SER MET GLN MET GLY MET ASP ASN GLY ALA ALA ALA LEU ALA GLN GLY MET ALA ALA GLN

ALA THR ALA SER PRO GLU ALA MET ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE
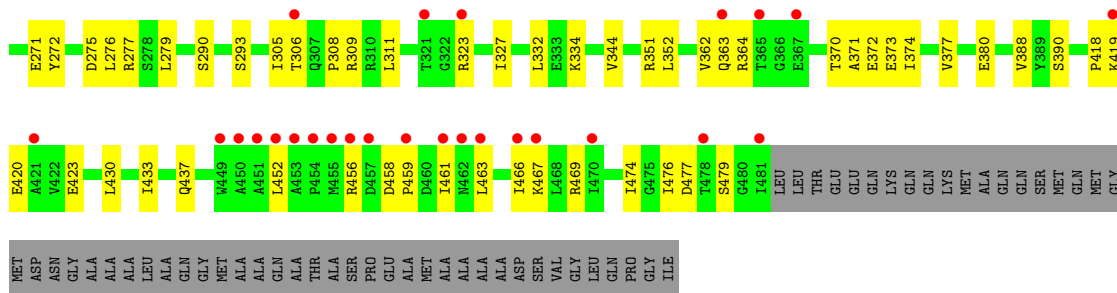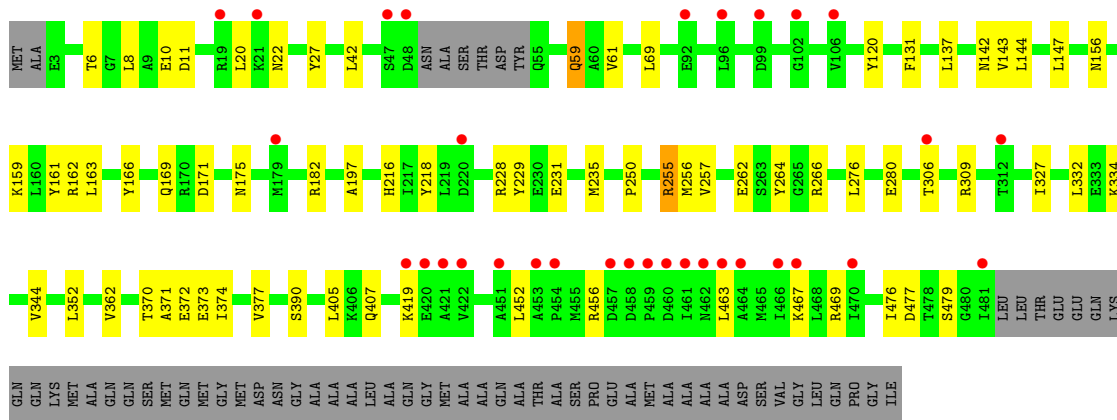
• Molecule 1: Portal protein

Chain D:

7%

73% 15% 12%

MET ALA E3 T6 G7 L8 D11 N22 D23 R24 Y27 E28 I39 F43 P44 K45 D46 S47 D48 ASN ALA SER THR ASP TYR Q55 Q59 A60 V61 L69 L73 Q81 Q95 S98 D101 G102 Y120 Y126 F131 E132 A133 L137

N142 V143 L144 L147 E151 G152 S153 N156 K159 L160 Y161 R162 L163 Y166 Q178 R182 A197 E204 A207 D208 I211 D212 R228 E231 M235 Y244 P250 R255 M256 V257 R258 L259 E262 S263 Y264 G265 R266 E271 L279

S293 T306 R309 R310 L311 I327 K334 F338 T339 V340 A341 K342 M357 V362 Q363 R364 T365 G366 E367 R368 V369 T370 A371 E372 E373 I374 V377 E380 V388 Y389 S390 L404 Q407 T411 Q412 Q413 K419 E420 A421 V422 E443 W449 A450 A451

L452 A453 P454 M455 R456 D457 P459 D460 I461 N462 L463 A464 M465 I466 K467 L468 R469 I470 A471 I476 D477 T478 S479 G480 I481 LEU LEU THR GLU GLU GLN LYS GLN GLN LYS MET ALA GLN GLN SER MET GLN MET GLY MET ASP ASN GLY ALA ALA ALA LEU ALA GLN GLY MET ALA ALA

GLN ALA THR ALA SER PRO GLU ALA MET ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE

• Molecule 1: Portal protein

Chain E:

9%

73% 15% 12%

MET ALA E3 K4 R5 T6 G7 L8 A9 E10 D11 G12 A13 Y17 Q36 K45 D46 S47 D48 ASN ALA SER THR ASP TYR Q55 Q59 A60 V61 L69 L73 P79 W83 I88 D99 Y120 F131 L137 N142 V143 L144 L147 E151

N156 K159 L160 Y161 R162 L163 Y166 Q169 R170 D171 N175 Q178 M179 R182 E192 D193 I194 A197 G203 V213 Y214 T215 H216 I217 Y218 L219 D220 E221 G224 Y226 L227 R228 Y229 E230 E231 V232 M235 Y244 P250 R255 L259 E271

D275 L279 E280 S293 I305 T306 R309 R323 I327 L332 E333 K334 F338 T339 V340 R351 V362 Q363 E367 R368 V369 T370 A371 E372 E373 I374 V377 V388 Y389 S390 I391 L398 R402 Q407 L417 P418 K419 E420 A421 G429

Q437 W449 A450 A451 L452 A453 P454 M455 R456 D457 D458 P459 D460 I461 N462 L463 A464 K467 L468 R469 I476 D477 T478 S479 G480 I481 LEU LEU THR GLU GLU GLN LYS GLN GLN LYS MET ALA GLN GLN SER MET GLN MET GLY MET ASP ASN GLY ALA ALA ALA LEU ALA GLN GLY MET

ALA ALA GLN ALA THR ALA SER PRO GLU ALA MET ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE

● Molecule 1: Portal protein

Chain F:

I198 G203 A207 D208 H216 I217 Y218 E221 R228 Y229 E230 V232 E233 D241 Y244 R255 M256 V257 R258

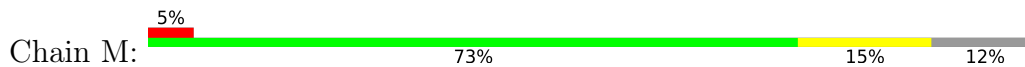● Molecule 1: Portal protein

Chain G:

• Molecule 1: Portal protein

Chain H:

• Molecule 1: Portal protein

Chain I:

• Molecule 1: Portal protein

Chain J:

E271 Y272 D275 L276 R277 S278 L279 S290 S293 I305 T306 Q307 P308 R309 R310 L311 T321 G322 R323 I327 L332 E333 K334 V344 R351 L352 V362 Q363 R364 T365 G366 E367 T370 A371 E372 E373 I374 V377 E380 V388 Y389 S390 P418 K419

E420 A421 V422 E423 L430 I433 Q437 W449 A450 A451 L452 A453 P454 M455 R456 D457 D458 P459 D460 I461 N462 L463 I466 K467 L468 R469 I470 I474 G475 I476 D477 T478 S479 G480 I481 LEU LEU THR GLU GLU GLN LYS GLN LYS MET ALA GLN SER MET GLN MET GLY

MET ASP ASN GLY ALA ALA LEU ALA GLN GLY MET ALA ALA GLN ALA THR ALA SER PRO GLU ALA MET ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE

● Molecule 1: Portal protein

Chain K:

MET ALA E3 T6 G7 L8 A9 E10 D11 R19 L20 K21 N22 Y27 L42 S47 D48 ASN ALA SER THR ASP TYR Q55 Q59 A60 V61 L69 E92 L96 D99 G102 V106 Y120 F131 L137 N142 V143 L144 L147 N156

K159 L160 Y161 R162 L163 Y166 Q169 R170 D171 N175 M179 R182 A197 H216 I217 Y218 L219 D220 R228 Y229 E230 E231 M235 P250 R255 M256 V257 E262 S263 Y264 G265 R266 L276 E280 T306 R309 T312 I327 L332 E333 K334

V344 L352 V362 T370 A371 E372 E373 I374 V377 S390 L405 K406 Q407 K419 E420 A421 V422 A451 L452 A453 P454 M455 R456 D457 D458 P459 D460 I461 N462 L463 A464 M465 I466 K467 L468 R469 I470 I476 D477 T478 S479 G480 I481 LEU LEU THR GLU GLU GLN LYS

GLN GLN LYS MET ALA GLN GLN SER MET GLN MET GLY MET ASP ASN GLY ALA ALA ALA LEU ALA GLN GLY MET ALA ALA GLN ALA THR ALA SER PRO GLU ALA MET ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE

● Molecule 1: Portal protein

Chain L:

MET ALA E3 L8 D11 N22 Y27 E28 L42 S47 D48 ASN ALA SER THR ASP TYR Q55 Q59 L73 E92 G102 K105 V106 Y120 A133 L134 K135 Q136 L137 V138 V139 N142 V143 L144 L147 E151 N156 Y161 R162 L163

Y166 R182 I185 P191 E192 D193 I194 R195 K205 K206 A207 D208 T211 D212 H216 I217 Y218 R228 Y229 E230 E231 V232 E233 S240 A248 C249 P250 R255 M256 V257 R258 L259 D260 G261 E262 S263 Y264 G265 R266 D275 L276 E280 V300 I305 T306 Q307

P308 R309 R310 L311 R323 I327 L332 E333 K334 F338 R351 L352 V362 R368 V369 T370 A371 E372 E373 I374 V388 Y389 S390 I391 L398 R402 K406 Q407 P415 E416 L417 P418 K419 E420 A421 V422 E423 Q437 A451 L452 A453 P454 M455 R456 D457 D458

P459 D460 I461 N462 L463 I466 K467 L468 R469 I476 D477 T478 S479 G480 I481 LEU LEU THR GLU GLU GLN LYS GLN LYS MET ALA GLN GLN SER MET GLN MET GLY MET ASP ASN GLY ALA ALA ALA LEU ALA LEU ALA GLN GLY MET ALA ALA GLN ALA THR ALA SER PRO GLU ALA MET ALA

ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE

● Molecule 1: Portal protein

Chain M:

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.85Å 238.57Å 265.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.74 49.47 – 3.74	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.47-3.74) 98.5 (49.47-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.244 , 0.286 0.257 , 0.289	Depositor DCC
R_{free} test set	3918 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	130.3	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 108.9	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	48126	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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 (i)

5.1 Standard geometry (i)

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	0.26	0/3760	0.46	0/5089
1	B	0.26	0/3760	0.46	0/5089
1	C	0.26	0/3760	0.47	0/5089
1	D	0.26	0/3760	0.46	0/5089
1	E	0.26	0/3760	0.47	0/5089
1	F	0.27	0/3760	0.47	0/5089
1	G	0.27	0/3760	0.47	0/5089
1	H	0.26	0/3760	0.46	0/5089
1	I	0.26	0/3760	0.47	0/5089
1	J	0.27	0/3760	0.47	0/5089
1	K	0.27	0/3760	0.47	0/5089
1	L	0.26	0/3760	0.47	0/5089
1	M	0.26	0/3760	0.47	0/5089
All	All	0.26	0/48880	0.47	0/66157

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 (i)

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	3702	0	3710	44	0
1	B	3702	0	3710	48	2
1	C	3702	0	3710	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3702	0	3710	52	1
1	E	3702	0	3710	54	0
1	F	3702	0	3710	67	0
1	G	3702	0	3710	63	0
1	H	3702	0	3710	61	0
1	I	3702	0	3710	60	0
1	J	3702	0	3710	60	0
1	K	3702	0	3710	55	0
1	L	3702	0	3710	53	0
1	M	3702	0	3710	55	1
All	All	48126	0	48230	620	2

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.

The worst 5 of 620 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:144:LEU:HB3	1:F:161:TYR:HB2	1.60	0.83
1:C:306:THR:HG21	1:C:327:ILE:HD11	1.66	0.78
1:C:479:SER:O	1:D:469:ARG:NH2	2.16	0.78
1:I:162:ARG:HH22	1:J:259:LEU:HD22	1.50	0.77
1:K:456:ARG:HA	1:K:463:LEU:HD11	1.66	0.76

All (2) 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:B:15:SER:OG	1:D:95:GLN:OE1[4_555]	2.15	0.05
1:B:193:ASP:OD2	1:M:309:ARG:NH1[4_455]	2.17	0.03

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	469/536 (88%)	423 (90%)	45 (10%)	1 (0%)	47	78
1	B	469/536 (88%)	424 (90%)	43 (9%)	2 (0%)	34	69
1	C	469/536 (88%)	420 (90%)	46 (10%)	3 (1%)	25	61
1	D	469/536 (88%)	420 (90%)	47 (10%)	2 (0%)	34	69
1	E	469/536 (88%)	421 (90%)	45 (10%)	3 (1%)	25	61
1	F	469/536 (88%)	421 (90%)	45 (10%)	3 (1%)	25	61
1	G	469/536 (88%)	420 (90%)	48 (10%)	1 (0%)	47	78
1	H	469/536 (88%)	421 (90%)	45 (10%)	3 (1%)	25	61
1	I	469/536 (88%)	421 (90%)	46 (10%)	2 (0%)	34	69
1	J	469/536 (88%)	421 (90%)	45 (10%)	3 (1%)	25	61
1	K	469/536 (88%)	422 (90%)	46 (10%)	1 (0%)	47	78
1	L	469/536 (88%)	420 (90%)	48 (10%)	1 (0%)	47	78
1	M	469/536 (88%)	423 (90%)	44 (9%)	2 (0%)	34	69
All	All	6097/6968 (88%)	5477 (90%)	593 (10%)	27 (0%)	34	69

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	419	LYS
1	A	419	LYS
1	B	419	LYS
1	C	419	LYS
1	D	419	LYS

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	400/442 (90%)	391 (98%)	9 (2%)	50	71
1	B	400/442 (90%)	391 (98%)	9 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	C	400/442 (90%)	390 (98%)	10 (2%)		47	70
1	D	400/442 (90%)	389 (97%)	11 (3%)		43	67
1	E	400/442 (90%)	391 (98%)	9 (2%)		50	71
1	F	400/442 (90%)	391 (98%)	9 (2%)		50	71
1	G	400/442 (90%)	392 (98%)	8 (2%)		55	75
1	H	400/442 (90%)	389 (97%)	11 (3%)		43	67
1	I	400/442 (90%)	388 (97%)	12 (3%)		41	65
1	J	400/442 (90%)	390 (98%)	10 (2%)		47	70
1	K	400/442 (90%)	391 (98%)	9 (2%)		50	71
1	L	400/442 (90%)	390 (98%)	10 (2%)		47	70
1	M	400/442 (90%)	391 (98%)	9 (2%)		50	71
All	All	5200/5746 (90%)	5074 (98%)	126 (2%)		49	71

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	59	GLN
1	L	151	GLU
1	H	255	ARG
1	L	147	LEU
1	M	23	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	184	GLN
1	M	136	GLN
1	C	156	ASN
1	F	184	GLN
1	J	184	GLN

5.3.3   RNA (i)

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	473/536 (88%)	0.30	31 (6%)	18	14	68, 139, 224, 386	1 (0%)
1	B	473/536 (88%)	0.27	26 (5%)	25	21	72, 141, 242, 294	1 (0%)
1	C	473/536 (88%)	0.40	49 (10%)	6	6	76, 144, 247, 328	1 (0%)
1	D	473/536 (88%)	0.43	40 (8%)	10	9	90, 160, 263, 353	1 (0%)
1	E	473/536 (88%)	0.57	46 (9%)	7	7	89, 164, 258, 310	1 (0%)
1	F	473/536 (88%)	0.32	32 (6%)	17	13	81, 164, 240, 285	1 (0%)
1	G	473/536 (88%)	0.19	29 (6%)	21	17	78, 149, 242, 341	1 (0%)
1	H	473/536 (88%)	0.23	22 (4%)	31	27	76, 137, 229, 294	1 (0%)
1	I	473/536 (88%)	0.19	26 (5%)	25	21	75, 129, 232, 316	1 (0%)
1	J	473/536 (88%)	0.32	42 (8%)	9	8	67, 128, 233, 363	1 (0%)
1	K	473/536 (88%)	0.30	32 (6%)	17	13	65, 132, 236, 321	1 (0%)
1	L	473/536 (88%)	0.33	34 (7%)	15	12	68, 138, 237, 287	1 (0%)
1	M	473/536 (88%)	0.21	29 (6%)	21	17	66, 141, 231, 329	1 (0%)
All	All	6149/6968 (88%)	0.31	438 (7%)	16	12	65, 145, 240, 386	13 (0%)

The worst 5 of 438 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	48	ASP	10.9
1	A	48	ASP	9.8
1	B	454	PRO	9.8
1	C	454	PRO	9.3
1	B	463	LEU	9.2

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.