



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:43 PM UTC

PDB ID : 6S32 / pdb_00006s32
Title : Crystal structure of ene-reductase CtOYE from *Chroococcidiopsis thermalis*.
Authors : Robescu, M.R.; Niero, M.; Hall, M.; Bergantino, E.; Cendron, L.
Deposited on : 2019-06-24
Resolution : 1.35 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

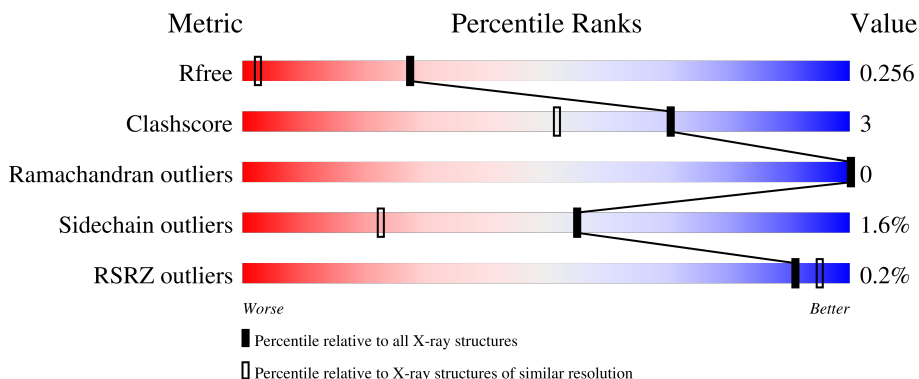
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

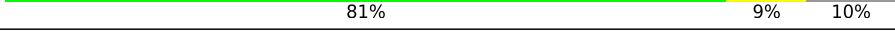
The reported resolution of this entry is 1.35 Å.

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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	390	 78% 10% 10%
1	B	390	 82% 8% 10%
1	C	390	 81% 8% 11%
1	D	390	 81% 9% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12468 atoms, of which 9 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 NADH:flavin oxidoreductase/NADH oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	1	0
			2718	1719	473	522	4			
1	B	350	Total	C	N	O	S	0	6	0
			2749	1739	479	527	4			
1	C	349	Total	C	N	O	S	0	1	0
			2713	1716	474	519	4			
1	D	352	Total	C	N	O	S	0	1	0
			2738	1730	480	523	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP K9TVC9
A	-18	GLY	-	expression tag	UNP K9TVC9
A	-17	SER	-	expression tag	UNP K9TVC9
A	-16	SER	-	expression tag	UNP K9TVC9
A	-15	HIS	-	expression tag	UNP K9TVC9
A	-14	HIS	-	expression tag	UNP K9TVC9
A	-13	HIS	-	expression tag	UNP K9TVC9
A	-12	HIS	-	expression tag	UNP K9TVC9
A	-11	HIS	-	expression tag	UNP K9TVC9
A	-10	HIS	-	expression tag	UNP K9TVC9
A	-9	SER	-	expression tag	UNP K9TVC9
A	-8	SER	-	expression tag	UNP K9TVC9
A	-7	GLY	-	expression tag	UNP K9TVC9
A	-6	LEU	-	expression tag	UNP K9TVC9
A	-5	VAL	-	expression tag	UNP K9TVC9
A	-4	PRO	-	expression tag	UNP K9TVC9
A	-3	ARG	-	expression tag	UNP K9TVC9
A	-2	GLY	-	expression tag	UNP K9TVC9
A	-1	SER	-	expression tag	UNP K9TVC9
A	0	HIS	-	expression tag	UNP K9TVC9
B	-19	MET	-	initiating methionine	UNP K9TVC9

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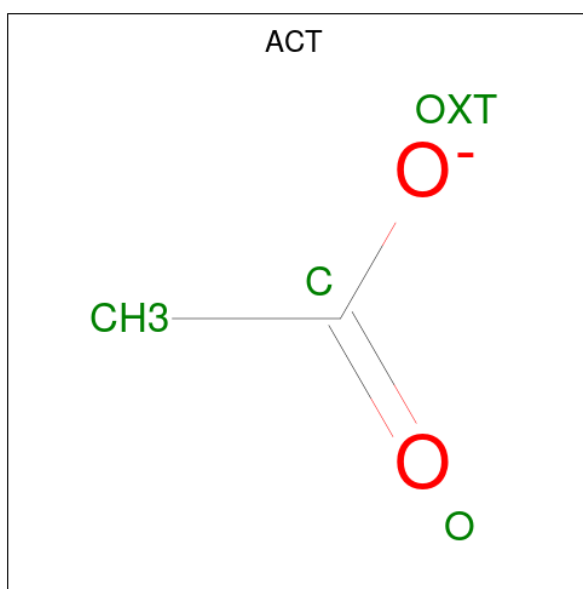
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP K9TVC9
B	-17	SER	-	expression tag	UNP K9TVC9
B	-16	SER	-	expression tag	UNP K9TVC9
B	-15	HIS	-	expression tag	UNP K9TVC9
B	-14	HIS	-	expression tag	UNP K9TVC9
B	-13	HIS	-	expression tag	UNP K9TVC9
B	-12	HIS	-	expression tag	UNP K9TVC9
B	-11	HIS	-	expression tag	UNP K9TVC9
B	-10	HIS	-	expression tag	UNP K9TVC9
B	-9	SER	-	expression tag	UNP K9TVC9
B	-8	SER	-	expression tag	UNP K9TVC9
B	-7	GLY	-	expression tag	UNP K9TVC9
B	-6	LEU	-	expression tag	UNP K9TVC9
B	-5	VAL	-	expression tag	UNP K9TVC9
B	-4	PRO	-	expression tag	UNP K9TVC9
B	-3	ARG	-	expression tag	UNP K9TVC9
B	-2	GLY	-	expression tag	UNP K9TVC9
B	-1	SER	-	expression tag	UNP K9TVC9
B	0	HIS	-	expression tag	UNP K9TVC9
C	-19	MET	-	initiating methionine	UNP K9TVC9
C	-18	GLY	-	expression tag	UNP K9TVC9
C	-17	SER	-	expression tag	UNP K9TVC9
C	-16	SER	-	expression tag	UNP K9TVC9
C	-15	HIS	-	expression tag	UNP K9TVC9
C	-14	HIS	-	expression tag	UNP K9TVC9
C	-13	HIS	-	expression tag	UNP K9TVC9
C	-12	HIS	-	expression tag	UNP K9TVC9
C	-11	HIS	-	expression tag	UNP K9TVC9
C	-10	HIS	-	expression tag	UNP K9TVC9
C	-9	SER	-	expression tag	UNP K9TVC9
C	-8	SER	-	expression tag	UNP K9TVC9
C	-7	GLY	-	expression tag	UNP K9TVC9
C	-6	LEU	-	expression tag	UNP K9TVC9
C	-5	VAL	-	expression tag	UNP K9TVC9
C	-4	PRO	-	expression tag	UNP K9TVC9
C	-3	ARG	-	expression tag	UNP K9TVC9
C	-2	GLY	-	expression tag	UNP K9TVC9
C	-1	SER	-	expression tag	UNP K9TVC9
C	0	HIS	-	expression tag	UNP K9TVC9
D	-19	MET	-	initiating methionine	UNP K9TVC9
D	-18	GLY	-	expression tag	UNP K9TVC9
D	-17	SER	-	expression tag	UNP K9TVC9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP K9TVC9
D	-15	HIS	-	expression tag	UNP K9TVC9
D	-14	HIS	-	expression tag	UNP K9TVC9
D	-13	HIS	-	expression tag	UNP K9TVC9
D	-12	HIS	-	expression tag	UNP K9TVC9
D	-11	HIS	-	expression tag	UNP K9TVC9
D	-10	HIS	-	expression tag	UNP K9TVC9
D	-9	SER	-	expression tag	UNP K9TVC9
D	-8	SER	-	expression tag	UNP K9TVC9
D	-7	GLY	-	expression tag	UNP K9TVC9
D	-6	LEU	-	expression tag	UNP K9TVC9
D	-5	VAL	-	expression tag	UNP K9TVC9
D	-4	PRO	-	expression tag	UNP K9TVC9
D	-3	ARG	-	expression tag	UNP K9TVC9
D	-2	GLY	-	expression tag	UNP K9TVC9
D	-1	SER	-	expression tag	UNP K9TVC9
D	0	HIS	-	expression tag	UNP K9TVC9

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



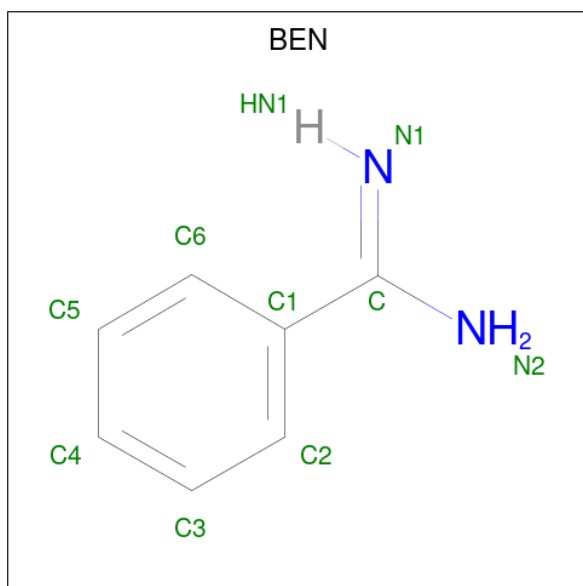
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

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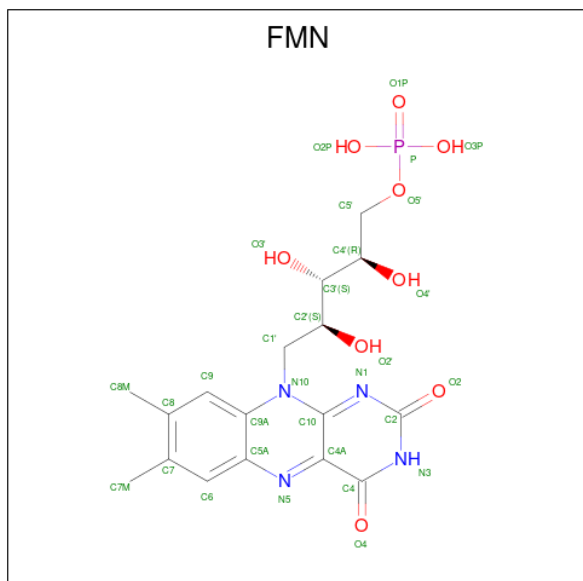
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			18	7	9	2		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	C	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	D	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	426	Total 426	O 426	0	0
5	B	356	Total 356	O 356	0	0
5	C	296	Total 296	O 296	0	0
5	D	314	Total 314	O 314	0	0

- Molecule 1: NADH:flavin oxidoreductase/NADH oxidase

- Molecule 1: NADH:flavin oxidoreductase/NADH oxidase

- Molecule 1: NADH:flavin oxidoreductase/NADH oxidase

- Molecule 1: NADH:flavin oxidoreductase/NADH oxidase

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	ARG	PRO	GLY	SER	HIS	M1	N4	I5	D6	E44	A47	Q48	R49	V50	A59	L67	R85	W103	L113	A125	P128	S129	V143	T144	I153	H178	Y200	E216	F249
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V253	L264	P269	R270	VAL	ALA	GLY	ASN	GLU	THR	VAL	GLU	ASN	PRO	THR	SER	E283	K287	Y293	L297	D316	F336	R347	F350	Y351	D354	L364	GLU	LEU	GLN	ALA	ALA	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.66Å 78.17Å 108.69Å 104.23° 99.98° 90.04°	Depositor
Resolution (Å)	48.86 – 1.35 48.86 – 1.35	Depositor EDS
% Data completeness (in resolution range)	90.9 (48.86-1.35) 90.9 (48.86-1.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.206 , 0.255 0.211 , 0.256	Depositor DCC
R_{free} test set	15465 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12468	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% 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: BEN, FMN, ACT

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	0.92	5/2783 (0.2%)	1.19	5/3784 (0.1%)
1	B	0.93	5/2814 (0.2%)	1.23	9/3825 (0.2%)
1	C	0.78	0/2778	1.18	3/3778 (0.1%)
1	D	0.81	2/2803 (0.1%)	1.15	9/3811 (0.2%)
All	All	0.86	12/11178 (0.1%)	1.19	26/15198 (0.2%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	HIS	CE1-NE2	8.97	1.41	1.32
1	A	227	VAL	C-O	-6.74	1.17	1.24
1	D	178	HIS	CE1-NE2	6.31	1.38	1.32
1	B	17	GLU	C-O	-6.07	1.17	1.24
1	D	269	PRO	C-O	-6.05	1.16	1.24

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ASP	CA-C-N	7.57	130.75	120.38
1	B	354	ASP	C-N-CA	7.57	130.75	120.38
1	B	140	LYS	O-C-N	-7.21	117.10	121.71
1	B	360	ASP	CA-CB-CG	7.10	119.70	112.60
1	D	4	ASN	CA-C-N	7.05	131.81	122.93

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	2718	0	2631	30	0
1	B	2749	0	2662	16	0
1	C	2713	0	2627	14	0
1	D	2738	0	2658	16	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	9	9	7	0	0
4	A	31	0	19	1	0
4	B	31	0	19	0	0
4	C	31	0	19	1	0
4	D	31	0	19	2	0
5	A	426	0	0	6	0
5	B	356	0	0	5	0
5	C	296	0	0	0	0
5	D	314	0	0	3	0
All	All	12459	9	10673	73	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 3.

The worst 5 of 73 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:355:LYS:HE2	1:D:143:VAL:HA	1.46	0.97
1:C:351:TYR:CE1	4:C:402:FMN:HM71	2.28	0.69
1:A:15:ARG:O	1:A:15:ARG:HG3	1.97	0.65
1:C:18:LEU:CD2	1:C:97:LYS:HD2	2.29	0.63
1:A:53:GLY:HA3	5:A:647:HOH:O	2.00	0.61

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/390 (89%)	333 (96%)	14 (4%)	0	100	100
1	B	350/390 (90%)	336 (96%)	14 (4%)	0	100	100
1	C	346/390 (89%)	332 (96%)	14 (4%)	0	100	100
1	D	349/390 (90%)	335 (96%)	14 (4%)	0	100	100
All	All	1392/1560 (89%)	1336 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/314 (90%)	279 (99%)	4 (1%)	59	28
1	B	286/314 (91%)	282 (99%)	4 (1%)	59	28
1	C	282/314 (90%)	276 (98%)	6 (2%)	47	15
1	D	285/314 (91%)	281 (99%)	4 (1%)	59	28
All	All	1136/1256 (90%)	1118 (98%)	18 (2%)	55	23

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	85	ARG
1	D	270	ARG
1	D	129	SER

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Mol	Chain	Res	Type
1	C	3	THR
1	C	294	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	36	ASN
1	C	36	ASN
1	D	30	ASN
1	D	258	GLN

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](#)

9 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	$\# Z > 2$
2	ACT	C	401	-	3,3,3	1.75	0	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMN	D	402	-	33,33,33	1.68	7 (21%)	48,50,50	1.99	16 (33%)
4	FMN	C	402	-	33,33,33	1.64	6 (18%)	48,50,50	1.85	15 (31%)
2	ACT	D	401	-	3,3,3	1.12	0	3,3,3	0.88	0
2	ACT	B	401	-	3,3,3	0.71	0	3,3,3	0.93	0
4	FMN	B	402	-	33,33,33	2.19	11 (33%)	48,50,50	2.45	15 (31%)
4	FMN	A	403	-	33,33,33	1.78	7 (21%)	48,50,50	1.54	9 (18%)
2	ACT	A	401	-	3,3,3	1.59	1 (33%)	3,3,3	0.77	0
3	BEN	A	402	-	9,9,9	0.67	0	7,11,11	0.85	1 (14%)

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	FMN	D	402	-	-	5/18/18/18	0/3/3/3
4	FMN	C	402	-	-	3/18/18/18	0/3/3/3
4	FMN	B	402	-	-	12/18/18/18	0/3/3/3
4	FMN	A	403	-	-	2/18/18/18	0/3/3/3
3	BEN	A	402	-	-	0/4/4/4	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	FMN	C5'-C4'	6.14	1.60	1.51
4	A	403	FMN	C9A-C5A	4.94	1.49	1.41
4	B	402	FMN	C9A-C5A	4.86	1.49	1.41
4	C	402	FMN	C1'-C2'	4.68	1.59	1.52
4	D	402	FMN	C9A-C5A	4.66	1.48	1.41

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	FMN	O4'-C4'-C3'	-6.26	94.59	109.25
4	B	402	FMN	O4'-C4'-C5'	6.00	123.21	109.99
4	D	402	FMN	O2'-C2'-C3'	-5.71	95.90	109.25
4	B	402	FMN	O2'-C2'-C3'	5.65	122.46	109.25
4	D	402	FMN	C5'-C4'-C3'	-5.56	101.72	112.22

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

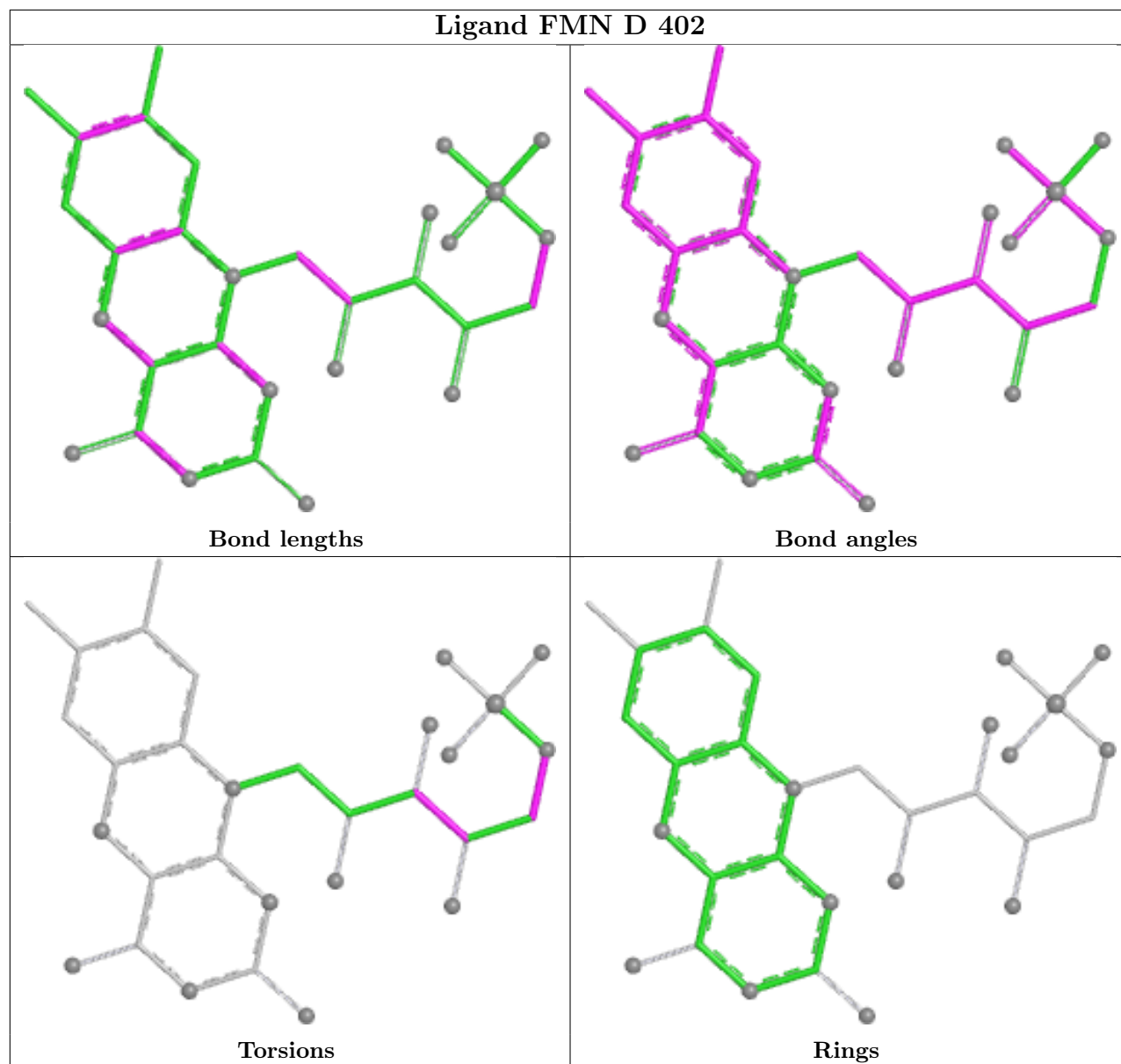
Mol	Chain	Res	Type	Atoms
4	B	402	FMN	N10-C1'-C2'-C3'
4	B	402	FMN	C1'-C2'-C3'-O3'
4	B	402	FMN	C1'-C2'-C3'-C4'
4	B	402	FMN	O2'-C2'-C3'-O3'
4	B	402	FMN	O2'-C2'-C3'-C4'

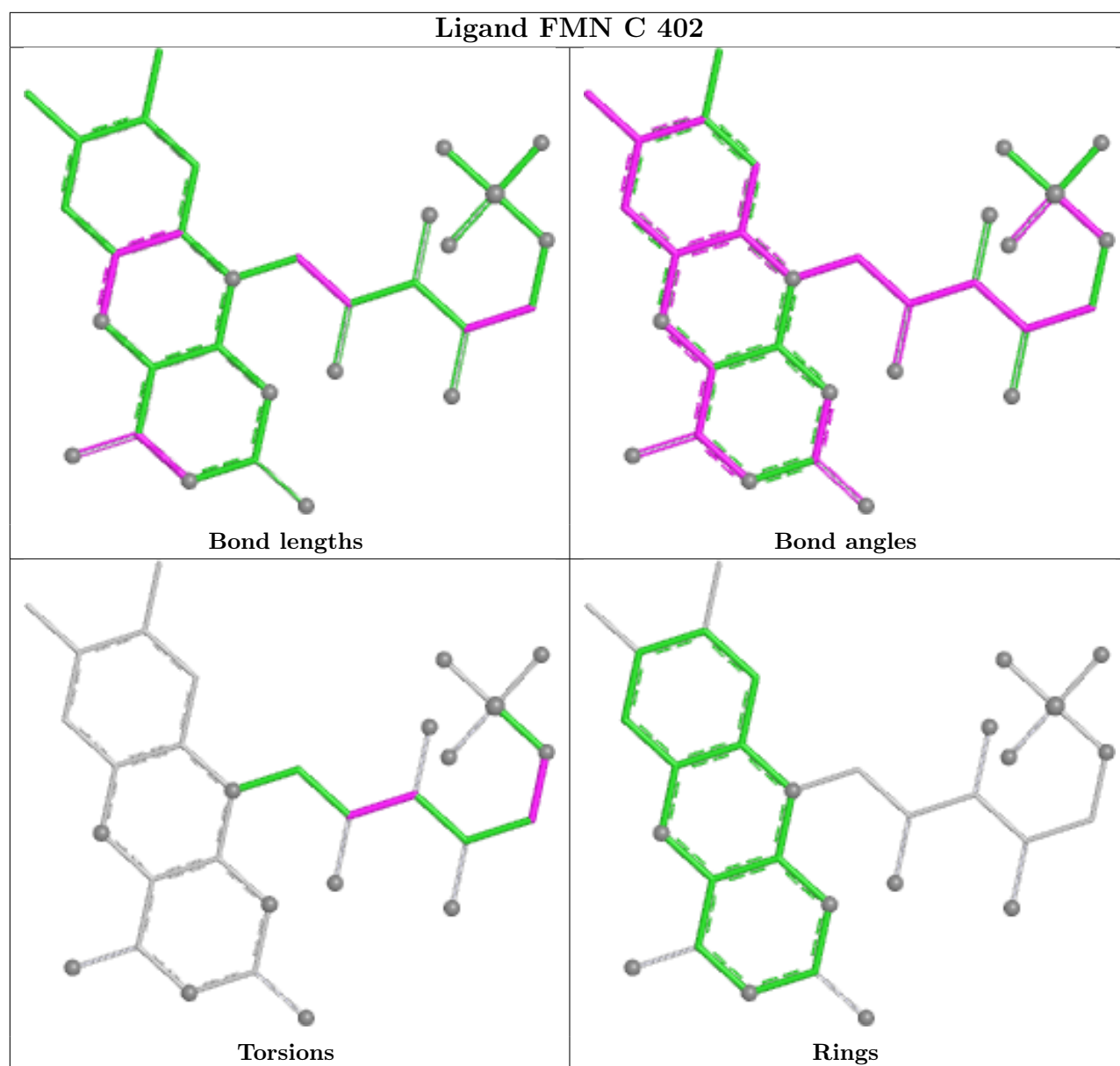
There are no ring outliers.

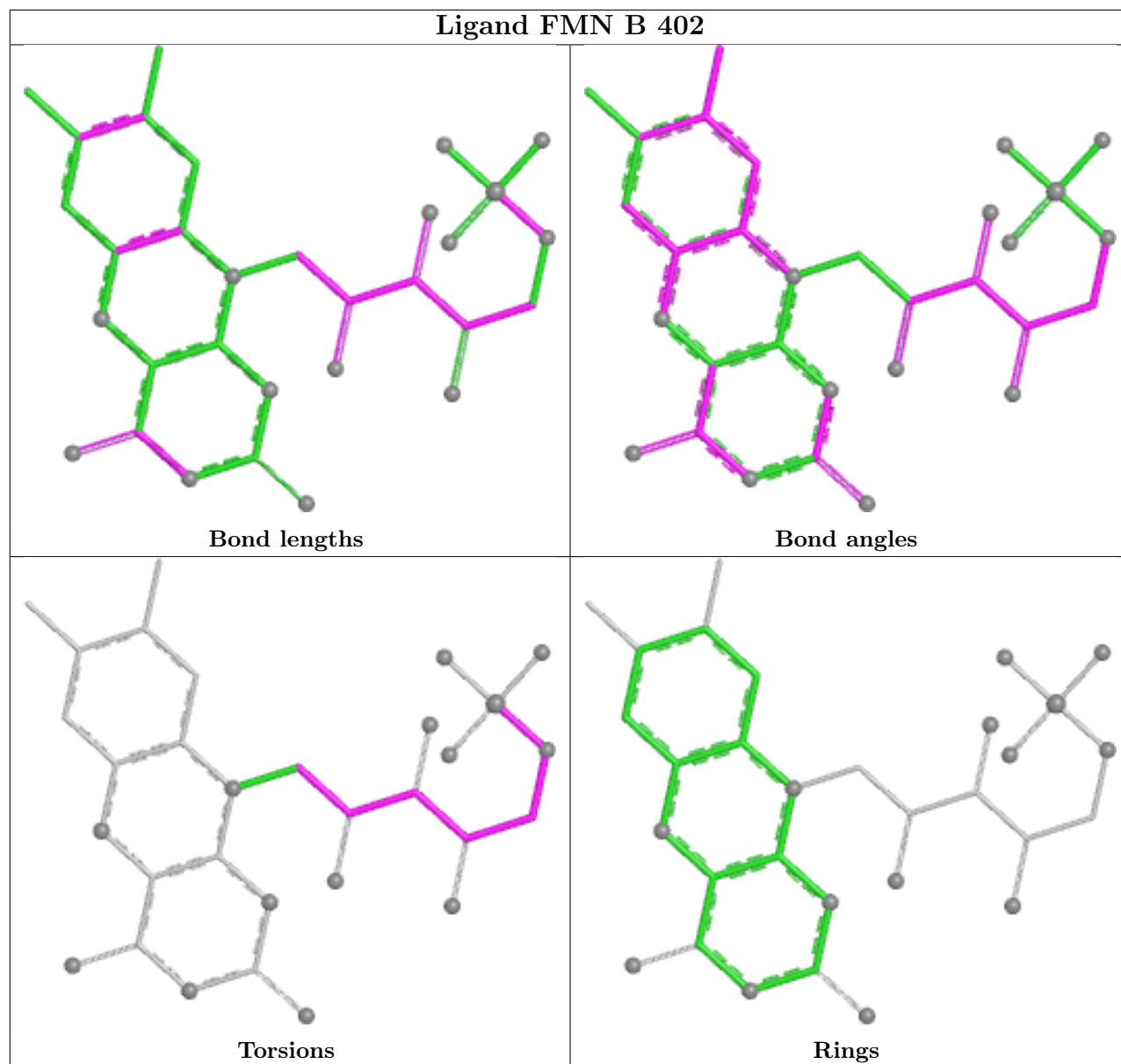
3 monomers are involved in 4 short contacts:

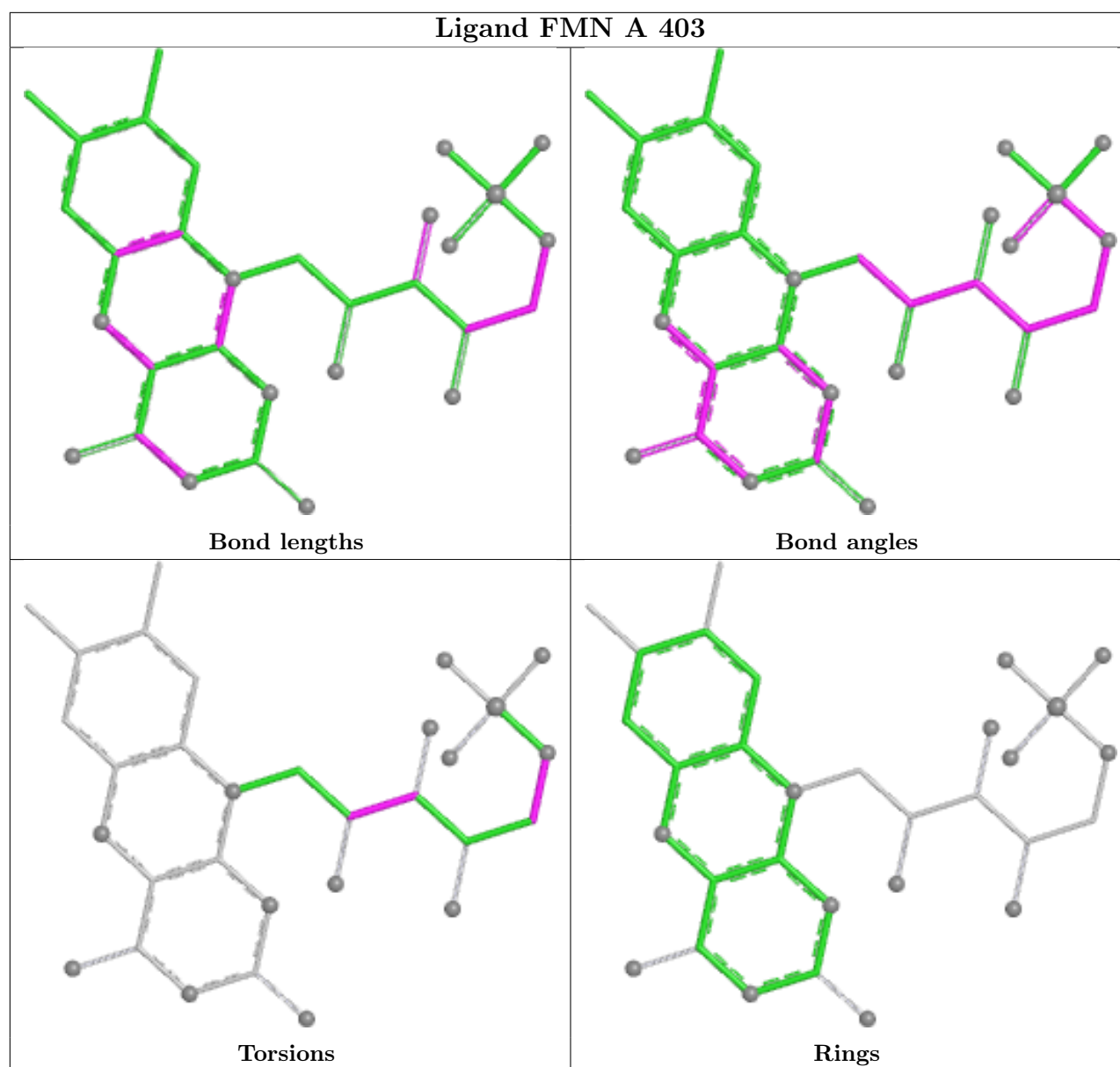
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402	FMN	2	0
4	C	402	FMN	1	0
4	A	403	FMN	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/390 (89%)	-0.82	1 (0%) 90 94	9, 13, 23, 48	1 (0%)
1	B	350/390 (89%)	-0.69	1 (0%) 90 94	6, 14, 34, 72	4 (1%)
1	C	349/390 (89%)	-0.64	1 (0%) 90 94	12, 17, 30, 41	1 (0%)
1	D	352/390 (90%)	-0.61	0 100 100	7, 18, 29, 47	1 (0%)
All	All	1401/1560 (89%)	-0.69	3 (0%) 91 95	6, 16, 30, 72	7 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	THR	3.0
1	A	235	GLY	2.4
1	C	3	THR	2.3

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

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

6.3 Carbohydrates [i](#)

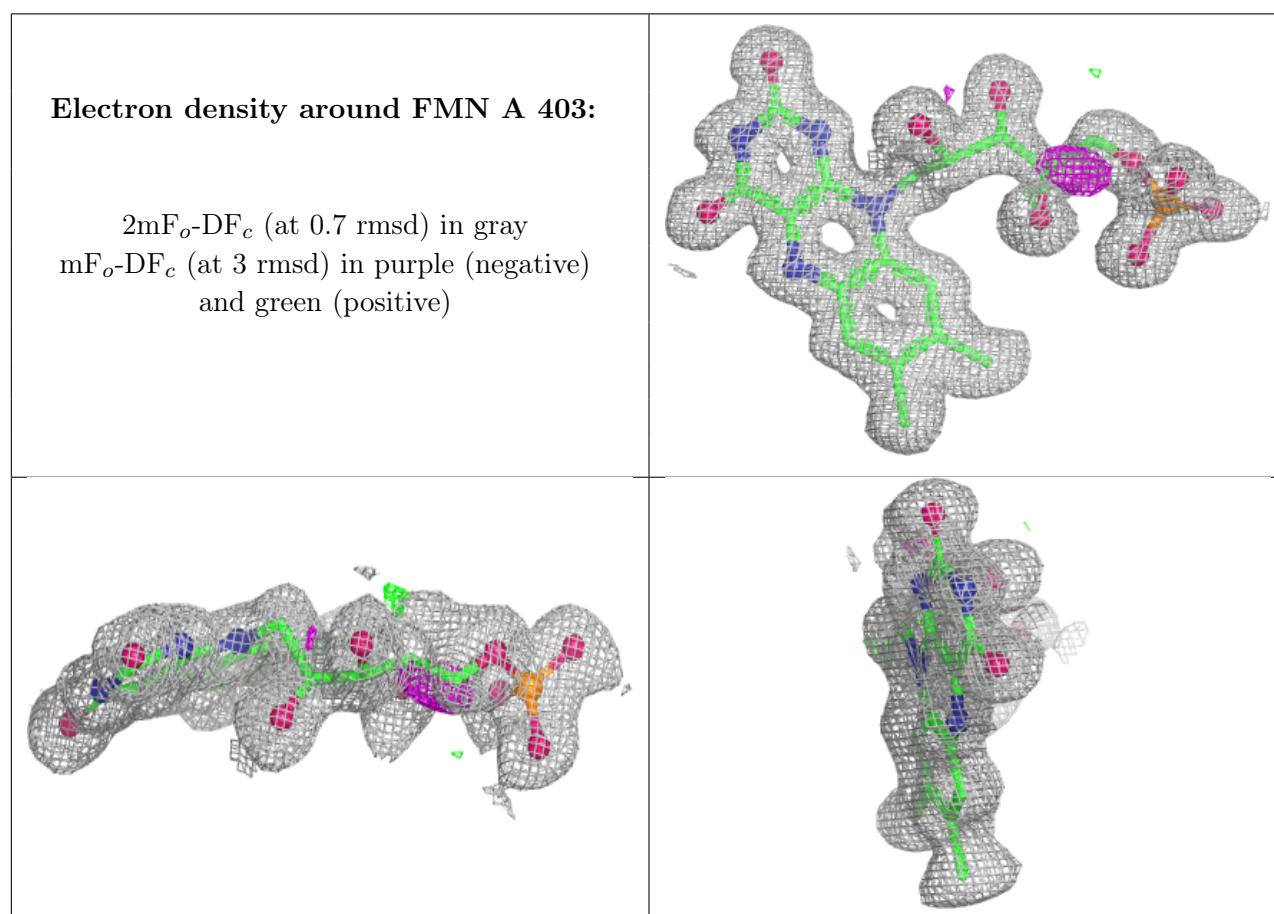
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

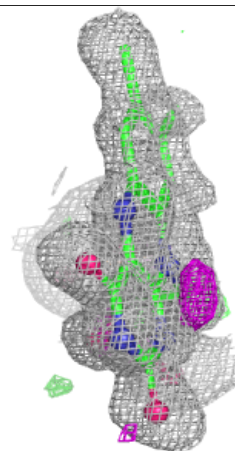
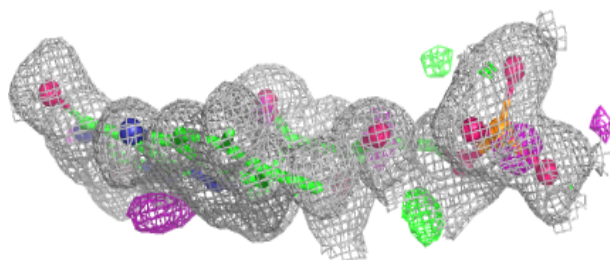
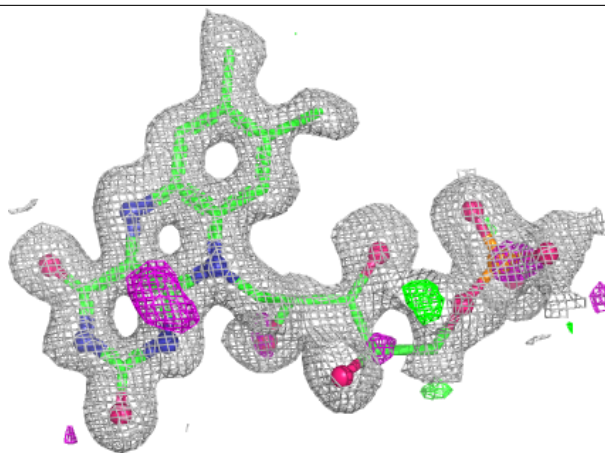
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BEN	A	402	9/9	0.98	0.04	20,20,20,20	0
2	ACT	B	401	4/4	0.99	0.05	15,19,20,24	0
2	ACT	C	401	4/4	0.99	0.06	15,17,21,21	0
2	ACT	D	401	4/4	0.99	0.03	15,17,19,22	0
2	ACT	A	401	4/4	0.99	0.03	11,13,16,19	0
4	FMN	A	403	31/31	0.99	0.03	8,11,16,17	0
4	FMN	B	402	31/31	0.99	0.04	11,15,25,26	0
4	FMN	C	402	31/31	0.99	0.04	10,14,18,20	0
4	FMN	D	402	31/31	0.99	0.04	11,14,21,26	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.



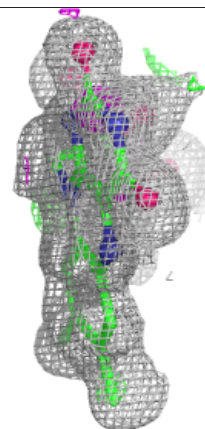
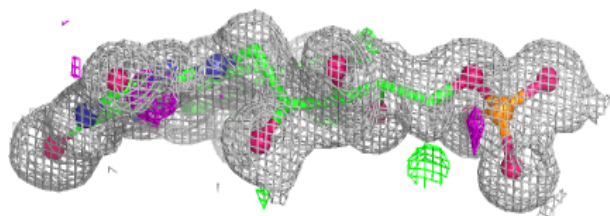
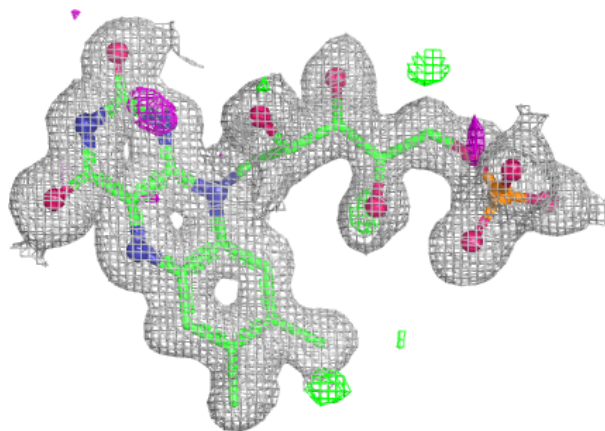
Electron density around FMN B 402:

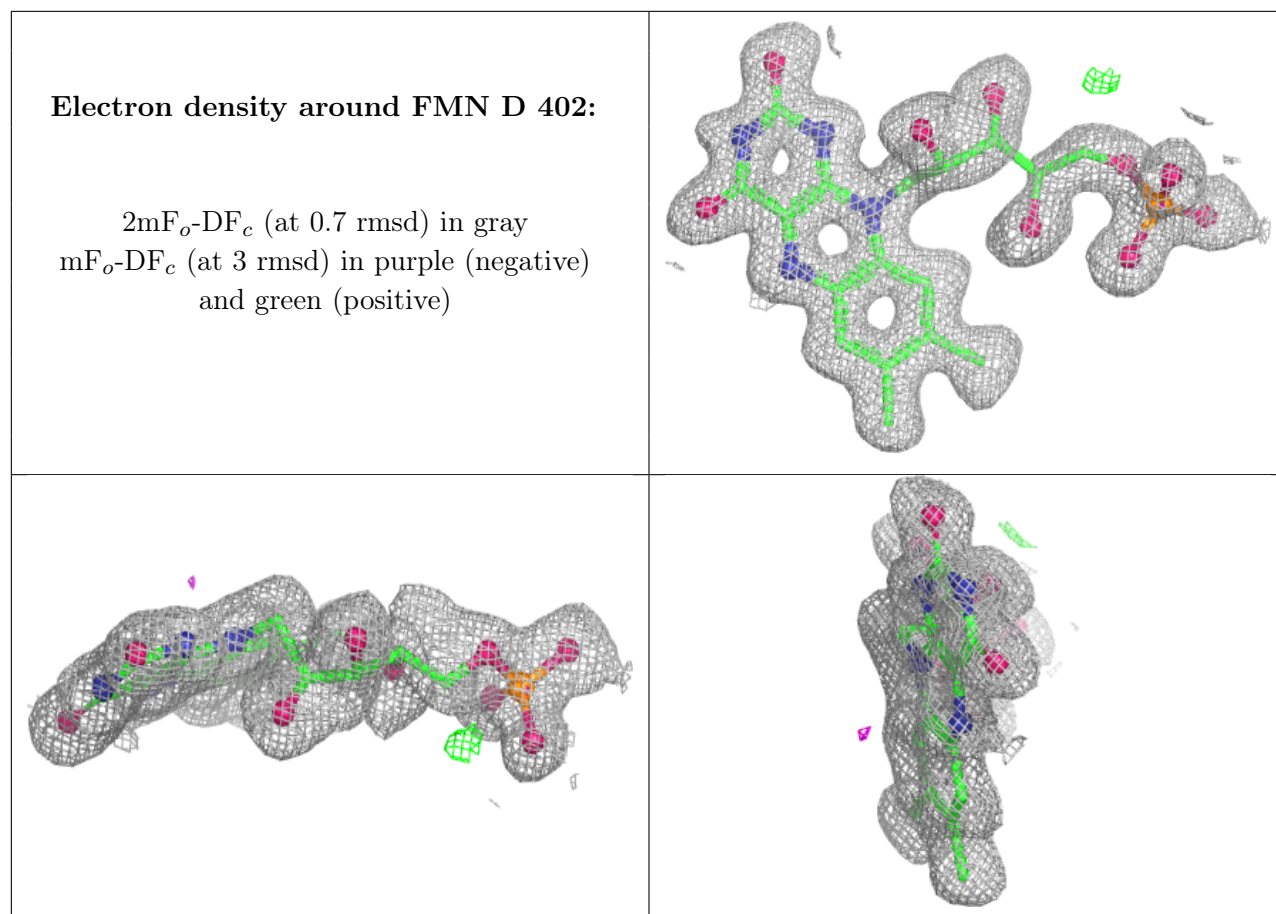
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.