



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 PM UTC

PDB ID : 1UKW / pdb_00001ukw
Title : Crystal structure of medium-chain acyl-CoA dehydrogenase from *Thermus thermophilus* HB8
Authors : Hamada, K.; Ago, H.; Kuramitsu, S.; Miyano, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-09-02
Resolution : 2.40 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

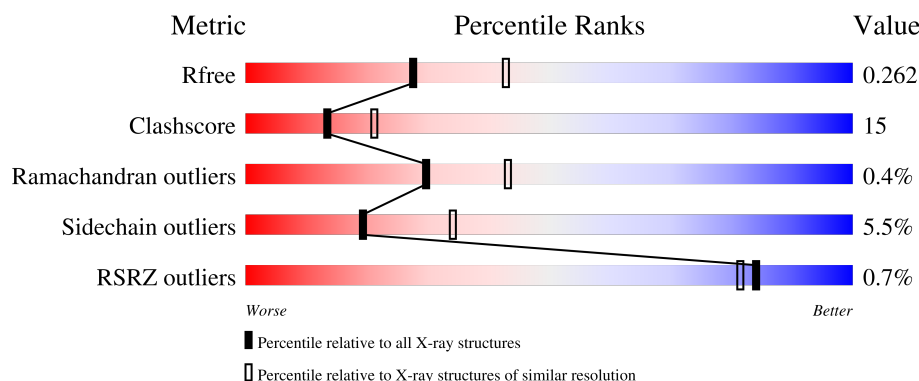
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	379	68% 27% .
1	B	379	68% 28% .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6221 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 acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2953	1888	509	546	10			
1	B	379	Total	C	N	O	S	0	0	0
			2953	1888	509	546	10			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Co 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total 99	O 99	0	0
4	B	109	Total 109	O 109	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.12Å 88.12Å 206.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.40 19.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.93-2.40) 99.7 (19.93-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.260 0.207 , 0.262	Depositor DCC
R_{free} test set	3255 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6221	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: CO, FAD

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	0.45	0/3011	0.95	10/4073 (0.2%)
1	B	0.45	0/3011	0.93	13/4073 (0.3%)
All	All	0.45	0/6022	0.94	23/8146 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	GLN	N-CA-C	-7.40	103.22	111.28
1	B	218	ARG	N-CA-C	7.20	120.04	111.33
1	A	54	VAL	N-CA-C	6.99	118.31	111.67
1	B	241	GLU	N-CA-C	-6.73	98.27	109.24
1	A	55	ILE	N-CA-C	6.65	116.67	110.42
1	B	391	ILE	N-CA-C	6.58	117.22	111.56
1	B	399	GLN	N-CA-C	-6.38	104.24	111.07
1	A	379	VAL	N-CA-C	6.37	117.16	110.72
1	A	194	GLU	N-CA-C	-6.35	103.88	111.69
1	A	391	ILE	N-CA-C	6.19	116.51	111.62
1	B	211	VAL	N-CA-C	6.06	117.45	109.21
1	B	220	THR	CA-C-N	5.96	126.31	119.93
1	B	220	THR	C-N-CA	5.96	126.31	119.93
1	B	54	VAL	N-CA-C	5.83	116.58	111.56
1	A	378	PRO	N-CA-C	5.80	122.24	114.18
1	B	378	PRO	N-CA-C	5.72	122.14	114.18
1	A	240	TYR	N-CA-C	5.71	118.36	109.52
1	B	376	GLU	N-CA-C	-5.30	106.08	112.54
1	B	240	TYR	N-CA-C	5.21	117.60	109.52
1	A	42	GLN	N-CA-C	-5.20	105.51	111.07
1	B	187	ILE	N-CA-C	5.14	115.17	107.51
1	A	202	VAL	N-CA-C	-5.12	106.92	113.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	GLU	N-CA-C	-5.10	107.12	113.19

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	2953	0	2977	94	0
1	B	2953	0	2977	91	0
2	A	53	0	31	8	0
2	B	53	0	31	5	0
3	B	1	0	0	0	0
4	A	99	0	0	6	0
4	B	109	0	0	4	0
All	All	6221	0	6016	177	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 15.

All (177) 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:34:PHE:HA	1:B:32:ILE:HG13	1.59	0.85
1:B:40:GLN:HE22	1:B:98:LEU:HD23	1.41	0.85
1:A:32:ILE:HG21	1:B:98:LEU:HD22	1.57	0.84
1:B:250:PRO:HB2	1:B:252:GLU:HG2	1.60	0.84
1:A:64:GLU:HG2	1:A:375:ARG:HH11	1.45	0.79
1:B:37:THR:OG1	1:B:40:GLN:HG3	1.82	0.79
1:B:273:ARG:NH1	4:B:1024:HOH:O	2.16	0.76
1:A:161:GLY:HA3	2:A:420:FAD:H5'2	1.68	0.75
1:A:263:LYS:O	1:A:267:GLN:HG3	1.89	0.73
1:A:380:GLU:OE2	1:A:384:ARG:NE	2.23	0.71
1:B:137:LYS:O	1:B:141:LEU:HB2	1.91	0.70
1:B:222:GLY:HA2	4:B:1117:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HB	1:A:275:PRO:HD3	1.73	0.68
1:A:40:GLN:HE22	1:A:98:LEU:HD23	1.59	0.67
1:B:274:ILE:HB	1:B:275:PRO:HD3	1.77	0.67
1:A:152:ALA:HB3	1:A:196:VAL:HG22	1.77	0.66
1:B:46:LEU:HD21	1:B:79:VAL:HG21	1.77	0.66
1:B:74:GLU:O	1:B:78:GLU:HG3	1.96	0.65
1:A:231:LYS:HE2	4:A:1173:HOH:O	1.97	0.64
1:B:46:LEU:HD21	1:B:79:VAL:CG2	2.28	0.63
1:A:84:ALA:CB	1:A:95:LEU:HD22	2.28	0.63
1:B:142:ARG:HB3	1:B:143:PRO:HD3	1.81	0.62
1:A:84:ALA:HB3	1:A:95:LEU:HD22	1.81	0.61
1:A:211:VAL:HG12	1:A:261:GLY:HA3	1.82	0.61
1:B:38:GLU:O	1:B:42:GLN:HG2	2.01	0.61
1:B:135:GLU:OE2	1:B:139:ARG:HD3	2.01	0.61
1:A:105:GLU:OE1	1:A:326:ARG:HD3	1.99	0.61
1:B:38:GLU:OE2	1:B:38:GLU:HA	2.01	0.61
1:A:272:THR:O	1:A:275:PRO:HD2	2.00	0.61
1:B:375:ARG:HG2	1:B:380:GLU:OE1	2.00	0.61
1:A:231:LYS:O	1:A:235:ARG:HD2	2.02	0.60
1:A:64:GLU:CG	1:A:375:ARG:HH11	2.15	0.60
1:B:105:GLU:OE1	1:B:326:ARG:HD3	2.03	0.59
1:B:40:GLN:HE22	1:B:98:LEU:CD2	2.15	0.59
1:A:272:THR:C	1:A:275:PRO:HD2	2.28	0.58
1:B:308:PHE:O	1:B:312:GLN:HG3	2.03	0.58
1:A:379:VAL:HA	1:A:382:LEU:HD22	1.84	0.58
1:B:272:THR:O	1:B:275:PRO:HD2	2.03	0.58
1:B:272:THR:C	1:B:275:PRO:HD2	2.29	0.58
1:B:395:THR:O	1:B:399:GLN:HG2	2.03	0.58
1:B:356:ILE:C	1:B:356:ILE:HD12	2.29	0.57
1:A:392:TYR:HA	2:A:420:FAD:H2'	1.87	0.57
1:A:32:ILE:HG21	1:B:98:LEU:CD2	2.33	0.56
1:A:70:TRP:CE3	1:A:73:ILE:HD12	2.39	0.56
1:B:380:GLU:OE2	1:B:384:ARG:NE	2.37	0.55
1:A:327:MET:HA	1:A:327:MET:HE2	1.89	0.55
1:A:46:LEU:HD21	1:A:79:VAL:HG22	1.88	0.55
2:A:420:FAD:H8A	2:A:420:FAD:H51A	1.89	0.55
1:A:397:GLU:HB2	2:A:420:FAD:O2B	2.07	0.54
1:A:129:LEU:CD2	1:A:141:LEU:HD21	2.38	0.54
1:A:154:ALA:HA	1:A:187:ILE:HD12	1.88	0.54
1:B:124:GLY:O	1:B:127:PRO:HD2	2.08	0.54
1:A:64:GLU:HG2	1:A:375:ARG:NH1	2.18	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:HB3	1:A:143:PRO:HD3	1.88	0.54
1:B:139:ARG:NH2	1:B:253:ASN:OD1	2.41	0.54
1:A:76:LEU:O	1:A:79:VAL:HG12	2.08	0.54
1:B:61:GLU:HG2	1:B:65:LYS:HE2	1.89	0.54
1:A:46:LEU:HD21	1:A:79:VAL:CG2	2.37	0.53
1:B:231:LYS:O	1:B:235:ARG:HD2	2.08	0.53
1:B:326:ARG:HG2	1:B:327:MET:HE2	1.91	0.53
1:B:40:GLN:NE2	1:B:98:LEU:HD23	2.20	0.52
1:B:392:TYR:HA	2:B:421:FAD:H2'	1.91	0.52
1:B:120:ALA:O	1:B:123:LEU:HB3	2.09	0.52
1:A:228:ILE:HD12	1:A:239:THR:HG22	1.91	0.52
1:A:132:GLY:O	1:A:137:LYS:HE3	2.11	0.51
1:A:176:ASP:OD2	1:A:176:ASP:O	2.28	0.51
1:B:123:LEU:HG	1:B:153:PHE:CB	2.40	0.51
1:A:156:SER:OG	2:A:420:FAD:H1'1	2.11	0.51
1:A:106:GLU:O	1:A:109:TYR:HB3	2.11	0.50
1:A:160:ASN:OD1	1:A:163:ASP:O	2.30	0.50
1:B:123:LEU:O	1:B:127:PRO:HD3	2.11	0.50
1:B:303:GLU:CG	1:B:307:ASN:HD22	2.25	0.50
1:B:95:LEU:HG	1:B:99:ASP:HB3	1.94	0.50
1:B:209:LYS:O	1:B:259:GLY:HA2	2.12	0.50
1:A:40:GLN:NE2	1:A:98:LEU:HD23	2.24	0.50
1:B:389:ASN:HD22	1:B:389:ASN:N	2.09	0.50
1:A:32:ILE:O	1:A:32:ILE:HG23	2.11	0.49
1:A:160:ASN:OD1	1:A:163:ASP:HB3	2.12	0.49
2:B:421:FAD:H8A	2:B:421:FAD:H51A	1.93	0.49
1:A:123:LEU:HD12	1:A:272:THR:HG21	1.94	0.49
1:A:312:GLN:O	1:A:316:VAL:HG23	2.13	0.49
1:A:186:TRP:O	2:A:420:FAD:N5	2.45	0.49
1:B:69:PRO:HB2	1:B:72:VAL:HG23	1.94	0.49
1:A:323:GLU:HB3	1:B:328:TYR:CE1	2.47	0.49
1:B:334:TRP:O	1:B:338:GLN:HG2	2.13	0.49
1:A:389:ASN:HD22	1:A:389:ASN:N	2.10	0.49
1:B:223:PHE:C	1:B:223:PHE:CD1	2.90	0.49
1:A:218:ARG:HG2	1:A:218:ARG:O	2.11	0.48
1:A:137:LYS:O	1:A:141:LEU:HB2	2.13	0.48
1:A:116:THR:OG1	1:A:234:GLN:NE2	2.47	0.48
1:B:56:LEU:HB3	1:B:57:PRO:HD3	1.96	0.48
1:B:70:TRP:N	1:B:71:PRO:CD	2.76	0.48
1:A:232:MET:HE3	1:A:384:ARG:HA	1.96	0.48
1:A:348:ILE:HG12	1:A:403:ILE:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ILE:HD13	1:B:122:ASP:HB3	1.95	0.48
1:B:379:VAL:HA	1:B:382:LEU:HD22	1.95	0.48
1:A:164:ALA:O	1:A:167:LEU:HG	2.14	0.48
1:A:176:ASP:HB2	4:A:1056:HOH:O	2.14	0.48
1:A:407:ILE:HG22	1:B:292:ARG:HD3	1.96	0.47
1:B:171:ALA:O	1:B:202:VAL:HG23	2.14	0.47
1:A:98:LEU:HD22	1:B:32:ILE:CG2	2.44	0.47
1:A:388:LEU:HD11	2:A:420:FAD:C7M	2.43	0.47
1:B:61:GLU:HB2	4:B:1131:HOH:O	2.13	0.47
1:B:404:ALA:O	1:B:408:LEU:HD22	2.14	0.47
1:B:37:THR:HG1	1:B:40:GLN:HG3	1.75	0.47
1:B:358:PHE:HA	1:B:386:VAL:HG11	1.95	0.47
1:A:98:LEU:HD22	1:B:32:ILE:HG22	1.96	0.47
1:A:157:GLU:HG2	1:A:184:LYS:HD3	1.96	0.47
1:A:209:LYS:O	1:A:259:GLY:HA2	2.15	0.47
1:A:203:ASN:OD1	1:A:205:GLU:HB2	2.15	0.46
1:A:388:LEU:HD11	2:A:420:FAD:HM73	1.97	0.46
1:A:363:GLN:HG3	4:A:1054:HOH:O	2.16	0.46
1:B:186:TRP:O	2:B:421:FAD:C4X	2.63	0.46
1:A:308:PHE:O	1:A:312:GLN:HG3	2.16	0.46
1:A:395:THR:O	1:A:399:GLN:HG2	2.15	0.46
1:A:328:TYR:CE1	1:B:323:GLU:HB3	2.51	0.46
1:A:38:GLU:O	1:A:42:GLN:HG2	2.16	0.45
1:B:397:GLU:HB2	2:B:421:FAD:O2B	2.16	0.45
1:A:36:LEU:N	1:A:36:LEU:HD12	2.31	0.45
1:B:156:SER:OG	2:B:421:FAD:H1'1	2.16	0.45
1:A:398:ILE:C	1:A:398:ILE:HD12	2.41	0.44
1:A:117:ILE:HB	1:A:118:PRO:CD	2.47	0.44
1:A:168:LYS:HB2	1:A:168:LYS:NZ	2.32	0.44
1:A:398:ILE:HA	1:A:401:LEU:HB2	1.98	0.44
1:B:116:THR:OG1	1:B:234:GLN:NE2	2.51	0.44
1:B:395:THR:O	1:B:398:ILE:HG13	2.17	0.44
1:A:133:THR:O	1:A:137:LYS:HG3	2.18	0.44
1:B:353:ALA:O	1:B:356:ILE:HG13	2.16	0.44
1:A:327:MET:HE2	1:A:327:MET:CA	2.48	0.44
1:A:129:LEU:HD21	1:A:141:LEU:HD21	2.00	0.43
1:A:138:GLU:CD	1:A:142:ARG:HH21	2.27	0.43
1:B:176:ASP:C	1:B:251:VAL:HG13	2.43	0.43
1:A:168:LYS:NZ	1:A:168:LYS:CB	2.82	0.43
1:B:69:PRO:HB2	1:B:72:VAL:CG2	2.49	0.43
1:A:35:SER:C	1:A:36:LEU:HD12	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ALA:HB3	1:B:262:PHE:CE1	2.53	0.43
1:B:220:THR:O	1:B:223:PHE:HB3	2.19	0.43
1:B:232:MET:O	1:B:384:ARG:HB3	2.19	0.43
1:A:211:VAL:HB	4:A:1035:HOH:O	2.19	0.43
1:A:33:ASP:O	1:B:32:ILE:HA	2.18	0.43
1:A:199:PHE:CE2	1:A:265:ALA:HB2	2.54	0.42
1:A:293:LYS:O	1:A:297:GLU:HG3	2.19	0.42
1:B:84:ALA:HB3	1:B:95:LEU:HD22	2.00	0.42
1:B:188:SER:O	1:B:189:ASN:HB2	2.18	0.42
1:B:245:GLU:O	1:B:246:ASP:C	2.60	0.42
1:B:388:LEU:HD13	1:B:392:TYR:CE2	2.54	0.42
1:A:84:ALA:HB1	1:A:95:LEU:HD22	1.99	0.42
1:A:327:MET:HE3	4:A:1157:HOH:O	2.19	0.42
1:B:89:GLU:H	1:B:89:GLU:CD	2.27	0.42
1:B:327:MET:HE3	4:B:1165:HOH:O	2.19	0.42
1:B:154:ALA:HA	1:B:187:ILE:HD12	2.00	0.42
1:B:220:THR:HA	1:B:221:PRO:HD3	1.88	0.42
1:B:228:ILE:HD12	1:B:239:THR:HG22	2.01	0.42
1:A:295:ALA:HA	1:A:305:ILE:HD11	2.01	0.42
1:B:388:LEU:HD22	1:B:388:LEU:O	2.20	0.42
1:A:124:GLY:O	1:A:127:PRO:HD2	2.19	0.42
1:B:398:ILE:O	1:B:402:ILE:HG12	2.18	0.42
1:A:173:ARG:CB	1:A:173:ARG:HH11	2.32	0.42
1:A:86:ILE:O	1:A:92:GLY:HA3	2.19	0.41
1:B:312:GLN:O	1:B:316:VAL:HG23	2.20	0.41
1:A:173:ARG:HH11	1:A:173:ARG:CG	2.31	0.41
1:A:173:ARG:HH11	1:A:173:ARG:HB3	1.85	0.41
1:B:117:ILE:HB	1:B:118:PRO:CD	2.50	0.41
1:B:135:GLU:CD	1:B:139:ARG:HH11	2.28	0.41
1:A:34:PHE:CA	1:B:32:ILE:HG13	2.40	0.41
1:A:184:LYS:HB3	1:A:187:ILE:HD11	2.02	0.41
1:B:70:TRP:CE3	1:B:73:ILE:HD12	2.54	0.41
1:B:157:GLU:HG2	1:B:184:LYS:HD3	2.03	0.41
1:A:289:ASP:OD1	1:A:292:ARG:NH2	2.53	0.41
1:A:381:LYS:NZ	4:A:1007:HOH:O	2.52	0.41
1:B:144:LEU:HD21	1:B:151:ALA:HB2	2.03	0.41
1:B:113:GLY:HA3	1:B:234:GLN:HA	2.03	0.41
1:B:84:ALA:CB	1:B:95:LEU:HD22	2.51	0.41
1:B:123:LEU:HG	1:B:153:PHE:HB2	2.02	0.41
1:A:260:GLU:O	1:A:264:ILE:HG13	2.22	0.40
1:A:34:PHE:CD1	1:A:34:PHE:N	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ARG:O	1:B:146:GLU:HG3	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	377/379 (100%)	362 (96%)	12 (3%)	3 (1%)	16	25
1	B	377/379 (100%)	363 (96%)	14 (4%)	0	100	100
All	All	754/758 (100%)	725 (96%)	26 (3%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	165	ALA
1	A	161	GLY

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	298/298 (100%)	280 (94%)	18 (6%)	17	31
1	B	298/298 (100%)	283 (95%)	15 (5%)	22	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	596/596 (100%)	563 (94%)	33 (6%)	19	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	82	LEU
1	A	95	LEU
1	A	141	LEU
1	A	144	LEU
1	A	150	LEU
1	A	168	LYS
1	A	173	ARG
1	A	180	LEU
1	A	209	LYS
1	A	255	LEU
1	A	260	GLU
1	A	382	LEU
1	A	386	VAL
1	A	388	LEU
1	A	392	TYR
1	A	401	LEU
1	A	408	LEU
1	B	46	LEU
1	B	56	LEU
1	B	82	LEU
1	B	95	LEU
1	B	141	LEU
1	B	168	LYS
1	B	180	LEU
1	B	235	ARG
1	B	252	GLU
1	B	255	LEU
1	B	382	LEU
1	B	386	VAL
1	B	388	LEU
1	B	392	TYR
1	B	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	189	ASN
1	A	208	HIS
1	A	234	GLN
1	A	389	ASN
1	A	390	GLN
1	A	406	HIS
1	B	40	GLN
1	B	174	GLN
1	B	189	ASN
1	B	234	GLN
1	B	307	ASN
1	B	389	ASN
1	B	390	GLN
1	B	406	HIS

5.3.3 RNA [i](#)

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	FAD	A	420	-	58,58,58	2.23	17 (29%)	85,89,89	1.87	20 (23%)
2	FAD	B	421	-	58,58,58	2.35	16 (27%)	85,89,89	1.91	21 (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
2	FAD	A	420	-	-	4/34/50/50	0/6/6/6
2	FAD	B	421	-	-	5/34/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	421	FAD	C4X-N5	6.53	1.44	1.30
2	B	421	FAD	PA-O3P	-6.35	1.52	1.59
2	A	420	FAD	C4X-N5	6.08	1.43	1.30
2	A	420	FAD	C9A-N10	5.51	1.50	1.41
2	B	421	FAD	C9A-N10	5.29	1.50	1.41
2	A	420	FAD	C9A-C5X	5.23	1.49	1.41
2	B	421	FAD	C9A-C5X	5.19	1.49	1.41
2	B	421	FAD	C4A-N3A	4.83	1.43	1.34
2	A	420	FAD	PA-O3P	-4.73	1.54	1.59
2	A	420	FAD	C4A-N3A	4.39	1.42	1.34
2	B	421	FAD	C2A-N3A	4.17	1.41	1.33
2	A	420	FAD	C5A-C4A	-3.94	1.32	1.39
2	A	420	FAD	C2A-N3A	3.92	1.40	1.33
2	A	420	FAD	C8A-N9A	3.84	1.44	1.37
2	B	421	FAD	C8A-N9A	3.83	1.44	1.37
2	B	421	FAD	C5A-C4A	-3.63	1.32	1.39
2	B	421	FAD	P-O3P	-3.42	1.55	1.59
2	A	420	FAD	C2B-C3B	-3.33	1.44	1.53
2	A	420	FAD	C5'-C4'	-3.27	1.47	1.51
2	B	421	FAD	C2B-C3B	-3.23	1.44	1.53
2	B	421	FAD	C4'-C3'	-2.89	1.48	1.53
2	A	420	FAD	C4'-C3'	-2.83	1.48	1.53
2	A	420	FAD	C1'-C2'	2.70	1.56	1.52
2	A	420	FAD	C10-N1	2.66	1.38	1.33
2	B	421	FAD	C10-N1	2.66	1.38	1.33
2	B	421	FAD	C1'-C2'	2.60	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	420	FAD	O4-C4	2.25	1.27	1.23
2	B	421	FAD	P-O5'	-2.24	1.50	1.59
2	A	420	FAD	C4-N3	2.16	1.42	1.38
2	B	421	FAD	C5'-C4'	-2.13	1.48	1.51
2	A	420	FAD	C6-C7	2.12	1.42	1.39
2	A	420	FAD	P-O5'	-2.12	1.51	1.59
2	B	421	FAD	O4-C4	2.11	1.27	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	421	FAD	C4A-N9A-C8A	-5.80	99.65	105.74
2	B	421	FAD	O2P-P-O3P	-5.76	91.71	107.27
2	A	420	FAD	C4A-N9A-C8A	-5.64	99.81	105.74
2	A	420	FAD	O2P-P-O3P	-5.22	93.17	107.27
2	A	420	FAD	C5A-C4A-N9A	5.03	111.29	105.81
2	B	421	FAD	C5A-C4A-N9A	4.93	111.19	105.81
2	A	420	FAD	N3A-C4A-N9A	-4.77	119.05	127.17
2	A	420	FAD	O4B-C4B-C5B	-4.73	94.19	109.33
2	B	421	FAD	N3A-C4A-N9A	-4.54	119.45	127.17
2	B	421	FAD	O4B-C4B-C5B	-4.44	95.11	109.33
2	B	421	FAD	O5'-C5'-C4'	-4.14	98.30	109.36
2	A	420	FAD	C5X-C9A-N10	-3.79	114.54	117.97
2	A	420	FAD	O5'-C5'-C4'	-3.74	99.39	109.36
2	A	420	FAD	C5'-C4'-C3'	3.35	118.54	112.22
2	B	421	FAD	C5X-C9A-N10	-3.20	115.07	117.97
2	B	421	FAD	C5'-C4'-C3'	3.17	118.20	112.22
2	B	421	FAD	O5B-C5B-C4B	3.12	119.61	108.99
2	A	420	FAD	C9-C9A-N10	3.09	126.01	121.85
2	A	420	FAD	O3P-P-O1P	2.96	119.62	110.70
2	B	421	FAD	O3P-PA-O1A	-2.84	102.16	110.70
2	B	421	FAD	O2B-C2B-C3B	2.82	120.85	111.82
2	A	420	FAD	O5B-C5B-C4B	2.80	118.52	108.99
2	B	421	FAD	C9-C9A-N10	2.76	125.56	121.85
2	A	420	FAD	O3P-PA-O1A	-2.73	102.48	110.70
2	A	420	FAD	N3A-C2A-N1A	-2.66	124.55	128.58
2	A	420	FAD	C4X-C10-N10	2.60	120.21	116.48
2	A	420	FAD	O2B-C2B-C3B	2.59	120.11	111.82
2	B	421	FAD	O2P-P-O5'	-2.59	95.84	107.57
2	B	421	FAD	O3P-P-O1P	2.51	118.26	110.70
2	B	421	FAD	PA-O5B-C5B	-2.45	107.30	121.35
2	B	421	FAD	N3A-C2A-N1A	-2.42	124.92	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	421	FAD	C4X-C10-N10	2.32	119.80	116.48
2	A	420	FAD	O2P-P-O5'	-2.29	97.19	107.57
2	B	421	FAD	C3B-C2B-C1B	2.29	105.79	101.46
2	B	421	FAD	C4-C4X-C10	2.19	120.69	116.93
2	B	421	FAD	C1'-C2'-C3'	2.14	115.45	109.66
2	A	420	FAD	C5A-C4A-N3A	2.14	129.66	126.72
2	A	420	FAD	PA-O5B-C5B	-2.13	109.16	121.35
2	B	421	FAD	O3'-C3'-C2'	2.10	113.69	108.93
2	A	420	FAD	C4-C4X-C10	2.09	120.52	116.93
2	A	420	FAD	O3'-C3'-C2'	2.00	113.48	108.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	420	FAD	P-O3P-PA-O5B
2	A	420	FAD	C5'-O5'-P-O3P
2	B	421	FAD	C5B-O5B-PA-O1A
2	B	421	FAD	C5'-O5'-P-O3P
2	B	421	FAD	P-O3P-PA-O5B
2	A	420	FAD	C5B-O5B-PA-O1A
2	B	421	FAD	O2'-C2'-C3'-C4'
2	B	421	FAD	P-O3P-PA-O2A
2	A	420	FAD	P-O3P-PA-O2A

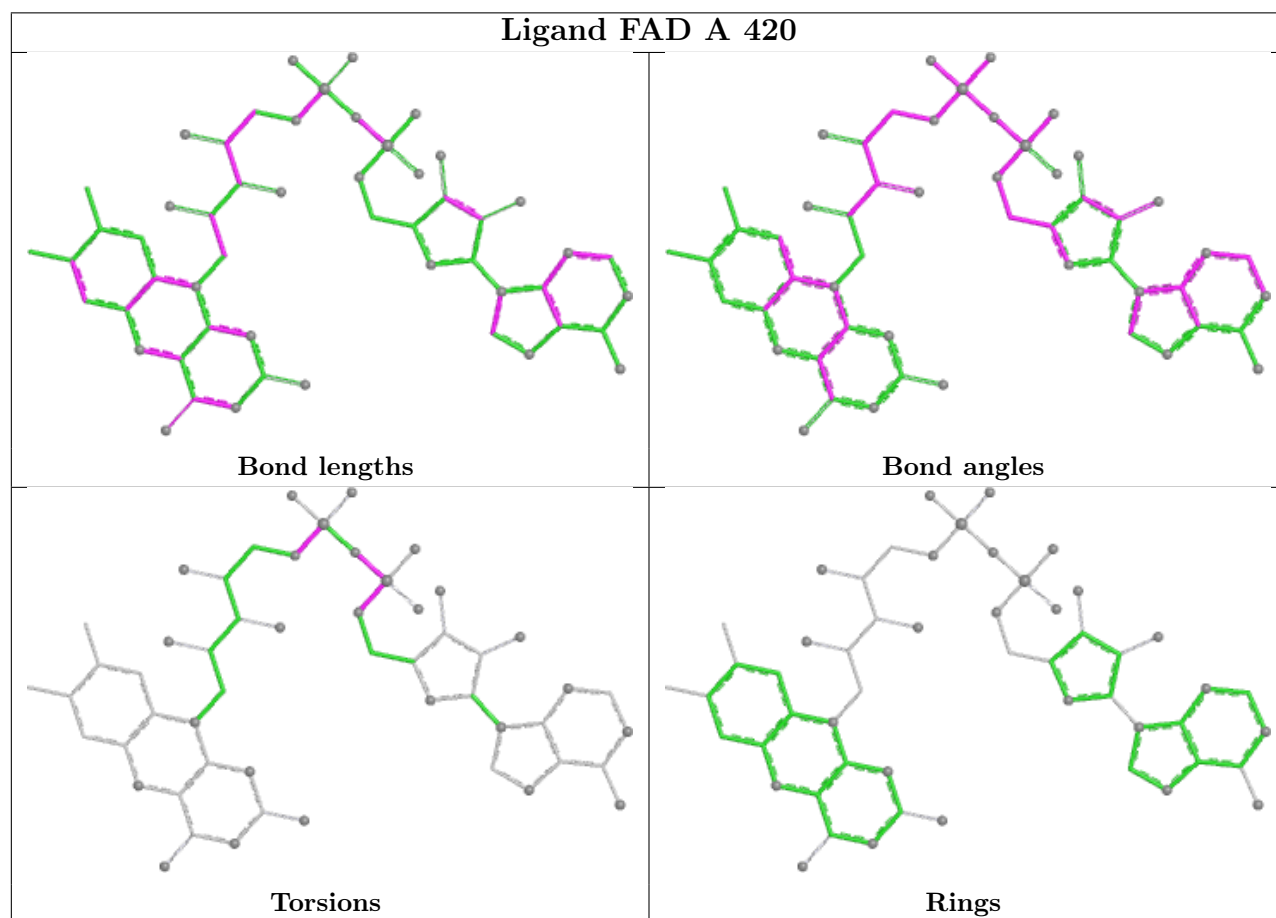
There are no ring outliers.

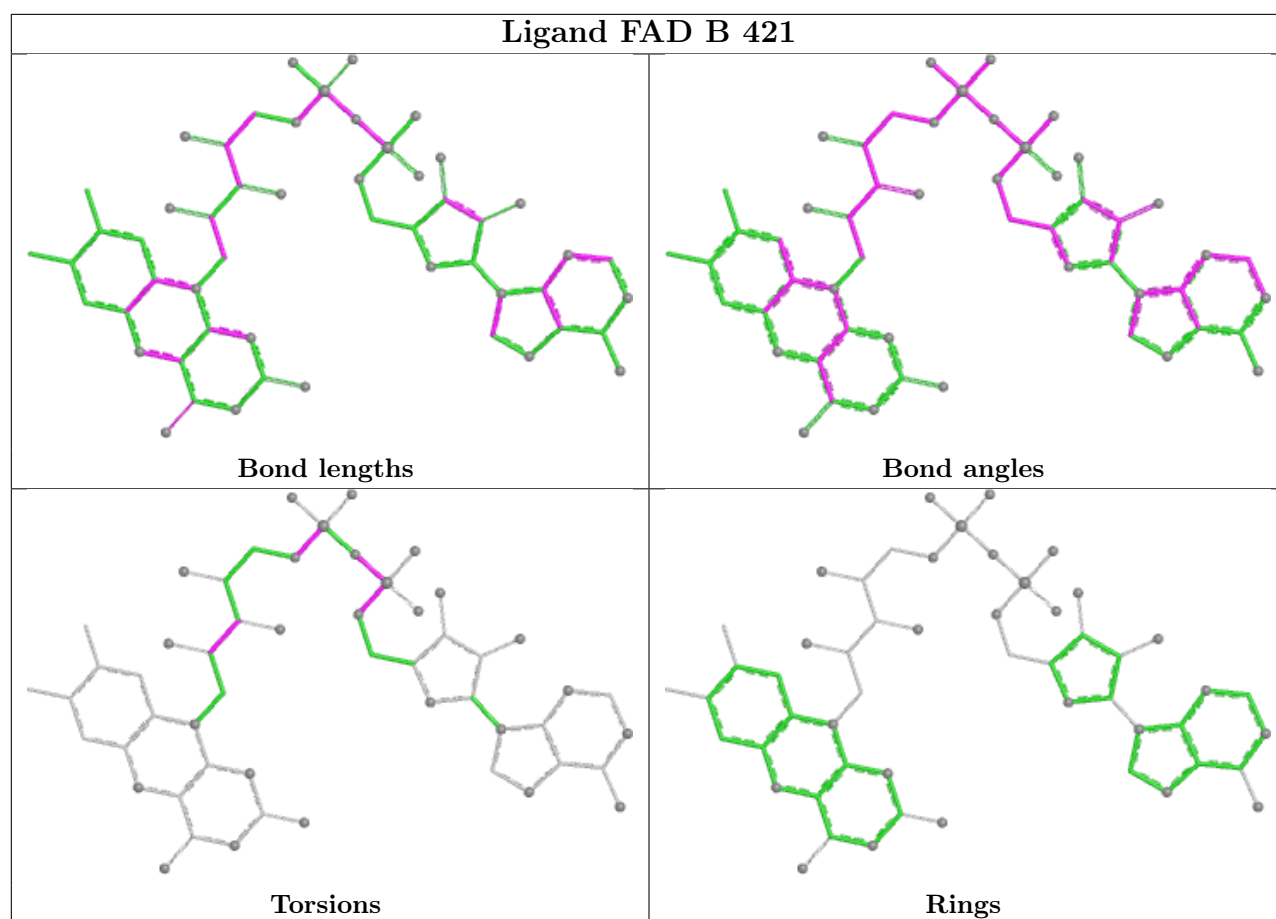
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	420	FAD	8	0
2	B	421	FAD	5	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	379/379 (100%)	-0.22	5 (1%) 75 71	21, 32, 48, 59	0
1	B	379/379 (100%)	-0.21	0 100 100	21, 32, 43, 53	0
All	All	758/758 (100%)	-0.21	5 (0%) 84 81	21, 32, 46, 59	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	ILE	3.4
1	A	176	ASP	3.0
1	A	410	ALA	2.8
1	A	35	SER	2.4
1	A	33	ASP	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

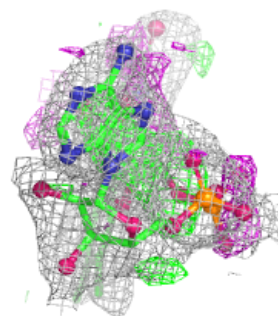
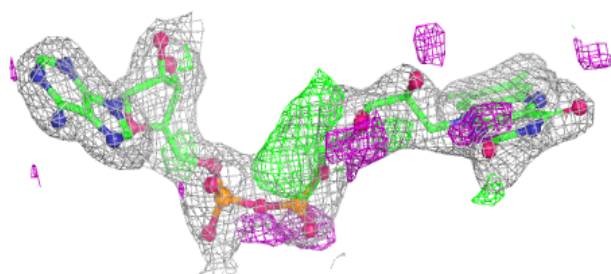
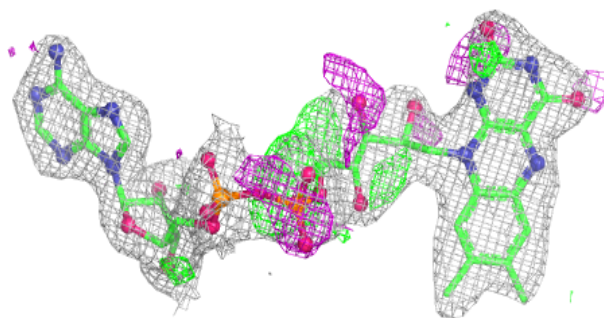
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

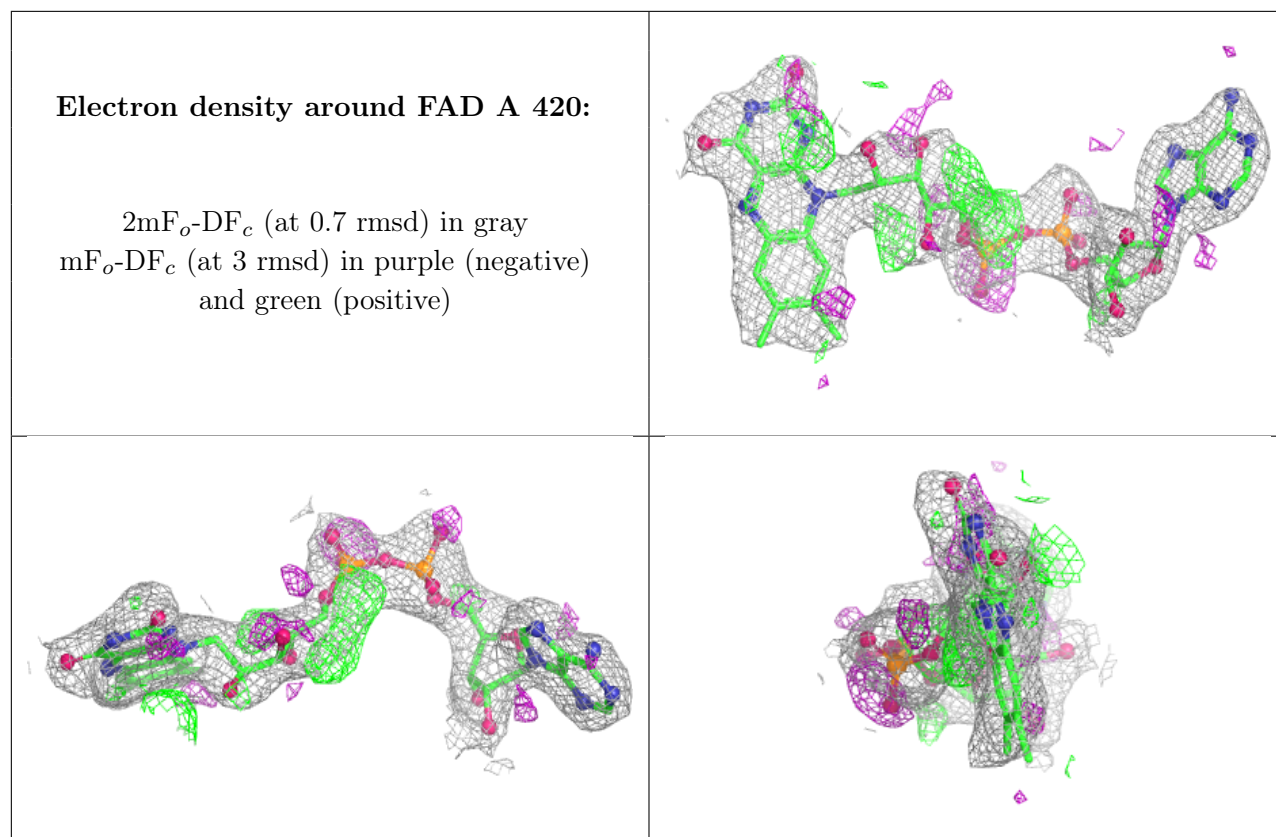
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	421	53/53	0.84	0.12	25,34,44,49	0
2	FAD	A	420	53/53	0.86	0.13	28,36,45,49	0
3	CO	B	411	1/1	0.97	0.04	55,55,55,55	0

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 FAD B 421:

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.