Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 07:26 PM EDT

PDB ID	:	1TFY
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 (i) 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 (i)) were used in the production of this report:

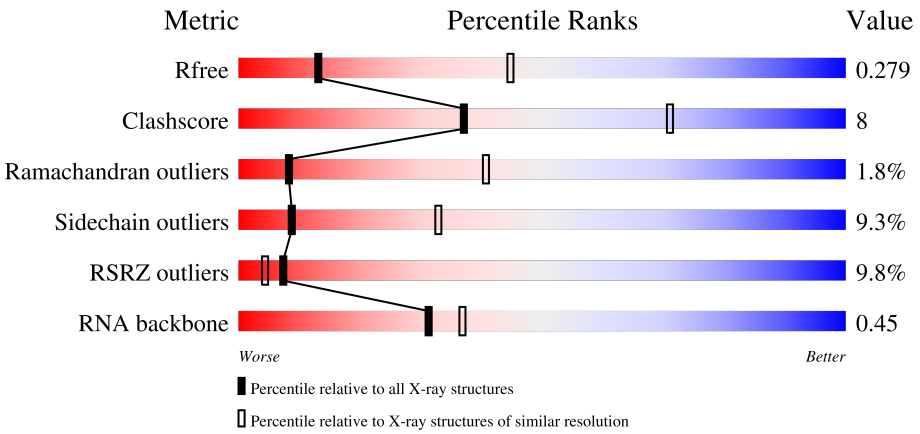
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (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 <=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	23% 62% 31% 8%
1	F	13	46% 46% 54%
2	H	14	29% 57% 21% 7% 14%
2	I	14	14% 36% 57% 7%

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Mol	Chain	Length	Quality of chain
3	G	11	27% 9% 27% 27% 36%
4	J	8	50% 12% 75% 12%
5	A	437	7% 79% 17%
5	B	437	14% 76% 21%
5	C	437	5% 72% 23%
5	D	437	9% 75% 22%

2 Entry composition (i)

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*CP*G)-3'.

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

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

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

- 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
			Total	C	N	O	P			
3	G	11	230	104	42	74	10	0	0	0

- 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
			Total	C	N	O	P			
4	J	8	168	76	31	54	7	0	0	0

- Molecule 5 is a protein called tRNA nucleotidyltransferase.

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

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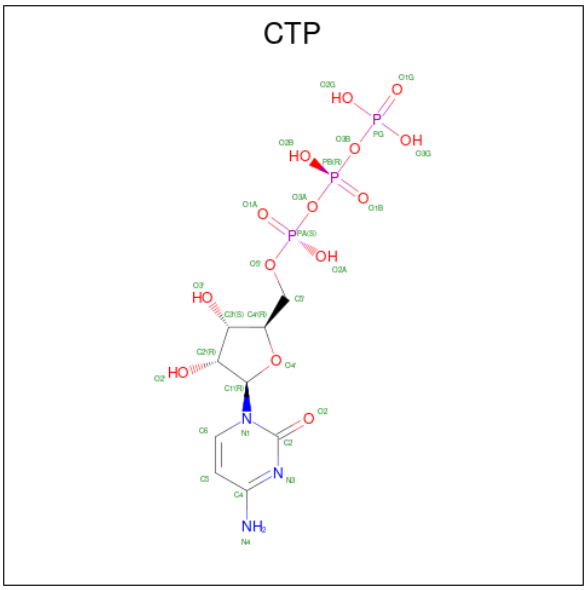
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	437	3630	2333	632	652	13	0	0	0
			Total	C	N	O	S			
5	C	437	3630	2333	632	652	13	0	0	0
			Total	C	N	O	S			
5	D	437	3630	2333	632	652	13	0	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



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

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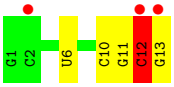
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	C	1	29	9	3	14	3	0	0
			Total	C	N	O	P		
7	D	1	29	9	3	14	3	0	0

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.

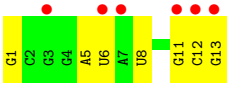
• Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'

Chain E:



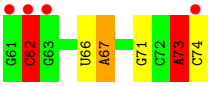
• Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'

Chain F:



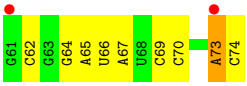
• Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*AP*C)-3'

Chain H:



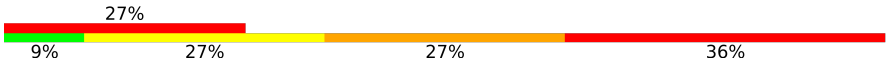
• Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*AP*C)-3'

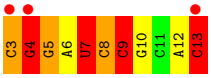
Chain I:



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

Chain G:





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

Chain J: 50% 12% 75% 12%

C61 G62 C63 G64 G65 A66 U67 C68

• Molecule 5: tRNA nucleotidyltransferase

Chain A: 7% 79% 17%

M1 K2 V3 E4 E5 I6 L11 E12 L13 V14 I15 P16 D17 E18 V21 R22 R25 R34 G39 V43 S47 R50 W53 L54 K55 I60 F63 L64 L65 F66 P67 E68 E69 F70 S71 K72 E73 E74 L75 R76 E77 R78 G79 G83 K84 A85 V86 L87

R93 Y94 A95 E96 H97 P98 Y99 G102 V109 V112 P113 C114 Y115 K116 L117 K118 E119 P120 K121 N122 I123 K124 S125 W136 K144 R149 F154 E176 F185 L186 R194 R197 R198 K210 E213 D218 E222 K223 R224 D233 R237

P249 S250 L251 L260 E263 P264 E265 K282 D287 I288 V289 D290 D291 N292 R299 K303 F307 E311 M314 Q334 R344 M345 Q348 F349 E350 K356 L359 S360 R361 A364 R373 R380 T383 S391 T395 T399 L400 G401 K402

I415 L420 F421 K422 E423 P424 K436 D437

• Molecule 5: tRNA nucleotidyltransferase

Chain B: 14% 76% 21%

M1 E8 K9 A10 L11 E12 L13 V14 D17 E18 E19 K23 G24 E29 E30 L31 R32 R33 E37 L38 E41 Y42 V43 Y48 A49 R50 N51 T52 W53 L54 I60 F63 L64 L65 E68 E69 F70 S71 K72 E73 E74 L75 R76 E77 R78 I82 G83 V86

L87 D88 S89 I92 R93 Y94 A95 Y99 V100 H101 G102 V103 V104 K105 G106 V107 E108 V109 D110 V111 V112 P113 C114 Y115 K116 L117 K118 E119 P120 K121 N122 I123 K124 S125 A126 R129 T130 P131 H134 K142 G143 K144 E145 N146 E147 V148 K152 G153 F154 E164 G183 S184

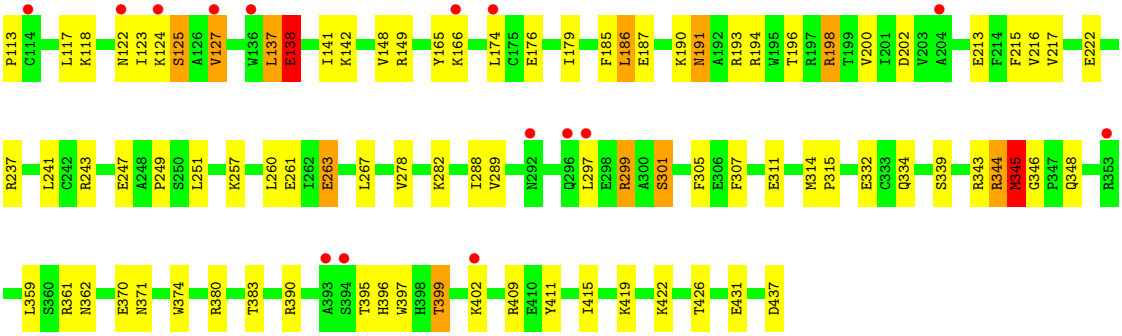
F185 L186 V200 E212 F215 D218 D221 L235 V239 M246 P249 F254 K257 L260 E261 R266 L267 R268 K269 I270 V271 E272 K282 F283 R284 I288 V289 D290 D291 R299 A300 S301 L308 N312 F313 M314 F320 E324 Y328

E332 C333 Q334 I335 S339 R340 R343 R344 M345 D351 V355 K356 L359 S360 R361 N362 E370 W375 E378 M379 R380 K381 E386 T399 N403 V404 I408 F412 E413 I414 M432 D437

• Molecule 5: tRNA nucleotidyltransferase

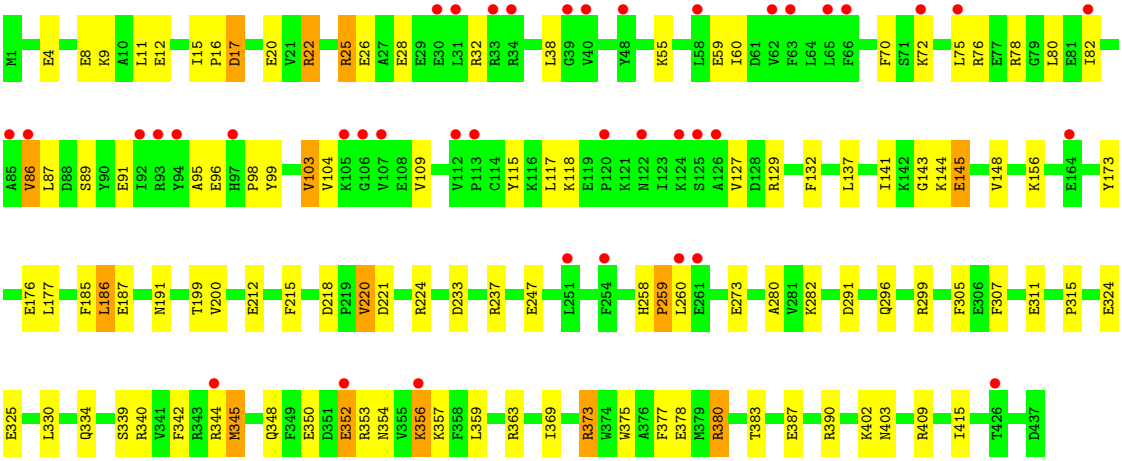
Chain C: 5% 72% 23%

M1 K2 V3 I6 L7 L11 V14 I15 P16 D17 E18 R25 E30 R33 R34 L35 L38 G39 R50 L54 K55 I60 F63 E69 F70 S71 K72 E73 E74 L75 R76 E77 R78 G79 L80 E81 V86 R93 Y94 A95 E96 H97 P98 Y99 V100



- Molecule 5: tRNA nucleotidyltransferase

Chain D:



4 Data and refinement statistics (i)

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 44.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.28-3.20) 98.8 (44.18-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.28 , 124.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.67	0/308	1.26	2/479 (0.4%)
1	F	0.72	0/308	1.17	0/479
2	H	0.78	0/329	1.39	3/511 (0.6%)
2	I	0.77	0/329	1.40	3/511 (0.6%)
3	G	0.99	1/256 (0.4%)	1.95	12/397 (3.0%)
4	J	0.77	0/187	1.46	1/290 (0.3%)
5	A	0.35	0/3713	0.52	1/4987 (0.0%)
5	B	0.36	0/3713	0.51	0/4987
5	C	0.36	0/3713	0.53	1/4987 (0.0%)
5	D	0.38	0/3713	0.53	0/4987
All	All	0.43	1/16569 (0.0%)	0.70	23/22615 (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	5.26	1.56	1.48

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5	G	P-O3'-C3'	-11.56	105.83	119.70
3	G	8	C	P-O3'-C3'	-9.96	107.75	119.70
3	G	6	A	P-O3'-C3'	-6.96	111.35	119.70
3	G	7	U	C5'-C4'-O4'	6.75	117.20	109.10
4	J	68	C	O4'-C1'-N1	6.46	113.37	108.20
1	E	12	C	O4'-C1'-N1	6.01	113.01	108.20
3	G	3	C	C2-N1-C1'	5.95	125.35	118.80
3	G	7	U	O4'-C4'-C3'	-5.93	98.07	104.00
1	E	10	C	O4'-C1'-N1	5.92	112.94	108.20
2	I	69	C	O4'-C1'-N1	5.83	112.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	75	LEU	CA-CB-CG	5.82	128.69	115.30
2	H	66	U	O4'-C1'-N1	5.79	112.83	108.20
3	G	8	C	O4'-C1'-N1	5.66	112.73	108.20
3	G	13	C	C6-N1-C2	-5.64	118.04	120.30
3	G	4	G	O4'-C1'-N9	5.54	112.64	108.20
2	H	73	A	C3'-C2'-C1'	5.51	105.91	101.50
3	G	3	C	N1-C2-O2	5.38	122.13	118.90
2	I	70	C	O4'-C1'-N1	5.37	112.50	108.20
3	G	13	C	O4'-C1'-N1	5.37	112.50	108.20
2	I	64	G	C4'-C3'-C2'	-5.32	97.28	102.60
2	H	62	C	O4'-C1'-N1	5.23	112.39	108.20
3	G	9	C	O4'-C1'-N1	5.16	112.33	108.20
5	C	75	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	60	0
5	B	3630	0	3633	55	0
5	C	3630	0	3633	71	0
5	D	3630	0	3633	60	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	29	0	12	0	0
7	D	29	0	12	1	0
All	All	16180	0	15385	244	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 (244) 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: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:71:SER:C	5:A:73:GLU:H	1.88	0.74
5:D:344:ARG:O	5:D:345:MET:HB3	1.88	0.74
5:A:198:ARG:HH11	5:A:198:ARG:CG	1.93	0.73
5:A:391:SER:O	5:A:395:THR:HG22	1.88	0.73
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:D:280:ALA:HB2	5:D:330:LEU:HD23	1.81	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
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:A:314:MET:HE3	5:B:312:ASN:HB3	1.87	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:A:71:SER:C	5:A:73:GLU:N	2.59	0.55
5:D:95:ALA:HB3	5:D:99:TYR:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:144:LYS:HZ1	5:B:183:GLY:HA2	1.76	0.50
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:B:314:MET:HE3	5:B:335:ILE:HD11	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:75:LEU:HD12	5:C:76:ARG:N	2.27	0.49
5:A:380:ARG:HH12	5:B:334:GLN:HE21	1.59	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: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: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:314:MET:CE	5:B:312:ASN:HB3	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: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: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: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: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
5:A:197:ARG:O	5:A:213:GLU:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:93:ARG:HD3	5:B:289:VAL:HG11	1.98	0.45
5:C:137:LEU:O	5:C:138:GLU:C	2.54	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: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:A:350:GLU:HG3	5:C:38:LEU:C	2.36	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:A:263:GLU:C	5:A:265:GLU:H	2.21	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:H	2.21	0.44
5:C:343:ARG:HH22	5:C:370:GLU:CD	2.21	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: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: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:B:332:GLU:HB2	5:B:432:MET:HE3	2.00	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:B:343:ARG:HH22	5:B:370:GLU:CD	2.22	0.43
5:B:332:GLU:HB2	5:B:432:MET:CE	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:142:LYS:HA	5:B:145:GLU:OE2	2.19	0.43
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: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: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: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: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:C:75:LEU:HD12	5:C:75:LEU:C	2.41	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:243:ARG:CZ	5:D:352:GLU:HG3	2.50	0.41
5:A:345:MET:HE3	5:C:70:PHE:CE1	2.57	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: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%)	8 41
5	B	435/437 (100%)	395 (91%)	32 (7%)	8 (2%)	8 41
5	C	435/437 (100%)	403 (93%)	23 (5%)	9 (2%)	7 37
5	D	435/437 (100%)	390 (90%)	39 (9%)	6 (1%)	11 46
All	All	1740/1748 (100%)	1592 (92%)	117 (7%)	31 (2%)	8 41

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	72	LYS
5	A	186	LEU
5	B	186	LEU
5	C	70	PHE
5	C	117	LEU
5	C	125	SER
5	C	186	LEU

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Mol	Chain	Res	Type
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 (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
5	A	387/387 (100%)	355 (92%)	32 (8%)	11 40
5	B	387/387 (100%)	354 (92%)	33 (8%)	10 38
5	C	387/387 (100%)	341 (88%)	46 (12%)	5 22
5	D	387/387 (100%)	354 (92%)	33 (8%)	10 38
All	All	1548/1548 (100%)	1404 (91%)	144 (9%)	9 33

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	2	LYS
5	A	5	GLU
5	A	13	LEU
5	A	22	ARG
5	A	47	SER
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	194	ARG
5	A	198	ARG
5	A	210	LYS
5	A	213	GLU
5	A	222	GLU
5	A	224	ARG
5	A	260	LEU
5	A	288	ILE
5	A	289	VAL
5	A	291	ASP
5	A	345	MET
5	A	350	GLU
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	1	MET
5	B	9	LYS
5	B	13	LEU
5	B	17	ASP
5	B	18	GLU
5	B	23	LYS
5	B	38	LEU
5	B	54	LEU
5	B	70	PHE
5	B	77	GLU

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Mol	Chain	Res	Type
5	B	78	ARG
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	212	GLU
5	B	246	MET
5	B	257	LYS
5	B	260	LEU
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
5	C	1	MET
5	C	6	ILE
5	C	11	LEU
5	C	14	VAL
5	C	18	GLU
5	C	25	ARG
5	C	54	LEU
5	C	69	GLU
5	C	75	LEU
5	C	78	ARG
5	C	80	LEU
5	C	93	ARG
5	C	118	LYS
5	C	122	ASN
5	C	123	ILE
5	C	127	VAL
5	C	137	LEU
5	C	138	GLU
5	C	142	LYS

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Mol	Chain	Res	Type
5	C	166	LYS
5	C	191	ASN
5	C	194	ARG
5	C	198	ARG
5	C	213	GLU
5	C	222	GLU
5	C	241	LEU
5	C	251	LEU
5	C	257	LYS
5	C	263	GLU
5	C	288	ILE
5	C	289	VAL
5	C	299	ARG
5	C	301	SER
5	C	314	MET
5	C	344	ARG
5	C	345	MET
5	C	359	LEU
5	C	361	ARG
5	C	362	ASN
5	C	383	THR
5	C	390	ARG
5	C	399	THR
5	C	411	TYR
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	38	LEU
5	D	55	LYS
5	D	59	GLU
5	D	70	PHE
5	D	72	LYS
5	D	78	ARG
5	D	91	GLU
5	D	103	VAL
5	D	118	LYS
5	D	127	VAL
5	D	144	LYS

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Mol	Chain	Res	Type
5	D	145	GLU
5	D	156	LYS
5	D	199	THR
5	D	220	VAL
5	D	247	GLU
5	D	260	LEU
5	D	273	GLU
5	D	299	ARG
5	D	324	GLU
5	D	325	GLU
5	D	340	ARG
5	D	352	GLU
5	D	353	ARG
5	D	356	LYS
5	D	373	ARG
5	D	380	ARG
5	D	383	THR
5	D	409	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	229	ASN
5	A	292	ASN
5	A	348	GLN
5	A	371	ASN
5	A	396	HIS
5	B	97	HIS
5	B	312	ASN
5	B	334	GLN
5	C	334	GLN
5	C	362	ASN
5	C	396	HIS
5	D	334	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	12/13 (92%)	1 (8%)	0
1	F	12/13 (92%)	3 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	13/14 (92%)	4 (30%)	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
All	All	67/73 (91%)	19 (28%)	2 (2%)

All (19) 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	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	26,30,30	0.81	1 (3%)	39,47,47	1.11	2 (5%)
7	CTP	B	502	6	26,30,30	0.70	0	39,47,47	1.06	3 (7%)
7	CTP	A	501	6	26,30,30	0.80	1 (3%)	39,47,47	0.96	3 (7%)
7	CTP	D	504	6	26,30,30	0.78	0	39,47,47	1.05	2 (5%)

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	-	3/22/38/38	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	CTP	C6-C5	2.25	1.40	1.35
7	A	501	CTP	C4-N3	2.02	1.38	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	504	CTP	PB-O3B-PG	-3.80	119.80	132.83
7	B	502	CTP	PB-O3B-PG	-3.29	121.55	132.83
7	C	503	CTP	O4'-C1'-N1	3.23	115.74	108.36
7	D	504	CTP	PB-O3A-PA	-3.01	122.50	132.83
7	A	501	CTP	PB-O3A-PA	-2.47	124.36	132.83
7	B	502	CTP	O2-C2-N3	-2.35	118.52	122.33
7	C	503	CTP	O2-C2-N3	-2.29	118.60	122.33
7	B	502	CTP	PB-O3A-PA	-2.25	125.12	132.83
7	A	501	CTP	C3'-C2'-C1'	2.04	105.30	101.43
7	A	501	CTP	O3G-PG-O3B	2.03	111.45	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

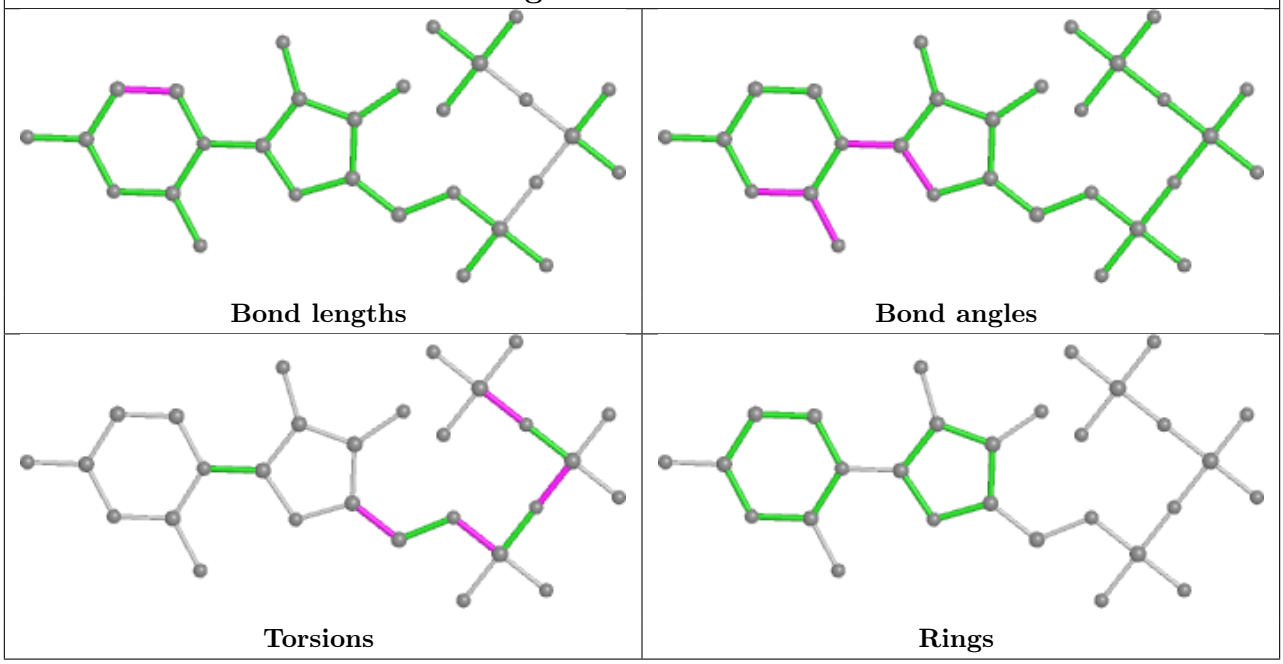
There are no ring outliers.

1 monomer is involved in 1 short contact:

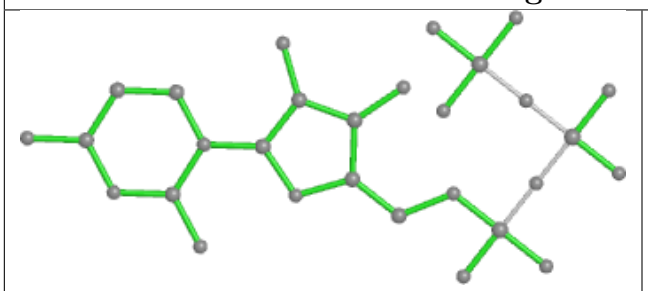
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	504	CTP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

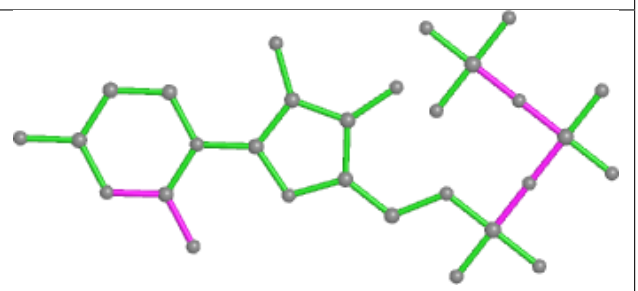
Ligand CTP C 503



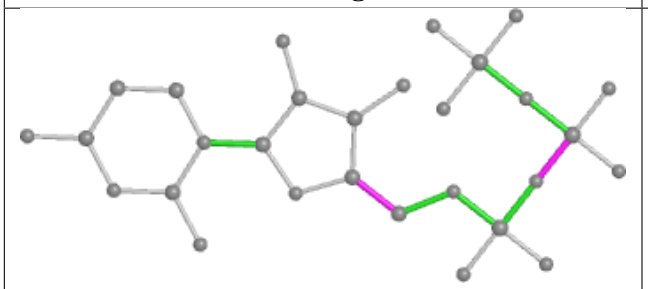
Ligand CTP B 502



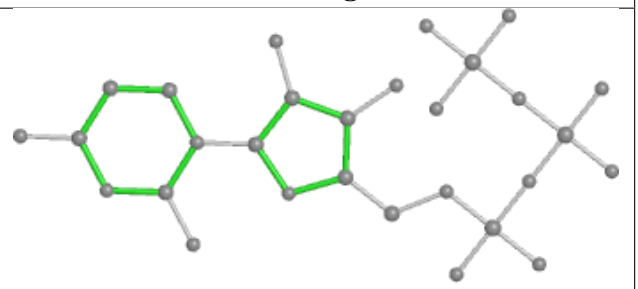
Bond lengths



Bond angles

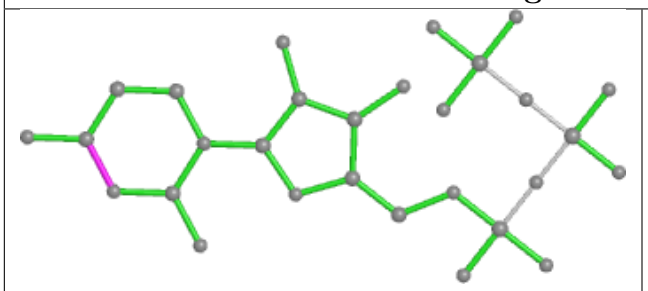


Torsions

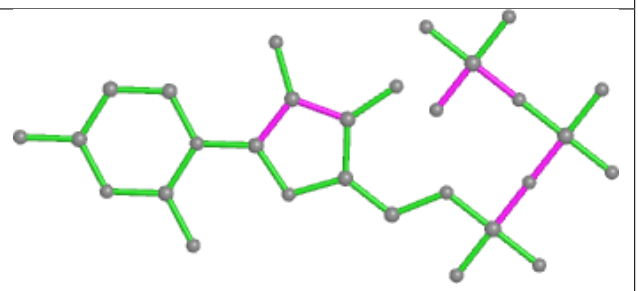


Rings

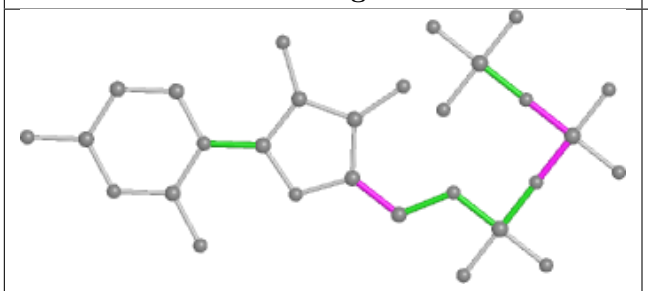
Ligand CTP A 501



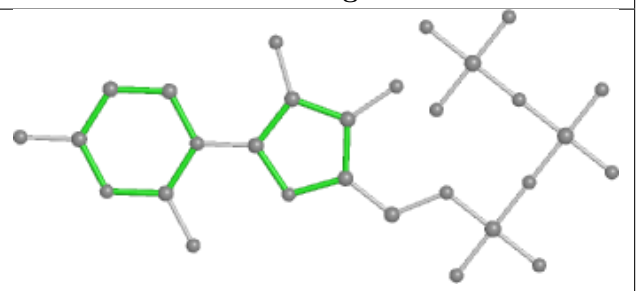
Bond lengths



Bond angles

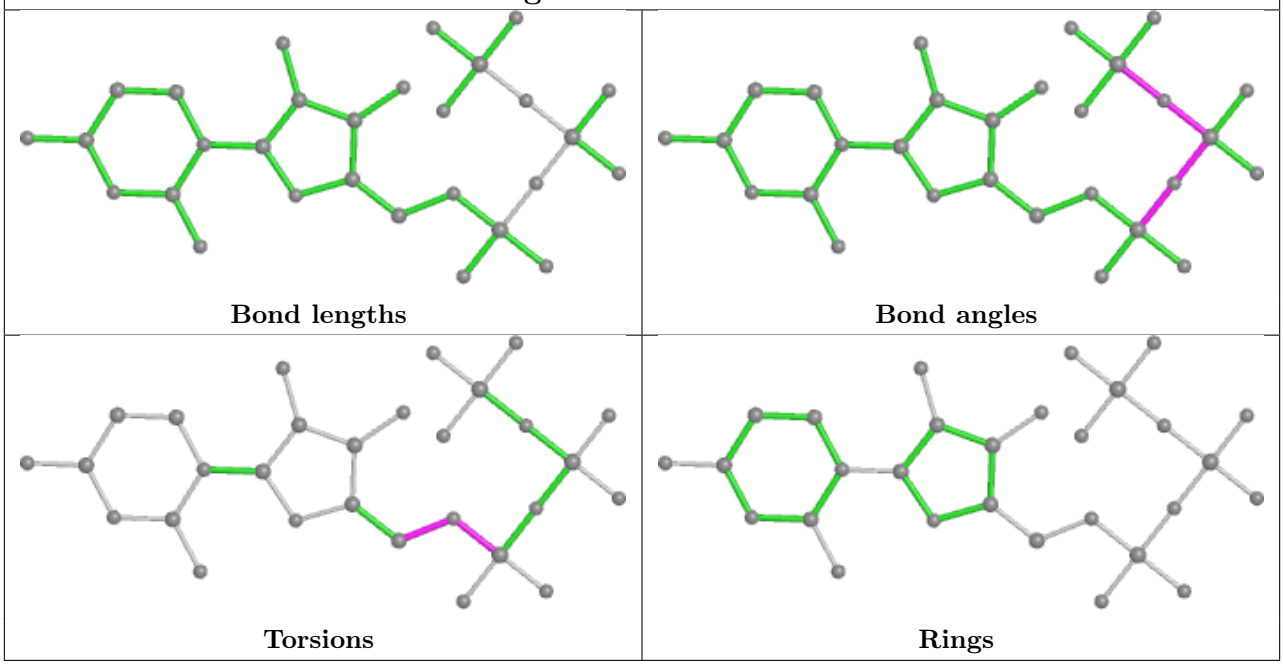


Torsions



Rings

Ligand CTP D 504



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%)	1.19	3 (23%)	0	0	130, 131, 132, 132	0
1	F	13/13 (100%)	1.76	6 (46%)	0	0	130, 131, 131, 132	0
2	H	14/14 (100%)	1.36	4 (28%)	0	0	129, 131, 133, 134	0
2	I	14/14 (100%)	1.49	2 (14%)	2	1	130, 131, 133, 133	0
3	G	11/11 (100%)	1.57	3 (27%)	0	0	130, 131, 132, 132	0
4	J	8/8 (100%)	2.09	4 (50%)	0	0	129, 130, 131, 131	0
5	A	437/437 (100%)	0.38	30 (6%)	16	9	130, 131, 132, 132	0
5	B	437/437 (100%)	0.72	62 (14%)	2	1	130, 131, 132, 132	0
5	C	437/437 (100%)	0.36	24 (5%)	25	14	130, 131, 132, 133	0
5	D	437/437 (100%)	0.61	40 (9%)	9	5	130, 131, 132, 132	0
All	All	1821/1821 (100%)	0.56	178 (9%)	7	4	129, 131, 132, 134	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	61	G	8.3
5	D	92	ILE	7.4
5	C	72	LYS	7.0
5	B	107	VAL	6.8
5	D	94	TYR	6.8
5	A	96	GLU	6.4
5	B	68	GLU	6.1
5	D	122	ASN	6.0
5	B	122	ASN	5.8
5	B	113	PRO	5.8
5	B	73	GLU	5.3
5	B	437	ASP	5.1
5	B	72	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
5	A	250	SER	4.9
5	A	84	LYS	4.8
5	D	125	SER	4.8
3	G	4	G	4.8
2	H	74	C	4.6
5	C	122	ASN	4.6
5	D	93	ARG	4.6
5	B	87	LEU	4.5
1	F	13	G	4.5
5	C	100	VAL	4.5
5	D	30	GLU	4.5
5	B	75	LEU	4.5
5	A	119	GLU	4.4
5	C	124	LYS	4.4
5	B	124	LYS	4.4
5	B	63	PHE	4.3
5	B	126	ALA	4.3
5	B	89	SER	4.3
5	D	85	ALA	4.2
5	B	120	PRO	4.2
5	D	126	ALA	4.1
2	H	63	G	4.1
5	A	122	ASN	4.1
5	D	58	LEU	4.0
5	D	124	LYS	4.0
5	B	267	LEU	4.0
2	H	61	G	4.0
5	B	88	ASP	4.0
5	B	123	ILE	3.9
3	G	13	C	3.9
5	D	251	LEU	3.9
5	C	1	MET	3.9
5	B	103	VAL	3.9
5	B	42	TYR	3.8
5	D	260	LEU	3.8
5	B	114	CYS	3.8
5	B	13	LEU	3.7
5	B	115	TYR	3.7
5	A	97	HIS	3.6
2	H	62	C	3.6
1	E	12	C	3.5
5	B	41	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
5	B	129	ARG	3.4
5	D	254	PHE	3.4
5	B	254	PHE	3.4
5	D	40	VAL	3.3
5	B	119	GLU	3.3
5	A	87	LEU	3.3
5	A	420	LEU	3.2
5	C	99	TYR	3.2
1	E	13	G	3.2
5	D	48	TYR	3.2
5	D	72	LYS	3.1
1	F	7	A	3.1
5	A	421	PHE	3.0
5	A	60	ILE	3.0
5	B	86	VAL	3.0
5	B	37	GLU	2.9
5	B	403	ASN	2.9
5	C	296	GLN	2.9
5	D	33	ARG	2.9
5	A	437	ASP	2.8
1	F	11	G	2.8
5	B	106	GLY	2.8
5	B	105	LYS	2.8
5	D	62	VAL	2.8
5	B	148	VAL	2.8
5	D	261	GLU	2.8
5	C	114	CYS	2.8
5	C	204	ALA	2.8
5	D	112	VAL	2.8
5	D	107	VAL	2.7
4	J	68	C	2.7
5	A	287	ASP	2.7
5	B	104	VAL	2.7
5	B	154	PHE	2.7
5	C	136	TRP	2.7
5	B	118	LYS	2.7
5	C	292	ASN	2.6
5	D	86	VAL	2.6
5	B	43	VAL	2.6
5	B	29	GLU	2.6
5	B	64	LEU	2.6
5	D	113	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
5	C	297	LEU	2.6
5	B	164	GLU	2.5
5	B	121	LYS	2.5
5	B	12	GLU	2.5
5	A	83	GLY	2.5
5	B	359	LEU	2.5
5	D	344	ARG	2.5
5	C	353	ARG	2.5
5	D	34	ARG	2.5
1	F	12	C	2.5
5	C	127	VAL	2.5
3	G	3	C	2.4
5	A	95	ALA	2.4
5	B	14	VAL	2.4
5	B	24	GLY	2.4
4	J	63	C	2.4
5	A	102	GLY	2.4
5	A	402	LYS	2.4
5	A	112	VAL	2.4
5	A	400	LEU	2.4
5	C	402	LYS	2.4
5	D	75	LEU	2.4
5	D	106	GLY	2.4
5	C	79	GLY	2.3
5	A	251	LEU	2.3
5	D	39	GLY	2.3
5	C	96	GLU	2.3
5	C	81	GLU	2.3
5	C	393	ALA	2.3
5	B	116	LYS	2.3
5	D	63	PHE	2.3
1	F	3	G	2.3
5	B	266	ARG	2.3
5	A	79	GLY	2.3
5	A	116	LYS	2.3
5	D	82	ILE	2.3
5	B	77	GLU	2.3
5	C	33	ARG	2.3
2	I	73	A	2.3
5	B	125	SER	2.3
5	C	394	SER	2.3
5	C	174	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
5	B	92	ILE	2.2
5	B	52	THR	2.2
5	A	72	LYS	2.2
5	B	30	GLU	2.2
5	D	66	PHE	2.2
1	F	6	U	2.2
5	B	112	VAL	2.2
5	C	166	LYS	2.2
5	D	31	LEU	2.1
5	B	33	ARG	2.1
5	B	31	LEU	2.1
5	D	97	HIS	2.1
5	B	111	VAL	2.1
5	A	401	GLY	2.1
5	A	136	TRP	2.1
4	J	62	G	2.1
5	C	60	ILE	2.1
5	B	48	TYR	2.1
5	B	76	ARG	2.1
5	D	356	LYS	2.1
5	B	70	PHE	2.1
5	B	146	ASN	2.1
5	B	282	LYS	2.1
5	A	154	PHE	2.1
5	A	99	TYR	2.1
5	A	364	ALA	2.1
5	D	352	GLU	2.1
5	B	17	ASP	2.1
4	J	64	G	2.0
5	D	65	LEU	2.0
5	D	105	LYS	2.0
5	B	82	ILE	2.0
5	A	63	PHE	2.0
5	A	120	PRO	2.0
1	E	2	C	2.0
5	D	120	PRO	2.0
5	D	426	THR	2.0
5	A	263	GLU	2.0
5	D	164	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

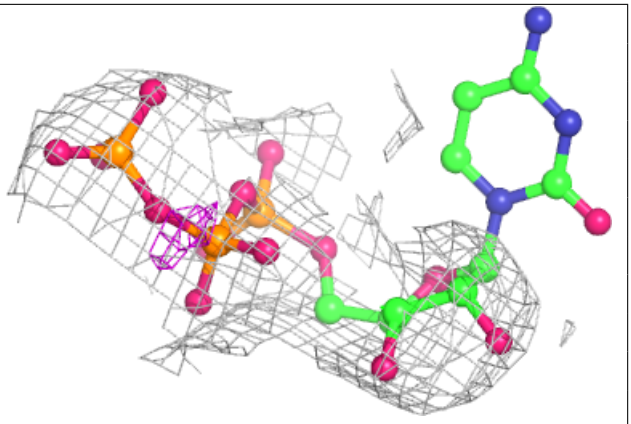
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

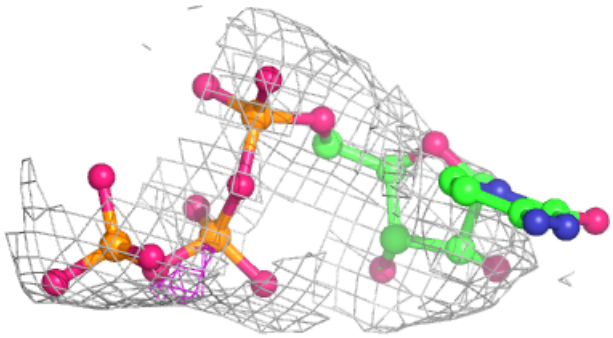
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	601	1/1	0.64	0.34	117,117,117,117	0
7	CTP	A	501	29/29	0.73	0.30	134,135,138,138	0
7	CTP	C	503	29/29	0.75	0.29	134,135,137,138	0
6	MG	B	602	1/1	0.83	0.22	95,95,95,95	0
6	MG	C	603	1/1	0.87	0.16	109,109,109,109	0
7	CTP	B	502	29/29	0.90	0.21	132,132,133,133	0
6	MG	D	604	1/1	0.90	0.19	102,102,102,102	0
7	CTP	D	504	29/29	0.91	0.24	131,131,132,132	0

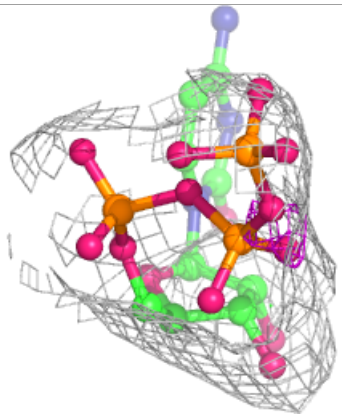
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

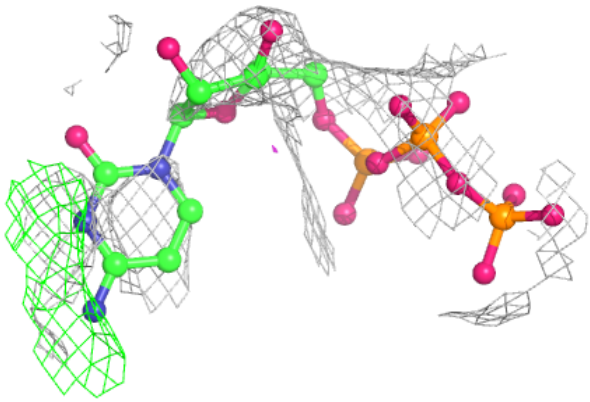


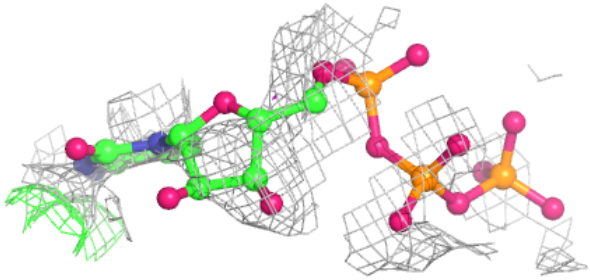


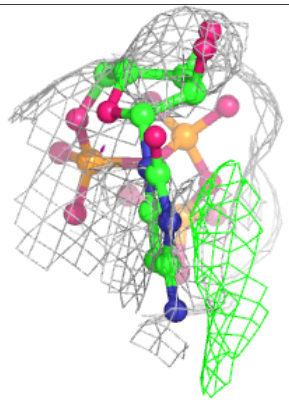


Electron density around CTP C 503:

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

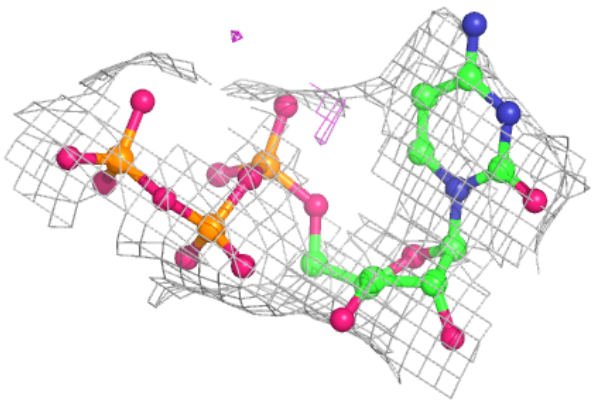


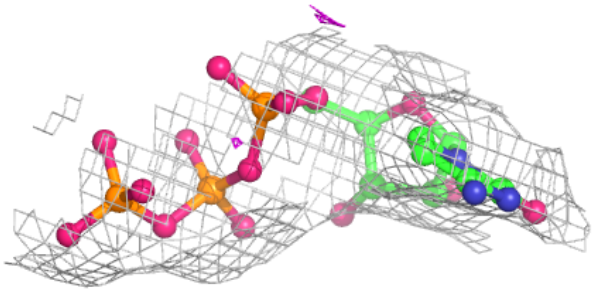


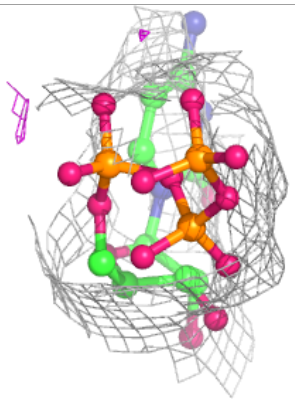


Electron density around CTP B 502:

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

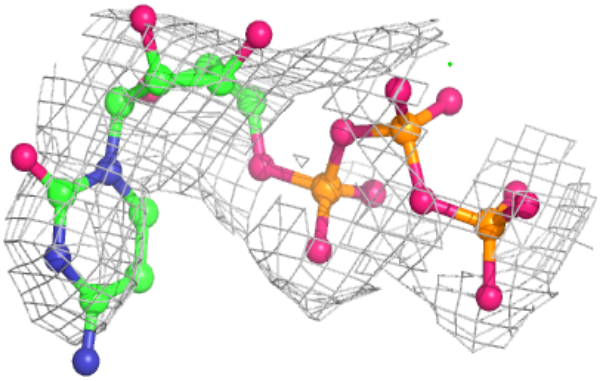


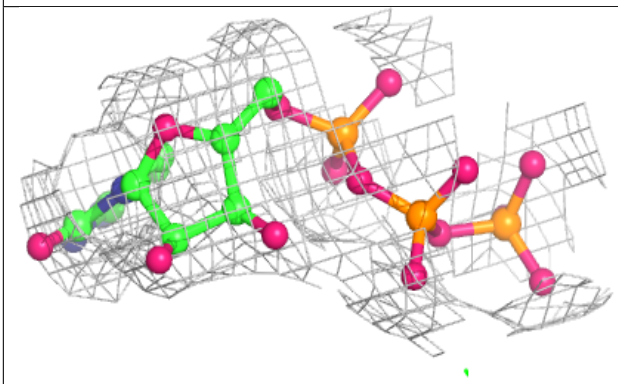


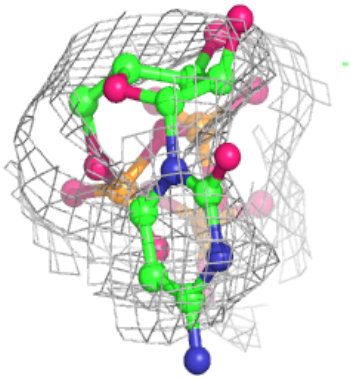


Electron density around CTP D 504:

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







6.5 Other polymers (i)

There are no such residues in this entry.