



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:32 AM UTC

PDB ID : 8C8J / pdb_00008c8j
Title : Long Interspersed Nuclear Element 1 (LINE-1) reverse transcriptase ternary complex with hybrid duplex and dTTP
Authors : Nichols, C.E.; Walpole, T.B.; Baldwin, E.
Deposited on : 2023-01-20
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

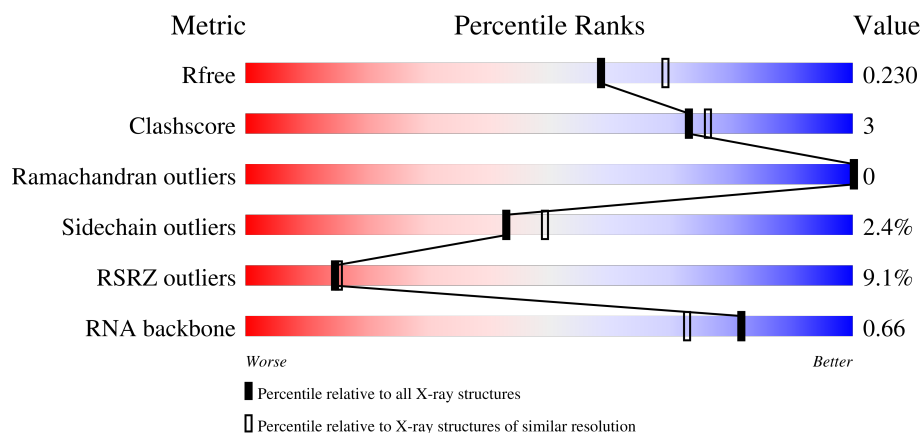
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

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	832	8% 77% 7% 16%
2	B	9	67% 33%
3	C	12	67% 25% 8%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6441 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 RNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	11	0
			5655	3665	940	1030	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	ASP	ASN	conflict	UNP G8I2S9
A	910	HIS	LEU	conflict	UNP G8I2S9
A	1062	HIS	-	expression tag	UNP G8I2S9
A	1063	HIS	-	expression tag	UNP G8I2S9
A	1064	HIS	-	expression tag	UNP G8I2S9
A	1065	HIS	-	expression tag	UNP G8I2S9
A	1066	HIS	-	expression tag	UNP G8I2S9
A	1067	HIS	-	expression tag	UNP G8I2S9
A	1068	HIS	-	expression tag	UNP G8I2S9
A	1069	HIS	-	expression tag	UNP G8I2S9

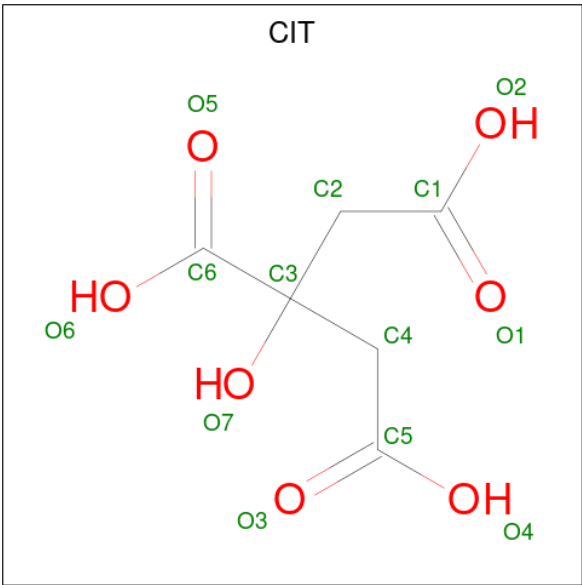
- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*GP*CP*TP*TP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			179	86	28	56	9			

- Molecule 3 is a RNA chain called RNA (5'-R(P*UP*UP*AP*GP*GP*AP*AP*AP*GP*CP*GP*C)-3').

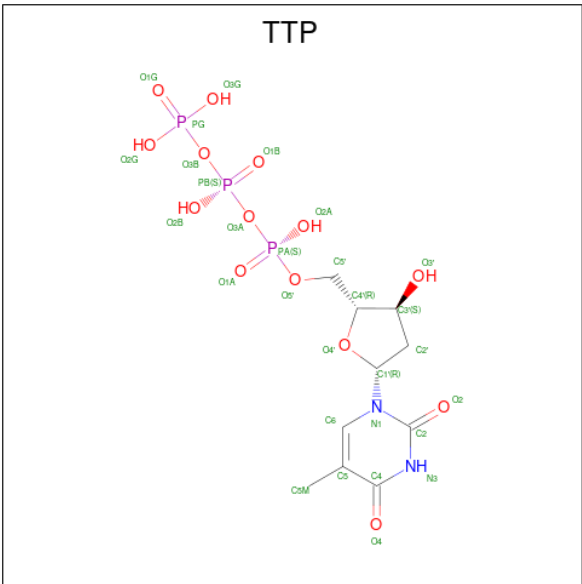
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			260	116	50	82	12			

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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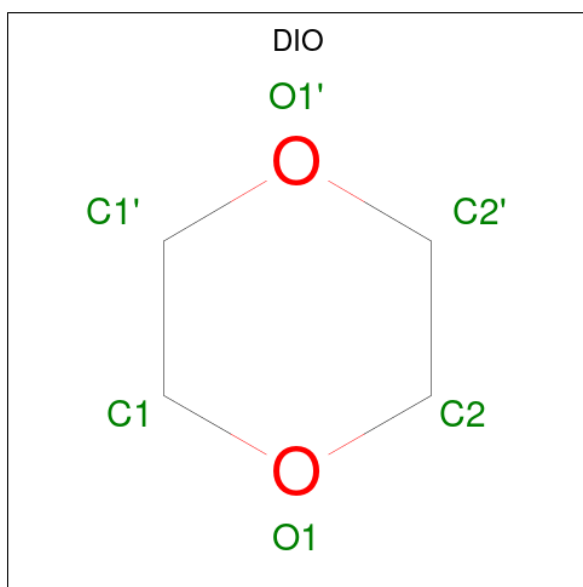
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	Mg	0	0
			2	2		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		

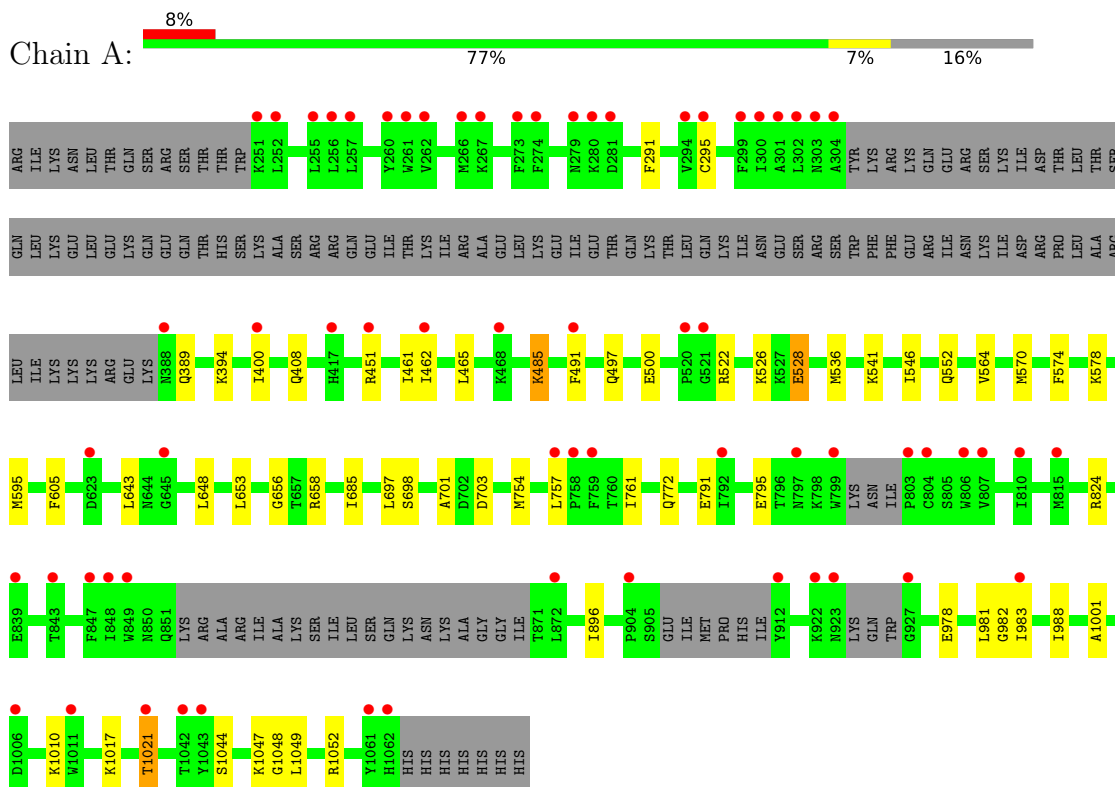
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	194	Total	O	0	0
			194	194		
11	B	10	Total	O	0	0
			10	10		
11	C	15	Total	O	0	0
			15	15		

3 Residue-property plots [i](#)

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

• Molecule 1: RNA-directed DNA polymerase



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



• Molecule 3: RNA (5'-R(P*UP*UP*AP*GP*GP*AP*AP*AP*GP*CP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.35Å 84.53Å 107.94Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	59.66 – 2.10 59.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.66-2.10) 100.0 (59.66-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.208 , 0.238 0.202 , 0.230	Depositor DCC
R_{free} test set	3001 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6441	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: CL, DIO, DMS, CIT, CSX, MG, EDO, TTP

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	0.70	1/5776 (0.0%)	0.99	4/7823 (0.1%)
2	B	0.40	0/198	0.59	0/302
3	C	0.68	1/291 (0.3%)	0.72	0/452
All	All	0.69	2/6265 (0.0%)	0.97	4/8577 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	701	ALA	CA-C	6.40	1.58	1.52
3	C	2	U	C1'-N1	5.46	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	PHE	CA-CB-CG	-7.40	106.40	113.80
1	A	656	GLY	N-CA-C	6.04	121.74	112.81
1	A	685	ILE	N-CA-C	-5.55	98.97	106.85
1	A	574	PHE	CA-CB-CG	5.46	119.25	113.80

There are no chirality outliers.

There are no planarity outliers.

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	5655	0	5616	34	0
2	B	179	0	101	6	0
3	C	260	0	131	6	0
4	A	26	0	10	0	0
5	A	29	0	13	1	0
6	A	52	0	78	7	0
6	C	4	0	6	0	0
7	A	8	0	12	0	0
8	A	6	0	8	0	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
11	A	194	0	0	1	0
11	B	10	0	0	0	0
11	C	15	0	0	0	0
All	All	6441	0	5975	39	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 (39) 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)
2:B:4:DC:H42	3:C:11:G:H1	1.07	0.99
2:B:3:DG:H1	3:C:12:C:H42	1.27	0.82
2:B:4:DC:N3	3:C:11:G:N2	2.29	0.78
2:B:4:DC:N4	3:C:11:G:H1	1.83	0.76
1:A:462[B]:ILE:HD11	1:A:485:LYS:HD3	1.67	0.74
1:A:408[A]:GLN:HG2	1:A:643:LEU:HD23	1.70	0.74
1:A:658:ARG:HG3	6:A:1103:EDO:H12	1.72	0.71
1:A:536:MET:HE3	1:A:541:LYS:HG2	1.70	0.71
1:A:643:LEU:HD12	6:A:1105:EDO:H21	1.73	0.70
1:A:1017:LYS:O	1:A:1021:THR:HB	1.97	0.63
1:A:595:MET:HE1	1:A:757:LEU:HD13	1.80	0.62
1:A:754:MET:HG2	1:A:761:ILE:HG13	1.82	0.62
1:A:978:GLU:HA	1:A:982:GLY:O	2.03	0.58
1:A:595:MET:HE1	1:A:757:LEU:CD1	2.34	0.57
1:A:772:GLN:HE21	6:A:1118:EDO:H21	1.73	0.54
1:A:536:MET:CE	1:A:541:LYS:HG2	2.37	0.52
2:B:3:DG:H1	3:C:12:C:N4	2.00	0.51
1:A:528:GLU:H	1:A:528:GLU:CD	2.17	0.51
1:A:461:ILE:CD1	1:A:546:ILE:HG12	2.41	0.50
1:A:981:LEU:HD21	1:A:1001:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ILE:HD13	1:A:546:ILE:HG13	1.94	0.49
1:A:896:ILE:O	6:A:1111:EDO:H22	2.15	0.47
1:A:461:ILE:CD1	1:A:546:ILE:CG1	2.93	0.47
1:A:1048:GLY:O	1:A:1052:ARG:HG3	2.15	0.47
1:A:564:VAL:HG12	1:A:570:MET:HE3	1.96	0.47
1:A:1047:LYS:HE3	3:C:8:A:OP2	2.15	0.46
1:A:408[B]:GLN:HG3	1:A:648:LEU:HD22	1.97	0.46
1:A:605:PHE:CG	5:A:1102:TTP:H2'1	2.52	0.44
1:A:824:ARG:HH12	6:A:1118:EDO:H11	1.82	0.44
1:A:394:LYS:HB2	1:A:400:ILE:HG22	2.00	0.43
1:A:552:GLN:NE2	11:A:1212:HOH:O	2.51	0.43
1:A:497:GLN:HA	1:A:500[A]:GLU:HG2	2.00	0.42
1:A:462[B]:ILE:HA	1:A:465:LEU:HG	2.02	0.42
1:A:291:PHE:CE1	1:A:295:CYS:SG	3.13	0.41
1:A:791:GLU:O	1:A:795:GLU:HG2	2.20	0.41
1:A:541:LYS:NZ	6:A:1107:EDO:H12	2.36	0.41
1:A:658:ARG:HG3	6:A:1103:EDO:C1	2.47	0.40
1:A:578:LYS:HE3	1:A:698:SER:OG	2.22	0.40
1:A:703:ASP:OD2	2:B:11:DC:H5"	2.21	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	A	696/832 (84%)	677 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	598/765 (78%)	584 (98%)	14 (2%)	44 51

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
1	A	451	ARG
1	A	485	LYS
1	A	522	ARG
1	A	526	LYS
1	A	528	GLU
1	A	653	LEU
1	A	697	LEU
1	A	983	ILE
1	A	988	ILE
1	A	1010	LYS
1	A	1021	THR
1	A	1044	SER
1	A	1049	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	552	GLN
1	A	716	GLN
1	A	748	GLN
1	A	772	GLN
1	A	892	GLN
1	A	898	GLN
1	A	900	ASN
1	A	913	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	11/12 (91%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	12	C

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSX	A	661	1	3,6,7	0.76	0	1,6,8	0.44	0

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
1	CSX	A	661	1	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	$\# Z > 2$
7	DMS	A	1110	-	3,3,3	0.67	0	3,3,3	0.21	0
5	TTP	A	1102	9	29,30,30	0.62	0	43,47,47	0.57	0
4	CIT	A	1113	-	12,12,12	1.03	0	17,17,17	1.11	1 (5%)
6	EDO	A	1109	-	3,3,3	0.26	0	2,2,2	0.32	0
6	EDO	A	1112	-	3,3,3	0.23	0	2,2,2	0.26	0
6	EDO	A	1114	-	3,3,3	0.28	0	2,2,2	0.25	0
6	EDO	A	1108	-	3,3,3	0.23	0	2,2,2	0.40	0
6	EDO	A	1105	-	3,3,3	0.19	0	2,2,2	0.29	0
6	EDO	A	1103	-	3,3,3	0.17	0	2,2,2	0.16	0
6	EDO	A	1107	-	3,3,3	0.19	0	2,2,2	0.56	0
6	EDO	A	1119	-	3,3,3	0.28	0	2,2,2	0.24	0
6	EDO	A	1116	-	3,3,3	0.18	0	2,2,2	0.31	0
6	EDO	A	1117	-	3,3,3	0.19	0	2,2,2	0.43	0
6	EDO	A	1106	-	3,3,3	0.26	0	2,2,2	0.26	0
4	CIT	A	1101	9	12,12,12	1.07	0	17,17,17	1.24	3 (17%)
8	DIO	A	1115	-	6,6,6	0.33	0	6,6,6	0.21	0
7	DMS	A	1104	-	3,3,3	0.63	0	3,3,3	0.27	0
6	EDO	A	1118	-	3,3,3	0.25	0	2,2,2	0.37	0
6	EDO	C	101	-	3,3,3	0.27	0	2,2,2	0.21	0
6	EDO	A	1111	-	3,3,3	0.27	0	2,2,2	0.25	0

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
6	EDO	A	1108	-	-	1/1/1/1	-
5	TTP	A	1102	9	-	3/22/34/34	0/2/2/2
8	DIO	A	1115	-	-	-	0/1/1/1
6	EDO	A	1105	-	-	0/1/1/1	-
6	EDO	A	1103	-	-	1/1/1/1	-
6	EDO	A	1107	-	-	1/1/1/1	-
6	EDO	A	1116	-	-	0/1/1/1	-
4	CIT	A	1113	-	-	6/16/16/16	-
6	EDO	A	1117	-	-	1/1/1/1	-
6	EDO	A	1106	-	-	0/1/1/1	-
6	EDO	A	1109	-	-	1/1/1/1	-
4	CIT	A	1101	9	-	8/16/16/16	-
6	EDO	A	1118	-	-	1/1/1/1	-
6	EDO	C	101	-	-	0/1/1/1	-
6	EDO	A	1112	-	-	0/1/1/1	-
6	EDO	A	1119	-	-	0/1/1/1	-
6	EDO	A	1111	-	-	0/1/1/1	-
6	EDO	A	1114	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1113	CIT	O5-C6-C3	-2.39	117.45	122.09
4	A	1101	CIT	C3-C2-C1	2.37	120.39	113.92
4	A	1101	CIT	O5-C6-C3	-2.29	117.65	122.09
4	A	1101	CIT	O3-C5-C4	-2.16	116.83	122.95

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	CIT	O7-C3-C6-O5
4	A	1101	CIT	O7-C3-C6-O6
4	A	1101	CIT	C4-C3-C6-O5
4	A	1101	CIT	C4-C3-C6-O6
4	A	1113	CIT	O7-C3-C6-O5
4	A	1113	CIT	O7-C3-C6-O6
4	A	1113	CIT	C4-C3-C6-O5
4	A	1113	CIT	C4-C3-C6-O6

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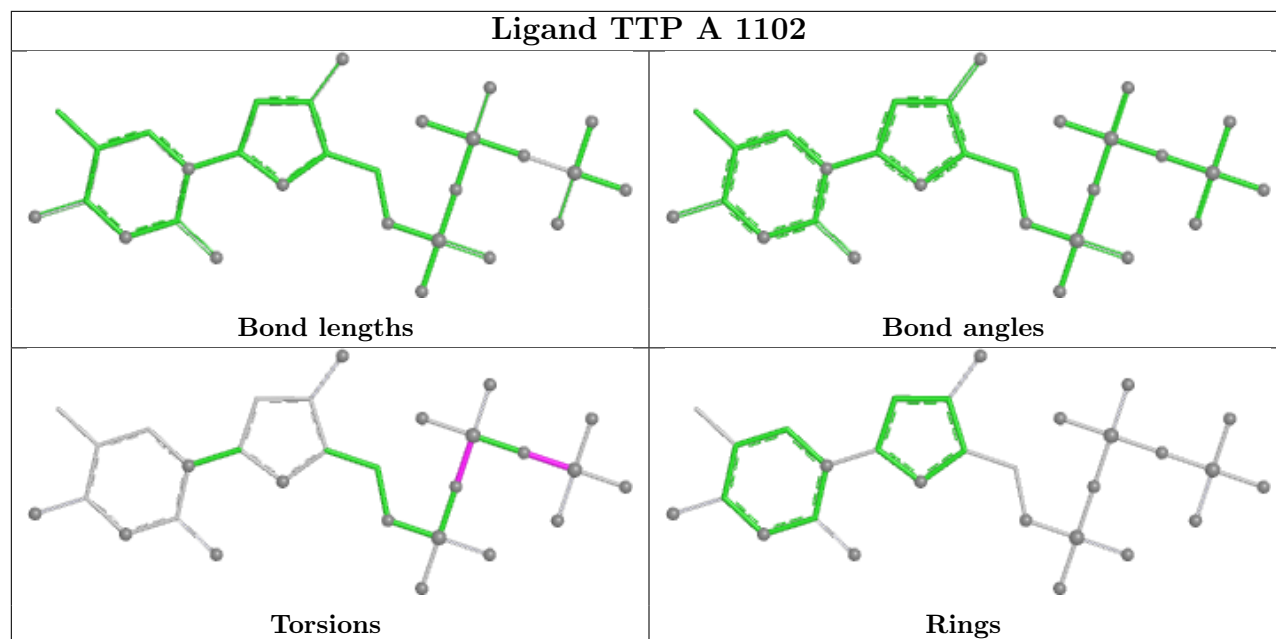
Mol	Chain	Res	Type	Atoms
5	A	1102	TTP	PB-O3B-PG-O2G
6	A	1109	EDO	O1-C1-C2-O2
6	A	1114	EDO	O1-C1-C2-O2
6	A	1117	EDO	O1-C1-C2-O2
6	A	1107	EDO	O1-C1-C2-O2
4	A	1101	CIT	C1-C2-C3-C4
4	A	1101	CIT	C1-C2-C3-O7
4	A	1113	CIT	C1-C2-C3-O7
4	A	1101	CIT	C3-C4-C5-O4
4	A	1101	CIT	C3-C4-C5-O3
6	A	1108	EDO	O1-C1-C2-O2
6	A	1118	EDO	O1-C1-C2-O2
5	A	1102	TTP	PB-O3B-PG-O3G
6	A	1103	EDO	O1-C1-C2-O2
4	A	1113	CIT	C3-C4-C5-O3
5	A	1102	TTP	PA-O3A-PB-O2B

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1102	TTP	1	0
6	A	1105	EDO	1	0
6	A	1103	EDO	2	0
6	A	1107	EDO	1	0
6	A	1118	EDO	2	0
6	A	1111	EDO	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.



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	697/832 (83%)	0.68	65 (9%) 14 15	24, 57, 95, 106	11 (1%)
2	B	9/9 (100%)	0.42	0 100 100	46, 55, 111, 121	0
3	C	12/12 (100%)	-0.49	0 100 100	46, 49, 86, 98	0
All	All	718/853 (84%)	0.66	65 (9%) 15 15	24, 57, 96, 121	11 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	6.7
1	A	923	ASN	5.3
1	A	260	TYR	5.2
1	A	303	ASN	5.0
1	A	257	LEU	4.6
1	A	274	PHE	4.5
1	A	803	PRO	4.4
1	A	815[A]	MET	4.4
1	A	927	GLY	4.3
1	A	252	LEU	4.2
1	A	417[A]	HIS	4.2
1	A	799	TRP	4.1
1	A	301	ALA	4.0
1	A	267	LYS	4.0
1	A	256	LEU	4.0
1	A	299	PHE	3.7
1	A	251	LYS	3.5
1	A	304	ALA	3.4
1	A	912	TYR	3.4
1	A	807	VAL	3.4
1	A	300	ILE	3.3
1	A	810	ILE	3.3
1	A	261	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	797	ASN	3.2
1	A	1042	THR	3.1
1	A	645	GLY	2.9
1	A	294	VAL	2.8
1	A	388	ASN	2.8
1	A	491	PHE	2.8
1	A	451	ARG	2.7
1	A	262	VAL	2.7
1	A	757	LEU	2.7
1	A	843	THR	2.7
1	A	462[A]	ILE	2.7
1	A	281	ASP	2.6
1	A	806	TRP	2.6
1	A	872	LEU	2.5
1	A	1011	TRP	2.5
1	A	849	TRP	2.5
1	A	295	CYS	2.4
1	A	904	PRO	2.4
1	A	1006	ASP	2.4
1	A	804	CYS	2.4
1	A	1061	TYR	2.3
1	A	266	MET	2.3
1	A	758	PRO	2.3
1	A	1043	TYR	2.3
1	A	400	ILE	2.3
1	A	848	ILE	2.3
1	A	1062	HIS	2.3
1	A	521	GLY	2.3
1	A	922	LYS	2.3
1	A	847	PHE	2.3
1	A	280	LYS	2.2
1	A	792	ILE	2.2
1	A	279	ASN	2.2
1	A	1021	THR	2.2
1	A	759	PHE	2.1
1	A	839	GLU	2.1
1	A	520	PRO	2.1
1	A	255	LEU	2.0
1	A	623	ASP	2.0
1	A	983	ILE	2.0
1	A	273	PHE	2.0
1	A	468	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSX	A	661	7/8	0.95	0.07	46,48,63,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	1109	4/4	0.70	0.18	91,92,92,92	0
6	EDO	A	1119	4/4	0.74	0.16	85,85,86,86	0
4	CIT	A	1113	13/13	0.75	0.14	91,93,94,94	0
6	EDO	A	1114	4/4	0.78	0.19	96,97,97,97	0
6	EDO	A	1106	4/4	0.81	0.20	81,81,82,82	0
6	EDO	A	1117	4/4	0.82	0.21	87,87,88,88	0
6	EDO	A	1116	4/4	0.82	0.21	74,75,75,76	0
6	EDO	C	101	4/4	0.82	0.18	89,89,89,90	0
6	EDO	A	1105	4/4	0.84	0.19	87,87,87,87	0
8	DIO	A	1115	6/6	0.84	0.23	94,95,95,95	0
7	DMS	A	1104	4/4	0.85	0.35	76,76,76,76	4
6	EDO	A	1111	4/4	0.85	0.22	64,64,64,64	0
6	EDO	A	1103	4/4	0.87	0.20	62,63,64,65	0
6	EDO	A	1118	4/4	0.87	0.19	87,87,87,87	0
6	EDO	A	1112	4/4	0.88	0.11	80,80,80,80	0
7	DMS	A	1110	4/4	0.89	0.22	90,90,90,90	0
6	EDO	A	1108	4/4	0.89	0.14	61,62,63,64	0
10	CL	A	1122	1/1	0.89	0.16	93,93,93,93	0
4	CIT	A	1101	13/13	0.90	0.10	76,78,79,79	0
6	EDO	A	1107	4/4	0.93	0.15	64,64,65,65	0
9	MG	A	1120	1/1	0.98	0.09	54,54,54,54	0

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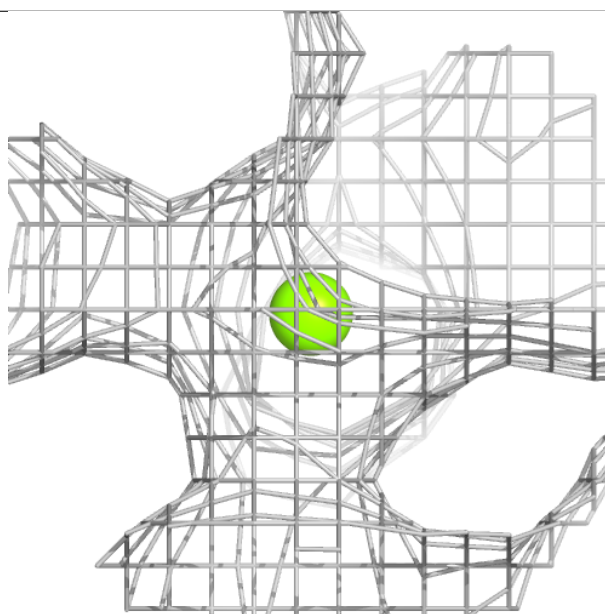
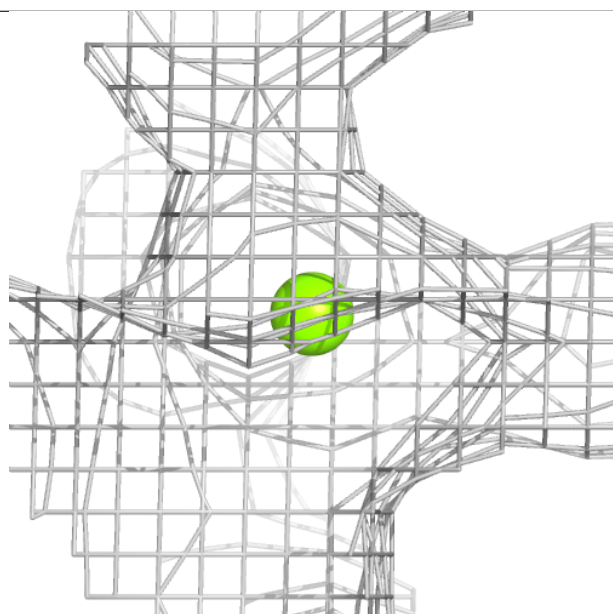
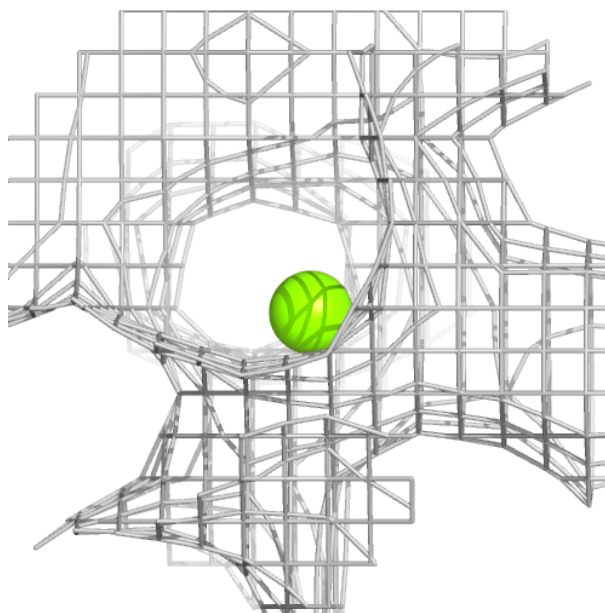
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TTP	A	1102	29/29	0.98	0.05	37,40,43,44	0
9	MG	A	1121	1/1	0.99	0.11	38,38,38,38	0

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.

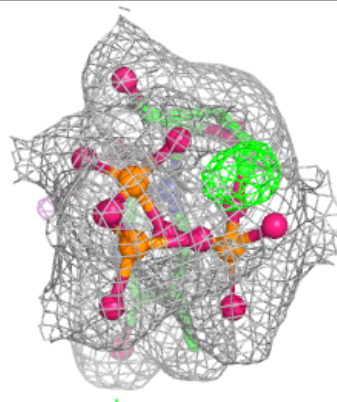
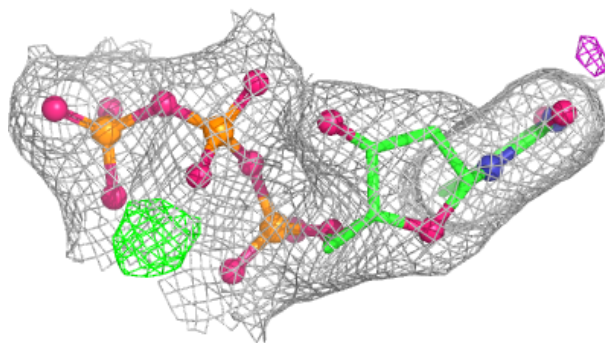
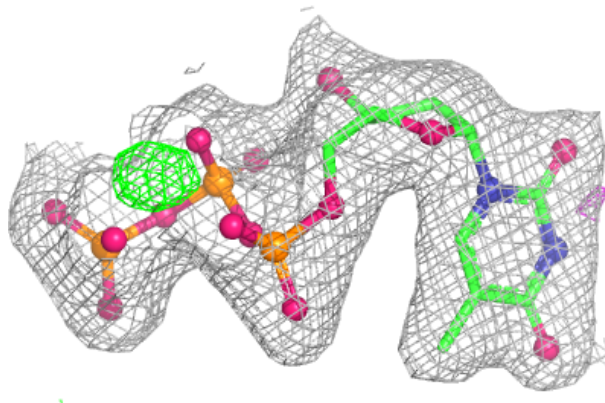
Electron density around MG A 1120:

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



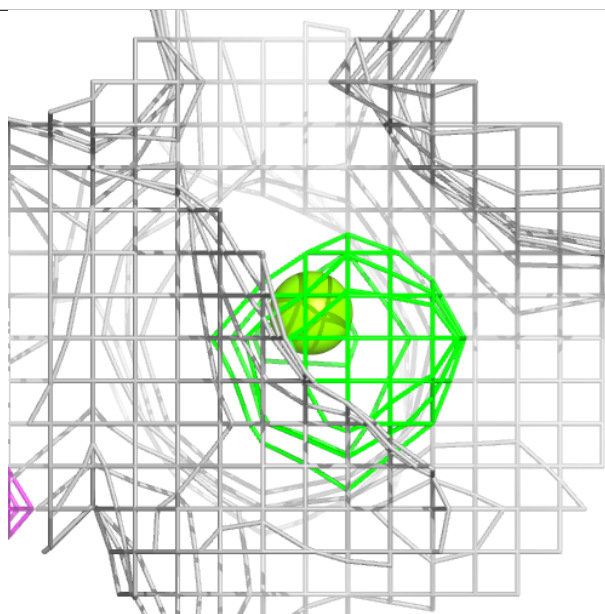
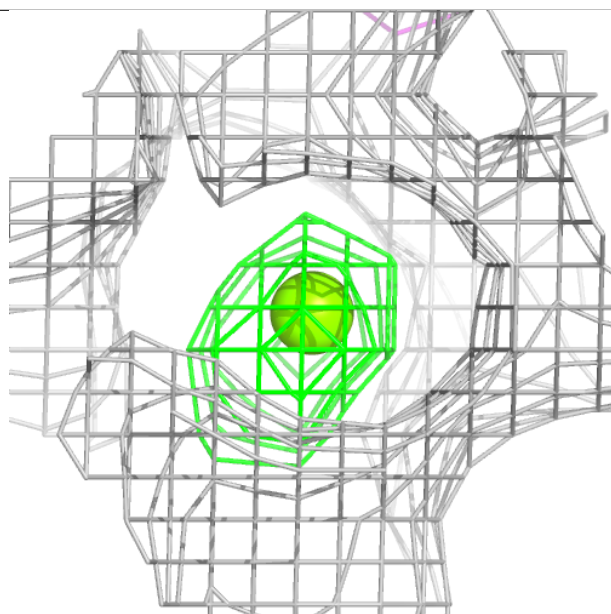
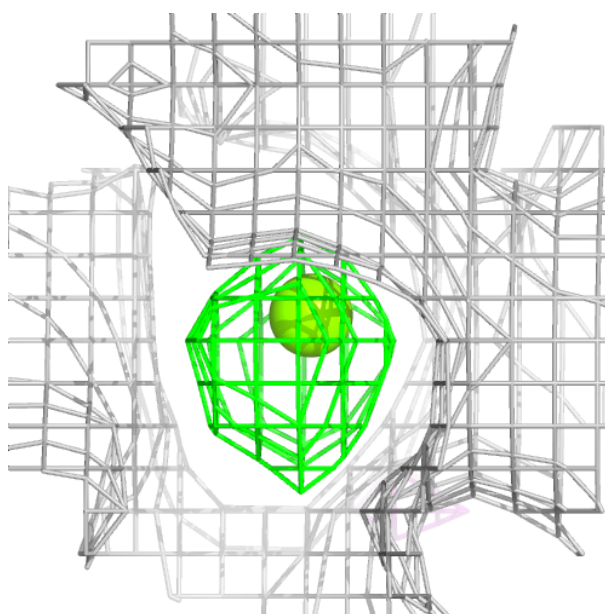
Electron density around TTP A 1102:

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



Electron density around MG A 1121:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.