



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:13 PM UTC

PDB ID : 5K0A / pdb_00005k0a
Title : Structure of an oxidoreductase from Synechocystis sp. PCC6803
Authors : Buey, R.M.; de Pereda, J.M.; Balsera, M.
Deposited on : 2016-05-17
Resolution : 1.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

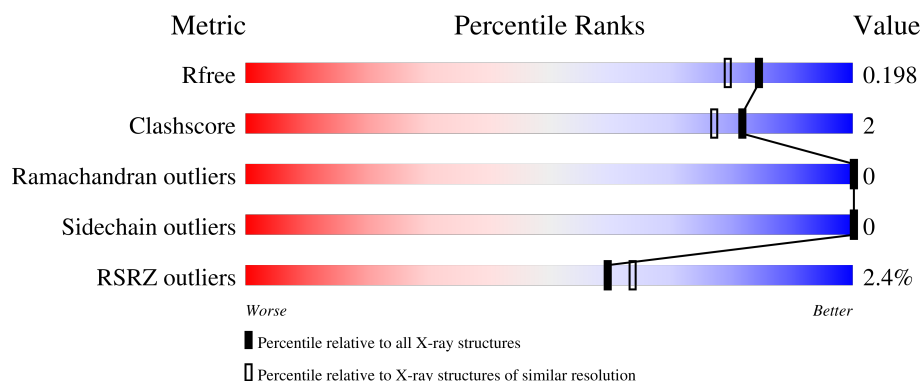
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	331	2% 94% ...
1	B	331	3% 92% 5% ..
1	C	331	% 89% 5% • 5%
1	D	331	2% 94% ...

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21583 atoms, of which 9962 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 Slr0600 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	H	N	O	S	0	1	0
			4817	1559	2375	418	450	15			
1	B	321	Total	C	H	N	O	S	0	1	0
			4831	1564	2372	421	459	15			
1	C	313	Total	C	H	N	O	S	0	1	0
			4751	1538	2343	408	448	14			
1	D	322	Total	C	H	N	O	S	0	2	0
			4885	1580	2407	420	463	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P74746
A	2	SER	-	expression tag	UNP P74746
A	3	HIS	-	expression tag	UNP P74746
A	4	MET	-	expression tag	UNP P74746
A	5	VAL	-	expression tag	UNP P74746
A	157	CSO	CYS	microheterogeneity/modified residue	UNP P74746
A	244	MET	VAL	conflict	UNP P74746
B	1	GLY	-	expression tag	UNP P74746
B	2	SER	-	expression tag	UNP P74746
B	3	HIS	-	expression tag	UNP P74746
B	4	MET	-	expression tag	UNP P74746
B	5	VAL	-	expression tag	UNP P74746
B	157	CSO	CYS	microheterogeneity/modified residue	UNP P74746
B	244	MET	VAL	conflict	UNP P74746
C	1	GLY	-	expression tag	UNP P74746
C	2	SER	-	expression tag	UNP P74746
C	3	HIS	-	expression tag	UNP P74746
C	4	MET	-	expression tag	UNP P74746
C	5	VAL	-	expression tag	UNP P74746
C	157	CSO	CYS	microheterogeneity/modified residue	UNP P74746
C	244	MET	VAL	conflict	UNP P74746

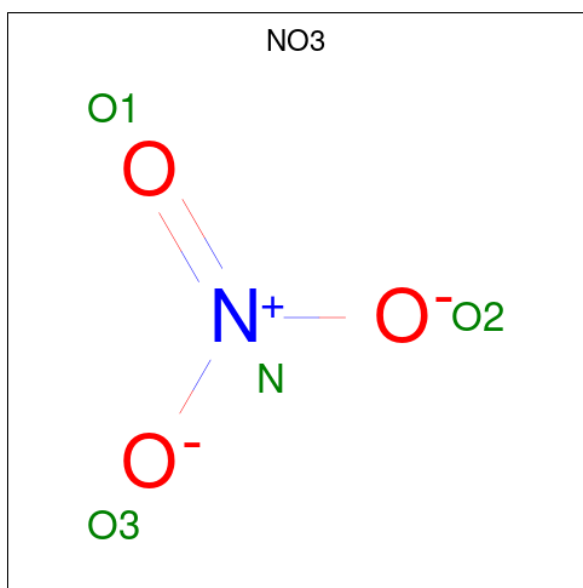
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP P74746
D	2	SER	-	expression tag	UNP P74746
D	3	HIS	-	expression tag	UNP P74746
D	4	MET	-	expression tag	UNP P74746
D	5	VAL	-	expression tag	UNP P74746
D	157	CSO	CYS	microheterogeneity/modified residue	UNP P74746
D	244	MET	VAL	conflict	UNP P74746

- # FAD

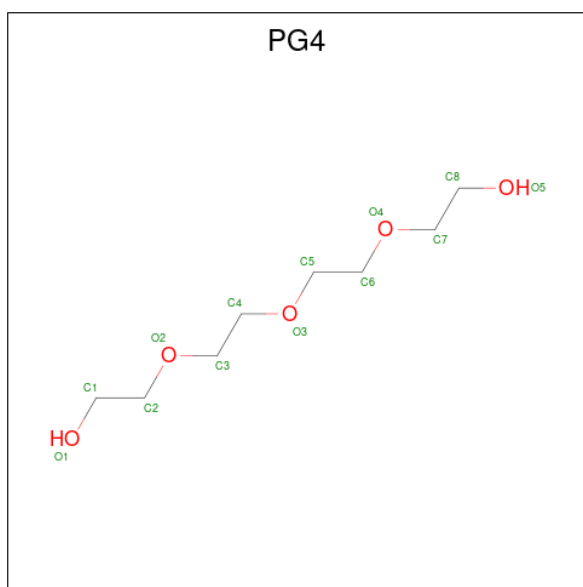
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	A	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	B	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	B	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	C	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	C	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	D	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	D	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



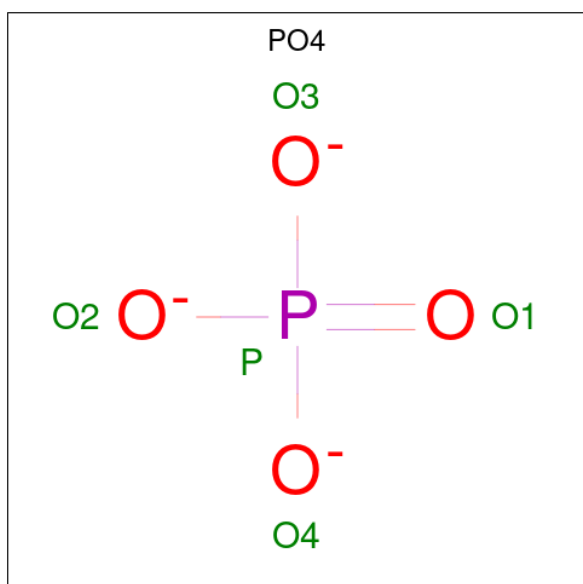
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $\text{C}_8\text{H}_{18}\text{O}_5$).



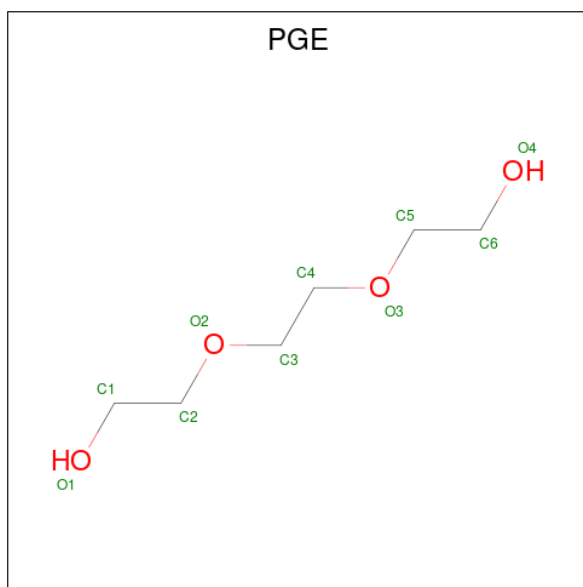
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			30	8	17	5		
4	A	1	Total	C	H	O	0	0
			30	8	17	5		
4	B	1	Total	C	H	O	0	0
			30	8	17	5		
4	B	1	Total	C	H	O	0	0
			30	8	17	5		
4	C	1	Total	C	H	O	0	0
			30	8	17	5		
4	D	1	Total	C	H	O	0	0
			30	8	17	5		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			23	6	13	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	285	Total	O	0	0
			285	285		
8	B	253	Total	O	0	0
			253	253		
8	C	308	Total	O	0	0
			308	308		
8	D	354	Total	O	0	0
			354	354		

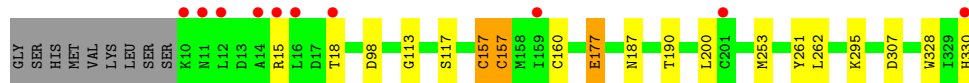
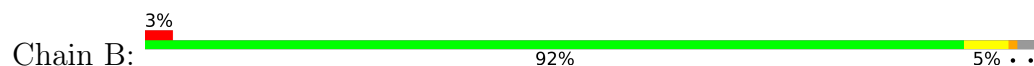
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Slr0600 protein



- Molecule 1: Slr0600 protein



- Molecule 1: Slr0600 protein



- Molecule 1: Slr0600 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.03Å 128.43Å 92.73Å 90.00° 91.61° 90.00°	Depositor
Resolution (Å)	49.04 – 1.71 49.04 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.04-1.71) 99.9 (49.04-1.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.71Å)	Xtriage
Refinement program	PHENIX (dev_2341: ???)	Depositor
R, R_{free}	0.165 , 0.193 0.172 , 0.198	Depositor DCC
R_{free} test set	8275 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21583	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8652e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NO3, PGE, 1PE, FAD, PO4, CSO, PG4

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	0.31	0/2487	0.48	0/3381
1	B	0.36	1/2504 (0.0%)	0.52	1/3403 (0.0%)
1	C	0.46	3/2453 (0.1%)	0.57	3/3333 (0.1%)
1	D	0.42	1/2526 (0.0%)	0.53	0/3433
All	All	0.39	5/9970 (0.1%)	0.53	4/13550 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	CYS	CA-C	5.42	1.59	1.52
1	C	159	ILE	CA-C	5.26	1.59	1.52
1	C	163	PHE	CA-C	5.22	1.59	1.52
1	D	10	LYS	CA-C	5.15	1.59	1.52
1	B	177	GLU	CA-C	5.02	1.59	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	THR	N-CA-C	-7.91	97.76	109.15
1	C	157[B]	CYS	CA-C-N	-6.66	111.38	120.44
1	C	157[B]	CYS	C-N-CA	-6.66	111.38	120.44
1	C	157[B]	CYS	O-C-N	6.01	130.31	123.27

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157[A]	CSO	Mainchain
1	B	157[A]	CSO	Mainchain
1	C	157[A]	CSO	Mainchain
1	D	157[A]	CSO	Mainchain

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	2442	2375	2370	4	0
1	B	2459	2372	2377	12	0
1	C	2408	2343	2338	12	0
1	D	2478	2407	2408	9	0
2	A	106	60	62	1	0
2	B	106	60	62	1	0
2	C	106	60	62	1	0
2	D	106	60	62	2	0
3	A	16	0	0	1	0
3	B	8	0	0	1	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	26	34	36	0	0
4	B	26	34	36	0	0
4	C	13	17	18	1	0
4	D	13	17	18	0	0
5	B	16	22	22	1	0
5	C	32	44	44	3	0
5	D	32	44	44	2	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	5	0	0	0	0
7	D	10	13	14	1	0
8	A	285	0	0	1	0
8	B	253	0	0	3	1
8	C	308	0	0	3	0
8	D	354	0	0	2	1
All	All	11621	9962	9973	45	1

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.

The worst 5 of 45 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)
3:A:404:NO3:O1	8:A:501:HOH:O	1.91	0.88
4:C:403:PG4:O1	8:C:501:HOH:O	1.99	0.79
3:B:405:NO3:O2	8:B:501:HOH:O	2.06	0.74
1:B:177:GLU:OE1	8:B:502:HOH:O	2.11	0.68
1:D:102:GLU:OE1	1:D:123:ARG:NH2	2.27	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:719:HOH:O	8:D:744:HOH:O[2_444]	2.15	0.05

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	317/331 (96%)	312 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	318/331 (96%)	313 (98%)	5 (2%)	0	100	100
1	C	310/331 (94%)	305 (98%)	5 (2%)	0	100	100
1	D	320/331 (97%)	315 (98%)	5 (2%)	0	100	100
All	All	1265/1324 (96%)	1245 (98%)	20 (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	244/269 (91%)	244 (100%)	0	100	100
1	B	247/269 (92%)	247 (100%)	0	100	100
1	C	242/269 (90%)	242 (100%)	0	100	100
1	D	251/269 (93%)	251 (100%)	0	100	100
All	All	984/1076 (91%)	984 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	274	ASN
1	D	260	HIS
1	C	260	HIS
1	C	139	GLN
1	D	86	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	B	157[A]	1	3,6,7	0.90	0	1,6,8	0.22	0
1	CSO	C	157[A]	1	3,6,7	1.06	0	1,6,8	0.10	0
1	CSO	D	157[A]	1	3,6,7	0.92	0	1,6,8	0.05	0
1	CSO	A	157[A]	1	3,6,7	0.90	0	1,6,8	0.35	0

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
1	CSO	B	157[A]	1	-	0/1/5/7	-
1	CSO	C	157[A]	1	-	0/1/5/7	-
1	CSO	D	157[A]	1	-	0/1/5/7	-
1	CSO	A	157[A]	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	157[A]	CSO	1	0
1	C	157[A]	CSO	1	0
1	D	157[A]	CSO	3	0
1	A	157[A]	CSO	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

30 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
5	1PE	B	404	-	15,15,15	0.53	0	14,14,14	0.26	0
4	PG4	B	406	-	12,12,12	0.54	0	11,11,11	0.36	0
2	FAD	C	402	-	58,58,58	1.43	7 (12%)	85,89,89	1.96	23 (27%)
2	FAD	D	402	-	58,58,58	1.41	7 (12%)	85,89,89	1.91	26 (30%)
3	NO3	A	407	-	1,3,3	0.59	0	0,3,3	-	-
4	PG4	C	403	-	12,12,12	0.53	0	11,11,11	0.40	0
2	FAD	D	403	-	58,58,58	1.47	7 (12%)	85,89,89	1.95	26 (30%)
3	NO3	A	403	-	1,3,3	0.56	0	0,3,3	-	-
3	NO3	D	405	-	1,3,3	0.60	0	0,3,3	-	-
3	NO3	B	405	-	1,3,3	0.69	0	0,3,3	-	-
4	PG4	B	407	-	12,12,12	0.53	0	11,11,11	0.35	0
6	PO4	B	408	-	4,4,4	0.92	0	6,6,6	0.49	0
2	FAD	B	402	-	58,58,58	1.47	8 (13%)	85,89,89	1.94	26 (30%)
3	NO3	A	404	-	1,3,3	0.58	0	0,3,3	-	-
2	FAD	C	401	-	58,58,58	1.41	8 (13%)	85,89,89	1.91	24 (28%)
3	NO3	A	408	-	1,3,3	0.59	0	0,3,3	-	-
5	1PE	C	405	-	15,15,15	0.52	0	14,14,14	0.42	0
6	PO4	D	404	-	4,4,4	0.90	0	6,6,6	0.49	0
5	1PE	D	401	-	15,15,15	0.54	0	14,14,14	0.28	0
5	1PE	D	407	-	15,15,15	0.56	0	14,14,14	0.40	0
3	NO3	B	403	-	1,3,3	0.53	0	0,3,3	-	-
7	PGE	D	408	-	9,9,9	0.49	0	8,8,8	0.28	0
3	NO3	C	404	-	1,3,3	0.74	0	0,3,3	-	-
5	1PE	C	406	-	15,15,15	0.56	0	14,14,14	0.40	0
2	FAD	B	401	-	58,58,58	1.69	14 (24%)	85,89,89	2.03	25 (29%)
4	PG4	A	405	-	12,12,12	0.52	0	11,11,11	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	401	-	58,58,58	1.40	7 (12%)	85,89,89	1.91	25 (29%)
4	PG4	D	406	-	12,12,12	0.53	0	11,11,11	0.36	0
2	FAD	A	402	-	58,58,58	1.46	6 (10%)	85,89,89	1.99	25 (29%)
4	PG4	A	406	-	12,12,12	0.57	0	11,11,11	0.29	0

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
5	1PE	B	404	-	-	8/13/13/13	-
4	PG4	B	406	-	-	4/10/10/10	-
2	FAD	C	402	-	-	4/34/50/50	0/6/6/6
2	FAD	D	402	-	-	0/34/50/50	0/6/6/6
4	PG4	C	403	-	-	2/10/10/10	-
2	FAD	D	403	-	-	3/34/50/50	0/6/6/6
4	PG4	B	407	-	-	3/10/10/10	-
2	FAD	B	402	-	-	5/34/50/50	0/6/6/6
2	FAD	C	401	-	-	0/34/50/50	0/6/6/6
5	1PE	C	405	-	-	7/13/13/13	-
5	1PE	D	401	-	-	2/13/13/13	-
5	1PE	D	407	-	-	8/13/13/13	-
7	PGE	D	408	-	-	4/7/7/7	-
5	1PE	C	406	-	-	7/13/13/13	-
2	FAD	B	401	-	-	0/34/50/50	0/6/6/6
4	PG4	A	405	-	-	4/10/10/10	-
2	FAD	A	401	-	-	0/34/50/50	0/6/6/6
4	PG4	D	406	-	-	3/10/10/10	-
2	FAD	A	402	-	-	4/34/50/50	0/6/6/6
4	PG4	A	406	-	-	4/10/10/10	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	FAD	C9A-C5X	5.26	1.49	1.41
2	B	402	FAD	C9A-C5X	5.25	1.49	1.41
2	C	401	FAD	C9A-C5X	5.22	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	FAD	C9A-C5X	5.21	1.49	1.41
2	A	401	FAD	C9A-C5X	4.99	1.49	1.41

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	FAD	O2-C2-N1	-5.96	111.91	121.80
2	B	402	FAD	O2-C2-N1	-5.92	111.97	121.80
2	D	403	FAD	O2-C2-N1	-5.90	112.00	121.80
2	C	401	FAD	O2-C2-N1	-5.87	112.05	121.80
2	C	402	FAD	C5A-C4A-N3A	-5.86	118.64	126.72

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	FAD	C5B-O5B-PA-O1A
2	B	402	FAD	C5B-O5B-PA-O2A
2	B	402	FAD	C5B-O5B-PA-O3P
5	B	404	1PE	OH4-C13-C23-OH3
5	C	405	1PE	OH5-C14-C24-OH4

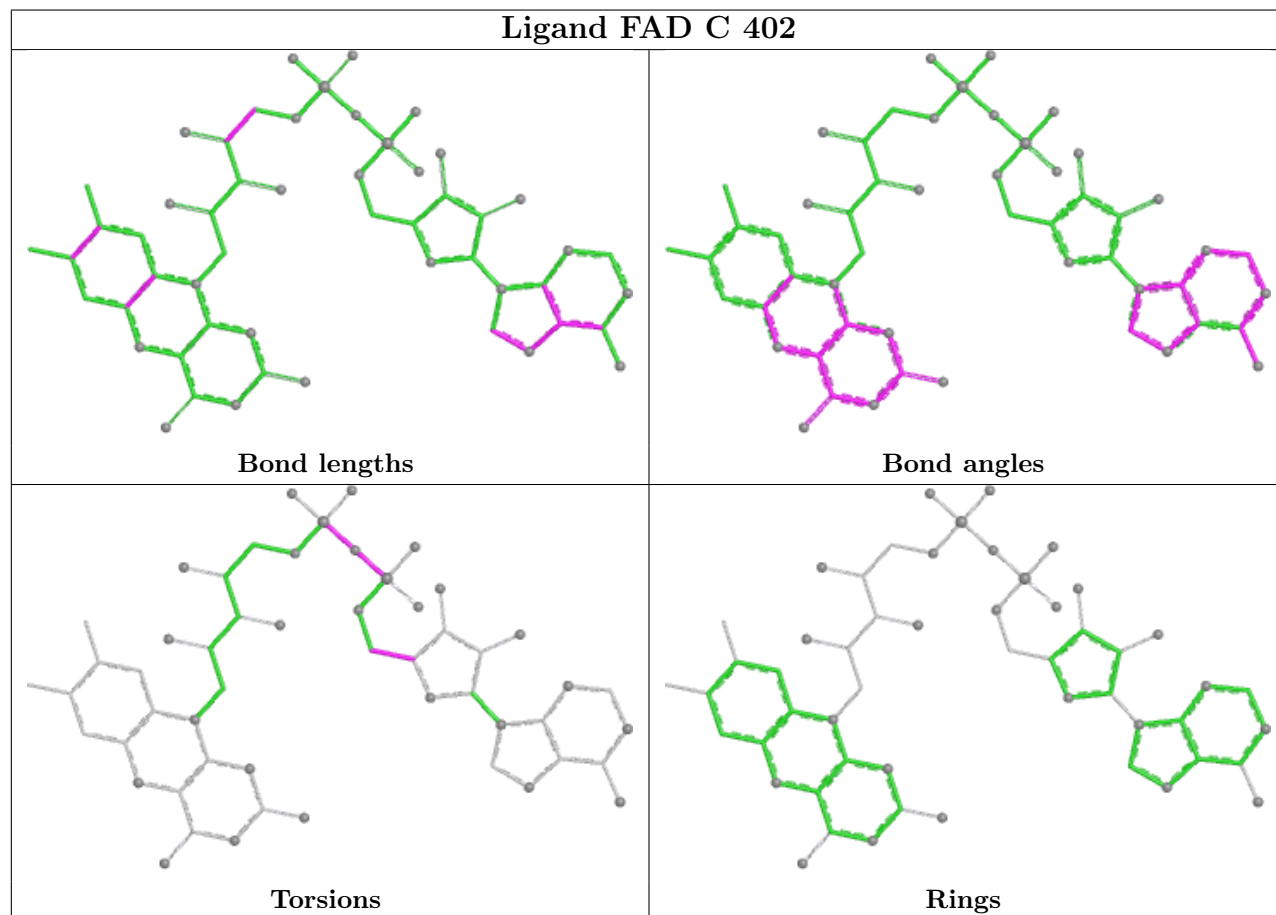
There are no ring outliers.

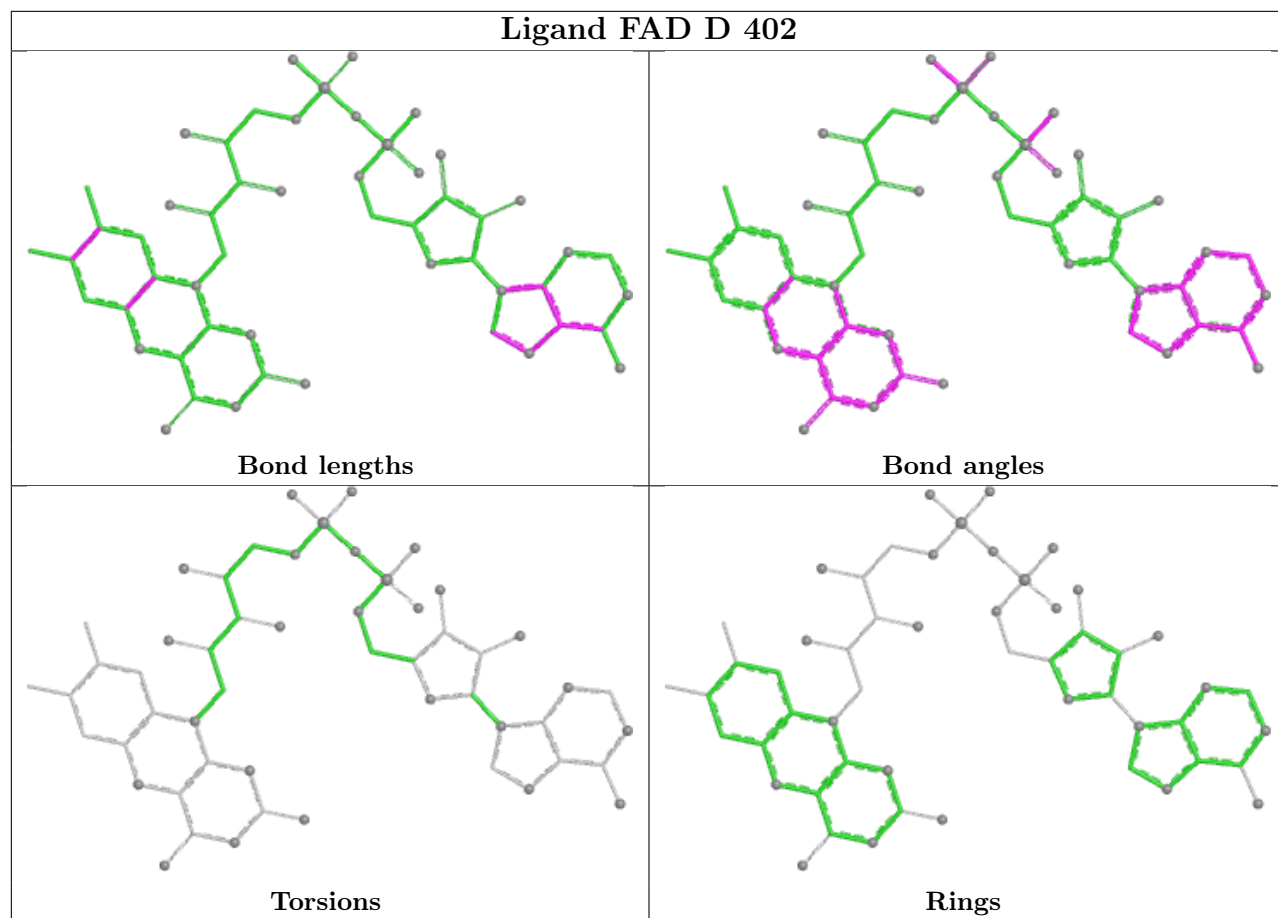
12 monomers are involved in 15 short contacts:

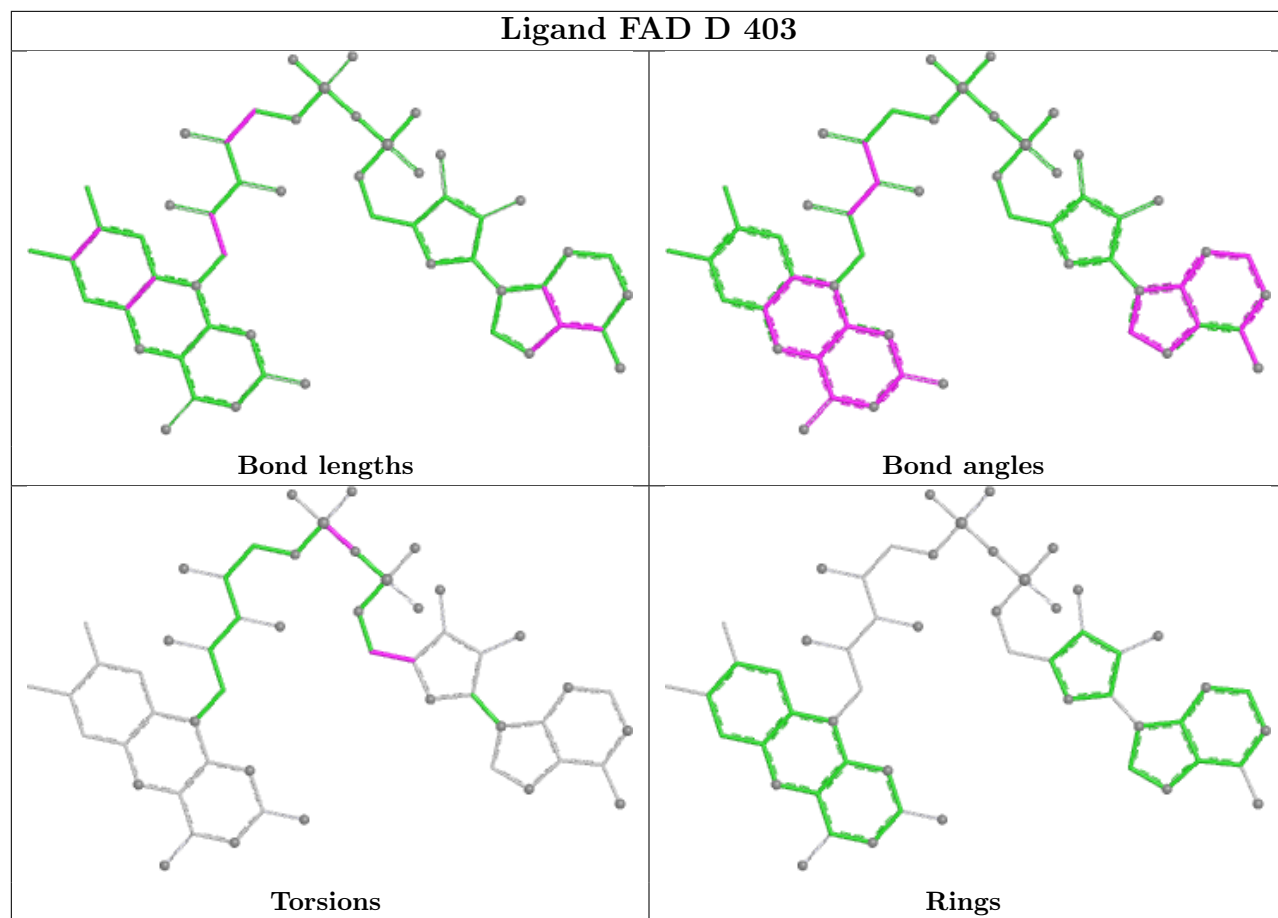
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	1PE	1	0
4	C	403	PG4	1	0
2	D	403	FAD	2	0
3	B	405	NO3	1	0
2	B	402	FAD	1	0
3	A	404	NO3	1	0
2	C	401	FAD	1	0
5	C	405	1PE	1	0
5	D	401	1PE	2	0
7	D	408	PGE	1	0
5	C	406	1PE	2	0
2	A	401	FAD	1	0

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

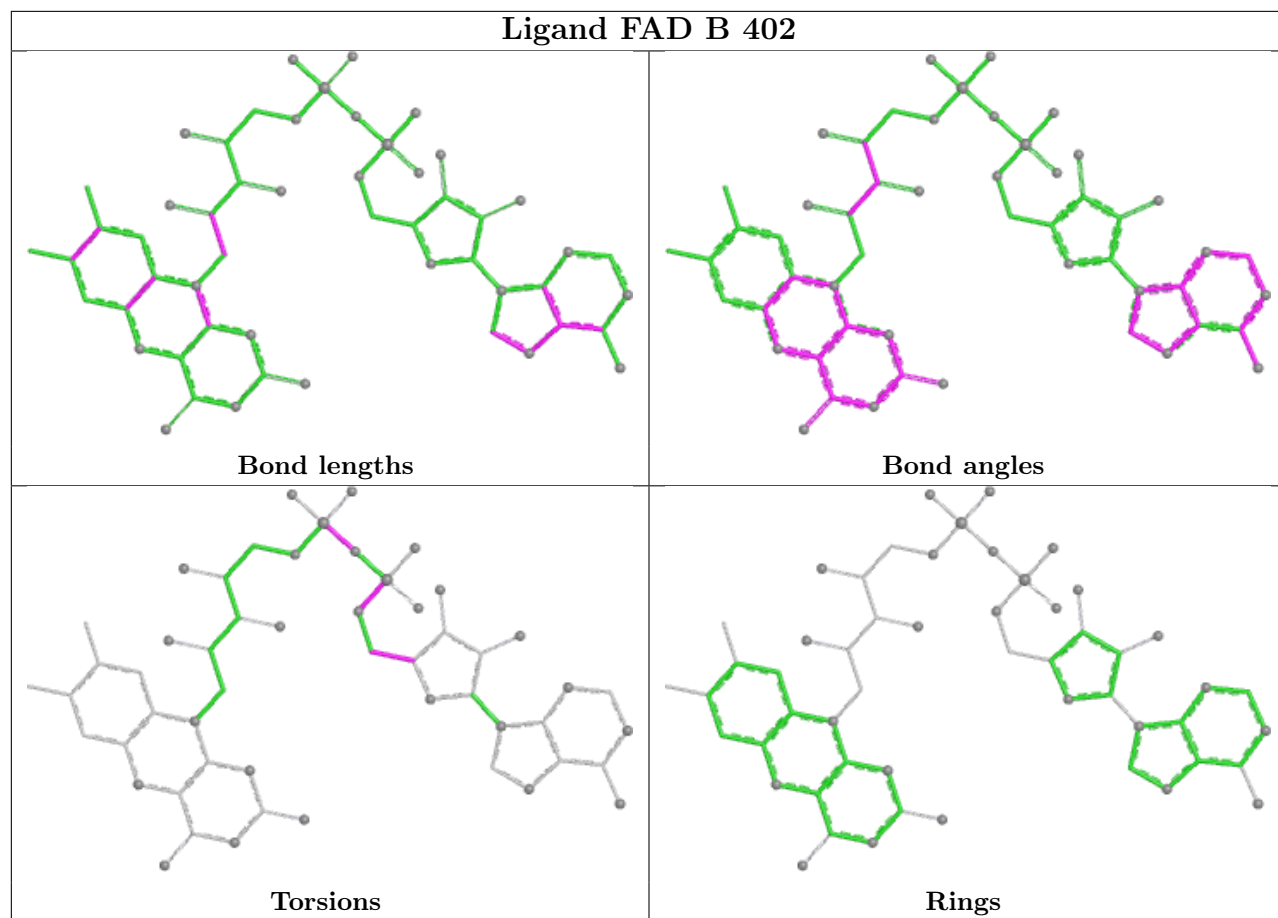
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

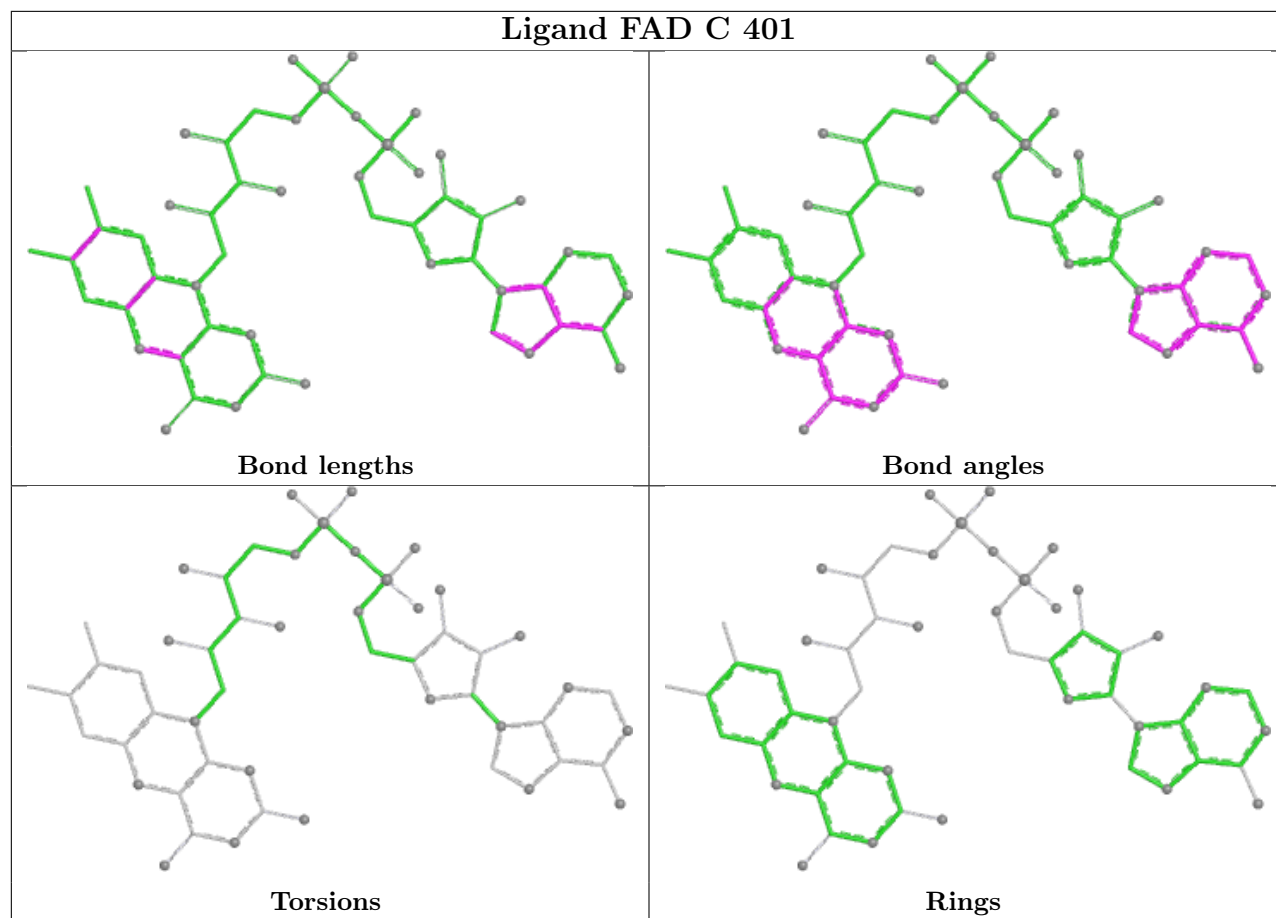


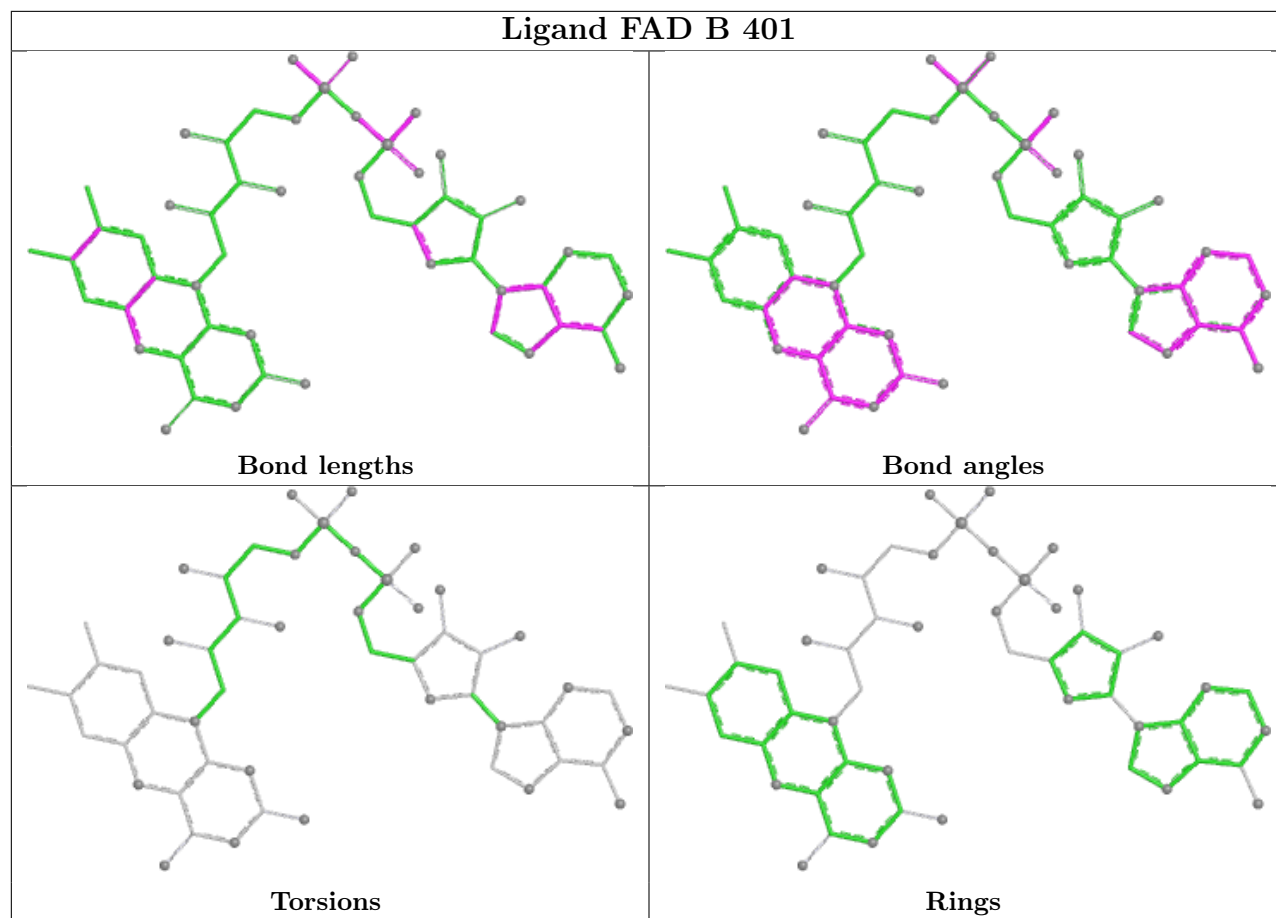




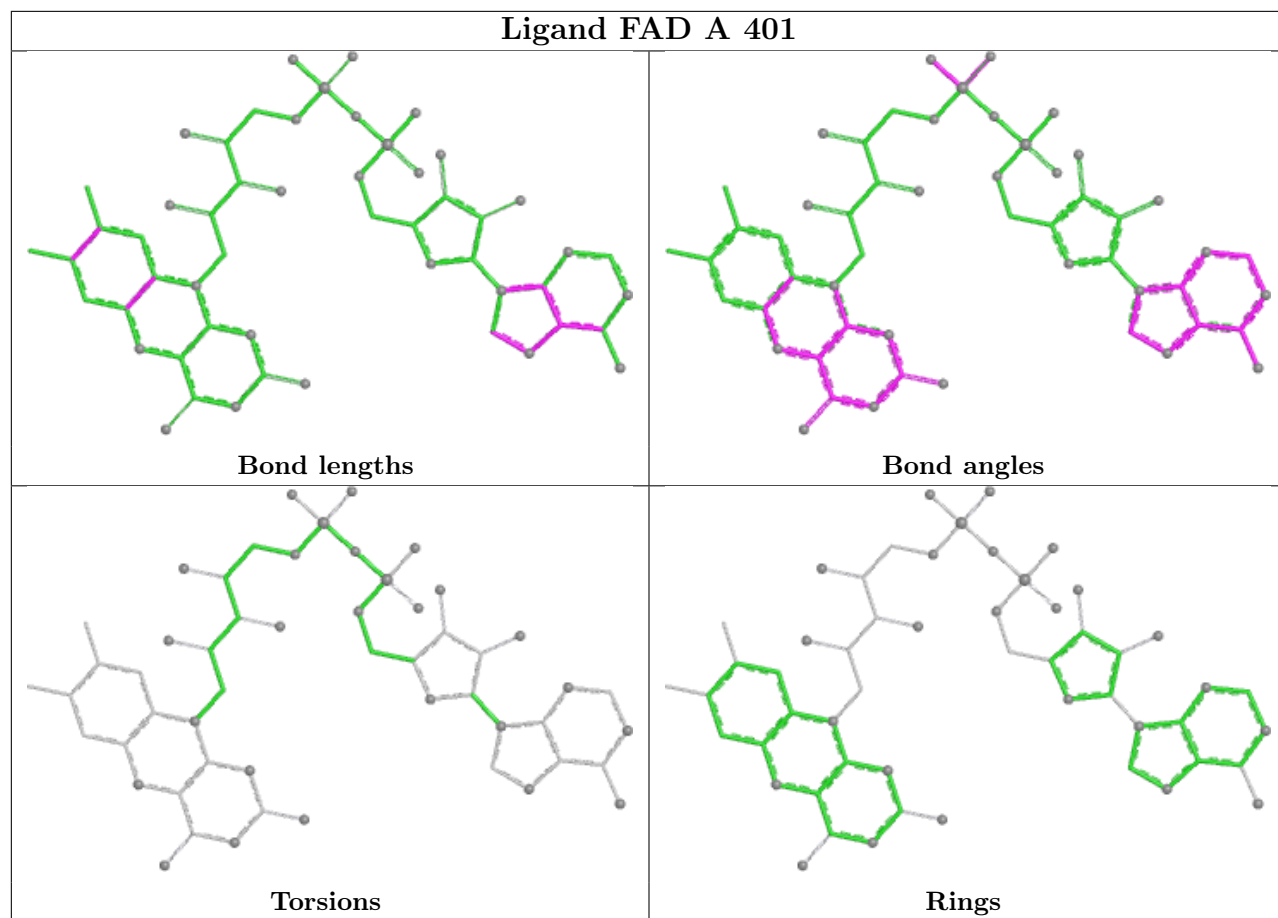
Ligand FAD B 402

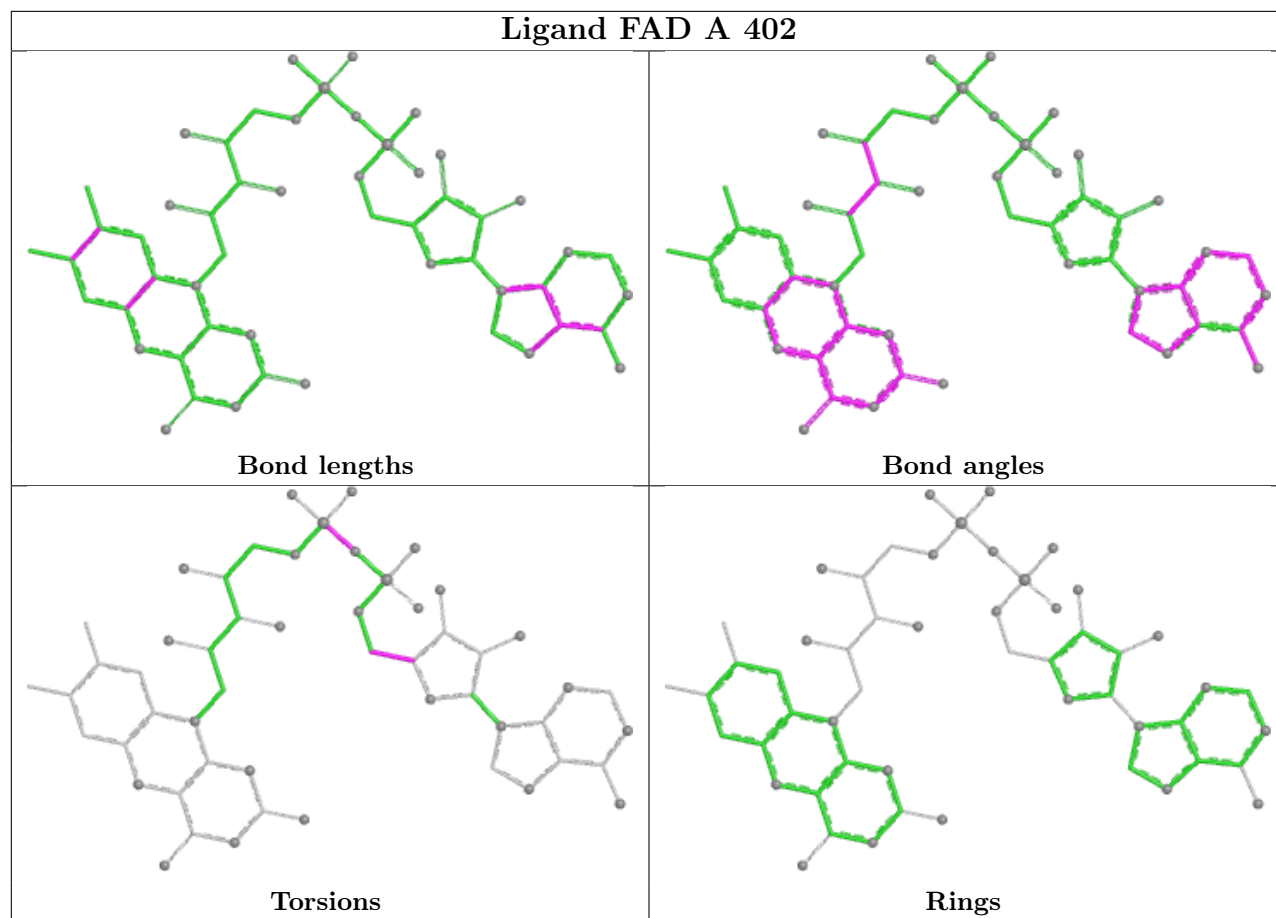






Ligand FAD A 401





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	319/331 (96%)	-0.16	8 (2%) 58 62	21, 33, 57, 101	0
1	B	320/331 (96%)	-0.06	10 (3%) 51 55	22, 37, 62, 106	0
1	C	312/331 (94%)	-0.23	4 (1%) 75 79	22, 31, 54, 69	0
1	D	321/331 (96%)	-0.20	8 (2%) 58 62	20, 31, 51, 91	1 (0%)
All	All	1272/1324 (96%)	-0.16	30 (2%) 59 64	20, 33, 57, 106	1 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	LYS	6.3
1	A	12	LEU	6.0
1	C	201	CYS	6.0
1	D	10	LYS	5.8
1	D	12	LEU	4.6

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSO	B	157[A]	7/8	0.86	0.17	25,30,39,79	10
1	CSO	A	157[A]	7/8	0.87	0.12	24,30,34,35	10
1	CSO	D	157[A]	7/8	0.87	0.15	27,34,54,60	10
1	CSO	C	157[A]	7/8	0.89	0.14	27,34,44,60	10

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

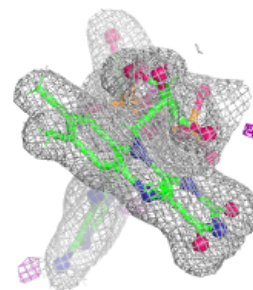
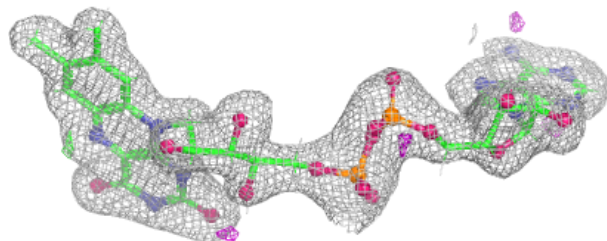
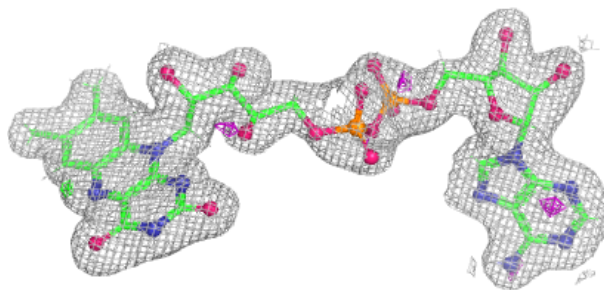
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	D	404	5/5	0.75	0.13	82,84,97,110	0
3	NO3	B	403	4/4	0.76	0.11	68,75,80,81	0
6	PO4	B	408	5/5	0.78	0.11	83,91,96,97	0
3	NO3	A	403	4/4	0.79	0.12	63,64,65,67	0
5	1PE	D	407	16/16	0.80	0.15	52,73,93,101	0
4	PG4	B	407	13/13	0.80	0.15	54,70,87,93	0
5	1PE	B	404	16/16	0.80	0.15	53,76,96,108	0
4	PG4	A	405	13/13	0.82	0.16	47,68,83,86	0
3	NO3	A	407	4/4	0.82	0.12	72,73,74,88	0
4	PG4	C	403	13/13	0.84	0.16	48,71,86,88	0
4	PG4	D	406	13/13	0.84	0.16	50,72,92,110	0
7	PGE	D	408	10/10	0.84	0.19	57,69,87,92	0
3	NO3	B	405	4/4	0.85	0.14	57,59,66,86	0
3	NO3	C	404	4/4	0.85	0.12	52,52,58,65	0
3	NO3	D	405	4/4	0.85	0.13	69,73,75,82	0
3	NO3	A	408	4/4	0.85	0.12	59,59,63,72	0
4	PG4	B	406	13/13	0.86	0.16	59,72,93,97	0
5	1PE	D	401	16/16	0.86	0.14	49,71,91,92	0
5	1PE	C	406	16/16	0.87	0.16	49,65,96,104	0
5	1PE	C	405	16/16	0.87	0.14	38,59,86,93	0
3	NO3	A	404	4/4	0.88	0.10	45,46,46,50	0
4	PG4	A	406	13/13	0.88	0.15	53,71,91,92	0
2	FAD	B	402	53/53	0.92	0.09	27,46,72,82	0
2	FAD	A	402	53/53	0.94	0.08	24,39,66,82	0
2	FAD	C	402	53/53	0.94	0.09	20,37,61,96	0
2	FAD	D	403	53/53	0.95	0.08	20,35,64,79	0
2	FAD	D	402	53/53	0.96	0.06	18,23,31,35	0
2	FAD	C	401	53/53	0.96	0.07	17,23,33,35	0
2	FAD	B	401	53/53	0.97	0.06	20,29,38,43	0
2	FAD	A	401	53/53	0.97	0.06	19,25,33,39	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.

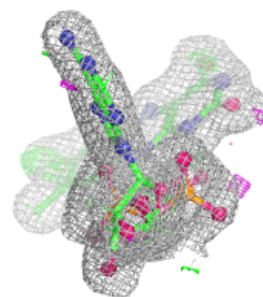
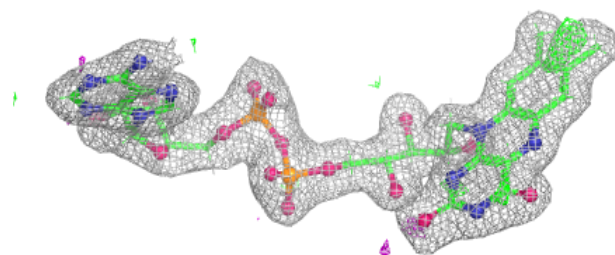
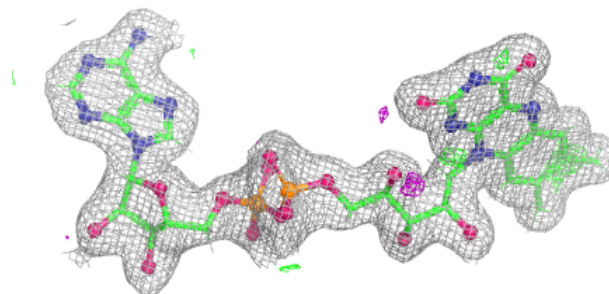
Electron density around FAD B 402:

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

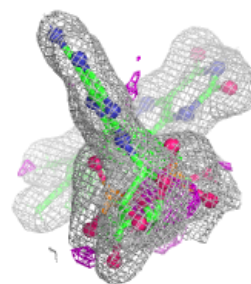
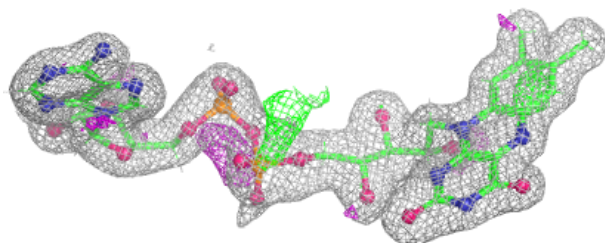
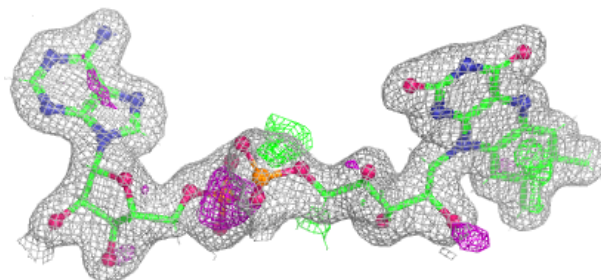


Electron density around FAD A 402:

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

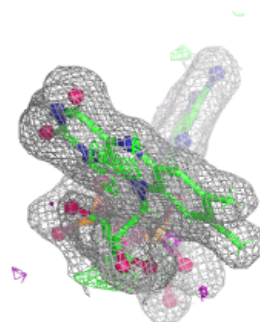
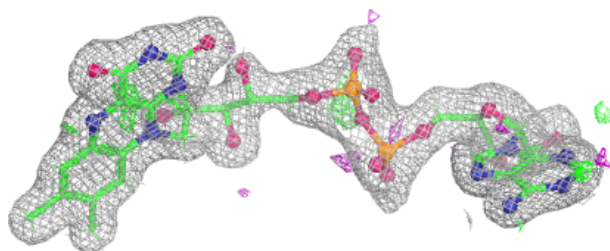
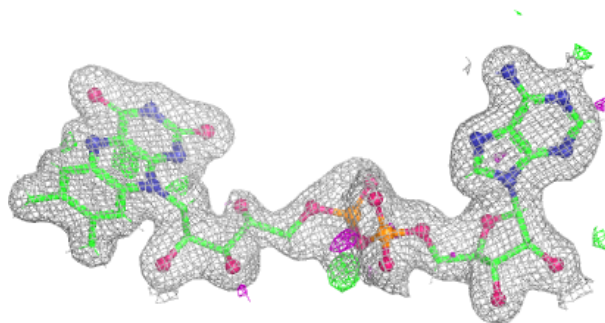
**Electron density around FAD C 402:**

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

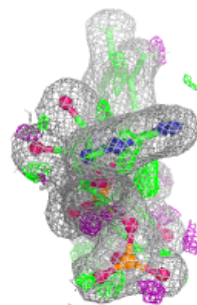
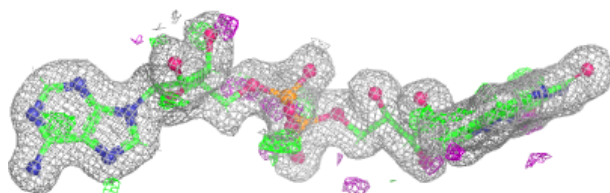
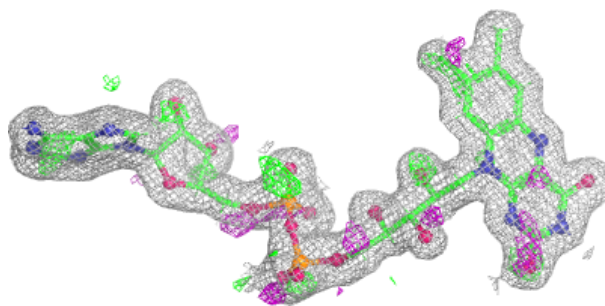


Electron density around FAD D 403:

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

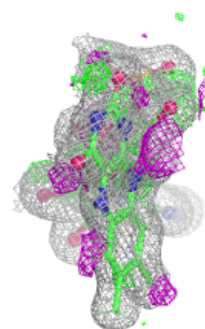
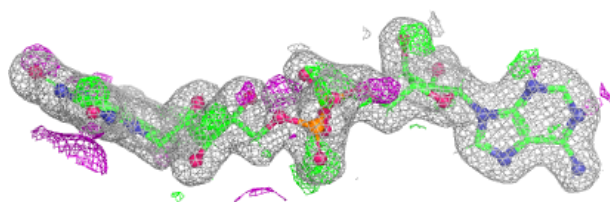
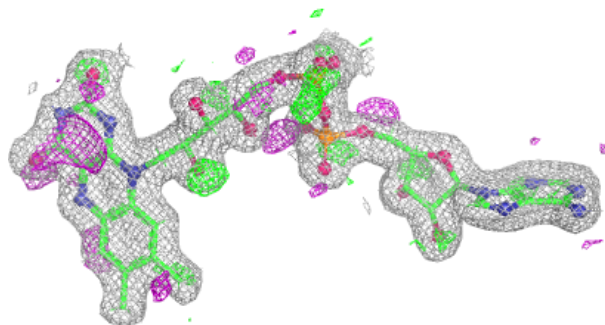
**Electron density around FAD D 402:**

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

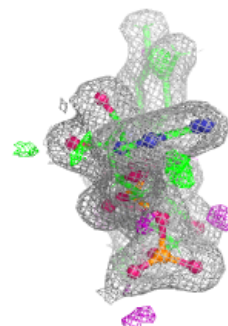
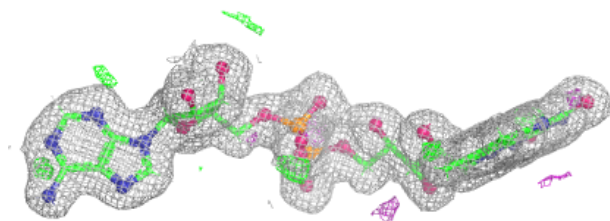
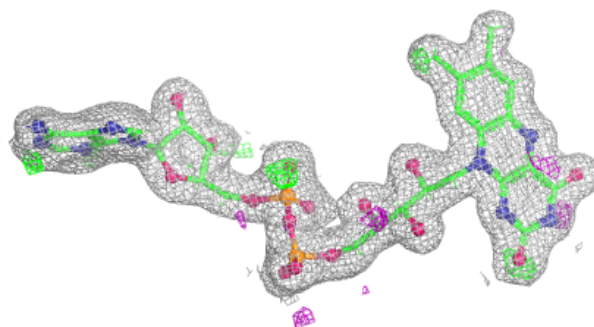


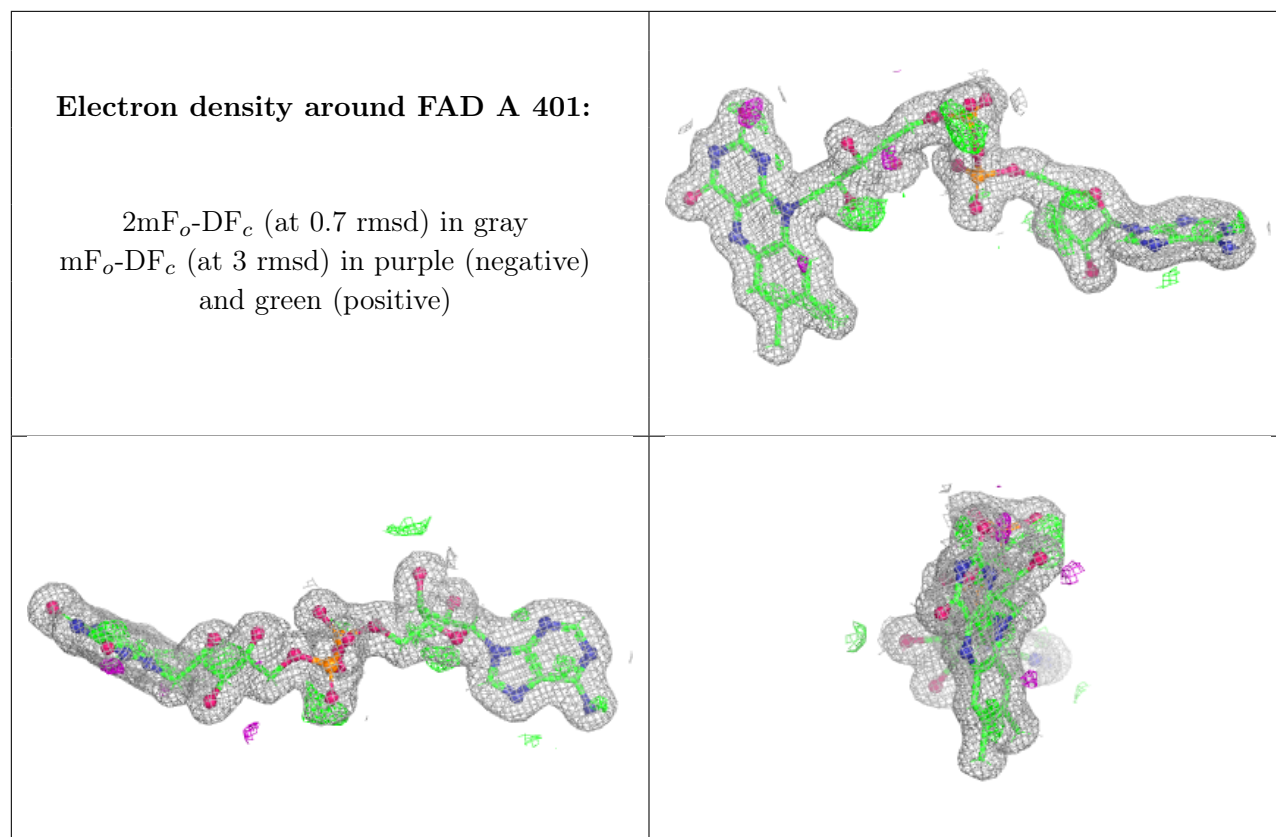
Electron density around FAD C 401:

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

**Electron density around FAD B 401:**

$2mF_o-DF_c$ (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.