



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2021 – 12:40 PM EDT

PDB ID : 7LHZ
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.18
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) : 2.18

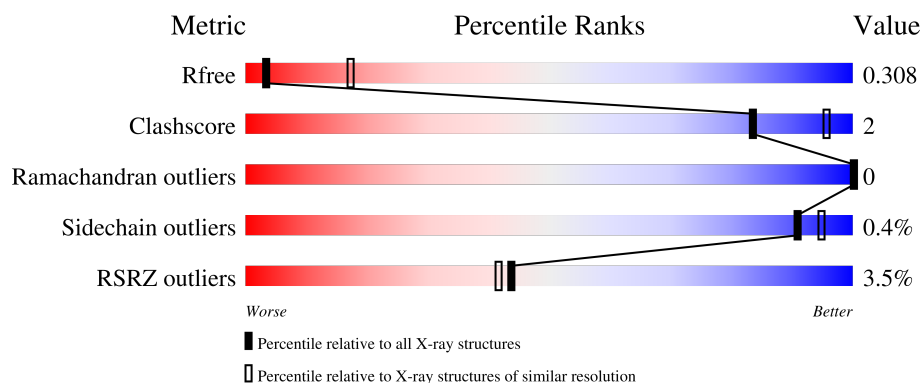
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	743	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	743	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
1	D	743	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
2	E	11	<div> <div></div> <div> <div>82%</div> <div>18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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

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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').

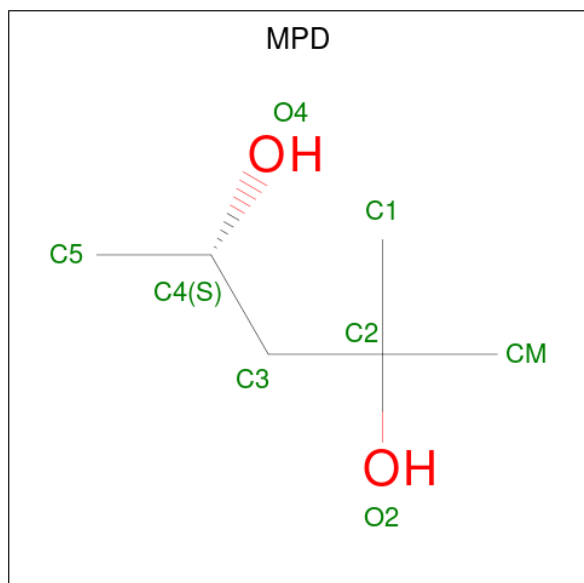
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	10	Total	C	H	N	O	P	0	0	0
			309	99	104	33	63	10			
2	J	10	Total	C	H	N	O	P	0	0	0
			321	99	116	33	63	10			
2	H	8	Total	C	H	N	O	P	0	0	0
			257	79	93	26	51	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			289	89	104	31	56	9			

- 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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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 (three-letter code: MG) (formula: Mg).

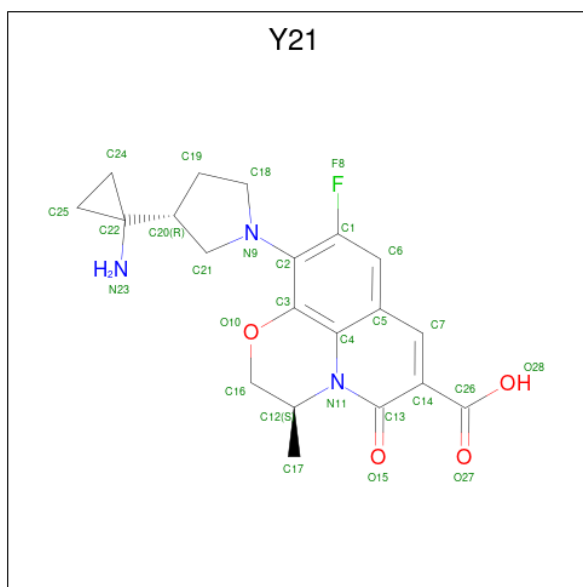
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
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 (three-letter code: Y21) (formula: C₂₀H₂₂FN₃O₄) (labeled as "Ligand of Interest" by depositor).



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

- 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		

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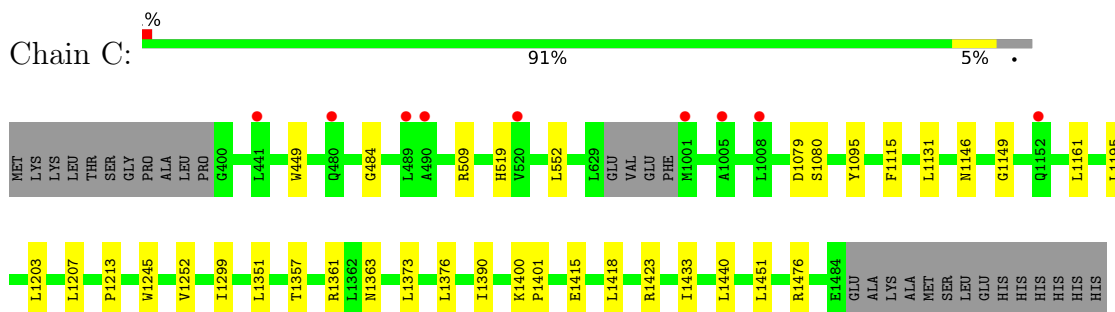
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	1	Total	O	0	0
			1	1		

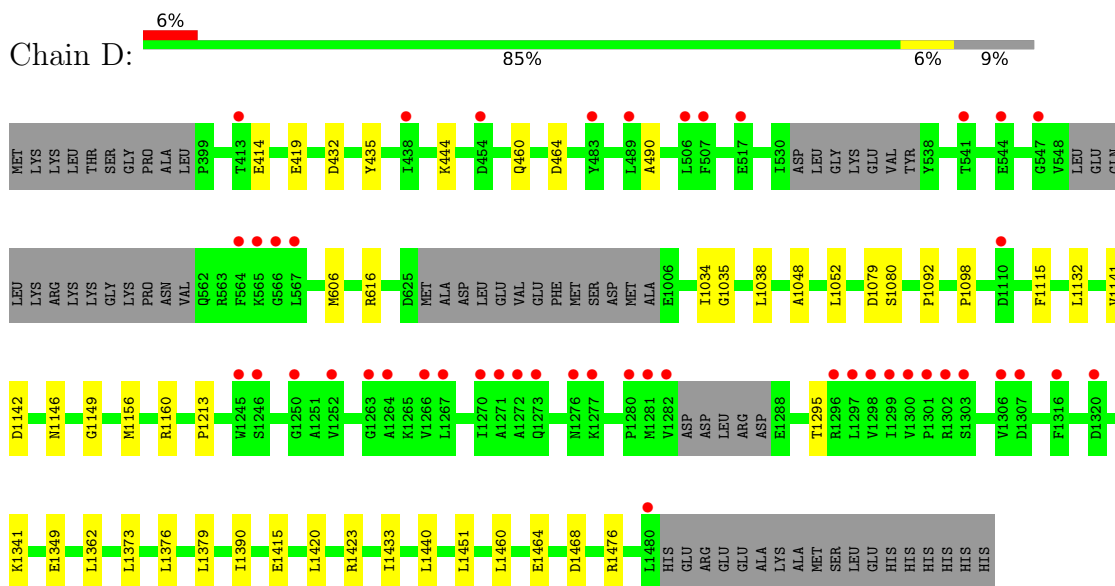
3 Residue-property plots

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.

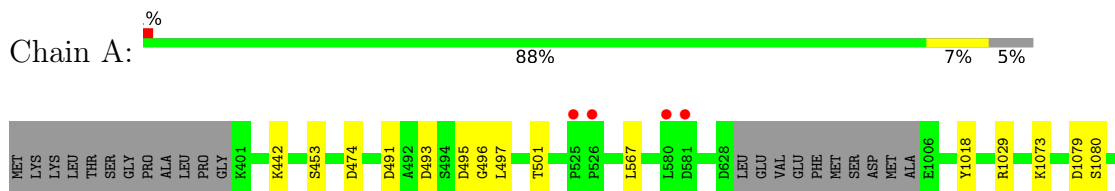
- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera

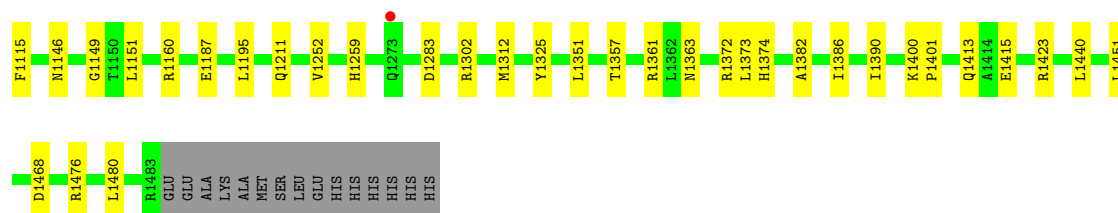


- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera

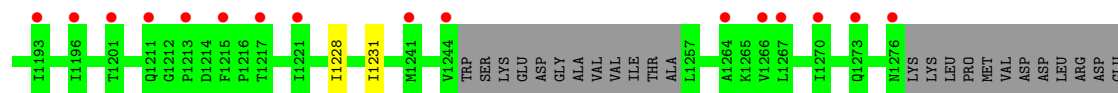
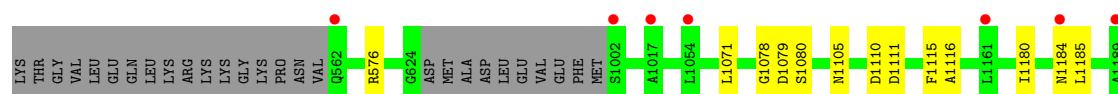
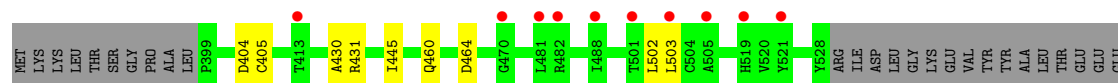
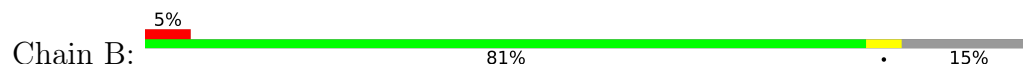


- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera

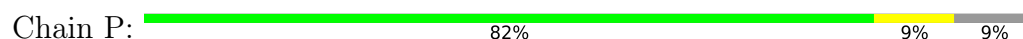




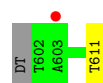
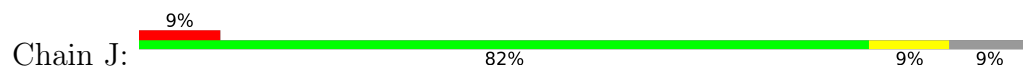
- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A chimera



- 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')

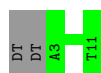


- Molecule 2: DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')



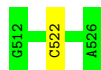
- Molecule 2: DNA (5'-D(P*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')

Chain E:  82% 18%




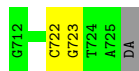
- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')

Chain K:  93% 7%




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

Chain I:  80% 13% 7%



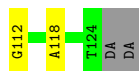
- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')

Chain G:  80% 7% 13%



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

Chain F:  73% 13% 13%



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 0.282 , 0.308	Depositor DCC
R_{free} test set	3287 reflections (5.17%)	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)	0.30 , 73.2	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: MG, MPD, 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	0.28	0/5073	0.44	0/6921
1	B	0.25	0/4357	0.41	0/5961
1	C	0.27	0/5196	0.43	0/7085
1	D	0.26	0/4718	0.43	0/6451
2	E	0.76	0/206	1.02	0/316
2	H	0.72	0/182	1.02	0/279
2	J	0.78	0/228	1.10	0/350
2	P	0.88	0/228	1.11	0/350
3	F	0.72	0/294	0.90	0/452
3	G	0.74	0/294	0.92	0/452
3	I	0.83	0/318	0.94	0/489
3	K	0.77	0/342	0.92	0/526
All	All	0.35	0/21436	0.52	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	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4285	3545	3554	17	0
1	C	5108	4502	4507	20	0
1	D	4639	3873	3900	28	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	92	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 2.

All (92) 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: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: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:D:419:GLU:HB2	1:D:490:ALA:HA	1.82	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1252:VAL:HG11	1:A:1312:MET:CE	2.35	0.57
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: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: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:A:1252:VAL:HG11	1:A:1312:MET:HE2	1.93	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:A:1211:GLN:HG2	1:A:1480:LEU:HD22	1.96	0.46
1:A:1259:HIS:O	1:A:1325:TYR:OH	2.23	0.46
1:A:493:ASP:HB2	1:A:496:GLY:H	1.81	0.46
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:C:484:GLY:O	1:C:519:HIS:ND1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1141:VAL:HG22	1:D:1142:ASP:N	2.32	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:A:1372:ARG:HH22	4:A:1501:MPD:HO4	1.65	0.45
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: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:1252:VAL:HG11	1:A:1312:MET:HE3	2.00	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1195:LEU:HD12	1:C:1351:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/640 (66%)	421 (100%)	1 (0%)	93	97
1	B	334/640 (52%)	332 (99%)	2 (1%)	86	91
1	C	447/640 (70%)	445 (100%)	2 (0%)	91	95
1	D	362/640 (57%)	361 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1565/2560 (61%)	1559 (100%)	6 (0%)	91 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1095	TYR
1	C	1115	PHE
1	D	1115	PHE
1	A	1115	PHE
1	B	431	ARG
1	B	1115	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	26,32,32	1.77	7 (26%)	25,51,51	2.01	5 (20%)
6	Y21	K	601	-	26,32,32	1.75	8 (30%)	25,51,51	1.99	5 (20%)
6	Y21	G	401	-	26,32,32	1.77	8 (30%)	25,51,51	1.98	5 (20%)
4	MPD	C	1501	-	7,7,7	0.25	0	9,10,10	0.47	0
4	MPD	A	1501	-	7,7,7	0.30	0	9,10,10	0.18	0
6	Y21	F	201	-	26,32,32	1.74	7 (26%)	25,51,51	1.97	6 (24%)

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	-	-	1/6/36/36	0/4/5/5
6	Y21	K	601	-	-	2/6/36/36	0/4/5/5
6	Y21	G	401	-	-	2/6/36/36	0/4/5/5
4	MPD	C	1501	-	-	0/5/5/5	-
4	MPD	A	1501	-	-	0/5/5/5	-
6	Y21	F	201	-	-	4/6/36/36	0/4/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	801	Y21	C7-C5	4.36	1.51	1.42
6	G	401	Y21	C7-C5	4.26	1.51	1.42
6	K	601	Y21	C7-C5	4.09	1.51	1.42
6	F	201	Y21	C7-C5	4.02	1.51	1.42
6	I	801	Y21	C6-C1	3.33	1.40	1.35
6	G	401	Y21	C6-C1	3.32	1.40	1.35
6	F	201	Y21	C6-C1	3.17	1.40	1.35
6	K	601	Y21	C6-C1	2.99	1.39	1.35
6	K	601	Y21	C24-C22	2.74	1.55	1.49
6	F	201	Y21	C24-C22	2.69	1.55	1.49
6	G	401	Y21	C24-C22	2.68	1.55	1.49
6	I	801	Y21	C24-C22	2.68	1.55	1.49
6	G	401	Y21	C25-C22	2.55	1.54	1.49
6	K	601	Y21	C25-C22	2.53	1.54	1.49
6	F	201	Y21	C25-C22	2.46	1.54	1.49
6	I	801	Y21	C25-C22	2.40	1.54	1.49
6	K	601	Y21	C7-C14	-2.24	1.34	1.37
6	K	601	Y21	O10-C3	2.24	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	401	Y21	C4-N11	2.19	1.42	1.39
6	G	401	Y21	C21-C20	2.17	1.55	1.52
6	I	801	Y21	O10-C3	2.17	1.39	1.36
6	I	801	Y21	C4-N11	2.16	1.42	1.39
6	F	201	Y21	C4-N11	2.12	1.42	1.39
6	K	601	Y21	C4-N11	2.09	1.42	1.39
6	F	201	Y21	C25-C24	2.04	1.55	1.50
6	K	601	Y21	C25-C24	2.04	1.55	1.50
6	I	801	Y21	C25-C24	2.01	1.55	1.50
6	G	401	Y21	O10-C3	2.00	1.39	1.36
6	F	201	Y21	C21-C20	2.00	1.55	1.52
6	G	401	Y21	C25-C24	2.00	1.55	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	401	Y21	C14-C13-N11	6.99	120.96	116.11
6	K	601	Y21	C14-C13-N11	6.97	120.94	116.11
6	I	801	Y21	C14-C13-N11	6.96	120.93	116.11
6	F	201	Y21	C14-C13-N11	6.08	120.33	116.11
6	F	201	Y21	C3-C2-C1	3.59	119.42	115.99
6	I	801	Y21	C3-C2-C1	3.59	119.42	115.99
6	F	201	Y21	C7-C14-C13	3.58	119.83	117.58
6	I	801	Y21	C17-C12-N11	-3.44	108.20	111.19
6	F	201	Y21	C17-C12-N11	-3.29	108.33	111.19
6	G	401	Y21	C17-C12-N11	-3.22	108.39	111.19
6	K	601	Y21	C3-C2-C1	3.21	119.06	115.99
6	G	401	Y21	C3-C2-C1	3.17	119.02	115.99
6	K	601	Y21	C7-C14-C13	2.76	119.32	117.58
6	K	601	Y21	O10-C3-C2	2.64	120.71	117.85
6	K	601	Y21	C17-C12-N11	-2.55	108.98	111.19
6	F	201	Y21	C19-C18-N9	-2.53	100.39	103.35
6	G	401	Y21	C19-C18-N9	-2.49	100.44	103.35
6	I	801	Y21	C19-C18-N9	-2.42	100.51	103.35
6	F	201	Y21	C6-C1-C2	-2.15	120.12	123.25
6	I	801	Y21	C6-C1-C2	-2.14	120.14	123.25
6	G	401	Y21	C6-C1-C2	-2.07	120.25	123.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

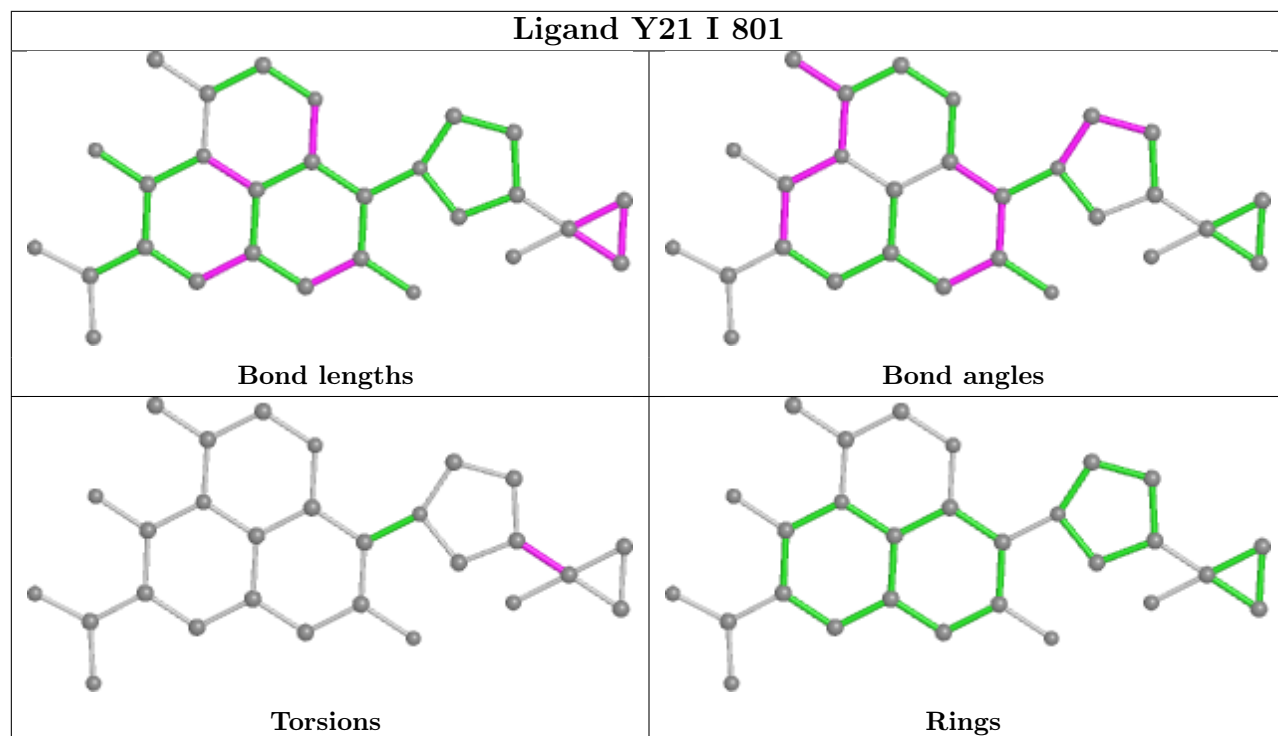
There are no ring outliers.

2 monomers are involved in 2 short contacts:

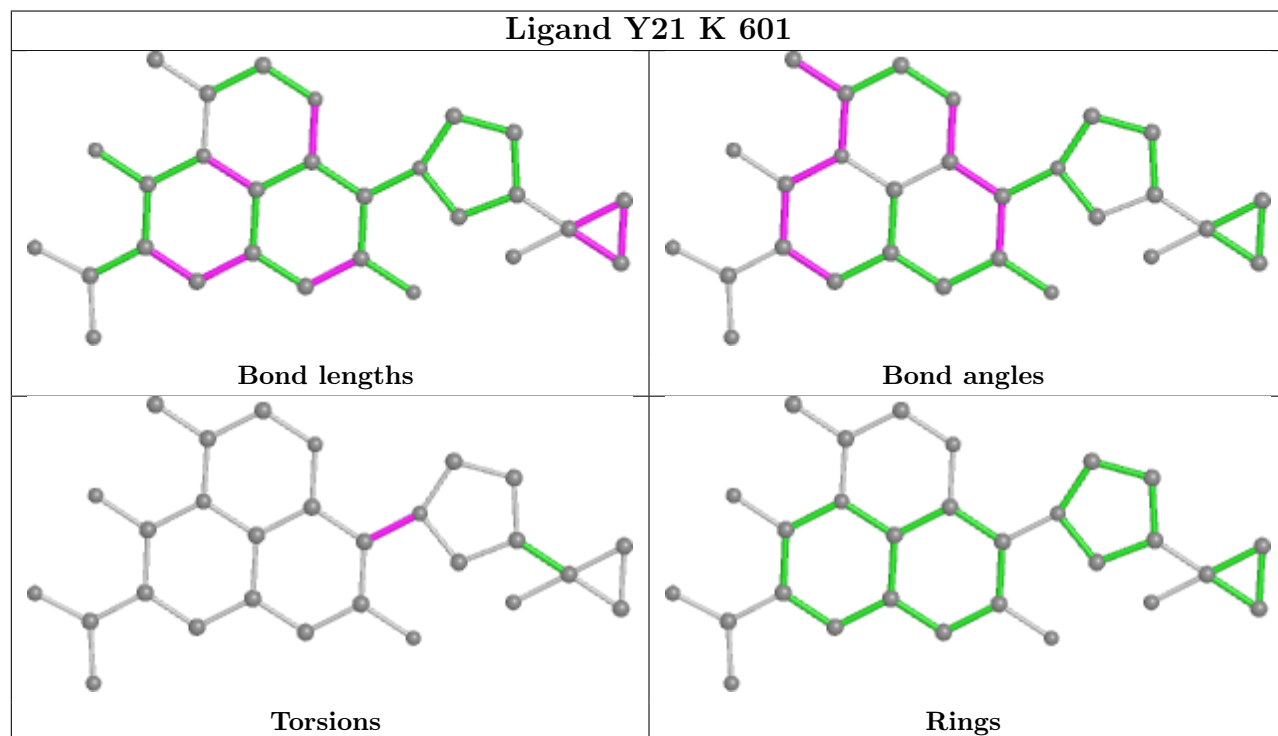
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	401	Y21	1	0
4	A	1501	MPD	1	0

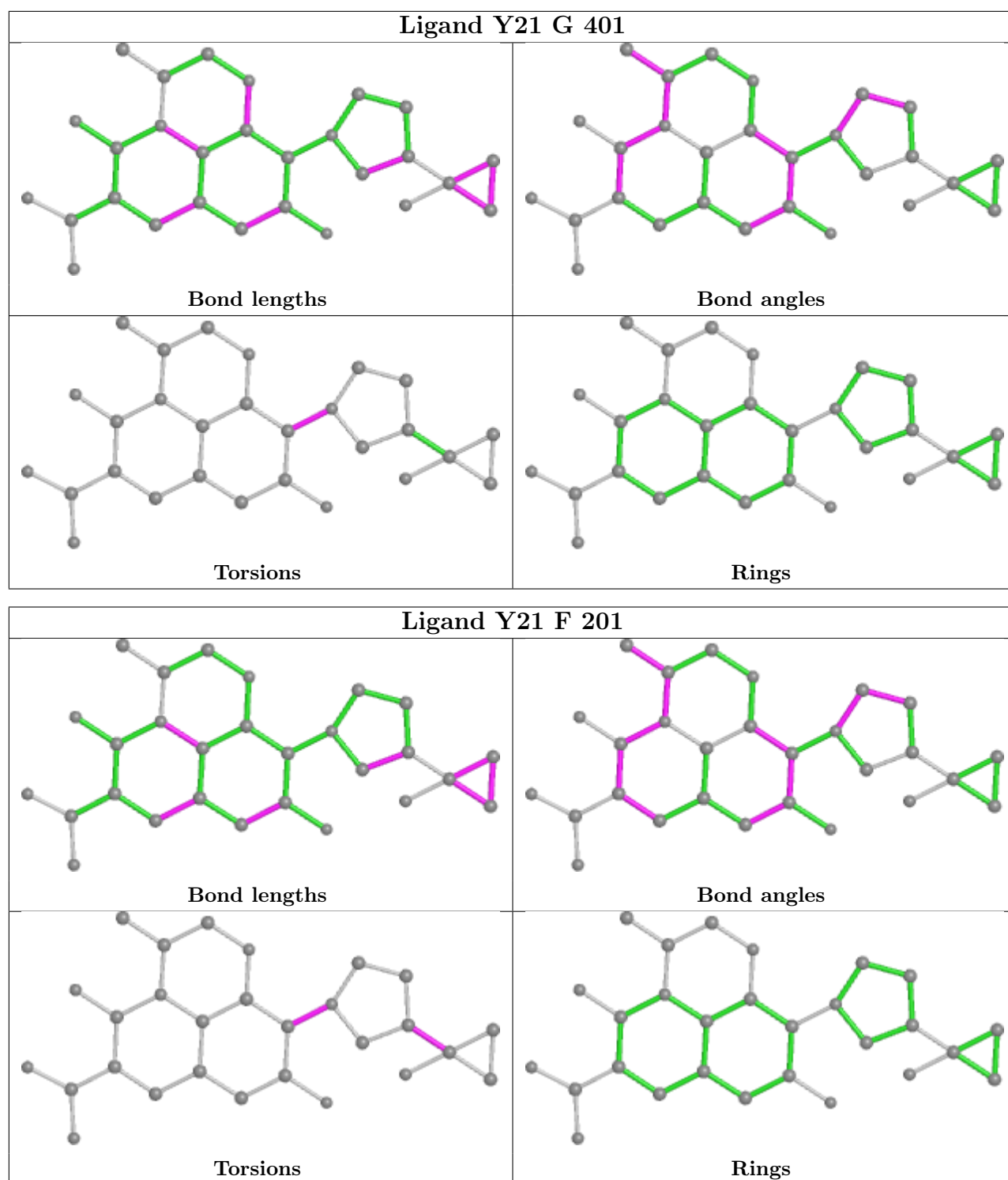
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 I 801



Ligand Y21 K 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	706/743 (95%)	-0.09	5 (0%) 87 88	49, 71, 110, 131	0
1	B	631/743 (84%)	0.30	38 (6%) 21 21	68, 106, 146, 175	0
1	C	714/743 (96%)	-0.05	9 (1%) 77 77	53, 73, 118, 144	0
1	D	677/743 (91%)	0.30	46 (6%) 17 17	57, 95, 161, 211	0
2	E	9/11 (81%)	0.15	0 100 100	60, 69, 126, 141	0
2	H	8/11 (72%)	0.31	0 100 100	93, 100, 133, 153	0
2	J	10/11 (90%)	0.84	1 (10%) 7 7	86, 105, 161, 168	0
2	P	10/11 (90%)	-0.05	0 100 100	61, 73, 107, 108	0
3	F	13/15 (86%)	0.32	0 100 100	86, 104, 164, 182	0
3	G	13/15 (86%)	0.15	0 100 100	65, 87, 104, 111	0
3	I	14/15 (93%)	0.11	0 100 100	67, 81, 90, 92	0
3	K	15/15 (100%)	0.42	0 100 100	85, 99, 195, 211	0
All	All	2820/3076 (91%)	0.11	99 (3%) 44 42	49, 87, 143, 211	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1301	PRO	5.9
1	D	1272	ALA	5.0
1	D	1270	ILE	4.8
1	D	1302	ARG	4.7
1	D	1271	ALA	4.7
1	D	566	GLY	4.6
1	D	541	THR	4.5
1	B	505	ALA	4.4
1	B	470	GLY	4.3
1	B	1312	MET	4.3
1	D	1277	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	1273	GLN	4.2
1	D	1300	VAL	3.9
1	B	482	ARG	3.8
1	D	413	THR	3.7
1	D	1246	SER	3.6
1	D	1263	GLY	3.6
1	D	565	LYS	3.6
1	B	1478	SER	3.6
1	B	1002	SER	3.6
1	A	1273	GLN	3.5
1	D	1245	TRP	3.5
1	B	1221	ILE	3.4
1	B	1217	THR	3.4
1	A	525	PRO	3.3
1	A	580	LEU	3.3
1	C	1005	ALA	3.3
1	B	413	THR	3.2
1	D	1252	VAL	3.2
1	B	1241	MET	3.2
1	D	544	GLU	3.2
1	B	488	ILE	3.1
1	B	1267	LEU	3.1
1	B	1266	VAL	3.1
1	D	506	LEU	3.1
1	B	519	HIS	3.0
1	C	520	VAL	2.9
1	B	1397	ASP	2.9
1	B	1273	GLN	2.9
1	B	521	TYR	2.9
1	D	547	GLY	2.8
1	B	501	THR	2.8
1	B	1270	ILE	2.8
1	D	1480	LEU	2.8
1	B	1479	PRO	2.8
1	B	1244	VAL	2.7
1	B	481	LEU	2.7
1	D	1299	ILE	2.7
1	D	564	PHE	2.6
1	D	1316	PHE	2.6
1	D	1297	LEU	2.6
1	B	1193	ILE	2.6
1	C	1152	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1266	VAL	2.5
1	D	507	PHE	2.5
1	D	1296	ARG	2.5
1	B	1458	ASN	2.4
1	B	1184	ASN	2.4
1	B	1201	THR	2.4
1	C	490	ALA	2.4
1	D	454	ASP	2.4
2	J	603	DA	2.4
1	D	1276	ASN	2.3
1	D	1307	ASP	2.3
1	B	1196	ILE	2.3
1	B	1215	PHE	2.3
1	D	517	GLU	2.3
1	D	1282	VAL	2.3
1	D	1267	LEU	2.3
1	B	1211	GLN	2.3
1	B	1189	ALA	2.3
1	B	1276	ASN	2.2
1	B	1054	LEU	2.2
1	A	581	ASP	2.2
1	D	1303	SER	2.2
1	D	1264	ALA	2.2
1	A	526	PRO	2.2
1	B	1017	ALA	2.2
1	D	1298	VAL	2.2
1	C	441	LEU	2.2
1	B	1213	PRO	2.1
1	C	1001	MET	2.1
1	D	1281	MET	2.1
1	D	1250	GLY	2.1
1	B	562	GLN	2.1
1	B	1161	LEU	2.1
1	D	1306	VAL	2.1
1	B	503	LEU	2.1
1	D	567	LEU	2.1
1	D	483	TYR	2.1
1	D	1280	PRO	2.1
1	C	489	LEU	2.1
1	D	438	ILE	2.1
1	D	1320	ASP	2.0
1	C	480	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1110	ASP	2.0
1	D	489	LEU	2.0
1	B	1264	ALA	2.0
1	C	1008	LEU	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](#)

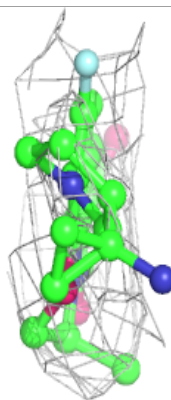
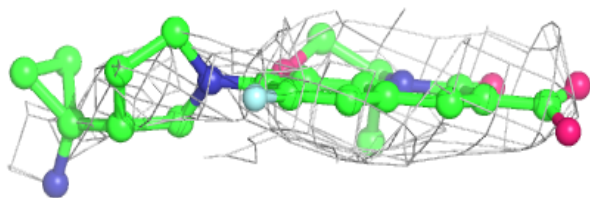
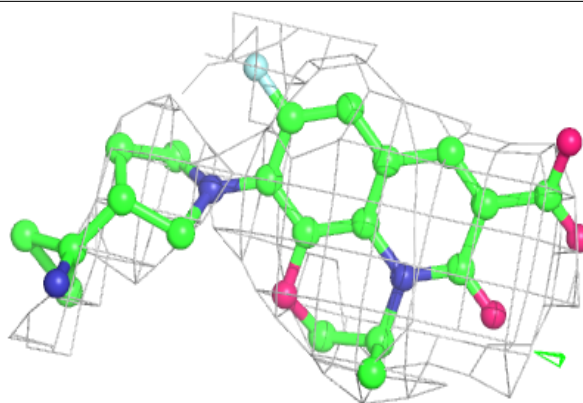
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	B	1501	1/1	0.47	0.26	108,108,108,108	0
5	MG	D	1501	1/1	0.74	0.29	91,91,91,91	0
6	Y21	F	201	28/28	0.77	0.40	98,102,104,105	0
5	MG	A	1502	1/1	0.82	0.17	82,82,82,82	0
6	Y21	K	601	28/28	0.85	0.33	90,93,94,94	0
4	MPD	C	1501	8/8	0.87	0.27	20,20,60,60	0
5	MG	C	1502	1/1	0.89	0.23	85,85,85,85	0
6	Y21	G	401	28/28	0.91	0.29	80,84,86,88	0
6	Y21	I	801	28/28	0.91	0.26	77,81,82,83	0
4	MPD	A	1501	8/8	0.92	0.26	20,20,70,70	0

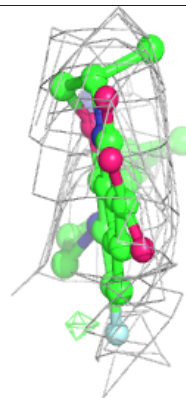
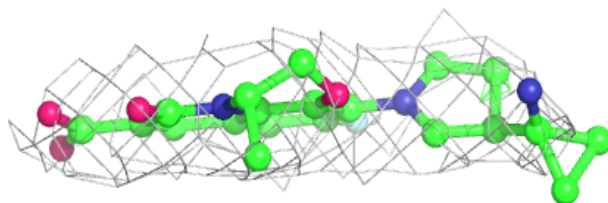
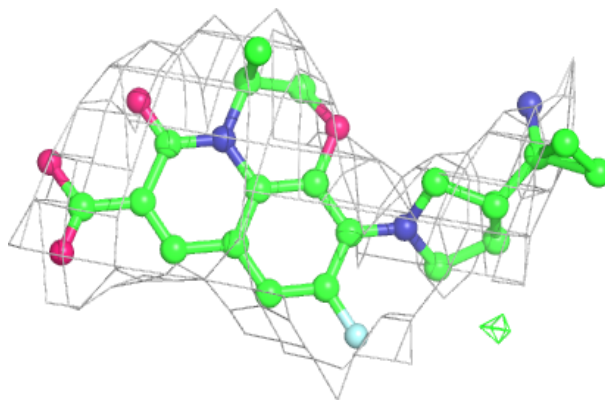
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

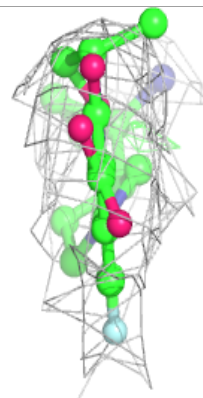
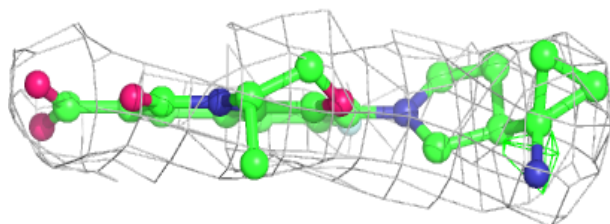
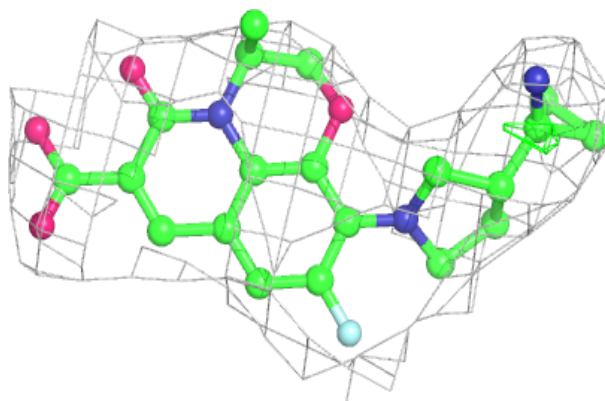
**Electron density around Y21 K 601:**

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

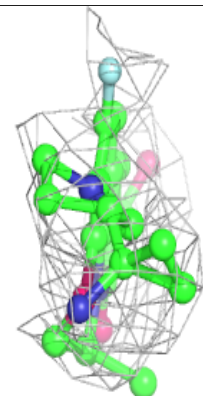
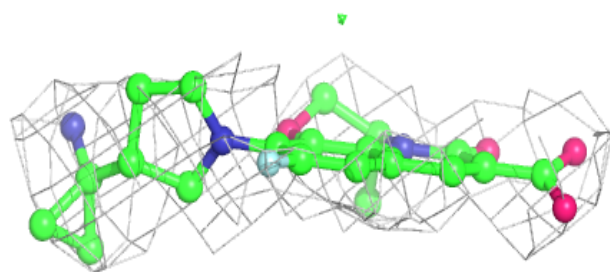
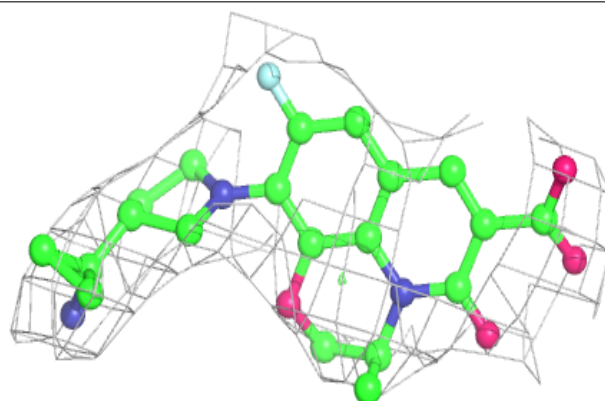


Electron density around Y21 G 401:

$2mF_o-DF_c$ (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.