



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 09:40 PM EDT

PDB ID : 4EQS
Title : Crystal structure of the Y419F mutant of Staphylococcus aureus CoADR
Authors : Wallace, B.D.; Edwards, J.S.; Wallen, J.R.; Claiborne, A.; Redinbo, M.R.
Deposited on : 2012-04-19
Resolution : 1.50 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

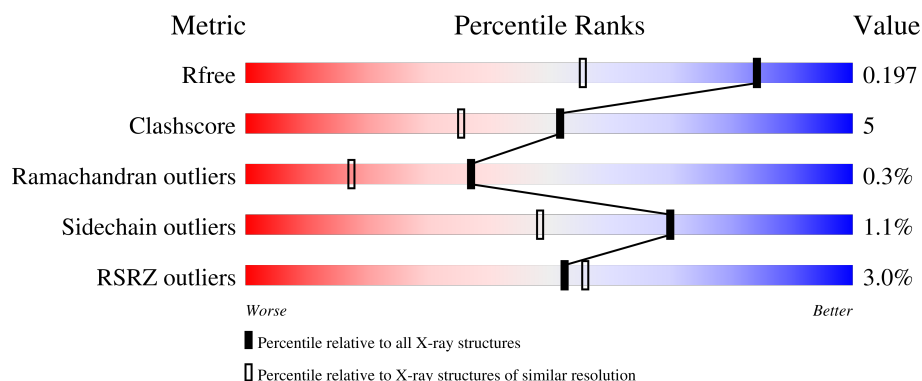
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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	437	 2% 92% 8%
1	B	437	 4% 90% 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8509 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 Coenzyme A disulfide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	8	0
			3496	2220	591	673	12			
1	B	437	Total	C	N	O	S	0	9	0
			3503	2226	593	672	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	PHE	TYR	engineered mutation	UNP Q2FIA5
B	419	PHE	TYR	engineered mutation	UNP Q2FIA5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

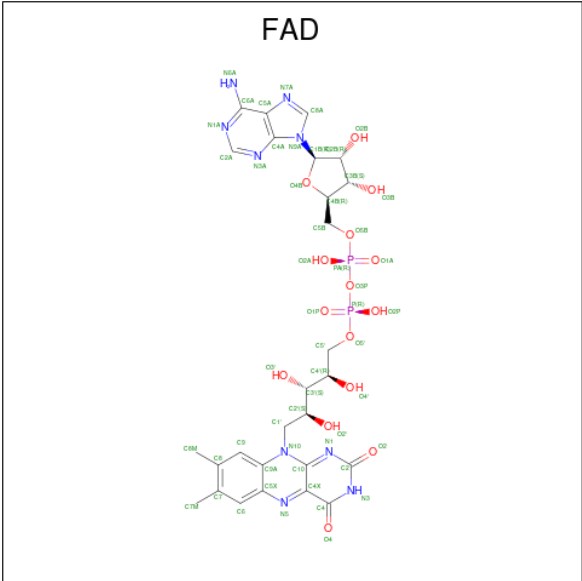
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	B	1	Total	C	N	O	P	S	0	1
			79	31	12	29	6	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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

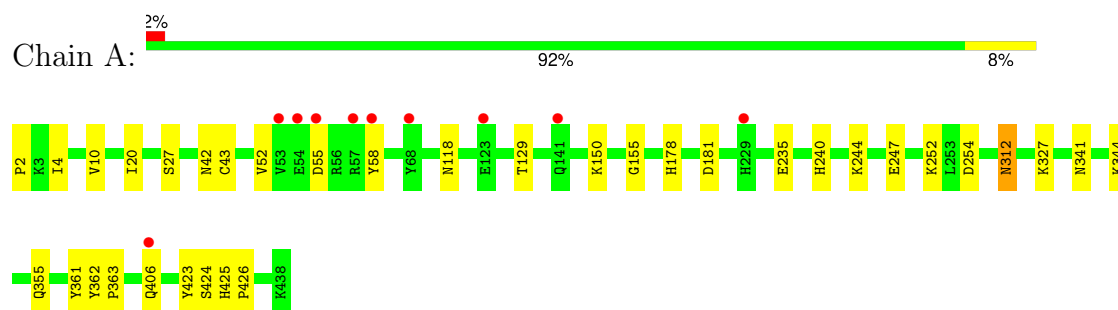
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	668	Total	O	0	0
			668	668		
6	B	600	Total	O	0	0
			600	600		

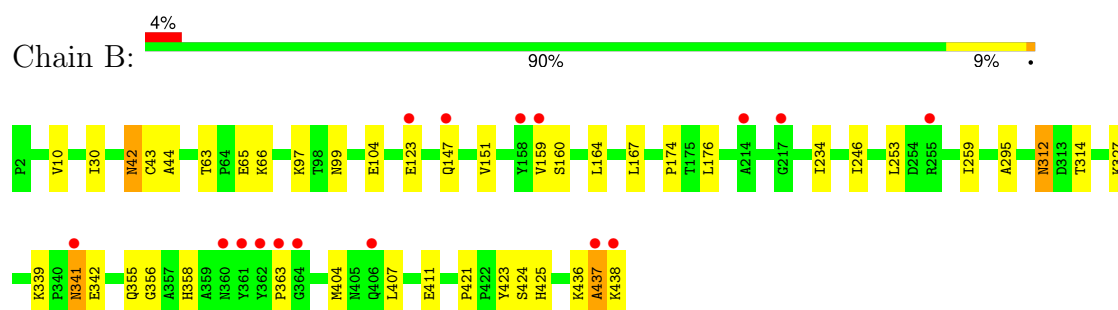
3 Residue-property plots

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: Coenzyme A disulfide reductase



- Molecule 1: Coenzyme A disulfide reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.18Å 65.42Å 94.57Å 90.00° 104.74° 90.00°	Depositor
Resolution (Å)	51.34 – 1.50 51.34 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (51.34-1.50) 95.4 (51.34-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.50Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.175 , 0.201 0.173 , 0.197	Depositor DCC
R_{free} test set	13234 reflections (9.65%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8509	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, MG, CL, COA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/3598	0.48	0/4871
1	B	0.27	0/3609	0.48	0/4886
All	All	0.27	0/7207	0.48	0/9757

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3496	0	3450	30	0
1	B	3503	0	3462	43	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	1	0
3	B	2	0	0	0	0
4	A	48	0	31	1	0
4	B	79	0	26	1	0
5	A	53	0	30	1	0
5	B	53	0	30	2	0
6	A	668	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	600	0	0	7	0
All	All	8509	0	7029	70	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 (70) 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:30[A]:ILE:HD11	1:B:104:GLU:HG2	1.65	0.77
1:A:129:THR:HG22	1:A:235[A]:GLU:HG3	1.67	0.77
1:B:356:GLY:O	1:B:425[B]:HIS:HE1	1.74	0.71
1:A:2:PRO:N	1:A:27:SER:HG	1.94	0.66
1:B:42:ASN:ND2	1:B:42:ASN:H	1.95	0.65
1:B:65[A]:GLU:HG3	6:B:2156:HOH:O	1.99	0.62
1:B:355:GLN:HG3	6:B:2367:HOH:O	1.99	0.62
1:A:118:ASN:OD1	1:A:240:HIS:HD2	1.83	0.62
1:A:424:SER:O	1:A:425[B]:HIS:HD2	1.83	0.61
1:B:424:SER:O	1:B:425[A]:HIS:HD2	1.84	0.61
1:B:159:VAL:HG22	6:B:2176:HOH:O	2.00	0.61
1:B:42:ASN:H	1:B:42:ASN:HD22	1.48	0.59
1:A:240:HIS:HE1	6:A:854:HOH:O	1.85	0.59
1:B:312:ASN:C	1:B:312:ASN:HD22	2.06	0.59
1:B:30[A]:ILE:CD1	1:B:104:GLU:HG2	2.31	0.58
1:B:97:LYS:HG3	6:B:2385:HOH:O	2.05	0.56
1:B:159:VAL:HG23	1:B:160:SER:N	2.22	0.55
1:A:43:CYS:SG	5:A:507:FAD:C4X	2.95	0.55
1:B:147:GLN:HG3	6:B:2699:HOH:O	2.05	0.55
1:B:43:CYS:SG	5:B:2006:FAD:C4X	2.96	0.54
6:A:831:HOH:O	1:B:404:MET:HG3	2.08	0.53
1:B:312:ASN:ND2	1:B:314:THR:H	2.07	0.53
1:A:129:THR:CG2	1:A:235[A]:GLU:HG3	2.37	0.52
1:A:4[A]:ILE:HD13	1:A:20:ILE:HD13	1.92	0.51
1:B:159:VAL:HG23	1:B:160:SER:H	1.75	0.51
1:A:312:ASN:HD22	1:A:312:ASN:C	2.14	0.51
1:A:362:TYR:OH	1:B:327:LYS:HE2	2.10	0.50
1:B:341:ASN:ND2	1:B:342:GLU:HG3	2.26	0.50
1:B:164:LEU:CD1	1:B:176:LEU:HB2	2.43	0.48
1:B:312:ASN:HD22	1:B:314:THR:H	1.61	0.48
1:A:355:GLN:HE21	1:A:425[B]:HIS:CE1	2.31	0.48
1:B:339:LYS:HB2	1:B:341:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LYS:HB2	6:B:2692:HOH:O	2.13	0.47
1:B:246:ILE:HD13	1:B:259:ILE:HD11	1.96	0.47
1:B:63:THR:H	1:B:66:LYS:HE3	1.80	0.46
1:A:327:LYS:HB2	1:B:423:TYR:OH	2.17	0.45
1:A:355:GLN:NE2	1:A:425[B]:HIS:ND1	2.64	0.45
1:A:355:GLN:HG3	6:A:731:HOH:O	2.16	0.45
1:A:52:VAL:HG13	1:B:363:PRO:HG2	1.99	0.44
1:A:55:ASP:O	1:A:58:TYR:HB2	2.17	0.44
1:A:362:TYR:HA	1:A:363:PRO:HD3	1.88	0.43
1:A:252:LYS:C	1:A:252:LYS:HD3	2.39	0.43
1:A:423:TYR:OH	1:B:327:LYS:HB2	2.19	0.43
1:A:244:LYS:HG2	6:A:1180:HOH:O	2.19	0.43
1:B:425[B]:HIS:HD2	6:B:2426:HOH:O	2.00	0.43
1:A:252:LYS:HZ3	1:A:254:ASP:HA	1.84	0.42
1:A:406:GLN:HG3	6:A:922:HOH:O	2.18	0.42
1:A:150:LYS:HE2	1:A:150:LYS:HB3	1.81	0.42
1:B:253:LEU:HD23	1:B:259:ILE:HG12	2.01	0.42
1:A:252:LYS:NZ	1:A:254:ASP:HA	2.35	0.42
1:A:244:LYS:HD2	1:A:247:GLU:OE2	2.19	0.42
3:A:503:CL:CL	4:A:506:COA:H21	2.57	0.41
1:A:155:GLY:HA2	1:A:178:HIS:HD2	1.85	0.41
1:B:151:VAL:O	1:B:174:PRO:HA	2.20	0.41
1:A:344:LYS:HD3	6:A:1053:HOH:O	2.20	0.41
1:B:123:GLU:O	1:B:123:GLU:HG3	2.20	0.41
1:B:355:GLN:OE1	1:B:425[A]:HIS:ND1	2.53	0.41
1:B:407:LEU:HG	1:B:411:GLU:HB2	2.03	0.41
1:B:164:LEU:C	1:B:164:LEU:HD23	2.41	0.41
1:B:358:HIS:HB2	1:B:421:PRO:O	2.20	0.41
1:B:436:LYS:O	1:B:437:ALA:O	2.38	0.41
1:A:424:SER:O	1:A:425[B]:HIS:CD2	2.69	0.41
1:B:43:CYS:SG	5:B:2006:FAD:C10	3.09	0.40
1:A:361:TYR:CZ	1:B:44:ALA:HB2	2.56	0.40
1:B:167:LEU:HD11	1:B:234[A]:ILE:HD12	2.02	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	443/437 (101%)	430 (97%)	12 (3%)	1 (0%)	44	22
1	B	444/437 (102%)	434 (98%)	8 (2%)	2 (0%)	25	8
All	All	887/874 (102%)	864 (97%)	20 (2%)	3 (0%)	37	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	437	ALA
1	A	10	VAL
1	B	10	VAL

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	384/376 (102%)	380 (99%)	4 (1%)	73	53
1	B	385/376 (102%)	381 (99%)	4 (1%)	73	53
All	All	769/752 (102%)	761 (99%)	8 (1%)	70	53

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	181	ASP
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	341	ASN
1	B	42	ASN
1	B	99	ASN
1	B	312	ASN
1	B	341	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	240	HIS
1	A	312	ASN
1	A	355	GLN
1	B	42	ASN
1	B	89	GLN
1	B	99	ASN
1	B	216	ASN
1	B	242	ASN
1	B	312	ASN
1	B	341	ASN

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 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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
4	COA	A	506	1	43,50,50	3.27	23 (53%)	56,75,75	1.46	7 (12%)
4	COA	B	2005[B]	-	43,50,50	3.46	24 (55%)	56,75,75	1.44	5 (8%)
5	FAD	A	507	-	54,58,58	3.30	24 (44%)	71,89,89	1.66	11 (15%)
5	FAD	B	2006	-	54,58,58	3.44	23 (42%)	71,89,89	1.61	10 (14%)
4	COA	B	2005[A]	-	43,50,50	3.55	24 (55%)	56,75,75	1.49	7 (12%)

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
4	COA	A	506	1	-	6/44/64/64	0/3/3/3
4	COA	B	2005[B]	-	-	13/44/64/64	0/3/3/3
5	FAD	A	507	-	-	2/30/50/50	0/6/6/6
5	FAD	B	2006	-	-	4/30/50/50	0/6/6/6
4	COA	B	2005[A]	-	-	10/44/64/64	0/3/3/3

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2006	FAD	O2'-C2'	-11.73	1.18	1.43
5	A	507	FAD	O2'-C2'	-11.31	1.19	1.43
4	B	2005[A]	COA	P1A-O3A	9.34	1.69	1.59
4	B	2005[A]	COA	P2A-O3A	8.95	1.69	1.59
4	B	2005[B]	COA	P1A-O3A	8.62	1.68	1.59
4	B	2005[A]	COA	C2A-N3A	8.32	1.45	1.32
4	B	2005[B]	COA	C2A-N3A	8.30	1.44	1.32
4	B	2005[B]	COA	P2A-O3A	8.11	1.68	1.59
5	B	2006	FAD	O4-C4	8.07	1.38	1.23
4	A	506	COA	C2A-N3A	7.98	1.44	1.32
5	A	507	FAD	O4-C4	7.90	1.38	1.23
4	A	506	COA	P1A-O3A	7.75	1.67	1.59
4	A	506	COA	P2A-O3A	7.73	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2006	FAD	PA-O3P	7.00	1.67	1.59
5	A	507	FAD	PA-O3P	6.93	1.67	1.59
5	B	2006	FAD	O2-C2	6.45	1.37	1.24
4	A	506	COA	C9P-N8P	6.01	1.47	1.33
4	B	2005[A]	COA	C9P-N8P	5.91	1.47	1.33
4	B	2005[B]	COA	C9P-N8P	5.91	1.47	1.33
5	A	507	FAD	O2-C2	5.74	1.35	1.24
5	B	2006	FAD	C2A-N3A	5.51	1.40	1.32
4	B	2005[A]	COA	C5P-N4P	5.44	1.46	1.33
4	B	2005[B]	COA	C5P-N4P	5.44	1.46	1.33
5	B	2006	FAD	C9-C9A	5.40	1.48	1.39
5	B	2006	FAD	C6-C5X	5.38	1.48	1.40
5	A	507	FAD	C2A-N3A	5.31	1.40	1.32
5	B	2006	FAD	P-O3P	5.26	1.65	1.59
5	A	507	FAD	C6-C5X	5.25	1.48	1.40
5	A	507	FAD	P-O3P	5.23	1.65	1.59
4	B	2005[B]	COA	P3B-O7A	5.04	1.66	1.50
4	B	2005[A]	COA	O4B-C1B	5.00	1.47	1.40
4	A	506	COA	P3B-O7A	5.00	1.66	1.50
4	B	2005[A]	COA	P3B-O7A	5.00	1.66	1.50
4	A	506	COA	C5P-N4P	5.00	1.45	1.33
5	B	2006	FAD	C4X-N5	4.92	1.41	1.30
5	A	507	FAD	C4X-N5	4.84	1.41	1.30
4	B	2005[A]	COA	C2A-N1A	4.84	1.42	1.33
4	B	2005[B]	COA	C2A-N1A	4.83	1.42	1.33
5	A	507	FAD	C9-C9A	4.76	1.47	1.39
4	B	2005[B]	COA	O4B-C1B	4.59	1.46	1.40
4	A	506	COA	C2A-N1A	4.58	1.42	1.33
5	B	2006	FAD	PA-O1A	4.46	1.66	1.50
4	A	506	COA	O4B-C1B	4.44	1.46	1.40
4	B	2005[B]	COA	P2A-O4A	4.25	1.65	1.50
4	B	2005[B]	COA	P1A-O1A	4.22	1.65	1.50
4	B	2005[A]	COA	C4A-N3A	4.20	1.41	1.35
4	B	2005[B]	COA	C4A-N3A	4.19	1.41	1.35
5	B	2006	FAD	C9-C8	4.19	1.45	1.39
4	B	2005[B]	COA	P3B-O3B	4.16	1.66	1.59
4	B	2005[A]	COA	P2A-O4A	4.15	1.65	1.50
4	B	2005[A]	COA	P1A-O1A	4.12	1.65	1.50
5	B	2006	FAD	C2A-N1A	4.10	1.41	1.33
4	B	2005[A]	COA	P3B-O3B	4.07	1.66	1.59
4	A	506	COA	P1A-O1A	4.01	1.64	1.50
5	A	507	FAD	C9-C8	4.01	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	COA	C4A-N3A	3.98	1.41	1.35
5	B	2006	FAD	C6-C7	3.92	1.45	1.39
4	A	506	COA	P2A-O4A	3.92	1.64	1.50
5	A	507	FAD	C8A-N7A	3.88	1.41	1.34
5	A	507	FAD	PA-O1A	3.85	1.64	1.50
5	A	507	FAD	C2A-N1A	3.73	1.40	1.33
4	B	2005[B]	COA	C8A-N7A	3.70	1.41	1.34
5	B	2006	FAD	C8A-N7A	3.68	1.41	1.34
5	B	2006	FAD	P-O1P	3.62	1.63	1.50
5	A	507	FAD	P-O1P	3.59	1.63	1.50
4	A	506	COA	P3B-O3B	3.59	1.65	1.59
4	B	2005[A]	COA	C8A-N7A	3.56	1.41	1.34
4	B	2005[A]	COA	C6A-N6A	3.55	1.46	1.34
5	A	507	FAD	C6-C7	3.53	1.44	1.39
4	B	2005[B]	COA	C6A-N6A	3.52	1.46	1.34
4	A	506	COA	C6A-N6A	3.46	1.46	1.34
4	A	506	COA	C8A-N7A	3.42	1.41	1.34
5	B	2006	FAD	C10-N10	3.31	1.44	1.37
5	A	507	FAD	O4B-C1B	3.19	1.45	1.40
5	B	2006	FAD	C6A-N6A	3.17	1.45	1.34
5	B	2006	FAD	O4B-C1B	3.15	1.45	1.40
5	A	507	FAD	C6A-N6A	3.14	1.45	1.34
5	B	2006	FAD	C8-C7	2.99	1.48	1.40
4	B	2005[B]	COA	P3B-O8A	2.94	1.65	1.54
4	A	506	COA	P3B-O8A	2.91	1.65	1.54
4	B	2005[A]	COA	P3B-O8A	2.89	1.65	1.54
5	A	507	FAD	C8-C7	2.87	1.47	1.40
4	B	2005[B]	COA	O4B-C4B	2.83	1.51	1.45
4	B	2005[A]	COA	O4B-C4B	2.81	1.51	1.45
5	B	2006	FAD	C10-N1	2.77	1.38	1.33
5	B	2006	FAD	C9A-C5X	2.63	1.45	1.41
4	A	506	COA	O4B-C4B	2.61	1.50	1.45
5	A	507	FAD	C10-N10	2.58	1.42	1.37
5	A	507	FAD	C10-N1	2.58	1.38	1.33
4	B	2005[A]	COA	CCP-CBP	2.44	1.56	1.52
4	B	2005[B]	COA	CCP-CBP	2.44	1.56	1.52
5	A	507	FAD	C1'-C2'	2.38	1.56	1.52
4	B	2005[A]	COA	O5P-C5P	-2.33	1.18	1.23
4	B	2005[B]	COA	O5P-C5P	-2.33	1.18	1.23
4	B	2005[A]	COA	P1A-O5B	2.31	1.68	1.59
5	B	2006	FAD	C3B-C4B	2.30	1.58	1.53
4	B	2005[A]	COA	P2A-O6A	2.26	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	COA	P3B-O9A	-2.25	1.46	1.54
5	B	2006	FAD	C1'-C2'	2.24	1.55	1.52
4	B	2005[A]	COA	O9P-C9P	-2.23	1.19	1.23
4	B	2005[B]	COA	O9P-C9P	-2.23	1.19	1.23
5	A	507	FAD	C9A-C5X	2.22	1.44	1.41
4	B	2005[A]	COA	P3B-O9A	-2.21	1.46	1.54
4	B	2005[B]	COA	P3B-O9A	-2.15	1.46	1.54
5	A	507	FAD	C3B-C4B	2.15	1.58	1.53
4	B	2005[B]	COA	P1A-O5B	2.15	1.67	1.59
4	A	506	COA	O5P-C5P	-2.14	1.19	1.23
4	B	2005[B]	COA	P2A-O6A	2.14	1.67	1.59
4	A	506	COA	P1A-O5B	2.11	1.67	1.59
4	B	2005[B]	COA	P1A-O2A	-2.08	1.45	1.55
4	A	506	COA	P1A-O2A	-2.08	1.45	1.55
4	B	2005[A]	COA	P1A-O2A	-2.08	1.45	1.55
4	B	2005[B]	COA	C6A-N1A	2.04	1.44	1.36
4	B	2005[A]	COA	C6A-N1A	2.03	1.44	1.36
5	A	507	FAD	C4A-N3A	-2.03	1.32	1.35
4	A	506	COA	C2B-C3B	-2.02	1.48	1.53
4	A	506	COA	C6A-N1A	2.01	1.44	1.36
4	A	506	COA	O9P-C9P	-2.00	1.19	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	507	FAD	N3A-C2A-N1A	-6.61	119.70	128.67
4	B	2005[B]	COA	N3A-C2A-N1A	-6.37	120.02	128.67
4	B	2005[A]	COA	N3A-C2A-N1A	-6.22	120.23	128.67
4	A	506	COA	N3A-C2A-N1A	-6.17	120.30	128.67
5	B	2006	FAD	N3A-C2A-N1A	-5.86	120.72	128.67
5	B	2006	FAD	C4B-O4B-C1B	-5.24	105.13	109.92
5	A	507	FAD	C4B-O4B-C1B	-4.85	105.48	109.92
5	B	2006	FAD	O2'-C2'-C3'	4.80	120.48	109.25
5	A	507	FAD	O2'-C2'-C3'	4.76	120.40	109.25
4	B	2005[A]	COA	O6A-CCP-CBP	3.93	116.87	110.55
4	B	2005[B]	COA	O6A-CCP-CBP	3.36	115.94	110.55
4	B	2005[B]	COA	C4B-O4B-C1B	-3.11	107.07	109.92
4	A	506	COA	C3P-N4P-C5P	-3.09	117.08	122.82
5	A	507	FAD	C4-N3-C2	-3.08	120.18	125.64
4	A	506	COA	P3B-O3B-C3B	-2.93	115.60	123.43
4	B	2005[A]	COA	C4B-O4B-C1B	-2.82	107.34	109.92
5	B	2006	FAD	C4X-C10-N10	2.81	120.50	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	COA	C4B-O4B-C1B	-2.77	107.39	109.92
4	A	506	COA	O5P-C5P-N4P	-2.76	117.61	123.03
5	B	2006	FAD	C4-N3-C2	-2.69	120.86	125.64
5	A	507	FAD	C4X-C10-N10	2.67	120.31	116.48
5	B	2006	FAD	O4B-C1B-N9A	-2.66	105.22	108.75
4	B	2005[A]	COA	O5B-C5B-C4B	2.50	117.50	108.99
5	A	507	FAD	O4-C4-C4X	-2.39	120.23	126.53
5	A	507	FAD	C4X-C4-N3	2.38	119.30	113.25
4	B	2005[B]	COA	O3B-C3B-C2B	2.35	120.12	111.68
5	B	2006	FAD	C4X-C4-N3	2.35	119.22	113.25
4	B	2005[A]	COA	C7P-N8P-C9P	-2.28	118.44	122.55
4	B	2005[B]	COA	C7P-N8P-C9P	-2.28	118.44	122.55
5	A	507	FAD	O3'-C3'-C2'	2.26	114.07	108.93
4	B	2005[A]	COA	O2B-C2B-C3B	2.25	117.49	111.19
4	A	506	COA	O3A-P2A-O4A	-2.21	104.07	110.70
5	B	2006	FAD	O4-C4-C4X	-2.19	120.75	126.53
4	B	2005[A]	COA	O4B-C4B-C5B	2.13	116.16	109.33
5	B	2006	FAD	O2'-C2'-C1'	2.10	118.85	110.20
5	A	507	FAD	O2-C2-N1	-2.06	118.37	121.80
4	A	506	COA	O2B-C2B-C3B	2.06	116.95	111.19
5	B	2006	FAD	C4'-C3'-C2'	-2.06	110.15	113.57
5	A	507	FAD	C4'-C3'-C2'	-2.05	110.15	113.57
5	A	507	FAD	C10-C4X-N5	-2.05	120.63	124.81

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	COA	CCP-O6A-P2A-O4A
4	A	506	COA	C5P-C6P-C7P-N8P
4	A	506	COA	S1P-C2P-C3P-N4P
4	B	2005[A]	COA	CCP-O6A-P2A-O5A
4	B	2005[A]	COA	CDP-CBP-CCP-O6A
4	B	2005[A]	COA	CEP-CBP-CCP-O6A
4	B	2005[A]	COA	CAP-CBP-CCP-O6A
4	B	2005[A]	COA	S1P-C2P-C3P-N4P
4	B	2005[B]	COA	C2B-C3B-O3B-P3B
4	B	2005[B]	COA	C5B-O5B-P1A-O1A
4	B	2005[B]	COA	C5B-O5B-P1A-O3A
4	B	2005[B]	COA	P1A-O3A-P2A-O6A
4	B	2005[B]	COA	CBP-CCP-O6A-P2A
4	B	2005[B]	COA	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
5	A	507	FAD	C3B-C4B-C5B-O5B
5	A	507	FAD	O4B-C4B-C5B-O5B
5	B	2006	FAD	O4B-C4B-C5B-O5B
4	A	506	COA	P1A-O3A-P2A-O6A
4	B	2005[A]	COA	P2A-O3A-P1A-O2A
4	B	2005[B]	COA	CEP-CBP-CCP-O6A
5	B	2006	FAD	N10-C1'-C2'-O2'
4	A	506	COA	CCP-O6A-P2A-O3A
4	B	2005[A]	COA	CCP-O6A-P2A-O3A
4	B	2005[A]	COA	CCP-O6A-P2A-O4A
4	B	2005[B]	COA	C5B-O5B-P1A-O2A
4	B	2005[B]	COA	P2A-O3A-P1A-O2A
4	A	506	COA	C6P-C5P-N4P-C3P
4	B	2005[A]	COA	O5P-C5P-N4P-C3P
4	B	2005[B]	COA	O5P-C5P-N4P-C3P
4	B	2005[A]	COA	C3B-O3B-P3B-O7A
5	B	2006	FAD	O2'-C2'-C3'-C4'
4	B	2005[B]	COA	P2A-O3A-P1A-O1A
5	B	2006	FAD	C3B-C4B-C5B-O5B
4	B	2005[B]	COA	C3B-O3B-P3B-O8A
4	B	2005[B]	COA	CDP-CBP-CCP-O6A

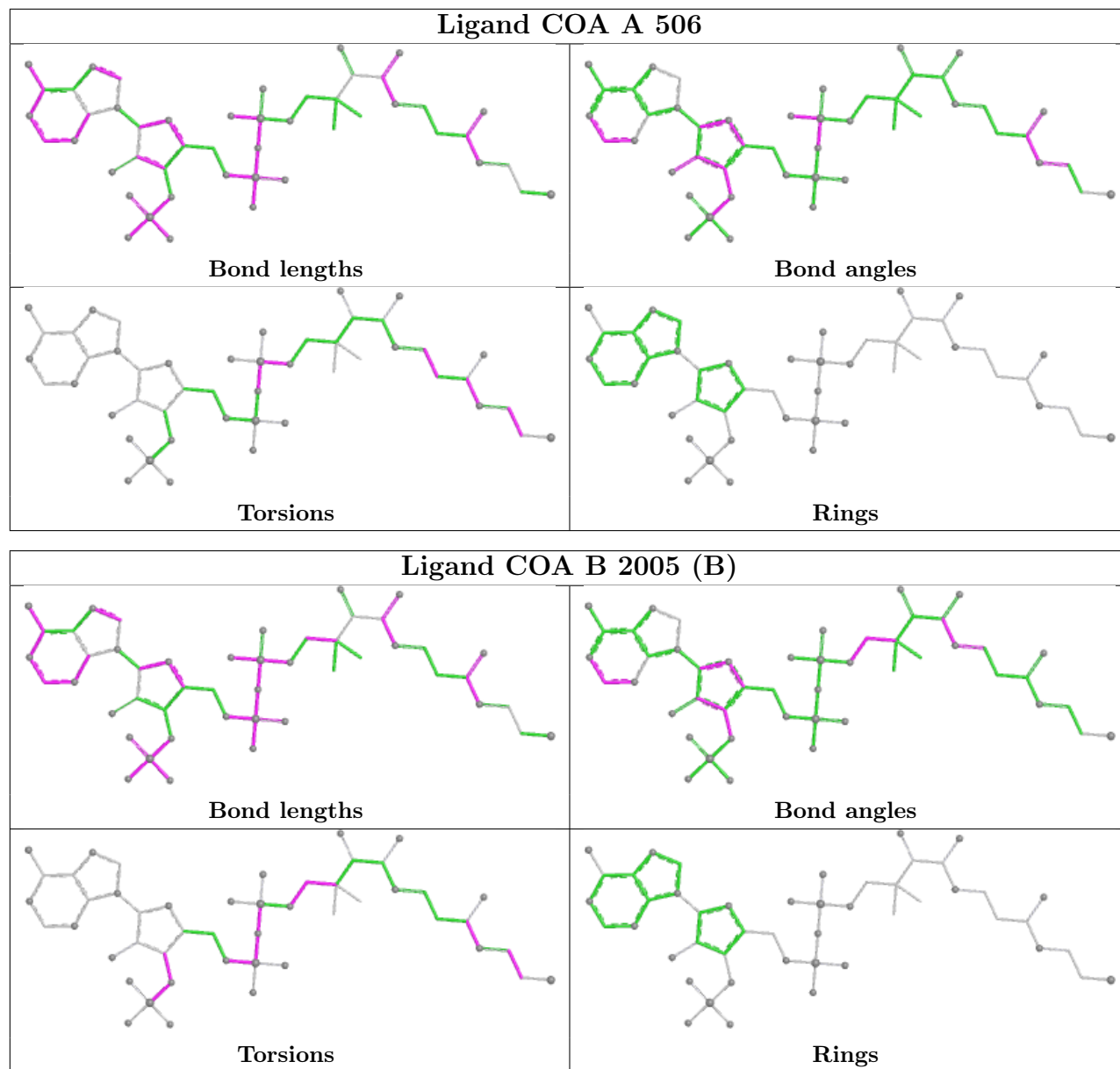
There are no ring outliers.

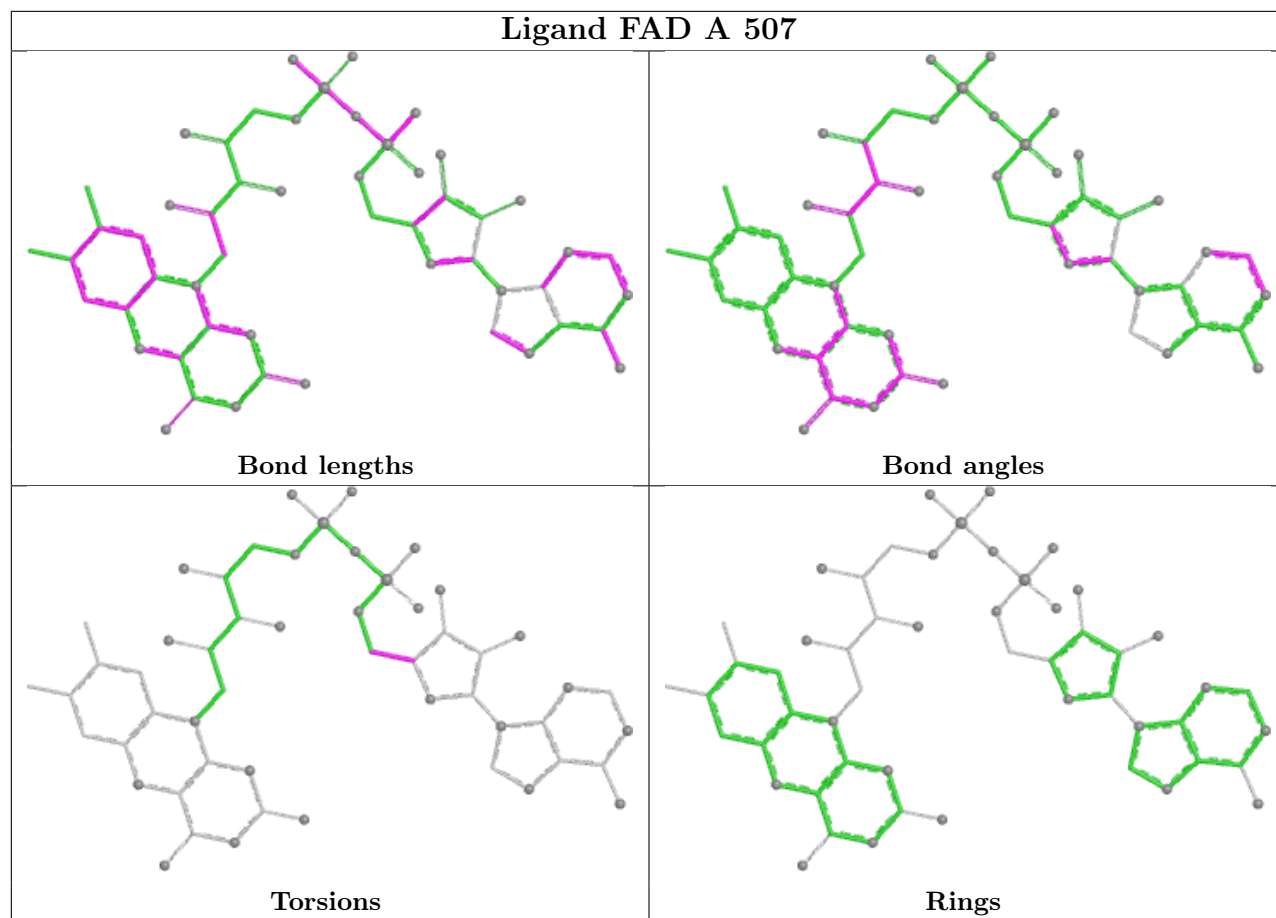
4 monomers are involved in 5 short contacts:

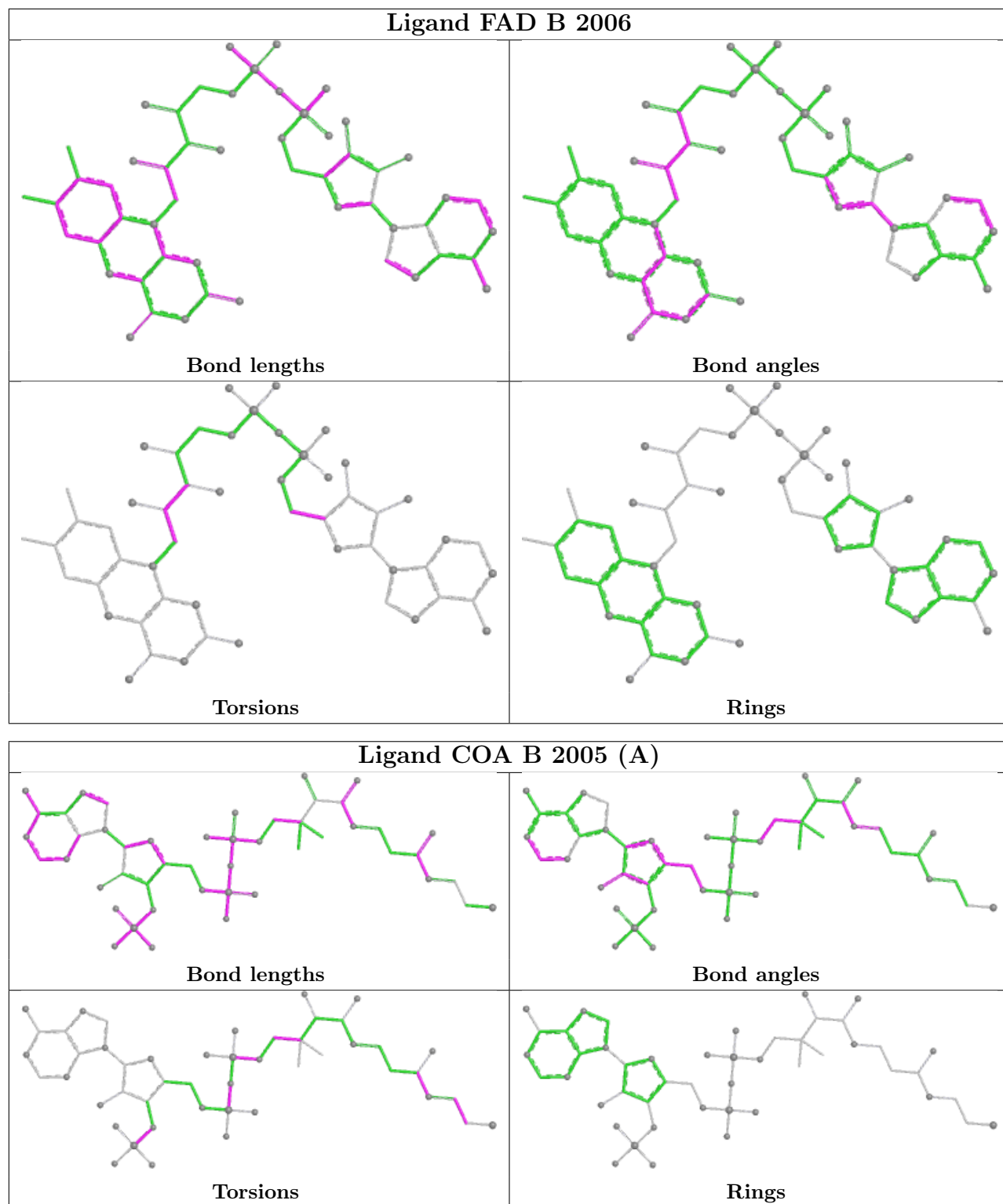
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	COA	1	0
4	B	2005[B]	COA	1	0
5	A	507	FAD	1	0
5	B	2006	FAD	2	0

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 ⓘ

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	437/437 (100%)	0.02	10 (2%) 61 64	11, 17, 32, 56	8 (1%)
1	B	437/437 (100%)	0.16	16 (3%) 45 49	11, 20, 32, 55	9 (2%)
All	All	874/874 (100%)	0.09	26 (2%) 52 56	11, 18, 32, 56	17 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	VAL	4.3
1	B	437	ALA	4.1
1	B	363	PRO	3.9
1	B	360	ASN	3.6
1	B	438	LYS	3.2
1	A	68	TYR	3.1
1	B	147	GLN	3.1
1	A	54	GLU	2.9
1	A	229	HIS	2.9
1	A	58	TYR	2.9
1	A	57	ARG	2.9
1	B	364	GLY	2.8
1	B	341	ASN	2.8
1	B	362	TYR	2.7
1	B	361	TYR	2.6
1	B	406	GLN	2.6
1	A	53	VAL	2.5
1	A	141	GLN	2.4
1	B	123	GLU	2.4
1	B	158	TYR	2.3
1	B	214	ALA	2.2
1	A	406	GLN	2.1
1	B	217	GLY	2.1
1	B	255	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	55	ASP	2.0
1	A	123	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

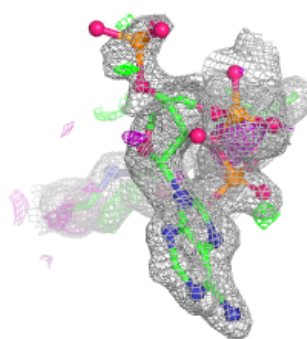
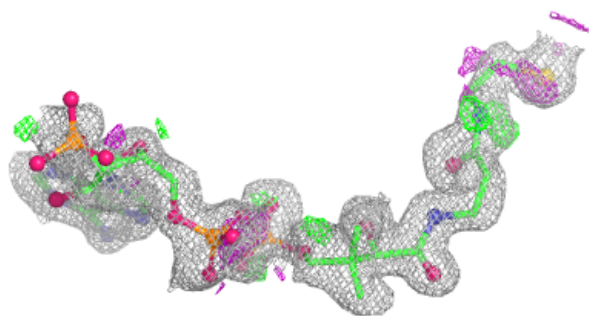
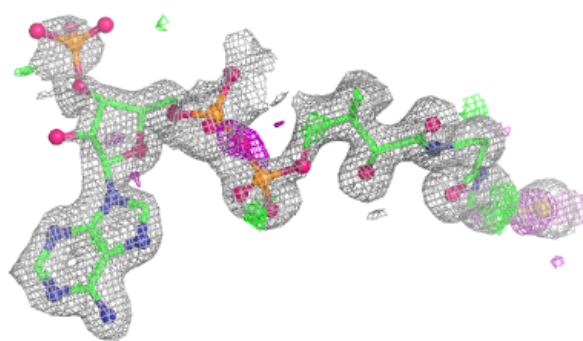
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	504	1/1	0.77	0.24	60,60,60,60	0
2	MG	B	2002	1/1	0.92	0.08	30,30,30,30	0
2	MG	A	501	1/1	0.92	0.08	35,35,35,35	0
4	COA	B	2005[A]	48/48	0.92	0.12	18,30,52,64	31
4	COA	B	2005[B]	48/48	0.92	0.12	18,32,49,55	31
4	COA	A	506	48/48	0.95	0.09	17,22,36,50	0
2	MG	B	2001	1/1	0.95	0.06	21,21,21,21	0
3	CL	B	2004	1/1	0.95	0.14	31,31,31,31	0
5	FAD	B	2006	53/53	0.96	0.06	12,15,19,20	0
5	FAD	A	507	53/53	0.97	0.06	11,13,15,17	0
3	CL	A	503	1/1	0.98	0.17	29,29,29,29	0
3	CL	A	505	1/1	0.98	0.07	23,23,23,23	0
3	CL	B	2003	1/1	0.98	0.06	27,27,27,27	0
3	CL	A	502	1/1	0.99	0.18	26,26,26,26	0

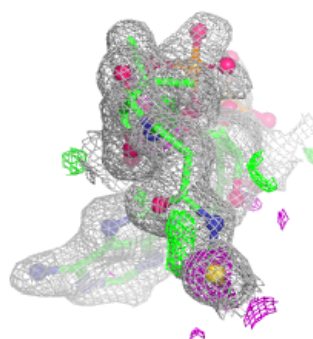
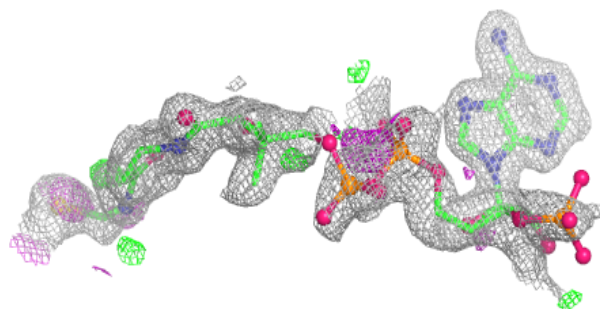
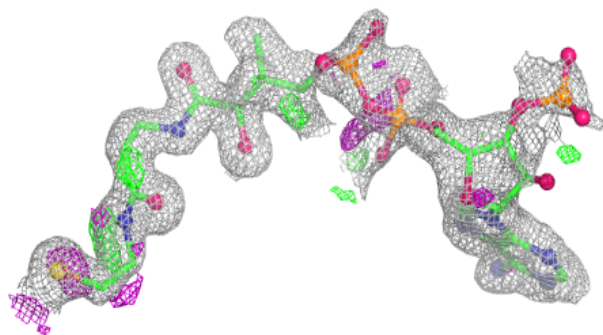
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA B 2005 (A):

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

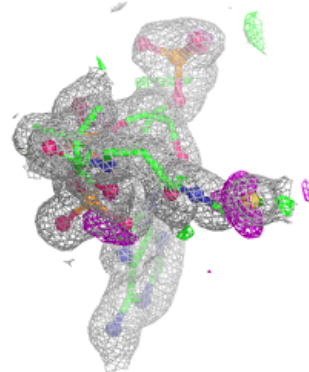
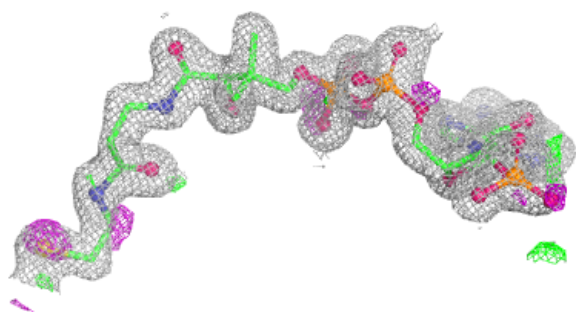
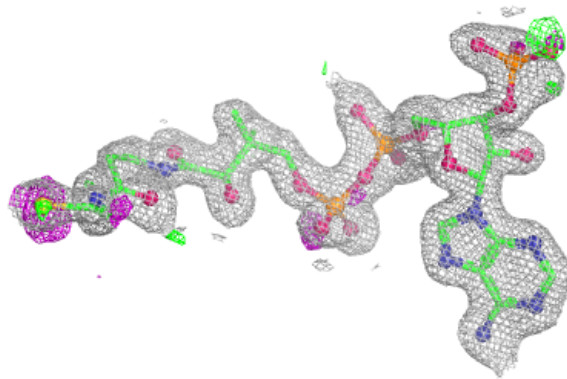
**Electron density around COA B 2005 (B):**

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

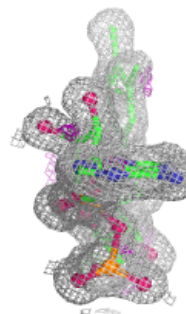
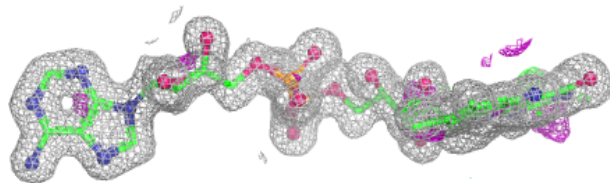
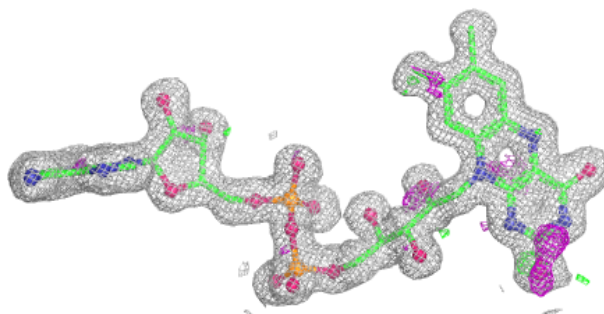


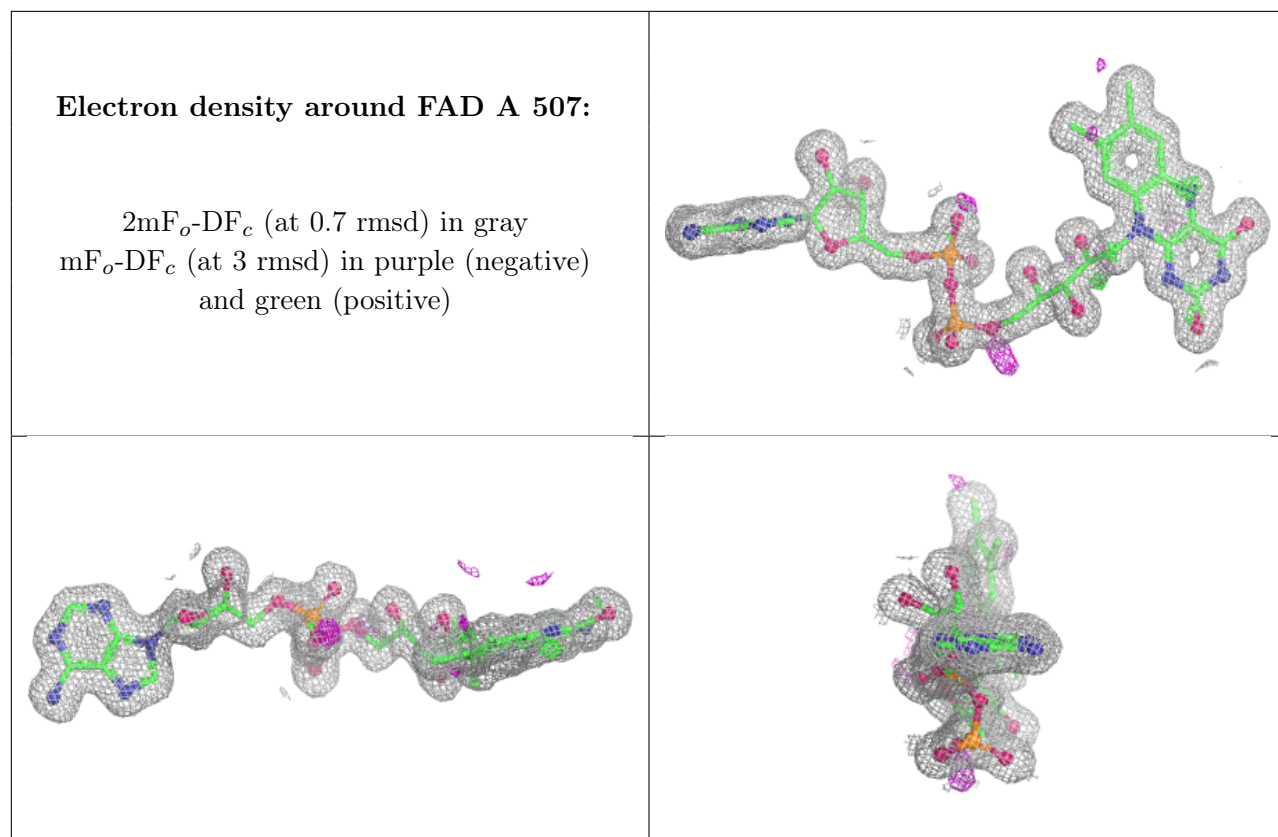
Electron density around COA A 506:

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

**Electron density around FAD B 2006:**

$2mF_o-DF_c$ (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.