



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:48 PM UTC

PDB ID : 1XT6 / pdb_00001xt6
Title : S35C Flavodoxin Mutant in the semiquinone state
Authors : Artali, R.; Marchini, N.; Meneghetti, F.; Cavazzini, D.; Cassetta, A.; Sassone, C.; Bombieri, G.; Rossi, G.L.; Gilardi, G.
Deposited on : 2004-10-21
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

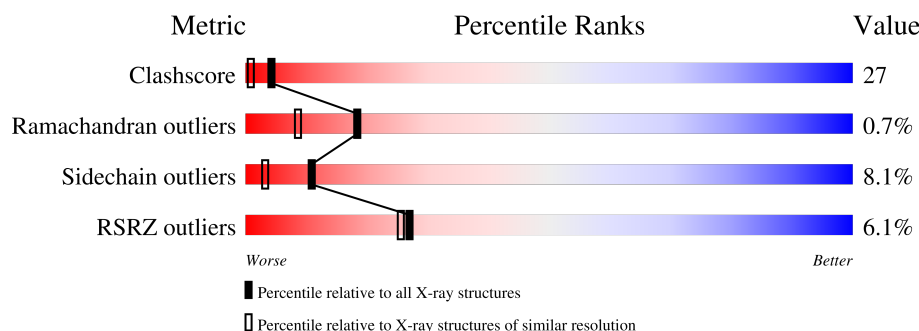
1 Overall quality at a glance

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))
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	147	6% 10% 59% 27% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	A	149	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1261 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.

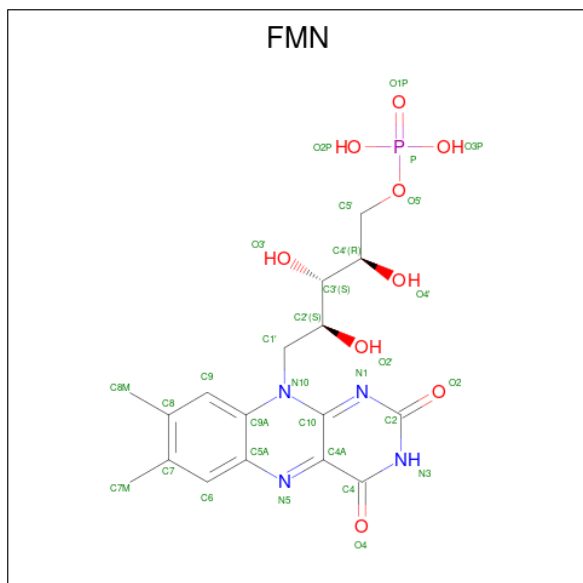
- Molecule 1 is a protein called Flavodoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1102	684	181	232	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	conflict	UNP P00323
A	35	CYS	SER	engineered mutation	UNP P00323

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: 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		

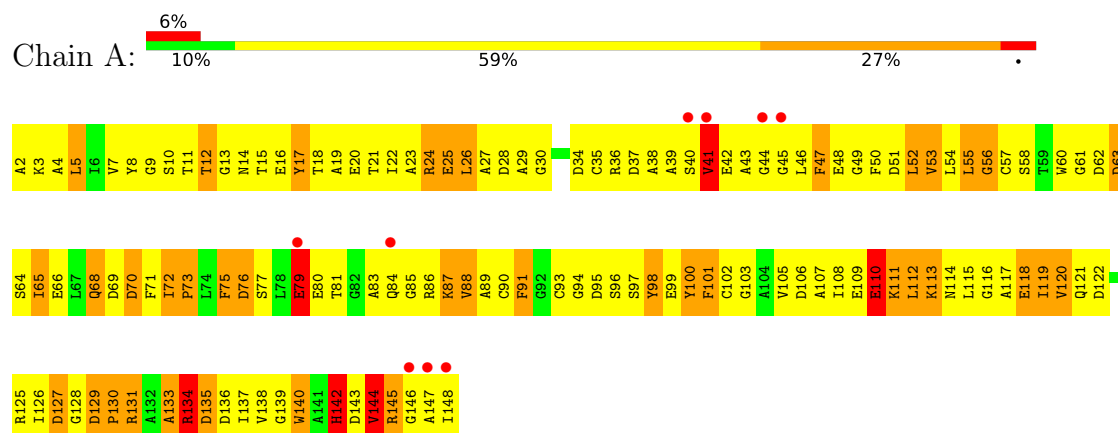
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0

3 Residue-property plots [i](#)

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

• Molecule 1: Flavodoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	51.08Å 51.08Å 138.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.80 19.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	79.4 (19.99-1.80) 98.7 (19.99-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.38Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.261 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 56.3	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	0.93	EDS
Total number of atoms	1261	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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

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	3.76	188/1119 (16.8%)	2.66	100/1514 (6.6%)

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	2

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ALA	CA-CB	16.52	1.76	1.53
1	A	24	ARG	C-O	15.25	1.42	1.24
1	A	119	ILE	CA-CB	14.16	1.69	1.53
1	A	131	ARG	C-O	13.29	1.40	1.24
1	A	118	GLU	CA-C	12.54	1.69	1.53
1	A	19	ALA	CA-C	11.97	1.68	1.52
1	A	27	ALA	N-CA	11.33	1.60	1.46
1	A	112	LEU	C-O	10.93	1.37	1.24
1	A	122	ASP	CA-C	10.72	1.66	1.52
1	A	110	GLU	CG-CD	10.54	1.78	1.52
1	A	47	PHE	C-O	-10.44	1.10	1.24
1	A	88	VAL	N-CA	10.18	1.57	1.46
1	A	90	CYS	CA-C	10.07	1.65	1.52
1	A	108	ILE	CA-C	10.05	1.65	1.52
1	A	79	GLU	CG-CD	9.93	1.76	1.52
1	A	137	ILE	CA-CB	-9.78	1.43	1.54
1	A	29	ALA	CA-C	9.73	1.66	1.52
1	A	75	PHE	C-O	9.62	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ILE	C-O	9.60	1.34	1.23
1	A	3	LYS	CA-C	9.58	1.63	1.52
1	A	20	GLU	N-CA	9.53	1.57	1.46
1	A	103	GLY	C-O	9.25	1.35	1.24
1	A	87	LYS	CA-CB	-9.22	1.40	1.53
1	A	97	SER	CA-C	9.22	1.65	1.52
1	A	9	GLY	C-O	9.21	1.36	1.23
1	A	54	LEU	CA-CB	9.06	1.71	1.53
1	A	131	ARG	N-CA	9.04	1.57	1.46
1	A	136	ASP	CA-C	9.04	1.65	1.52
1	A	131	ARG	CZ-NH1	8.96	1.45	1.32
1	A	87	LYS	CA-C	8.96	1.63	1.52
1	A	133	ALA	C-O	-8.96	1.11	1.24
1	A	145	ARG	CA-C	8.93	1.64	1.52
1	A	94	GLY	C-O	8.83	1.29	1.23
1	A	101	PHE	CA-C	8.75	1.64	1.52
1	A	23	ALA	C-O	-8.74	1.13	1.24
1	A	77	SER	CA-C	-8.66	1.42	1.53
1	A	100	TYR	CA-C	8.57	1.63	1.52
1	A	121	GLN	CA-CB	8.50	1.68	1.53
1	A	131	ARG	CA-CB	-8.48	1.39	1.53
1	A	107	ALA	CA-CB	-8.47	1.39	1.53
1	A	34	ASP	N-CA	8.46	1.56	1.46
1	A	121	GLN	C-O	-8.41	1.13	1.23
1	A	38	ALA	CA-CB	8.36	1.68	1.53
1	A	101	PHE	C-O	8.30	1.33	1.24
1	A	83	ALA	CA-C	-8.28	1.41	1.52
1	A	117	ALA	C-O	8.26	1.33	1.23
1	A	16	GLU	N-CA	8.25	1.56	1.46
1	A	95	ASP	N-CA	-8.22	1.36	1.46
1	A	72	ILE	CA-CB	-8.20	1.50	1.54
1	A	19	ALA	N-CA	8.18	1.56	1.46
1	A	107	ALA	N-CA	8.13	1.56	1.46
1	A	29	ALA	N-CA	-8.10	1.35	1.46
1	A	95	ASP	CB-CG	8.08	1.72	1.52
1	A	137	ILE	N-CA	8.04	1.56	1.46
1	A	10	SER	CA-C	7.93	1.61	1.52
1	A	99	GLU	CA-C	7.87	1.63	1.52
1	A	145	ARG	CZ-NH1	7.77	1.43	1.32
1	A	16	GLU	CA-C	7.66	1.62	1.52
1	A	93	CYS	CA-C	7.66	1.61	1.52
1	A	109	GLU	CA-C	7.63	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	ALA	N-CA	7.62	1.60	1.46
1	A	111	LYS	N-CA	-7.52	1.37	1.46
1	A	69	ASP	N-CA	7.43	1.55	1.46
1	A	106	ASP	N-CA	7.41	1.55	1.46
1	A	125	ARG	CZ-NH2	7.41	1.43	1.33
1	A	134	ARG	C-O	7.41	1.32	1.24
1	A	79	GLU	CD-OE2	7.36	1.39	1.25
1	A	79	GLU	C-O	-7.35	1.14	1.24
1	A	25	GLU	CG-CD	7.28	1.70	1.52
1	A	93	CYS	N-CA	7.28	1.54	1.45
1	A	85	GLY	C-O	7.23	1.34	1.24
1	A	101	PHE	N-CA	7.22	1.55	1.46
1	A	8	TYR	C-O	-7.14	1.14	1.23
1	A	101	PHE	CA-CB	-7.12	1.42	1.53
1	A	75	PHE	CA-C	7.12	1.62	1.52
1	A	42	GLU	CA-C	-7.09	1.44	1.52
1	A	26	LEU	CA-CB	7.03	1.64	1.53
1	A	56	GLY	CA-C	7.00	1.57	1.52
1	A	100	TYR	C-N	-6.98	1.23	1.33
1	A	30	GLY	C-O	6.92	1.33	1.24
1	A	106	ASP	CG-OD2	6.91	1.38	1.25
1	A	42	GLU	C-O	6.89	1.31	1.24
1	A	72	ILE	CA-C	6.87	1.60	1.52
1	A	5	LEU	CA-C	6.86	1.60	1.52
1	A	113	LYS	CE-NZ	6.85	1.70	1.49
1	A	97	SER	N-CA	6.85	1.55	1.46
1	A	52	LEU	N-CA	6.84	1.54	1.46
1	A	80	GLU	CA-C	6.77	1.63	1.52
1	A	27	ALA	CA-CB	-6.75	1.42	1.53
1	A	89	ALA	N-CA	6.73	1.54	1.45
1	A	70	ASP	N-CA	6.69	1.54	1.46
1	A	91	PHE	C-O	6.68	1.32	1.23
1	A	18	THR	CA-CB	6.66	1.63	1.53
1	A	75	PHE	N-CA	6.62	1.54	1.46
1	A	23	ALA	CA-CB	6.62	1.63	1.53
1	A	135	ASP	CG-OD1	6.58	1.37	1.25
1	A	125	ARG	N-CA	6.50	1.54	1.46
1	A	145	ARG	N-CA	6.47	1.54	1.46
1	A	38	ALA	CA-C	6.45	1.61	1.52
1	A	53	VAL	CB-CG2	6.44	1.73	1.52
1	A	52	LEU	CA-C	6.42	1.60	1.52
1	A	64	SER	CA-C	6.38	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	THR	CA-C	-6.38	1.44	1.52
1	A	39	ALA	CA-C	6.35	1.61	1.52
1	A	120	VAL	C-O	6.35	1.32	1.24
1	A	113	LYS	CA-C	6.31	1.60	1.52
1	A	17	TYR	C-O	6.31	1.31	1.24
1	A	136	ASP	N-CA	6.31	1.54	1.46
1	A	26	LEU	CA-C	6.28	1.60	1.52
1	A	7	VAL	CA-CB	-6.26	1.46	1.54
1	A	113	LYS	CD-CE	6.26	1.71	1.52
1	A	94	GLY	CA-C	6.25	1.65	1.51
1	A	129	ASP	CA-CB	6.21	1.65	1.53
1	A	144	VAL	N-CA	6.20	1.54	1.46
1	A	107	ALA	C-O	6.20	1.31	1.24
1	A	97	SER	C-O	6.19	1.32	1.24
1	A	134	ARG	CZ-NH2	6.18	1.41	1.33
1	A	63	ASP	C-O	-6.17	1.15	1.24
1	A	113	LYS	CB-CG	-6.13	1.34	1.52
1	A	73	PRO	CG-CD	6.12	1.71	1.50
1	A	79	GLU	CD-OE1	6.12	1.36	1.25
1	A	40	SER	CB-OG	6.08	1.54	1.42
1	A	110	GLU	CD-OE1	6.06	1.36	1.25
1	A	4	ALA	C-N	6.05	1.42	1.33
1	A	126	ILE	CB-CG2	6.05	1.72	1.52
1	A	125	ARG	CA-C	6.04	1.60	1.52
1	A	105	VAL	CB-CG1	6.04	1.72	1.52
1	A	87	LYS	C-O	6.01	1.31	1.24
1	A	142	HIS	N-CA	6.01	1.53	1.46
1	A	35	CYS	CB-SG	5.98	2.00	1.81
1	A	43	ALA	CA-CB	-5.97	1.43	1.53
1	A	120	VAL	CB-CG1	5.95	1.72	1.52
1	A	21	THR	CA-CB	5.93	1.62	1.53
1	A	52	LEU	C-O	5.92	1.30	1.23
1	A	51	ASP	CG-OD2	5.92	1.36	1.25
1	A	143	ASP	C-O	5.90	1.31	1.24
1	A	4	ALA	CA-CB	5.88	1.63	1.53
1	A	71	PHE	CD1-CE1	5.86	1.56	1.38
1	A	134	ARG	CZ-NH1	5.82	1.40	1.32
1	A	73	PRO	C-N	5.80	1.41	1.33
1	A	13	GLY	C-O	5.77	1.32	1.24
1	A	55	LEU	CA-CB	5.76	1.64	1.53
1	A	86	ARG	CZ-NH2	5.75	1.41	1.33
1	A	22	ILE	CA-CB	5.75	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ASP	C-O	5.74	1.31	1.24
1	A	46	LEU	N-CA	5.65	1.53	1.46
1	A	125	ARG	CG-CD	5.64	1.69	1.52
1	A	13	GLY	C-N	5.62	1.41	1.33
1	A	45	GLY	C-O	5.58	1.31	1.23
1	A	39	ALA	CA-CB	-5.55	1.44	1.53
1	A	118	GLU	CA-CB	-5.51	1.45	1.53
1	A	18	THR	N-CA	5.49	1.52	1.46
1	A	49	GLY	CA-C	5.49	1.59	1.51
1	A	48	GLU	CD-OE1	5.48	1.35	1.25
1	A	145	ARG	C-O	-5.46	1.17	1.24
1	A	66	GLU	C-N	-5.46	1.25	1.33
1	A	81	THR	CA-CB	5.45	1.62	1.53
1	A	30	GLY	CA-C	5.39	1.59	1.51
1	A	99	GLU	CD-OE1	5.38	1.35	1.25
1	A	76	ASP	CA-C	5.35	1.59	1.52
1	A	61	GLY	C-O	-5.29	1.17	1.23
1	A	137	ILE	C-O	-5.28	1.18	1.24
1	A	68	GLN	CG-CD	5.28	1.65	1.52
1	A	62	ASP	CG-OD1	-5.27	1.15	1.25
1	A	15	THR	C-N	5.27	1.41	1.33
1	A	13	GLY	N-CA	5.25	1.53	1.45
1	A	89	ALA	CA-C	-5.25	1.46	1.52
1	A	134	ARG	N-CA	5.25	1.52	1.46
1	A	34	ASP	CG-OD2	5.25	1.35	1.25
1	A	17	TYR	CA-C	5.24	1.59	1.52
1	A	42	GLU	CD-OE1	5.23	1.35	1.25
1	A	45	GLY	C-N	5.19	1.41	1.33
1	A	71	PHE	N-CA	-5.18	1.39	1.46
1	A	91	PHE	CB-CG	5.18	1.62	1.50
1	A	42	GLU	CD-OE2	5.17	1.35	1.25
1	A	100	TYR	CZ-OH	5.17	1.49	1.38
1	A	91	PHE	CD2-CE2	5.13	1.54	1.38
1	A	100	TYR	CD1-CE1	5.12	1.54	1.38
1	A	57	CYS	C-N	5.10	1.40	1.33
1	A	5	LEU	CG-CD2	5.09	1.69	1.52
1	A	47	PHE	CG-CD2	5.09	1.49	1.38
1	A	102	CYS	CA-C	5.09	1.59	1.53
1	A	68	GLN	CA-CB	5.04	1.61	1.53
1	A	93	CYS	C-O	-5.04	1.17	1.23
1	A	144	VAL	CB-CG2	-5.04	1.35	1.52
1	A	55	LEU	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	CYS	CA-CB	5.04	1.61	1.53
1	A	58	SER	C-O	5.01	1.30	1.23

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ALA	N-CA-C	-12.45	96.23	112.41
1	A	19	ALA	N-CA-C	-10.47	99.95	111.36
1	A	99	GLU	CA-C-N	-10.02	108.44	123.07
1	A	99	GLU	C-N-CA	-10.02	108.44	123.07
1	A	38	ALA	N-CA-C	-8.80	101.80	112.54
1	A	65	ILE	CB-CG1-CD1	-8.29	96.39	113.80
1	A	41	VAL	N-CA-C	7.97	120.60	109.29
1	A	81	THR	N-CA-C	7.85	123.15	113.50
1	A	138	VAL	N-CA-C	7.81	118.56	110.36
1	A	114	ASN	N-CA-C	-7.81	102.77	111.28
1	A	119	ILE	CB-CA-C	-7.51	103.12	111.23
1	A	114	ASN	N-CA-CB	7.44	121.06	110.12
1	A	145	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	A	118	GLU	CB-CA-C	-7.39	98.90	111.31
1	A	40	SER	CA-C-N	-7.31	114.22	122.48
1	A	40	SER	C-N-CA	-7.31	114.22	122.48
1	A	144	VAL	CG1-CB-CG2	7.26	126.77	110.80
1	A	131	ARG	CD-NE-CZ	-7.20	114.31	124.40
1	A	110	GLU	CB-CG-CD	6.87	124.28	112.60
1	A	23	ALA	CA-C-O	-6.87	113.27	120.55
1	A	103	GLY	CA-C-N	-6.82	111.14	120.28
1	A	103	GLY	C-N-CA	-6.82	111.14	120.28
1	A	105	VAL	N-CA-C	-6.81	103.67	110.62
1	A	43	ALA	N-CA-C	6.72	120.36	111.75
1	A	117	ALA	CA-C-O	6.57	128.54	121.44
1	A	87	LYS	N-CA-C	-6.42	98.81	109.46
1	A	137	ILE	N-CA-C	-6.40	104.40	110.42
1	A	22	ILE	CB-CA-C	-6.40	103.39	112.22
1	A	90	CYS	CB-CA-C	-6.33	96.82	109.79
1	A	27	ALA	N-CA-C	-6.24	104.48	111.28
1	A	62	ASP	CA-C-N	-6.20	111.89	122.56
1	A	62	ASP	C-N-CA	-6.20	111.89	122.56
1	A	21	THR	N-CA-C	6.19	118.03	111.28
1	A	117	ALA	CA-C-N	-6.17	114.27	122.85
1	A	117	ALA	C-N-CA	-6.17	114.27	122.85
1	A	140	TRP	N-CA-C	-6.17	104.64	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ASP	OD1-CG-OD2	-6.15	108.14	122.90
1	A	95	ASP	CB-CG-OD1	6.14	132.52	118.40
1	A	93	CYS	N-CA-C	-6.13	100.20	109.95
1	A	52	LEU	CA-C-N	-6.12	114.48	122.99
1	A	52	LEU	C-N-CA	-6.12	114.48	122.99
1	A	38	ALA	CA-C-N	-6.11	111.48	120.28
1	A	38	ALA	C-N-CA	-6.11	111.48	120.28
1	A	16	GLU	N-CA-C	-6.11	104.70	111.36
1	A	20	GLU	CB-CA-C	-6.02	101.43	110.88
1	A	63	ASP	N-CA-C	6.02	120.24	113.02
1	A	8	TYR	N-CA-C	5.99	118.97	109.50
1	A	135	ASP	N-CA-CB	5.99	118.66	109.91
1	A	96	SER	CA-CB-OG	-5.98	99.14	111.10
1	A	48	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	130	PRO	O-C-N	5.95	129.08	122.24
1	A	5	LEU	N-CA-C	-5.93	98.74	108.76
1	A	23	ALA	O-C-N	5.93	128.40	122.12
1	A	24	ARG	CB-CG-CD	-5.84	97.86	111.30
1	A	91	PHE	CA-C-N	-5.81	113.36	120.92
1	A	91	PHE	C-N-CA	-5.81	113.36	120.92
1	A	87	LYS	CB-CG-CD	-5.78	98.01	111.30
1	A	127	ASP	CB-CG-OD2	-5.77	105.12	118.40
1	A	22	ILE	CA-C-O	-5.72	114.79	120.85
1	A	9	GLY	N-CA-C	-5.70	99.68	113.18
1	A	139	GLY	N-CA-C	5.67	120.66	113.24
1	A	36	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	A	138	VAL	O-C-N	-5.64	116.30	121.94
1	A	58	SER	CA-C-O	-5.60	115.50	121.94
1	A	99	GLU	CA-CB-CG	-5.55	103.00	114.10
1	A	87	LYS	CA-C-N	-5.53	114.39	122.58
1	A	87	LYS	C-N-CA	-5.53	114.39	122.58
1	A	93	CYS	N-CA-CB	-5.52	102.01	110.85
1	A	26	LEU	CA-C-O	-5.51	114.71	120.55
1	A	79	GLU	N-CA-C	-5.51	105.82	112.54
1	A	65	ILE	CA-C-N	-5.49	114.19	122.81
1	A	65	ILE	C-N-CA	-5.49	114.19	122.81
1	A	98	TYR	N-CA-C	-5.45	101.98	110.42
1	A	134	ARG	CA-CB-CG	-5.42	103.25	114.10
1	A	47	PHE	N-CA-C	5.41	119.87	113.16
1	A	88	VAL	CG1-CB-CG2	5.40	122.68	110.80
1	A	107	ALA	CA-C-O	5.39	126.17	119.97
1	A	131	ARG	N-CA-CB	-5.38	101.93	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASP	CB-CA-C	-5.32	100.78	110.63
1	A	140	TRP	CA-C-O	-5.32	114.78	120.42
1	A	98	TYR	CA-CB-CG	-5.28	104.40	113.90
1	A	34	ASP	N-CA-C	-5.26	99.83	108.41
1	A	87	LYS	CA-C-O	5.25	126.47	120.54
1	A	100	TYR	O-C-N	5.24	130.03	123.12
1	A	72	ILE	CA-C-O	5.23	122.68	118.71
1	A	122	ASP	N-CA-C	-5.22	103.45	110.24
1	A	71	PHE	CA-C-N	-5.20	115.44	120.43
1	A	71	PHE	C-N-CA	-5.20	115.44	120.43
1	A	135	ASP	CB-CG-OD2	-5.19	106.47	118.40
1	A	110	GLU	CA-C-O	-5.12	115.10	120.63
1	A	63	ASP	CA-C-O	-5.10	113.26	119.43
1	A	127	ASP	CA-C-O	-5.08	115.15	120.58
1	A	3	LYS	CA-CB-CG	-5.07	103.95	114.10
1	A	108	ILE	N-CA-C	-5.07	105.60	110.72
1	A	128	GLY	CA-C-O	5.07	129.38	120.57
1	A	109	GLU	N-CA-C	-5.06	105.66	111.07
1	A	111	LYS	CD-CE-NZ	5.06	128.08	111.90
1	A	42	GLU	CA-C-O	5.04	125.58	120.24
1	A	5	LEU	CB-CG-CD2	-5.03	95.61	110.70
1	A	29	ALA	O-C-N	5.01	129.53	122.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	PHE	Sidechain
1	A	98	TYR	Sidechain

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	1102	0	1029	56	1
2	A	31	0	19	3	0
3	A	128	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1261	0	1048	59	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (59) 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:79:GLU:CD	1:A:79:GLU:CG	1.76	1.57
1:A:110:GLU:CD	1:A:110:GLU:CG	1.78	1.56
1:A:133:ALA:CA	1:A:133:ALA:CB	1.76	1.56
1:A:113:LYS:CE	1:A:113:LYS:NZ	1.69	1.55
2:A:149:FMN:O4'	2:A:149:FMN:C4'	1.65	1.39
1:A:68:GLN:HE22	1:A:70:ASP:HB2	1.31	0.92
1:A:25:GLU:HB3	3:A:157:HOH:O	1.69	0.91
1:A:120:VAL:HB	1:A:147:ALA:CB	2.09	0.82
1:A:120:VAL:HB	1:A:147:ALA:HB1	1.64	0.76
1:A:25:GLU:OE1	3:A:182:HOH:O	2.07	0.73
1:A:142:HIS:CD2	1:A:142:HIS:C	2.66	0.73
1:A:110:GLU:OE1	1:A:113:LYS:NZ	2.19	0.72
1:A:146:GLY:O	1:A:148:ILE:N	2.24	0.70
1:A:118:GLU:OE2	3:A:241:HOH:O	2.11	0.68
1:A:87:LYS:NZ	1:A:118:GLU:OE2	2.27	0.68
1:A:53:VAL:HB	1:A:88:VAL:HG12	1.75	0.67
2:A:149:FMN:O4'	2:A:149:FMN:C3'	2.44	0.66
1:A:133:ALA:CB	1:A:133:ALA:N	2.54	0.66
1:A:52:LEU:HD13	1:A:148:ILE:HD11	1.78	0.65
1:A:120:VAL:HB	1:A:147:ALA:HB3	1.80	0.63
1:A:146:GLY:C	1:A:148:ILE:H	2.05	0.63
1:A:146:GLY:C	1:A:148:ILE:N	2.57	0.62
1:A:76:ASP:OD2	3:A:190:HOH:O	2.16	0.61
1:A:129:ASP:OD1	1:A:131:ARG:NH1	2.34	0.60
1:A:26:LEU:HD23	1:A:145:ARG:HD3	1.85	0.59
1:A:65:ILE:HA	3:A:223:HOH:O	2.01	0.58
1:A:140:TRP:O	1:A:144:VAL:HG13	2.04	0.57
1:A:84:GLN:NE2	1:A:116:GLY:HA3	2.20	0.57
1:A:56:GLY:HA2	1:A:91:PHE:O	2.06	0.56
1:A:72:ILE:HB	1:A:73:PRO:HD3	1.88	0.56
1:A:84:GLN:HE22	1:A:116:GLY:HA3	1.71	0.55
1:A:11:THR:HG22	1:A:12:THR:HG22	1.89	0.55
1:A:68:GLN:HE22	1:A:70:ASP:CB	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:FMN:C4'	2:A:149:FMN:HO4'	2.09	0.52
1:A:129:ASP:OD1	1:A:130:PRO:HD2	2.10	0.51
1:A:47:PHE:N	1:A:47:PHE:CD1	2.75	0.51
1:A:101:PHE:CZ	1:A:127:ASP:HB2	2.46	0.51
1:A:84:GLN:NE2	1:A:115:LEU:O	2.45	0.50
1:A:5:LEU:HB2	1:A:50:PHE:CE1	2.49	0.47
1:A:84:GLN:HB3	3:A:270:HOH:O	2.12	0.47
1:A:14:ASN:HB3	1:A:130:PRO:HG3	1.97	0.47
1:A:111:LYS:O	1:A:111:LYS:HG3	2.14	0.47
1:A:65:ILE:HD13	1:A:65:ILE:HG21	1.55	0.47
1:A:146:GLY:O	1:A:147:ALA:C	2.55	0.47
1:A:5:LEU:HB2	1:A:50:PHE:CD1	2.51	0.46
1:A:37:ASP:O	1:A:41:VAL:HG13	2.17	0.45
1:A:110:GLU:CD	1:A:110:GLU:HA	2.40	0.45
1:A:11:THR:HB	1:A:60:TRP:CZ2	2.53	0.44
1:A:142:HIS:C	1:A:142:HIS:HD2	2.23	0.43
1:A:24:ARG:HE	1:A:28:ASP:CG	2.27	0.43
1:A:133:ALA:CB	1:A:133:ALA:C	2.77	0.42
1:A:55:LEU:HD12	1:A:112:LEU:HD11	2.02	0.42
1:A:134:ARG:HG2	1:A:135:ASP:N	2.25	0.41
1:A:17:TYR:CD1	1:A:17:TYR:C	2.97	0.41
1:A:68:GLN:NE2	1:A:70:ASP:HB2	2.15	0.41
1:A:120:VAL:HG11	1:A:148:ILE:HD13	2.03	0.41
1:A:120:VAL:O	1:A:147:ALA:CB	2.69	0.41
1:A:84:GLN:CB	3:A:270:HOH:O	2.69	0.40
1:A:113:LYS:HE3	1:A:113:LYS:HB2	1.78	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:OH	3:A:169:HOH:O[6_455]	2.11	0.09

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	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	18 8

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLY

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	111/111 (100%)	102 (92%)	9 (8%)	11 3

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

Mol	Chain	Res	Type
1	A	12	THR
1	A	41	VAL
1	A	63	ASP
1	A	79	GLU
1	A	110	GLU
1	A	119	ILE
1	A	134	ARG
1	A	142	HIS
1	A	144	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	84	GLN
1	A	121	GLN
1	A	142	HIS

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](#)

1 ligand is 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	A	149	-	33,33,33	4.29	21 (63%)	48,50,50	2.85	26 (54%)

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	A	149	-	-	4/18/18/18	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	O4'-C4'	10.55	1.65	1.43
2	A	149	FMN	C9A-C5A	8.07	1.54	1.41
2	A	149	FMN	C6-C5A	7.58	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C1'-C2'	-6.72	1.43	1.52
2	A	149	FMN	C6-C7	-6.55	1.30	1.39
2	A	149	FMN	C8M-C8	6.54	1.63	1.51
2	A	149	FMN	C5'-C4'	6.27	1.60	1.51
2	A	149	FMN	O4-C4	5.83	1.34	1.23
2	A	149	FMN	C10-N10	-4.83	1.26	1.37
2	A	149	FMN	C8-C7	4.59	1.52	1.40
2	A	149	FMN	C4'-C3'	4.18	1.60	1.53
2	A	149	FMN	P-O1P	4.15	1.63	1.50
2	A	149	FMN	C4A-C10	4.06	1.56	1.44
2	A	149	FMN	P-O5'	-3.64	1.48	1.60
2	A	149	FMN	C9A-N10	3.42	1.47	1.41
2	A	149	FMN	C2-N3	3.29	1.46	1.39
2	A	149	FMN	O2-C2	-3.07	1.18	1.24
2	A	149	FMN	C10-N1	2.89	1.39	1.33
2	A	149	FMN	C2'-C3'	2.41	1.57	1.53
2	A	149	FMN	C4-N3	2.31	1.43	1.38
2	A	149	FMN	C1'-N10	2.18	1.53	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C9A-N10-C10	6.18	130.16	120.75
2	A	149	FMN	C5A-C9A-N10	-6.16	112.40	117.97
2	A	149	FMN	C9-C9A-N10	5.24	128.90	121.85
2	A	149	FMN	O4'-C4'-C3'	-5.20	97.08	109.25
2	A	149	FMN	C6-C5A-N5	4.72	126.28	118.44
2	A	149	FMN	C9A-C5A-N5	-4.34	117.85	122.45
2	A	149	FMN	C7M-C7-C8	-4.13	112.33	120.76
2	A	149	FMN	O2P-P-O1P	4.03	126.55	110.83
2	A	149	FMN	C4-C4A-N5	4.02	123.77	118.21
2	A	149	FMN	C5'-C4'-C3'	3.64	119.08	112.22
2	A	149	FMN	C5A-N5-C4A	3.62	123.94	118.09
2	A	149	FMN	O3'-C3'-C2'	-3.31	101.41	108.93
2	A	149	FMN	O5'-P-O1P	3.09	114.79	106.44
2	A	149	FMN	C7M-C7-C6	3.06	124.96	119.57
2	A	149	FMN	O3P-P-O1P	-3.02	99.06	110.83
2	A	149	FMN	O2-C2-N1	3.00	126.78	121.80
2	A	149	FMN	O4-C4-C4A	-2.97	118.68	126.53
2	A	149	FMN	O2'-C2'-C3'	-2.89	102.49	109.25
2	A	149	FMN	O3P-P-O5'	-2.81	99.35	106.67
2	A	149	FMN	C1'-N10-C9A	-2.69	115.41	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C4A-C10-N10	-2.65	112.69	116.48
2	A	149	FMN	C4A-C4-N3	2.60	119.87	113.25
2	A	149	FMN	O5'-C5'-C4'	-2.45	102.81	109.36
2	A	149	FMN	C6-C5A-C9A	-2.35	115.82	119.05
2	A	149	FMN	C9A-C9-C8	2.25	123.74	119.22
2	A	149	FMN	C6-C7-C8	2.05	122.69	119.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

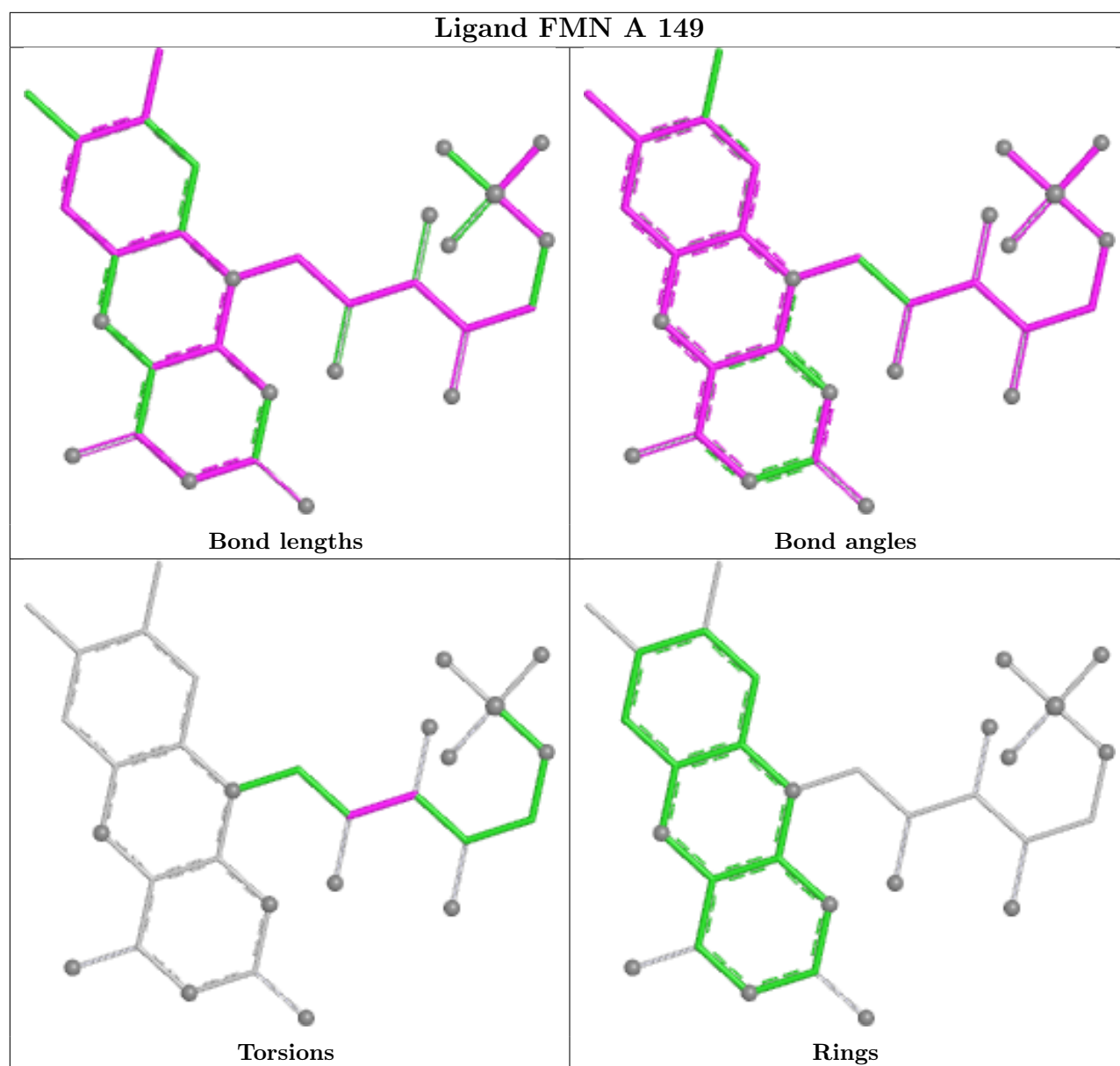
Mol	Chain	Res	Type	Atoms
2	A	149	FMN	C1'-C2'-C3'-O3'
2	A	149	FMN	C1'-C2'-C3'-C4'
2	A	149	FMN	O2'-C2'-C3'-C4'
2	A	149	FMN	O2'-C2'-C3'-O3'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	149	FMN	3	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	147/147 (100%)	0.49	9 (6%)	27 25	14, 26, 40, 47	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	GLN	3.0
1	A	41	VAL	2.5
1	A	44	GLY	2.3
1	A	148	ILE	2.3
1	A	147	ALA	2.2
1	A	79	GLU	2.2
1	A	40	SER	2.1
1	A	45	GLY	2.1
1	A	146	GLY	2.1

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](#)

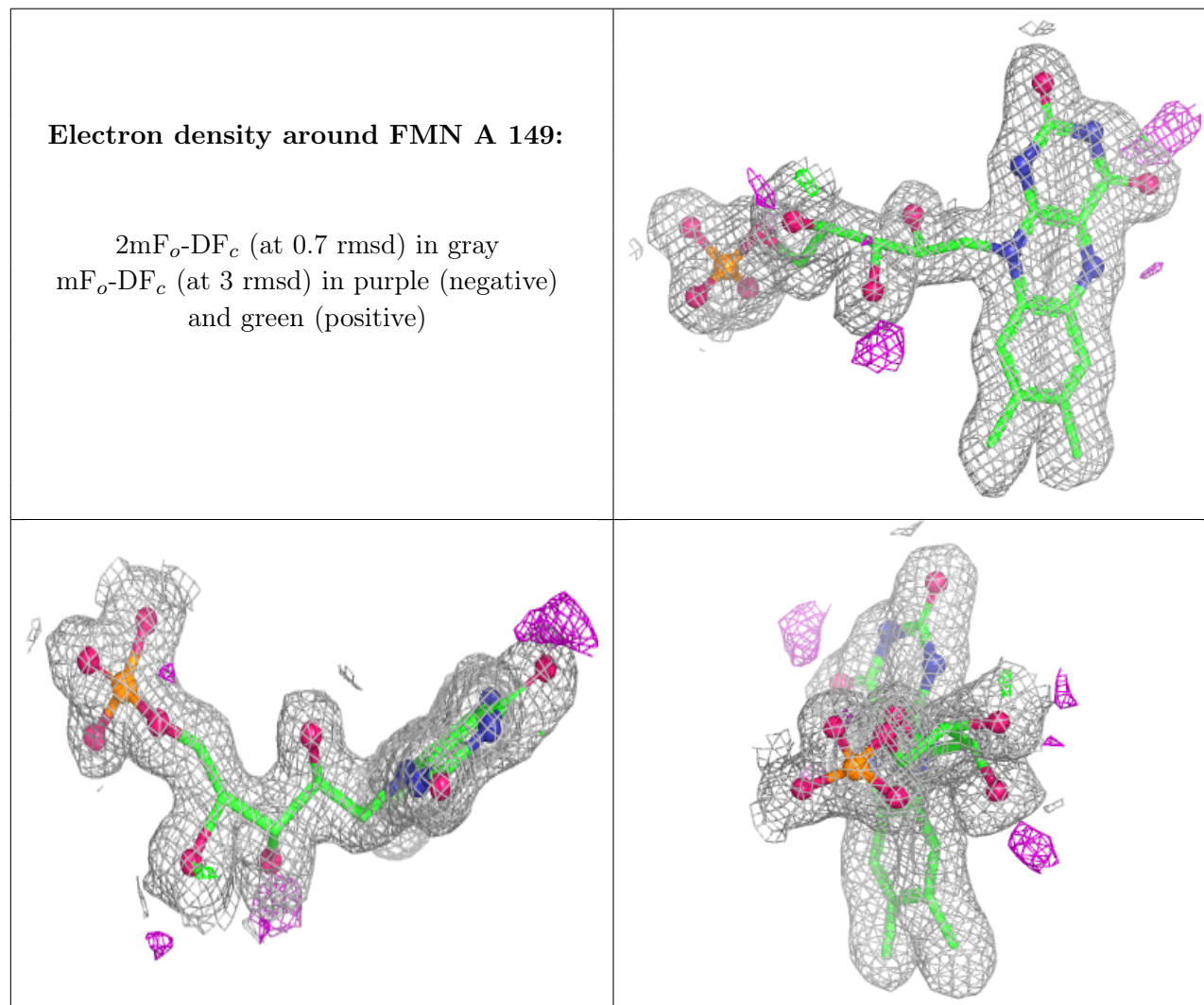
There are no oligosaccharides in this entry.

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
2	FMN	A	149	31/31	0.96	0.07	12,19,22,23	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.