



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:59 AM GMT

PDB ID : 3GLI
Title : Crystal Structure of the E. coli clamp loader bound to Primer-Template DNA and Psi Peptide
Authors : Simonetta, K.R.; Cantor, A.J.; Kuriyan, J.
Deposited on : 2009-03-12
Resolution : 3.50 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

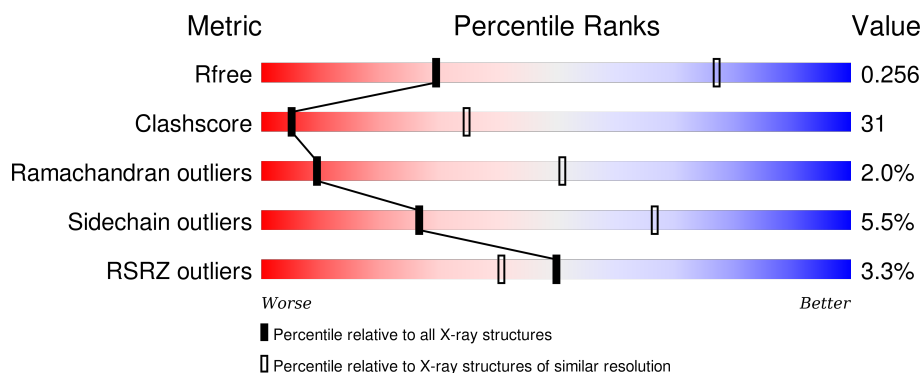
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	343	<div> <div>11%</div> <div>48%</div> <div>45%</div> <div>• •</div> </div>
1	F	343	<div> <div>14%</div> <div>45%</div> <div>48%</div> <div>• •</div> </div>
2	B	395	<div> <div>50%</div> <div>36%</div> <div>•</div> <div>9%</div> </div>
2	C	395	<div> <div>47%</div> <div>41%</div> <div>5%</div> <div>8%</div> </div>
2	D	395	<div> <div>%</div> <div>44%</div> <div>44%</div> <div>•</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	395	
2	H	395	
2	I	395	
3	E	334	
3	J	334	
4	K	15	
4	M	15	
5	L	10	
5	N	10	
6	O	27	
6	P	27	

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
9	MG	B	412	-	-	-	X
9	MG	H	416	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29139 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	334	Total	C	N	O	S	0	0	0
			2659	1684	484	481	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	359	Total	C	N	O	S	0	0	0
			2791	1753	506	516	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	373	Total	C	N	O	S	0	0	0
			2903	1826	524	536	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			

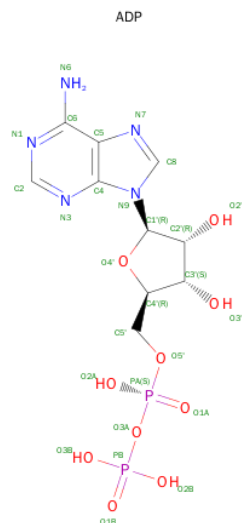
- Molecule 5 is a DNA chain called DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3').

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 a protein called DNA polymerase III subunit psi.

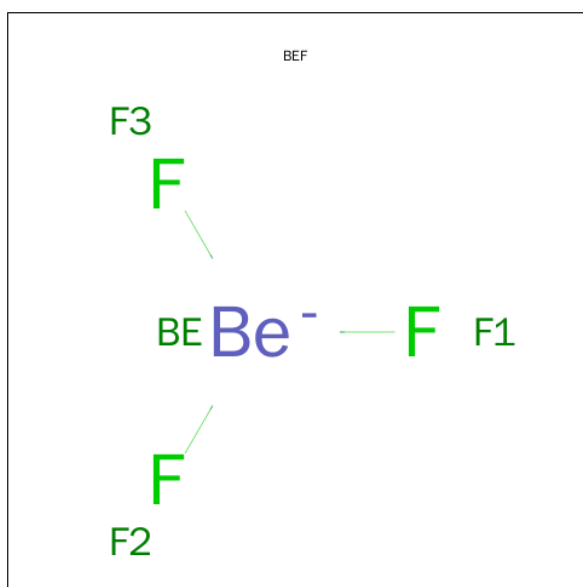
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	27	Total	C	N	O	0	0	0
			224	138	46	40			
6	P	27	Total	C	N	O	0	0	0
			224	138	46	40			

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 8 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

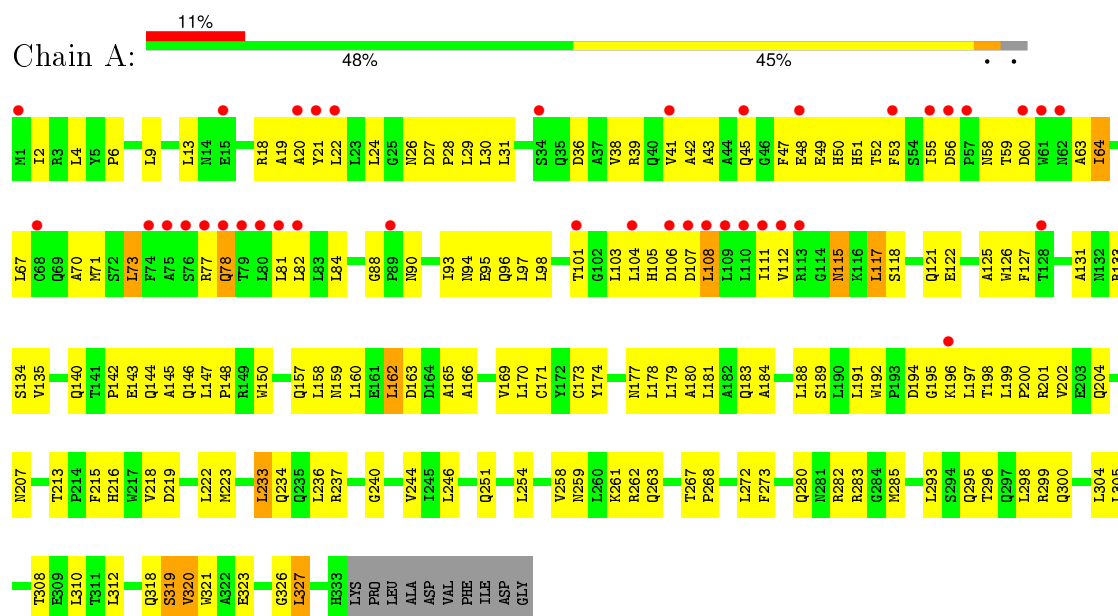
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

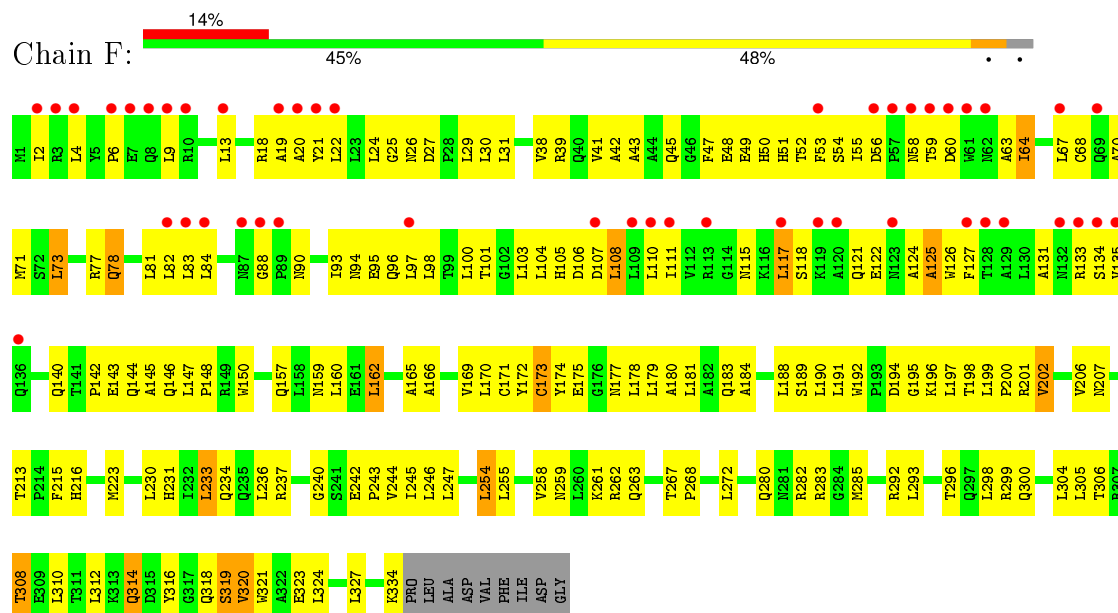
3 Residue-property plots

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.

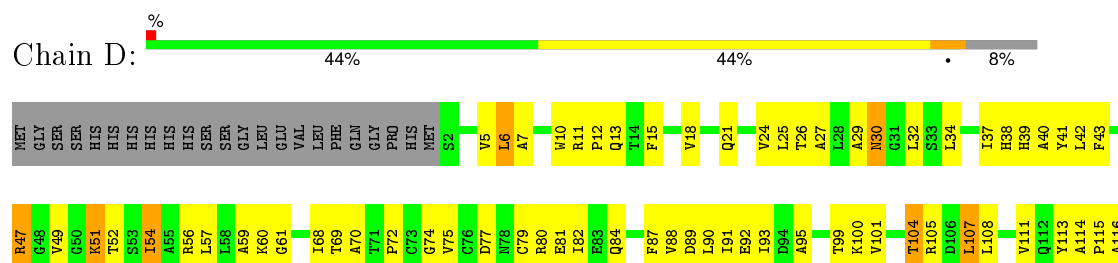
• Molecule 1: DNA polymerase III subunit delta

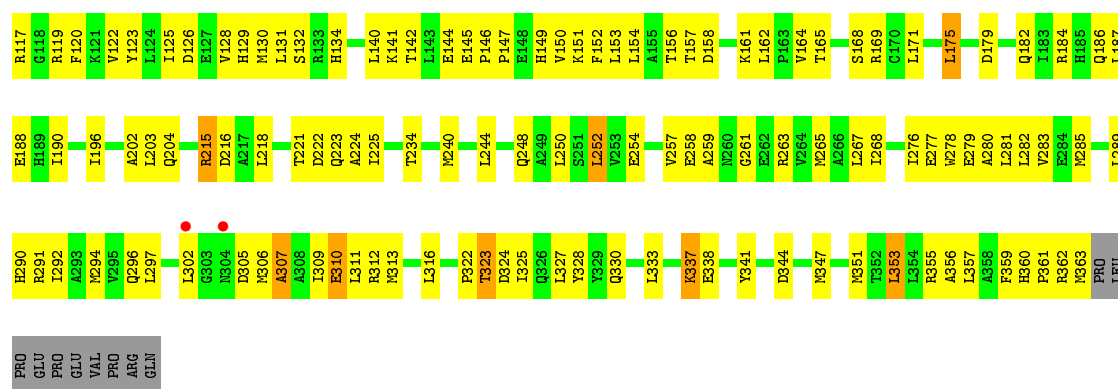


• Molecule 1: DNA polymerase III subunit delta

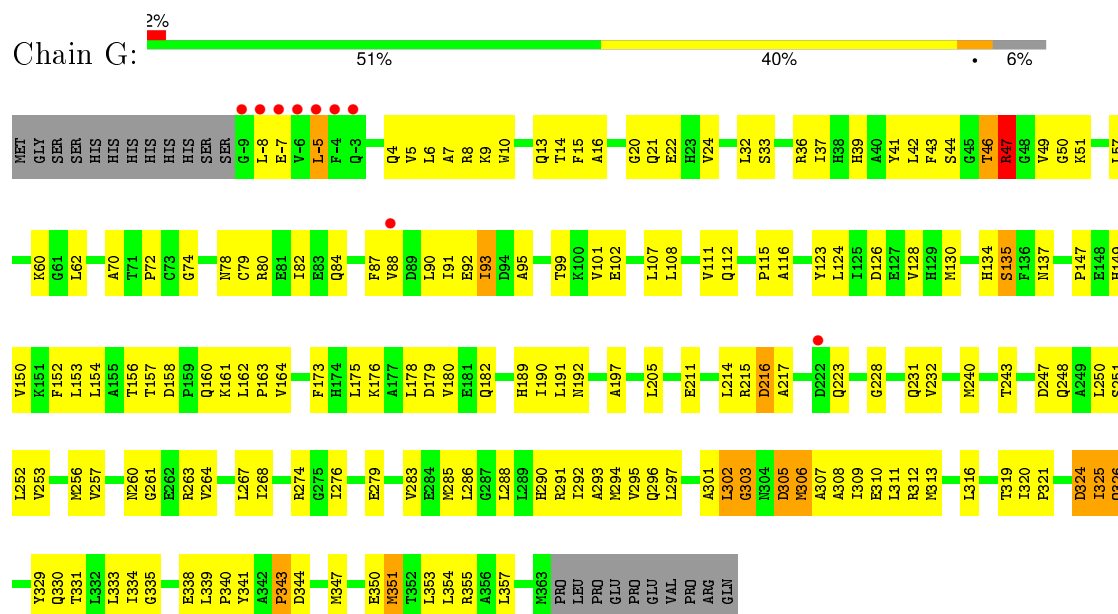


Chain B: 50% 36% 9%

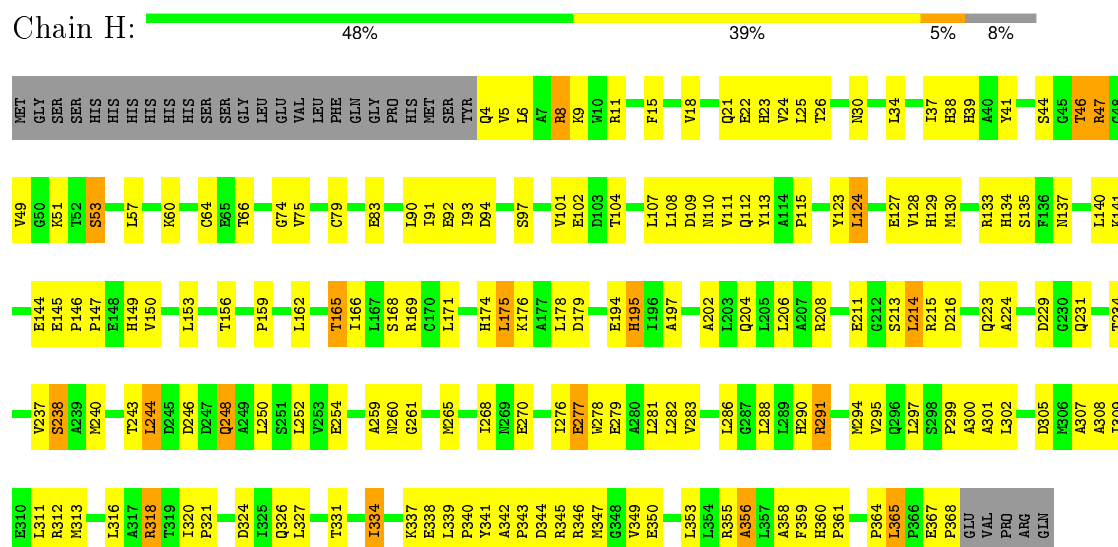




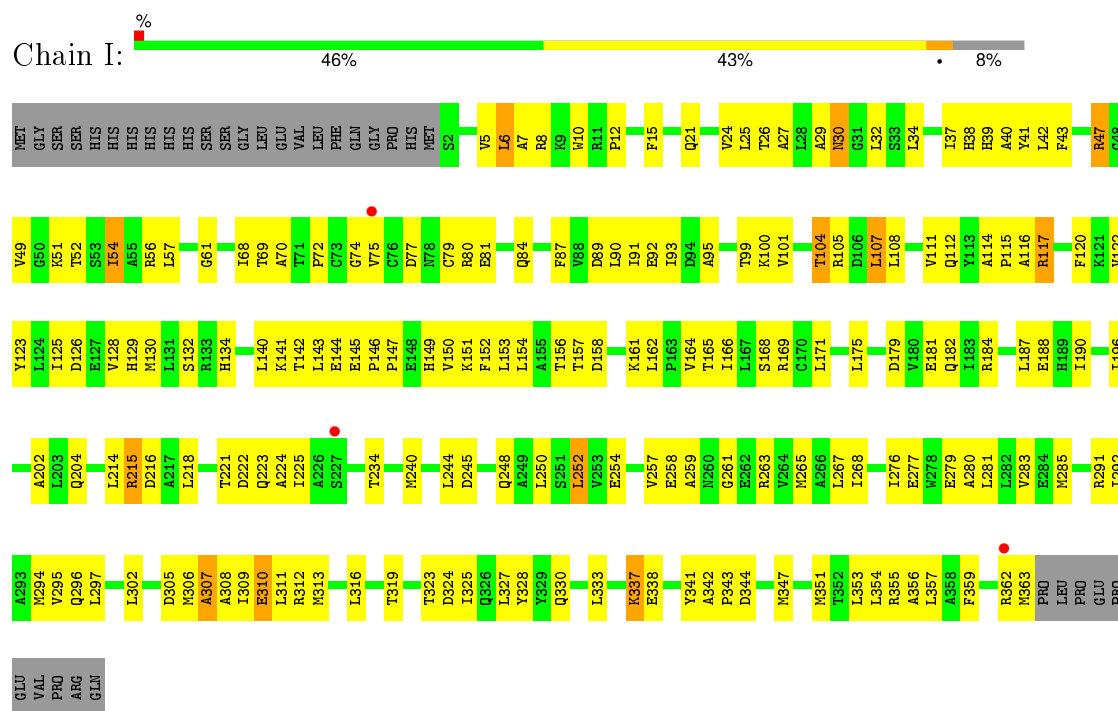
• Molecule 2: DNA polymerase III subunit tau



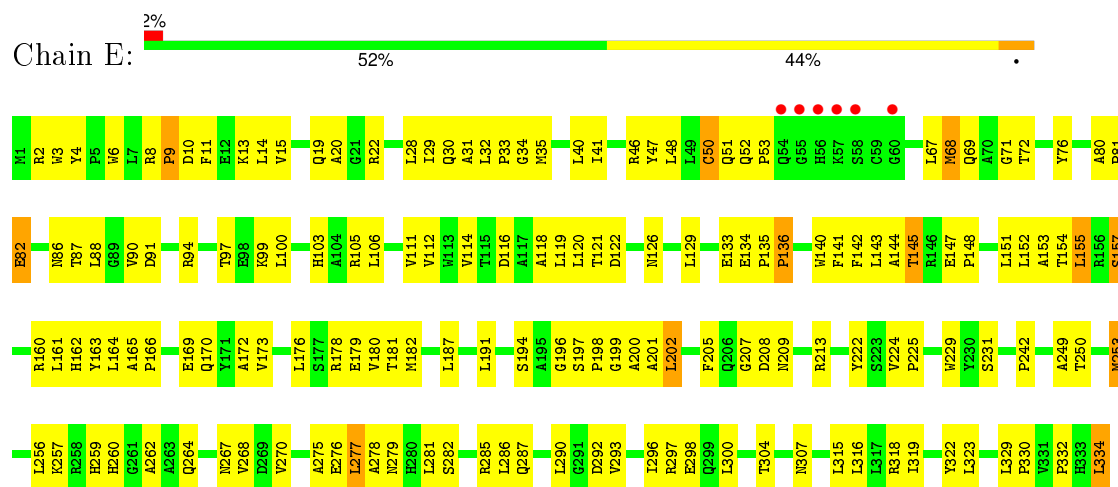
• Molecule 2: DNA polymerase III subunit tau



- Molecule 2: DNA polymerase III subunit tau

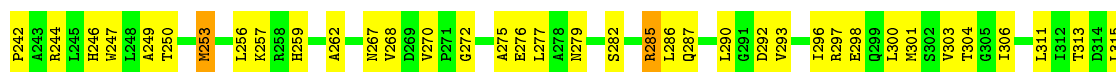


- Molecule 3: DNA polymerase III subunit delta'

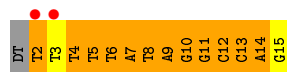


- Molecule 3: DNA polymerase III subunit delta'





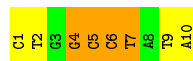
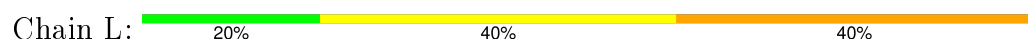
- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')



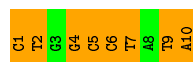
- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')



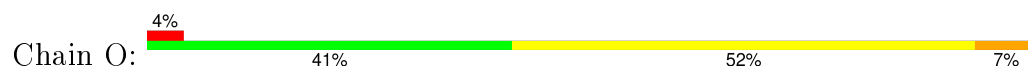
- Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')



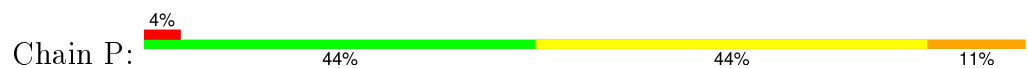
- Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')



- Molecule 6: DNA polymerase III subunit psi



- Molecule 6: DNA polymerase III subunit psi



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.69Å 217.18Å 275.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.03 – 3.50 85.42 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (73.03-3.50) 97.5 (85.42-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.222 , 0.257 0.221 , 0.256	Depositor DCC
R_{free} test set	3721 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	95.9	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 73562 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29139	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 ⓘ

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	0.53	0/2697	0.66	0/3664
1	F	0.53	0/2706	0.65	1/3675 (0.0%)
2	B	0.57	2/2835 (0.1%)	0.72	0/3841
2	C	0.57	0/2885	0.74	0/3912
2	D	0.58	0/2863	0.78	3/3879 (0.1%)
2	G	0.59	2/2951 (0.1%)	0.75	0/3998
2	H	0.67	2/2885 (0.1%)	0.78	0/3912
2	I	0.67	0/2863	0.82	0/3879
3	E	0.68	0/2666	0.78	1/3639 (0.0%)
3	J	0.66	0/2666	0.77	1/3639 (0.0%)
4	K	1.60	3/320 (0.9%)	2.54	28/492 (5.7%)
4	M	1.65	4/320 (1.2%)	2.53	29/492 (5.9%)
5	L	1.32	1/223 (0.4%)	2.48	22/342 (6.4%)
5	N	1.44	2/223 (0.9%)	2.50	18/342 (5.3%)
6	O	0.60	0/228	0.72	0/307
6	P	0.65	0/228	0.79	0/307
All	All	0.66	16/29559 (0.1%)	0.89	103/40320 (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	G	0	1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	127	GLU	CG-CD	6.26	1.61	1.51
4	M	9	DA	C3'-O3'	-6.08	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	326	GLN	CB-CG	5.90	1.68	1.52
4	K	12	DC	C3'-O3'	-5.81	1.36	1.44
5	L	6	DC	C3'-O3'	-5.76	1.36	1.44

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	5	DT	O4'-C1'-N1	-15.54	97.13	108.00
4	K	5	DT	O4'-C1'-N1	-14.21	98.05	108.00
5	L	5	DC	O4'-C4'-C3'	-12.67	98.40	106.00
5	N	5	DC	O4'-C4'-C3'	-12.08	98.75	106.00
5	N	1	DC	O4'-C4'-C3'	-11.92	98.85	106.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	303	GLY	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	173	0
1	F	2659	0	2716	181	0
2	B	2791	0	2841	165	1
2	C	2838	0	2886	208	0
2	D	2818	0	2863	205	1
2	G	2903	0	2949	171	1
2	H	2838	0	2886	217	1
2	I	2818	0	2863	212	1
3	E	2601	0	2603	163	1
3	J	2601	0	2603	183	0
4	K	287	0	161	22	0
4	M	287	0	161	22	0
5	L	200	0	115	3	0
5	N	200	0	115	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	224	0	221	26	0
6	P	224	0	221	31	0
7	B	27	0	12	4	0
7	C	27	0	12	4	0
7	D	27	0	12	5	0
7	G	27	0	12	5	0
7	H	27	0	12	4	0
7	I	27	0	12	4	0
8	B	4	0	0	0	0
8	C	4	0	0	0	0
8	D	4	0	0	0	0
8	G	4	0	0	0	0
8	H	4	0	0	0	0
8	I	4	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	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
All	All	29139	0	28979	1785	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 31.

The worst 5 of 1785 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:216:ASP:OD1	3:J:157:SER:HB3	1.35	1.25
2:D:361:PRO:HB2	3:J:272:GLY:HA2	1.23	1.17
2:I:90:LEU:CD1	2:I:122:VAL:HG12	1.86	1.05
3:J:114:VAL:HB	3:J:143:LEU:HD23	1.33	1.05
3:E:114:VAL:HB	3:E:143:LEU:HD23	1.39	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)
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.03	0.17
2:D:88:VAL:CG2	2:G:88:VAL:CG2[2_555]	2.05	0.15
2:B:117:ARG:NH2	2:I:117:ARG:NE[2_555]	2.12	0.08

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	331/343 (96%)	293 (88%)	29 (9%)	9 (3%)	6	44
1	F	332/343 (97%)	295 (89%)	30 (9%)	7 (2%)	9	50
2	B	357/395 (90%)	314 (88%)	37 (10%)	6 (2%)	11	54
2	C	363/395 (92%)	317 (87%)	42 (12%)	4 (1%)	17	63
2	D	360/395 (91%)	310 (86%)	40 (11%)	10 (3%)	6	43
2	G	371/395 (94%)	334 (90%)	30 (8%)	7 (2%)	10	51
2	H	363/395 (92%)	315 (87%)	43 (12%)	5 (1%)	14	58
2	I	360/395 (91%)	315 (88%)	38 (11%)	7 (2%)	10	51
3	E	332/334 (99%)	299 (90%)	28 (8%)	5 (2%)	13	56
3	J	332/334 (99%)	299 (90%)	29 (9%)	4 (1%)	16	61
6	O	25/27 (93%)	20 (80%)	1 (4%)	4 (16%)	0	3
6	P	25/27 (93%)	20 (80%)	2 (8%)	3 (12%)	0	6
All	All	3551/3778 (94%)	3131 (88%)	349 (10%)	71 (2%)	9	51

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	159	ASN

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Mol	Chain	Res	Type
1	A	320	VAL
2	B	247	ASP
2	B	248	GLN

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	283/291 (97%)	271 (96%)	12 (4%)	36	74
1	F	284/291 (98%)	271 (95%)	13 (5%)	33	72
2	B	296/329 (90%)	280 (95%)	16 (5%)	27	67
2	C	302/329 (92%)	280 (93%)	22 (7%)	17	57
2	D	299/329 (91%)	286 (96%)	13 (4%)	35	74
2	G	308/329 (94%)	290 (94%)	18 (6%)	25	65
2	H	302/329 (92%)	281 (93%)	21 (7%)	19	59
2	I	299/329 (91%)	286 (96%)	13 (4%)	35	74
3	E	270/270 (100%)	255 (94%)	15 (6%)	26	66
3	J	270/270 (100%)	253 (94%)	17 (6%)	22	63
6	O	23/23 (100%)	22 (96%)	1 (4%)	35	74
6	P	23/23 (100%)	22 (96%)	1 (4%)	35	74
All	All	2959/3142 (94%)	2797 (94%)	162 (6%)	27	67

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	208	ASP
1	F	319	SER
3	J	160	ARG
3	E	253	MET
1	F	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such

sidechains are listed below:

Mol	Chain	Res	Type
3	E	56	HIS
1	F	105	HIS
3	J	54	GLN
3	E	103	HIS
3	E	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no 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$
7	ADP	B	400	9,8	22,29,29	1.05	1 (4%)	27,45,45	2.01	6 (22%)
8	BEF	B	401	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	C	402	9,8	22,29,29	1.05	1 (4%)	27,45,45	2.12	6 (22%)
8	BEF	C	403	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	D	404	9,8	22,29,29	1.10	1 (4%)	27,45,45	1.94	6 (22%)
8	BEF	D	405	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	G	406	9,8	22,29,29	1.10	1 (4%)	27,45,45	2.04	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BEF	G	407	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	H	408	9,8	22,29,29	1.17	2 (9%)	27,45,45	2.22	5 (18%)
8	BEF	H	409	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	I	410	9,8	22,29,29	1.10	2 (9%)	27,45,45	1.99	6 (22%)
8	BEF	I	411	7	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
7	ADP	B	400	9,8	-	0/12/32/32	0/3/3/3
8	BEF	B	401	7	-	0/0/0/0	0/0/0/0
7	ADP	C	402	9,8	-	0/12/32/32	0/3/3/3
8	BEF	C	403	7	-	0/0/0/0	0/0/0/0
7	ADP	D	404	9,8	-	0/12/32/32	0/3/3/3
8	BEF	D	405	7	-	0/0/0/0	0/0/0/0
7	ADP	G	406	9,8	-	0/12/32/32	0/3/3/3
8	BEF	G	407	7	-	0/0/0/0	0/0/0/0
7	ADP	H	408	9,8	-	0/12/32/32	0/3/3/3
8	BEF	H	409	7	-	0/0/0/0	0/0/0/0
7	ADP	I	410	9,8	-	0/12/32/32	0/3/3/3
8	BEF	I	411	7	-	0/0/0/0	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	410	ADP	C5-N7	-2.01	1.32	1.39
7	I	410	ADP	C5-C4	2.32	1.45	1.40
7	H	408	ADP	PB-O3B	2.34	1.63	1.54
7	B	400	ADP	C5-C4	2.86	1.47	1.40
7	D	404	ADP	C5-C4	3.03	1.47	1.40

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	408	ADP	N3-C2-N1	-6.67	123.79	128.89
7	G	406	ADP	N3-C2-N1	-6.52	123.90	128.89
7	B	400	ADP	N3-C2-N1	-6.33	124.05	128.89
7	C	402	ADP	N3-C2-N1	-6.33	124.05	128.89
7	D	404	ADP	N3-C2-N1	-5.37	124.78	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	400	ADP	4	0
7	C	402	ADP	4	0
7	D	404	ADP	5	0
7	G	406	ADP	5	0
7	H	408	ADP	4	0
7	I	410	ADP	4	0

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	333/343 (97%)	0.75	39 (11%) 6 6	75, 139, 217, 248	0
1	F	334/343 (97%)	0.80	47 (14%) 4 4	78, 147, 225, 251	0
2	B	359/395 (90%)	0.05	1 (0%) 94 91	81, 116, 159, 175	0
2	C	365/395 (92%)	-0.09	1 (0%) 94 91	76, 116, 166, 198	0
2	D	362/395 (91%)	0.12	2 (0%) 90 85	77, 111, 154, 195	0
2	G	373/395 (94%)	0.07	9 (2%) 62 52	71, 113, 164, 236	0
2	H	365/395 (92%)	-0.21	0 100 100	68, 88, 131, 164	0
2	I	362/395 (91%)	0.00	3 (0%) 87 80	64, 86, 131, 171	0
3	E	334/334 (100%)	0.04	6 (1%) 71 62	71, 92, 164, 216	0
3	J	334/334 (100%)	0.22	7 (2%) 67 58	71, 92, 160, 222	0
4	K	14/15 (93%)	0.38	2 (14%) 4 4	89, 99, 195, 205	0
4	M	14/15 (93%)	0.10	0 100 100	90, 95, 197, 219	0
5	L	10/10 (100%)	-0.43	0 100 100	96, 104, 110, 110	0
5	N	10/10 (100%)	-0.42	0 100 100	88, 97, 117, 119	0
6	O	27/27 (100%)	0.31	1 (3%) 45 36	83, 125, 187, 193	0
6	P	27/27 (100%)	0.15	1 (3%) 45 36	69, 105, 163, 168	0
All	All	3623/3828 (94%)	0.16	119 (3%) 50 41	64, 107, 188, 251	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TRP	7.3
3	J	56	HIS	7.0
1	F	57	PRO	6.5
3	J	55	GLY	6.3
3	J	54	GLN	6.0

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 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, 95th 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
9	MG	H	416	1/1	0.96	0.34	5.02	66,66,66,66	0
9	MG	B	412	1/1	0.96	0.26	2.27	86,86,86,86	0
8	BEF	C	403	4/4	0.96	0.28	1.93	85,86,86,87	0
9	MG	C	413	1/1	0.96	0.27	1.64	83,83,83,83	0
8	BEF	H	409	4/4	0.94	0.26	0.92	74,74,74,75	0
9	MG	D	414	1/1	0.92	0.28	0.67	83,83,83,83	0
9	MG	I	417	1/1	0.96	0.28	0.66	67,67,67,67	0
9	MG	G	415	1/1	0.89	0.28	0.49	92,92,92,92	0
7	ADP	H	408	27/27	0.98	0.25	0.14	70,73,78,78	0
7	ADP	B	400	27/27	0.95	0.25	-0.32	92,101,107,110	0
7	ADP	C	402	27/27	0.97	0.23	-0.33	87,94,101,102	0
10	ZN	H	423	1/1	0.98	0.13	-0.44	153,153,153,153	0
8	BEF	D	405	4/4	0.91	0.21	-0.54	81,82,82,83	0
7	ADP	G	406	27/27	0.95	0.24	-0.55	93,100,105,107	0
7	ADP	I	410	27/27	0.96	0.25	-0.63	67,74,77,79	0
8	BEF	B	401	4/4	0.97	0.21	-0.65	96,96,96,97	0
8	BEF	I	411	4/4	0.95	0.21	-0.72	81,81,82,83	0
7	ADP	D	404	27/27	0.95	0.21	-0.87	84,93,99,101	0
10	ZN	E	421	1/1	0.85	0.17	-1.04	267,267,267,267	0
10	ZN	I	424	1/1	0.97	0.11	-1.22	107,107,107,107	0
10	ZN	C	419	1/1	0.99	0.12	-1.25	146,146,146,146	0
8	BEF	G	407	4/4	0.95	0.20	-1.41	94,94,94,95	0
10	ZN	J	425	1/1	0.79	0.21	-1.68	253,253,253,253	0
10	ZN	B	418	1/1	0.98	0.06	-1.93	162,162,162,162	0
10	ZN	G	422	1/1	1.00	0.08	-2.10	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	ZN	D	420	1/1	0.98	0.06	-2.41	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.