



# Full wwPDB X-ray Structure Validation Report i

Oct 6, 2022 – 04:52 pm BST

PDB ID : 7ZX1  
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](mailto: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 i symbol.

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

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The following versions of software and data (see [references](#) ①) 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

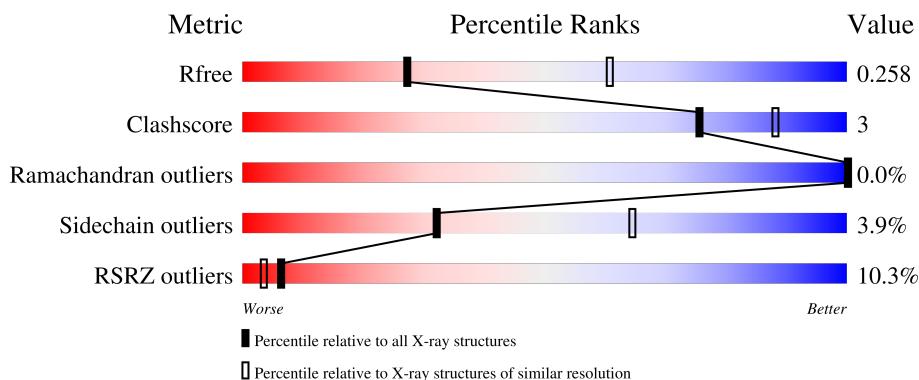
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

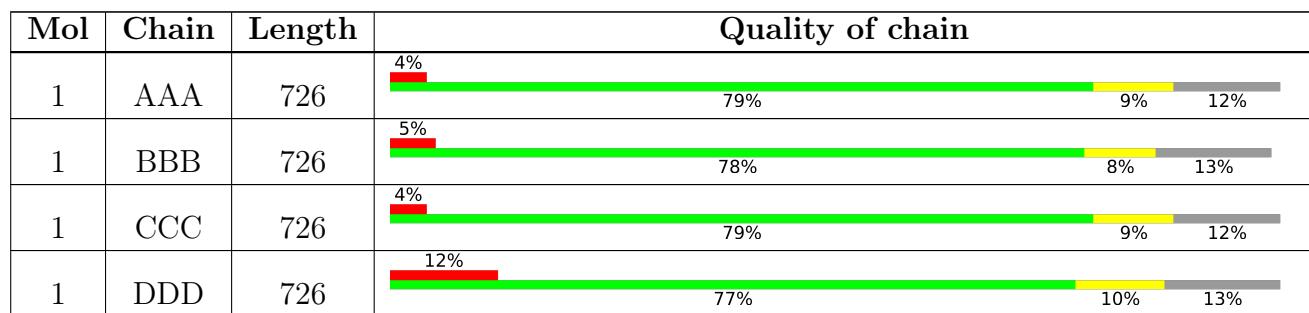
The reported resolution of this entry is 2.83 Å.

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))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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  $\geq 3$ , 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.



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## 2 Entry composition (i)

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			

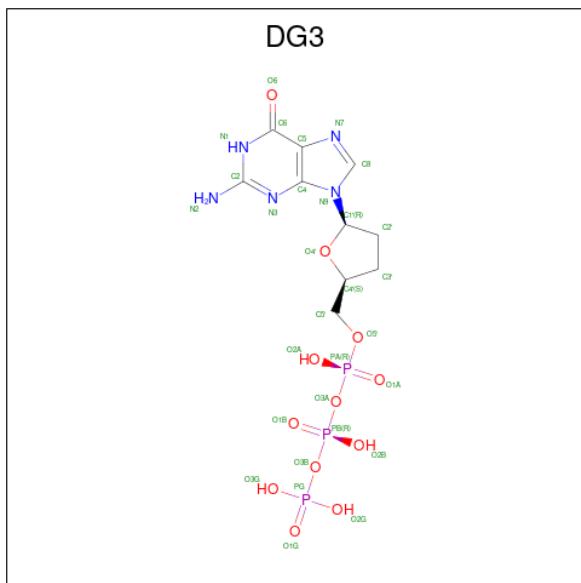
- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*(DDG))-3').

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 (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<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



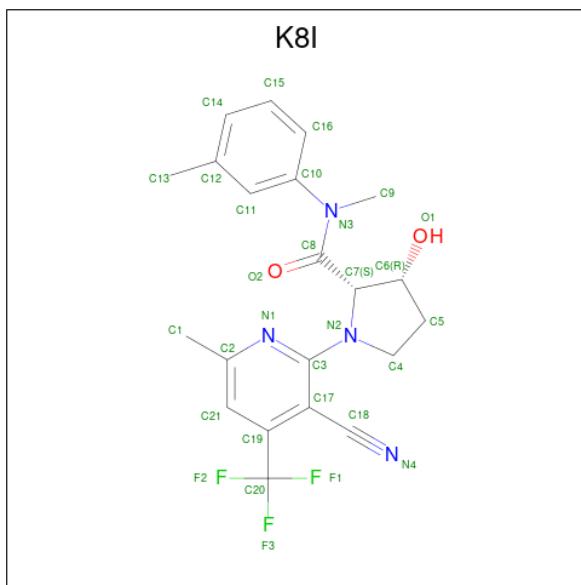
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C N O P 30 10 5 12 3	0	0
5	BBB	1	Total C N O P 30 10 5 12 3	0	0
5	DDD	1	Total C N O P 30 10 5 12 3	0	0
5	EEE	1	Total C N O P 30 10 5 12 3	0	0

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

- 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 (three-letter code: K8I) (formula: C<sub>21</sub>H<sub>21</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

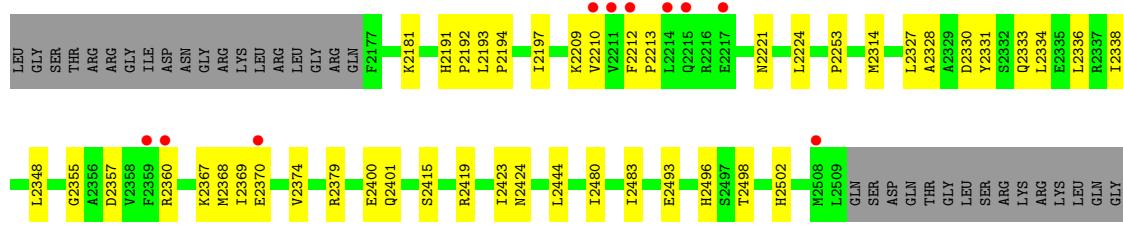
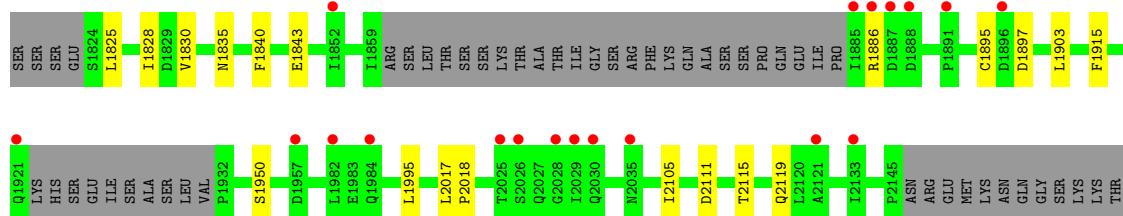
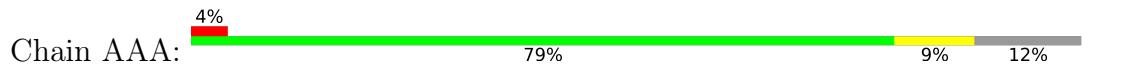
- Molecule 7 is water.

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

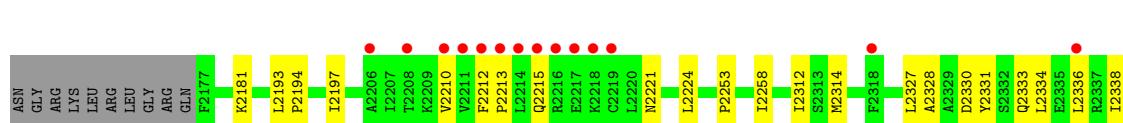
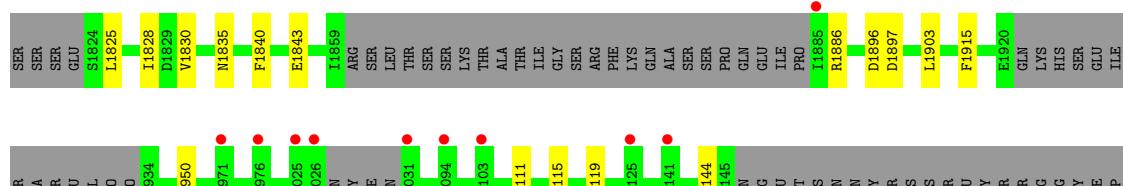
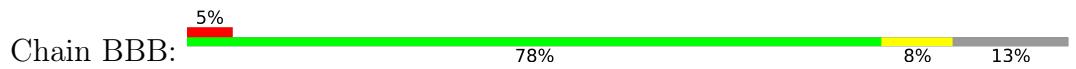
### 3 Residue-property plots

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

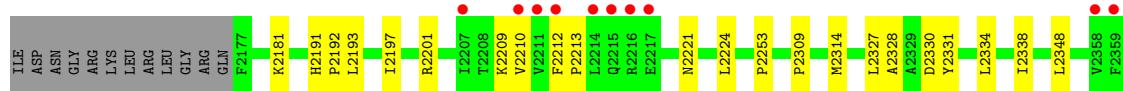
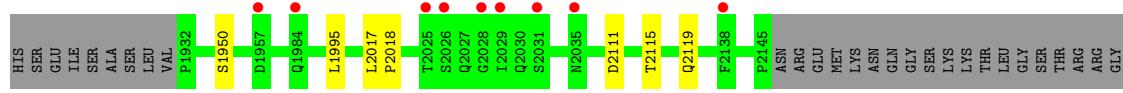
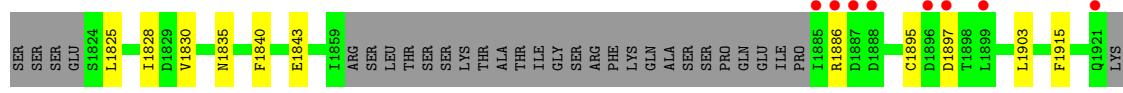
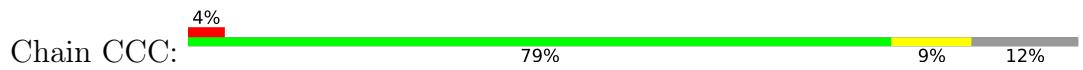


- Molecule 1: DNA polymerase theta

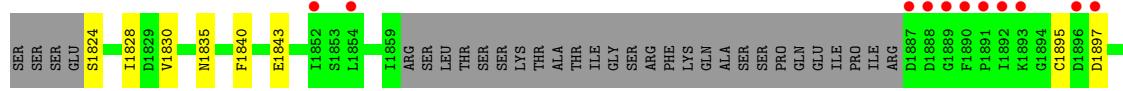
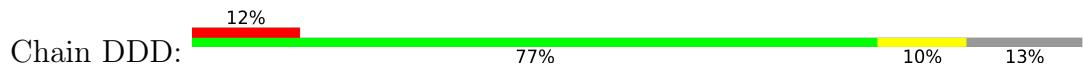


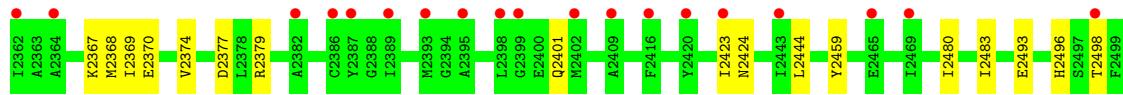


- Molecule 1: DNA polymerase theta



- Molecule 1: DNA polymerase theta

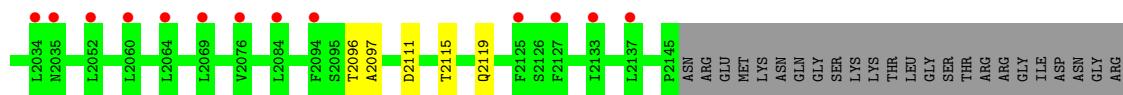
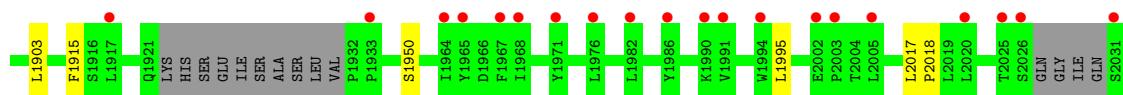
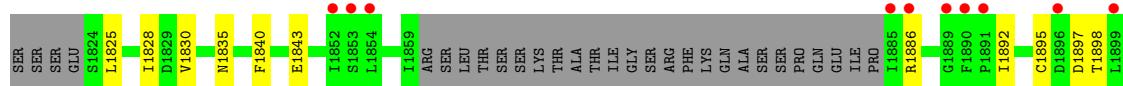




- Molecule 1c-DNA polymers that

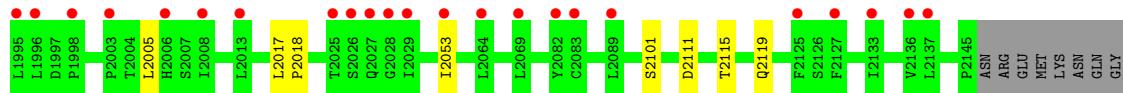
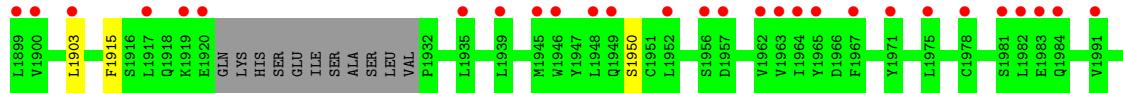
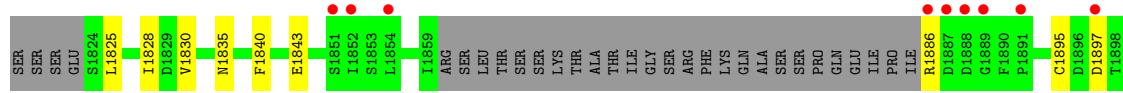
A horizontal bar chart illustrating the composition of Chain EEE. The total length of the bar is 100%, divided into four segments: 13% (red), 77% (green), 10% (yellow), and 13% (grey).

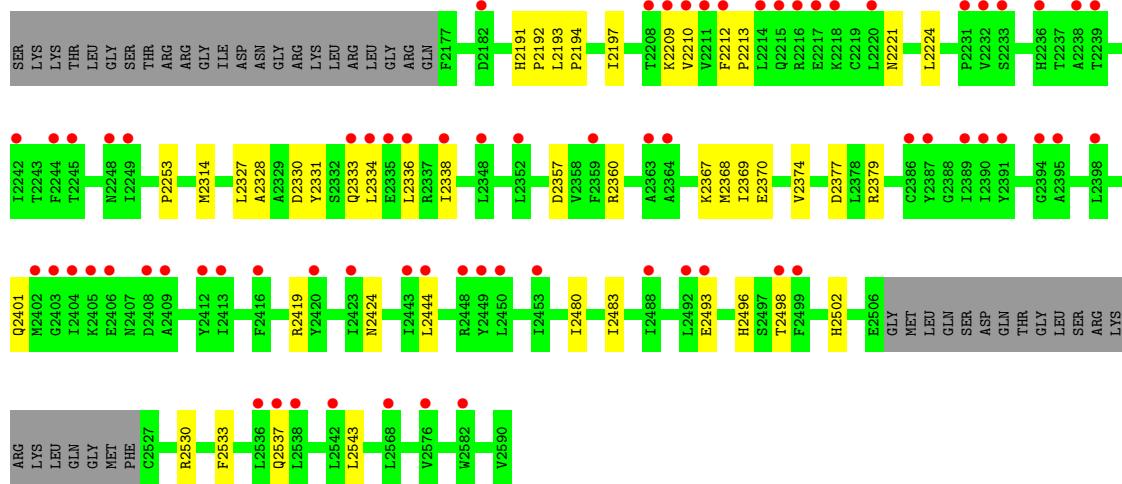
Component	Percentage
Red	13%
Green	77%
Yellow	10%
Grey	13%



- Molecule 1: DNA polymerase theta

Chain FFF: 18%  79% 9% 13%





- 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:  56% 38% 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:  50%  44%  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:  44% 50% 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:  44% 50%  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: 



- 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: 



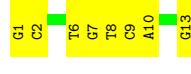
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*(DDG))-3')

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:  38% 62%



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.59 Å    172.29 Å    289.21 Å 90.00°    91.22°    90.00°	Depositor
Resolution (Å)	50.01 – 2.83 110.75 – 2.83	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.01-2.83) 97.5 (110.75-2.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.38 (at 2.82 Å)	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 <sup>2</sup> )	79.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32843	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

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

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	0.69	0/4904	0.76	0/6649
1	CCC	0.69	0/4952	0.76	0/6717
1	DDD	0.70	0/4905	0.76	0/6659
1	EEE	0.68	0/4919	0.75	0/6672
1	FFF	0.68	0/4919	0.75	0/6676
2	GGG	1.03	0/362	1.47	6/555 (1.1%)
2	III	1.01	1/362 (0.3%)	1.45	6/555 (1.1%)
2	KKK	1.02	0/362	1.44	8/555 (1.4%)
2	MMM	1.01	0/362	1.44	7/555 (1.3%)
2	OOO	0.95	0/362	1.44	5/555 (0.9%)
2	QQQ	0.95	0/362	1.46	6/555 (1.1%)
3	HHH	1.02	0/271	1.46	7/417 (1.7%)
3	JJJ	1.00	0/271	1.45	6/417 (1.4%)
3	LLL	1.01	0/271	1.47	6/417 (1.4%)
3	NNN	0.97	0/271	1.43	6/417 (1.4%)
3	PPP	0.93	0/271	1.46	7/417 (1.7%)
3	RRR	0.91	0/271	1.45	7/417 (1.7%)
All	All	0.73	1/33377 (0.0%)	0.88	77/45956 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	III	7	DA	P-O5'	5.32	1.65	1.59

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GGG	3	DT	P-O3'-C3'	-9.60	108.18	119.70
3	LLL	7	DG	P-O3'-C3'	-9.16	108.71	119.70
3	NNN	7	DG	P-O3'-C3'	-9.06	108.83	119.70
2	QQQ	3	DT	P-O3'-C3'	-8.99	108.91	119.70
2	III	15	DC	P-O3'-C3'	-8.64	109.33	119.70
2	KKK	3	DT	P-O3'-C3'	-8.63	109.34	119.70
3	HHH	7	DG	P-O3'-C3'	-8.63	109.34	119.70
3	PPP	7	DG	P-O3'-C3'	-8.61	109.37	119.70
3	PPP	6	DT	P-O3'-C3'	-8.53	109.47	119.70
3	RRR	6	DT	P-O3'-C3'	-8.52	109.48	119.70
2	OOO	15	DC	P-O3'-C3'	-8.51	109.49	119.70
3	RRR	7	DG	P-O3'-C3'	-8.50	109.50	119.70
2	KKK	15	DC	P-O3'-C3'	-8.46	109.55	119.70
3	JJJ	7	DG	P-O3'-C3'	-8.40	109.62	119.70
2	GGG	15	DC	P-O3'-C3'	-8.38	109.64	119.70
2	MMM	15	DC	P-O3'-C3'	-8.37	109.66	119.70
3	LLL	6	DT	P-O3'-C3'	-8.34	109.70	119.70
3	NNN	6	DT	P-O3'-C3'	-8.31	109.73	119.70
3	HHH	6	DT	P-O3'-C3'	-8.26	109.79	119.70
2	OOO	3	DT	P-O3'-C3'	-8.21	109.84	119.70
2	QQQ	15	DC	P-O3'-C3'	-8.20	109.86	119.70
3	JJJ	6	DT	P-O3'-C3'	-8.20	109.87	119.70
2	MMM	3	DT	P-O3'-C3'	-7.48	110.72	119.70
2	III	3	DT	P-O3'-C3'	-7.19	111.07	119.70
3	JJJ	1	DG	P-O3'-C3'	-6.99	111.31	119.70
2	GGG	12	DA	P-O3'-C3'	-6.85	111.48	119.70
3	HHH	9	DC	P-O3'-C3'	-6.84	111.49	119.70
3	PPP	1	DG	P-O3'-C3'	-6.71	111.65	119.70
3	PPP	9	DC	P-O3'-C3'	-6.65	111.72	119.70
2	III	12	DA	P-O3'-C3'	-6.58	111.80	119.70
3	RRR	9	DC	P-O3'-C3'	-6.46	111.95	119.70
3	HHH	1	DG	P-O3'-C3'	-6.42	112.00	119.70
2	MMM	12	DA	P-O3'-C3'	-6.39	112.03	119.70
3	JJJ	2	DC	P-O3'-C3'	-6.37	112.06	119.70
3	LLL	1	DG	P-O3'-C3'	-6.36	112.07	119.70
3	RRR	1	DG	P-O3'-C3'	-6.32	112.12	119.70
2	OOO	12	DA	P-O3'-C3'	-6.30	112.14	119.70
2	QQQ	12	DA	P-O3'-C3'	-6.30	112.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KKK	12	DA	P-O3'-C3'	-6.22	112.24	119.70
3	RRR	2	DC	P-O3'-C3'	-6.20	112.27	119.70
3	NNN	1	DG	P-O3'-C3'	-6.18	112.28	119.70
3	PPP	2	DC	P-O3'-C3'	-6.18	112.29	119.70
3	LLL	9	DC	P-O3'-C3'	-6.12	112.36	119.70
2	OOO	5	DC	P-O3'-C3'	-6.08	112.40	119.70
3	NNN	9	DC	P-O3'-C3'	-6.05	112.43	119.70
2	QQQ	4	DC	P-O3'-C3'	-6.04	112.46	119.70
2	QQQ	5	DC	P-O3'-C3'	-6.04	112.46	119.70
3	LLL	2	DC	P-O3'-C3'	-5.95	112.56	119.70
3	HHH	2	DC	P-O3'-C3'	-5.94	112.57	119.70
2	III	4	DC	P-O3'-C3'	-5.92	112.60	119.70
2	OOO	4	DC	P-O3'-C3'	-5.91	112.61	119.70
2	KKK	5	DC	P-O3'-C3'	-5.88	112.64	119.70
2	MMM	5	DC	P-O3'-C3'	-5.87	112.66	119.70
3	HHH	10	DA	P-O3'-C3'	-5.86	112.67	119.70
3	JJJ	10	DA	P-O3'-C3'	-5.86	112.67	119.70
3	NNN	2	DC	P-O3'-C3'	-5.80	112.74	119.70
2	III	5	DC	P-O3'-C3'	-5.62	112.95	119.70
3	RRR	10	DA	P-O3'-C3'	-5.51	113.09	119.70
3	HHH	8	DT	P-O3'-C3'	-5.50	113.09	119.70
3	LLL	10	DA	P-O3'-C3'	-5.50	113.10	119.70
2	GGG	4	DC	P-O3'-C3'	-5.46	113.15	119.70
3	NNN	10	DA	P-O3'-C3'	-5.45	113.16	119.70
3	JJJ	9	DC	P-O3'-C3'	-5.42	113.19	119.70
2	KKK	4	DC	P-O3'-C3'	-5.38	113.25	119.70
2	MMM	4	DC	P-O3'-C3'	-5.29	113.36	119.70
3	PPP	10	DA	P-O3'-C3'	-5.28	113.37	119.70
2	MMM	6	DA	P-O3'-C3'	-5.25	113.39	119.70
2	KKK	10	DA	P-O3'-C3'	-5.24	113.41	119.70
2	GGG	5	DC	P-O3'-C3'	-5.24	113.41	119.70
2	GGG	10	DA	P-O3'-C3'	-5.14	113.53	119.70
2	QQQ	10	DA	P-O3'-C3'	-5.13	113.54	119.70
2	KKK	6	DA	P-O3'-C3'	-5.11	113.57	119.70
2	KKK	7	DA	OP2-P-O3'	5.09	116.39	105.20
3	RRR	8	DT	P-O3'-C3'	-5.08	113.61	119.70
2	III	10	DA	P-O3'-C3'	-5.07	113.62	119.70
3	PPP	8	DT	P-O3'-C3'	-5.02	113.67	119.70
2	MMM	10	DA	P-O3'-C3'	-5.01	113.68	119.70

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	31	0
1	BBB	4811	0	4625	28	0
1	CCC	4856	0	4667	27	0
1	DDD	4810	0	4593	37	0
1	EEE	4824	0	4632	32	0
1	FFF	4823	0	4617	28	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	196	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 (196) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:EEE:2360:ARG:HG2	1:EEE:2374:VAL:HG21	1.90	0.54
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:DDD:2013:LEU:HD11	1:DDD:2055:ASN:CG	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:DDD:1931:VAL:HB	1:DDD:1932:PRO:HD3	1.98	0.45
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2096:THR:O	1:EEE:2097:ALA:C	2.58	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:2327:LEU:HD23	1:EEE:2327:LEU:C	2.41	0.41
1:EEE:2533:PHE:CD1	1:EEE:2533:PHE:N	2.89	0.41
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:CCC:2327:LEU:HD23	1:CCC:2327:LEU:C	2.41	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: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:AAA:2327:LEU:HD23	1:AAA:2327:LEU:C	2.42	0.41
1:BBB:2327:LEU:HD23	1:BBB:2327:LEU:C	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:2327:LEU:HD23	1:FFF:2327:LEU:C	2.41	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 [\(i\)](#)

### 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%)	612 (97%)	16 (2%)	1 (0%)	47 76
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 [\(i\)](#)

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%)	483 (96%)	19 (4%)	33 65
1	BBB	494/638 (77%)	475 (96%)	19 (4%)	33 65
1	CCC	494/638 (77%)	473 (96%)	21 (4%)	29 60
1	DDD	491/638 (77%)	472 (96%)	19 (4%)	32 64
1	EEE	493/638 (77%)	473 (96%)	20 (4%)	30 63
1	FFF	490/638 (77%)	471 (96%)	19 (4%)	32 64
All	All	2964/3828 (77%)	2847 (96%)	117 (4%)	32 64

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [\(i\)](#)

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	NNN	13	3,2	17,23,24	1.18	1 (5%)	15,33,36	1.32	3 (20%)
3	DDG	PPP	13	3,2	17,23,24	1.20	2 (11%)	15,33,36	1.45	3 (20%)
3	DDG	JJJ	13	3,2	17,23,24	1.18	1 (5%)	15,33,36	1.36	3 (20%)
3	DDG	HHH	13	3,2	17,23,24	1.36	3 (17%)	15,33,36	1.39	3 (20%)
3	DDG	LLL	13	3,2	17,23,24	1.31	1 (5%)	15,33,36	1.71	4 (26%)
3	DDG	RRR	13	3,2	17,23,24	1.22	1 (5%)	15,33,36	1.43	3 (20%)

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	NNN	13	3,2	-	2/3/18/19	0/3/3/3
3	DDG	PPP	13	3,2	-	2/3/18/19	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DDG	JJJ	13	3,2	-	2/3/18/19	0/3/3/3
3	DDG	HHH	13	3,2	-	2/3/18/19	0/3/3/3
3	DDG	LLL	13	3,2	-	2/3/18/19	0/3/3/3
3	DDG	RRR	13	3,2	-	2/3/18/19	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	RRR	13	DDG	C6-N1	-3.72	1.32	1.37
3	LLL	13	DDG	C6-N1	-3.48	1.32	1.37
3	PPP	13	DDG	C6-N1	-3.37	1.32	1.37
3	JJJ	13	DDG	C6-N1	-3.30	1.33	1.37
3	NNN	13	DDG	C6-N1	-2.86	1.33	1.37
3	HHH	13	DDG	C6-N1	-2.80	1.33	1.37
3	HHH	13	DDG	O4'-C4'	-2.48	1.39	1.44
3	HHH	13	DDG	O5'-C5'	-2.27	1.39	1.44
3	PPP	13	DDG	O5'-C5'	-2.09	1.39	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LLL	13	DDG	O4'-C1'-C2'	3.06	109.99	106.67
3	NNN	13	DDG	C8-N7-C5	2.83	108.38	102.99
3	LLL	13	DDG	C8-N7-C5	2.82	108.36	102.99
3	JJJ	13	DDG	C8-N7-C5	2.72	108.18	102.99
3	PPP	13	DDG	C8-N7-C5	2.69	108.12	102.99
3	RRR	13	DDG	C8-N7-C5	2.68	108.09	102.99
3	HHH	13	DDG	C8-N7-C5	2.61	107.96	102.99
3	PPP	13	DDG	C3'-C2'-C1'	2.55	105.72	102.78
3	LLL	13	DDG	C2'-C3'-C4'	2.52	107.45	102.72
3	NNN	13	DDG	C3'-C2'-C1'	2.46	105.62	102.78
3	RRR	13	DDG	C3'-C2'-C1'	2.28	105.41	102.78
3	LLL	13	DDG	C5-C6-N1	2.26	117.94	113.95
3	NNN	13	DDG	C5-C6-N1	2.15	117.74	113.95
3	JJJ	13	DDG	C3'-C2'-C1'	2.14	105.25	102.78
3	JJJ	13	DDG	C5-C6-N1	2.13	117.72	113.95
3	RRR	13	DDG	C5-C6-N1	2.12	117.70	113.95
3	HHH	13	DDG	C5-C6-N1	2.10	117.65	113.95
3	PPP	13	DDG	C5-C6-N1	2.08	117.62	113.95
3	HHH	13	DDG	C2'-C3'-C4'	2.07	106.61	102.72

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'
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 monosaccharides 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	AAA	2602	4	25,32,32	0.96	1 (4%)	28,50,50	0.98	2 (7%)
5	DG3	DDD	2602	4	25,32,32	1.00	2 (8%)	28,50,50	1.10	2 (7%)
6	K8I	BBB	2603	-	31,32,32	0.84	1 (3%)	39,48,48	0.68	1 (2%)
6	K8I	CCC	2602	-	31,32,32	0.88	1 (3%)	39,48,48	0.75	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	K8I	DDD	2603	-	31,32,32	0.92	1 (3%)	39,48,48	0.83	2 (5%)
5	DG3	BBB	2602	4	25,32,32	1.01	2 (8%)	28,50,50	1.23	4 (14%)
5	DG3	FFF	2602	4	25,32,32	0.95	2 (8%)	28,50,50	1.14	2 (7%)
5	DG3	KKK	101	4	25,32,32	1.02	3 (12%)	28,50,50	0.99	1 (3%)
6	K8I	AAA	2603	-	31,32,32	0.97	1 (3%)	39,48,48	0.84	1 (2%)
5	DG3	EEE	2602	4	25,32,32	0.98	1 (4%)	28,50,50	1.42	3 (10%)

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	AAA	2602	4	-	5/18/31/31	0/3/3/3
5	DG3	DDD	2602	4	-	7/18/31/31	0/3/3/3
6	K8I	BBB	2603	-	-	0/22/37/37	0/3/3/3
6	K8I	CCC	2602	-	-	1/22/37/37	0/3/3/3
6	K8I	DDD	2603	-	-	0/22/37/37	0/3/3/3
5	DG3	BBB	2602	4	-	3/18/31/31	0/3/3/3
5	DG3	FFF	2602	4	-	5/18/31/31	0/3/3/3
5	DG3	KKK	101	4	-	6/18/31/31	0/3/3/3
6	K8I	AAA	2603	-	-	0/22/37/37	0/3/3/3
5	DG3	EEE	2602	4	-	2/18/31/31	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	K8I	C10-N3	-4.32	1.36	1.43
6	CCC	2602	K8I	C10-N3	-3.85	1.37	1.43
6	DDD	2603	K8I	C10-N3	-3.81	1.37	1.43
6	BBB	2603	K8I	C10-N3	-3.72	1.37	1.43
5	KKK	101	DG3	C5-C6	-3.16	1.41	1.47
5	BBB	2602	DG3	C5-C6	-2.93	1.41	1.47
5	EEE	2602	DG3	C5-C6	-2.77	1.41	1.47
5	AAA	2602	DG3	C5-C6	-2.69	1.41	1.47
5	DDD	2602	DG3	C5-C6	-2.69	1.42	1.47
5	FFF	2602	DG3	C5-C6	-2.50	1.42	1.47
5	KKK	101	DG3	C5-C4	-2.18	1.37	1.43
5	DDD	2602	DG3	C8-N7	-2.09	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	KKK	101	DG3	C8-N7	-2.05	1.31	1.35
5	FFF	2602	DG3	C8-N7	-2.03	1.31	1.35
5	BBB	2602	DG3	C5-C4	-2.02	1.37	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	EEE	2602	DG3	PA-O3A-PB	-4.33	117.96	132.83
6	DDD	2603	K8I	C17-C18-N4	-3.30	169.92	177.40
5	BBB	2602	DG3	PA-O3A-PB	-3.15	122.03	132.83
5	FFF	2602	DG3	PA-O3A-PB	-2.88	122.96	132.83
5	EEE	2602	DG3	PB-O3B-PG	-2.59	123.95	132.83
5	AAA	2602	DG3	O6-C6-C5	2.43	129.12	124.37
5	EEE	2602	DG3	C4'-O4'-C1'	-2.34	107.60	109.81
5	FFF	2602	DG3	O6-C6-C5	2.28	128.83	124.37
6	CCC	2602	K8I	C3-N1-C2	2.24	120.80	116.58
5	DDD	2602	DG3	O6-C6-C5	2.23	128.73	124.37
6	DDD	2603	K8I	C3-N1-C2	2.20	120.73	116.58
5	AAA	2602	DG3	O2A-PA-O1A	2.20	123.13	112.24
5	BBB	2602	DG3	O2A-PA-O1A	2.19	123.05	112.24
6	AAA	2603	K8I	C3-N1-C2	2.15	120.63	116.58
6	CCC	2602	K8I	C17-C18-N4	-2.08	172.67	177.40
5	KKK	101	DG3	O2A-PA-O1A	2.08	122.53	112.24
5	BBB	2602	DG3	O6-C6-C5	2.07	128.42	124.37
5	DDD	2602	DG3	O2A-PA-O1A	2.05	122.35	112.24
5	BBB	2602	DG3	O3B-PG-O1G	-2.01	100.04	111.19
6	BBB	2603	K8I	C3-N1-C2	2.00	120.34	116.58

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-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
5	KKK	101	DG3	C5'-O5'-PA-O3A
5	AAA	2602	DG3	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
5	AAA	2602	DG3	PB-O3A-PA-O2A
5	DDD	2602	DG3	PB-O3A-PA-O2A
5	KKK	101	DG3	C5'-O5'-PA-O1A
6	CCC	2602	K8I	C19-C17-C18-N4
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	EEE	2602	DG3	C4'-C5'-O5'-PA
5	DDD	2602	DG3	C3'-C4'-C5'-O5'
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

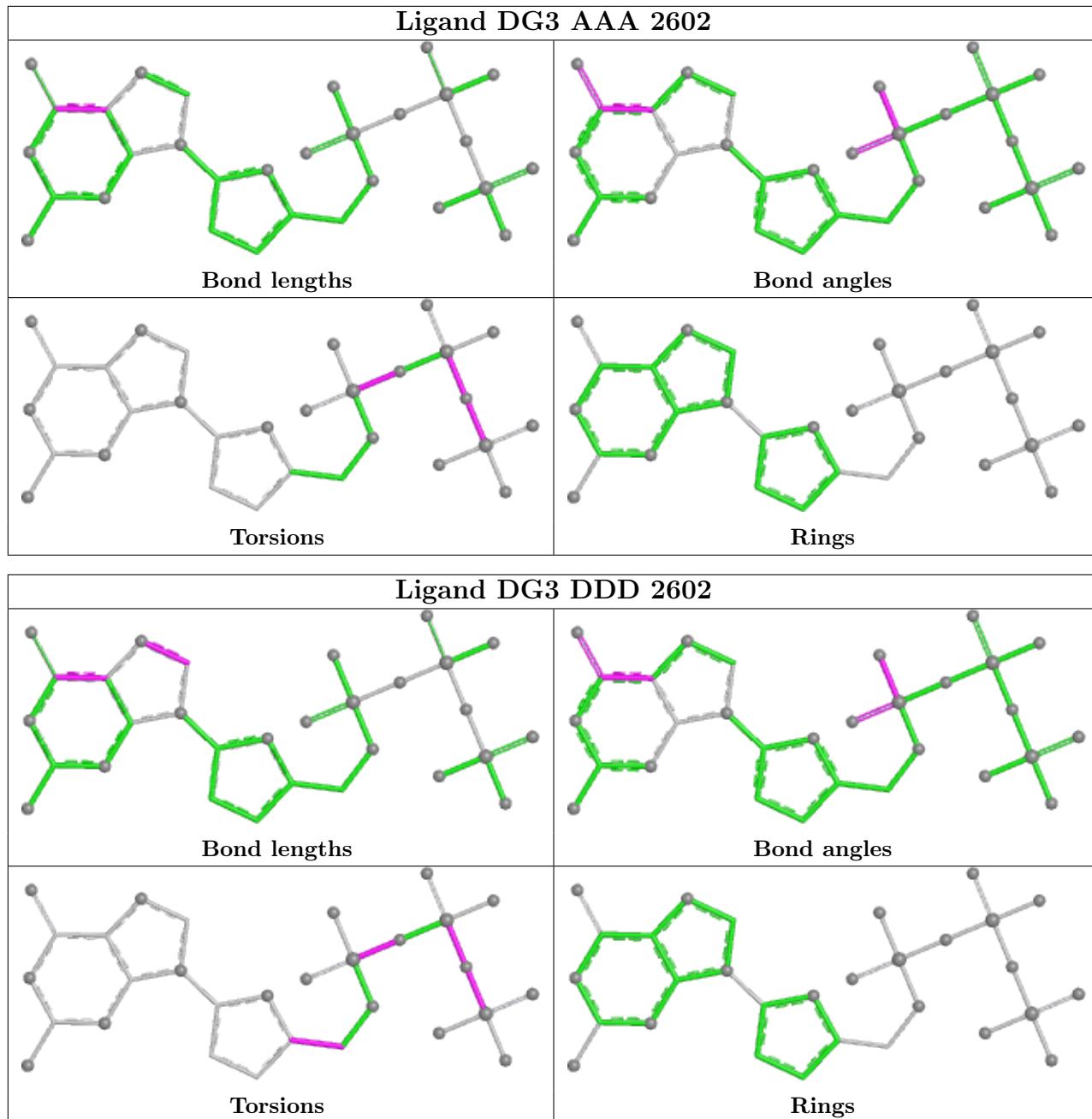
There are no ring outliers.

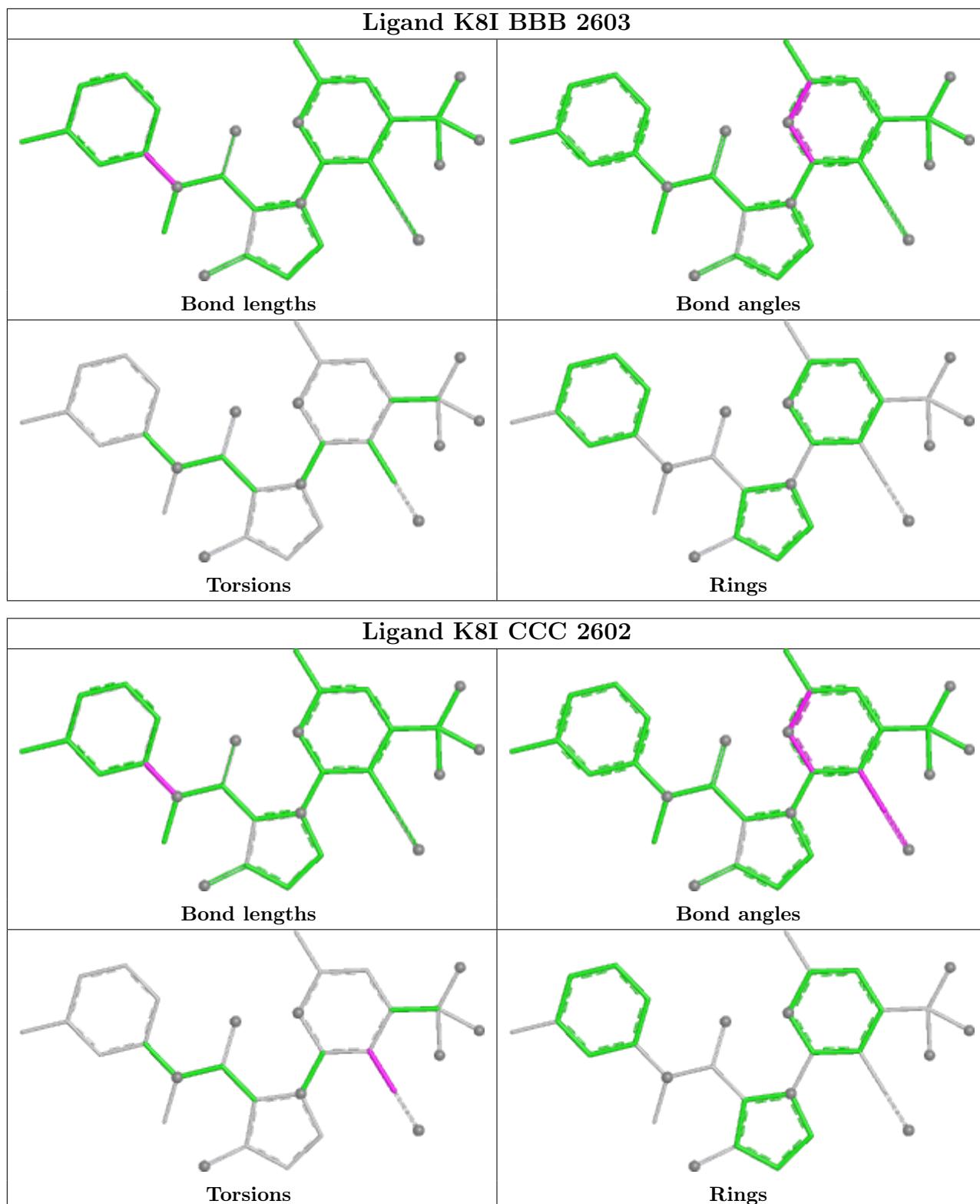
6 monomers are involved in 10 short contacts:

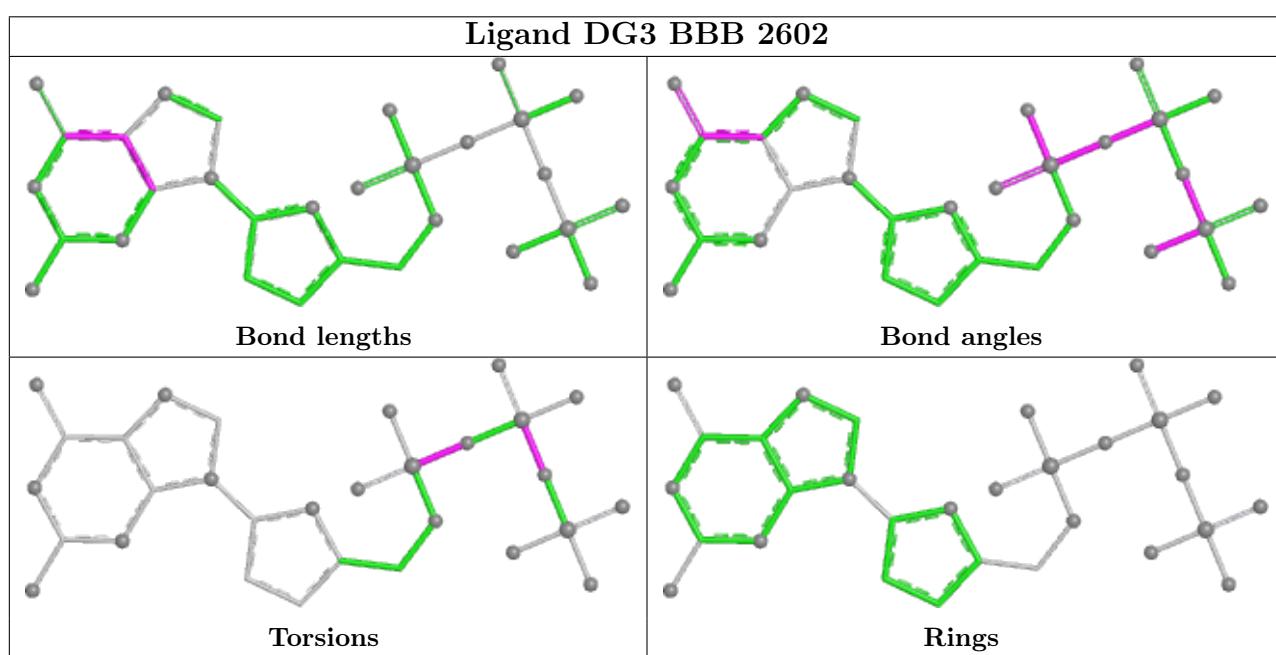
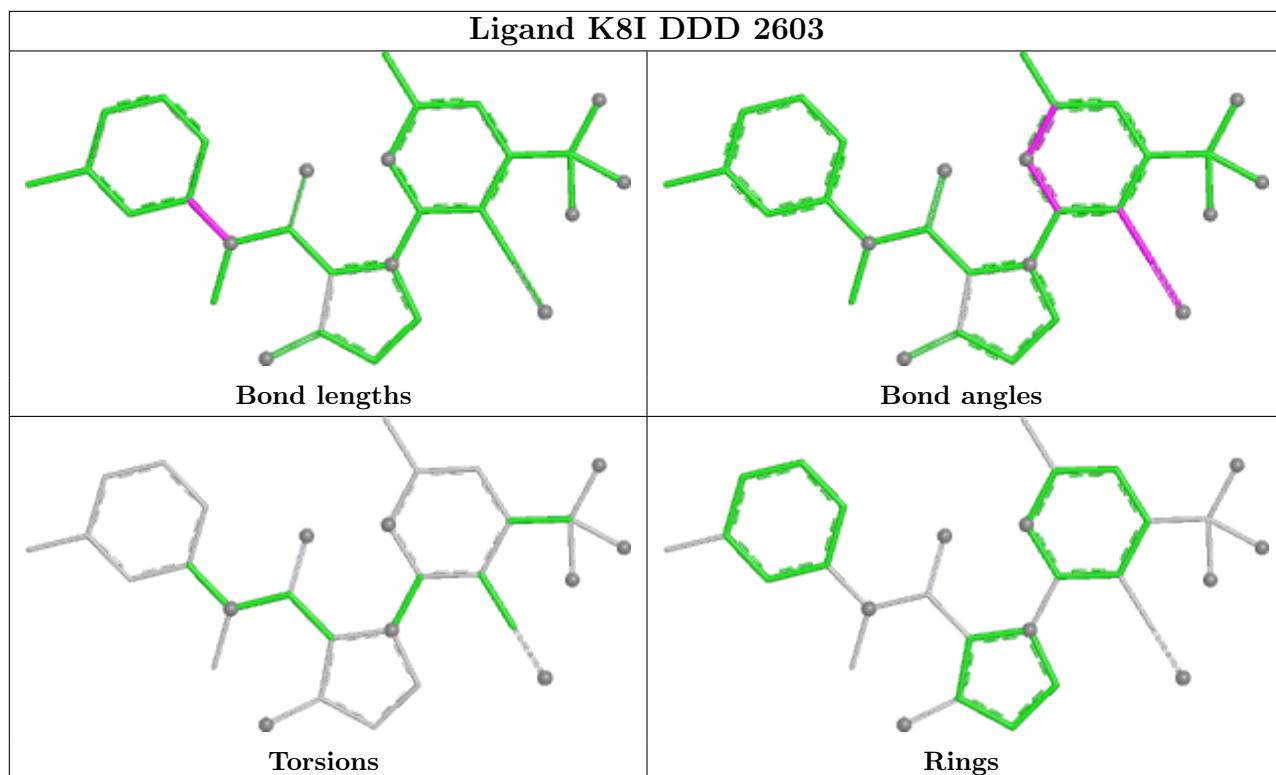
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	2603	K8I	2	0
6	CCC	2602	K8I	2	0
6	DDD	2603	K8I	1	0
5	KKK	101	DG3	1	0
6	AAA	2603	K8I	2	0
5	EEE	2602	DG3	2	0

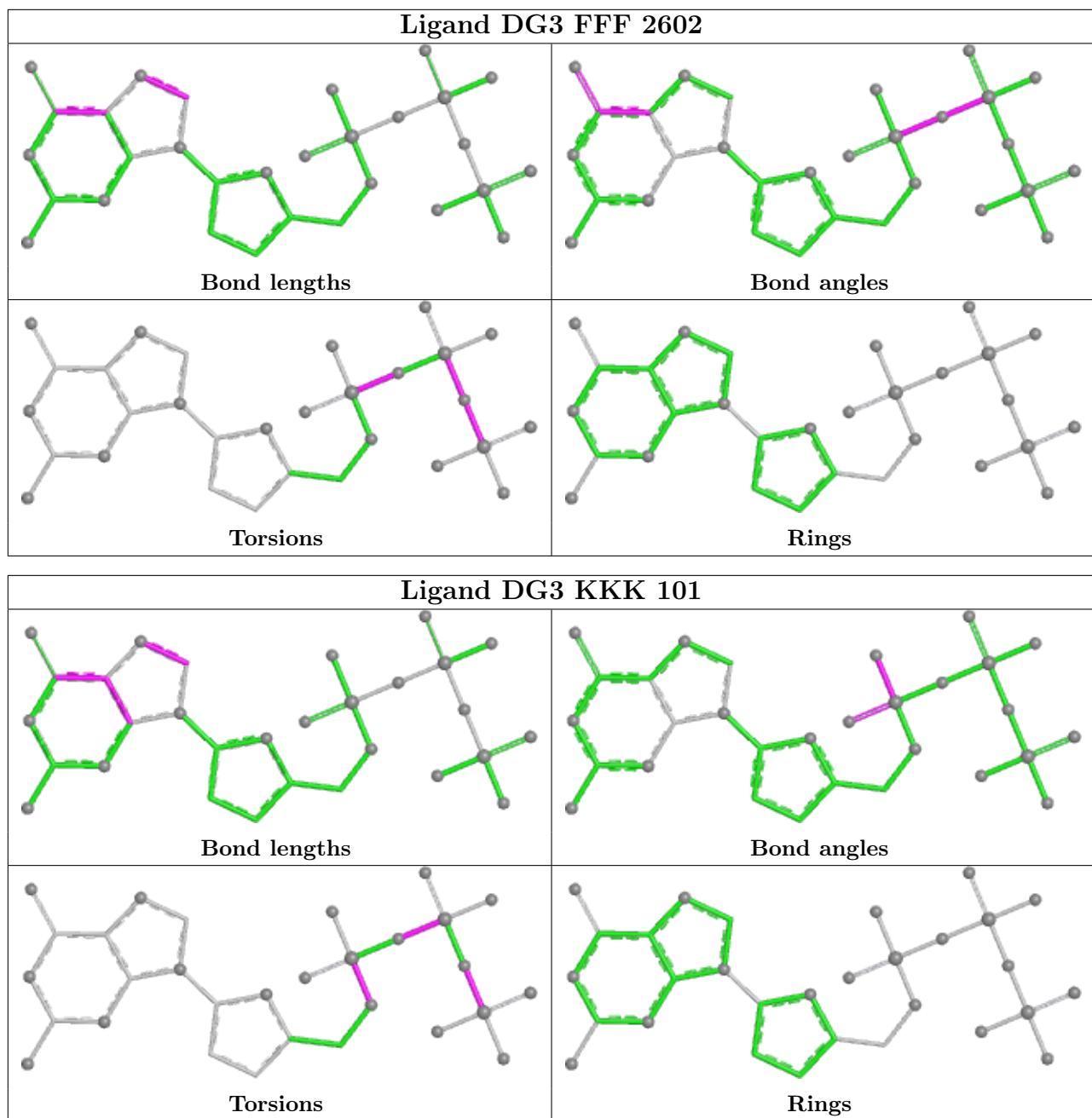
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

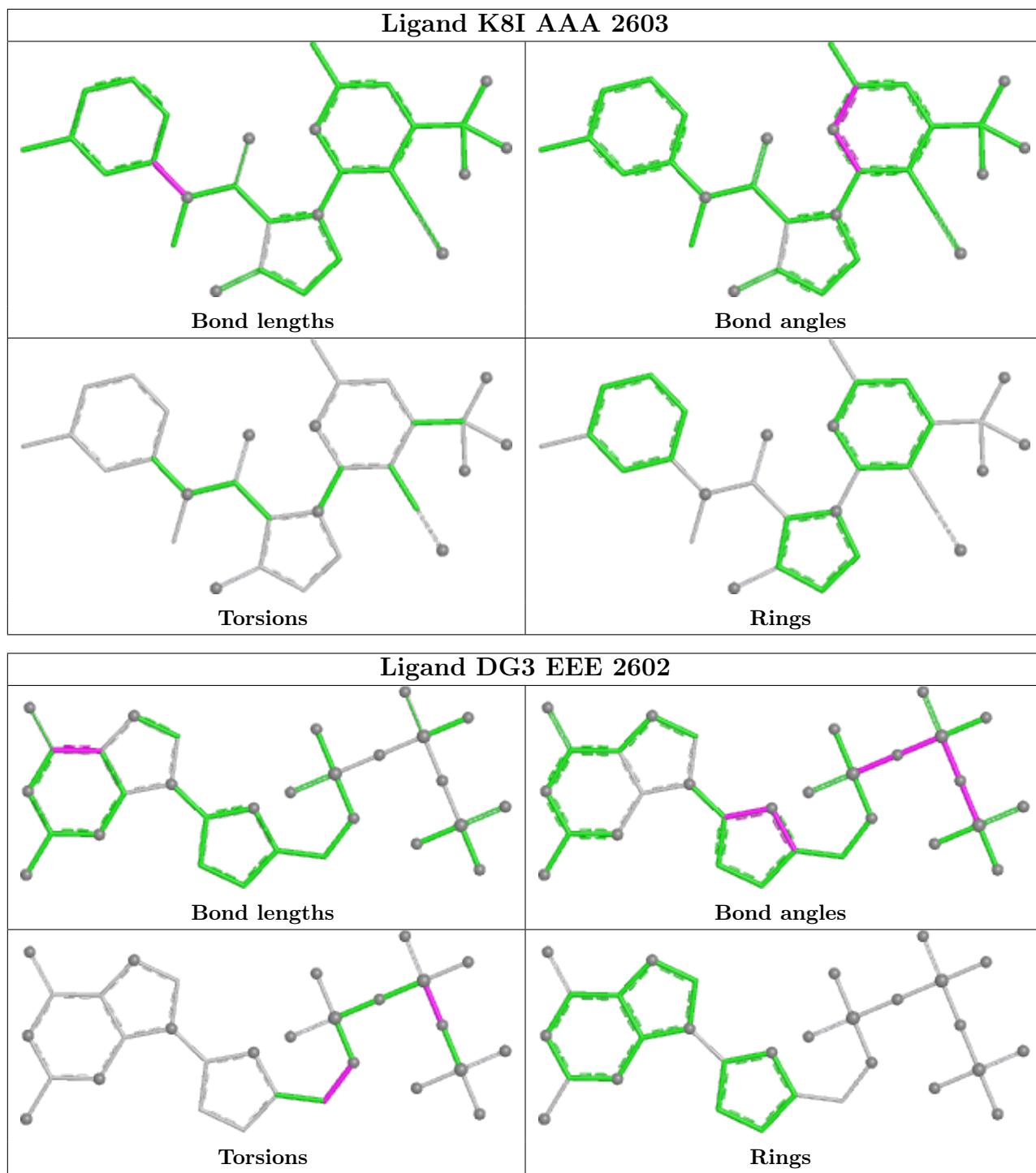
equivalents in the CSD to analyse the geometry.











## 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	639/726 (88%)	0.47	29 (4%)	33	23	39, 74, 135, 198	0
1	BBB	629/726 (86%)	0.49	33 (5%)	27	18	45, 84, 140, 194	0
1	CCC	638/726 (87%)	0.45	31 (4%)	29	20	45, 87, 145, 197	0
1	DDD	633/726 (87%)	0.81	88 (13%)	2	1	56, 103, 176, 219	0
1	EEE	632/726 (87%)	0.80	96 (15%)	2	1	62, 114, 169, 208	0
1	FFF	634/726 (87%)	0.97	131 (20%)	1	0	73, 129, 177, 227	0
2	GGG	16/16 (100%)	-0.22	0	100	100	43, 94, 155, 158	0
2	III	16/16 (100%)	-0.12	0	100	100	60, 112, 173, 177	0
2	KKK	16/16 (100%)	-0.17	0	100	100	54, 110, 172, 174	0
2	MMM	16/16 (100%)	-0.05	0	100	100	61, 100, 168, 179	0
2	OOO	16/16 (100%)	-0.14	0	100	100	93, 148, 225, 232	0
2	QQQ	16/16 (100%)	0.01	1 (6%)	20	12	93, 154, 226, 237	0
3	HHH	12/13 (92%)	-0.24	0	100	100	41, 100, 155, 160	0
3	JJJ	12/13 (92%)	-0.25	0	100	100	50, 134, 160, 176	0
3	LLL	12/13 (92%)	-0.35	0	100	100	58, 107, 160, 162	0
3	NNN	12/13 (92%)	-0.15	0	100	100	57, 117, 153, 155	0
3	PPP	12/13 (92%)	-0.35	0	100	100	74, 171, 238, 248	0
3	RRR	12/13 (92%)	0.11	0	100	100	83, 168, 218, 220	0
All	All	3973/4530 (87%)	0.63	409 (10%)	6	3	39, 100, 168, 248	0

All (409) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	2031	SER	14.3
1	DDD	2026	SER	12.2
1	DDD	2028	GLY	12.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	2212	PHE	9.3
1	FFF	2212	PHE	9.2
1	AAA	1896	ASP	8.8
1	DDD	2027	GLN	8.6
1	EEE	2210	VAL	8.4
1	EEE	2212	PHE	8.3
1	FFF	2416	PHE	8.2
1	EEE	2217	GLU	8.1
1	DDD	2025	THR	7.9
1	DDD	2029	ILE	7.7
1	EEE	2211	VAL	7.6
1	BBB	2026	SER	7.4
1	FFF	2210	VAL	7.4
1	FFF	2215	GLN	6.6
1	FFF	2209	LYS	6.5
1	EEE	2026	SER	6.3
1	EEE	2404	ILE	6.3
1	BBB	2211	VAL	6.1
1	BBB	2210	VAL	6.0
1	FFF	2449	TYR	6.0
1	FFF	2027	GLN	6.0
1	FFF	1891	PRO	5.9
1	FFF	1996	LEU	5.9
1	DDD	2210	VAL	5.7
1	CCC	2212	PHE	5.7
1	FFF	2386	CYS	5.7
1	EEE	2005	LEU	5.7
1	EEE	2209	LYS	5.6
1	EEE	2375	GLY	5.6
1	FFF	2409	ALA	5.5
1	BBB	2404	ILE	5.4
1	DDD	2030	GLN	5.3
1	EEE	2025	THR	5.3
1	FFF	2499	PHE	5.3
1	FFF	2404	ILE	5.3
1	DDD	1952	LEU	5.2
1	BBB	2217	GLU	5.2
1	DDD	2336	LEU	5.2
1	FFF	2211	VAL	5.1
1	CCC	2215	GLN	5.0
1	FFF	2395	ALA	5.0
1	DDD	2217	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	2216	ARG	5.0
1	EEE	2133	ILE	5.0
1	DDD	1897	ASP	5.0
1	EEE	1886	ARG	5.0
1	DDD	1939	LEU	4.9
1	FFF	1889	GLY	4.9
1	FFF	2216	ARG	4.9
1	FFF	1887	ASP	4.9
1	FFF	2137	LEU	4.9
1	EEE	2216	ARG	4.9
1	CCC	1888	ASP	4.8
1	CCC	1957	ASP	4.8
1	DDD	2182	ASP	4.7
1	EEE	2034	LEU	4.7
1	FFF	1920	GLU	4.7
1	FFF	2335	GLU	4.6
1	DDD	2333	GLN	4.6
1	DDD	2214	LEU	4.6
1	AAA	2214	LEU	4.6
1	EEE	2394	GLY	4.6
1	FFF	1888	ASP	4.6
1	CCC	1896	ASP	4.6
1	CCC	2211	VAL	4.5
1	CCC	2214	LEU	4.5
1	FFF	1949	GLN	4.5
1	BBB	2214	LEU	4.5
1	EEE	2506	GLU	4.5
1	FFF	2412	TYR	4.5
1	CCC	1886	ARG	4.5
1	FFF	1900	VAL	4.4
1	FFF	1984	GLN	4.4
1	EEE	2214	LEU	4.4
1	FFF	2336	LEU	4.4
1	AAA	2212	PHE	4.4
1	DDD	1890	PHE	4.4
1	EEE	2412	TYR	4.4
1	BBB	2506	GLU	4.3
1	EEE	2409	ALA	4.2
1	CCC	1885	ILE	4.2
1	FFF	1952	LEU	4.2
1	CCC	2217	GLU	4.2
1	FFF	1852	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	FFF	2453	ILE	4.2
1	FFF	2443	ILE	4.2
1	CCC	2210	VAL	4.1
1	EEE	1889	GLY	4.1
1	FFF	2214	LEU	4.1
1	FFF	1981	SER	4.1
1	FFF	2348	LEU	4.1
1	FFF	1982	LEU	4.1
1	EEE	2376	ASP	4.1
1	BBB	2215	GLN	4.0
1	FFF	1964	ILE	4.0
1	EEE	1965	TYR	4.0
1	DDD	1891	PRO	3.9
1	EEE	2395	ALA	3.9
1	AAA	1921	GLN	3.9
1	CCC	2029	ILE	3.9
1	BBB	2218	LYS	3.9
1	FFF	1939	LEU	3.9
1	DDD	1945	MET	3.8
1	DDD	2215	GLN	3.8
1	EEE	1853	SER	3.8
1	EEE	2402	MET	3.8
1	FFF	2053	ILE	3.8
1	DDD	2356	ALA	3.8
1	FFF	2133	ILE	3.7
1	DDD	1896	ASP	3.7
1	DDD	2359	PHE	3.7
1	DDD	1938	SER	3.7
1	FFF	2064	LEU	3.7
1	DDD	1889	GLY	3.7
1	FFF	2182	ASP	3.7
1	DDD	1888	ASP	3.7
1	FFF	2408	ASP	3.6
1	BBB	2364	ALA	3.6
1	DDD	2395	ALA	3.6
1	EEE	1968	ILE	3.6
1	EEE	2242	ILE	3.6
1	EEE	1885	ILE	3.6
1	AAA	2217	GLU	3.6
1	EEE	2568	LEU	3.6
1	AAA	2029	ILE	3.6
1	AAA	1888	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	FFF	2242	ILE	3.6
1	FFF	1965	TYR	3.6
1	FFF	2402	MET	3.5
1	DDD	2211	VAL	3.5
1	FFF	2338	ILE	3.5
1	AAA	1887	ASP	3.5
1	BBB	2031	SER	3.5
1	FFF	1854	LEU	3.5
1	EEE	2218	LYS	3.4
1	AAA	2210	VAL	3.4
1	DDD	2035	ASN	3.4
1	FFF	2387	TYR	3.4
1	BBB	2219	CYS	3.4
1	DDD	1996	LEU	3.4
1	FFF	1917	LEU	3.4
1	FFF	1991	VAL	3.4
1	FFF	2218	LYS	3.4
1	DDD	2398	LEU	3.4
1	EEE	2434	CYS	3.4
1	CCC	2359	PHE	3.3
1	EEE	2403	GLY	3.3
1	EEE	1991	VAL	3.3
1	FFF	2498	THR	3.3
1	DDD	2386	CYS	3.3
1	AAA	2030	GLN	3.3
1	DDD	2504	HIS	3.3
1	EEE	1852	ILE	3.3
1	DDD	2393	MET	3.3
1	FFF	2405	LYS	3.2
1	CCC	2025	THR	3.2
1	EEE	1933	PRO	3.2
1	BBB	2025	THR	3.2
1	DDD	1940	THR	3.2
1	FFF	1956	SER	3.2
1	DDD	2416	PHE	3.2
1	EEE	2127	PHE	3.2
1	FFF	2220	LEU	3.2
1	CCC	2507	GLY	3.1
1	BBB	2402	MET	3.1
1	BBB	2363	ALA	3.1
1	EEE	2340	ALA	3.1
1	FFF	2359	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	1962	VAL	3.1
1	AAA	2215	GLN	3.1
1	CCC	1887	ASP	3.1
1	EEE	2003	PRO	3.1
1	CCC	2216	ARG	3.1
1	EEE	2249	ILE	3.1
1	FFF	2233	SER	3.1
1	DDD	2137	LEU	3.1
1	EEE	2336	LEU	3.1
1	FFF	2389	ILE	3.1
1	DDD	2399	GLY	3.0
1	DDD	2209	LYS	3.0
1	EEE	2020	LEU	3.0
1	DDD	1984	GLN	3.0
1	FFF	2364	ALA	3.0
1	BBB	2125	PHE	3.0
1	EEE	1854	LEU	3.0
1	CCC	2138	PHE	3.0
1	EEE	2399	GLY	3.0
1	DDD	2216	ARG	3.0
1	AAA	1984	GLN	3.0
1	EEE	2137	LEU	3.0
1	FFF	1967	PHE	3.0
1	FFF	2013	LEU	3.0
1	DDD	2364	ALA	2.9
1	AAA	1886	ARG	2.9
1	CCC	2031	SER	2.9
1	FFF	2008	ILE	2.9
1	FFF	2420	TYR	2.9
1	FFF	2248	ASN	2.9
1	FFF	2239	THR	2.9
1	EEE	1899	LEU	2.9
1	BBB	2412	TYR	2.9
1	FFF	1975	LEU	2.9
1	FFF	2208	THR	2.9
1	CCC	1921	GLN	2.9
1	FFF	2537	GLN	2.9
1	BBB	1885	ILE	2.9
1	DDD	2084	LEU	2.9
1	FFF	2125	PHE	2.9
1	EEE	1971	TYR	2.8
1	CCC	1984	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	EEE	1967	PHE	2.8
1	FFF	2003	PRO	2.8
1	FFF	1946	TRP	2.8
1	FFF	2450	LEU	2.8
1	AAA	1885	ILE	2.8
1	FFF	2025	THR	2.8
1	DDD	2500	LYS	2.8
1	FFF	1995	LEU	2.8
1	FFF	2026	SER	2.8
1	FFF	2217	GLU	2.8
1	FFF	2568	LEU	2.8
1	FFF	2363	ALA	2.8
1	FFF	1886	ARG	2.8
1	AAA	2035	ASN	2.8
1	EEE	2334	LEU	2.8
1	AAA	2508	MET	2.7
1	DDD	2024	GLU	2.7
1	EEE	2398	LEU	2.7
1	DDD	1852	ILE	2.7
1	EEE	2245	THR	2.7
1	FFF	2492	LEU	2.7
1	CCC	2026	SER	2.7
1	DDD	2387	TYR	2.7
1	FFF	1963	VAL	2.7
1	CCC	2028	GLY	2.7
1	DDD	2219	CYS	2.7
1	EEE	2366	TRP	2.7
1	DDD	2402	MET	2.7
1	DDD	2362	ILE	2.7
1	FFF	1971	TYR	2.7
1	AAA	2211	VAL	2.7
1	EEE	2064	LEU	2.7
1	FFF	2398	LEU	2.7
1	FFF	2406	GLU	2.6
1	DDD	2348	LEU	2.6
1	DDD	2034	LEU	2.6
1	FFF	2542	LEU	2.6
1	DDD	2531	GLY	2.6
1	FFF	1919	LYS	2.6
1	EEE	1964	ILE	2.6
1	AAA	1982	LEU	2.6
1	FFF	2403	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	DDD	2218	LYS	2.6
1	DDD	2208	THR	2.6
1	AAA	2359	PHE	2.6
1	FFF	1945	MET	2.6
1	DDD	1962	VAL	2.6
1	EEE	2035	ASN	2.6
1	DDD	1942	LYS	2.6
1	FFF	2333	GLN	2.6
1	AAA	2028	GLY	2.6
1	FFF	1948	LEU	2.6
1	EEE	2233	SER	2.6
1	EEE	1994	TRP	2.6
1	FFF	2238	ALA	2.6
1	EEE	2240	GLY	2.6
1	CCC	2035	ASN	2.6
1	FFF	2394	GLY	2.5
1	FFF	2576	VAL	2.5
1	DDD	1967	PHE	2.5
1	FFF	2413	ILE	2.5
1	DDD	2334	LEU	2.5
1	BBB	1971	TYR	2.5
1	DDD	2409	ALA	2.5
1	BBB	2213	PRO	2.5
1	EEE	2181	LYS	2.5
1	FFF	2231	PRO	2.5
1	EEE	2338	ILE	2.5
1	BBB	2366	TRP	2.5
1	DDD	1976	LEU	2.5
1	BBB	2403	GLY	2.5
1	DDD	1892	ILE	2.5
1	DDD	2177	PHE	2.5
1	CCC	2364	ALA	2.5
1	EEE	2208	THR	2.5
1	DDD	2089	LEU	2.5
1	DDD	2389	ILE	2.5
1	EEE	2405	LYS	2.5
1	EEE	1976	LEU	2.5
1	EEE	2084	LEU	2.5
1	DDD	1946	TRP	2.5
1	FFF	1899	LEU	2.5
1	FFF	2493	GLU	2.4
1	FFF	2334	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	2360	ARG	2.4
1	BBB	2504	HIS	2.4
1	CCC	2207	ILE	2.4
1	DDD	2179	THR	2.4
1	FFF	2089	LEU	2.4
1	EEE	2496	HIS	2.4
1	FFF	1983	GLU	2.4
1	DDD	2423	ILE	2.4
1	EEE	2125	PHE	2.4
1	DDD	2229	ILE	2.4
1	FFF	2249	ILE	2.4
1	FFF	2444	LEU	2.4
1	EEE	2215	GLN	2.4
1	EEE	1986	TYR	2.4
1	FFF	2448	ARG	2.4
1	DDD	2443	ILE	2.4
1	EEE	2378	LEU	2.4
1	FFF	2236	HIS	2.4
1	DDD	2357	ASP	2.4
1	EEE	1896	ASP	2.4
1	DDD	1968	ILE	2.4
1	FFF	2136	VAL	2.4
1	AAA	2121	ALA	2.4
1	FFF	2069	LEU	2.4
1	BBB	1976	LEU	2.3
1	AAA	1891	PRO	2.3
1	EEE	1891	PRO	2.3
1	FFF	2082	TYR	2.3
1	EEE	1890	PHE	2.3
1	AAA	2133	ILE	2.3
1	BBB	2141	LEU	2.3
1	DDD	2352	LEU	2.3
1	EEE	2401	GLN	2.3
1	BBB	2208	THR	2.3
1	EEE	2472	ILE	2.3
1	EEE	2416	PHE	2.3
1	EEE	1990	LYS	2.3
1	BBB	2206	ALA	2.3
1	CCC	1899	LEU	2.3
1	FFF	2029	ILE	2.3
1	EEE	2076	VAL	2.3
1	CCC	1897	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	2336	LEU	2.3
1	EEE	1982	LEU	2.3
1	FFF	2244	PHE	2.3
1	DDD	1978	CYS	2.2
1	FFF	2352	LEU	2.2
1	EEE	2465	GLU	2.2
1	FFF	1851	SER	2.2
1	FFF	1935	LEU	2.2
1	DDD	1951	CYS	2.2
1	AAA	2026	SER	2.2
1	FFF	1903	LEU	2.2
1	EEE	2179	THR	2.2
1	BBB	2094	PHE	2.2
1	CCC	2363	ALA	2.2
1	EEE	2480	ILE	2.2
1	AAA	2025	THR	2.2
1	CCC	2362	ILE	2.2
1	FFF	2488	ILE	2.2
1	DDD	2178	SER	2.2
1	FFF	1998	PRO	2.2
1	FFF	2391	TYR	2.2
1	EEE	2069	LEU	2.1
1	DDD	1893	LYS	2.1
1	FFF	2245	THR	2.1
1	EEE	2449	TYR	2.1
1	EEE	2094	PHE	2.1
1	BBB	2103	LYS	2.1
1	EEE	2386	CYS	2.1
1	DDD	2249	ILE	2.1
1	FFF	2390	ILE	2.1
1	EEE	2232	VAL	2.1
1	FFF	1978	CYS	2.1
1	EEE	2060	LEU	2.1
1	DDD	1887	ASP	2.1
1	DDD	2469	ILE	2.1
1	DDD	2498	THR	2.1
1	EEE	2204	THR	2.1
1	EEE	2538	LEU	2.1
1	FFF	2127	PHE	2.1
1	FFF	2538	LEU	2.1
1	EEE	2248	ASN	2.1
1	DDD	1854	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	DDD	1943	ASP	2.1
1	DDD	2133	ILE	2.1
1	EEE	2207	ILE	2.1
1	FFF	2028	GLY	2.1
1	EEE	2002	GLU	2.1
1	DDD	2536	LEU	2.1
1	DDD	2382	ALA	2.1
1	BBB	2318	PHE	2.1
1	EEE	1917	LEU	2.0
1	FFF	1957	ASP	2.0
1	EEE	2363	ALA	2.0
1	FFF	2006	HIS	2.0
1	EEE	2443	ILE	2.0
1	FFF	2423	ILE	2.0
1	FFF	2582	TRP	2.0
1	DDD	2465	GLU	2.0
1	FFF	2083	CYS	2.0
1	EEE	2052	LEU	2.0
2	QQQ	11	DC	2.0
1	AAA	1852	ILE	2.0
1	AAA	2370	GLU	2.0
1	DDD	2420	TYR	2.0
1	CCC	2358	VAL	2.0
1	AAA	1957	ASP	2.0
1	FFF	1897	ASP	2.0
1	DDD	2565	ALA	2.0
1	FFF	2232	VAL	2.0
1	FFF	2536	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	DDG	RRR	13	21/22	0.95	0.17	72,85,98,100	0
3	DDG	NNN	13	21/22	0.96	0.23	48,55,66,69	0
3	DDG	PPP	13	21/22	0.97	0.19	61,76,95,97	0
3	DDG	LLL	13	21/22	0.97	0.18	42,51,60,62	0
3	DDG	HHH	13	21/22	0.98	0.22	30,38,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DDG	JJJ	13	21/22	0.99	0.19	43,51,55,57	0

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

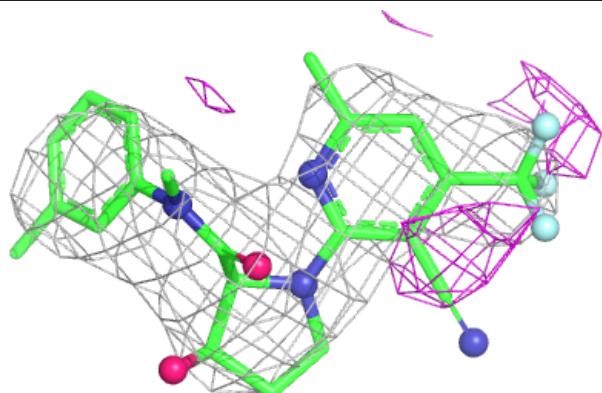
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	AAA	2601	1/1	0.62	0.11	59,59,59,59	0
4	MG	EEE	2601	1/1	0.83	0.07	99,99,99,99	0
6	K8I	DDD	2603	30/30	0.85	0.51	94,114,136,144	0
4	MG	DDD	2601	1/1	0.87	0.07	84,84,84,84	0
4	MG	CCC	2601	1/1	0.91	0.12	59,59,59,59	0
4	MG	BBB	2601	1/1	0.91	0.15	66,66,66,66	0
6	K8I	CCC	2602	30/30	0.92	0.34	80,95,111,117	0
6	K8I	BBB	2603	30/30	0.93	0.35	78,93,115,119	0
6	K8I	AAA	2603	30/30	0.94	0.30	71,95,113,119	0
4	MG	FFF	2601	1/1	0.94	0.05	111,111,111,111	0
5	DG3	FFF	2602	30/30	0.95	0.17	89,102,119,121	0
5	DG3	EEE	2602	30/30	0.96	0.16	71,91,108,109	0
5	DG3	DDD	2602	30/30	0.96	0.17	51,63,86,93	0
5	DG3	BBB	2602	30/30	0.97	0.20	50,62,73,75	0
5	DG3	KKK	101	30/30	0.97	0.17	41,49,83,91	0
5	DG3	AAA	2602	30/30	0.98	0.18	39,44,64,76	0

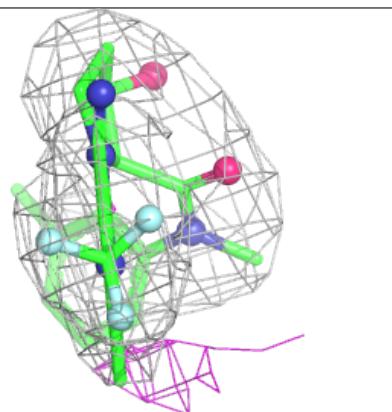
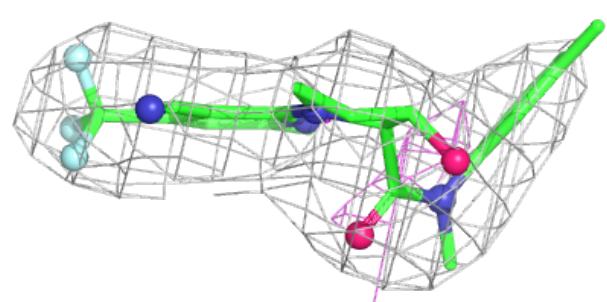
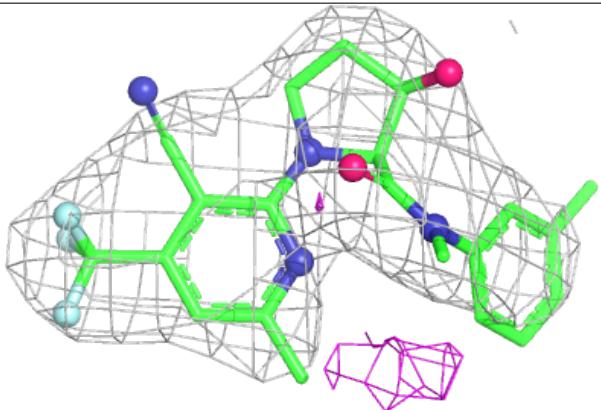
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around K8I DDD 2603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

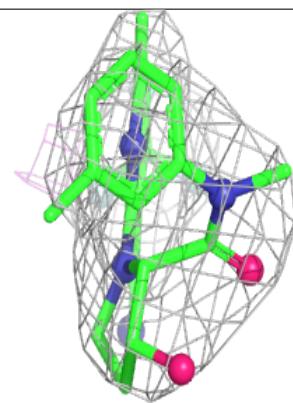
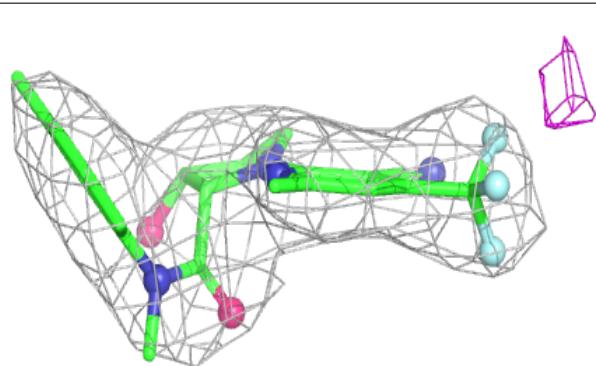
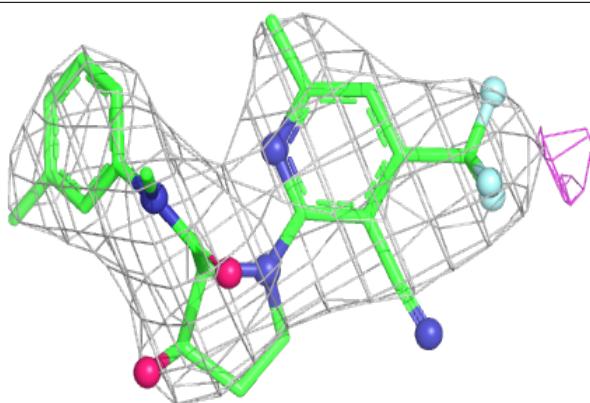
**Electron density around K8I CCC 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

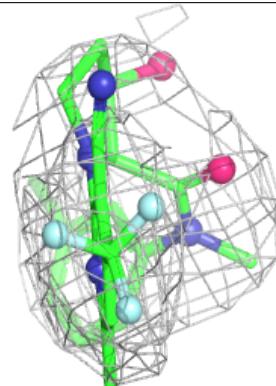
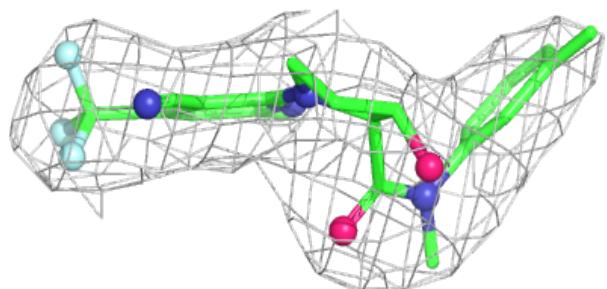
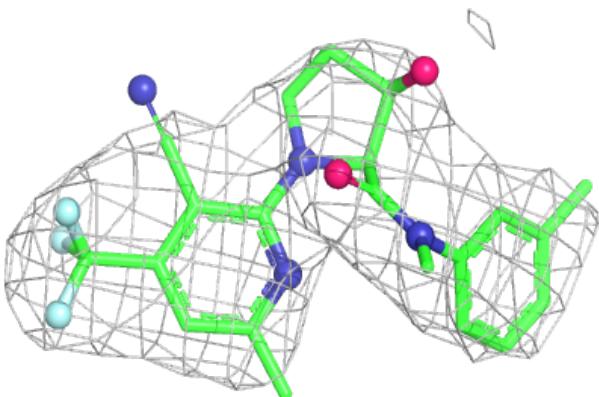


**Electron density around K8I BBB 2603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

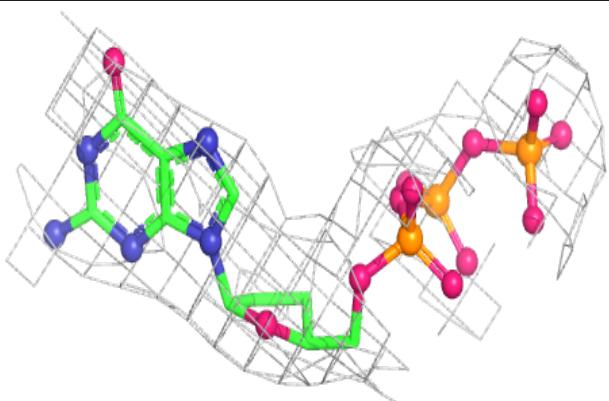
**Electron density around K8I AAA 2603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

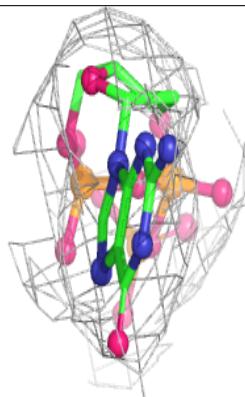
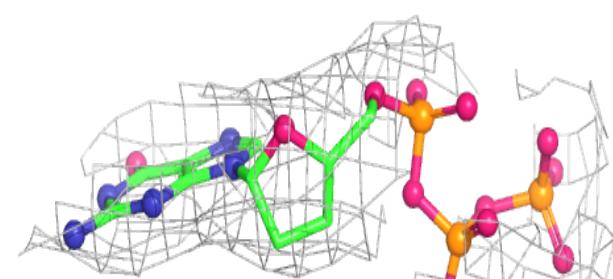
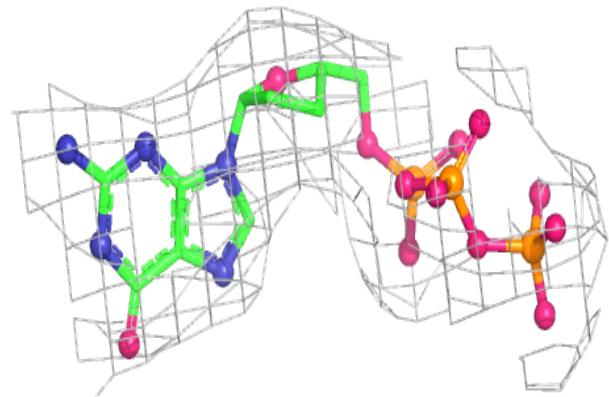


**Electron density around DG3 FFF 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

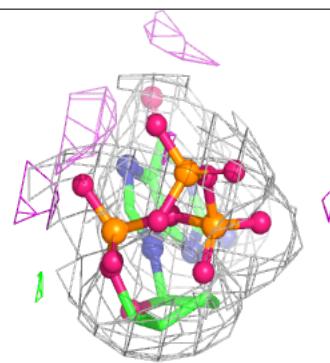
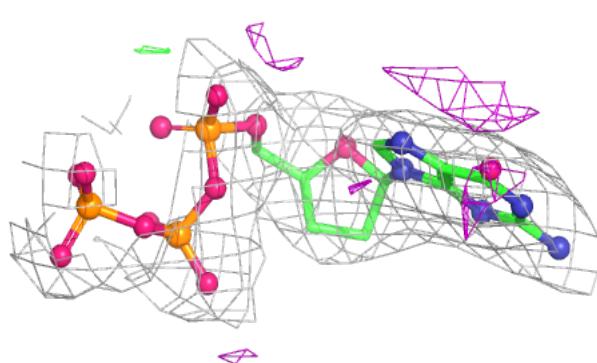
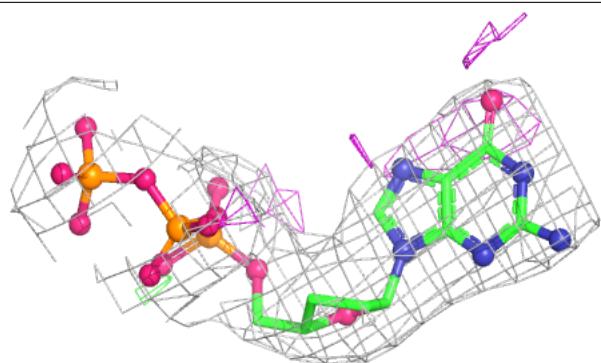
**Electron density around DG3 EEE 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

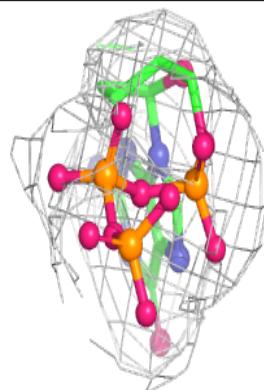
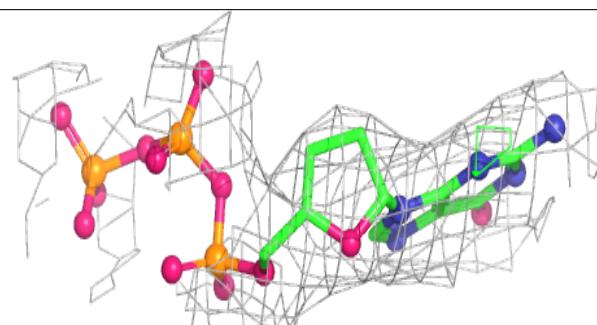
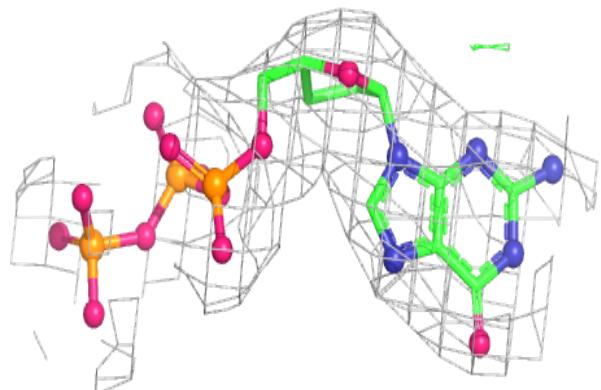


**Electron density around DG3 DDD 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

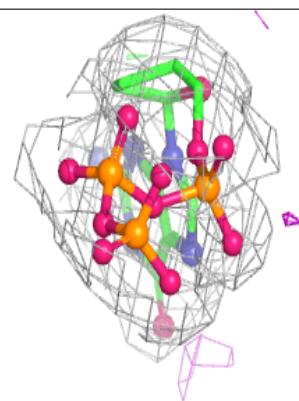
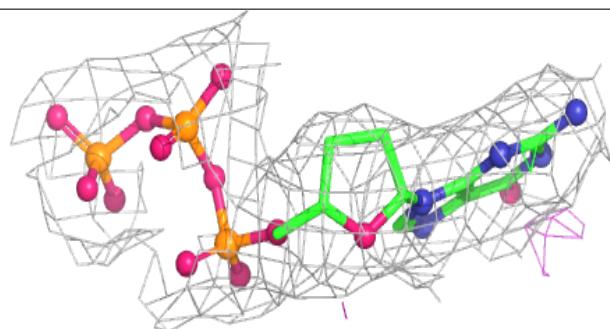
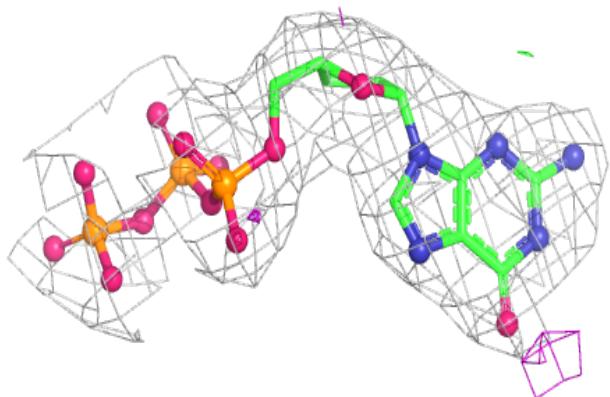
**Electron density around DG3 BBB 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

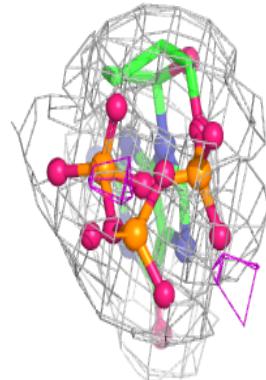
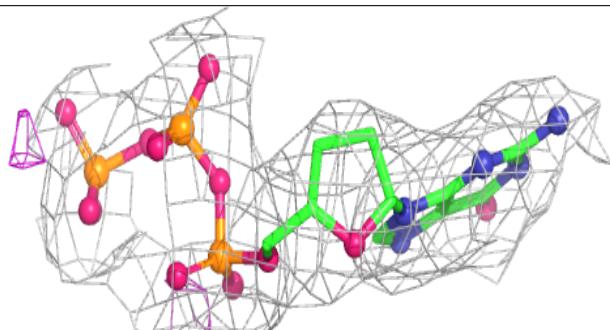
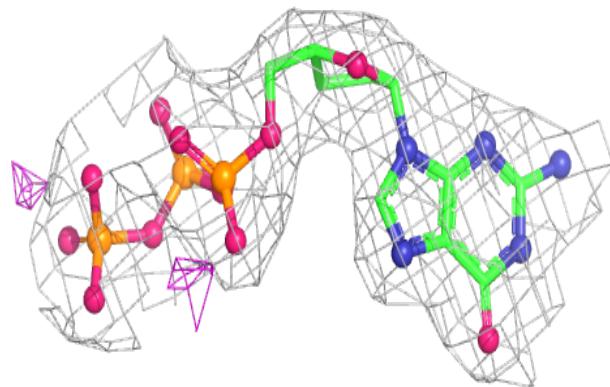


**Electron density around DG3 KKK 101:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DG3 AAA 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.