



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 09:55 AM UTC

PDB ID : 8QA8 / pdb_00008qa8
Title : Crystal structure of the C-terminally truncated transcriptional repressor protein KorB from the RK2 plasmid complexed with CTP-gamma-S
Authors : McLean, T.C.; Mundy, J.E.A.; Lawson, D.M.; Le, T.B.K.
Deposited on : 2023-08-22
Resolution : 2.30 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 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

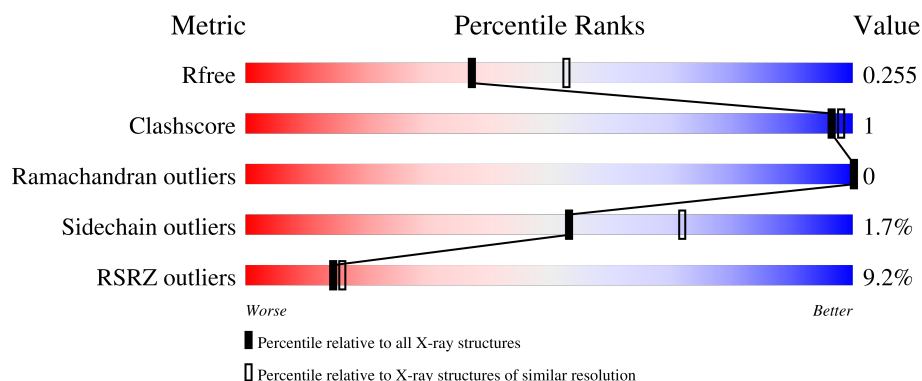
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



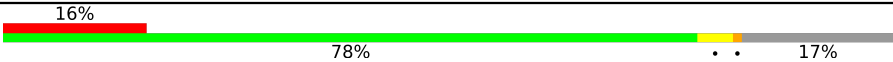
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	237	5% 81% 15%
1	B	237	5% 82% 15%
1	C	237	6% 79% 5% 16%
1	D	237	6% 82% 15%
1	E	237	8% 79% 16%

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Mol	Chain	Length	Quality of chain
1	F	237	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment on the left labeled '16%', a green segment in the middle labeled '78%', and a grey segment on the right labeled '17%'. There are two small black dots on the boundary between the green and grey segments.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9992 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 Transcriptional repressor protein KorB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	0	3	0
			1610	1010	284	316			
1	B	202	Total	C	N	O	0	3	0
			1615	1011	287	317			
1	C	200	Total	C	N	O	0	3	0
			1614	1011	288	315			
1	D	201	Total	C	N	O	0	2	0
			1602	1003	284	315			
1	E	200	Total	C	N	O	0	3	0
			1610	1008	287	315			
1	F	197	Total	C	N	O	0	3	0
			1538	962	279	297			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P07674
A	254	LYS	-	expression tag	UNP P07674
A	255	LEU	-	expression tag	UNP P07674
A	256	ALA	-	expression tag	UNP P07674
A	257	ALA	-	expression tag	UNP P07674
A	258	ALA	-	expression tag	UNP P07674
A	259	LEU	-	expression tag	UNP P07674
A	260	GLU	-	expression tag	UNP P07674
A	261	HIS	-	expression tag	UNP P07674
A	262	HIS	-	expression tag	UNP P07674
A	263	HIS	-	expression tag	UNP P07674
A	264	HIS	-	expression tag	UNP P07674
A	265	HIS	-	expression tag	UNP P07674
A	266	HIS	-	expression tag	UNP P07674
B	30	MET	-	initiating methionine	UNP P07674
B	254	LYS	-	expression tag	UNP P07674
B	255	LEU	-	expression tag	UNP P07674

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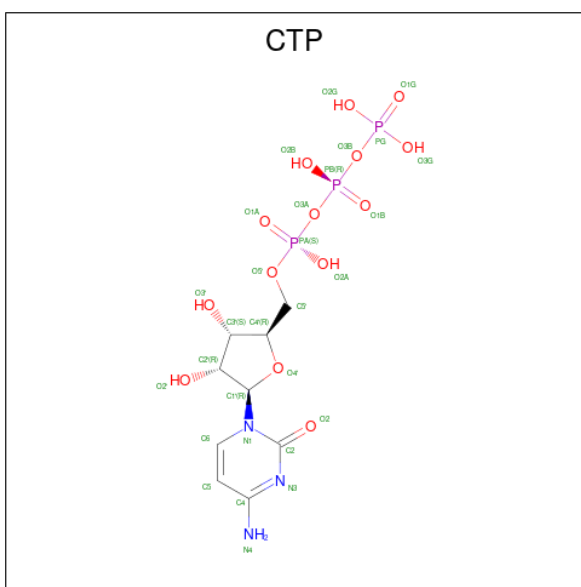
Chain	Residue	Modelled	Actual	Comment	Reference
B	256	ALA	-	expression tag	UNP P07674
B	257	ALA	-	expression tag	UNP P07674
B	258	ALA	-	expression tag	UNP P07674
B	259	LEU	-	expression tag	UNP P07674
B	260	GLU	-	expression tag	UNP P07674
B	261	HIS	-	expression tag	UNP P07674
B	262	HIS	-	expression tag	UNP P07674
B	263	HIS	-	expression tag	UNP P07674
B	264	HIS	-	expression tag	UNP P07674
B	265	HIS	-	expression tag	UNP P07674
B	266	HIS	-	expression tag	UNP P07674
C	30	MET	-	initiating methionine	UNP P07674
C	254	LYS	-	expression tag	UNP P07674
C	255	LEU	-	expression tag	UNP P07674
C	256	ALA	-	expression tag	UNP P07674
C	257	ALA	-	expression tag	UNP P07674
C	258	ALA	-	expression tag	UNP P07674
C	259	LEU	-	expression tag	UNP P07674
C	260	GLU	-	expression tag	UNP P07674
C	261	HIS	-	expression tag	UNP P07674
C	262	HIS	-	expression tag	UNP P07674
C	263	HIS	-	expression tag	UNP P07674
C	264	HIS	-	expression tag	UNP P07674
C	265	HIS	-	expression tag	UNP P07674
C	266	HIS	-	expression tag	UNP P07674
D	30	MET	-	initiating methionine	UNP P07674
D	254	LYS	-	expression tag	UNP P07674
D	255	LEU	-	expression tag	UNP P07674
D	256	ALA	-	expression tag	UNP P07674
D	257	ALA	-	expression tag	UNP P07674
D	258	ALA	-	expression tag	UNP P07674
D	259	LEU	-	expression tag	UNP P07674
D	260	GLU	-	expression tag	UNP P07674
D	261	HIS	-	expression tag	UNP P07674
D	262	HIS	-	expression tag	UNP P07674
D	263	HIS	-	expression tag	UNP P07674
D	264	HIS	-	expression tag	UNP P07674
D	265	HIS	-	expression tag	UNP P07674
D	266	HIS	-	expression tag	UNP P07674
E	30	MET	-	initiating methionine	UNP P07674
E	254	LYS	-	expression tag	UNP P07674
E	255	LEU	-	expression tag	UNP P07674

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Chain	Residue	Modelled	Actual	Comment	Reference
E	256	ALA	-	expression tag	UNP P07674
E	257	ALA	-	expression tag	UNP P07674
E	258	ALA	-	expression tag	UNP P07674
E	259	LEU	-	expression tag	UNP P07674
E	260	GLU	-	expression tag	UNP P07674
E	261	HIS	-	expression tag	UNP P07674
E	262	HIS	-	expression tag	UNP P07674
E	263	HIS	-	expression tag	UNP P07674
E	264	HIS	-	expression tag	UNP P07674
E	265	HIS	-	expression tag	UNP P07674
E	266	HIS	-	expression tag	UNP P07674
F	30	MET	-	initiating methionine	UNP P07674
F	254	LYS	-	expression tag	UNP P07674
F	255	LEU	-	expression tag	UNP P07674
F	256	ALA	-	expression tag	UNP P07674
F	257	ALA	-	expression tag	UNP P07674
F	258	ALA	-	expression tag	UNP P07674
F	259	LEU	-	expression tag	UNP P07674
F	260	GLU	-	expression tag	UNP P07674
F	261	HIS	-	expression tag	UNP P07674
F	262	HIS	-	expression tag	UNP P07674
F	263	HIS	-	expression tag	UNP P07674
F	264	HIS	-	expression tag	UNP P07674
F	265	HIS	-	expression tag	UNP P07674
F	266	HIS	-	expression tag	UNP P07674

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	B	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	C	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	D	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	E	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	F	1	Total 29	C 9	N 3	O 14	P 3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cl 4 4	0	0
3	B	4	Total Cl 4 4	0	0
3	C	3	Total Cl 3 3	0	0
3	D	4	Total Cl 4 4	0	0
3	E	4	Total Cl 4 4	0	0
3	F	3	Total Cl 3 3	0	0

- Molecule 4 is water.

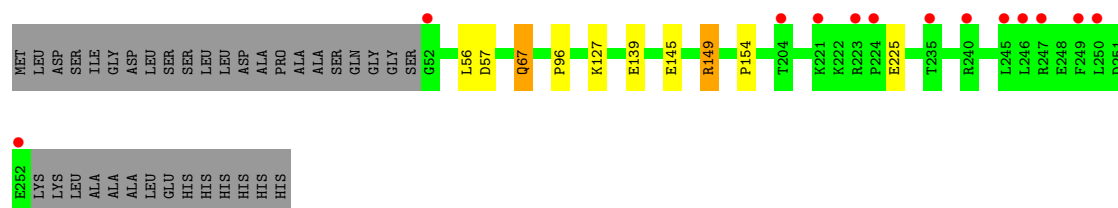
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total 53	O 53	0	1
4	B	44	Total 45	O 45	0	1
4	C	26	Total 26	O 26	0	0
4	D	23	Total 23	O 23	0	0
4	E	26	Total 27	O 27	0	1
4	F	33	Total 33	O 33	0	0

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.

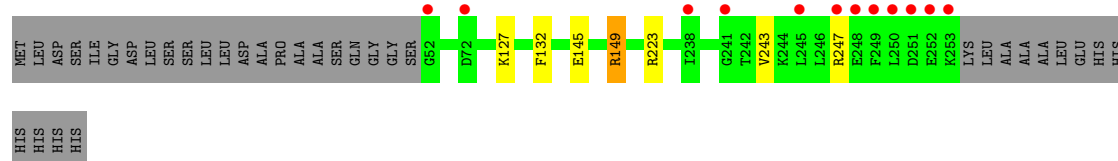
- Molecule 1: Transcriptional repressor protein KorB

Chain A: 



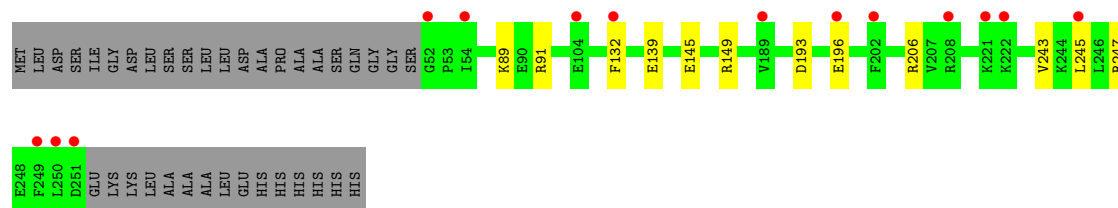
- Molecule 1: Transcriptional repressor protein KorB

Chain B: 



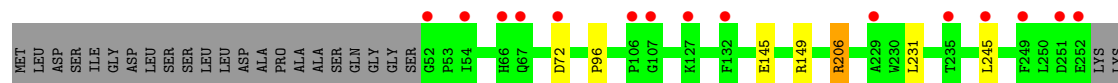
- Molecule 1: Transcriptional repressor protein KorB

Chain C: 



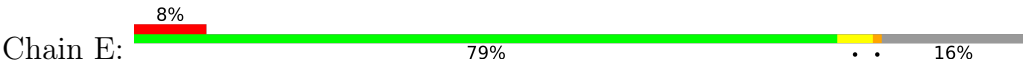
- Molecule 1: Transcriptional repressor protein KorB

Chain D: 



LEU
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

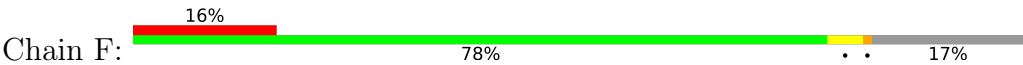
● Molecule 1: Transcriptional repressor protein KorB



MET LEU ASP SER ILE GLY ASP LEU SER SER LEU LEU ASP ALA PRO ALA ALA SER GLN GLY SER G52 P53 I54 Q67 E79 G107 E139 I144 E145 R149 K197 R206 F220 K221 K222 E225 A229 W230 L231 D232 D233 D234 T235 Q236 E237 I238 T239

E240 V243 R244 L245 L246 E247 E248 F249 L250 D251 GLU LYS LEU LYS ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

● Molecule 1: Transcriptional repressor protein KorB



MET LEU ASP SER ILE GLY ASP LEU SER SER LEU LEU ASP ALA PRO ALA ALA SER GLN GLY SER G52 P53 I54 Q67 P68 D72 E79 F132 E145 N146 R149 K170 E177 A201 T204 G205 R206 V207 R208 V212 L216 F220 K221 K222 R223

P224 E225 V227 E228 A229 V230 L231 D232 D233 D234 L235 Q236 E237 I238 T239 R240 G241 T242 V243 K244 L245 L246 R247 E248 PHE LEU ASP GLU LYS LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.69Å 152.71Å 198.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.28 – 2.30 120.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (121.28-2.30) 100.0 (120.98-2.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.227 , 0.256 0.228 , 0.255	Depositor DCC
R_{free} test set	4000 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9992	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: CTP, CL

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	0.67	0/1639	0.98	2/2219 (0.1%)
1	B	0.66	0/1644	1.00	1/2227 (0.0%)
1	C	0.62	0/1643	1.05	3/2222 (0.1%)
1	D	0.59	0/1630	0.99	2/2206 (0.1%)
1	E	0.62	0/1639	1.01	3/2218 (0.1%)
1	F	0.66	0/1566	1.03	3/2123 (0.1%)
All	All	0.64	0/9761	1.01	14/13215 (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	A	0	1
1	B	0	2
1	C	0	3
1	D	0	2
1	F	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	ASP	CA-CB-CG	8.81	121.41	112.60
1	F	145	GLU	CB-CG-CD	6.44	123.55	112.60
1	C	145	GLU	CB-CG-CD	6.21	123.15	112.60
1	A	145	GLU	CB-CG-CD	6.19	123.13	112.60
1	E	145	GLU	CB-CG-CD	6.07	122.92	112.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149[A]	ARG	Sidechain
1	B	149[A]	ARG	Sidechain
1	B	223	ARG	Sidechain
1	C	149[A]	ARG	Sidechain
1	C	91	ARG	Sidechain

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	1610	0	1578	6	0
1	B	1615	0	1576	4	0
1	C	1614	0	1599	2	0
1	D	1602	0	1579	2	0
1	E	1610	0	1588	8	0
1	F	1538	0	1486	8	0
2	A	29	0	12	1	0
2	B	29	0	12	0	0
2	C	29	0	12	0	0
2	D	29	0	12	0	0
2	E	29	0	12	1	0
2	F	29	0	12	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	A	53	0	0	1	0
4	B	45	0	0	0	0
4	C	26	0	0	0	0
4	D	23	0	0	0	0
4	E	27	0	0	0	0
4	F	33	0	0	0	0
All	All	9992	0	9478	20	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 1.

The worst 5 of 20 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:E:149[B]:ARG:HD3	1:F:149[B]:ARG:CZ	2.33	0.59
1:A:96:PRO:HG2	1:B:132[B]:PHE:CE2	2.39	0.58
1:A:67[A]:GLN:NE2	2:A:301:CTP:O1G	2.41	0.51
1:C:132[B]:PHE:CE2	1:D:96:PRO:HG2	2.45	0.51
1:B:243:VAL:O	1:B:247:ARG:HG2	2.12	0.49

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	202/237 (85%)	196 (97%)	6 (3%)	0	100	100
1	B	203/237 (86%)	198 (98%)	5 (2%)	0	100	100
1	C	201/237 (85%)	197 (98%)	4 (2%)	0	100	100
1	D	201/237 (85%)	196 (98%)	5 (2%)	0	100	100
1	E	201/237 (85%)	196 (98%)	5 (2%)	0	100	100
1	F	198/237 (84%)	192 (97%)	6 (3%)	0	100	100
All	All	1206/1422 (85%)	1175 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	170/199 (85%)	165 (97%)	5 (3%)	37	55
1	B	170/199 (85%)	169 (99%)	1 (1%)	78	89
1	C	173/199 (87%)	170 (98%)	3 (2%)	53	72
1	D	170/199 (85%)	169 (99%)	1 (1%)	78	89
1	E	172/199 (86%)	167 (97%)	5 (3%)	37	55
1	F	156/199 (78%)	153 (98%)	3 (2%)	50	69
All	All	1011/1194 (85%)	993 (98%)	18 (2%)	53	70

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	236	GLN
1	F	239	THR
1	F	225	GLU
1	C	245	LEU
1	E	235	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	150	ASN
1	E	142	GLN
1	F	142	GLN
1	E	187	GLN
1	C	150	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 22 are monoatomic - leaving 6 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	CTP	B	301	-	29,30,30	1.17	2 (6%)	43,47,47	0.87	1 (2%)
2	CTP	F	301	-	29,30,30	1.27	4 (13%)	43,47,47	0.96	4 (9%)
2	CTP	C	301	-	29,30,30	1.19	4 (13%)	43,47,47	1.07	4 (9%)
2	CTP	A	301	-	29,30,30	0.97	2 (6%)	43,47,47	0.91	2 (4%)
2	CTP	E	301	-	29,30,30	1.09	3 (10%)	43,47,47	0.82	0
2	CTP	D	301	-	29,30,30	0.83	0	43,47,47	0.86	2 (4%)

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	CTP	B	301	-	-	2/22/38/38	0/2/2/2
2	CTP	F	301	-	-	3/22/38/38	0/2/2/2
2	CTP	C	301	-	-	2/22/38/38	0/2/2/2
2	CTP	A	301	-	-	6/22/38/38	0/2/2/2
2	CTP	E	301	-	-	6/22/38/38	0/2/2/2
2	CTP	D	301	-	-	5/22/38/38	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	CTP	PA-O3A	4.22	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CTP	PA-O3A	3.73	1.63	1.59
2	C	301	CTP	PA-O3A	3.50	1.63	1.59
2	C	301	CTP	PG-O1G	3.32	1.60	1.50
2	B	301	CTP	PG-O1G	3.25	1.60	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	CTP	O2B-PB-O3B	2.59	114.28	107.27
2	C	301	CTP	O3A-PA-O1A	-2.58	102.94	110.70
2	A	301	CTP	O3G-PG-O3B	2.53	113.11	104.64
2	F	301	CTP	O3G-PG-O2G	2.39	116.78	107.80
2	F	301	CTP	O2B-PB-O3B	2.39	113.74	107.27

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	CTP	PB-O3A-PA-O5'
2	D	301	CTP	C5'-O5'-PA-O1A
2	D	301	CTP	C5'-O5'-PA-O3A
2	E	301	CTP	PB-O3B-PG-O2G
2	F	301	CTP	O4'-C4'-C5'-O5'

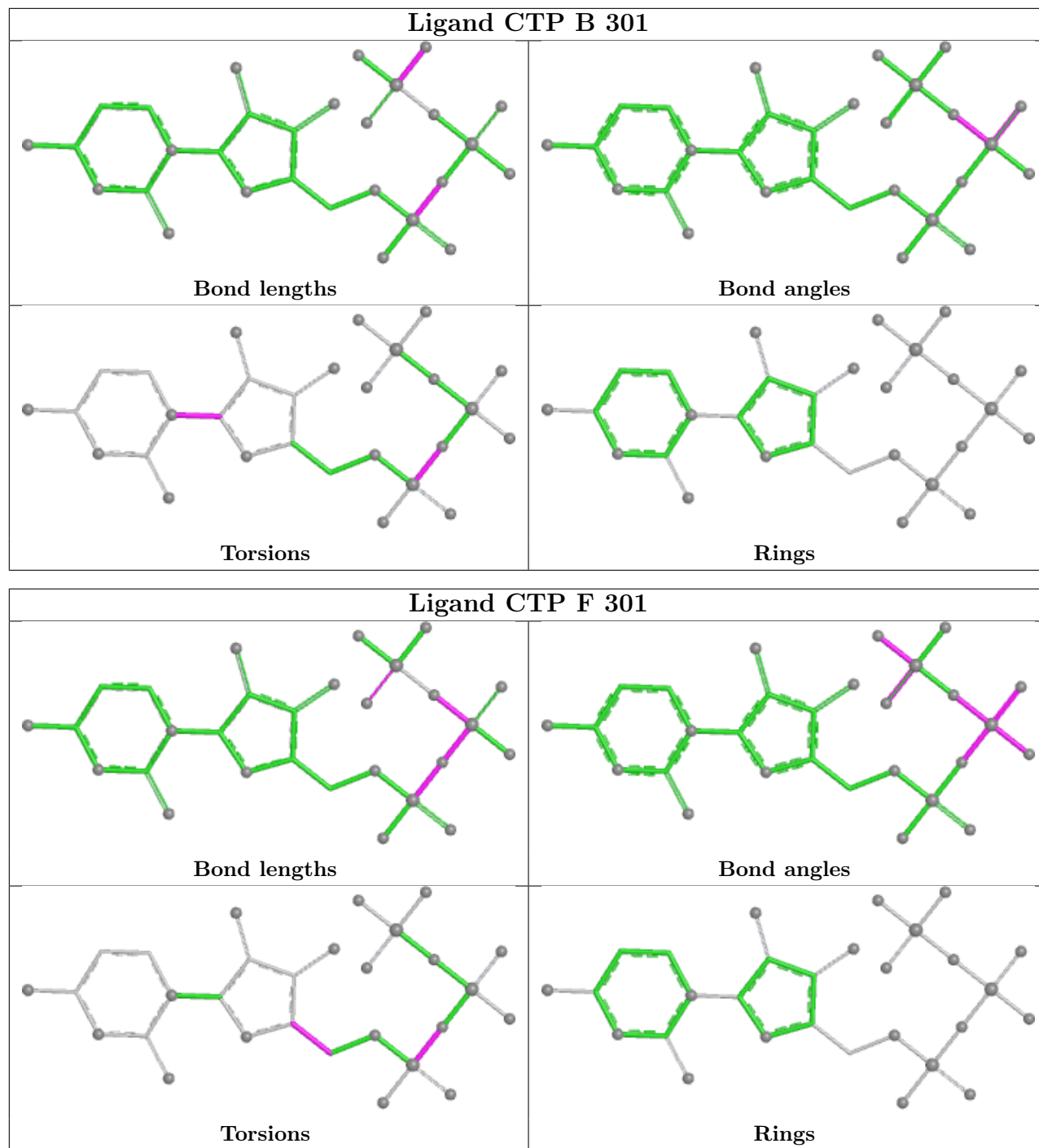
There are no ring outliers.

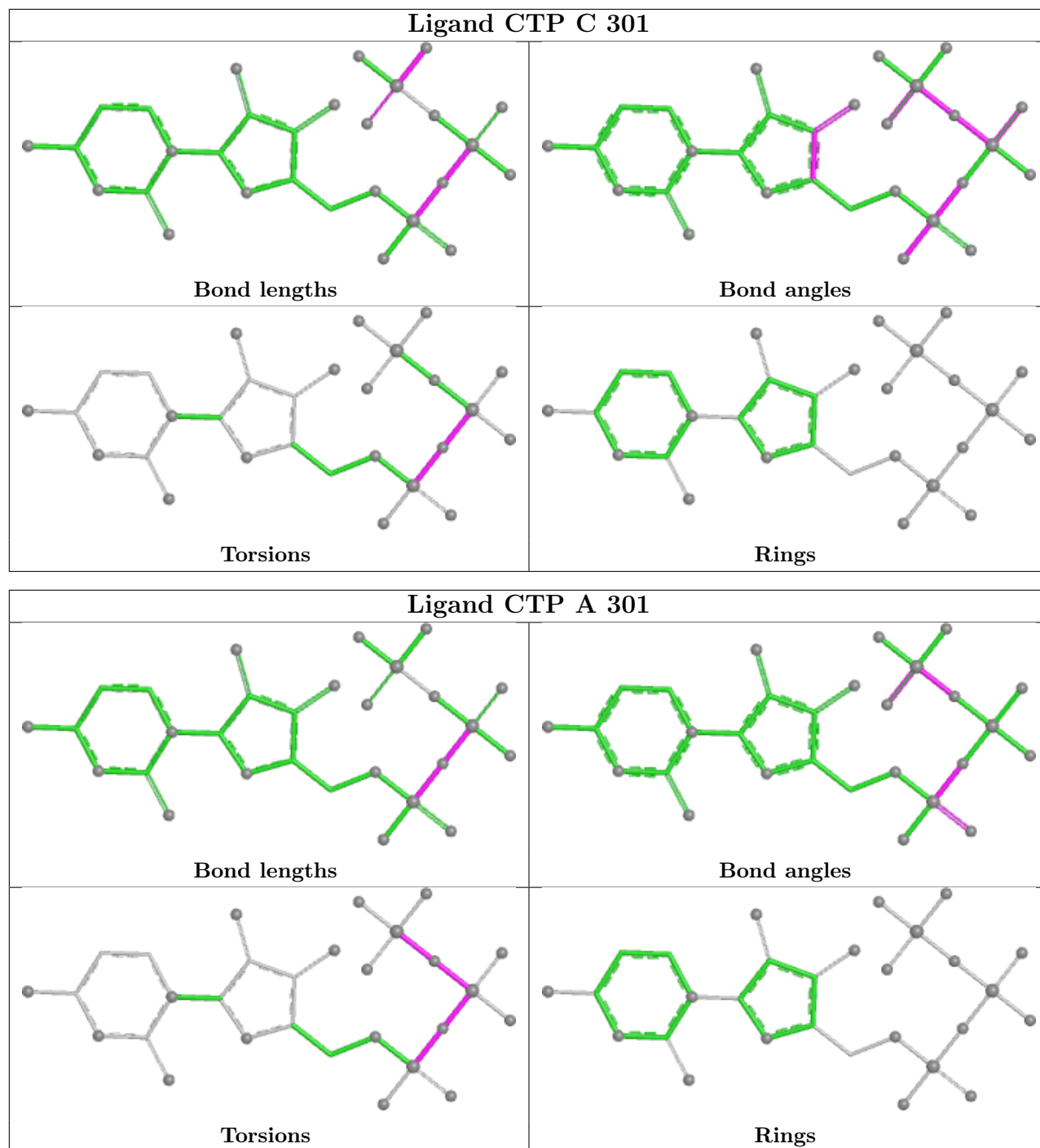
2 monomers are involved in 2 short contacts:

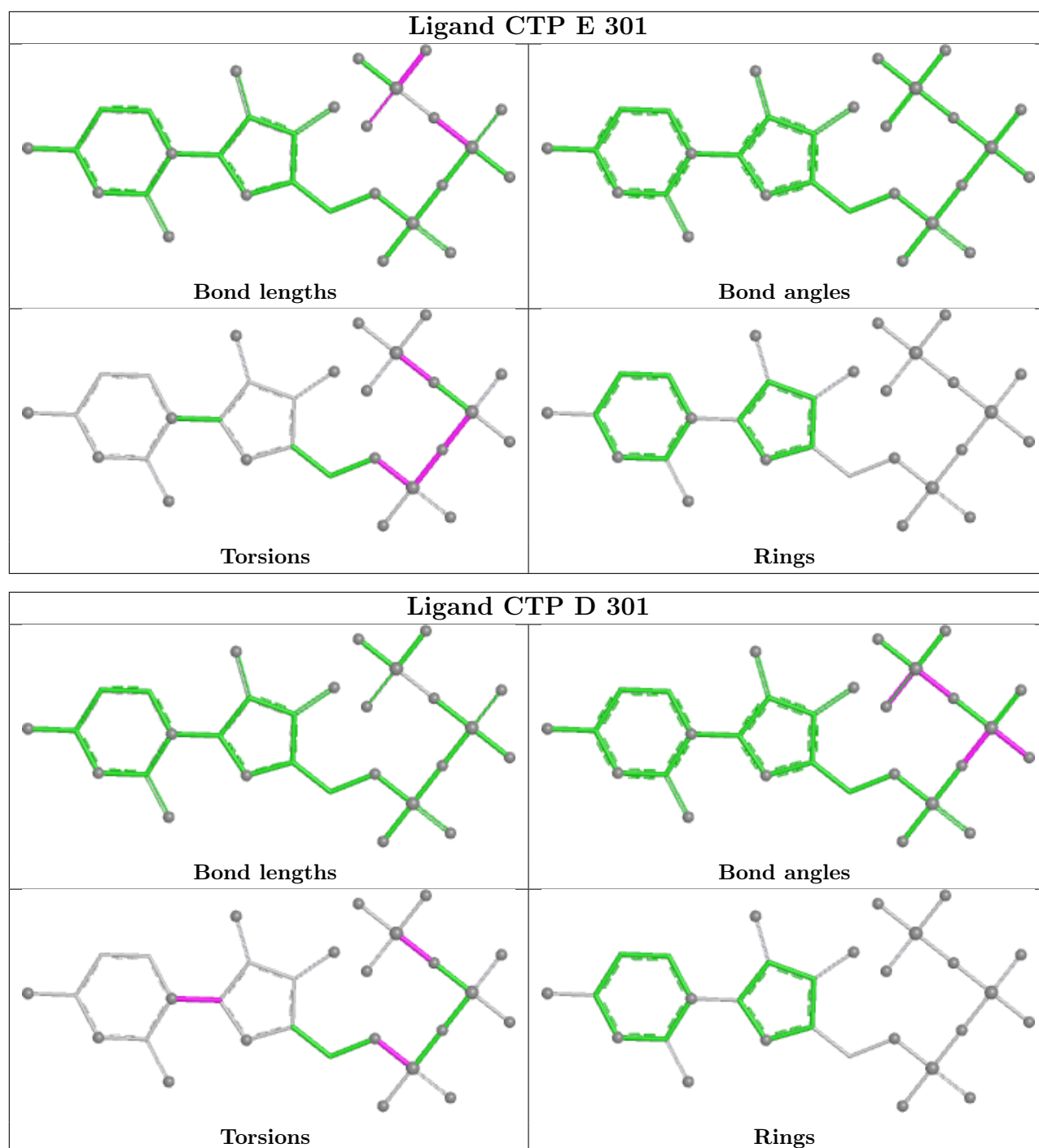
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CTP	1	0
2	E	301	CTP	1	0

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 [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	201/237 (84%)	0.23	13 (6%)	25 27	14, 44, 98, 132	3 (1%)
1	B	202/237 (85%)	0.25	12 (5%)	28 30	15, 43, 103, 132	3 (1%)
1	C	200/237 (84%)	0.54	14 (7%)	22 24	17, 51, 97, 119	3 (1%)
1	D	201/237 (84%)	0.65	15 (7%)	20 22	18, 60, 107, 124	2 (0%)
1	E	200/237 (84%)	0.65	19 (9%)	14 15	15, 52, 121, 143	3 (1%)
1	F	197/237 (83%)	0.80	38 (19%)	3 3	15, 48, 148, 179	3 (1%)
All	All	1201/1422 (84%)	0.52	111 (9%)	14 16	14, 50, 113, 179	17 (1%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	LYS	6.4
1	F	230	TRP	5.7
1	D	52	GLY	5.7
1	F	248	GLU	5.3
1	D	252	GLU	5.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

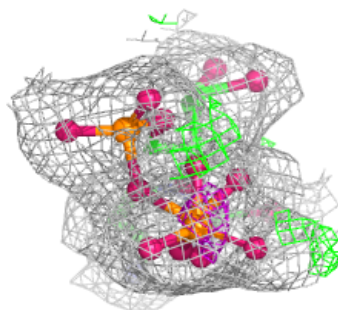
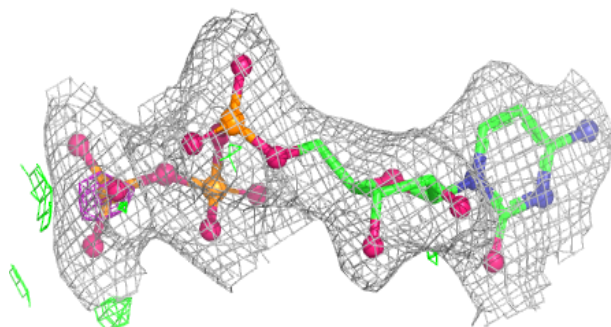
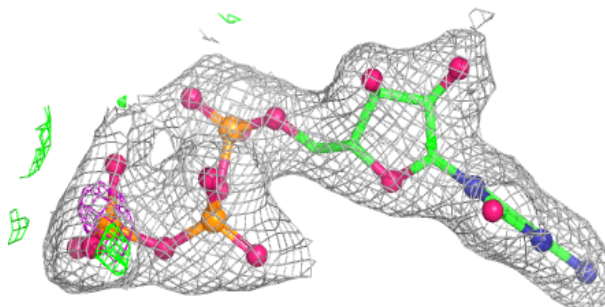
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	E	304	1/1	0.77	0.18	86,86,86,86	0
3	CL	D	304	1/1	0.78	0.16	83,83,83,83	0
3	CL	B	304	1/1	0.88	0.17	70,70,70,70	0
3	CL	F	304	1/1	0.88	0.14	61,61,61,61	0
3	CL	C	302	1/1	0.89	0.18	65,65,65,65	0
3	CL	A	302	1/1	0.89	0.12	53,53,53,53	0
3	CL	E	302	1/1	0.90	0.20	72,72,72,72	0
3	CL	C	304	1/1	0.90	0.10	78,78,78,78	0
3	CL	F	302	1/1	0.90	0.12	63,63,63,63	0
3	CL	A	304	1/1	0.90	0.19	64,64,64,64	0
3	CL	D	302	1/1	0.91	0.15	75,75,75,75	0
3	CL	E	305	1/1	0.91	0.10	62,62,62,62	0
3	CL	A	305	1/1	0.91	0.19	71,71,71,71	0
3	CL	B	305	1/1	0.91	0.16	70,70,70,70	0
3	CL	D	305	1/1	0.92	0.17	72,72,72,72	0
3	CL	C	303	1/1	0.92	0.16	56,56,56,56	0
3	CL	B	302	1/1	0.92	0.11	61,61,61,61	0
3	CL	B	303	1/1	0.94	0.15	52,52,52,52	0
3	CL	E	303	1/1	0.95	0.14	55,55,55,55	0
3	CL	A	303	1/1	0.96	0.11	57,57,57,57	0
2	CTP	C	301	29/29	0.97	0.06	30,36,41,47	0
2	CTP	D	301	29/29	0.97	0.06	35,42,58,68	0
2	CTP	E	301	29/29	0.97	0.06	28,32,37,43	0
3	CL	D	303	1/1	0.97	0.16	72,72,72,72	0
2	CTP	B	301	29/29	0.98	0.05	24,27,46,55	0
2	CTP	A	301	29/29	0.98	0.05	25,28,36,49	0
3	CL	F	303	1/1	0.98	0.16	58,58,58,58	0
2	CTP	F	301	29/29	0.98	0.05	30,33,40,46	0

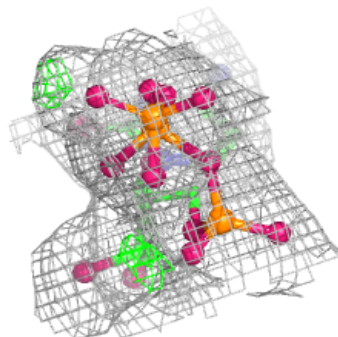
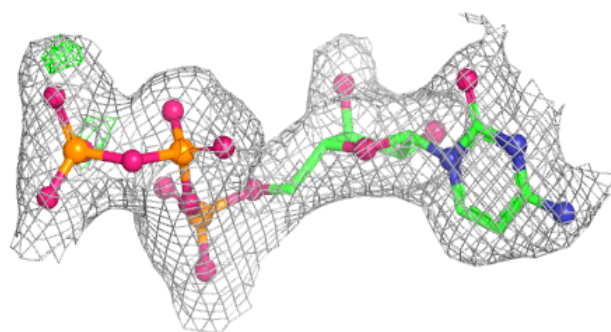
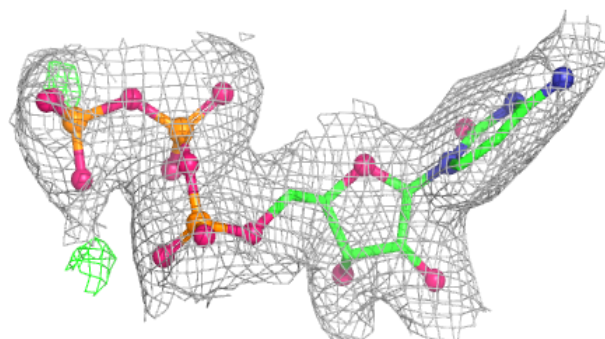
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CTP C 301:

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

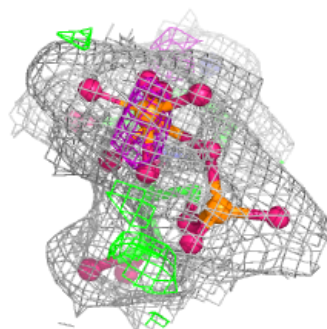
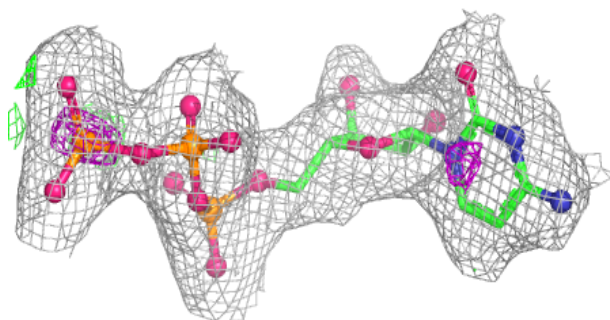
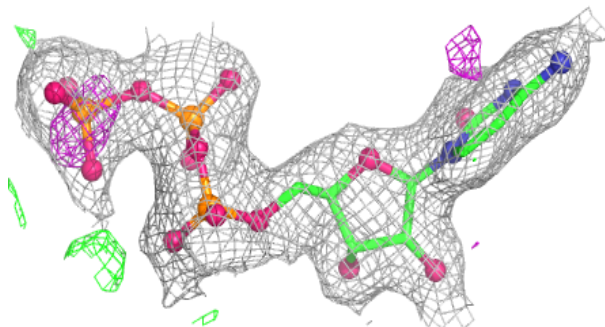
**Electron density around CTP D 301:**

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

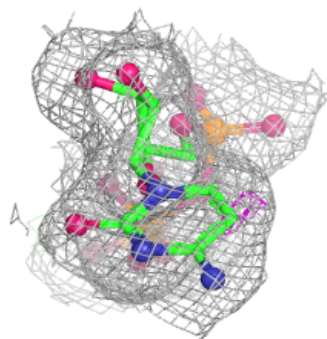
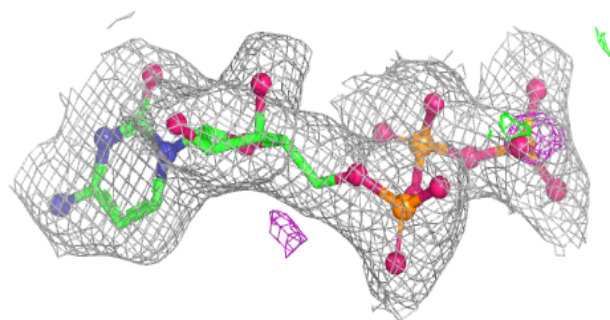
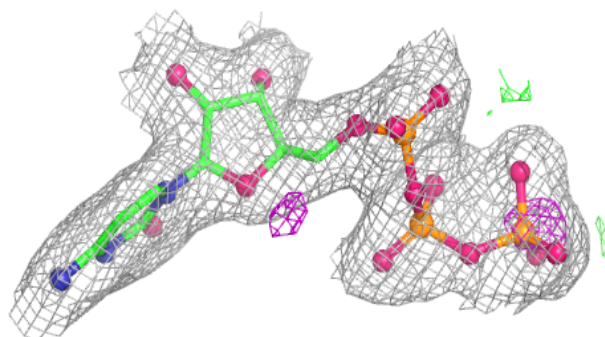


Electron density around CTP E 301:

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

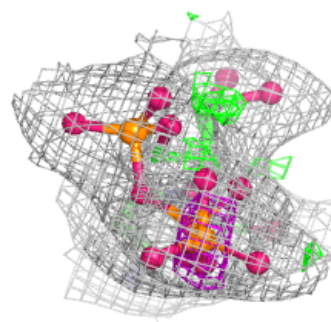
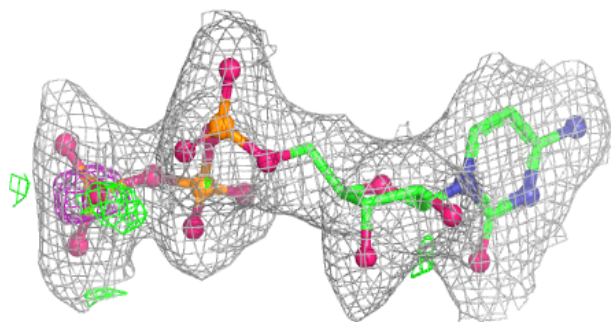
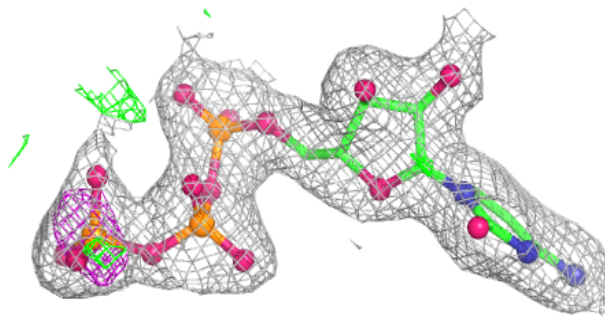
**Electron density around CTP B 301:**

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

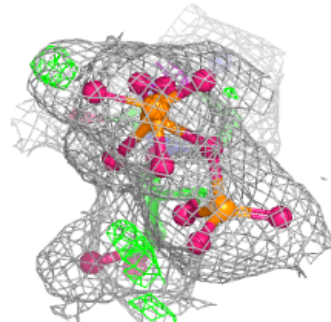
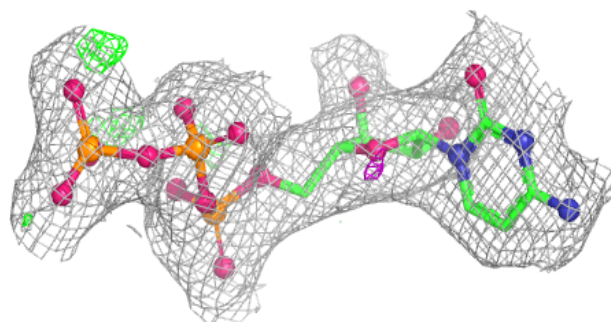
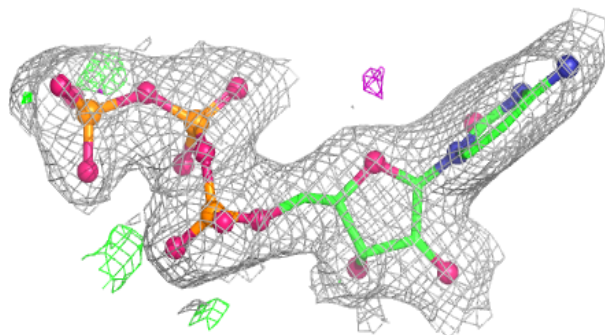


Electron density around CTP A 301:

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

**Electron density around CTP F 301:**

$2mF_o-DF_c$ (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.