



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:02 PM UTC

PDB ID : 1TFY / pdb_00001tfy
Title : How CCA is added to the 3' end of immature tRNA without the use of an oligonucleotide template
Authors : Xiong, Y.; Steitz, T.A.
Deposited on : 2004-05-27
Resolution : 3.20 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

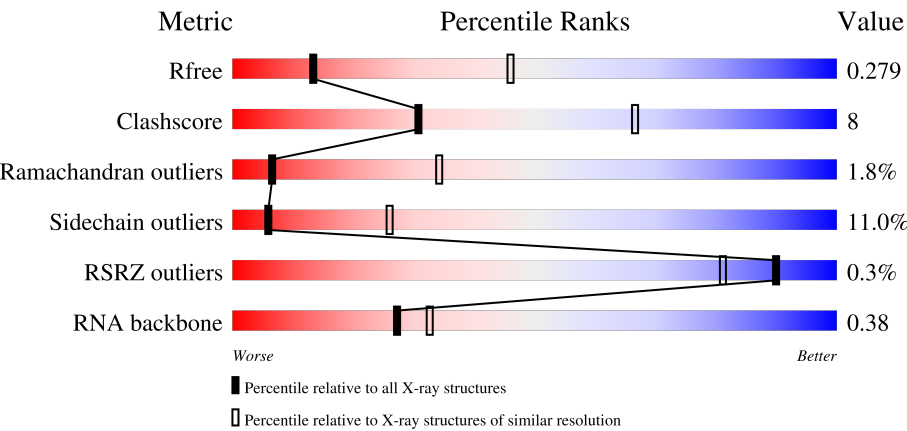
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	E	13	8% 69% 23% 8%
1	F	13	46% 54%
2	H	14	14% 64% 14% 21%
2	I	14	50% 43% 7%

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Mol	Chain	Length	Quality of chain
3	G	11	9%36%36%18%
4	J	8	12%12%88%
5	A	437	78%17%5%
5	B	437	74%23%•
5	C	437	70%26%•
5	D	437	73%23%•

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16180 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 RNA chain called 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*C P*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			276	124	51	89	12			
1	F	13	Total	C	N	O	P	0	0	0
			276	124	51	89	12			

- Molecule 2 is a RNA chain called 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*C P*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	14	Total	C	N	O	P	0	0	0
			295	133	54	95	13			
2	I	14	Total	C	N	O	P	0	0	0
			295	133	54	95	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	11	Total	C	N	O	P	0	0	0
			230	104	42	74	10			

- Molecule 4 is a RNA chain called 5'-R(*CP*GP*CP*GP*GP*AP*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	8	Total	C	N	O	P	0	0	0
			168	76	31	54	7			

- Molecule 5 is a protein called tRNA nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

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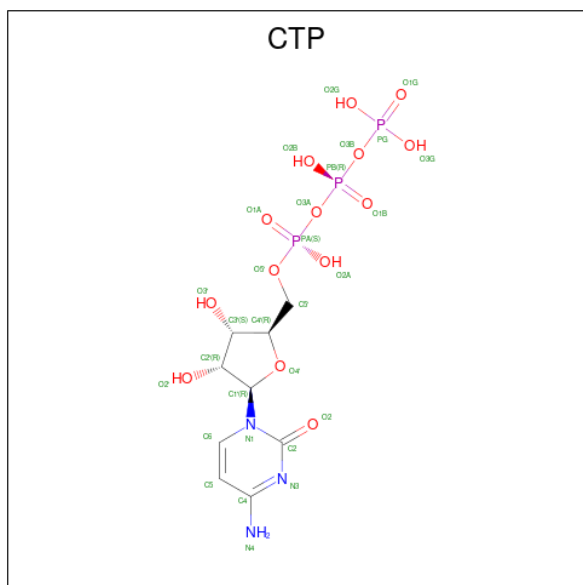
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	C	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	D	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
7	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

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.

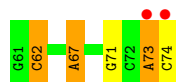
- Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'



- Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'



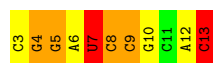
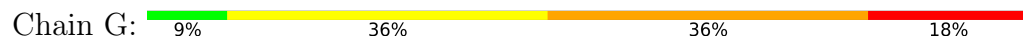
- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*AP*C)-3'



- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*AP*C)-3'



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



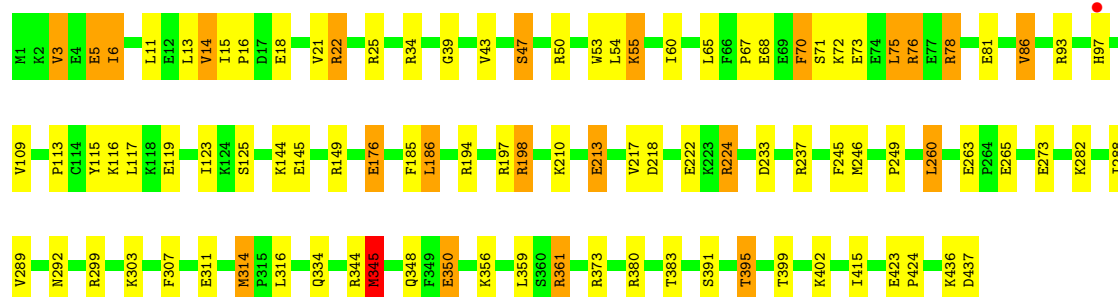
- Molecule 4: 5'-R(*CP*GP*CP*GP*GP*AP*UP*C)-3'



C61
G62
G63
G64
G65
A66
U67
C68

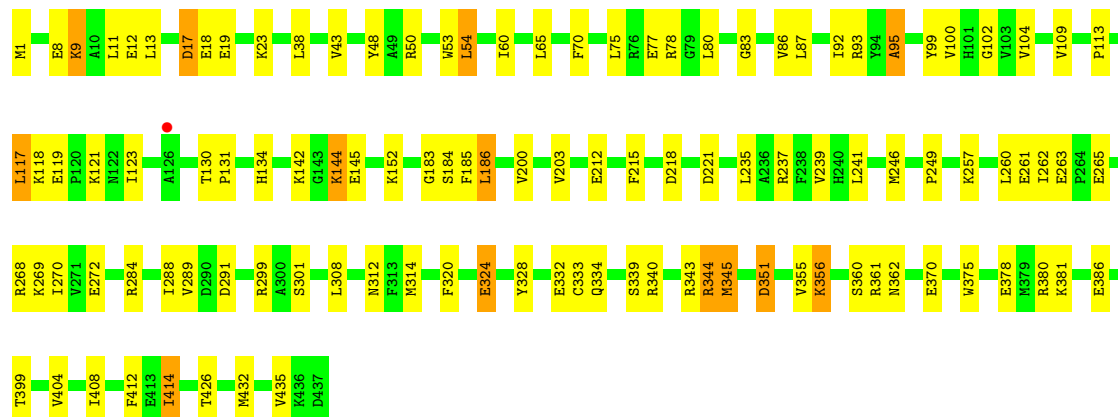
• Molecule 5: tRNA nucleotidyltransferase

Chain A: 78% 17% 5%



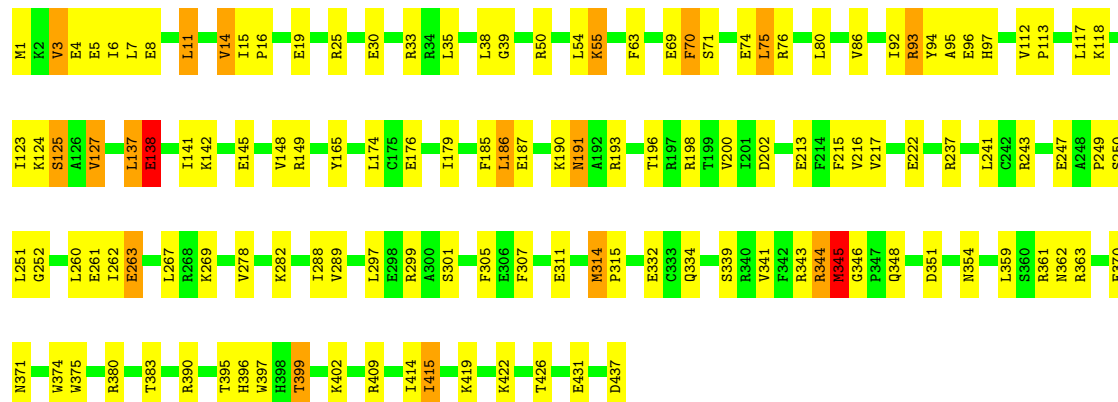
• Molecule 5: tRNA nucleotidyltransferase

Chain B: 74% 23% .

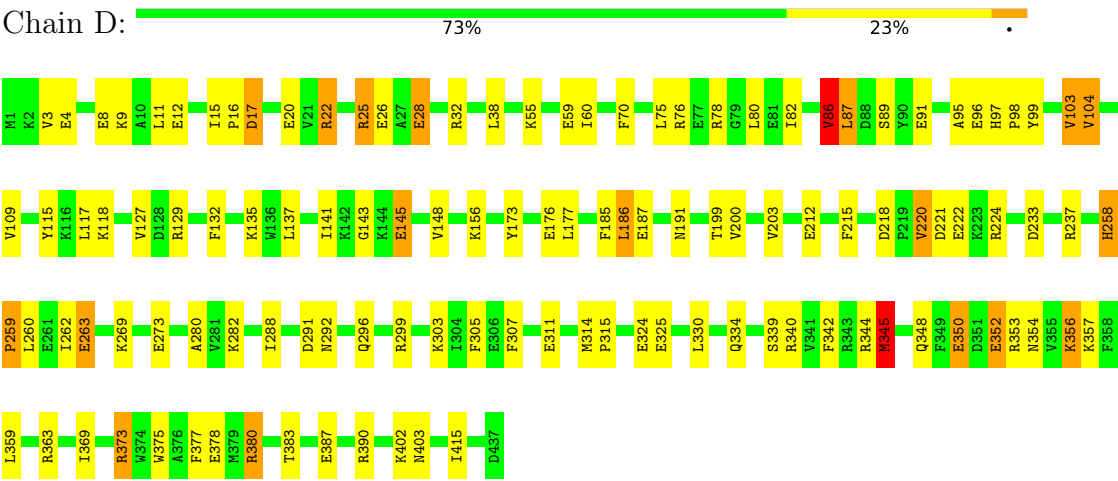


• Molecule 5: tRNA nucleotidyltransferase

Chain C: 70% 26% .



● Molecule 5: tRNA nucleotidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.09Å 84.02Å 134.56Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	44.28 – 3.20 44.28 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.28-3.20) 98.8 (44.28-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.235 , 0.290 0.226 , 0.279	Depositor DCC
R_{free} test set	2053 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	103.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 120.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16180	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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, CTP

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	E	0.55	0/308	0.92	0/479
1	F	0.60	0/308	0.81	0/479
2	H	0.62	0/329	1.03	0/511
2	I	0.60	0/329	1.05	1/511 (0.2%)
3	G	0.80	1/256 (0.4%)	1.56	6/397 (1.5%)
4	J	0.61	0/187	0.97	0/290
5	A	0.42	0/3713	0.82	0/4987
5	B	0.44	0/3713	0.81	0/4987
5	C	0.42	0/3713	0.82	1/4987 (0.0%)
5	D	0.46	0/3713	0.85	4/4987 (0.1%)
All	All	0.46	1/16569 (0.0%)	0.86	12/22615 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	13	C	C1'-N1	6.13	1.56	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5	G	P-O3'-C3'	-9.58	105.83	120.20
3	G	8	C	P-O3'-C3'	-8.30	107.75	120.20
3	G	7	U	C4'-C3'-O3'	-6.90	102.65	113.00
5	D	258	HIS	CA-C-N	6.75	128.28	119.84
5	D	258	HIS	C-N-CA	6.75	128.28	119.84
3	G	7	U	O4'-C4'-C3'	-5.93	98.07	104.00
3	G	6	A	P-O3'-C3'	-5.90	111.35	120.20
5	D	350	GLU	N-CA-C	5.89	117.57	111.03
5	D	3	VAL	N-CA-C	5.37	115.82	110.23
2	I	64	G	C4'-C3'-C2'	-5.32	97.28	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	6	A	O5'-C5'-C4'	-5.07	103.89	111.50
5	C	363	ARG	N-CA-C	5.01	115.92	108.86

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	E	276	0	143	4	0
1	F	276	0	143	3	0
2	H	295	0	154	3	0
2	I	295	0	154	2	0
3	G	230	0	122	12	0
4	J	168	0	89	11	0
5	A	3630	0	3633	65	0
5	B	3630	0	3633	58	0
5	C	3630	0	3633	80	0
5	D	3630	0	3633	65	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	29	0	12	0	0
7	B	29	0	12	0	0
7	C	29	0	12	0	0
7	D	29	0	12	1	0
All	All	16180	0	15385	261	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.

All (261) 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)
5:A:198:ARG:HG2	5:A:198:ARG:HH11	1.02	1.11
5:A:198:ARG:HG2	5:A:198:ARG:NH1	1.78	0.89
5:C:395:THR:HG23	5:C:396:HIS:HD2	1.40	0.87
5:D:132:PHE:HB3	5:D:220:VAL:HG21	1.55	0.87
5:D:22:ARG:HE	5:D:25:ARG:HG2	1.39	0.87
5:A:345:MET:HE1	5:C:70:PHE:CZ	2.13	0.83
5:A:71:SER:C	5:A:73:GLU:H	1.88	0.80
5:C:14:VAL:HG13	5:C:149:ARG:HB3	1.64	0.79
3:G:7:U:H3	4:J:66:A:H61	1.31	0.79
5:C:186:LEU:O	5:C:190:LYS:HB2	1.83	0.78
5:A:16:PRO:HA	5:A:55:LYS:HG2	1.66	0.77
5:C:267:LEU:HD22	5:C:426:THR:HG23	1.66	0.76
5:C:299:ARG:NH1	5:C:399:THR:O	2.18	0.75
5:D:141:ILE:HD11	5:D:148:VAL:HG21	1.67	0.74
5:A:198:ARG:HH11	5:A:198:ARG:CG	1.93	0.73
5:D:344:ARG:O	5:D:345:MET:HB3	1.88	0.73
5:A:391:SER:O	5:A:395:THR:HG22	1.88	0.73
5:A:314:MET:HE1	5:B:312:ASN:HB3	1.72	0.72
5:B:268:ARG:HH21	5:B:269:LYS:HE2	1.55	0.71
5:C:380:ARG:HH12	5:D:334:GLN:NE2	1.89	0.70
5:A:299:ARG:NH1	5:A:399:THR:O	2.24	0.70
5:A:314:MET:HE3	5:B:314:MET:HE2	1.74	0.70
1:E:12:C:H2'	1:E:13:G:O4'	1.92	0.69
5:D:87:LEU:HD23	5:D:104:VAL:HG23	1.76	0.68
5:C:380:ARG:HH12	5:D:334:GLN:HE21	1.41	0.68
5:C:14:VAL:CG1	5:C:149:ARG:HB3	2.24	0.68
5:C:395:THR:HG23	5:C:396:HIS:CD2	2.24	0.68
5:B:83:GLY:HA3	5:B:100:VAL:HG21	1.76	0.67
5:B:95:ALA:HB3	5:B:99:TYR:HE2	1.60	0.66
5:A:380:ARG:HH22	5:B:334:GLN:HE22	1.42	0.66
5:A:43:VAL:HG22	5:A:65:LEU:HD11	1.77	0.66
5:C:124:LYS:O	5:C:125:SER:HB3	1.95	0.66
5:B:344:ARG:O	5:B:345:MET:HB3	1.96	0.65
5:C:16:PRO:HA	5:C:55:LYS:HG2	1.78	0.65
5:C:50:ARG:HD3	5:C:137:LEU:HB3	1.77	0.65
5:B:185:PHE:O	5:B:186:LEU:CB	2.44	0.65
5:C:30:GLU:HA	5:C:33:ARG:NH1	2.12	0.65
4:J:62:G:N2	5:C:165:TYR:HE1	1.95	0.65
5:B:345:MET:HB2	5:B:375:TRP:CZ3	2.32	0.64
5:A:3:VAL:HG22	5:A:249:PRO:HG2	1.80	0.64
5:D:82:ILE:O	5:D:86:VAL:HB	1.98	0.63
5:D:173:TYR:HB2	7:D:504:CTP:H2'	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:280:ALA:HB2	5:D:330:LEU:HD23	1.81	0.63
5:B:332:GLU:HB2	5:B:432:MET:HE3	1.79	0.63
5:C:185:PHE:O	5:C:186:LEU:CB	2.47	0.63
3:G:5:G:O2'	5:A:292:ASN:ND2	2.32	0.62
5:D:95:ALA:HB3	5:D:99:TYR:HE2	1.63	0.62
3:G:9:C:OP2	3:G:9:C:H6	1.82	0.62
3:G:7:U:H3	4:J:66:A:N6	1.98	0.61
5:B:19:GLU:O	5:B:23:LYS:HB2	2.01	0.61
5:C:344:ARG:O	5:C:345:MET:HB3	1.99	0.61
5:B:87:LEU:HD23	5:B:104:VAL:HG23	1.83	0.60
3:G:9:C:OP2	3:G:9:C:C6	2.54	0.60
5:B:339:SER:O	5:B:380:ARG:HD2	2.01	0.60
5:A:47:SER:HB3	5:A:53:TRP:HB3	1.83	0.60
3:G:12:A:H61	4:J:61:C:H42	1.49	0.60
5:C:185:PHE:O	5:C:186:LEU:HB3	2.02	0.60
5:C:63:PHE:CE2	5:C:127:VAL:HG12	2.37	0.59
4:J:62:G:N2	5:C:165:TYR:CE1	2.71	0.59
5:A:71:SER:O	5:A:73:GLU:N	2.35	0.59
5:C:282:LYS:HD2	5:C:415:ILE:HD11	1.85	0.59
5:A:22:ARG:HA	5:A:25:ARG:HB2	1.85	0.58
5:D:11:LEU:HB3	5:D:15:ILE:HD12	1.84	0.58
5:C:96:GLU:HG2	5:C:127:VAL:CG2	2.34	0.58
5:A:198:ARG:NH1	5:A:198:ARG:CG	2.61	0.57
5:A:68:GLU:HA	5:A:115:TYR:CD2	2.40	0.57
5:D:22:ARG:HA	5:D:25:ARG:HB3	1.87	0.57
5:A:345:MET:HE1	5:C:70:PHE:CE1	2.39	0.57
4:J:63:C:H2'	4:J:64:G:C8	2.39	0.56
5:A:380:ARG:HH22	5:B:334:GLN:NE2	2.01	0.56
5:C:371:ASN:N	5:D:233:ASP:OD1	2.39	0.56
5:D:129:ARG:NH1	5:D:224:ARG:HD3	2.21	0.56
5:B:17:ASP:OD2	5:B:19:GLU:HB3	2.06	0.56
2:H:73:A:O2'	5:B:291:ASP:OD2	2.25	0.55
5:D:95:ALA:HB3	5:D:99:TYR:CE2	2.42	0.55
5:D:233:ASP:HB3	5:D:237:ARG:NH1	2.22	0.55
5:D:129:ARG:CZ	5:D:224:ARG:HD3	2.37	0.55
5:A:380:ARG:HH12	5:B:334:GLN:NE2	2.05	0.55
5:A:65:LEU:HD23	5:A:116:LYS:HG3	1.89	0.54
5:A:307:PHE:CE1	5:A:311:GLU:HG3	2.42	0.54
5:D:305:PHE:CE1	5:D:315:PRO:HB2	2.42	0.54
5:C:187:GLU:O	5:C:191:ASN:HB2	2.07	0.54
5:B:43:VAL:HG22	5:B:65:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:11:LEU:O	5:C:15:ILE:HG12	2.08	0.54
3:G:12:A:N6	4:J:61:C:H42	2.07	0.53
5:B:50:ARG:HE	5:B:134:HIS:HA	1.72	0.53
5:A:34:ARG:HB3	5:A:86:VAL:HG22	1.91	0.53
5:A:185:PHE:O	5:A:186:LEU:CB	2.56	0.53
5:A:348:GLN:NE2	5:C:39:GLY:O	2.42	0.53
5:C:196:THR:HG23	5:C:198:ARG:H	1.72	0.53
5:C:278:VAL:HG22	5:C:332:GLU:HG3	1.91	0.53
5:D:185:PHE:O	5:D:186:LEU:CB	2.57	0.52
5:D:185:PHE:O	5:D:186:LEU:HB3	2.10	0.52
5:D:354:ASN:HA	5:D:357:LYS:HG2	1.91	0.52
5:A:14:VAL:HG13	5:A:149:ARG:HB3	1.92	0.52
4:J:67:U:OP1	5:A:224:ARG:NH1	2.42	0.52
5:B:53:TRP:HD1	5:B:54:LEU:O	1.93	0.52
5:C:334:GLN:HG2	5:D:339:SER:OG	2.10	0.52
5:B:144:LYS:HZ1	5:B:183:GLY:HA2	1.75	0.51
5:B:356:LYS:O	5:B:360:SER:HB3	2.10	0.51
5:C:200:VAL:HG22	5:C:215:PHE:HB3	1.92	0.51
5:D:89:SER:HB3	5:D:103:VAL:HG12	1.92	0.51
5:A:218:ASP:HB2	5:A:224:ARG:HG2	1.93	0.51
5:C:93:ARG:HD3	5:C:94:TYR:H	1.76	0.51
5:D:17:ASP:HB2	5:D:20:GLU:HB2	1.92	0.51
5:D:22:ARG:NE	5:D:25:ARG:HG2	2.19	0.50
5:D:200:VAL:HG13	5:D:215:PHE:HB3	1.93	0.50
1:E:11:G:H1	2:H:62:C:H42	1.59	0.50
4:J:63:C:H2'	4:J:64:G:H8	1.76	0.50
5:C:137:LEU:O	5:C:138:GLU:C	2.54	0.50
5:B:185:PHE:O	5:B:186:LEU:HB2	2.11	0.50
5:D:4:GLU:O	5:D:8:GLU:HG3	2.11	0.50
5:A:350:GLU:HG3	5:C:38:LEU:C	2.36	0.50
5:A:299:ARG:O	5:A:303:LYS:HG2	2.12	0.50
3:G:13:C:H2'	5:C:95:ALA:HA	1.94	0.49
5:A:423:GLU:HB3	5:A:424:PRO:HD2	1.94	0.49
5:B:83:GLY:O	5:B:87:LEU:HD12	2.11	0.49
5:C:75:LEU:HD12	5:C:76:ARG:N	2.27	0.49
5:C:314:MET:HE1	5:D:314:MET:HE1	1.94	0.49
5:A:380:ARG:HH12	5:B:334:GLN:HE21	1.59	0.49
5:C:345:MET:HE2	5:C:375:TRP:CH2	2.47	0.49
5:C:307:PHE:CE1	5:C:311:GLU:HG3	2.47	0.49
3:G:3:C:H3'	3:G:4:G:C5'	2.42	0.49
5:C:343:ARG:HH22	5:C:370:GLU:CD	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:263:GLU:C	5:A:265:GLU:H	2.21	0.49
5:A:75:LEU:HD22	5:A:113:PRO:HB2	1.95	0.49
5:A:314:MET:HB2	5:A:334:GLN:HB2	1.94	0.49
5:C:35:LEU:HD23	5:C:86:VAL:HG21	1.94	0.48
5:C:190:LYS:HG2	5:C:193:ARG:HH21	1.78	0.48
5:C:260:LEU:HD23	5:C:437:ASP:HB2	1.94	0.48
5:C:314:MET:HE1	5:D:314:MET:CE	2.42	0.48
5:C:124:LYS:O	5:C:125:SER:CB	2.61	0.48
5:D:218:ASP:HB2	5:D:224:ARG:O	2.14	0.48
5:B:87:LEU:HD22	5:B:102:GLY:HA3	1.96	0.48
5:D:187:GLU:O	5:D:191:ASN:HB2	2.13	0.48
5:A:47:SER:HB3	5:A:53:TRP:CB	2.44	0.48
5:A:50:ARG:NH1	5:A:176:GLU:OE2	2.46	0.48
5:B:269:LYS:HA	5:B:272:GLU:HB3	1.94	0.48
5:D:9:LYS:O	5:D:12:GLU:HG2	2.13	0.48
2:I:73:A:O2'	5:D:291:ASP:OD2	2.27	0.48
5:B:343:ARG:HH22	5:B:370:GLU:CD	2.22	0.48
5:A:345:MET:HG2	5:A:373:ARG:HD3	1.95	0.48
5:D:356:LYS:HA	5:D:359:LEU:HB2	1.96	0.48
5:D:387:GLU:HA	5:D:390:ARG:NH2	2.28	0.48
3:G:7:U:H5'	5:A:299:ARG:HD2	1.96	0.47
5:B:386:GLU:HB3	5:B:414:ILE:HG21	1.96	0.47
5:B:185:PHE:O	5:B:186:LEU:HB3	2.14	0.47
5:C:174:LEU:HD11	5:C:216:VAL:HG21	1.95	0.47
5:D:348:GLN:C	5:D:350:GLU:H	2.21	0.47
5:B:60:ILE:HB	5:B:109:VAL:HG22	1.96	0.47
5:C:148:VAL:HA	5:C:179:ILE:HG13	1.95	0.47
5:C:237:ARG:HG3	5:D:369:ILE:HD12	1.97	0.47
5:C:297:LEU:O	5:C:301:SER:HB2	2.14	0.47
5:C:305:PHE:CE1	5:C:315:PRO:HB2	2.50	0.47
5:B:235:LEU:O	5:B:239:VAL:HG23	2.14	0.47
5:C:75:LEU:HD12	5:C:75:LEU:C	2.41	0.46
5:B:144:LYS:NZ	5:B:183:GLY:HA2	2.31	0.46
5:D:296:GLN:HE22	5:D:403:ASN:H	1.64	0.46
5:C:63:PHE:HE2	5:C:127:VAL:HG12	1.77	0.46
5:C:314:MET:HE3	5:C:314:MET:HB2	1.71	0.46
5:C:243:ARG:NH2	5:D:350:GLU:O	2.32	0.46
5:C:30:GLU:HA	5:C:33:ARG:HH11	1.80	0.46
5:C:397:TRP:CE2	5:C:409:ARG:HD2	2.51	0.46
5:A:344:ARG:O	5:A:345:MET:CB	2.64	0.46
5:D:60:ILE:HB	5:D:109:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:197:ARG:O	5:A:213:GLU:HA	2.15	0.45
5:B:93:ARG:HD3	5:B:289:VAL:HG11	1.98	0.45
5:D:345:MET:HB2	5:D:375:TRP:CZ3	2.51	0.45
5:A:282:LYS:HD3	5:A:415:ILE:HD11	1.98	0.45
5:B:324:GLU:OE2	5:B:324:GLU:HA	2.16	0.45
5:C:141:ILE:HD11	5:C:148:VAL:HG21	1.99	0.45
5:B:340:ARG:O	5:B:380:ARG:HG3	2.17	0.45
5:A:314:MET:CE	5:B:312:ASN:HB3	2.44	0.45
5:B:54:LEU:HD11	5:B:152:LYS:HB2	1.99	0.45
5:A:76:ARG:HG2	5:A:97:HIS:HB3	1.98	0.45
5:B:344:ARG:HG3	5:B:378:GLU:OE2	2.16	0.44
5:B:351:ASP:O	5:B:355:VAL:HG23	2.17	0.44
5:C:75:LEU:HD13	5:C:113:PRO:HB2	1.99	0.44
5:C:346:GLY:N	5:C:374:TRP:O	2.45	0.44
5:C:334:GLN:HE21	5:D:380:ARG:HH12	1.63	0.44
5:D:15:ILE:HA	5:D:16:PRO:HD3	1.90	0.44
5:D:307:PHE:CE1	5:D:311:GLU:HG3	2.53	0.44
5:D:348:GLN:C	5:D:350:GLU:N	2.76	0.44
5:D:258:HIS:HA	5:D:259:PRO:HD3	1.90	0.44
5:A:361:ARG:H	5:A:361:ARG:HG2	1.65	0.44
5:B:320:PHE:HA	5:B:328:TYR:O	2.18	0.44
5:C:339:SER:O	5:C:380:ARG:HD2	2.17	0.44
5:D:342:PHE:O	5:D:377:PHE:HA	2.18	0.44
1:F:8:U:H3	2:I:65:A:H61	1.66	0.43
5:D:263:GLU:CD	5:D:263:GLU:H	2.26	0.43
5:C:3:VAL:HG22	5:C:249:PRO:HG2	1.99	0.43
5:D:369:ILE:HA	5:D:373:ARG:O	2.18	0.43
5:C:263:GLU:H	5:C:263:GLU:HG2	1.53	0.43
5:C:345:MET:HE2	5:C:345:MET:HB2	1.91	0.43
5:D:212:GLU:OE1	5:D:212:GLU:HA	2.18	0.43
5:B:8:GLU:HA	5:B:11:LEU:HD12	2.00	0.43
5:B:48:TYR:HA	5:B:53:TRP:CE3	2.54	0.43
5:C:70:PHE:HB3	5:C:71:SER:H	1.60	0.43
5:A:18:GLU:O	5:A:21:VAL:HG12	2.17	0.43
5:A:233:ASP:O	5:A:237:ARG:HB2	2.19	0.43
5:B:1:MET:HG3	5:B:249:PRO:HD2	2.01	0.43
5:D:143:GLY:N	5:D:145:GLU:OE1	2.51	0.43
5:A:14:VAL:CG1	5:A:149:ARG:HB3	2.49	0.43
5:A:245:PHE:O	5:A:246:MET:C	2.62	0.43
5:B:142:LYS:HA	5:B:145:GLU:OE2	2.19	0.43
5:A:78:ARG:HH22	5:A:81:GLU:CD	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:185:PHE:O	5:A:186:LEU:HB2	2.18	0.42
5:D:218:ASP:HB3	5:D:221:ASP:O	2.19	0.42
5:D:282:LYS:HD3	5:D:415:ILE:HD11	2.01	0.42
5:C:137:LEU:HD23	5:C:141:ILE:HB	2.01	0.42
5:C:397:TRP:CE2	5:C:409:ARG:CD	3.02	0.42
5:C:250:SER:C	5:C:252:GLY:H	2.27	0.42
5:D:75:LEU:HD11	5:D:115:TYR:CE1	2.54	0.42
1:F:1:G:H5'	5:D:402:LYS:HE3	2.01	0.42
5:A:67:PRO:HG2	5:A:70:PHE:CE1	2.54	0.42
5:B:75:LEU:HD22	5:B:113:PRO:HB2	2.01	0.42
5:C:344:ARG:HA	5:C:344:ARG:HD2	1.88	0.42
4:J:62:G:H22	5:C:165:TYR:HE1	1.66	0.42
5:B:408:ILE:HG23	5:B:412:PHE:HB3	2.00	0.42
3:G:3:C:H3'	3:G:4:G:H5'	2.02	0.42
5:C:202:ASP:HA	5:C:217:VAL:HB	2.01	0.42
5:C:351:ASP:CG	5:C:354:ASN:HB2	2.45	0.42
5:A:314:MET:HE1	5:B:312:ASN:CB	2.43	0.42
5:A:345:MET:SD	5:C:74:GLU:HG2	2.59	0.42
5:C:7:LEU:HD11	5:C:186:LEU:HD13	2.02	0.42
5:C:247:GLU:C	5:C:249:PRO:HD3	2.45	0.42
5:D:282:LYS:HD3	5:D:415:ILE:CD1	2.50	0.42
1:F:5:A:H2'	1:F:6:U:C6	2.54	0.42
5:D:76:ARG:O	5:D:80:LEU:HB2	2.19	0.42
5:A:260:LEU:HD23	5:A:437:ASP:OD2	2.20	0.41
5:B:185:PHE:CD1	5:B:185:PHE:C	2.98	0.41
5:A:39:GLY:O	5:C:348:GLN:NE2	2.53	0.41
5:B:130:THR:N	5:B:131:PRO:HD2	2.35	0.41
5:D:137:LEU:HD21	5:D:177:LEU:HD23	2.01	0.41
1:E:6:U:H3	2:H:67:A:H61	1.69	0.41
3:G:12:A:H61	4:J:61:C:N4	2.15	0.41
5:B:200:VAL:HA	5:B:215:PHE:O	2.20	0.41
5:D:80:LEU:HD11	5:D:98:PRO:HB2	2.02	0.41
5:D:137:LEU:HD13	5:D:176:GLU:OE1	2.20	0.41
5:A:11:LEU:HD22	5:A:15:ILE:HD11	2.03	0.41
5:B:53:TRP:CD1	5:B:54:LEU:O	2.72	0.41
5:C:137:LEU:HD21	5:C:176:GLU:HB3	2.02	0.41
5:A:60:ILE:HB	5:A:109:VAL:HG13	2.02	0.41
5:D:345:MET:HE3	5:D:373:ARG:HH12	1.85	0.41
5:A:71:SER:C	5:A:73:GLU:N	2.59	0.41
5:B:218:ASP:HB3	5:B:221:ASP:O	2.20	0.41
5:B:299:ARG:NH1	5:B:399:THR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:75:LEU:HD13	5:A:76:ARG:N	2.36	0.41
5:C:76:ARG:HE	5:C:97:HIS:CE1	2.39	0.41
5:C:247:GLU:O	5:C:249:PRO:HD3	2.20	0.41
5:A:5:GLU:HG3	5:A:6:ILE:N	2.34	0.41
5:B:9:LYS:O	5:B:12:GLU:HG2	2.20	0.41
5:C:243:ARG:CZ	5:D:352:GLU:HG3	2.50	0.41
5:B:221:ASP:OD1	5:B:221:ASP:C	2.65	0.40
5:A:350:GLU:H	5:A:350:GLU:HG2	1.65	0.40
5:B:308:LEU:HD13	5:B:333:CYS:SG	2.61	0.40
5:D:28:GLU:OE2	5:D:32:ARG:NE	2.51	0.40
5:A:68:GLU:HA	5:A:115:TYR:HD2	1.83	0.40
1:E:13:G:H5"	1:E:13:G:H8	1.87	0.40
5:B:263:GLU:C	5:B:265:GLU:H	2.30	0.40
5:D:363:ARG:NE	5:D:378:GLU:OE2	2.52	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	
5	A	435/437 (100%)	404 (93%)	23 (5%)	8 (2%)	6	34
5	B	435/437 (100%)	395 (91%)	32 (7%)	8 (2%)	6	34
5	C	435/437 (100%)	403 (93%)	23 (5%)	9 (2%)	5	31
5	D	435/437 (100%)	390 (90%)	39 (9%)	6 (1%)	9	39
All	All	1740/1748 (100%)	1592 (92%)	117 (7%)	31 (2%)	6	34

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	72	LYS

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Mol	Chain	Res	Type
5	A	186	LEU
5	B	186	LEU
5	C	70	PHE
5	C	117	LEU
5	C	125	SER
5	C	186	LEU
5	D	186	LEU
5	A	117	LEU
5	B	184	SER
5	B	351	ASP
5	D	86	VAL
5	A	70	PHE
5	B	261	GLU
5	C	261	GLU
5	D	96	GLU
5	D	117	LEU
5	D	345	MET
5	A	125	SER
5	C	138	GLU
5	C	402	LYS
5	A	3	VAL
5	A	345	MET
5	B	95	ALA
5	B	345	MET
5	A	402	LYS
5	B	117	LEU
5	C	345	MET
5	C	3	VAL
5	D	259	PRO
5	B	123	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
5	A	387/387 (100%)	348 (90%)	39 (10%)	7 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	387/387 (100%)	348 (90%)	39 (10%)	7	30
5	C	387/387 (100%)	338 (87%)	49 (13%)	4	20
5	D	387/387 (100%)	343 (89%)	44 (11%)	5	24
All	All	1548/1548 (100%)	1377 (89%)	171 (11%)	6	26

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	5	GLU
5	A	6	ILE
5	A	13	LEU
5	A	14	VAL
5	A	22	ARG
5	A	47	SER
5	A	54	LEU
5	A	55	LYS
5	A	75	LEU
5	A	76	ARG
5	A	78	ARG
5	A	86	VAL
5	A	93	ARG
5	A	119	GLU
5	A	123	ILE
5	A	144	LYS
5	A	145	GLU
5	A	176	GLU
5	A	194	ARG
5	A	198	ARG
5	A	210	LYS
5	A	213	GLU
5	A	217	VAL
5	A	222	GLU
5	A	224	ARG
5	A	260	LEU
5	A	273	GLU
5	A	288	ILE
5	A	289	VAL
5	A	314	MET
5	A	316	LEU
5	A	345	MET
5	A	350	GLU

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Mol	Chain	Res	Type
5	A	356	LYS
5	A	359	LEU
5	A	361	ARG
5	A	383	THR
5	A	395	THR
5	A	436	LYS
5	B	9	LYS
5	B	13	LEU
5	B	17	ASP
5	B	18	GLU
5	B	38	LEU
5	B	54	LEU
5	B	70	PHE
5	B	77	GLU
5	B	78	ARG
5	B	80	LEU
5	B	86	VAL
5	B	92	ILE
5	B	117	LEU
5	B	118	LYS
5	B	119	GLU
5	B	121	LYS
5	B	144	LYS
5	B	203	VAL
5	B	212	GLU
5	B	237	ARG
5	B	241	LEU
5	B	246	MET
5	B	257	LYS
5	B	260	LEU
5	B	262	ILE
5	B	270	ILE
5	B	284	ARG
5	B	288	ILE
5	B	301	SER
5	B	324	GLU
5	B	344	ARG
5	B	356	LYS
5	B	361	ARG
5	B	362	ASN
5	B	381	LYS
5	B	404	VAL

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Mol	Chain	Res	Type
5	B	414	ILE
5	B	426	THR
5	B	435	VAL
5	C	1	MET
5	C	4	GLU
5	C	5	GLU
5	C	6	ILE
5	C	8	GLU
5	C	11	LEU
5	C	14	VAL
5	C	19	GLU
5	C	25	ARG
5	C	54	LEU
5	C	55	LYS
5	C	69	GLU
5	C	75	LEU
5	C	80	LEU
5	C	92	ILE
5	C	93	ARG
5	C	112	VAL
5	C	118	LYS
5	C	123	ILE
5	C	127	VAL
5	C	137	LEU
5	C	138	GLU
5	C	142	LYS
5	C	145	GLU
5	C	191	ASN
5	C	213	GLU
5	C	222	GLU
5	C	241	LEU
5	C	251	LEU
5	C	262	ILE
5	C	263	GLU
5	C	269	LYS
5	C	288	ILE
5	C	289	VAL
5	C	314	MET
5	C	341	VAL
5	C	344	ARG
5	C	345	MET
5	C	359	LEU

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Mol	Chain	Res	Type
5	C	361	ARG
5	C	362	ASN
5	C	383	THR
5	C	390	ARG
5	C	399	THR
5	C	414	ILE
5	C	415	ILE
5	C	419	LYS
5	C	422	LYS
5	C	431	GLU
5	D	17	ASP
5	D	22	ARG
5	D	25	ARG
5	D	26	GLU
5	D	28	GLU
5	D	38	LEU
5	D	55	LYS
5	D	59	GLU
5	D	70	PHE
5	D	78	ARG
5	D	86	VAL
5	D	87	LEU
5	D	91	GLU
5	D	97	HIS
5	D	103	VAL
5	D	104	VAL
5	D	118	LYS
5	D	127	VAL
5	D	135	LYS
5	D	145	GLU
5	D	156	LYS
5	D	199	THR
5	D	203	VAL
5	D	220	VAL
5	D	222	GLU
5	D	260	LEU
5	D	262	ILE
5	D	263	GLU
5	D	269	LYS
5	D	273	GLU
5	D	288	ILE
5	D	292	ASN

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Mol	Chain	Res	Type
5	D	299	ARG
5	D	303	LYS
5	D	324	GLU
5	D	325	GLU
5	D	340	ARG
5	D	345	MET
5	D	352	GLU
5	D	353	ARG
5	D	356	LYS
5	D	373	ARG
5	D	380	ARG
5	D	383	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	229	ASN
5	A	292	ASN
5	A	348	GLN
5	A	396	HIS
5	B	97	HIS
5	B	312	ASN
5	B	334	GLN
5	B	348	GLN
5	C	191	ASN
5	C	240	HIS
5	C	334	GLN
5	C	362	ASN
5	C	396	HIS
5	D	334	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	12/13 (92%)	1 (8%)	0
1	F	12/13 (92%)	3 (25%)	0
2	H	13/14 (92%)	5 (38%)	1 (7%)
2	I	13/14 (92%)	4 (30%)	1 (7%)
3	G	10/11 (90%)	6 (60%)	0
4	J	7/8 (87%)	1 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	67/73 (91%)	20 (29%)	2 (2%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	12	C
2	H	62	C
2	H	67	A
2	H	71	G
2	H	73	A
2	H	74	C
1	F	11	G
1	F	12	C
1	F	13	G
2	I	62	C
2	I	66	U
2	I	67	A
2	I	74	C
3	G	4	G
3	G	7	U
3	G	8	C
3	G	9	C
3	G	10	G
3	G	13	C
4	J	68	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	73	A
2	I	73	A

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 oligosaccharides 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
7	CTP	C	503	6	29,30,30	1.44	4 (13%)	43,47,47	1.12	4 (9%)
7	CTP	B	502	6	29,30,30	1.10	3 (10%)	43,47,47	0.87	1 (2%)
7	CTP	A	501	6	29,30,30	1.47	4 (13%)	43,47,47	0.89	2 (4%)
7	CTP	D	504	6	29,30,30	0.81	0	43,47,47	0.73	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
7	CTP	C	503	6	-	10/22/38/38	0/2/2/2
7	CTP	B	502	6	-	2/22/38/38	0/2/2/2
7	CTP	A	501	6	-	5/22/38/38	0/2/2/2
7	CTP	D	504	6	-	2/22/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	CTP	PB-O3B	4.28	1.64	1.59
7	C	503	CTP	PA-O3A	4.05	1.63	1.59
7	C	503	CTP	PB-O3B	3.84	1.63	1.59
7	A	501	CTP	PA-O3A	3.81	1.63	1.59
7	A	501	CTP	PB-O3A	3.57	1.63	1.59
7	C	503	CTP	PB-O3A	3.41	1.63	1.59
7	B	502	CTP	PA-O3A	2.93	1.62	1.59
7	B	502	CTP	PB-O3A	2.89	1.62	1.59
7	C	503	CTP	C6-C5	2.23	1.40	1.35
7	B	502	CTP	PB-O3B	2.21	1.61	1.59
7	A	501	CTP	C4-N3	2.04	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	503	CTP	O4'-C1'-N1	3.26	115.74	108.36
7	B	502	CTP	O2-C2-N3	-2.42	118.52	122.33
7	C	503	CTP	O2-C2-N3	-2.37	118.60	122.33
7	C	503	CTP	O2B-PB-O3A	2.07	112.87	107.27
7	A	501	CTP	O3G-PG-O3B	2.03	111.45	104.64
7	A	501	CTP	C3'-C2'-C1'	2.03	105.30	101.46
7	C	503	CTP	O4'-C4'-C5'	2.01	115.76	109.33

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	501	CTP	O4'-C4'-C5'-O5'
7	C	503	CTP	O4'-C4'-C5'-O5'
7	C	503	CTP	C5'-O5'-PA-O3A
7	C	503	CTP	PB-O3B-PG-O3G
7	D	504	CTP	C5'-O5'-PA-O1A
7	C	503	CTP	C3'-C4'-C5'-O5'
7	A	501	CTP	C3'-C4'-C5'-O5'
7	C	503	CTP	C5'-O5'-PA-O1A
7	C	503	CTP	C5'-O5'-PA-O2A
7	A	501	CTP	PA-O3A-PB-O2B
7	B	502	CTP	PA-O3A-PB-O2B
7	C	503	CTP	PA-O3A-PB-O2B
7	B	502	CTP	O4'-C4'-C5'-O5'
7	A	501	CTP	PG-O3B-PB-O1B
7	D	504	CTP	C4'-C5'-O5'-PA
7	C	503	CTP	PB-O3B-PG-O1G
7	C	503	CTP	PB-O3B-PG-O2G
7	A	501	CTP	PA-O3A-PB-O1B
7	C	503	CTP	PA-O3A-PB-O1B

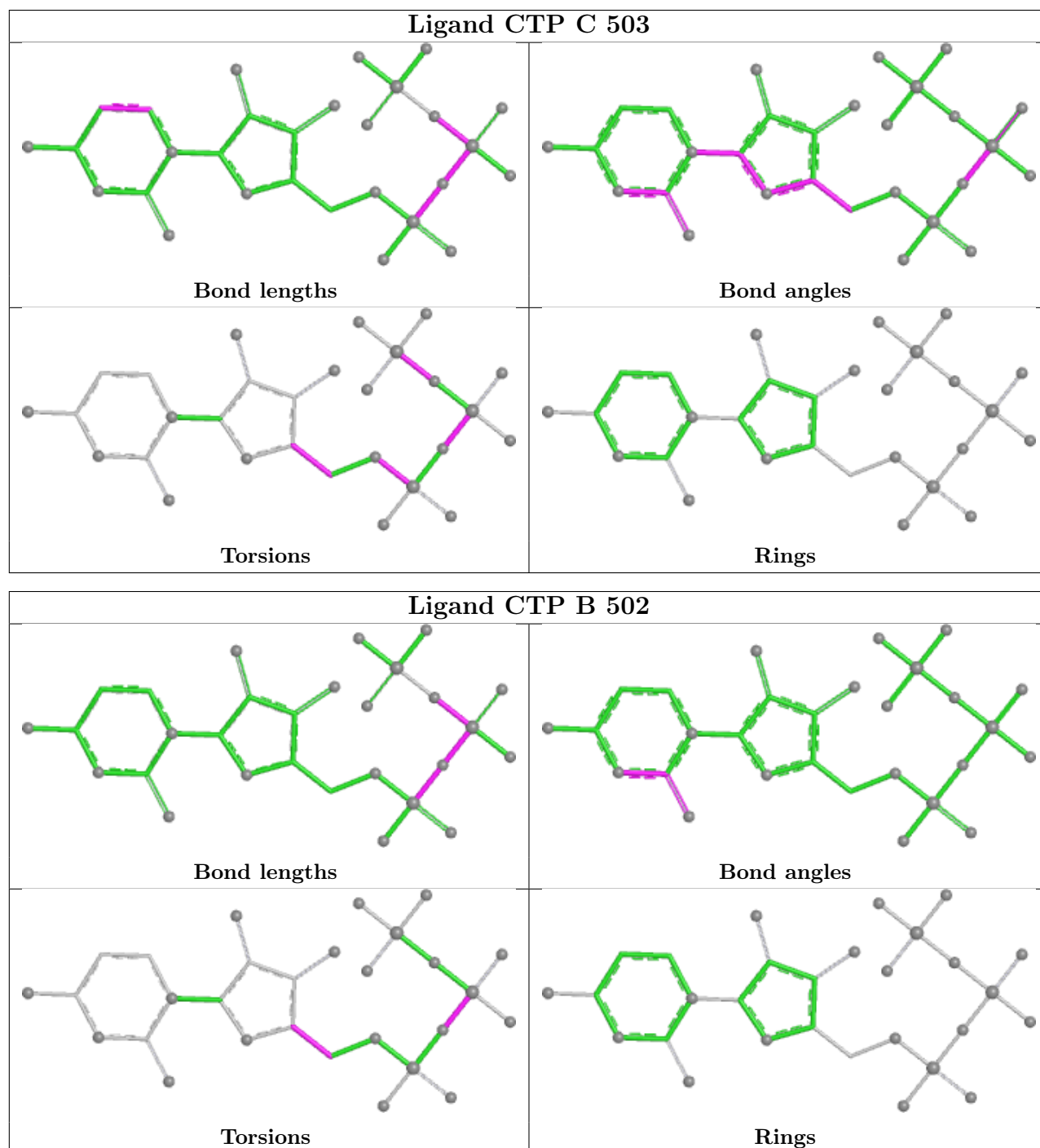
There are no ring outliers.

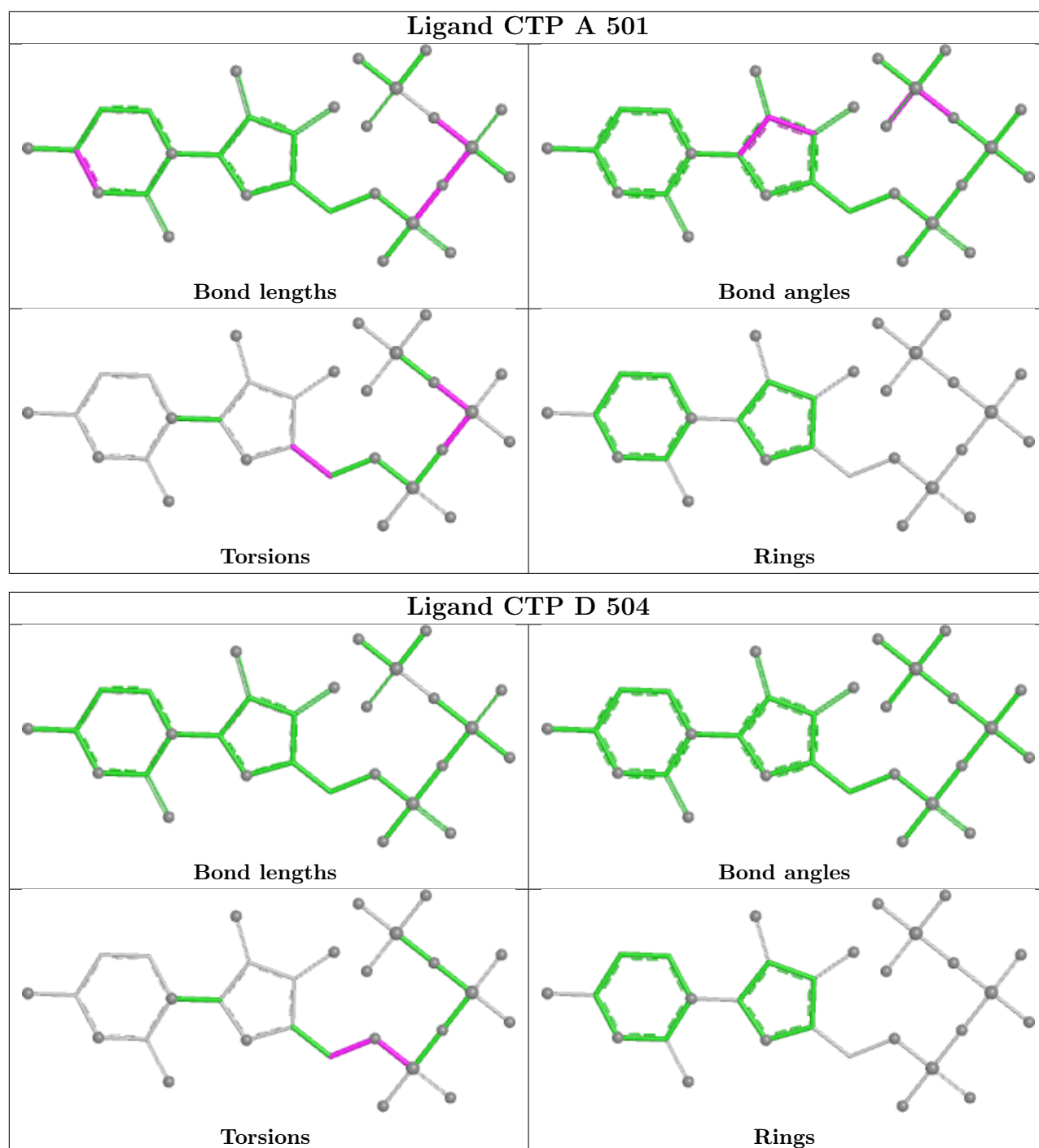
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	504	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	E	13/13 (100%)	-0.30	1 (7%) 19 13	130, 131, 132, 132	0
1	F	13/13 (100%)	-0.21	0 100 100	130, 131, 131, 132	0
2	H	14/14 (100%)	0.12	2 (14%) 6 5	129, 131, 133, 134	0
2	I	14/14 (100%)	-0.27	0 100 100	130, 131, 133, 133	0
3	G	11/11 (100%)	0.09	0 100 100	130, 131, 132, 132	0
4	J	8/8 (100%)	1.06	1 (12%) 8 6	129, 130, 131, 131	0
5	A	437/437 (100%)	-0.22	1 (0%) 91 85	130, 131, 132, 132	0
5	B	437/437 (100%)	-0.24	1 (0%) 91 85	130, 131, 132, 132	0
5	C	437/437 (100%)	-0.23	0 100 100	130, 131, 132, 133	0
5	D	437/437 (100%)	-0.26	0 100 100	130, 131, 132, 132	0
All	All	1821/1821 (100%)	-0.23	6 (0%) 90 81	129, 131, 132, 134	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	74	C	4.2
5	A	97	HIS	2.7
2	H	73	A	2.5
4	J	68	C	2.4
1	E	1	G	2.2
5	B	126	ALA	2.1

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 [i](#)

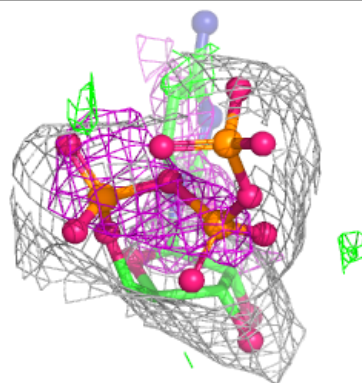
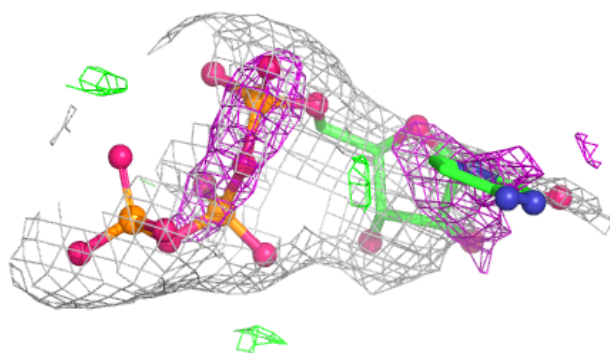
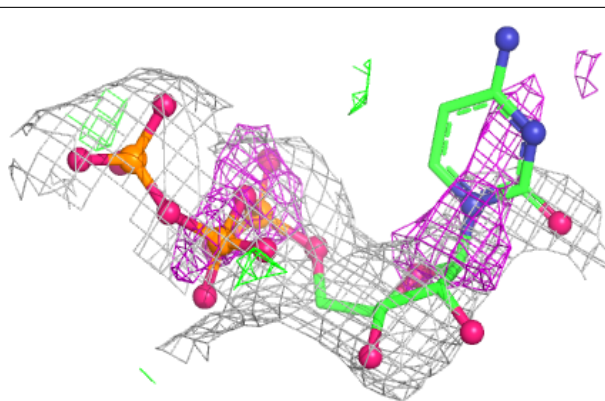
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CTP	A	501	29/29	0.76	0.13	134,135,138,138	0
6	MG	A	601	1/1	0.80	0.11	117,117,117,117	0
7	CTP	C	503	29/29	0.82	0.12	134,135,137,138	0
7	CTP	D	504	29/29	0.91	0.09	131,131,132,132	0
7	CTP	B	502	29/29	0.92	0.09	132,132,133,133	0
6	MG	C	603	1/1	0.96	0.05	109,109,109,109	0
6	MG	B	602	1/1	0.98	0.07	95,95,95,95	0
6	MG	D	604	1/1	0.99	0.09	102,102,102,102	0

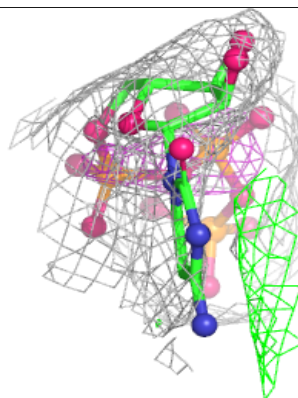
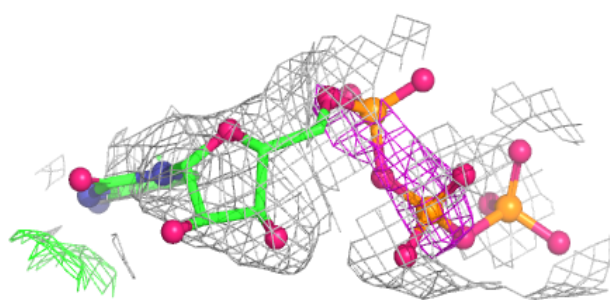
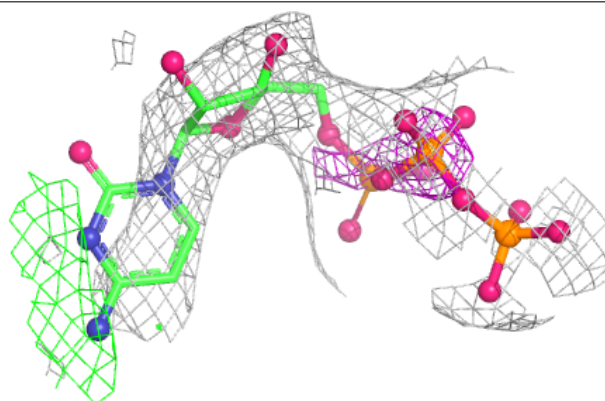
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CTP A 501:

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

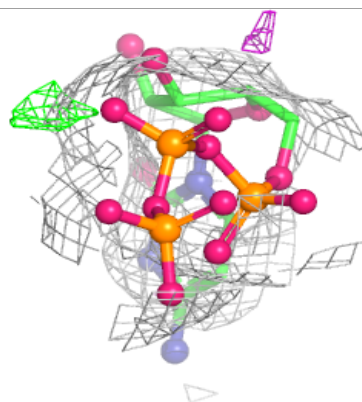
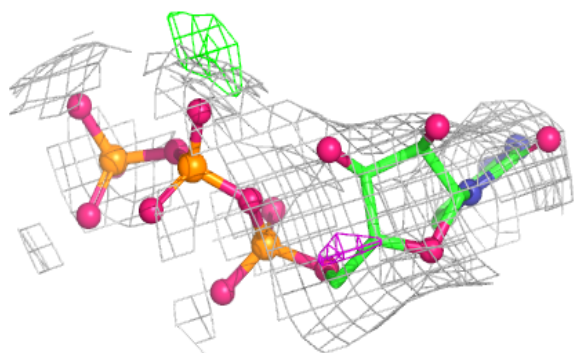
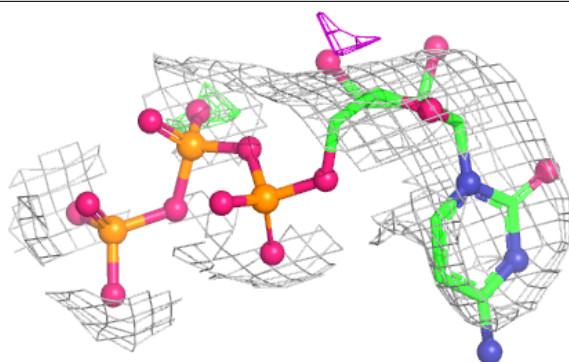
**Electron density around CTP C 503:**

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

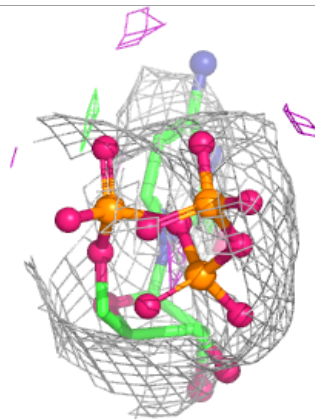
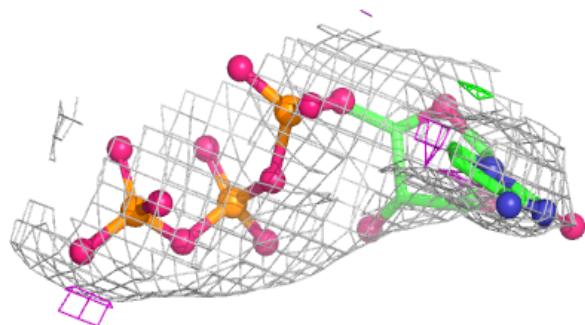
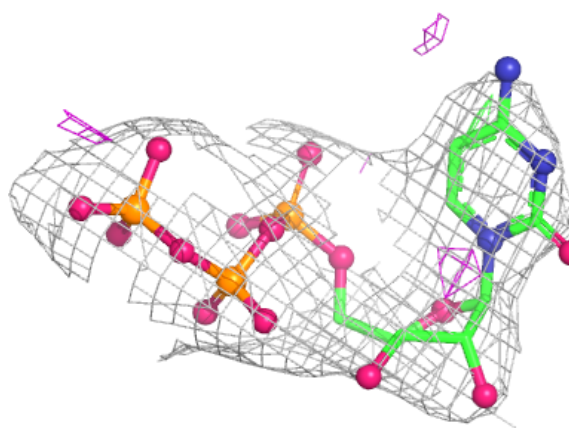


Electron density around CTP D 504:

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

**Electron density around CTP B 502:**

$2mF_o-DF_c$ (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.