



wwPDB X-ray Structure Validation Summary Report

Feb 12, 2024 – 03:17 AM EST

PDB ID : 3GLH
Title : Crystal Structure of the E. coli clamp loader bound to Psi Peptide
Authors : Kazmirski, S.L.; Simonetta, K.R.; Kuriyan, J.
Deposited on : 2009-03-12
Resolution : 3.89 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  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](#) ) 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

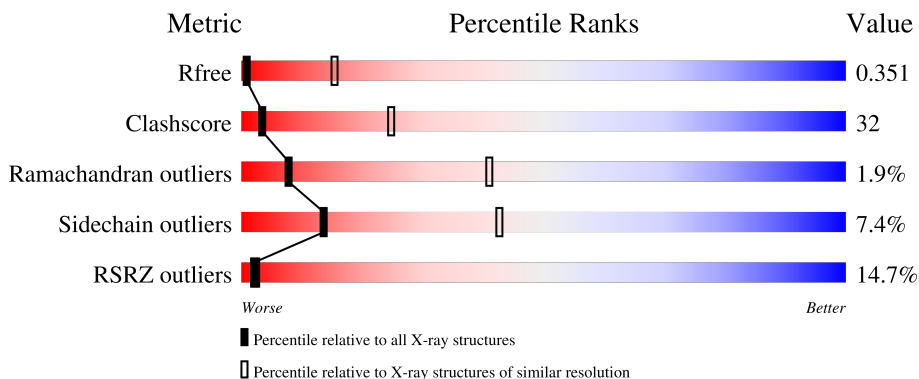
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.89 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 $\leq 5\%$. 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	343	
1	F	343	
1	K	343	
2	B	376	
2	C	376	

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Mol	Chain	Length	Quality of chain
2	D	376	
2	G	376	
2	H	376	
2	I	376	
2	L	376	
2	M	376	
2	N	376	
3	E	334	
3	J	334	
3	O	334	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41322 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 DNA polymerase III subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2670	1692	484	484	10	0	0	0
1	F	336	2670	1692	484	484	10	0	0	0
1	K	336	2670	1692	484	484	10	0	0	0

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	364	2841	1788	512	525	16	0	0	0
2	C	364	2841	1788	512	525	16	0	0	0
2	D	363	2829	1779	511	523	16	0	0	0
2	G	364	2841	1788	512	525	16	0	0	0
2	H	364	2841	1788	512	525	16	0	0	0
2	I	363	2829	1779	511	523	16	0	0	0
2	L	364	2841	1788	512	525	16	0	0	0
2	M	364	2841	1788	512	525	16	0	0	0
2	N	363	2829	1779	511	523	16	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	expression tag	UNP P06710
B	0	HIS	-	expression tag	UNP P06710
C	-2	GLY	-	expression tag	UNP P06710
C	-1	PRO	-	expression tag	UNP P06710
C	0	HIS	-	expression tag	UNP P06710
D	-2	GLY	-	expression tag	UNP P06710
D	-1	PRO	-	expression tag	UNP P06710
D	0	HIS	-	expression tag	UNP P06710
G	-2	GLY	-	expression tag	UNP P06710
G	-1	PRO	-	expression tag	UNP P06710
G	0	HIS	-	expression tag	UNP P06710
H	-2	GLY	-	expression tag	UNP P06710
H	-1	PRO	-	expression tag	UNP P06710
H	0	HIS	-	expression tag	UNP P06710
I	-2	GLY	-	expression tag	UNP P06710
I	-1	PRO	-	expression tag	UNP P06710
I	0	HIS	-	expression tag	UNP P06710
L	-2	GLY	-	expression tag	UNP P06710
L	-1	PRO	-	expression tag	UNP P06710
L	0	HIS	-	expression tag	UNP P06710
M	-2	GLY	-	expression tag	UNP P06710
M	-1	PRO	-	expression tag	UNP P06710
M	0	HIS	-	expression tag	UNP P06710
N	-2	GLY	-	expression tag	UNP P06710
N	-1	PRO	-	expression tag	UNP P06710
N	0	HIS	-	expression tag	UNP P06710

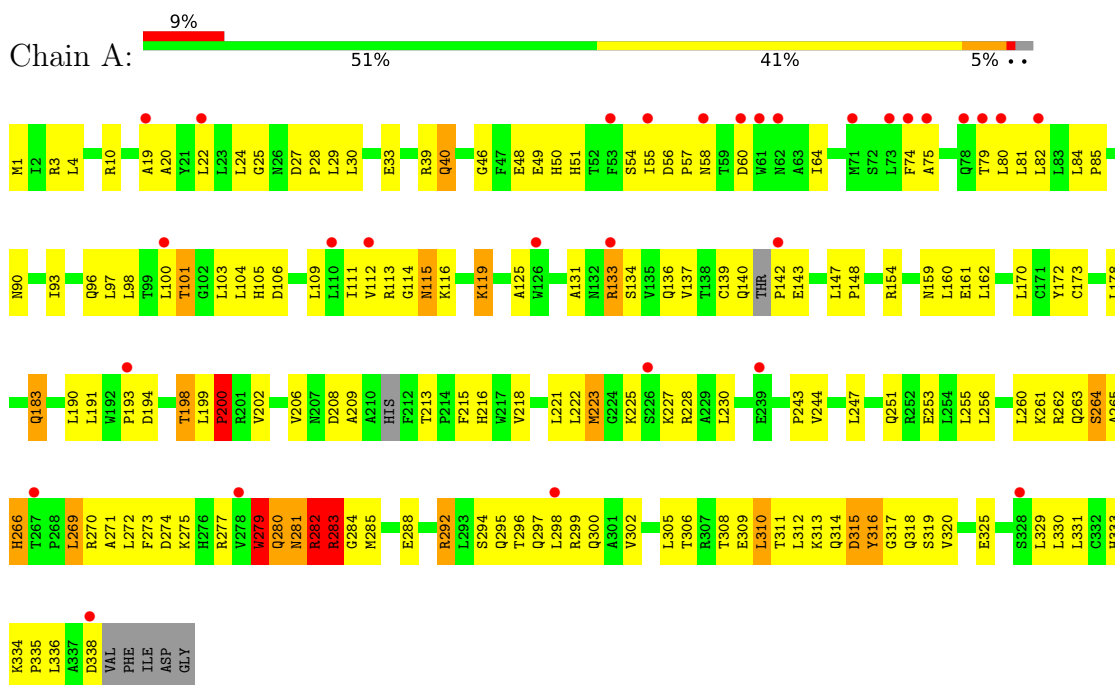
- Molecule 3 is a protein called DNA polymerase III subunit delta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	332	Total	C	N	O	S	0	0	0
			2593	1650	466	464	13			
3	J	332	Total	C	N	O	S	0	0	0
			2593	1650	466	464	13			
3	O	332	Total	C	N	O	S	0	0	0
			2593	1650	466	464	13			

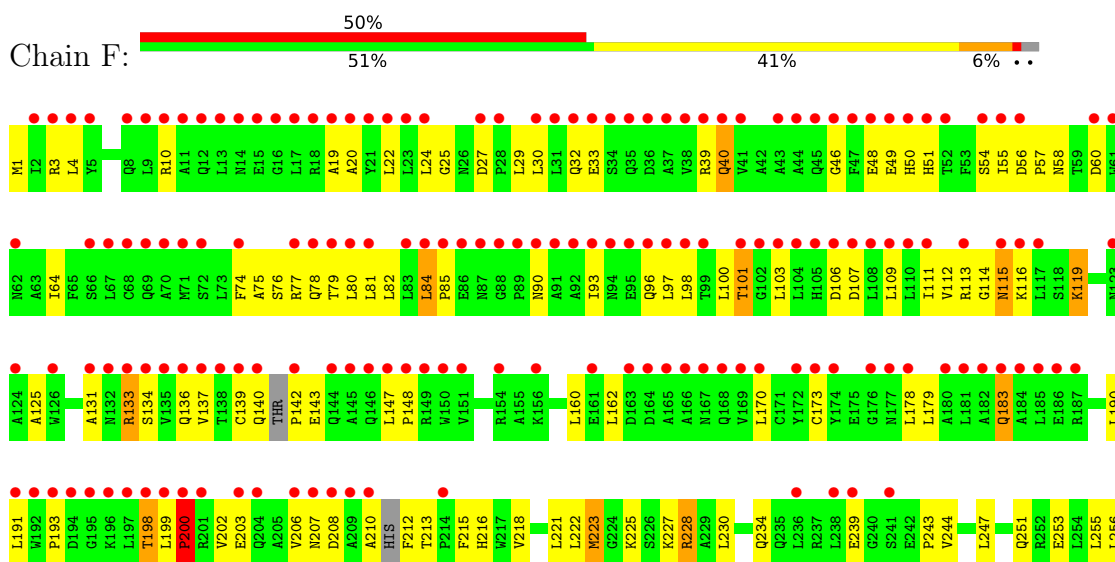
3 Residue-property plots [i](#)

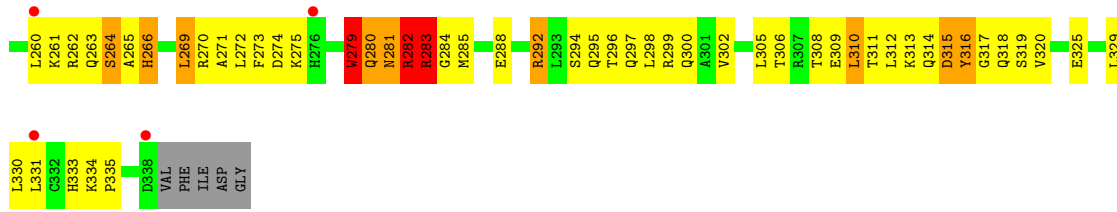
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase III subunit delta

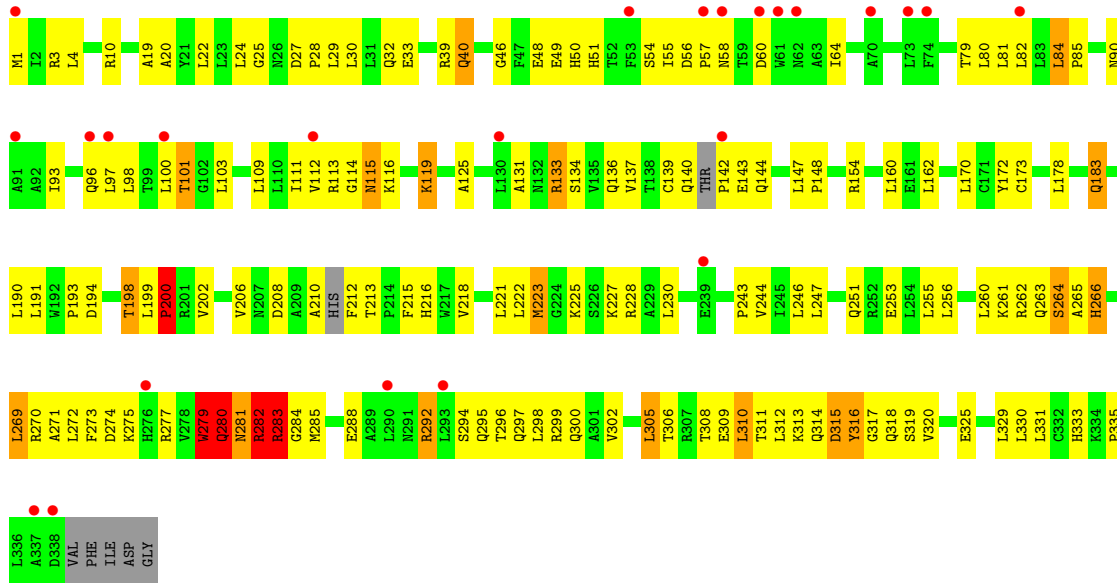


- Molecule 1: DNA polymerase III subunit delta

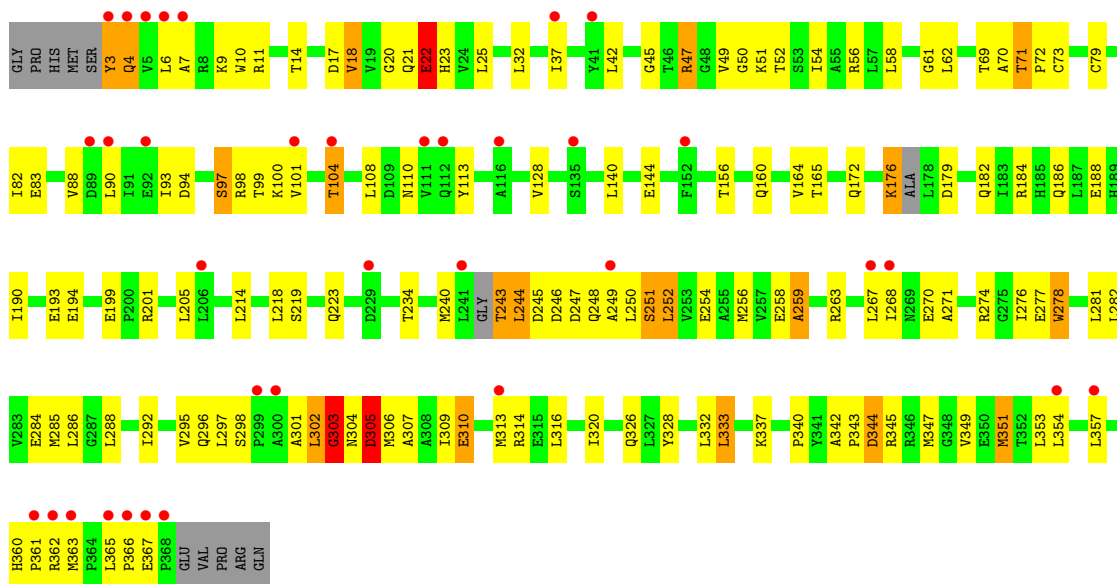




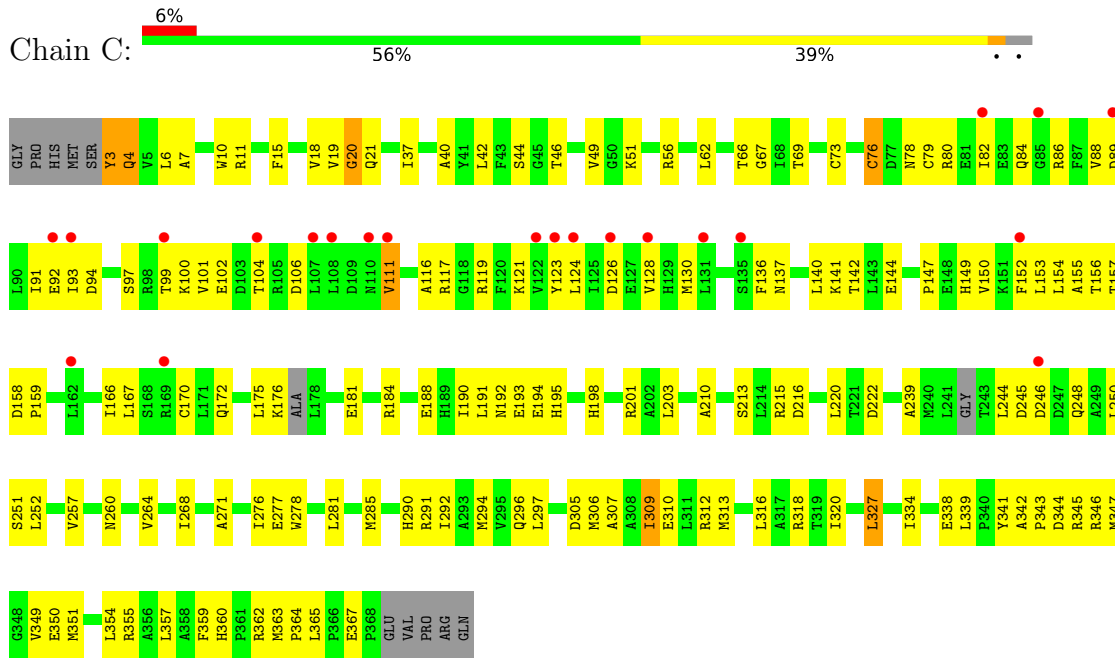
● Molecule 1: DNA polymerase III subunit delta



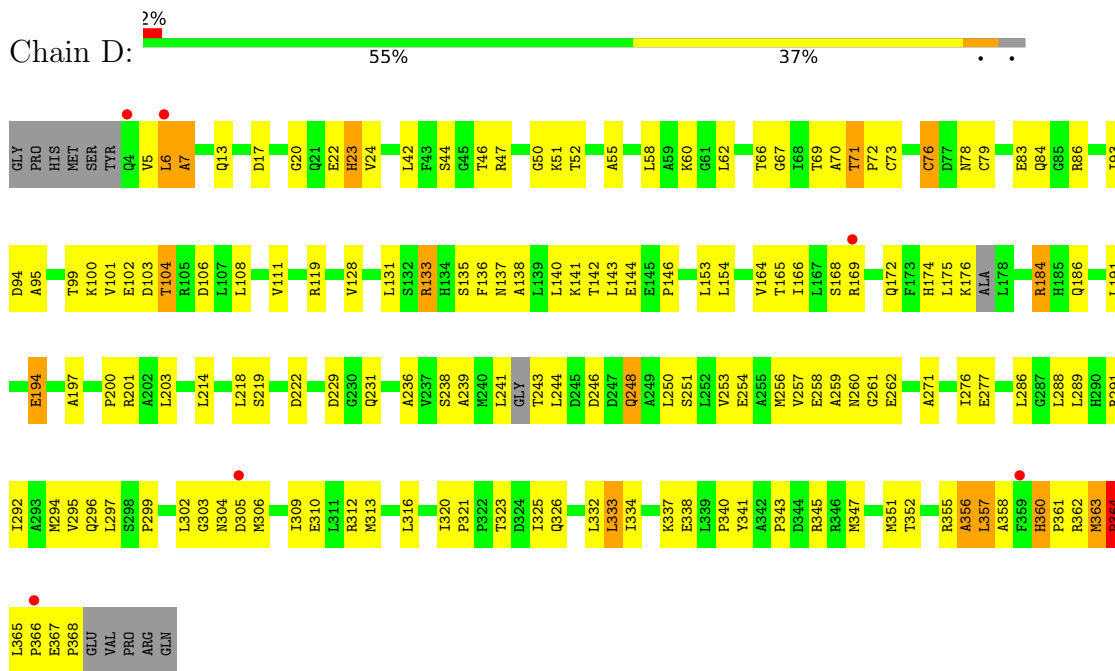
● Molecule 2: DNA polymerase III subunit tau



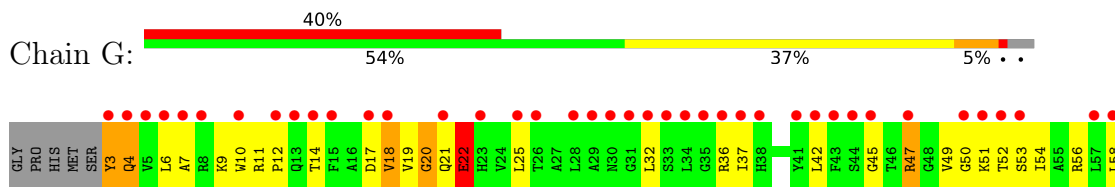
• Molecule 2: DNA polymerase III subunit tau

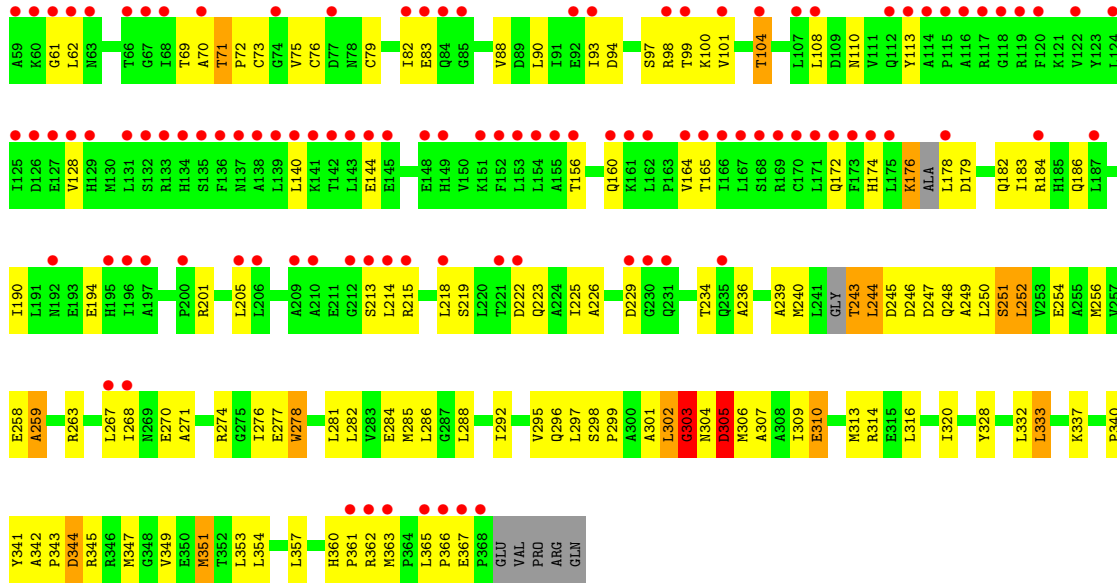


• Molecule 2: DNA polymerase III subunit tau

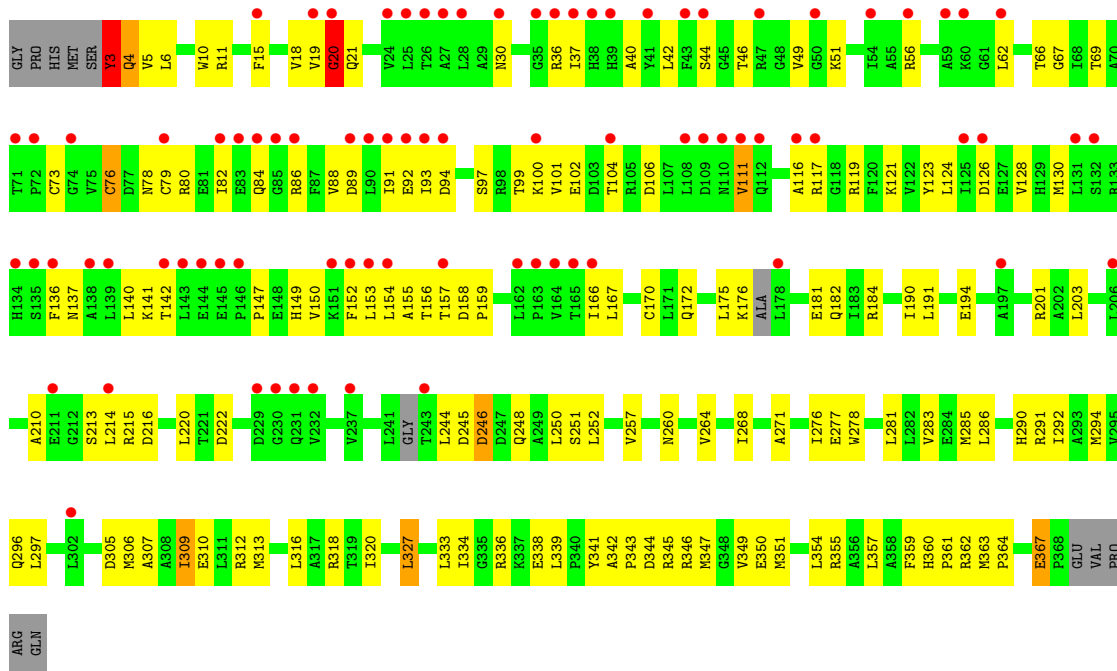


• Molecule 2: DNA polymerase III subunit tau

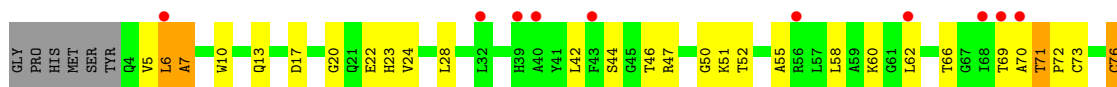


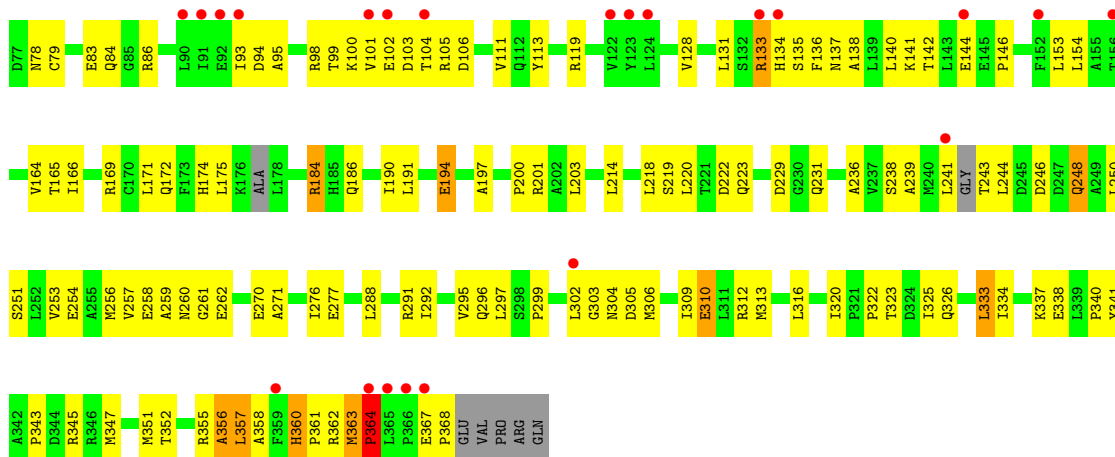


• Molecule 2: DNA polymerase III subunit tau

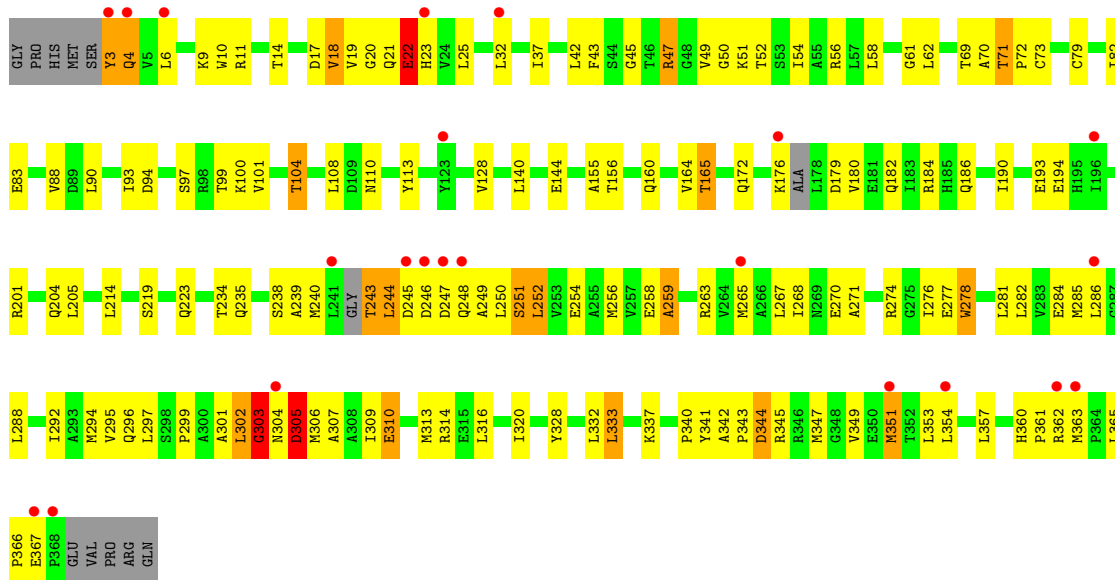


• Molecule 2: DNA polymerase III subunit tau

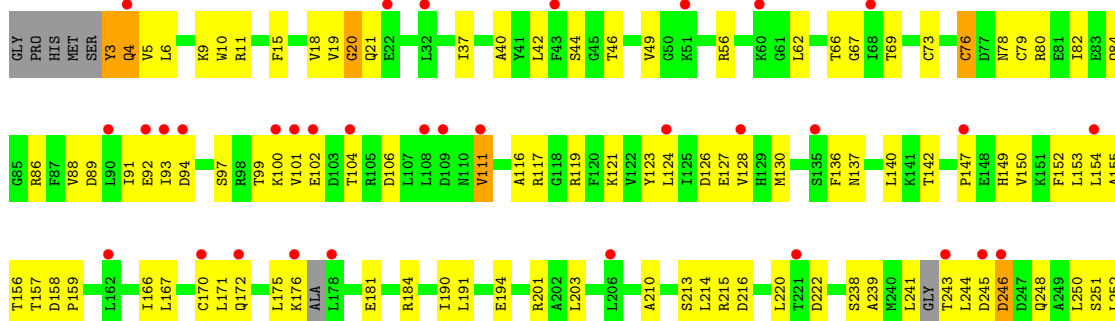


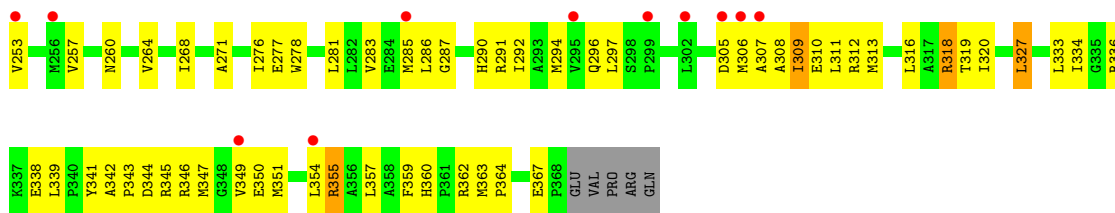


• Molecule 2: DNA polymerase III subunit tau

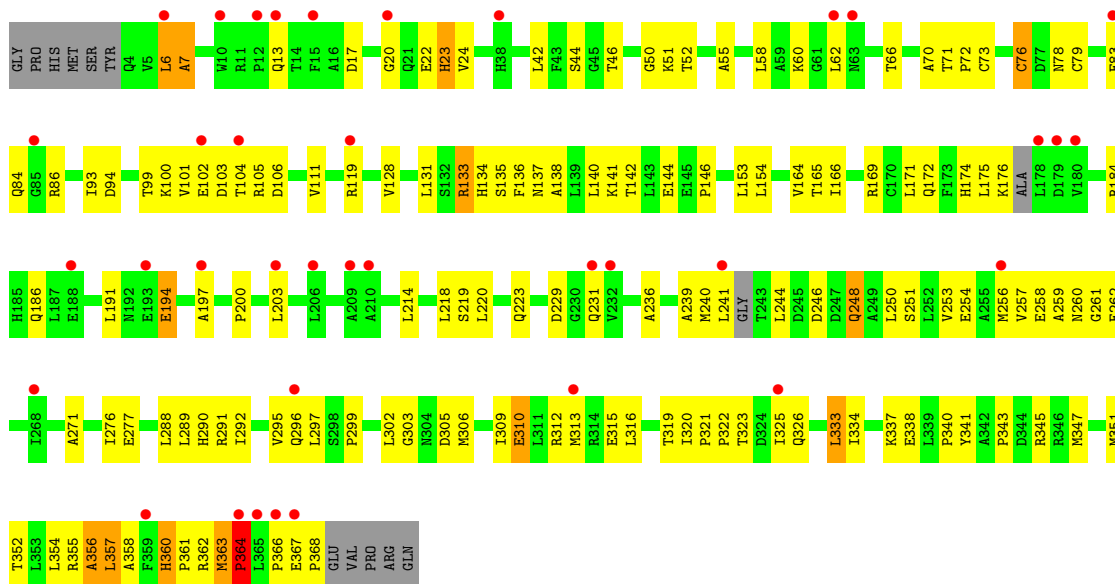


• Molecule 2: DNA polymerase III subunit tau

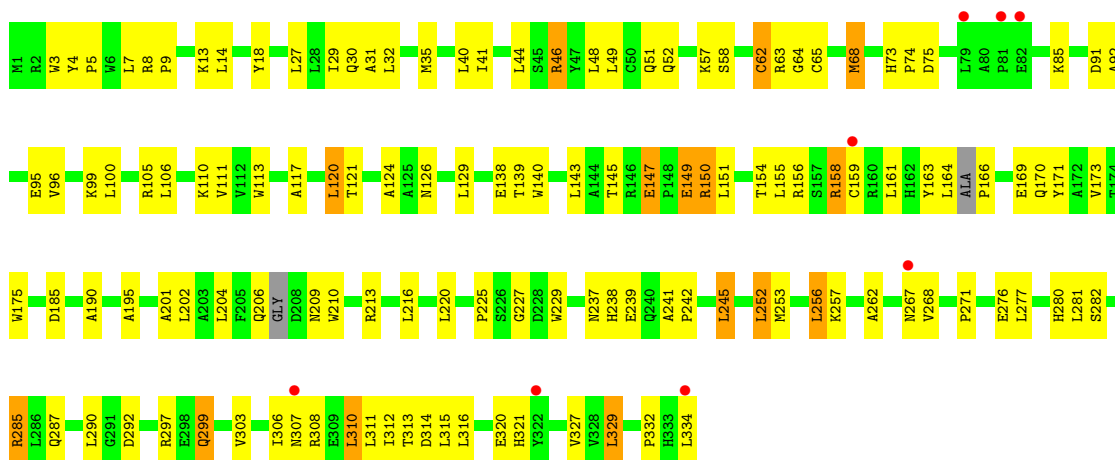




• Molecule 2: DNA polymerase III subunit tau

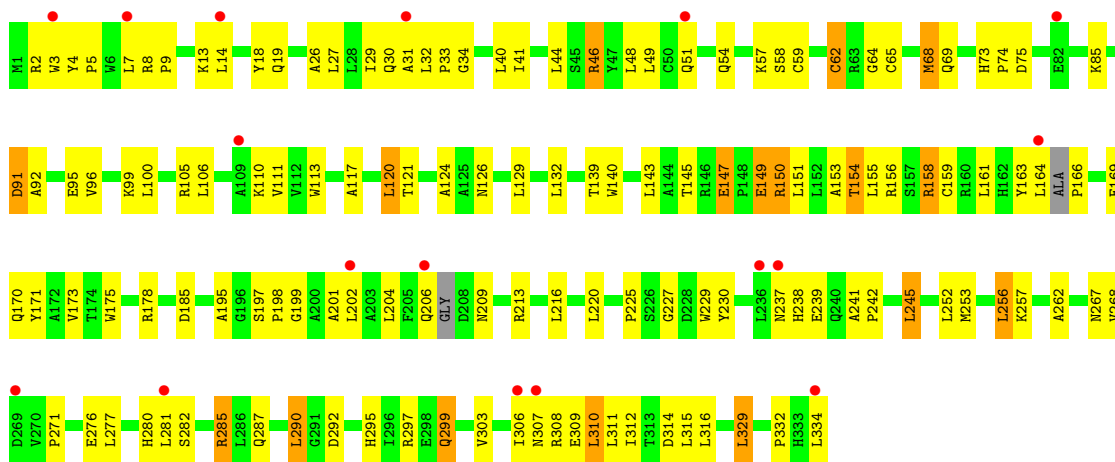


• Molecule 3: DNA polymerase III subunit delta'

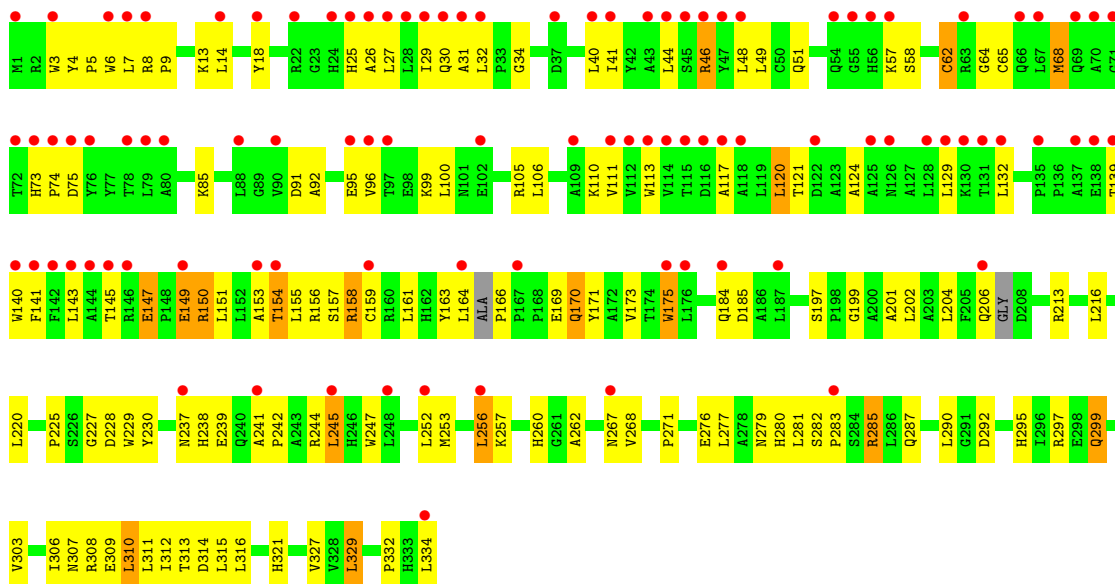


• Molecule 3: DNA polymerase III subunit delta'





• Molecule 3: DNA polymerase III subunit delta'



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.16Å 228.49Å 164.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 3.89 49.62 – 3.89	Depositor EDS
% Data completeness (in resolution range)	89.9 (49.62-3.89) 94.7 (49.62-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.88Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.359 , 0.361 0.347 , 0.351	Depositor DCC
R_{free} test set	6264 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	134.9	Xtrriage
Anisotropy	0.190	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	41322	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, 0.333 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	0.86	8/2715 (0.3%)	0.93	10/3684 (0.3%)
1	F	0.86	8/2715 (0.3%)	0.93	10/3684 (0.3%)
1	K	0.86	8/2715 (0.3%)	0.93	10/3684 (0.3%)
2	B	0.57	0/2887	0.88	11/3912 (0.3%)
2	C	0.47	0/2887	0.74	2/3912 (0.1%)
2	D	0.66	7/2874 (0.2%)	0.95	14/3894 (0.4%)
2	G	0.57	0/2887	0.88	11/3912 (0.3%)
2	H	0.50	1/2887 (0.0%)	0.75	2/3912 (0.1%)
2	I	0.66	7/2874 (0.2%)	0.95	14/3894 (0.4%)
2	L	0.57	0/2887	0.88	10/3912 (0.3%)
2	M	0.47	0/2887	0.75	2/3912 (0.1%)
2	N	0.66	7/2874 (0.2%)	0.95	14/3894 (0.4%)
3	E	0.49	0/2656	0.70	0/3620
3	J	0.49	0/2656	0.70	0/3620
3	O	0.49	0/2656	0.70	0/3620
All	All	0.63	46/42057 (0.1%)	0.85	110/57066 (0.2%)

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	4
1	F	0	4
1	K	0	4
2	D	0	1
2	H	0	1
2	I	0	1
2	N	0	1
All	All	0	16

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	315	ASP	CB-CG	29.17	2.13	1.51
1	K	315	ASP	CB-CG	29.14	2.12	1.51
1	A	315	ASP	CB-CG	29.08	2.12	1.51
2	D	133	ARG	CZ-NH2	-11.05	1.18	1.33
2	N	133	ARG	CZ-NH2	-10.98	1.18	1.33

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	363	MET	CG-SD-CE	17.07	127.52	100.20
2	I	363	MET	CG-SD-CE	17.07	127.52	100.20
2	N	363	MET	CG-SD-CE	17.05	127.48	100.20
1	F	283	ARG	C-N-CA	12.41	148.35	122.30
1	A	283	ARG	C-N-CA	12.38	148.29	122.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	GLN	Peptide
1	A	281	ASN	Mainchain
1	A	282	ARG	Mainchain
1	A	319	SER	Mainchain
2	D	23	HIS	Sidechain

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	2670	0	2724	226	5
1	F	2670	0	2719	258	36
1	K	2670	0	2726	183	5
2	B	2841	0	2890	185	15
2	C	2841	0	2888	187	36
2	D	2829	0	2878	250	5
2	G	2841	0	2887	240	5
2	H	2841	0	2889	220	13
2	I	2829	0	2880	272	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2841	0	2888	245	7
2	M	2841	0	2886	270	1
2	N	2829	0	2876	312	3
3	E	2593	0	2598	127	14
3	J	2593	0	2598	139	21
3	O	2593	0	2598	178	1
All	All	41322	0	41925	2686	87

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 32.

The worst 5 of 2686 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)
2:I:277:GLU:HB3	3:J:149:GLU:CG	1.24	1.60
2:G:10:TRP:CH2	2:G:190:ILE:HG23	1.37	1.57
2:D:277:GLU:HB3	3:E:149:GLU:CG	1.33	1.57
2:B:6:LEU:HD13	2:B:190:ILE:CG2	1.08	1.51
2:B:6:LEU:HD21	2:B:194:GLU:CG	1.37	1.50

The worst 5 of 87 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)
3:E:63:ARG:NH1	2:H:361:PRO:CA[1_455]	0.61	1.59
2:C:193:GLU:O	1:F:75:ALA:CA[2_546]	0.77	1.43
3:J:19:GLN:OE1	2:L:299:PRO:CB[2_756]	0.81	1.39
2:C:195:HIS:CD2	1:F:74:PHE:O[2_546]	0.91	1.29
2:C:193:GLU:O	1:F:75:ALA:CB[2_546]	0.94	1.26

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	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	7	39
1	F	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	7	39
1	K	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	7	39
2	B	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	6	38
2	C	358/376 (95%)	329 (92%)	23 (6%)	6 (2%)	9	43
2	D	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	5	34
2	G	358/376 (95%)	328 (92%)	22 (6%)	8 (2%)	6	38
2	H	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	7	40
2	I	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	5	34
2	L	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	6	38
2	M	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	7	40
2	N	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	5	34
3	E	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	25	63
3	J	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	25	63
3	O	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	25	63
All	All	5187/5415 (96%)	4720 (91%)	366 (7%)	101 (2%)	8	41

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	TRP
2	B	104	THR
2	B	310	GLU
2	C	20	GLY
2	C	104	THR

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	285/291 (98%)	259 (91%)	26 (9%)	9	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	285/291 (98%)	259 (91%)	26 (9%)	9	35
1	K	285/291 (98%)	259 (91%)	26 (9%)	9	35
2	B	303/312 (97%)	280 (92%)	23 (8%)	13	42
2	C	303/312 (97%)	288 (95%)	15 (5%)	24	53
2	D	302/312 (97%)	289 (96%)	13 (4%)	29	57
2	G	303/312 (97%)	280 (92%)	23 (8%)	13	42
2	H	303/312 (97%)	288 (95%)	15 (5%)	24	53
2	I	302/312 (97%)	289 (96%)	13 (4%)	29	57
2	L	303/312 (97%)	280 (92%)	23 (8%)	13	42
2	M	303/312 (97%)	288 (95%)	15 (5%)	24	53
2	N	302/312 (97%)	289 (96%)	13 (4%)	29	57
3	E	270/270 (100%)	239 (88%)	31 (12%)	5	26
3	J	270/270 (100%)	239 (88%)	31 (12%)	5	26
3	O	270/270 (100%)	239 (88%)	31 (12%)	5	26
All	All	4389/4491 (98%)	4065 (93%)	324 (7%)	13	43

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	208	ASP
2	N	184	ARG
1	K	283	ARG
2	L	305	ASP
3	O	147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	240	GLN
1	K	276	HIS
3	J	280	HIS
1	K	94	ASN
1	K	314	GLN

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 monosaccharides 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	336/343 (97%)	0.52	30 (8%) 9 7	69, 78, 90, 90	0
1	F	336/343 (97%)	2.75	170 (50%) 0 0	127, 241, 267, 267	0
1	K	336/343 (97%)	0.46	24 (7%) 16 11	56, 67, 79, 79	0
2	B	364/376 (96%)	0.66	35 (9%) 8 6	85, 90, 111, 111	0
2	C	364/376 (96%)	0.39	22 (6%) 21 16	61, 66, 76, 85	0
2	D	363/376 (96%)	0.33	6 (1%) 70 60	57, 67, 70, 70	0
2	G	364/376 (96%)	2.37	149 (40%) 0 0	84, 208, 291, 291	0
2	H	364/376 (96%)	1.18	84 (23%) 0 0	59, 171, 228, 228	0
2	I	363/376 (96%)	0.50	32 (8%) 10 7	66, 67, 151, 151	0
2	L	364/376 (96%)	0.49	22 (6%) 21 16	66, 94, 101, 101	0
2	M	364/376 (96%)	0.72	44 (12%) 4 4	79, 127, 140, 140	0
2	N	363/376 (96%)	0.60	37 (10%) 6 6	102, 107, 133, 133	0
3	E	332/334 (99%)	0.21	8 (2%) 59 48	30, 46, 62, 62	0
3	J	332/334 (99%)	0.39	17 (5%) 28 23	52, 66, 71, 71	0
3	O	332/334 (99%)	1.44	98 (29%) 0 0	75, 182, 266, 266	0
All	All	5277/5415 (97%)	0.87	778 (14%) 2 2	30, 79, 267, 291	0

The worst 5 of 778 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	181	LEU	20.0
3	O	55	GLY	18.9
2	G	104	THR	17.5
1	F	55	ILE	14.6
3	O	56	HIS	14.0

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 [i](#)

There are no monosaccharides 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.