



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:32 PM UTC

PDB ID : 1JRC / pdb_00001jrc
Title : The N67A mutant of Lactococcus lactis dihydroorotate dehydrogenase A
Authors : Norager, S.; Arent, S.; Bjornberg, O.; Ottosen, M.; Lo Leggio, L.; Jensen, K.F.; Larsen, S.
Deposited on : 2001-08-13
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

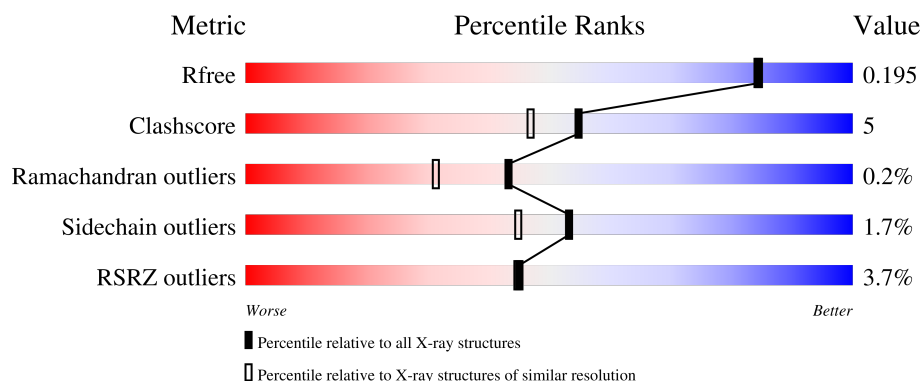
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	311	5% 81% 14% • •
1	B	311	3% 80% 16% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5554 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2406	1551	386	457	12			
1	B	311	Total	C	N	O	S	0	1	0
			2410	1553	387	458	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	ASN	engineered mutation	UNP P54321
B	67	ALA	ASN	engineered mutation	UNP P54321

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



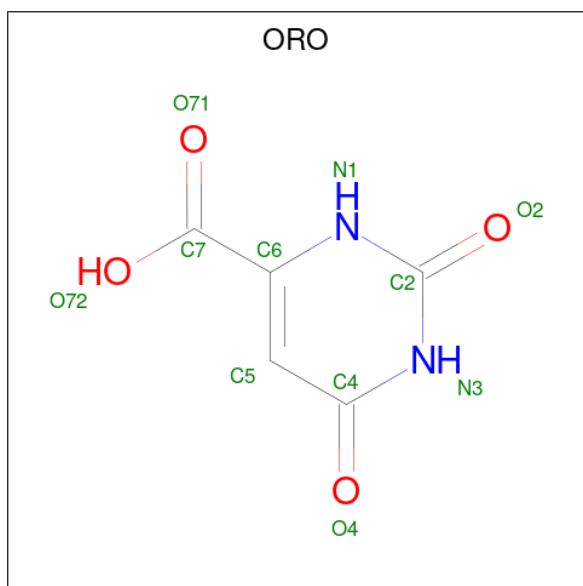
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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

- Molecule 3 is OROTIC ACID (CCD ID: 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		

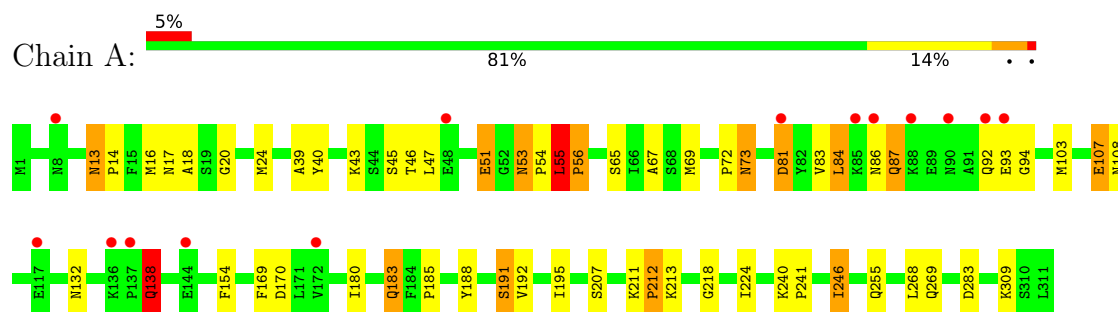
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	342	Total	O	0	0
			342	342		
4	B	312	Total	O	0	0
			312	312		

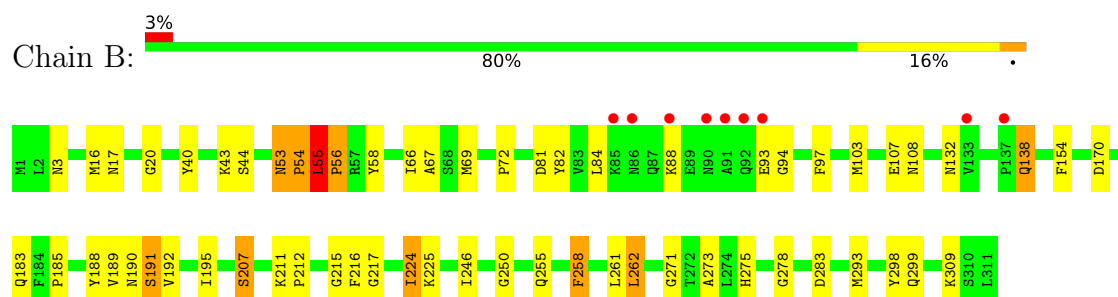
3 Residue-property plots

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

- Molecule 1: dihydroorotate dehydrogenase A



- Molecule 1: dihydroorotate dehydrogenase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.80Å 108.09Å 65.80Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.80) 99.1 (20.00-1.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.84Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.220 0.160 , 0.195	Depositor DCC
R_{free} test set	6195 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5554	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, 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	1.15	0/2458	1.90	63/3322 (1.9%)
1	B	1.13	2/2466 (0.1%)	1.87	62/3333 (1.9%)
All	All	1.14	2/4924 (0.0%)	1.89	125/6655 (1.9%)

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	4
1	B	0	4
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	LEU	C-O	-5.63	1.17	1.24
1	B	217	GLY	N-CA	5.53	1.51	1.45

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	LEU	CA-C-O	-13.79	107.37	120.19
1	B	191	SER	O-C-N	-13.63	105.30	123.01
1	A	55	LEU	CA-C-N	13.09	136.20	119.84
1	A	55	LEU	C-N-CA	13.09	136.20	119.84
1	B	56	PRO	N-CA-CB	12.30	116.13	102.60
1	A	191	SER	O-C-N	-12.14	107.23	123.01
1	B	271	GLY	O-C-N	-10.61	115.91	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LEU	O-C-N	10.34	135.34	120.96
1	A	56	PRO	N-CA-CB	10.18	113.94	103.25
1	A	53	ASN	OD1-CG-ND2	-10.15	112.45	122.60
1	B	53	ASN	OD1-CG-ND2	-9.87	112.73	122.60
1	A	191	SER	CA-C-O	-9.86	109.46	120.70
1	B	261	LEU	CA-C-O	9.63	130.63	120.42
1	A	55	LEU	CA-C-O	-9.06	108.13	121.46
1	B	191	SER	CA-C-O	-8.96	110.49	120.70
1	B	56	PRO	CA-N-CD	-8.85	99.12	111.50
1	B	258	PHE	CA-C-O	-8.59	111.45	120.55
1	B	261	LEU	O-C-N	-8.13	112.88	122.15
1	A	56	PRO	CA-N-CD	-8.01	100.79	112.00
1	A	132	ASN	CA-C-N	-7.98	116.84	122.59
1	A	132	ASN	C-N-CA	-7.98	116.84	122.59
1	A	55	LEU	N-CA-CB	7.94	118.47	109.49
1	B	40	TYR	CD1-CG-CD2	-7.85	106.33	118.10
1	A	40	TYR	CD1-CG-CD2	-7.63	106.66	118.10
1	A	73	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	192	VAL	N-CA-CB	7.40	124.08	111.50
1	B	44	SER	CA-C-N	-7.18	110.75	122.81
1	B	44	SER	C-N-CA	-7.18	110.75	122.81
1	B	3	ASN	OD1-CG-ND2	7.12	129.72	122.60
1	B	132	ASN	CA-C-N	-7.10	117.48	122.59
1	B	132	ASN	C-N-CA	-7.10	117.48	122.59
1	A	183	GLN	OE1-CD-NE2	-7.02	115.58	122.60
1	B	154	PHE	CA-CB-CG	-7.01	106.79	113.80
1	A	94	GLY	CA-C-N	6.88	126.86	119.78
1	A	94	GLY	C-N-CA	6.88	126.86	119.78
1	B	190	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	A	40	TYR	CE1-CZ-CE2	-6.74	106.82	120.30
1	A	81	ASP	O-C-N	-6.73	115.09	122.09
1	A	154	PHE	CA-CB-CG	-6.70	107.10	113.80
1	A	81	ASP	CA-C-N	6.70	129.15	120.44
1	A	81	ASP	C-N-CA	6.70	129.15	120.44
1	B	192	VAL	N-CA-CB	6.59	122.69	111.50
1	A	87	GLN	CA-C-N	6.57	129.73	120.28
1	A	87	GLN	C-N-CA	6.57	129.73	120.28
1	A	67	ALA	O-C-N	-6.56	116.13	123.48
1	A	283	ASP	CA-CB-CG	-6.52	106.08	112.60
1	B	185	PRO	CA-C-O	6.45	126.08	121.31
1	A	107	GLU	CB-CG-CD	6.44	123.55	112.60
1	B	189	VAL	O-C-N	-6.40	116.27	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	40	TYR	CA-C-O	6.38	128.22	121.33
1	B	225	LYS	CA-C-O	6.38	124.53	118.34
1	A	65	SER	O-C-N	-6.35	116.16	123.33
1	A	212	PRO	CA-C-O	-6.29	113.99	121.67
1	B	82	TYR	CA-C-O	-6.27	114.23	120.82
1	B	40	TYR	CE1-CZ-CE2	-6.25	107.80	120.30
1	A	67	ALA	CA-C-O	6.25	127.76	120.89
1	B	72	PRO	N-CA-CB	6.20	108.85	103.27
1	A	86	ASN	CA-CB-CG	-6.20	106.40	112.60
1	B	16	MET	CA-CB-CG	6.18	126.46	114.10
1	B	66	ILE	O-C-N	6.17	129.71	123.10
1	B	94	GLY	CA-C-N	6.17	126.08	119.85
1	B	94	GLY	C-N-CA	6.17	126.08	119.85
1	A	13	ASN	CA-C-O	6.16	126.17	120.56
1	A	40	TYR	CB-CG-CD1	6.15	130.02	120.80
1	A	46	THR	CA-C-O	-6.12	114.46	121.68
1	A	255	GLN	O-C-N	-6.11	115.65	122.12
1	A	83	VAL	O-C-N	6.10	128.69	121.80
1	A	65	SER	CA-C-O	6.09	127.81	120.99
1	B	108	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	B	283	ASP	CA-CB-CG	-6.09	106.51	112.60
1	A	17	ASN	CA-C-O	6.04	128.88	121.87
1	B	298	TYR	CA-C-O	-6.03	113.86	120.43
1	B	273	ALA	O-C-N	5.93	128.91	122.15
1	B	293	MET	CA-C-O	-5.92	114.27	120.55
1	B	215	GLY	CA-C-O	-5.89	112.46	119.06
1	B	17	ASN	CA-C-O	5.84	128.65	121.87
1	A	185	PRO	N-CA-CB	5.81	106.63	102.79
1	A	108	ASN	CA-CB-CG	-5.80	106.80	112.60
1	B	97	PHE	O-C-N	5.80	130.58	123.21
1	B	67	ALA	CA-C-O	5.79	127.26	120.89
1	B	261	LEU	CA-C-N	5.69	128.17	120.38
1	B	261	LEU	C-N-CA	5.69	128.17	120.38
1	A	241	PRO	N-CA-CB	5.68	108.96	103.51
1	A	240	LYS	CA-C-N	5.66	125.28	119.56
1	A	240	LYS	C-N-CA	5.66	125.28	119.56
1	A	169	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	255	GLN	CA-C-O	5.61	126.71	120.82
1	A	218	GLY	O-C-N	-5.58	117.09	122.84
1	A	84	LEU	CA-C-O	-5.57	112.53	119.38
1	A	268	LEU	CA-C-O	-5.56	114.15	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLN	O-C-N	-5.51	116.39	122.07
1	A	17	ASN	O-C-N	-5.50	116.52	122.79
1	B	275	HIS	O-C-N	-5.49	116.30	122.12
1	A	132	ASN	OD1-CG-ND2	5.47	128.07	122.60
1	B	211	LYS	O-C-N	-5.44	115.06	121.32
1	A	45	SER	CA-C-O	5.40	128.09	121.56
1	A	40	TYR	O-C-N	-5.39	117.11	123.25
1	B	53	ASN	CA-C-N	5.39	125.33	119.78
1	B	53	ASN	C-N-CA	5.39	125.33	119.78
1	B	299	GLN	CB-CG-CD	-5.37	103.48	112.60
1	A	211	LYS	O-C-N	-5.35	115.16	121.32
1	A	13	ASN	O-C-N	-5.35	116.26	121.56
1	B	278	GLY	CA-C-N	5.31	125.40	119.87
1	B	278	GLY	C-N-CA	5.31	125.40	119.87
1	A	73	ASN	CB-CG-ND2	5.29	124.33	116.40
1	B	81	ASP	CA-C-N	5.25	127.27	120.44
1	B	81	ASP	C-N-CA	5.25	127.27	120.44
1	B	54	PRO	N-CA-CB	5.24	107.91	103.35
1	A	138	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	298	TYR	O-C-N	5.18	129.12	123.27
1	B	107	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	258	PHE	N-CA-C	-5.17	105.64	111.28
1	A	191	SER	CA-CB-OG	-5.13	100.84	111.10
1	A	51	GLU	CA-C-N	-5.12	112.58	121.39
1	A	51	GLU	C-N-CA	-5.12	112.58	121.39
1	A	246	ILE	CA-C-N	-5.12	116.70	121.62
1	A	246	ILE	C-N-CA	-5.12	116.70	121.62
1	B	224	ILE	CA-C-N	-5.10	113.72	120.09
1	B	224	ILE	C-N-CA	-5.10	113.72	120.09
1	B	216	PHE	CA-C-O	-5.09	114.89	120.69
1	B	108	ASN	CA-CB-CG	-5.07	107.53	112.60
1	B	250	GLY	CA-C-N	-5.06	116.04	122.37
1	B	250	GLY	C-N-CA	-5.06	116.04	122.37
1	A	191	SER	CB-CA-C	-5.01	102.60	111.22

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	SER	Mainchain,Peptide
1	A	55	LEU	Mainchain,Peptide
1	B	191	SER	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	B	55	LEU	Mainchain,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	2406	0	2406	30	0
1	B	2410	0	2408	20	0
2	A	31	0	19	2	0
2	B	31	0	19	2	0
3	A	11	0	3	0	0
3	B	11	0	3	0	0
4	A	342	0	0	9	0
4	B	312	0	0	5	0
All	All	5554	0	4858	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (46) 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:258:PHE:O	4:B:2606:HOH:O	1.67	1.11
1:B:262:LEU:HB2	4:B:2606:HOH:O	1.72	0.89
1:A:84:LEU:O	4:A:1642:HOH:O	1.98	0.81
1:B:138:GLN:HE21	1:B:138:GLN:H	1.30	0.80
1:A:138:GLN:HE21	1:A:138:GLN:H	1.31	0.78
1:A:81:ASP:HB3	4:A:1628:HOH:O	1.93	0.68
1:A:309:LYS:HB2	1:B:207:SER:HB2	1.75	0.68
1:A:195:ILE:HD12	1:A:224:ILE:HG22	1.78	0.66
1:B:195:ILE:HD12	1:B:224:ILE:HG22	1.80	0.64
1:A:92:GLN:NE2	4:A:1433:HOH:O	2.32	0.62
1:B:53:ASN:HB3	1:B:54:PRO:HD2	1.81	0.61
1:A:207:SER:HB2	1:B:309:LYS:HB2	1.84	0.59
1:A:53:ASN:HB3	1:A:54:PRO:HD2	1.86	0.57
1:A:103:MET:HB2	4:A:1637:HOH:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLY:HA3	2:A:1312:FMN:N5	2.20	0.56
1:B:53:ASN:HB3	1:B:212:PRO:HG3	1.88	0.56
1:B:262:LEU:N	4:B:2606:HOH:O	1.79	0.54
1:A:170:ASP:OD2	1:B:138:GLN:NE2	2.42	0.53
1:A:138:GLN:NE2	1:B:170:ASP:OD2	2.42	0.53
1:A:69:MET:HG2	4:A:1414:HOH:O	2.13	0.49
1:A:24:MET:SD	1:A:73:ASN:HA	2.53	0.48
1:A:87:GLN:HB3	4:A:1642:HOH:O	2.13	0.48
1:B:20:GLY:HA3	2:B:2312:FMN:N5	2.28	0.48
1:B:103:MET:HB2	4:B:2479:HOH:O	2.12	0.48
1:A:53:ASN:HB3	1:A:212:PRO:HG3	1.97	0.47
1:B:55:LEU:HB3	1:B:56:PRO:HA	1.99	0.45
1:A:43:LYS:HE2	1:A:72:PRO:O	2.17	0.45
1:A:92:GLN:HG2	4:A:1651:HOH:O	2.17	0.44
1:B:20:GLY:HA2	1:B:43:LYS:HD2	1.98	0.44
1:A:180:ILE:O	1:A:183:GLN:HG2	2.18	0.44
1:A:47:LEU:HD12	1:A:107:GLU:HG3	2.01	0.43
1:A:138:GLN:HE21	1:A:138:GLN:N	2.08	0.43
1:B:58:TYR:CD1	1:B:58:TYR:C	2.95	0.43
1:A:87:GLN:HB2	4:A:1440:HOH:O	2.19	0.43
1:A:138:GLN:H	1:A:138:GLN:NE2	2.08	0.43
1:A:18:ALA:HB1	2:A:1312:FMN:O2'	2.19	0.42
1:A:13:ASN:HB2	1:A:14:PRO:HD2	2.02	0.42
2:B:2312:FMN:HM83	2:B:2312:FMN:HM71	1.95	0.41
1:A:188:TYR:CE1	1:A:246:ILE:HD12	2.55	0.41
1:B:69:MET:HG2	4:B:2407:HOH:O	2.20	0.41
1:A:207:SER:CB	1:B:309:LYS:HB2	2.49	0.41
1:A:16:MET:HB2	1:A:269:GLN:HG2	2.03	0.41
1:A:213:LYS:HD3	4:A:1497:HOH:O	2.20	0.41
1:A:16:MET:HG2	1:A:39:ALA:HB3	2.03	0.40
1:B:84:LEU:O	1:B:88:LYS:HG3	2.22	0.40
1:B:188:TYR:CE1	1:B:246:ILE:HD12	2.57	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	309/311 (99%)	297 (96%)	11 (4%)	1 (0%)	36	25
1	B	310/311 (100%)	300 (97%)	10 (3%)	0	100	100
All	All	619/622 (100%)	597 (96%)	21 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	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	258/258 (100%)	254 (98%)	4 (2%)	55	47
1	B	259/258 (100%)	254 (98%)	5 (2%)	50	41
All	All	517/516 (100%)	508 (98%)	9 (2%)	53	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	55	LEU
1	A	93	GLU
1	A	138	GLN
1	B	55	LEU
1	B	93	GLU
1	B	138	GLN
1	B	207	SER
1	B	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	305	HIS
1	B	90	ASN
1	B	138	GLN
1	B	183	GLN
1	B	295	GLN
1	B	305	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ORO	A	1313	-	11,11,11	1.32	1 (9%)	14,15,15	2.06	5 (35%)
2	FMN	A	1312	-	33,33,33	1.96	7 (21%)	48,50,50	2.24	18 (37%)
2	FMN	B	2312	-	33,33,33	2.00	11 (33%)	48,50,50	2.13	13 (27%)
3	ORO	B	2313	-	11,11,11	1.41	2 (18%)	14,15,15	2.20	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ORO	A	1313	-	-	4/4/4/4	0/1/1/1
2	FMN	A	1312	-	-	2/18/18/18	0/3/3/3
2	FMN	B	2312	-	-	1/18/18/18	0/3/3/3
3	ORO	B	2313	-	-	4/4/4/4	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1312	FMN	C4'-C3'	5.72	1.63	1.53
2	B	2312	FMN	C9-C8	-5.03	1.32	1.39
2	A	1312	FMN	C7M-C7	4.41	1.59	1.51
2	A	1312	FMN	C4A-N5	4.40	1.40	1.30
2	A	1312	FMN	C1'-N10	-3.62	1.39	1.47
2	B	2312	FMN	C5'-C4'	3.52	1.56	1.51
2	B	2312	FMN	C4'-C3'	3.32	1.59	1.53
2	B	2312	FMN	C6-C5A	-3.28	1.35	1.40
2	B	2312	FMN	C1'-C2'	3.27	1.57	1.52
2	B	2312	FMN	C4A-N5	3.07	1.37	1.30
3	B	2313	ORO	C2-N1	2.87	1.42	1.37
3	A	1313	ORO	C2-N1	2.79	1.42	1.37
2	B	2312	FMN	C9-C9A	-2.74	1.35	1.39
2	A	1312	FMN	C6-C5A	-2.46	1.36	1.40
3	B	2313	ORO	C6-C7	2.35	1.54	1.48
2	A	1312	FMN	C9-C9A	-2.17	1.36	1.39
2	B	2312	FMN	C7M-C7	2.11	1.55	1.51
2	A	1312	FMN	P-O3P	-2.11	1.47	1.54
2	B	2312	FMN	C1'-N10	-2.10	1.42	1.47
2	B	2312	FMN	C9A-C5A	2.08	1.44	1.41
2	B	2312	FMN	O2-C2	-2.00	1.20	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2312	FMN	C4A-C10-N1	-5.90	110.11	124.59
2	A	1312	FMN	C5'-C4'-C3'	-5.90	101.09	112.22
2	B	2312	FMN	C10-N1-C2	5.17	128.05	116.85
2	B	2312	FMN	C5'-C4'-C3'	-5.15	102.50	112.22
2	A	1312	FMN	C4A-C10-N1	-4.83	112.74	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1312	FMN	C4-C4A-C10	4.55	124.74	116.93
3	B	2313	ORO	C6-N1-C2	-4.41	117.93	122.65
2	A	1312	FMN	C10-N1-C2	4.40	126.38	116.85
2	A	1312	FMN	C4'-C3'-C2'	-4.24	106.52	113.57
2	B	2312	FMN	C9A-C5A-N5	-3.84	118.38	122.45
3	A	1313	ORO	C6-N1-C2	-3.83	118.55	122.65
3	A	1313	ORO	C5-C6-N1	3.83	125.36	120.87
2	A	1312	FMN	O3'-C3'-C2'	-3.77	100.36	108.93
2	B	2312	FMN	N10-C10-N1	3.69	129.38	118.51
3	B	2313	ORO	O71-C7-C6	-3.69	113.53	121.01
2	A	1312	FMN	C9-C9A-N10	-3.67	116.92	121.85
3	B	2313	ORO	C5-C6-N1	3.61	125.11	120.87
3	B	2313	ORO	C4-N3-C2	3.54	128.98	125.55
2	B	2312	FMN	C7M-C7-C6	3.48	125.70	119.57
2	B	2312	FMN	N3-C2-N1	-3.48	112.11	119.50
2	B	2312	FMN	C4-C4A-C10	3.42	122.81	116.93
2	A	1312	FMN	C4A-C10-N10	3.28	121.17	116.48
3	A	1313	ORO	O71-C7-C6	-3.26	114.39	121.01
2	A	1312	FMN	C7M-C7-C8	-3.06	114.50	120.76
2	B	2312	FMN	O3'-C3'-C2'	-3.03	102.05	108.93
2	A	1312	FMN	C1'-C2'-C3'	3.02	117.86	109.66
2	B	2312	FMN	C10-C4A-N5	-2.97	118.75	124.81
3	A	1313	ORO	O72-C7-O71	2.85	130.68	123.90
2	A	1312	FMN	C7M-C7-C6	2.58	124.12	119.57
2	A	1312	FMN	N10-C10-N1	2.50	125.86	118.51
2	A	1312	FMN	C5A-C6-C7	-2.48	116.23	120.83
2	A	1312	FMN	C4-C4A-N5	-2.45	114.82	118.21
2	A	1312	FMN	O3P-P-O2P	2.44	116.97	107.80
2	A	1312	FMN	C10-C4A-N5	-2.27	120.17	124.81
2	B	2312	FMN	C7M-C7-C8	-2.25	116.17	120.76
3	A	1313	ORO	C4-N3-C2	2.12	127.60	125.55
2	A	1312	FMN	O5'-C5'-C4'	2.09	114.94	109.36
2	A	1312	FMN	O2P-P-O5'	-2.03	101.39	106.67
2	B	2312	FMN	O4'-C4'-C3'	2.01	113.96	109.25
2	B	2312	FMN	C5A-N5-C4A	2.01	121.33	118.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1313	ORO	N1-C6-C7-O71
3	A	1313	ORO	N1-C6-C7-O72

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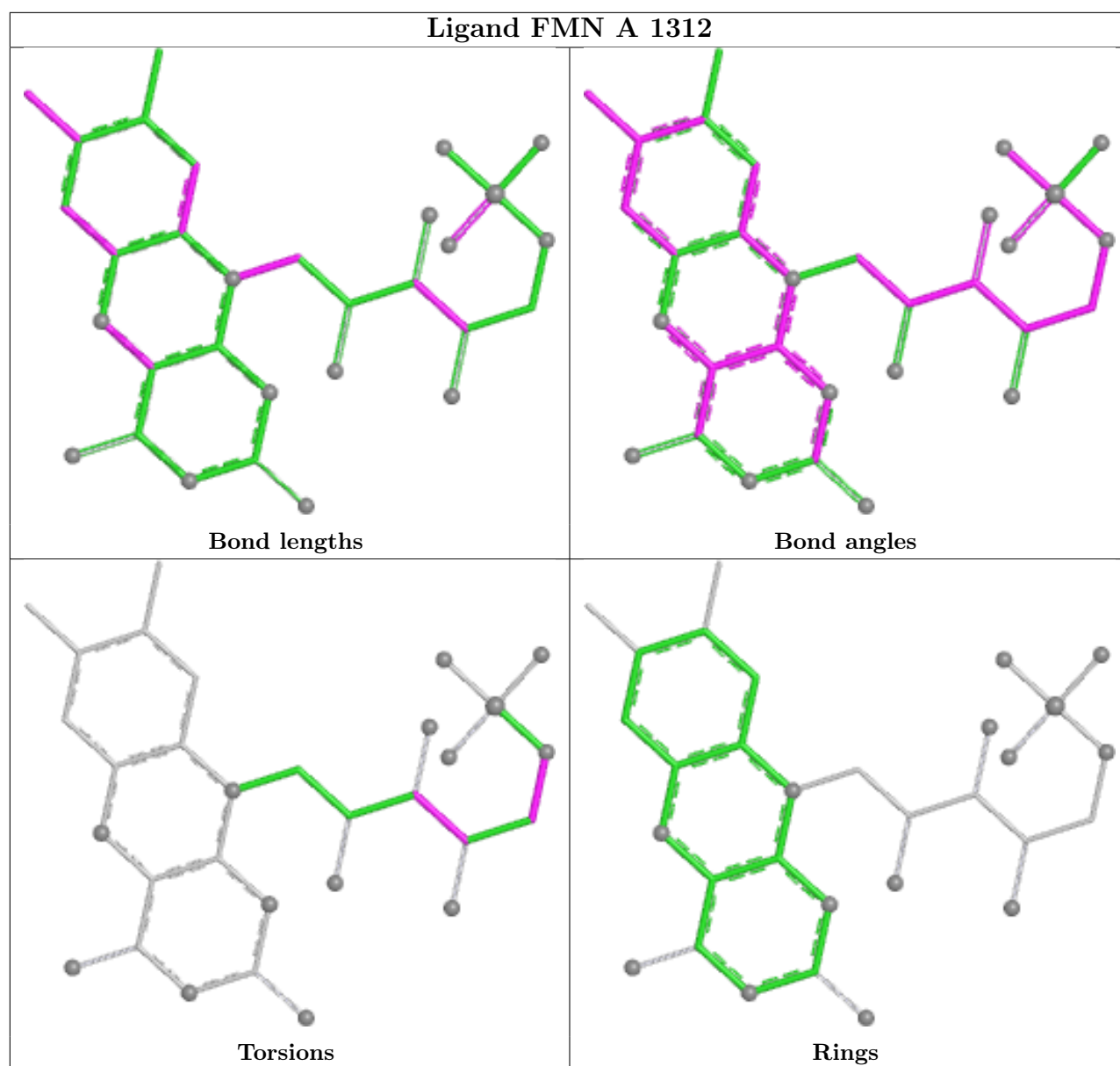
Mol	Chain	Res	Type	Atoms
3	A	1313	ORO	C5-C6-C7-O71
3	A	1313	ORO	C5-C6-C7-O72
3	B	2313	ORO	N1-C6-C7-O71
3	B	2313	ORO	N1-C6-C7-O72
3	B	2313	ORO	C5-C6-C7-O71
3	B	2313	ORO	C5-C6-C7-O72
2	A	1312	FMN	C4'-C5'-O5'-P
2	B	2312	FMN	C4'-C5'-O5'-P
2	A	1312	FMN	O3'-C3'-C4'-C5'

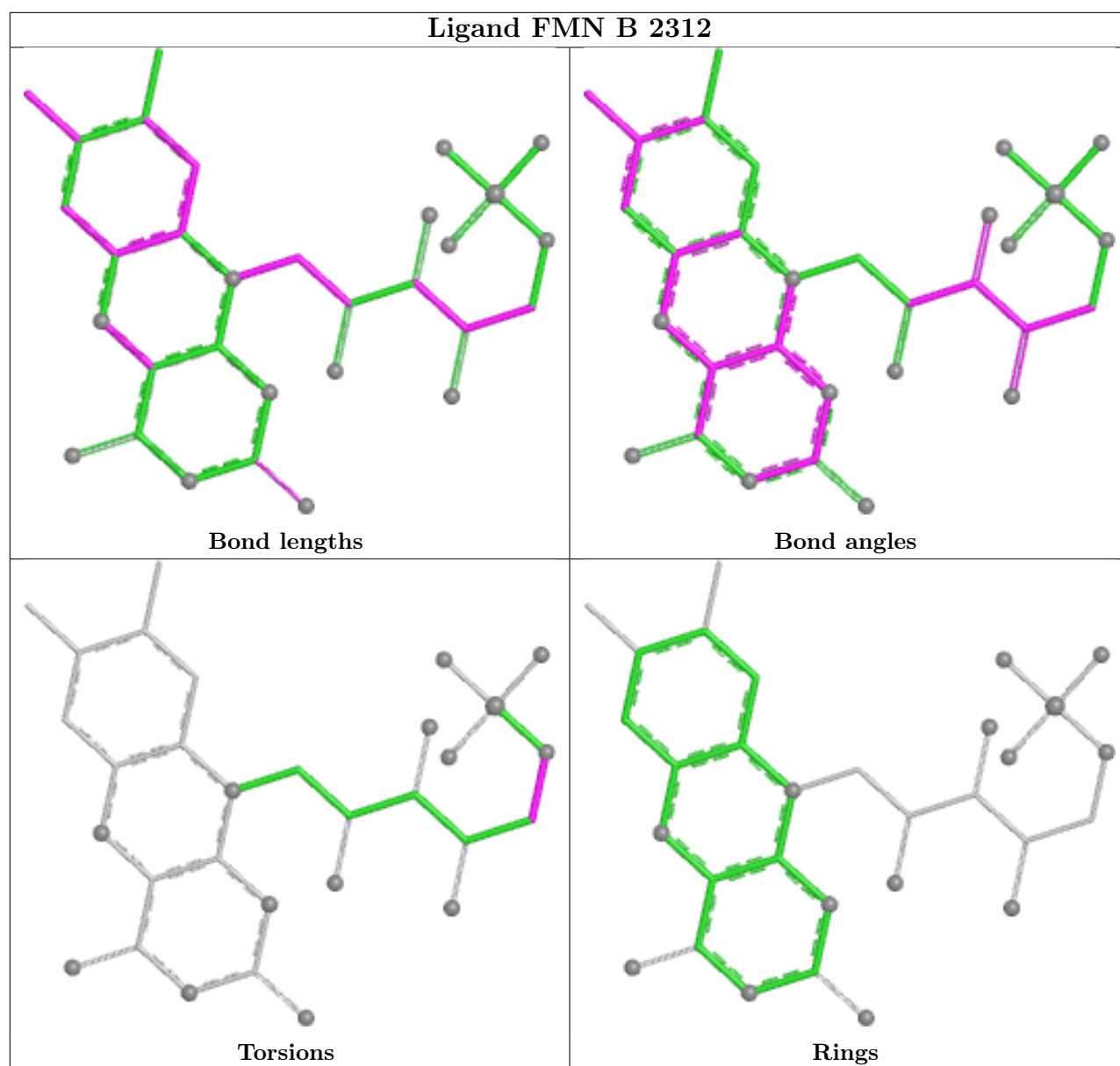
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1312	FMN	2	0
2	B	2312	FMN	2	0

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





5.7 Other polymers [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	311/311 (100%)	-0.32	14 (4%) 38 37	7, 13, 24, 45	25 (8%)
1	B	311/311 (100%)	-0.39	9 (2%) 53 53	7, 13, 24, 39	26 (8%)
All	All	622/622 (100%)	-0.35	23 (3%) 45 45	7, 13, 24, 45	51 (8%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	LYS	7.4
1	A	85	LYS	6.6
1	A	88	LYS	6.0
1	B	85	LYS	5.7
1	B	93	GLU	5.1
1	A	8	ASN	4.4
1	A	92	GLN	3.5
1	A	81	ASP	3.4
1	B	92	GLN	3.2
1	A	90	ASN	3.0
1	B	88	LYS	3.0
1	A	117	GLU	2.9
1	A	48	GLU	2.8
1	B	86[A]	ASN	2.8
1	A	93	GLU	2.6
1	B	90	ASN	2.6
1	B	91	ALA	2.4
1	B	133	VAL	2.4
1	A	137	PRO	2.4
1	A	86	ASN	2.2
1	A	144	GLU	2.2
1	A	172	VAL	2.1
1	B	137	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

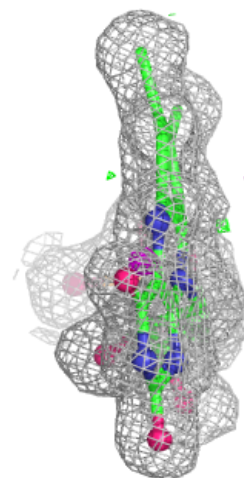
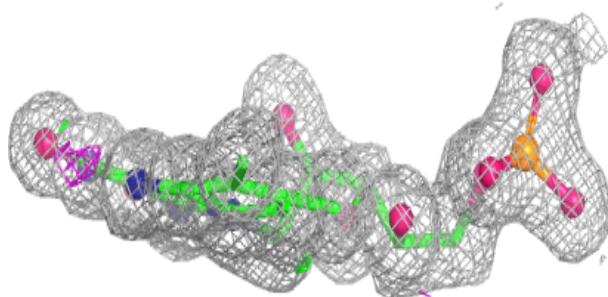
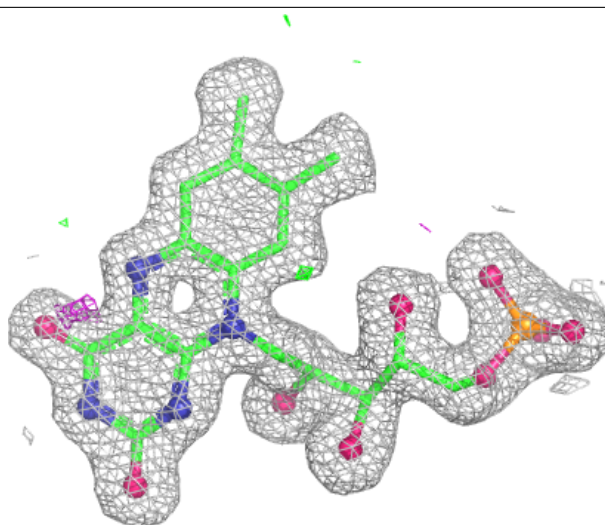
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ORO	A	1313	11/11	0.92	0.13	14,16,18,20	0
3	ORO	B	2313	11/11	0.96	0.07	13,15,18,19	0
2	FMN	A	1312	31/31	0.98	0.04	6,9,11,11	0
2	FMN	B	2312	31/31	0.98	0.04	6,9,11,11	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.

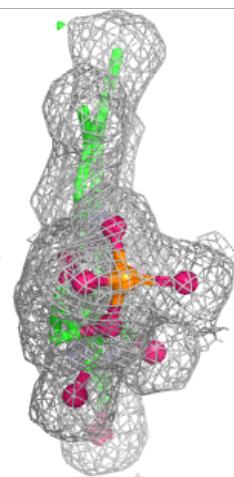
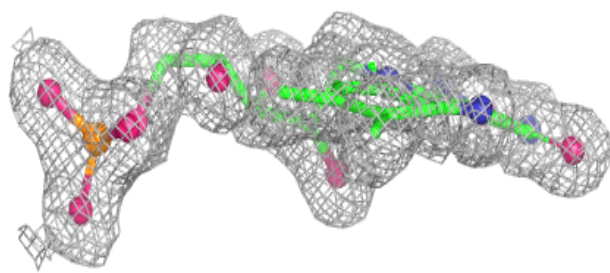
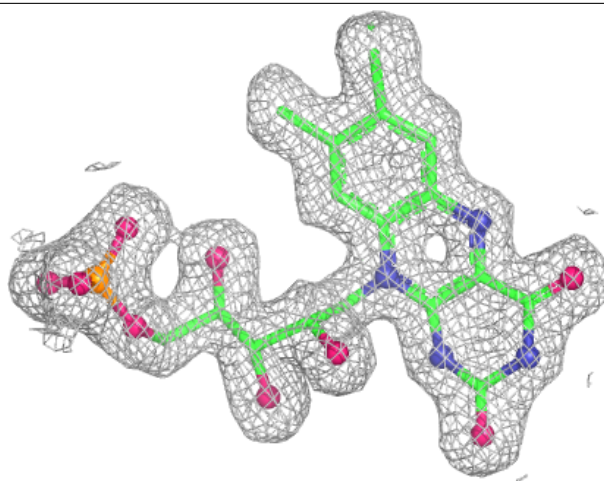
Electron density around FMN A 1312:

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



Electron density around FMN B 2312:

$2mF_o-DF_c$ (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.