wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:58 AM GMT

PDB ID	:	3GLF
Title	:	Crystal Structure of the Ecoli Clamp Loader Bound to Primer-Template DNA
Authors	:	Simonetta, K.R.; Kuriyan, J.
Deposited on	:	2009-03-12
Resolution	:	3.39 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 (i) symbol.

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

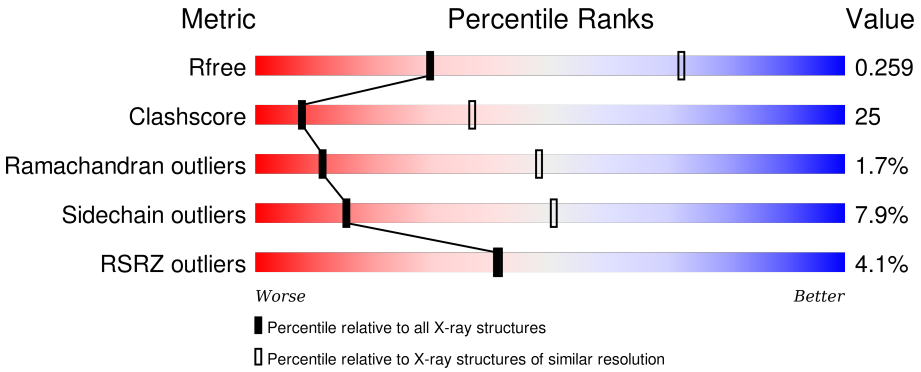
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 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	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

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 <=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	16% 48% 44% 5% •
1	F	343	8% 50% 42% 5% •
2	B	395	4% 54% 35% • 8%
2	C	395	4% 52% 33% 7% • 8%
2	D	395	3% 50% 37% • 8%

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Mol	Chain	Length	Quality of chain
2	G	395	2% 59% 34%
2	H	395	% 50% 36% 6% 8%
2	I	395	% 49% 38% 8%
3	E	334	2% 63% 34%
3	J	334	% 66% 30%
4	K	15	13% 80% 7%
4	M	15	7% 13% 73% 7%
5	L	10	40% 60%
5	N	10	60% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BEF	B	401	-	-	-	X
7	BEF	I	411	-	-	-	X
8	MG	D	414	-	-	-	X
8	MG	I	417	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28758 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
1	A	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			
1	F	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	C	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	D	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			
2	G	378	Total	C	N	O	S	0	0	0
			2941	1852	529	543	17			
2	H	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	I	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	EXPRESSION TAG	UNP P06710
B	-20	GLY	-	EXPRESSION TAG	UNP P06710
B	-19	SER	-	EXPRESSION TAG	UNP P06710
B	-18	SER	-	EXPRESSION TAG	UNP P06710
B	-17	HIS	-	EXPRESSION TAG	UNP P06710
B	-16	HIS	-	EXPRESSION TAG	UNP P06710
B	-15	HIS	-	EXPRESSION TAG	UNP P06710
B	-14	HIS	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	EXPRESSION TAG	UNP P06710
B	-12	HIS	-	EXPRESSION TAG	UNP P06710
B	-11	SER	-	EXPRESSION TAG	UNP P06710
B	-10	SER	-	EXPRESSION TAG	UNP P06710
B	-9	GLY	-	EXPRESSION TAG	UNP P06710
B	-8	LEU	-	EXPRESSION TAG	UNP P06710
B	-7	GLU	-	EXPRESSION TAG	UNP P06710
B	-6	VAL	-	EXPRESSION TAG	UNP P06710
B	-5	LEU	-	EXPRESSION TAG	UNP P06710
B	-4	PHE	-	EXPRESSION TAG	UNP P06710
B	-3	GLN	-	EXPRESSION TAG	UNP P06710
B	-2	GLY	-	EXPRESSION TAG	UNP P06710
B	-1	PRO	-	EXPRESSION TAG	UNP P06710
B	0	HIS	-	EXPRESSION TAG	UNP P06710
C	-21	MET	-	EXPRESSION TAG	UNP P06710
C	-20	GLY	-	EXPRESSION TAG	UNP P06710
C	-19	SER	-	EXPRESSION TAG	UNP P06710
C	-18	SER	-	EXPRESSION TAG	UNP P06710
C	-17	HIS	-	EXPRESSION TAG	UNP P06710
C	-16	HIS	-	EXPRESSION TAG	UNP P06710
C	-15	HIS	-	EXPRESSION TAG	UNP P06710
C	-14	HIS	-	EXPRESSION TAG	UNP P06710
C	-13	HIS	-	EXPRESSION TAG	UNP P06710
C	-12	HIS	-	EXPRESSION TAG	UNP P06710
C	-11	SER	-	EXPRESSION TAG	UNP P06710
C	-10	SER	-	EXPRESSION TAG	UNP P06710
C	-9	GLY	-	EXPRESSION TAG	UNP P06710
C	-8	LEU	-	EXPRESSION TAG	UNP P06710
C	-7	GLU	-	EXPRESSION TAG	UNP P06710
C	-6	VAL	-	EXPRESSION TAG	UNP P06710
C	-5	LEU	-	EXPRESSION TAG	UNP P06710
C	-4	PHE	-	EXPRESSION TAG	UNP P06710
C	-3	GLN	-	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	-21	MET	-	EXPRESSION TAG	UNP P06710
D	-20	GLY	-	EXPRESSION TAG	UNP P06710
D	-19	SER	-	EXPRESSION TAG	UNP P06710
D	-18	SER	-	EXPRESSION TAG	UNP P06710
D	-17	HIS	-	EXPRESSION TAG	UNP P06710
D	-16	HIS	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	EXPRESSION TAG	UNP P06710
D	-14	HIS	-	EXPRESSION TAG	UNP P06710
D	-13	HIS	-	EXPRESSION TAG	UNP P06710
D	-12	HIS	-	EXPRESSION TAG	UNP P06710
D	-11	SER	-	EXPRESSION TAG	UNP P06710
D	-10	SER	-	EXPRESSION TAG	UNP P06710
D	-9	GLY	-	EXPRESSION TAG	UNP P06710
D	-8	LEU	-	EXPRESSION TAG	UNP P06710
D	-7	GLU	-	EXPRESSION TAG	UNP P06710
D	-6	VAL	-	EXPRESSION TAG	UNP P06710
D	-5	LEU	-	EXPRESSION TAG	UNP P06710
D	-4	PHE	-	EXPRESSION TAG	UNP P06710
D	-3	GLN	-	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	-21	MET	-	EXPRESSION TAG	UNP P06710
G	-20	GLY	-	EXPRESSION TAG	UNP P06710
G	-19	SER	-	EXPRESSION TAG	UNP P06710
G	-18	SER	-	EXPRESSION TAG	UNP P06710
G	-17	HIS	-	EXPRESSION TAG	UNP P06710
G	-16	HIS	-	EXPRESSION TAG	UNP P06710
G	-15	HIS	-	EXPRESSION TAG	UNP P06710
G	-14	HIS	-	EXPRESSION TAG	UNP P06710
G	-13	HIS	-	EXPRESSION TAG	UNP P06710
G	-12	HIS	-	EXPRESSION TAG	UNP P06710
G	-11	SER	-	EXPRESSION TAG	UNP P06710
G	-10	SER	-	EXPRESSION TAG	UNP P06710
G	-9	GLY	-	EXPRESSION TAG	UNP P06710
G	-8	LEU	-	EXPRESSION TAG	UNP P06710
G	-7	GLU	-	EXPRESSION TAG	UNP P06710
G	-6	VAL	-	EXPRESSION TAG	UNP P06710
G	-5	LEU	-	EXPRESSION TAG	UNP P06710
G	-4	PHE	-	EXPRESSION TAG	UNP P06710
G	-3	GLN	-	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	-21	MET	-	EXPRESSION TAG	UNP P06710
H	-20	GLY	-	EXPRESSION TAG	UNP P06710
H	-19	SER	-	EXPRESSION TAG	UNP P06710
H	-18	SER	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	EXPRESSION TAG	UNP P06710
H	-16	HIS	-	EXPRESSION TAG	UNP P06710
H	-15	HIS	-	EXPRESSION TAG	UNP P06710
H	-14	HIS	-	EXPRESSION TAG	UNP P06710
H	-13	HIS	-	EXPRESSION TAG	UNP P06710
H	-12	HIS	-	EXPRESSION TAG	UNP P06710
H	-11	SER	-	EXPRESSION TAG	UNP P06710
H	-10	SER	-	EXPRESSION TAG	UNP P06710
H	-9	GLY	-	EXPRESSION TAG	UNP P06710
H	-8	LEU	-	EXPRESSION TAG	UNP P06710
H	-7	GLU	-	EXPRESSION TAG	UNP P06710
H	-6	VAL	-	EXPRESSION TAG	UNP P06710
H	-5	LEU	-	EXPRESSION TAG	UNP P06710
H	-4	PHE	-	EXPRESSION TAG	UNP P06710
H	-3	GLN	-	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	-21	MET	-	EXPRESSION TAG	UNP P06710
I	-20	GLY	-	EXPRESSION TAG	UNP P06710
I	-19	SER	-	EXPRESSION TAG	UNP P06710
I	-18	SER	-	EXPRESSION TAG	UNP P06710
I	-17	HIS	-	EXPRESSION TAG	UNP P06710
I	-16	HIS	-	EXPRESSION TAG	UNP P06710
I	-15	HIS	-	EXPRESSION TAG	UNP P06710
I	-14	HIS	-	EXPRESSION TAG	UNP P06710
I	-13	HIS	-	EXPRESSION TAG	UNP P06710
I	-12	HIS	-	EXPRESSION TAG	UNP P06710
I	-11	SER	-	EXPRESSION TAG	UNP P06710
I	-10	SER	-	EXPRESSION TAG	UNP P06710
I	-9	GLY	-	EXPRESSION TAG	UNP P06710
I	-8	LEU	-	EXPRESSION TAG	UNP P06710
I	-7	GLU	-	EXPRESSION TAG	UNP P06710
I	-6	VAL	-	EXPRESSION TAG	UNP P06710
I	-5	LEU	-	EXPRESSION TAG	UNP P06710
I	-4	PHE	-	EXPRESSION TAG	UNP P06710
I	-3	GLN	-	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			
3	J	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

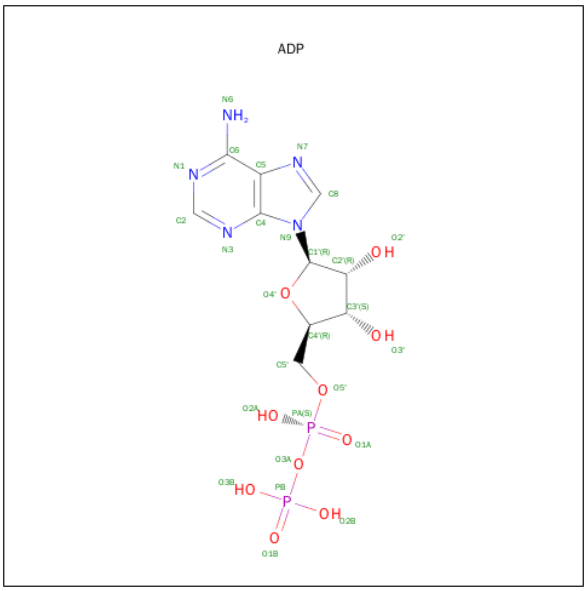
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			
4	M	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			

- Molecule 5 is a DNA chain called DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3').

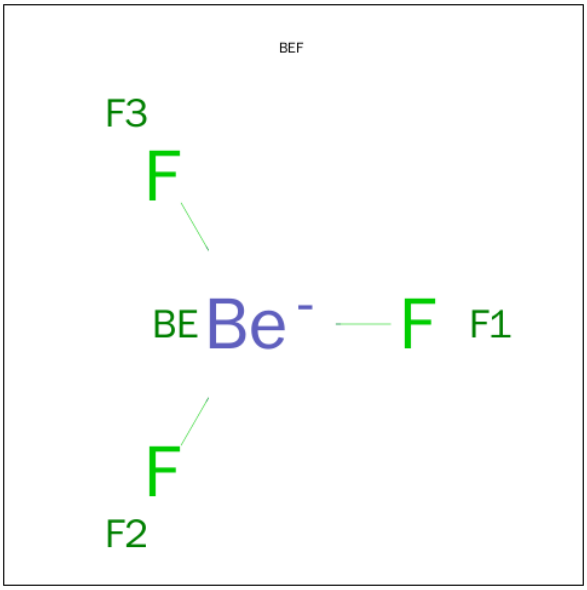
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Be	F		0	0
			4	1	3			
7	C	1	Total	Be	F		0	0
			4	1	3			
7	D	1	Total	Be	F		0	0
			4	1	3			
7	G	1	Total	Be	F		0	0
			4	1	3			
7	H	1	Total	Be	F		0	0
			4	1	3			
7	I	1	Total	Be	F		0	0
			4	1	3			

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0
8	B	1	Total Mg 1 1	0	0
8	I	1	Total Mg 1 1	0	0
8	C	1	Total Mg 1 1	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

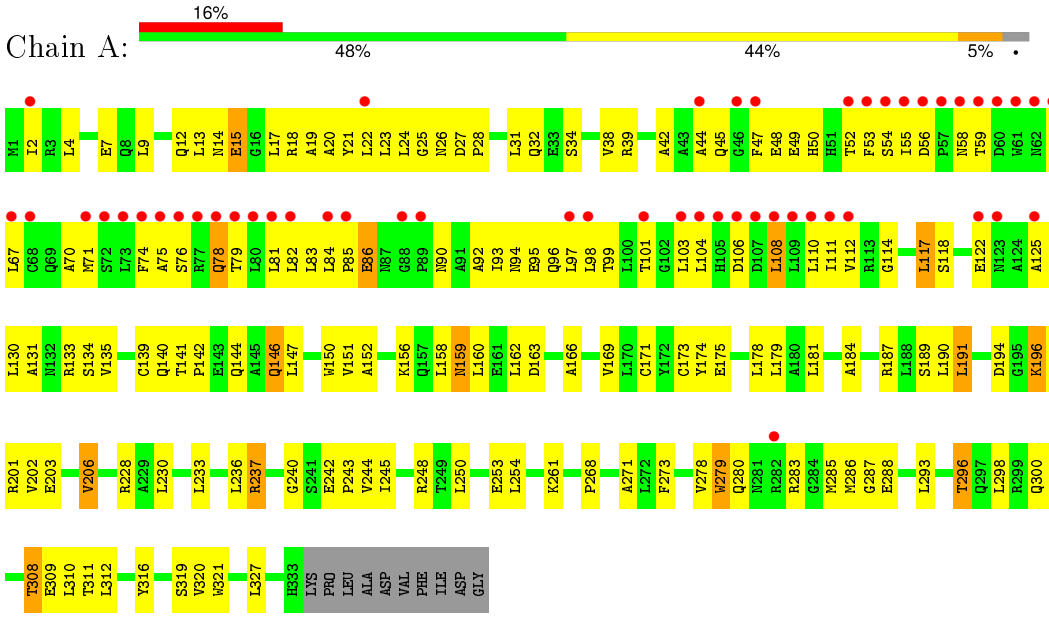
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total Zn 1 1	0	0
9	J	1	Total Zn 1 1	0	0
9	D	1	Total Zn 1 1	0	0
9	E	1	Total Zn 1 1	0	0
9	H	1	Total Zn 1 1	0	0
9	B	1	Total Zn 1 1	0	0
9	I	1	Total Zn 1 1	0	0
9	C	1	Total Zn 1 1	0	0

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 (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.

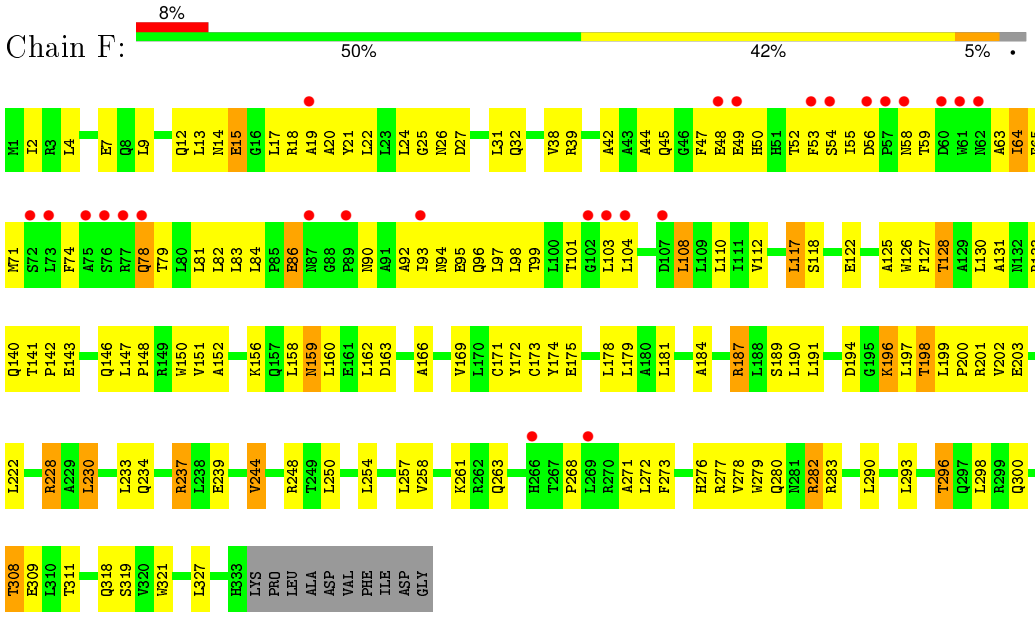
- Molecule 1: DNA polymerase III subunit delta

Chain A:



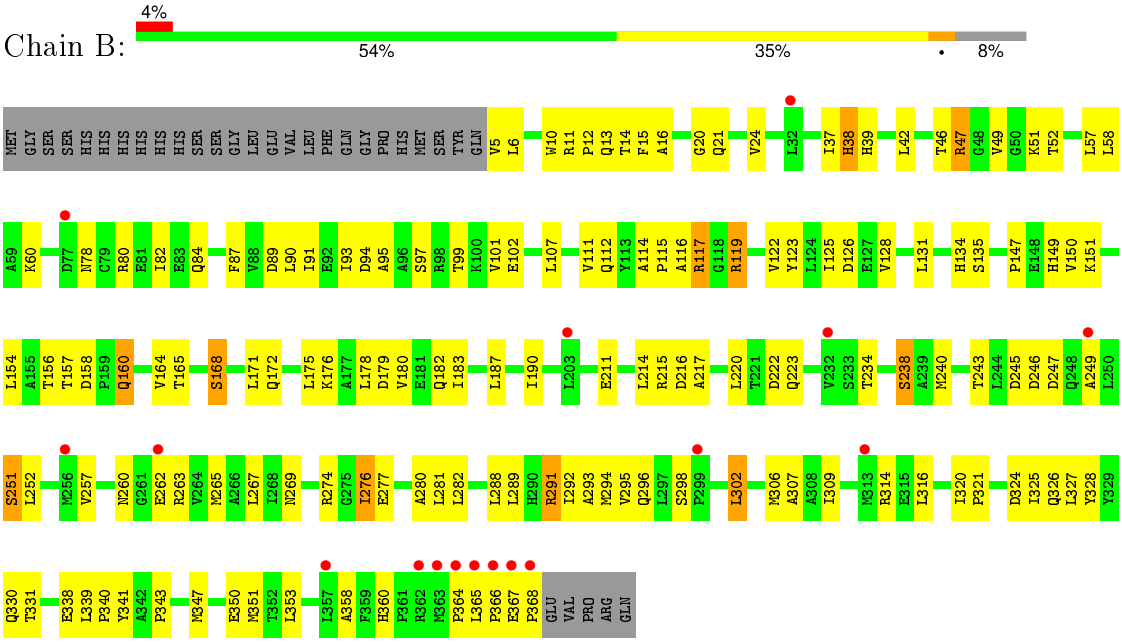
- Molecule 1: DNA polymerase III subunit delta

Chain F:



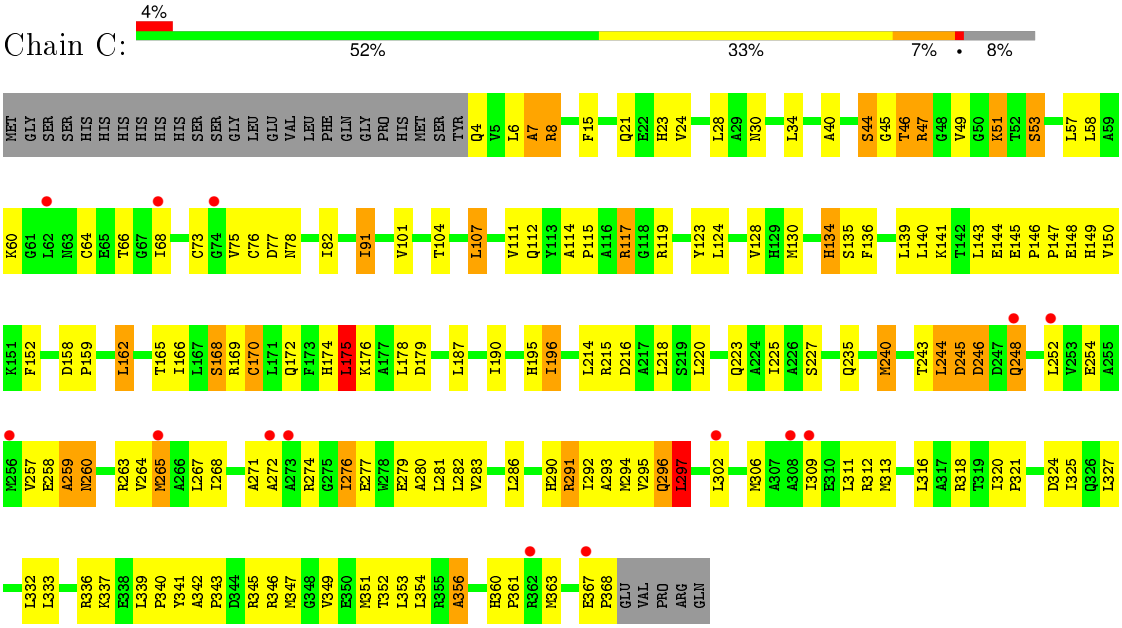
• Molecule 2: DNA polymerase III subunit tau

Chain B:



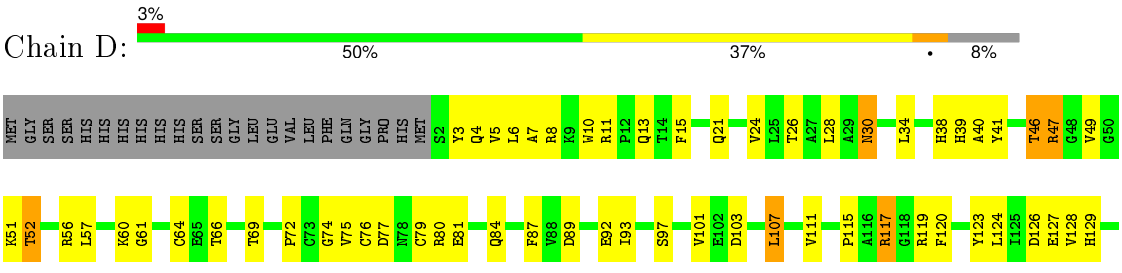
• Molecule 2: DNA polymerase III subunit tau

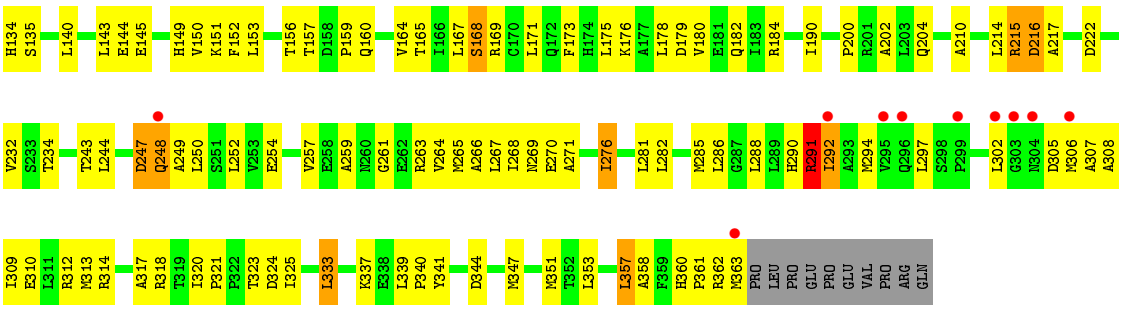
Chain C:



• Molecule 2: DNA polymerase III subunit tau

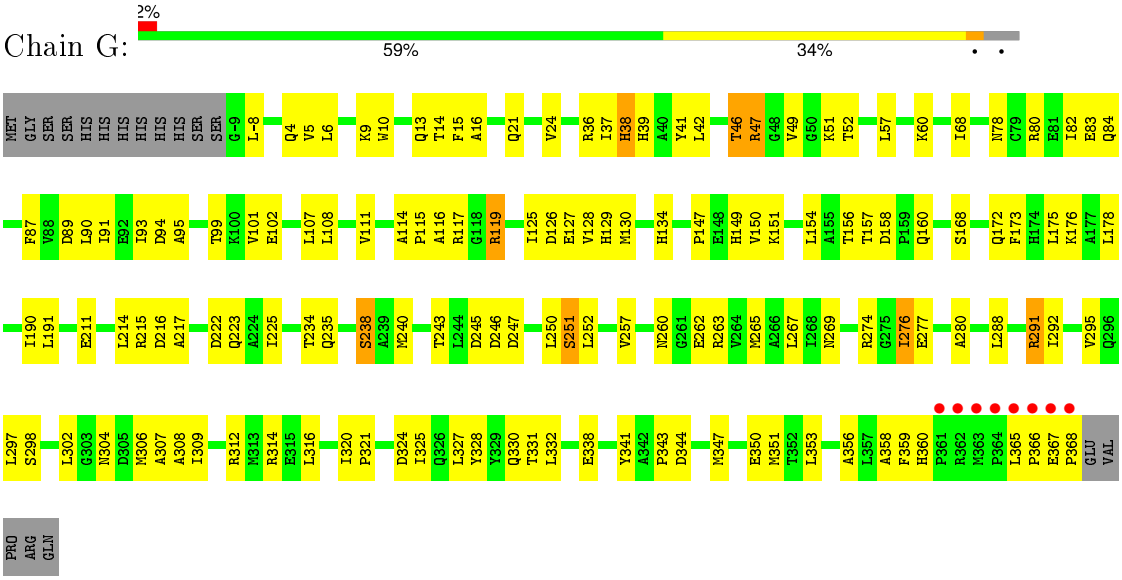
Chain D:





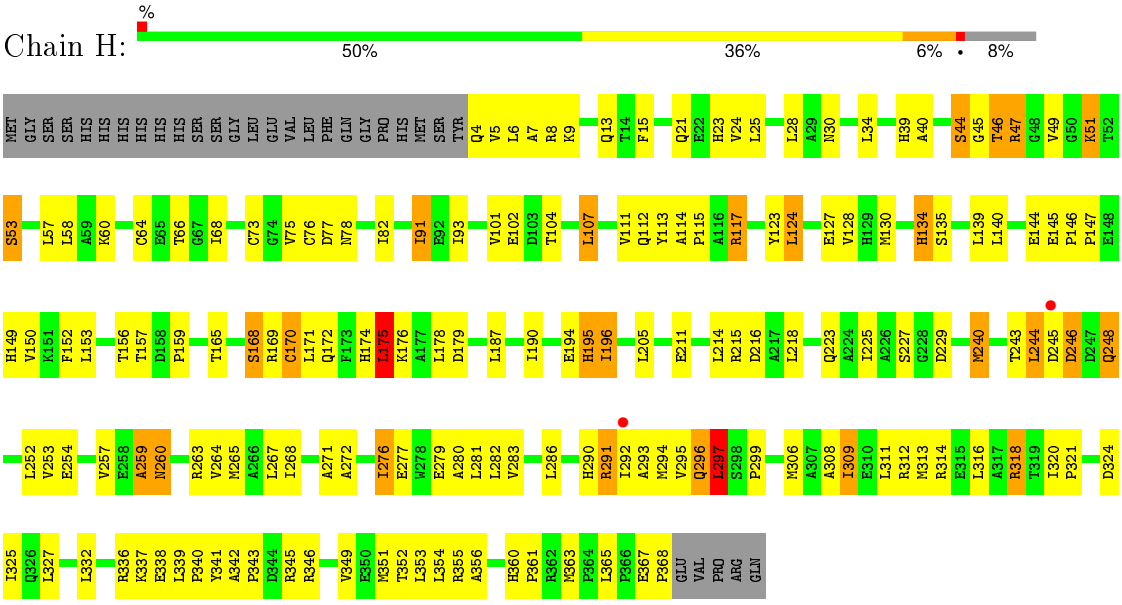
• Molecule 2: DNA polymerase III subunit tau

Chain G:



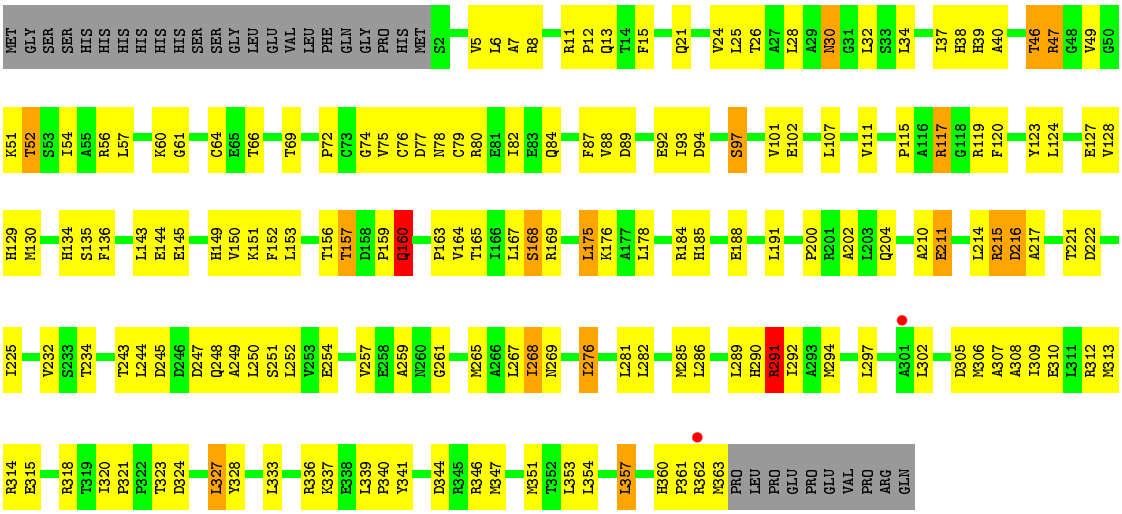
• Molecule 2: DNA polymerase III subunit tau

Chain H:



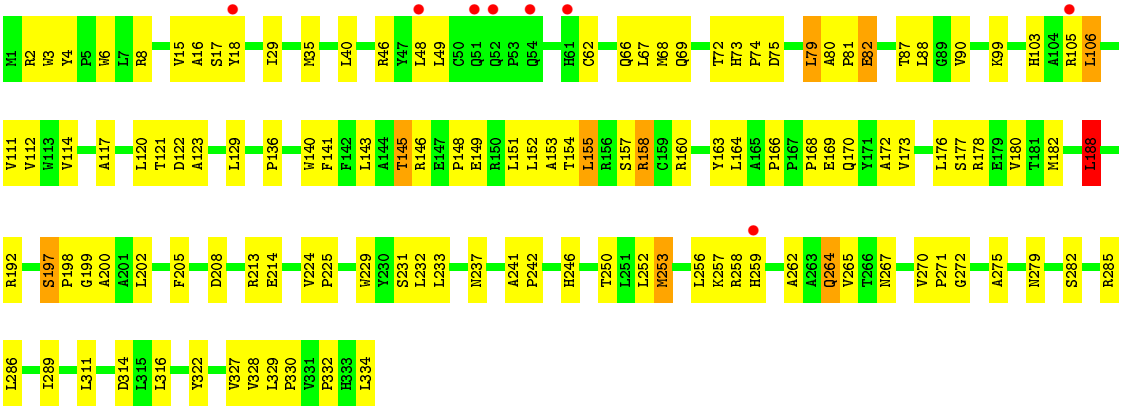
• Molecule 2: DNA polymerase III subunit tau

Chain I:



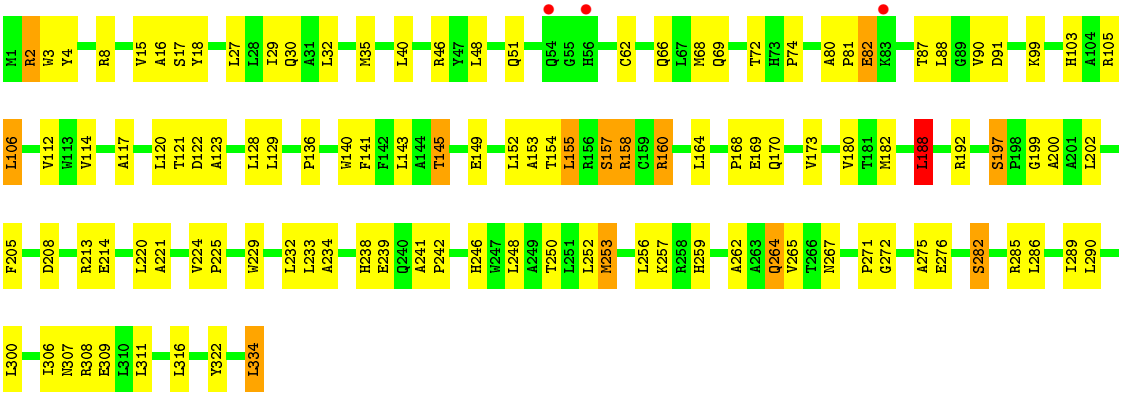
• Molecule 3: DNA polymerase III subunit delta'

Chain E:



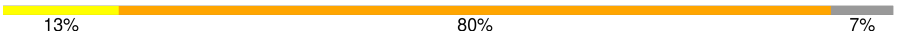
• Molecule 3: DNA polymerase III subunit delta'

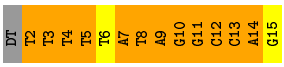
Chain J:



• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain K:





• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

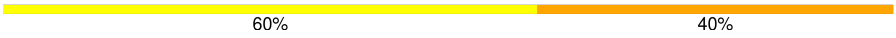
Chain M:

• Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

Chain L:

• Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.26Å 219.95Å 273.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.39 49.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.97-3.39) 97.5 (49.97-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.221 , 0.260 0.221 , 0.259	Depositor DCC
R_{free} test set	4166 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	92.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 82685 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28758	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BEF, MG, ADP

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	0.72	0/2697	0.78	3/3664 (0.1%)
1	F	0.73	0/2697	0.78	3/3664 (0.1%)
2	B	0.72	0/2876	0.81	0/3900
2	C	0.72	1/2885 (0.0%)	0.86	6/3912 (0.2%)
2	D	0.77	1/2863 (0.0%)	0.89	0/3879
2	G	0.75	2/2992 (0.1%)	0.83	1/4057 (0.0%)
2	H	0.86	4/2885 (0.1%)	0.92	4/3912 (0.1%)
2	I	0.92	4/2863 (0.1%)	0.96	2/3879 (0.1%)
3	E	0.89	2/2666 (0.1%)	0.91	5/3639 (0.1%)
3	J	0.89	1/2666 (0.0%)	0.91	2/3639 (0.1%)
4	K	1.97	6/320 (1.9%)	2.68	32/492 (6.5%)
4	M	1.96	5/320 (1.6%)	2.58	27/492 (5.5%)
5	L	1.76	3/223 (1.3%)	2.80	28/342 (8.2%)
5	N	1.76	2/223 (0.9%)	2.75	25/342 (7.3%)
All	All	0.87	31/29176 (0.1%)	1.01	138/39813 (0.3%)

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
2	B	0	1
2	C	0	1
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	11	DG	C3'-O3'	-8.40	1.33	1.44
2	H	127	GLU	CG-CD	8.31	1.64	1.51
4	M	9	DA	C3'-O3'	-8.17	1.33	1.44
5	N	6	DC	C3'-O3'	-7.52	1.34	1.44
2	G	127	GLU	CG-CD	7.35	1.62	1.51

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	5	DT	O4'-C1'-N1	-11.71	99.80	108.00
4	K	5	DT	O4'-C1'-N1	-11.64	99.85	108.00
5	L	5	DC	O4'-C4'-C3'	-11.36	99.19	106.00
5	N	2	DT	N3-C4-O4	10.52	126.21	119.90
5	N	5	DC	O4'-C4'-C3'	-10.37	99.78	106.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	246	ASP	Peptide
2	C	245	ASP	Peptide
2	G	246	ASP	Peptide
2	H	245	ASP	Peptide
2	I	157	THR	Peptide

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	2650	0	2703	168	0
1	F	2650	0	2703	158	0
2	B	2829	0	2879	153	1
2	C	2838	0	2886	165	1
2	D	2818	0	2863	173	0
2	G	2941	0	2987	139	0
2	H	2838	0	2886	160	2
2	I	2818	0	2863	165	1
3	E	2601	0	2603	108	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	2601	0	2603	119	0
4	K	287	0	161	17	0
4	M	287	0	161	14	0
5	L	200	0	115	5	0
5	N	200	0	115	4	0
6	B	27	0	12	3	0
6	C	27	0	12	3	0
6	D	27	0	12	3	0
6	G	27	0	12	2	0
6	H	27	0	12	4	0
6	I	27	0	12	2	0
7	B	4	0	0	1	0
7	C	4	0	0	0	0
7	D	4	0	0	0	0
7	G	4	0	0	1	0
7	H	4	0	0	0	0
7	I	4	0	0	1	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
All	All	28758	0	28600	1426	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 25.

The worst 5 of 1426 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:H:351:MET:CE	2:I:290:HIS:HA	1.75	1.15
1:F:95:GLU:HA	1:F:98:LEU:HD12	1.33	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HA	1:A:98:LEU:HD12	1.35	1.07
2:H:351:MET:HE1	2:I:290:HIS:HA	1.13	1.06
2:I:216:ASP:OD1	3:J:157:SER:HB2	1.57	1.03

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)
2:B:117:ARG:NH2	2:I:117:ARG:NE[2_555]	1.99	0.21
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.02	0.18
2:C:117:ARG:NE	2:H:117:ARG:NH2[2_555]	2.03	0.17

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	331/343 (96%)	292 (88%)	34 (10%)	5 (2%)	13	50
1	F	331/343 (96%)	298 (90%)	29 (9%)	4 (1%)	16	56
2	B	362/395 (92%)	323 (89%)	36 (10%)	3 (1%)	24	65
2	C	363/395 (92%)	326 (90%)	31 (8%)	6 (2%)	11	48
2	D	360/395 (91%)	317 (88%)	34 (9%)	9 (2%)	7	40
2	G	376/395 (95%)	340 (90%)	33 (9%)	3 (1%)	24	65
2	H	363/395 (92%)	320 (88%)	37 (10%)	6 (2%)	11	48
2	I	360/395 (91%)	318 (88%)	33 (9%)	9 (2%)	7	40
3	E	332/334 (99%)	300 (90%)	24 (7%)	8 (2%)	7	41
3	J	332/334 (99%)	298 (90%)	28 (8%)	6 (2%)	11	47
All	All	3510/3724 (94%)	3132 (89%)	319 (9%)	59 (2%)	11	48

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
2	B	307	ALA
2	C	297	LEU
2	D	307	ALA
3	E	153	ALA

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	283/291 (97%)	256 (90%)	27 (10%)	11 38
1	F	283/291 (97%)	256 (90%)	27 (10%)	11 38
2	B	301/329 (92%)	282 (94%)	19 (6%)	22 61
2	C	302/329 (92%)	267 (88%)	35 (12%)	7 28
2	D	299/329 (91%)	280 (94%)	19 (6%)	22 60
2	G	313/329 (95%)	296 (95%)	17 (5%)	27 66
2	H	302/329 (92%)	266 (88%)	36 (12%)	6 26
2	I	299/329 (91%)	283 (95%)	16 (5%)	27 66
3	E	270/270 (100%)	254 (94%)	16 (6%)	24 63
3	J	270/270 (100%)	252 (93%)	18 (7%)	20 59
All	All	2922/3096 (94%)	2692 (92%)	230 (8%)	15 50

5 of 230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	158	ARG
1	F	191	LEU
3	J	2	ARG
3	E	188	LEU
1	F	7	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	246	HIS
1	F	216	HIS
3	J	54	GLN
3	E	267	ASN
1	F	45	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

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	B	400	8,7	22,29,29	1.26	1 (4%)	27,45,45	2.01	9 (33%)
7	BEF	B	401	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	C	402	8,7	22,29,29	1.08	1 (4%)	27,45,45	2.39	8 (29%)
7	BEF	C	403	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	D	404	8,7	22,29,29	1.14	1 (4%)	27,45,45	2.02	8 (29%)
7	BEF	D	405	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	G	406	8,7	22,29,29	1.14	2 (9%)	27,45,45	2.07	9 (33%)
7	BEF	G	407	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	H	408	8,7	22,29,29	1.29	5 (22%)	27,45,45	1.97	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BEF	H	409	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	I	410	8,7	22,29,29	1.36	3 (13%)	27,45,45	1.92	8 (29%)
7	BEF	I	411	6	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	400	8,7	-	0/12/32/32	0/3/3/3
7	BEF	B	401	6	-	0/0/0/0	0/0/0/0
6	ADP	C	402	8,7	-	0/12/32/32	0/3/3/3
7	BEF	C	403	6	-	0/0/0/0	0/0/0/0
6	ADP	D	404	8,7	-	0/12/32/32	0/3/3/3
7	BEF	D	405	6	-	0/0/0/0	0/0/0/0
6	ADP	G	406	8,7	-	0/12/32/32	0/3/3/3
7	BEF	G	407	6	-	0/0/0/0	0/0/0/0
6	ADP	H	408	8,7	-	0/12/32/32	0/3/3/3
7	BEF	H	409	6	-	0/0/0/0	0/0/0/0
6	ADP	I	410	8,7	-	0/12/32/32	0/3/3/3
7	BEF	I	411	6	-	0/0/0/0	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	410	ADP	PB-O2B	-2.27	1.46	1.54
6	I	410	ADP	C4-N3	-2.21	1.32	1.35
6	H	408	ADP	PB-O2B	-2.06	1.47	1.54
6	H	408	ADP	O4'-C1'	2.15	1.43	1.41
6	H	408	ADP	PB-O1B	2.25	1.58	1.51

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	402	ADP	N3-C2-N1	-6.76	123.72	128.89
6	D	404	ADP	N3-C2-N1	-5.58	124.62	128.89
6	C	402	ADP	C2'-C1'-N9	-5.01	106.64	114.29
6	B	400	ADP	N3-C2-N1	-4.59	125.38	128.89
6	G	406	ADP	C2'-C1'-N9	-4.55	107.34	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	400	ADP	3	0
7	B	401	BEF	1	0
6	C	402	ADP	3	0
6	D	404	ADP	3	0
6	G	406	ADP	2	0
7	G	407	BEF	1	0
6	H	408	ADP	4	0
6	I	410	ADP	2	0
7	I	411	BEF	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	333/343 (97%)	0.93	56 (16%) 2 2	73, 127, 209, 244	0
1	F	333/343 (97%)	0.44	26 (7%) 16 17	67, 127, 197, 222	0
2	B	364/395 (92%)	0.32	17 (4%) 35 37	76, 119, 164, 189	0
2	C	365/395 (92%)	0.26	14 (3%) 44 45	68, 114, 180, 208	0
2	D	362/395 (91%)	0.23	10 (2%) 56 58	69, 106, 156, 198	0
2	G	378/395 (95%)	0.10	8 (2%) 67 68	76, 101, 146, 182	0
2	H	365/395 (92%)	-0.02	2 (0%) 91 93	58, 88, 125, 165	0
2	I	362/395 (91%)	-0.00	2 (0%) 90 91	56, 80, 125, 184	0
3	E	334/334 (100%)	0.09	8 (2%) 62 63	67, 86, 134, 175	0
3	J	334/334 (100%)	0.04	3 (0%) 85 88	63, 84, 133, 172	0
4	K	14/15 (93%)	0.10	0 100 100	79, 87, 169, 171	0
4	M	14/15 (93%)	-0.13	0 100 100	76, 84, 174, 181	0
5	L	10/10 (100%)	-0.38	0 100 100	85, 88, 95, 105	0
5	N	10/10 (100%)	-0.38	0 100 100	81, 86, 98, 99	0
All	All	3578/3774 (94%)	0.23	146 (4%) 41 41	56, 101, 175, 244	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	11.3
1	A	55	ILE	9.7
1	A	61	TRP	9.0
1	F	61	TRP	8.6
1	A	62	ASN	7.2

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MG	D	414	1/1	0.84	0.39	12.09	75,75,75,75	0
8	MG	I	417	1/1	0.97	0.39	8.20	58,58,58,58	0
7	BEF	B	401	4/4	0.97	0.28	3.37	79,80,80,81	0
7	BEF	I	411	4/4	0.97	0.29	3.24	62,63,63,64	0
8	MG	C	413	1/1	0.95	0.29	1.97	77,77,77,77	0
7	BEF	C	403	4/4	0.97	0.25	1.77	77,78,78,79	0
8	MG	H	416	1/1	0.93	0.26	1.48	57,57,57,57	0
7	BEF	D	405	4/4	0.97	0.23	0.67	85,85,86,87	0
7	BEF	H	409	4/4	0.97	0.22	0.46	57,57,57,58	0
6	ADP	I	410	27/27	0.98	0.23	0.33	62,68,72,73	0
7	BEF	G	407	4/4	0.95	0.22	0.21	79,79,80,80	0
6	ADP	C	402	27/27	0.96	0.21	-0.14	78,86,91,93	0
6	ADP	G	406	27/27	0.96	0.23	-0.21	81,87,92,94	0
6	ADP	B	400	27/27	0.95	0.22	-0.31	86,94,99,100	0
6	ADP	D	404	27/27	0.95	0.21	-0.36	80,89,95,96	0
6	ADP	H	408	27/27	0.97	0.20	-0.40	60,62,67,67	0
9	ZN	G	422	1/1	0.99	0.12	-0.69	160,160,160,160	0
9	ZN	I	424	1/1	0.99	0.10	-1.23	99,99,99,99	0
9	ZN	H	423	1/1	0.98	0.10	-1.27	112,112,112,112	0
9	ZN	D	420	1/1	0.97	0.07	-1.28	133,133,133,133	0
9	ZN	B	418	1/1	0.98	0.07	-1.43	144,144,144,144	0
9	ZN	J	425	1/1	0.87	0.09	-1.58	146,146,146,146	0
9	ZN	E	421	1/1	0.98	0.06	-1.66	161,161,161,161	0
9	ZN	C	419	1/1	0.99	0.06	-2.13	130,130,130,130	0
8	MG	G	415	1/1	0.92	0.35	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MG	B	412	1/1	0.92	0.38	-	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.