



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:03 PM GMT

PDB ID : 1W4C
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI12 APO STATE
Authors : Mancini, E.J.; Kainov, D.E.; Grimes, J.M.; Tuma, R.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2004-07-22
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

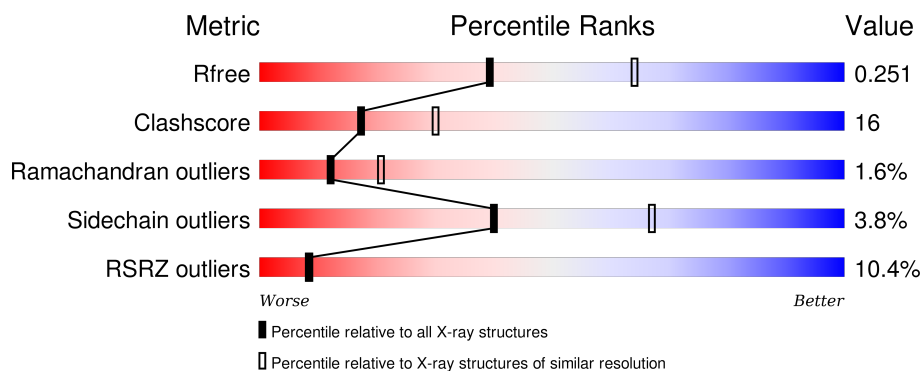
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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 $\leq 5\%$. 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	331	<div> <div>8%</div> <div>67% 18% • 13%</div> </div>
1	B	331	<div> <div>13%</div> <div>66% 23% • 8%</div> </div>
1	C	331	<div> <div>8%</div> <div>67% 22% • 8%</div> </div>
1	D	331	<div> <div>6%</div> <div>66% 19% • 13%</div> </div>
1	E	331	<div> <div>11%</div> <div>66% 23% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	331	
1	G	331	
1	H	331	
1	I	331	
1	J	331	
1	K	331	
1	L	331	
1	M	331	
1	N	331	
1	O	331	
1	P	331	
1	Q	331	
1	R	331	
1	S	331	
1	T	331	
1	U	331	
1	V	331	
1	W	331	
1	X	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57270 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 NTPASE P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	B	304	Total	C	N	O	S	0	0	0
			2288	1434	399	448	7			
1	C	304	Total	C	N	O	S	0	0	0
			2288	1433	399	449	7			
1	D	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	E	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	F	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	G	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	H	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	I	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	J	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	K	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	L	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	M	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	N	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	O	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	P	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	R	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	S	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	T	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	U	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	V	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	W	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	X	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	119	Total	O	0	0
			119	119		
2	C	129	Total	O	0	0
			129	129		
2	D	145	Total	O	0	0
			145	145		
2	E	143	Total	O	0	0
			143	143		
2	F	151	Total	O	0	0
			151	151		
2	G	101	Total	O	0	0
			101	101		
2	H	178	Total	O	0	0
			178	178		
2	I	193	Total	O	0	0
			193	193		
2	J	159	Total	O	0	0
			159	159		
2	K	122	Total	O	0	0
			122	122		

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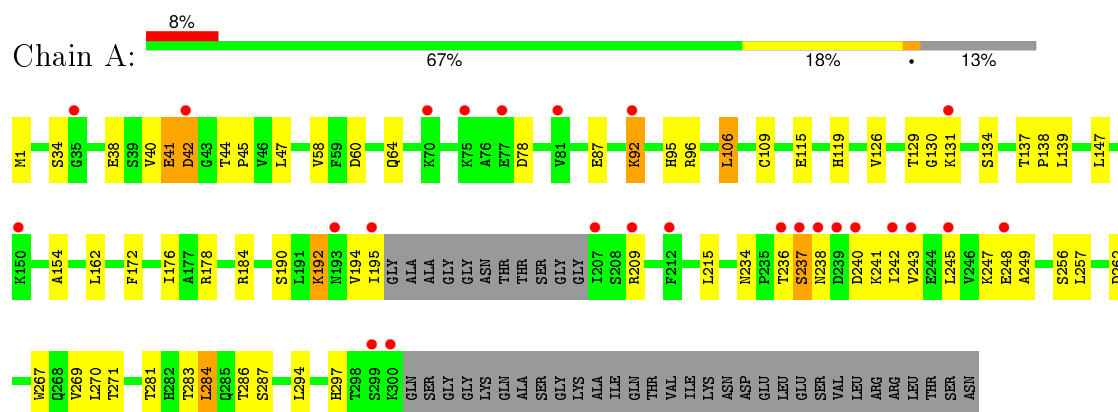
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	93	Total 93	O 93	0	0
2	M	169	Total 169	O 169	0	0
2	N	202	Total 202	O 202	0	0
2	O	144	Total 144	O 144	0	0
2	P	103	Total 103	O 103	0	0
2	Q	93	Total 93	O 93	0	0
2	R	110	Total 110	O 110	0	0
2	S	146	Total 146	O 146	0	0
2	T	88	Total 88	O 88	0	0
2	U	73	Total 73	O 73	0	0
2	V	118	Total 118	O 118	0	0
2	W	120	Total 120	O 120	0	0
2	X	153	Total 153	O 153	0	0

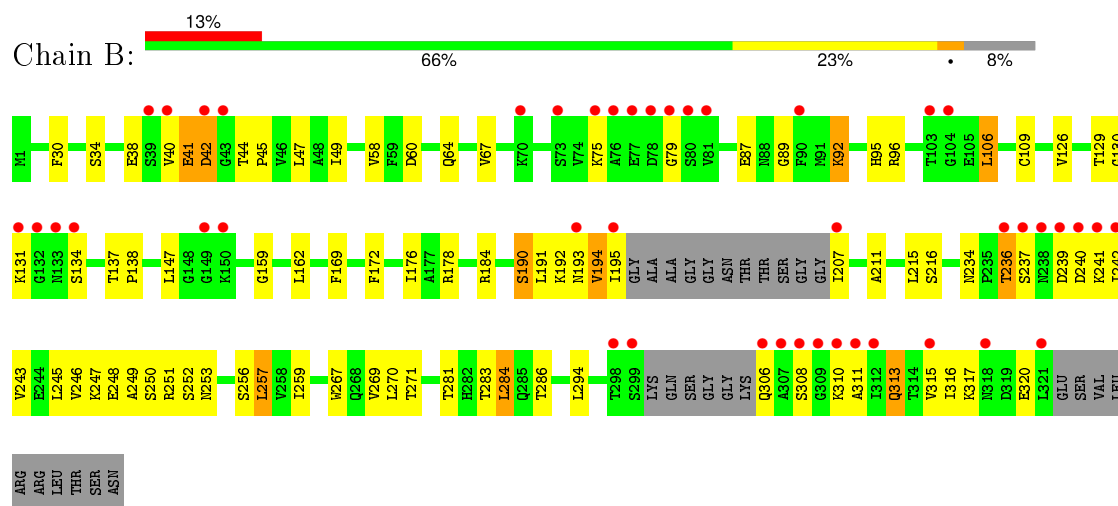
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

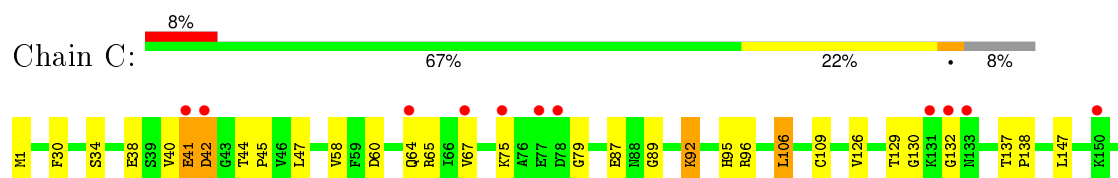
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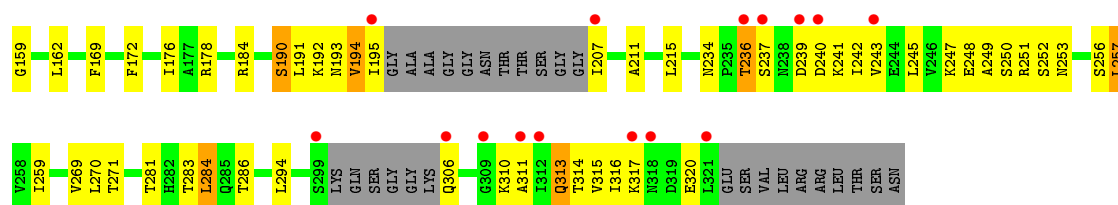


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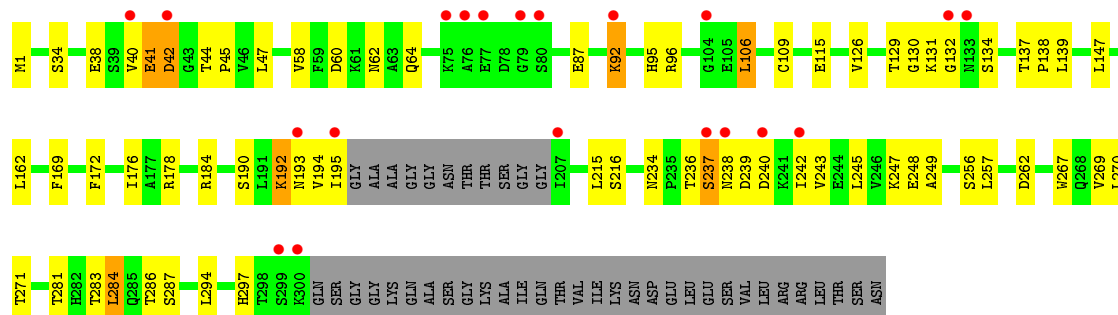


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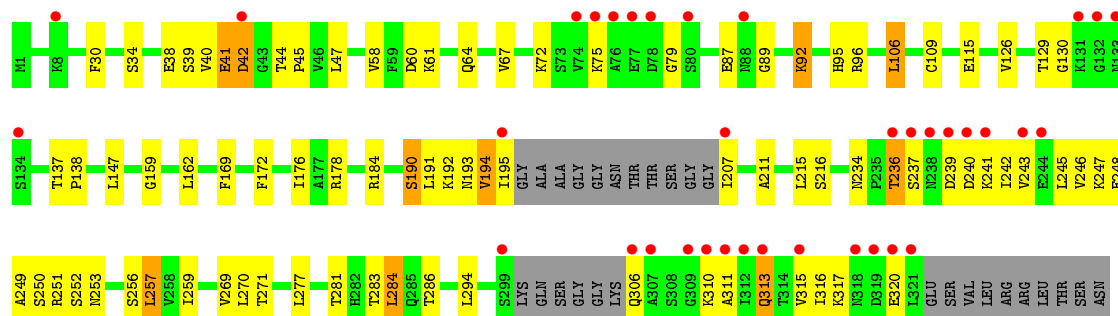




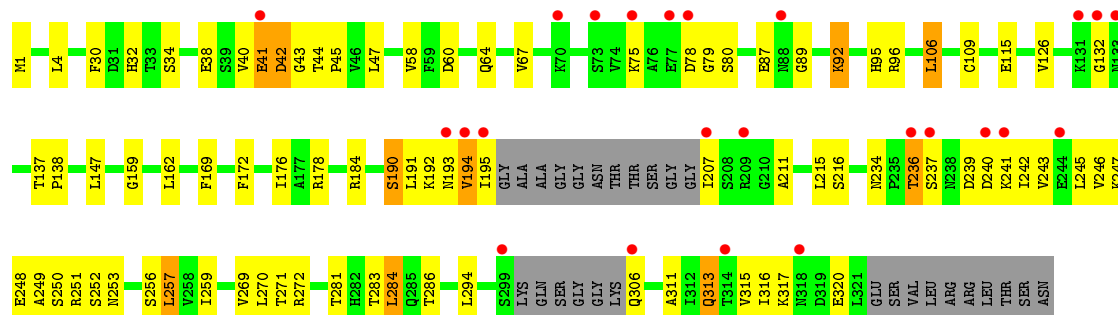
• Molecule 1: NTPASE P4



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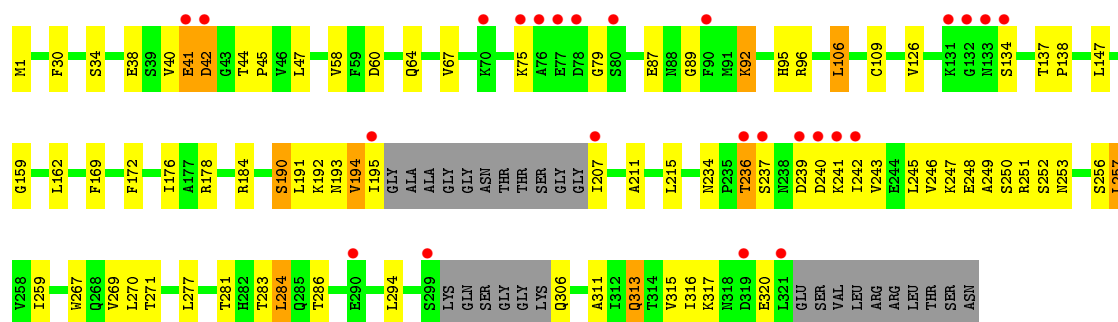


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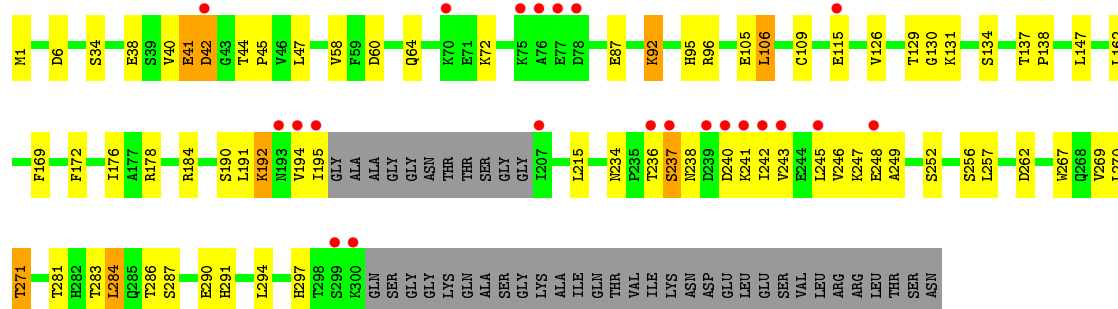


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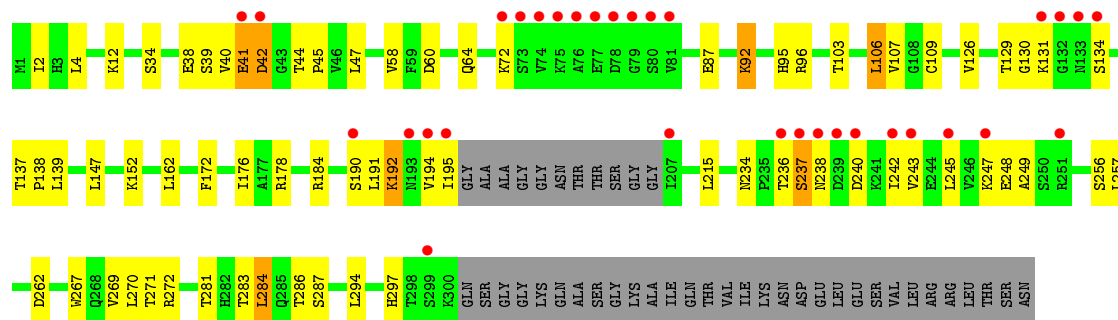




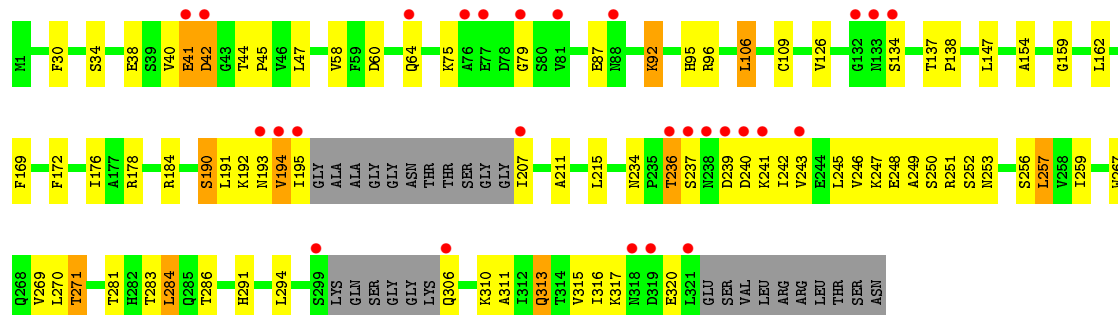
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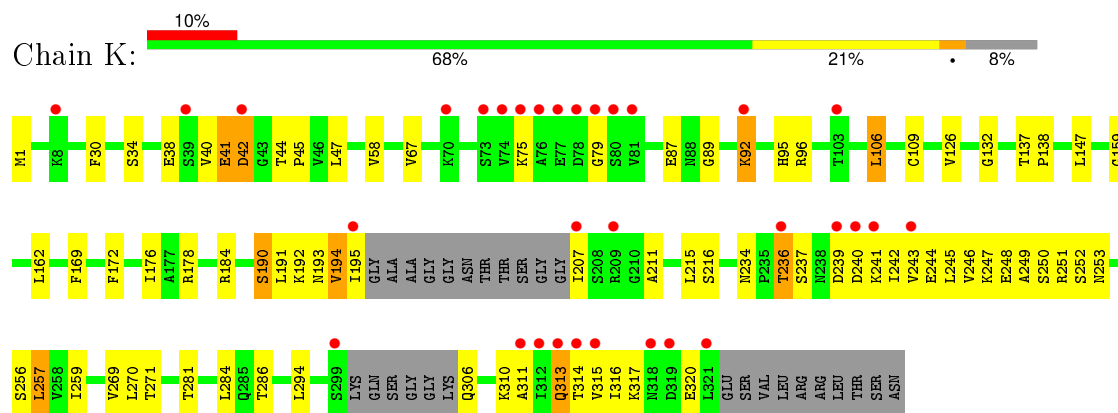
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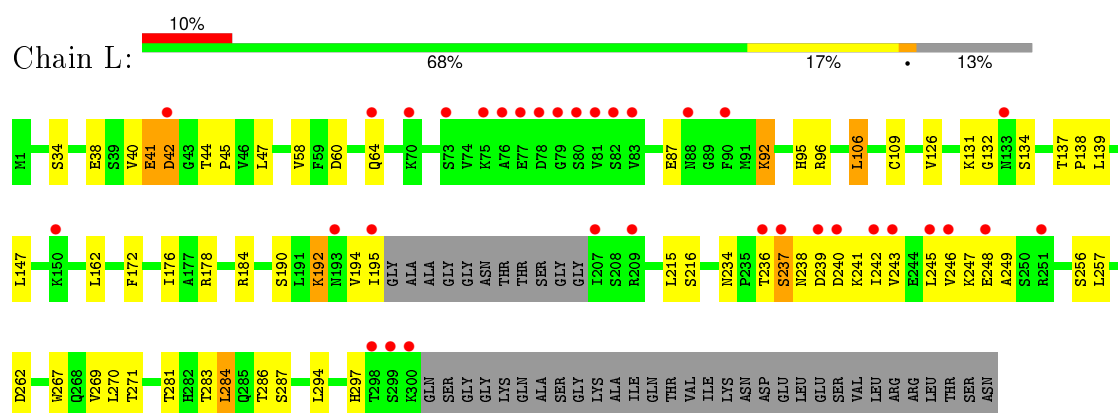
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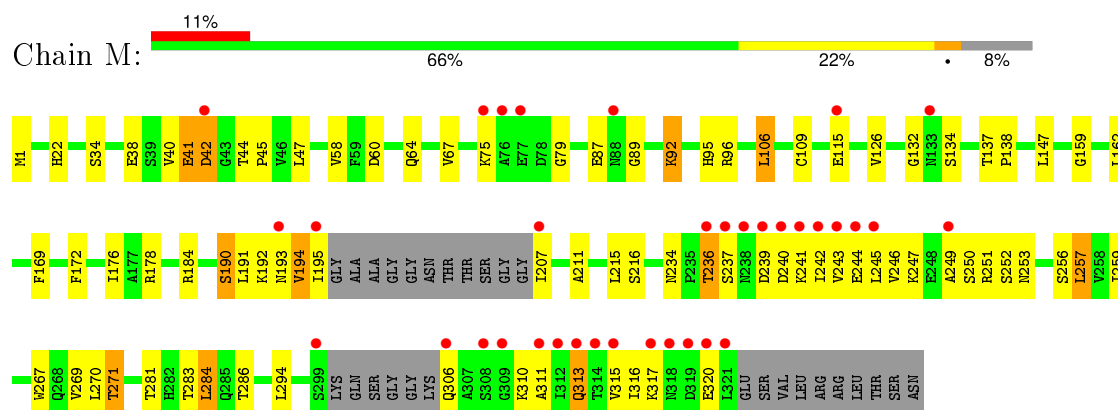
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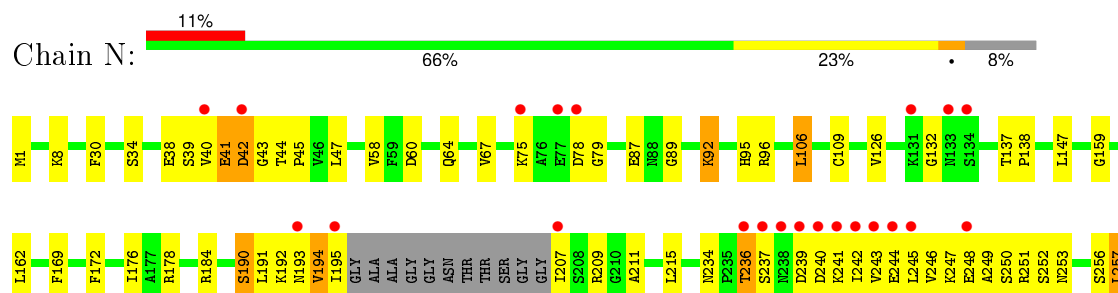
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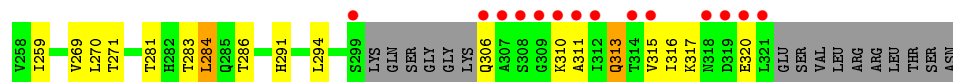


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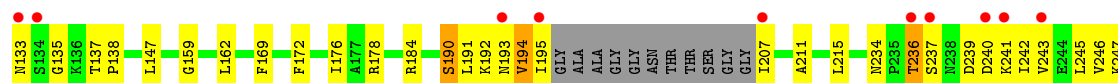
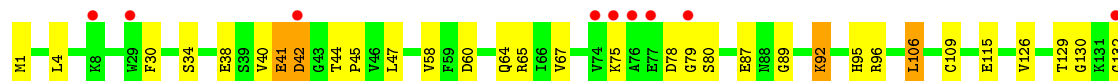


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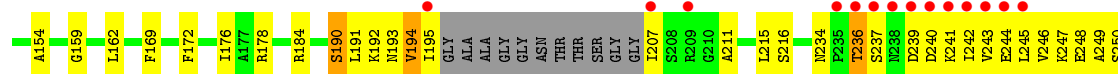
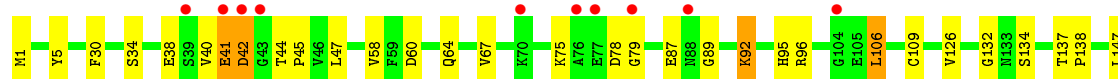




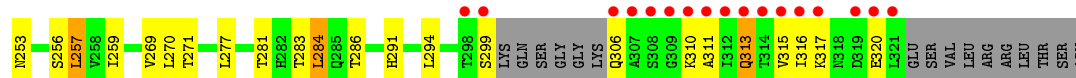
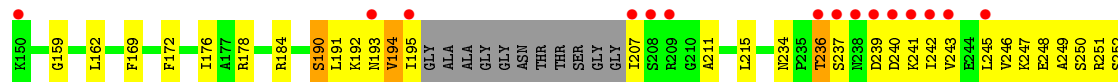
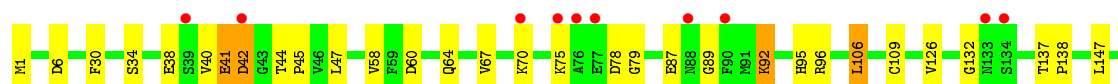
• Molecule 1: NTPASE P4



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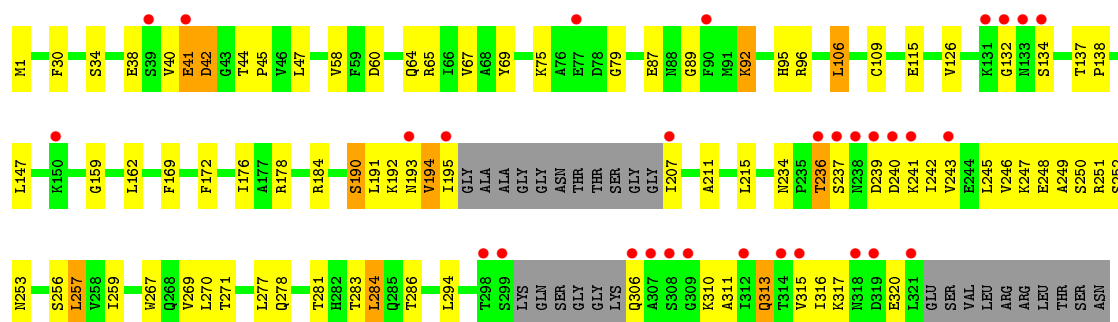


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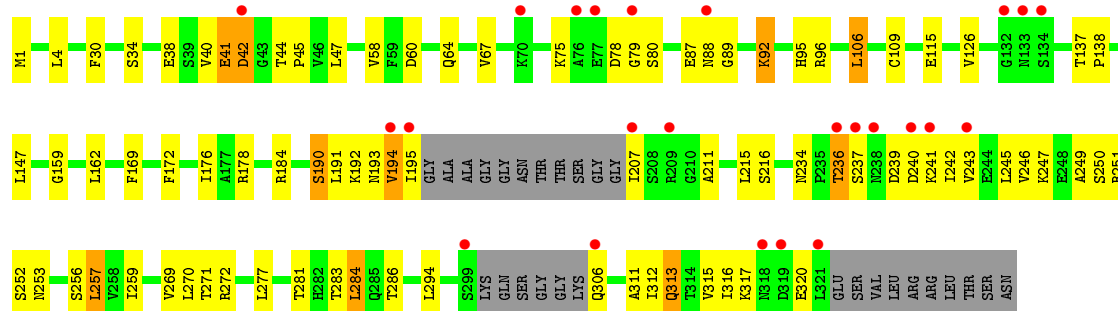


• Molecule 1: NTPASE P4

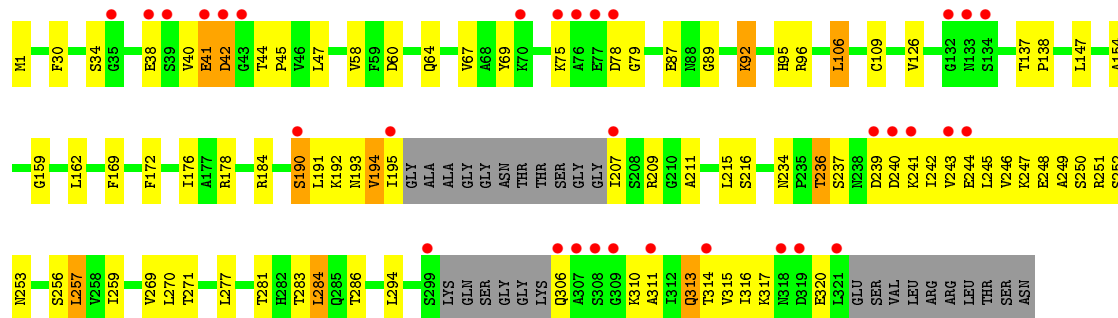




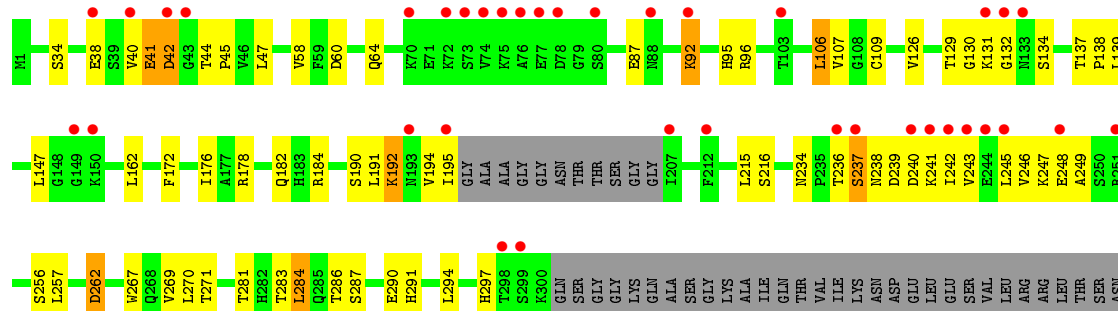
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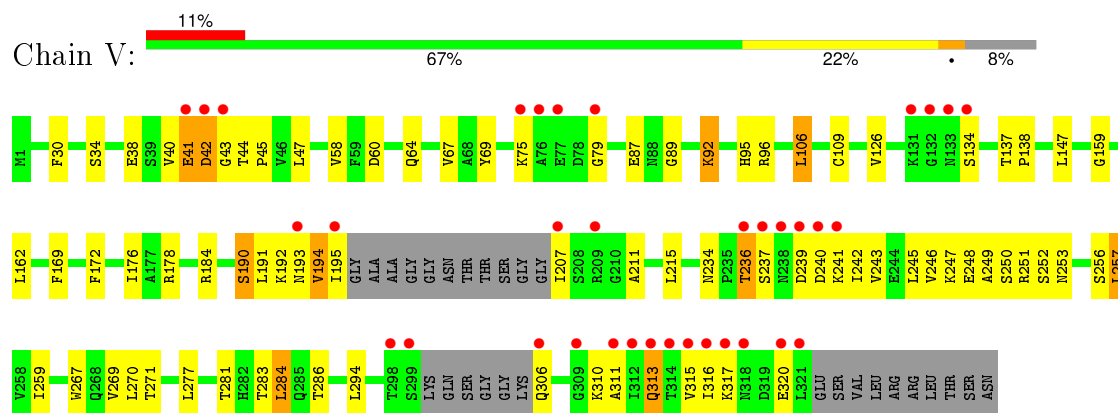
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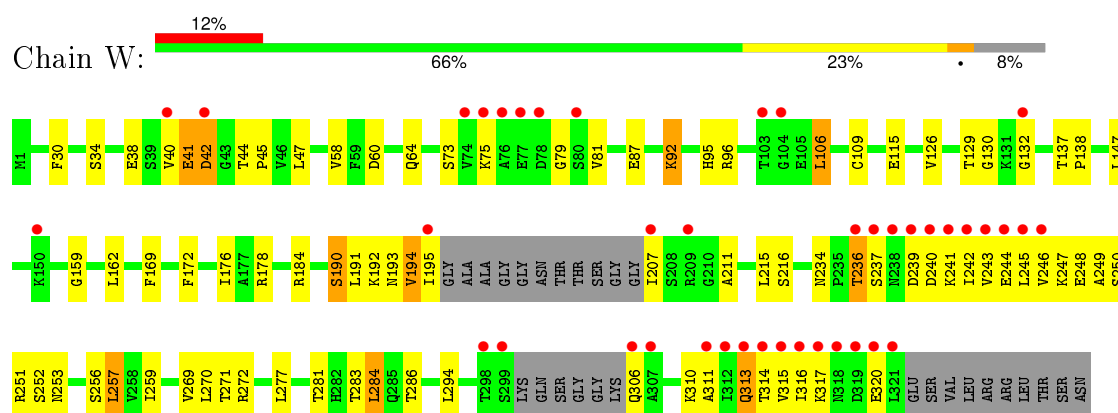
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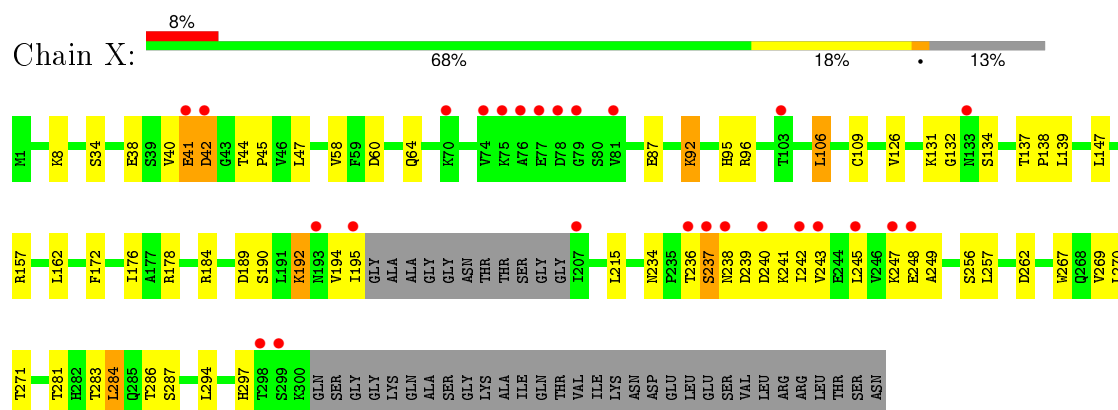
- Molecule 1: NTPASE P4



- Molecule 1: NTPASE P4



- Molecule 1: NTPASE P4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	115.40Å 126.30Å 155.60Å 90.00° 91.60° 90.50°	Depositor
Resolution (Å)	20.00 – 2.50 20.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.50) 95.9 (20.01-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.224 0.225 , 0.251	Depositor DCC
R_{free} test set	14482 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.2	EDS
Estimated twinning fraction	0.004 for h,-k,-l 0.006 for -h,k,-l 0.001 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 291711 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57270	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/2208	0.66	0/2991
1	B	0.34	0/2324	0.65	0/3145
1	C	0.35	0/2323	0.64	0/3142
1	D	0.37	0/2208	0.65	0/2991
1	E	0.36	0/2325	0.65	0/3146
1	F	0.36	0/2325	0.65	0/3146
1	G	0.36	0/2325	0.64	0/3146
1	H	0.39	0/2208	0.66	0/2991
1	I	0.40	0/2208	0.67	0/2991
1	J	0.37	0/2325	0.65	0/3146
1	K	0.35	0/2325	0.65	0/3146
1	L	0.36	0/2208	0.66	0/2991
1	M	0.37	0/2325	0.65	0/3146
1	N	0.36	0/2325	0.65	0/3146
1	O	0.36	0/2325	0.64	0/3146
1	P	0.34	0/2325	0.65	0/3146
1	Q	0.35	0/2325	0.64	0/3146
1	R	0.35	0/2325	0.64	0/3146
1	S	0.36	0/2325	0.64	0/3146
1	T	0.35	0/2325	0.64	0/3146
1	U	0.36	0/2208	0.65	0/2991
1	V	0.35	0/2325	0.64	0/3146
1	W	0.35	0/2325	0.65	0/3146
1	X	0.38	0/2208	0.66	0/2991
All	All	0.36	0/54978	0.65	0/74414

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	2171	0	2147	70	0
1	B	2288	0	2271	75	0
1	C	2288	0	2266	81	0
1	D	2171	0	2147	72	1
1	E	2289	0	2271	80	1
1	F	2289	0	2271	83	0
1	G	2289	0	2271	66	0
1	H	2171	0	2147	74	1
1	I	2171	0	2147	82	0
1	J	2289	0	2271	66	0
1	K	2289	0	2271	78	0
1	L	2171	0	2147	69	0
1	M	2289	0	2271	98	0
1	N	2289	0	2271	90	1
1	O	2289	0	2271	91	0
1	P	2289	0	2271	90	0
1	Q	2289	0	2271	88	0
1	R	2289	0	2271	86	0
1	S	2289	0	2271	78	0
1	T	2289	0	2271	82	0
1	U	2171	0	2147	80	0
1	V	2289	0	2271	76	0
1	W	2289	0	2271	89	1
1	X	2171	0	2147	76	1
2	A	110	0	0	6	0
2	B	119	0	0	5	0
2	C	129	0	0	3	0
2	D	145	0	0	4	0
2	E	143	0	0	11	0
2	F	151	0	0	9	0
2	G	101	0	0	1	0
2	H	178	0	0	9	0
2	I	193	0	0	11	0
2	J	159	0	0	2	0
2	K	122	0	0	2	0
2	L	93	0	0	4	0
2	M	169	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	202	0	0	5	0
2	O	144	0	0	6	0
2	P	103	0	0	8	0
2	Q	93	0	0	6	0
2	R	110	0	0	3	0
2	S	146	0	0	8	0
2	T	88	0	0	4	0
2	U	73	0	0	7	0
2	V	118	0	0	5	0
2	W	120	0	0	7	0
2	X	153	0	0	6	0
All	All	57270	0	53631	1731	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 16.

The worst 5 of 1731 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:I:39:SER:HA	1:M:115:GLU:OE2	1.15	1.28
1:I:39:SER:HA	1:M:115:GLU:CD	1.56	1.26
1:S:251:ARG:HD2	1:T:236:THR:HG23	1.27	1.15
1:T:251:ARG:HD2	1:U:236:THR:HG23	1.15	1.13
1:K:251:ARG:HD2	1:L:236:THR:HG23	1.14	1.13

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:H:115:GLU:OE2	1:N:39:SER:OG[1_655]	1.92	0.28
1:E:39:SER:CB	1:W:115:GLU:OE1[1_645]	2.04	0.16
1:D:115:GLU:OE2	1:X:38:GLU:O[1_545]	2.17	0.03

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	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	14	24
1	B	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	11	19
1	C	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	11	19
1	D	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	14	24
1	E	298/331 (90%)	288 (97%)	5 (2%)	5 (2%)	11	19
1	F	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	11	19
1	G	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	11	19
1	H	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	14	24
1	I	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	14	24
1	J	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	11	19
1	K	298/331 (90%)	284 (95%)	9 (3%)	5 (2%)	11	19
1	L	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	14	24
1	M	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	11	19
1	N	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	11	19
1	O	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	11	19
1	P	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	11	19
1	Q	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	11	19
1	R	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	11	19
1	S	298/331 (90%)	288 (97%)	5 (2%)	5 (2%)	11	19
1	T	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	11	19
1	U	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	14	24
1	V	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	11	19
1	W	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	11	19
1	X	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	14	24
All	All	7061/7944 (89%)	6723 (95%)	225 (3%)	113 (2%)	12	21

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	THR
1	C	236	THR

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Mol	Chain	Res	Type
1	E	236	THR
1	F	236	THR
1	G	236	THR

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	234/265 (88%)	225 (96%)	9 (4%)	40	67
1	B	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	C	246/265 (93%)	237 (96%)	9 (4%)	41	68
1	D	234/265 (88%)	225 (96%)	9 (4%)	40	67
1	E	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	F	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	G	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	H	234/265 (88%)	225 (96%)	9 (4%)	40	67
1	I	234/265 (88%)	225 (96%)	9 (4%)	40	67
1	J	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	K	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	L	234/265 (88%)	225 (96%)	9 (4%)	40	67
1	M	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	N	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	O	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	P	247/265 (93%)	238 (96%)	9 (4%)	42	69
1	Q	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	R	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	S	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	T	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	U	234/265 (88%)	225 (96%)	9 (4%)	40	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	W	247/265 (93%)	237 (96%)	10 (4%)	38	64
1	X	234/265 (88%)	225 (96%)	9 (4%)	40	67
All	All	5836/6360 (92%)	5612 (96%)	224 (4%)	40	67

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	47	LEU
1	N	271	THR
1	W	106	LEU
1	L	162	LEU
1	M	162	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 265 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	313	GLN
1	N	297	HIS
1	W	62	ASN
1	L	193	ASN
1	M	268	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 carbohydrates 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, 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(Å ²)	Q<0.9
1	A	289/331 (87%)	0.28	25 (8%) 13 13	25, 38, 90, 114	0
1	B	304/331 (91%)	0.51	44 (14%) 3 3	26, 39, 89, 118	0
1	C	304/331 (91%)	0.26	26 (8%) 13 14	24, 37, 89, 119	0
1	D	289/331 (87%)	0.18	20 (6%) 20 22	22, 36, 90, 113	0
1	E	304/331 (91%)	0.39	36 (11%) 6 6	23, 37, 90, 119	0
1	F	304/331 (91%)	0.21	24 (7%) 15 17	23, 37, 89, 118	0
1	G	304/331 (91%)	0.36	25 (8%) 14 15	25, 38, 88, 119	0
1	H	289/331 (87%)	0.24	22 (7%) 17 18	20, 34, 90, 113	0
1	I	289/331 (87%)	0.46	32 (11%) 7 7	19, 33, 90, 113	0
1	J	304/331 (91%)	0.28	27 (8%) 12 13	20, 34, 88, 118	0
1	K	304/331 (91%)	0.36	32 (10%) 8 8	24, 38, 89, 119	0
1	L	289/331 (87%)	0.46	34 (11%) 6 6	25, 39, 91, 114	0
1	M	304/331 (91%)	0.49	35 (11%) 6 6	18, 34, 89, 119	0
1	N	304/331 (91%)	0.51	36 (11%) 6 6	19, 34, 90, 119	0
1	O	304/331 (91%)	0.26	25 (8%) 14 15	23, 36, 89, 119	0
1	P	304/331 (91%)	0.44	40 (13%) 4 4	26, 39, 90, 119	0
1	Q	304/331 (91%)	0.61	42 (13%) 4 4	27, 40, 90, 119	0
1	R	304/331 (91%)	0.42	31 (10%) 9 9	23, 37, 89, 119	0
1	S	304/331 (91%)	0.26	24 (7%) 15 17	22, 37, 89, 118	0
1	T	304/331 (91%)	0.39	32 (10%) 8 8	24, 40, 89, 118	0
1	U	289/331 (87%)	0.49	37 (12%) 5 5	27, 40, 91, 114	0
1	V	304/331 (91%)	0.37	35 (11%) 6 6	26, 39, 89, 119	0
1	W	304/331 (91%)	0.33	41 (13%) 4 4	25, 38, 90, 118	0
1	X	289/331 (87%)	0.30	26 (8%) 12 12	21, 36, 91, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(\AA^2)	Q<0.9
All	All	7191/7944 (90%)	0.37	751 (10%) 8 8	18, 37, 91, 119	0

The worst 5 of 751 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ASN	9.1
1	I	79	GLY	8.8
1	K	240	ASP	8.2
1	T	240	ASP	8.2
1	N	309	GLY	8.1

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 [i](#)

There are no carbohydrates 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.