



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2021 – 04:06 PM EDT

PDB ID : 6U6Y
Title : Human SAMHD1 bound to ribo(CGCCU)-oligonucleotide
Authors : Taylor, A.B.; Bhattacharya, A.; Wang, Z.; Ivanov, D.N.
Deposited on : 2019-08-30
Resolution : 2.47 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.1
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) : 2.23.1

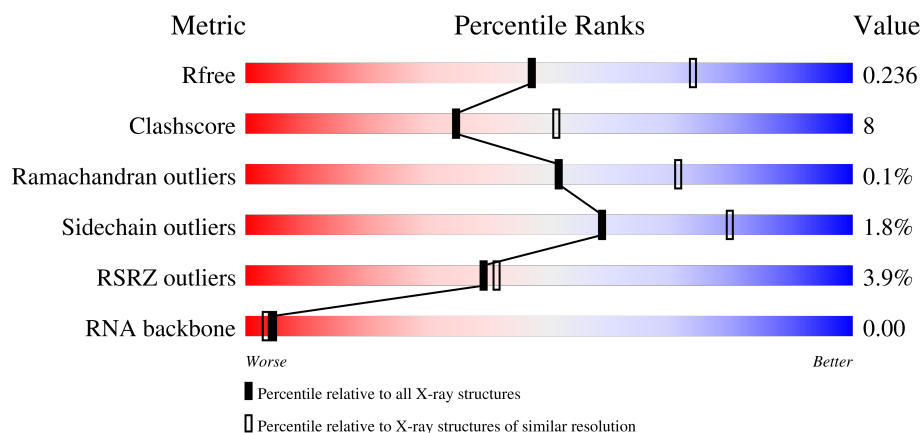
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)
RNA backbone	3102	1002 (2.82-2.14)

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

Mol	Chain	Length	Quality of chain
1	A	533	<div> <div>3%</div> <div>70% 11% 19%</div> </div>
1	B	533	<div> <div>4%</div> <div>65% 16% 18%</div> </div>
1	C	533	<div> <div>3%</div> <div>67% 14% 19%</div> </div>
1	D	533	<div> <div>3%</div> <div>65% 15% 19%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	5	
2	F	5	
2	G	5	
2	H	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTP	C	702	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14671 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 triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3559	2283	623	634	19			
1	B	437	Total	C	N	O	S	0	0	0
			3572	2287	623	643	19			
1	C	431	Total	C	N	O	S	0	1	0
			3529	2265	614	631	19			
1	D	430	Total	C	N	O	S	0	0	0
			3513	2250	611	633	19			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	-	initiating methionine	UNP Q9Y3Z3
A	95	TRP	-	expression tag	UNP Q9Y3Z3
A	96	SER	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	PRO	-	expression tag	UNP Q9Y3Z3
A	99	GLN	-	expression tag	UNP Q9Y3Z3
A	100	PHE	-	expression tag	UNP Q9Y3Z3
A	101	GLU	-	expression tag	UNP Q9Y3Z3
A	102	LYS	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	SER	-	expression tag	UNP Q9Y3Z3
A	105	GLY	-	expression tag	UNP Q9Y3Z3
A	106	SER	-	expression tag	UNP Q9Y3Z3
A	107	GLU	-	expression tag	UNP Q9Y3Z3
A	108	ASN	-	expression tag	UNP Q9Y3Z3
A	109	LEU	-	expression tag	UNP Q9Y3Z3
A	110	TYR	-	expression tag	UNP Q9Y3Z3
A	111	PHE	-	expression tag	UNP Q9Y3Z3
A	112	GLN	-	expression tag	UNP Q9Y3Z3
A	113	GLY	-	expression tag	UNP Q9Y3Z3
A	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	94	MET	-	initiating methionine	UNP Q9Y3Z3
B	95	TRP	-	expression tag	UNP Q9Y3Z3
B	96	SER	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	PRO	-	expression tag	UNP Q9Y3Z3
B	99	GLN	-	expression tag	UNP Q9Y3Z3
B	100	PHE	-	expression tag	UNP Q9Y3Z3
B	101	GLU	-	expression tag	UNP Q9Y3Z3
B	102	LYS	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	SER	-	expression tag	UNP Q9Y3Z3
B	105	GLY	-	expression tag	UNP Q9Y3Z3
B	106	SER	-	expression tag	UNP Q9Y3Z3
B	107	GLU	-	expression tag	UNP Q9Y3Z3
B	108	ASN	-	expression tag	UNP Q9Y3Z3
B	109	LEU	-	expression tag	UNP Q9Y3Z3
B	110	TYR	-	expression tag	UNP Q9Y3Z3
B	111	PHE	-	expression tag	UNP Q9Y3Z3
B	112	GLN	-	expression tag	UNP Q9Y3Z3
B	113	GLY	-	expression tag	UNP Q9Y3Z3
B	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3
C	94	MET	-	initiating methionine	UNP Q9Y3Z3
C	95	TRP	-	expression tag	UNP Q9Y3Z3
C	96	SER	-	expression tag	UNP Q9Y3Z3
C	97	HIS	-	expression tag	UNP Q9Y3Z3
C	98	PRO	-	expression tag	UNP Q9Y3Z3
C	99	GLN	-	expression tag	UNP Q9Y3Z3
C	100	PHE	-	expression tag	UNP Q9Y3Z3
C	101	GLU	-	expression tag	UNP Q9Y3Z3
C	102	LYS	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	SER	-	expression tag	UNP Q9Y3Z3
C	105	GLY	-	expression tag	UNP Q9Y3Z3
C	106	SER	-	expression tag	UNP Q9Y3Z3
C	107	GLU	-	expression tag	UNP Q9Y3Z3
C	108	ASN	-	expression tag	UNP Q9Y3Z3
C	109	LEU	-	expression tag	UNP Q9Y3Z3
C	110	TYR	-	expression tag	UNP Q9Y3Z3
C	111	PHE	-	expression tag	UNP Q9Y3Z3
C	112	GLN	-	expression tag	UNP Q9Y3Z3
C	113	GLY	-	expression tag	UNP Q9Y3Z3
C	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	MET	-	initiating methionine	UNP Q9Y3Z3
D	95	TRP	-	expression tag	UNP Q9Y3Z3
D	96	SER	-	expression tag	UNP Q9Y3Z3
D	97	HIS	-	expression tag	UNP Q9Y3Z3
D	98	PRO	-	expression tag	UNP Q9Y3Z3
D	99	GLN	-	expression tag	UNP Q9Y3Z3
D	100	PHE	-	expression tag	UNP Q9Y3Z3
D	101	GLU	-	expression tag	UNP Q9Y3Z3
D	102	LYS	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	SER	-	expression tag	UNP Q9Y3Z3
D	105	GLY	-	expression tag	UNP Q9Y3Z3
D	106	SER	-	expression tag	UNP Q9Y3Z3
D	107	GLU	-	expression tag	UNP Q9Y3Z3
D	108	ASN	-	expression tag	UNP Q9Y3Z3
D	109	LEU	-	expression tag	UNP Q9Y3Z3
D	110	TYR	-	expression tag	UNP Q9Y3Z3
D	111	PHE	-	expression tag	UNP Q9Y3Z3
D	112	GLN	-	expression tag	UNP Q9Y3Z3
D	113	GLY	-	expression tag	UNP Q9Y3Z3
D	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is a RNA chain called RNA CGCCU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			62	27	11	21	3			
2	G	3	Total	C	N	O	P	0	0	0
			42	19	5	16	2			
2	F	4	Total	C	N	O	P	0	0	0
			46	19	5	19	3			
2	H	4	Total	C	N	O	P	0	0	0
			47	19	6	19	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

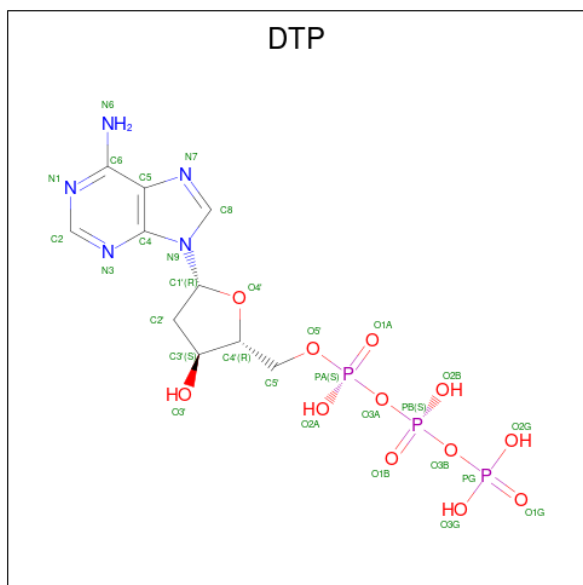
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	52	Total	O	0	0
			52	52		
5	C	61	Total	O	0	0
			61	61		
5	D	46	Total	O	0	0
			46	46		

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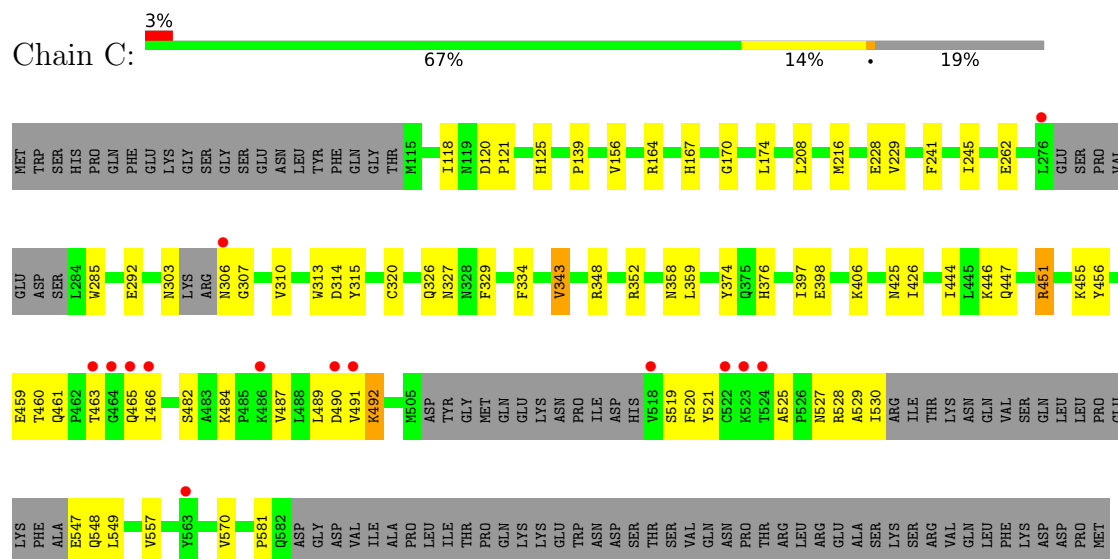
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	O	0	0
			2	2		
5	G	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		

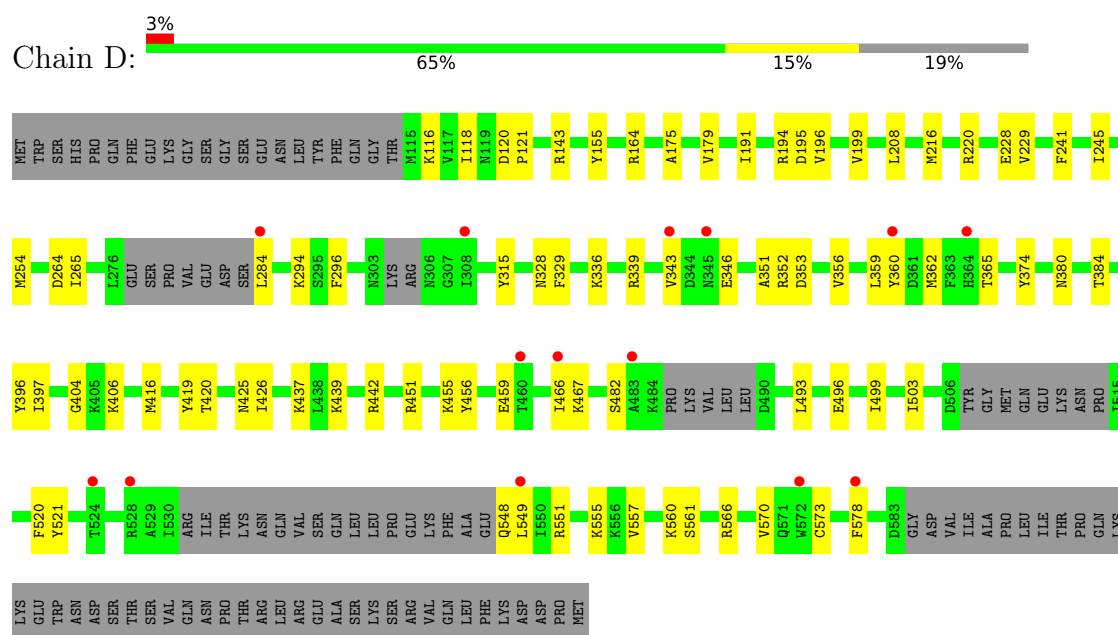
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



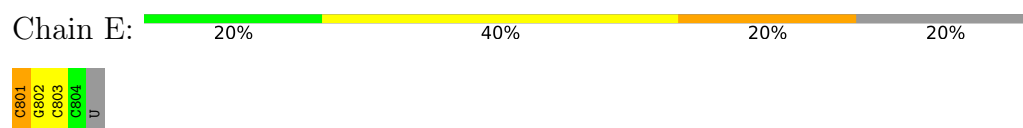
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



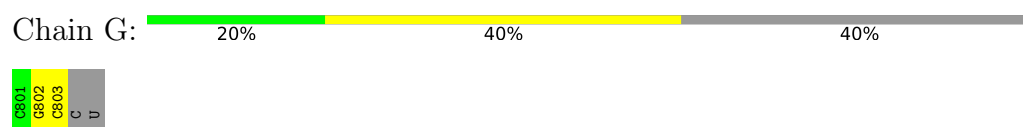
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 2: RNA CGCCU

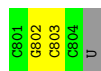


- Molecule 2: RNA CGCCU



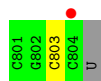
- Molecule 2: RNA CGCCU

Chain F:  40% 40% 20%



- Molecule 2: RNA CGCCU

Chain H:  20% 60% 20% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.34Å 183.62Å 81.56Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	75.96 – 2.47 75.96 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.96-2.47) 99.9 (75.96-2.47)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.180 , 0.235 0.180 , 0.236	Depositor DCC
R_{free} test set	3816 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14671	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DTP

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	0.45	0/3643	0.59	0/4912
1	B	0.43	0/3655	0.57	0/4929
1	C	0.50	0/3611	0.61	0/4869
1	D	0.43	0/3593	0.57	0/4843
2	E	0.48	0/68	1.12	0/105
2	F	0.45	0/50	0.90	0/77
2	G	0.67	0/46	1.41	0/70
2	H	0.41	0/51	1.03	0/79
All	All	0.45	0/14717	0.60	0/19884

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	3559	0	3544	49	0
1	B	3572	0	3546	68	0
1	C	3529	0	3510	61	0
1	D	3513	0	3476	59	0
2	E	62	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	46	0	20	1	0
2	G	42	0	21	3	0
2	H	47	0	21	0	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
4	A	22	0	12	3	0
4	B	22	0	12	4	0
4	C	22	0	12	6	0
4	D	22	0	12	5	0
5	A	46	0	0	1	0
5	B	52	0	0	0	0
5	C	61	0	0	0	0
5	D	46	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
All	All	14671	0	14216	237	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 8.

The worst 5 of 237 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:A:466:ILE:HD11	1:A:576:ARG:HH22	1.29	0.94
1:C:484:LYS:HZ1	1:C:492:LYS:HD2	1.35	0.91
1:C:527:ASN:H	1:C:528:ARG:HH11	1.16	0.90
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.58	0.85
1:A:466:ILE:HD11	1:A:576:ARG:NH2	1.91	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/533 (80%)	421 (99%)	6 (1%)	0	100	100
1	B	429/533 (80%)	424 (99%)	5 (1%)	0	100	100
1	C	422/533 (79%)	408 (97%)	13 (3%)	1 (0%)	47	66
1	D	418/533 (78%)	410 (98%)	8 (2%)	0	100	100
All	All	1696/2132 (80%)	1663 (98%)	32 (2%)	1 (0%)	51	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	466	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/474 (81%)	377 (98%)	7 (2%)	59	80
1	B	386/474 (81%)	376 (97%)	10 (3%)	46	70
1	C	381/474 (80%)	374 (98%)	7 (2%)	59	80
1	D	379/474 (80%)	376 (99%)	3 (1%)	81	92
All	All	1530/1896 (81%)	1503 (98%)	27 (2%)	59	80

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	553	TYR
1	C	125	HIS
1	D	284	LEU
1	B	582	GLN
1	C	262	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	ASN
1	C	358	ASN
1	D	119	ASN
1	D	548	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	2/5 (40%)	1 (50%)	2 (100%)
2	F	1/5 (20%)	1 (100%)	0
2	G	1/5 (20%)	1 (100%)	0
2	H	1/5 (20%)	1 (100%)	0
All	All	5/20 (25%)	4 (80%)	2 (40%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	803	C
2	G	803	C
2	F	803	C
2	H	803	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	801	C
2	E	803	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
4	DTP	D	702	-	22,24,32	0.92	1 (4%)	24,36,50	1.05	3 (12%)
4	DTP	A	702	-	22,24,32	0.65	0	24,36,50	1.04	2 (8%)
4	DTP	C	702	-	22,24,32	0.66	0	24,36,50	0.99	2 (8%)
4	DTP	B	702	-	22,24,32	0.90	1 (4%)	24,36,50	1.08	3 (12%)

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
4	DTP	D	702	-	-	0/6/22/34	0/3/3/3
4	DTP	A	702	-	-	0/6/22/34	0/3/3/3
4	DTP	C	702	-	-	2/6/22/34	0/3/3/3
4	DTP	B	702	-	-	1/6/22/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	DTP	PA-O1A	3.30	1.61	1.50
4	B	702	DTP	PA-O1A	3.19	1.60	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	DTP	O3A-PA-O2A	2.74	118.09	107.64
4	B	702	DTP	O3A-PA-O2A	2.69	117.92	107.64
4	B	702	DTP	O5'-PA-O1A	-2.67	98.97	106.47
4	D	702	DTP	C5-C6-N6	2.49	124.13	120.35
4	C	702	DTP	O3A-PA-O5'	-2.42	100.29	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

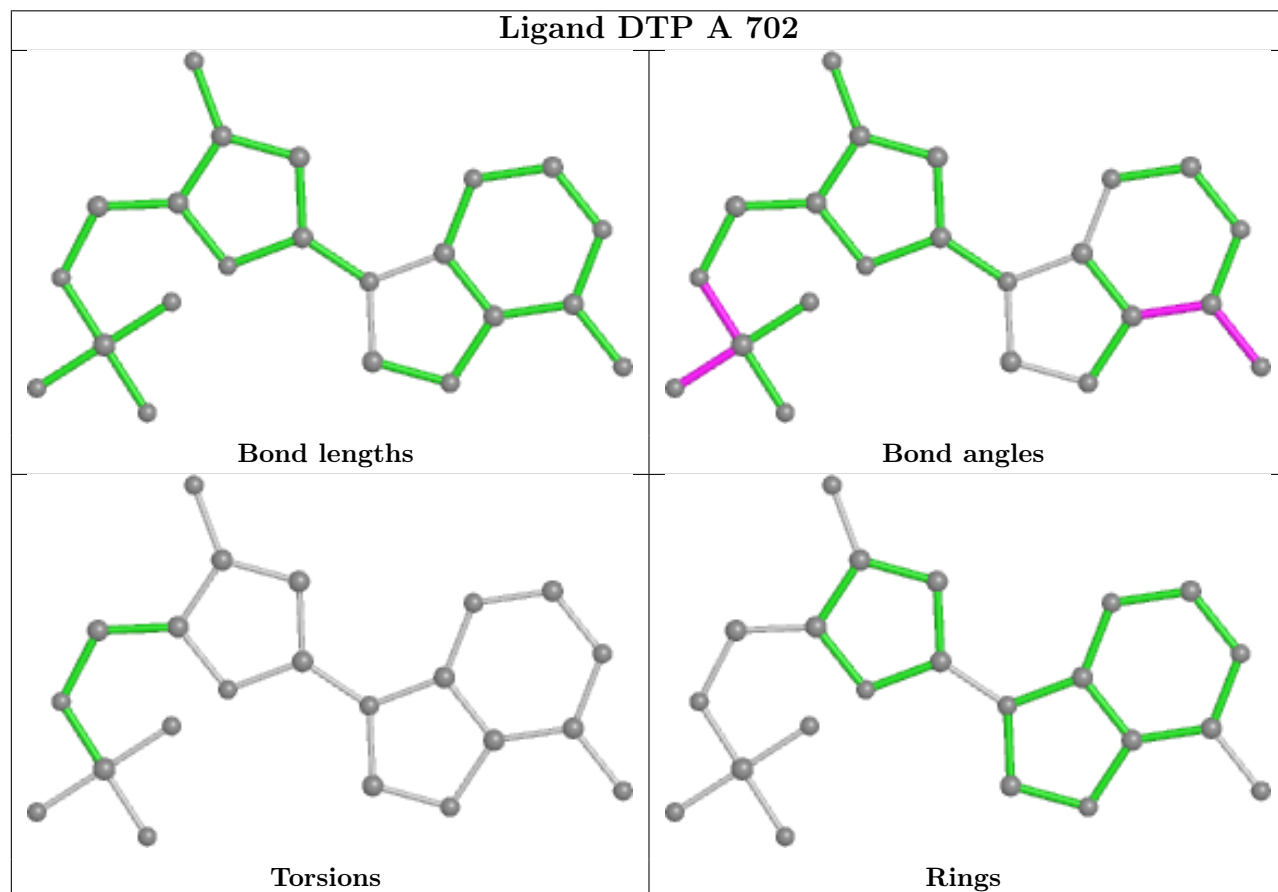
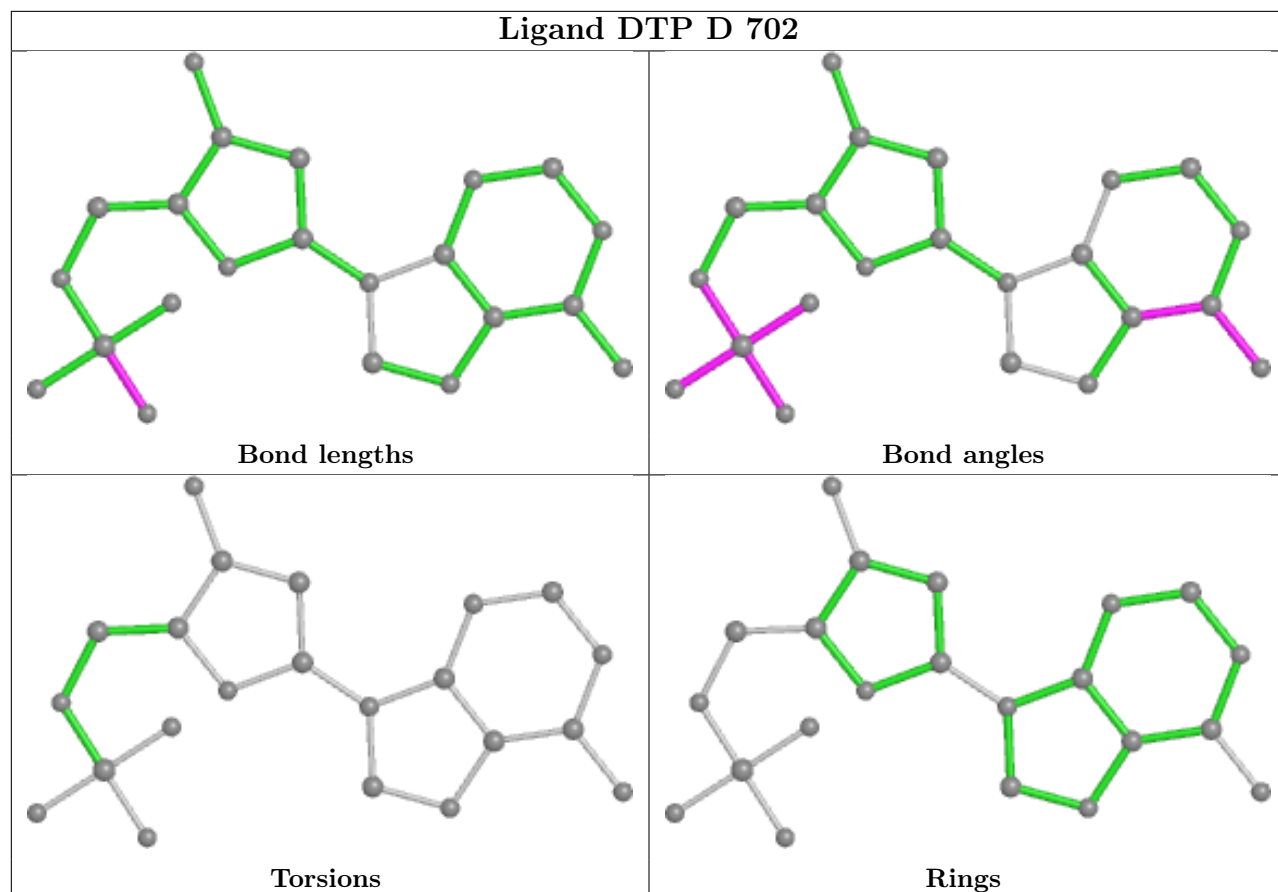
Mol	Chain	Res	Type	Atoms
4	C	702	DTP	C3'-C4'-C5'-O5'
4	C	702	DTP	O4'-C4'-C5'-O5'
4	B	702	DTP	C3'-C4'-C5'-O5'

There are no ring outliers.

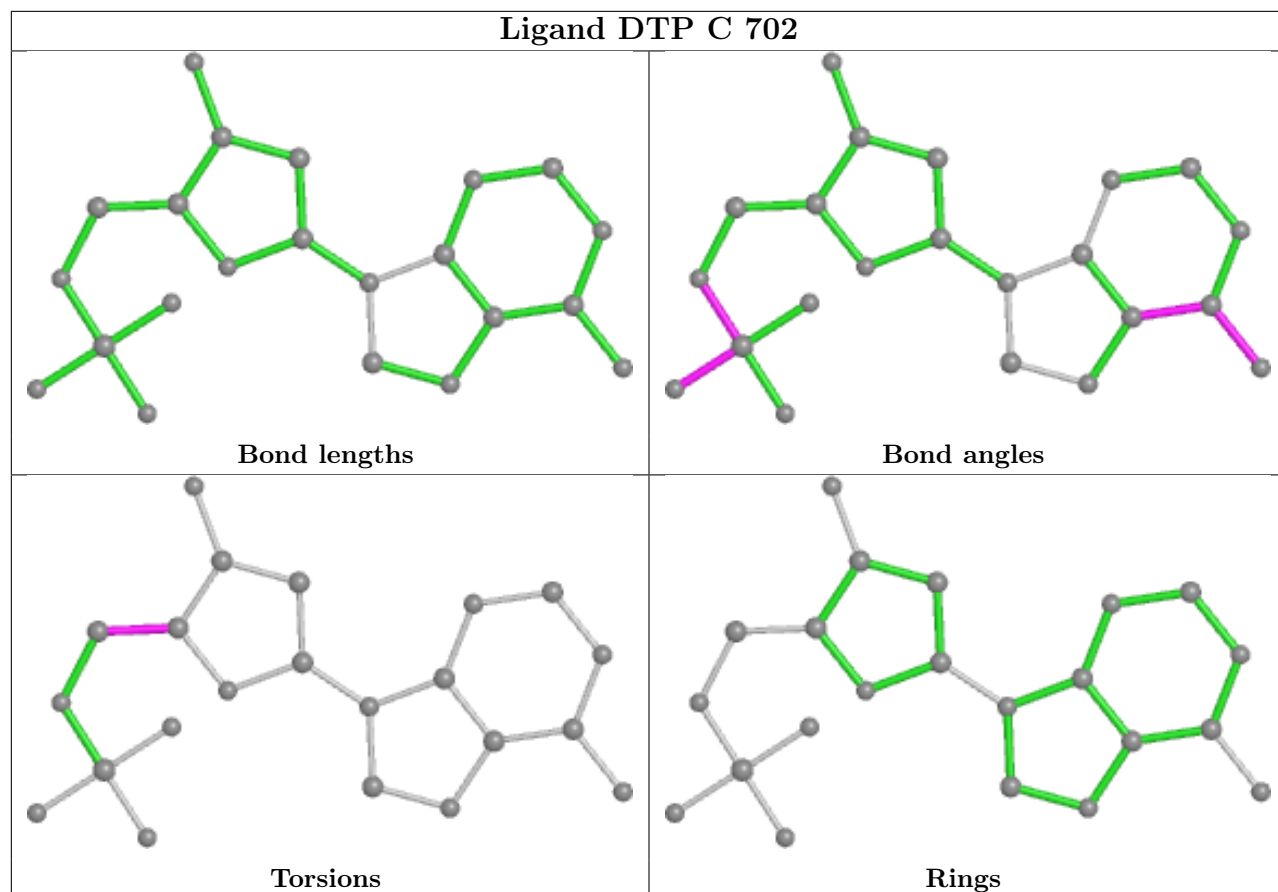
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	DTP	5	0
4	A	702	DTP	3	0
4	C	702	DTP	6	0
4	B	702	DTP	4	0

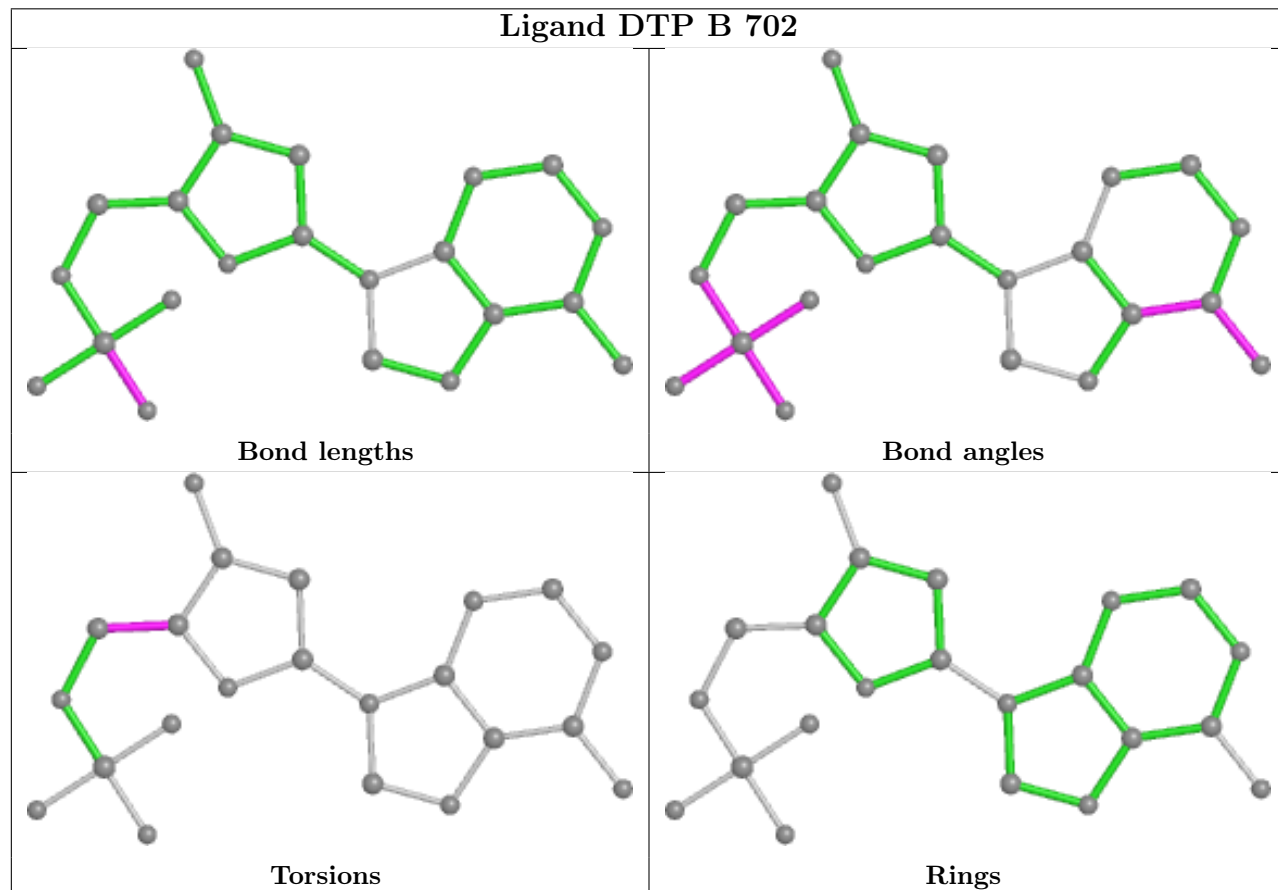
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 DTP C 702



Ligand DTP B 702



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, 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	434/533 (81%)	0.09	17 (3%) 39 41	30, 56, 120, 150	0
1	B	437/533 (81%)	0.11	23 (5%) 26 27	29, 57, 116, 158	0
1	C	431/533 (80%)	0.02	14 (3%) 47 50	26, 49, 113, 146	0
1	D	430/533 (80%)	0.09	14 (3%) 46 49	32, 60, 118, 146	0
2	E	4/5 (80%)	0.19	0 100 100	75, 105, 131, 158	0
2	F	4/5 (80%)	1.33	0 100 100	90, 123, 129, 132	0
2	G	3/5 (60%)	0.35	0 100 100	83, 83, 126, 129	0
2	H	4/5 (80%)	1.49	1 (25%) 0 0	101, 128, 130, 176	0
All	All	1747/2152 (81%)	0.09	69 (3%) 39 41	26, 56, 118, 176	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	GLN	6.8
1	A	466	ILE	5.7
1	A	463	THR	5.5
1	C	490	ASP	4.9
1	A	486	LYS	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

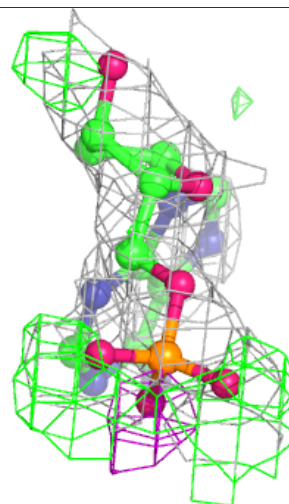
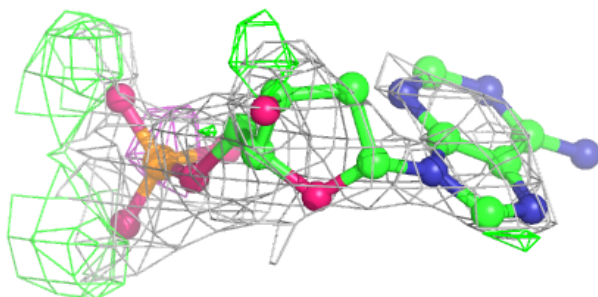
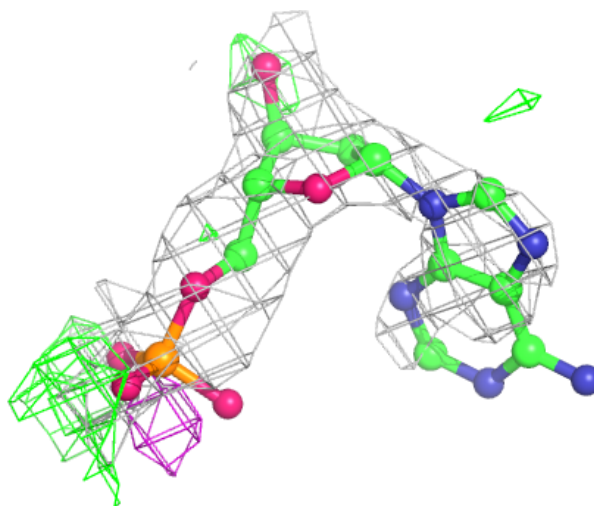
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DTP	C	702	22/30	0.69	0.40	59,73,87,90	22
4	DTP	A	702	22/30	0.75	0.27	57,84,90,94	22
4	DTP	B	702	22/30	0.77	0.21	54,69,82,90	22
4	DTP	D	702	22/30	0.79	0.24	56,78,90,101	22
3	ZN	D	701	1/1	0.96	0.13	54,54,54,54	1
3	ZN	B	701	1/1	0.97	0.19	52,52,52,52	1
3	ZN	A	701	1/1	0.98	0.10	61,61,61,61	1
3	ZN	C	701	1/1	0.99	0.07	64,64,64,64	1

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.

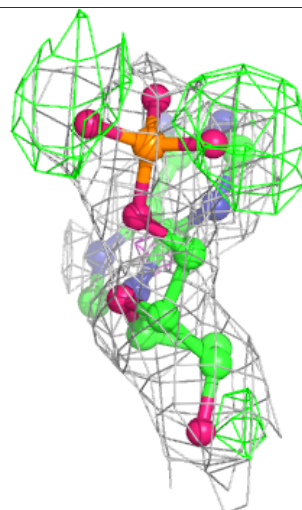
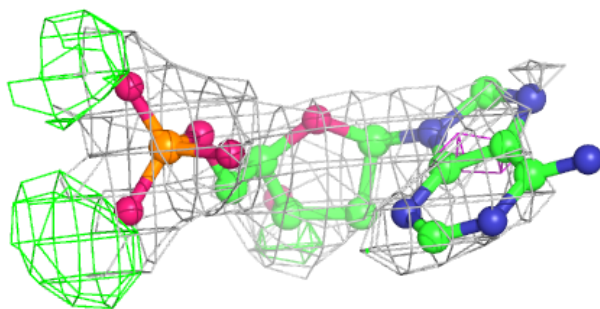
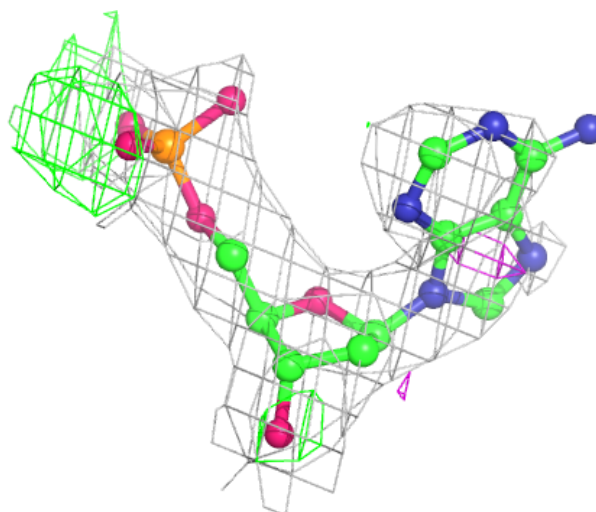
Electron density around DTP C 702:

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



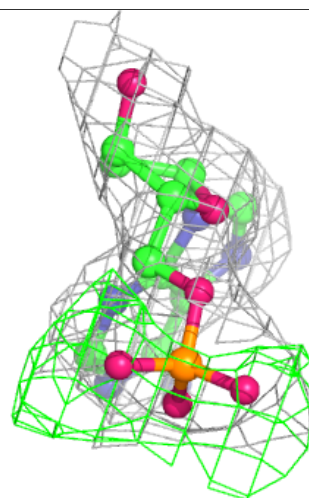
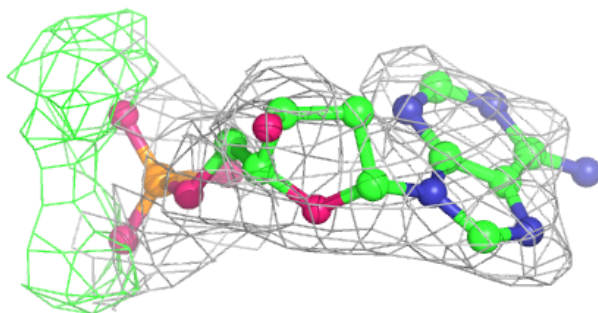
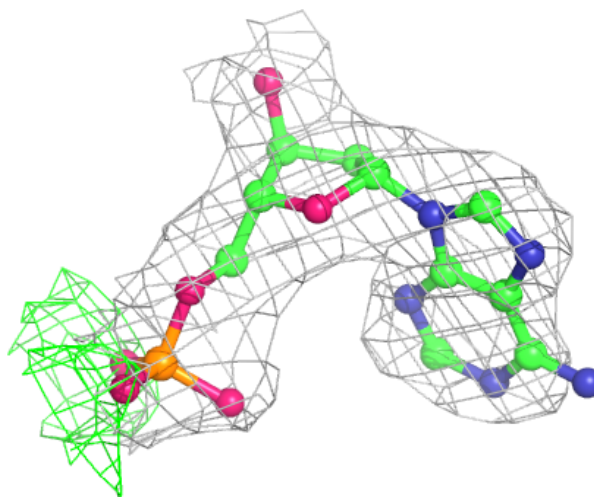
Electron density around DTP A 702:

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



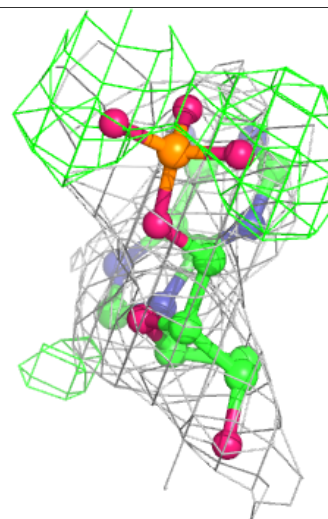
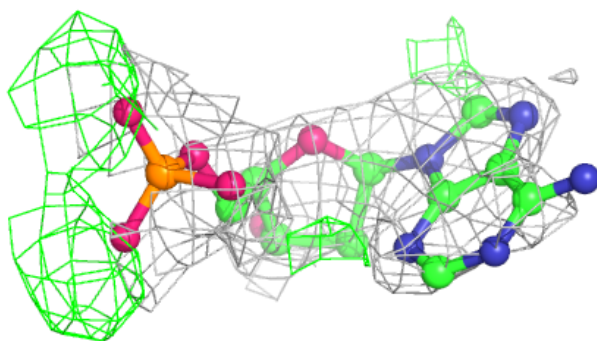
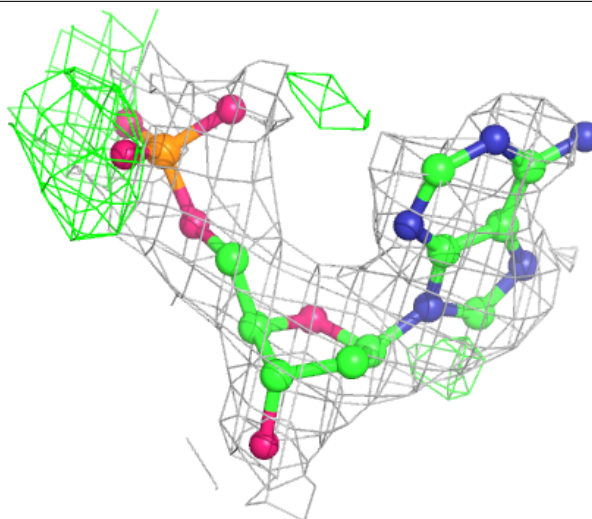
Electron density around DTP B 702:

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



Electron density around DTP D 702:

$2mF_o-DF_c$ (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.