



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:46 am BST

PDB ID : 4BZC
Title : Crystal structure of the tetrameric dGTP-bound wild type SAMHD1 catalytic core
Authors : Ji, X.; Yang, H.; Wu, Y.; Yan, J.; Mehrens, J.; DeLucia, M.; Hao, C.; Gronenborn, A.M.; Skowronski, J.; Ahn, J.; Xiong, Y.
Deposited on : 2013-07-25
Resolution : 2.88 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

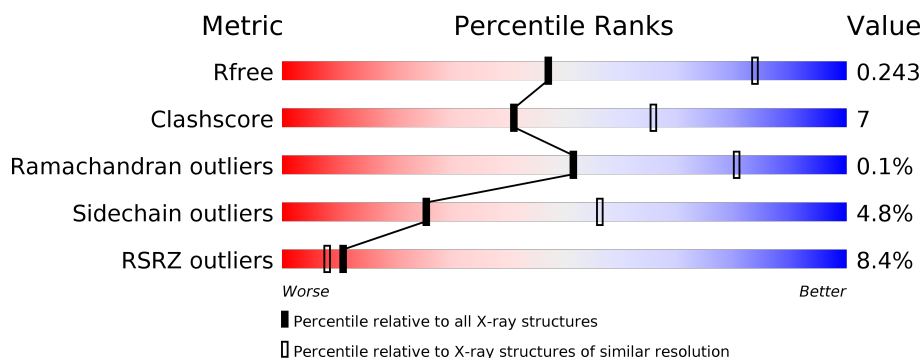
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A	550	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	550	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	550	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	550	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15954 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 DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHO-HYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3880	2483	672	705	20			
1	B	477	Total	C	N	O	S	0	0	0
			3887	2489	678	700	20			
1	C	481	Total	C	N	O	S	0	0	0
			3932	2517	683	712	20			
1	D	470	Total	C	N	O	S	0	0	0
			3841	2462	666	693	20			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	UNP Q9Y3Z3
A	78	GLY	-	expression tag	UNP Q9Y3Z3
A	79	SER	-	expression tag	UNP Q9Y3Z3
A	80	SER	-	expression tag	UNP Q9Y3Z3
A	81	HIS	-	expression tag	UNP Q9Y3Z3
A	82	HIS	-	expression tag	UNP Q9Y3Z3
A	83	HIS	-	expression tag	UNP Q9Y3Z3
A	84	HIS	-	expression tag	UNP Q9Y3Z3
A	85	HIS	-	expression tag	UNP Q9Y3Z3
A	86	HIS	-	expression tag	UNP Q9Y3Z3
A	87	SER	-	expression tag	UNP Q9Y3Z3
A	88	SER	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	LEU	-	expression tag	UNP Q9Y3Z3
A	91	VAL	-	expression tag	UNP Q9Y3Z3
A	92	PRO	-	expression tag	UNP Q9Y3Z3
A	93	ARG	-	expression tag	UNP Q9Y3Z3
A	94	GLY	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	expression tag	UNP Q9Y3Z3
A	98	ALA	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	MET	-	expression tag	UNP Q9Y3Z3
A	101	THR	-	expression tag	UNP Q9Y3Z3
A	102	GLY	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	GLN	-	expression tag	UNP Q9Y3Z3
A	105	GLN	-	expression tag	UNP Q9Y3Z3
A	106	MET	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	ARG	-	expression tag	UNP Q9Y3Z3
A	109	ASP	-	expression tag	UNP Q9Y3Z3
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
B	77	MET	-	expression tag	UNP Q9Y3Z3
B	78	GLY	-	expression tag	UNP Q9Y3Z3
B	79	SER	-	expression tag	UNP Q9Y3Z3
B	80	SER	-	expression tag	UNP Q9Y3Z3
B	81	HIS	-	expression tag	UNP Q9Y3Z3
B	82	HIS	-	expression tag	UNP Q9Y3Z3
B	83	HIS	-	expression tag	UNP Q9Y3Z3
B	84	HIS	-	expression tag	UNP Q9Y3Z3
B	85	HIS	-	expression tag	UNP Q9Y3Z3
B	86	HIS	-	expression tag	UNP Q9Y3Z3
B	87	SER	-	expression tag	UNP Q9Y3Z3
B	88	SER	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	LEU	-	expression tag	UNP Q9Y3Z3
B	91	VAL	-	expression tag	UNP Q9Y3Z3
B	92	PRO	-	expression tag	UNP Q9Y3Z3
B	93	ARG	-	expression tag	UNP Q9Y3Z3
B	94	GLY	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	MET	-	expression tag	UNP Q9Y3Z3
B	98	ALA	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	MET	-	expression tag	UNP Q9Y3Z3
B	101	THR	-	expression tag	UNP Q9Y3Z3
B	102	GLY	-	expression tag	UNP Q9Y3Z3

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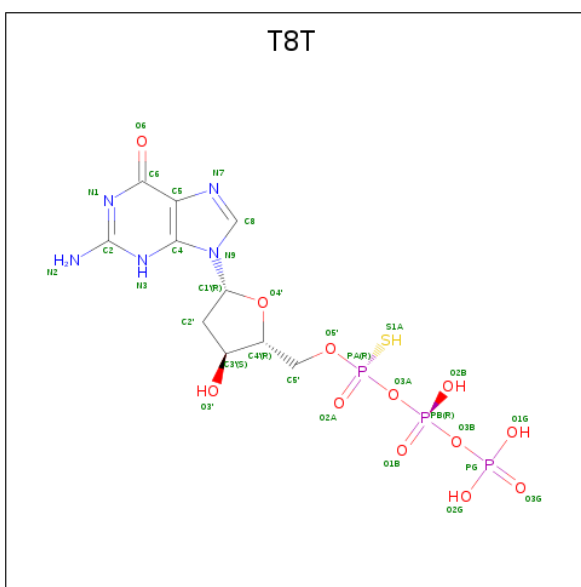
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	GLN	-	expression tag	UNP Q9Y3Z3
B	105	GLN	-	expression tag	UNP Q9Y3Z3
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag	UNP Q9Y3Z3
C	77	MET	-	expression tag	UNP Q9Y3Z3
C	78	GLY	-	expression tag	UNP Q9Y3Z3
C	79	SER	-	expression tag	UNP Q9Y3Z3
C	80	SER	-	expression tag	UNP Q9Y3Z3
C	81	HIS	-	expression tag	UNP Q9Y3Z3
C	82	HIS	-	expression tag	UNP Q9Y3Z3
C	83	HIS	-	expression tag	UNP Q9Y3Z3
C	84	HIS	-	expression tag	UNP Q9Y3Z3
C	85	HIS	-	expression tag	UNP Q9Y3Z3
C	86	HIS	-	expression tag	UNP Q9Y3Z3
C	87	SER	-	expression tag	UNP Q9Y3Z3
C	88	SER	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	LEU	-	expression tag	UNP Q9Y3Z3
C	91	VAL	-	expression tag	UNP Q9Y3Z3
C	92	PRO	-	expression tag	UNP Q9Y3Z3
C	93	ARG	-	expression tag	UNP Q9Y3Z3
C	94	GLY	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	MET	-	expression tag	UNP Q9Y3Z3
C	98	ALA	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	MET	-	expression tag	UNP Q9Y3Z3
C	101	THR	-	expression tag	UNP Q9Y3Z3
C	102	GLY	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	GLN	-	expression tag	UNP Q9Y3Z3
C	105	GLN	-	expression tag	UNP Q9Y3Z3
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
D	77	MET	-	expression tag	UNP Q9Y3Z3
D	78	GLY	-	expression tag	UNP Q9Y3Z3
D	79	SER	-	expression tag	UNP Q9Y3Z3
D	80	SER	-	expression tag	UNP Q9Y3Z3
D	81	HIS	-	expression tag	UNP Q9Y3Z3
D	82	HIS	-	expression tag	UNP Q9Y3Z3
D	83	HIS	-	expression tag	UNP Q9Y3Z3
D	84	HIS	-	expression tag	UNP Q9Y3Z3
D	85	HIS	-	expression tag	UNP Q9Y3Z3
D	86	HIS	-	expression tag	UNP Q9Y3Z3
D	87	SER	-	expression tag	UNP Q9Y3Z3
D	88	SER	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	LEU	-	expression tag	UNP Q9Y3Z3
D	91	VAL	-	expression tag	UNP Q9Y3Z3
D	92	PRO	-	expression tag	UNP Q9Y3Z3
D	93	ARG	-	expression tag	UNP Q9Y3Z3
D	94	GLY	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	MET	-	expression tag	UNP Q9Y3Z3
D	98	ALA	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	MET	-	expression tag	UNP Q9Y3Z3
D	101	THR	-	expression tag	UNP Q9Y3Z3
D	102	GLY	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	GLN	-	expression tag	UNP Q9Y3Z3
D	105	GLN	-	expression tag	UNP Q9Y3Z3
D	106	MET	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
D	109	ASP	-	expression tag	UNP Q9Y3Z3
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3

- Molecule 2 is 2'-deoxyguanosine-5'-O-(1-thiotriphosphate) (three-letter code: T8T) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	B	9	Total O 9 9	0	0
5	C	7	Total O 7 7	0	0
5	D	4	Total O 4 4	0	0

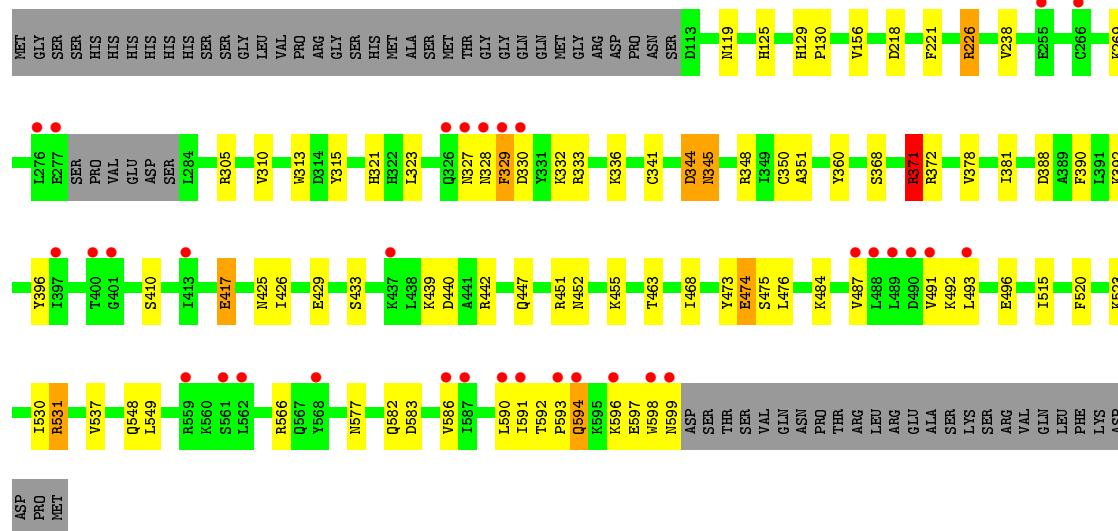
• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1



GLN
ASN
PRO
THR
ARG
LEU
ARG
GLU
ALA
SER
SER
SER
SER
VAL
GLN
LEU
PHE
LYS
ASP
ASP
PRO
MET

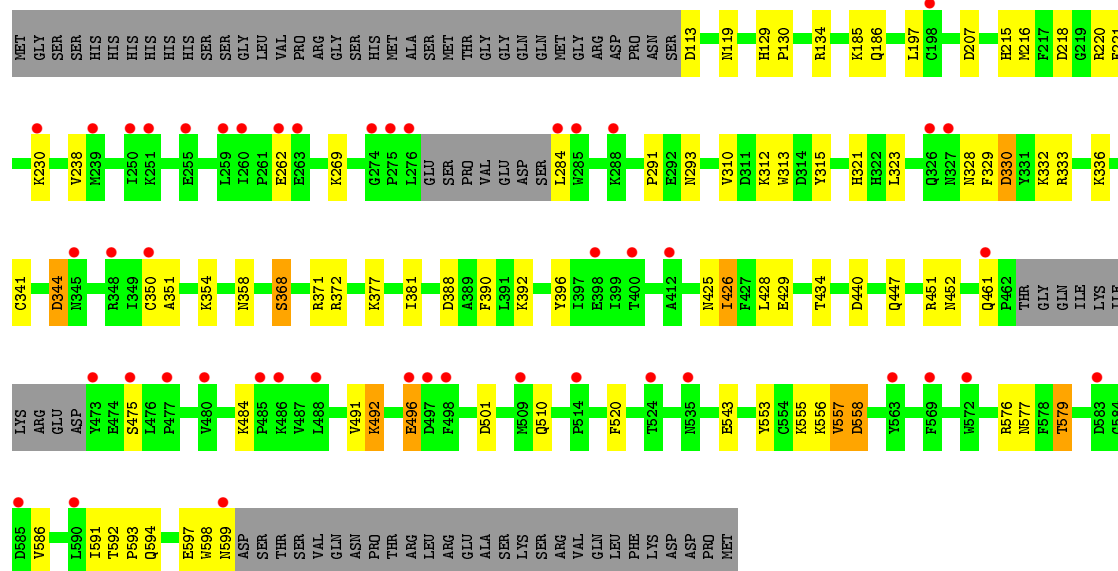
● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

Chain C: 



● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.00Å 138.73Å 93.72Å 90.00° 113.56° 90.00°	Depositor
Resolution (Å)	49.71 – 2.88 49.66 – 2.88	Depositor EDS
% Data completeness (in resolution range)	77.5 (49.71-2.88) 77.5 (49.66-2.88)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.245 0.193 , 0.243	Depositor DCC
R_{free} test set	1668 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15954	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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, T8T, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/3972	0.84	10/5364 (0.2%)
1	B	0.61	0/3978	0.85	9/5369 (0.2%)
1	C	0.65	0/4025	0.82	5/5434 (0.1%)
1	D	0.62	0/3933	0.78	2/5311 (0.0%)
All	All	0.63	0/15908	0.82	26/21478 (0.1%)

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	D	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ARG	NE-CZ-NH1	12.89	126.74	120.30
1	B	451	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	C	226	ARG	CG-CD-NE	8.26	129.14	111.80
1	B	366	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	531	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	531	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	115	MET	CB-CG-SD	6.47	131.82	112.40
1	B	371	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	216	MET	CG-SD-CE	-6.22	90.25	100.20
1	B	405	LYS	CB-CA-C	-6.06	98.27	110.40
1	D	451	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	473	TYR	CB-CG-CD1	-5.76	117.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	368	SER	N-CA-CB	-5.74	101.89	110.50
1	A	333	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	451	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	451	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	371	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	325	ILE	CB-CA-C	-5.40	100.80	111.60
1	A	440	ASP	N-CA-CB	5.36	120.25	110.60
1	A	473	TYR	CB-CG-CD2	5.34	124.20	121.00
1	C	333	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	352	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	325	ILE	CB-CA-C	-5.15	101.30	111.60
1	B	442	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	559	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	330	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3880	0	3844	76	0
1	B	3887	0	3872	54	0
1	C	3932	0	3913	59	2
1	D	3841	0	3817	69	2
2	A	93	0	39	3	0
2	B	93	0	39	4	0
2	C	93	0	39	12	0
2	D	93	0	39	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	14	0	0	1	0
5	B	9	0	0	1	0
5	C	7	0	0	0	0
5	D	4	0	0	0	0
All	All	15954	0	15602	225	2

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 7.

All (225) 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:D:556:LYS:O	1:D:557:VAL:HG22	1.44	1.17
1:D:215:HIS:NE2	2:D:700:T8T:O2A	1.84	1.09
1:A:325:ILE:C	1:C:328:ASN:HB2	1.77	1.04
1:B:402:ALA:O	1:B:405:LYS:HD2	1.60	0.99
1:D:368:SER:OG	1:D:372:ARG:NH1	1.97	0.97
1:A:328:ASN:HB2	1:A:365:THR:OG1	1.71	0.89
1:B:143:ARG:NH2	1:B:210:HIS:O	2.05	0.89
1:B:328:ASN:HB2	1:B:365:THR:OG1	1.73	0.88
1:B:325:ILE:C	1:D:328:ASN:HB2	1.93	0.88
1:D:207:ASP:OD1	2:D:700:T8T:S1A	2.32	0.88
1:C:474:GLU:HA	1:C:474:GLU:OE1	1.73	0.88
1:D:598:TRP:O	1:D:599:ASN:HB2	1.76	0.86
1:A:429:GLU:OE2	1:D:429:GLU:HG3	1.75	0.85
1:A:523:LYS:NZ	2:C:800:T8T:O3G	2.10	0.84
1:B:325:ILE:O	1:D:328:ASN:HB2	1.78	0.84
1:B:226:ARG:O	1:B:229:VAL:HG12	1.77	0.83
1:B:155:TYR:O	1:B:451:ARG:NH2	2.13	0.81
1:B:325:ILE:HG22	1:B:326:GLN:N	1.95	0.80
1:A:215:HIS:HB2	5:A:2007:HOH:O	1.82	0.79
1:A:325:ILE:HG22	1:A:326:GLN:N	1.97	0.78
1:D:113:ASP:HB3	1:D:130:PRO:HB3	1.67	0.75
1:A:325:ILE:O	1:C:328:ASN:HB2	1.86	0.74
1:D:556:LYS:O	1:D:557:VAL:CG2	2.30	0.74
1:B:325:ILE:CG2	1:B:326:GLN:N	2.50	0.74
1:A:325:ILE:CG2	1:A:326:GLN:N	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HZ2	2:C:800:T8T:PG	2.13	0.70
1:A:597:GLU:OE1	1:A:597:GLU:N	2.21	0.70
2:A:700:T8T:H5'	2:A:700:T8T:H8	1.73	0.70
2:B:800:T8T:O3G	2:B:900:T8T:O2B	2.10	0.69
1:B:238:VAL:HG13	1:B:269:LYS:HG2	1.75	0.69
1:B:597:GLU:N	1:B:597:GLU:OE1	2.23	0.68
1:A:305:ARG:NE	1:A:348:ARG:HH11	1.89	0.68
1:D:238:VAL:HG13	1:D:269:LYS:HG2	1.75	0.68
1:D:461:GLN:H	1:D:579:THR:CG2	2.08	0.67
1:A:585:ASP:OD1	1:A:592:THR:HG21	1.95	0.67
1:A:238:VAL:HG13	1:A:269:LYS:HG2	1.75	0.67
1:D:597:GLU:N	1:D:597:GLU:OE1	2.22	0.67
1:C:238:VAL:HG13	1:C:269:LYS:HG2	1.77	0.66
1:A:400:THR:HG21	1:D:434:THR:HG21	1.78	0.66
1:A:524:THR:HG21	1:C:566:ARG:CZ	2.26	0.66
1:C:597:GLU:OE1	1:C:597:GLU:N	2.25	0.66
1:B:164:ARG:NH1	2:B:700:T8T:S1A	2.67	0.65
1:B:524:THR:OG1	1:D:586:VAL:HG11	1.96	0.65
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.79	0.65
1:B:558:ASP:OD1	1:B:561:SER:CB	2.46	0.64
1:D:558:ASP:N	1:D:558:ASP:OD1	2.30	0.63
1:B:372:ARG:NE	1:D:358:ASN:OD1	2.31	0.63
1:B:333:ARG:NH2	2:D:800:T8T:S1A	2.71	0.63
2:C:700:T8T:S1A	2:C:700:T8T:O2B	2.57	0.62
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.00	0.62
1:D:556:LYS:C	1:D:557:VAL:HG13	2.20	0.61
1:A:523:LYS:NZ	2:C:900:T8T:O1G	2.26	0.61
1:A:326:GLN:N	1:C:328:ASN:HB2	2.15	0.61
1:B:342:GLU:OE2	1:B:345:ASN:HA	2.01	0.61
1:B:333:ARG:NH1	1:B:355:GLU:OE2	2.33	0.61
1:B:342:GLU:OE2	1:B:345:ASN:N	2.35	0.60
1:B:469:LYS:CD	1:B:469:LYS:N	2.65	0.60
1:A:342:GLU:OE2	1:A:345:ASN:N	2.34	0.59
1:A:325:ILE:C	1:C:328:ASN:CB	2.65	0.58
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.04	0.58
1:A:343:VAL:HB	1:A:348:ARG:HE	1.68	0.58
1:C:455:LYS:NZ	2:C:900:T8T:O3G	2.34	0.58
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.03	0.58
1:A:531:ARG:NH1	1:A:531:ARG:HB3	2.20	0.57
1:C:473:TYR:HA	1:C:476:LEU:HD12	1.87	0.57
1:D:329:PHE:CG	1:D:330:ASP:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:CYS:SG	1:C:583:ASP:CB	2.94	0.56
1:D:555:LYS:O	1:D:557:VAL:HG13	2.05	0.56
1:A:325:ILE:O	1:C:328:ASN:CB	2.53	0.56
1:B:376:HIS:CD2	1:B:378:VAL:H	2.24	0.56
1:A:525:ALA:HB3	1:C:586:VAL:CG1	2.35	0.56
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.06	0.55
1:B:358:ASN:OD1	1:D:372:ARG:NH2	2.40	0.54
1:B:323:LEU:O	1:C:119:ASN:ND2	2.41	0.53
1:D:461:GLN:H	1:D:579:THR:HG23	1.74	0.53
1:B:377:LYS:HE2	5:B:2007:HOH:O	2.08	0.53
1:B:325:ILE:O	1:D:328:ASN:CB	2.55	0.52
1:B:376:HIS:HD2	1:B:378:VAL:H	1.57	0.52
1:B:558:ASP:OD1	1:B:561:SER:OG	2.27	0.52
1:A:530:ILE:HD12	1:C:582:GLN:O	2.09	0.51
1:A:425:ASN:HB2	1:D:428:LEU:CD1	2.40	0.51
1:A:119:ASN:ND2	1:D:323:LEU:O	2.43	0.51
1:A:342:GLU:OE2	1:A:345:ASN:HA	2.10	0.51
1:A:352:ARG:HH22	2:C:800:T8T:PG	2.34	0.51
1:A:328:ASN:HB2	1:A:365:THR:HG1	1.75	0.51
1:A:305:ARG:NE	1:A:348:ARG:NH1	2.56	0.51
2:B:800:T8T:O2A	1:D:354:LYS:NZ	2.32	0.51
1:B:377:LYS:NZ	2:B:800:T8T:O1B	2.44	0.50
1:A:522:CYS:SG	1:C:583:ASP:HB3	2.51	0.50
1:A:524:THR:HG21	1:C:566:ARG:NH2	2.27	0.50
1:C:372:ARG:NE	2:C:800:T8T:O6	2.39	0.50
1:B:321:HIS:CE1	1:C:321:HIS:CE1	3.00	0.50
1:B:116:LYS:HE3	2:C:900:T8T:S1A	2.52	0.50
1:D:461:GLN:HB2	1:D:579:THR:CG2	2.42	0.50
1:B:558:ASP:OD1	1:B:561:SER:HB2	2.10	0.50
1:B:155:TYR:HB3	1:B:451:ARG:NH2	2.26	0.49
1:B:469:LYS:N	1:B:469:LYS:HD2	2.27	0.49
1:C:439:LYS:HA	1:C:442:ARG:NH1	2.28	0.49
1:A:323:LEU:O	1:D:119:ASN:ND2	2.45	0.49
1:C:371:ARG:HG3	1:C:371:ARG:HH11	1.78	0.49
1:D:461:GLN:O	1:D:579:THR:HG22	2.12	0.49
1:C:433:SER:C	1:C:442:ARG:HH21	2.16	0.49
1:A:524:THR:CG2	1:C:566:ARG:NH2	2.76	0.49
1:A:425:ASN:HB2	1:D:428:LEU:HD12	1.94	0.48
1:A:428:LEU:CD1	1:D:425:ASN:HB2	2.43	0.48
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.67	0.48
1:A:571:GLN:HE22	1:A:594:GLN:HE22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:O	1:A:384:THR:HG23	2.14	0.48
1:A:525:ALA:HB3	1:C:586:VAL:HG11	1.96	0.48
1:D:576:ARG:O	1:D:577:ASN:HB2	2.14	0.48
1:B:469:LYS:H	1:B:469:LYS:HD3	1.78	0.48
1:D:461:GLN:H	1:D:579:THR:HG22	1.78	0.48
1:D:591:ILE:O	1:D:594:GLN:HB2	2.13	0.48
1:A:207:ASP:OD1	2:A:700:T8T:S1A	2.71	0.48
1:B:469:LYS:CD	1:B:469:LYS:H	2.27	0.48
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.96	0.47
1:C:345:ASN:C	1:C:345:ASN:OD1	2.52	0.47
1:A:522:CYS:SG	1:C:583:ASP:HB2	2.54	0.47
1:D:134:ARG:NE	1:D:134:ARG:HA	2.28	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.47
1:D:330:ASP:HB3	1:D:332:LYS:HB2	1.97	0.47
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.50	0.47
1:A:216:MET:HG3	1:A:217:PHE:N	2.22	0.47
1:A:371:ARG:NH2	1:C:537:VAL:O	2.48	0.47
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.50	0.47
1:C:591:ILE:O	1:C:594:GLN:HB2	2.15	0.47
1:D:492:LYS:CG	1:D:492:LYS:O	2.62	0.47
1:A:472:ASP:OD2	1:A:473:TYR:CZ	2.68	0.47
1:C:327:ASN:ND2	1:C:329:PHE:CD1	2.82	0.47
1:D:381:ILE:HD13	1:D:553:TYR:CG	2.50	0.47
1:A:543:GLU:OE1	1:A:543:GLU:N	2.30	0.46
1:C:371:ARG:HH11	1:C:371:ARG:CG	2.28	0.46
1:A:320:CYS:SG	1:A:327:ASN:HB2	2.55	0.46
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.46
1:D:207:ASP:CG	2:D:700:T8T:S1A	2.93	0.46
1:C:125:HIS:CE1	1:D:333:ARG:HB2	2.50	0.46
1:C:330:ASP:HB3	1:C:332:LYS:HB2	1.97	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.15	0.46
1:D:341:CYS:CB	1:D:350:CYS:HG	2.29	0.46
1:B:325:ILE:CG2	1:B:326:GLN:H	2.27	0.46
1:B:342:GLU:OE2	1:B:345:ASN:CA	2.64	0.46
1:C:548:GLN:O	1:C:549:LEU:HD23	2.16	0.45
1:D:496:GLU:O	1:D:555:LYS:HE3	2.15	0.45
1:A:325:ILE:CG2	1:A:326:GLN:H	2.27	0.45
1:A:497:ASP:OD2	1:A:556:LYS:CE	2.65	0.45
1:A:313:TRP:CD1	1:A:329:PHE:CE2	3.04	0.45
2:C:800:T8T:O3G	2:C:900:T8T:O2B	2.35	0.45
1:B:328:ASN:HB2	1:B:365:THR:HG1	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLU:O	1:C:417:GLU:OE1	2.34	0.45
1:A:305:ARG:CZ	1:A:348:ARG:HH11	2.30	0.45
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:A:221:PHE:CE1	1:A:390:PHE:HB3	2.52	0.45
2:C:700:T8T:H8	2:C:700:T8T:H5'	1.99	0.44
1:C:417:GLU:HA	1:C:417:GLU:OE1	2.17	0.44
1:C:463:THR:HG21	1:C:577:ASN:O	2.17	0.44
1:D:312:LYS:HE3	2:D:700:T8T:O1G	2.17	0.44
1:A:463:THR:OG1	1:A:464:GLY:N	2.50	0.44
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.51	0.44
1:B:221:PHE:CE1	1:B:390:PHE:HB3	2.52	0.44
1:B:320:CYS:SG	1:B:327:ASN:HB2	2.58	0.44
1:A:342:GLU:OE2	1:A:345:ASN:CA	2.66	0.44
1:C:315:TYR:CE2	2:C:700:T8T:H5'A	2.53	0.44
1:A:525:ALA:HB3	1:C:586:VAL:HG13	1.98	0.44
1:B:598:TRP:O	1:B:599:ASN:CB	2.65	0.44
1:D:221:PHE:CE1	1:D:390:PHE:HB3	2.53	0.43
1:D:344:ASP:N	1:D:344:ASP:OD1	2.50	0.43
1:B:114:THR:OG1	1:B:115:MET:N	2.51	0.43
1:A:114:THR:HG22	1:A:115:MET:N	2.33	0.43
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.86	0.43
1:C:221:PHE:CE1	1:C:390:PHE:HB3	2.52	0.43
1:A:494:LYS:HB2	1:A:497:ASP:OD1	2.19	0.43
2:A:900:T8T:O3G	1:C:523:LYS:NZ	2.47	0.43
1:B:344:ASP:OD1	1:B:344:ASP:N	2.52	0.43
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.86	0.43
1:C:378:VAL:O	1:C:381:ILE:HG22	2.18	0.43
1:D:341:CYS:HB2	1:D:350:CYS:HG	1.84	0.43
1:C:341:CYS:CB	1:C:350:CYS:HG	2.31	0.43
1:B:388:ASP:O	1:B:392:LYS:HG3	2.19	0.43
1:A:426:ILE:HA	1:A:426:ILE:HD13	1.88	0.43
1:B:119:ASN:ND2	1:C:323:LEU:O	2.52	0.43
1:C:426:ILE:HD13	1:C:426:ILE:HA	1.91	0.43
1:C:368:SER:O	1:C:372:ARG:HG2	2.19	0.42
1:C:388:ASP:O	1:C:392:LYS:HG3	2.20	0.42
1:A:582:GLN:O	1:C:530:ILE:HD12	2.19	0.42
1:B:313:TRP:CD1	1:B:329:PHE:CE2	3.08	0.42
1:A:284:LEU:HG	1:A:292:GLU:OE2	2.20	0.42
1:A:371:ARG:CZ	1:A:549:LEU:HD11	2.50	0.42
1:B:598:TRP:O	1:B:599:ASN:CG	2.58	0.42
1:D:388:ASP:O	1:D:392:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:LYS:HG2	1:D:492:LYS:O	2.20	0.42
1:A:388:ASP:O	1:A:392:LYS:HG3	2.20	0.42
1:C:305:ARG:NE	1:C:348:ARG:HH11	2.17	0.42
1:D:310:VAL:HG12	1:D:313:TRP:CZ3	2.54	0.42
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.55	0.41
1:A:425:ASN:OD1	1:D:425:ASN:OD1	2.37	0.41
1:D:426:ILE:HD13	1:D:426:ILE:HA	1.94	0.41
1:B:467:LYS:O	1:B:469:LYS:NZ	2.38	0.41
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.93	0.41
1:D:461:GLN:N	1:D:579:THR:CG2	2.81	0.41
1:C:226:ARG:NE	1:C:410:SER:O	2.53	0.41
1:D:461:GLN:HB2	1:D:579:THR:HG22	2.03	0.41
1:A:213:PHE:HB2	1:A:216:MET:HG2	2.03	0.41
1:A:487:VAL:HG13	1:A:590:LEU:HD12	2.03	0.41
1:D:461:GLN:HB2	1:D:579:THR:HG21	2.02	0.41
1:B:487:VAL:HG13	1:B:590:LEU:HD12	2.03	0.41
1:C:310:VAL:HG12	1:C:313:TRP:CZ3	2.56	0.41
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.21	0.41
1:D:262:GLU:H	1:D:262:GLU:CD	2.23	0.41
1:A:524:THR:HG21	1:C:566:ARG:NH1	2.36	0.41
1:A:531:ARG:HB3	1:A:531:ARG:HH11	1.83	0.41
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.09	0.41
1:A:431:LEU:HD23	1:A:432:TYR:CE1	2.56	0.40
1:D:185:LYS:HG3	1:D:186:GLN:HG3	2.02	0.40
1:A:439:LYS:HG3	1:A:442:ARG:NH2	2.36	0.40
1:A:556:LYS:HB3	1:A:561:SER:CB	2.52	0.40
1:C:360:TYR:CE2	1:C:515:ILE:HG21	2.56	0.40
2:D:800:T8T:O2B	2:D:900:T8T:H5'	2.21	0.40
1:C:487:VAL:HG13	1:C:590:LEU:HD12	2.04	0.40
1:C:598:TRP:O	1:C:599:ASN:CB	2.69	0.40
1:C:156:VAL:O	2:C:900:T8T:H8	2.21	0.40
1:A:344:ASP:OD1	1:A:344:ASP:N	2.53	0.40
1:C:344:ASP:N	1:C:344:ASP:OD1	2.55	0.40
1:D:291:PRO:CG	1:D:293:ASN:OD1	2.69	0.40
1:D:293:ASN:N	1:D:293:ASN:OD1	2.52	0.40
1:D:220:ARG:NH1	1:D:501:ASP:OD2	2.42	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:O	1:D:396:TYR:OH[1_454]	2.10	0.10
1:C:396:TYR:OH	1:D:230:LYS:NZ[1_454]	2.10	0.10

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	A	470/550 (86%)	464 (99%)	6 (1%)	0	100	100
1	B	471/550 (86%)	466 (99%)	5 (1%)	0	100	100
1	C	477/550 (87%)	471 (99%)	6 (1%)	0	100	100
1	D	464/550 (84%)	458 (99%)	5 (1%)	1 (0%)	47	76
All	All	1882/2200 (86%)	1859 (99%)	22 (1%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	557	VAL

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	A	421/488 (86%)	402 (96%)	19 (4%)	27	59
1	B	421/488 (86%)	400 (95%)	21 (5%)	24	54
1	C	427/488 (88%)	405 (95%)	22 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	417/488 (86%)	398 (95%)	19 (5%)	27	58
All	All	1686/1952 (86%)	1605 (95%)	81 (5%)	25	56

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	MET
1	A	283	SER
1	A	293	ASN
1	A	336	LYS
1	A	342	GLU
1	A	344	ASP
1	A	371	ARG
1	A	377	LYS
1	A	425	ASN
1	A	426	ILE
1	A	443	GLU
1	A	447	GLN
1	A	452	ASN
1	A	475	SER
1	A	491	VAL
1	A	496	GLU
1	A	510	GLN
1	A	528	ARG
1	A	531	ARG
1	B	276	LEU
1	B	323	LEU
1	B	336	LYS
1	B	342	GLU
1	B	344	ASP
1	B	345	ASN
1	B	366	ARG
1	B	377	LYS
1	B	425	ASN
1	B	426	ILE
1	B	440	ASP
1	B	447	GLN
1	B	452	ASN
1	B	466	ILE
1	B	467	LYS
1	B	469	LYS
1	B	475	SER

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Mol	Chain	Res	Type
1	B	491	VAL
1	B	496	GLU
1	B	510	GLN
1	B	594	GLN
1	C	218	ASP
1	C	329	PHE
1	C	336	LYS
1	C	344	ASP
1	C	345	ASN
1	C	371	ARG
1	C	417	GLU
1	C	425	ASN
1	C	429	GLU
1	C	440	ASP
1	C	447	GLN
1	C	452	ASN
1	C	468	ILE
1	C	474	GLU
1	C	475	SER
1	C	484	LYS
1	C	491	VAL
1	C	492	LYS
1	C	496	GLU
1	C	531	ARG
1	C	594	GLN
1	C	596	LYS
1	D	216	MET
1	D	284	LEU
1	D	315	TYR
1	D	336	LYS
1	D	344	ASP
1	D	371	ARG
1	D	377	LYS
1	D	426	ILE
1	D	440	ASP
1	D	447	GLN
1	D	452	ASN
1	D	475	SER
1	D	484	LYS
1	D	491	VAL
1	D	492	LYS
1	D	496	GLU

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Mol	Chain	Res	Type
1	D	510	GLN
1	D	558	ASP
1	D	579	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	293	ASN
1	A	425	ASN
1	A	594	GLN
1	A	599	ASN
1	B	215	HIS
1	B	243	HIS
1	B	376	HIS
1	B	425	ASN
1	C	235	GLN
1	C	243	HIS
1	C	328	ASN
1	C	425	ASN
1	D	235	GLN
1	D	243	HIS
1	D	364	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	T8T	C	900	4	24,33,33	1.13	2 (8%)	30,52,52	2.30	8 (26%)
2	T8T	B	800	4	24,33,33	1.39	3 (12%)	30,52,52	2.27	8 (26%)
2	T8T	A	900	4	24,33,33	0.96	1 (4%)	30,52,52	2.25	9 (30%)
2	T8T	D	800	4	24,33,33	1.00	1 (4%)	30,52,52	1.87	7 (23%)
2	T8T	C	800	4	24,33,33	1.22	3 (12%)	30,52,52	1.84	8 (26%)
2	T8T	A	700	-	24,33,33	1.06	1 (4%)	30,52,52	2.17	11 (36%)
2	T8T	B	700	-	24,33,33	1.58	2 (8%)	30,52,52	2.24	10 (33%)
2	T8T	C	700	-	24,33,33	0.97	1 (4%)	30,52,52	2.03	9 (30%)
2	T8T	D	700	-	24,33,33	1.20	3 (12%)	30,52,52	1.95	7 (23%)
2	T8T	A	800	4	24,33,33	0.98	1 (4%)	30,52,52	2.53	12 (40%)
2	T8T	D	900	4	24,33,33	1.10	2 (8%)	30,52,52	2.36	10 (33%)
2	T8T	B	900	4	24,33,33	0.89	1 (4%)	30,52,52	1.69	7 (23%)

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
2	T8T	C	900	4	-	5/14/34/34	0/3/3/3
2	T8T	B	800	4	-	3/14/34/34	0/3/3/3
2	T8T	A	900	4	-	3/14/34/34	0/3/3/3
2	T8T	D	800	4	-	1/14/34/34	0/3/3/3
2	T8T	C	800	4	-	2/14/34/34	0/3/3/3
2	T8T	A	700	-	-	5/14/34/34	0/3/3/3
2	T8T	B	700	-	-	6/14/34/34	0/3/3/3
2	T8T	C	700	-	-	3/14/34/34	0/3/3/3
2	T8T	D	700	-	-	4/14/34/34	0/3/3/3
2	T8T	A	800	4	-	4/14/34/34	0/3/3/3
2	T8T	D	900	4	-	2/14/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	T8T	B	900	4	-	1/14/34/34	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	T8T	C6-C5	5.06	1.50	1.41
2	B	700	T8T	PA-O5'	4.22	1.64	1.57
2	D	700	T8T	C6-C5	3.78	1.47	1.41
2	C	900	T8T	C6-C5	3.73	1.47	1.41
2	B	800	T8T	PA-O5'	3.52	1.63	1.57
2	B	800	T8T	C6-C5	3.18	1.46	1.41
2	A	900	T8T	C6-C5	2.89	1.46	1.41
2	A	700	T8T	C6-C5	2.86	1.46	1.41
2	C	700	T8T	C6-C5	2.85	1.46	1.41
2	D	900	T8T	C6-C5	2.82	1.46	1.41
2	C	800	T8T	PA-O5'	2.77	1.62	1.57
2	C	800	T8T	C6-C5	2.61	1.45	1.41
2	B	900	T8T	C6-C5	2.60	1.45	1.41
2	C	900	T8T	C5-C4	2.55	1.47	1.40
2	C	800	T8T	C5-C4	2.34	1.47	1.40
2	D	700	T8T	C5-C4	2.31	1.47	1.40
2	D	800	T8T	C4-N3	-2.20	1.32	1.35
2	A	800	T8T	C6-N1	2.17	1.36	1.33
2	D	700	T8T	PA-O5'	2.10	1.61	1.57
2	D	900	T8T	C4-N3	-2.04	1.32	1.35
2	B	800	T8T	C4-N3	-2.01	1.32	1.35

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	T8T	C6-C5-C4	-6.41	114.68	120.80
2	A	800	T8T	N2-C2-N1	6.41	127.22	117.25
2	A	900	T8T	C2-N3-C4	6.24	122.48	115.36
2	D	900	T8T	C5-C6-N1	-5.82	115.47	123.43
2	A	800	T8T	C5-C6-N1	-5.45	115.98	123.43
2	D	700	T8T	C6-C5-C4	-5.40	115.64	120.80
2	B	800	T8T	C5-C6-N1	-5.12	116.43	123.43
2	A	800	T8T	N2-C2-N3	-5.11	109.47	117.79
2	C	800	T8T	C5-C6-N1	-5.11	116.44	123.43
2	B	800	T8T	N2-C2-N1	4.94	124.93	117.25
2	D	800	T8T	C6-C5-C4	-4.86	116.16	120.80
2	A	900	T8T	N3-C2-N1	-4.85	120.75	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	T8T	C6-C5-C4	-4.85	116.17	120.80
2	D	900	T8T	C6-N1-C2	4.72	123.42	115.93
2	A	700	T8T	C5-C6-N1	-4.68	117.03	123.43
2	B	700	T8T	PB-O3B-PG	-4.66	116.83	132.83
2	D	900	T8T	PB-O3B-PG	-4.61	116.99	132.83
2	B	800	T8T	N2-C2-N3	-4.60	110.29	117.79
2	A	900	T8T	C6-C5-C4	-4.57	116.43	120.80
2	B	800	T8T	C4-C5-N7	-4.53	104.68	109.40
2	A	700	T8T	C6-N1-C2	4.51	123.10	115.93
2	C	900	T8T	C2-N3-C4	4.51	120.51	115.36
2	C	800	T8T	C6-N1-C2	4.49	123.06	115.93
2	B	700	T8T	C4-C5-N7	-4.37	104.84	109.40
2	B	700	T8T	C6-C5-C4	-4.37	116.63	120.80
2	B	700	T8T	C2-N3-C4	4.35	120.33	115.36
2	B	700	T8T	C5-C6-N1	-4.35	117.49	123.43
2	C	900	T8T	C6-N1-C2	4.28	122.73	115.93
2	D	900	T8T	C2-N3-C4	4.27	120.23	115.36
2	C	700	T8T	C5-C6-N1	-4.13	117.78	123.43
2	B	800	T8T	C2-N3-C4	4.05	119.98	115.36
2	A	700	T8T	C6-C5-C4	-4.00	116.98	120.80
2	D	700	T8T	C2-N3-C4	3.86	119.77	115.36
2	C	800	T8T	C6-C5-C4	-3.83	117.14	120.80
2	D	700	T8T	C6-N1-C2	3.79	121.95	115.93
2	B	900	T8T	PB-O3B-PG	-3.79	119.82	132.83
2	C	900	T8T	N3-C2-N1	-3.71	122.28	127.22
2	C	900	T8T	PB-O3B-PG	-3.71	120.11	132.83
2	B	700	T8T	C6-N1-C2	3.70	121.81	115.93
2	A	900	T8T	C6-N1-C2	3.68	121.77	115.93
2	D	900	T8T	N3-C2-N1	-3.67	122.32	127.22
2	B	900	T8T	C5-C6-N1	-3.65	118.44	123.43
2	A	800	T8T	C6-N1-C2	3.63	121.69	115.93
2	D	700	T8T	PB-O3B-PG	-3.61	120.45	132.83
2	D	800	T8T	C2-N3-C4	3.57	119.43	115.36
2	D	700	T8T	C5-C6-N1	-3.55	118.58	123.43
2	A	800	T8T	C2-N3-C4	3.43	119.27	115.36
2	B	800	T8T	PB-O3B-PG	-3.42	121.08	132.83
2	A	700	T8T	PB-O3B-PG	-3.42	121.10	132.83
2	C	700	T8T	C6-N1-C2	3.34	121.23	115.93
2	A	800	T8T	O3'-C3'-C2'	-3.33	99.00	110.90
2	D	900	T8T	N2-C2-N1	3.33	122.42	117.25
2	A	700	T8T	N3-C2-N1	-3.26	122.88	127.22
2	C	900	T8T	C5-C6-N1	-3.12	119.17	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	T8T	N3-C2-N1	-3.11	123.07	127.22
2	C	900	T8T	O2G-PG-O3G	3.10	122.83	110.68
2	C	700	T8T	PB-O3B-PG	-3.00	122.54	132.83
2	A	700	T8T	O4'-C1'-C2'	2.97	111.85	106.25
2	D	800	T8T	PB-O3B-PG	-2.96	122.65	132.83
2	A	800	T8T	N3-C2-N1	-2.94	123.30	127.22
2	D	800	T8T	C4-C5-N7	-2.91	106.36	109.40
2	B	900	T8T	C6-N1-C2	2.91	120.55	115.93
2	C	700	T8T	O2G-PG-O1G	2.88	118.65	107.64
2	A	900	T8T	C5-C6-N1	-2.88	119.49	123.43
2	C	800	T8T	PB-O3B-PG	-2.86	123.00	132.83
2	C	700	T8T	C2-N3-C4	2.86	118.62	115.36
2	A	800	T8T	O2G-PG-O3B	-2.85	95.07	104.64
2	B	900	T8T	C2-N3-C4	2.83	118.58	115.36
2	D	900	T8T	C4-C5-N7	-2.81	106.47	109.40
2	D	900	T8T	C2'-C3'-C4'	2.81	108.61	102.76
2	C	700	T8T	PA-O5'-C5'	2.75	128.86	120.16
2	B	700	T8T	O2B-PB-O1B	2.73	125.74	112.24
2	A	900	T8T	PB-O3B-PG	-2.68	123.64	132.83
2	A	700	T8T	C2-N3-C4	2.67	118.41	115.36
2	B	800	T8T	O2G-PG-O3B	-2.62	95.83	104.64
2	A	700	T8T	O2B-PB-O1B	2.61	125.14	112.24
2	A	800	T8T	C4-C5-N7	-2.59	106.70	109.40
2	D	900	T8T	C6-C5-C4	-2.58	118.33	120.80
2	B	700	T8T	O3A-PA-O5'	2.56	110.52	101.37
2	A	800	T8T	C6-C5-C4	-2.53	118.38	120.80
2	C	700	T8T	O5'-C5'-C4'	-2.53	100.28	108.99
2	B	900	T8T	C4-C5-N7	-2.44	106.85	109.40
2	A	700	T8T	C2'-C1'-N9	-2.43	108.66	114.27
2	C	800	T8T	O4'-C1'-C2'	2.42	110.81	106.25
2	A	900	T8T	O2G-PG-O1G	2.41	116.86	107.64
2	B	800	T8T	C6-N1-C2	2.37	119.69	115.93
2	A	800	T8T	PB-O3B-PG	-2.35	124.75	132.83
2	C	800	T8T	C2'-C3'-C4'	2.35	107.66	102.76
2	B	900	T8T	C6-C5-C4	-2.35	118.56	120.80
2	C	700	T8T	O4'-C4'-C5'	-2.34	101.66	109.37
2	B	700	T8T	N3-C2-N1	-2.32	124.14	127.22
2	D	900	T8T	O4'-C4'-C5'	2.30	116.94	109.37
2	A	800	T8T	O2G-PG-O1G	2.25	116.22	107.64
2	D	800	T8T	O4'-C1'-C2'	2.24	110.47	106.25
2	C	800	T8T	N3-C2-N1	-2.20	124.29	127.22
2	D	800	T8T	O5'-PA-O2A	-2.19	106.35	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	T8T	C2'-C3'-C4'	2.16	107.27	102.76
2	C	900	T8T	O1G-PG-O3B	2.16	111.86	104.64
2	B	700	T8T	C2'-C1'-N9	-2.15	109.31	114.27
2	A	700	T8T	C2'-C3'-C4'	2.13	107.19	102.76
2	A	700	T8T	PA-O5'-C5'	2.13	126.88	120.16
2	B	900	T8T	O1G-PG-O3G	2.06	118.75	110.68
2	D	800	T8T	O2G-PG-O1G	2.06	115.50	107.64
2	A	900	T8T	C2'-C1'-N9	2.05	119.00	114.27
2	C	800	T8T	O3'-C3'-C2'	-2.03	103.63	110.90
2	D	700	T8T	N2-C2-N1	2.03	120.41	117.25

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	900	T8T	PB-O3B-PG-O1G
2	C	900	T8T	PB-O3B-PG-O2G
2	B	700	T8T	C3'-C4'-C5'-O5'
2	B	700	T8T	O4'-C4'-C5'-O5'
2	B	700	T8T	C4'-C5'-O5'-PA
2	D	700	T8T	C3'-C4'-C5'-O5'
2	D	700	T8T	O4'-C4'-C5'-O5'
2	A	700	T8T	C3'-C4'-C5'-O5'
2	B	700	T8T	C5'-O5'-PA-O2A
2	A	700	T8T	PB-O3B-PG-O3G
2	D	700	T8T	C4'-C5'-O5'-PA
2	C	800	T8T	PB-O3B-PG-O2G
2	A	700	T8T	PB-O3B-PG-O2G
2	A	700	T8T	O4'-C4'-C5'-O5'
2	C	700	T8T	C3'-C4'-C5'-O5'
2	B	900	T8T	C4'-C5'-O5'-PA
2	C	700	T8T	PA-O3A-PB-O2B
2	B	700	T8T	PB-O3B-PG-O3G
2	C	900	T8T	C4'-C5'-O5'-PA
2	C	700	T8T	C4'-C5'-O5'-PA
2	A	900	T8T	PG-O3B-PB-O2B
2	A	800	T8T	C5'-O5'-PA-O2A
2	D	900	T8T	C4'-C5'-O5'-PA
2	D	700	T8T	PA-O3A-PB-O2B
2	A	800	T8T	PB-O3B-PG-O3G
2	B	800	T8T	PB-O3B-PG-O2G
2	A	800	T8T	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
2	A	800	T8T	PB-O3B-PG-O2G
2	A	700	T8T	PA-O3A-PB-O2B
2	C	900	T8T	PG-O3B-PB-O1B
2	C	900	T8T	PG-O3B-PB-O2B
2	B	800	T8T	PG-O3B-PB-O2B
2	A	900	T8T	PG-O3B-PB-O1B
2	D	900	T8T	PG-O3B-PB-O2B
2	B	800	T8T	C5'-O5'-PA-O2A
2	A	900	T8T	C4'-C5'-O5'-PA
2	B	700	T8T	PB-O3A-PA-O2A
2	D	800	T8T	C5'-O5'-PA-O2A
2	C	800	T8T	C5'-O5'-PA-O2A

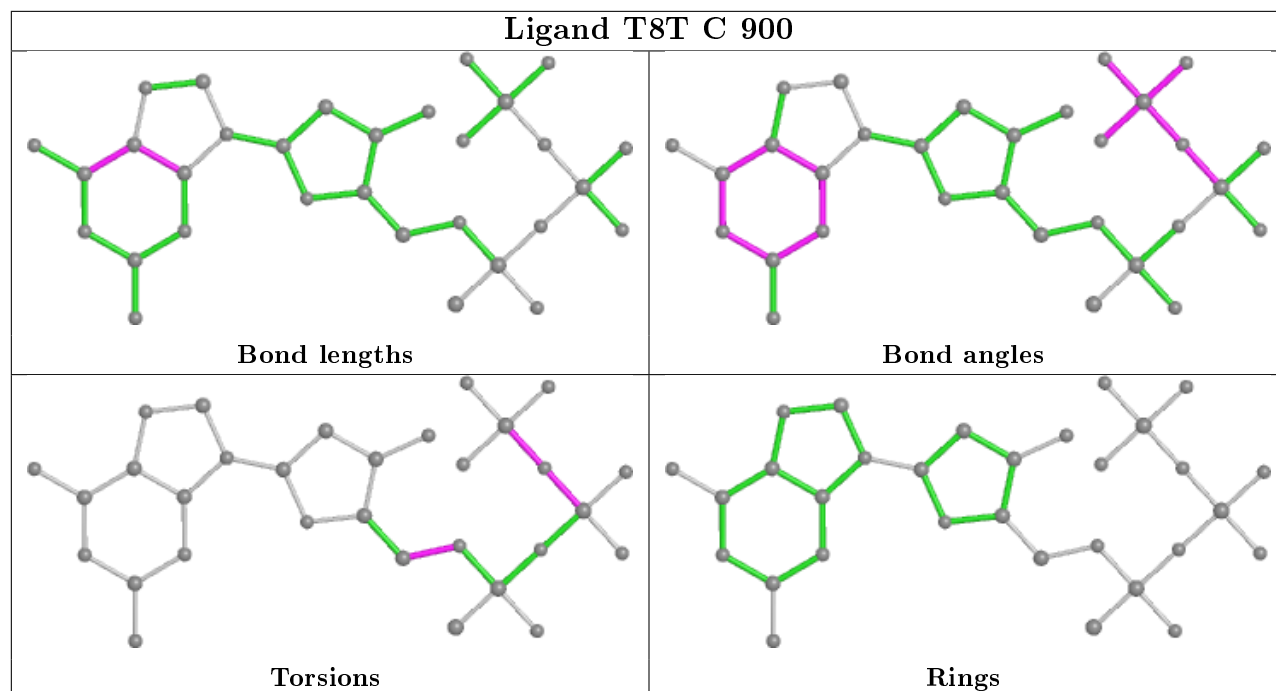
There are no ring outliers.

11 monomers are involved in 25 short contacts:

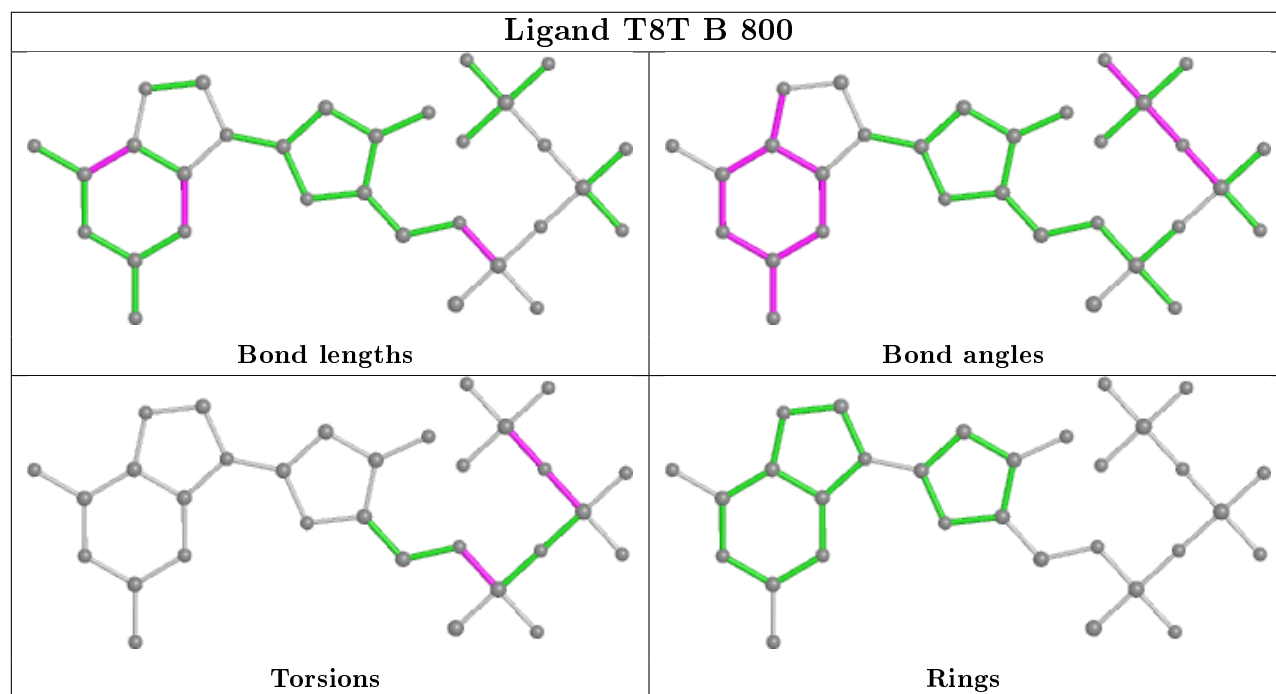
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	T8T	5	0
2	B	800	T8T	3	0
2	A	900	T8T	1	0
2	D	800	T8T	2	0
2	C	800	T8T	5	0
2	A	700	T8T	2	0
2	B	700	T8T	1	0
2	C	700	T8T	3	0
2	D	700	T8T	4	0
2	D	900	T8T	1	0
2	B	900	T8T	1	0

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.

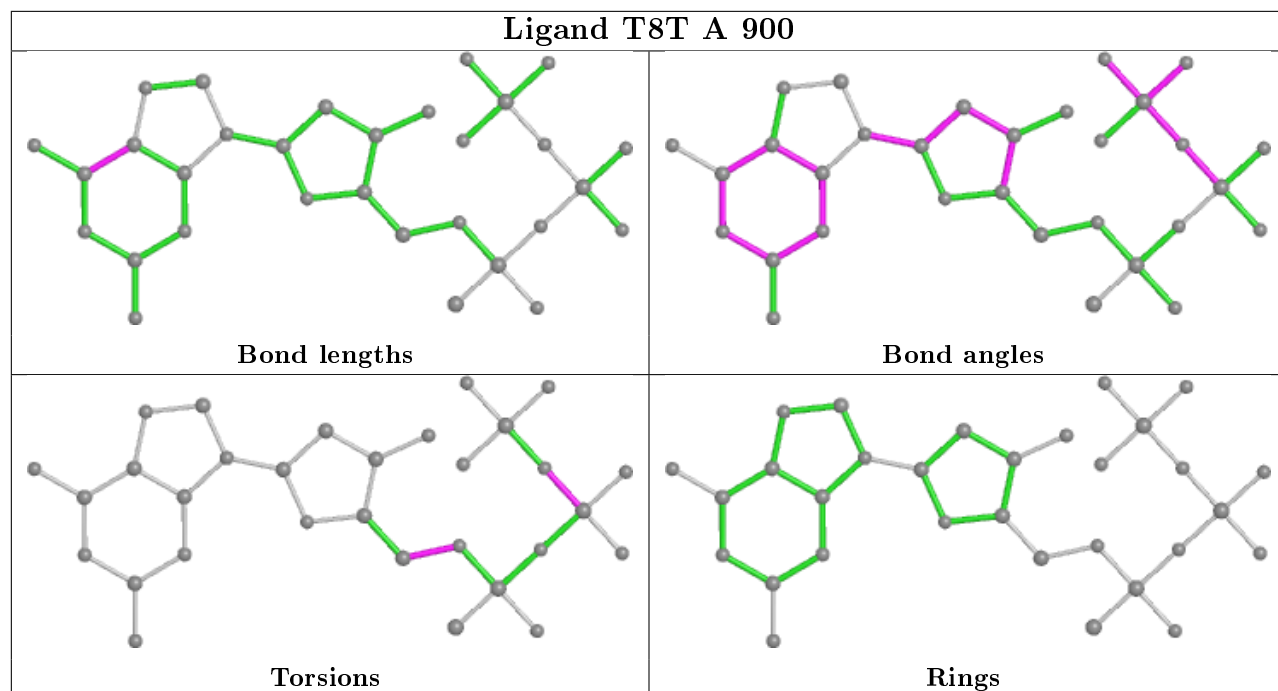
Ligand T8T C 900



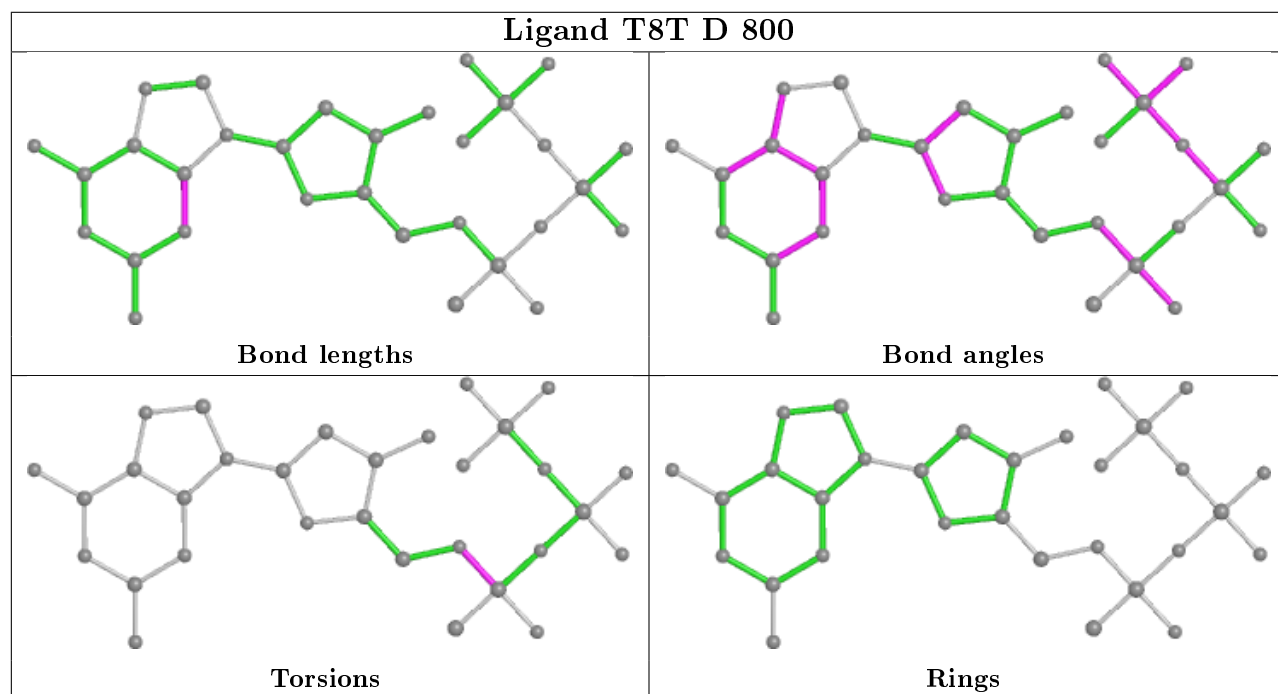
Ligand T8T B 800



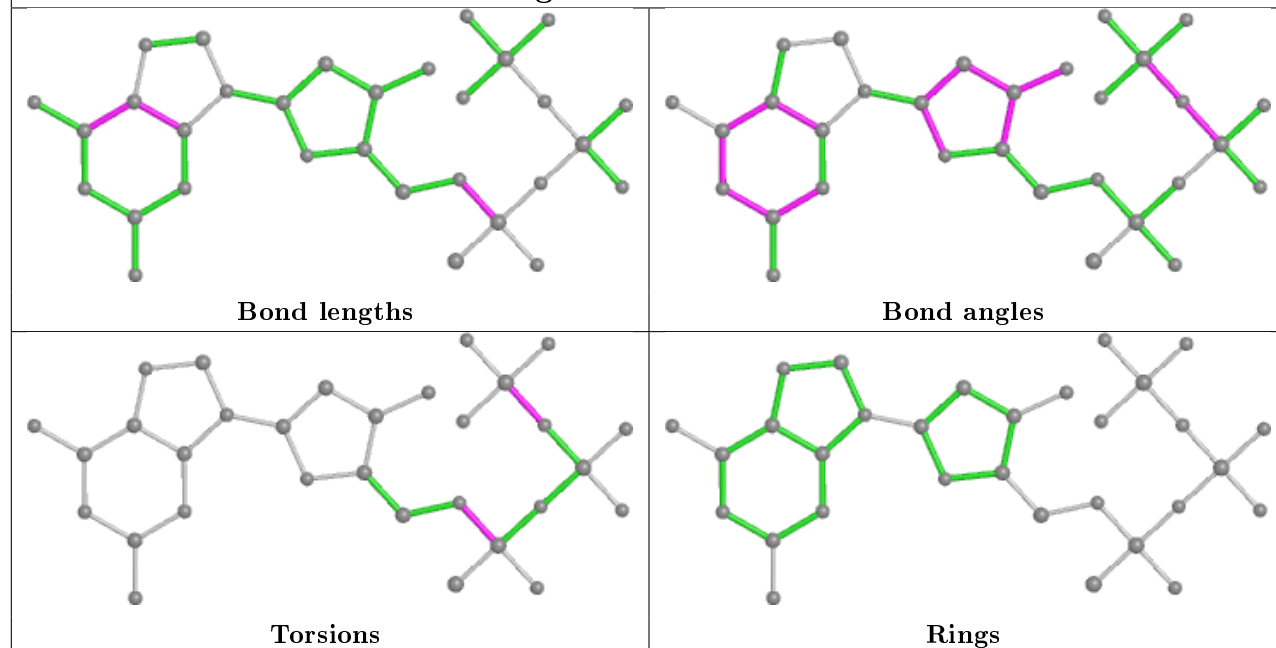
Ligand T8T A 900



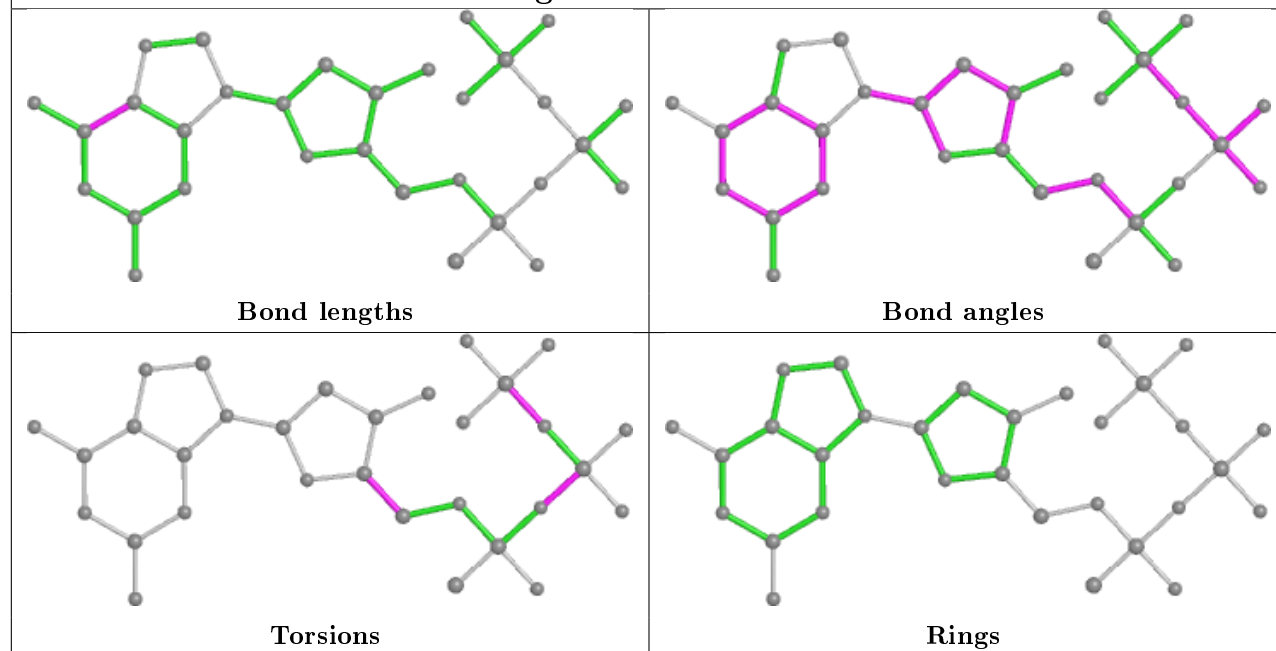
Ligand T8T D 800



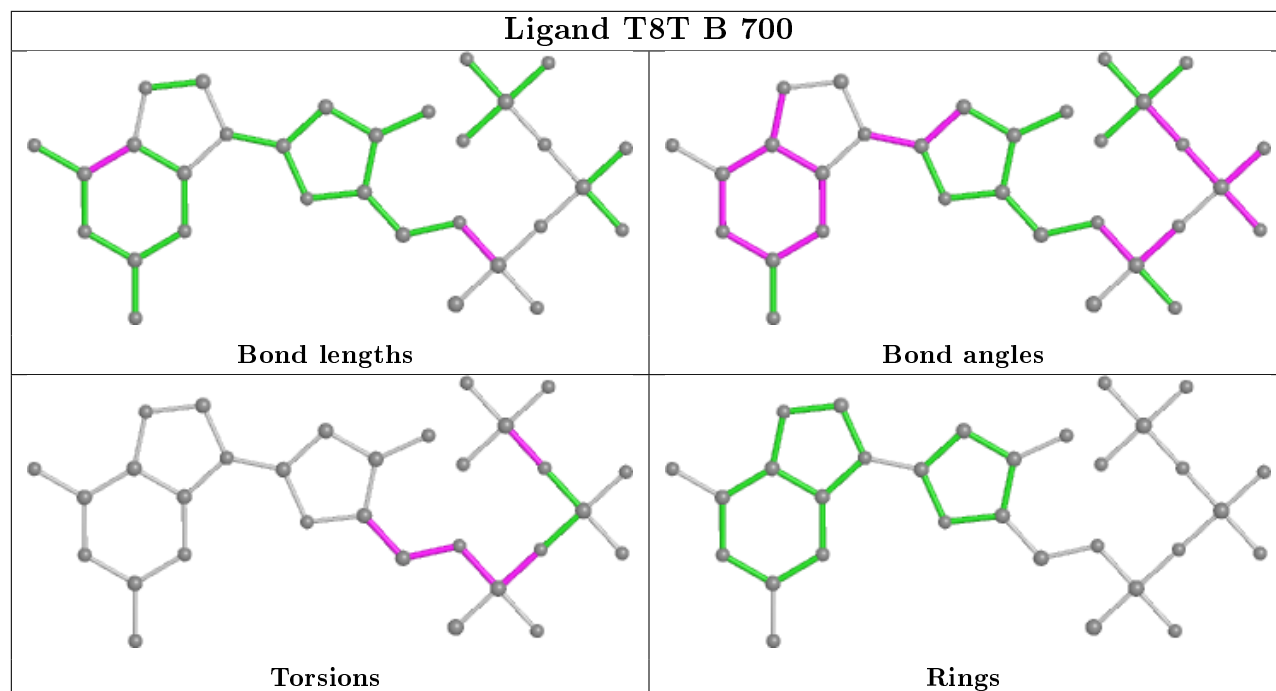
Ligand T8T C 800



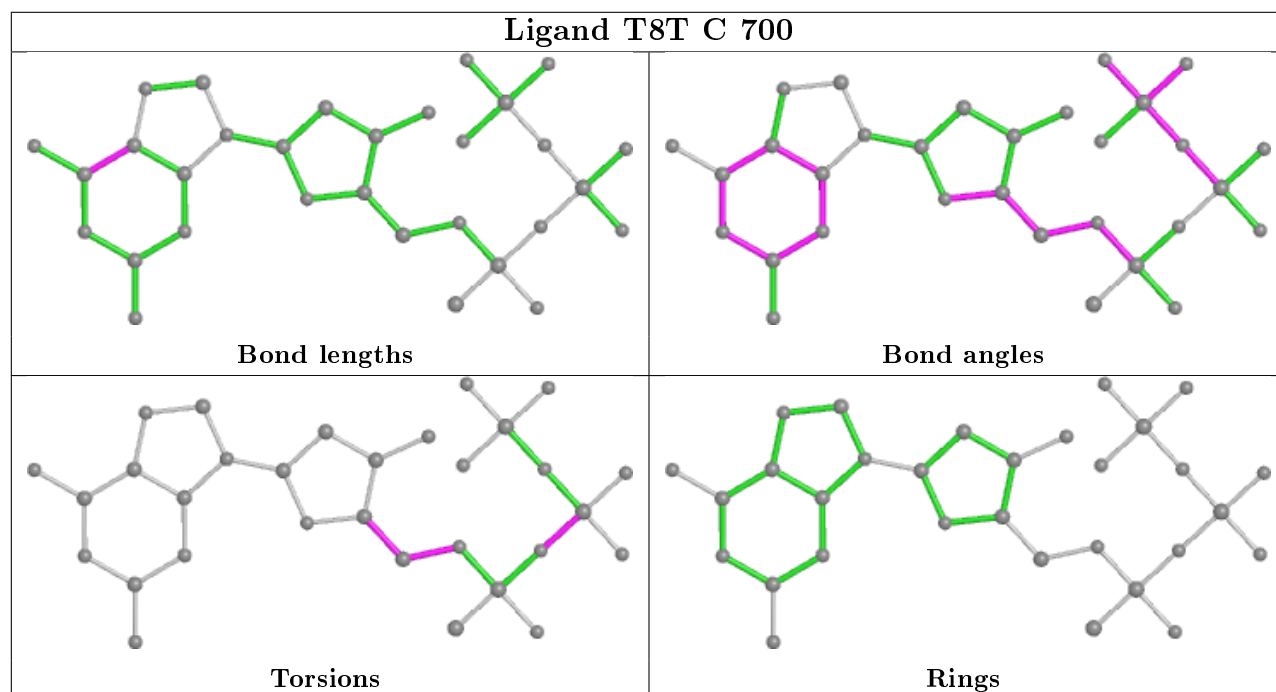
Ligand T8T A 700



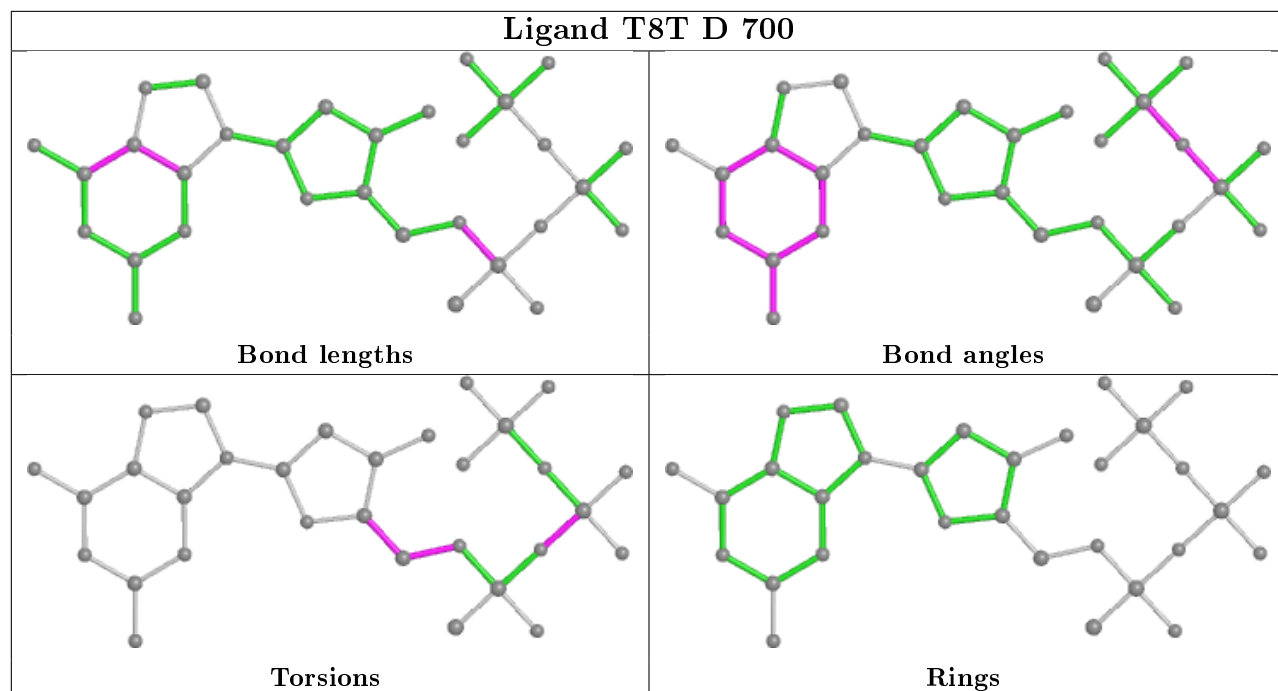
Ligand T8T B 700



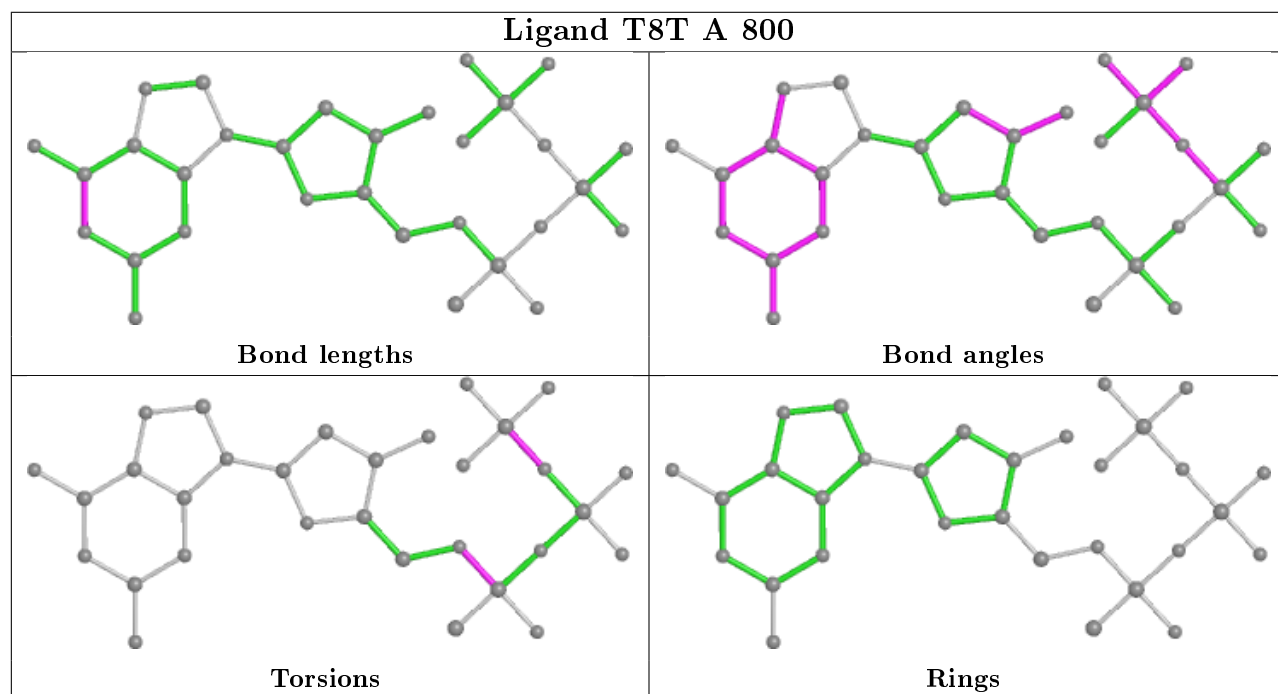
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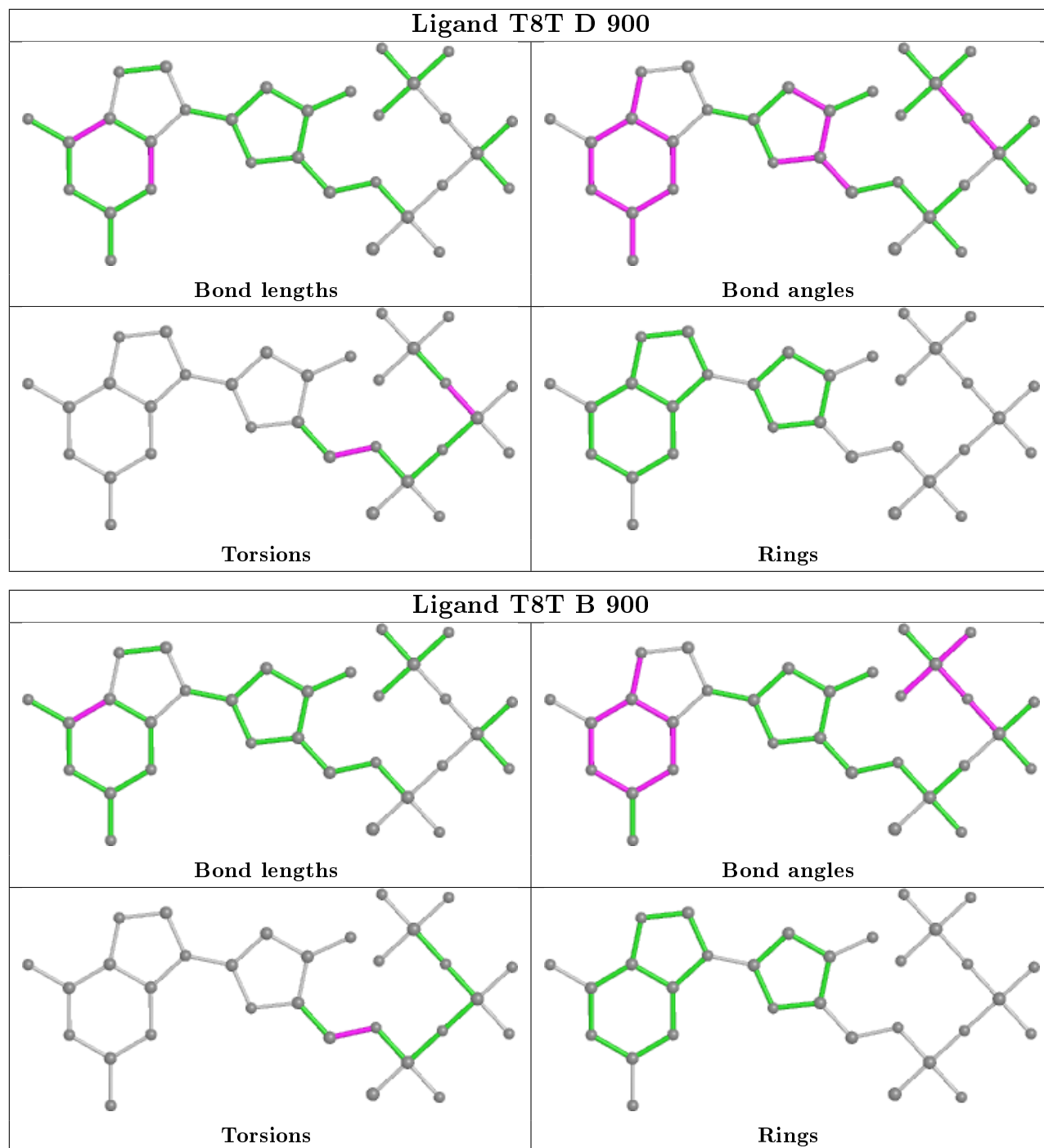


Ligand T8T D 700



Ligand T8T A 800





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	476/550 (86%)	0.26	22 (4%) 32 28	29, 53, 94, 127	0
1	B	477/550 (86%)	0.74	58 (12%) 4 2	40, 76, 117, 137	0
1	C	481/550 (87%)	0.34	33 (6%) 16 13	28, 56, 102, 140	0
1	D	470/550 (85%)	0.60	46 (9%) 7 5	39, 73, 108, 140	0
All	All	1904/2200 (86%)	0.48	159 (8%) 11 8	28, 65, 107, 140	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	490	ASP	9.2
1	B	488	LEU	6.9
1	B	491	VAL	6.4
1	A	345	ASN	5.7
1	D	412	ALA	5.5
1	B	486	LYS	5.4
1	A	490	ASP	5.0
1	D	274	GLY	5.0
1	B	345	ASN	5.0
1	B	571	GLN	4.9
1	B	489	LEU	4.9
1	C	489	LEU	4.9
1	B	465	GLN	4.6
1	B	585	ASP	4.5
1	B	575	ASP	4.5
1	A	344	ASP	4.4
1	B	293	ASN	4.4
1	C	594	GLN	4.2
1	B	592	THR	4.0
1	D	262	GLU	4.0
1	C	590	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	190	GLN	4.0
1	D	480	VAL	4.0
1	B	493	LEU	4.0
1	D	263	GLU	3.9
1	D	198	CYS	3.8
1	B	464	GLY	3.8
1	B	393	ALA	3.8
1	D	285	TRP	3.8
1	D	276	LEU	3.7
1	B	593	PRO	3.7
1	A	590	LEU	3.7
1	B	492	LYS	3.6
1	D	488	LEU	3.6
1	C	413	ILE	3.5
1	B	285	TRP	3.5
1	C	593	PRO	3.5
1	D	288	LYS	3.5
1	C	326	GLN	3.5
1	B	255	GLU	3.4
1	C	568	TYR	3.4
1	B	573	CYS	3.4
1	B	482	SER	3.4
1	B	562	LEU	3.4
1	C	587	ILE	3.3
1	B	344	ASP	3.3
1	B	590	LEU	3.3
1	C	491	VAL	3.3
1	C	255	GLU	3.3
1	D	599	ASN	3.3
1	B	348	ARG	3.3
1	B	485	PRO	3.3
1	A	488	LEU	3.3
1	C	561	SER	3.2
1	D	255	GLU	3.2
1	B	498	PHE	3.2
1	B	190	GLN	3.2
1	B	588	ALA	3.2
1	C	488	LEU	3.2
1	B	463	THR	3.2
1	B	414	ASP	3.2
1	B	572	TRP	3.2
1	B	556	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	346	GLU	3.1
1	C	493	LEU	3.1
1	C	329	PHE	3.0
1	B	594	GLN	3.0
1	D	326	GLN	3.0
1	C	327	ASN	3.0
1	C	596	LYS	3.0
1	A	593	PRO	2.9
1	B	487	VAL	2.9
1	D	572	TRP	2.9
1	D	345	ASN	2.9
1	C	598	TRP	2.9
1	C	277	GLU	2.9
1	B	408	ARG	2.9
1	C	599	ASN	2.8
1	B	397	ILE	2.8
1	B	259	LEU	2.8
1	B	484	LYS	2.8
1	D	398	GLU	2.8
1	A	434	THR	2.8
1	B	490	ASP	2.8
1	D	485	PRO	2.8
1	C	276	LEU	2.7
1	C	401	GLY	2.7
1	B	260	ILE	2.7
1	D	585	ASP	2.7
1	D	327	ASN	2.7
1	D	230	LYS	2.7
1	D	486	LYS	2.7
1	A	522	CYS	2.6
1	C	487	VAL	2.6
1	D	583	ASP	2.6
1	D	477	PRO	2.6
1	D	461	GLN	2.6
1	B	473	TYR	2.6
1	B	587	ILE	2.6
1	A	487	VAL	2.5
1	B	256	GLN	2.5
1	A	441	ALA	2.5
1	C	562	LEU	2.5
1	D	260	ILE	2.5
1	D	563	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	397	ILE	2.5
1	B	440	ASP	2.5
1	B	563	TYR	2.4
1	C	586	VAL	2.4
1	B	574	ALA	2.4
1	A	486	LYS	2.4
1	B	496	GLU	2.4
1	B	262	GLU	2.4
1	B	554	CYS	2.4
1	D	475	SER	2.4
1	A	530	ILE	2.4
1	D	509	MET	2.3
1	D	251	LYS	2.3
1	D	498	PHE	2.3
1	D	569	PHE	2.3
1	C	400	THR	2.3
1	D	284	LEU	2.3
1	C	437	LYS	2.3
1	D	275	PRO	2.2
1	B	598	TRP	2.2
1	A	343	VAL	2.2
1	B	497	ASP	2.2
1	C	591	ILE	2.2
1	D	239	MET	2.2
1	A	489	LEU	2.2
1	D	590	LEU	2.2
1	D	524	THR	2.2
1	D	259	LEU	2.2
1	D	350	CYS	2.2
1	D	400	THR	2.2
1	A	347	LEU	2.2
1	D	497	ASP	2.2
1	A	495	ALA	2.2
1	D	496	GLU	2.1
1	C	266	CYS	2.1
1	D	535	ASN	2.1
1	B	439	LYS	2.1
1	A	591	ILE	2.1
1	D	473	TYR	2.1
1	A	403	GLY	2.1
1	C	559	ARG	2.1
1	B	567	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	476	LEU	2.0
1	B	474	GLU	2.0
1	C	328	ASN	2.0
1	D	514	PRO	2.0
1	A	284	LEU	2.0
1	B	195	ASP	2.0
1	A	402	ALA	2.0
1	D	348	ARG	2.0
1	A	295	SER	2.0
1	D	250	ILE	2.0
1	C	330	ASP	2.0
1	B	483	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	T8T	B	700	31/31	0.93	0.18	59,69,80,85	0
2	T8T	D	700	31/31	0.94	0.15	63,72,80,88	0
2	T8T	A	700	31/31	0.96	0.12	36,41,62,73	0
2	T8T	C	700	31/31	0.97	0.12	42,46,51,59	0
2	T8T	A	900	31/31	0.97	0.13	27,29,31,31	0
4	MG	B	950	1/1	0.97	0.11	36,36,36,36	0
2	T8T	C	800	31/31	0.98	0.11	30,32,36,37	0
2	T8T	D	800	31/31	0.98	0.13	39,43,49,55	0
2	T8T	B	900	31/31	0.98	0.11	36,40,46,47	0
2	T8T	C	900	31/31	0.99	0.10	36,39,41,42	0
2	T8T	B	800	31/31	0.99	0.11	37,40,48,48	0

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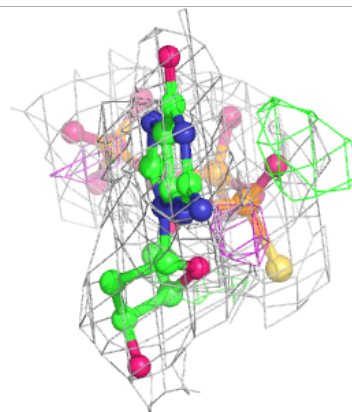
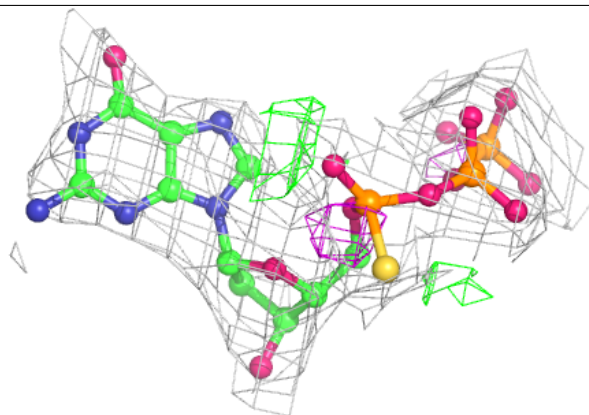
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	C	950	1/1	0.99	0.10	28,28,28,28	0
4	MG	A	950	1/1	0.99	0.10	25,25,25,25	0
2	T8T	A	800	31/31	0.99	0.13	23,24,25,26	0
3	MN	C	750	1/1	0.99	0.16	25,25,25,25	0
2	T8T	D	900	31/31	0.99	0.10	36,38,42,43	0
4	MG	D	950	1/1	0.99	0.09	34,34,34,34	0
3	MN	B	750	1/1	0.99	0.15	51,51,51,51	0
3	MN	D	750	1/1	1.00	0.15	43,43,43,43	0
3	MN	A	750	1/1	1.00	0.16	25,25,25,25	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.

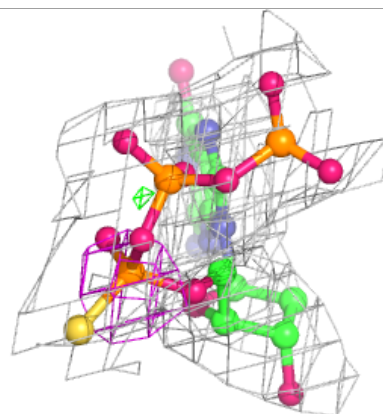
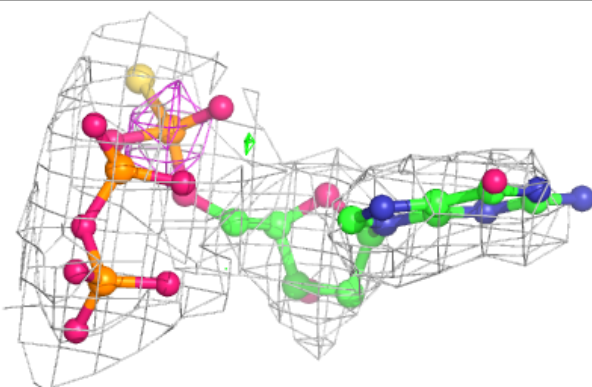
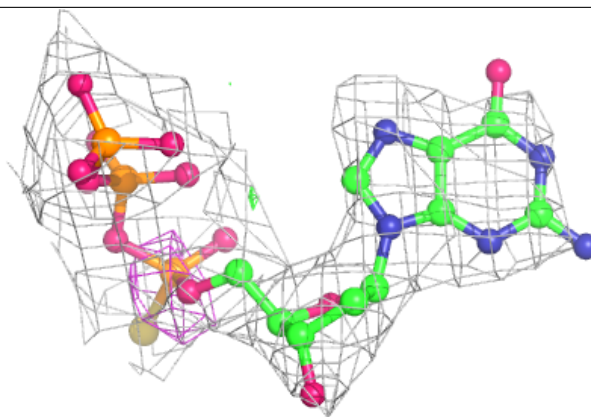
Electron density around T8T B 700:

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

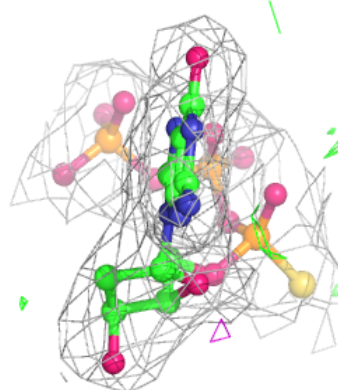
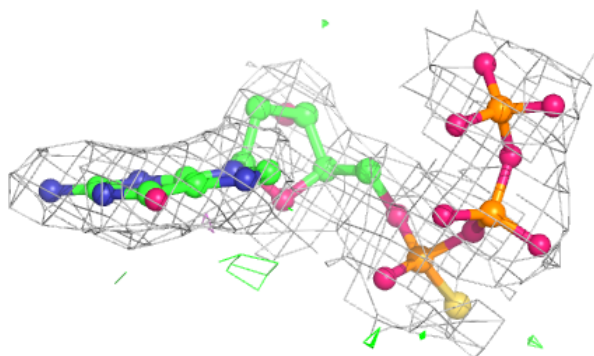
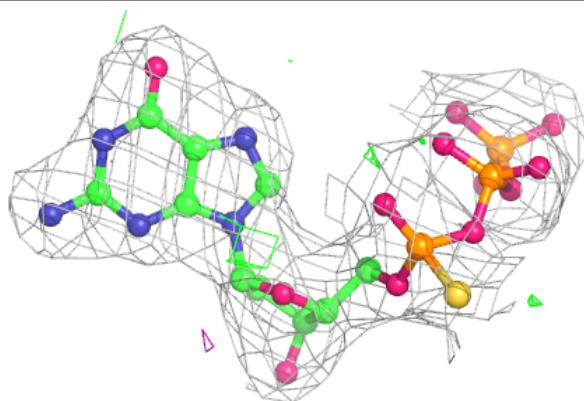


Electron density around T8T D 700:

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

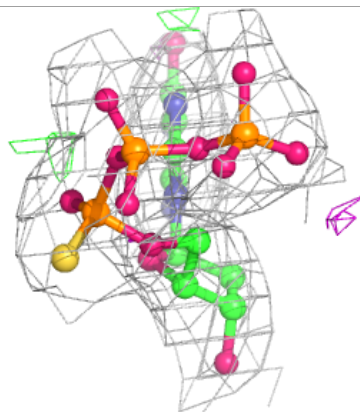
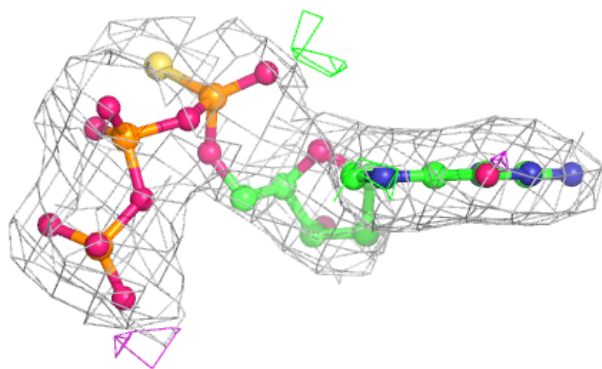
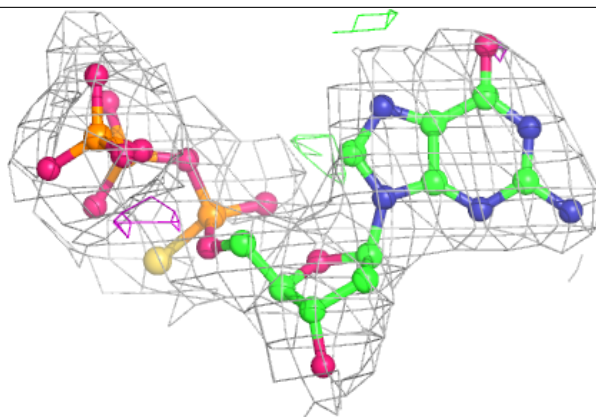
**Electron density around T8T A 700:**

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

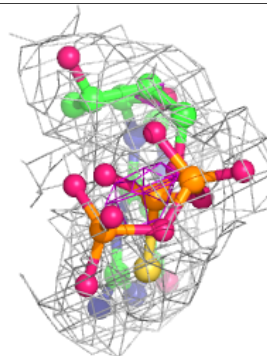
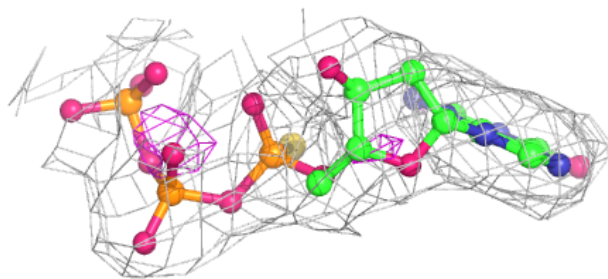
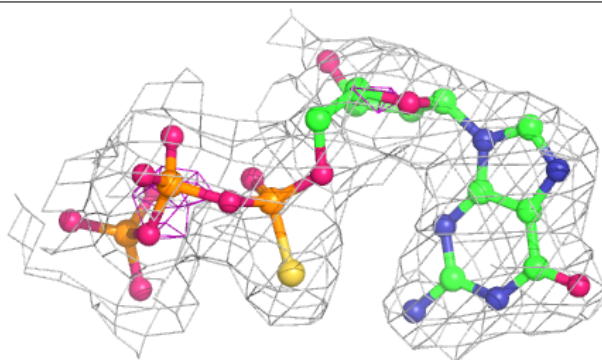


Electron density around T8T C 700:

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

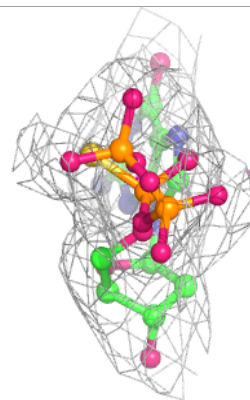
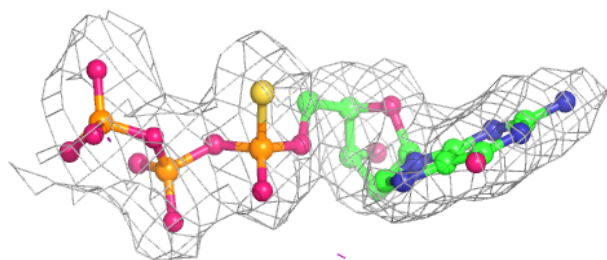
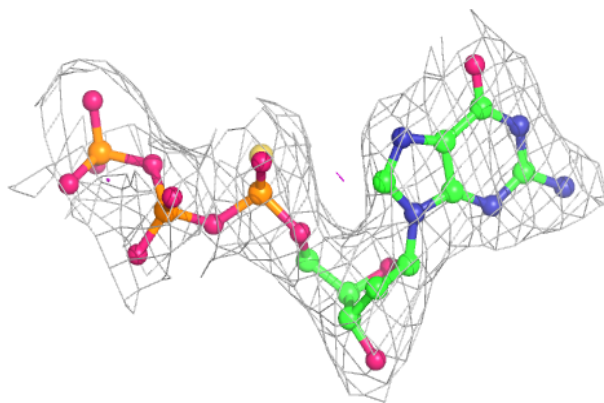
**Electron density around T8T A 900:**

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

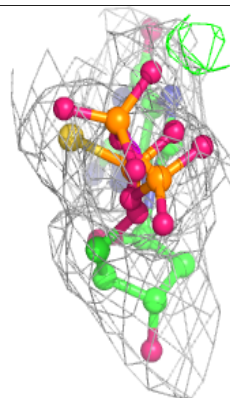
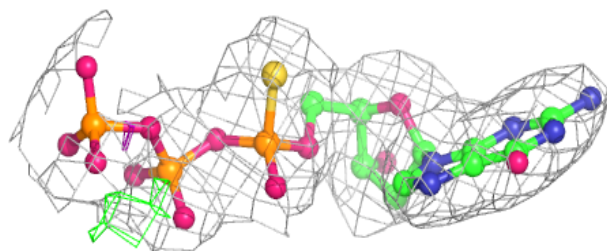
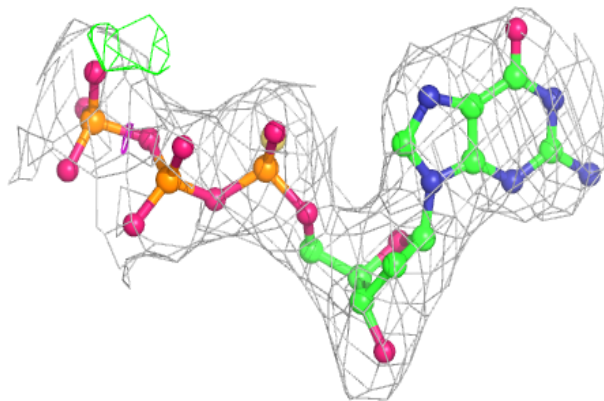


Electron density around T8T C 800:

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

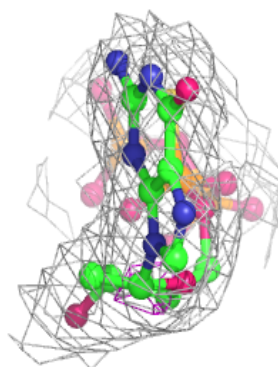
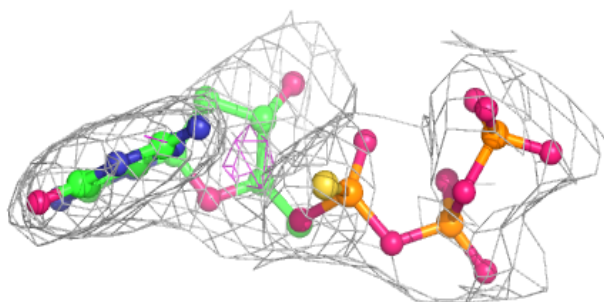
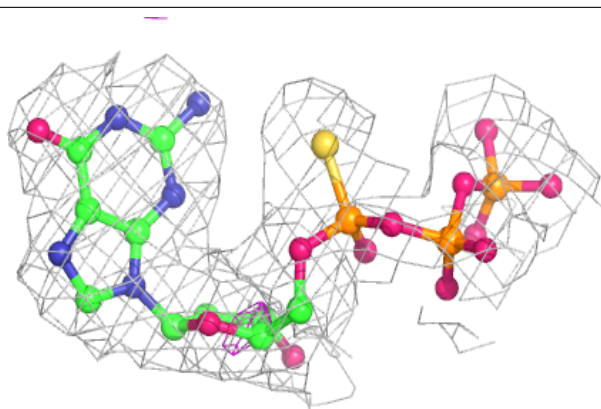
**Electron density around T8T D 800:**

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

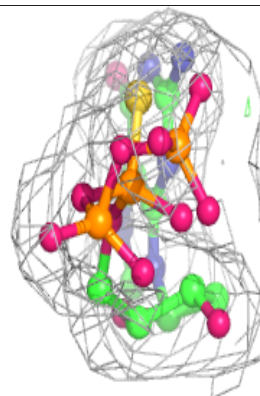
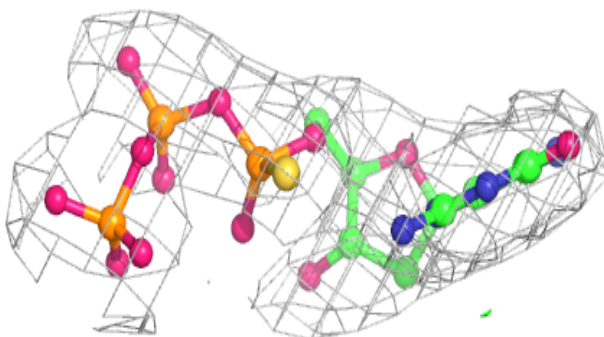
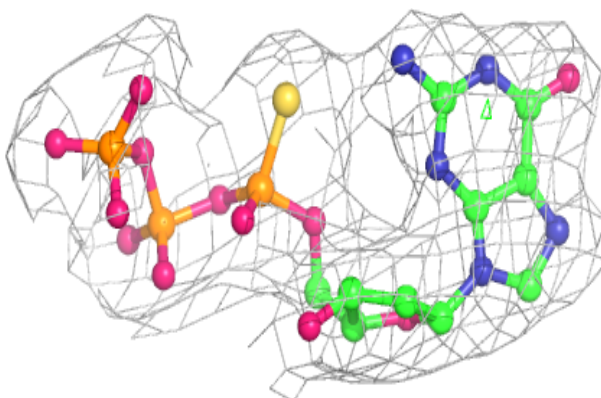


Electron density around T8T B 900:

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and green (positive)

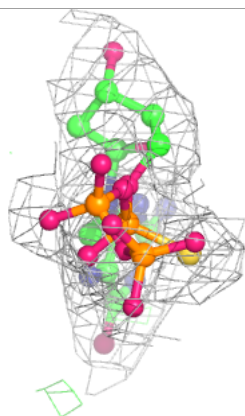
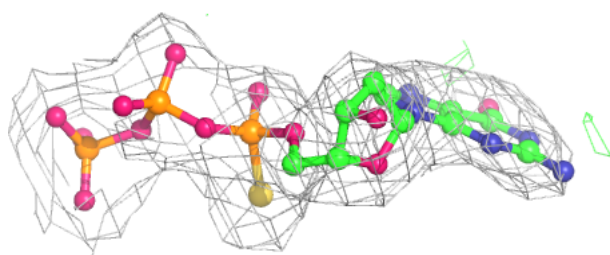
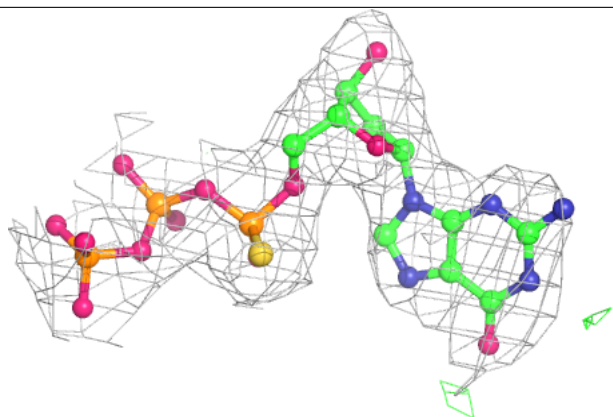
**Electron density around T8T C 900:**

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

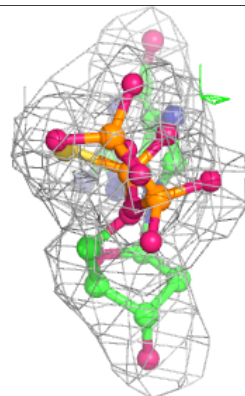
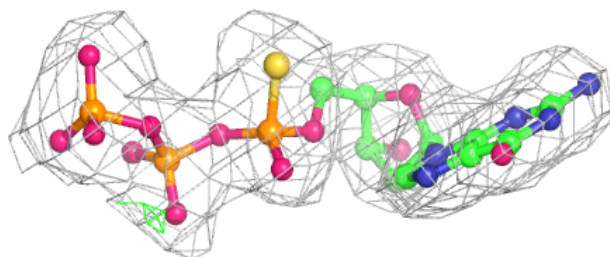
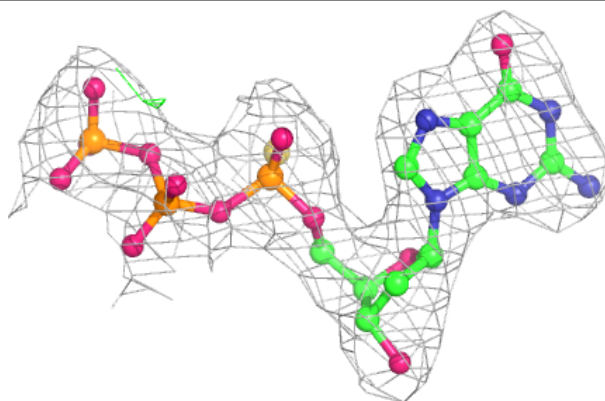


Electron density around T8T B 800:

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

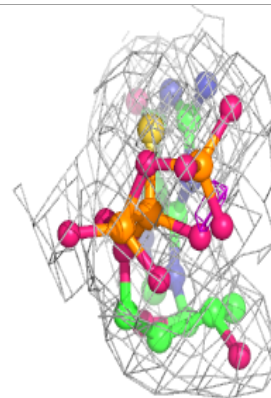
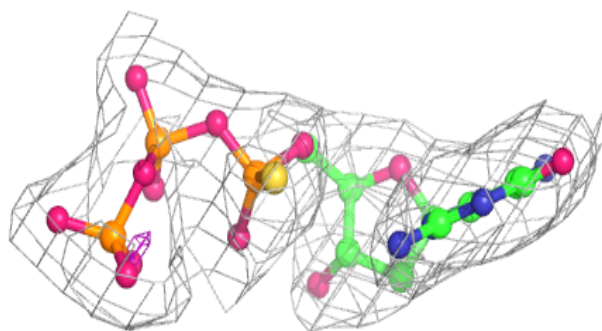
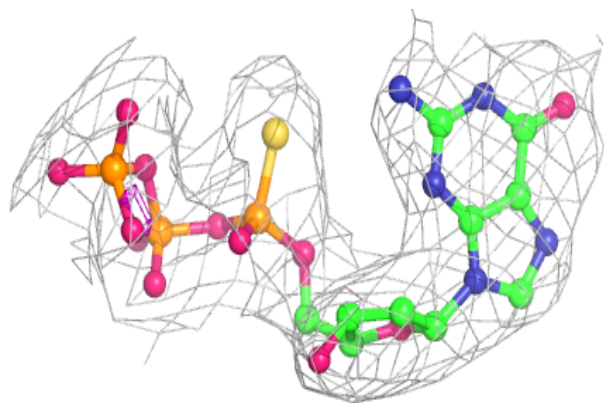
**Electron density around T8T A 800:**

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



Electron density around T8T D 900:

$2mF_o-DF_c$ (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.