Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 04:22 pm BST

PDB ID	:	7ZX0
Title	:	Crystal structure of Pol theta polymerase domain in complex with compound 5
Authors	:	Krajewski, W.W.; Turnbull, A.P.; Willis, S.; Charles, M.; Stockley, M.; Heald, R.A.
Deposited on	:	2022-05-19
Resolution	:	2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

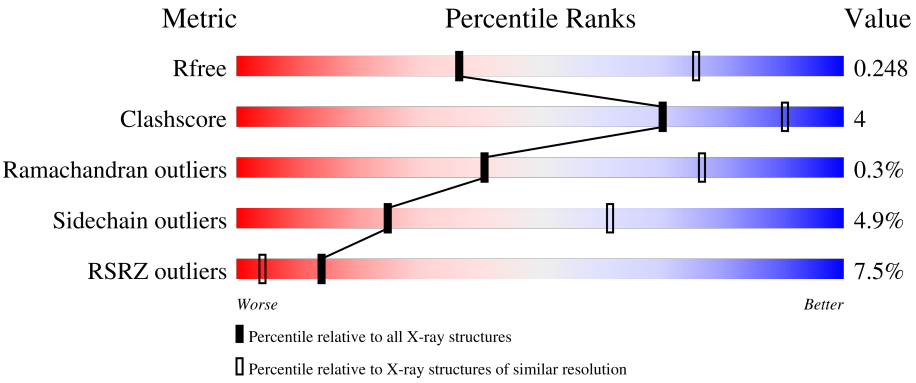
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AAA	726	2% 76% 11% 12%
1	BBB	726	5% 76% 10% 13%
1	CCC	726	5% 77% 10% 12%
1	DDD	726	8% 76% 11% 13%

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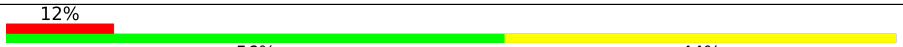
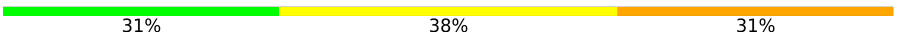
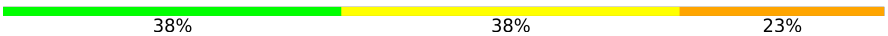
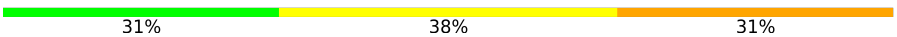
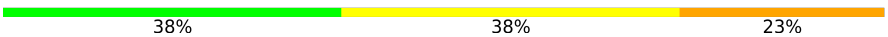
Mol	Chain	Length	Quality of chain
1	EEE	726	
1	FFF	726	
2	GGG	16	
2	III	16	
2	KKK	16	
2	MMM	16	
2	OOO	16	
2	QQQ	16	
3	HHH	13	
3	JJJ	13	
3	LLL	13	
3	NNN	13	
3	PPP	13	
3	RRR	13	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 32751 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 theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	639	Total	C	N	O	S	0	0	0
			4884	3123	825	906	30			
1	BBB	629	Total	C	N	O	S	0	0	0
			4811	3075	811	896	29			
1	CCC	638	Total	C	N	O	S	0	0	0
			4856	3107	822	897	30			
1	DDD	633	Total	C	N	O	S	0	0	0
			4810	3072	808	901	29			
1	EEE	632	Total	C	N	O	S	0	0	0
			4824	3086	814	896	28			
1	FFF	634	Total	C	N	O	S	0	0	0
			4823	3086	813	896	28			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2261	GLY	PRO	engineered mutation	UNP O75417
AAA	?	-	THR	deletion	UNP O75417
AAA	?	-	LEU	deletion	UNP O75417
AAA	?	-	VAL	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	GLU	deletion	UNP O75417
AAA	?	-	SER	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	SER	deletion	UNP O75417
AAA	?	-	GLN	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	VAL	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	LEU	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	LEU	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	MET	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	TYR	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	PHE	deletion	UNP O75417
AAA	?	-	SER	deletion	UNP O75417
AAA	?	-	VAL	deletion	UNP O75417
AAA	?	-	ASN	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
AAA	?	-	CYS	deletion	UNP O75417
AAA	?	-	GLN	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	GLN	deletion	UNP O75417
AAA	?	-	MET	deletion	UNP O75417
AAA	?	-	GLU	deletion	UNP O75417
AAA	?	-	GLU	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	ASP	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
BBB	2261	GLY	PRO	engineered mutation	UNP O75417
BBB	?	-	THR	deletion	UNP O75417
BBB	?	-	LEU	deletion	UNP O75417
BBB	?	-	VAL	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	GLU	deletion	UNP O75417
BBB	?	-	SER	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	SER	deletion	UNP O75417
BBB	?	-	GLN	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	VAL	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	LEU	deletion	UNP O75417
BBB	?	-	LEU	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	MET	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	TYR	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	PHE	deletion	UNP O75417
BBB	?	-	SER	deletion	UNP O75417
BBB	?	-	VAL	deletion	UNP O75417
BBB	?	-	ASN	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
BBB	?	-	CYS	deletion	UNP O75417
BBB	?	-	GLN	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	GLN	deletion	UNP O75417
BBB	?	-	MET	deletion	UNP O75417
BBB	?	-	GLU	deletion	UNP O75417
BBB	?	-	GLU	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	ASP	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
CCC	2261	GLY	PRO	engineered mutation	UNP O75417
CCC	?	-	THR	deletion	UNP O75417
CCC	?	-	LEU	deletion	UNP O75417
CCC	?	-	VAL	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	GLU	deletion	UNP O75417
CCC	?	-	SER	deletion	UNP O75417
CCC	?	-	PRO	deletion	UNP O75417
CCC	?	-	PRO	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	?	-	SER	deletion	UNP O75417
CCC	?	-	GLN	deletion	UNP O75417
CCC	?	-	ALA	deletion	UNP O75417
CCC	?	-	VAL	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	LYS	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	LEU	deletion	UNP O75417
CCC	?	-	LEU	deletion	UNP O75417
CCC	?	-	PRO	deletion	UNP O75417
CCC	?	-	MET	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	ARG	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	LYS	deletion	UNP O75417
CCC	?	-	TYR	deletion	UNP O75417
CCC	?	-	LYS	deletion	UNP O75417
CCC	?	-	LYS	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	PHE	deletion	UNP O75417
CCC	?	-	SER	deletion	UNP O75417
CCC	?	-	VAL	deletion	UNP O75417
CCC	?	-	ASN	deletion	UNP O75417
CCC	?	-	PRO	deletion	UNP O75417
CCC	?	-	ARG	deletion	UNP O75417
CCC	?	-	CYS	deletion	UNP O75417
CCC	?	-	GLN	deletion	UNP O75417
CCC	?	-	ALA	deletion	UNP O75417
CCC	?	-	GLN	deletion	UNP O75417
CCC	?	-	MET	deletion	UNP O75417
CCC	?	-	GLU	deletion	UNP O75417
CCC	?	-	GLU	deletion	UNP O75417
CCC	?	-	ARG	deletion	UNP O75417
CCC	?	-	ALA	deletion	UNP O75417
CCC	?	-	ALA	deletion	UNP O75417
CCC	?	-	ASP	deletion	UNP O75417
CCC	?	-	ARG	deletion	UNP O75417
DDD	2261	GLY	PRO	engineered mutation	UNP O75417
DDD	?	-	THR	deletion	UNP O75417
DDD	?	-	LEU	deletion	UNP O75417
DDD	?	-	VAL	deletion	UNP O75417
DDD	?	-	GLY	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	?	-	GLU	deletion	UNP O75417
DDD	?	-	SER	deletion	UNP O75417
DDD	?	-	PRO	deletion	UNP O75417
DDD	?	-	PRO	deletion	UNP O75417
DDD	?	-	SER	deletion	UNP O75417
DDD	?	-	GLN	deletion	UNP O75417
DDD	?	-	ALA	deletion	UNP O75417
DDD	?	-	VAL	deletion	UNP O75417
DDD	?	-	GLY	deletion	UNP O75417
DDD	?	-	LYS	deletion	UNP O75417
DDD	?	-	GLY	deletion	UNP O75417
DDD	?	-	LEU	deletion	UNP O75417
DDD	?	-	LEU	deletion	UNP O75417
DDD	?	-	PRO	deletion	UNP O75417
DDD	?	-	MET	deletion	UNP O75417
DDD	?	-	GLY	deletion	UNP O75417
DDD	?	-	ARG	deletion	UNP O75417
DDD	?	-	GLY	deletion	UNP O75417
DDD	?	-	LYS	deletion	UNP O75417
DDD	?	-	TYR	deletion	UNP O75417
DDD	?	-	LYS	deletion	UNP O75417
DDD	?	-	LYS	deletion	UNP O75417
DDD	?	-	GLY	deletion	UNP O75417
DDD	?	-	PHE	deletion	UNP O75417
DDD	?	-	SER	deletion	UNP O75417
DDD	?	-	VAL	deletion	UNP O75417
DDD	?	-	ASN	deletion	UNP O75417
DDD	?	-	PRO	deletion	UNP O75417
DDD	?	-	ARG	deletion	UNP O75417
DDD	?	-	CYS	deletion	UNP O75417
DDD	?	-	GLN	deletion	UNP O75417
DDD	?	-	ALA	deletion	UNP O75417
DDD	?	-	GLN	deletion	UNP O75417
DDD	?	-	MET	deletion	UNP O75417
DDD	?	-	GLU	deletion	UNP O75417
DDD	?	-	GLU	deletion	UNP O75417
DDD	?	-	ARG	deletion	UNP O75417
DDD	?	-	ALA	deletion	UNP O75417
DDD	?	-	ALA	deletion	UNP O75417
DDD	?	-	ASP	deletion	UNP O75417
DDD	?	-	ARG	deletion	UNP O75417
EEE	2261	GLY	PRO	engineered mutation	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	?	-	THR	deletion	UNP O75417
EEE	?	-	LEU	deletion	UNP O75417
EEE	?	-	VAL	deletion	UNP O75417
EEE	?	-	GLY	deletion	UNP O75417
EEE	?	-	GLU	deletion	UNP O75417
EEE	?	-	SER	deletion	UNP O75417
EEE	?	-	PRO	deletion	UNP O75417
EEE	?	-	PRO	deletion	UNP O75417
EEE	?	-	SER	deletion	UNP O75417
EEE	?	-	GLN	deletion	UNP O75417
EEE	?	-	ALA	deletion	UNP O75417
EEE	?	-	VAL	deletion	UNP O75417
EEE	?	-	GLY	deletion	UNP O75417
EEE	?	-	LYS	deletion	UNP O75417
EEE	?	-	GLY	deletion	UNP O75417
EEE	?	-	LEU	deletion	UNP O75417
EEE	?	-	LEU	deletion	UNP O75417
EEE	?	-	PRO	deletion	UNP O75417
EEE	?	-	MET	deletion	UNP O75417
EEE	?	-	GLY	deletion	UNP O75417
EEE	?	-	ARG	deletion	UNP O75417
EEE	?	-	GLY	deletion	UNP O75417
EEE	?	-	LYS	deletion	UNP O75417
EEE	?	-	TYR	deletion	UNP O75417
EEE	?	-	LYS	deletion	UNP O75417
EEE	?	-	LYS	deletion	UNP O75417
EEE	?	-	GLY	deletion	UNP O75417
EEE	?	-	PHE	deletion	UNP O75417
EEE	?	-	SER	deletion	UNP O75417
EEE	?	-	VAL	deletion	UNP O75417
EEE	?	-	ASN	deletion	UNP O75417
EEE	?	-	PRO	deletion	UNP O75417
EEE	?	-	ARG	deletion	UNP O75417
EEE	?	-	CYS	deletion	UNP O75417
EEE	?	-	GLN	deletion	UNP O75417
EEE	?	-	ALA	deletion	UNP O75417
EEE	?	-	GLN	deletion	UNP O75417
EEE	?	-	MET	deletion	UNP O75417
EEE	?	-	GLU	deletion	UNP O75417
EEE	?	-	GLU	deletion	UNP O75417
EEE	?	-	ARG	deletion	UNP O75417
EEE	?	-	ALA	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	?	-	ALA	deletion	UNP O75417
EEE	?	-	ASP	deletion	UNP O75417
EEE	?	-	ARG	deletion	UNP O75417
FFF	2261	GLY	PRO	engineered mutation	UNP O75417
FFF	?	-	THR	deletion	UNP O75417
FFF	?	-	LEU	deletion	UNP O75417
FFF	?	-	VAL	deletion	UNP O75417
FFF	?	-	GLY	deletion	UNP O75417
FFF	?	-	GLU	deletion	UNP O75417
FFF	?	-	SER	deletion	UNP O75417
FFF	?	-	PRO	deletion	UNP O75417
FFF	?	-	PRO	deletion	UNP O75417
FFF	?	-	SER	deletion	UNP O75417
FFF	?	-	GLN	deletion	UNP O75417
FFF	?	-	ALA	deletion	UNP O75417
FFF	?	-	VAL	deletion	UNP O75417
FFF	?	-	GLY	deletion	UNP O75417
FFF	?	-	LYS	deletion	UNP O75417
FFF	?	-	GLY	deletion	UNP O75417
FFF	?	-	LEU	deletion	UNP O75417
FFF	?	-	LEU	deletion	UNP O75417
FFF	?	-	PRO	deletion	UNP O75417
FFF	?	-	MET	deletion	UNP O75417
FFF	?	-	GLY	deletion	UNP O75417
FFF	?	-	ARG	deletion	UNP O75417
FFF	?	-	GLY	deletion	UNP O75417
FFF	?	-	LYS	deletion	UNP O75417
FFF	?	-	TYR	deletion	UNP O75417
FFF	?	-	LYS	deletion	UNP O75417
FFF	?	-	LYS	deletion	UNP O75417
FFF	?	-	GLY	deletion	UNP O75417
FFF	?	-	PHE	deletion	UNP O75417
FFF	?	-	SER	deletion	UNP O75417
FFF	?	-	VAL	deletion	UNP O75417
FFF	?	-	ASN	deletion	UNP O75417
FFF	?	-	PRO	deletion	UNP O75417
FFF	?	-	ARG	deletion	UNP O75417
FFF	?	-	CYS	deletion	UNP O75417
FFF	?	-	GLN	deletion	UNP O75417
FFF	?	-	ALA	deletion	UNP O75417
FFF	?	-	GLN	deletion	UNP O75417
FFF	?	-	MET	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
FFF	?	-	GLU	deletion	UNP O75417
FFF	?	-	GLU	deletion	UNP O75417
FFF	?	-	ARG	deletion	UNP O75417
FFF	?	-	ALA	deletion	UNP O75417
FFF	?	-	ALA	deletion	UNP O75417
FFF	?	-	ASP	deletion	UNP O75417
FFF	?	-	ARG	deletion	UNP O75417

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP *AP*GP*CP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GGG	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	III	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	KKK	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	MMM	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	OOO	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	QQQ	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			

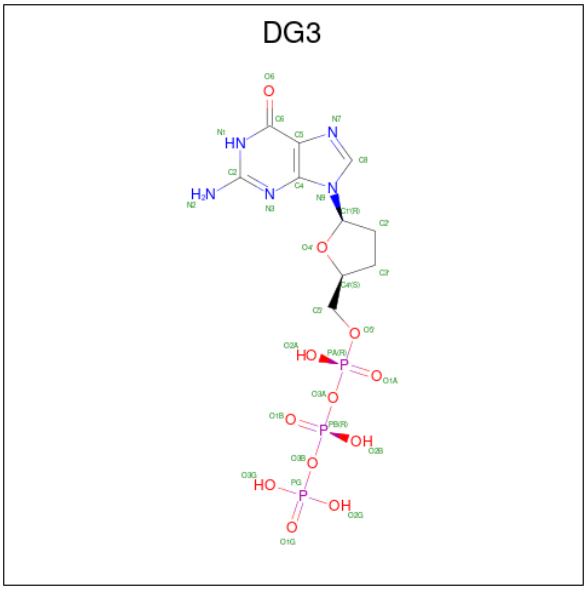
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP* TP*TP*(DDG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	HHH	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	JJJ	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	LLL	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	NNN	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	PPP	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	RRR	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Mg 1 1	0	0
4	BBB	1	Total Mg 1 1	0	0
4	CCC	1	Total Mg 1 1	0	0
4	DDD	1	Total Mg 1 1	0	0
4	EEE	1	Total Mg 1 1	0	0
4	FFF	1	Total Mg 1 1	0	0

- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C N O P 30 10 5 12 3	0	0
5	BBB	1	Total C N O P 30 10 5 12 3	0	0
5	CCC	1	Total C N O P 30 10 5 12 3	0	0
5	DDD	1	Total C N O P 30 10 5 12 3	0	0

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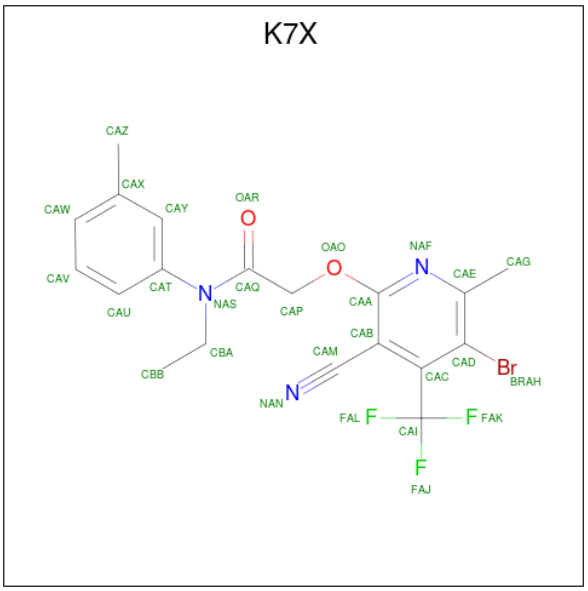
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	EEE	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	FFF	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is 2-[5-bromanyl-3-cyano-6-methyl-4-(trifluoromethyl)pyridin-2-yl]oxy- {N}-ethyl- {N}-(3-methylphenyl)ethanamide (three-letter code: K7X) (formula: $C_{19}H_{17}BrF_3N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	AAA	1	Total	Br	C	F	N	O	0	0
			28	1	19	3	3	2		

- Molecule 7 is water.

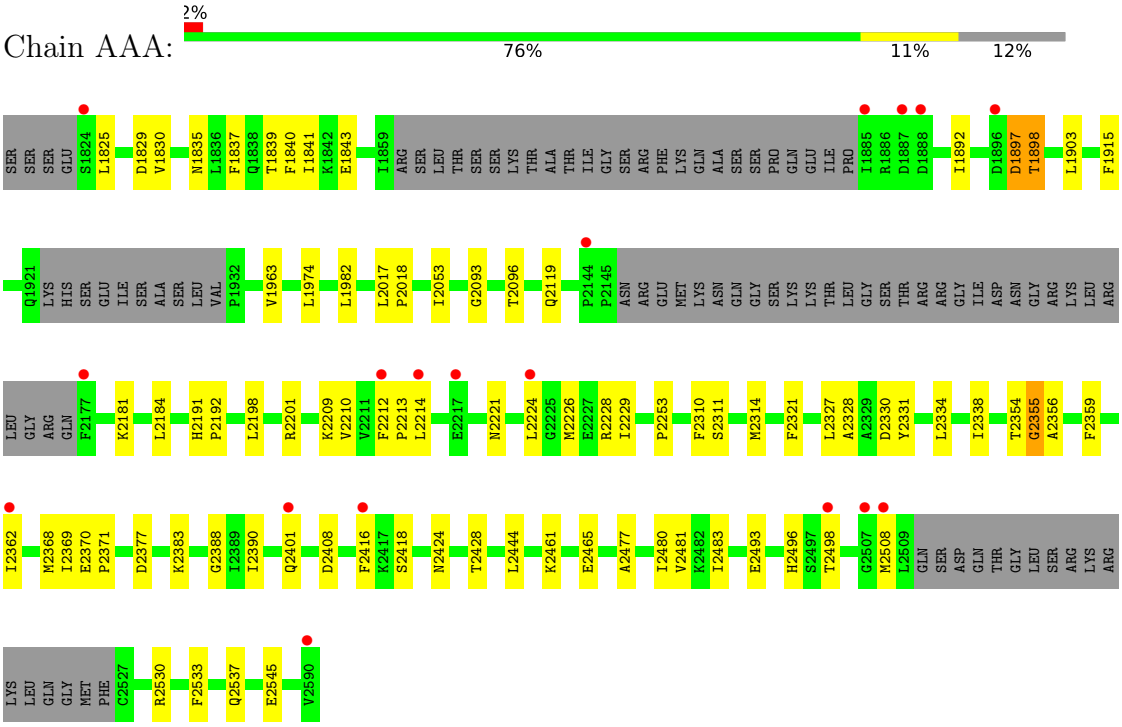
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

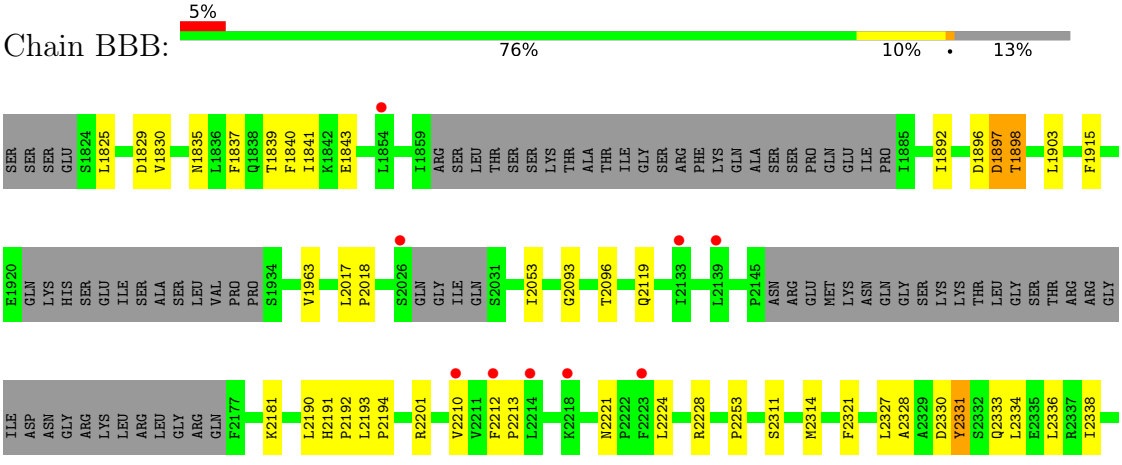
• Molecule 1: DNA polymerase theta

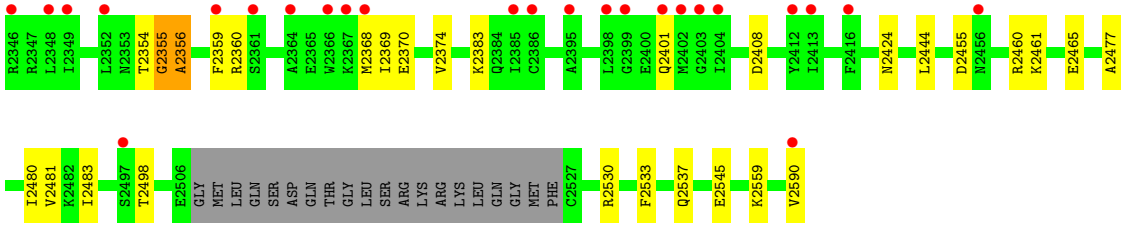
Chain AAA:



• Molecule 1: DNA polymerase theta

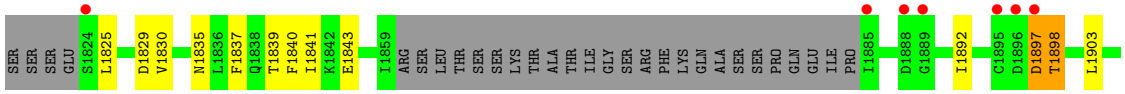
Chain BBB:

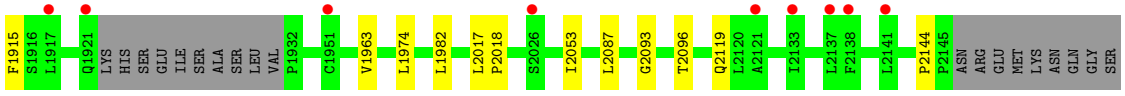


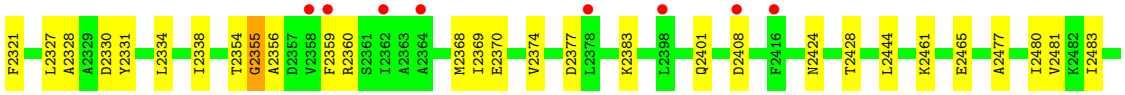


• Molecule 1: DNA polymerase theta

Chain CCC:

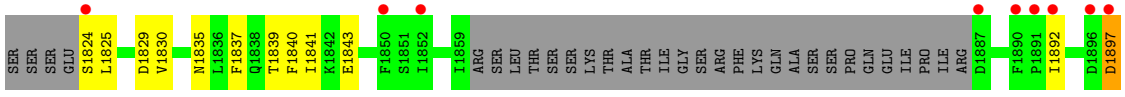


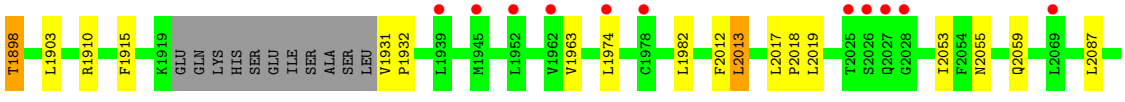


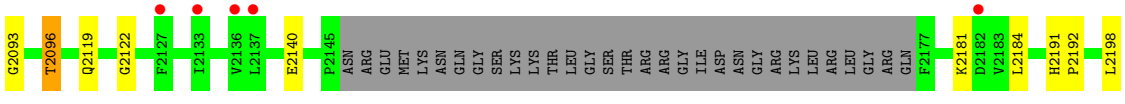


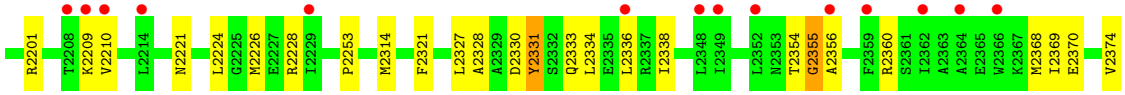
• Molecule 1: DNA polymerase theta

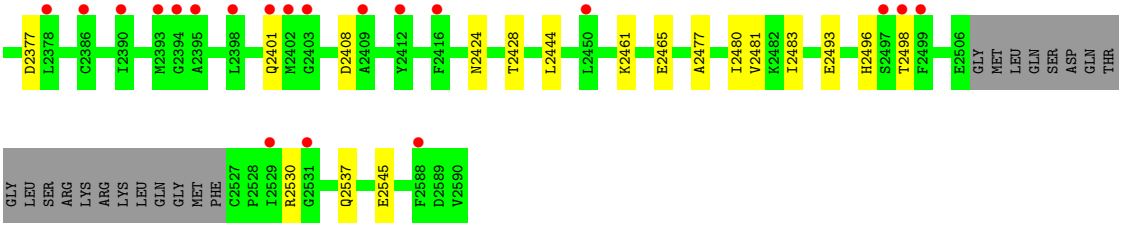
Chain DDD:





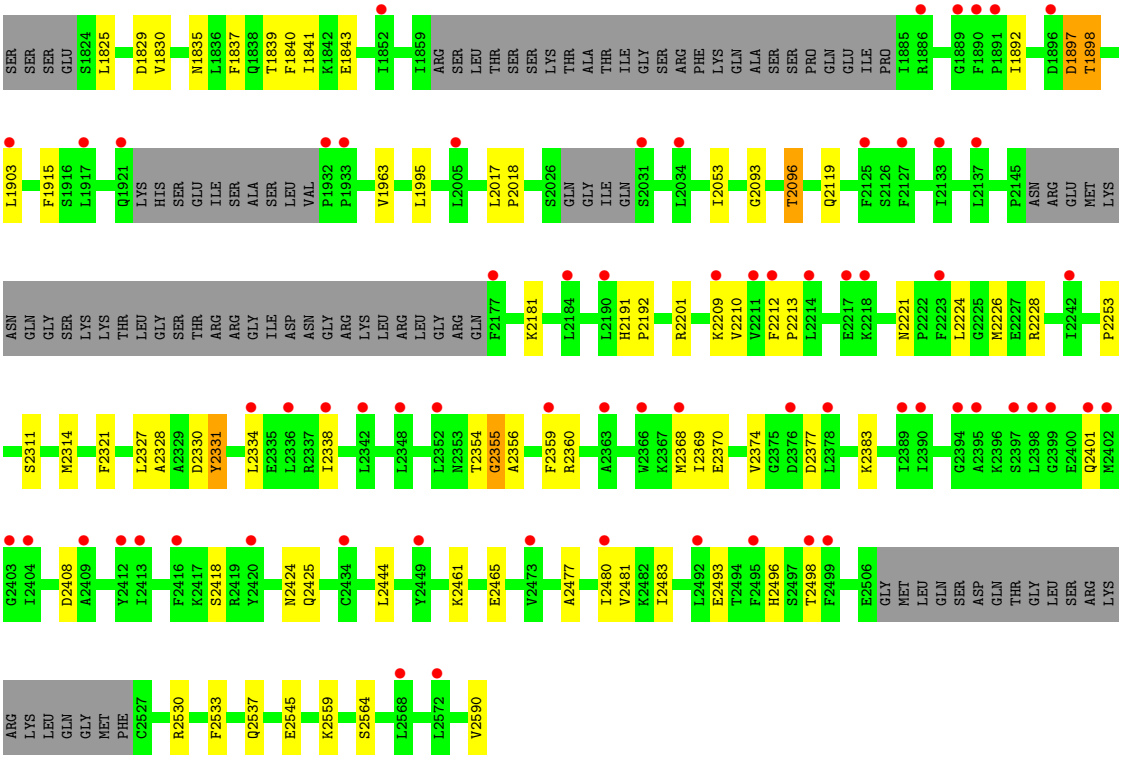






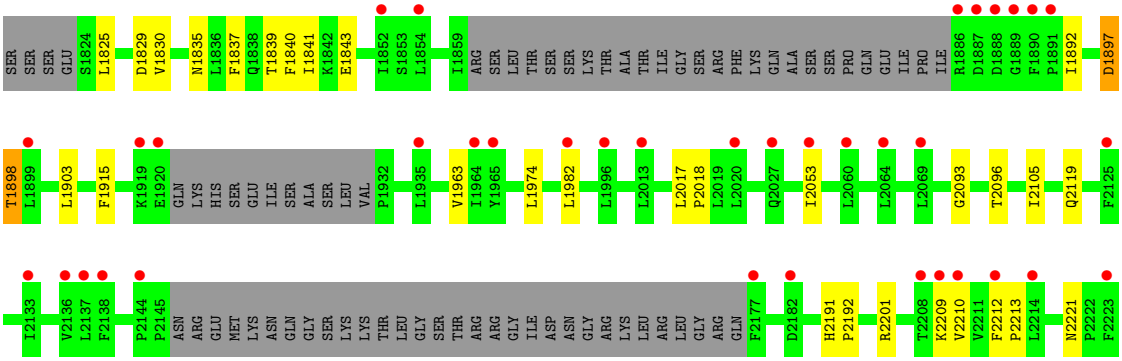
• Molecule 1: DNA polymerase theta

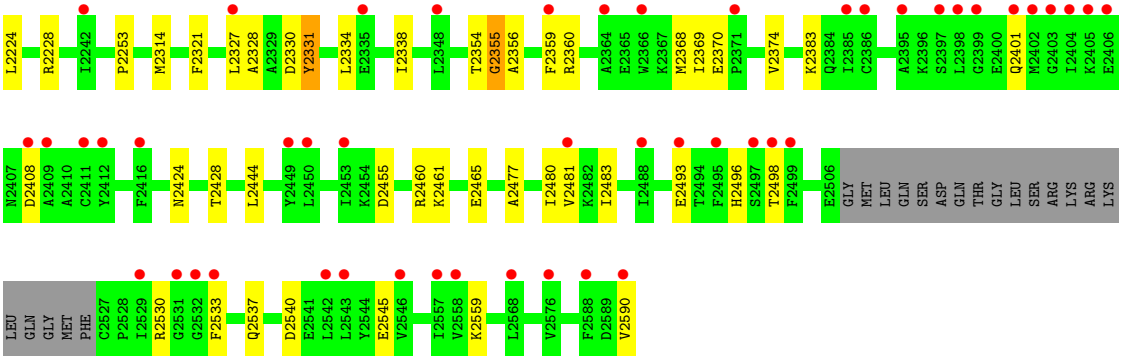
Chain EEE:



• Molecule 1: DNA polymerase theta

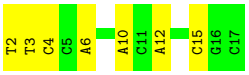
Chain FFF:





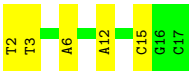
• Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain GGG:



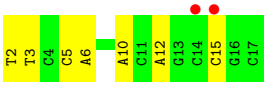
• Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain III:



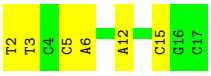
• Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain KKK:



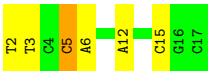
• Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain MMM:



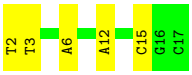
• Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain OOO:



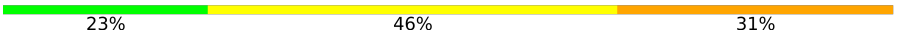
• Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain QQQ:



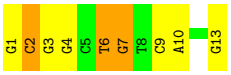
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')

Chain HHH:



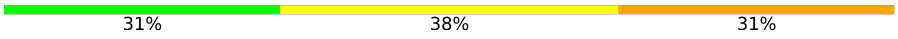
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')

Chain JJJ:



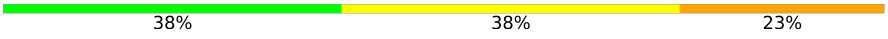
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')

Chain LLL:



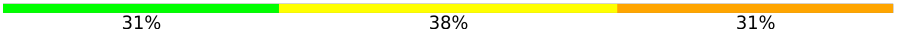
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')

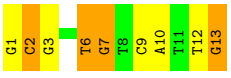
Chain NNN:



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

Chain PPP:





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

Chain RRR:


G1
C2
G3
T6
G7
T8
C9
A10
G13

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.05Å 172.02Å 288.61Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	50.01 – 2.99 147.75 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.01-2.99) 99.2 (147.75-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.252 0.217 , 0.248	Depositor DCC
R_{free} test set	6234 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	83.4	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32751	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 18.53% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: DDG, MG, DG3, K7X

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	AAA	0.71	0/4980	0.77	0/6751
1	BBB	0.70	1/4904 (0.0%)	0.76	0/6649
1	CCC	0.68	0/4952	0.75	0/6717
1	DDD	0.69	1/4905 (0.0%)	0.76	0/6659
1	EEE	0.68	1/4919 (0.0%)	0.75	0/6672
1	FFF	0.68	1/4919 (0.0%)	0.74	0/6676
2	GGG	1.06	0/362	1.43	5/555 (0.9%)
2	III	1.01	0/362	1.45	4/555 (0.7%)
2	KKK	1.00	0/362	1.43	6/555 (1.1%)
2	MMM	1.05	0/362	1.45	5/555 (0.9%)
2	OOO	0.94	0/362	1.46	5/555 (0.9%)
2	QQQ	0.95	0/362	1.46	4/555 (0.7%)
3	HHH	1.07	0/271	1.51	7/417 (1.7%)
3	JJJ	1.12	0/271	1.54	8/417 (1.9%)
3	LLL	1.04	0/271	1.49	7/417 (1.7%)
3	NNN	1.02	0/271	1.47	7/417 (1.7%)
3	PPP	0.98	0/271	1.52	7/417 (1.7%)
3	RRR	0.98	0/271	1.50	7/417 (1.7%)
All	All	0.73	4/33377 (0.0%)	0.88	72/45956 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DDD	0	1
1	EEE	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	2331	TYR	C-O	6.90	1.36	1.23
1	EEE	2331	TYR	C-O	5.62	1.34	1.23
1	DDD	2331	TYR	C-O	5.59	1.33	1.23
1	FFF	2331	TYR	C-O	5.51	1.33	1.23

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	QQQ	3	DT	P-O3'-C3'	-10.96	106.54	119.70
2	GGG	3	DT	P-O3'-C3'	-10.33	107.30	119.70
3	NNN	7	DG	P-O3'-C3'	-10.24	107.41	119.70
3	LLL	7	DG	P-O3'-C3'	-10.01	107.69	119.70
3	HHH	7	DG	P-O3'-C3'	-10.00	107.70	119.70
2	III	3	DT	P-O3'-C3'	-9.90	107.83	119.70
2	OOO	3	DT	P-O3'-C3'	-9.76	107.98	119.70
3	RRR	7	DG	P-O3'-C3'	-9.67	108.09	119.70
3	PPP	7	DG	P-O3'-C3'	-9.67	108.10	119.70
3	JJJ	7	DG	P-O3'-C3'	-9.61	108.17	119.70
2	KKK	3	DT	P-O3'-C3'	-9.46	108.36	119.70
2	III	15	DC	P-O3'-C3'	-9.13	108.74	119.70
2	OOO	15	DC	P-O3'-C3'	-9.10	108.78	119.70
2	KKK	15	DC	P-O3'-C3'	-9.00	108.90	119.70
2	GGG	15	DC	P-O3'-C3'	-8.94	108.98	119.70
3	NNN	6	DT	P-O3'-C3'	-8.89	109.03	119.70
2	MMM	15	DC	P-O3'-C3'	-8.84	109.10	119.70
3	RRR	6	DT	P-O3'-C3'	-8.84	109.10	119.70
2	QQQ	15	DC	P-O3'-C3'	-8.80	109.14	119.70
2	MMM	3	DT	P-O3'-C3'	-8.76	109.18	119.70
3	PPP	6	DT	P-O3'-C3'	-8.67	109.30	119.70
3	HHH	6	DT	P-O3'-C3'	-8.63	109.34	119.70
3	LLL	6	DT	P-O3'-C3'	-8.61	109.36	119.70
3	JJJ	6	DT	P-O3'-C3'	-8.34	109.69	119.70
3	LLL	9	DC	P-O3'-C3'	-7.95	110.16	119.70
3	RRR	9	DC	P-O3'-C3'	-7.86	110.26	119.70
3	JJJ	10	DA	P-O3'-C3'	-7.82	110.32	119.70
3	PPP	9	DC	P-O3'-C3'	-7.78	110.36	119.70
3	HHH	10	DA	P-O3'-C3'	-7.39	110.83	119.70
3	HHH	9	DC	P-O3'-C3'	-7.37	110.85	119.70
3	JJJ	9	DC	P-O3'-C3'	-7.23	111.03	119.70
3	RRR	10	DA	P-O3'-C3'	-7.09	111.19	119.70
3	PPP	10	DA	P-O3'-C3'	-7.07	111.22	119.70
2	MMM	12	DA	P-O3'-C3'	-7.03	111.26	119.70
2	GGG	12	DA	P-O3'-C3'	-7.02	111.28	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	III	12	DA	P-O3'-C3'	-6.92	111.39	119.70
3	JJJ	1	DG	P-O3'-C3'	-6.91	111.40	119.70
2	OOO	6	DA	P-O3'-C3'	-6.90	111.42	119.70
3	PPP	1	DG	P-O3'-C3'	-6.82	111.52	119.70
3	NNN	9	DC	P-O3'-C3'	-6.80	111.55	119.70
2	OOO	12	DA	P-O3'-C3'	-6.75	111.60	119.70
3	LLL	10	DA	P-O3'-C3'	-6.74	111.61	119.70
2	MMM	6	DA	P-O3'-C3'	-6.74	111.62	119.70
2	QQQ	12	DA	P-O3'-C3'	-6.73	111.63	119.70
3	RRR	1	DG	P-O3'-C3'	-6.73	111.63	119.70
2	QQQ	6	DA	P-O3'-C3'	-6.65	111.72	119.70
3	NNN	10	DA	P-O3'-C3'	-6.63	111.74	119.70
2	KKK	12	DA	P-O3'-C3'	-6.61	111.77	119.70
3	LLL	1	DG	P-O3'-C3'	-6.59	111.79	119.70
2	KKK	6	DA	P-O3'-C3'	-6.55	111.84	119.70
3	JJJ	9	DC	O4'-C4'-C3'	-6.55	101.88	104.50
3	NNN	1	DG	P-O3'-C3'	-6.24	112.22	119.70
3	JJJ	2	DC	P-O3'-C3'	-6.19	112.27	119.70
3	RRR	9	DC	O4'-C4'-C3'	-6.10	102.06	104.50
3	RRR	2	DC	P-O3'-C3'	-6.07	112.42	119.70
3	PPP	2	DC	P-O3'-C3'	-5.96	112.55	119.70
3	HHH	1	DG	P-O3'-C3'	-5.95	112.56	119.70
3	LLL	9	DC	O4'-C4'-C3'	-5.89	102.15	104.50
3	LLL	2	DC	P-O3'-C3'	-5.85	112.68	119.70
3	HHH	2	DC	P-O3'-C3'	-5.74	112.81	119.70
3	NNN	2	DC	P-O3'-C3'	-5.73	112.83	119.70
2	III	6	DA	P-O3'-C3'	-5.71	112.84	119.70
3	PPP	9	DC	O4'-C4'-C3'	-5.62	102.25	104.50
2	GGG	6	DA	P-O3'-C3'	-5.60	112.98	119.70
2	KKK	5	DC	P-O3'-C3'	-5.30	113.34	119.70
3	NNN	9	DC	O4'-C4'-C3'	-5.27	102.39	104.50
2	OOO	5	DC	P-O3'-C3'	-5.24	113.41	119.70
2	GGG	10	DA	P-O3'-C3'	-5.19	113.47	119.70
2	MMM	5	DC	P-O3'-C3'	-5.18	113.48	119.70
3	HHH	8	DT	P-O3'-C3'	-5.06	113.63	119.70
2	KKK	10	DA	P-O3'-C3'	-5.05	113.64	119.70
3	JJJ	4	DG	P-O3'-C3'	-5.00	113.69	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	2096	THR	Mainchain
1	EEE	2096	THR	Mainchain
1	EEE	2425	GLN	Mainchain

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	AAA	4884	0	4714	37	0
1	BBB	4811	0	4625	33	0
1	CCC	4856	0	4667	33	0
1	DDD	4810	0	4593	39	0
1	EEE	4824	0	4632	30	0
1	FFF	4823	0	4617	33	0
2	GGG	324	0	180	2	0
2	III	324	0	180	1	0
2	KKK	324	0	180	1	0
2	MMM	324	0	180	1	0
2	OOO	324	0	180	3	0
2	QQQ	324	0	180	1	0
3	HHH	264	0	149	3	0
3	JJJ	264	0	149	2	0
3	LLL	264	0	149	3	0
3	NNN	264	0	149	2	0
3	PPP	264	0	149	3	0
3	RRR	264	0	149	2	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	1	0	0	0	0
5	AAA	30	0	12	0	0
5	BBB	30	0	12	0	0
5	CCC	30	0	12	1	0
5	DDD	30	0	12	0	0
5	EEE	30	0	12	2	0
5	FFF	30	0	12	2	0
6	AAA	28	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AAA	1	0	0	0	0
All	All	32751	0	29894	226	0

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 4.

All (226) 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)
6:AAA:2603:K7X:BRAH	6:AAA:2603:K7X:FAK	2.27	0.98
1:CCC:2383:LYS:NZ	5:CCC:2602:DG3:O1G	2.09	0.86
1:DDD:2013:LEU:HD11	1:DDD:2055:ASN:OD1	1.81	0.81
1:AAA:2390:ILE:HD11	6:AAA:2603:K7X:BRAH	2.36	0.80
1:BBB:2338:ILE:HD11	1:BBB:2480:ILE:HD12	1.65	0.79
1:DDD:2013:LEU:CD1	1:DDD:2055:ASN:OD1	2.32	0.78
1:FFF:2338:ILE:HD11	1:FFF:2480:ILE:HD12	1.65	0.78
1:CCC:2338:ILE:HD11	1:CCC:2480:ILE:HD12	1.64	0.78
1:DDD:2338:ILE:HD11	1:DDD:2480:ILE:HD12	1.65	0.77
1:AAA:2338:ILE:HD11	1:AAA:2480:ILE:HD12	1.65	0.77
1:EEE:2338:ILE:HD11	1:EEE:2480:ILE:HD12	1.65	0.76
1:DDD:2013:LEU:HD11	1:DDD:2055:ASN:CG	2.15	0.67
1:DDD:2210:VAL:HG21	1:DDD:2253:PRO:HD3	1.76	0.66
1:AAA:2498:THR:HG21	1:AAA:2530:ARG:HB2	1.79	0.64
1:DDD:2498:THR:HG21	1:DDD:2530:ARG:HB2	1.79	0.64
1:FFF:2498:THR:HG21	1:FFF:2530:ARG:HB2	1.78	0.64
1:CCC:2493:GLU:HA	1:CCC:2496:HIS:HB2	1.80	0.64
1:FFF:2493:GLU:HA	1:FFF:2496:HIS:HB2	1.80	0.64
1:CCC:2498:THR:HG21	1:CCC:2530:ARG:HB2	1.80	0.63
1:EEE:2493:GLU:HA	1:EEE:2496:HIS:HB2	1.80	0.63
1:AAA:2210:VAL:HG21	1:AAA:2253:PRO:HD3	1.81	0.63
1:DDD:2493:GLU:HA	1:DDD:2496:HIS:HB2	1.81	0.63
1:AAA:2493:GLU:HA	1:AAA:2496:HIS:HB2	1.81	0.63
1:EEE:2210:VAL:HG21	1:EEE:2253:PRO:HD3	1.80	0.63
1:EEE:2498:THR:HG21	1:EEE:2530:ARG:HB2	1.79	0.63
1:BBB:2498:THR:HG21	1:BBB:2530:ARG:HB2	1.80	0.62
1:CCC:2210:VAL:HG21	1:CCC:2253:PRO:HD3	1.82	0.62
1:BBB:2210:VAL:HG21	1:BBB:2253:PRO:HD3	1.83	0.60
1:FFF:2210:VAL:HG21	1:FFF:2253:PRO:HD3	1.84	0.59
5:EEE:2602:DG3:N2	2:OOO:5:DC:C2	2.72	0.58
1:BBB:2354:THR:CB	1:DDD:2140:GLU:HG2	2.37	0.55
5:EEE:2602:DG3:N2	2:OOO:5:DC:O2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:2212:PHE:HB3	1:CCC:2213:PRO:HD3	1.90	0.54
1:EEE:2212:PHE:HB3	1:EEE:2213:PRO:HD3	1.90	0.53
1:FFF:2212:PHE:HB3	1:FFF:2213:PRO:HD3	1.90	0.52
1:AAA:2212:PHE:HB3	1:AAA:2213:PRO:HD3	1.92	0.52
1:DDD:2012:PHE:O	1:DDD:2059:GLN:NE2	2.41	0.52
1:DDD:1931:VAL:HB	1:DDD:1932:PRO:CD	2.39	0.52
1:DDD:1824:SER:O	1:DDD:2019:LEU:HD21	2.10	0.52
1:DDD:1824:SER:C	1:DDD:1910:ARG:HH22	2.14	0.51
1:BBB:2212:PHE:HB3	1:BBB:2213:PRO:HD3	1.92	0.51
1:BBB:1897:ASP:OD1	1:BBB:1897:ASP:N	2.44	0.51
1:EEE:1897:ASP:OD1	1:EEE:1897:ASP:N	2.44	0.50
1:AAA:1897:ASP:OD1	1:AAA:1897:ASP:N	2.44	0.50
1:FFF:1897:ASP:N	1:FFF:1897:ASP:OD1	2.44	0.50
3:JJJ:2:DC:H2"	3:JJJ:3:DG:C8	2.47	0.50
1:CCC:1897:ASP:N	1:CCC:1897:ASP:OD1	2.44	0.50
3:RRR:2:DC:H2"	3:RRR:3:DG:C8	2.47	0.50
1:DDD:1897:ASP:OD1	1:DDD:1897:ASP:N	2.44	0.49
1:EEE:2369:ILE:HG22	1:EEE:2370:GLU:O	2.13	0.49
3:NNN:2:DC:H2"	3:NNN:3:DG:C8	2.48	0.49
3:PPP:2:DC:H2"	3:PPP:3:DG:C8	2.47	0.49
3:HHH:2:DC:H2"	3:HHH:3:DG:C8	2.48	0.49
3:LLL:2:DC:H2"	3:LLL:3:DG:C8	2.47	0.48
1:BBB:1830:VAL:HG11	1:BBB:1840:PHE:CG	2.49	0.48
1:FFF:2369:ILE:HG22	1:FFF:2370:GLU:O	2.13	0.48
1:EEE:2221:ASN:HD22	1:EEE:2224:LEU:HB2	1.78	0.48
1:BBB:2327:LEU:HD23	1:BBB:2328:ALA:N	2.28	0.48
1:CCC:2221:ASN:HD22	1:CCC:2224:LEU:HB2	1.79	0.48
1:EEE:1830:VAL:HG11	1:EEE:1840:PHE:CG	2.49	0.48
1:AAA:1830:VAL:HG11	1:AAA:1840:PHE:CG	2.49	0.48
1:DDD:1830:VAL:HG11	1:DDD:1840:PHE:CG	2.49	0.48
1:EEE:2327:LEU:HD23	1:EEE:2328:ALA:N	2.29	0.48
1:BBB:2369:ILE:HG22	1:BBB:2370:GLU:O	2.14	0.48
1:FFF:2221:ASN:HD22	1:FFF:2224:LEU:HB2	1.79	0.48
1:AAA:2221:ASN:HD22	1:AAA:2224:LEU:HB2	1.79	0.48
1:CCC:2327:LEU:HD23	1:CCC:2328:ALA:N	2.29	0.48
1:AAA:2191:HIS:CG	1:AAA:2192:PRO:HD2	2.49	0.48
1:CCC:2444:LEU:HD11	1:CCC:2483:ILE:HD11	1.96	0.48
1:BBB:2221:ASN:HD22	1:BBB:2224:LEU:HB2	1.79	0.48
1:BBB:2461:LYS:HG2	1:BBB:2465:GLU:OE1	2.14	0.48
1:DDD:2327:LEU:HD23	1:DDD:2328:ALA:N	2.29	0.47
1:EEE:2461:LYS:HG2	1:EEE:2465:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:2327:LEU:HD23	1:AAA:2328:ALA:N	2.29	0.47
1:CCC:1830:VAL:HG11	1:CCC:1840:PHE:CG	2.49	0.47
1:FFF:2191:HIS:CG	1:FFF:2192:PRO:HD2	2.50	0.47
1:EEE:1963:VAL:HG12	1:EEE:2053:ILE:CG2	2.45	0.47
1:EEE:2191:HIS:CG	1:EEE:2192:PRO:HD2	2.50	0.47
1:FFF:2327:LEU:HD23	1:FFF:2328:ALA:N	2.29	0.47
1:CCC:2191:HIS:CG	1:CCC:2192:PRO:HD2	2.50	0.47
1:DDD:2221:ASN:HD22	1:DDD:2224:LEU:HB2	1.79	0.47
1:DDD:2461:LYS:HG2	1:DDD:2465:GLU:OE1	2.15	0.47
1:FFF:1830:VAL:HG11	1:FFF:1840:PHE:CG	2.49	0.47
1:BBB:2331:TYR:CD2	1:BBB:2334:LEU:HD22	2.50	0.47
1:DDD:1974:LEU:HD13	1:DDD:1982:LEU:HD21	1.97	0.47
1:DDD:2191:HIS:CG	1:DDD:2192:PRO:HD2	2.50	0.47
1:AAA:2369:ILE:HG22	1:AAA:2370:GLU:O	2.14	0.46
1:DDD:2360:ARG:HG2	1:DDD:2374:VAL:HG21	1.97	0.46
1:CCC:2369:ILE:HG22	1:CCC:2370:GLU:O	2.14	0.46
1:AAA:2461:LYS:HG2	1:AAA:2465:GLU:OE1	2.15	0.46
1:EEE:2444:LEU:HD11	1:EEE:2483:ILE:HD11	1.96	0.46
1:AAA:2331:TYR:CD2	1:AAA:2334:LEU:HD22	2.51	0.46
1:BBB:1963:VAL:HG12	1:BBB:2053:ILE:CG2	2.46	0.46
1:BBB:2444:LEU:HD11	1:BBB:2483:ILE:HD11	1.97	0.46
1:CCC:2461:LYS:HG2	1:CCC:2465:GLU:OE1	2.15	0.46
1:DDD:2331:TYR:CD2	1:DDD:2334:LEU:HD22	2.50	0.46
1:DDD:2444:LEU:HD11	1:DDD:2483:ILE:HD11	1.96	0.46
1:BBB:1837:PHE:O	1:BBB:1841:ILE:HG12	2.16	0.46
1:AAA:2416:PHE:HE1	6:AAA:2603:K7X:BRAH	2.53	0.46
1:AAA:2444:LEU:HD11	1:AAA:2483:ILE:HD11	1.98	0.46
1:DDD:1837:PHE:O	1:DDD:1841:ILE:HG12	2.16	0.46
1:DDD:2496:HIS:CG	1:DDD:2498:THR:O	2.69	0.46
1:FFF:2496:HIS:CG	1:FFF:2498:THR:O	2.69	0.46
1:AAA:2496:HIS:CG	1:AAA:2498:THR:O	2.69	0.46
1:BBB:2191:HIS:CG	1:BBB:2192:PRO:HD2	2.51	0.46
1:CCC:2496:HIS:CG	1:CCC:2498:THR:O	2.68	0.46
1:AAA:1837:PHE:O	1:AAA:1841:ILE:HG12	2.16	0.46
1:CCC:1963:VAL:HG12	1:CCC:2053:ILE:CG2	2.46	0.46
1:CCC:2017:LEU:N	1:CCC:2018:PRO:CD	2.79	0.46
1:DDD:1963:VAL:HG12	1:DDD:2053:ILE:CG2	2.46	0.46
1:EEE:2496:HIS:CG	1:EEE:2498:THR:O	2.69	0.46
1:FFF:2331:TYR:CD2	1:FFF:2334:LEU:HD22	2.51	0.45
1:CCC:2331:TYR:CD2	1:CCC:2334:LEU:HD22	2.51	0.45
1:FFF:2444:LEU:HD11	1:FFF:2483:ILE:HD11	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:2369:ILE:HG22	1:DDD:2370:GLU:O	2.17	0.45
1:EEE:2331:TYR:CD2	1:EEE:2334:LEU:HD22	2.51	0.45
1:FFF:2461:LYS:HG2	1:FFF:2465:GLU:OE1	2.16	0.45
1:CCC:1837:PHE:O	1:CCC:1841:ILE:HG12	2.17	0.45
1:AAA:2017:LEU:N	1:AAA:2018:PRO:CD	2.80	0.45
1:FFF:2383:LYS:NZ	5:FFF:2602:DG3:O1G	2.48	0.45
1:AAA:1963:VAL:HG12	1:AAA:2053:ILE:CG2	2.47	0.45
1:AAA:2388:GLY:HA2	2:GGG:4:DC:C2	2.52	0.45
3:NNN:6:DT:H2"	3:NNN:7:DG:C8	2.52	0.45
1:BBB:2017:LEU:N	1:BBB:2018:PRO:CD	2.80	0.45
3:HHH:12:DT:H2'	3:HHH:13:DDG:H8	1.99	0.45
1:DDD:2017:LEU:N	1:DDD:2018:PRO:CD	2.80	0.45
2:GGG:2:DT:H6	2:GGG:2:DT:P	2.39	0.44
3:LLL:6:DT:H2"	3:LLL:7:DG:C8	2.51	0.44
3:RRR:6:DT:H2"	3:RRR:7:DG:C8	2.53	0.44
2:KKK:2:DT:P	2:KKK:2:DT:H6	2.41	0.44
1:EEE:2017:LEU:N	1:EEE:2018:PRO:CD	2.80	0.44
1:FFF:1963:VAL:HG12	1:FFF:2053:ILE:CG2	2.46	0.44
2:III:2:DT:P	2:III:2:DT:H6	2.41	0.44
1:EEE:1837:PHE:O	1:EEE:1841:ILE:HG12	2.17	0.44
1:EEE:2559:LYS:HD3	1:EEE:2590:VAL:HB	1.99	0.44
1:CCC:2477:ALA:O	1:CCC:2481:VAL:HG23	2.18	0.44
1:AAA:2310:PHE:CE2	1:BBB:2190:LEU:HD11	2.52	0.44
1:FFF:1837:PHE:O	1:FFF:1841:ILE:HG12	2.17	0.44
2:OOO:2:DT:P	2:OOO:2:DT:H6	2.41	0.44
2:QQQ:2:DT:P	2:QQQ:2:DT:H6	2.41	0.44
1:DDD:2477:ALA:O	1:DDD:2481:VAL:HG23	2.18	0.43
1:FFF:2017:LEU:N	1:FFF:2018:PRO:CD	2.80	0.43
3:HHH:6:DT:H2"	3:HHH:7:DG:C8	2.52	0.43
1:AAA:2338:ILE:HD11	1:AAA:2480:ILE:CD1	2.42	0.43
1:AAA:2354:THR:O	1:AAA:2355:GLY:O	2.36	0.43
1:BBB:2093:GLY:HA2	1:BBB:2228:ARG:HG2	2.01	0.43
1:CCC:2360:ARG:HG2	1:CCC:2374:VAL:HG21	2.01	0.43
1:FFF:2360:ARG:HG2	1:FFF:2374:VAL:HG21	2.00	0.43
1:FFF:2354:THR:O	1:FFF:2355:GLY:O	2.37	0.43
2:MMM:2:DT:H6	2:MMM:2:DT:P	2.41	0.43
3:PPP:6:DT:H2"	3:PPP:7:DG:C8	2.53	0.43
1:DDD:2184:LEU:HB2	1:DDD:2198:LEU:HD21	2.01	0.43
1:BBB:2559:LYS:HD3	1:BBB:2590:VAL:HB	2.00	0.43
1:BBB:2354:THR:O	1:BBB:2355:GLY:O	2.37	0.42
1:BBB:2477:ALA:O	1:BBB:2481:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:2354:THR:O	1:DDD:2355:GLY:O	2.37	0.42
3:JJJ:6:DT:H2"	3:JJJ:7:DG:C8	2.54	0.42
1:CCC:2144:PRO:HG3	1:FFF:2105:ILE:HD11	2.00	0.42
1:CCC:2354:THR:O	1:CCC:2355:GLY:O	2.37	0.42
1:FFF:2477:ALA:O	1:FFF:2481:VAL:HG23	2.19	0.42
1:CCC:1974:LEU:HD13	1:CCC:1982:LEU:HD21	2.02	0.42
1:EEE:2354:THR:O	1:EEE:2355:GLY:O	2.37	0.42
1:AAA:2093:GLY:HA2	1:AAA:2228:ARG:HG2	2.01	0.42
1:CCC:2359:PHE:CD1	1:CCC:2383:LYS:HA	2.55	0.42
1:EEE:2093:GLY:HA2	1:EEE:2228:ARG:HG2	1.99	0.42
1:BBB:2327:LEU:HD23	1:BBB:2327:LEU:C	2.40	0.42
1:FFF:2093:GLY:HA2	1:FFF:2228:ARG:HG2	2.01	0.42
3:LLL:12:DT:H2'	3:LLL:13:DDG:H8	2.02	0.42
1:AAA:2477:ALA:O	1:AAA:2481:VAL:HG23	2.19	0.42
6:AAA:2603:K7X:CAU	6:AAA:2603:K7X:CAP	2.94	0.42
1:CCC:2184:LEU:HB2	1:CCC:2198:LEU:HD21	2.01	0.42
1:BBB:1892:ILE:HD12	1:BBB:1898:THR:HB	2.02	0.42
1:DDD:2321:PHE:CE2	1:DDD:2545:GLU:HG2	2.55	0.42
1:AAA:2184:LEU:HB2	1:AAA:2198:LEU:HD21	2.02	0.41
1:EEE:2327:LEU:HD23	1:EEE:2327:LEU:C	2.41	0.41
1:AAA:2390:ILE:CD1	6:AAA:2603:K7X:BRAH	3.18	0.41
1:EEE:1892:ILE:HD12	1:EEE:1898:THR:HB	2.01	0.41
1:EEE:2477:ALA:O	1:EEE:2481:VAL:HG23	2.19	0.41
1:AAA:2321:PHE:CE2	1:AAA:2545:GLU:HG2	2.55	0.41
1:BBB:2321:PHE:CE2	1:BBB:2545:GLU:HG2	2.55	0.41
1:BBB:2338:ILE:HD11	1:BBB:2480:ILE:CD1	2.44	0.41
1:BBB:2356:ALA:HB3	1:DDD:2122:GLY:O	2.20	0.41
1:CCC:2093:GLY:HA2	1:CCC:2228:ARG:HG2	2.01	0.41
1:EEE:2321:PHE:CE2	1:EEE:2545:GLU:HG2	2.55	0.41
1:AAA:2359:PHE:CD1	1:AAA:2383:LYS:HA	2.56	0.41
1:CCC:1892:ILE:HD12	1:CCC:1898:THR:HB	2.01	0.41
1:CCC:2327:LEU:HD23	1:CCC:2327:LEU:C	2.41	0.41
1:DDD:2093:GLY:HA2	1:DDD:2228:ARG:HG2	2.02	0.41
1:EEE:2360:ARG:HG2	1:EEE:2374:VAL:HG21	2.03	0.41
1:FFF:2359:PHE:CD1	1:FFF:2383:LYS:HA	2.56	0.41
1:AAA:2214:LEU:HD22	1:AAA:2229:ILE:HD13	2.01	0.41
1:BBB:2455:ASP:OD2	1:BBB:2460:ARG:NH1	2.51	0.41
1:DDD:2210:VAL:HG21	1:DDD:2253:PRO:CD	2.49	0.41
1:AAA:2226:MET:SD	1:AAA:2321:PHE:HA	2.60	0.41
1:AAA:2327:LEU:HD23	1:AAA:2327:LEU:C	2.41	0.41
1:AAA:2362:ILE:HG12	6:AAA:2603:K7X:CAP	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:2359:PHE:CD1	1:BBB:2383:LYS:HA	2.56	0.41
1:DDD:1892:ILE:HD12	1:DDD:1898:THR:HB	2.02	0.41
1:DDD:2226:MET:SD	1:DDD:2321:PHE:HA	2.61	0.41
1:AAA:1892:ILE:HD12	1:AAA:1898:THR:HB	2.01	0.41
1:BBB:2193:LEU:HB3	1:BBB:2194:PRO:HD3	2.03	0.41
1:BBB:2333:GLN:HB3	1:BBB:2336:LEU:HB2	2.03	0.41
1:BBB:2360:ARG:HG2	1:BBB:2374:VAL:HG21	2.02	0.41
1:CCC:2226:MET:SD	1:CCC:2321:PHE:HA	2.61	0.41
1:DDD:2327:LEU:HD23	1:DDD:2327:LEU:C	2.41	0.41
1:EEE:1995:LEU:HD12	1:EEE:1995:LEU:HA	1.94	0.41
1:EEE:2359:PHE:CD1	1:EEE:2383:LYS:HA	2.55	0.41
1:EEE:2533:PHE:CD1	1:EEE:2533:PHE:N	2.89	0.41
1:FFF:1892:ILE:HD12	1:FFF:1898:THR:HB	2.02	0.41
1:FFF:2559:LYS:HD3	1:FFF:2590:VAL:HB	2.03	0.41
1:AAA:1974:LEU:HD13	1:AAA:1982:LEU:HD21	2.03	0.41
1:BBB:2533:PHE:CD1	1:BBB:2533:PHE:N	2.89	0.41
1:CCC:2087:LEU:C	1:CCC:2087:LEU:HD23	2.42	0.41
1:FFF:2321:PHE:CE2	1:FFF:2545:GLU:HG2	2.55	0.41
1:FFF:2540:ASP:OD2	5:FFF:2602:DG3:O2A	2.39	0.41
1:CCC:2321:PHE:CE2	1:CCC:2545:GLU:HG2	2.56	0.40
1:FFF:2455:ASP:OD2	1:FFF:2460:ARG:NH1	2.52	0.40
1:FFF:2533:PHE:CD1	1:FFF:2533:PHE:N	2.89	0.40
1:CCC:2338:ILE:HD11	1:CCC:2480:ILE:CD1	2.41	0.40
1:DDD:2087:LEU:C	1:DDD:2087:LEU:HD23	2.42	0.40
1:EEE:2226:MET:SD	1:EEE:2321:PHE:HA	2.61	0.40
1:FFF:2327:LEU:HD23	1:FFF:2327:LEU:C	2.41	0.40
1:AAA:2533:PHE:N	1:AAA:2533:PHE:CD1	2.89	0.40
1:DDD:2333:GLN:HB3	1:DDD:2336:LEU:HB2	2.03	0.40
1:FFF:1974:LEU:HD13	1:FFF:1982:LEU:HD21	2.04	0.40
3:PPP:12:DT:H2'	3:PPP:13:DDG:H8	2.03	0.40

There are no symmetry-related clashes.

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	AAA	629/726 (87%)	610 (97%)	17 (3%)	2 (0%)	41	76
1	BBB	617/726 (85%)	598 (97%)	17 (3%)	2 (0%)	41	76
1	CCC	628/726 (86%)	607 (97%)	19 (3%)	2 (0%)	41	76
1	DDD	623/726 (86%)	602 (97%)	18 (3%)	3 (0%)	29	68
1	EEE	620/726 (85%)	599 (97%)	19 (3%)	2 (0%)	41	76
1	FFF	624/726 (86%)	604 (97%)	18 (3%)	2 (0%)	41	76
All	All	3741/4356 (86%)	3620 (97%)	108 (3%)	13 (0%)	41	76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	1825	LEU
1	AAA	2355	GLY
1	BBB	2355	GLY
1	CCC	2355	GLY
1	DDD	2355	GLY
1	EEE	2355	GLY
1	FFF	2355	GLY
1	AAA	2356	ALA
1	BBB	2356	ALA
1	DDD	2356	ALA
1	EEE	2356	ALA
1	FFF	2356	ALA
1	CCC	2356	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	AAA	502/638 (79%)	475 (95%)	27 (5%)	22	57
1	BBB	494/638 (77%)	472 (96%)	22 (4%)	27	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CCC	494/638 (77%)	468 (95%)	26 (5%)	22 58
1	DDD	491/638 (77%)	468 (95%)	23 (5%)	26 63
1	EEE	493/638 (77%)	468 (95%)	25 (5%)	24 60
1	FFF	490/638 (77%)	469 (96%)	21 (4%)	29 66
All	All	2964/3828 (77%)	2820 (95%)	144 (5%)	25 61

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1825	LEU
1	AAA	1829	ASP
1	AAA	1835	ASN
1	AAA	1839	THR
1	AAA	1843	GLU
1	AAA	1897	ASP
1	AAA	1898	THR
1	AAA	1903	LEU
1	AAA	1915	PHE
1	AAA	2096	THR
1	AAA	2119	GLN
1	AAA	2181	LYS
1	AAA	2201	ARG
1	AAA	2209	LYS
1	AAA	2311	SER
1	AAA	2314	MET
1	AAA	2330	ASP
1	AAA	2368	MET
1	AAA	2371	PRO
1	AAA	2377	ASP
1	AAA	2401	GLN
1	AAA	2408	ASP
1	AAA	2418	SER
1	AAA	2424	ASN
1	AAA	2428	THR
1	AAA	2508	MET
1	AAA	2537	GLN
1	BBB	1825	LEU
1	BBB	1829	ASP
1	BBB	1835	ASN
1	BBB	1839	THR
1	BBB	1843	GLU

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Mol	Chain	Res	Type
1	BBB	1896	ASP
1	BBB	1897	ASP
1	BBB	1898	THR
1	BBB	1903	LEU
1	BBB	1915	PHE
1	BBB	2096	THR
1	BBB	2119	GLN
1	BBB	2181	LYS
1	BBB	2201	ARG
1	BBB	2311	SER
1	BBB	2314	MET
1	BBB	2330	ASP
1	BBB	2368	MET
1	BBB	2401	GLN
1	BBB	2408	ASP
1	BBB	2424	ASN
1	BBB	2537	GLN
1	CCC	1825	LEU
1	CCC	1829	ASP
1	CCC	1835	ASN
1	CCC	1839	THR
1	CCC	1843	GLU
1	CCC	1897	ASP
1	CCC	1898	THR
1	CCC	1903	LEU
1	CCC	1915	PHE
1	CCC	2096	THR
1	CCC	2119	GLN
1	CCC	2181	LYS
1	CCC	2201	ARG
1	CCC	2209	LYS
1	CCC	2311	SER
1	CCC	2314	MET
1	CCC	2330	ASP
1	CCC	2368	MET
1	CCC	2377	ASP
1	CCC	2401	GLN
1	CCC	2408	ASP
1	CCC	2424	ASN
1	CCC	2428	THR
1	CCC	2508	MET
1	CCC	2537	GLN

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Mol	Chain	Res	Type
1	CCC	2564	SER
1	DDD	1829	ASP
1	DDD	1835	ASN
1	DDD	1839	THR
1	DDD	1843	GLU
1	DDD	1897	ASP
1	DDD	1898	THR
1	DDD	1903	LEU
1	DDD	1915	PHE
1	DDD	2013	LEU
1	DDD	2096	THR
1	DDD	2119	GLN
1	DDD	2181	LYS
1	DDD	2201	ARG
1	DDD	2209	LYS
1	DDD	2314	MET
1	DDD	2330	ASP
1	DDD	2368	MET
1	DDD	2377	ASP
1	DDD	2401	GLN
1	DDD	2408	ASP
1	DDD	2424	ASN
1	DDD	2428	THR
1	DDD	2537	GLN
1	EEE	1825	LEU
1	EEE	1829	ASP
1	EEE	1835	ASN
1	EEE	1839	THR
1	EEE	1843	GLU
1	EEE	1897	ASP
1	EEE	1898	THR
1	EEE	1903	LEU
1	EEE	1915	PHE
1	EEE	2096	THR
1	EEE	2119	GLN
1	EEE	2181	LYS
1	EEE	2201	ARG
1	EEE	2209	LYS
1	EEE	2311	SER
1	EEE	2314	MET
1	EEE	2330	ASP
1	EEE	2368	MET

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Mol	Chain	Res	Type
1	EEE	2377	ASP
1	EEE	2401	GLN
1	EEE	2408	ASP
1	EEE	2418	SER
1	EEE	2424	ASN
1	EEE	2537	GLN
1	EEE	2564	SER
1	FFF	1825	LEU
1	FFF	1829	ASP
1	FFF	1835	ASN
1	FFF	1839	THR
1	FFF	1843	GLU
1	FFF	1897	ASP
1	FFF	1898	THR
1	FFF	1903	LEU
1	FFF	1915	PHE
1	FFF	2096	THR
1	FFF	2119	GLN
1	FFF	2201	ARG
1	FFF	2209	LYS
1	FFF	2314	MET
1	FFF	2330	ASP
1	FFF	2368	MET
1	FFF	2401	GLN
1	FFF	2408	ASP
1	FFF	2424	ASN
1	FFF	2428	THR
1	FFF	2537	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
3	DDG	JJJ	13	2,3	17,23,24	1.04	1 (5%)	15,33,36	1.65	2 (13%)
3	DDG	HHH	13	2,3	17,23,24	1.14	2 (11%)	15,33,36	1.74	3 (20%)
3	DDG	NNN	13	2,3	17,23,24	1.15	2 (11%)	15,33,36	1.45	2 (13%)
3	DDG	LLL	13	2,3	17,23,24	1.04	1 (5%)	15,33,36	1.76	6 (40%)
3	DDG	RRR	13	2,3	17,23,24	1.01	1 (5%)	15,33,36	1.67	2 (13%)
3	DDG	PPP	13	2,3	17,23,24	1.02	1 (5%)	15,33,36	1.67	2 (13%)

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
3	DDG	JJJ	13	2,3	-	2/3/18/19	0/3/3/3
3	DDG	HHH	13	2,3	-	2/3/18/19	0/3/3/3
3	DDG	NNN	13	2,3	-	2/3/18/19	0/3/3/3
3	DDG	LLL	13	2,3	-	2/3/18/19	0/3/3/3
3	DDG	RRR	13	2,3	-	2/3/18/19	0/3/3/3
3	DDG	PPP	13	2,3	-	2/3/18/19	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	JJJ	13	DDG	C6-N1	-2.98	1.33	1.37
3	LLL	13	DDG	C6-N1	-2.93	1.33	1.37
3	PPP	13	DDG	C6-N1	-2.84	1.33	1.37
3	HHH	13	DDG	C6-N1	-2.78	1.33	1.37
3	RRR	13	DDG	C6-N1	-2.72	1.33	1.37
3	NNN	13	DDG	C6-N1	-2.53	1.34	1.37
3	NNN	13	DDG	C8-N7	2.09	1.38	1.35
3	HHH	13	DDG	O5'-C5'	-2.00	1.39	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	PPP	13	DDG	C3'-C2'-C1'	3.75	107.12	102.78
3	JJJ	13	DDG	C3'-C2'-C1'	3.54	106.87	102.78
3	HHH	13	DDG	C3'-C2'-C1'	3.40	106.71	102.78
3	RRR	13	DDG	C3'-C2'-C1'	3.04	106.29	102.78
3	NNN	13	DDG	C8-N7-C5	2.78	108.28	102.99
3	JJJ	13	DDG	C8-N7-C5	2.75	108.23	102.99
3	LLL	13	DDG	C8-N7-C5	2.70	108.13	102.99
3	RRR	13	DDG	C8-N7-C5	2.67	108.08	102.99
3	PPP	13	DDG	C8-N7-C5	2.62	107.98	102.99
3	NNN	13	DDG	C3'-C2'-C1'	2.55	105.73	102.78
3	LLL	13	DDG	C2'-C3'-C4'	2.53	107.47	102.72
3	HHH	13	DDG	C8-N7-C5	2.31	107.40	102.99
3	HHH	13	DDG	O6-C6-C5	-2.23	120.01	124.37
3	LLL	13	DDG	O4'-C1'-C2'	2.16	109.01	106.67
3	LLL	13	DDG	O6-C6-C5	-2.12	120.22	124.37
3	LLL	13	DDG	C5-C6-N1	2.10	117.66	113.95
3	LLL	13	DDG	N2-C2-N3	-2.02	115.81	119.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	HHH	13	DDG	O4'-C4'-C5'-O5'
3	JJJ	13	DDG	O4'-C4'-C5'-O5'
3	LLL	13	DDG	O4'-C4'-C5'-O5'
3	NNN	13	DDG	O4'-C4'-C5'-O5'
3	PPP	13	DDG	O4'-C4'-C5'-O5'
3	RRR	13	DDG	O4'-C4'-C5'-O5'
3	HHH	13	DDG	C3'-C4'-C5'-O5'
3	JJJ	13	DDG	C3'-C4'-C5'-O5'
3	LLL	13	DDG	C3'-C4'-C5'-O5'
3	NNN	13	DDG	C3'-C4'-C5'-O5'
3	PPP	13	DDG	C3'-C4'-C5'-O5'
3	RRR	13	DDG	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	HHH	13	DDG	1	0
3	LLL	13	DDG	1	0
3	PPP	13	DDG	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	DG3	DDD	2602	4	25,32,32	0.94	1 (4%)	28,50,50	1.01	2 (7%)
5	DG3	CCC	2602	4	25,32,32	0.98	3 (12%)	28,50,50	1.28	3 (10%)
5	DG3	AAA	2602	4	25,32,32	0.99	2 (8%)	28,50,50	1.07	2 (7%)
5	DG3	EEE	2602	4	25,32,32	0.99	2 (8%)	28,50,50	1.23	1 (3%)
5	DG3	FFF	2602	4	25,32,32	0.93	2 (8%)	28,50,50	1.17	3 (10%)
6	K7X	AAA	2603	-	28,29,29	1.14	2 (7%)	37,42,42	1.60	7 (18%)
5	DG3	BBB	2602	4	25,32,32	0.99	3 (12%)	28,50,50	1.21	4 (14%)

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
5	DG3	DDD	2602	4	-	9/18/31/31	0/3/3/3
5	DG3	CCC	2602	4	-	7/18/31/31	0/3/3/3
5	DG3	AAA	2602	4	-	1/18/31/31	0/3/3/3
5	DG3	EEE	2602	4	-	9/18/31/31	0/3/3/3
5	DG3	FFF	2602	4	-	9/18/31/31	0/3/3/3
6	K7X	AAA	2603	-	-	1/22/23/23	0/2/2/2
5	DG3	BBB	2602	4	-	5/18/31/31	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AAA	2603	K7X	CAT-NAS	-4.82	1.33	1.43
5	CCC	2602	DG3	C5-C6	-3.05	1.41	1.47
5	DDD	2602	DG3	C5-C6	-2.70	1.41	1.47
5	AAA	2602	DG3	C5-C6	-2.70	1.41	1.47
5	BBB	2602	DG3	C5-C6	-2.68	1.42	1.47
5	EEE	2602	DG3	C5-C6	-2.65	1.42	1.47
5	FFF	2602	DG3	C5-C6	-2.55	1.42	1.47
5	BBB	2602	DG3	C8-N7	-2.22	1.31	1.35
5	CCC	2602	DG3	C5-C4	-2.20	1.37	1.43
6	AAA	2603	K7X	CAA-NAF	2.13	1.35	1.32
5	CCC	2602	DG3	C8-N7	-2.13	1.31	1.35
5	BBB	2602	DG3	C5-C4	-2.08	1.37	1.43
5	EEE	2602	DG3	C8-N7	-2.08	1.31	1.35
5	FFF	2602	DG3	C8-N7	-2.07	1.31	1.35
5	AAA	2602	DG3	C5-C4	-2.01	1.37	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	EEE	2602	DG3	PA-O3A-PB	-3.92	119.39	132.83
6	AAA	2603	K7X	CAI-CAC-CAD	-3.56	117.73	122.38
5	BBB	2602	DG3	O2A-PA-O1A	3.17	127.89	112.24
5	FFF	2602	DG3	PA-O3A-PB	-3.13	122.08	132.83
6	AAA	2603	K7X	CAA-NAF-CAE	2.97	120.95	118.11
6	AAA	2603	K7X	CAZ-CAX-CAY	-2.77	116.84	120.94
5	CCC	2602	DG3	C3'-C2'-C1'	2.72	105.92	102.78
6	AAA	2603	K7X	CAY-CAT-NAS	-2.72	115.95	119.85
5	FFF	2602	DG3	PB-O3B-PG	-2.62	123.84	132.83
5	CCC	2602	DG3	PB-O3B-PG	-2.60	123.92	132.83
6	AAA	2603	K7X	BRAH-CAD-CAC	-2.52	117.04	121.17
6	AAA	2603	K7X	CAP-OAO-CAA	-2.36	113.58	116.86
5	AAA	2602	DG3	O6-C6-C5	2.35	128.96	124.37
5	DDD	2602	DG3	O6-C6-C5	2.33	128.93	124.37
5	CCC	2602	DG3	O6-C6-C5	2.26	128.78	124.37
5	AAA	2602	DG3	PB-O3B-PG	-2.20	125.29	132.83
6	AAA	2603	K7X	CAG-CAE-NAF	2.19	119.87	116.49
5	FFF	2602	DG3	O6-C6-C5	2.15	128.57	124.37
5	BBB	2602	DG3	C4'-O4'-C1'	-2.10	107.82	109.81
5	DDD	2602	DG3	PA-O3A-PB	-2.10	125.63	132.83
5	BBB	2602	DG3	O6-C6-C5	2.05	128.37	124.37
5	BBB	2602	DG3	O3B-PG-O1G	-2.02	99.96	111.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CCC	2602	DG3	PB-O3B-PG-O2G
5	CCC	2602	DG3	PB-O3B-PG-O3G
5	CCC	2602	DG3	C5'-O5'-PA-O2A
5	DDD	2602	DG3	PB-O3B-PG-O2G
5	DDD	2602	DG3	C5'-O5'-PA-O1A
5	DDD	2602	DG3	C5'-O5'-PA-O2A
5	EEE	2602	DG3	PB-O3B-PG-O2G
5	EEE	2602	DG3	C5'-O5'-PA-O2A
5	FFF	2602	DG3	PB-O3B-PG-O2G
5	FFF	2602	DG3	C5'-O5'-PA-O2A
5	BBB	2602	DG3	PB-O3B-PG-O1G
5	EEE	2602	DG3	PA-O3A-PB-O1B
5	FFF	2602	DG3	PA-O3A-PB-O1B
6	AAA	2603	K7X	CBB-CBA-NAS-CAQ
5	CCC	2602	DG3	C5'-O5'-PA-O3A
5	EEE	2602	DG3	C5'-O5'-PA-O3A
5	FFF	2602	DG3	C5'-O5'-PA-O3A
5	CCC	2602	DG3	PA-O3A-PB-O2B
5	DDD	2602	DG3	PA-O3A-PB-O2B
5	DDD	2602	DG3	PB-O3A-PA-O1A
5	EEE	2602	DG3	PB-O3A-PA-O2A
5	FFF	2602	DG3	PB-O3A-PA-O2A
5	CCC	2602	DG3	C5'-O5'-PA-O1A
5	EEE	2602	DG3	C5'-O5'-PA-O1A
5	FFF	2602	DG3	C5'-O5'-PA-O1A
5	BBB	2602	DG3	PB-O3A-PA-O2A
5	EEE	2602	DG3	PA-O3A-PB-O2B
5	FFF	2602	DG3	PA-O3A-PB-O2B
5	BBB	2602	DG3	PG-O3B-PB-O1B
5	DDD	2602	DG3	PA-O3A-PB-O1B
5	DDD	2602	DG3	PB-O3A-PA-O2A
5	EEE	2602	DG3	PB-O3A-PA-O1A
5	FFF	2602	DG3	PB-O3A-PA-O1A
5	DDD	2602	DG3	PB-O3B-PG-O3G
5	EEE	2602	DG3	PB-O3B-PG-O3G
5	FFF	2602	DG3	PB-O3B-PG-O3G
5	DDD	2602	DG3	C5'-O5'-PA-O3A
5	AAA	2602	DG3	PG-O3B-PB-O2B
5	BBB	2602	DG3	PG-O3B-PB-O2B
5	BBB	2602	DG3	PB-O3A-PA-O1A
5	CCC	2602	DG3	PB-O3A-PA-O2A

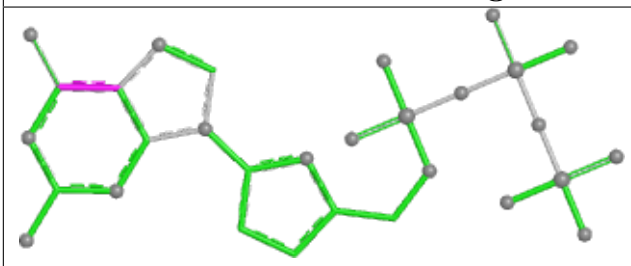
There are no ring outliers.

4 monomers are involved in 11 short contacts:

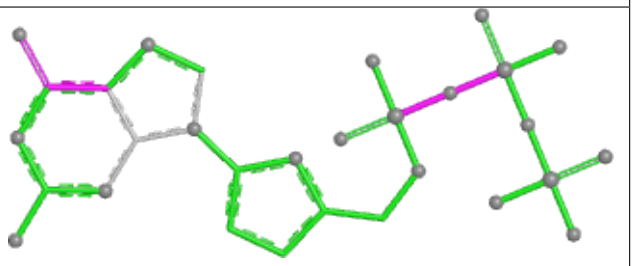
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	2602	DG3	1	0
5	EEE	2602	DG3	2	0
5	FFF	2602	DG3	2	0
6	AAA	2603	K7X	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

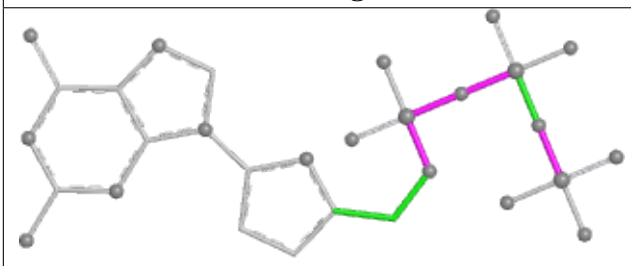
Ligand DG3 DDD 2602



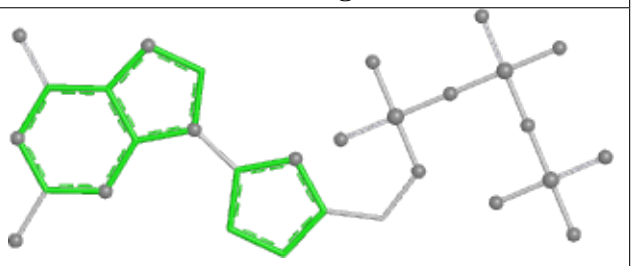
Bond lengths



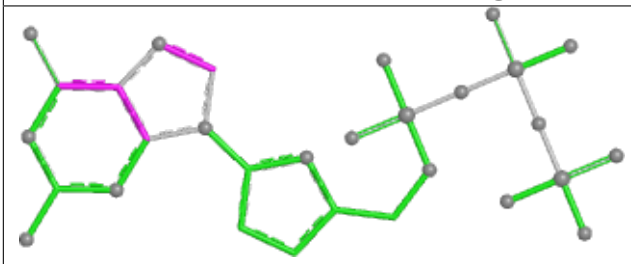
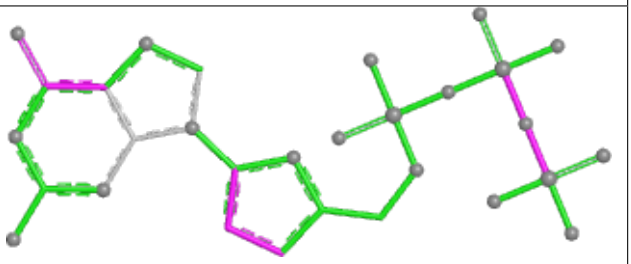
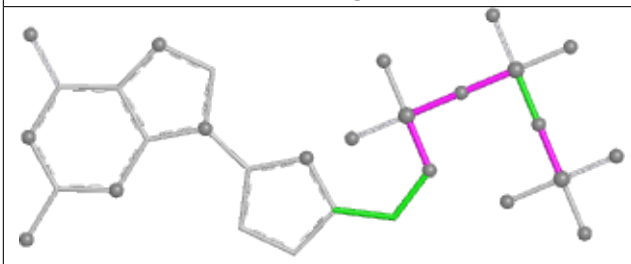
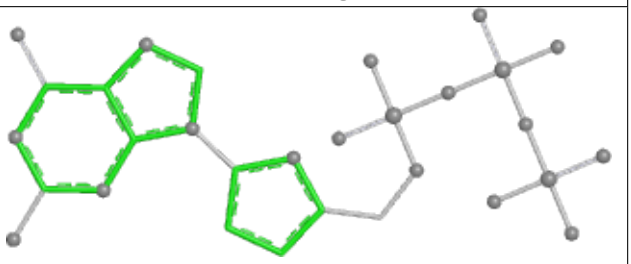
Bond angles

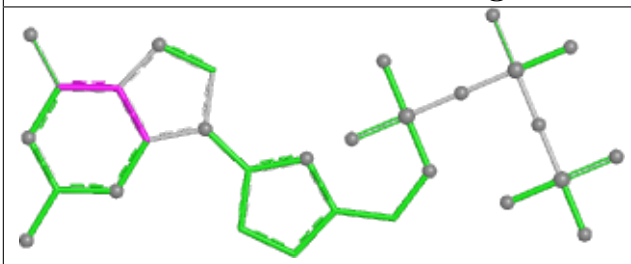
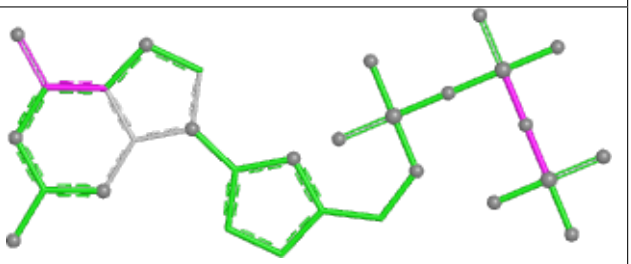
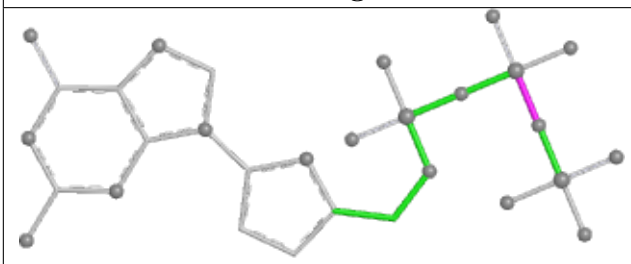
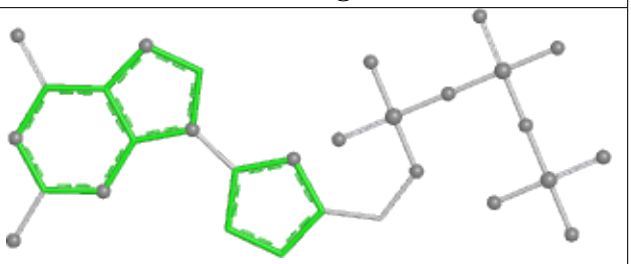


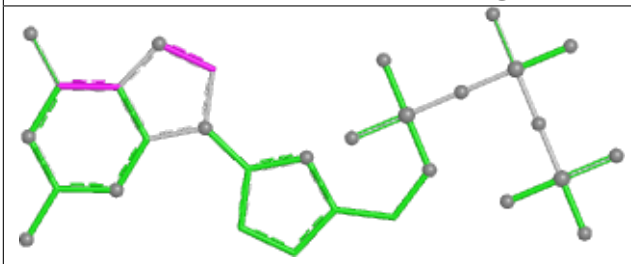
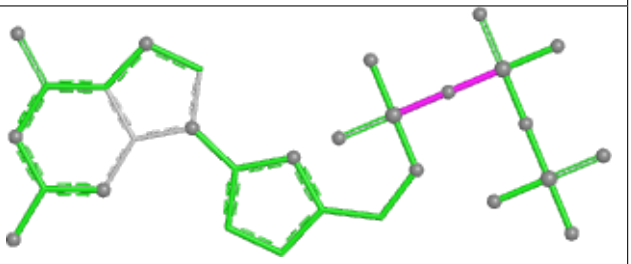
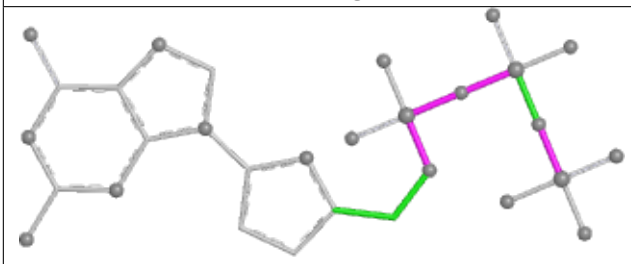
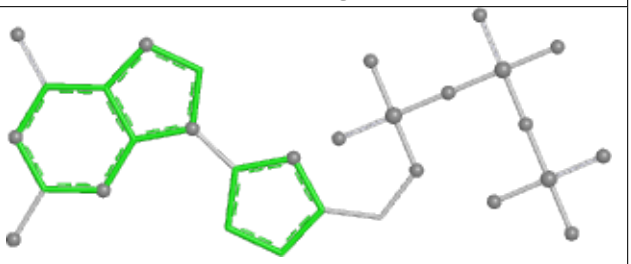
Torsions

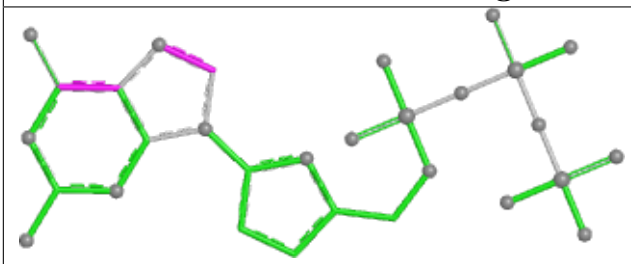
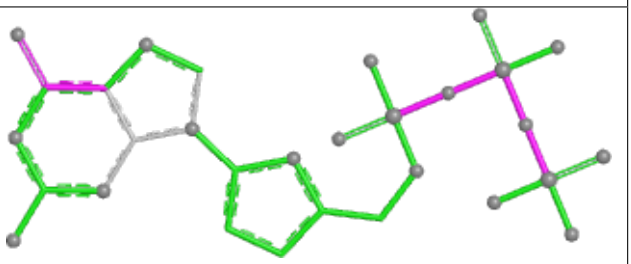
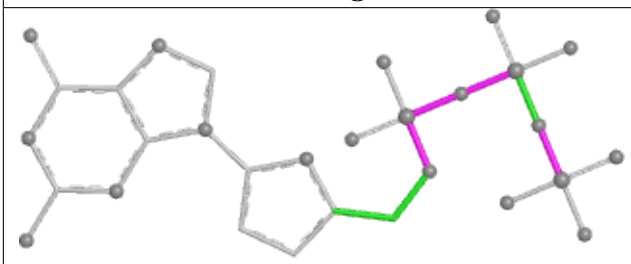
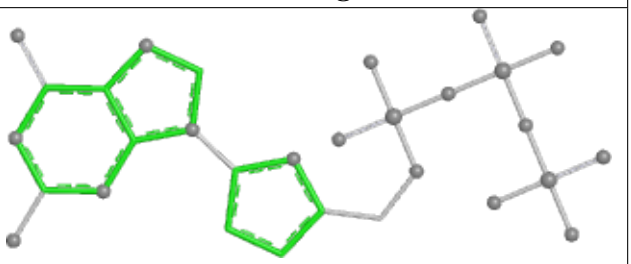


Rings

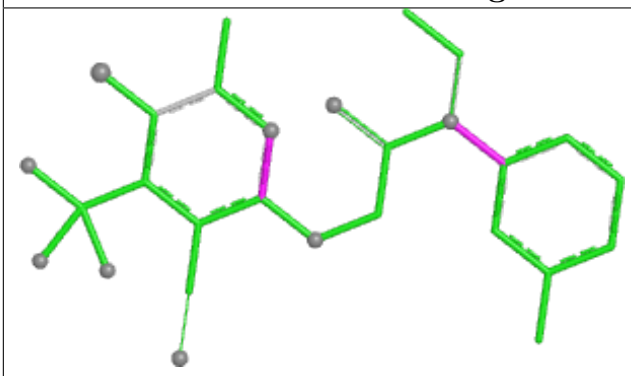
Ligand DG3 CCC 2602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DG3 AAA 2602	
 Bond lengths	 Bond angles
 Torsions	 Rings

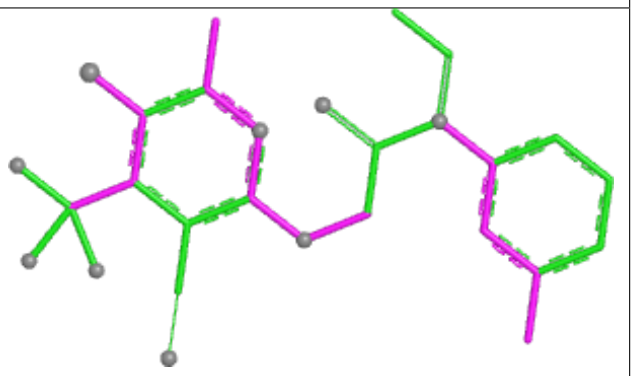
Ligand DG3 EEE 2602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DG3 FFF 2602	
 Bond lengths	 Bond angles
 Torsions	 Rings

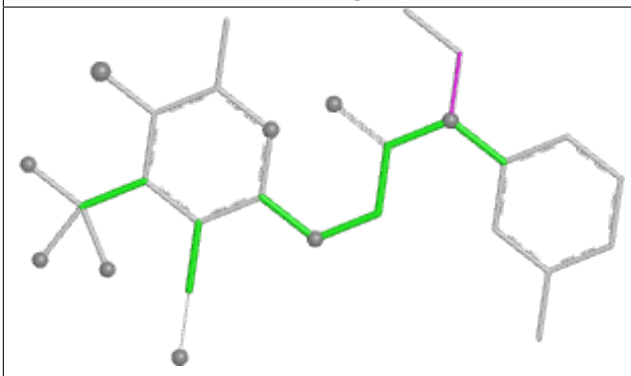
Ligand K7X AAA 2603



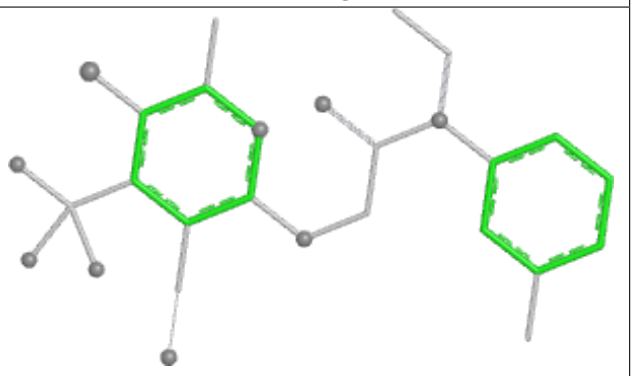
Bond lengths



Bond angles

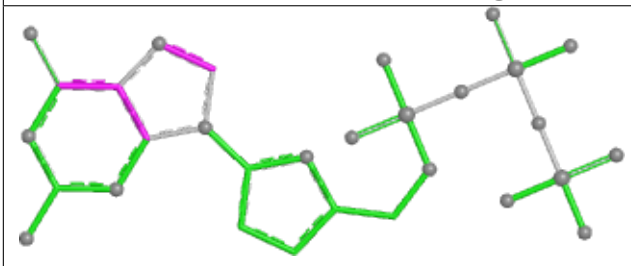


Torsions

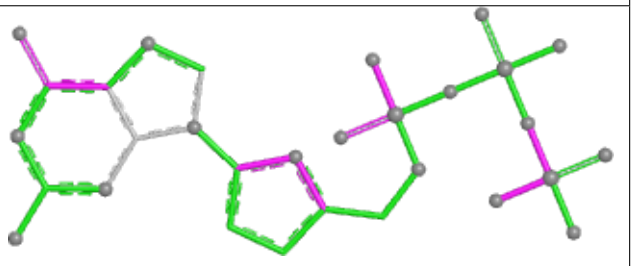


Rings

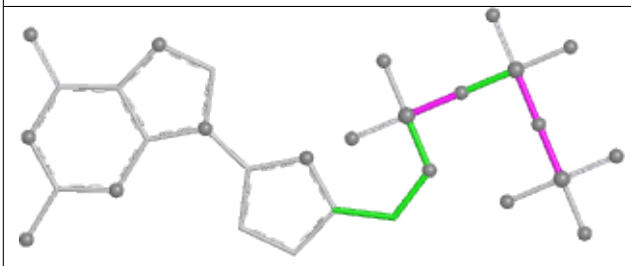
Ligand DG3 BBB 2602



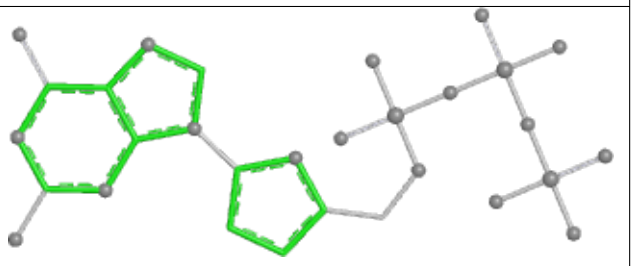
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 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	AAA	639/726 (88%)	0.30	18 (2%) 53 25	43, 79, 138, 199	0
1	BBB	629/726 (86%)	0.41	34 (5%) 25 9	49, 88, 154, 193	0
1	CCC	638/726 (87%)	0.35	34 (5%) 26 10	50, 93, 156, 211	0
1	DDD	633/726 (87%)	0.53	59 (9%) 8 3	59, 104, 169, 232	0
1	EEE	632/726 (87%)	0.54	67 (10%) 6 2	62, 116, 173, 211	0
1	FFF	634/726 (87%)	0.72	85 (13%) 3 1	75, 134, 188, 230	0
2	GGG	16/16 (100%)	-0.12	0 100 100	47, 96, 160, 170	0
2	III	16/16 (100%)	-0.31	0 100 100	57, 113, 151, 179	0
2	KKK	16/16 (100%)	0.07	2 (12%) 3 1	63, 124, 198, 200	0
2	MMM	16/16 (100%)	-0.21	0 100 100	60, 105, 167, 205	0
2	OOO	16/16 (100%)	-0.39	0 100 100	83, 146, 206, 207	0
2	QQQ	16/16 (100%)	-0.50	0 100 100	82, 154, 221, 229	0
3	HHH	12/13 (92%)	-0.28	0 100 100	50, 104, 151, 170	0
3	JJJ	12/13 (92%)	-0.34	0 100 100	50, 135, 155, 172	0
3	LLL	12/13 (92%)	-0.34	0 100 100	66, 117, 161, 162	0
3	NNN	12/13 (92%)	-0.51	0 100 100	59, 118, 148, 157	0
3	PPP	12/13 (92%)	-0.64	0 100 100	73, 161, 225, 229	0
3	RRR	12/13 (92%)	-0.08	0 100 100	85, 178, 212, 219	0
All	All	3973/4530 (87%)	0.44	299 (7%) 14 4	43, 103, 173, 232	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	2404	ILE	14.6
1	AAA	1896	ASP	11.7
1	FFF	2403	GLY	11.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	2412	TYR	8.6
1	FFF	2404	ILE	8.6
1	EEE	2416	PHE	8.6
1	CCC	1896	ASP	8.4
1	EEE	2404	ILE	8.0
1	FFF	2416	PHE	7.9
1	FFF	2412	TYR	7.7
1	EEE	2412	TYR	7.6
1	BBB	2403	GLY	7.5
1	FFF	2498	THR	7.4
1	BBB	2416	PHE	7.3
1	DDD	2026	SER	7.1
1	DDD	2531	GLY	6.7
1	EEE	2403	GLY	6.2
1	BBB	2401	GLN	6.1
1	EEE	2402	MET	6.1
1	FFF	2409	ALA	6.0
1	FFF	2395	ALA	5.4
1	FFF	2359	PHE	5.3
1	FFF	2405	LYS	5.0
1	FFF	1889	GLY	5.0
1	FFF	1886	ARG	5.0
1	EEE	2366	TRP	5.0
1	FFF	2402	MET	5.0
1	DDD	1897	ASP	4.9
1	FFF	2497	SER	4.9
1	BBB	2026	SER	4.8
1	EEE	2398	LEU	4.8
1	DDD	2588	PHE	4.7
1	FFF	2064	LEU	4.6
1	FFF	2408	ASP	4.6
1	DDD	2409	ALA	4.6
1	FFF	2495	PHE	4.6
1	DDD	2398	LEU	4.5
1	FFF	2406	GLU	4.5
1	FFF	2137	LEU	4.4
1	DDD	2027	GLN	4.4
1	DDD	2362	ILE	4.4
1	FFF	2348	LEU	4.4
1	DDD	1896	ASP	4.3
1	FFF	2364	ALA	4.3
1	DDD	2497	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	CCC	1885	ILE	4.3
1	CCC	2507	GLY	4.2
1	DDD	2498	THR	4.2
1	DDD	2025	THR	4.2
1	CCC	1895	CYS	4.2
1	FFF	1891	PRO	4.1
1	CCC	2590	VAL	4.1
1	FFF	1888	ASP	4.1
1	FFF	2531	GLY	4.1
1	FFF	2449	TYR	4.0
1	DDD	2359	PHE	4.0
1	CCC	2138	PHE	4.0
1	CCC	2212	PHE	4.0
1	FFF	2144	PRO	3.9
1	DDD	2214	LEU	3.9
1	BBB	2364	ALA	3.9
1	EEE	2498	THR	3.9
1	BBB	2399	GLY	3.9
1	DDD	1890	PHE	3.8
1	DDD	2401	GLN	3.8
1	CCC	2217	GLU	3.8
1	FFF	2209	LYS	3.8
1	BBB	2348	LEU	3.8
1	FFF	2401	GLN	3.7
1	FFF	2223	PHE	3.7
1	AAA	1888	ASP	3.7
1	FFF	2212	PHE	3.7
1	DDD	2028	GLY	3.7
1	EEE	2399	GLY	3.7
1	FFF	2133	ILE	3.6
1	EEE	2409	ALA	3.6
1	EEE	2005	LEU	3.6
1	FFF	2398	LEU	3.6
1	CCC	2177	PHE	3.6
1	CCC	2362	ILE	3.5
1	AAA	2214	LEU	3.5
1	BBB	2366	TRP	3.5
1	EEE	1896	ASP	3.5
1	DDD	1892	ILE	3.5
1	EEE	2348	LEU	3.5
1	FFF	1964	ILE	3.4
1	FFF	1890	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	DDD	2336	LEU	3.4
1	BBB	2368	MET	3.4
1	CCC	2364	ALA	3.3
1	CCC	2416	PHE	3.3
1	EEE	2368	MET	3.3
1	AAA	2507	GLY	3.3
1	FFF	2499	PHE	3.3
1	EEE	2338	ILE	3.3
1	CCC	2214	LEU	3.3
1	DDD	2416	PHE	3.3
1	BBB	2590	VAL	3.2
1	FFF	2335	GLU	3.2
1	EEE	2127	PHE	3.2
1	EEE	1933	PRO	3.2
1	EEE	2568	LEU	3.2
1	FFF	2588	PHE	3.1
1	FFF	2532	GLY	3.1
1	FFF	2450	LEU	3.1
1	DDD	1887	ASP	3.1
1	EEE	2434	CYS	3.1
1	FFF	2386	CYS	3.1
1	CCC	2218	LYS	3.1
1	DDD	2412	TYR	3.1
1	BBB	2456	ASN	3.1
1	EEE	2031	SER	3.1
1	CCC	2508	MET	3.1
1	AAA	2217	GLU	3.0
1	BBB	2361	SER	3.0
1	FFF	2453	ILE	3.0
1	FFF	2533	PHE	3.0
1	BBB	2352	LEU	3.0
1	EEE	2413	ILE	3.0
1	DDD	2402	MET	3.0
1	EEE	1889	GLY	2.9
1	FFF	2557	ILE	2.9
1	AAA	2590	VAL	2.9
1	AAA	1824	SER	2.9
1	FFF	1982	LEU	2.9
1	CCC	1824	SER	2.9
1	FFF	2366	TRP	2.9
1	DDD	2348	LEU	2.9
2	KKK	14	DC	2.9

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Mol	Chain	Res	Type	RSRZ
1	EEE	1886	ARG	2.9
1	FFF	1920	GLU	2.9
1	BBB	2395	ALA	2.9
1	FFF	2590	VAL	2.8
1	AAA	2508	MET	2.8
1	DDD	2393	MET	2.8
1	EEE	2401	GLN	2.8
1	AAA	1885	ILE	2.8
1	DDD	2529	ILE	2.8
1	FFF	2481	VAL	2.8
1	EEE	2217	GLU	2.8
2	KKK	15	DC	2.8
1	DDD	2137	LEU	2.8
1	EEE	2363	ALA	2.8
1	EEE	1932	PRO	2.8
1	EEE	2334	LEU	2.8
1	EEE	2395	ALA	2.8
1	DDD	2366	TRP	2.7
1	EEE	2376	ASP	2.7
1	FFF	1935	LEU	2.7
1	DDD	1939	LEU	2.7
1	AAA	2416	PHE	2.7
1	EEE	2495	PHE	2.7
1	CCC	2408	ASP	2.7
1	DDD	2403	GLY	2.7
1	BBB	2402	MET	2.7
1	EEE	2378	LEU	2.7
1	CCC	1888	ASP	2.7
1	BBB	2359	PHE	2.6
1	EEE	1890	PHE	2.6
1	DDD	2378	LEU	2.6
1	CCC	2359	PHE	2.6
1	EEE	2449	TYR	2.6
1	BBB	2386	CYS	2.6
1	FFF	2210	VAL	2.6
1	FFF	2371	PRO	2.6
1	BBB	2212	PHE	2.6
1	DDD	1850	PHE	2.6
1	BBB	2497	SER	2.6
1	DDD	2352	LEU	2.6
1	DDD	2386	CYS	2.6
1	BBB	2367	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	DDD	2349	ILE	2.6
1	EEE	2133	ILE	2.6
1	DDD	2182	ASP	2.6
1	DDD	2210	VAL	2.5
1	EEE	2420	TYR	2.5
1	CCC	2378	LEU	2.5
1	EEE	2218	LYS	2.5
1	FFF	2177	PHE	2.5
1	EEE	1921	GLN	2.5
1	EEE	2572	LEU	2.5
1	EEE	2177	PHE	2.5
1	BBB	2133	ILE	2.5
1	AAA	2401	GLN	2.5
1	FFF	2543	LEU	2.5
1	FFF	2136	VAL	2.5
1	CCC	2137	LEU	2.5
1	FFF	2242	ILE	2.5
1	CCC	2121	ALA	2.4
1	BBB	2385	ILE	2.4
1	DDD	2356	ALA	2.4
1	AAA	2498	THR	2.4
1	EEE	2397	SER	2.4
1	DDD	2229	ILE	2.4
1	DDD	1952	LEU	2.4
1	FFF	2013	LEU	2.4
1	DDD	1978	CYS	2.4
1	FFF	2493	GLU	2.4
1	DDD	1824	SER	2.4
1	CCC	2572	LEU	2.4
1	EEE	2389	ILE	2.4
1	FFF	1852	ILE	2.4
1	FFF	1996	LEU	2.4
1	EEE	2211	VAL	2.3
1	FFF	2399	GLY	2.3
1	FFF	1965	TYR	2.3
1	DDD	2395	ALA	2.3
1	EEE	1852	ILE	2.3
1	EEE	2190	LEU	2.3
1	EEE	2394	GLY	2.3
1	EEE	2034	LEU	2.3
1	FFF	2069	LEU	2.3
1	BBB	2223	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	FFF	2125	PHE	2.3
1	BBB	2346	ARG	2.3
1	EEE	2209	LYS	2.3
1	EEE	2336	LEU	2.3
1	EEE	2499	PHE	2.3
1	FFF	1919	LYS	2.3
1	FFF	2488	ILE	2.3
1	CCC	2215	GLN	2.3
1	FFF	2546	VAL	2.3
1	FFF	2576	VAL	2.3
1	FFF	2542	LEU	2.3
1	EEE	2212	PHE	2.3
1	CCC	1951	CYS	2.2
1	DDD	2136	VAL	2.2
1	CCC	2141	LEU	2.2
1	DDD	2364	ALA	2.2
1	EEE	2390	ILE	2.2
1	FFF	2138	PHE	2.2
1	FFF	2529	ILE	2.2
1	CCC	1917	LEU	2.2
1	DDD	2394	GLY	2.2
1	FFF	2060	LEU	2.2
1	CCC	1921	GLN	2.2
1	FFF	2327	LEU	2.2
1	EEE	2125	PHE	2.2
1	FFF	1899	LEU	2.2
1	CCC	2133	ILE	2.2
1	DDD	2208	THR	2.2
1	EEE	2223	PHE	2.2
1	EEE	2242	ILE	2.2
1	DDD	2127	PHE	2.2
1	DDD	2209	LYS	2.2
1	EEE	2137	LEU	2.2
1	FFF	2214	LEU	2.2
1	BBB	2214	LEU	2.2
1	FFF	2411	CYS	2.2
1	CCC	2398	LEU	2.2
1	DDD	2499	PHE	2.2
1	EEE	1903	LEU	2.2
1	FFF	1887	ASP	2.2
1	FFF	2208	THR	2.2
1	AAA	2177	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	DDD	2069	LEU	2.1
1	EEE	2214	LEU	2.1
1	FFF	2020	LEU	2.1
1	FFF	2182	ASP	2.1
1	DDD	2390	ILE	2.1
1	FFF	2385	ILE	2.1
1	AAA	1887	ASP	2.1
1	AAA	2362	ILE	2.1
1	DDD	1852	ILE	2.1
1	BBB	2210	VAL	2.1
1	AAA	2212	PHE	2.1
1	DDD	1962	VAL	2.1
1	BBB	1854	LEU	2.1
1	CCC	2358	VAL	2.1
1	DDD	2133	ILE	2.1
1	CCC	2026	SER	2.1
1	DDD	1974	LEU	2.1
1	FFF	1854	LEU	2.1
1	CCC	1897	ASP	2.1
1	FFF	2027	GLN	2.1
1	BBB	2413	ILE	2.1
1	EEE	2480	ILE	2.1
1	CCC	1889	GLY	2.1
1	AAA	2144	PRO	2.1
1	DDD	1945	MET	2.1
1	BBB	2398	LEU	2.1
1	EEE	1917	LEU	2.1
1	EEE	2473	VAL	2.1
1	FFF	2053	ILE	2.1
1	DDD	1891	PRO	2.1
1	EEE	2342	LEU	2.0
1	BBB	2349	ILE	2.0
1	EEE	2492	LEU	2.0
1	FFF	2397	SER	2.0
1	AAA	2224	LEU	2.0
1	BBB	2139	LEU	2.0
1	DDD	2450	LEU	2.0
1	BBB	2218	LYS	2.0
1	FFF	2558	VAL	2.0
1	EEE	2359	PHE	2.0
1	EEE	1891	PRO	2.0
1	EEE	2184	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	EEE	2352	LEU	2.0
1	FFF	2568	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
3	DDG	RRR	13	21/22	0.96	0.14	72,92,102,117	0
3	DDG	JJJ	13	21/22	0.98	0.17	42,56,60,63	0
3	DDG	LLL	13	21/22	0.98	0.15	43,59,66,71	0
3	DDG	NNN	13	21/22	0.98	0.19	44,53,63,64	0
3	DDG	PPP	13	21/22	0.98	0.18	49,83,103,107	0
3	DDG	HHH	13	21/22	0.98	0.16	38,44,50,58	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	MG	EEE	2601	1/1	0.72	0.14	140,140,140,140	0
4	MG	FFF	2601	1/1	0.85	0.11	139,139,139,139	0
4	MG	BBB	2601	1/1	0.89	0.09	83,83,83,83	0
4	MG	CCC	2601	1/1	0.91	0.04	100,100,100,100	0
5	DG3	BBB	2602	30/30	0.95	0.17	55,66,87,88	0
5	DG3	DDD	2602	30/30	0.95	0.15	51,62,103,119	0
5	DG3	FFF	2602	30/30	0.95	0.14	93,109,134,142	0
6	K7X	AAA	2603	28/28	0.95	0.56	79,107,119,134	1
4	MG	DDD	2601	1/1	0.96	0.07	102,102,102,102	0
5	DG3	EEE	2602	30/30	0.96	0.15	74,97,120,125	0

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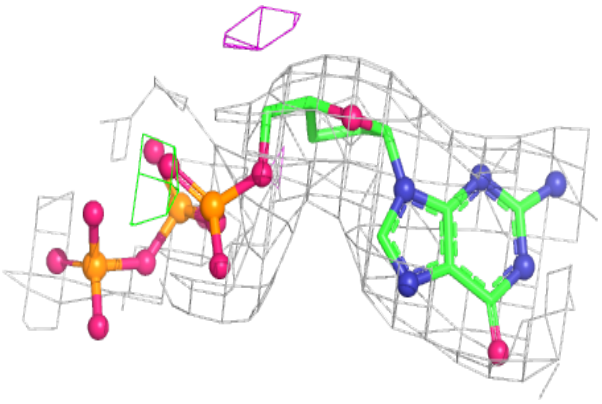
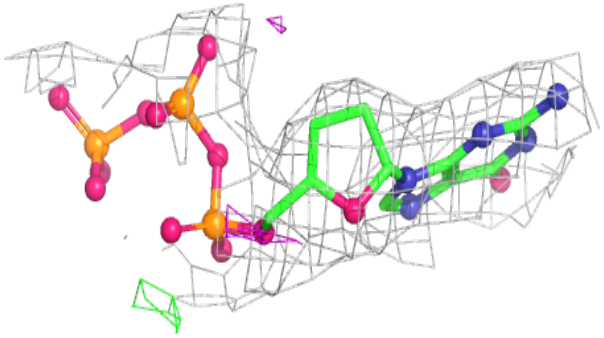
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	AAA	2601	1/1	0.97	0.06	86,86,86,86	0
5	DG3	CCC	2602	30/30	0.97	0.16	51,61,93,108	0
5	DG3	AAA	2602	30/30	0.98	0.17	42,52,73,77	0

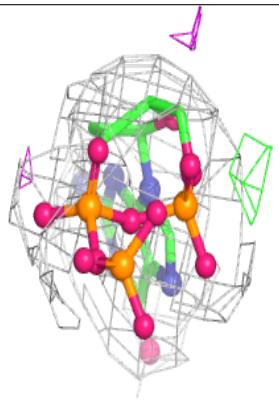
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DG3 BBB 2602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

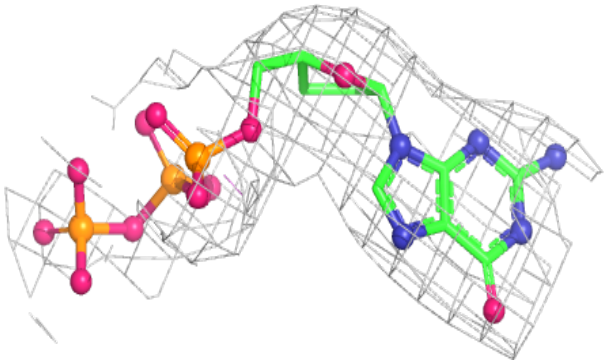


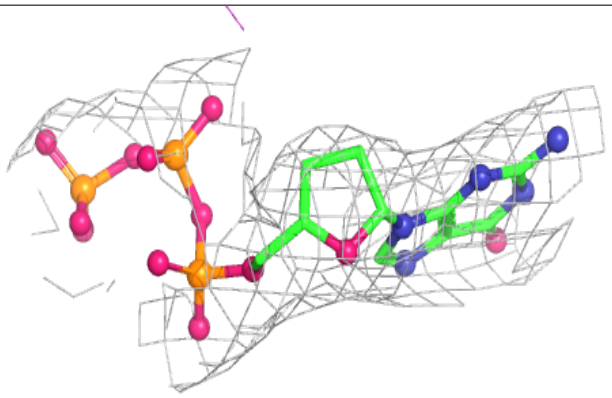


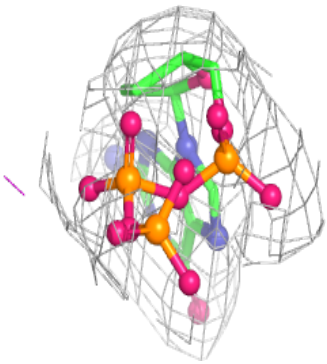


Electron density around DG3 DDD 2602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

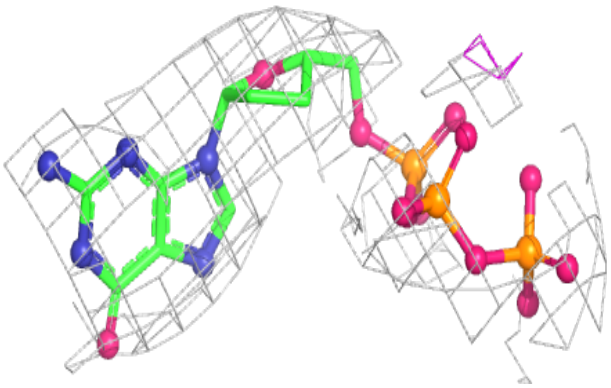


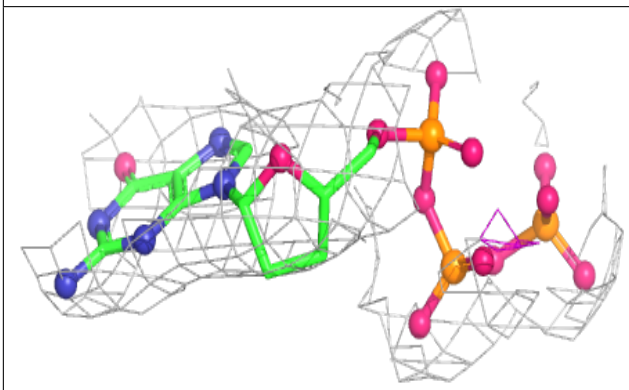


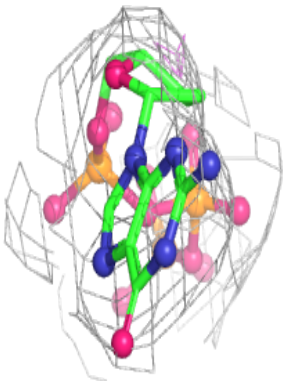


Electron density around DG3 FFF 2602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

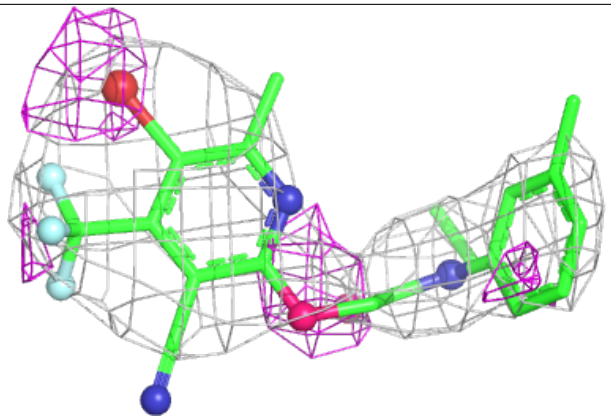


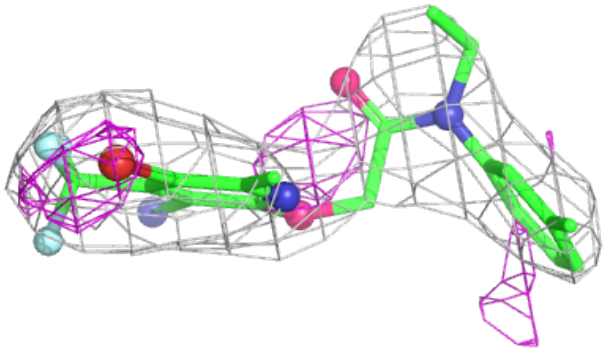


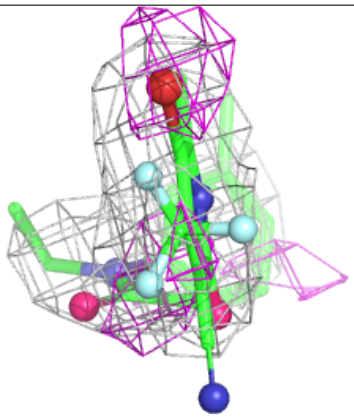


Electron density around K7X AAA 2603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

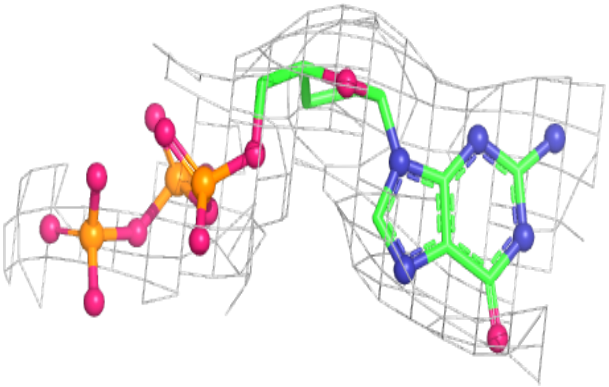


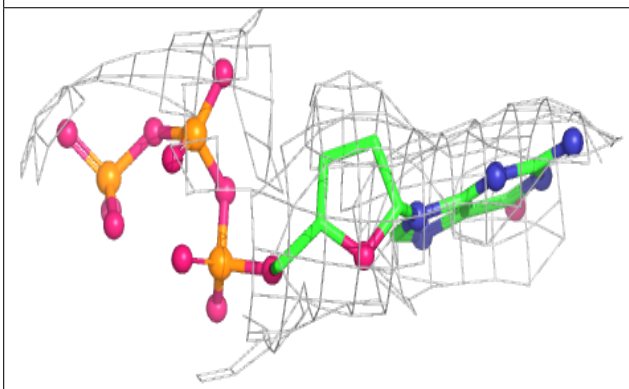


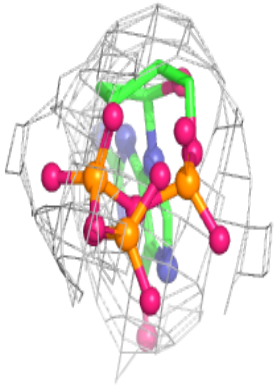


Electron density around DG3 EEE 2602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

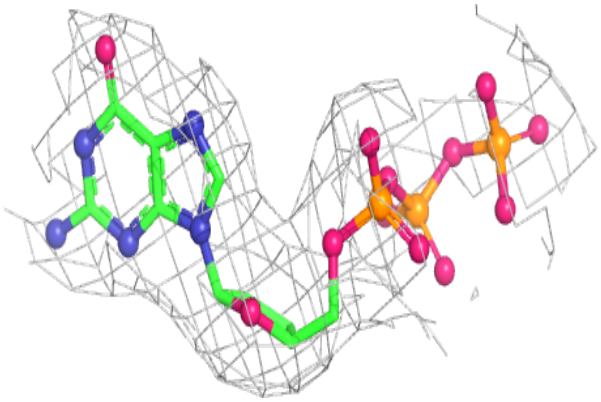


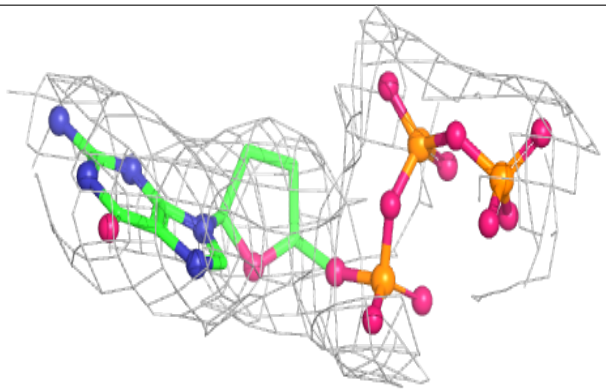


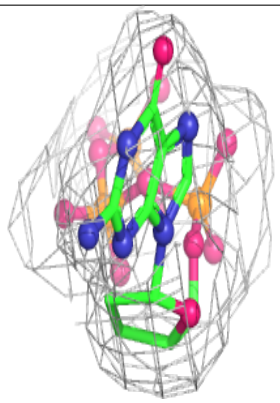


Electron density around DG3 CCC 2602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

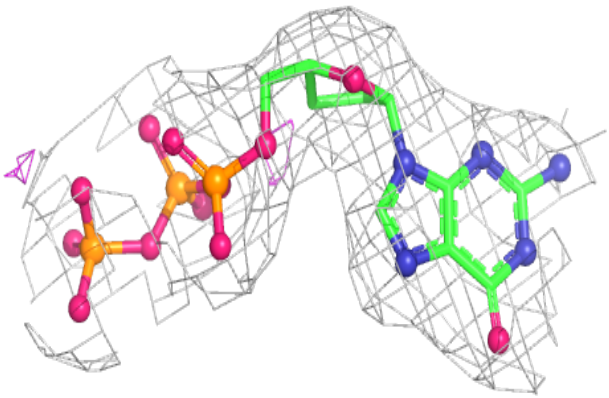


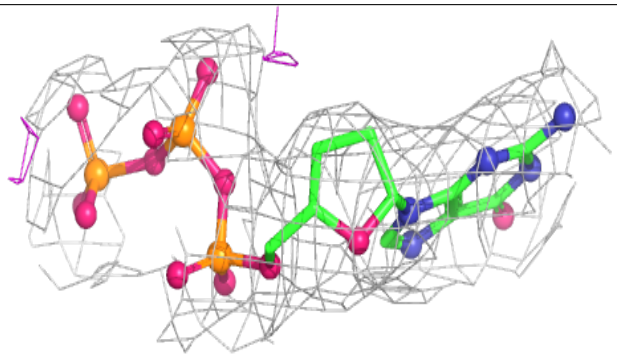


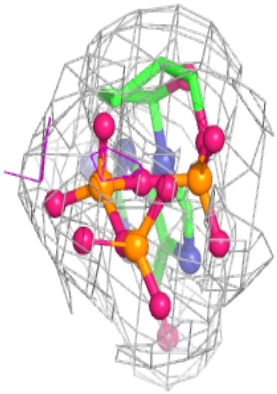


Electron density around DG3 AAA 2602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.