Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2023 – 05:50 pm BST

PDB ID	:	8CIW
Title	:	Methylsuccinyl-CoA dehydrogenase from Pseudomonas migulae with bound FAD and (2S)-methylsuccinyl-CoA
Authors	:	Zarzycki, J.; McLean, R.; Erb, T.J.
Deposited on	:	2023-02-10
Resolution	:	1.93 Å(reported)

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

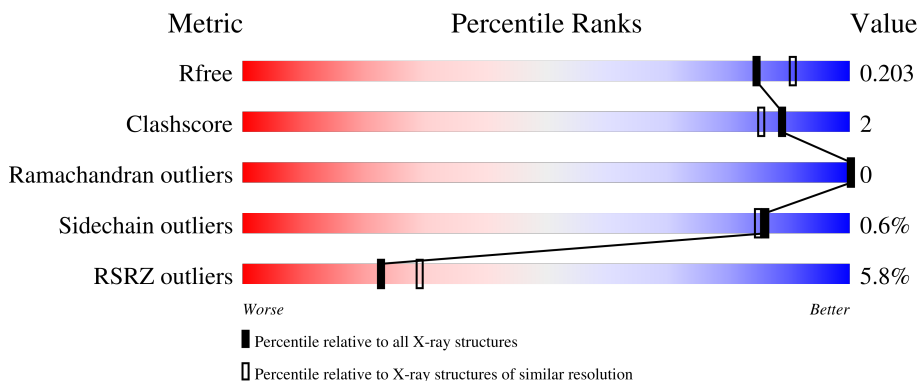|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	Percentile Ranks	Value
Rfree		0.203
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		5.8%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	7% / 95% / 5%
1	B	555	5% / 95% / 5%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 9225 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 (2S)-methylsuccinyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4185	2631	740	792	22			
1	B	555	Total	C	N	O	S	0	0	0
			4185	2631	740	792	22			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).


FAD

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 (2S)-Methylsuccinyl-CoA (three-letter code: ZKK) (formula: $C_{26}H_{42}N_7O_{19}P_3S$) (labeled as "Ligand of Interest" by depositor).
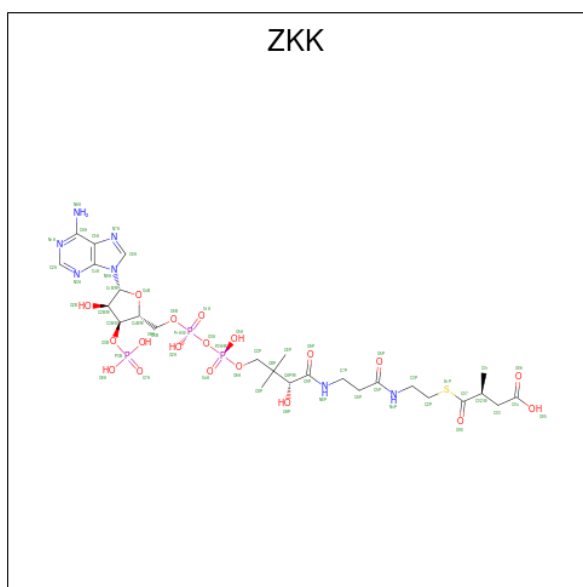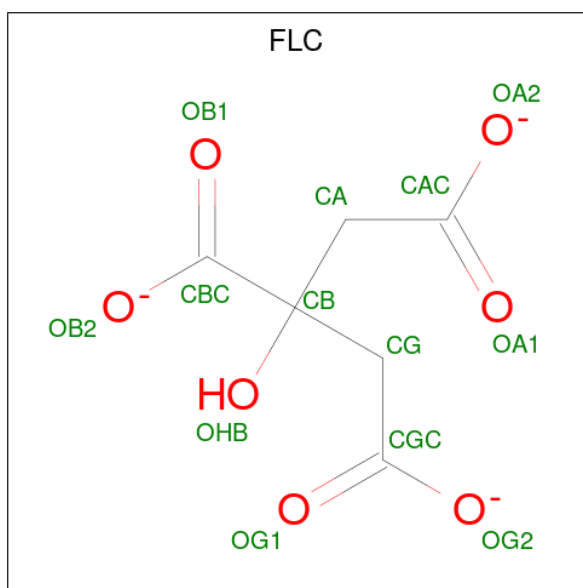
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).
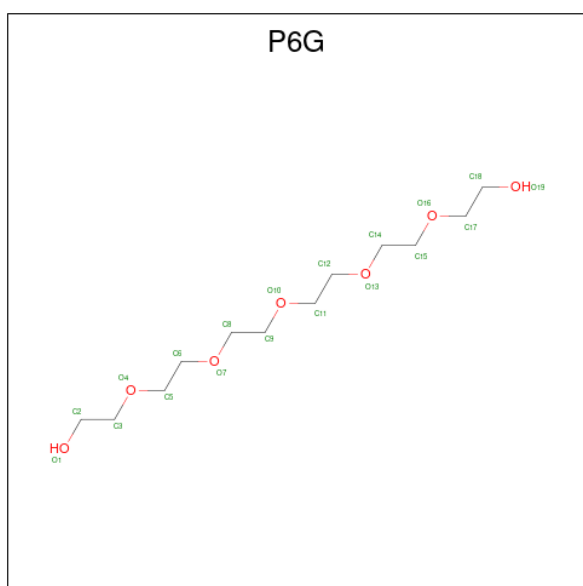
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 13	C 6	O 7	0	0

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
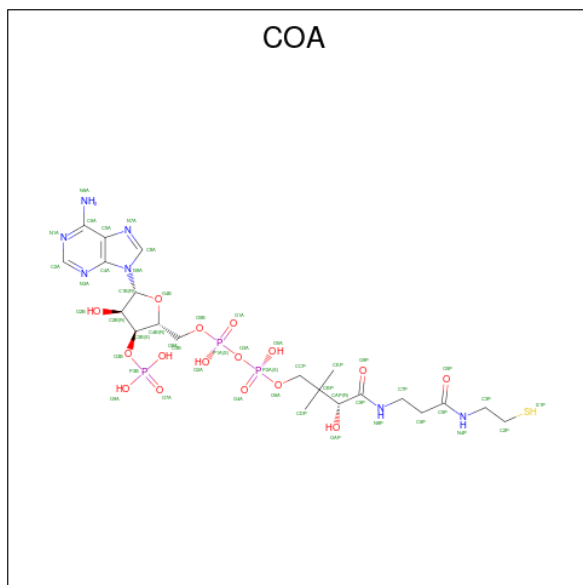
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	272	Total 272	O 272	0	0
7	B	295	Total 295	O 295	0	0

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: (2S)-methylsuccinyl-CoA dehydrogenase
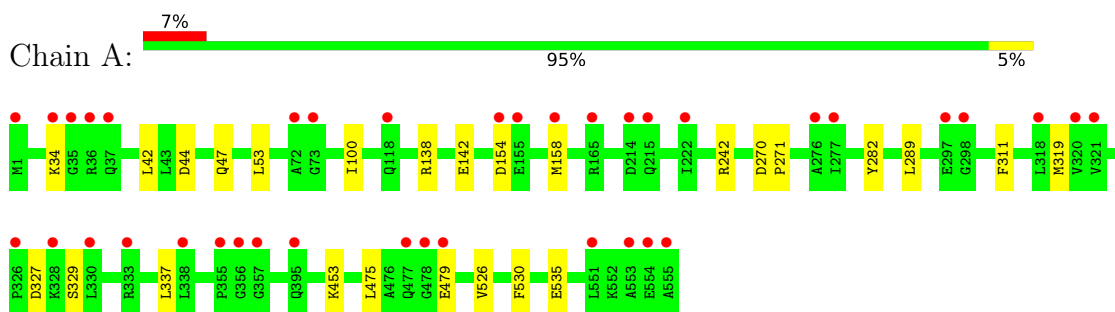
• Molecule 1: (2S)-methylsuccinyl-CoA dehydrogenase
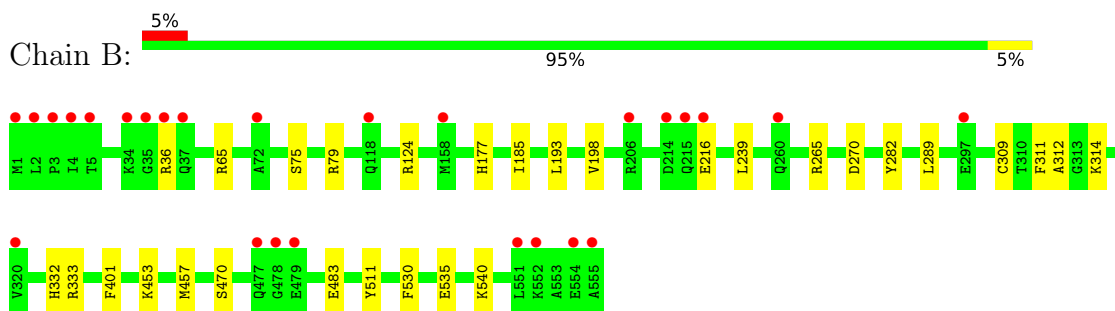
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.81Å 169.56Å 118.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.01 – 1.93 25.01 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.01-1.93) 99.7 (25.01-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.93Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.174 , 0.203 0.174 , 0.203	Depositor DCC
R_{free} test set	1997 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.864	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9225	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5　Model quality ⓘ

5.1　Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA, P6G, FAD, FLC, ZKK

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	0.43	0/4252	0.63	0/5751
1	B	0.44	0/4252	0.63	0/5751
All	All	0.44	0/8504	0.63	0/11502

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 ⓘ

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	4185	0	4230	13	0
1	B	4185	0	4230	20	0
2	A	53	0	30	1	0
2	B	53	0	30	1	0
3	A	56	0	0	0	0
3	B	56	0	0	0	0
4	A	13	0	16	0	0
4	B	13	0	16	0	0
5	B	13	0	5	0	0
6	B	31	0	11	0	0
7	A	272	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	295	0	0	7	0
All	All	9225	0	8568	32	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 (32) 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:216:GLU:N	1:B:216:GLU:OE1	2.35	0.60
1:B:282:TYR:HB2	1:B:289:LEU:HD23	1.89	0.55
1:B:314:LYS:HE2	7:B:751:HOH:O	2.07	0.54
1:B:75:SER:O	1:B:79:ARG:HG3	2.08	0.54
1:B:332:HIS:HB2	1:B:401:PHE:CG	2.45	0.51
1:A:453:LYS:NZ	7:A:703:HOH:O	2.30	0.50
1:B:124:ARG:NH2	7:B:707:HOH:O	2.45	0.50
1:B:483:GLU:HG3	7:B:844:HOH:O	2.13	0.48
1:B:270:ASP:HB2	7:B:790:HOH:O	2.14	0.48
1:B:193:LEU:HD22	1:B:198:VAL:HG21	1.97	0.47
1:A:44:ASP:O	1:A:47:GLN:HG3	2.15	0.46
1:B:177:HIS:HB3	7:B:924:HOH:O	2.16	0.46
1:A:138:ARG:O	1:A:142:GLU:HG3	2.16	0.45
1:A:475:LEU:HD23	1:A:479:GLU:O	2.17	0.45
1:A:535:GLU:HB2	2:A:601:FAD:O2B	2.17	0.44
1:A:53:LEU:HD23	1:A:100:ILE:HD13	2.00	0.43
1:B:65:ARG:HD2	1:B:470:SER:OG	2.18	0.43
1:B:333:ARG:HD3	7:B:949:HOH:O	2.17	0.43
1:B:265:ARG:HB3	1:B:270:ASP:O	2.19	0.43
1:A:526:VAL:HB	1:B:511:TYR:CZ	2.54	0.43
1:B:185:ILE:CD1	1:B:239:LEU:HD21	2.48	0.43
1:A:154:ASP:O	1:A:158:MET:HG2	2.19	0.43
1:A:34:LYS:HD3	1:A:42:LEU:HD11	2.02	0.42
1:B:453:LYS:O	1:B:457:MET:HG3	2.20	0.42
1:B:535:GLU:HB2	2:B:603:FAD:O2B	2.20	0.42
1:A:282:TYR:HB2	1:A:289:LEU:HD23	2.02	0.41
1:A:327:ASP:OD1	1:A:329:SER:HB3	2.21	0.41
1:A:270:ASP:HA	1:A:271:PRO:HA	1.84	0.41
1:A:319:MET:HG2	1:A:337:LEU:HD22	2.02	0.41
1:B:36:ARG:HG2	1:B:36:ARG:HH21	1.86	0.41
1:B:540:LYS:HE3	7:B:895:HOH:O	2.21	0.40
1:B:309:CYS:SG	1:B:312:ALA:HB2	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/555 (100%)	543 (98%)	10 (2%)	0	100	100
1	B	553/555 (100%)	544 (98%)	9 (2%)	0	100	100
All	All	1106/1110 (100%)	1087 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/429 (100%)	426 (99%)	3 (1%)	84	81
1	B	429/429 (100%)	427 (100%)	2 (0%)	88	88
All	All	858/858 (100%)	853 (99%)	5 (1%)	86	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	ARG
1	A	311	PHE
1	A	530	PHE
1	B	311	PHE
1	B	530	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 ⓘ

8 ligands are modelled in this entry.

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	$\#|Z| > 2$
3	ZKK	B	604	-	49,58,58	1.98	15 (30%)	59,86,86	1.34	7 (11%)
4	P6G	A	603	-	12,12,18	0.13	0	11,11,17	0.17	0
2	FAD	B	603	-	53,58,58	2.34	16 (30%)	68,89,89	1.67	13 (19%)
6	COA	B	605	-	28,33,50	2.30	10 (35%)	35,52,75	1.68	8 (22%)
3	ZKK	A	602	-	49,58,58	1.99	15 (30%)	59,86,86	1.31	8 (13%)
4	P6G	B	602	-	12,12,18	0.11	0	11,11,17	0.16	0
5	FLC	B	601	-	12,12,12	1.10	2 (16%)	17,17,17	1.21	2 (11%)
2	FAD	A	601	-	53,58,58	2.32	16 (30%)	68,89,89	1.68	12 (17%)

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
3	ZKK	B	604	-	-	11/54/75/75	0/3/3/3
4	P6G	A	603	-	-	1/10/10/16	-
2	FAD	B	603	-	-	1/30/50/50	0/6/6/6
6	COA	B	605	-	-	4/17/37/64	0/3/3/3
3	ZKK	A	602	-	-	12/54/75/75	0/3/3/3
4	P6G	B	602	-	-	0/10/10/16	-
5	FLC	B	601	-	-	2/16/16/16	-
2	FAD	A	601	-	-	0/30/50/50	0/6/6/6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	605	COA	O4B-C1B	7.26	1.51	1.41
2	B	603	FAD	C4X-N5	7.17	1.44	1.30
2	A	601	FAD	C4X-N5	7.09	1.44	1.30
2	B	603	FAD	C10-N1	5.80	1.45	1.33
2	A	601	FAD	C10-N1	5.74	1.45	1.33
3	A	602	ZKK	C9P-N8P	5.48	1.45	1.33
3	B	604	ZKK	C9P-N8P	5.48	1.45	1.33
3	A	602	ZKK	C5P-N4P	5.03	1.44	1.33
3	B	604	ZKK	C5P-N4P	5.00	1.44	1.33
2	A	601	FAD	C5X-N5	4.87	1.48	1.39
2	B	603	FAD	C5X-N5	4.78	1.48	1.39
2	B	603	FAD	C9A-N10	4.56	1.49	1.41
2	A	601	FAD	C9A-N10	4.41	1.48	1.41
3	A	602	ZKK	O4B-C1B	4.36	1.47	1.41
2	B	603	FAD	C2-N1	4.35	1.47	1.36
2	A	601	FAD	C2-N1	4.24	1.46	1.36
3	B	604	ZKK	O4B-C1B	4.14	1.46	1.41
2	B	603	FAD	C2-N3	4.07	1.48	1.39
2	A	601	FAD	C2-N3	4.05	1.48	1.39
2	A	601	FAD	O2-C2	-3.60	1.17	1.24
2	A	601	FAD	C4-N3	3.47	1.45	1.38
6	B	605	COA	P2A-O6A	3.44	1.68	1.54
2	B	603	FAD	O3B-C3B	-3.44	1.34	1.43
2	B	603	FAD	C4-N3	3.44	1.45	1.38
2	B	603	FAD	O2-C2	-3.43	1.17	1.24
2	B	603	FAD	C6A-N6A	3.36	1.46	1.34
2	A	601	FAD	C6A-N6A	3.31	1.46	1.34
6	B	605	COA	C6A-N6A	3.19	1.45	1.34
2	B	603	FAD	C10-N10	3.15	1.44	1.37
3	A	602	ZKK	C6A-N6A	3.14	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	605	COA	C2B-C1B	-3.13	1.49	1.53
2	A	601	FAD	O4-C4	-3.13	1.17	1.23
2	A	601	FAD	O3B-C3B	-3.11	1.35	1.43
2	B	603	FAD	O4-C4	-3.11	1.17	1.23
3	B	604	ZKK	C6A-N6A	3.10	1.45	1.34
3	A	602	ZKK	C2B-C1B	-3.08	1.49	1.53
6	B	605	COA	P3B-O3B	3.07	1.65	1.59
2	A	601	FAD	C5A-C4A	-3.04	1.32	1.40
2	A	601	FAD	C10-N10	2.94	1.43	1.37
3	B	604	ZKK	C2B-C1B	-2.89	1.49	1.53
2	B	603	FAD	C5A-C4A	-2.89	1.33	1.40
3	B	604	ZKK	C2B-C3B	-2.78	1.46	1.52
3	A	602	ZKK	P3B-O3B	2.78	1.64	1.59
3	A	602	ZKK	C5A-N7A	2.74	1.49	1.39
3	B	604	ZKK	C5A-N7A	2.71	1.49	1.39
6	B	605	COA	C2B-C3B	-2.68	1.47	1.52
5	B	601	FLC	OG1-CGC	2.68	1.31	1.22
3	B	604	ZKK	P3B-O3B	2.65	1.64	1.59
3	B	604	ZKK	P3B-O8A	-2.63	1.44	1.54
3	A	602	ZKK	C2B-C3B	-2.63	1.47	1.52
2	A	601	FAD	O2B-C2B	2.62	1.49	1.43
3	B	604	ZKK	O5P-C5P	-2.61	1.18	1.23
3	B	604	ZKK	P3B-O9A	-2.60	1.44	1.54
2	B	603	FAD	O2B-C2B	2.59	1.49	1.43
3	A	602	ZKK	O5P-C5P	-2.54	1.18	1.23
3	A	602	ZKK	P3B-O9A	-2.53	1.45	1.54
3	A	602	ZKK	O9P-C9P	-2.52	1.18	1.23
3	A	602	ZKK	P3B-O8A	-2.48	1.45	1.54
5	B	601	FLC	OG2-CGC	-2.46	1.22	1.30
3	B	604	ZKK	O9P-C9P	-2.45	1.18	1.23
6	B	605	COA	O4B-C4B	2.38	1.50	1.45
3	B	604	ZKK	P2A-O5A	-2.28	1.44	1.55
3	A	602	ZKK	P2A-O5A	-2.26	1.44	1.55
2	B	603	FAD	O4'-C4'	-2.19	1.38	1.43
3	A	602	ZKK	P1A-O2A	-2.19	1.45	1.55
3	B	604	ZKK	P1A-O2A	-2.18	1.45	1.55
2	B	603	FAD	O2'-C2'	-2.15	1.38	1.43
3	A	602	ZKK	C4A-N3A	-2.14	1.32	1.35
6	B	605	COA	P3B-O9A	-2.13	1.46	1.54
6	B	605	COA	C4A-N3A	-2.11	1.32	1.35
3	B	604	ZKK	C4A-N3A	-2.11	1.32	1.35
6	B	605	COA	P2A-O5A	-2.10	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O4'-C4'	-2.09	1.38	1.43
2	A	601	FAD	O2'-C2'	-2.09	1.38	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	N3A-C2A-N1A	-5.67	119.82	128.68
2	B	603	FAD	N3A-C2A-N1A	-5.57	119.97	128.68
2	A	601	FAD	C7M-C7-C6	-5.36	109.58	119.49
2	B	603	FAD	C7M-C7-C6	-5.24	109.81	119.49
2	A	601	FAD	C7M-C7-C8	4.67	130.31	120.74
2	B	603	FAD	C7M-C7-C8	4.49	129.94	120.74
6	B	605	COA	C4A-C5A-N7A	-4.31	104.91	109.40
6	B	605	COA	N3A-C2A-N1A	-4.08	122.31	128.68
2	A	601	FAD	C4X-C10-N10	3.77	121.99	116.48
2	B	603	FAD	C4X-C10-N10	3.61	121.75	116.48
5	B	601	FLC	OG1-CGC-CG	-3.54	112.60	122.94
3	B	604	ZKK	O08-C07-S1P	-3.49	119.11	123.80
3	A	602	ZKK	O08-C07-S1P	-3.34	119.30	123.80
3	B	604	ZKK	C6P-C7P-N8P	-3.15	105.54	111.90
5	B	601	FLC	OG2-CGC-CG	3.09	124.28	114.35
2	B	603	FAD	C4-N3-C2	-3.04	120.03	125.64
2	A	601	FAD	C4-N3-C2	-3.03	120.04	125.64
6	B	605	COA	P1A-O3A-P2A	-3.01	122.51	132.83
3	A	602	ZKK	C1B-N9A-C4A	-2.85	121.64	126.64
3	B	604	ZKK	C1B-N9A-C4A	-2.85	121.64	126.64
2	A	601	FAD	P-O3P-PA	-2.79	123.26	132.83
6	B	605	COA	C1B-N9A-C4A	-2.74	121.83	126.64
2	B	603	FAD	C5X-C9A-N10	2.73	120.77	117.95
2	B	603	FAD	P-O3P-PA	-2.72	123.48	132.83
2	B	603	FAD	C9A-N10-C10	-2.72	116.53	120.77
2	A	601	FAD	C9A-N10-C10	-2.70	116.56	120.77
2	A	601	FAD	C5X-C9A-N10	2.61	120.65	117.95
2	B	603	FAD	C4X-C4-N3	2.61	119.81	113.19
2	A	601	FAD	C4X-C4-N3	2.47	119.47	113.19
3	A	602	ZKK	C2A-N1A-C6A	-2.44	114.57	118.75
3	B	604	ZKK	C2A-N1A-C6A	-2.44	114.59	118.75
2	B	603	FAD	C10-N1-C2	2.42	121.74	116.90
3	A	602	ZKK	C4A-C5A-N7A	-2.42	106.88	109.40
2	B	603	FAD	O4-C4-C4X	-2.42	120.19	126.60
3	B	604	ZKK	P1A-O3A-P2A	-2.40	124.61	132.83
3	A	602	ZKK	P1A-O3A-P2A	-2.37	124.69	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	O4-C4-C4X	-2.37	120.32	126.60
6	B	605	COA	O5A-P2A-O4A	-2.30	101.67	110.68
3	B	604	ZKK	C4A-C5A-N7A	-2.28	107.03	109.40
6	B	605	COA	O2A-P1A-O1A	-2.26	101.05	112.24
6	B	605	COA	O8A-P3B-O7A	-2.19	102.11	110.68
2	B	603	FAD	C10-C4X-N5	-2.18	120.23	124.86
3	A	602	ZKK	C6P-C7P-N8P	-2.18	107.50	111.90
3	A	602	ZKK	O2A-P1A-O1A	-2.16	101.56	112.24
6	B	605	COA	O8A-P3B-O3B	2.12	115.47	105.99
2	A	601	FAD	C10-C4X-N5	-2.11	120.38	124.86
3	B	604	ZKK	O2A-P1A-O1A	-2.10	101.86	112.24
3	A	602	ZKK	O8A-P3B-O3B	2.08	115.33	105.99
2	B	603	FAD	C4X-C10-N1	-2.03	120.01	124.73
2	A	601	FAD	C10-N1-C2	2.01	120.91	116.90

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ZKK	N8P-C9P-CAP-OAP
3	A	602	ZKK	C5B-O5B-P1A-O3A
3	A	602	ZKK	C5B-O5B-P1A-O2A
3	B	604	ZKK	N8P-C9P-CAP-OAP
3	B	604	ZKK	O9P-C9P-CAP-OAP
3	B	604	ZKK	C5B-O5B-P1A-O3A
3	B	604	ZKK	C3B-O3B-P3B-O9A
6	B	605	COA	C5B-O5B-P1A-O3A
6	B	605	COA	P1A-O3A-P2A-O6A
3	A	602	ZKK	O9P-C9P-CAP-OAP
6	B	605	COA	P1A-O3A-P2A-O4A
3	B	604	ZKK	S1P-C2P-C3P-N4P
3	A	602	ZKK	C3B-O3B-P3B-O7A
3	B	604	ZKK	C9P-CAP-CBP-CDP
3	A	602	ZKK	C3B-O3B-P3B-O9A
3	A	602	ZKK	C5B-O5B-P1A-O1A
3	B	604	ZKK	C5B-O5B-P1A-O2A
6	B	605	COA	C5B-O5B-P1A-O1A
3	B	604	ZKK	C9P-CAP-CBP-CCP
3	B	604	ZKK	OAP-CAP-CBP-CCP
3	B	604	ZKK	OAP-CAP-CBP-CEP
3	A	602	ZKK	C2P-C3P-N4P-C5P
5	B	601	FLC	CB-CG-CGC-OG2

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Mol	Chain	Res	Type	Atoms
5	B	601	FLC	CB-CG-CGC-OG1
3	A	602	ZKK	S1P-C2P-C3P-N4P
4	A	603	P6G	C5-C6-O7-C8
3	A	602	ZKK	C9P-CAP-CBP-CDP
3	B	604	ZKK	C9P-CAP-CBP-CEP
3	A	602	ZKK	OAP-CAP-CBP-CEP
3	A	602	ZKK	C9P-CAP-CBP-CCP
2	B	603	FAD	C2'-C1'-N10-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	FAD	1	0
2	A	601	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ZKK B 604

Bond lengths

Bond angles

Torsions

Rings

Ligand P6G A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 603

Bond lengths

Bond angles

Torsions

Rings

Ligand COA B 605

Bond lengths

Bond angles

Torsions

Rings

Ligand ZKK A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 601

Bond lengths

Bond angles

Torsions

Rings
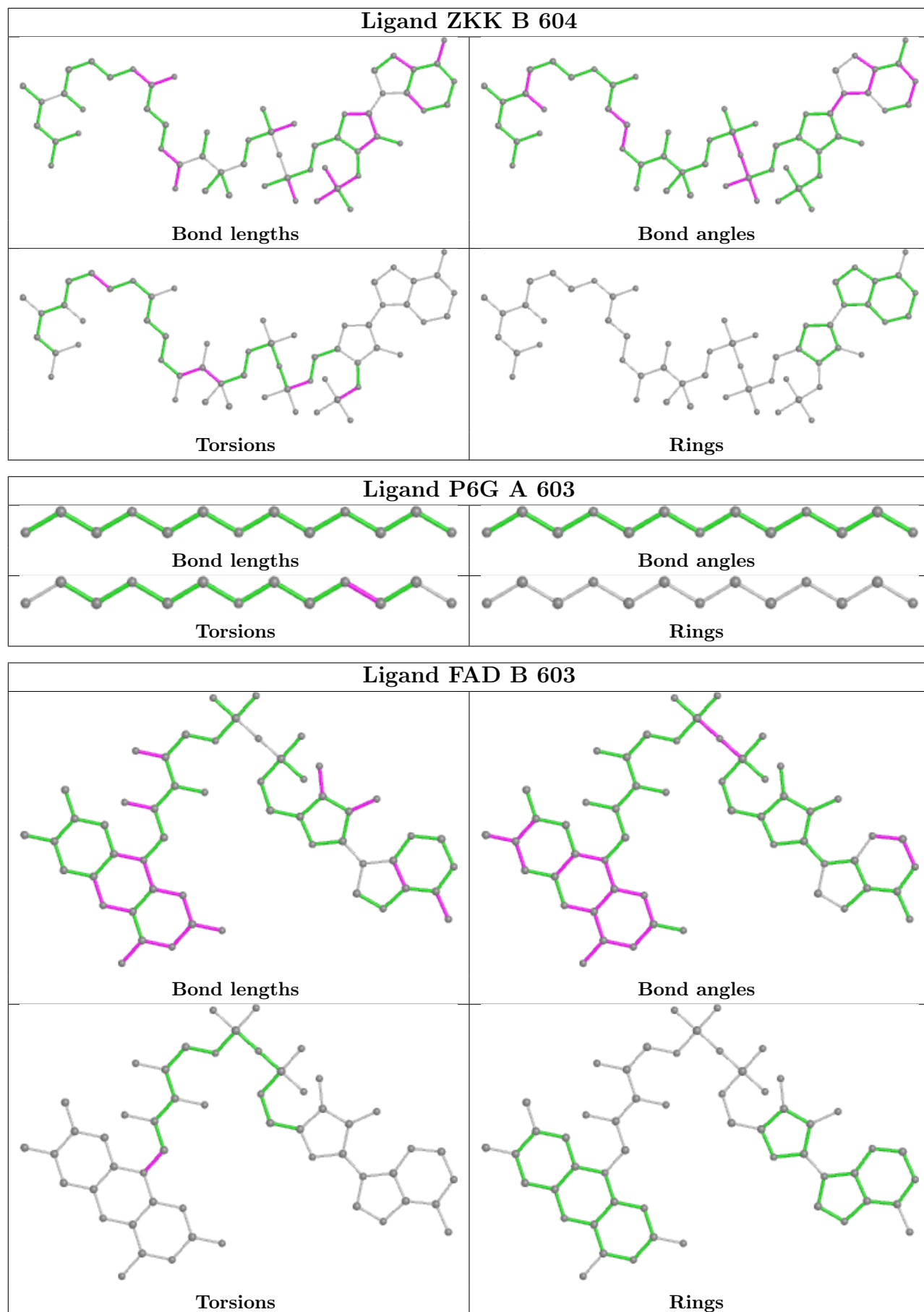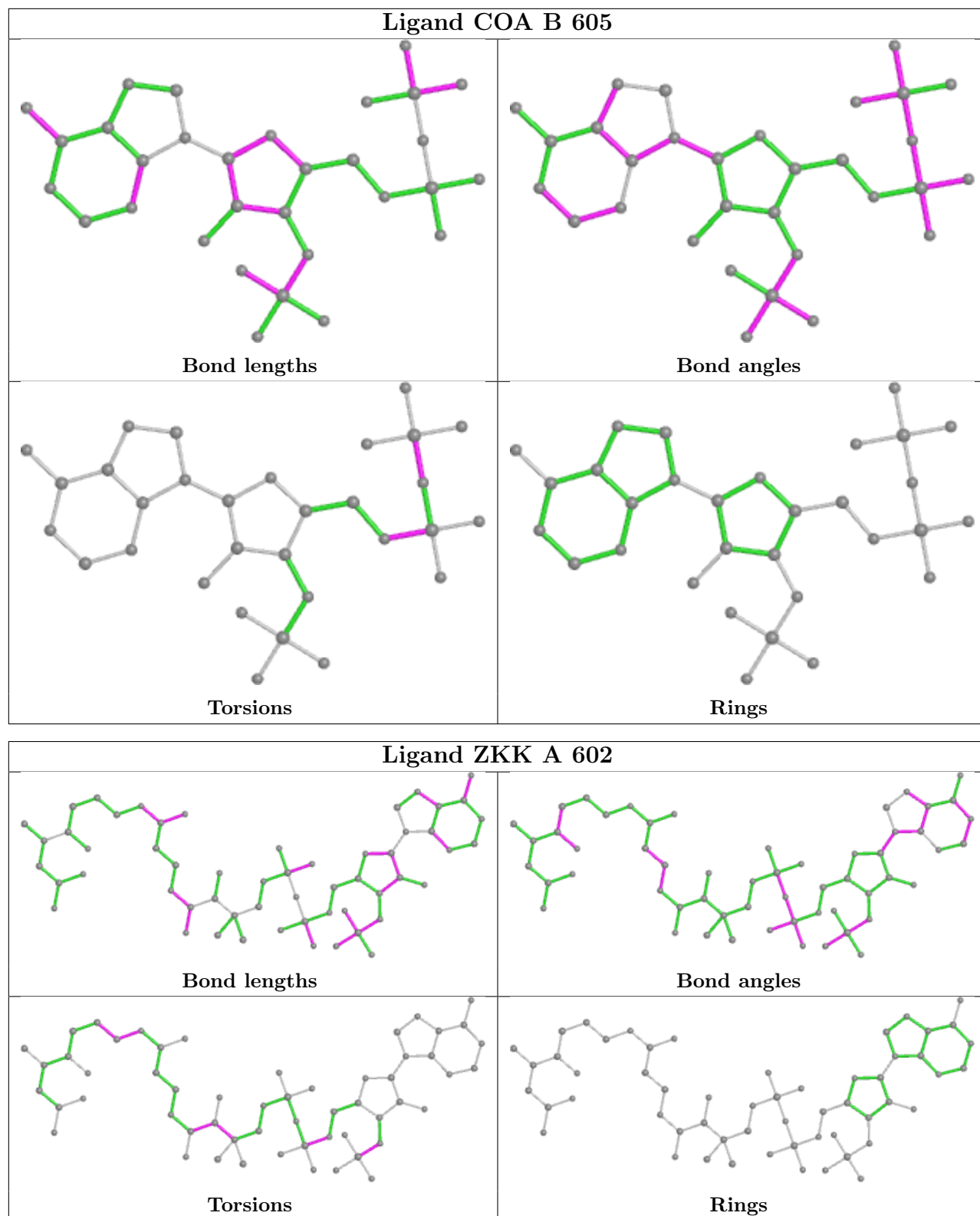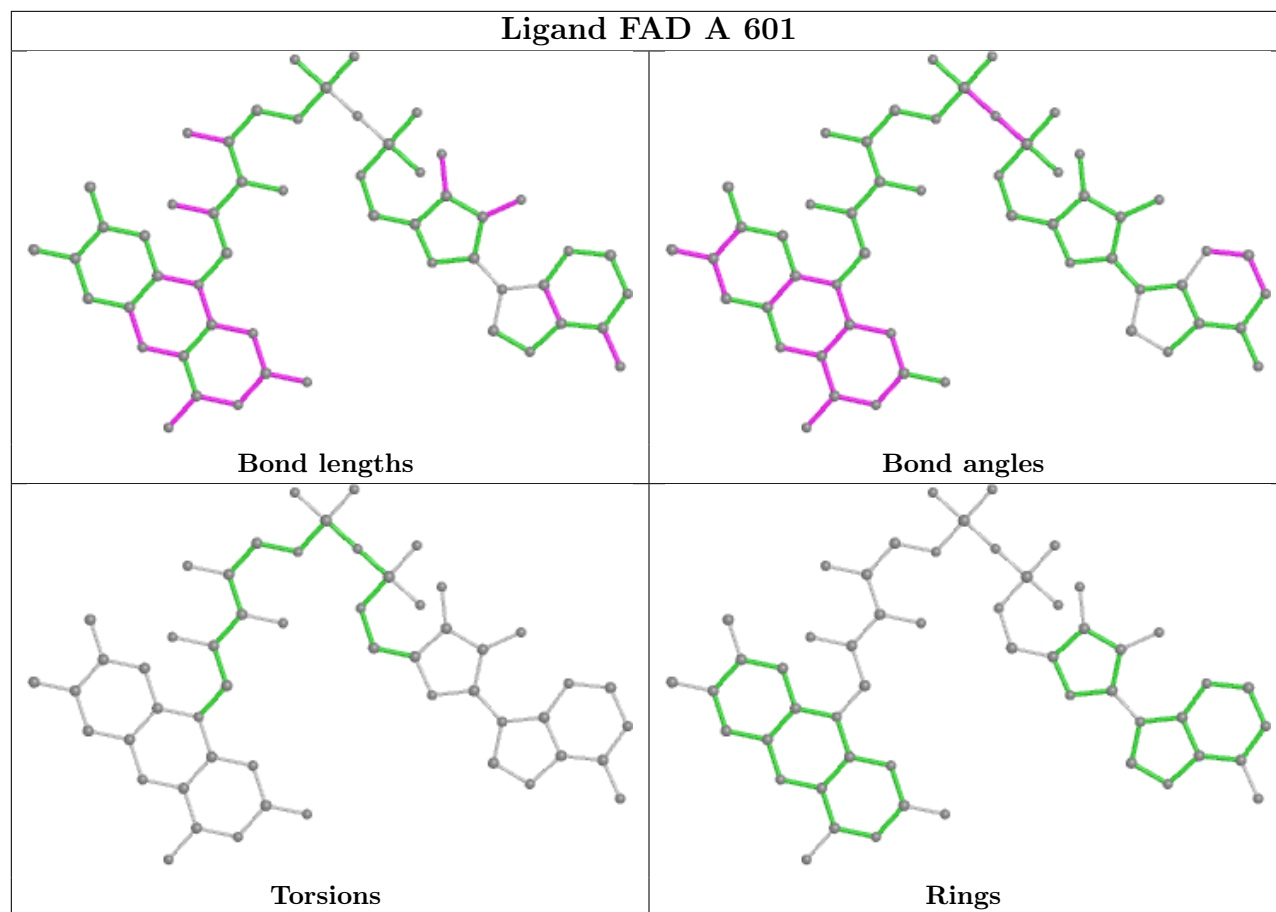
5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	555/555 (100%)	0.33	38 (6%)	17	23	24, 39, 59, 90	0
1	B	555/555 (100%)	0.19	26 (4%)	31	39	24, 36, 57, 89	0
All	All	1110/1110 (100%)	0.26	64 (5%)	23	29	24, 38, 58, 90	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	ALA	6.9
1	B	4	ILE	6.8
1	A	555	ALA	6.7
1	B	36	ARG	6.6
1	B	1	MET	6.5
1	B	2	LEU	5.4
1	A	36	ARG	4.9
1	B	3	PRO	4.7
1	A	35	GLY	4.7
1	B	35	GLY	4.5
1	B	37	GLN	4.3
1	A	72	ALA	4.3
1	A	356	GLY	4.2
1	A	154	ASP	4.1
1	A	320	VAL	4.0
1	A	553	ALA	3.9
1	B	215	GLN	3.8
1	A	330	LEU	3.8
1	A	158	MET	3.7
1	B	118	GLN	3.6
1	A	328	LYS	3.5
1	A	477	GLN	3.4
1	A	297	GLU	3.4
1	B	297	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	338	LEU	3.3
1	A	318	LEU	3.3
1	A	165	ARG	3.2
1	A	214	ASP	3.2
1	B	478	GLY	3.2
1	A	554	GLU	3.1
1	A	357	GLY	3.1
1	A	298	GLY	3.1
1	B	260	GLN	3.0
1	A	73	GLY	3.0
1	A	155	GLU	3.0
1	B	216	GLU	3.0
1	A	478	GLY	2.9
1	B	158	MET	2.9
1	B	479	GLU	2.9
1	A	276	ALA	2.9
1	B	552	LYS	2.9
1	A	277	ILE	2.8
1	A	395	GLN	2.8
1	B	5	THR	2.8
1	A	355	PRO	2.8
1	A	479	GLU	2.8
1	B	214	ASP	2.7
1	A	551	LEU	2.7
1	B	477	GLN	2.7
1	B	554	GLU	2.7
1	A	326	PRO	2.7
1	B	72	ALA	2.6
1	A	222	ILE	2.6
1	A	215	GLN	2.6
1	B	34	LYS	2.5
1	A	321	VAL	2.5
1	A	1	MET	2.5
1	A	37	GLN	2.5
1	A	118	GLN	2.4
1	B	551	LEU	2.2
1	B	320	VAL	2.2
1	A	34	LYS	2.1
1	A	333	ARG	2.0
1	B	206	ARG	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
6	COA	B	605	31/48	0.83	0.20	38,55,70,75	31
4	P6G	A	603	13/19	0.86	0.12	58,63,67,67	0
5	FLC	B	601	13/13	0.88	0.14	32,34,36,40	13
4	P6G	B	602	13/19	0.88	0.17	60,64,68,68	0
3	ZKK	B	604	56/56	0.91	0.13	29,39,49,51	0
3	ZKK	A	602	56/56	0.93	0.11	33,44,54,57	0
2	FAD	A	601	53/53	0.97	0.12	28,32,35,37	0
2	FAD	B	603	53/53	0.97	0.10	23,28,31,32	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 COA B 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
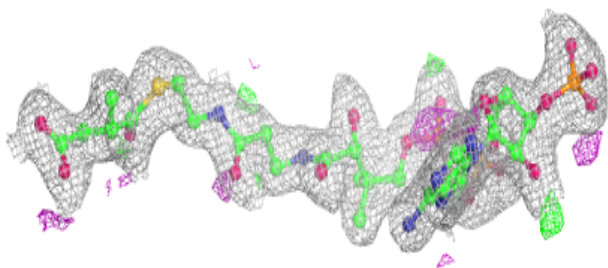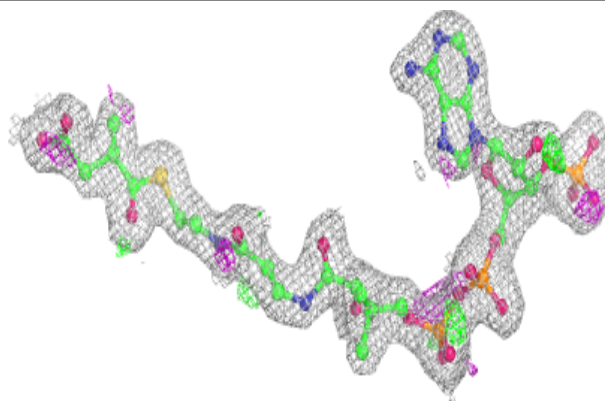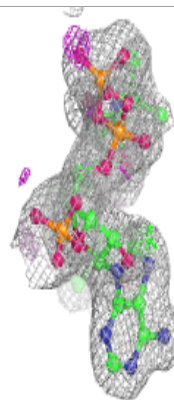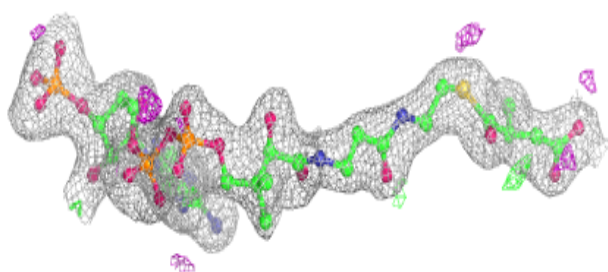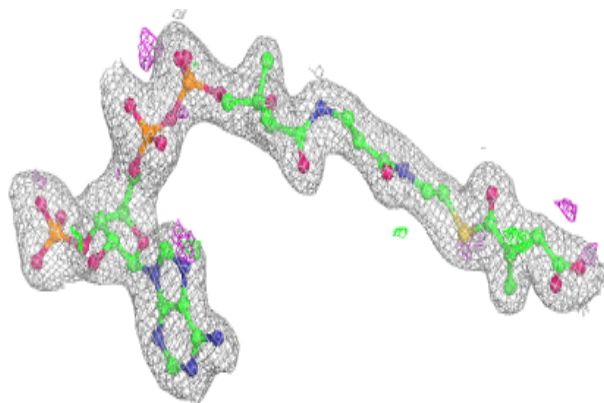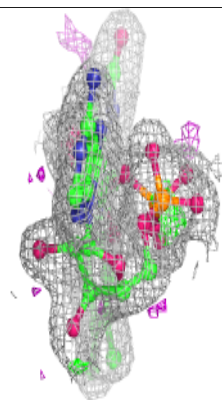and green (positive)
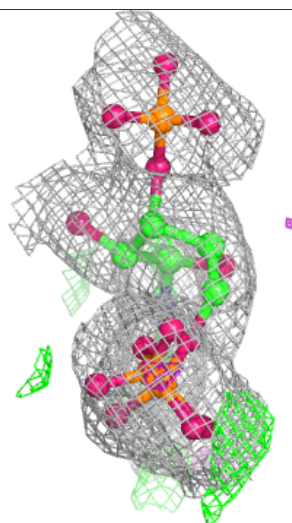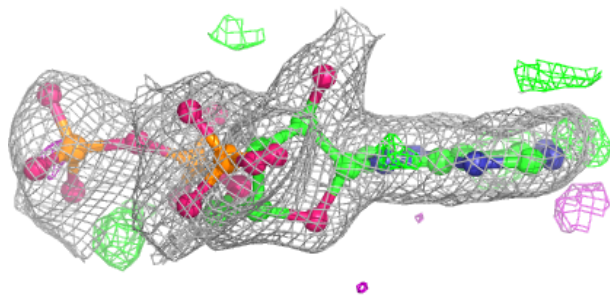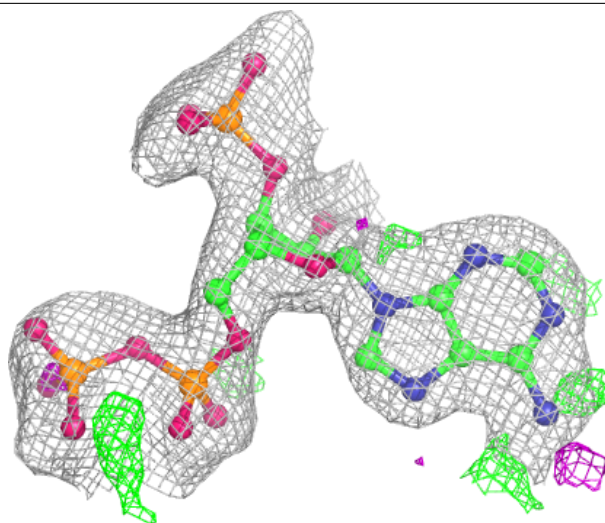
Electron density around P6G A 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
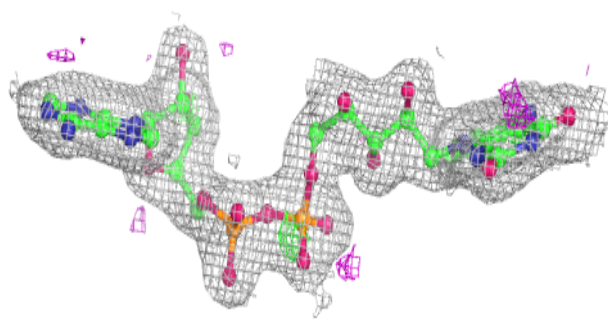and green (positive)
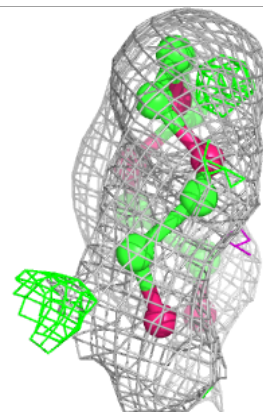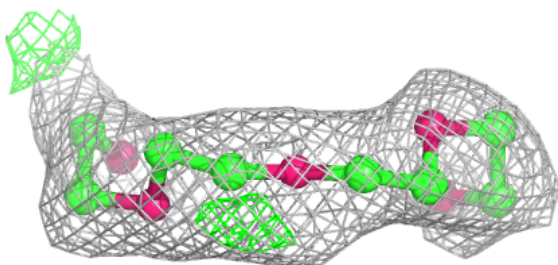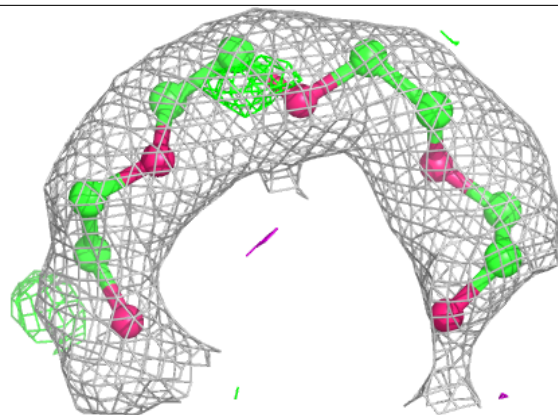
Electron density around ZKK B 604:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
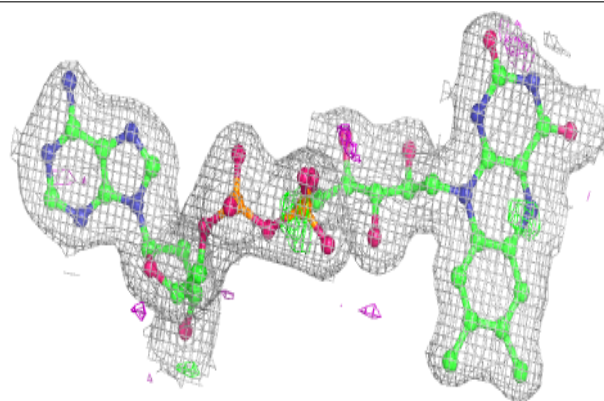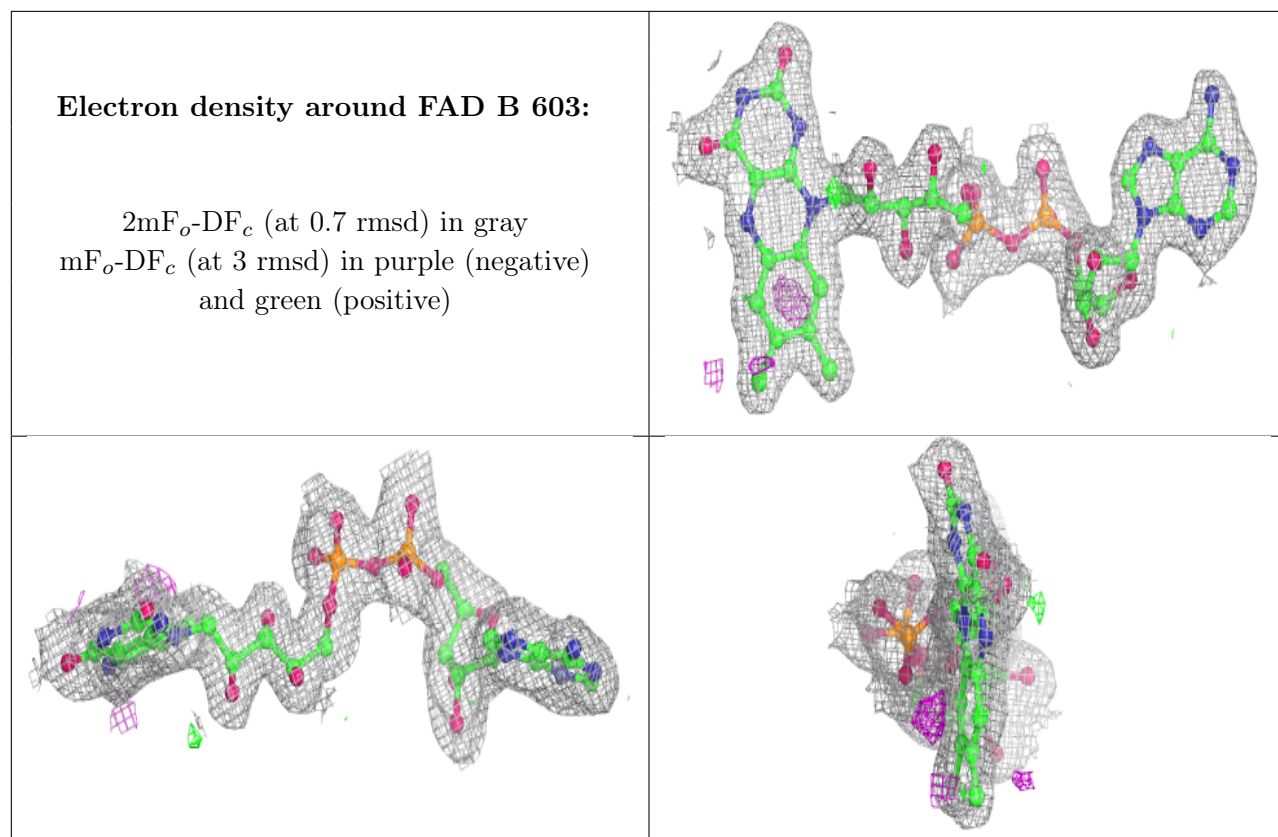and green (positive)
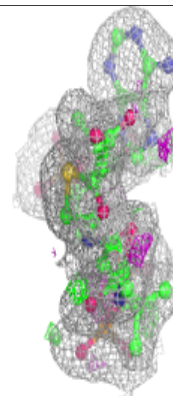
Electron density around ZKK A 602:

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

Electron density around FAD A 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 FAD B 603:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.