



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:05 am BST

PDB ID : 6AJE
Title : Crystal structure of DHODH in complex with ferulenol from Eimeria tenella
Authors : Shiba, T.; Inaoka, D.K.; Sato, D.; Hartuti, E.D.; Amalia, E.; Nagahama, M.; Yoshioka, Y.; Matsubayashi, M.; Balogun, E.O.; Tsuji, N.; Kita, K.; Harada, S.
Deposited on : 2018-08-27
Resolution : 3.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

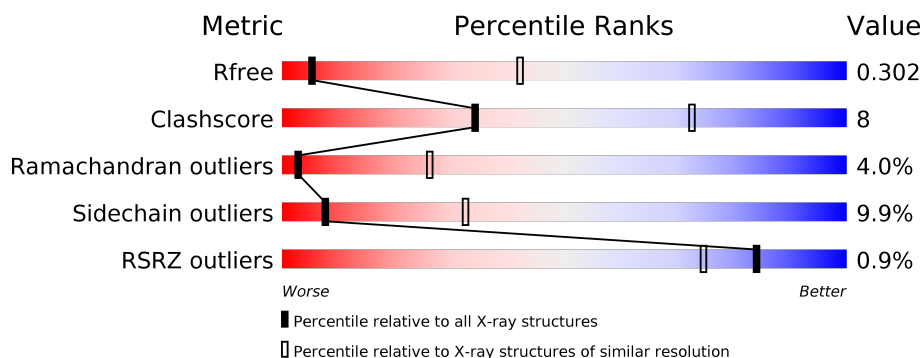
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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 on 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	436	
1	B	436	
1	C	436	
1	D	436	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12040 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 Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2953	1855	533	554	11			
1	B	376	Total	C	N	O	S	0	0	0
			2937	1846	528	552	11			
1	C	376	Total	C	N	O	S	0	0	0
			2937	1846	528	552	11			
1	D	376	Total	C	N	O	S	0	0	0
			2937	1846	528	552	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP U6KL66
A	-20	GLY	-	expression tag	UNP U6KL66
A	-19	HIS	-	expression tag	UNP U6KL66
A	-18	HIS	-	expression tag	UNP U6KL66
A	-17	HIS	-	expression tag	UNP U6KL66
A	-16	HIS	-	expression tag	UNP U6KL66
A	-15	HIS	-	expression tag	UNP U6KL66
A	-14	HIS	-	expression tag	UNP U6KL66
A	-13	HIS	-	expression tag	UNP U6KL66
A	-12	HIS	-	expression tag	UNP U6KL66
A	-11	HIS	-	expression tag	UNP U6KL66
A	-10	SER	-	expression tag	UNP U6KL66
A	-9	SER	-	expression tag	UNP U6KL66
A	-8	GLY	-	expression tag	UNP U6KL66
A	-7	HIS	-	expression tag	UNP U6KL66
A	-6	ILE	-	expression tag	UNP U6KL66
A	-5	ASP	-	expression tag	UNP U6KL66
A	-4	ASP	-	expression tag	UNP U6KL66
A	-3	ASP	-	expression tag	UNP U6KL66
A	-2	ASP	-	expression tag	UNP U6KL66
A	-1	LYS	-	expression tag	UNP U6KL66

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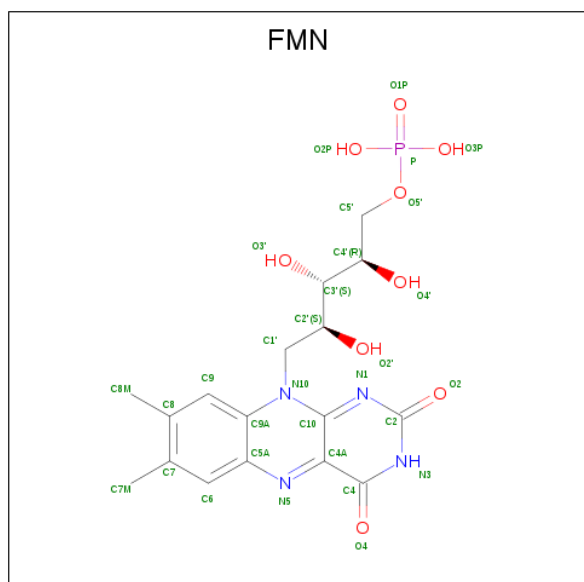
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP U6KL66
B	-21	MET	-	initiating methionine	UNP U6KL66
B	-20	GLY	-	expression tag	UNP U6KL66
B	-19	HIS	-	expression tag	UNP U6KL66
B	-18	HIS	-	expression tag	UNP U6KL66
B	-17	HIS	-	expression tag	UNP U6KL66
B	-16	HIS	-	expression tag	UNP U6KL66
B	-15	HIS	-	expression tag	UNP U6KL66
B	-14	HIS	-	expression tag	UNP U6KL66
B	-13	HIS	-	expression tag	UNP U6KL66
B	-12	HIS	-	expression tag	UNP U6KL66
B	-11	HIS	-	expression tag	UNP U6KL66
B	-10	SER	-	expression tag	UNP U6KL66
B	-9	SER	-	expression tag	UNP U6KL66
B	-8	GLY	-	expression tag	UNP U6KL66
B	-7	HIS	-	expression tag	UNP U6KL66
B	-6	ILE	-	expression tag	UNP U6KL66
B	-5	ASP	-	expression tag	UNP U6KL66
B	-4	ASP	-	expression tag	UNP U6KL66
B	-3	ASP	-	expression tag	UNP U6KL66
B	-2	ASP	-	expression tag	UNP U6KL66
B	-1	LYS	-	expression tag	UNP U6KL66
B	0	HIS	-	expression tag	UNP U6KL66
C	-21	MET	-	initiating methionine	UNP U6KL66
C	-20	GLY	-	expression tag	UNP U6KL66
C	-19	HIS	-	expression tag	UNP U6KL66
C	-18	HIS	-	expression tag	UNP U6KL66
C	-17	HIS	-	expression tag	UNP U6KL66
C	-16	HIS	-	expression tag	UNP U6KL66
C	-15	HIS	-	expression tag	UNP U6KL66
C	-14	HIS	-	expression tag	UNP U6KL66
C	-13	HIS	-	expression tag	UNP U6KL66
C	-12	HIS	-	expression tag	UNP U6KL66
C	-11	HIS	-	expression tag	UNP U6KL66
C	-10	SER	-	expression tag	UNP U6KL66
C	-9	SER	-	expression tag	UNP U6KL66
C	-8	GLY	-	expression tag	UNP U6KL66
C	-7	HIS	-	expression tag	UNP U6KL66
C	-6	ILE	-	expression tag	UNP U6KL66
C	-5	ASP	-	expression tag	UNP U6KL66
C	-4	ASP	-	expression tag	UNP U6KL66
C	-3	ASP	-	expression tag	UNP U6KL66

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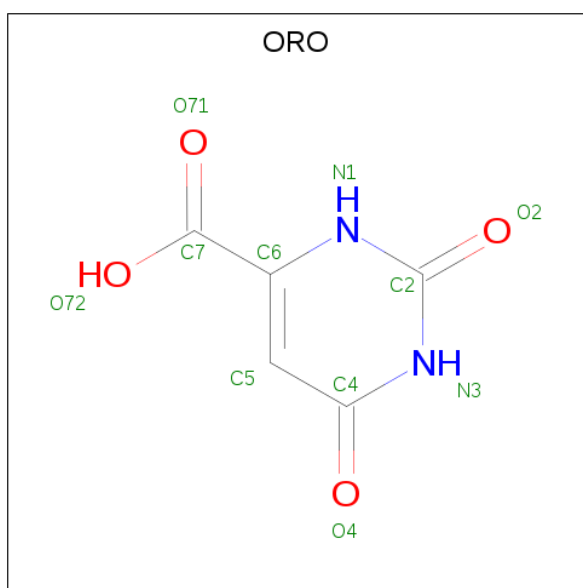
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ASP	-	expression tag	UNP U6KL66
C	-1	LYS	-	expression tag	UNP U6KL66
C	0	HIS	-	expression tag	UNP U6KL66
D	-21	MET	-	initiating methionine	UNP U6KL66
D	-20	GLY	-	expression tag	UNP U6KL66
D	-19	HIS	-	expression tag	UNP U6KL66
D	-18	HIS	-	expression tag	UNP U6KL66
D	-17	HIS	-	expression tag	UNP U6KL66
D	-16	HIS	-	expression tag	UNP U6KL66
D	-15	HIS	-	expression tag	UNP U6KL66
D	-14	HIS	-	expression tag	UNP U6KL66
D	-13	HIS	-	expression tag	UNP U6KL66
D	-12	HIS	-	expression tag	UNP U6KL66
D	-11	HIS	-	expression tag	UNP U6KL66
D	-10	SER	-	expression tag	UNP U6KL66
D	-9	SER	-	expression tag	UNP U6KL66
D	-8	GLY	-	expression tag	UNP U6KL66
D	-7	HIS	-	expression tag	UNP U6KL66
D	-6	ILE	-	expression tag	UNP U6KL66
D	-5	ASP	-	expression tag	UNP U6KL66
D	-4	ASP	-	expression tag	UNP U6KL66
D	-3	ASP	-	expression tag	UNP U6KL66
D	-2	ASP	-	expression tag	UNP U6KL66
D	-1	LYS	-	expression tag	UNP U6KL66
D	0	HIS	-	expression tag	UNP U6KL66

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



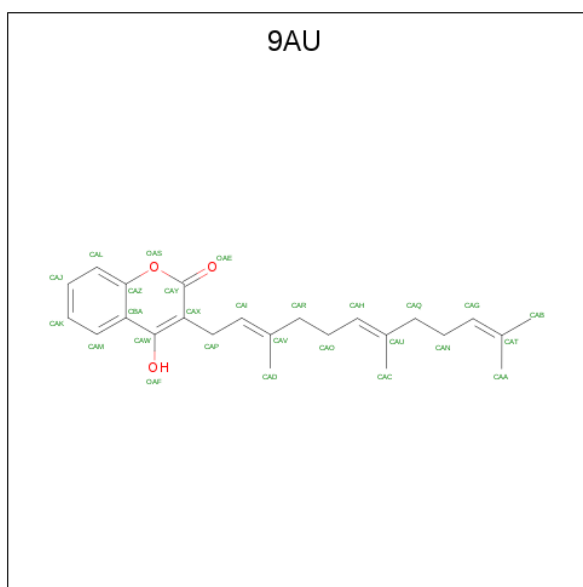
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		
3	B	1	Total	C	N	O	0	0
			11	5	2	4		
3	C	1	Total	C	N	O	0	0
			11	5	2	4		
3	D	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is 4-oxidanyl-3-[(2 {E},6 {E})-3,7,11-trimethyldodeca-2,6,10-trienyl]chromen-2-one (three-letter code: 9AU) (formula: $C_{24}H_{30}O_3$).

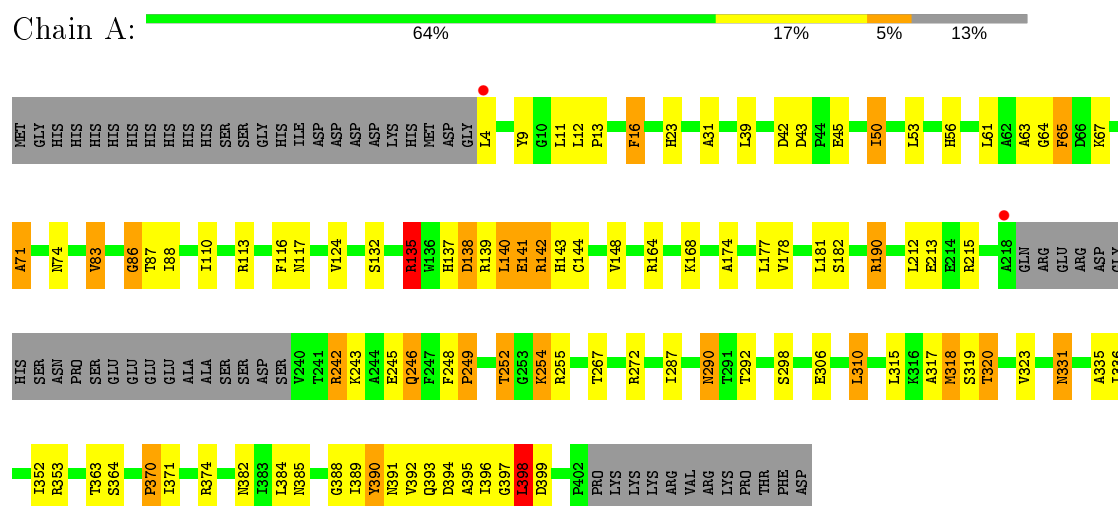


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 27	C 24	O 3	0	0
4	B	1	Total 27	C 24	O 3	0	0
4	C	1	Total 27	C 24	O 3	0	0
4	D	1	Total 27	C 24	O 3	0	0

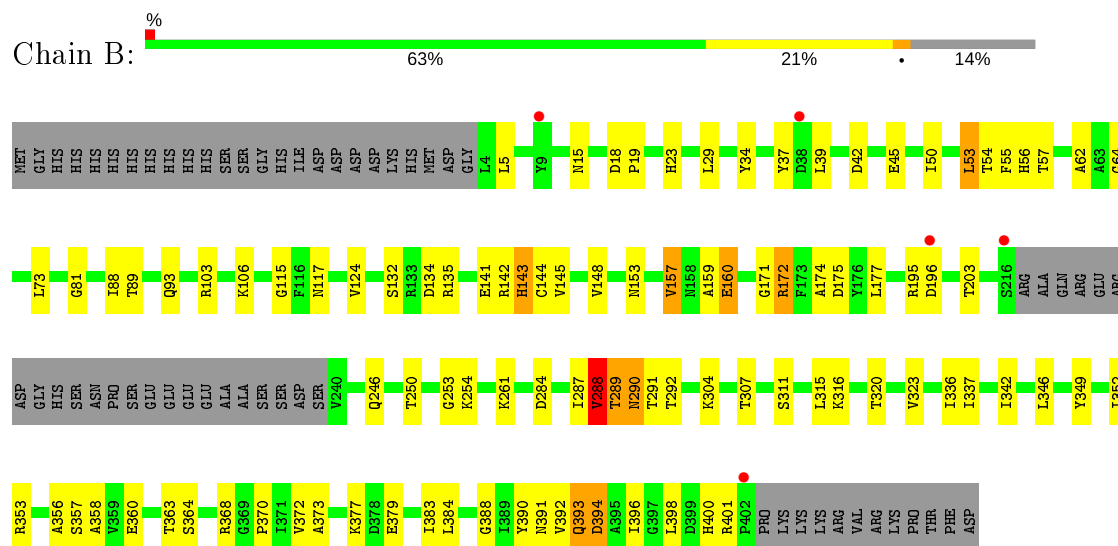
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Dihydroorotate dehydrogenase (quinone), mitochondrial

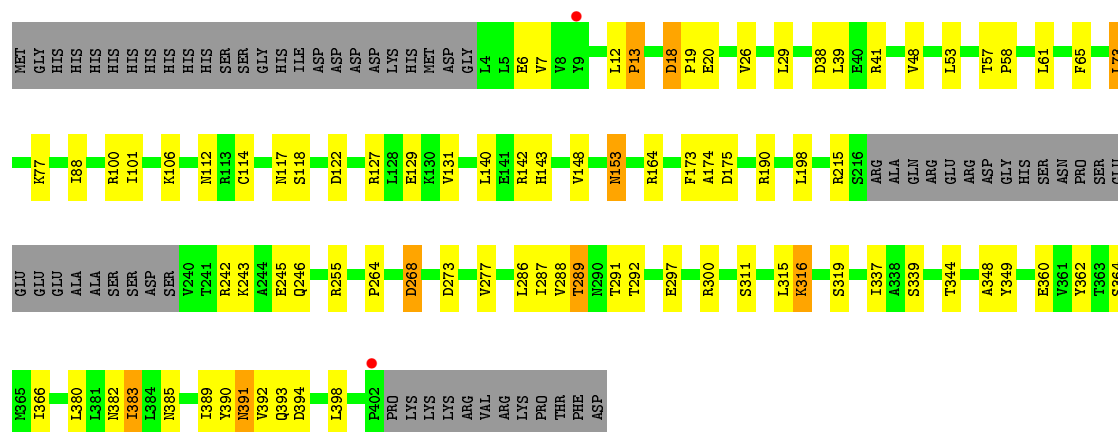


- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial

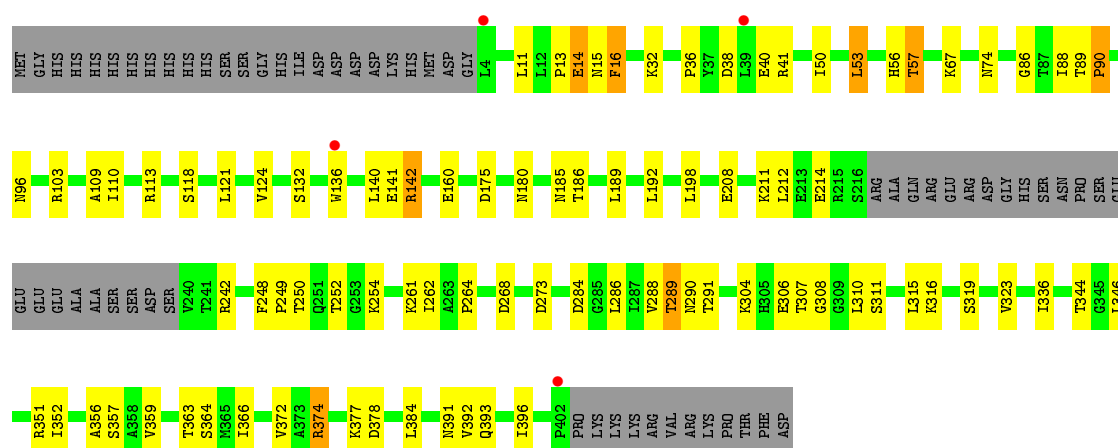


- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial





- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	132.98Å 132.98Å 215.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.65 19.87 – 3.65	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-3.65) 93.0 (19.87-3.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.303 0.224 , 0.302	Depositor DCC
R_{free} test set	1089 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12040	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: FMN, 9AU, ORO

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	0.48	0/3004	0.78	1/4060 (0.0%)
1	B	0.47	0/2988	0.77	2/4039 (0.0%)
1	C	0.46	0/2988	0.75	0/4039
1	D	0.47	0/2988	0.73	0/4039
All	All	0.47	0/11968	0.76	3/16177 (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	3
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	VAL	N-CA-C	7.29	130.70	111.00
1	B	288	VAL	CB-CA-C	-5.04	101.82	111.40
1	A	135	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	PHE	Peptide
1	A	248	PHE	Peptide
1	A	86	GLY	Peptide
1	B	134	ASP	Peptide
1	B	246	GLN	Peptide
1	B	37	TYR	Peptide
1	C	39	LEU	Peptide
1	D	16	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2953	0	2990	69	0
1	B	2937	0	2974	63	0
1	C	2937	0	2972	39	0
1	D	2937	0	2972	42	0
2	A	31	0	19	2	0
2	B	31	0	19	2	0
2	C	31	0	19	0	0
2	D	31	0	19	1	0
3	A	11	0	3	0	0
3	B	11	0	3	1	0
3	C	11	0	3	0	0
3	D	11	0	3	0	0
4	A	27	0	0	1	0
4	B	27	0	0	2	0
4	C	27	0	0	1	0
4	D	27	0	0	1	0
All	All	12040	0	11996	201	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 8.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:NH2	1:B:391:ASN:ND2	1.89	1.20
1:B:45:GLU:O	1:B:392:VAL:HG12	1.56	1.04
1:A:272:ARG:NH2	1:B:391:ASN:HD22	1.49	1.03
1:A:272:ARG:HH21	1:B:391:ASN:HD22	1.01	0.99
1:B:288:VAL:HG12	1:B:289:THR:N	1.79	0.96
1:A:272:ARG:CZ	1:B:391:ASN:ND2	2.29	0.96
1:A:388:GLY:O	1:A:390:TYR:CE1	2.19	0.95
1:C:390:TYR:O	1:C:391:ASN:ND2	2.07	0.88
1:D:391:ASN:OD1	1:D:393:GLN:N	2.10	0.85
1:B:288:VAL:HG21	1:B:323:VAL:HG22	1.59	0.83
1:A:396:ILE:HD12	1:A:396:ILE:H	1.43	0.81
1:A:272:ARG:HH21	1:B:391:ASN:ND2	1.63	0.75
1:C:385:ASN:HA	1:C:390:TYR:CE1	2.21	0.75
1:A:385:ASN:HA	1:A:390:TYR:CE1	2.22	0.74
1:B:56:HIS:HB2	1:B:143:HIS:HB2	1.68	0.74
1:A:272:ARG:CZ	1:B:391:ASN:HD22	1.98	0.74
1:B:288:VAL:HG23	1:B:336:ILE:HG23	1.70	0.73
1:B:288:VAL:CG1	1:B:289:THR:N	2.53	0.70
1:D:391:ASN:HD21	1:D:393:GLN:HB3	1.56	0.70
1:A:272:ARG:NH2	1:B:394:ASP:OD1	2.25	0.68
1:D:391:ASN:ND2	1:D:393:GLN:HB3	2.09	0.68
1:A:397:GLY:O	1:A:399:ASP:N	2.27	0.68
1:C:288:VAL:HG12	1:C:289:THR:HG23	1.77	0.66
1:B:357:SER:HA	1:B:396:ILE:HD13	1.78	0.66
1:B:171:GLY:HA2	1:B:177:LEU:HD21	1.75	0.66
1:A:272:ARG:CZ	1:B:391:ASN:HD21	2.08	0.65
1:A:393:GLN:HA	1:A:396:ILE:CD1	2.27	0.64
1:C:391:ASN:HB2	1:C:394:ASP:HB2	1.80	0.63
1:A:384:LEU:HD11	1:A:392:VAL:CG1	2.30	0.62
1:A:272:ARG:NE	1:B:391:ASN:ND2	2.47	0.62
1:B:53:LEU:HD11	1:B:175:ASP:HB3	1.80	0.62
1:C:292:THR:HG22	1:C:315:LEU:HD11	1.83	0.61
1:A:390:TYR:O	1:A:391:ASN:HB2	2.01	0.61
1:C:291:THR:HG22	1:C:311:SER:HB3	1.83	0.61
1:D:88:ILE:HG12	1:D:124:VAL:HG11	1.82	0.61
1:A:393:GLN:HA	1:A:396:ILE:HD11	1.83	0.60
1:A:397:GLY:O	1:A:398:LEU:C	2.40	0.59
1:B:388:GLY:HA2	1:B:390:TYR:HE2	1.67	0.59
1:A:392:VAL:O	1:A:396:ILE:HD12	2.02	0.59
1:A:178:VAL:HG11	1:A:287:ILE:HD12	1.84	0.58
1:B:390:TYR:H	1:B:390:TYR:HD2	1.50	0.58
1:D:175:ASP:HA	1:D:250:THR:HG23	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLY:HA2	1:B:390:TYR:CE2	2.39	0.58
1:D:288:VAL:HG11	1:D:323:VAL:HG22	1.85	0.58
1:C:48:VAL:HG22	1:C:392:VAL:HG23	1.86	0.57
1:B:357:SER:CB	1:B:396:ILE:HD13	2.34	0.57
1:C:122:ASP:O	1:D:307:THR:HG21	2.04	0.57
1:A:135:ARG:HD3	1:A:143:HIS:CE1	2.40	0.56
1:D:393:GLN:HA	1:D:393:GLN:OE1	2.05	0.56
1:B:390:TYR:N	1:B:390:TYR:CD2	2.73	0.56
1:D:140:LEU:HD12	1:D:140:LEU:O	2.06	0.55
1:A:384:LEU:HD11	1:A:392:VAL:HG12	1.87	0.55
1:C:6:GLU:HG3	1:C:7:VAL:HG23	1.88	0.55
1:B:391:ASN:OD1	1:B:392:VAL:N	2.39	0.55
1:C:100:ARG:HD2	1:C:114:CYS:HA	1.88	0.55
1:A:323:VAL:HG13	1:A:336:ILE:HG21	1.88	0.54
1:B:394:ASP:N	1:B:394:ASP:OD1	2.36	0.54
1:A:292:THR:HG23	1:A:310:LEU:HD23	1.90	0.54
1:B:88:ILE:HD13	1:B:124:VAL:HG11	1.90	0.54
1:A:390:TYR:N	1:A:390:TYR:CD1	2.73	0.54
1:B:352:ILE:HG23	1:B:396:ILE:HG12	1.89	0.54
1:B:148:VAL:CG2	1:B:174:ALA:HB2	2.37	0.54
1:A:87:THR:HG21	1:A:116:PHE:CZ	2.43	0.53
1:B:103:ARG:NH2	4:B:503:9AU:OAF	2.41	0.53
1:C:289:THR:HG21	1:C:319:SER:HA	1.90	0.53
1:B:288:VAL:CG2	1:B:336:ILE:HG23	2.36	0.53
1:B:45:GLU:OE1	1:B:391:ASN:HB2	2.09	0.53
1:A:389:ILE:HD12	1:A:395:ALA:HB2	1.91	0.53
1:D:323:VAL:HG13	1:D:336:ILE:HG21	1.90	0.53
1:B:261:LYS:HD3	1:B:290:ASN:HD22	1.74	0.52
1:C:385:ASN:HA	1:C:390:TYR:HE1	1.73	0.52
1:B:349:TYR:CE1	1:B:384:LEU:HD23	2.45	0.52
1:D:38:ASP:HB2	1:D:374:ARG:NH1	2.24	0.52
1:B:57:THR:HG21	1:B:377:LYS:CD	2.39	0.52
1:B:288:VAL:HG23	1:B:336:ILE:CG2	2.37	0.52
1:B:57:THR:HG21	1:B:377:LYS:HD3	1.91	0.52
1:D:261:LYS:NZ	2:D:501:FMN:O2'	2.42	0.52
1:D:67:LYS:HA	1:D:86:GLY:CA	2.40	0.52
1:A:148:VAL:HB	1:A:174:ALA:HB2	1.91	0.51
1:C:289:THR:HG21	1:C:319:SER:CB	2.40	0.51
1:A:272:ARG:NE	1:B:391:ASN:HD22	2.06	0.51
1:D:208:GLU:HA	1:D:211:LYS:HD2	1.93	0.51
1:D:57:THR:HG21	1:D:377:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:HA	1:A:86:GLY:CA	2.41	0.51
1:C:392:VAL:HG23	1:C:393:GLN:N	2.25	0.51
1:B:62:ALA:HB2	1:B:360:GLU:HB3	1.93	0.50
1:D:103:ARG:NH1	4:D:503:9AU:OAF	2.40	0.50
1:D:113:ARG:NH2	1:D:306:GLU:OE2	2.44	0.50
1:D:357:SER:HA	1:D:396:ILE:HD13	1.92	0.50
1:A:67:LYS:HA	1:A:86:GLY:HA2	1.93	0.50
1:A:181:LEU:O	1:A:190:ARG:HA	2.11	0.49
1:D:288:VAL:HG12	1:D:289:THR:HG23	1.93	0.49
1:A:138:ASP:OD1	1:A:139:ARG:N	2.39	0.49
1:B:357:SER:CA	1:B:396:ILE:HD13	2.41	0.49
1:B:288:VAL:CG2	1:B:336:ILE:CG2	2.90	0.49
1:C:129:GLU:HA	1:C:173:PHE:CE1	2.48	0.49
1:D:212:LEU:HD13	1:D:254:LYS:HD2	1.94	0.49
1:B:171:GLY:CA	1:B:177:LEU:HD21	2.42	0.48
1:B:373:ALA:O	1:B:377:LYS:HG3	2.13	0.48
1:C:339:SER:HB3	1:C:360:GLU:HB2	1.96	0.48
1:A:61:LEU:HB3	1:A:83:VAL:HG12	1.94	0.48
1:A:113:ARG:NH2	1:A:306:GLU:OE2	2.47	0.48
1:C:153:ASN:OD1	1:C:153:ASN:N	2.47	0.48
1:B:89:THR:HB	1:B:153:ASN:OD1	2.14	0.48
1:B:346:LEU:HA	1:B:383:ILE:HD13	1.96	0.47
1:B:363:THR:HG23	2:B:501:FMN:O3P	2.15	0.47
1:D:89:THR:OG1	1:D:118:SER:OG	2.32	0.47
1:B:56:HIS:CD2	1:B:143:HIS:CD2	3.03	0.47
1:A:87:THR:HG21	1:A:116:PHE:CE2	2.49	0.47
1:D:67:LYS:HA	1:D:86:GLY:HA3	1.95	0.47
1:A:315:LEU:HD12	1:A:318:MET:CB	2.45	0.47
1:A:353:ARG:O	1:A:397:GLY:HA2	2.14	0.46
1:A:397:GLY:C	1:A:399:ASP:N	2.69	0.46
1:A:74:ASN:N	1:A:74:ASN:HD22	2.14	0.46
1:A:246:GLN:HE21	1:A:246:GLN:HA	1.79	0.46
1:A:389:ILE:C	1:A:390:TYR:CD1	2.89	0.46
1:B:291:THR:HG22	1:B:311:SER:HB3	1.97	0.46
1:D:289:THR:HG21	1:D:319:SER:HA	1.97	0.46
1:D:50:ILE:HD12	1:D:357:SER:HB2	1.98	0.46
1:A:331:ASN:ND2	1:B:393:GLN:OE1	2.48	0.46
1:A:395:ALA:O	1:A:398:LEU:HB2	2.15	0.46
1:B:353:ARG:NH2	1:B:398:LEU:HD12	2.31	0.45
1:B:368:ARG:HG2	1:B:372:VAL:HG23	1.97	0.45
1:C:12:LEU:N	1:C:13:PRO:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD11	1:A:335:ALA:HB1	1.98	0.45
1:A:353:ARG:O	1:A:397:GLY:CA	2.64	0.45
1:A:65:PHE:O	1:A:67:LYS:N	2.50	0.45
1:B:337:ILE:HG23	1:B:358:ALA:HB3	1.99	0.45
1:A:56:HIS:CE1	1:A:142:ARG:HB3	2.52	0.45
1:D:110:ILE:HD12	1:D:363:THR:HG23	1.99	0.45
1:C:385:ASN:HA	1:C:390:TYR:CD1	2.52	0.45
1:A:132:SER:OG	1:A:249:PRO:HG2	2.17	0.44
1:A:392:VAL:O	1:A:395:ALA:N	2.50	0.44
1:D:262:ILE:HD11	1:D:286:LEU:HD22	1.98	0.44
1:A:148:VAL:CG2	1:A:174:ALA:HB2	2.48	0.44
1:C:315:LEU:O	1:C:316:LYS:C	2.56	0.44
1:D:185:ASN:HD21	1:D:308:GLY:HA2	1.83	0.43
1:C:61:LEU:HD21	1:C:65:PHE:HB3	1.99	0.43
1:B:352:ILE:HA	1:B:356:ALA:O	2.18	0.43
1:C:366:ILE:HG22	1:C:366:ILE:O	2.19	0.43
1:D:248:PHE:N	1:D:249:PRO:HD3	2.33	0.43
1:C:73:LEU:HD22	1:C:77:LYS:NZ	2.33	0.43
1:A:393:GLN:CA	1:A:396:ILE:CD1	2.95	0.43
1:A:12:LEU:N	1:A:13:PRO:CD	2.82	0.43
1:B:357:SER:HB2	1:B:396:ILE:HD13	2.01	0.43
1:B:357:SER:HA	1:B:396:ILE:CD1	2.47	0.43
1:C:287:ILE:HA	1:C:337:ILE:O	2.19	0.43
1:D:291:THR:HG22	1:D:311:SER:HB3	2.00	0.43
1:A:182:SER:HB2	1:A:290:ASN:HB2	2.01	0.43
1:C:26:VAL:HG21	4:C:503:9AU:OAE	2.19	0.43
1:D:248:PHE:N	1:D:249:PRO:CD	2.82	0.43
1:A:317:ALA:HA	1:A:320:THR:HG22	2.01	0.43
1:A:64:GLY:HA2	2:A:501:FMN:N5	2.34	0.43
1:B:55:PHE:CZ	1:B:145:VAL:HG11	2.54	0.42
1:D:109:ALA:HB1	1:D:310:LEU:HD11	2.01	0.42
1:D:56:HIS:ND1	1:D:142:ARG:HG2	2.34	0.42
1:C:101:ILE:HG22	1:C:112:ASN:HB2	2.01	0.42
1:A:31:ALA:HA	1:A:71:ALA:HB2	2.02	0.42
1:C:148:VAL:CG2	1:C:174:ALA:HB2	2.49	0.42
1:A:45:GLU:HA	1:A:391:ASN:OD1	2.19	0.42
1:C:53:LEU:HD11	1:C:175:ASP:HB3	2.00	0.42
1:A:61:LEU:HD21	1:A:65:PHE:HB3	2.02	0.42
1:C:77:LYS:HG2	1:C:140:LEU:HD22	2.01	0.42
1:A:110:ILE:HG13	1:A:363:THR:HG23	2.01	0.42
1:D:384:LEU:HD11	1:D:392:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:O	1:A:177:LEU:HD23	2.20	0.42
1:B:23:HIS:HB2	4:B:503:9AU:CAJ	2.50	0.42
1:D:90:PRO:HA	1:D:121:LEU:HD12	2.01	0.42
1:D:391:ASN:CG	1:D:393:GLN:HB3	2.40	0.42
1:A:141:GLU:O	1:A:143:HIS:N	2.53	0.42
1:C:48:VAL:CG2	1:C:392:VAL:HG23	2.49	0.42
1:A:63:ALA:HB3	2:A:501:FMN:C2	2.50	0.42
1:C:127:ARG:O	1:C:131:VAL:HG23	2.20	0.42
1:C:289:THR:HG21	1:C:319:SER:CA	2.50	0.42
1:B:261:LYS:HA	1:B:287:ILE:O	2.20	0.41
1:C:117:ASN:N	1:C:117:ASN:OD1	2.53	0.41
1:B:57:THR:HB	1:B:81:GLY:HA3	2.02	0.41
1:A:88:ILE:HD13	1:A:124:VAL:HG11	2.02	0.41
1:C:392:VAL:CG2	1:C:393:GLN:N	2.83	0.41
1:B:115:GLY:N	3:B:502:ORO:O71	2.46	0.41
1:D:352:ILE:HA	1:D:356:ALA:O	2.19	0.41
1:C:390:TYR:O	1:C:391:ASN:CB	2.68	0.41
1:D:180:ASN:O	1:D:189:LEU:HD21	2.21	0.41
1:A:254:LYS:O	1:A:255:ARG:C	2.58	0.41
1:A:352:ILE:O	1:A:396:ILE:HA	2.20	0.41
1:C:18:ASP:OD2	1:C:20:GLU:N	2.53	0.41
1:B:323:VAL:HG13	1:B:336:ILE:HG21	2.03	0.41
1:D:74:ASN:N	1:D:74:ASN:HD22	2.19	0.41
1:B:288:VAL:HG12	1:B:289:THR:CA	2.49	0.41
1:B:292:THR:HG22	1:B:315:LEU:HD11	2.03	0.41
1:B:64:GLY:HA3	2:B:501:FMN:N5	2.36	0.41
1:D:50:ILE:HD12	1:D:357:SER:CB	2.51	0.40
1:C:273:ASP:O	1:C:277:VAL:HG23	2.21	0.40
1:C:349:TYR:HB2	1:C:383:ILE:HD13	2.03	0.40
1:D:53:LEU:HD11	1:D:175:ASP:HB3	2.03	0.40
1:A:212:LEU:HD11	1:A:255:ARG:NH2	2.36	0.40
1:A:23:HIS:HB2	4:A:503:9AU:CAL	2.52	0.40
1:D:185:ASN:HD21	1:D:308:GLY:CA	2.35	0.40
1:C:348:ALA:HB3	1:C:380:LEU:HD13	2.03	0.40
1:A:315:LEU:HD12	1:A:318:MET:HB2	2.04	0.40
1:D:366:ILE:N	1:D:366:ILE:HD13	2.37	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	374/436 (86%)	303 (81%)	54 (14%)	17 (4%)	2	23
1	B	372/436 (85%)	306 (82%)	50 (13%)	16 (4%)	2	24
1	C	372/436 (85%)	309 (83%)	47 (13%)	16 (4%)	2	24
1	D	372/436 (85%)	325 (87%)	37 (10%)	10 (3%)	5	33
All	All	1490/1744 (85%)	1243 (83%)	188 (13%)	59 (4%)	3	26

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASP
1	A	242	ARG
1	A	252	THR
1	A	254	LYS
1	B	34	TYR
1	B	135	ARG
1	C	344	THR
1	D	316	LYS
1	A	140	LEU
1	A	144	CYS
1	A	298	SER
1	A	370	PRO
1	A	398	LEU
1	B	117	ASN
1	B	172	ARG
1	B	253	GLY
1	B	288	VAL
1	B	289	THR
1	C	41	ARG
1	C	215	ARG
1	C	391	ASN
1	D	15	ASN

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Mol	Chain	Res	Type
1	D	264	PRO
1	A	42	ASP
1	A	249	PRO
1	B	290	ASN
1	B	304	LYS
1	C	18	ASP
1	C	243	LYS
1	C	264	PRO
1	D	36	PRO
1	D	289	THR
1	D	290	ASN
1	A	117	ASN
1	B	15	ASN
1	B	19	PRO
1	C	143	HIS
1	C	389	ILE
1	D	14	GLU
1	A	142	ARG
1	B	18	ASP
1	B	159	ALA
1	B	160	GLU
1	C	289	THR
1	C	316	LYS
1	A	50	ILE
1	A	331	ASN
1	C	58	PRO
1	C	268	ASP
1	B	157	VAL
1	A	371	ILE
1	B	370	PRO
1	C	255	ARG
1	C	19	PRO
1	D	90	PRO
1	D	372	VAL
1	A	71	ALA
1	C	13	PRO
1	D	13	PRO

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	319/371 (86%)	283 (89%)	36 (11%)	6	28
1	B	318/371 (86%)	284 (89%)	34 (11%)	6	30
1	C	318/371 (86%)	294 (92%)	24 (8%)	13	44
1	D	318/371 (86%)	286 (90%)	32 (10%)	7	31
All	All	1273/1484 (86%)	1147 (90%)	126 (10%)	8	32

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	9	TYR
1	A	11	LEU
1	A	16	PHE
1	A	39	LEU
1	A	43	ASP
1	A	53	LEU
1	A	65	PHE
1	A	83	VAL
1	A	135	ARG
1	A	137	HIS
1	A	140	LEU
1	A	141	GLU
1	A	164	ARG
1	A	168	LYS
1	A	190	ARG
1	A	213	GLU
1	A	215	ARG
1	A	242	ARG
1	A	243	LYS
1	A	245	GLU
1	A	246	GLN
1	A	252	THR
1	A	267	THR
1	A	290	ASN
1	A	310	LEU
1	A	318	MET
1	A	319	SER

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Mol	Chain	Res	Type
1	A	320	THR
1	A	364	SER
1	A	370	PRO
1	A	374	ARG
1	A	382	ASN
1	A	390	TYR
1	A	394	ASP
1	A	398	LEU
1	B	5	LEU
1	B	29	LEU
1	B	39	LEU
1	B	42	ASP
1	B	50	ILE
1	B	53	LEU
1	B	54	THR
1	B	73	LEU
1	B	93	GLN
1	B	106	LYS
1	B	132	SER
1	B	141	GLU
1	B	142	ARG
1	B	143	HIS
1	B	144	CYS
1	B	157	VAL
1	B	160	GLU
1	B	172	ARG
1	B	195	ARG
1	B	196	ASP
1	B	203	THR
1	B	250	THR
1	B	254	LYS
1	B	284	ASP
1	B	307	THR
1	B	316	LYS
1	B	320	THR
1	B	342	ILE
1	B	364	SER
1	B	379	GLU
1	B	393	GLN
1	B	394	ASP
1	B	400	HIS
1	B	401	ARG

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	38	ASP
1	C	57	THR
1	C	73	LEU
1	C	88	ILE
1	C	106	LYS
1	C	118	SER
1	C	142	ARG
1	C	153	ASN
1	C	164	ARG
1	C	190	ARG
1	C	198	LEU
1	C	242	ARG
1	C	245	GLU
1	C	246	GLN
1	C	268	ASP
1	C	286	LEU
1	C	297	GLU
1	C	300	ARG
1	C	362	TYR
1	C	364	SER
1	C	382	ASN
1	C	383	ILE
1	C	398	LEU
1	D	11	LEU
1	D	14	GLU
1	D	16	PHE
1	D	32	LYS
1	D	40	GLU
1	D	41	ARG
1	D	53	LEU
1	D	57	THR
1	D	96	ASN
1	D	132	SER
1	D	136	TRP
1	D	141	GLU
1	D	142	ARG
1	D	160	GLU
1	D	186	THR
1	D	192	LEU
1	D	198	LEU
1	D	214	GLU

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Mol	Chain	Res	Type
1	D	242	ARG
1	D	252	THR
1	D	268	ASP
1	D	273	ASP
1	D	284	ASP
1	D	304	LYS
1	D	315	LEU
1	D	344	THR
1	D	346	LEU
1	D	351	ARG
1	D	359	VAL
1	D	364	SER
1	D	374	ARG
1	D	378	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	56	HIS
1	A	68	ASN
1	A	74	ASN
1	A	206	GLN
1	A	246	GLN
1	A	382	ASN
1	B	56	HIS
1	B	143	HIS
1	B	158	ASN
1	B	194	GLN
1	B	290	ASN
1	B	391	ASN
1	C	68	ASN
1	C	74	ASN
1	C	333	GLN
1	C	382	ASN
1	C	385	ASN
1	C	386	GLN
1	D	68	ASN
1	D	74	ASN
1	D	137	HIS
1	D	185	ASN
1	D	294	GLN

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Mol	Chain	Res	Type
1	D	386	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	FMN	D	501	-	31,33,33	2.41	6 (19%)	40,50,50	2.22	9 (22%)
2	FMN	B	501	-	31,33,33	2.14	6 (19%)	40,50,50	2.28	7 (17%)
3	ORO	A	502	-	6,11,11	1.06	0	3,15,15	2.41	1 (33%)
3	ORO	C	502	-	6,11,11	1.10	0	3,15,15	2.97	2 (66%)
4	9AU	D	503	-	25,28,28	1.00	1 (4%)	29,37,37	2.29	4 (13%)
4	9AU	A	503	-	25,28,28	0.89	0	29,37,37	1.86	2 (6%)
4	9AU	C	503	-	25,28,28	0.92	1 (4%)	29,37,37	2.08	4 (13%)
3	ORO	D	502	-	6,11,11	1.24	0	3,15,15	2.86	2 (66%)
2	FMN	C	501	-	31,33,33	2.40	5 (16%)	40,50,50	2.46	7 (17%)
3	ORO	B	502	-	6,11,11	1.00	0	3,15,15	2.80	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	A	501	-	31,33,33	2.40	6 (19%)	40,50,50	2.29	9 (22%)
4	9AU	B	503	-	25,28,28	0.87	0	29,37,37	2.34	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	D	501	-	-	2/18/18/18	0/3/3/3
2	FMN	B	501	-	-	3/18/18/18	0/3/3/3
3	ORO	A	502	-	-	0/0/4/4	0/1/1/1
3	ORO	C	502	-	-	0/0/4/4	0/1/1/1
4	9AU	D	503	-	-	6/17/17/17	0/2/2/2
4	9AU	A	503	-	-	8/17/17/17	0/2/2/2
4	9AU	C	503	-	-	3/17/17/17	0/2/2/2
3	ORO	D	502	-	-	0/0/4/4	0/1/1/1
2	FMN	C	501	-	-	6/18/18/18	0/3/3/3
3	ORO	B	502	-	-	0/0/4/4	0/1/1/1
2	FMN	A	501	-	-	4/18/18/18	0/3/3/3
4	9AU	B	503	-	-	10/17/17/17	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FMN	C4A-C10	10.12	1.48	1.38
2	A	501	FMN	C4A-C10	10.04	1.48	1.38
2	C	501	FMN	C4A-C10	10.03	1.48	1.38
2	B	501	FMN	C4A-C10	8.89	1.47	1.38
2	C	501	FMN	C4-C4A	4.72	1.49	1.41
2	D	501	FMN	C4-C4A	4.57	1.49	1.41
2	A	501	FMN	C8-C7	4.33	1.51	1.40
2	A	501	FMN	C4-C4A	4.20	1.48	1.41
2	C	501	FMN	C9A-C5A	4.06	1.50	1.42
2	A	501	FMN	C9A-C5A	3.97	1.50	1.42
2	B	501	FMN	C4-C4A	3.81	1.47	1.41
2	D	501	FMN	C9A-C5A	3.62	1.49	1.42
2	D	501	FMN	C9A-N10	3.50	1.43	1.38
2	B	501	FMN	C9A-C5A	3.44	1.49	1.42
2	D	501	FMN	C8-C7	3.32	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C8-C7	3.31	1.49	1.40
2	C	501	FMN	C8-C7	3.31	1.49	1.40
2	C	501	FMN	C9A-N10	3.18	1.42	1.38
2	B	501	FMN	C9A-N10	2.98	1.42	1.38
2	A	501	FMN	C9A-N10	2.95	1.42	1.38
4	D	503	9AU	CAI-CAV	2.67	1.39	1.33
4	C	503	9AU	CAI-CAV	2.35	1.38	1.33
2	A	501	FMN	C6-C5A	-2.10	1.38	1.41
2	D	501	FMN	C10-N1	2.09	1.36	1.33
2	B	501	FMN	C6-C5A	-2.08	1.38	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	9AU	CAX-CAP-CAI	10.44	128.57	112.15
4	B	503	9AU	CAX-CAP-CAI	10.04	127.92	112.15
4	C	503	9AU	CAX-CAP-CAI	9.17	126.56	112.15
2	C	501	FMN	C4-N3-C2	8.86	122.62	115.14
2	A	501	FMN	C4-N3-C2	8.41	122.24	115.14
4	A	503	9AU	CAX-CAP-CAI	8.18	125.00	112.15
2	B	501	FMN	C4-N3-C2	8.03	121.92	115.14
2	D	501	FMN	C4-N3-C2	7.90	121.82	115.14
2	B	501	FMN	C1'-N10-C9A	7.05	123.84	118.29
2	C	501	FMN	C4-C4A-C10	-6.50	115.64	119.95
2	C	501	FMN	C1'-N10-C9A	5.92	122.95	118.29
2	A	501	FMN	C1'-N10-C9A	5.70	122.78	118.29
2	D	501	FMN	C4A-N5-C5A	5.11	121.88	116.77
2	D	501	FMN	C1'-N10-C9A	4.88	122.14	118.29
2	C	501	FMN	C4-C4A-N5	4.84	124.13	118.60
2	A	501	FMN	C4-C4A-C10	-4.66	116.86	119.95
2	B	501	FMN	C4-C4A-C10	-4.63	116.89	119.95
2	C	501	FMN	C4A-N5-C5A	4.51	121.27	116.77
2	D	501	FMN	C4-C4A-C10	-4.48	116.98	119.95
2	B	501	FMN	C4A-N5-C5A	4.15	120.92	116.77
3	C	502	ORO	C5-C4-N3	-3.91	119.52	124.08
2	A	501	FMN	C4A-N5-C5A	3.85	120.62	116.77
2	A	501	FMN	C4A-C4-N3	-3.81	118.22	123.43
3	D	502	ORO	C5-C4-N3	-3.78	119.67	124.08
2	B	501	FMN	C4A-C4-N3	-3.59	118.53	123.43
2	C	501	FMN	C4A-C4-N3	-3.54	118.58	123.43
2	D	501	FMN	C4A-C4-N3	-3.47	118.69	123.43
3	A	502	ORO	C5-C4-N3	-3.43	120.07	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	ORO	C5-C4-N3	-3.18	120.37	124.08
4	C	503	9AU	OAS-CAZ-CBA	-3.06	118.25	121.20
4	B	503	9AU	CAP-CAX-CAW	3.00	124.74	120.80
4	B	503	9AU	OAF-CAW-CAX	2.95	121.83	118.68
2	D	501	FMN	C4-C4A-N5	2.95	121.97	118.60
3	C	502	ORO	C4-C5-C6	2.94	118.63	116.73
2	A	501	FMN	C4-C4A-N5	2.87	121.88	118.60
2	B	501	FMN	C4-C4A-N5	2.86	121.87	118.60
2	A	501	FMN	C9A-N10-C10	-2.86	118.16	121.91
2	B	501	FMN	C9A-N10-C10	-2.85	118.18	121.91
2	C	501	FMN	C9A-N10-C10	-2.78	118.27	121.91
4	B	503	9AU	CAM-CBA-CAZ	2.70	119.63	116.50
4	D	503	9AU	CAP-CAX-CAY	2.69	126.08	121.28
3	D	502	ORO	C4-C5-C6	2.66	118.45	116.73
4	B	503	9AU	CAR-CAV-CAI	2.65	126.48	121.12
3	B	502	ORO	C4-C5-C6	2.62	118.42	116.73
3	B	502	ORO	C5-C6-N1	-2.58	119.29	122.35
2	A	501	FMN	P-O5'-C5'	2.47	125.09	118.30
4	B	503	9AU	CAD-CAV-CAI	-2.46	117.36	123.68
2	D	501	FMN	C9A-N10-C10	-2.35	118.83	121.91
4	D	503	9AU	OAS-CAZ-CBA	-2.31	118.98	121.20
4	C	503	9AU	CAP-CAX-CAY	2.25	125.31	121.28
2	D	501	FMN	O4'-C4'-C3'	2.16	114.36	109.10
2	D	501	FMN	O3P-P-O2P	2.10	115.68	107.64
4	C	503	9AU	CAC-CAU-CAQ	2.07	118.76	115.27
4	D	503	9AU	CAP-CAX-CAW	-2.03	118.14	120.80
2	A	501	FMN	C7M-C7-C6	-2.02	115.52	120.34
4	A	503	9AU	CAC-CAU-CAH	-2.01	118.53	123.68

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	503	9AU	CAI-CAP-CAX-CAY
4	D	503	9AU	CAI-CAP-CAX-CAW
4	D	503	9AU	CAG-CAN-CAQ-CAU
4	A	503	9AU	CAI-CAP-CAX-CAY
4	A	503	9AU	CAI-CAP-CAX-CAW
4	A	503	9AU	CAG-CAN-CAQ-CAU
4	C	503	9AU	CAI-CAP-CAX-CAY
4	C	503	9AU	CAI-CAP-CAX-CAW
2	A	501	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	A	501	FMN	C5'-O5'-P-O3P
4	B	503	9AU	CAI-CAP-CAX-CAY
4	B	503	9AU	CAI-CAP-CAX-CAW
4	B	503	9AU	CAH-CAO-CAR-CAV
4	B	503	9AU	CAG-CAN-CAQ-CAU
4	A	503	9AU	CAH-CAO-CAR-CAV
2	C	501	FMN	O3'-C3'-C4'-C5'
2	C	501	FMN	C2'-C3'-C4'-C5'
2	C	501	FMN	C2'-C3'-C4'-O4'
4	A	503	9AU	CAO-CAR-CAV-CAD
4	A	503	9AU	CAO-CAR-CAV-CAI
2	C	501	FMN	O3'-C3'-C4'-O4'
4	B	503	9AU	CAN-CAQ-CAU-CAC
4	B	503	9AU	CAN-CAQ-CAU-CAH
2	A	501	FMN	C5'-O5'-P-O1P
2	B	501	FMN	C4'-C5'-O5'-P
4	B	503	9AU	CAO-CAR-CAV-CAD
2	D	501	FMN	C5'-O5'-P-O3P
4	D	503	9AU	CAN-CAQ-CAU-CAC
4	D	503	9AU	CAN-CAQ-CAU-CAH
2	C	501	FMN	C4'-C5'-O5'-P
4	B	503	9AU	CAO-CAR-CAV-CAI
2	D	501	FMN	C4'-C5'-O5'-P
4	A	503	9AU	CAV-CAI-CAP-CAX
4	B	503	9AU	CAV-CAI-CAP-CAX
4	D	503	9AU	CAO-CAR-CAV-CAI
2	B	501	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	C5'-O5'-P-O2P
2	C	501	FMN	C5'-O5'-P-O2P
4	A	503	9AU	CAU-CAH-CAO-CAR
2	A	501	FMN	C4'-C5'-O5'-P
4	B	503	9AU	CAU-CAH-CAO-CAR
4	C	503	9AU	CAG-CAN-CAQ-CAU

There are no ring outliers.

8 monomers are involved in 11 short contacts:

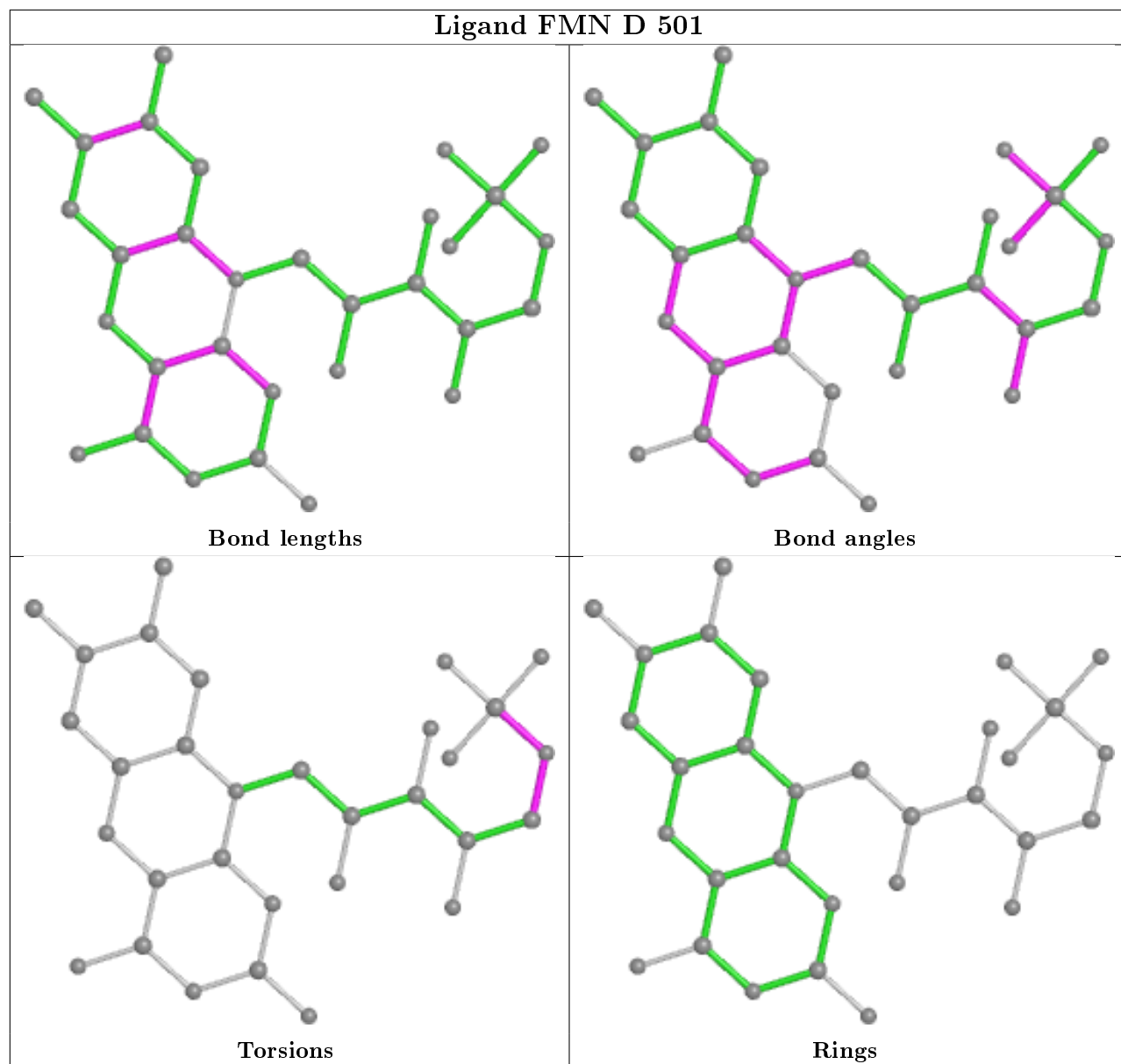
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FMN	1	0
2	B	501	FMN	2	0
4	D	503	9AU	1	0
4	A	503	9AU	1	0

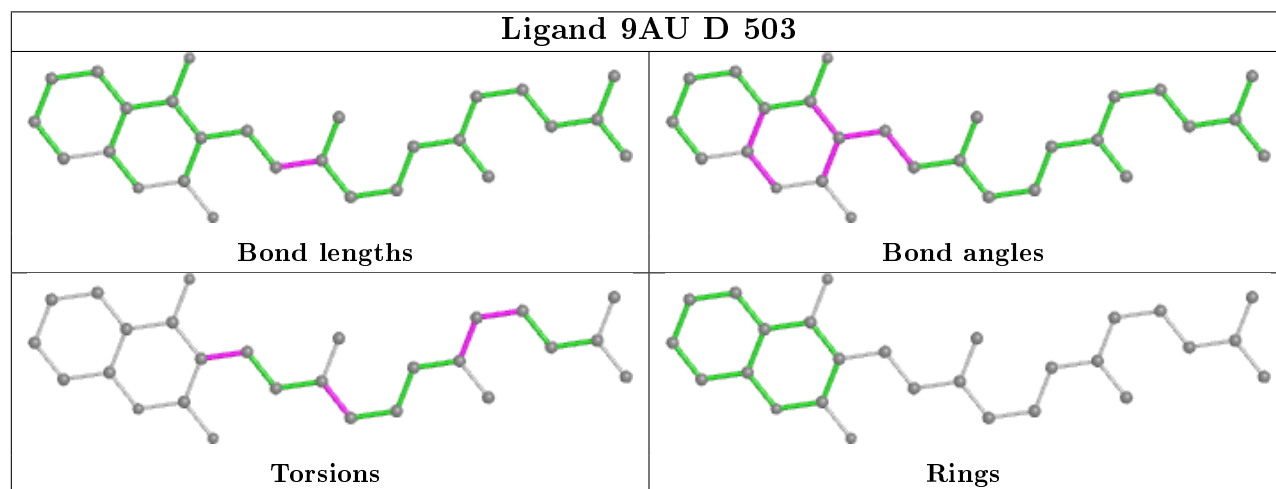
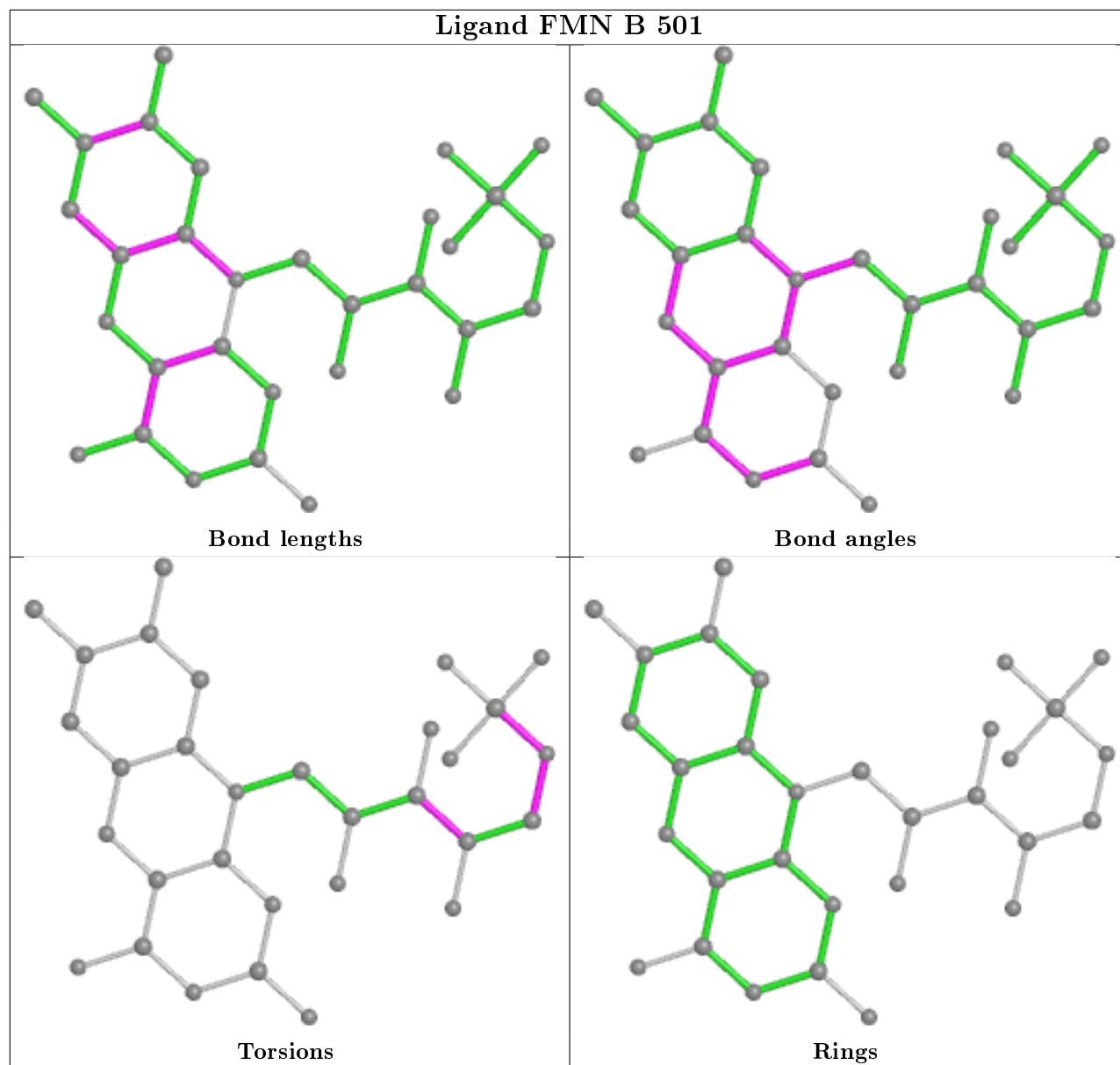
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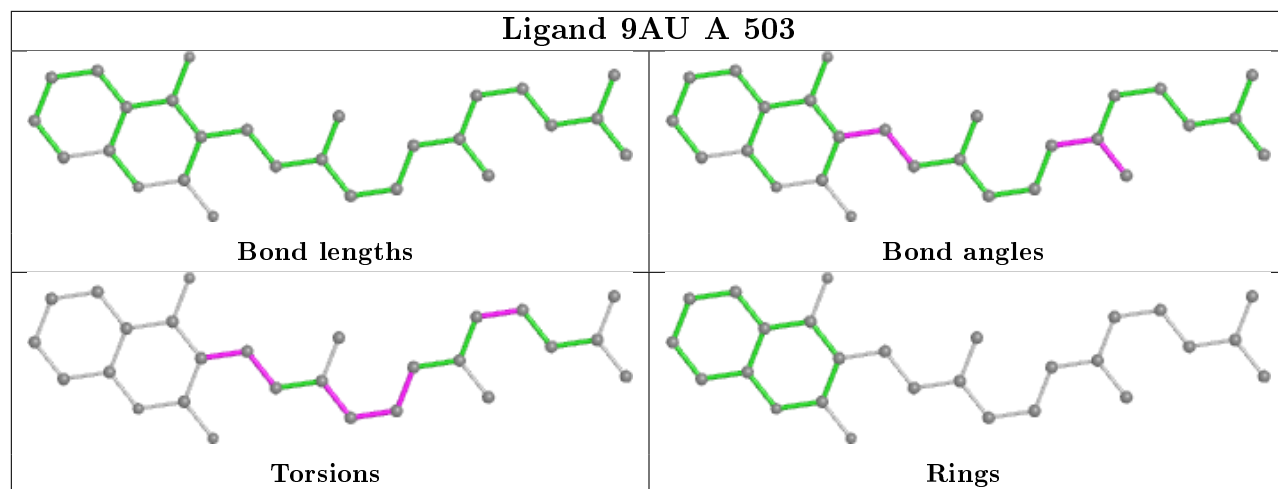
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	9AU	1	0
3	B	502	ORO	1	0
2	A	501	FMN	2	0
4	B	503	9AU	2	0

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.

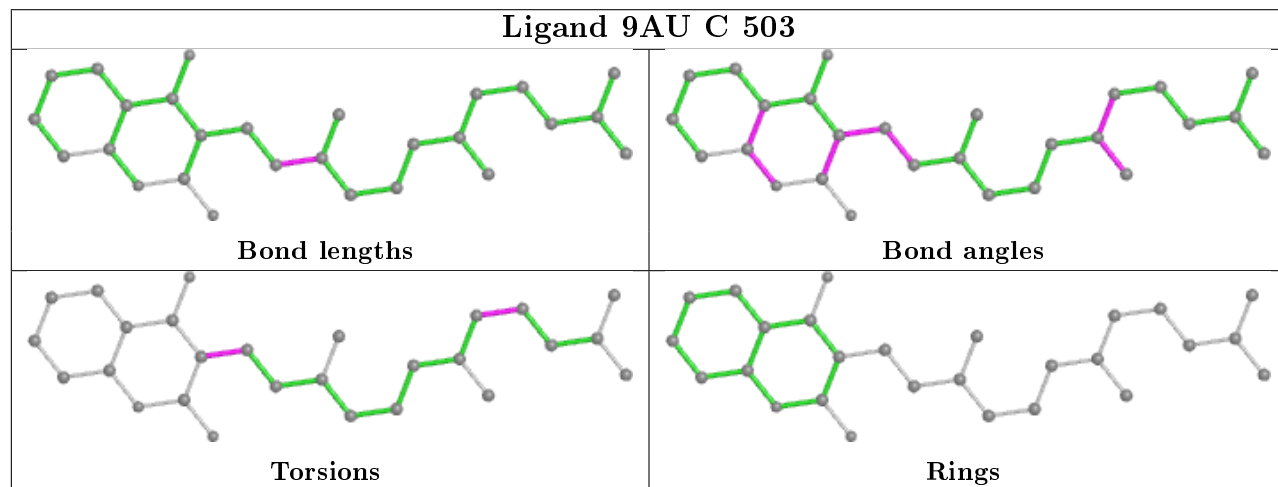


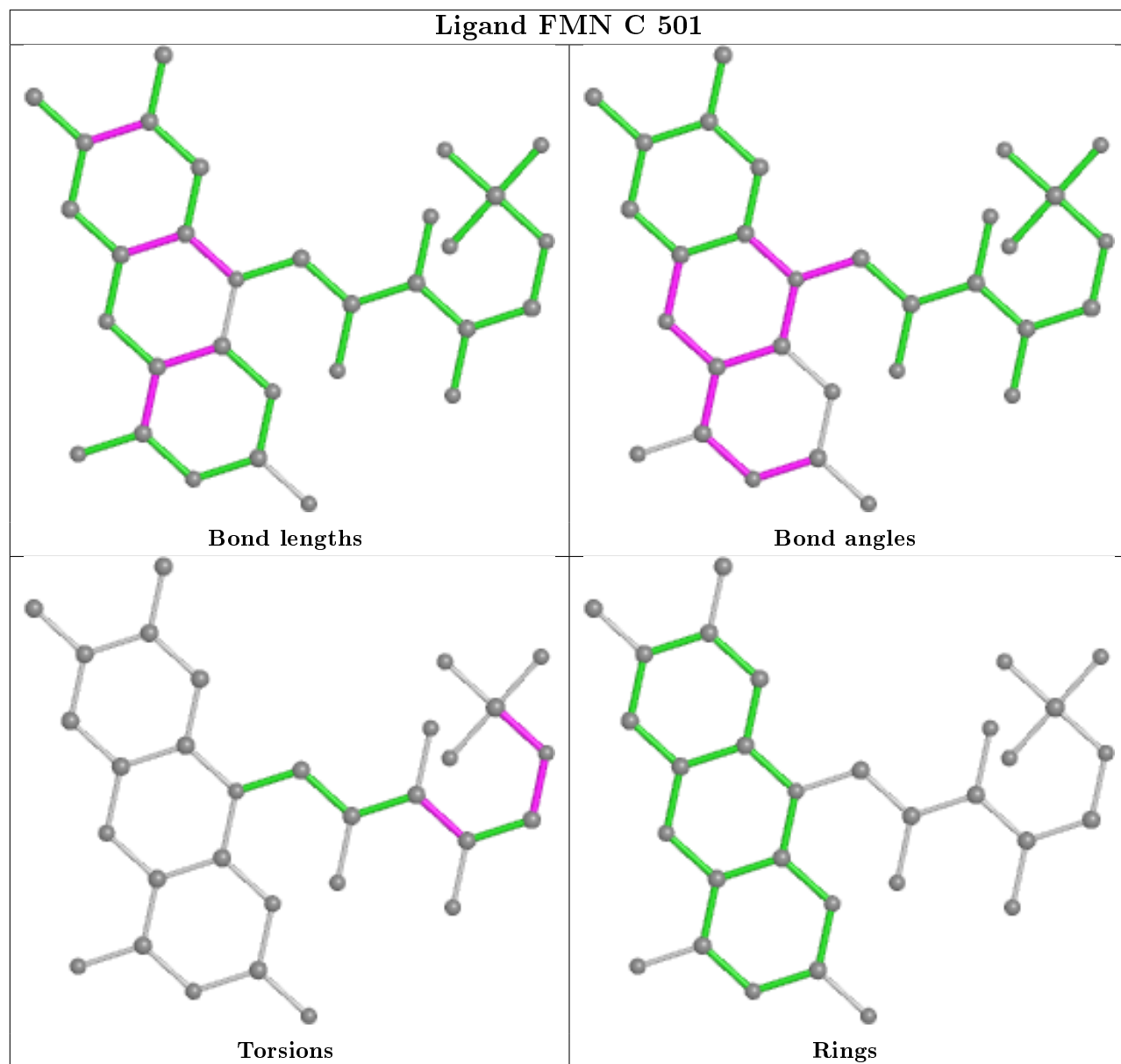


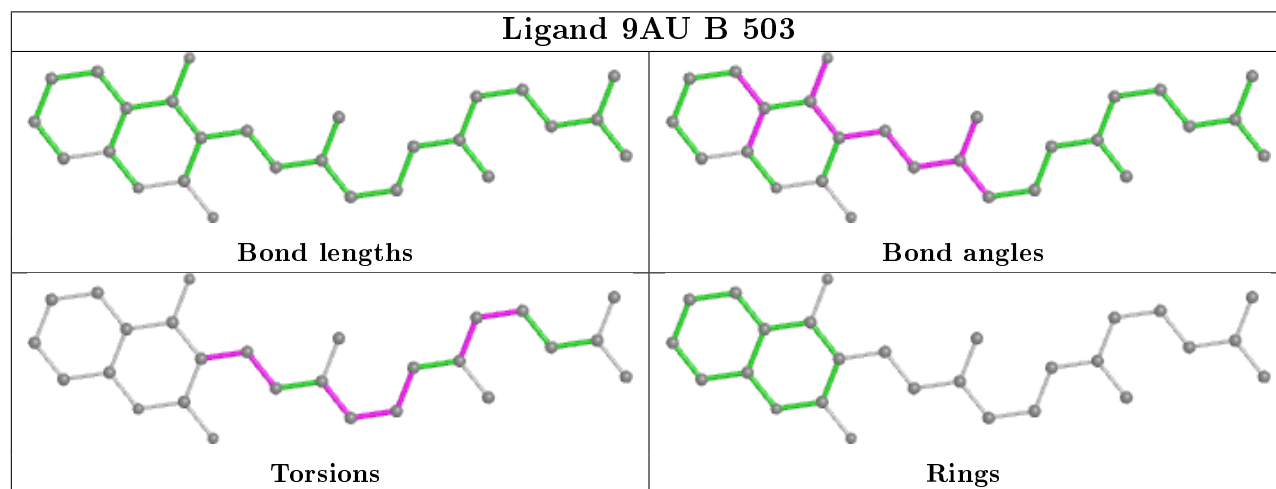
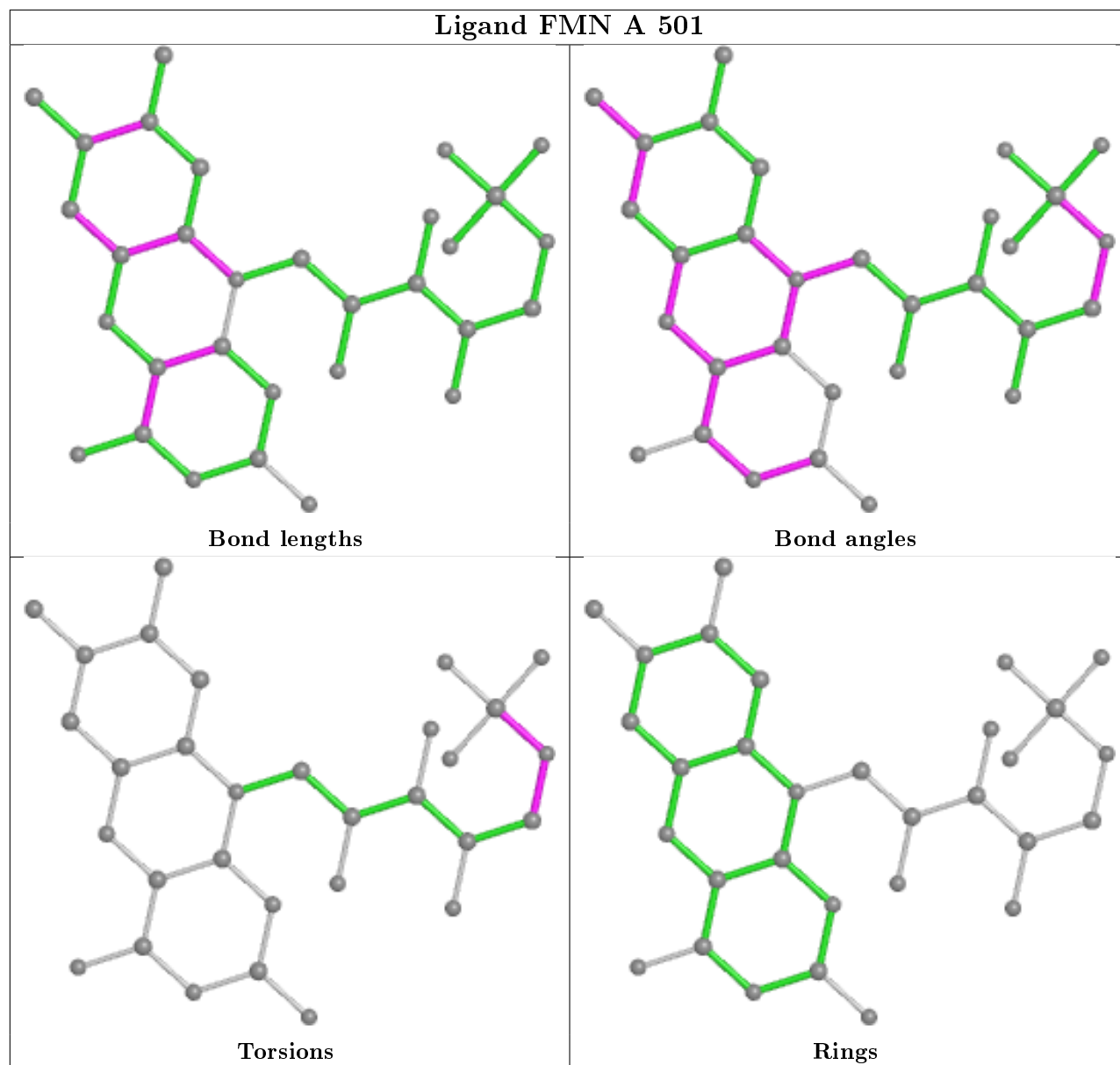
Ligand 9AU A 503



Ligand 9AU C 503







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 ⓘ

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	378/436 (86%)	-0.55	2 (0%) 91 85	28, 52, 95, 113	0
1	B	376/436 (86%)	-0.52	5 (1%) 77 65	30, 54, 85, 155	0
1	C	376/436 (86%)	-0.50	2 (0%) 91 85	33, 57, 96, 125	0
1	D	376/436 (86%)	-0.34	4 (1%) 80 70	42, 73, 104, 135	0
All	All	1506/1744 (86%)	-0.48	13 (0%) 84 74	28, 58, 99, 155	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	LEU	3.5
1	B	216	SER	3.0
1	D	39	LEU	2.9
1	B	196	ASP	2.4
1	A	218	ALA	2.4
1	B	402	PRO	2.3
1	D	136	TRP	2.3
1	B	9	TYR	2.3
1	C	9	TYR	2.2
1	C	402	PRO	2.1
1	D	402	PRO	2.1
1	B	38	ASP	2.1
1	A	4	LEU	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 carbohydrates in this entry.

6.4 Ligands ⓘ

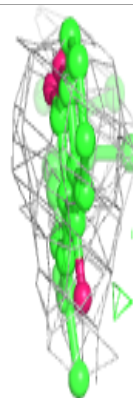
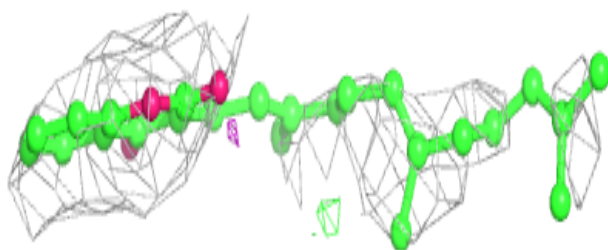
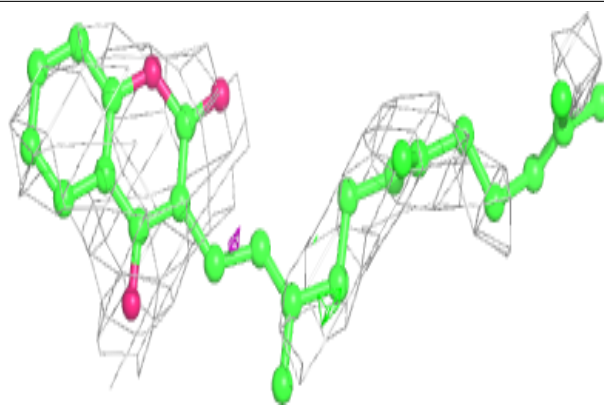
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	9AU	C	503	27/27	0.80	0.39	63,73,85,85	0
4	9AU	A	503	27/27	0.81	0.36	55,65,73,73	0
4	9AU	B	503	27/27	0.82	0.33	62,68,78,79	0
4	9AU	D	503	27/27	0.84	0.34	55,62,71,72	0
2	FMN	D	501	31/31	0.95	0.18	52,55,57,57	0
3	ORO	B	502	11/11	0.96	0.15	37,38,38,38	0
2	FMN	A	501	31/31	0.96	0.16	29,30,33,33	0
3	ORO	D	502	11/11	0.96	0.17	46,48,49,50	0
3	ORO	A	502	11/11	0.97	0.15	30,30,31,31	0
3	ORO	C	502	11/11	0.97	0.14	29,29,30,30	0
2	FMN	C	501	31/31	0.97	0.14	33,34,37,38	0
2	FMN	B	501	31/31	0.98	0.13	35,36,42,42	0

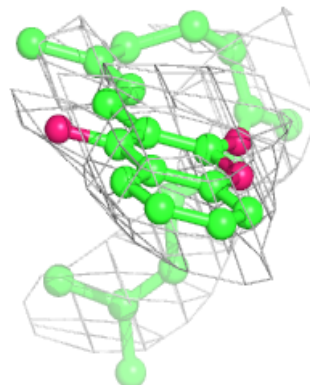
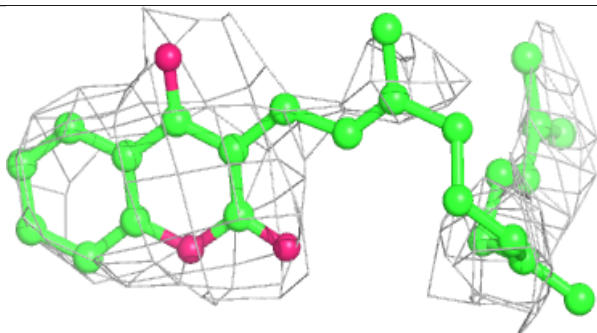
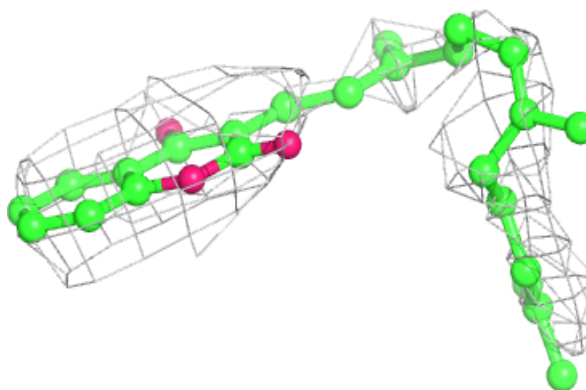
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9AU C 503:

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

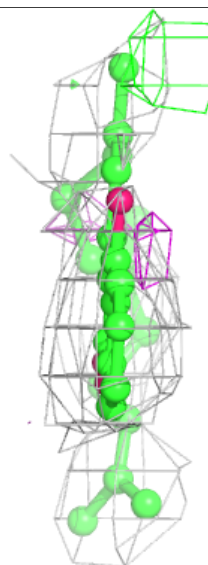
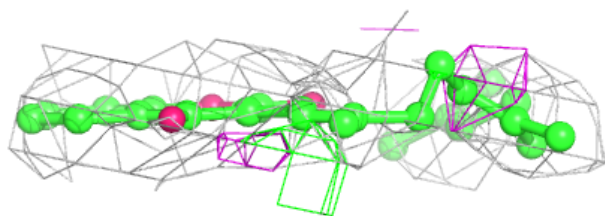
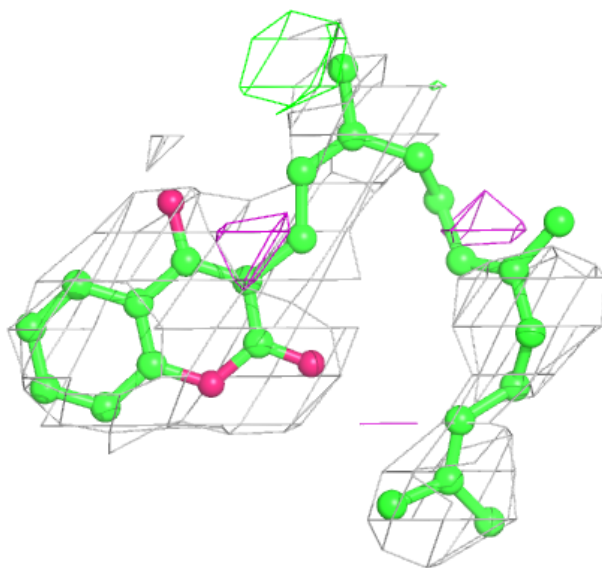
**Electron density around 9AU A 503:**

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



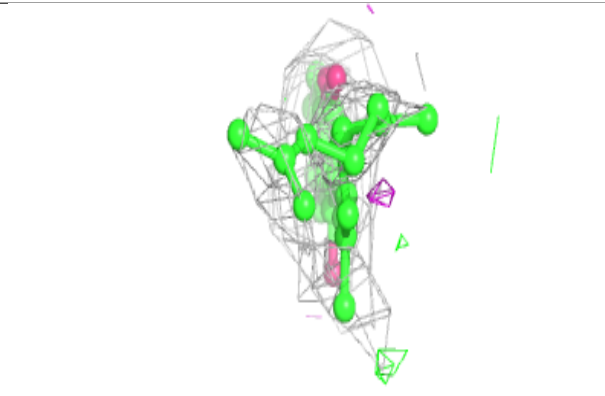
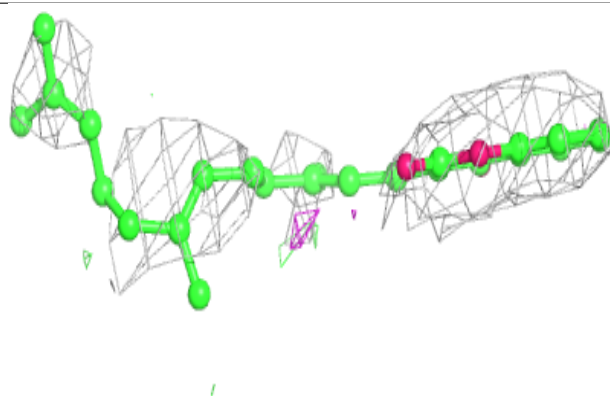
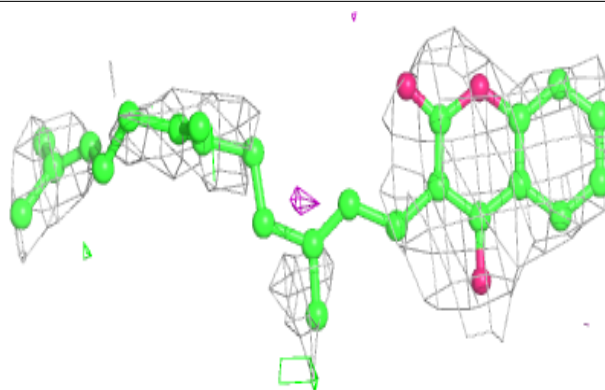
Electron density around 9AU B 503:

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

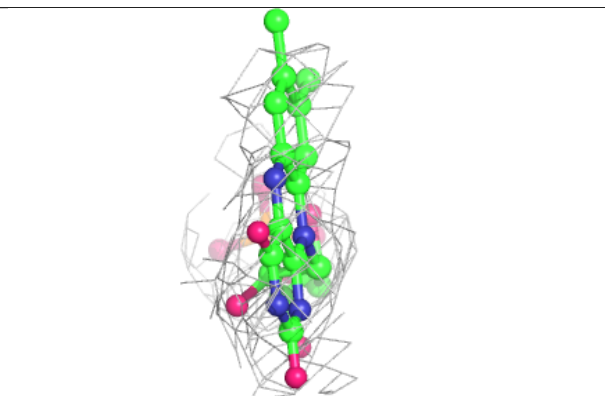
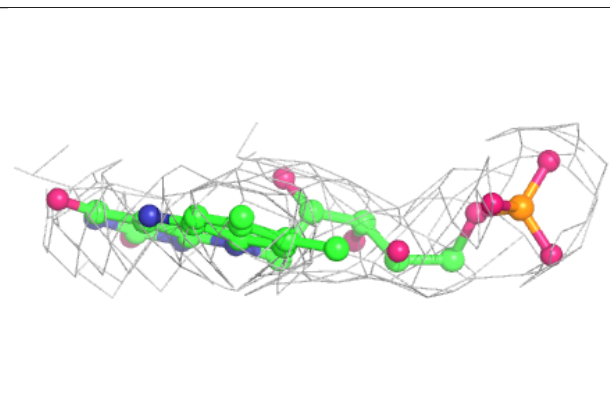
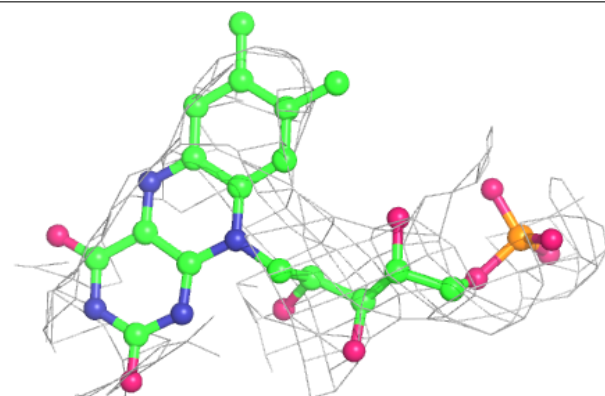


Electron density around 9AU D 503:

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

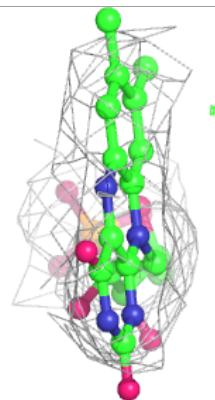
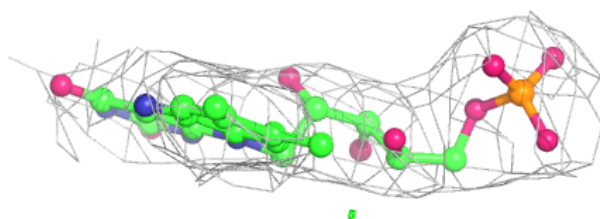
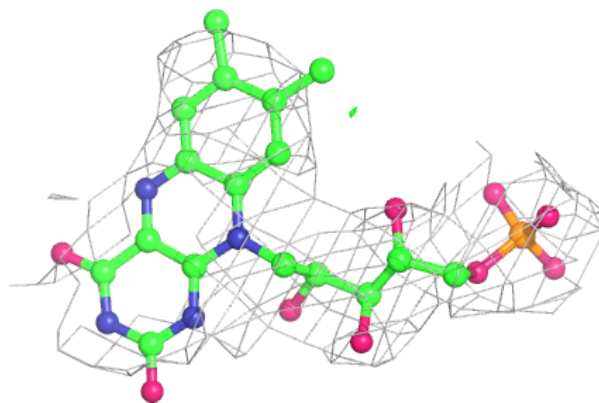
**Electron density around FMN D 501:**

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

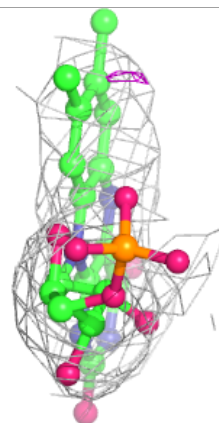
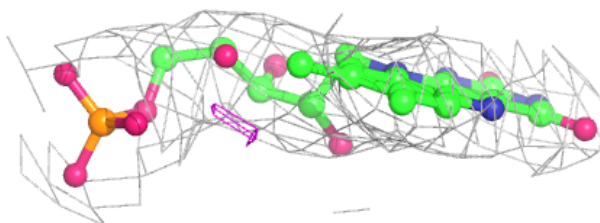
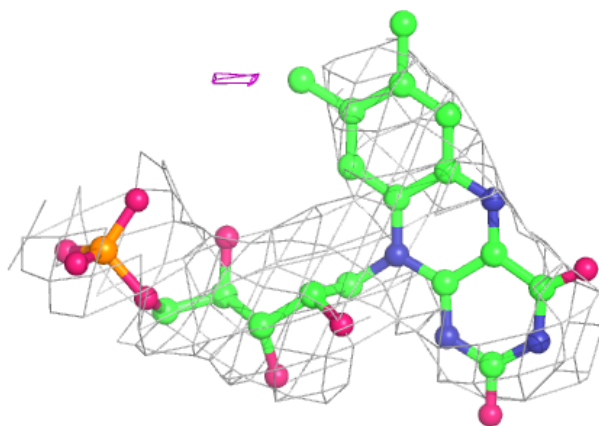


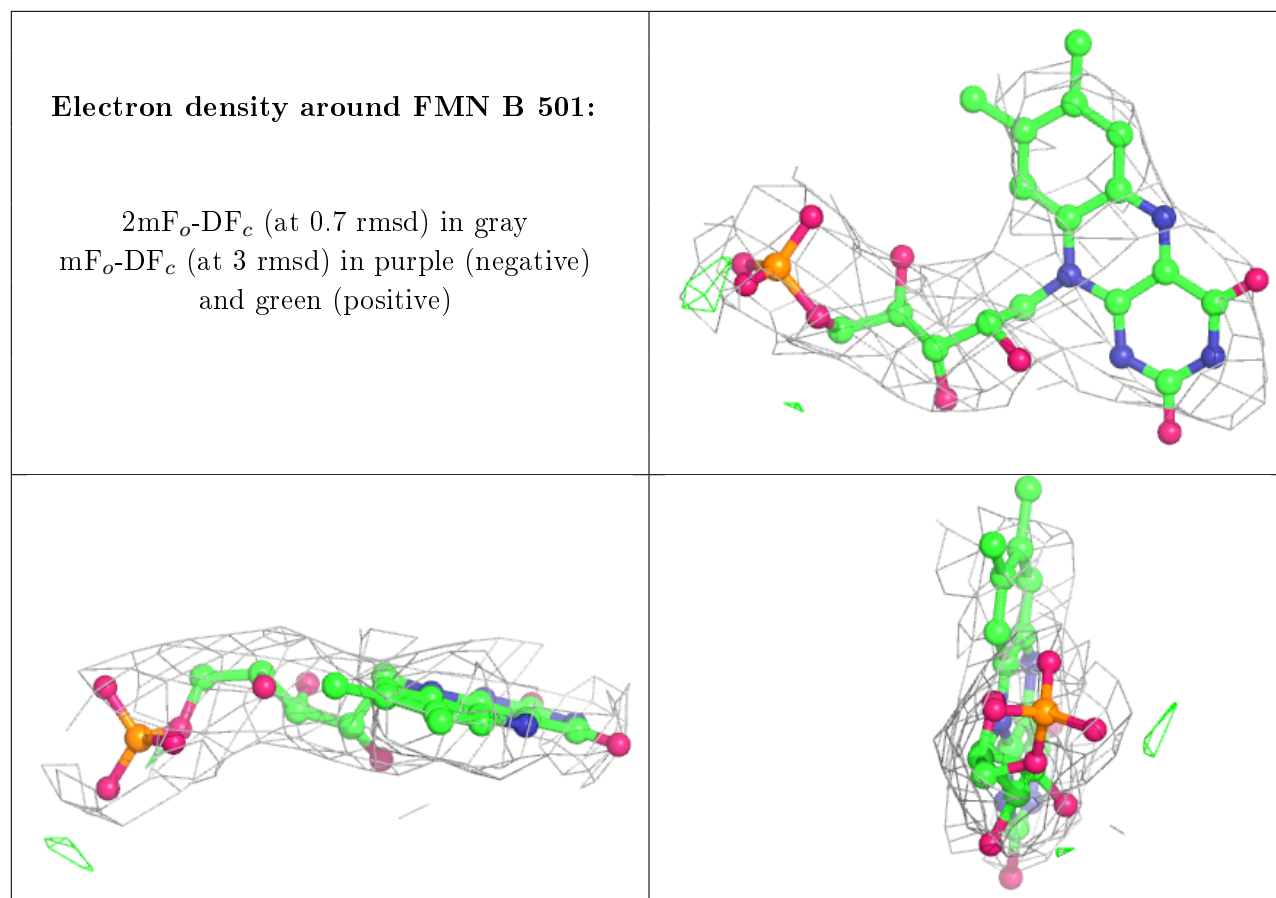
Electron density around FMN A 501:

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

**Electron density around FMN C 501:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.