



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:52 PM UTC

PDB ID : 7LHZ / pdb_00007lhz
Title : K. pneumoniae Topoisomerase IV (ParE-ParC) in complex with DNA and (3S)-10-[(3R)-3-(1-aminocyclopropyl)pyrrolidin-1-yl]-9-fluoro-3-methyl-5-oxo-2,3-dihydro-5H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (compound 25)
Authors : Noeske, J.; Shu, W.; Bellamacina, C.
Deposited on : 2021-01-26
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

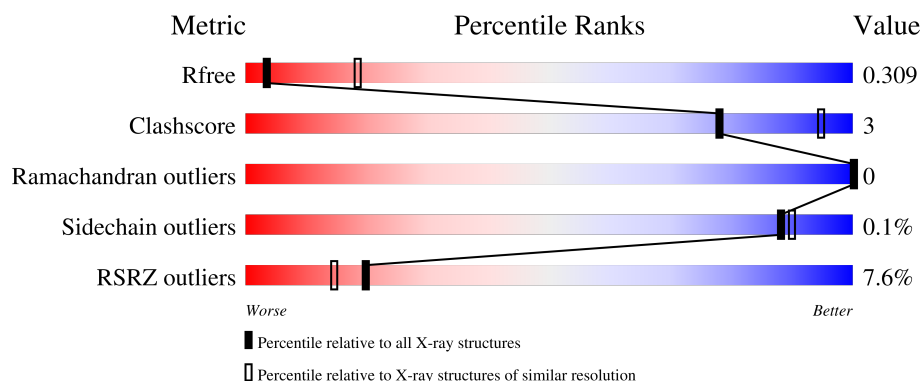
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



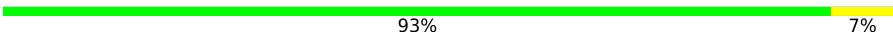
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	743	5% 88% 7% 5%
1	B	743	10% 80% 5% 15%
1	C	743	5% 91% 5% .
1	D	743	9% 84% 7% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	11	 82% 18%
2	H	11	 45% 27% 27%
2	J	11	 9% 82% 9% 9%
2	P	11	 82% 9% 9%
3	F	15	 73% 13% 13%
3	G	15	 80% 7% 13%
3	I	15	 80% 13% 7%
3	K	15	 93% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 38321 atoms, of which 17296 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 DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	714	Total	C	H	N	O	S	0	0	0
			9610	3190	4502	898	995	25			
1	D	677	Total	C	H	N	O	S	0	0	0
			8512	2904	3873	824	896	15			
1	A	706	Total	C	H	N	O	S	0	0	0
			9319	3109	4332	890	963	25			
1	B	631	Total	C	H	N	O	S	0	0	0
			7830	2666	3545	761	838	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	389	MET	-	initiating methionine	UNP A0A377Y395
C	999	GLU	-	linker	UNP A0A377Y395
C	1000	PHE	-	linker	UNP A0A377Y395
C	1255	THR	SER	conflict	UNP A0A486EJ79
C	1491	LEU	-	expression tag	UNP A0A486EJ79
C	1492	GLU	-	expression tag	UNP A0A486EJ79
C	1493	HIS	-	expression tag	UNP A0A486EJ79
C	1494	HIS	-	expression tag	UNP A0A486EJ79
C	1495	HIS	-	expression tag	UNP A0A486EJ79
C	1496	HIS	-	expression tag	UNP A0A486EJ79
C	1497	HIS	-	expression tag	UNP A0A486EJ79
C	1498	HIS	-	expression tag	UNP A0A486EJ79
D	389	MET	-	initiating methionine	UNP A0A377Y395
D	999	GLU	-	linker	UNP A0A377Y395
D	1000	PHE	-	linker	UNP A0A377Y395
D	1255	THR	SER	conflict	UNP A0A486EJ79
D	1491	LEU	-	expression tag	UNP A0A486EJ79
D	1492	GLU	-	expression tag	UNP A0A486EJ79
D	1493	HIS	-	expression tag	UNP A0A486EJ79
D	1494	HIS	-	expression tag	UNP A0A486EJ79

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1495	HIS	-	expression tag	UNP A0A486EJ79
D	1496	HIS	-	expression tag	UNP A0A486EJ79
D	1497	HIS	-	expression tag	UNP A0A486EJ79
D	1498	HIS	-	expression tag	UNP A0A486EJ79
A	389	MET	-	initiating methionine	UNP A0A377Y395
A	999	GLU	-	linker	UNP A0A377Y395
A	1000	PHE	-	linker	UNP A0A377Y395
A	1255	THR	SER	conflict	UNP A0A486EJ79
A	1491	LEU	-	expression tag	UNP A0A486EJ79
A	1492	GLU	-	expression tag	UNP A0A486EJ79
A	1493	HIS	-	expression tag	UNP A0A486EJ79
A	1494	HIS	-	expression tag	UNP A0A486EJ79
A	1495	HIS	-	expression tag	UNP A0A486EJ79
A	1496	HIS	-	expression tag	UNP A0A486EJ79
A	1497	HIS	-	expression tag	UNP A0A486EJ79
A	1498	HIS	-	expression tag	UNP A0A486EJ79
B	389	MET	-	initiating methionine	UNP A0A377Y395
B	999	GLU	-	linker	UNP A0A377Y395
B	1000	PHE	-	linker	UNP A0A377Y395
B	1255	THR	SER	conflict	UNP A0A486EJ79
B	1491	LEU	-	expression tag	UNP A0A486EJ79
B	1492	GLU	-	expression tag	UNP A0A486EJ79
B	1493	HIS	-	expression tag	UNP A0A486EJ79
B	1494	HIS	-	expression tag	UNP A0A486EJ79
B	1495	HIS	-	expression tag	UNP A0A486EJ79
B	1496	HIS	-	expression tag	UNP A0A486EJ79
B	1497	HIS	-	expression tag	UNP A0A486EJ79
B	1498	HIS	-	expression tag	UNP A0A486EJ79

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3').

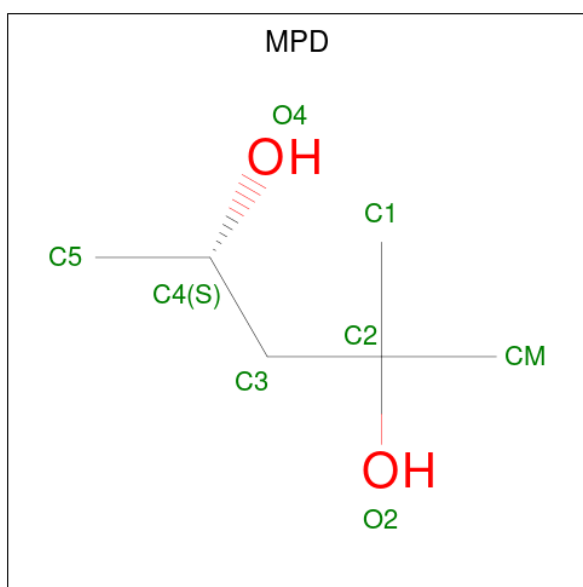
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	10	Total	C	H	N	O	P	0	0	0
			309	99	104	33	63	10			
2	J	10	Total	C	H	N	O	P	0	0	0
			321	99	116	33	63	10			
2	H	8	Total	C	H	N	O	P	0	0	0
			257	79	93	26	51	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			289	89	104	31	56	9			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*

CP*GP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	K	15	Total	C	H	N	O	P	0	0	0
			471	147	167	60	83	14			
3	I	14	Total	C	H	N	O	P	0	0	0
			427	137	144	55	78	13			
3	G	13	Total	C	H	N	O	P	0	0	0
			406	127	144	50	73	12			
3	F	13	Total	C	H	N	O	P	0	0	0
			406	127	144	50	73	12			

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			22	6	14	2		
4	A	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

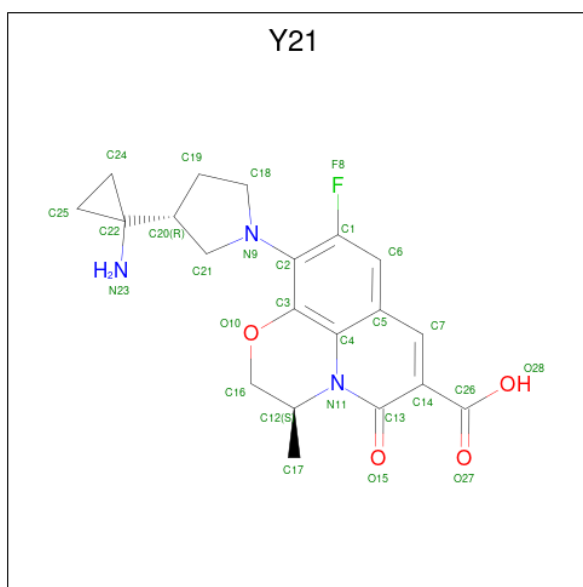
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is (3S)-10-[(3R)-3-(1-aminocyclopropyl)pyrrolidin-1-yl]-9-fluoro-3-methyl-5-oxo-2,3-dihydro-5H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (CCD ID: Y21) (formula: $C_{20}H_{22}FN_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	K	1	Total	C	F	N	O	0	0
			28	20	1	3	4		
6	I	1	Total	C	F	N	O	0	0
			28	20	1	3	4		
6	G	1	Total	C	F	N	O	0	0
			28	20	1	3	4		
6	F	1	Total	C	F	N	O	0	0
			28	20	1	3	4		

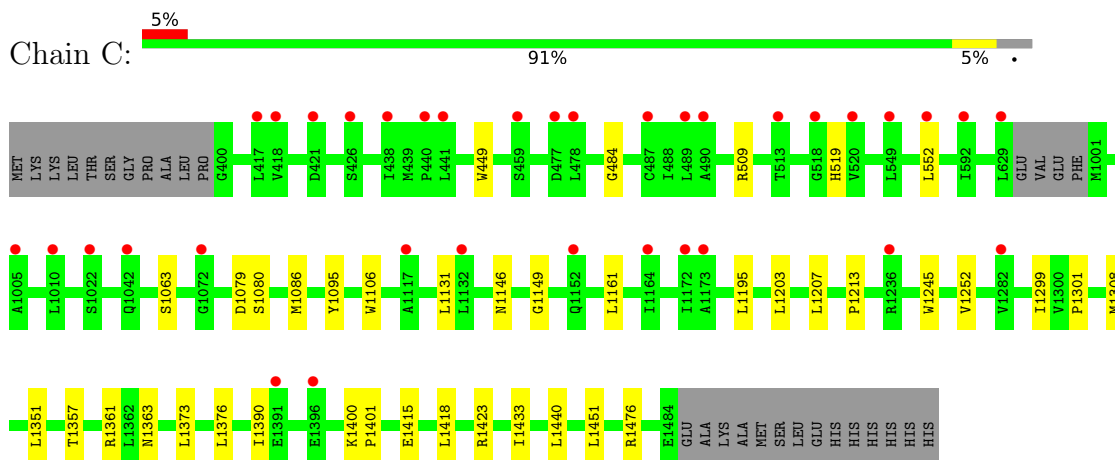
- Molecule 7 is water.

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

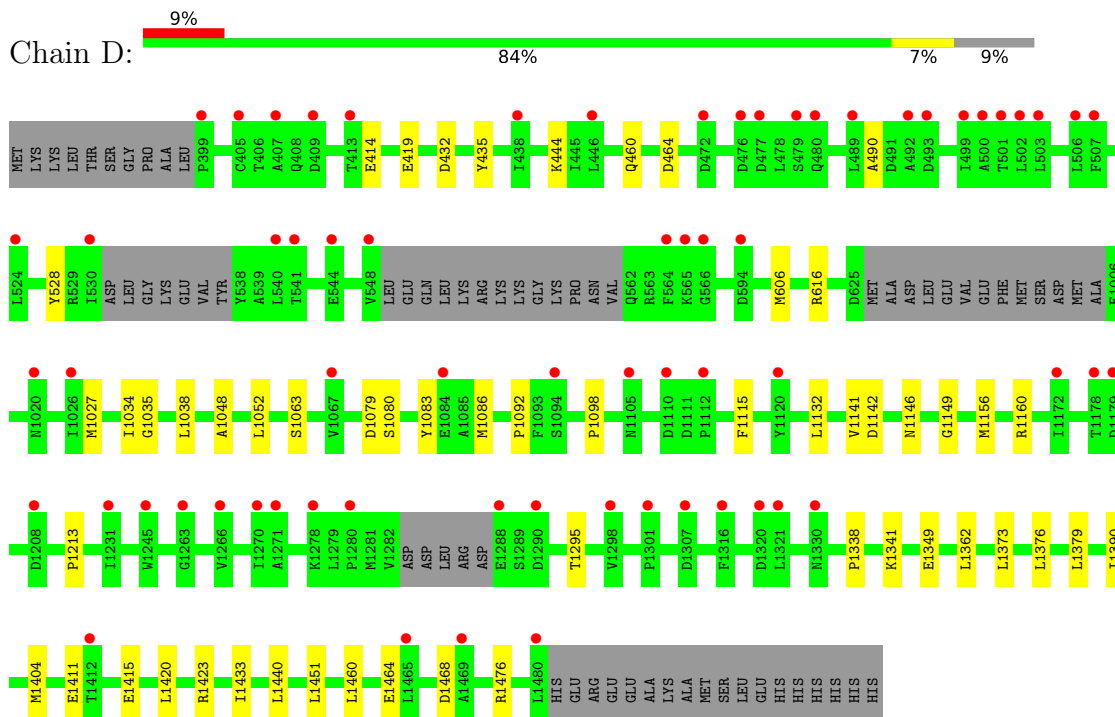
3 Residue-property plots [i](#)

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.

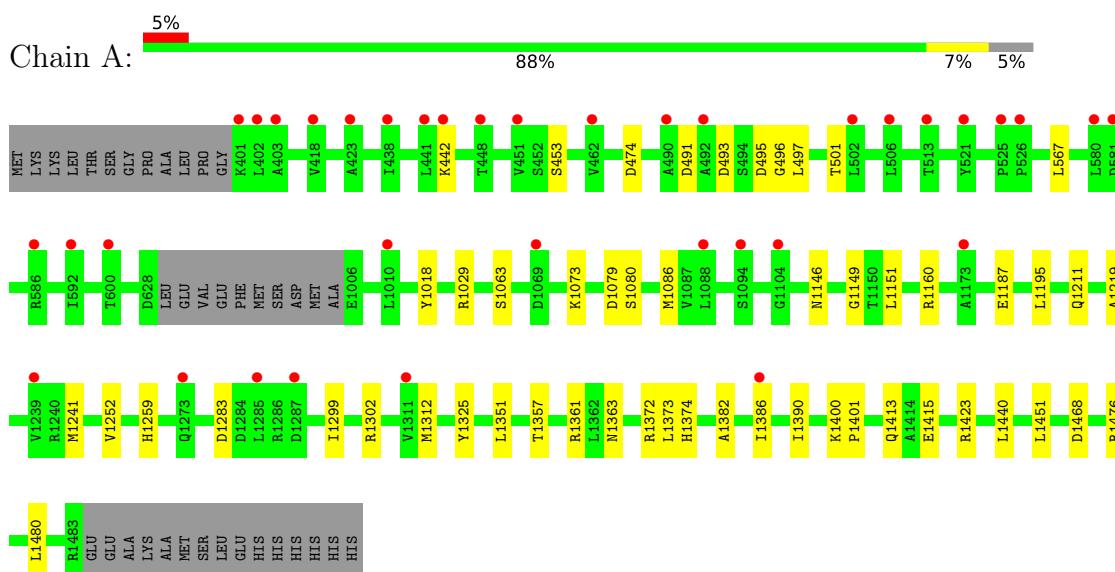
- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera



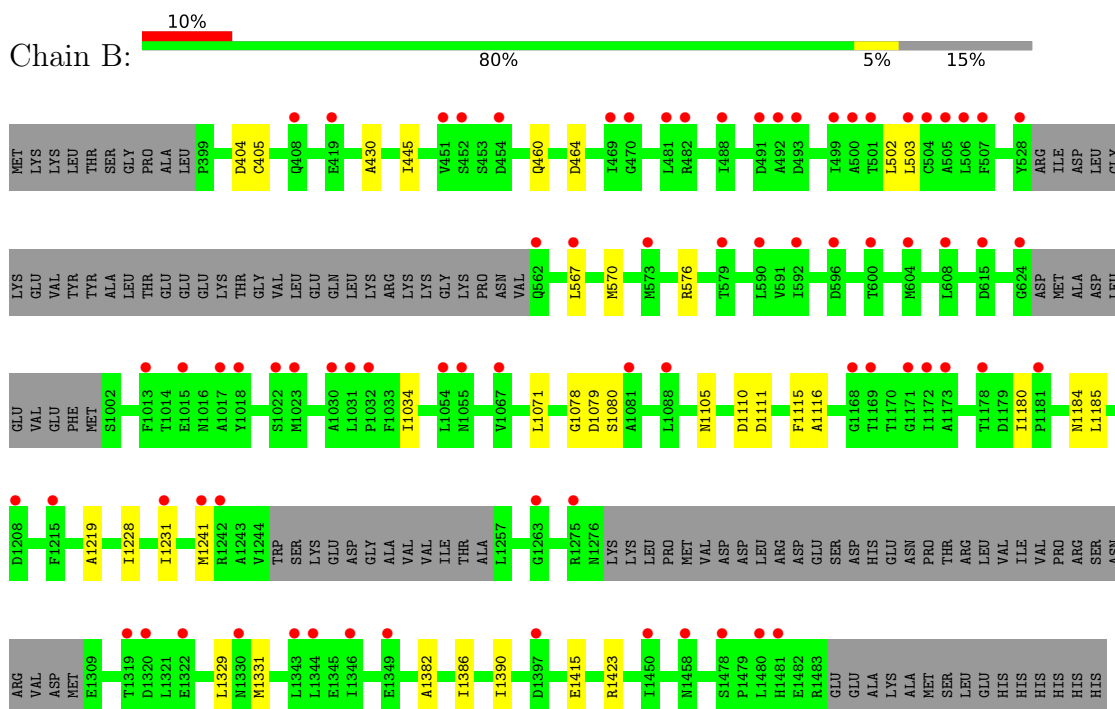
- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera



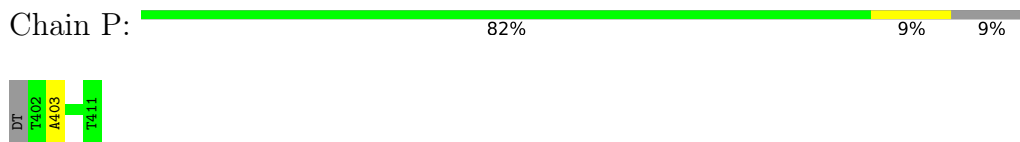
- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera



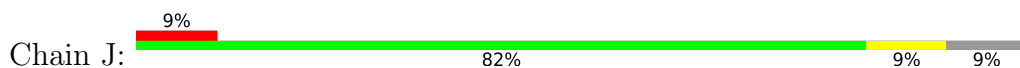
- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera

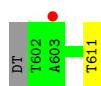


- Molecule 2: DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')



- Molecule 2: DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')

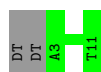
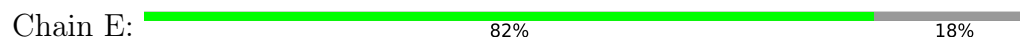




- Molecule 2: DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')



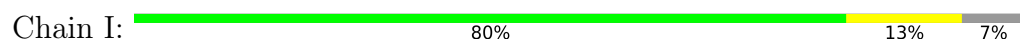
- Molecule 2: DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')



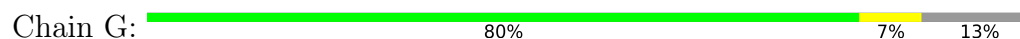
- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')



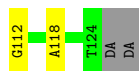
- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')



- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')



- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.19Å 159.82Å 144.06Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	46.92 – 3.30 46.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.92-3.30) 99.4 (46.92-3.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.283 , 0.308 0.283 , 0.309	Depositor DCC
R_{free} test set	3301 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	86.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	38321	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MG, Y21

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	0.17	0/5073	0.28	0/6921
1	B	0.12	0/4357	0.25	0/5961
1	C	0.16	0/5196	0.28	0/7085
1	D	0.15	0/4718	0.28	0/6451
2	E	0.31	0/206	0.49	0/316
2	H	0.27	0/182	0.43	0/279
2	J	0.33	0/228	0.50	0/350
2	P	0.37	0/228	0.52	0/350
3	F	0.28	0/294	0.43	0/452
3	G	0.29	0/294	0.44	0/452
3	I	0.38	0/318	0.57	0/489
3	K	0.31	0/342	0.44	0/526
All	All	0.18	0/21436	0.30	0/29632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4987	4332	4332	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4285	3545	3554	20	0
1	C	5108	4502	4507	23	0
1	D	4639	3873	3900	35	0
2	E	185	104	104	0	0
2	H	164	93	93	2	0
2	J	205	116	116	1	0
2	P	205	104	116	1	0
3	F	262	144	145	2	0
3	G	262	144	145	1	0
3	I	283	144	156	2	0
3	K	304	167	167	1	0
4	A	8	14	14	1	0
4	C	8	14	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	F	28	0	0	0	0
6	G	28	0	0	1	0
6	I	28	0	0	0	0
6	K	28	0	0	0	0
7	A	2	0	0	0	0
7	C	1	0	0	0	0
7	P	1	0	0	0	0
All	All	21025	17296	17363	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:VAL:HG11	1:A:1312:MET:HE3	1.38	1.02
1:A:1283:ASP:OD1	1:A:1302:ARG:NH1	2.18	0.75
1:B:460:GLN:NE2	1:B:464:ASP:OD2	2.20	0.75
1:D:1404:MET:HE2	1:D:1411:GLU:HA	1.75	0.69
1:A:495:ASP:OD1	1:A:1029:ARG:NH2	2.30	0.65
1:C:1423:ARG:NH2	1:D:1415:GLU:OE2	2.31	0.64
1:D:1079:ASP:OD1	1:D:1080:SER:N	2.33	0.62
1:C:1301:PRO:HB3	1:C:1308:MET:HE2	1.81	0.62
1:D:419:GLU:HB2	1:D:490:ALA:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:SER:OG	1:A:474:ASP:OD2	2.19	0.61
1:A:497:LEU:O	1:A:501:THR:N	2.33	0.61
1:A:1160:ARG:NH1	1:A:1468:ASP:OD1	2.35	0.60
1:D:414:GLU:OE2	1:D:435:TYR:HE1	1.84	0.60
1:D:1160:ARG:NH1	1:D:1468:ASP:OD1	2.35	0.59
1:D:1213:PRO:O	1:D:1476:ARG:NH2	2.36	0.59
1:B:404:ASP:OD1	1:B:405:CYS:N	2.36	0.58
2:P:403:DA:N6	3:I:723:DG:O6	2.37	0.58
1:D:414:GLU:OE2	1:D:435:TYR:CE1	2.57	0.57
1:D:1027:MET:HE1	1:D:1338:PRO:HD3	1.87	0.56
1:A:1259:HIS:O	1:A:1325:TYR:OH	2.23	0.56
1:C:552:LEU:O	1:C:552:LEU:HD12	2.06	0.56
1:A:1423:ARG:NH2	1:B:1415:GLU:OE2	2.40	0.55
1:D:1146:ASN:OD1	1:D:1149:GLY:N	2.40	0.55
1:A:491:ASP:HA	1:A:567:LEU:HD13	1.88	0.55
1:D:1341:LYS:HE2	1:D:1349:GLU:OE1	2.07	0.55
1:B:1079:ASP:OD1	1:B:1080:SER:N	2.37	0.54
1:C:1146:ASN:OD1	1:C:1149:GLY:N	2.38	0.54
1:A:442:LYS:O	6:G:401:Y21:N23	2.41	0.54
1:B:1219:ALA:HB3	1:B:1241:MET:HE2	1.89	0.54
1:B:567:LEU:HA	1:B:570:MET:HE3	1.89	0.53
1:C:1079:ASP:OD1	1:C:1080:SER:N	2.40	0.53
1:C:1203:LEU:O	1:C:1207:LEU:HD13	2.09	0.53
1:D:606:MET:O	1:D:616:ARG:NH1	2.42	0.52
1:A:1219:ALA:HB3	1:A:1241:MET:HE2	1.92	0.52
1:A:1252:VAL:CG1	1:A:1312:MET:HE3	2.25	0.51
1:B:1071:LEU:HD11	1:B:1079:ASP:HA	1.94	0.50
1:B:1382:ALA:O	1:B:1386:ILE:N	2.44	0.50
1:D:432:ASP:OD2	1:D:435:TYR:CE2	2.64	0.50
1:B:1034:ILE:HD12	1:B:1331:MET:HE3	1.94	0.50
1:C:1245:TRP:CE3	1:C:1252:VAL:HG23	2.49	0.48
1:C:1213:PRO:O	1:C:1476:ARG:NH2	2.46	0.48
1:C:1390:ILE:HD13	1:D:1390:ILE:HD13	1.95	0.48
1:D:1379:LEU:HD22	1:D:1420:LEU:HD21	1.97	0.47
1:C:1415:GLU:OE2	1:D:1423:ARG:NH1	2.47	0.47
1:D:1048:ALA:O	1:D:1052:LEU:HD13	2.14	0.47
1:D:1295:THR:HG23	1:D:1295:THR:O	2.14	0.47
1:D:1373:LEU:HD21	1:D:1440:LEU:HB2	1.97	0.47
1:D:1063:SER:HB3	1:D:1086:MET:HE1	1.97	0.46
1:A:1211:GLN:HG2	1:A:1480:LEU:HD22	1.96	0.46
1:A:493:ASP:HB2	1:A:496:GLY:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ALA:HB1	1:B:576:ARG:HB2	1.96	0.46
1:A:1374:HIS:O	1:A:1413:GLN:NE2	2.45	0.46
3:K:522:DC:O2	3:K:522:DC:O4'	2.34	0.46
1:C:1131:LEU:HD13	1:C:1161:LEU:HD12	1.98	0.46
1:A:1079:ASP:OD1	1:A:1080:SER:N	2.45	0.46
1:C:1418:LEU:HB3	1:D:1423:ARG:HG2	1.97	0.46
1:B:1105:ASN:HB3	1:B:1116:ALA:HB2	1.98	0.46
1:A:1299:ILE:HD12	1:A:1312:MET:HE1	1.98	0.45
1:D:1141:VAL:HG23	1:D:1156:MET:HE2	1.99	0.45
1:C:484:GLY:O	1:C:519:HIS:ND1	2.50	0.45
1:D:1141:VAL:HG22	1:D:1142:ASP:N	2.32	0.45
1:A:1372:ARG:HH22	4:A:1501:MPD:HO4	1.64	0.45
1:A:1390:ILE:HD13	1:B:1390:ILE:HD13	1.99	0.45
1:B:502:LEU:HD21	3:F:118:DA:H4'	1.98	0.45
1:C:1376:LEU:HD22	1:C:1433:ILE:HG23	1.98	0.45
1:C:1086:MET:HE3	1:C:1106:TRP:HH2	1.82	0.44
1:A:1063:SER:HB3	1:A:1086:MET:HE1	1.99	0.44
1:A:1373:LEU:HD21	1:A:1440:LEU:HB2	2.00	0.44
1:B:445:ILE:HD13	1:B:503:LEU:HD23	2.00	0.44
1:D:460:GLN:NE2	1:D:464:ASP:OD2	2.50	0.44
1:C:449:TRP:HA	1:C:509:ARG:HG3	2.00	0.44
1:A:1195:LEU:HD22	1:A:1351:LEU:HD12	1.99	0.44
3:G:314:DT:O4	3:F:112:DG:N1	2.50	0.44
1:D:1034:ILE:HG23	1:D:1035:GLY:N	2.33	0.43
1:A:1363:ASN:OD1	1:A:1451:LEU:HD13	2.18	0.43
1:C:1063:SER:HB3	1:C:1086:MET:HE1	1.99	0.43
1:D:1376:LEU:HD22	1:D:1433:ILE:HG23	2.00	0.43
1:B:1078:GLY:N	2:H:211:DT:OP2	2.50	0.43
1:C:1252:VAL:CG1	1:C:1299:ILE:HB	2.48	0.43
1:B:1180:ILE:HG12	1:B:1329:LEU:HD13	2.00	0.43
1:D:1141:VAL:HG23	1:D:1156:MET:HB2	2.01	0.43
1:A:1382:ALA:O	1:A:1386:ILE:N	2.52	0.43
1:C:1400:LYS:HB3	1:C:1401:PRO:HD3	2.01	0.43
1:B:1184:ASN:OD1	1:B:1185:LEU:N	2.52	0.43
1:D:444:LYS:HG3	2:J:611:DT:H1'	2.01	0.43
1:A:501:THR:HG21	1:A:1018:TYR:CD1	2.54	0.42
1:A:1357:THR:O	1:A:1361:ARG:N	2.42	0.42
1:C:1357:THR:O	1:C:1361:ARG:N	2.41	0.42
1:A:1187:GLU:OE1	1:A:1476:ARG:NH1	2.52	0.42
1:A:1415:GLU:OE2	1:B:1423:ARG:NH2	2.51	0.42
1:D:1115:PHE:C	1:D:1115:PHE:CD1	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:205:DG:H2'	2:H:206:DT:H72	2.02	0.41
1:D:1038:LEU:HD11	1:D:1132:LEU:HD13	2.01	0.41
1:D:528:TYR:C	1:D:528:TYR:CD1	2.99	0.41
1:B:1110:ASP:OD1	1:B:1111:ASP:N	2.54	0.41
1:A:1146:ASN:OD1	1:A:1149:GLY:N	2.50	0.41
1:C:1373:LEU:HD21	1:C:1440:LEU:HB2	2.02	0.41
1:A:1073:LYS:HD2	1:A:1151:LEU:HD22	2.02	0.41
1:A:1400:LYS:HB2	1:A:1401:PRO:HD3	2.03	0.41
3:I:722:DC:H2'	3:I:723:DG:C8	2.55	0.41
1:D:1092:PRO:HA	1:D:1098:PRO:HG3	2.03	0.40
1:D:1362:LEU:HB2	1:D:1451:LEU:HD21	2.03	0.40
1:B:1228:ILE:HA	1:B:1231:ILE:HD12	2.04	0.40
1:D:1083:TYR:CD1	1:D:1086:MET:HE2	2.56	0.40
1:D:1460:LEU:O	1:D:1464:GLU:N	2.43	0.40
1:C:1363:ASN:OD1	1:C:1451:LEU:HD13	2.22	0.40
1:C:1195:LEU:HD12	1:C:1351:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	702/743 (94%)	680 (97%)	22 (3%)	0	100	100
1	B	621/743 (84%)	605 (97%)	16 (3%)	0	100	100
1	C	710/743 (96%)	688 (97%)	22 (3%)	0	100	100
1	D	667/743 (90%)	647 (97%)	20 (3%)	0	100	100
All	All	2700/2972 (91%)	2620 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/640 (66%)	422 (100%)	0	100	100
1	B	334/640 (52%)	333 (100%)	1 (0%)	86	86
1	C	447/640 (70%)	446 (100%)	1 (0%)	87	88
1	D	362/640 (57%)	362 (100%)	0	100	100
All	All	1565/2560 (61%)	1563 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1095	TYR
1	B	1115	PHE

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

Mol	Chain	Res	Type
1	C	583	ASN
1	C	1273	GLN
1	C	1424	HIS
1	D	463	HIS
1	D	583	ASN
1	D	1152	GLN
1	A	583	ASN
1	A	1075	HIS
1	A	1152	GLN
1	A	1259	HIS
1	B	519	HIS
1	B	583	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

Of 10 ligands modelled in this entry, 4 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$
6	Y21	I	801	-	30,32,32	1.43	4 (13%)	38,51,51	1.60	7 (18%)
4	MPD	C	1501	-	7,7,7	0.27	0	9,10,10	0.44	0
6	Y21	K	601	-	30,32,32	1.42	4 (13%)	38,51,51	1.53	8 (21%)
6	Y21	G	401	-	30,32,32	1.43	5 (16%)	38,51,51	1.58	7 (18%)
4	MPD	A	1501	-	7,7,7	0.33	0	9,10,10	0.20	0
6	Y21	F	201	-	30,32,32	1.42	5 (16%)	38,51,51	1.59	9 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y21	I	801	-	-	7/12/36/36	0/5/5/5
4	MPD	C	1501	-	-	0/5/5/5	-
6	Y21	K	601	-	-	2/12/36/36	0/5/5/5
6	Y21	G	401	-	-	2/12/36/36	0/5/5/5
4	MPD	A	1501	-	-	0/5/5/5	-
6	Y21	F	201	-	-	7/12/36/36	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	801	Y21	C5-C7	4.12	1.51	1.43
6	G	401	Y21	C5-C7	4.01	1.51	1.43
6	K	601	Y21	C5-C7	3.81	1.51	1.43
6	F	201	Y21	C5-C7	3.72	1.51	1.43
6	K	601	Y21	C24-C22	2.87	1.55	1.49
6	F	201	Y21	C24-C22	2.81	1.55	1.49
6	G	401	Y21	C24-C22	2.81	1.55	1.49
6	I	801	Y21	C24-C22	2.81	1.55	1.49
6	G	401	Y21	C25-C22	2.67	1.54	1.49
6	K	601	Y21	C25-C22	2.65	1.54	1.49
6	F	201	Y21	C25-C22	2.57	1.54	1.49
6	I	801	Y21	C25-C22	2.51	1.54	1.49
6	G	401	Y21	C21-C20	2.20	1.55	1.52
6	F	201	Y21	C25-C24	2.07	1.55	1.50
6	K	601	Y21	C25-C24	2.07	1.55	1.50
6	I	801	Y21	C25-C24	2.04	1.55	1.50
6	G	401	Y21	C25-C24	2.04	1.55	1.50
6	F	201	Y21	C21-C20	2.02	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	401	Y21	C16-C12-N11	3.77	109.54	106.70
6	I	801	Y21	O15-C13-C14	-3.66	117.20	124.96
6	G	401	Y21	O15-C13-C14	-3.64	117.24	124.96
6	F	201	Y21	C3-C2-C1	3.60	119.42	115.92
6	I	801	Y21	C3-C2-C1	3.59	119.42	115.92
6	I	801	Y21	C16-C12-N11	3.58	109.39	106.70
6	I	801	Y21	C17-C12-N11	-3.31	108.20	111.14
6	K	601	Y21	C3-C2-C1	3.23	119.06	115.92
6	F	201	Y21	O15-C13-C14	-3.22	118.13	124.96
6	G	401	Y21	C3-C2-C1	3.18	119.02	115.92
6	F	201	Y21	C17-C12-N11	-3.17	108.33	111.14
6	G	401	Y21	C17-C12-N11	-3.10	108.39	111.14
6	K	601	Y21	O15-C13-C14	-3.09	118.41	124.96
6	F	201	Y21	C16-C12-N11	2.94	108.91	106.70
6	F	201	Y21	C6-C5-C4	2.79	120.41	117.85
6	K	601	Y21	C16-C12-N11	2.75	108.77	106.70
6	K	601	Y21	O10-C3-C2	2.68	120.71	117.90
6	G	401	Y21	C14-C13-N11	2.66	120.96	115.93
6	K	601	Y21	C14-C13-N11	2.65	120.94	115.93
6	I	801	Y21	C14-C13-N11	2.64	120.93	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	601	Y21	C6-C5-C4	2.60	120.22	117.85
6	K	601	Y21	C17-C12-N11	-2.44	108.98	111.14
6	F	201	Y21	C14-C13-N11	2.32	120.33	115.93
6	K	601	Y21	C5-C7-C14	-2.25	119.87	122.06
6	F	201	Y21	C5-C7-C14	-2.25	119.87	122.06
6	F	201	Y21	C6-C1-C2	-2.16	120.12	123.34
6	I	801	Y21	C6-C1-C2	-2.15	120.14	123.34
6	I	801	Y21	C6-C5-C4	2.12	119.79	117.85
6	G	401	Y21	C6-C1-C2	-2.08	120.25	123.34
6	G	401	Y21	C6-C5-C4	2.05	119.73	117.85
6	F	201	Y21	C20-C21-N9	-2.02	101.24	103.51

There are no chirality outliers.

All (18) torsion outliers are listed below:

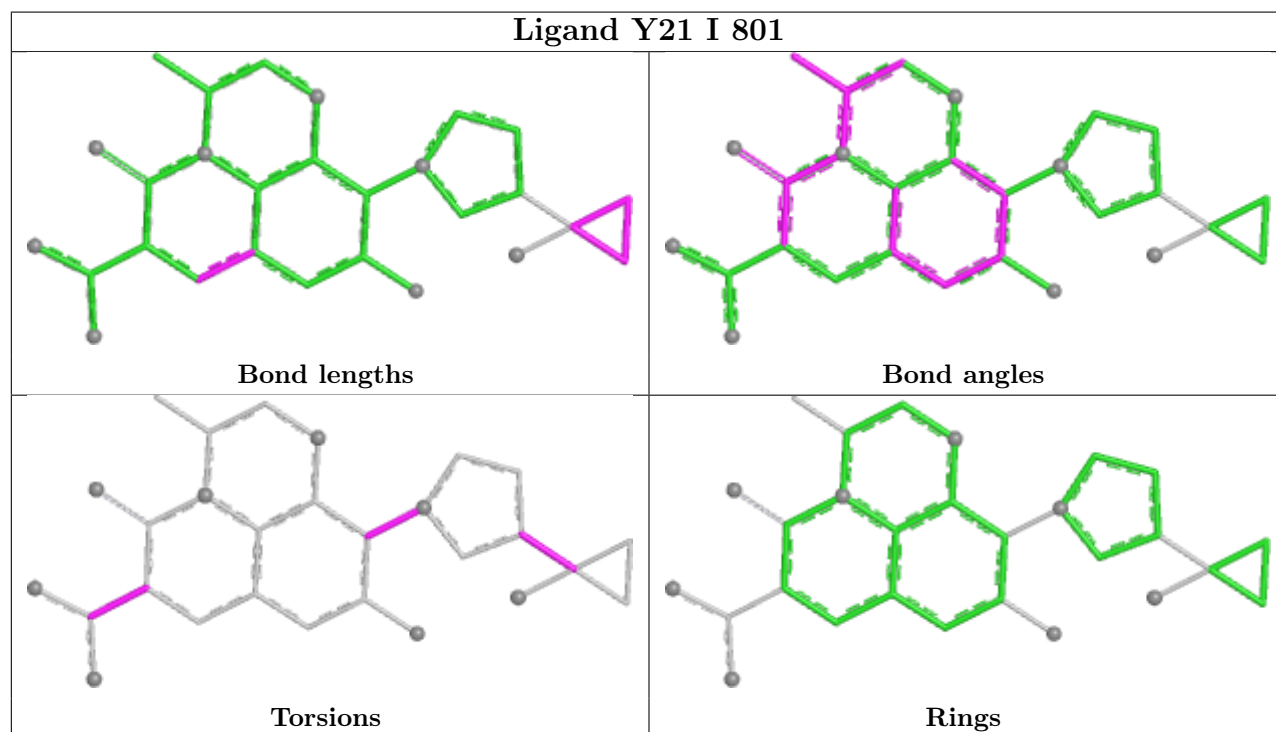
Mol	Chain	Res	Type	Atoms
6	K	601	Y21	C3-C2-N9-C18
6	I	801	Y21	C1-C2-N9-C18
6	I	801	Y21	C21-C20-C22-C25
6	G	401	Y21	C3-C2-N9-C18
6	F	201	Y21	C1-C2-N9-C18
6	F	201	Y21	C19-C20-C22-C24
6	K	601	Y21	C1-C2-N9-C18
6	I	801	Y21	C1-C2-N9-C21
6	G	401	Y21	C1-C2-N9-C18
6	F	201	Y21	C1-C2-N9-C21
6	I	801	Y21	C13-C14-C26-O28
6	I	801	Y21	C7-C14-C26-O27
6	I	801	Y21	C7-C14-C26-O28
6	F	201	Y21	C7-C14-C26-O27
6	F	201	Y21	C7-C14-C26-O28
6	F	201	Y21	C3-C2-N9-C18
6	I	801	Y21	C19-C20-C22-C25
6	F	201	Y21	C21-C20-C22-C24

There are no ring outliers.

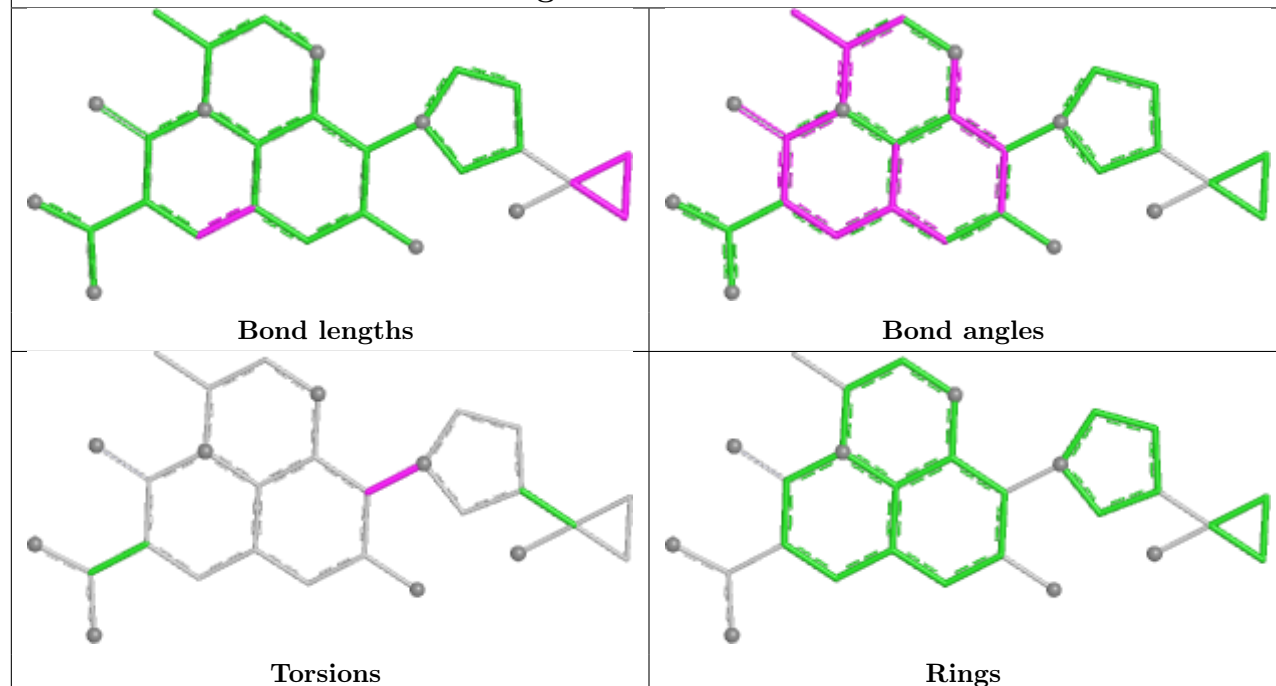
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	401	Y21	1	0
4	A	1501	MPD	1	0

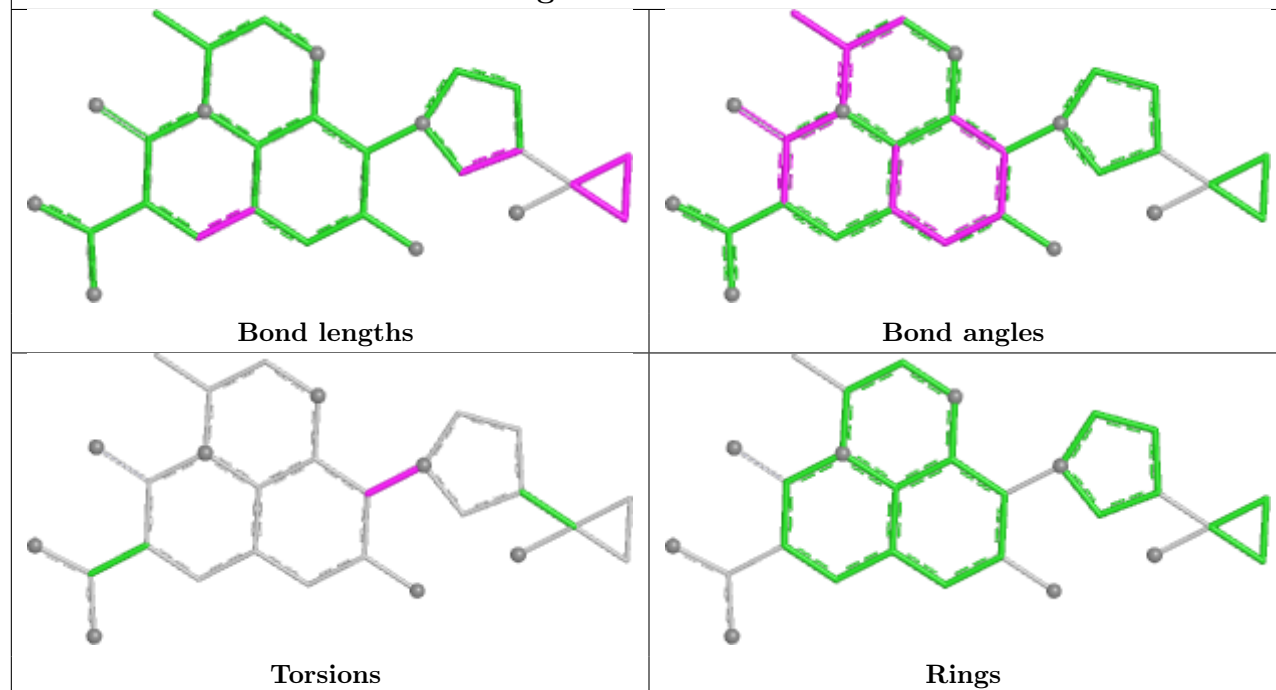
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

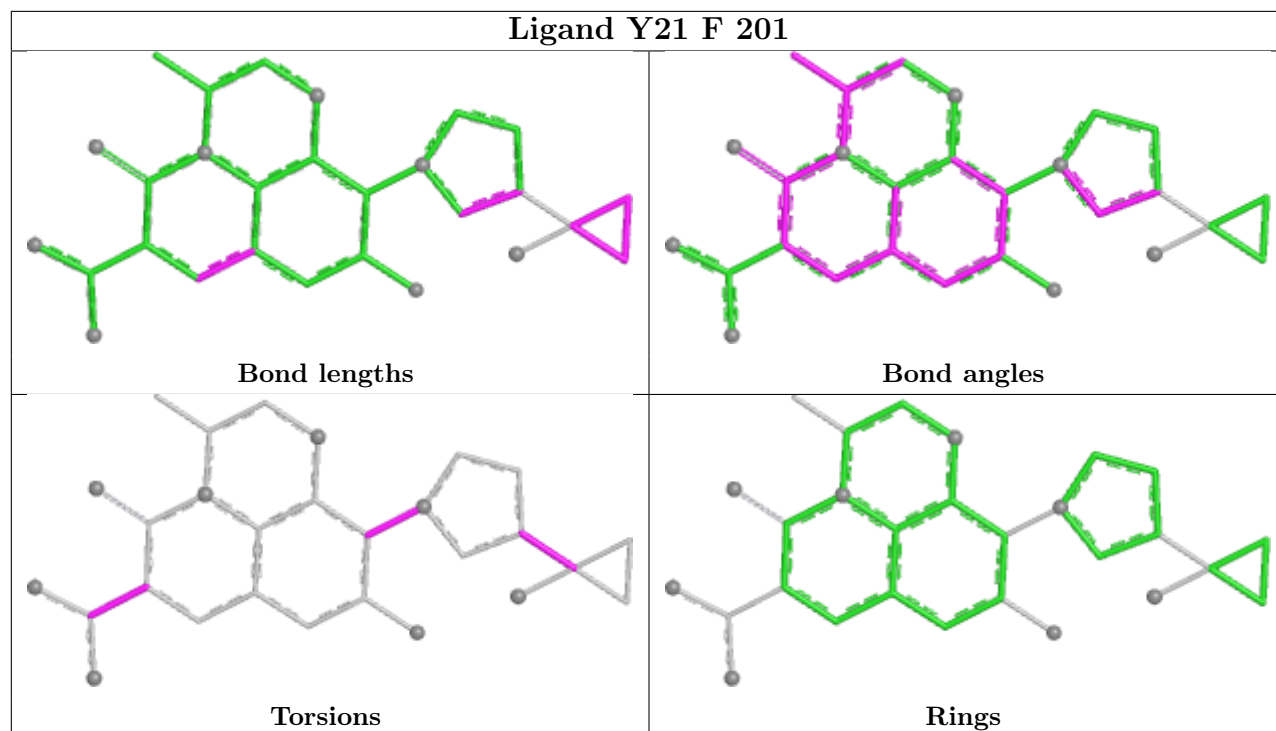


Ligand Y21 K 601



Ligand Y21 G 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	706/743 (95%)	0.54	36 (5%) 33 22	43, 66, 105, 124	0
1	B	631/743 (84%)	0.89	76 (12%) 9 7	45, 100, 142, 171	0
1	C	714/743 (96%)	0.55	35 (4%) 35 23	49, 67, 113, 137	0
1	D	677/743 (91%)	0.75	66 (9%) 13 11	53, 90, 155, 203	0
2	E	9/11 (81%)	0.70	0 100 100	57, 65, 117, 131	0
2	H	8/11 (72%)	1.08	0 100 100	89, 95, 130, 147	0
2	J	10/11 (90%)	1.16	1 (10%) 12 10	81, 99, 160, 166	0
2	P	10/11 (90%)	0.39	0 100 100	56, 67, 104, 108	0
3	F	13/15 (86%)	0.85	0 100 100	85, 102, 160, 176	0
3	G	13/15 (86%)	0.44	0 100 100	62, 81, 99, 105	0
3	I	14/15 (93%)	0.50	0 100 100	63, 76, 89, 92	0
3	K	15/15 (100%)	0.94	0 100 100	81, 95, 191, 205	0
All	All	2820/3076 (91%)	0.68	214 (7%) 20 14	43, 82, 137, 205	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	THR	5.4
1	B	504	CYS	5.2
1	D	566	GLY	5.2
1	B	503	LEU	4.5
1	B	1320	ASP	4.4
1	D	565	LYS	4.4
1	A	580	LEU	4.2
1	C	1152	GLN	4.2
1	A	525	PRO	4.2
1	C	441	LEU	4.0
1	D	530	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	501	THR	3.8
1	B	488	ILE	3.8
1	D	541	THR	3.8
1	C	490	ALA	3.7
1	C	1117	ALA	3.7
1	A	448	THR	3.7
1	A	1273	GLN	3.6
1	B	1397	ASP	3.5
1	B	1171	GLY	3.5
1	B	1030	ALA	3.4
1	C	1010	LEU	3.4
1	B	505	ALA	3.4
1	B	579	THR	3.4
1	B	590	LEU	3.4
1	D	1270	ILE	3.3
1	C	520	VAL	3.3
1	C	459	SER	3.3
1	B	1478	SER	3.3
1	D	1067	VAL	3.3
1	A	581	ASP	3.2
1	D	548	VAL	3.2
1	A	418	VAL	3.2
1	A	438	ILE	3.2
1	A	441	LEU	3.2
1	A	451	VAL	3.2
1	B	507	PHE	3.2
1	D	1094	SER	3.2
1	C	518	GLY	3.0
1	C	417	LEU	3.0
1	C	421	ASP	3.0
1	B	1330	ASN	3.0
1	B	1173	ALA	2.9
1	D	1321	LEU	2.9
1	D	564	PHE	2.9
1	C	418	VAL	2.9
1	A	402	LEU	2.9
1	B	1242	ARG	2.8
1	D	1288	GLU	2.8
1	D	1263	GLY	2.8
1	C	513	THR	2.8
1	B	1031	LEU	2.8
1	C	489	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1072	GLY	2.7
1	A	1173	ALA	2.7
1	D	1412	THR	2.7
1	D	409	ASP	2.7
1	B	470	GLY	2.7
1	A	513	THR	2.7
1	D	540	LEU	2.7
1	D	507	PHE	2.7
1	B	1319	THR	2.7
1	C	549	LEU	2.7
1	B	500	ALA	2.6
1	B	1458	ASN	2.6
1	D	413	THR	2.6
1	D	506	LEU	2.6
1	D	1465	LEU	2.6
1	D	500	ALA	2.6
1	A	586	ARG	2.6
1	D	476	ASP	2.6
1	D	479	SER	2.6
1	D	477	ASP	2.6
1	C	1396	GLU	2.6
1	C	629	LEU	2.5
1	B	1169	THR	2.5
1	D	493	ASP	2.5
1	D	438	ILE	2.5
1	B	1215	PHE	2.5
1	C	440	PRO	2.5
1	B	1343	LEU	2.5
1	A	1094	SER	2.5
1	B	408	GLN	2.5
1	B	451	VAL	2.5
1	A	403	ALA	2.5
1	A	592	ILE	2.5
1	D	1026	ILE	2.5
1	D	1178	THR	2.5
1	C	1132	LEU	2.5
1	A	502	LEU	2.5
1	B	492	ALA	2.4
1	B	499	ILE	2.4
1	C	478	LEU	2.4
1	D	489	LEU	2.4
1	A	1285	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1173	ALA	2.4
1	D	1271	ALA	2.4
1	C	592	ILE	2.4
1	D	594	ASP	2.4
1	B	615	ASP	2.4
1	B	1168	GLY	2.4
1	D	499	ILE	2.4
1	B	469	ILE	2.4
1	B	1346	ILE	2.4
1	A	401	LYS	2.4
1	A	526	PRO	2.4
1	B	454	ASP	2.4
1	A	490	ALA	2.4
1	B	1172	ILE	2.4
1	C	552	LEU	2.4
1	B	452	SER	2.4
1	D	492	ALA	2.3
1	D	1330	ASN	2.3
1	B	1018	TYR	2.3
1	B	1344	LEU	2.3
1	D	1290	ASP	2.3
1	D	1320	ASP	2.3
1	A	1069	ASP	2.3
1	B	506	LEU	2.3
1	B	1480	LEU	2.3
1	B	1015	GLU	2.3
1	B	1178	THR	2.3
1	C	477	ASP	2.3
1	D	1298	VAL	2.3
1	A	462	VAL	2.3
1	D	1112	PRO	2.3
1	C	1005	ALA	2.3
1	D	407	ALA	2.3
1	B	1017	ALA	2.3
1	C	426	SER	2.3
1	D	503	LEU	2.3
1	A	1104	GLY	2.3
1	B	1023	MET	2.3
1	A	506	LEU	2.3
1	B	608	LEU	2.3
1	C	1022	SER	2.3
1	C	1282	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1311	VAL	2.3
1	D	1231	ILE	2.2
1	A	1386	ILE	2.2
1	B	1081	ALA	2.2
1	B	1241	MET	2.2
1	D	524	LEU	2.2
1	D	1316	PHE	2.2
1	A	442	LYS	2.2
1	B	1055	ASN	2.2
1	B	1067	VAL	2.2
1	B	493	ASP	2.2
1	C	438	ILE	2.2
1	C	1172	ILE	2.2
1	B	592	ILE	2.2
1	D	1280	PRO	2.2
1	D	480	GLN	2.2
1	D	1179	ASP	2.2
1	D	399	PRO	2.2
1	B	1088	LEU	2.2
1	D	1266	VAL	2.2
1	C	487	CYS	2.2
1	D	1469	ALA	2.2
1	B	1231	ILE	2.2
1	D	1480	LEU	2.2
1	C	1391	GLU	2.2
1	D	1245	TRP	2.2
1	A	600	THR	2.1
1	B	1450	ILE	2.1
1	A	1088	LEU	2.1
1	D	544	GLU	2.1
1	B	624	GLY	2.1
1	B	1032	PRO	2.1
1	D	472	ASP	2.1
1	D	1110	ASP	2.1
1	D	1208	ASP	2.1
1	B	1208	ASP	2.1
1	C	1164	ILE	2.1
1	A	521	TYR	2.1
1	B	528	TYR	2.1
1	D	1278	LYS	2.1
1	A	1010	LEU	2.1
1	B	562	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	2.1
1	D	1120	TYR	2.1
1	B	567	LEU	2.1
1	B	482	ARG	2.1
1	D	1105	ASN	2.1
1	A	1287	ASP	2.1
1	B	491	ASP	2.1
1	B	1481	HIS	2.1
1	C	1236	ARG	2.1
1	D	1172	ILE	2.1
1	B	596	ASP	2.1
1	D	405	CYS	2.1
1	A	423	ALA	2.1
1	C	1042	GLN	2.1
1	B	1013	PHE	2.1
1	B	1022	SER	2.0
1	B	573	MET	2.0
1	B	604	MET	2.0
1	B	600	THR	2.0
1	D	1084	GLU	2.0
1	B	1322	GLU	2.0
1	B	1349	GLU	2.0
1	A	1239	VAL	2.0
1	D	502	LEU	2.0
1	D	1020	ASN	2.0
2	J	603	DA	2.0
1	D	1307	ASP	2.0
1	B	1263	GLY	2.0
1	D	1301	PRO	2.0
1	B	1181	PRO	2.0
1	B	419	GLU	2.0
1	B	1275	ARG	2.0
1	D	446	LEU	2.0
1	B	481	LEU	2.0
1	B	1054	LEU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

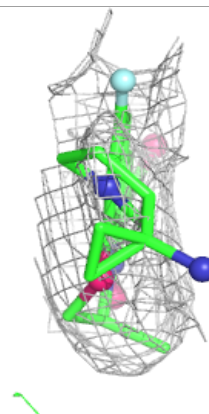
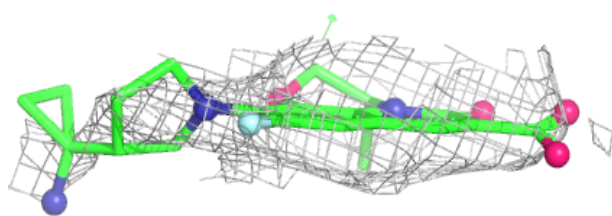
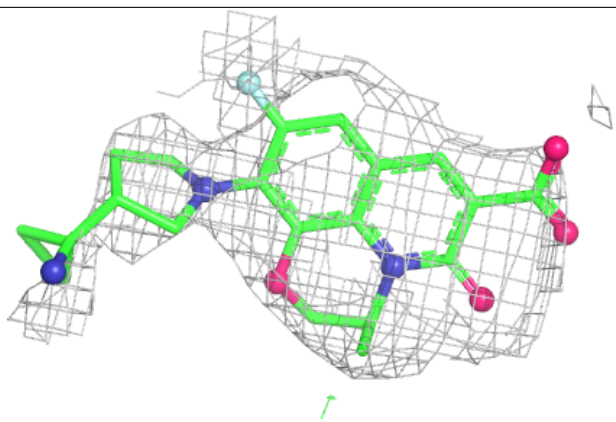
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	1501	1/1	0.63	0.26	108,108,108,108	0
5	MG	D	1501	1/1	0.69	0.25	91,91,91,91	0
5	MG	A	1502	1/1	0.74	0.14	82,82,82,82	0
6	Y21	F	201	28/28	0.75	0.22	98,102,104,105	0
4	MPD	C	1501	8/8	0.80	0.15	20,20,60,60	0
4	MPD	A	1501	8/8	0.82	0.14	20,20,70,70	0
5	MG	C	1502	1/1	0.87	0.18	85,85,85,85	0
6	Y21	K	601	28/28	0.89	0.16	90,93,94,94	0
6	Y21	G	401	28/28	0.91	0.15	80,84,86,88	0
6	Y21	I	801	28/28	0.91	0.13	77,81,82,83	0

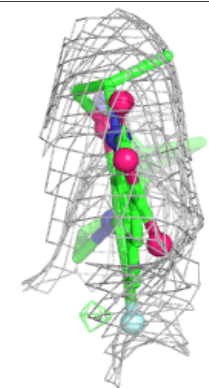
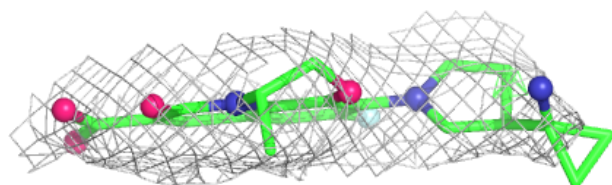
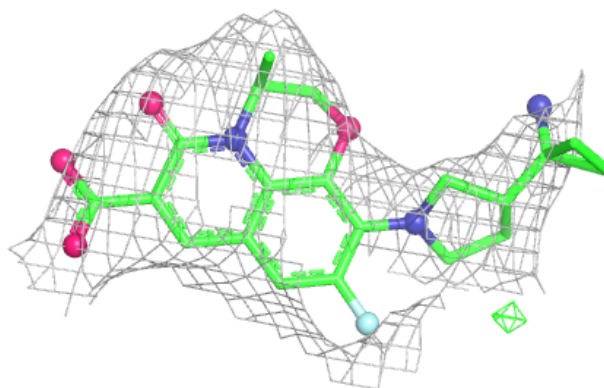
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y21 F 201:

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

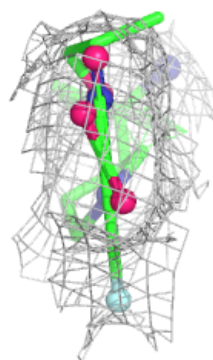
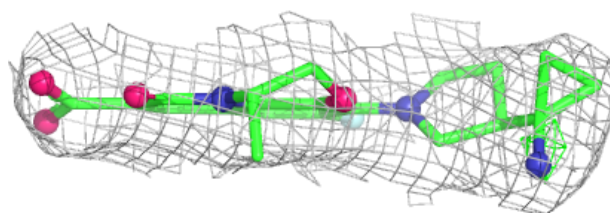
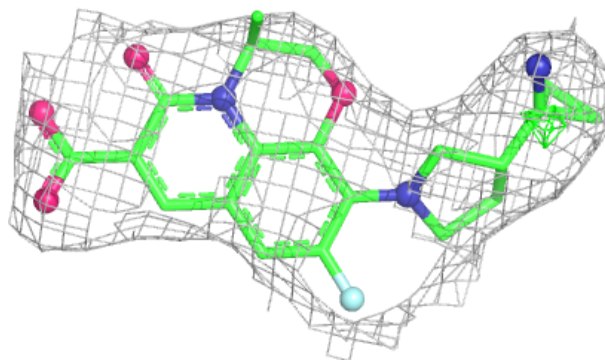
**Electron density around Y21 K 601:**

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

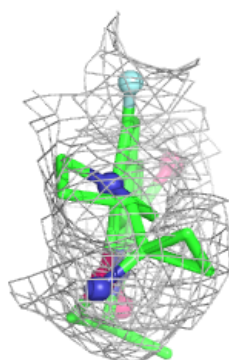
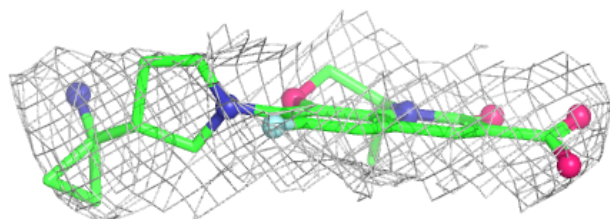
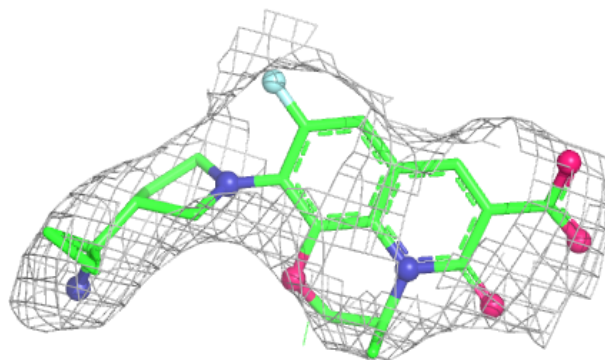


Electron density around Y21 G 401:

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

**Electron density around Y21 I 801:**

$2mF_o-DF_c$ (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.