



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:34 AM UTC

PDB ID : 7ZX1 / pdb_00007zx1
Title : Crystal structure of Pol theta polymerase domain in complex with compound 22
Authors : Krajewski, W.W.; Turnbull, A.P.; Willis, S.; Charles, M.; Stockley, M.; Heald, R.A.
Deposited on : 2022-05-19
Resolution : 2.83 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

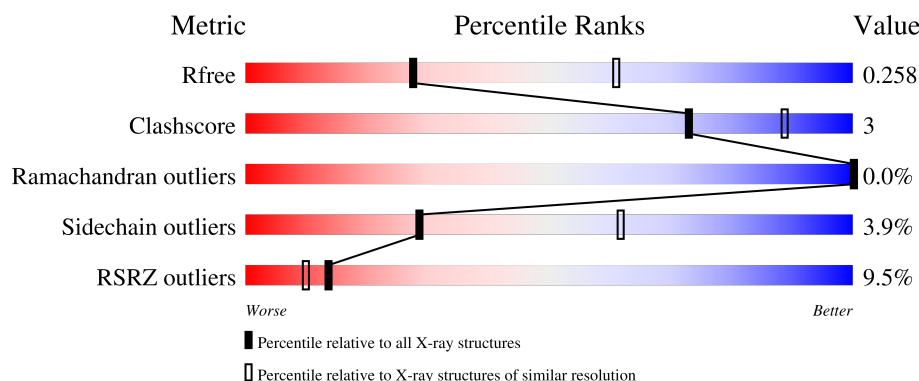
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	726	5% 78% 10% • 12%
1	BBB	726	6% 78% 8% • 13%
1	CCC	726	4% 78% 9% 12%
1	DDD	726	10% 77% 10% 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

There are 7 unique types of molecules in this entry. The entry contains 32843 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			

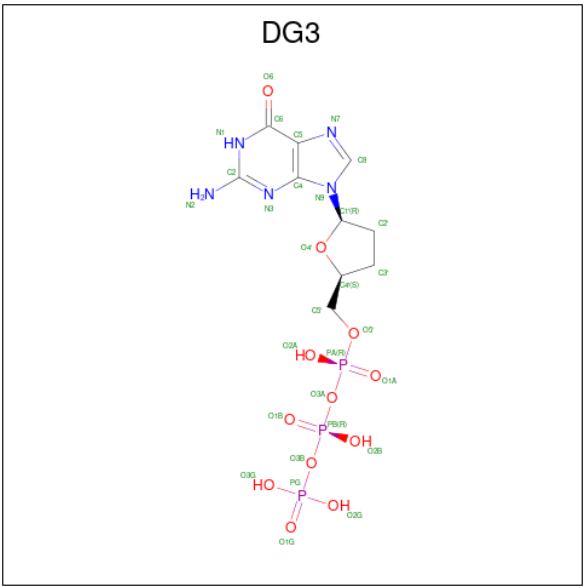
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3').

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



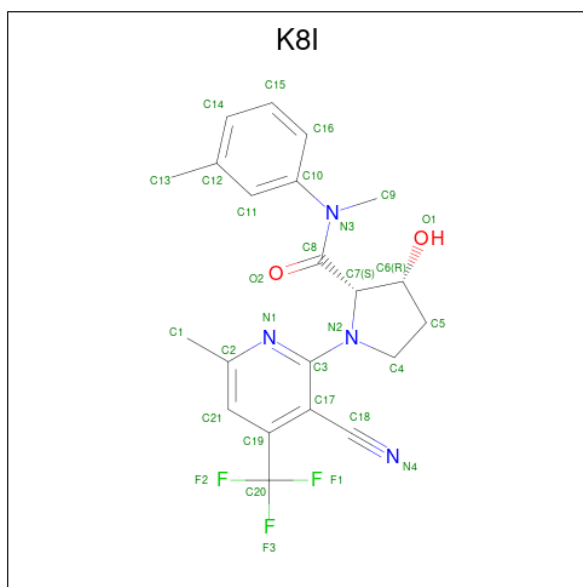
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	BBB	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	DDD	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	EEE	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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

- Molecule 6 is (2 {S},3 {R})-1-[3-cyano-6-methyl-4-(trifluoromethyl)pyridin-2-yl]- {N}-methyl- {N}-(3-methylphenyl)-3-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: K8I) (formula: C₂₁H₂₁F₃N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	AAA	1	Total	C	F	N	O	0	0
			30	21	3	4	2		
6	BBB	1	Total	C	F	N	O	0	0
			30	21	3	4	2		
6	CCC	1	Total	C	F	N	O	0	0
			30	21	3	4	2		
6	DDD	1	Total	C	F	N	O	0	0
			30	21	3	4	2		

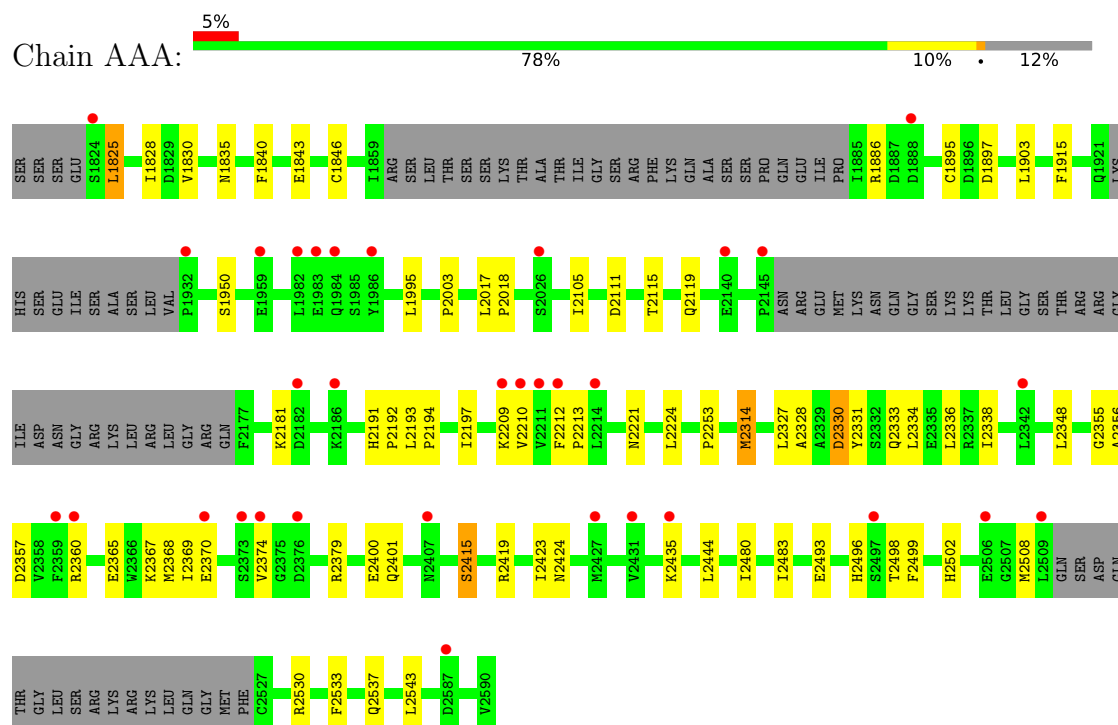
- Molecule 7 is water.

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

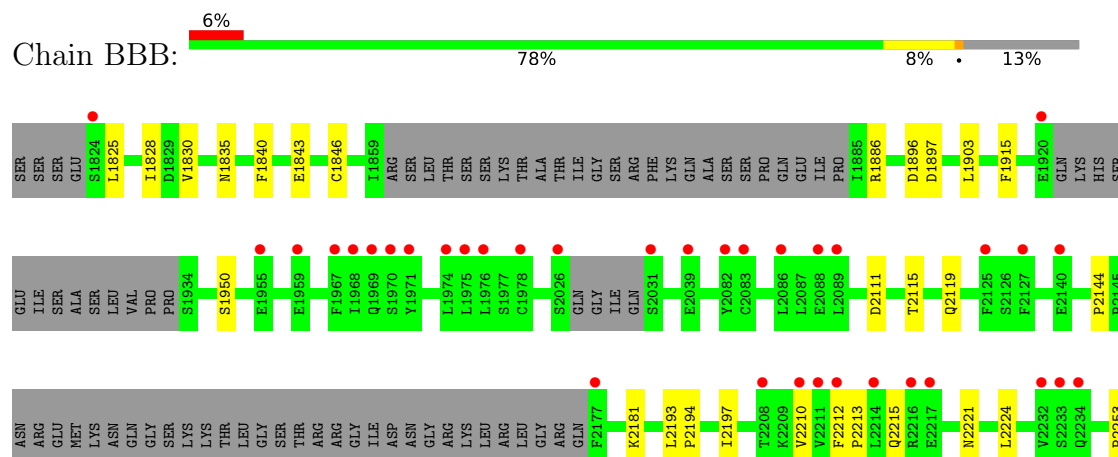
3 Residue-property plots [i](#)

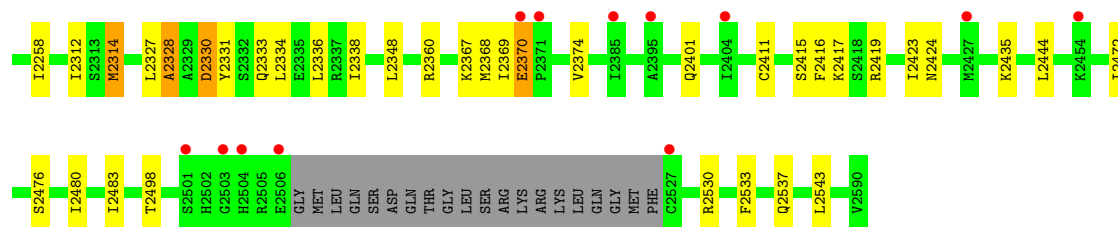
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

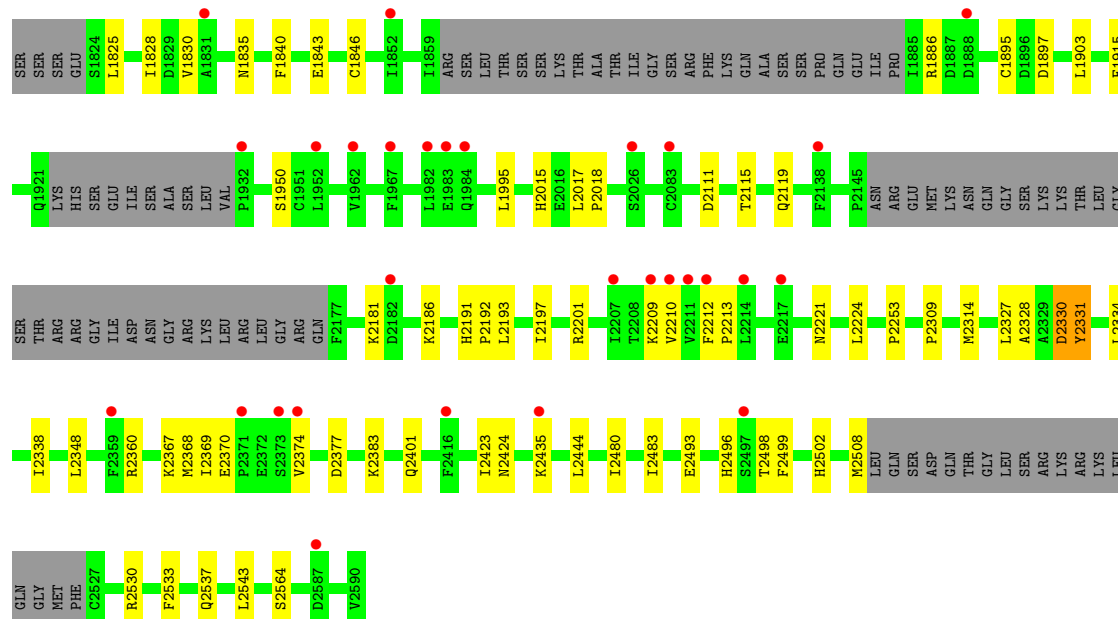
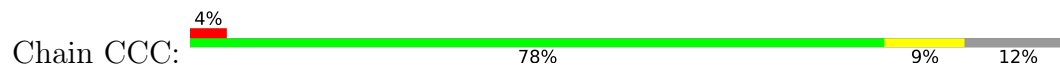


- Molecule 1: DNA polymerase theta

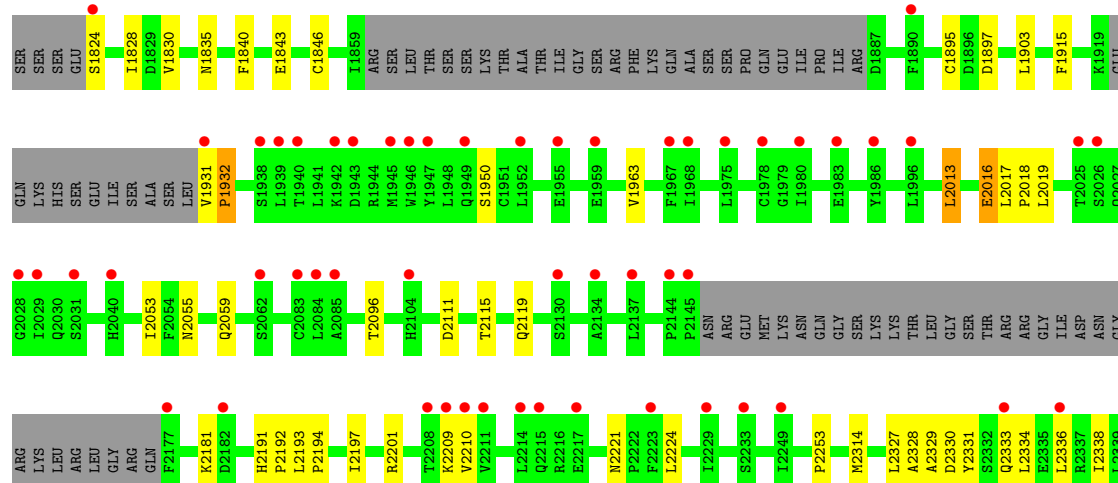
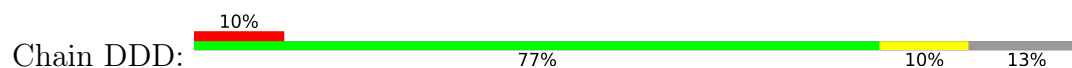


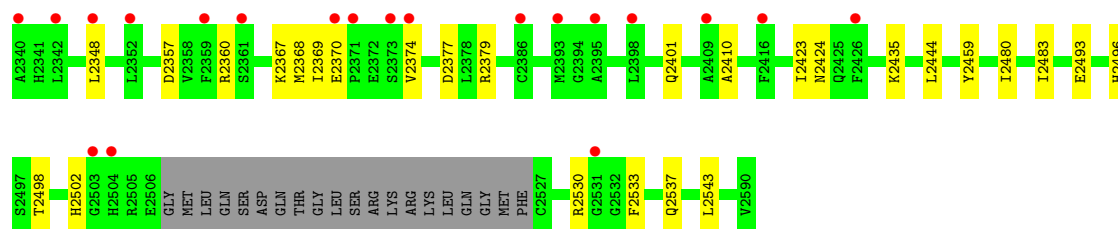


• Molecule 1: DNA polymerase theta

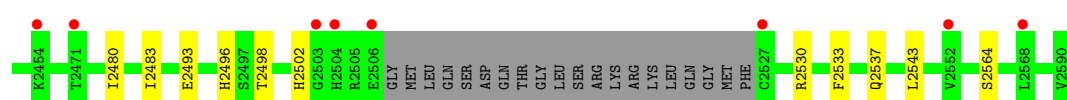
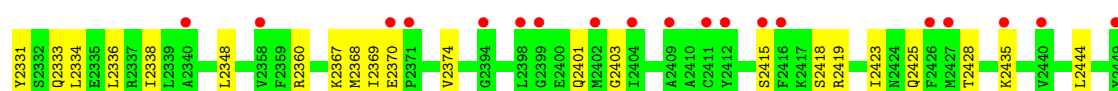
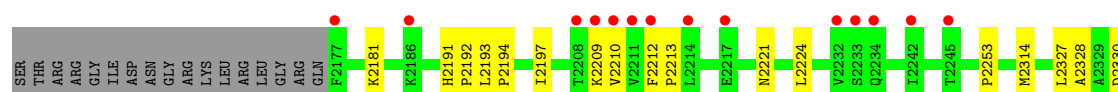
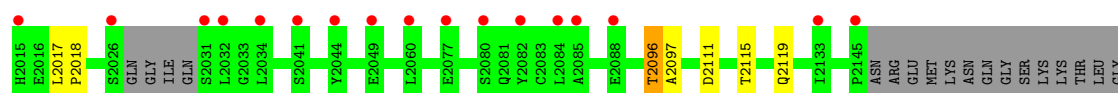
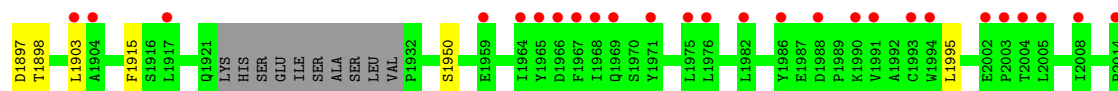
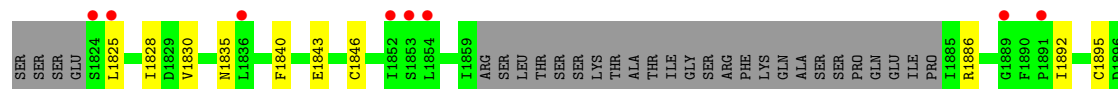
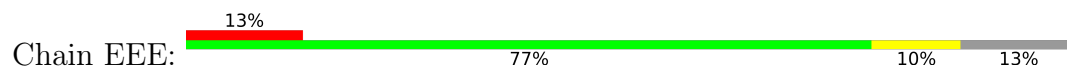


• Molecule 1: DNA polymerase theta

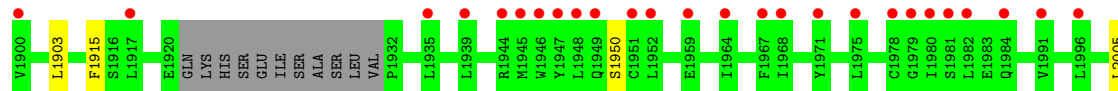
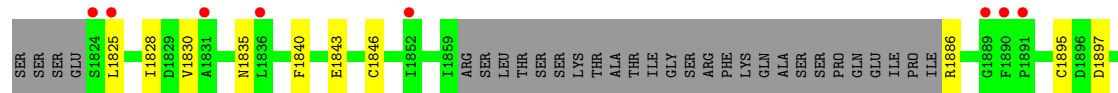
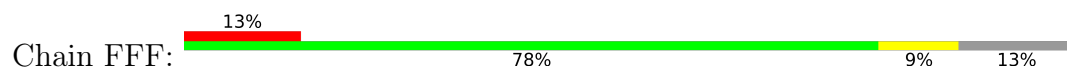


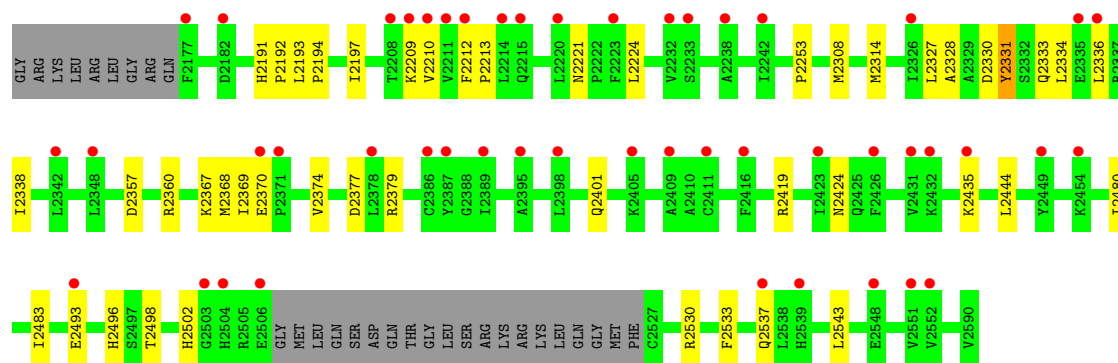


• Molecule 1: DNA polymerase theta



• Molecule 1: DNA polymerase theta





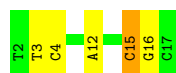
- Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain GGG: 75% 19% 6%



- 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: 69% 25% 6%



- 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: 69% 25% 6%



- 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: 62% 31% 6%

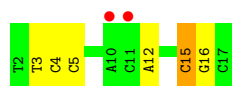


- Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

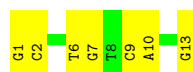
Chain OOO: 6% 62% 25% 12%



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



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



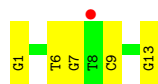
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')



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



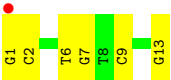
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.59Å 172.29Å 289.21Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	50.01 – 2.83 50.01 – 2.83	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.01-2.83) 97.5 (50.01-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.228 , 0.260 0.229 , 0.258	Depositor DCC
R_{free} test set	6878 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32843	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4445e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DG3, K8I, DDG

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	1.08	3/4980 (0.1%)	1.41	6/6751 (0.1%)
1	BBB	1.06	3/4904 (0.1%)	1.40	4/6649 (0.1%)
1	CCC	1.06	2/4952 (0.0%)	1.40	4/6717 (0.1%)
1	DDD	1.07	3/4905 (0.1%)	1.41	5/6659 (0.1%)
1	EEE	1.05	2/4919 (0.0%)	1.39	3/6672 (0.0%)
1	FFF	1.05	1/4919 (0.0%)	1.41	4/6676 (0.1%)
2	GGG	0.77	0/362	1.18	3/555 (0.5%)
2	III	0.72	0/362	1.16	4/555 (0.7%)
2	KKK	0.75	0/362	1.16	4/555 (0.7%)
2	MMM	0.74	0/362	1.15	4/555 (0.7%)
2	OOO	0.69	0/362	1.16	5/555 (0.9%)
2	QQQ	0.71	0/362	1.16	5/555 (0.9%)
3	HHH	0.73	0/271	1.18	6/417 (1.4%)
3	JJJ	0.74	0/271	1.17	5/417 (1.2%)
3	LLL	0.72	0/271	1.17	5/417 (1.2%)
3	NNN	0.70	0/271	1.16	4/417 (1.0%)
3	PPP	0.68	0/271	1.18	5/417 (1.2%)
3	RRR	0.69	0/271	1.17	5/417 (1.2%)
All	All	1.03	14/33377 (0.0%)	1.38	81/45956 (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	BBB	0	1
1	FFF	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	2329	ALA	C-O	-6.79	1.16	1.24
1	CCC	2331	TYR	C-O	6.64	1.32	1.23
1	AAA	2356	ALA	C-O	6.46	1.32	1.24
1	BBB	2416	PHE	C-O	6.25	1.31	1.24
1	FFF	2331	TYR	C-O	5.95	1.31	1.23
1	AAA	1825	LEU	C-O	-5.79	1.17	1.24
1	EEE	2096	THR	C-O	5.74	1.31	1.23
1	CCC	2015	HIS	CE1-NE2	5.57	1.38	1.32
1	EEE	2425	GLN	C-O	5.57	1.30	1.24
1	BBB	2417	LYS	C-O	5.47	1.30	1.24
1	AAA	2003	PRO	C-O	-5.40	1.17	1.23
1	BBB	2328	ALA	C-O	-5.23	1.17	1.24
1	DDD	2096	THR	C-O	5.16	1.30	1.24
1	DDD	2410	ALA	C-O	5.16	1.30	1.24

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GGG	3	DT	P-O3'-C3'	-8.02	108.18	120.20
3	LLL	7	DG	P-O3'-C3'	-7.66	108.71	120.20
3	NNN	7	DG	P-O3'-C3'	-7.58	108.83	120.20
2	QQQ	3	DT	P-O3'-C3'	-7.53	108.91	120.20
1	FFF	2101	SER	CA-C-O	-7.46	112.52	120.42
2	III	15	DC	P-O3'-C3'	-7.25	109.33	120.20
2	KKK	3	DT	P-O3'-C3'	-7.24	109.34	120.20
3	HHH	7	DG	P-O3'-C3'	-7.24	109.34	120.20
3	PPP	7	DG	P-O3'-C3'	-7.22	109.37	120.20
3	PPP	6	DT	P-O3'-C3'	-7.16	109.47	120.20
3	RRR	6	DT	P-O3'-C3'	-7.15	109.48	120.20
2	OOO	15	DC	P-O3'-C3'	-7.14	109.49	120.20
3	RRR	7	DG	P-O3'-C3'	-7.13	109.50	120.20
2	KKK	15	DC	P-O3'-C3'	-7.10	109.55	120.20
3	JJJ	7	DG	P-O3'-C3'	-7.05	109.62	120.20
2	GGG	15	DC	P-O3'-C3'	-7.04	109.64	120.20
2	MMM	15	DC	P-O3'-C3'	-7.03	109.66	120.20
3	LLL	6	DT	P-O3'-C3'	-7.00	109.70	120.20
3	NNN	6	DT	P-O3'-C3'	-6.98	109.73	120.20
3	HHH	6	DT	P-O3'-C3'	-6.94	109.79	120.20
2	OOO	3	DT	P-O3'-C3'	-6.91	109.84	120.20
2	QQQ	15	DC	P-O3'-C3'	-6.89	109.86	120.20
3	JJJ	6	DT	P-O3'-C3'	-6.89	109.87	120.20
2	MMM	3	DT	P-O3'-C3'	-6.32	110.72	120.20
1	CCC	2330	ASP	CA-CB-CG	6.18	118.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	III	3	DT	P-O3'-C3'	-6.08	111.07	120.20
3	JJJ	1	DG	P-O3'-C3'	-5.93	111.31	120.20
2	GGG	12	DA	P-O3'-C3'	-5.81	111.48	120.20
3	HHH	9	DC	P-O3'-C3'	-5.81	111.49	120.20
3	PPP	1	DG	P-O3'-C3'	-5.70	111.65	120.20
3	PPP	9	DC	P-O3'-C3'	-5.65	111.72	120.20
2	III	12	DA	P-O3'-C3'	-5.60	111.80	120.20
3	RRR	9	DC	P-O3'-C3'	-5.50	111.95	120.20
1	BBB	1846	CYS	CB-CA-C	5.47	119.86	110.01
1	AAA	1846	CYS	CB-CA-C	5.47	119.85	110.01
3	HHH	1	DG	P-O3'-C3'	-5.47	112.00	120.20
2	MMM	12	DA	P-O3'-C3'	-5.45	112.03	120.20
3	JJJ	2	DC	P-O3'-C3'	-5.43	112.06	120.20
3	LLL	1	DG	P-O3'-C3'	-5.42	112.07	120.20
3	RRR	1	DG	P-O3'-C3'	-5.39	112.12	120.20
1	CCC	1846	CYS	CB-CA-C	5.38	119.69	110.01
2	OOO	12	DA	P-O3'-C3'	-5.37	112.14	120.20
2	QQQ	12	DA	P-O3'-C3'	-5.37	112.14	120.20
2	KKK	12	DA	P-O3'-C3'	-5.31	112.24	120.20
3	RRR	2	DC	P-O3'-C3'	-5.29	112.27	120.20
1	EEE	1846	CYS	CB-CA-C	5.28	119.52	110.01
3	NNN	1	DG	P-O3'-C3'	-5.28	112.28	120.20
1	AAA	2330	ASP	CA-CB-CG	5.28	117.88	112.60
3	PPP	2	DC	P-O3'-C3'	-5.28	112.29	120.20
1	DDD	1846	CYS	CB-CA-C	5.27	119.50	110.01
1	AAA	2365	GLU	CA-C-O	-5.25	114.98	120.55
1	CCC	2435	LYS	CA-C-N	5.23	127.24	120.44
1	CCC	2435	LYS	C-N-CA	5.23	127.24	120.44
3	LLL	9	DC	P-O3'-C3'	-5.23	112.36	120.20
1	AAA	2435	LYS	CA-C-N	5.23	127.23	120.44
1	AAA	2435	LYS	C-N-CA	5.23	127.23	120.44
1	FFF	2435	LYS	CA-C-N	5.23	127.23	120.44
1	FFF	2435	LYS	C-N-CA	5.23	127.23	120.44
1	BBB	2435	LYS	CA-C-N	5.20	127.20	120.44
1	BBB	2435	LYS	C-N-CA	5.20	127.20	120.44
2	OOO	5	DC	P-O3'-C3'	-5.20	112.40	120.20
3	NNN	9	DC	P-O3'-C3'	-5.18	112.43	120.20
1	EEE	2435	LYS	CA-C-N	5.16	127.15	120.44
1	EEE	2435	LYS	C-N-CA	5.16	127.15	120.44
2	QQQ	4	DC	P-O3'-C3'	-5.16	112.46	120.20
2	QQQ	5	DC	P-O3'-C3'	-5.16	112.46	120.20
1	DDD	2435	LYS	CA-C-N	5.10	127.07	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	2435	LYS	C-N-CA	5.10	127.07	120.44
3	LLL	2	DC	P-O3'-C3'	-5.09	112.56	120.20
3	HHH	2	DC	P-O3'-C3'	-5.08	112.57	120.20
1	AAA	2415	SER	CA-C-O	-5.07	115.50	120.82
1	DDD	2016	GLU	N-CA-C	-5.07	106.78	113.17
2	III	4	DC	P-O3'-C3'	-5.07	112.60	120.20
1	DDD	1932	PRO	CB-CA-C	-5.06	104.74	110.92
2	OOO	4	DC	P-O3'-C3'	-5.06	112.61	120.20
2	KKK	5	DC	P-O3'-C3'	-5.04	112.64	120.20
2	MMM	5	DC	P-O3'-C3'	-5.03	112.66	120.20
3	HHH	10	DA	P-O3'-C3'	-5.02	112.67	120.20
3	JJJ	10	DA	P-O3'-C3'	-5.02	112.67	120.20
1	FFF	1846	CYS	CB-CA-C	5.02	119.04	110.01
1	BBB	2330	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	2215	GLN	Mainchain
1	FFF	2101	SER	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	33	0
1	BBB	4811	0	4625	29	0
1	CCC	4856	0	4667	29	0
1	DDD	4810	0	4593	38	0
1	EEE	4824	0	4632	32	0
1	FFF	4823	0	4617	29	0
2	GGG	324	0	180	1	0
2	III	324	0	180	1	0
2	KKK	324	0	180	1	0
2	MMM	324	0	180	2	0
2	OOO	324	0	180	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	QQQ	324	0	180	1	0
3	HHH	264	0	149	0	0
3	JJJ	264	0	149	0	0
3	LLL	264	0	149	0	0
3	NNN	264	0	149	0	0
3	PPP	264	0	149	0	0
3	RRR	264	0	149	0	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	DDD	30	0	12	0	0
5	EEE	30	0	12	2	0
5	FFF	30	0	12	0	0
5	KKK	30	0	12	1	0
6	AAA	30	0	0	2	0
6	BBB	30	0	0	2	0
6	CCC	30	0	0	2	0
6	DDD	30	0	0	1	0
7	AAA	1	0	0	0	0
All	All	32843	0	29894	202	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 3.

All (202) 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)
1:DDD:2013:LEU:HD11	1:DDD:2055:ASN:OD1	1.49	1.13
5:EEE:2602:DG3:N2	2:OOO:5:DC:C2	2.53	0.76
1:DDD:2210:VAL:HG21	1:DDD:2253:PRO:HD3	1.71	0.72
1:BBB:2210:VAL:HG21	1:BBB:2253:PRO:HD3	1.73	0.69
1:EEE:2210:VAL:HG21	1:EEE:2253:PRO:HD3	1.75	0.69
1:FFF:2210:VAL:HG21	1:FFF:2253:PRO:HD3	1.74	0.68
1:CCC:2210:VAL:HG21	1:CCC:2253:PRO:HD3	1.74	0.68
1:AAA:2210:VAL:HG21	1:AAA:2253:PRO:HD3	1.74	0.68
1:CCC:2338:ILE:HD11	1:CCC:2480:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:2338:ILE:HD11	1:FFF:2480:ILE:HD12	1.78	0.64
1:BBB:2338:ILE:HD11	1:BBB:2480:ILE:HD12	1.80	0.64
1:CCC:2493:GLU:HA	1:CCC:2496:HIS:HB2	1.80	0.64
1:EEE:2493:GLU:HA	1:EEE:2496:HIS:HB2	1.80	0.64
1:DDD:2338:ILE:HD11	1:DDD:2480:ILE:HD12	1.78	0.64
1:EEE:2338:ILE:HD11	1:EEE:2480:ILE:HD12	1.78	0.64
1:AAA:2338:ILE:HD11	1:AAA:2480:ILE:HD12	1.79	0.63
1:FFF:2493:GLU:HA	1:FFF:2496:HIS:HB2	1.80	0.63
1:AAA:2493:GLU:HA	1:AAA:2496:HIS:HB2	1.81	0.62
1:DDD:2493:GLU:HA	1:DDD:2496:HIS:HB2	1.81	0.62
1:BBB:2498:THR:HG21	1:BBB:2530:ARG:HB2	1.81	0.62
1:FFF:2498:THR:HG21	1:FFF:2530:ARG:HB2	1.84	0.60
5:EEE:2602:DG3:N2	2:OOO:5:DC:O2	2.35	0.60
6:DDD:2603:K8I:C18	6:DDD:2603:K8I:C4	2.80	0.60
1:AAA:2498:THR:HG21	1:AAA:2530:ARG:HB2	1.82	0.59
1:DDD:2498:THR:HG21	1:DDD:2530:ARG:HB2	1.84	0.59
1:EEE:2498:THR:HG21	1:EEE:2530:ARG:HB2	1.84	0.59
1:DDD:2013:LEU:HD23	1:DDD:2016:GLU:HG3	1.84	0.59
1:CCC:2498:THR:HG21	1:CCC:2530:ARG:HB2	1.84	0.58
1:CCC:2212:PHE:HB3	1:CCC:2213:PRO:HD3	1.86	0.57
1:FFF:2212:PHE:HB3	1:FFF:2213:PRO:HD3	1.86	0.57
6:AAA:2603:K8I:C4	6:AAA:2603:K8I:C18	2.83	0.56
6:CCC:2602:K8I:C18	6:CCC:2602:K8I:C4	2.83	0.56
1:EEE:2212:PHE:HB3	1:EEE:2213:PRO:HD3	1.86	0.56
1:BBB:2210:VAL:HG21	1:BBB:2253:PRO:CD	2.34	0.56
1:BBB:2212:PHE:HB3	1:BBB:2213:PRO:HD3	1.85	0.56
1:EEE:2444:LEU:HD11	1:EEE:2483:ILE:HD11	1.86	0.56
1:DDD:2444:LEU:HD11	1:DDD:2483:ILE:HD11	1.86	0.56
1:AAA:2212:PHE:HB3	1:AAA:2213:PRO:HD3	1.87	0.56
1:BBB:2444:LEU:HD11	1:BBB:2483:ILE:HD11	1.88	0.56
1:DDD:2210:VAL:HG21	1:DDD:2253:PRO:CD	2.35	0.56
1:AAA:2444:LEU:HD11	1:AAA:2483:ILE:HD11	1.87	0.56
1:DDD:2360:ARG:HG2	1:DDD:2374:VAL:HG21	1.87	0.56
1:FFF:2444:LEU:HD11	1:FFF:2483:ILE:HD11	1.87	0.56
1:CCC:2444:LEU:HD11	1:CCC:2483:ILE:HD11	1.87	0.56
1:CCC:2360:ARG:HG2	1:CCC:2374:VAL:HG21	1.89	0.55
1:FFF:2360:ARG:HG2	1:FFF:2374:VAL:HG21	1.88	0.55
1:EEE:2210:VAL:HG21	1:EEE:2253:PRO:CD	2.37	0.55
1:FFF:2210:VAL:HG21	1:FFF:2253:PRO:CD	2.37	0.55
1:DDD:2013:LEU:HD11	1:DDD:2055:ASN:CG	2.28	0.54
1:EEE:2360:ARG:HG2	1:EEE:2374:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BBB:2603:K8I:C4	6:BBB:2603:K8I:C18	2.86	0.53
1:BBB:2360:ARG:HG2	1:BBB:2374:VAL:HG21	1.91	0.53
1:AAA:2360:ARG:HG2	1:AAA:2374:VAL:HG21	1.91	0.53
1:AAA:2210:VAL:HG21	1:AAA:2253:PRO:CD	2.39	0.52
6:BBB:2603:K8I:C7	6:BBB:2603:K8I:C11	2.88	0.52
1:DDD:1824:SER:O	1:DDD:2019:LEU:HD21	2.09	0.52
1:CCC:2383:LYS:NZ	5:KKK:101:DG3:O1G	2.35	0.52
1:DDD:2369:ILE:HG22	1:DDD:2370:GLU:O	2.12	0.50
1:DDD:2013:LEU:CD1	1:DDD:2055:ASN:OD1	2.41	0.49
1:AAA:2331:TYR:CD2	1:AAA:2334:LEU:HD22	2.48	0.49
1:AAA:2369:ILE:HG22	1:AAA:2370:GLU:O	2.13	0.49
1:BBB:2369:ILE:HG22	1:BBB:2370:GLU:O	2.13	0.49
1:FFF:2331:TYR:CD2	1:FFF:2334:LEU:HD22	2.48	0.49
1:BBB:2258:ILE:HD12	1:BBB:2312:ILE:HG13	1.94	0.49
1:FFF:2369:ILE:HG22	1:FFF:2370:GLU:O	2.12	0.49
1:CCC:2210:VAL:HG21	1:CCC:2253:PRO:CD	2.39	0.48
1:CCC:2369:ILE:HG22	1:CCC:2370:GLU:O	2.13	0.48
1:CCC:2331:TYR:CD2	1:CCC:2334:LEU:HD22	2.49	0.48
1:DDD:1931:VAL:HB	1:DDD:1932:PRO:CD	2.44	0.48
1:EEE:2369:ILE:HG22	1:EEE:2370:GLU:O	2.14	0.48
1:DDD:2331:TYR:CD2	1:DDD:2334:LEU:HD22	2.49	0.47
1:BBB:2331:TYR:CD2	1:BBB:2334:LEU:HD22	2.49	0.47
1:BBB:1828:ILE:HD12	1:BBB:1828:ILE:N	2.30	0.47
1:EEE:1828:ILE:HD12	1:EEE:1828:ILE:N	2.30	0.47
1:AAA:1828:ILE:HD12	1:AAA:1828:ILE:N	2.30	0.47
1:FFF:1828:ILE:HD12	1:FFF:1828:ILE:N	2.30	0.47
1:FFF:2193:LEU:O	1:FFF:2197:ILE:HG12	2.15	0.46
1:EEE:2331:TYR:CD2	1:EEE:2334:LEU:HD22	2.49	0.46
1:DDD:1828:ILE:N	1:DDD:1828:ILE:HD12	2.31	0.46
1:BBB:2111:ASP:O	1:BBB:2115:THR:HG23	2.16	0.46
1:CCC:2193:LEU:O	1:CCC:2197:ILE:HG12	2.16	0.46
1:BBB:2193:LEU:O	1:BBB:2197:ILE:HG12	2.16	0.46
1:EEE:2327:LEU:C	1:EEE:2327:LEU:HD23	2.41	0.46
1:AAA:2193:LEU:O	1:AAA:2197:ILE:HG12	2.16	0.46
1:BBB:2333:GLN:HB3	1:BBB:2336:LEU:HB2	1.98	0.46
1:EEE:2193:LEU:O	1:EEE:2197:ILE:HG12	2.16	0.46
1:AAA:2369:ILE:HG22	1:AAA:2370:GLU:N	2.31	0.46
1:CCC:1828:ILE:HD12	1:CCC:1828:ILE:N	2.30	0.46
1:DDD:2013:LEU:HD12	1:DDD:2059:GLN:NE2	2.31	0.46
1:CCC:2327:LEU:C	1:CCC:2327:LEU:HD23	2.41	0.46
1:DDD:1931:VAL:HB	1:DDD:1932:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:2111:ASP:O	1:DDD:2115:THR:HG23	2.16	0.45
1:FFF:2111:ASP:O	1:FFF:2115:THR:HG23	2.16	0.45
1:EEE:2096:THR:O	1:EEE:2097:ALA:C	2.58	0.45
1:EEE:2367:LYS:O	1:EEE:2369:ILE:HG13	2.17	0.45
1:AAA:2221:ASN:HD22	1:AAA:2224:LEU:HB2	1.82	0.45
1:AAA:2327:LEU:C	1:AAA:2327:LEU:HD23	2.42	0.45
1:BBB:2327:LEU:C	1:BBB:2327:LEU:HD23	2.41	0.45
1:CCC:2221:ASN:HD22	1:CCC:2224:LEU:HB2	1.81	0.45
1:CCC:2369:ILE:HG22	1:CCC:2370:GLU:N	2.31	0.45
1:DDD:2193:LEU:O	1:DDD:2197:ILE:HG12	2.16	0.45
1:EEE:2369:ILE:HG22	1:EEE:2370:GLU:N	2.31	0.45
1:AAA:2367:LYS:O	1:AAA:2369:ILE:HG13	2.17	0.45
1:AAA:2415:SER:O	1:AAA:2419:ARG:HG3	2.17	0.45
1:DDD:2013:LEU:HD12	1:DDD:2059:GLN:HE21	1.81	0.45
1:BBB:2221:ASN:HD22	1:BBB:2224:LEU:HB2	1.82	0.45
1:EEE:2111:ASP:O	1:EEE:2115:THR:HG23	2.17	0.45
1:BBB:2369:ILE:HG22	1:BBB:2370:GLU:N	2.32	0.45
1:BBB:2327:LEU:HD23	1:BBB:2328:ALA:N	2.32	0.45
1:BBB:2328:ALA:HB2	1:BBB:2543:LEU:HD22	1.99	0.45
1:DDD:2367:LYS:O	1:DDD:2369:ILE:HG13	2.17	0.45
1:CCC:2367:LYS:O	1:CCC:2369:ILE:HG13	2.16	0.45
1:EEE:2327:LEU:HD23	1:EEE:2328:ALA:N	2.32	0.45
1:AAA:2111:ASP:O	1:AAA:2115:THR:HG23	2.16	0.44
1:CCC:2111:ASP:O	1:CCC:2115:THR:HG23	2.17	0.44
1:DDD:2327:LEU:C	1:DDD:2327:LEU:HD23	2.41	0.44
1:EEE:2221:ASN:HD22	1:EEE:2224:LEU:HB2	1.82	0.44
1:EEE:2348:LEU:HD22	1:EEE:2423:ILE:HD11	2.00	0.44
1:FFF:2367:LYS:O	1:FFF:2369:ILE:HG13	2.17	0.44
1:FFF:2369:ILE:HG22	1:FFF:2370:GLU:N	2.33	0.44
1:FFF:2221:ASN:HD22	1:FFF:2224:LEU:HB2	1.82	0.44
1:FFF:2327:LEU:C	1:FFF:2327:LEU:HD23	2.41	0.44
1:BBB:2367:LYS:O	1:BBB:2369:ILE:HG13	2.17	0.44
6:CCC:2602:K8I:C7	6:CCC:2602:K8I:C11	2.96	0.44
1:BBB:2415:SER:O	1:BBB:2419:ARG:HG3	2.18	0.44
1:DDD:2327:LEU:HD23	1:DDD:2328:ALA:N	2.33	0.43
1:AAA:2499:PHE:CZ	1:AAA:2508:MET:HE2	2.52	0.43
1:DDD:2221:ASN:HD22	1:DDD:2224:LEU:HB2	1.82	0.43
1:DDD:2328:ALA:HB2	1:DDD:2543:LEU:HD22	2.01	0.43
1:DDD:2459:TYR:CE2	2:MMM:2:DT:O2	2.72	0.43
1:FFF:2327:LEU:HD23	1:FFF:2328:ALA:N	2.33	0.43
2:III:15:DC:H2"	2:III:16:DG:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:2327:LEU:HD23	1:CCC:2328:ALA:N	2.33	0.43
1:EEE:1830:VAL:HG11	1:EEE:1840:PHE:CG	2.54	0.43
1:AAA:2327:LEU:HD23	1:AAA:2328:ALA:N	2.33	0.43
1:BBB:1830:VAL:HG11	1:BBB:1840:PHE:CG	2.54	0.43
1:BBB:2348:LEU:HD22	1:BBB:2423:ILE:HD11	2.01	0.43
1:EEE:2333:GLN:HB3	1:EEE:2336:LEU:HB2	2.01	0.43
1:CCC:1995:LEU:HD12	1:CCC:1995:LEU:HA	1.89	0.43
1:DDD:1830:VAL:HG11	1:DDD:1840:PHE:CG	2.54	0.43
1:EEE:2415:SER:O	1:EEE:2419:ARG:HG3	2.18	0.42
1:DDD:2333:GLN:HB3	1:DDD:2336:LEU:HB2	2.01	0.42
1:AAA:2348:LEU:HD22	1:AAA:2423:ILE:HD11	2.02	0.42
1:CCC:2499:PHE:CZ	1:CCC:2508:MET:HE2	2.54	0.42
1:FFF:2328:ALA:HB2	1:FFF:2543:LEU:HD22	2.01	0.42
1:CCC:2309:PRO:HD3	1:EEE:2403:GLY:O	2.19	0.42
1:DDD:2369:ILE:HG22	1:DDD:2370:GLU:N	2.34	0.42
1:AAA:1830:VAL:HG11	1:AAA:1840:PHE:CG	2.54	0.42
1:AAA:2357:ASP:OD2	1:AAA:2379:ARG:NE	2.43	0.42
1:DDD:2357:ASP:OD2	1:DDD:2379:ARG:NE	2.44	0.42
1:CCC:1830:VAL:HG11	1:CCC:1840:PHE:CG	2.54	0.42
1:EEE:1995:LEU:HD12	1:EEE:1995:LEU:HA	1.90	0.42
1:FFF:1830:VAL:HG11	1:FFF:1840:PHE:CG	2.54	0.42
2:QQQ:15:DC:H2"	2:QQQ:16:DG:C8	2.55	0.42
1:BBB:2193:LEU:HB3	1:BBB:2194:PRO:HD3	2.02	0.42
1:CCC:2348:LEU:HD22	1:CCC:2423:ILE:HD11	2.02	0.42
1:FFF:2017:LEU:N	1:FFF:2018:PRO:CD	2.83	0.42
1:BBB:2472:ILE:O	1:BBB:2476:SER:OG	2.35	0.42
1:CCC:2186:LYS:HA	1:FFF:2308:MET:HE2	2.02	0.42
1:EEE:2328:ALA:HB2	1:EEE:2543:LEU:HD22	2.01	0.42
1:AAA:2105:ILE:HD11	1:BBB:2144:PRO:HG3	2.02	0.41
2:OOO:15:DC:H2"	2:OOO:16:DG:C8	2.54	0.41
1:EEE:1892:ILE:HD12	1:EEE:1898:THR:HB	2.02	0.41
2:GGG:15:DC:H2"	2:GGG:16:DG:C8	2.54	0.41
1:AAA:2191:HIS:CG	1:AAA:2192:PRO:HD2	2.55	0.41
1:BBB:2333:GLN:HG2	1:BBB:2336:LEU:HD12	2.02	0.41
1:AAA:2333:GLN:HB3	1:AAA:2336:LEU:HB2	2.01	0.41
1:CCC:2328:ALA:HB2	1:CCC:2543:LEU:HD22	2.01	0.41
1:EEE:2191:HIS:CG	1:EEE:2192:PRO:HD2	2.56	0.41
2:KKK:15:DC:H2"	2:KKK:16:DG:C8	2.55	0.41
1:AAA:2193:LEU:HB3	1:AAA:2194:PRO:HD3	2.02	0.41
1:DDD:2348:LEU:HD22	1:DDD:2423:ILE:HD11	2.03	0.41
1:EEE:2533:PHE:CD1	1:EEE:2533:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:2357:ASP:OD2	1:FFF:2379:ARG:NE	2.44	0.41
1:FFF:2502:HIS:CE1	1:FFF:2533:PHE:CD2	3.09	0.41
1:AAA:2017:LEU:N	1:AAA:2018:PRO:CD	2.84	0.41
1:CCC:2191:HIS:CG	1:CCC:2192:PRO:HD2	2.56	0.41
1:CCC:2502:HIS:CE1	1:CCC:2533:PHE:CD2	3.09	0.41
1:EEE:2193:LEU:HB3	1:EEE:2194:PRO:HD3	2.03	0.41
1:FFF:2193:LEU:HB3	1:FFF:2194:PRO:HD3	2.03	0.41
1:FFF:2191:HIS:CG	1:FFF:2192:PRO:HD2	2.56	0.41
1:AAA:1995:LEU:HD12	1:AAA:1995:LEU:HA	1.89	0.41
1:AAA:2533:PHE:CD1	1:AAA:2533:PHE:N	2.89	0.41
1:BBB:2314:MET:HA	1:BBB:2314:MET:HE2	2.02	0.41
1:BBB:2533:PHE:CD1	1:BBB:2533:PHE:N	2.89	0.41
1:DDD:2502:HIS:CE1	1:DDD:2533:PHE:CD2	3.09	0.41
1:CCC:2017:LEU:N	1:CCC:2018:PRO:CD	2.83	0.41
2:MMM:15:DC:H2"	2:MMM:16:DG:C8	2.56	0.41
6:AAA:2603:K8I:C11	6:AAA:2603:K8I:C7	2.99	0.40
1:DDD:2193:LEU:HB3	1:DDD:2194:PRO:HD3	2.03	0.40
1:EEE:2502:HIS:CE1	1:EEE:2533:PHE:CD2	3.09	0.40
1:AAA:2328:ALA:HB2	1:AAA:2543:LEU:HD22	2.02	0.40
1:FFF:2533:PHE:CD1	1:FFF:2533:PHE:N	2.89	0.40
1:DDD:2533:PHE:CD1	1:DDD:2533:PHE:N	2.89	0.40
1:EEE:2017:LEU:N	1:EEE:2018:PRO:CD	2.83	0.40
1:FFF:2005:LEU:HD13	1:FFF:2053:ILE:HD11	2.04	0.40
1:AAA:2314:MET:HA	1:AAA:2314:MET:HE2	2.03	0.40
1:AAA:2502:HIS:CE1	1:AAA:2533:PHE:CD2	3.09	0.40
1:DDD:1963:VAL:HG12	1:DDD:2053:ILE:CG2	2.52	0.40
1:DDD:2017:LEU:N	1:DDD:2018:PRO:CD	2.85	0.40
1:DDD:2191:HIS:CG	1:DDD:2192:PRO:HD2	2.57	0.40
1:FFF:2333:GLN:HB3	1:FFF:2336:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

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	AAA	629/726 (87%)	612 (97%)	16 (2%)	1 (0%)	43	71
1	BBB	617/726 (85%)	600 (97%)	17 (3%)	0	100	100
1	CCC	628/726 (86%)	607 (97%)	21 (3%)	0	100	100
1	DDD	623/726 (86%)	604 (97%)	19 (3%)	0	100	100
1	EEE	620/726 (85%)	599 (97%)	21 (3%)	0	100	100
1	FFF	624/726 (86%)	604 (97%)	20 (3%)	0	100	100
All	All	3741/4356 (86%)	3626 (97%)	114 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	2355	GLY

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	AAA	502/638 (79%)	483 (96%)	19 (4%)	29	62
1	BBB	494/638 (77%)	475 (96%)	19 (4%)	29	62
1	CCC	494/638 (77%)	473 (96%)	21 (4%)	26	58
1	DDD	491/638 (77%)	472 (96%)	19 (4%)	28	62
1	EEE	493/638 (77%)	473 (96%)	20 (4%)	27	60
1	FFF	490/638 (77%)	471 (96%)	19 (4%)	28	62
All	All	2964/3828 (77%)	2847 (96%)	117 (4%)	28	62

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1825	LEU
1	AAA	1835	ASN
1	AAA	1843	GLU
1	AAA	1886	ARG

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Mol	Chain	Res	Type
1	AAA	1895	CYS
1	AAA	1897	ASP
1	AAA	1903	LEU
1	AAA	1915	PHE
1	AAA	1950	SER
1	AAA	2119	GLN
1	AAA	2181	LYS
1	AAA	2209	LYS
1	AAA	2314	MET
1	AAA	2330	ASP
1	AAA	2368	MET
1	AAA	2400	GLU
1	AAA	2401	GLN
1	AAA	2424	ASN
1	AAA	2537	GLN
1	BBB	1825	LEU
1	BBB	1835	ASN
1	BBB	1843	GLU
1	BBB	1886	ARG
1	BBB	1896	ASP
1	BBB	1897	ASP
1	BBB	1903	LEU
1	BBB	1915	PHE
1	BBB	1950	SER
1	BBB	2119	GLN
1	BBB	2181	LYS
1	BBB	2314	MET
1	BBB	2330	ASP
1	BBB	2368	MET
1	BBB	2370	GLU
1	BBB	2401	GLN
1	BBB	2411	CYS
1	BBB	2424	ASN
1	BBB	2537	GLN
1	CCC	1825	LEU
1	CCC	1835	ASN
1	CCC	1843	GLU
1	CCC	1886	ARG
1	CCC	1895	CYS
1	CCC	1897	ASP
1	CCC	1903	LEU
1	CCC	1915	PHE

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Mol	Chain	Res	Type
1	CCC	1950	SER
1	CCC	2119	GLN
1	CCC	2181	LYS
1	CCC	2201	ARG
1	CCC	2209	LYS
1	CCC	2314	MET
1	CCC	2330	ASP
1	CCC	2368	MET
1	CCC	2377	ASP
1	CCC	2401	GLN
1	CCC	2424	ASN
1	CCC	2537	GLN
1	CCC	2564	SER
1	DDD	1835	ASN
1	DDD	1843	GLU
1	DDD	1895	CYS
1	DDD	1897	ASP
1	DDD	1903	LEU
1	DDD	1915	PHE
1	DDD	1950	SER
1	DDD	2013	LEU
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	2424	ASN
1	DDD	2537	GLN
1	EEE	1825	LEU
1	EEE	1835	ASN
1	EEE	1843	GLU
1	EEE	1886	ARG
1	EEE	1895	CYS
1	EEE	1897	ASP
1	EEE	1903	LEU
1	EEE	1915	PHE
1	EEE	1950	SER
1	EEE	2119	GLN

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Mol	Chain	Res	Type
1	EEE	2181	LYS
1	EEE	2209	LYS
1	EEE	2314	MET
1	EEE	2330	ASP
1	EEE	2368	MET
1	EEE	2401	GLN
1	EEE	2418	SER
1	EEE	2428	THR
1	EEE	2537	GLN
1	EEE	2564	SER
1	FFF	1825	LEU
1	FFF	1835	ASN
1	FFF	1843	GLU
1	FFF	1886	ARG
1	FFF	1895	CYS
1	FFF	1897	ASP
1	FFF	1903	LEU
1	FFF	1915	PHE
1	FFF	1950	SER
1	FFF	2119	GLN
1	FFF	2209	LYS
1	FFF	2314	MET
1	FFF	2330	ASP
1	FFF	2368	MET
1	FFF	2377	ASP
1	FFF	2401	GLN
1	FFF	2419	ARG
1	FFF	2424	ASN
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 ⓘ

There are no RNA molecules in this entry.

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

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	RRR	13	2,3	20,23,24	1.44	4 (20%)	27,33,36	2.14	7 (25%)
3	DDG	NNN	13	2,3	20,23,24	1.46	4 (20%)	27,33,36	2.11	8 (29%)
3	DDG	LLL	13	2,3	20,23,24	1.56	5 (25%)	27,33,36	2.29	8 (29%)
3	DDG	HHH	13	2,3	20,23,24	1.70	6 (30%)	27,33,36	2.09	8 (29%)
3	DDG	JJJ	13	2,3	20,23,24	1.55	5 (25%)	27,33,36	2.14	7 (25%)
3	DDG	PPP	13	2,3	20,23,24	1.47	4 (20%)	27,33,36	2.17	7 (25%)

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	RRR	13	2,3	-	2/7/18/19	0/3/3/3
3	DDG	NNN	13	2,3	-	2/7/18/19	0/3/3/3
3	DDG	LLL	13	2,3	-	2/7/18/19	0/3/3/3
3	DDG	HHH	13	2,3	-	2/7/18/19	0/3/3/3
3	DDG	JJJ	13	2,3	-	2/7/18/19	0/3/3/3
3	DDG	PPP	13	2,3	-	2/7/18/19	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	HHH	13	DDG	C5-N7	-3.54	1.32	1.39
3	RRR	13	DDG	C6-N1	-3.48	1.32	1.38
3	LLL	13	DDG	C6-N1	-3.30	1.32	1.38
3	PPP	13	DDG	C6-N1	-3.20	1.32	1.38
3	JJJ	13	DDG	C5-N7	-3.16	1.32	1.39
3	JJJ	13	DDG	C6-N1	-3.15	1.33	1.38
3	NNN	13	DDG	C5-N7	-3.10	1.32	1.39
3	LLL	13	DDG	C5-N7	-3.03	1.33	1.39
3	PPP	13	DDG	C5-N7	-2.89	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	NNN	13	DDG	C6-N1	-2.80	1.33	1.38
3	RRR	13	DDG	C5-N7	-2.77	1.33	1.39
3	HHH	13	DDG	C6-N1	-2.75	1.33	1.38
3	NNN	13	DDG	C5-C4	2.72	1.46	1.38
3	JJJ	13	DDG	C4-N9	-2.60	1.31	1.38
3	HHH	13	DDG	O4'-C4'	-2.59	1.39	1.44
3	HHH	13	DDG	C4-N9	-2.56	1.31	1.38
3	PPP	13	DDG	C5-C4	2.56	1.45	1.38
3	LLL	13	DDG	C5-C4	2.52	1.45	1.38
3	JJJ	13	DDG	C5-C4	2.51	1.45	1.38
3	RRR	13	DDG	C5-C4	2.48	1.45	1.38
3	PPP	13	DDG	C4-N9	-2.46	1.31	1.38
3	RRR	13	DDG	C4-N9	-2.27	1.32	1.38
3	HHH	13	DDG	C5-C4	2.27	1.44	1.38
3	HHH	13	DDG	C8-N9	-2.26	1.32	1.37
3	LLL	13	DDG	C8-N9	-2.25	1.32	1.37
3	LLL	13	DDG	C4-N9	-2.20	1.32	1.38
3	JJJ	13	DDG	C8-N9	-2.20	1.32	1.37
3	NNN	13	DDG	C8-N7	2.00	1.38	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LLL	13	DDG	C5-C4-N3	-5.95	118.91	128.39
3	PPP	13	DDG	C5-C4-N3	-5.93	118.96	128.39
3	RRR	13	DDG	C5-C4-N3	-5.85	119.08	128.39
3	JJJ	13	DDG	C5-C4-N3	-5.82	119.12	128.39
3	HHH	13	DDG	C5-C4-N3	-5.81	119.15	128.39
3	NNN	13	DDG	C5-C4-N3	-5.80	119.16	128.39
3	PPP	13	DDG	C2-N3-C4	4.51	120.07	112.30
3	RRR	13	DDG	C2-N3-C4	4.49	120.03	112.30
3	LLL	13	DDG	C2-N3-C4	4.48	120.02	112.30
3	NNN	13	DDG	C2-N3-C4	4.48	120.01	112.30
3	JJJ	13	DDG	C2-N3-C4	4.39	119.86	112.30
3	HHH	13	DDG	C2-N3-C4	4.19	119.51	112.30
3	PPP	13	DDG	N9-C4-N3	4.08	134.11	125.95
3	NNN	13	DDG	N9-C4-N3	4.03	134.01	125.95
3	HHH	13	DDG	N9-C4-N3	4.00	133.94	125.95
3	RRR	13	DDG	N9-C4-N3	3.99	133.93	125.95
3	JJJ	13	DDG	N9-C4-N3	3.98	133.91	125.95
3	LLL	13	DDG	N9-C4-N3	3.85	133.66	125.95
3	LLL	13	DDG	C6-C5-N7	3.43	136.53	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	JJJ	13	DDG	C6-C5-N7	3.32	136.33	130.29
3	LLL	13	DDG	C4-C5-N7	-3.24	105.54	110.67
3	RRR	13	DDG	C6-C5-N7	3.18	136.07	130.29
3	PPP	13	DDG	C6-C5-N7	3.15	136.03	130.29
3	NNN	13	DDG	C6-C5-N7	3.14	136.01	130.29
3	JJJ	13	DDG	C4-C5-N7	-3.10	105.76	110.67
3	LLL	13	DDG	O4'-C1'-C2'	3.02	109.99	106.41
3	HHH	13	DDG	C6-C5-N7	2.99	135.73	130.29
3	PPP	13	DDG	C4-C5-N7	-2.94	106.01	110.67
3	NNN	13	DDG	C4-C5-N7	-2.86	106.14	110.67
3	RRR	13	DDG	C4-C5-N7	-2.84	106.17	110.67
3	HHH	13	DDG	C4-C5-N7	-2.77	106.28	110.67
3	LLL	13	DDG	C2'-C3'-C4'	2.53	107.45	102.75
3	PPP	13	DDG	C3'-C2'-C1'	2.47	105.72	102.87
3	NNN	13	DDG	C3'-C2'-C1'	2.38	105.62	102.87
3	NNN	13	DDG	C8-N7-C5	2.31	108.38	104.26
3	LLL	13	DDG	C8-N7-C5	2.30	108.36	104.26
3	RRR	13	DDG	C3'-C2'-C1'	2.21	105.41	102.87
3	JJJ	13	DDG	C8-N7-C5	2.20	108.18	104.26
3	PPP	13	DDG	C8-N7-C5	2.17	108.12	104.26
3	NNN	13	DDG	N9-C8-N7	-2.16	109.39	113.40
3	RRR	13	DDG	C8-N7-C5	2.15	108.09	104.26
3	HHH	13	DDG	O6-C6-C5	-2.08	121.03	126.53
3	HHH	13	DDG	C8-N7-C5	2.08	107.96	104.26
3	HHH	13	DDG	C2'-C3'-C4'	2.08	106.61	102.75
3	JJJ	13	DDG	C3'-C2'-C1'	2.07	105.25	102.87

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	PPP	13	DDG	C3'-C4'-C5'-O5'
3	RRR	13	DDG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	NNN	13	DDG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	BBB	2602	4	31,32,32	0.57	0	44,50,50	0.97	4 (9%)
6	K8I	AAA	2603	-	32,32,32	0.98	1 (3%)	43,48,48	0.90	3 (6%)
6	K8I	DDD	2603	-	32,32,32	0.94	1 (3%)	43,48,48	1.09	4 (9%)
5	DG3	EEE	2602	4	31,32,32	0.50	0	44,50,50	0.86	2 (4%)
5	DG3	AAA	2602	4	31,32,32	0.53	0	44,50,50	0.90	2 (4%)
6	K8I	BBB	2603	-	32,32,32	0.86	1 (3%)	43,48,48	0.79	2 (4%)
5	DG3	KKK	101	4	31,32,32	0.49	0	44,50,50	0.88	2 (4%)
5	DG3	FFF	2602	4	31,32,32	0.53	0	44,50,50	0.76	0
5	DG3	DDD	2602	4	31,32,32	0.59	0	44,50,50	0.80	1 (2%)
6	K8I	CCC	2602	-	32,32,32	0.90	1 (3%)	43,48,48	0.94	4 (9%)

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	BBB	2602	4	-	3/22/31/31	0/3/3/3
6	K8I	AAA	2603	-	-	0/22/37/37	0/3/3/3
6	K8I	DDD	2603	-	-	0/22/37/37	0/3/3/3
5	DG3	EEE	2602	4	-	2/22/31/31	0/3/3/3
5	DG3	AAA	2602	4	-	5/22/31/31	0/3/3/3
6	K8I	BBB	2603	-	-	0/22/37/37	0/3/3/3
5	DG3	KKK	101	4	-	6/22/31/31	0/3/3/3
5	DG3	FFF	2602	4	-	5/22/31/31	0/3/3/3
5	DG3	DDD	2602	4	-	7/22/31/31	0/3/3/3
6	K8I	CCC	2602	-	-	1/22/37/37	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AAA	2603	K8I	C10-N3	-4.40	1.36	1.43
6	CCC	2602	K8I	C10-N3	-3.92	1.37	1.43
6	DDD	2603	K8I	C10-N3	-3.88	1.37	1.43
6	BBB	2603	K8I	C10-N3	-3.79	1.37	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	DDD	2603	K8I	C5-C6-C7	3.59	106.86	102.57
6	DDD	2603	K8I	C17-C18-N4	-3.41	169.92	177.46
6	DDD	2603	K8I	C6-C7-C8	2.95	115.58	110.19
6	CCC	2602	K8I	C6-C7-C8	2.83	115.36	110.19
6	CCC	2602	K8I	C5-C6-C7	2.42	105.45	102.57
5	EEE	2602	DG3	C4'-O4'-C1'	-2.34	107.60	109.81
5	BBB	2602	DG3	O3A-PB-O1B	-2.31	103.76	110.70
5	AAA	2602	DG3	O2A-PA-O1A	2.30	123.13	112.44
5	BBB	2602	DG3	O2A-PA-O1A	2.28	123.05	112.44
6	CCC	2602	K8I	C3-N1-C2	2.26	120.80	116.85
6	DDD	2603	K8I	C3-N1-C2	2.22	120.73	116.85
5	KKK	101	DG3	O3A-PB-O1B	-2.20	104.08	110.70
5	KKK	101	DG3	O2A-PA-O1A	2.17	122.53	112.44
6	AAA	2603	K8I	C3-N1-C2	2.17	120.63	116.85
6	CCC	2602	K8I	C17-C18-N4	-2.17	172.67	177.46
5	DDD	2602	DG3	O2A-PA-O1A	2.13	122.35	112.44
5	BBB	2602	DG3	O3A-PA-O1A	-2.13	104.30	110.70
6	BBB	2603	K8I	C5-C6-C7	2.11	105.09	102.57
5	BBB	2602	DG3	O3B-PG-O1G	-2.09	100.04	111.04
5	AAA	2602	DG3	O3A-PB-O1B	-2.06	104.49	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AAA	2603	K8I	C5-C4-N2	-2.03	102.43	104.15
6	AAA	2603	K8I	C17-C18-N4	-2.02	173.00	177.46
5	EEE	2602	DG3	O2A-PA-O1A	2.02	121.83	112.44
6	BBB	2603	K8I	C3-N1-C2	2.00	120.34	116.85

There are no chirality outliers.

All (29) torsion outliers are listed below:

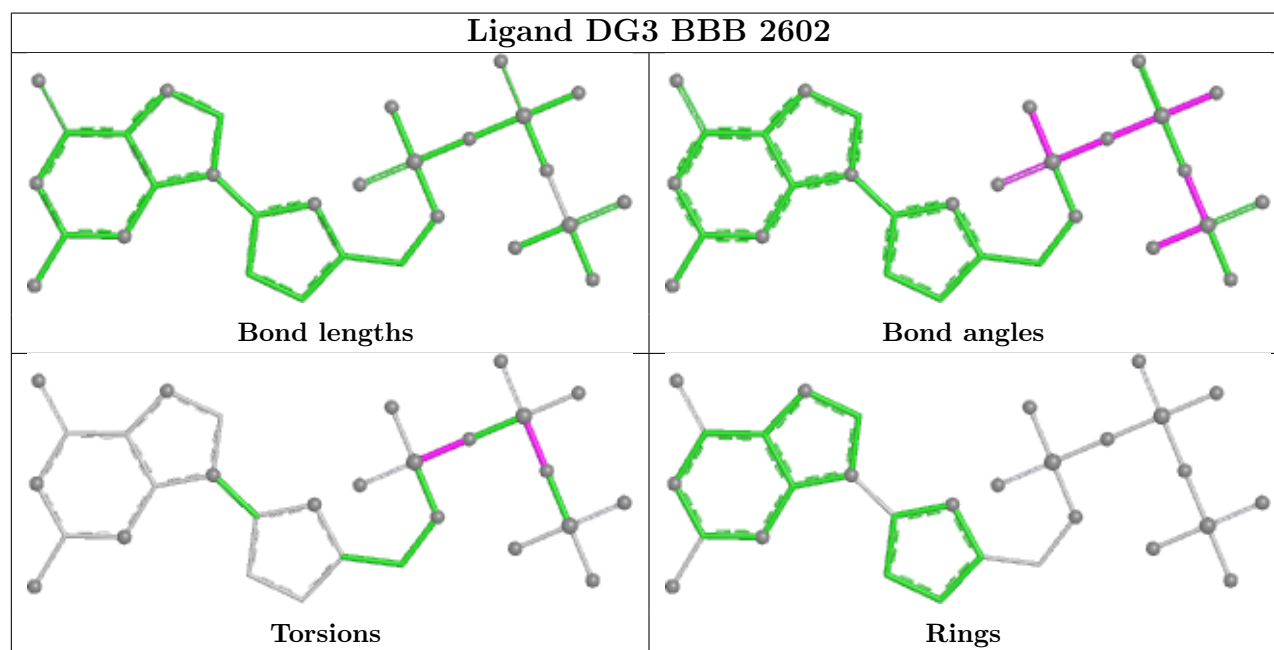
Mol	Chain	Res	Type	Atoms
5	FFF	2602	DG3	PB-O3B-PG-O2G
5	KKK	101	DG3	C5'-O5'-PA-O3A
5	KKK	101	DG3	C5'-O5'-PA-O2A
5	DDD	2602	DG3	PB-O3B-PG-O1G
5	AAA	2602	DG3	PG-O3B-PB-O1B
5	DDD	2602	DG3	PG-O3B-PB-O1B
5	FFF	2602	DG3	PG-O3B-PB-O1B
5	KKK	101	DG3	PB-O3B-PG-O2G
5	KKK	101	DG3	PB-O3B-PG-O3G
6	CCC	2602	K8I	C19-C17-C18-N4
5	AAA	2602	DG3	PG-O3B-PB-O2B
5	AAA	2602	DG3	PB-O3A-PA-O2A
5	DDD	2602	DG3	PB-O3A-PA-O2A
5	KKK	101	DG3	C5'-O5'-PA-O1A
5	FFF	2602	DG3	PB-O3B-PG-O1G
5	BBB	2602	DG3	PG-O3B-PB-O2B
5	BBB	2602	DG3	PB-O3A-PA-O2A
5	DDD	2602	DG3	PG-O3B-PB-O2B
5	FFF	2602	DG3	PG-O3B-PB-O2B
5	FFF	2602	DG3	PB-O3A-PA-O2A
5	KKK	101	DG3	PA-O3A-PB-O2B
5	AAA	2602	DG3	PB-O3B-PG-O1G
5	DDD	2602	DG3	O4'-C4'-C5'-O5'
5	DDD	2602	DG3	C3'-C4'-C5'-O5'
5	EEE	2602	DG3	C4'-C5'-O5'-PA
5	AAA	2602	DG3	PB-O3A-PA-O1A
5	BBB	2602	DG3	PG-O3B-PB-O1B
5	DDD	2602	DG3	PB-O3A-PA-O1A
5	EEE	2602	DG3	PG-O3B-PB-O1B

There are no ring outliers.

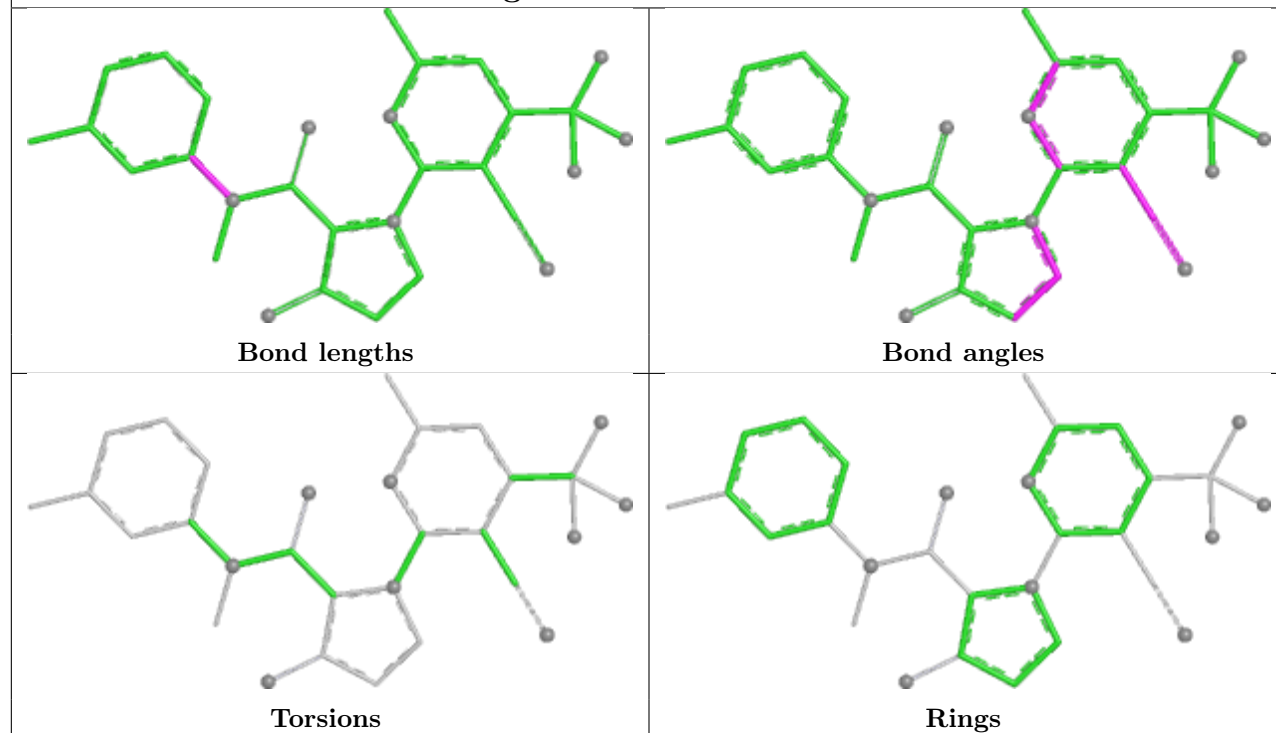
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	2603	K8I	2	0
6	DDD	2603	K8I	1	0
5	EEE	2602	DG3	2	0
6	BBB	2603	K8I	2	0
5	KKK	101	DG3	1	0
6	CCC	2602	K8I	2	0

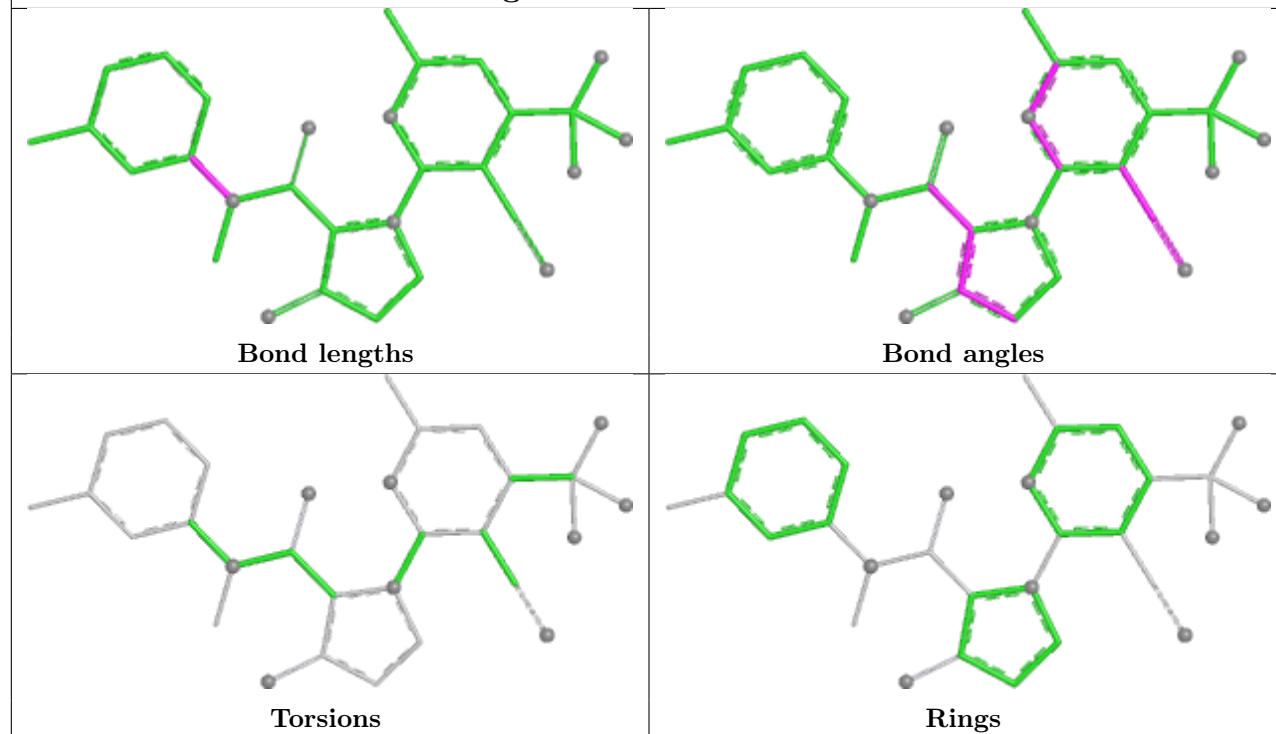
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



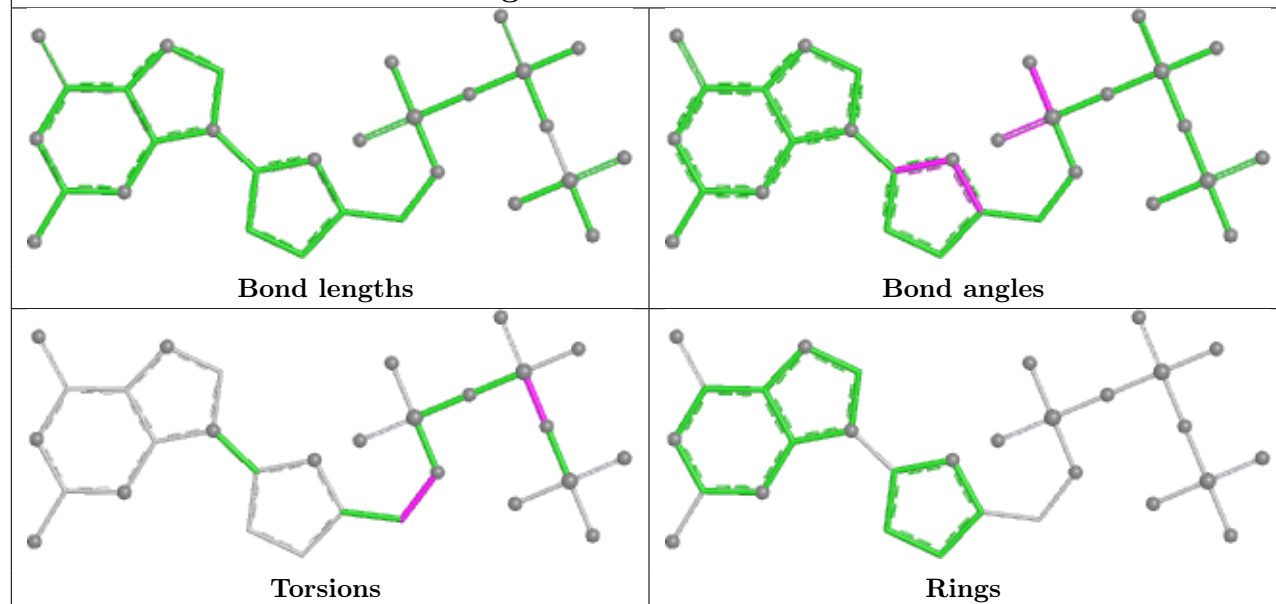
Ligand K8I AAA 2603



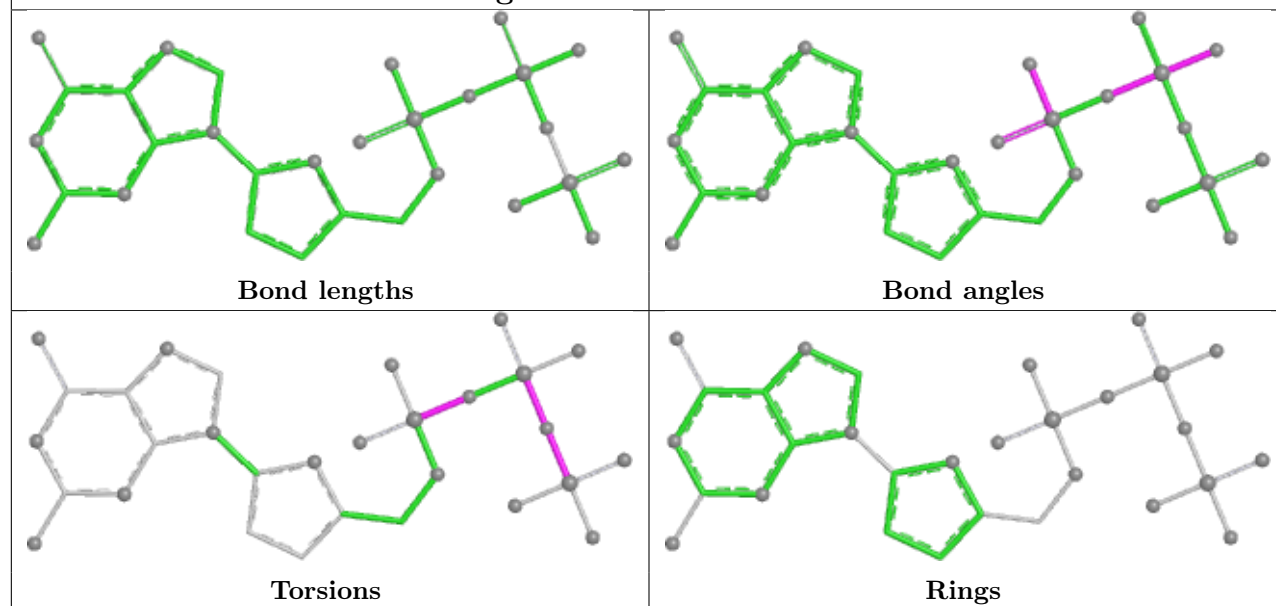
Ligand K8I DDD 2603



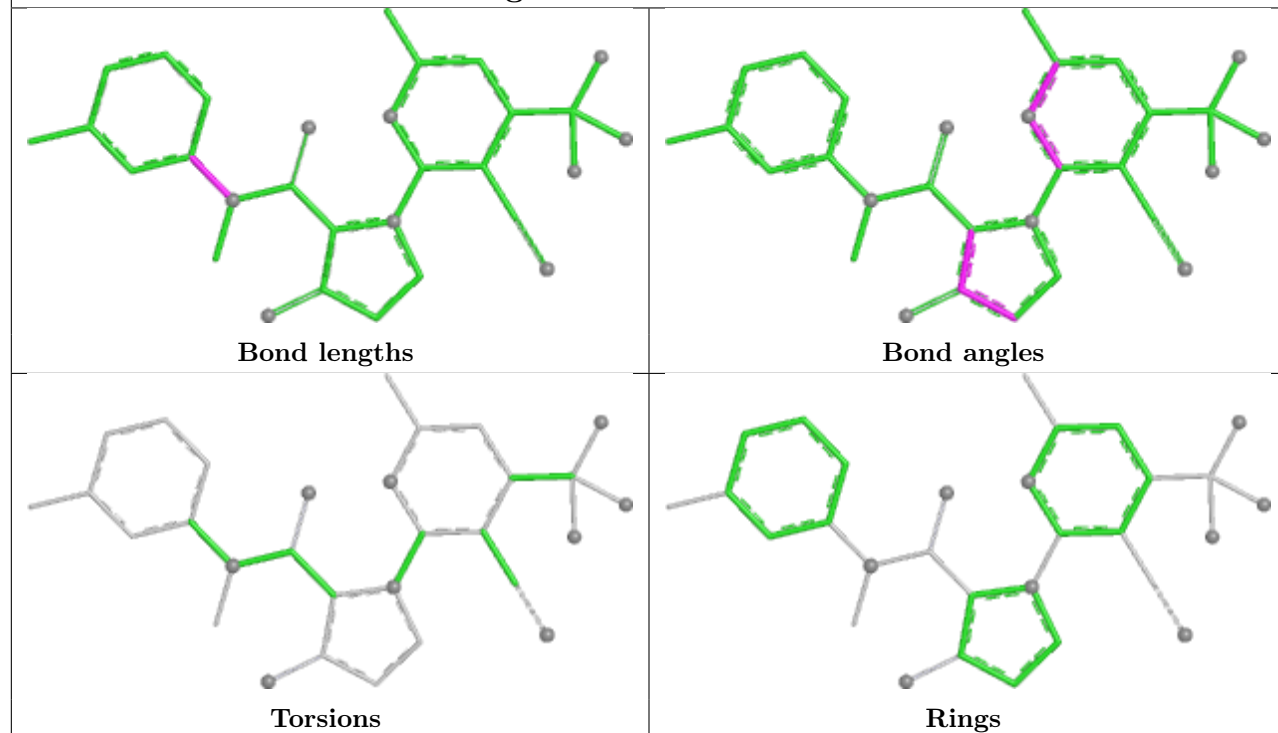
Ligand DG3 EEE 2602



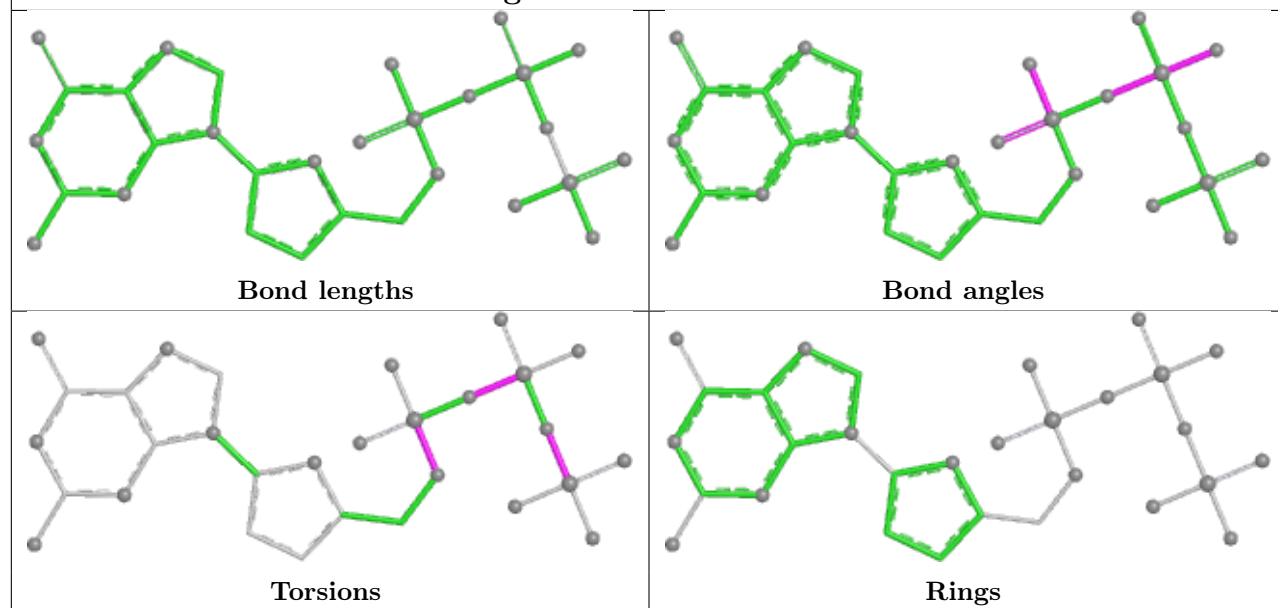
Ligand DG3 AAA 2602



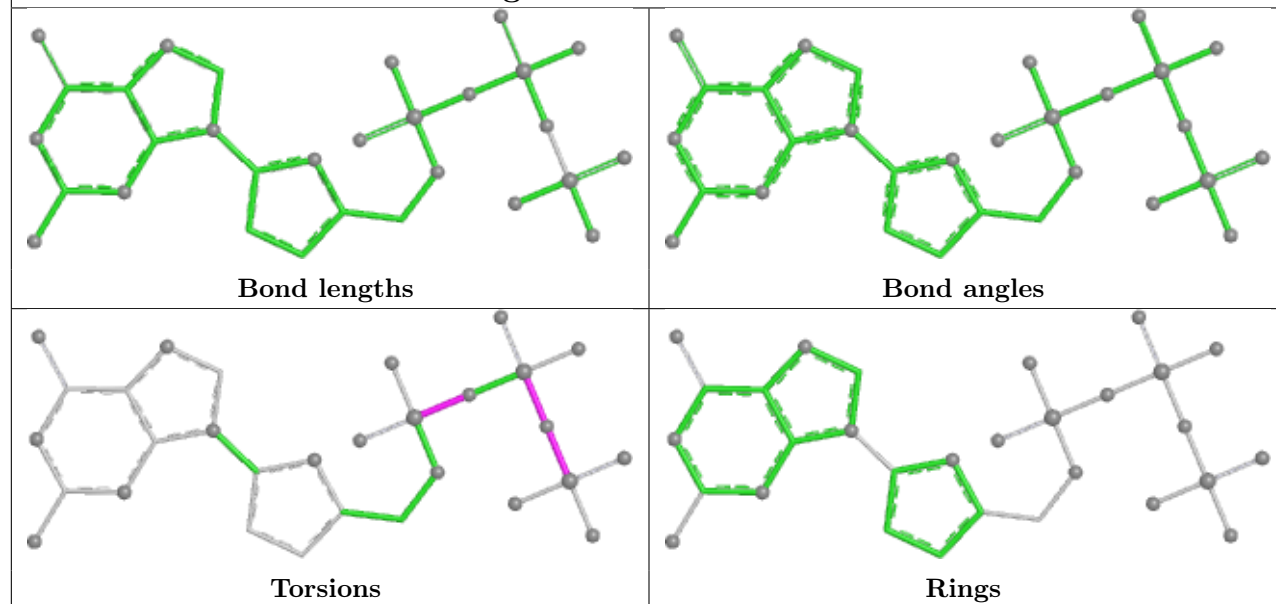
Ligand K8I BBB 2603



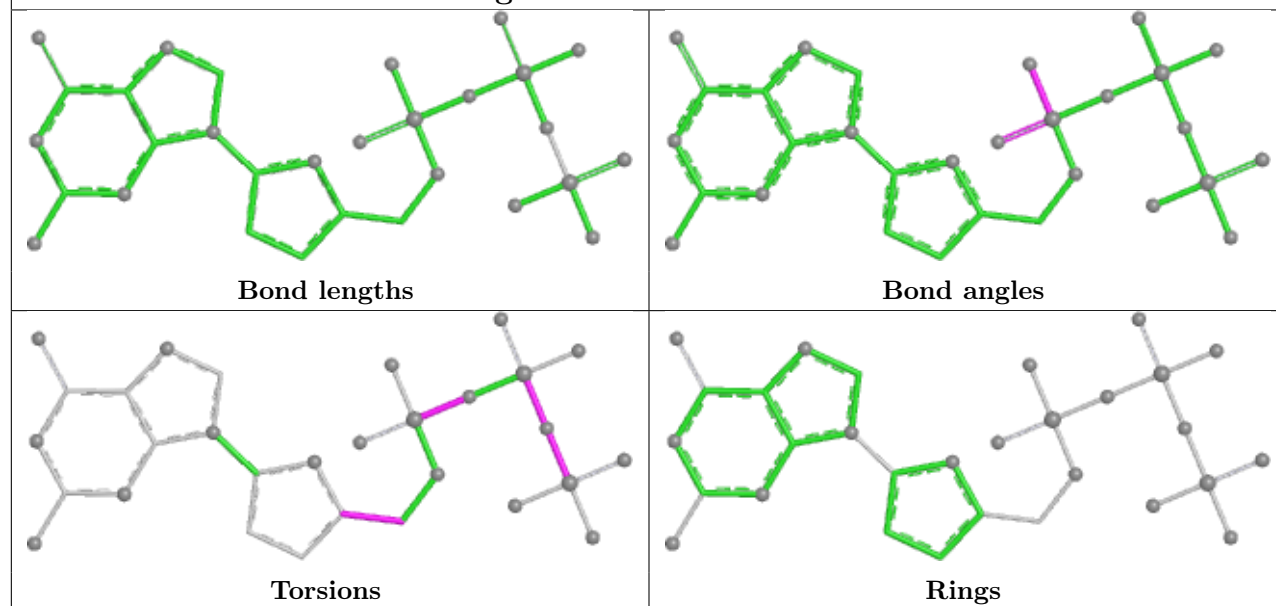
Ligand DG3 KKK 101

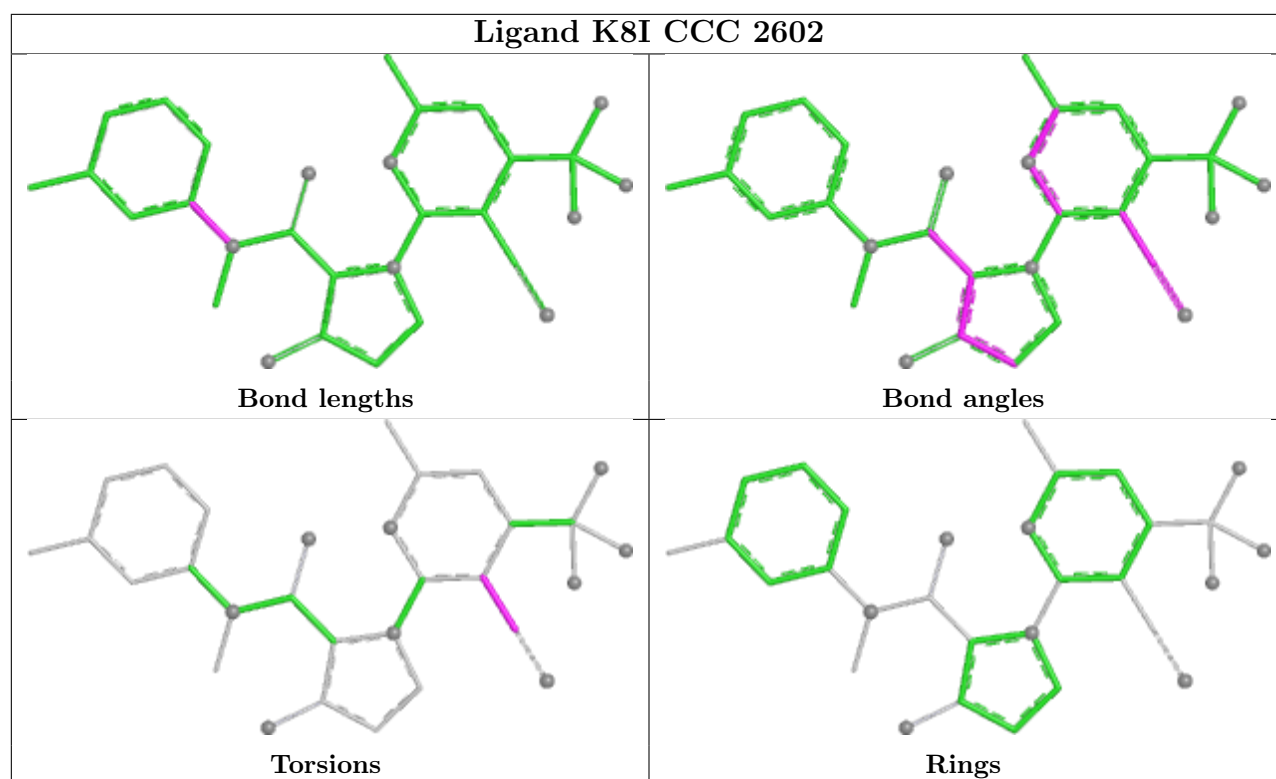


Ligand DG3 FFF 2602



Ligand DG3 DDD 2602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AAA	639/726 (88%)	0.29	33 (5%)	33	24	39, 74, 135, 198	0
1	BBB	629/726 (86%)	0.55	47 (7%)	20	14	45, 84, 140, 194	0
1	CCC	638/726 (87%)	0.40	29 (4%)	38	30	45, 87, 145, 197	0
1	DDD	633/726 (87%)	0.81	74 (11%)	9	7	56, 103, 176, 219	0
1	EEE	632/726 (87%)	0.94	92 (14%)	6	4	62, 114, 169, 208	0
1	FFF	634/726 (87%)	0.98	97 (15%)	5	4	73, 129, 177, 227	0
2	GGG	16/16 (100%)	0.03	0	100	100	43, 94, 155, 158	0
2	III	16/16 (100%)	0.15	0	100	100	60, 112, 173, 177	0
2	KKK	16/16 (100%)	0.16	0	100	100	54, 110, 172, 174	0
2	MMM	16/16 (100%)	0.13	0	100	100	61, 100, 168, 179	0
2	OOO	16/16 (100%)	0.48	1 (6%)	26	19	93, 148, 225, 232	0
2	QQQ	16/16 (100%)	0.74	2 (12%)	8	6	93, 154, 226, 237	0
3	HHH	12/13 (92%)	-0.04	0	100	100	41, 100, 155, 160	0
3	JJJ	12/13 (92%)	0.19	0	100	100	50, 134, 160, 176	0
3	LLL	12/13 (92%)	0.21	0	100	100	58, 107, 160, 162	0
3	NNN	12/13 (92%)	0.33	1 (8%)	17	12	57, 117, 153, 155	0
3	PPP	12/13 (92%)	0.10	0	100	100	74, 171, 238, 248	0
3	RRR	12/13 (92%)	0.55	1 (8%)	17	12	83, 168, 218, 220	0
All	All	3973/4530 (87%)	0.64	377 (9%)	14	10	39, 100, 168, 248	0

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	2416	PHE	6.4
1	EEE	1965	TYR	6.3
1	EEE	2031	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	DDD	1943	ASP	6.2
1	FFF	1949	GLN	6.1
1	EEE	2003	PRO	5.9
1	BBB	2217	GLU	5.4
1	DDD	2026	SER	5.2
1	FFF	1981	SER	5.2
1	DDD	1945	MET	5.1
1	EEE	2005	LEU	5.0
1	EEE	1967	PHE	5.0
1	EEE	1852	ILE	5.0
1	DDD	1952	LEU	5.0
1	EEE	2210	VAL	5.0
1	EEE	2233	SER	4.9
1	FFF	1964	ILE	4.9
1	FFF	2209	LYS	4.9
1	DDD	2336	LEU	4.8
1	FFF	1979	GLY	4.8
1	EEE	1968	ILE	4.8
1	FFF	2210	VAL	4.8
1	FFF	2386	CYS	4.7
1	FFF	2208	THR	4.7
1	DDD	1939	LEU	4.7
1	BBB	2212	PHE	4.7
1	FFF	1946	TRP	4.7
1	BBB	2214	LEU	4.6
1	BBB	2233	SER	4.6
1	BBB	2504	HIS	4.5
1	EEE	1964	ILE	4.5
1	DDD	2386	CYS	4.5
1	DDD	1931	VAL	4.5
1	EEE	2209	LYS	4.5
1	FFF	1889	GLY	4.5
1	DDD	2028	GLY	4.4
1	FFF	2409	ALA	4.4
1	EEE	2211	VAL	4.4
1	EEE	1969	GLN	4.4
1	CCC	2587	ASP	4.3
1	FFF	2395	ALA	4.3
1	FFF	1996	LEU	4.3
1	DDD	2395	ALA	4.2
1	CCC	2214	LEU	4.1
1	EEE	2212	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	1959	GLU	4.1
1	DDD	2409	ALA	4.1
1	FFF	2212	PHE	4.0
1	BBB	1969	GLN	4.0
1	DDD	1996	LEU	4.0
1	FFF	1991	VAL	4.0
1	EEE	1853	SER	4.0
1	DDD	1946	TRP	4.0
1	BBB	1971	TYR	4.0
1	DDD	2210	VAL	3.9
1	DDD	2208	THR	3.9
1	EEE	2409	ALA	3.9
1	EEE	2214	LEU	3.9
1	EEE	2398	LEU	3.9
1	CCC	1984	GLN	3.9
1	FFF	1967	PHE	3.8
1	FFF	2137	LEU	3.8
1	BBB	2427	MET	3.8
1	FFF	1891	PRO	3.8
1	EEE	1971	TYR	3.8
1	BBB	1976	LEU	3.8
1	DDD	2029	ILE	3.8
1	FFF	1978	CYS	3.8
1	AAA	1984	GLN	3.7
1	DDD	2214	LEU	3.7
1	DDD	2177	PHE	3.7
1	EEE	1889	GLY	3.7
1	AAA	2210	VAL	3.7
1	BBB	2371	PRO	3.7
1	CCC	2212	PHE	3.7
1	EEE	1991	VAL	3.7
1	DDD	1978	CYS	3.6
1	FFF	2233	SER	3.6
1	BBB	1959	GLU	3.6
1	BBB	1978	CYS	3.6
1	EEE	2370	GLU	3.6
1	EEE	1904	ALA	3.6
1	FFF	2053	ILE	3.6
1	BBB	2211	VAL	3.6
1	FFF	1900	VAL	3.5
1	CCC	1983	GLU	3.5
1	EEE	2133	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	DDD	2211	VAL	3.5
1	AAA	2214	LEU	3.5
1	BBB	2216	ARG	3.5
1	BBB	2503	GLY	3.5
1	DDD	1942	LYS	3.5
1	EEE	2034	LEU	3.4
1	EEE	1959	GLU	3.4
1	AAA	1932	PRO	3.4
1	EEE	1990	LYS	3.4
1	DDD	2342	LEU	3.4
1	AAA	2370	GLU	3.4
1	CCC	2083	CYS	3.4
1	FFF	2133	ILE	3.4
1	FFF	1982	LEU	3.4
1	BBB	2088	GLU	3.4
1	DDD	2504	HIS	3.4
1	FFF	1945	MET	3.4
1	FFF	2177	PHE	3.4
1	DDD	2371	PRO	3.4
1	FFF	1980	ILE	3.4
1	EEE	2208	THR	3.4
1	AAA	2435	LYS	3.3
1	DDD	2145	PRO	3.3
1	BBB	2501	SER	3.3
1	EEE	1966	ASP	3.3
1	BBB	2370	GLU	3.3
1	DDD	2104	HIS	3.3
2	QQQ	11	DC	3.2
1	FFF	1975	LEU	3.2
1	BBB	1967	PHE	3.2
1	CCC	1932	PRO	3.2
1	BBB	1975	LEU	3.2
1	DDD	2340	ALA	3.2
1	BBB	2125	PHE	3.2
1	DDD	2333	GLN	3.2
1	BBB	1824	SER	3.2
1	FFF	1971	TYR	3.2
1	EEE	1825	LEU	3.2
1	FFF	2214	LEU	3.2
1	DDD	2025	THR	3.2
1	FFF	2145	PRO	3.1
1	EEE	2060	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	1935	LEU	3.1
1	FFF	1952	LEU	3.1
1	FFF	2336	LEU	3.1
1	EEE	1975	LEU	3.1
1	AAA	1982	LEU	3.1
1	DDD	2217	GLU	3.1
1	DDD	2348	LEU	3.1
1	EEE	2145	PRO	3.1
1	FFF	2431	VAL	3.0
1	BBB	1970	SER	3.0
1	EEE	2371	PRO	3.0
1	DDD	2134	ALA	3.0
1	DDD	1824	SER	3.0
1	EEE	2008	ILE	3.0
1	EEE	2242	ILE	3.0
1	AAA	2407	ASN	3.0
1	EEE	2399	GLY	3.0
1	AAA	1983	GLU	3.0
1	BBB	2208	THR	3.0
1	FFF	2449	TYR	3.0
1	FFF	2242	ILE	3.0
1	CCC	1888	ASP	3.0
1	FFF	2182	ASP	3.0
1	EEE	1986	TYR	2.9
1	FFF	2024	GLU	2.9
2	QQQ	10	DA	2.9
1	EEE	2084	LEU	2.9
1	BBB	2527	CYS	2.9
2	OOO	11	DC	2.9
1	FFF	2398	LEU	2.9
1	BBB	2506	GLU	2.9
1	AAA	2212	PHE	2.9
1	DDD	1940	THR	2.9
1	EEE	2404	ILE	2.9
1	EEE	2416	PHE	2.9
1	FFF	1824	SER	2.9
1	EEE	1976	LEU	2.9
1	FFF	1917	LEU	2.9
1	DDD	2370	GLU	2.8
1	FFF	2370	GLU	2.8
1	DDD	2503	GLY	2.8
1	EEE	2427	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	DDD	1949	GLN	2.8
1	FFF	2548	GLU	2.8
1	BBB	2082	TYR	2.8
1	CCC	2210	VAL	2.8
1	EEE	1824	SER	2.8
1	CCC	2138	PHE	2.8
1	DDD	1980	ILE	2.8
1	BBB	2031	SER	2.8
1	EEE	2245	THR	2.8
1	FFF	1968	ILE	2.8
1	DDD	2233	SER	2.8
1	EEE	2527	CYS	2.7
1	FFF	2064	LEU	2.7
1	CCC	2497	SER	2.7
1	EEE	2506	GLU	2.7
1	FFF	1831	ALA	2.7
1	DDD	2531	GLY	2.7
1	DDD	2144	PRO	2.7
1	BBB	2177	PHE	2.7
1	DDD	2209	LYS	2.7
1	EEE	2471	THR	2.7
1	EEE	2435	LYS	2.7
1	FFF	2503	GLY	2.7
1	AAA	2587	ASP	2.7
1	BBB	2210	VAL	2.7
1	FFF	2232	VAL	2.7
1	DDD	2398	LEU	2.7
1	EEE	1854	LEU	2.7
1	FFF	1939	LEU	2.7
1	DDD	1967	PHE	2.6
1	FFF	2134	ALA	2.6
1	FFF	2022	GLY	2.6
1	FFF	2371	PRO	2.6
1	BBB	2232	VAL	2.6
1	DDD	1959	GLU	2.6
1	BBB	1968	ILE	2.6
1	AAA	1824	SER	2.6
1	CCC	1831	ALA	2.6
1	DDD	2373	SER	2.6
1	FFF	2504	HIS	2.6
1	AAA	2360	ARG	2.6
1	CCC	2209	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	1959	GLU	2.6
1	BBB	2234	GLN	2.6
1	FFF	1852	ILE	2.6
1	FFF	2389	ILE	2.6
1	DDD	2393	MET	2.6
1	EEE	2454	LYS	2.6
1	AAA	2374	VAL	2.6
1	DDD	1983	GLU	2.6
1	AAA	1888	ASP	2.6
1	CCC	2026	SER	2.6
1	FFF	1947	TYR	2.6
1	FFF	2387	TYR	2.6
1	EEE	1982	LEU	2.6
1	DDD	2229	ILE	2.6
1	EEE	2402	MET	2.6
1	EEE	2217	GLU	2.6
1	CCC	2435	LYS	2.5
1	DDD	2084	LEU	2.5
1	EEE	2358	VAL	2.5
1	EEE	2049	GLU	2.5
1	EEE	2411	CYS	2.5
1	EEE	2041	SER	2.5
1	FFF	1825	LEU	2.5
1	FFF	2342	LEU	2.5
1	AAA	1986	TYR	2.5
1	FFF	2335	GLU	2.5
1	FFF	2085	ALA	2.5
1	DDD	2361	SER	2.5
1	CCC	1982	LEU	2.5
1	CCC	2374	VAL	2.5
1	EEE	2232	VAL	2.5
1	EEE	2394	GLY	2.5
1	FFF	2506	GLU	2.5
1	FFF	2537	GLN	2.5
1	AAA	2509	LEU	2.4
1	EEE	1836	LEU	2.4
1	EEE	2026	SER	2.4
1	EEE	2177	PHE	2.4
1	BBB	2089	LEU	2.4
1	DDD	1975	LEU	2.4
1	DDD	2352	LEU	2.4
3	RRR	1	DG	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	2211	VAL	2.4
1	FFF	1944	ARG	2.4
1	FFF	2426	PHE	2.4
1	EEE	2044	TYR	2.4
1	EEE	2412	TYR	2.4
1	FFF	1984	GLN	2.4
1	FFF	2082	TYR	2.4
1	CCC	2371	PRO	2.4
1	DDD	2249	ILE	2.4
1	AAA	2431	VAL	2.4
1	CCC	2182	ASP	2.4
1	FFF	2211	VAL	2.4
1	FFF	2551	VAL	2.4
1	AAA	2209	LYS	2.4
1	AAA	2373	SER	2.4
1	AAA	2506	GLU	2.4
1	BBB	2026	SER	2.4
1	DDD	2130	SER	2.4
1	AAA	2342	LEU	2.4
1	FFF	2060	LEU	2.4
1	FFF	2378	LEU	2.4
1	EEE	2014	PRO	2.4
1	AAA	2182	ASP	2.4
1	CCC	1952	LEU	2.4
1	CCC	1967	PHE	2.3
1	EEE	2088	GLU	2.3
1	AAA	2497	SER	2.3
1	EEE	2415	SER	2.3
1	DDD	1986	TYR	2.3
1	EEE	1917	LEU	2.3
1	FFF	2435	LYS	2.3
1	DDD	1890	PHE	2.3
1	AAA	2376	ASP	2.3
1	DDD	2062	SER	2.3
1	DDD	1968	ILE	2.3
1	BBB	2127	PHE	2.3
1	FFF	1890	PHE	2.3
1	BBB	2395	ALA	2.3
1	FFF	2215	GLN	2.3
1	CCC	2359	PHE	2.3
1	DDD	2223	PHE	2.3
1	BBB	1974	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	EEE	1988	ASP	2.3
1	FFF	2081	GLN	2.3
1	DDD	2083	CYS	2.3
1	FFF	2432	LYS	2.3
1	EEE	2504	HIS	2.3
1	DDD	1947	TYR	2.3
1	CCC	1962	VAL	2.3
1	CCC	2211	VAL	2.3
1	CCC	2217	GLU	2.2
1	DDD	1955	GLU	2.2
1	EEE	2340	ALA	2.2
1	BBB	2086	LEU	2.2
1	EEE	2440	VAL	2.2
1	EEE	2082	TYR	2.2
1	EEE	2449	TYR	2.2
1	EEE	2426	PHE	2.2
1	BBB	1920	GLU	2.2
1	FFF	1948	LEU	2.2
1	AAA	2427	MET	2.2
1	AAA	2186	LYS	2.2
1	FFF	2348	LEU	2.2
1	CCC	1852	ILE	2.2
1	FFF	2423	ILE	2.2
1	EEE	2552	VAL	2.2
1	EEE	1993	CYS	2.2
1	FFF	1951	CYS	2.2
1	DDD	1938	SER	2.2
1	DDD	2031	SER	2.2
1	DDD	2426	PHE	2.2
1	DDD	2137	LEU	2.2
1	FFF	2493	GLU	2.2
1	BBB	2385	ILE	2.2
1	BBB	1955	GLU	2.2
1	FFF	2238	ALA	2.2
1	EEE	2234	GLN	2.1
1	DDD	2374	VAL	2.1
1	EEE	1891	PRO	2.1
1	DDD	2416	PHE	2.1
1	FFF	1836	LEU	2.1
1	CCC	2373	SER	2.1
1	EEE	2080	SER	2.1
1	AAA	2145	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	2405	LYS	2.1
1	CCC	2416	PHE	2.1
1	FFF	2013	LEU	2.1
1	FFF	2223	PHE	2.1
1	DDD	2085	ALA	2.1
1	EEE	2077	GLU	2.1
1	FFF	2539	HIS	2.1
1	FFF	2454	LYS	2.1
1	FFF	2220	LEU	2.1
1	EEE	1994	TRP	2.1
1	BBB	2140	GLU	2.1
1	EEE	2002	GLU	2.1
1	FFF	2326	ILE	2.1
3	NNN	8	DT	2.1
1	FFF	2552	VAL	2.1
1	EEE	2503	GLY	2.1
1	DDD	2182	ASP	2.1
1	AAA	2140	GLU	2.1
1	AAA	2026	SER	2.0
1	BBB	2083	CYS	2.0
1	BBB	2454	LYS	2.0
1	DDD	2040	HIS	2.0
1	EEE	2015	HIS	2.0
1	FFF	2411	CYS	2.0
1	EEE	2032	LEU	2.0
1	EEE	2568	LEU	2.0
1	BBB	2404	ILE	2.0
1	CCC	2207	ILE	2.0
1	EEE	2004	THR	2.0
1	EEE	2085	ALA	2.0
1	DDD	2215	GLN	2.0
1	FFF	2059	GLN	2.0
1	EEE	1903	LEU	2.0
1	FFF	2089	LEU	2.0
1	AAA	2359	PHE	2.0
1	DDD	2359	PHE	2.0
1	BBB	2039	GLU	2.0
1	EEE	2186	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DDG	NNN	13	21/22	0.94	0.08	48,55,66,69	0
3	DDG	RRR	13	21/22	0.94	0.09	72,85,98,100	0
3	DDG	PPP	13	21/22	0.95	0.07	61,76,95,97	0
3	DDG	LLL	13	21/22	0.96	0.07	42,51,60,62	0
3	DDG	HHH	13	21/22	0.98	0.06	30,38,43,44	0
3	DDG	JJJ	13	21/22	0.98	0.05	43,51,55,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

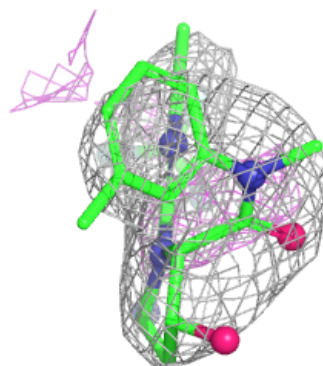
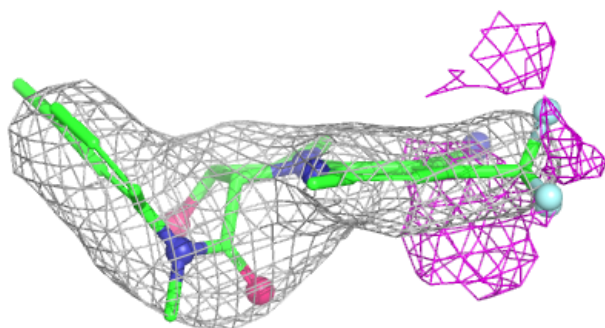
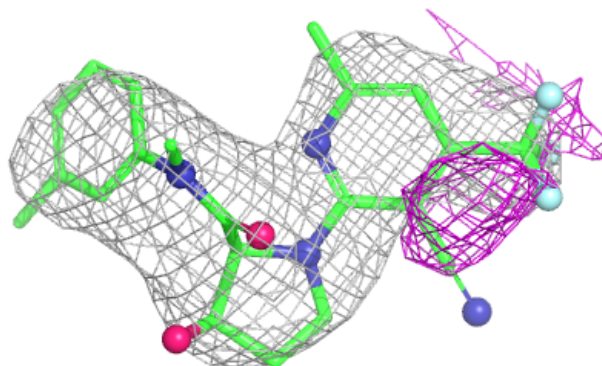
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	K8I	DDD	2603	30/30	0.88	0.15	94,114,136,144	0
6	K8I	AAA	2603	30/30	0.92	0.12	71,95,113,119	0
5	DG3	FFF	2602	30/30	0.92	0.07	89,102,119,121	0
6	K8I	BBB	2603	30/30	0.93	0.10	78,93,115,119	0
6	K8I	CCC	2602	30/30	0.93	0.12	80,95,111,117	0
4	MG	AAA	2601	1/1	0.93	0.06	59,59,59,59	0
5	DG3	DDD	2602	30/30	0.95	0.06	51,63,86,93	0
4	MG	EEE	2601	1/1	0.95	0.05	99,99,99,99	0
5	DG3	EEE	2602	30/30	0.96	0.06	71,91,108,109	0
5	DG3	KKK	101	30/30	0.96	0.06	41,49,83,91	0
4	MG	FFF	2601	1/1	0.97	0.07	111,111,111,111	0
5	DG3	BBB	2602	30/30	0.97	0.06	50,62,73,75	0
4	MG	CCC	2601	1/1	0.98	0.03	59,59,59,59	0
4	MG	DDD	2601	1/1	0.98	0.04	84,84,84,84	0
5	DG3	AAA	2602	30/30	0.98	0.05	39,44,64,76	0
4	MG	BBB	2601	1/1	0.99	0.05	66,66,66,66	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.

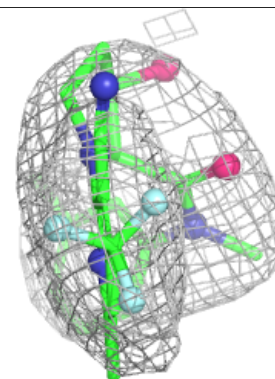
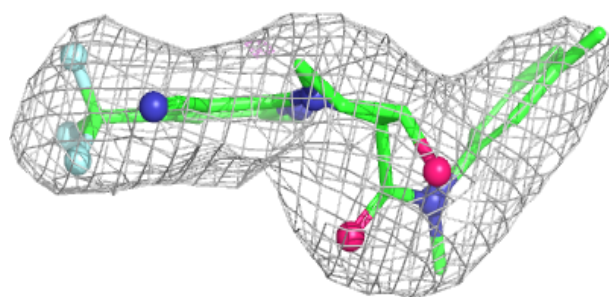
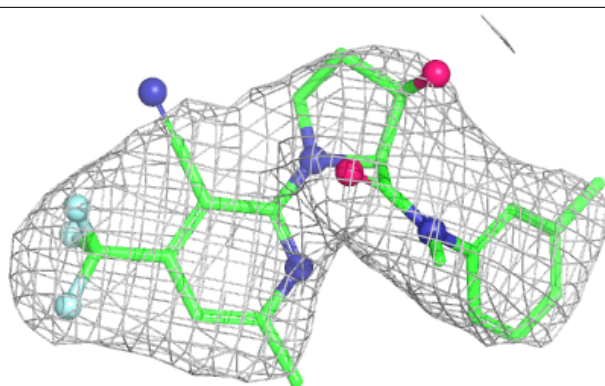
Electron density around K8I DDD 2603:

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

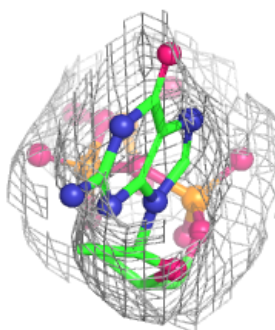
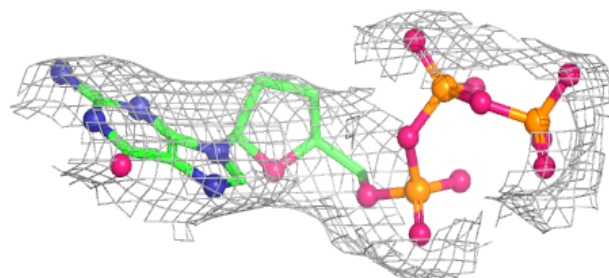
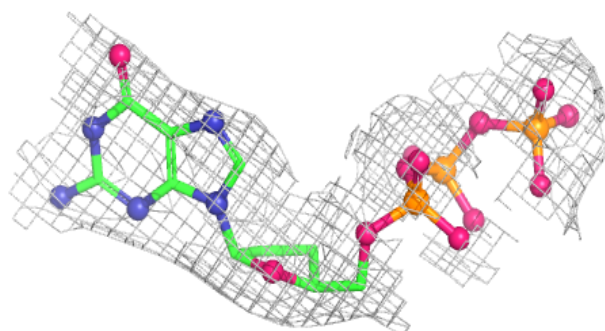


Electron density around K8I AAA 2603:

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

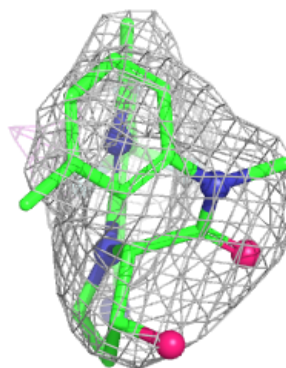
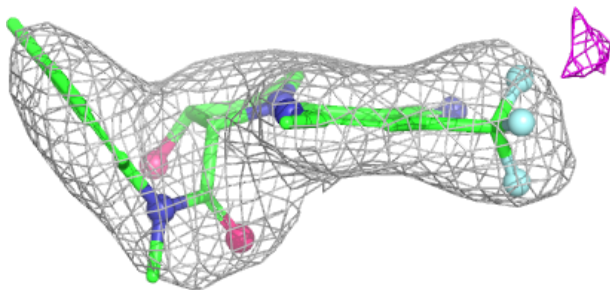
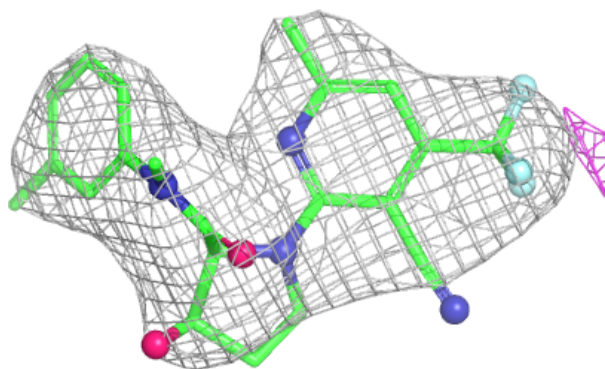
**Electron density around DG3 FFF 2602:**

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

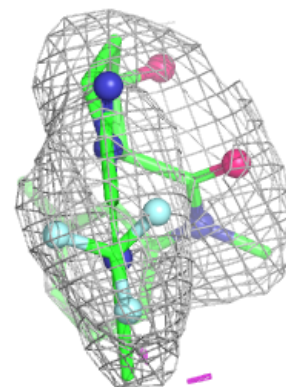
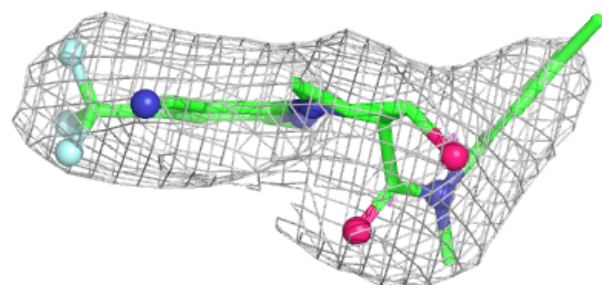
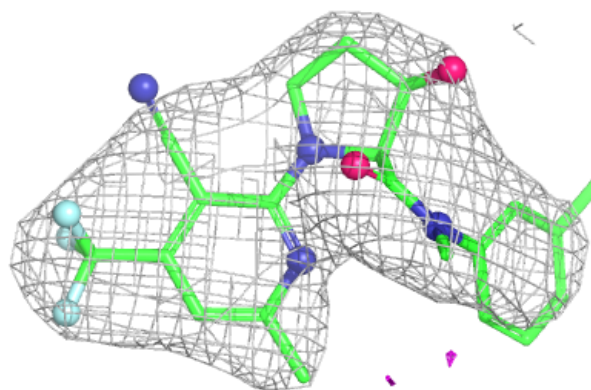


Electron density around K8I BBB 2603:

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

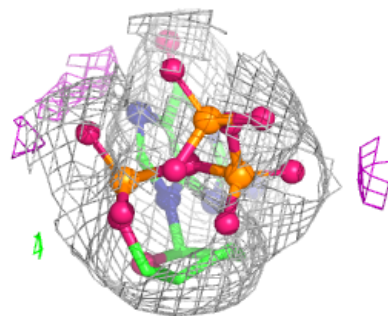
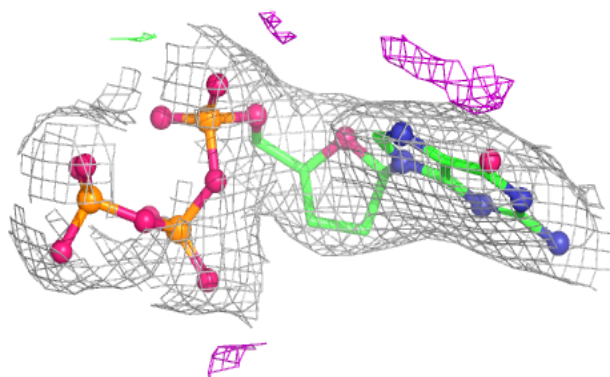
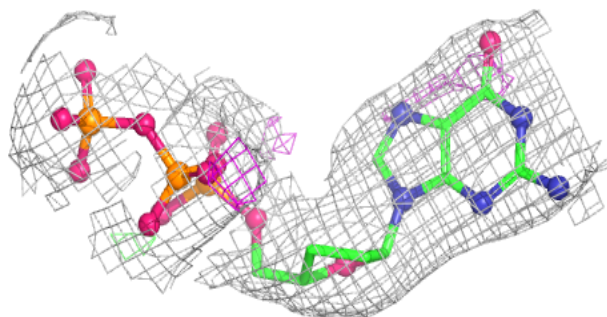
**Electron density around K8I CCC 2602:**

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

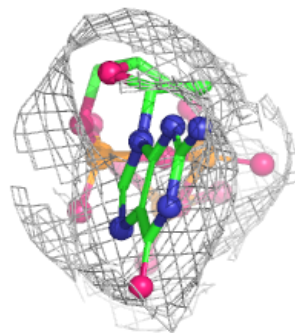
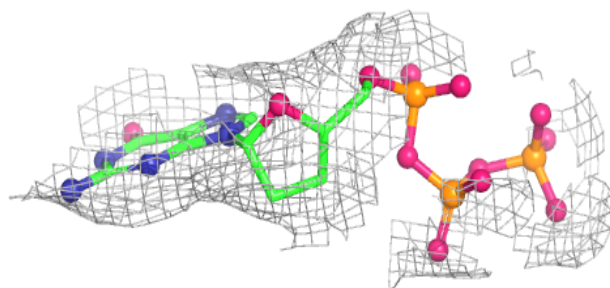
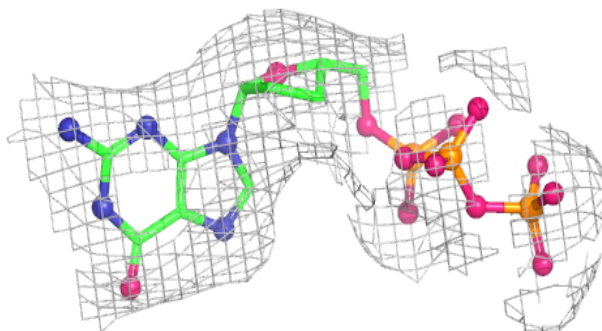


Electron density around DG3 DDD 2602:

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

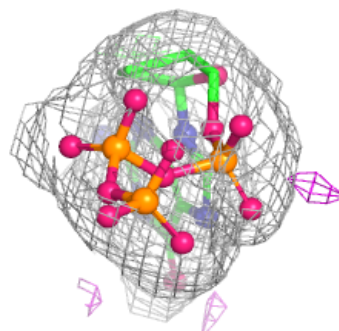
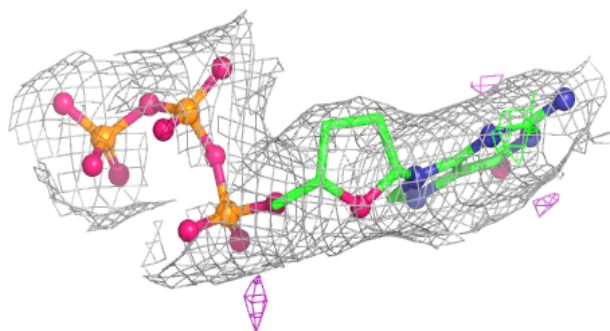
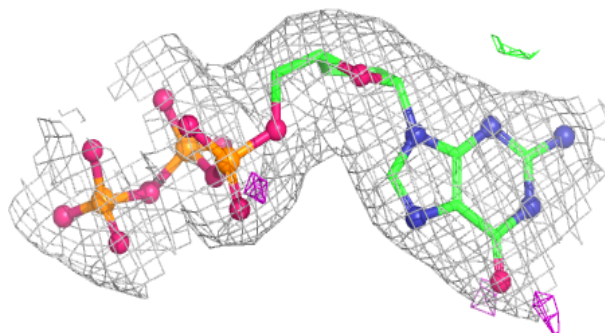
**Electron density around DG3 EEE 2602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

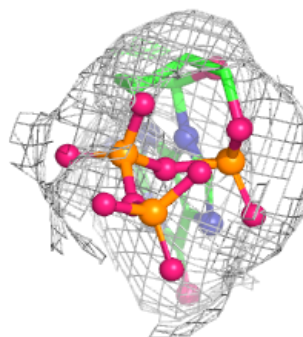
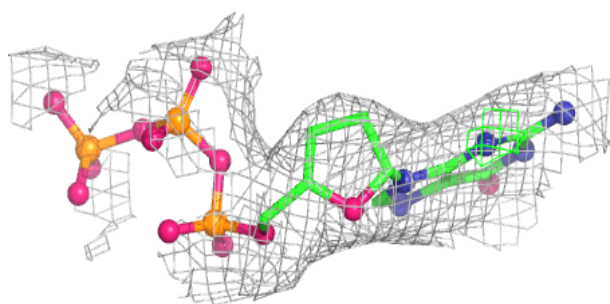
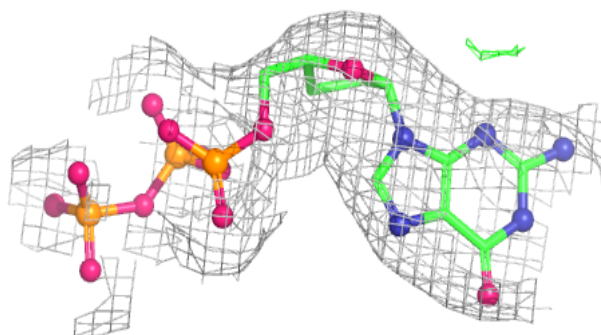


Electron density around DG3 KKK 101:

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

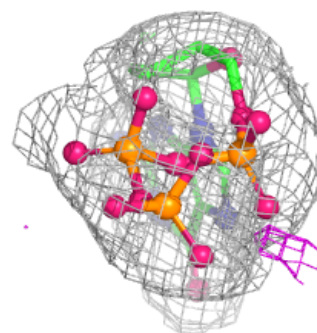
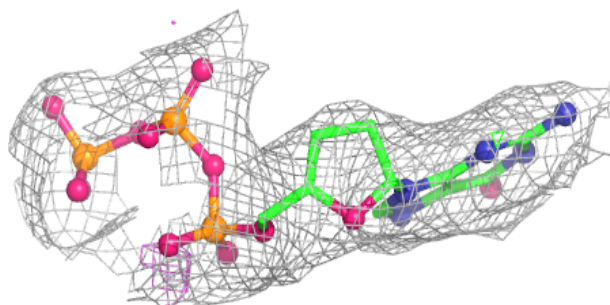
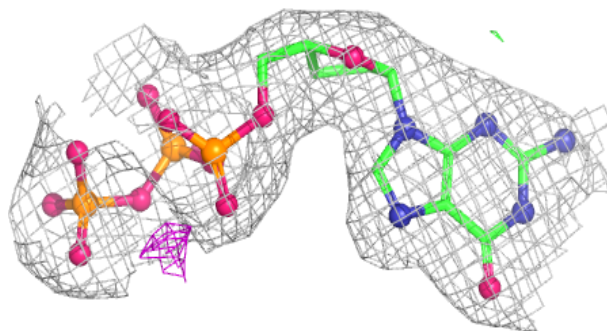
**Electron density around DG3 BBB 2602:**

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



Electron density around DG3 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.