



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:55 AM UTC

PDB ID : 3R7K / pdb_00003r7k
Title : Crystal structure of a probable acyl CoA dehydrogenase from Mycobacterium abscessus ATCC 19977 / DSM 44196
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2011-03-22
Resolution : 2.50 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

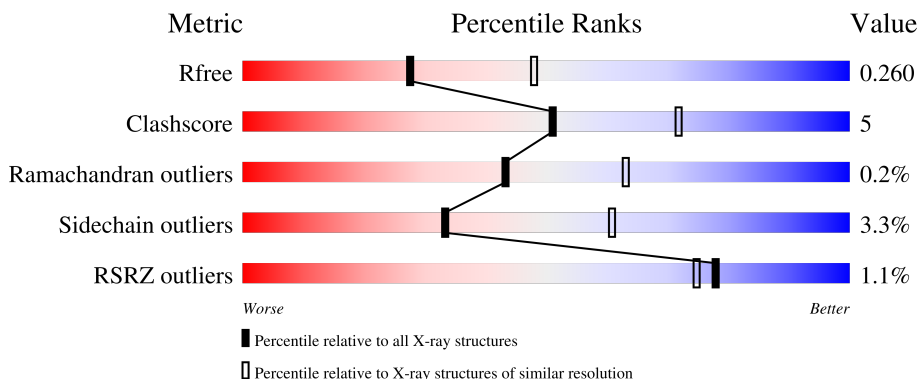
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	403	81% 12% • 6%
1	B	403	79% 14% 6%
1	C	403	82% 10% • 6%
1	D	403	83% 10% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11294 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

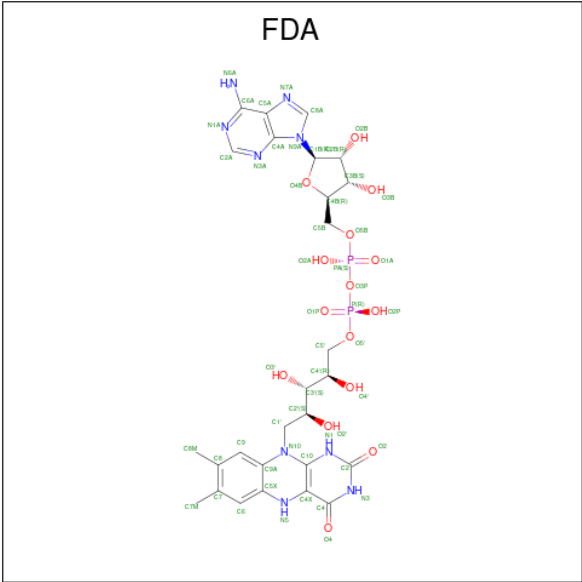
- Molecule 1 is a protein called Probable acyl CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2792	1741	508	528	15			
1	B	378	Total	C	N	O	S	0	0	0
			2736	1706	496	519	15			
1	C	377	Total	C	N	O	S	0	0	0
			2774	1731	506	523	14			
1	D	376	Total	C	N	O	S	0	0	0
			2722	1691	496	521	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP B1MPB5
A	-2	PRO	-	expression tag	UNP B1MPB5
A	-1	GLY	-	expression tag	UNP B1MPB5
A	0	SER	-	expression tag	UNP B1MPB5
B	-3	GLY	-	expression tag	UNP B1MPB5
B	-2	PRO	-	expression tag	UNP B1MPB5
B	-1	GLY	-	expression tag	UNP B1MPB5
B	0	SER	-	expression tag	UNP B1MPB5
C	-3	GLY	-	expression tag	UNP B1MPB5
C	-2	PRO	-	expression tag	UNP B1MPB5
C	-1	GLY	-	expression tag	UNP B1MPB5
C	0	SER	-	expression tag	UNP B1MPB5
D	-3	GLY	-	expression tag	UNP B1MPB5
D	-2	PRO	-	expression tag	UNP B1MPB5
D	-1	GLY	-	expression tag	UNP B1MPB5
D	0	SER	-	expression tag	UNP B1MPB5

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	1	Total	K	0	0
			1	1		
3	C	2	Total	K	0	0
			2	2		
3	D	1	Total	K	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		

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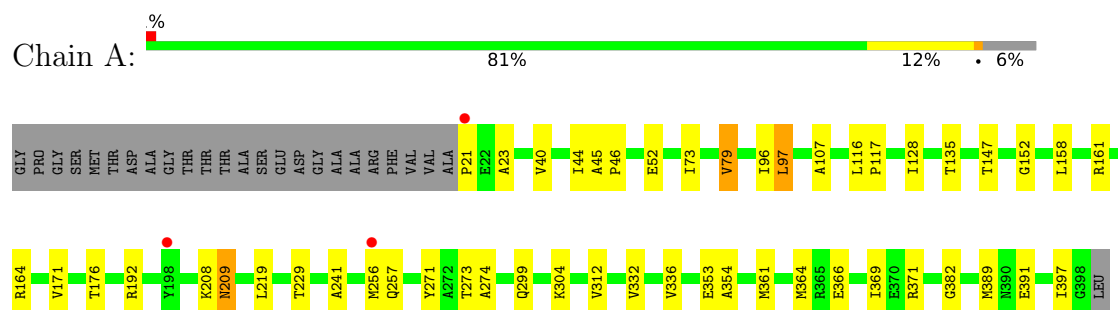
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	11	Total 11	O 11	0	0
4	C	13	Total 13	O 13	0	0
4	D	12	Total 12	O 12	0	0

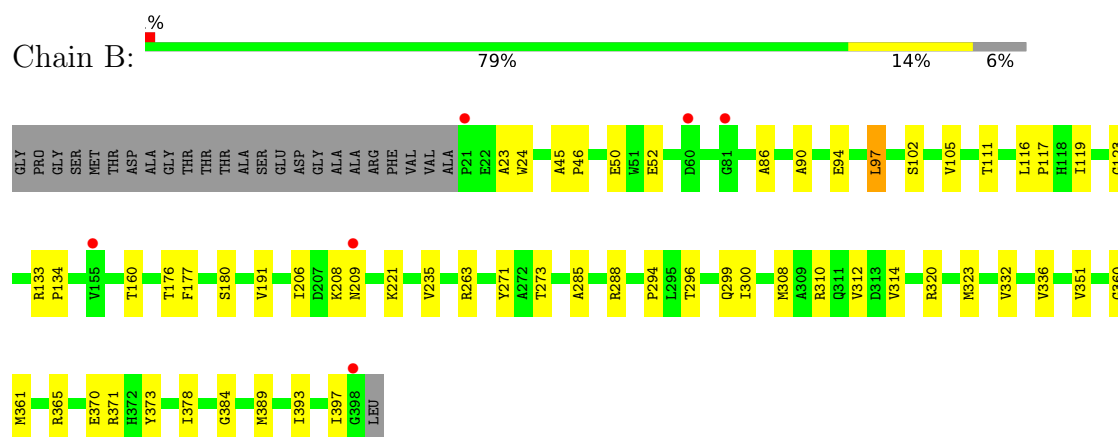
3 Residue-property plots [i](#)

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.

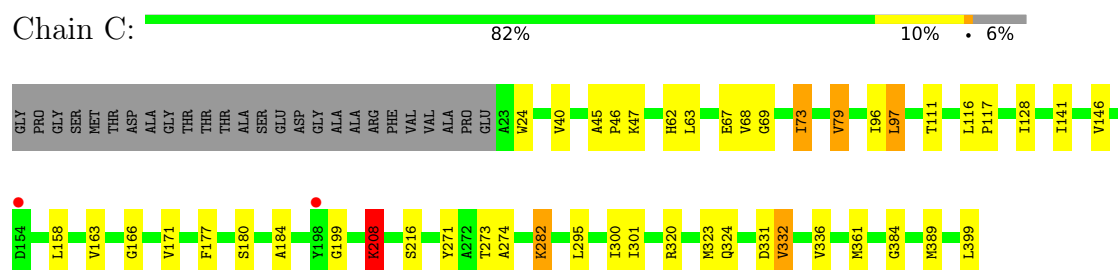
- Molecule 1: Probable acyl CoA dehydrogenase



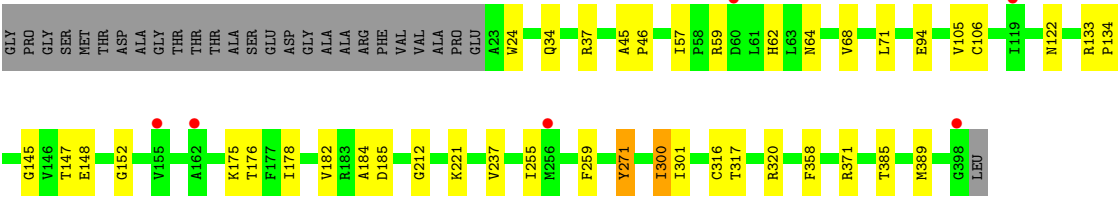
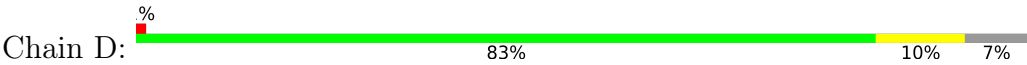
- Molecule 1: Probable acyl CoA dehydrogenase



- Molecule 1: Probable acyl CoA dehydrogenase



- Molecule 1: Probable acyl CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.25Å 121.12Å 172.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.50 49.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.52-2.50) 99.7 (49.52-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.259 0.214 , 0.260	Depositor DCC
R_{free} test set	4843 reflections (7.76%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11294	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.05	1/2838 (0.0%)	1.02	1/3848 (0.0%)
1	B	1.01	0/2782	1.07	2/3780 (0.1%)
1	C	1.07	2/2819 (0.1%)	1.05	3/3821 (0.1%)
1	D	0.90	1/2767 (0.0%)	1.01	3/3758 (0.1%)
All	All	1.01	4/11206 (0.0%)	1.04	9/15207 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	274	ALA	CA-CB	6.70	1.63	1.53
1	C	171	VAL	CA-CB	6.24	1.61	1.54
1	A	382	GLY	C-O	5.31	1.31	1.23
1	D	358	PHE	C-O	-5.11	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ALA	N-CA-C	-7.39	104.26	113.20
1	C	146	VAL	CB-CA-C	-6.51	106.17	111.71
1	C	208	LYS	N-CA-C	6.03	117.52	111.07
1	B	97	LEU	N-CA-C	5.88	117.77	111.36
1	C	199	GLY	N-CA-C	5.75	120.99	114.67
1	D	184	ALA	N-CA-C	5.57	118.54	110.42
1	D	182	VAL	CB-CA-C	-5.42	104.94	112.04
1	D	221	LYS	N-CA-C	5.35	118.30	109.85
1	A	107	ALA	N-CA-C	-5.19	105.70	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2733	33	0
1	B	2736	0	2620	36	0
1	C	2774	0	2712	30	0
1	D	2722	0	2585	24	0
2	A	53	0	33	1	0
2	B	53	0	33	2	0
2	C	53	0	33	1	0
2	D	53	0	33	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	0	0	0
4	B	11	0	0	0	0
4	C	13	0	0	0	0
4	D	12	0	0	0	0
All	All	11294	0	10782	115	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 5.

All (115) 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:B:86:ALA:HB1	1:B:323:MET:HE2	1.32	1.07
1:A:304:LYS:HZ2	1:A:353:GLU:CD	1.99	0.71
1:D:34:GLN:OE1	1:D:37:ARG:NH1	2.24	0.70
1:B:102:SER:HB3	1:B:105:VAL:HG23	1.75	0.68
1:A:97:LEU:HD22	1:A:273:THR:HA	1.77	0.67
1:B:299:GLN:HG2	1:C:300:ILE:HD13	1.77	0.66
1:B:97:LEU:HD22	1:B:273:THR:HA	1.78	0.65
1:A:79:VAL:HG22	1:A:128:ILE:CG2	2.27	0.65
1:A:158:LEU:C	1:A:158:LEU:HD12	2.22	0.65
1:C:45:ALA:HB3	1:C:46:PRO:HD3	1.78	0.64
1:C:295:LEU:HB3	1:C:301:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLN:CG	1:C:300:ILE:HD13	2.30	0.62
1:D:62:HIS:O	1:D:71:LEU:HD22	2.01	0.61
1:D:389:MET:HA	1:D:389:MET:HE2	1.81	0.61
1:C:320:ARG:O	1:C:324:GLN:HG3	2.01	0.61
1:A:79:VAL:HG13	1:A:79:VAL:O	2.01	0.61
1:C:158:LEU:C	1:C:158:LEU:HD12	2.27	0.60
1:A:332:VAL:O	1:A:336:VAL:HG23	2.03	0.59
1:C:332:VAL:HG23	1:C:336:VAL:HG23	1.84	0.59
1:B:308:MET:O	1:B:312:VAL:HG23	2.04	0.57
1:C:24:TRP:CH2	1:C:323:MET:CE	2.87	0.57
1:C:24:TRP:CZ2	1:C:323:MET:CE	2.88	0.56
1:A:79:VAL:HG22	1:A:128:ILE:HG21	1.87	0.56
1:C:24:TRP:CZ2	1:C:323:MET:HE2	2.40	0.56
1:D:59:ARG:NH2	1:D:185:ASP:OD2	2.36	0.56
1:A:299:GLN:HG2	1:D:300:ILE:CD1	2.35	0.56
1:A:208:LYS:O	1:A:209:ASN:CB	2.54	0.56
1:B:263:ARG:CZ	1:B:389:MET:HE1	2.37	0.55
1:D:68:VAL:HG12	1:D:68:VAL:O	2.05	0.55
1:B:300:ILE:HA	1:C:300:ILE:HD11	1.89	0.55
1:A:147:THR:HG23	1:A:152:GLY:HA2	1.90	0.54
1:A:40:VAL:HG21	1:A:96:ILE:HA	1.90	0.53
1:B:97:LEU:CD2	1:B:273:THR:HA	2.39	0.53
1:A:299:GLN:HG2	1:D:300:ILE:HD12	1.91	0.52
1:B:365:ARG:HG2	1:B:370:GLU:OE1	2.10	0.52
1:C:97:LEU:HD22	1:C:273:THR:HA	1.91	0.52
2:A:420:FDA:H2A	1:B:300:ILE:HD11	1.92	0.51
1:A:299:GLN:CG	1:D:300:ILE:HD12	2.41	0.51
1:A:274:ALA:HB1	1:A:312:VAL:HG22	1.92	0.51
1:A:389:MET:HE2	1:A:389:MET:HA	1.92	0.50
1:B:111:THR:HG21	1:B:180:SER:HB2	1.92	0.50
1:A:158:LEU:O	1:A:192:ARG:NH2	2.43	0.50
1:A:364:MET:HE1	1:B:221:LYS:HG2	1.95	0.49
1:C:40:VAL:HG21	1:C:96:ILE:HA	1.93	0.49
1:D:45:ALA:HB3	1:D:46:PRO:HD3	1.94	0.49
1:B:86:ALA:CB	1:B:323:MET:HE2	2.23	0.49
1:B:52:GLU:OE1	1:B:371:ARG:HD3	2.12	0.49
1:C:24:TRP:CH2	1:C:323:MET:HE1	2.47	0.49
1:B:208:LYS:O	1:B:209:ASN:CB	2.61	0.48
1:A:79:VAL:CG2	1:A:128:ILE:HG21	2.44	0.48
1:D:94:GLU:OE2	1:D:271:TYR:OH	2.17	0.48
1:C:24:TRP:CZ2	1:C:320:ARG:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ALA:O	1:C:208:LYS:HG3	2.13	0.48
1:C:24:TRP:HZ2	1:C:323:MET:HE2	1.79	0.48
1:A:208:LYS:O	1:A:209:ASN:HB2	2.14	0.47
1:B:332:VAL:O	1:B:336:VAL:HG23	2.15	0.47
1:B:160:THR:CG2	1:B:191:VAL:HG12	2.45	0.47
1:C:62:HIS:CE1	1:C:141:ILE:CD1	2.98	0.47
1:B:119:ILE:O	1:B:123:GLY:N	2.48	0.47
1:B:24:TRP:CZ2	1:B:320:ARG:HG2	2.50	0.46
1:D:57:ILE:C	1:D:57:ILE:HD12	2.40	0.46
1:B:393:ILE:O	1:B:397:ILE:HG12	2.15	0.46
1:B:97:LEU:HD22	1:B:273:THR:CA	2.45	0.46
1:B:45:ALA:HB3	1:B:46:PRO:HD3	1.99	0.45
1:A:116:LEU:N	1:A:117:PRO:CD	2.79	0.45
1:D:145:GLY:HA2	1:D:178:ILE:HD12	1.98	0.45
1:A:52:GLU:OE1	1:A:371:ARG:HD3	2.17	0.45
1:D:64:ASN:O	1:D:68:VAL:HG23	2.17	0.45
1:A:79:VAL:O	1:A:79:VAL:CG1	2.63	0.45
1:B:86:ALA:HB1	1:B:323:MET:CE	2.24	0.45
1:A:116:LEU:HD21	1:A:135:THR:HB	1.99	0.45
1:B:351:VAL:HG11	1:B:373:TYR:HA	1.98	0.45
2:D:420:FDA:HM83	2:D:420:FDA:HM71	1.79	0.44
1:B:160:THR:HG22	1:B:191:VAL:HG12	1.99	0.44
1:B:384:GLY:HA3	1:B:389:MET:HE3	1.98	0.44
1:C:384:GLY:HA3	1:C:389:MET:HE3	1.99	0.44
1:B:116:LEU:N	1:B:117:PRO:CD	2.81	0.44
1:D:148:GLU:HG2	1:D:175:LYS:HD3	2.00	0.44
1:A:364:MET:CE	1:B:221:LYS:HG2	2.48	0.43
1:B:90:ALA:O	1:B:94:GLU:HG3	2.19	0.43
1:A:164:ARG:HH12	1:A:241:ALA:HB1	1.84	0.43
1:B:177:PHE:HB3	2:B:420:FDA:C9	2.49	0.43
1:D:24:TRP:CZ2	1:D:320:ARG:HG2	2.54	0.43
1:A:45:ALA:HB3	1:A:46:PRO:HD3	2.00	0.42
1:B:177:PHE:O	2:B:420:FDA:C4X	2.66	0.42
1:C:24:TRP:HH2	1:C:323:MET:HE1	1.83	0.42
1:C:332:VAL:HG23	1:C:332:VAL:O	2.19	0.42
1:A:21:PRO:C	1:A:23:ALA:N	2.77	0.42
1:A:397:ILE:HB	1:C:282:LYS:NZ	2.35	0.42
1:D:105:VAL:O	1:D:106:CYS:C	2.61	0.42
1:D:147:THR:HG23	1:D:152:GLY:HA2	2.02	0.42
1:D:212:GLY:C	1:D:237:VAL:HG22	2.44	0.42
1:C:69:GLY:O	1:C:73:ILE:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:N	1:C:117:PRO:CD	2.83	0.42
1:D:133:ARG:HB3	1:D:134:PRO:HD3	2.01	0.42
1:A:40:VAL:HG22	1:A:44:ILE:HD12	2.02	0.41
1:D:316:CYS:O	1:D:317:THR:C	2.62	0.41
1:C:79:VAL:CG2	1:C:128:ILE:HG23	2.51	0.41
1:A:161:ARG:O	1:A:171:VAL:HA	2.20	0.41
1:C:331:ASP:OD1	1:C:331:ASP:C	2.63	0.41
1:D:389:MET:HE2	1:D:389:MET:CA	2.48	0.41
1:A:219:LEU:HD12	1:A:229:THR:HG22	2.02	0.41
1:C:111:THR:HG21	1:C:180:SER:HB2	2.03	0.41
1:C:177:PHE:HB3	2:C:420:FDA:C9	2.51	0.41
1:B:285:ALA:C	1:B:296:THR:HG23	2.46	0.41
1:B:288:ARG:O	1:B:294:PRO:HA	2.21	0.41
1:C:361:MET:HE2	1:C:361:MET:HA	2.02	0.41
1:D:255:ILE:HG22	1:D:259:PHE:CZ	2.56	0.41
1:C:389:MET:HA	1:C:389:MET:HE2	2.03	0.41
1:A:354:ALA:HB3	1:A:369:ILE:HD11	2.02	0.40
1:A:361:MET:HE1	1:A:366:GLU:OE2	2.20	0.40
1:D:24:TRP:CE2	1:D:320:ARG:HD3	2.56	0.40
1:D:385:THR:O	1:D:389:MET:HG2	2.20	0.40
1:B:133:ARG:HB3	1:B:134:PRO:HD3	2.03	0.40
1:B:310:ARG:O	1:B:314:VAL:HG23	2.22	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	376/403 (93%)	365 (97%)	10 (3%)	1 (0%)	36 55
1	B	376/403 (93%)	365 (97%)	10 (3%)	1 (0%)	36 55
1	C	375/403 (93%)	363 (97%)	11 (3%)	1 (0%)	36 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	374/403 (93%)	358 (96%)	16 (4%)	0	100	100
All	All	1501/1612 (93%)	1451 (97%)	47 (3%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	C	166	GLY
1	B	360	GLY

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	275/304 (90%)	267 (97%)	8 (3%)	37	65
1	B	259/304 (85%)	252 (97%)	7 (3%)	39	67
1	C	270/304 (89%)	256 (95%)	14 (5%)	21	42
1	D	256/304 (84%)	250 (98%)	6 (2%)	44	72
All	All	1060/1216 (87%)	1025 (97%)	35 (3%)	33	61

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	79	VAL
1	A	97	LEU
1	A	176	THR
1	A	256	MET
1	A	257	GLN
1	A	271	TYR
1	A	391	GLU
1	B	50	GLU
1	B	176	THR
1	B	206	ILE

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Mol	Chain	Res	Type
1	B	235	VAL
1	B	271	TYR
1	B	361	MET
1	B	378	ILE
1	C	47	LYS
1	C	63	LEU
1	C	67	GLU
1	C	68	VAL
1	C	73	ILE
1	C	79	VAL
1	C	97	LEU
1	C	163	VAL
1	C	208	LYS
1	C	216	SER
1	C	271	TYR
1	C	282	LYS
1	C	332	VAL
1	C	399	LEU
1	D	122	ASN
1	D	176	THR
1	D	271	TYR
1	D	300	ILE
1	D	301	ILE
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	C	34	GLN
1	C	62	HIS
1	C	260	GLN
1	C	386	ASN
1	D	258	GLN
1	D	386	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, 6 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$
2	FDA	B	420	-	57,58,58	1.04	7 (12%)	78,89,89	1.72	17 (21%)
2	FDA	C	420	-	57,58,58	1.08	6 (10%)	78,89,89	1.72	17 (21%)
2	FDA	D	420	-	57,58,58	1.06	2 (3%)	78,89,89	1.77	19 (24%)
2	FDA	A	420	-	57,58,58	1.10	5 (8%)	78,89,89	1.65	15 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDA	B	420	-	-	7/34/50/50	0/6/6/6
2	FDA	C	420	-	-	2/34/50/50	0/6/6/6
2	FDA	D	420	-	-	2/34/50/50	0/6/6/6
2	FDA	A	420	-	-	0/34/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	420	FDA	C10-N10	3.30	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	420	FDA	O2-C2	3.04	1.29	1.23
2	C	420	FDA	PA-O3P	3.04	1.62	1.59
2	A	420	FDA	PA-O3P	2.96	1.62	1.59
2	D	420	FDA	C8A-N7A	2.87	1.37	1.31
2	B	420	FDA	C5X-N5	-2.74	1.35	1.39
2	C	420	FDA	C10-N10	2.65	1.43	1.38
2	C	420	FDA	C8A-N7A	2.61	1.36	1.31
2	A	420	FDA	C10-N10	2.53	1.42	1.38
2	B	420	FDA	PA-O3P	2.43	1.62	1.59
2	A	420	FDA	P-O3P	2.22	1.61	1.59
2	C	420	FDA	C4A-N3A	2.22	1.38	1.34
2	B	420	FDA	P-O3P	2.15	1.61	1.59
2	B	420	FDA	C5A-N7A	-2.13	1.35	1.39
2	C	420	FDA	P-O3P	2.10	1.61	1.59
2	B	420	FDA	C10-N10	2.07	1.42	1.38
2	A	420	FDA	C5X-N5	-2.04	1.36	1.39
2	B	420	FDA	C8A-N9A	-2.04	1.34	1.37
2	C	420	FDA	C5X-N5	-2.03	1.36	1.39
2	B	420	FDA	C8A-N7A	2.00	1.35	1.31

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	420	FDA	C5A-C4A-N3A	-5.62	118.98	126.72
2	D	420	FDA	N3A-C2A-N1A	-5.44	120.35	128.58
2	C	420	FDA	C5A-C4A-N3A	-4.94	119.91	126.72
2	C	420	FDA	N3A-C2A-N1A	-4.76	121.38	128.58
2	D	420	FDA	C5A-C4A-N3A	-4.58	120.41	126.72
2	A	420	FDA	N3A-C2A-N1A	-4.42	121.89	128.58
2	B	420	FDA	N3A-C2A-N1A	-4.24	122.17	128.58
2	D	420	FDA	C4-N3-C2	-4.16	120.64	126.37
2	A	420	FDA	C5A-C4A-N3A	-4.15	121.00	126.72
2	B	420	FDA	C4A-C5A-N7A	-3.90	106.13	110.58
2	B	420	FDA	N9A-C8A-N7A	-3.87	108.44	113.94
2	A	420	FDA	C4-N3-C2	-3.86	121.06	126.37
2	D	420	FDA	C2A-N3A-C4A	3.75	120.99	111.83
2	D	420	FDA	N9A-C8A-N7A	-3.74	108.64	113.94
2	B	420	FDA	C5A-N7A-C8A	3.69	109.25	103.45
2	B	420	FDA	N3A-C4A-N9A	3.64	133.36	127.17
2	C	420	FDA	N3A-C4A-N9A	3.64	133.35	127.17
2	C	420	FDA	N9A-C8A-N7A	-3.57	108.87	113.94
2	A	420	FDA	N9A-C8A-N7A	-3.55	108.89	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	420	FDA	C4A-C5A-N7A	-3.50	106.58	110.58
2	A	420	FDA	C4A-N9A-C8A	3.44	109.35	105.74
2	B	420	FDA	C4-N3-C2	-3.43	121.65	126.37
2	A	420	FDA	C4X-C4-N3	3.38	121.40	112.13
2	C	420	FDA	C2A-N3A-C4A	3.25	119.78	111.83
2	C	420	FDA	C4-N3-C2	-3.20	121.97	126.37
2	A	420	FDA	O4-C4-C4X	-3.20	119.55	127.26
2	A	420	FDA	O3P-PA-O1A	-3.18	101.14	110.70
2	B	420	FDA	C2A-N3A-C4A	3.17	119.58	111.83
2	D	420	FDA	C4X-C4-N3	3.13	120.73	112.13
2	A	420	FDA	N3A-C4A-N9A	3.05	132.36	127.17
2	A	420	FDA	C4A-C5A-N7A	-2.97	107.19	110.58
2	A	420	FDA	C2A-N3A-C4A	2.95	119.04	111.83
2	C	420	FDA	C5A-N7A-C8A	2.94	108.07	103.45
2	B	420	FDA	C4-C4X-N5	2.92	123.84	116.37
2	C	420	FDA	C4A-N9A-C8A	2.91	108.79	105.74
2	D	420	FDA	C4A-N9A-C1B	-2.89	119.86	126.63
2	D	420	FDA	O4B-C1B-N9A	2.88	113.61	108.09
2	A	420	FDA	C5A-N7A-C8A	2.85	107.93	103.45
2	C	420	FDA	C4-C4X-N5	2.84	123.65	116.37
2	C	420	FDA	O2B-C2B-C1B	2.84	119.88	110.10
2	D	420	FDA	C5A-N7A-C8A	2.78	107.83	103.45
2	D	420	FDA	C4A-N9A-C8A	2.78	108.66	105.74
2	D	420	FDA	C4-C4X-N5	2.76	123.42	116.37
2	B	420	FDA	C4X-C4-N3	2.74	119.65	112.13
2	C	420	FDA	C9-C9A-N10	-2.71	118.21	121.85
2	C	420	FDA	C4A-C5A-N7A	-2.67	107.52	110.58
2	B	420	FDA	C4A-N9A-C8A	2.65	108.52	105.74
2	C	420	FDA	N3-C2-N1	2.64	119.89	115.74
2	A	420	FDA	O4B-C1B-N9A	2.63	113.15	108.09
2	C	420	FDA	C4X-C4-N3	2.56	119.17	112.13
2	D	420	FDA	N3-C2-N1	2.51	119.69	115.74
2	D	420	FDA	N3A-C4A-N9A	2.43	131.30	127.17
2	B	420	FDA	O4-C4-C4X	-2.37	121.55	127.26
2	C	420	FDA	O5'-P-O1P	2.35	118.27	108.94
2	D	420	FDA	C5A-C4A-N9A	2.27	108.29	105.81
2	D	420	FDA	C6A-C5A-N7A	2.24	136.41	132.09
2	B	420	FDA	O4B-C1B-N9A	2.20	112.32	108.09
2	C	420	FDA	O2A-PA-O1A	2.20	122.68	112.44
2	D	420	FDA	O3'-C3'-C2'	-2.14	104.06	108.93
2	A	420	FDA	C4-C4X-N5	2.14	121.83	116.37
2	B	420	FDA	O4'-C4'-C3'	2.09	114.14	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	420	FDA	O4-C4-C4X	-2.08	122.24	127.26
2	B	420	FDA	O2A-PA-O1A	2.07	122.07	112.44
2	C	420	FDA	O2-C2-N3	-2.07	118.19	121.86
2	D	420	FDA	O3P-P-O1P	-2.06	104.51	110.70
2	B	420	FDA	C6A-C5A-C4A	2.05	119.97	117.18
2	A	420	FDA	O2A-PA-O1A	2.02	121.84	112.44
2	B	420	FDA	C4'-C3'-C2'	2.00	116.90	113.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	420	FDA	C5B-O5B-PA-O2A
2	B	420	FDA	C5B-O5B-PA-O3P
2	D	420	FDA	C5B-O5B-PA-O2A
2	B	420	FDA	O4B-C4B-C5B-O5B
2	B	420	FDA	PA-O3P-P-O1P
2	C	420	FDA	PA-O3P-P-O1P
2	B	420	FDA	C3B-C4B-C5B-O5B
2	B	420	FDA	C5B-O5B-PA-O1A
2	C	420	FDA	PA-O3P-P-O2P
2	B	420	FDA	PA-O3P-P-O2P
2	D	420	FDA	N10-C1'-C2'-O2'

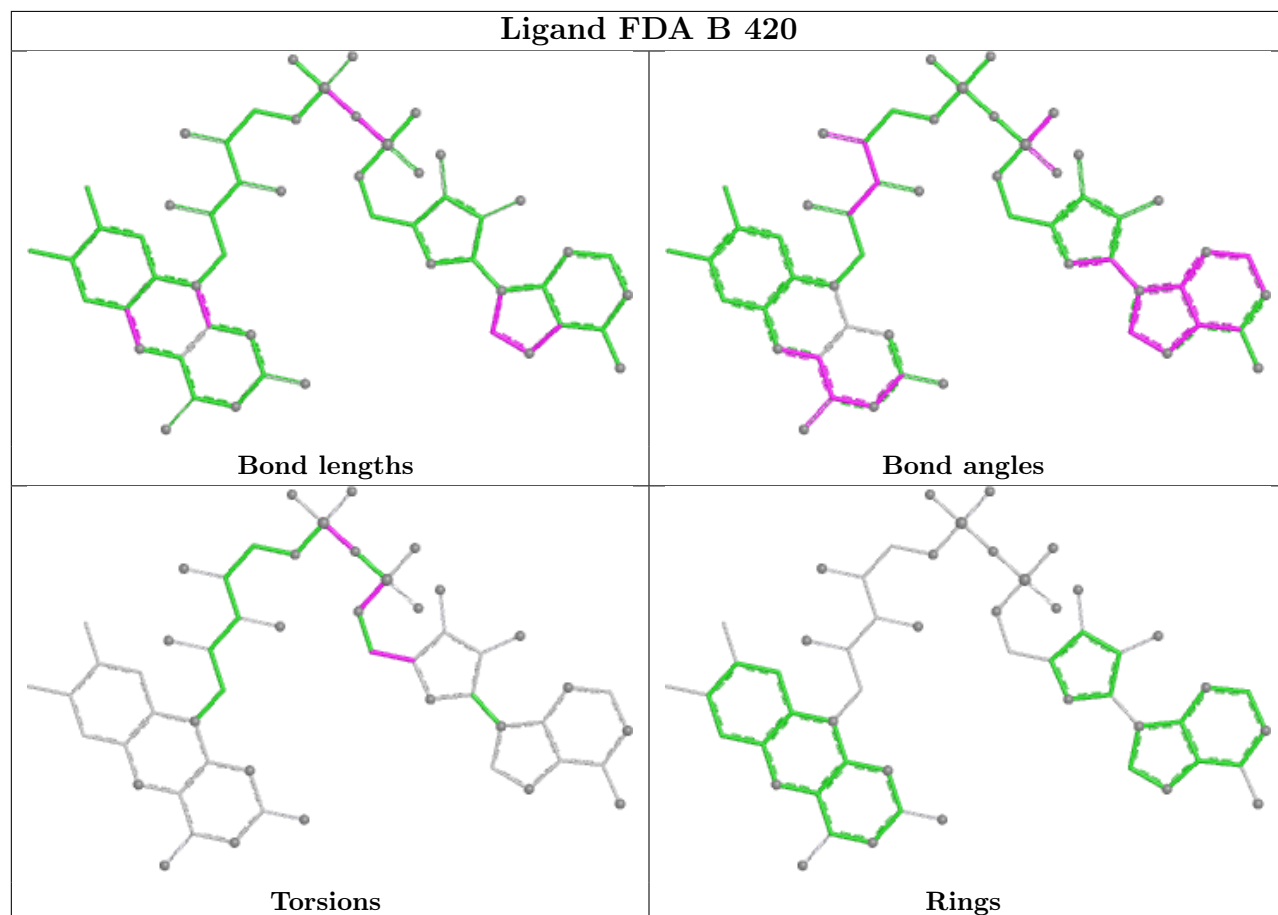
There are no ring outliers.

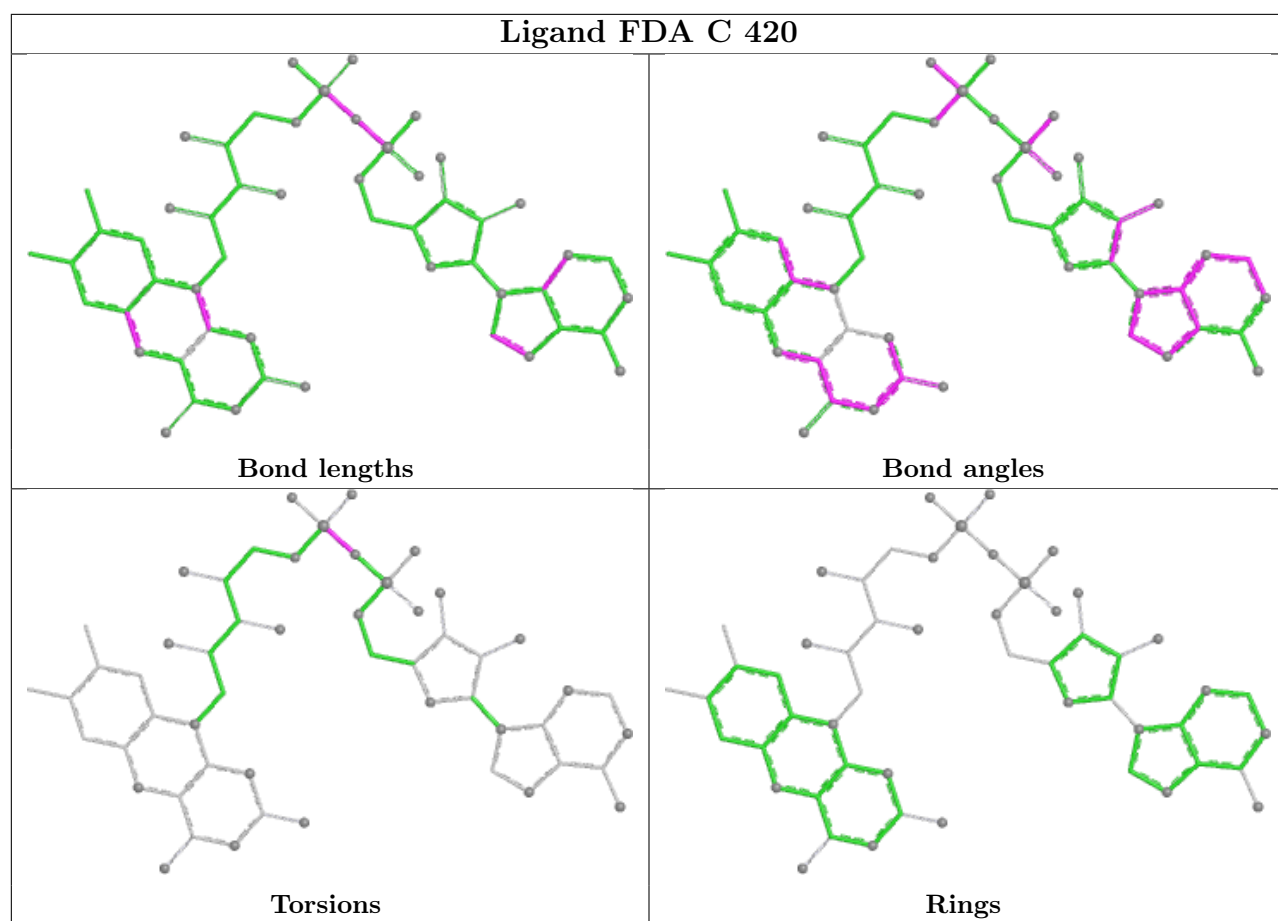
4 monomers are involved in 5 short contacts:

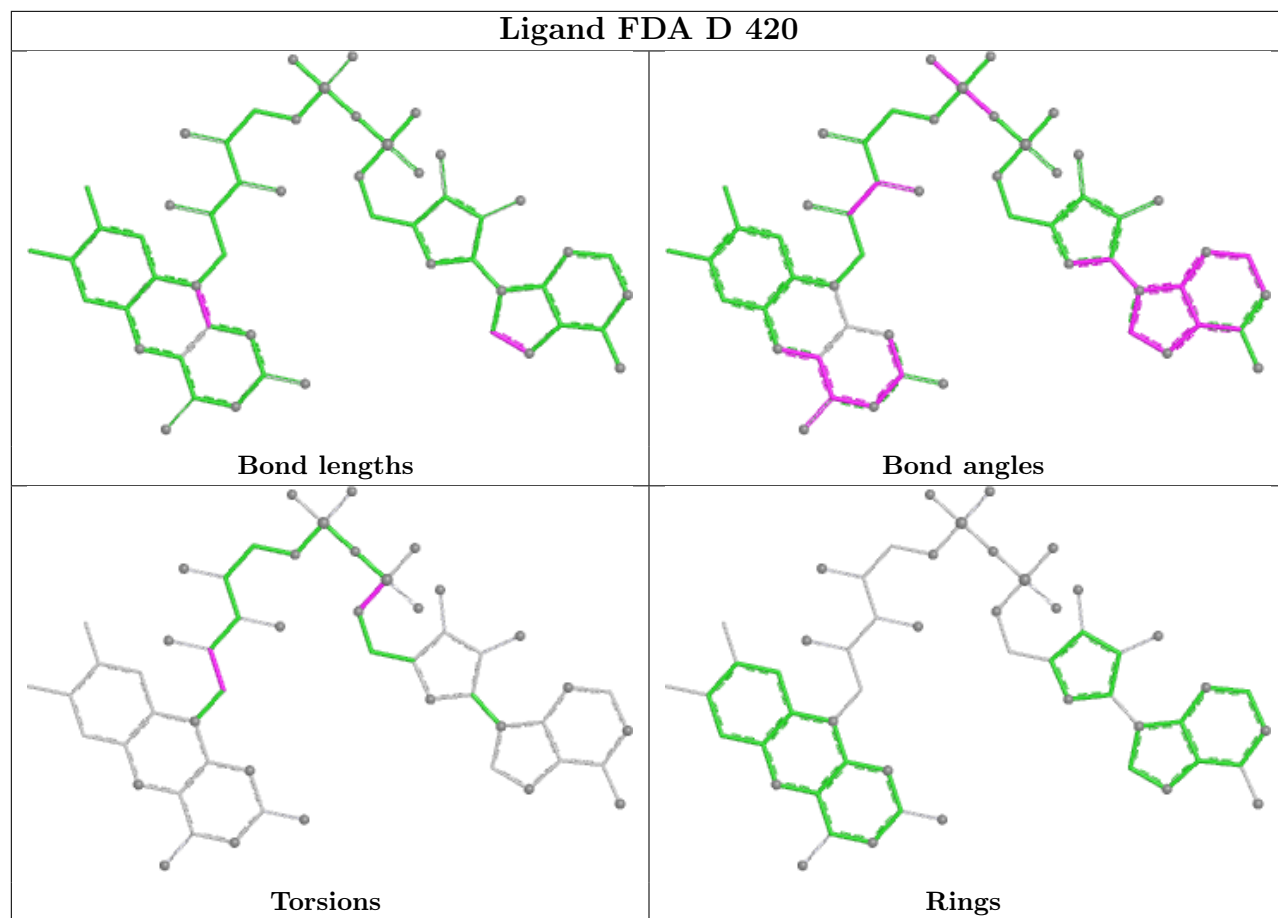
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	420	FDA	2	0
2	C	420	FDA	1	0
2	D	420	FDA	1	0
2	A	420	FDA	1	0

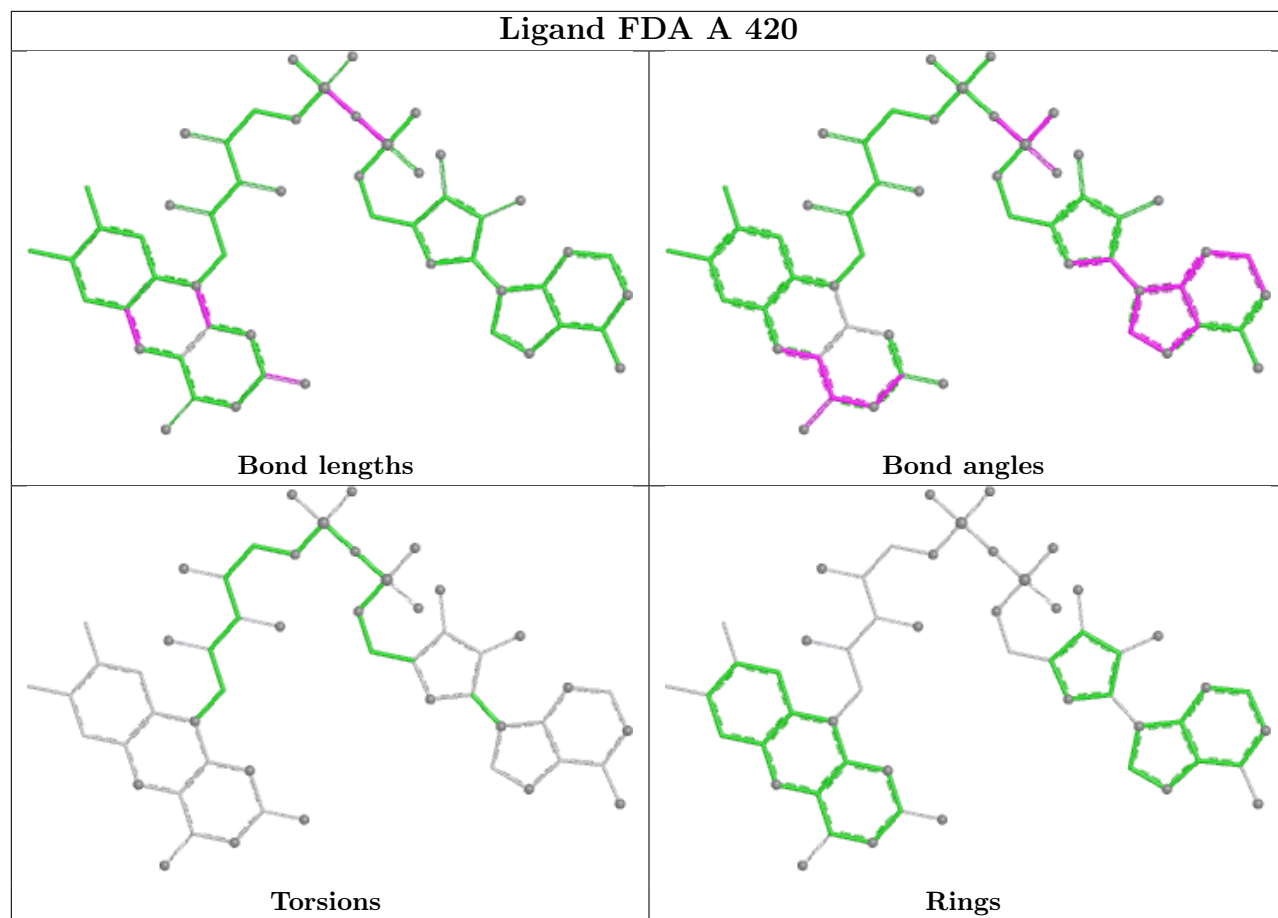
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/403 (93%)	-0.16	3 (0%) 82 80	36, 55, 77, 89	0
1	B	378/403 (93%)	-0.04	6 (1%) 70 67	38, 58, 78, 92	0
1	C	377/403 (93%)	-0.12	2 (0%) 87 85	36, 54, 83, 102	0
1	D	376/403 (93%)	0.16	6 (1%) 70 67	40, 66, 91, 107	0
All	All	1509/1612 (93%)	-0.04	17 (1%) 78 75	36, 58, 84, 107	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	GLY	3.7
1	D	162	ALA	3.3
1	D	119	ILE	3.1
1	B	81	GLY	3.1
1	C	198	TYR	3.0
1	C	154	ASP	2.7
1	B	21	PRO	2.5
1	D	256	MET	2.4
1	A	21	PRO	2.4
1	B	209	ASN	2.2
1	B	398	GLY	2.1
1	A	198	TYR	2.1
1	D	60	ASP	2.1
1	D	155	VAL	2.1
1	B	60	ASP	2.1
1	B	155	VAL	2.0
1	A	256	MET	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

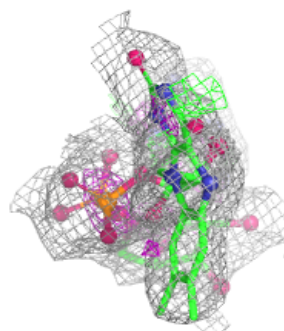
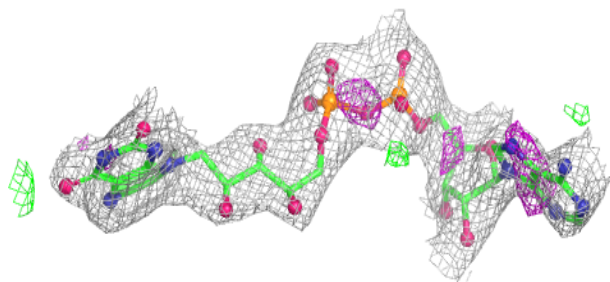
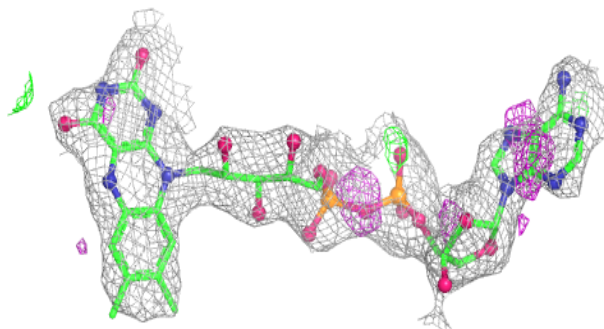
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	K	C	400	1/1	0.78	0.14	69,69,69,69	0
3	K	D	400	1/1	0.85	0.12	78,78,78,78	0
3	K	A	400	1/1	0.87	0.20	83,83,83,83	0
3	K	B	400	1/1	0.87	0.09	72,72,72,72	0
2	FDA	B	420	53/53	0.88	0.12	60,68,80,81	0
2	FDA	D	420	53/53	0.90	0.10	56,61,66,67	0
2	FDA	C	420	53/53	0.90	0.11	54,62,70,71	0
3	K	A	401	1/1	0.90	0.09	53,53,53,53	0
3	K	C	401	1/1	0.91	0.08	54,54,54,54	0
2	FDA	A	420	53/53	0.92	0.09	46,55,60,61	0

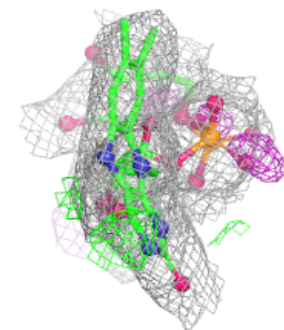
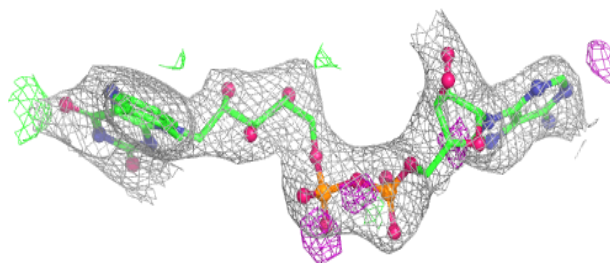
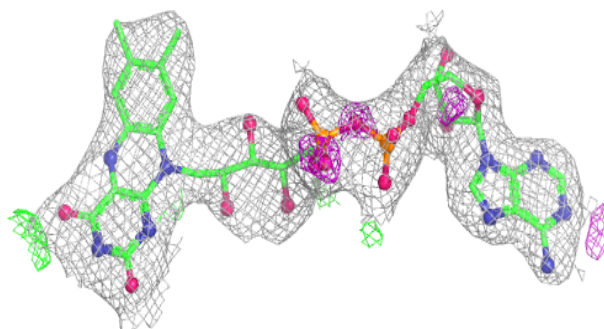
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA B 420:

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

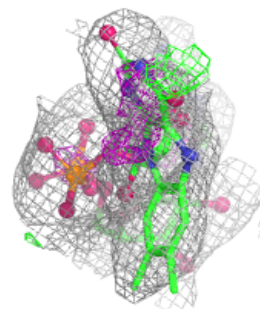
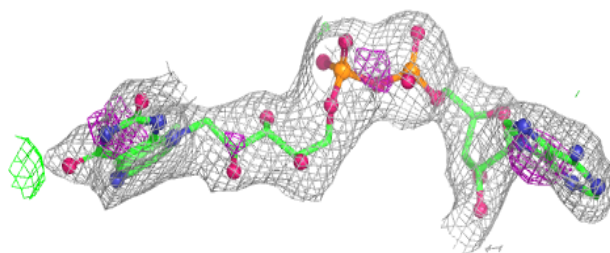
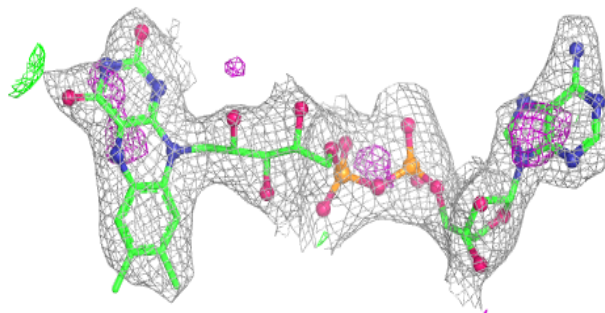
**Electron density around FDA D 420:**

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

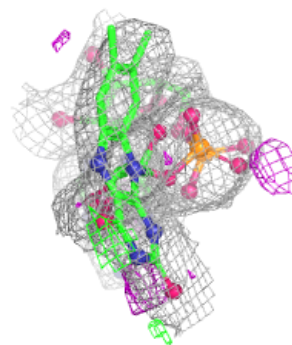
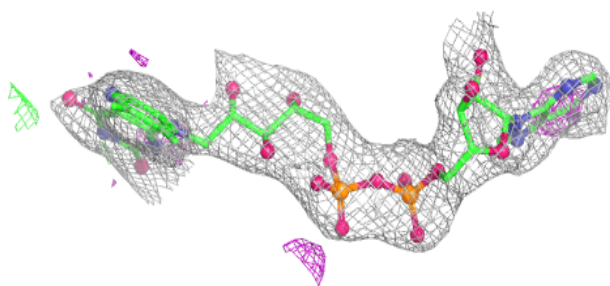
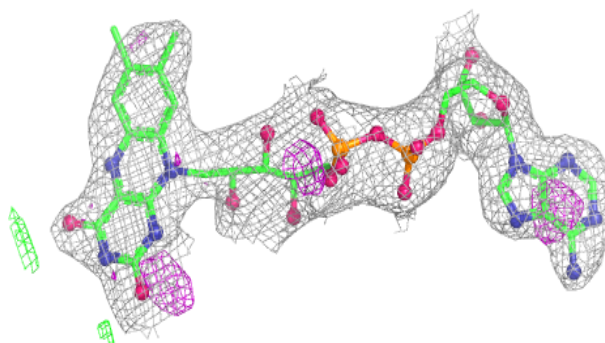


Electron density around FDA C 420:

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

**Electron density around FDA A 420:**

$2mF_o-DF_c$ (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.