



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:12 AM GMT

PDB ID : 3GLG
Title : Crystal Structure of a Mutant (gammaT157A) E. coli Clamp Loader Bound to Primer-Template DNA
Authors : Simonetta, K.R.; Seyedin, S.N.; Kuriyan, J.
Deposited on : 2009-03-12
Resolution : 3.25 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

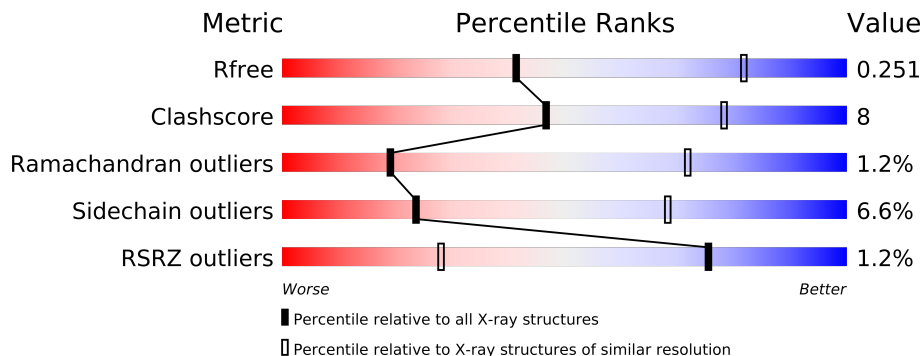
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.25 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}	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	343	
1	F	343	
2	B	395	
2	C	395	
2	D	395	
2	G	395	
2	H	395	
2	I	395	
3	E	334	
3	J	334	
4	K	20	
4	M	20	
5	L	10	
5	N	10	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	BEF	B	401	-	X
7	BEF	D	405	-	X
7	BEF	G	407	-	X
7	BEF	I	409	-	X
7	BEF	I	411	-	X
8	MG	B	412	-	X
8	MG	C	413	-	X
8	MG	D	414	-	X
8	MG	G	415	-	X
8	MG	H	416	-	X
8	MG	I	417	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28746 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			2827	1778	511	522	16			
2	C	365	Total	C	N	O	S	0	0	0
			2836	1783	513	524	16			
2	D	362	Total	C	N	O	S	0	0	0
			2816	1769	510	521	16			
2	G	378	Total	C	N	O	S	0	0	0
			2939	1851	529	542	17			
2	H	365	Total	C	N	O	S	0	0	0
			2836	1783	513	524	16			
2	I	362	Total	C	N	O	S	0	0	0
			2816	1769	510	521	16			

There are 138 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
B	157	ALA	THR	ENGINEERED	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
C	157	ALA	THR	ENGINEERED	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	HIS	-	EXPRESSION TAG	UNP P06710
D	-16	HIS	-	EXPRESSION TAG	UNP P06710
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
D	157	ALA	THR	ENGINEERED	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
G	157	ALA	THR	ENGINEERED	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
H	157	ALA	THR	ENGINEERED	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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	EXPRESSION TAG	UNP P06710
I	-1	PRO	-	EXPRESSION TAG	UNP P06710
I	0	HIS	-	EXPRESSION TAG	UNP P06710
I	157	ALA	THR	ENGINEERED	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			

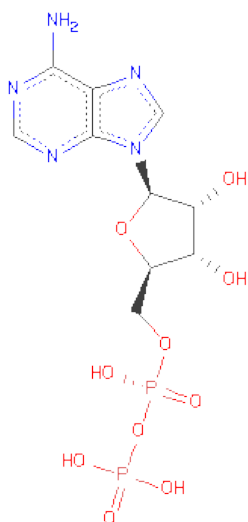
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3').

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').

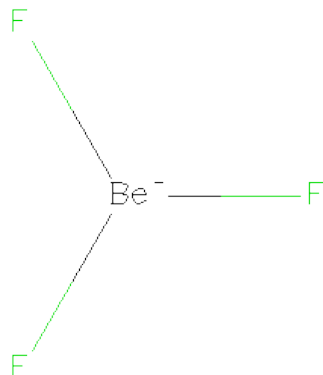
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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: BeF₃).



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	I	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	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	I	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		

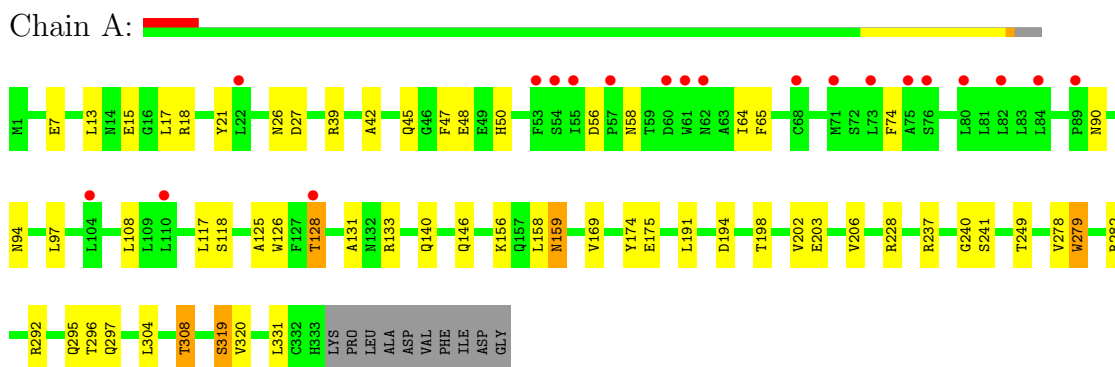
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

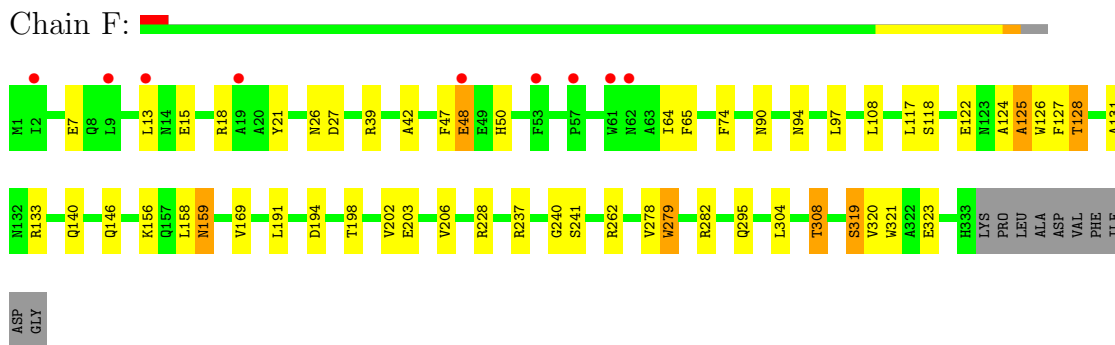
3 Residue-property plots

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 ($RSRZ > 2$). 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.

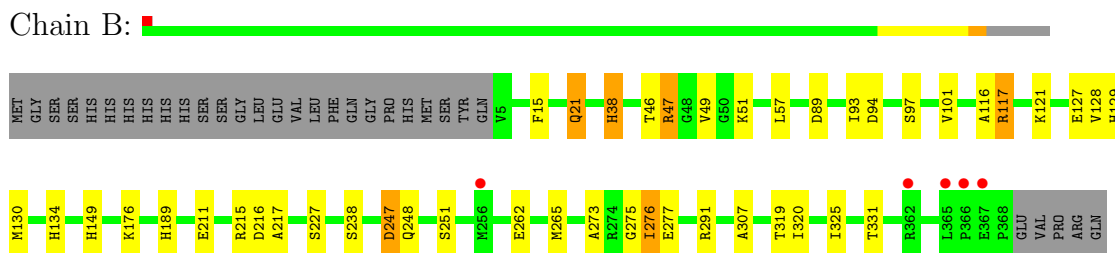
- Molecule 1: DNA polymerase III subunit delta



- Molecule 1: DNA polymerase III subunit delta

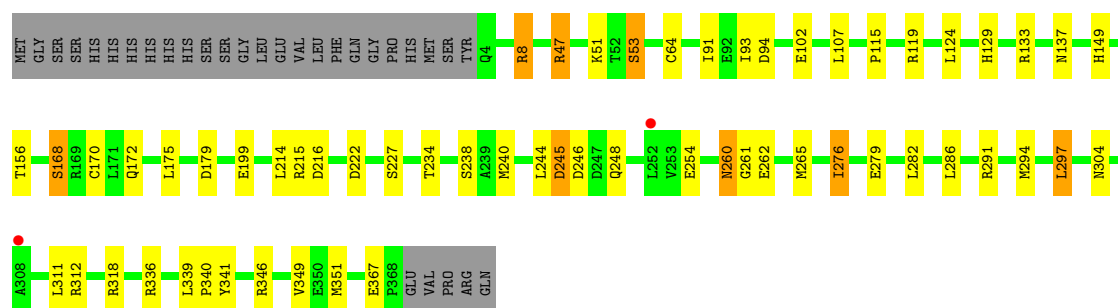


- Molecule 2: DNA polymerase III subunit tau



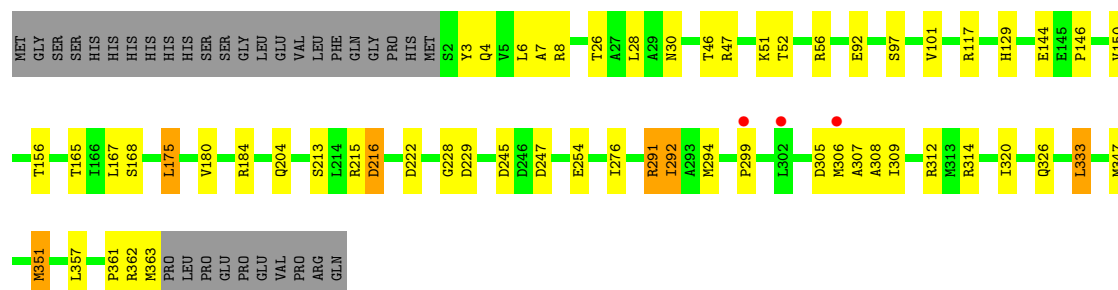
- Molecule 2: DNA polymerase III subunit tau





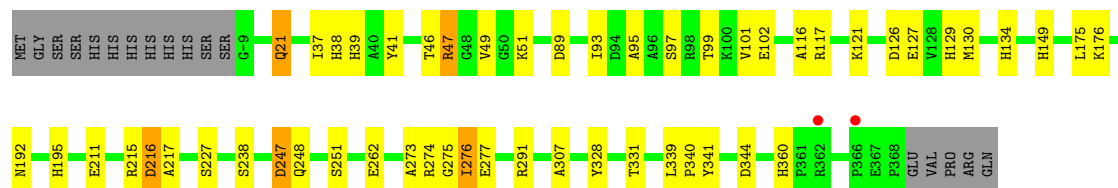
- Molecule 2: DNA polymerase III subunit tau

Chain D:



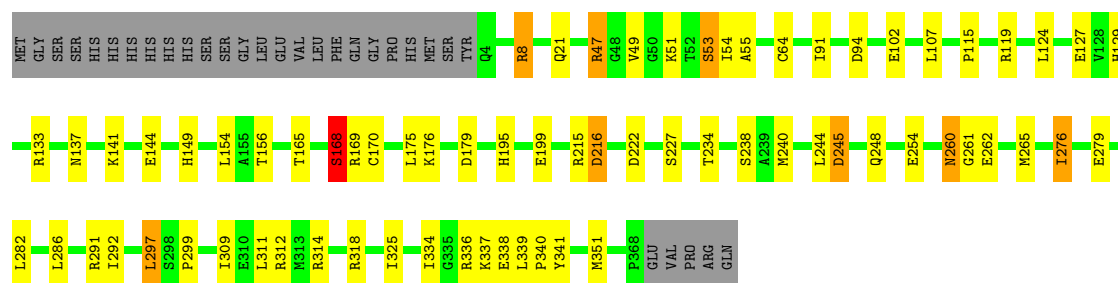
- Molecule 2: DNA polymerase III subunit tau

Chain G:



- Molecule 2: DNA polymerase III subunit tau

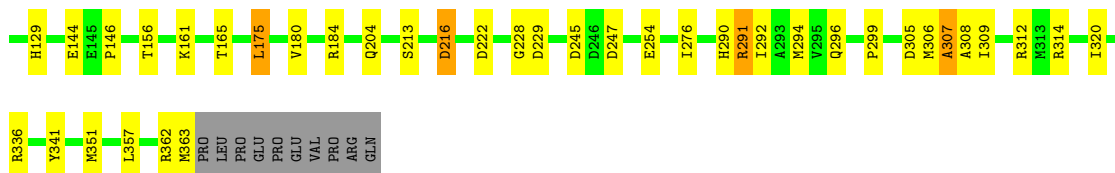
Chain H:



- Molecule 2: DNA polymerase III subunit tau

Chain I:





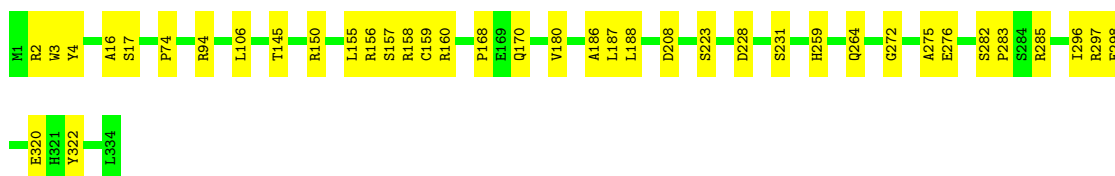
- Molecule 3: DNA polymerase III subunit delta'

Chain E:



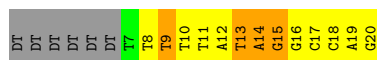
- Molecule 3: DNA polymerase III subunit delta'

Chain J:



- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*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*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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.10Å 219.10Å 274.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.25 49.24 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.24-3.25) 98.6 (49.24-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.224 , 0.263 0.211 , 0.251	Depositor DCC
R_{free} test set	4744 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 94557 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28746	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.66	0/2697	0.73	0/3664
1	F	0.68	0/2697	0.73	0/3664
2	B	0.68	1/2874 (0.0%)	0.78	0/3897
2	C	0.66	1/2883 (0.0%)	0.82	2/3909 (0.1%)
2	D	0.68	0/2861	0.86	1/3876 (0.0%)
2	G	0.68	1/2990 (0.0%)	0.78	1/4054 (0.0%)
2	H	0.82	4/2883 (0.1%)	0.90	2/3909 (0.1%)
2	I	0.86	2/2861 (0.1%)	0.93	2/3876 (0.1%)
3	E	0.85	0/2666	0.89	1/3639 (0.0%)
3	J	0.84	1/2666 (0.0%)	0.88	0/3639
4	K	1.92	6/320 (1.9%)	2.63	39/492 (7.9%)
4	M	1.81	3/320 (0.9%)	2.51	21/492 (4.3%)
5	L	1.58	4/223 (1.8%)	2.69	24/342 (7.0%)
5	N	1.76	4/223 (1.8%)	2.58	25/342 (7.3%)
All	All	0.81	27/29164 (0.1%)	0.97	118/39795 (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	C	0	1
2	H	0	1
3	E	0	1
3	J	0	1
All	All	0	4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	14	DA	C3'-O3'	-8.93	1.32	1.44
2	B	127	GLU	CG-CD	7.35	1.62	1.51
2	H	127	GLU	CD-OE1	7.06	1.33	1.25
4	K	11	DT	C3'-O3'	-7.03	1.34	1.44
4	K	14	DA	C3'-O3'	-6.89	1.34	1.44

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	10	DT	O4'-C1'-N1	-13.46	98.58	108.00
4	M	10	DT	O4'-C1'-N1	-13.27	98.71	108.00
4	K	19	DA	O4'-C1'-N9	-11.97	99.62	108.00
4	M	11	DT	O5'-P-OP2	-10.33	96.40	105.70
5	L	7	DT	N3-C4-O4	10.13	125.98	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	245	ASP	Peptide
3	E	264	GLN	Peptide
2	H	245	ASP	Peptide
3	J	264	GLN	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2650	0	0	24	0
1	F	2650	0	0	23	0
2	B	2827	0	0	18	1
2	C	2836	0	0	27	0
2	D	2816	0	0	29	0
2	G	2939	0	0	28	0
2	H	2836	0	0	36	1
2	I	2816	0	0	30	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2601	0	0	15	1
3	J	2601	0	0	19	0
4	K	287	0	0	3	0
4	M	287	0	0	3	0
5	L	200	0	0	1	0
5	N	200	0	0	1	0
6	B	27	0	0	1	0
6	C	27	0	0	2	0
6	D	27	0	0	1	0
6	G	27	0	0	1	0
6	H	27	0	0	2	0
6	I	27	0	0	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	I	8	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	28746	0	0	231	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 231 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:362:ARG:O	2:D:363:MET:CG	2.35	0.75
2:I:216:ASP:OD1	3:J:157:SER:CB	2.34	0.74
2:I:362:ARG:O	2:I:363:MET:CG	2.36	0.72
1:F:74:PHE:CD1	1:F:74:PHE:O	2.48	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:215:ARG:NH2	7:B:401:BEF:F2	2.20	0.64

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:117:ARG:NH2	2:I:117:ARG:NE[2_555]	1.94	0.26
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.06	0.14

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%)	292 (88%)	33 (10%)	6 (2%)	13	62
1	F	331/343 (96%)	291 (88%)	34 (10%)	6 (2%)	13	62
2	B	362/395 (92%)	330 (91%)	28 (8%)	4 (1%)	21	74
2	C	363/395 (92%)	337 (93%)	22 (6%)	4 (1%)	21	74
2	D	360/395 (91%)	328 (91%)	28 (8%)	4 (1%)	21	74
2	G	376/395 (95%)	343 (91%)	30 (8%)	3 (1%)	27	79
2	H	363/395 (92%)	331 (91%)	29 (8%)	3 (1%)	27	79
2	I	360/395 (91%)	326 (91%)	28 (8%)	6 (2%)	14	63
3	E	332/334 (99%)	305 (92%)	24 (7%)	3 (1%)	25	77
3	J	332/334 (99%)	303 (91%)	26 (8%)	3 (1%)	25	77
All	All	3510/3724 (94%)	3186 (91%)	282 (8%)	42 (1%)	19	72

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	159	ASN
1	A	319	SER
2	D	307	ALA

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Mol	Chain	Res	Type
3	E	74	PRO

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%)	261 (92%)	22 (8%)	18	60
1	F	283/291 (97%)	261 (92%)	22 (8%)	18	60
2	B	300/328 (92%)	283 (94%)	17 (6%)	29	75
2	C	301/328 (92%)	276 (92%)	25 (8%)	16	56
2	D	298/328 (91%)	277 (93%)	21 (7%)	21	66
2	G	312/328 (95%)	295 (95%)	17 (5%)	31	76
2	H	301/328 (92%)	278 (92%)	23 (8%)	19	61
2	I	298/328 (91%)	279 (94%)	19 (6%)	25	69
3	E	270/270 (100%)	256 (95%)	14 (5%)	32	76
3	J	270/270 (100%)	259 (96%)	11 (4%)	41	83
All	All	2916/3090 (94%)	2725 (93%)	191 (7%)	24	68

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	50	CYS
1	F	146	GLN
2	I	305	ASP
3	E	143	LEU
3	E	231	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	29,29,29	1.37	3 (10%)	45,45,45	1.82	9 (20%)
7	BEF	B	401	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	C	402	8,7	29,29,29	1.22	3 (10%)	45,45,45	2.08	10 (22%)
7	BEF	C	403	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	D	404	8,7	29,29,29	1.40	4 (13%)	45,45,45	1.71	9 (20%)
7	BEF	D	405	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	G	406	8,7	29,29,29	1.30	4 (13%)	45,45,45	1.73	8 (17%)
7	BEF	G	407	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	H	408	8,7	29,29,29	1.37	4 (13%)	45,45,45	1.85	11 (24%)
7	BEF	I	409	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	I	410	8,7	29,29,29	1.67	5 (17%)	45,45,45	1.76	8 (17%)
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	-	0/16/32/32	0/1/3/3
7	BEF	B	401	6	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	C	402	8,7	-	0/16/32/32	0/1/3/3
7	BEF	C	403	6	-	0/0/0/0	0/0/0/0
6	ADP	D	404	8,7	-	0/16/32/32	0/1/3/3
7	BEF	D	405	6	-	0/0/0/0	0/0/0/0
6	ADP	G	406	8,7	-	0/16/32/32	0/1/3/3
7	BEF	G	407	6	-	0/0/0/0	0/0/0/0
6	ADP	H	408	8,7	-	0/16/32/32	0/1/3/3
7	BEF	I	409	6	-	0/0/0/0	0/0/0/0
6	ADP	I	410	8,7	-	0/16/32/32	0/1/3/3
7	BEF	I	411	6	-	0/0/0/0	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	410	ADP	C4-N9	-4.74	1.30	1.37
6	D	404	ADP	C4-N9	-4.10	1.31	1.37
6	H	408	ADP	C4-N9	-3.76	1.32	1.37
6	I	410	ADP	C2'-C1'	-3.72	1.48	1.53
6	B	400	ADP	C5-C4	3.39	1.48	1.40

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	402	ADP	N3-C2-N1	-7.30	122.61	128.71
6	C	402	ADP	N3-C4-N9	5.36	135.11	125.43
6	H	408	ADP	N3-C4-N9	5.04	134.54	125.43
6	H	408	ADP	N3-C2-N1	-5.00	124.53	128.71
6	D	404	ADP	N3-C4-N9	4.77	134.04	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	333/343 (97%)	0.32	20 (6%)	21	5	81, 139, 220, 252	0
1	F	333/343 (97%)	0.09	9 (2%)	52	12	76, 140, 204, 232	0
2	B	364/395 (92%)	0.02	5 (1%)	72	24	85, 134, 185, 215	0
2	C	365/395 (92%)	0.03	2 (0%)	88	48	76, 127, 197, 216	0
2	D	362/395 (91%)	0.03	3 (0%)	83	37	77, 117, 173, 206	0
2	G	378/395 (95%)	-0.07	2 (0%)	88	48	87, 118, 166, 207	0
2	H	365/395 (92%)	-0.16	0	100	100	68, 99, 141, 168	0
2	I	362/395 (91%)	-0.12	0	100	100	63, 92, 135, 203	0
3	E	334/334 (100%)	-0.13	0	100	100	74, 95, 145, 184	0
3	J	334/334 (100%)	-0.18	0	100	100	71, 93, 140, 186	0
4	K	14/20 (70%)	-0.36	0	100	100	84, 95, 192, 198	0
4	M	14/20 (70%)	-0.33	0	100	100	82, 96, 193, 210	0
5	L	10/10 (100%)	-0.81	0	100	100	92, 95, 102, 105	0
5	N	10/10 (100%)	-0.76	0	100	100	83, 92, 107, 109	0
All	All	3578/3784 (94%)	-0.02	41 (1%)	75	30	63, 112, 191, 252	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	6.2
1	A	55	ILE	6.1
2	D	302	LEU	4.5
1	A	61	TRP	4.1
1	F	53	PHE	3.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	MG	I	417	1/1	0.36	10.85	67,67,67,67	0
8	MG	D	414	1/1	0.42	10.24	85,85,85,85	0
8	MG	C	413	1/1	0.36	8.77	88,88,88,88	0
8	MG	B	412	1/1	0.47	8.26	89,89,89,89	0
7	BEF	I	411	4/4	0.34	6.36	76,76,77,78	0
8	MG	G	415	1/1	0.35	4.69	89,89,89,89	0
8	MG	H	416	1/1	0.29	4.55	63,63,63,63	0
7	BEF	B	401	4/4	0.38	4.17	94,95,95,95	0
7	BEF	D	405	4/4	0.27	3.81	105,105,106,107	0
7	BEF	G	407	4/4	0.27	2.39	96,96,97,97	0
7	BEF	I	409	4/4	0.23	2.08	72,72,72,72	0
7	BEF	C	403	4/4	0.26	1.52	95,96,96,97	0
6	ADP	I	410	27/27	0.23	0.46	67,74,78,79	0
6	ADP	B	400	27/27	0.26	0.41	100,109,115,117	0
6	ADP	G	406	27/27	0.23	0.07	91,98,104,105	0
6	ADP	C	402	27/27	0.20	-0.21	90,99,104,106	0
6	ADP	D	404	27/27	0.20	-0.25	92,103,109,111	0
6	ADP	H	408	27/27	0.19	-0.29	74,76,81,82	0
9	ZN	J	425	1/1	0.13	-0.33	143,143,143,143	0
9	ZN	H	423	1/1	0.13	-0.46	121,121,121,121	0
9	ZN	G	422	1/1	0.11	-0.56	198,198,198,198	0
9	ZN	E	421	1/1	0.13	-0.65	146,146,146,146	0
9	ZN	D	420	1/1	0.11	-0.65	157,157,157,157	0
9	ZN	I	424	1/1	0.13	-0.76	117,117,117,117	0
9	ZN	B	418	1/1	0.09	-1.27	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	ZN	C	419	1/1	0.07	-1.51	149,149,149,149	0

6.5 Other polymers ⓘ

There are no such residues in this entry.