



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:12 AM UTC

PDB ID : 6JXN / pdb_00006jxn
Title : Crystal Structure of Indigo reductase from *Bacillus smithii* type strain DSM 4216
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.
Deposited on : 2019-04-24
Resolution : 1.97 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

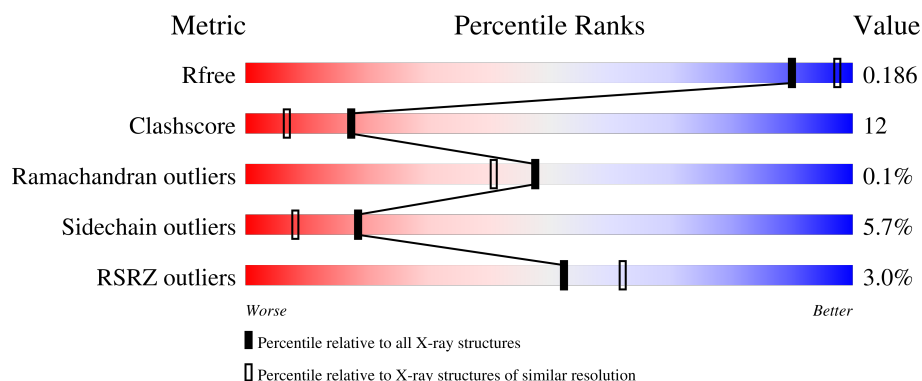
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	231	5% 56% 26% 8% 9%
1	B	231	2% 59% 28% 8%
1	C	231	0% 51% 36% 10%
1	D	231	3% 55% 30% 5% 8%

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
3	PE8	A	302	-	-	X	-
3	PE8	C	302	-	-	X	-
4	NHE	B	302	-	-	X	-
4	NHE	B	303	-	-	X	-
4	NHE	D	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7273 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 FMN-dependent NADH-azoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1649	1062	266	313	8			
1	B	212	Total	C	N	O	S	0	0	0
			1658	1067	268	315	8			
1	C	208	Total	C	N	O	S	0	0	0
			1629	1051	263	307	8			
1	D	212	Total	C	N	O	S	0	0	0
			1658	1067	268	315	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP G9QLG5
A	-18	GLY	-	expression tag	UNP G9QLG5
A	-17	SER	-	expression tag	UNP G9QLG5
A	-16	SER	-	expression tag	UNP G9QLG5
A	-15	HIS	-	expression tag	UNP G9QLG5
A	-14	HIS	-	expression tag	UNP G9QLG5
A	-13	HIS	-	expression tag	UNP G9QLG5
A	-12	HIS	-	expression tag	UNP G9QLG5
A	-11	HIS	-	expression tag	UNP G9QLG5
A	-10	HIS	-	expression tag	UNP G9QLG5
A	-9	SER	-	expression tag	UNP G9QLG5
A	-8	SER	-	expression tag	UNP G9QLG5
A	-7	GLY	-	expression tag	UNP G9QLG5
A	-6	LEU	-	expression tag	UNP G9QLG5
A	-5	VAL	-	expression tag	UNP G9QLG5
A	-4	PRO	-	expression tag	UNP G9QLG5
A	-3	ARG	-	expression tag	UNP G9QLG5
A	-2	GLY	-	expression tag	UNP G9QLG5
A	-1	SER	-	expression tag	UNP G9QLG5
A	0	HIS	-	expression tag	UNP G9QLG5
B	-19	MET	-	expression tag	UNP G9QLG5

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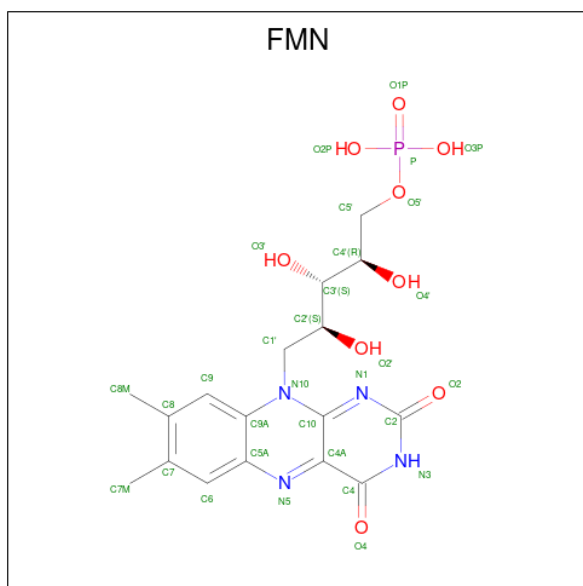
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP G9QLG5
B	-17	SER	-	expression tag	UNP G9QLG5
B	-16	SER	-	expression tag	UNP G9QLG5
B	-15	HIS	-	expression tag	UNP G9QLG5
B	-14	HIS	-	expression tag	UNP G9QLG5
B	-13	HIS	-	expression tag	UNP G9QLG5
B	-12	HIS	-	expression tag	UNP G9QLG5
B	-11	HIS	-	expression tag	UNP G9QLG5
B	-10	HIS	-	expression tag	UNP G9QLG5
B	-9	SER	-	expression tag	UNP G9QLG5
B	-8	SER	-	expression tag	UNP G9QLG5
B	-7	GLY	-	expression tag	UNP G9QLG5
B	-6	LEU	-	expression tag	UNP G9QLG5
B	-5	VAL	-	expression tag	UNP G9QLG5
B	-4	PRO	-	expression tag	UNP G9QLG5
B	-3	ARG	-	expression tag	UNP G9QLG5
B	-2	GLY	-	expression tag	UNP G9QLG5
B	-1	SER	-	expression tag	UNP G9QLG5
B	0	HIS	-	expression tag	UNP G9QLG5
C	-19	MET	-	expression tag	UNP G9QLG5
C	-18	GLY	-	expression tag	UNP G9QLG5
C	-17	SER	-	expression tag	UNP G9QLG5
C	-16	SER	-	expression tag	UNP G9QLG5
C	-15	HIS	-	expression tag	UNP G9QLG5
C	-14	HIS	-	expression tag	UNP G9QLG5
C	-13	HIS	-	expression tag	UNP G9QLG5
C	-12	HIS	-	expression tag	UNP G9QLG5
C	-11	HIS	-	expression tag	UNP G9QLG5
C	-10	HIS	-	expression tag	UNP G9QLG5
C	-9	SER	-	expression tag	UNP G9QLG5
C	-8	SER	-	expression tag	UNP G9QLG5
C	-7	GLY	-	expression tag	UNP G9QLG5
C	-6	LEU	-	expression tag	UNP G9QLG5
C	-5	VAL	-	expression tag	UNP G9QLG5
C	-4	PRO	-	expression tag	UNP G9QLG5
C	-3	ARG	-	expression tag	UNP G9QLG5
C	-2	GLY	-	expression tag	UNP G9QLG5
C	-1	SER	-	expression tag	UNP G9QLG5
C	0	HIS	-	expression tag	UNP G9QLG5
D	-19	MET	-	expression tag	UNP G9QLG5
D	-18	GLY	-	expression tag	UNP G9QLG5
D	-17	SER	-	expression tag	UNP G9QLG5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9QLG5
D	-15	HIS	-	expression tag	UNP G9QLG5
D	-14	HIS	-	expression tag	UNP G9QLG5
D	-13	HIS	-	expression tag	UNP G9QLG5
D	-12	HIS	-	expression tag	UNP G9QLG5
D	-11	HIS	-	expression tag	UNP G9QLG5
D	-10	HIS	-	expression tag	UNP G9QLG5
D	-9	SER	-	expression tag	UNP G9QLG5
D	-8	SER	-	expression tag	UNP G9QLG5
D	-7	GLY	-	expression tag	UNP G9QLG5
D	-6	LEU	-	expression tag	UNP G9QLG5
D	-5	VAL	-	expression tag	UNP G9QLG5
D	-4	PRO	-	expression tag	UNP G9QLG5
D	-3	ARG	-	expression tag	UNP G9QLG5
D	-2	GLY	-	expression tag	UNP G9QLG5
D	-1	SER	-	expression tag	UNP G9QLG5
D	0	HIS	-	expression tag	UNP G9QLG5

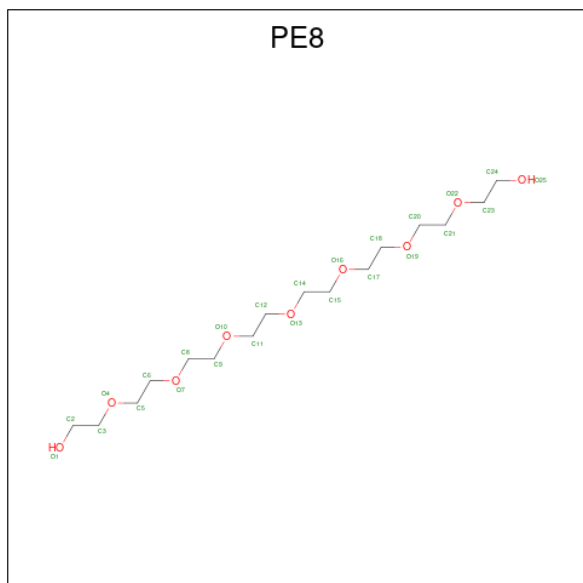
- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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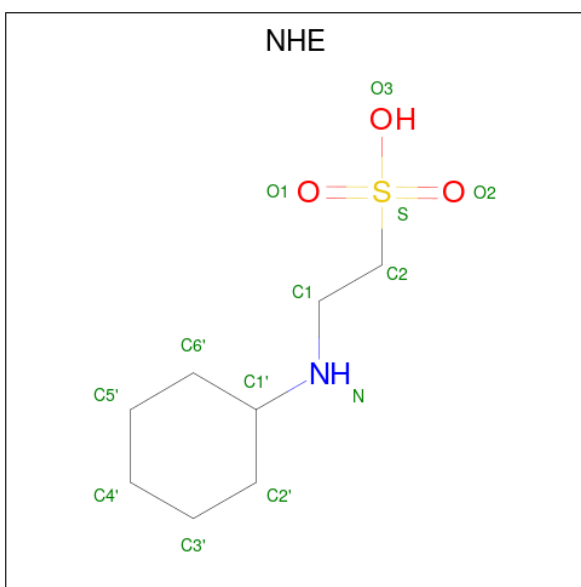
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		
3	C	1	Total	C	O	0	0
			25	16	9		

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$) (labeled as "Ligand of Interest" by depositor).



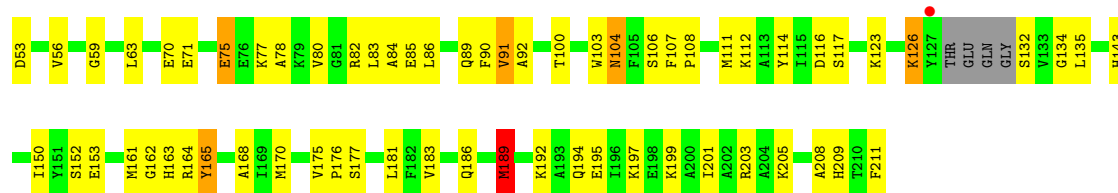
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	D	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

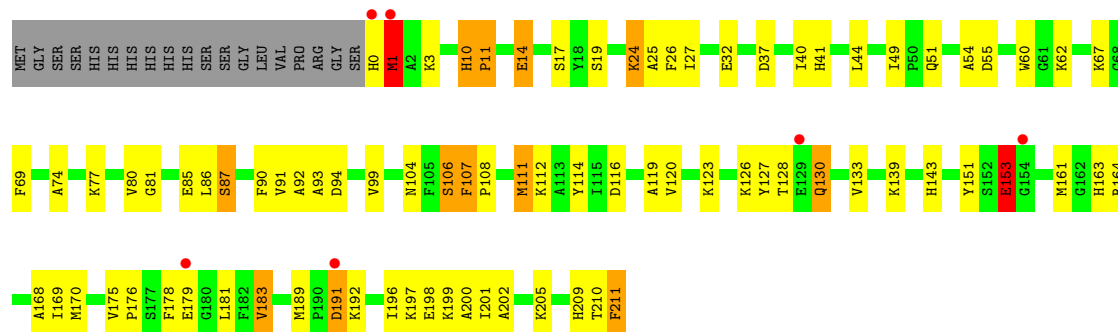
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	119	Total	O	0	0
			119	119		
5	C	119	Total	O	0	0
			119	119		
5	D	123	Total	O	0	0
			123	123		

- Molecule 1: FMN-dependent NADH-azoreductase





● Molecule 1: FMN-dependent NADH-azoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.48Å 105.14Å 87.78Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	35.62 – 1.97 35.62 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.62-1.97) 99.9 (35.62-1.97)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 1.97Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.178 , 0.186 0.178 , 0.186	Depositor DCC
R_{free} test set	3132 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7273	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, NHE, PE8

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	1.98	53/1688 (3.1%)	1.18	6/2277 (0.3%)
1	B	1.97	59/1698 (3.5%)	1.15	1/2292 (0.0%)
1	C	2.02	69/1668 (4.1%)	1.11	3/2250 (0.1%)
1	D	2.02	69/1698 (4.1%)	1.15	5/2292 (0.2%)
All	All	2.00	250/6752 (3.7%)	1.15	15/9111 (0.2%)

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	D	0	1

All (250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	PHE	C-OXT	-9.91	1.03	1.23
1	A	211	PHE	C-OXT	-9.87	1.03	1.23
1	B	107	PHE	C-O	-9.65	1.16	1.24
1	C	107	PHE	C-O	-9.46	1.16	1.24
1	C	108	PRO	CA-C	8.92	1.56	1.51
1	C	108	PRO	C-O	-8.36	1.18	1.25
1	A	0	HIS	CD2-NE2	-8.06	1.28	1.37
1	C	208	ALA	C-O	-7.70	1.14	1.24
1	A	10	HIS	CG-ND1	-7.69	1.29	1.38
1	D	108	PRO	C-O	-7.54	1.18	1.25
1	A	23	GLY	C-O	-7.43	1.14	1.23
1	C	19	SER	C-O	-7.41	1.15	1.24
1	D	201	ILE	C-O	-7.39	1.15	1.24
1	A	99	VAL	C-O	-7.31	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	HIS	CG-ND1	-7.29	1.30	1.38
1	A	0	HIS	CG-CD2	7.26	1.43	1.35
1	C	23	GLY	C-O	-7.14	1.15	1.23
1	B	0	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	163	HIS	CG-ND1	-7.09	1.30	1.38
1	D	209	HIS	CG-ND1	-7.09	1.30	1.38
1	A	19	SER	C-O	-7.09	1.15	1.24
1	B	163	HIS	CD2-NE2	-7.09	1.30	1.37
1	B	23	GLY	C-O	-7.08	1.15	1.23
1	A	54	ALA	C-O	-7.04	1.16	1.24
1	C	8	THR	C-O	-7.01	1.15	1.24
1	C	181	LEU	C-O	-7.00	1.16	1.24
1	D	27	ILE	C-O	-6.98	1.15	1.24
1	C	10	HIS	CG-ND1	-6.93	1.30	1.38
1	A	57	PHE	C-O	-6.92	1.16	1.24
1	A	163	HIS	CD2-NE2	-6.92	1.30	1.37
1	C	199	LYS	C-O	-6.90	1.16	1.24
1	B	52	ILE	C-O	-6.90	1.17	1.24
1	B	7	ILE	C-O	-6.89	1.16	1.24
1	B	143	HIS	CG-ND1	-6.88	1.30	1.38
1	C	32	GLU	C-O	-6.88	1.16	1.24
1	B	108	PRO	C-O	-6.85	1.19	1.25
1	C	10	HIS	CD2-NE2	-6.84	1.30	1.37
1	D	175	VAL	C-O	-6.80	1.15	1.24
1	D	163	HIS	CG-ND1	-6.79	1.30	1.38
1	A	170	MET	C-O	-6.72	1.16	1.24
1	B	106	SER	C-O	-6.71	1.17	1.24
1	D	69	PHE	C-O	-6.70	1.16	1.24
1	C	106	SER	C-O	-6.70	1.15	1.24
1	A	0	HIS	CE1-NE2	6.69	1.39	1.32
1	D	74	ALA	C-O	-6.67	1.16	1.24
1	C	41	HIS	CG-ND1	-6.66	1.30	1.38
1	D	108	PRO	CA-C	6.59	1.55	1.51
1	B	163	HIS	CG-ND1	-6.59	1.31	1.38
1	D	163	HIS	CD2-NE2	-6.58	1.30	1.37
1	D	11	PRO	C-O	-6.52	1.15	1.24
1	D	116	ASP	C-O	-6.49	1.16	1.24
1	B	49	ILE	C-O	-6.47	1.16	1.24
1	B	209	HIS	CG-ND1	-6.46	1.31	1.38
1	C	112	LYS	C-O	-6.44	1.16	1.24
1	D	205	LYS	C-O	-6.40	1.16	1.24
1	B	100	THR	C-O	-6.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	GLY	C-O	-6.37	1.16	1.23
1	A	112	LYS	C-O	-6.34	1.16	1.24
1	C	90	PHE	C-O	-6.33	1.16	1.24
1	D	196	ILE	C-O	-6.29	1.17	1.24
1	A	209	HIS	CG-ND1	-6.28	1.31	1.38
1	A	104	ASN	C-O	-6.28	1.16	1.23
1	A	114	TYR	C-O	-6.27	1.16	1.24
1	D	92	ALA	C-O	-6.24	1.16	1.24
1	B	48	ASN	C-O	-6.21	1.16	1.24
1	D	80	VAL	C-O	-6.21	1.17	1.24
1	D	111	MET	C-O	-6.19	1.16	1.24
1	B	22	VAL	C-O	-6.19	1.17	1.24
1	C	209	HIS	CG-ND1	-6.15	1.31	1.38
1	D	127	TYR	C-O	-6.15	1.16	1.23
1	A	107	PHE	C-O	-6.15	1.16	1.24
1	D	91	VAL	C-O	-6.12	1.16	1.24
1	A	25	ALA	C-O	-6.12	1.17	1.24
1	B	19	SER	C-O	-6.09	1.17	1.24
1	B	50	PRO	C-O	-6.09	1.16	1.23
1	C	52	ILE	C-O	-6.08	1.18	1.24
1	C	56	VAL	C-O	-6.08	1.17	1.24
1	A	10	HIS	CD2-NE2	-6.07	1.31	1.37
1	C	150	ILE	C-O	-6.06	1.17	1.24
1	C	49	ILE	C-O	-6.05	1.16	1.24
1	C	20	MET	C-O	-6.05	1.17	1.24
1	A	205	LYS	C-O	-6.03	1.17	1.24
1	B	125	PHE	C-O	-6.02	1.16	1.23
1	C	27	ILE	C-O	-6.02	1.17	1.24
1	C	117	SER	C-O	-6.02	1.16	1.24
1	D	32	GLU	C-O	-6.01	1.17	1.24
1	C	50	PRO	C-O	-6.01	1.16	1.23
1	B	208	ALA	C-O	-5.98	1.16	1.24
1	D	40	ILE	C-O	-5.96	1.17	1.24
1	A	1	MET	C-O	-5.95	1.17	1.24
1	C	163	HIS	CG-ND1	-5.94	1.31	1.38
1	D	24	LYS	C-O	-5.92	1.17	1.24
1	C	164	ARG	C-O	-5.90	1.17	1.24
1	A	168	ALA	C-O	-5.89	1.17	1.24
1	B	24	LYS	C-O	-5.89	1.17	1.24
1	D	202	ALA	C-O	-5.88	1.17	1.24
1	C	189	MET	C-O	-5.87	1.17	1.24
1	B	209	HIS	CD2-NE2	-5.87	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	LYS	C-O	-5.86	1.17	1.24
1	C	177	SER	C-O	-5.84	1.17	1.23
1	B	0	HIS	CG-ND1	-5.84	1.31	1.38
1	B	207	LEU	C-O	-5.83	1.16	1.24
1	D	200	ALA	C-O	-5.82	1.17	1.24
1	D	55	ASP	C-O	-5.82	1.17	1.24
1	D	44	LEU	C-O	-5.81	1.16	1.24
1	C	80	VAL	C-O	-5.80	1.17	1.24
1	C	134	GLY	C-O	-5.79	1.17	1.23
1	D	106	SER	C-O	-5.79	1.16	1.24
1	B	114	TYR	C-O	-5.79	1.17	1.24
1	C	91	VAL	C-O	-5.79	1.16	1.24
1	D	26	PHE	C-O	-5.79	1.17	1.24
1	A	41	HIS	CD2-NE2	-5.78	1.31	1.37
1	B	10	HIS	CG-ND1	-5.78	1.31	1.38
1	C	201	ILE	C-O	-5.75	1.17	1.24
1	D	114	TYR	C-O	-5.75	1.17	1.24
1	C	29	THR	C-O	-5.75	1.17	1.24
1	A	8	THR	C-O	-5.75	1.17	1.24
1	B	32	GLU	C-O	-5.74	1.17	1.24
1	C	44	LEU	C-O	-5.74	1.16	1.24
1	C	78	ALA	C-O	-5.74	1.17	1.24
1	D	164	ARG	C-O	-5.73	1.17	1.24
1	A	48	ASN	C-O	-5.73	1.17	1.24
1	D	143	HIS	CD2-NE2	-5.72	1.31	1.37
1	C	195	GLU	C-O	-5.72	1.17	1.24
1	B	41	HIS	CG-ND1	-5.71	1.31	1.38
1	D	86	LEU	C-O	-5.70	1.17	1.24
1	D	199	LYS	C-O	-5.70	1.17	1.24
1	C	77	LYS	C-O	-5.69	1.17	1.24
1	A	86	LEU	C-O	-5.67	1.17	1.24
1	D	139	LYS	C-O	-5.63	1.16	1.23
1	A	38	GLU	C-O	-5.62	1.17	1.24
1	D	19	SER	C-O	-5.62	1.17	1.24
1	A	157	ALA	C-O	-5.61	1.17	1.24
1	D	51	GLN	C-O	-5.61	1.16	1.23
1	A	11	PRO	C-O	-5.60	1.17	1.24
1	D	104	ASN	C-O	-5.58	1.16	1.23
1	D	198	GLU	C-O	-5.58	1.17	1.24
1	C	22	VAL	C-O	-5.58	1.17	1.24
1	D	112	LYS	C-O	-5.58	1.17	1.24
1	C	89	GLN	C-O	-5.57	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	LYS	C-O	-5.57	1.17	1.24
1	A	143	HIS	CD2-NE2	-5.56	1.31	1.37
1	C	143	HIS	CG-ND1	-5.56	1.32	1.38
1	B	11	PRO	C-O	-5.56	1.17	1.24
1	D	153	GLU	C-O	-5.56	1.17	1.23
1	C	83	LEU	C-O	-5.54	1.17	1.24
1	A	40	ILE	C-O	-5.54	1.18	1.24
1	B	116	ASP	C-O	-5.53	1.17	1.24
1	B	168	ALA	C-O	-5.53	1.17	1.24
1	A	55	ASP	C-O	-5.53	1.17	1.24
1	B	177	SER	C-O	-5.51	1.17	1.23
1	C	170	MET	C-O	-5.50	1.17	1.24
1	C	30	TYR	C-O	-5.50	1.17	1.24
1	B	135	LEU	C-O	-5.49	1.16	1.24
1	B	202	ALA	C-O	-5.49	1.17	1.24
1	A	111	MET	C-O	-5.49	1.17	1.24
1	B	10	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	46	LYS	C-O	-5.49	1.16	1.23
1	C	186	GLN	C-O	-5.49	1.17	1.24
1	C	34	ASN	C-O	-5.47	1.17	1.24
1	D	85	GLU	C-O	-5.45	1.17	1.24
1	C	92	ALA	C-O	-5.45	1.17	1.24
1	B	28	ASP	C-O	-5.43	1.17	1.24
1	C	116	ASP	C-O	-5.43	1.17	1.24
1	D	94	ASP	C-O	-5.43	1.16	1.24
1	B	211	PHE	C-OXT	-5.42	1.12	1.23
1	D	17	SER	C-O	-5.42	1.17	1.24
1	D	60	TRP	NE1-CE2	-5.42	1.31	1.37
1	A	164	ARG	C-O	-5.42	1.17	1.24
1	B	39	VAL	C-O	-5.42	1.18	1.24
1	D	54	ALA	C-O	-5.41	1.17	1.24
1	A	198	GLU	C-O	-5.40	1.17	1.24
1	D	49	ILE	C-O	-5.39	1.17	1.24
1	B	4	VAL	C-O	-5.38	1.18	1.24
1	D	209	HIS	CD2-NE2	-5.38	1.31	1.37
1	C	168	ALA	C-O	-5.38	1.18	1.24
1	A	134	GLY	C-O	-5.38	1.18	1.23
1	A	202	ALA	C-O	-5.36	1.17	1.24
1	D	151	TYR	C-O	-5.36	1.17	1.24
1	B	111	MET	C-O	-5.35	1.17	1.24
1	C	205	LYS	C-O	-5.35	1.17	1.24
1	A	20	MET	C-O	-5.33	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ALA	C-O	-5.33	1.17	1.24
1	B	159	MET	C-O	-5.33	1.17	1.24
1	D	176	PRO	C-O	-5.33	1.17	1.24
1	B	112	LYS	C-O	-5.31	1.18	1.24
1	C	163	HIS	CD2-NE2	-5.31	1.32	1.37
1	C	31	LYS	C-O	-5.29	1.17	1.24
1	D	168	ALA	C-O	-5.29	1.18	1.24
1	C	5	LEU	C-O	-5.29	1.17	1.24
1	A	17	SER	C-O	-5.28	1.18	1.24
1	C	143	HIS	C-O	-5.28	1.18	1.24
1	C	103	TRP	NE1-CE2	-5.27	1.31	1.37
1	C	84	ALA	C-O	-5.27	1.17	1.24
1	C	24	LYS	C-O	-5.26	1.18	1.24
1	D	189	MET	C-O	-5.26	1.18	1.24
1	D	90	PHE	C-O	-5.25	1.18	1.24
1	C	104	ASN	C-O	-5.24	1.17	1.23
1	B	87	SER	C-O	-5.24	1.17	1.24
1	C	26	PHE	C-O	-5.22	1.18	1.24
1	B	37	ASP	C-O	-5.22	1.17	1.23
1	B	143	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	35	PRO	C-O	-5.21	1.17	1.24
1	A	139	LYS	C-O	-5.20	1.16	1.23
1	A	49	ILE	C-O	-5.20	1.17	1.24
1	B	41	HIS	CD2-NE2	-5.20	1.32	1.37
1	D	10	HIS	CD2-NE2	-5.18	1.32	1.37
1	A	186	GLN	C-O	-5.17	1.17	1.24
1	D	41	HIS	CG-ND1	-5.17	1.32	1.38
1	B	189	MET	C-O	-5.17	1.18	1.24
1	C	41	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	209	HIS	CD2-NE2	-5.16	1.32	1.37
1	B	160	GLU	C-O	-5.15	1.17	1.23
1	C	165	TYR	C-O	-5.14	1.18	1.24
1	D	10	HIS	CG-ND1	-5.14	1.32	1.38
1	B	54	ALA	C-O	-5.13	1.18	1.24
1	C	18	TYR	C-O	-5.13	1.18	1.24
1	A	32	GLU	C-O	-5.12	1.18	1.24
1	C	85	GLU	C-O	-5.12	1.18	1.24
1	C	162	GLY	C-O	-5.12	1.17	1.23
1	C	211	PHE	C-OXT	-5.12	1.13	1.23
1	D	87	SER	C-O	-5.11	1.18	1.24
1	D	169	ILE	C-O	-5.11	1.18	1.24
1	B	79	LYS	C-O	-5.10	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	MET	C-O	-5.10	1.18	1.24
1	D	25	ALA	C-O	-5.10	1.18	1.24
1	B	25	ALA	C-O	-5.09	1.18	1.24
1	B	146	ALA	C-O	-5.09	1.17	1.24
1	D	107	PHE	C-O	-5.08	1.19	1.24
1	D	178	PHE	C-O	-5.08	1.18	1.23
1	B	80	VAL	C-O	-5.08	1.18	1.24
1	D	77	LYS	C-O	-5.07	1.18	1.24
1	C	114	TYR	C-O	-5.07	1.18	1.24
1	B	194	GLN	C-O	-5.07	1.18	1.24
1	C	86	LEU	C-O	-5.07	1.18	1.24
1	B	121	ALA	C-O	-5.06	1.17	1.23
1	D	197	LYS	C-O	-5.06	1.18	1.24
1	A	90	PHE	C-O	-5.05	1.18	1.24
1	A	148	GLY	C-O	-5.04	1.17	1.23
1	D	119	ALA	C-O	-5.04	1.16	1.23
1	B	99	VAL	C-O	-5.04	1.18	1.24
1	B	74	ALA	C-O	-5.04	1.18	1.24
1	B	175	VAL	C-O	-5.03	1.18	1.24
1	D	14	GLU	C-O	-5.03	1.17	1.24
1	A	120	VAL	C-O	-5.02	1.18	1.24
1	D	99	VAL	C-O	-5.02	1.18	1.24
1	C	11	PRO	C-O	-5.01	1.18	1.24
1	D	170	MET	C-O	-5.01	1.18	1.24
1	D	41	HIS	CD2-NE2	-5.01	1.32	1.37
1	B	115	ILE	C-O	-5.00	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	GLN	N-CA-C	8.85	122.84	112.93
1	A	1	MET	N-CA-C	7.37	119.96	111.11
1	A	127	TYR	CA-C-N	-6.83	110.64	123.27
1	A	127	TYR	C-N-CA	-6.83	110.64	123.27
1	C	108	PRO	O-C-N	6.68	124.38	121.31
1	D	183	VAL	CB-CA-C	-6.58	102.98	111.53
1	D	108	PRO	O-C-N	6.14	124.13	121.31
1	A	108	PRO	O-C-N	5.76	123.86	121.15
1	D	1	MET	CB-CG-SD	-5.61	95.87	112.70
1	D	0	HIS	CB-CA-C	5.52	120.60	110.10
1	A	154	GLY	CA-C-N	5.45	125.27	119.28
1	A	154	GLY	C-N-CA	5.45	125.27	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	40	ILE	N-CA-C	5.40	115.36	107.37
1	C	100	THR	N-CA-C	5.15	117.53	108.82
1	C	53	ASP	N-CA-C	5.02	114.92	108.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	153	GLU	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	1649	0	1615	68	0
1	B	1658	0	1624	46	0
1	C	1629	0	1599	33	0
1	D	1658	0	1624	24	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	2	0
2	D	31	0	19	0	0
3	A	25	0	34	16	0
3	C	25	0	34	11	0
4	B	26	0	32	22	0
4	D	13	0	16	9	0
5	A	105	0	0	4	0
5	B	119	0	0	2	0
5	C	119	0	0	3	0
5	D	123	0	0	5	0
All	All	7273	0	6654	168	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 12.

All (168) 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:0:HIS:HB2	1:A:36:ASN:O	1.54	1.08
1:A:40:ILE:HD11	1:B:40:ILE:HD11	1.37	1.03
1:A:89:GLN:HE22	1:B:0:HIS:CE1	1.77	1.02
1:A:197:LYS:HZ2	3:A:302:PE8:H182	1.24	1.00
1:A:192:LYS:O	1:A:195:GLU:HG2	1.68	0.94
1:D:123:LYS:HE3	5:D:403:HOH:O	1.68	0.93
1:A:165:TYR:HB2	4:D:302:NHE:HC12	1.51	0.92
1:B:192:LYS:O	1:B:195:GLU:HG2	1.70	0.90
1:A:197:LYS:NZ	3:A:302:PE8:H182	1.88	0.89
1:A:89:GLN:NE2	1:B:0:HIS:ND1	2.22	0.88
1:B:107:PHE:CE1	4:B:303:NHE:H3'1	2.09	0.86
1:A:0:HIS:HB3	1:B:82:ARG:HH12	1.43	0.84
1:A:0:HIS:CB	1:A:36:ASN:O	2.26	0.83
1:A:67:LYS:HB3	1:A:71:GLU:HG3	1.61	0.83
1:B:3:LYS:HE3	1:B:93:ALA:HB2	1.61	0.81
1:A:197:LYS:NZ	3:A:302:PE8:H121	1.96	0.80
1:B:0:HIS:HB2	1:B:38:GLU:HG3	1.62	0.80
1:A:161:MET:HB3	4:D:302:NHE:O2	1.81	0.80
1:A:197:LYS:HZ3	3:A:302:PE8:H121	1.44	0.80
1:C:197:LYS:HZ2	3:C:302:PE8:C20	1.95	0.79
1:D:106:SER:OG	4:D:302:NHE:H5'1	1.81	0.79
1:A:197:LYS:HZ2	3:A:302:PE8:C15	1.96	0.78
1:A:197:LYS:HZ2	3:A:302:PE8:H152	1.49	0.78
1:A:0:HIS:CG	1:A:36:ASN:O	2.40	0.75
1:A:197:LYS:HZ3	3:A:302:PE8:C12	1.99	0.75
1:D:107:PHE:CE1	4:D:302:NHE:H4'2	2.22	0.74
1:C:197:LYS:NZ	3:C:302:PE8:H172	2.01	0.74
1:C:152:SER:O	1:C:153:GLU:HG3	1.88	0.73
1:D:24:LYS:NZ	5:D:401:HOH:O	2.21	0.73
1:A:68:GLY:H	1:A:71:GLU:HG3	1.54	0.72
4:B:303:NHE:O1	1:C:161:MET:HB3	1.89	0.72
1:B:0:HIS:CB	1:B:38:GLU:HG3	2.19	0.72
1:B:165:TYR:HB2	4:B:303:NHE:HC12	1.69	0.72
1:A:40:ILE:CD1	1:B:40:ILE:HD11	2.15	0.72
1:A:0:HIS:CD2	1:A:36:ASN:O	2.43	0.72
1:D:161:MET:HB3	4:D:302:NHE:S	2.30	0.71
1:B:161:MET:SD	4:B:303:NHE:O3	2.48	0.71
4:B:302:NHE:HC22	4:B:302:NHE:H6'1	1.74	0.70
1:B:0:HIS:CD2	1:B:38:GLU:HG2	2.28	0.69
1:C:197:LYS:HZ2	3:C:302:PE8:H202	1.58	0.69
1:C:197:LYS:HZ2	3:C:302:PE8:H201	1.58	0.68
1:A:68:GLY:O	1:A:71:GLU:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LYS:HZ3	3:C:302:PE8:H172	1.58	0.67
1:A:14:GLU:HG3	1:A:24:LYS:HE2	1.75	0.67
1:A:89:GLN:HE22	1:B:0:HIS:CG	2.10	0.67
1:B:127:TYR:HE1	4:B:302:NHE:H5'1	1.59	0.66
1:B:112:LYS:HB2	4:B:303:NHE:H4'1	1.78	0.65
1:D:10:HIS:ND1	1:D:11:PRO:HD2	2.12	0.65
1:C:126:LYS:O	1:C:132:SER:HA	1.96	0.65
1:D:62:LYS:O	1:D:67:LYS:HD2	1.97	0.64
1:C:197:LYS:HZ3	3:C:302:PE8:C17	2.10	0.64
1:C:197:LYS:NZ	3:C:302:PE8:H232	2.12	0.64
1:C:197:LYS:NZ	3:C:302:PE8:C17	2.61	0.63
1:A:10:HIS:ND1	1:A:11:PRO:HD2	2.13	0.63
4:B:303:NHE:HC22	1:C:165:TYR:HB2	1.79	0.62
1:A:197:LYS:HZ2	3:A:302:PE8:C18	2.08	0.62
1:B:161:MET:O	4:B:303:NHE:HC11	2.00	0.61
1:A:48:ASN:HD22	1:B:36:ASN:HD21	1.49	0.60
1:A:68:GLY:H	1:A:71:GLU:CG	2.15	0.60
4:B:303:NHE:O1	1:C:161:MET:CB	2.51	0.59
1:B:107:PHE:CE1	4:B:303:NHE:C3'	2.82	0.59
4:B:302:NHE:H6'1	4:B:302:NHE:C2	2.32	0.58
1:D:106:SER:CB	4:D:302:NHE:H5'1	2.33	0.58
1:A:70:GLU:HG3	1:A:71:GLU:N	2.17	0.58
4:B:303:NHE:O1	1:C:161:MET:O	2.21	0.57
1:B:189:MET:HE2	1:B:192:LYS:NZ	2.20	0.57
1:C:197:LYS:HZ2	3:C:302:PE8:H232	1.67	0.57
1:A:198:GLU:OE2	3:A:302:PE8:O25	2.23	0.57
1:A:197:LYS:HZ2	3:A:302:PE8:H151	1.70	0.56
1:B:189:MET:HE2	1:B:192:LYS:HZ3	1.70	0.56
1:D:120:VAL:HG11	1:D:123:LYS:HD2	1.86	0.56
1:A:0:HIS:HB3	1:B:82:ARG:NH1	2.16	0.56
1:A:68:GLY:O	1:A:70:GLU:N	2.38	0.56
1:A:89:GLN:NE2	1:B:0:HIS:CE1	2.61	0.55
1:B:3:LYS:HE3	1:B:93:ALA:CB	2.34	0.55
1:C:0:HIS:CE1	1:C:36:ASN:OD1	2.59	0.55
1:A:165:TYR:CB	4:D:302:NHE:HC12	2.30	0.55
1:A:89:GLN:NE2	1:B:0:HIS:CG	2.72	0.55
4:B:302:NHE:H6'2	2:C:301:FMN:C4A	2.37	0.55
4:B:303:NHE:O1	1:C:161:MET:CA	2.55	0.54
1:B:161:MET:HE1	1:B:164:ARG:NH1	2.22	0.54
1:C:47:GLU:OE1	1:C:82:ARG:NH2	2.38	0.54
1:A:138:ASP:O	1:A:138:ASP:OD1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:SER:C	1:C:153:GLU:HG3	2.33	0.54
1:A:0:HIS:CD2	1:B:89:GLN:HE22	2.26	0.54
1:C:194:GLN:HG3	3:C:302:PE8:H112	1.90	0.54
1:A:128:THR:N	1:A:131:GLY:O	2.32	0.53
1:B:87:SER:HB2	5:B:481:HOH:O	2.09	0.53
1:B:189:MET:HE2	1:B:192:LYS:CE	2.39	0.52
1:A:112:LYS:HG2	4:D:302:NHE:H4'1	1.92	0.52
1:A:197:LYS:NZ	3:A:302:PE8:H152	2.24	0.52
3:A:302:PE8:H211	3:A:302:PE8:H51	1.92	0.51
4:B:302:NHE:HC21	2:C:301:FMN:C5A	2.40	0.51
4:B:303:NHE:C2	1:C:165:TYR:HB2	2.40	0.51
1:A:0:HIS:CE1	1:B:89:GLN:OE1	2.63	0.51
1:A:68:GLY:O	1:A:71:GLU:N	2.33	0.51
1:C:91:VAL:HG21	1:C:123:LYS:HB3	1.93	0.50
1:B:22:VAL:HG21	1:B:183:VAL:HG21	1.94	0.50
1:D:126:LYS:HG2	1:D:133:VAL:CG1	2.42	0.50
1:B:189:MET:HE2	1:B:192:LYS:HE2	1.92	0.50
1:A:77:LYS:HB2	5:A:407:HOH:O	2.10	0.50
1:B:189:MET:CE	1:B:192:LYS:NZ	2.75	0.49
1:B:10:HIS:ND1	1:B:11:PRO:HD2	2.28	0.49
1:A:0:HIS:CE1	1:B:89:GLN:HE22	2.31	0.49
1:C:189:MET:HG3	1:C:192:LYS:HD2	1.93	0.49
1:A:14:GLU:CG	1:A:24:LYS:HE2	2.43	0.49
1:A:91:VAL:HG11	1:A:123:LYS:HB3	1.95	0.49
1:D:120:VAL:CG1	1:D:123:LYS:HD2	2.42	0.49
1:B:0:HIS:CG	1:B:36:ASN:O	2.66	0.48
1:A:68:GLY:O	1:A:69:PHE:C	2.55	0.48
1:A:68:GLY:N	1:A:71:GLU:HG3	2.26	0.47
1:B:165:TYR:HB2	4:B:303:NHE:C1	2.43	0.47
1:D:107:PHE:CD1	1:D:111:MET:HB3	2.49	0.47
1:B:192:LYS:HA	1:B:195:GLU:CD	2.40	0.47
1:A:73:THR:HG23	1:A:76:GLU:OE1	2.15	0.47
1:A:68:GLY:C	1:A:70:GLU:N	2.69	0.47
1:A:77:LYS:HE2	5:A:407:HOH:O	2.15	0.47
1:A:192:LYS:HA	1:A:195:GLU:CD	2.40	0.47
1:D:128:THR:C	1:D:130:GLN:N	2.70	0.47
1:B:91:VAL:HG11	1:B:123:LYS:HB3	1.97	0.46
1:A:87:SER:OG	1:A:123:LYS:HD2	2.15	0.46
1:C:75:GLU:CG	5:C:411:HOH:O	2.62	0.46
1:A:192:LYS:C	1:A:195:GLU:HG2	2.37	0.46
1:C:203:ARG:HH11	1:C:203:ARG:HG3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:HIS:H3	1:A:38:GLU:HG3	1.80	0.46
1:B:0:HIS:CG	1:B:38:GLU:HG2	2.51	0.45
1:A:126:LYS:HE2	5:A:430:HOH:O	2.17	0.45
1:B:0:HIS:CD2	1:B:36:ASN:O	2.70	0.45
1:D:210:THR:O	1:D:211:PHE:C	2.59	0.45
1:D:191:ASP:O	1:D:191:ASP:CG	2.60	0.44
1:B:189:MET:CE	1:B:192:LYS:HZ3	2.30	0.44
1:B:0:HIS:CD2	1:B:38:GLU:CG	2.99	0.44
1:A:138:ASP:OD1	1:A:138:ASP:C	2.60	0.44
1:D:14:GLU:H	1:D:14:GLU:HG3	1.67	0.44
1:C:59:GLY:O	1:C:63:LEU:HD23	2.18	0.43
1:C:175:VAL:HA	1:C:176:PRO:HD3	1.90	0.43
1:B:0:HIS:CG	1:B:38:GLU:CG	3.02	0.43
1:C:126:LYS:HD3	1:C:135:LEU:HD21	2.01	0.43
1:B:126:LYS:HE2	1:B:133:VAL:HG11	2.00	0.43
1:D:179:GLU:HG3	5:D:440:HOH:O	2.19	0.43
1:D:3:LYS:HE3	1:D:93:ALA:HB2	1.99	0.43
1:A:77:LYS:HB2	1:A:77:LYS:HE2	1.70	0.43
1:A:197:LYS:NZ	3:A:302:PE8:C12	2.69	0.43
1:A:14:GLU:HG3	1:A:24:LYS:CE	2.47	0.42
1:D:126:LYS:HG2	1:D:133:VAL:HG12	2.01	0.42
4:B:302:NHE:O2	5:B:401:HOH:O	2.21	0.42
1:A:181:LEU:C	1:A:181:LEU:HD23	2.44	0.42
1:D:1:MET:HB3	1:D:37:ASP:OD1	2.20	0.42
3:A:302:PE8:H91	3:A:302:PE8:H122	1.65	0.42
1:C:75:GLU:HG3	5:C:411:HOH:O	2.18	0.41
1:A:199:LYS:HG2	5:A:495:HOH:O	2.20	0.41
4:B:302:NHE:C2	4:B:302:NHE:C6'	2.96	0.41
1:D:87:SER:OG	1:D:123:LYS:HE3	2.21	0.41
1:A:197:LYS:CD	3:A:302:PE8:H151	2.50	0.41
1:C:27:ILE:HD12	1:C:27:ILE:HA	1.96	0.41
1:A:71:GLU:HG2	1:A:71:GLU:H	1.59	0.41
1:B:107:PHE:HB2	1:B:108:PRO:HD2	2.03	0.41
4:B:302:NHE:H5'2	5:C:496:HOH:O	2.20	0.41
1:A:140:LYS:HE3	1:A:211:PHE:OXT	2.21	0.41
1:A:197:LYS:HD2	3:A:302:PE8:H151	2.03	0.41
4:D:302:NHE:HC22	4:D:302:NHE:HC'1	1.73	0.41
1:A:159:MET:HB2	1:A:159:MET:HE2	1.14	0.40
1:C:197:LYS:CD	3:C:302:PE8:H201	2.51	0.40
1:D:14:GLU:CD	1:D:24:LYS:HD2	2.46	0.40
4:B:302:NHE:HC12	1:C:104:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LYS:CD	1:C:135:LEU:HD21	2.52	0.40
1:D:67:LYS:CE	5:D:413:HOH:O	2.69	0.40
1:D:191:ASP:HB3	5:D:508:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/231 (90%)	196 (95%)	11 (5%)	0	100	100
1	B	210/231 (91%)	203 (97%)	7 (3%)	0	100	100
1	C	204/231 (88%)	199 (98%)	4 (2%)	1 (0%)	24	14
1	D	210/231 (91%)	203 (97%)	7 (3%)	0	100	100
All	All	831/924 (90%)	801 (96%)	29 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/188 (91%)	154 (90%)	17 (10%)	7	1
1	B	172/188 (92%)	165 (96%)	7 (4%)	27	16
1	C	169/188 (90%)	161 (95%)	8 (5%)	23	12
1	D	172/188 (92%)	165 (96%)	7 (4%)	27	16
All	All	684/752 (91%)	645 (94%)	39 (6%)	18	8

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MET
1	A	3	LYS
1	A	24	LYS
1	A	31	LYS
1	A	70	GLU
1	A	71	GLU
1	A	73	THR
1	A	75	GLU
1	A	77	LYS
1	A	128	THR
1	A	140	LYS
1	A	153	GLU
1	A	159	MET
1	A	177	SER
1	A	192	LYS
1	A	195	GLU
1	B	0	HIS
1	B	16	GLN
1	B	17	SER
1	B	48	ASN
1	B	70	GLU
1	B	195	GLU
1	B	203	ARG
1	C	12	LEU
1	C	36	ASN
1	C	70	GLU
1	C	71	GLU
1	C	75	GLU
1	C	126	LYS
1	C	183	VAL
1	C	189	MET
1	D	1	MET

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Mol	Chain	Res	Type
1	D	130	GLN
1	D	153	GLU
1	D	181	LEU
1	D	183	VAL
1	D	191	ASP
1	D	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	48	ASN
1	A	64	GLN
1	A	89	GLN
1	A	104	ASN
1	A	167	GLN
1	A	194	GLN
1	B	0	HIS
1	B	48	ASN
1	B	89	GLN
1	B	167	GLN
1	C	145	GLN
1	C	194	GLN
1	D	36	ASN
1	D	89	GLN
1	D	194	GLN

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

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NHE	B	302	-	13,13,13	2.96	3 (23%)	16,17,17	2.19	6 (37%)
2	FMN	B	301	-	33,33,33	1.88	9 (27%)	48,50,50	1.59	9 (18%)
3	PE8	C	302	-	24,24,24	0.46	0	23,23,23	0.81	0
3	PE8	A	302	-	24,24,24	0.45	0	23,23,23	0.59	0
2	FMN	C	301	-	33,33,33	1.77	7 (21%)	48,50,50	1.34	5 (10%)
4	NHE	B	303	-	13,13,13	3.14	2 (15%)	16,17,17	1.67	5 (31%)
4	NHE	D	302	-	13,13,13	3.52	4 (30%)	16,17,17	6.69	7 (43%)
2	FMN	D	301	-	33,33,33	1.79	7 (21%)	48,50,50	1.49	8 (16%)
2	FMN	A	301	-	33,33,33	1.72	8 (24%)	48,50,50	1.49	10 (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
4	NHE	B	302	-	-	4/7/15/15	0/1/1/1
2	FMN	B	301	-	-	2/18/18/18	0/3/3/3
3	PE8	C	302	-	-	10/22/22/22	-
3	PE8	A	302	-	-	13/22/22/22	-
2	FMN	C	301	-	-	2/18/18/18	0/3/3/3
4	NHE	B	303	-	-	4/7/15/15	0/1/1/1
4	NHE	D	302	-	-	3/7/15/15	0/1/1/1
2	FMN	D	301	-	-	2/18/18/18	0/3/3/3
2	FMN	A	301	-	-	3/18/18/18	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	302	NHE	C2-S	-10.01	1.63	1.77
4	B	303	NHE	C2-S	-8.83	1.65	1.77
4	B	302	NHE	C2-S	-8.53	1.65	1.77
4	D	302	NHE	O2-S	6.76	1.64	1.45
4	B	303	NHE	O2-S	6.53	1.63	1.45
2	B	301	FMN	C9A-C5A	6.09	1.51	1.41
2	D	301	FMN	C9A-C5A	5.89	1.50	1.41
2	C	301	FMN	C9A-C5A	5.74	1.50	1.41
4	B	302	NHE	O2-S	5.47	1.60	1.45
2	A	301	FMN	C9A-C5A	4.89	1.49	1.41
2	A	301	FMN	C4-N3	-3.50	1.32	1.38
2	C	301	FMN	C4-N3	-3.24	1.32	1.38
2	B	301	FMN	C4-N3	-3.16	1.32	1.38
2	C	301	FMN	C8-C7	3.14	1.48	1.40
2	D	301	FMN	P-O2P	-2.86	1.44	1.54
2	B	301	FMN	P-O2P	-2.85	1.44	1.54
2	A	301	FMN	P-O2P	-2.81	1.44	1.54
2	C	301	FMN	C5A-N5	-2.78	1.34	1.39
2	C	301	FMN	P-O2P	-2.78	1.44	1.54
2	A	301	FMN	C8-C7	2.72	1.47	1.40
2	A	301	FMN	C5A-N5	-2.71	1.34	1.39
2	B	301	FMN	C8-C7	2.60	1.47	1.40
4	D	302	NHE	C1-N	-2.60	1.41	1.47
2	B	301	FMN	C5A-N5	-2.54	1.34	1.39
2	D	301	FMN	C5A-N5	-2.48	1.34	1.39
2	D	301	FMN	C4-N3	-2.43	1.34	1.38
2	C	301	FMN	P-O3P	-2.43	1.45	1.54
2	A	301	FMN	C2-N3	-2.42	1.33	1.39
2	B	301	FMN	P-O3P	-2.42	1.45	1.54
2	A	301	FMN	P-O3P	-2.41	1.45	1.54
2	B	301	FMN	O4-C4	-2.34	1.19	1.23
2	C	301	FMN	C2-N3	-2.31	1.33	1.39
4	D	302	NHE	C1'-N	-2.30	1.41	1.48
4	B	302	NHE	C1'-N	-2.22	1.41	1.48
2	D	301	FMN	C6-C7	-2.21	1.36	1.39
2	B	301	FMN	C10-N10	2.20	1.42	1.37
2	D	301	FMN	C8-C7	2.12	1.46	1.40
2	A	301	FMN	C5'-C4'	2.05	1.54	1.51
2	D	301	FMN	C4A-N5	2.01	1.35	1.30
2	B	301	FMN	C2-N3	-2.01	1.34	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	NHE	O2-S-C2	-20.65	75.53	106.73
4	D	302	NHE	O1-S-C2	10.67	122.85	106.73
4	D	302	NHE	O2-S-O1	-7.93	88.04	113.82
4	D	302	NHE	O3-S-O2	-7.90	91.64	111.40
4	D	302	NHE	O3-S-C2	5.77	117.30	106.00
2	B	301	FMN	C4-C4A-N5	5.00	125.12	118.21
4	B	302	NHE	C3'-C2'-C1'	-4.80	102.49	111.09
2	A	301	FMN	C4-C4A-N5	4.33	124.19	118.21
2	C	301	FMN	C4-C4A-N5	4.23	124.06	118.21
2	D	301	FMN	C4-C4A-N5	4.23	124.05	118.21
4	B	302	NHE	O3-S-O2	-3.86	101.73	111.40
4	B	303	NHE	O3-S-C2	3.75	113.33	106.00
2	D	301	FMN	O2-C2-N1	-3.66	115.73	121.80
4	B	302	NHE	O2-S-C2	3.39	111.85	106.73
4	B	302	NHE	O3-S-C2	3.13	112.14	106.00
2	A	301	FMN	O2P-P-O5'	-2.95	98.98	106.67
4	B	303	NHE	O2-S-C2	-2.75	102.58	106.73
2	B	301	FMN	O2-C2-N1	-2.63	117.43	121.80
2	D	301	FMN	C10-C4A-N5	-2.60	119.49	124.81
2	D	301	FMN	C5A-N5-C4A	2.59	122.28	118.09
2	D	301	FMN	C4A-C10-N1	-2.55	118.33	124.59
2	C	301	FMN	O2-C2-N1	-2.51	117.63	121.80
2	B	301	FMN	C4A-C10-N10	2.47	120.02	116.48
2	B	301	FMN	C4A-C4-N3	2.46	119.53	113.25
4	D	302	NHE	O3-S-O1	2.45	117.52	111.40
2	A	301	FMN	C4A-C4-N3	2.40	119.36	113.25
4	B	303	NHE	C4'-C3'-C2'	-2.39	106.52	111.42
2	B	301	FMN	C10-C4A-N5	-2.36	120.00	124.81
2	A	301	FMN	C10-N1-C2	2.34	121.92	116.85
2	B	301	FMN	C8M-C8-C9	2.33	123.68	119.57
2	D	301	FMN	C10-N1-C2	2.32	121.86	116.85
2	A	301	FMN	O3P-P-O2P	2.31	116.47	107.80
4	B	302	NHE	O1-S-C2	-2.31	103.24	106.73
2	B	301	FMN	C10-N1-C2	2.31	121.84	116.85
4	B	303	NHE	O3-S-O1	-2.26	105.74	111.40
2	B	301	FMN	C4A-C10-N1	-2.26	119.05	124.59
2	D	301	FMN	C4A-C10-N10	2.25	119.71	116.48
2	A	301	FMN	O4-C4-C4A	-2.24	120.61	126.53
2	A	301	FMN	C9A-C5A-N5	-2.20	120.12	122.45
4	B	302	NHE	C1-N-C1'	2.20	118.41	114.18
2	A	301	FMN	C4A-C10-N1	-2.18	119.26	124.59
2	A	301	FMN	C5A-N5-C4A	2.16	121.58	118.09
2	B	301	FMN	O2P-P-O1P	2.15	119.21	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FMN	C5A-N5-C4A	2.13	121.54	118.09
2	C	301	FMN	O5'-C5'-C4'	2.10	114.97	109.36
2	D	301	FMN	O4-C4-C4A	-2.07	121.06	126.53
2	C	301	FMN	C4A-C10-N10	2.06	119.43	116.48
2	A	301	FMN	O2-C2-N1	-2.05	118.40	121.80
4	D	302	NHE	C4'-C5'-C6'	-2.03	107.26	111.42
4	B	303	NHE	C6'-C1'-C2'	2.02	114.28	110.80

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FMN	O4'-C4'-C5'-O5'
4	B	302	NHE	C1-C2-S-O2
4	B	302	NHE	C1-C2-S-O3
4	B	303	NHE	C2-C1-N-C1'
4	B	303	NHE	C1-C2-S-O1
4	B	303	NHE	C1-C2-S-O2
4	B	303	NHE	C1-C2-S-O3
4	D	302	NHE	C2-C1-N-C1'
4	D	302	NHE	C1-C2-S-O1
4	D	302	NHE	C1-C2-S-O3
3	A	302	PE8	C15-C14-O13-C12
3	A	302	PE8	C18-C17-O16-C15
3	C	302	PE8	C17-C18-O19-C20
3	C	302	PE8	O7-C8-C9-O10
3	C	302	PE8	C20-C21-O22-C23
3	A	302	PE8	O7-C8-C9-O10
3	A	302	PE8	O19-C20-C21-O22
3	A	302	PE8	O22-C23-C24-O25
3	A	302	PE8	O4-C5-C6-O7
3	A	302	PE8	C12-C11-O10-C9
3	C	302	PE8	O16-C17-C18-O19
2	A	301	FMN	C2'-C3'-C4'-C5'
3	C	302	PE8	O10-C11-C12-O13
4	B	302	NHE	C1-C2-S-O1
3	A	302	PE8	C24-C23-O22-C21
3	A	302	PE8	C6-C5-O4-C3
3	C	302	PE8	C12-C11-O10-C9
2	B	301	FMN	C2'-C3'-C4'-C5'
3	C	302	PE8	C14-C15-O16-C17
2	A	301	FMN	C4'-C5'-O5'-P

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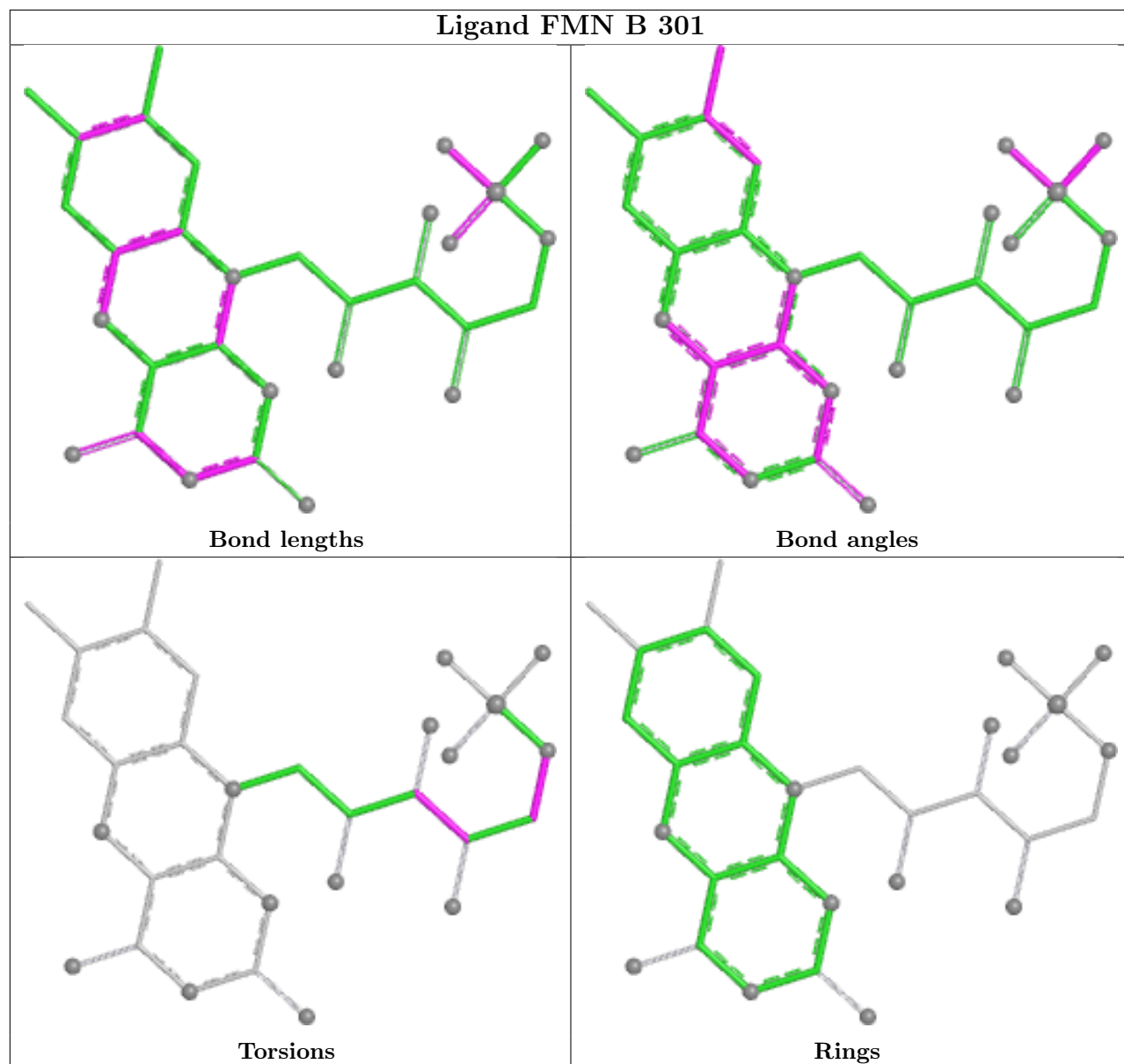
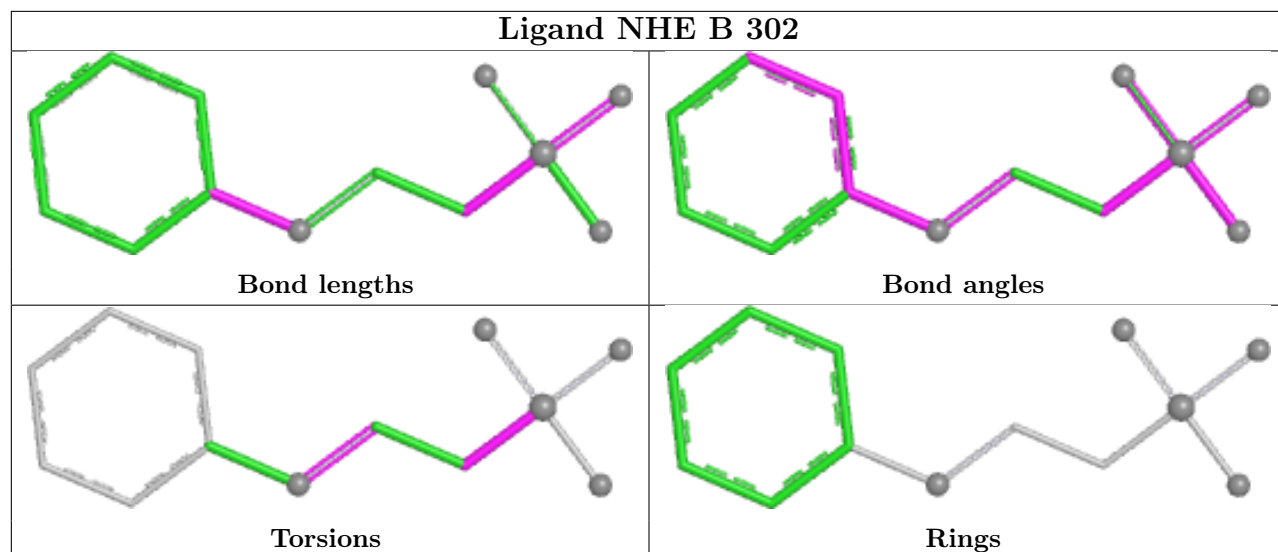
Mol	Chain	Res	Type	Atoms
3	A	302	PE8	C21-C20-O19-C18
3	C	302	PE8	O19-C20-C21-O22
3	A	302	PE8	C17-C18-O19-C20
2	D	301	FMN	C4'-C5'-O5'-P
2	C	301	FMN	C4'-C5'-O5'-P
2	B	301	FMN	C4'-C5'-O5'-P
2	D	301	FMN	C2'-C3'-C4'-C5'
2	C	301	FMN	C2'-C3'-C4'-C5'
3	C	302	PE8	C21-C20-O19-C18
3	C	302	PE8	C15-C14-O13-C12
4	B	302	NHE	C2-C1-N-C1'
3	A	302	PE8	O16-C17-C18-O19
3	A	302	PE8	O10-C11-C12-O13

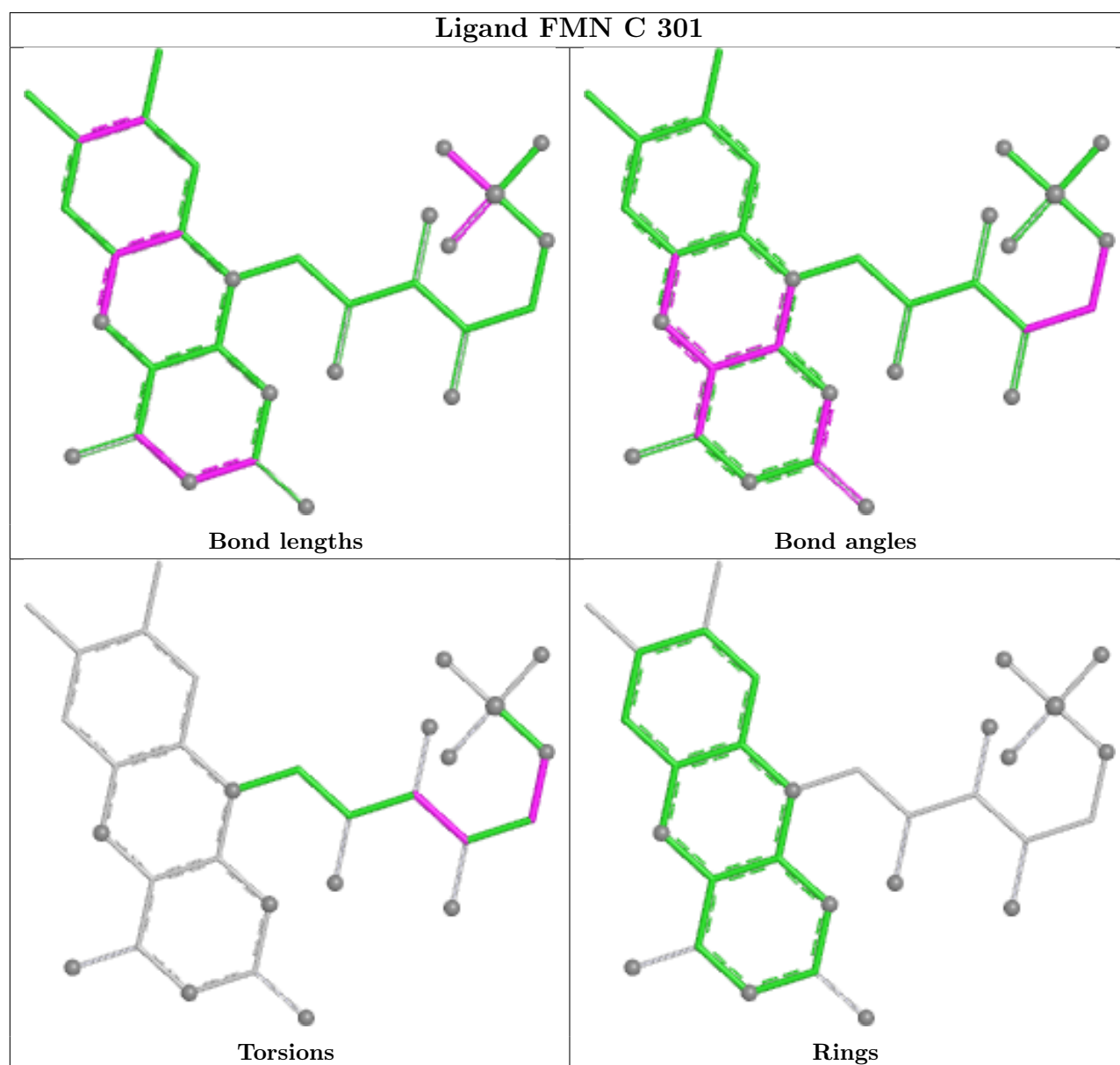
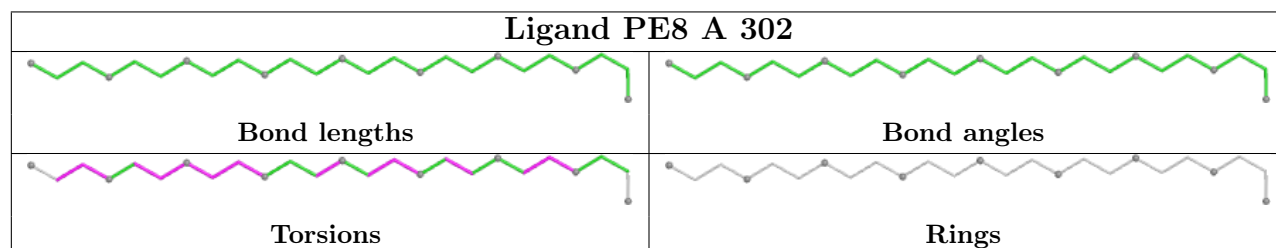
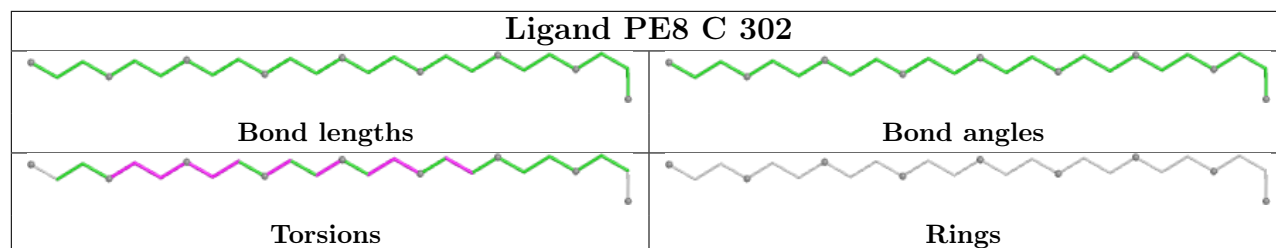
There are no ring outliers.

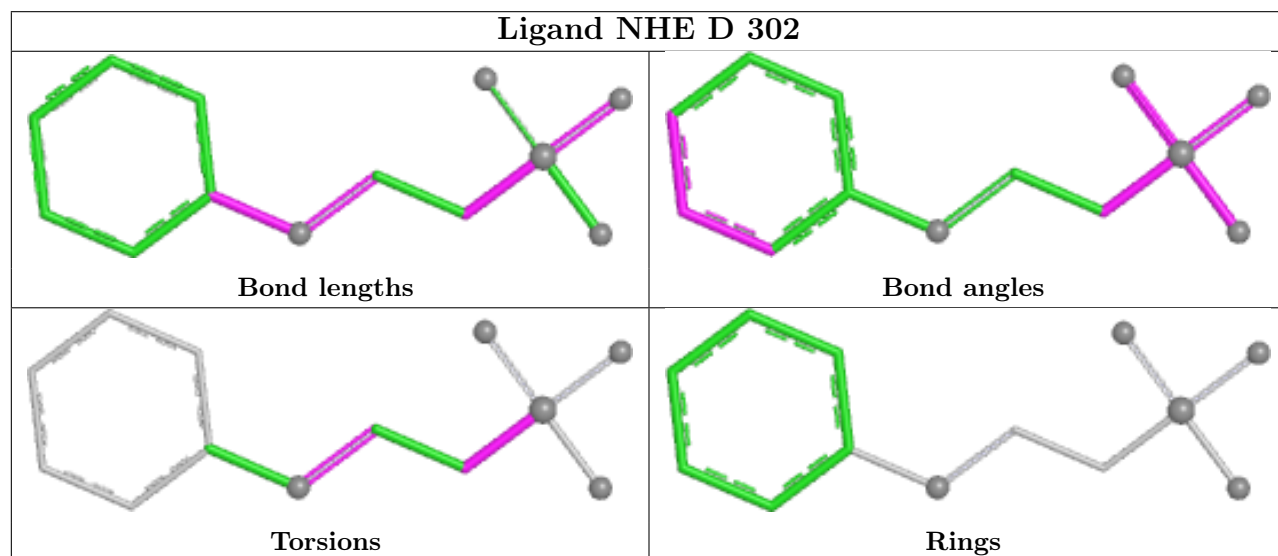
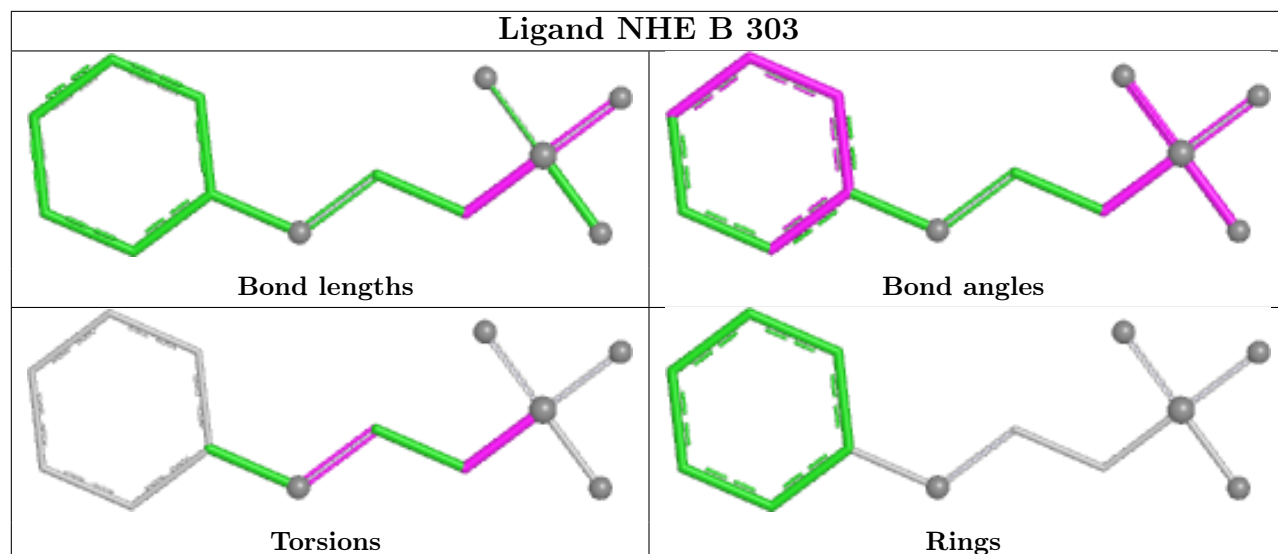
6 monomers are involved in 58 short contacts:

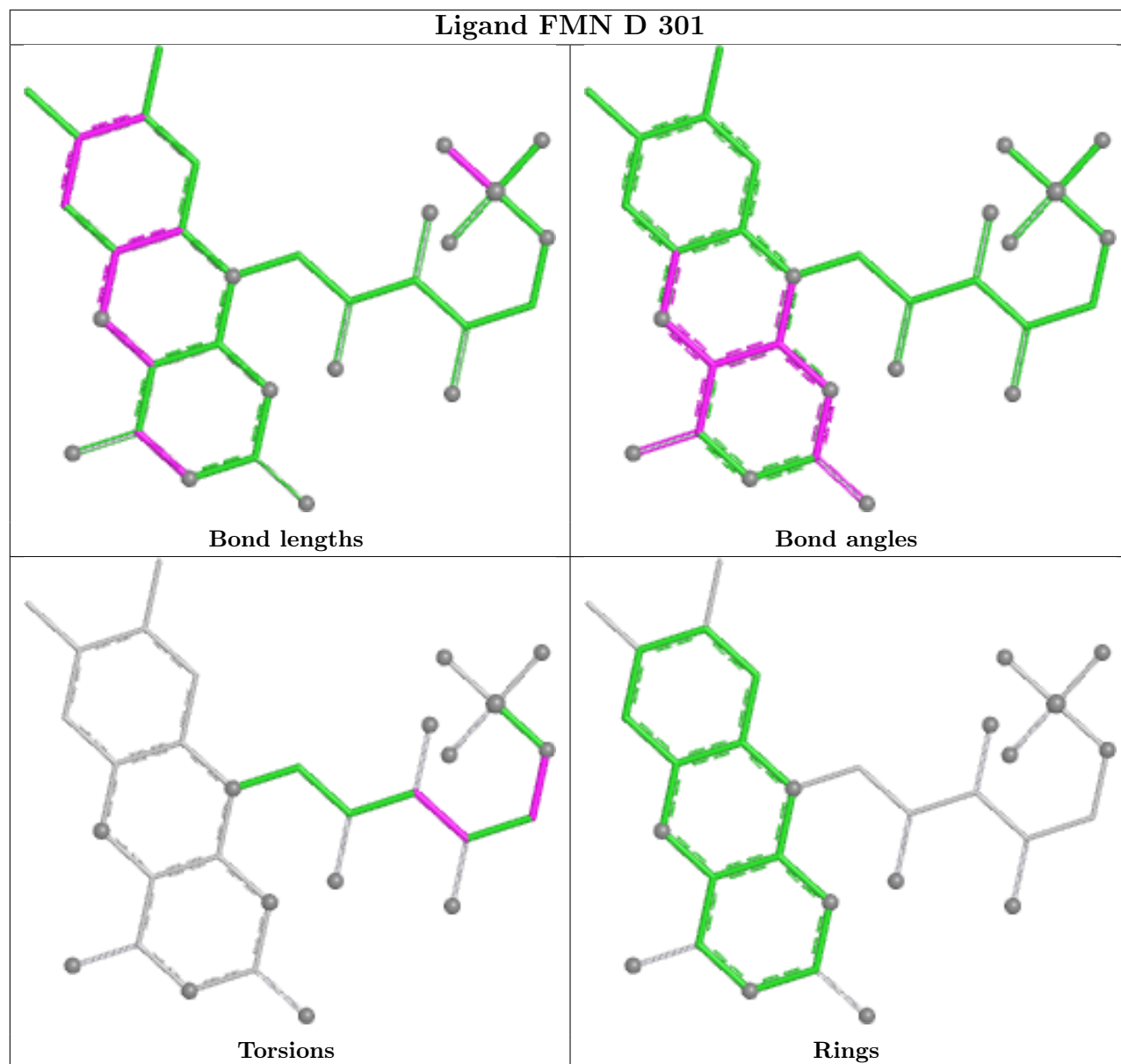
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	NHE	9	0
3	C	302	PE8	11	0
3	A	302	PE8	16	0
2	C	301	FMN	2	0
4	B	303	NHE	13	0
4	D	302	NHE	9	0

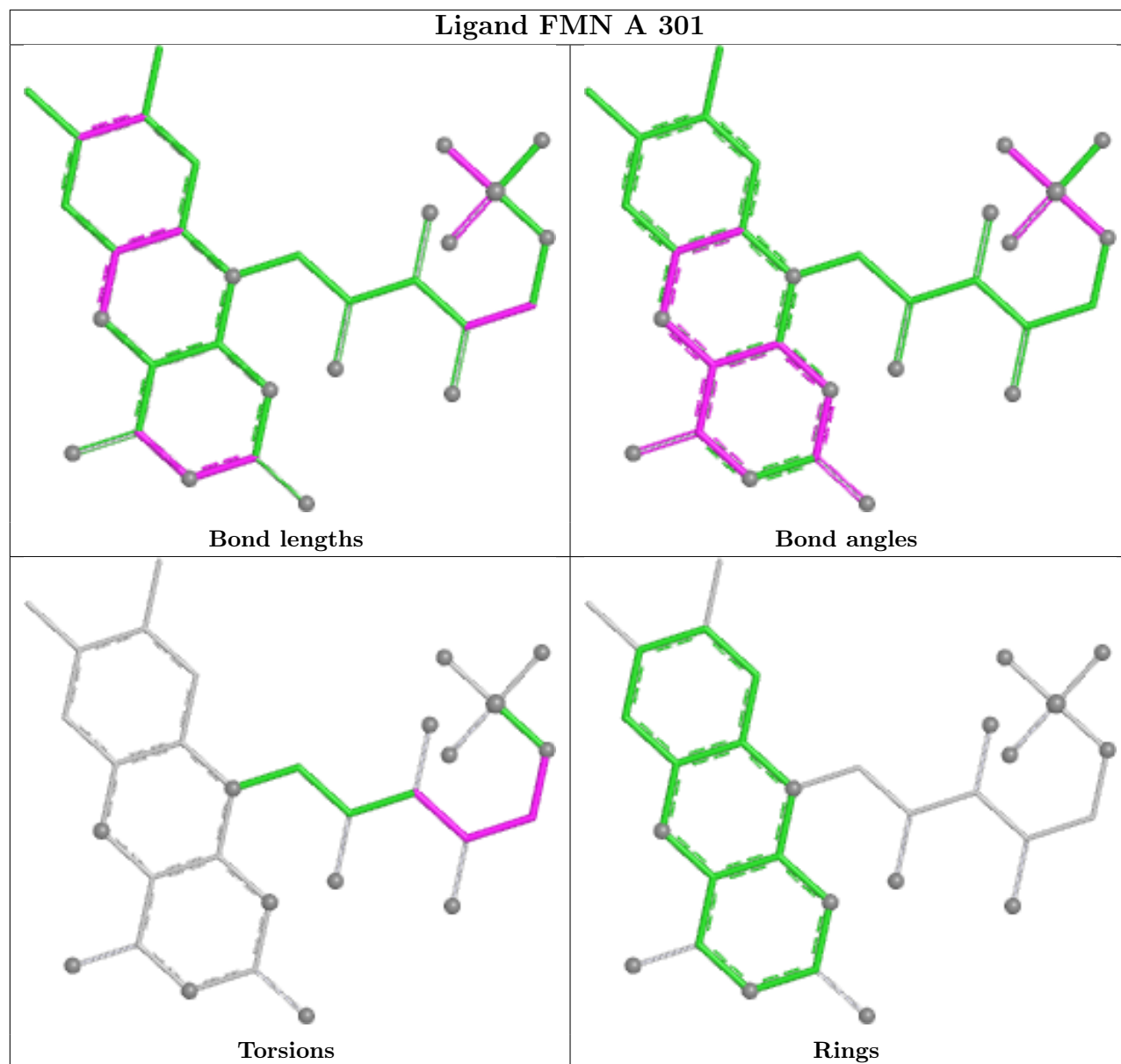
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	211/231 (91%)	0.09	12 (5%) 29 38	11, 21, 48, 73	0
1	B	212/231 (91%)	-0.15	4 (1%) 66 75	10, 19, 37, 55	0
1	C	208/231 (90%)	-0.23	3 (1%) 73 81	10, 17, 38, 50	0
1	D	212/231 (91%)	-0.25	6 (2%) 55 65	10, 16, 37, 63	0
All	All	843/924 (91%)	-0.14	25 (2%) 52 62	10, 18, 40, 73	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	HIS	5.6
1	A	0	HIS	5.4
1	D	0	HIS	5.2
1	B	0	HIS	4.9
1	A	66	GLY	3.3
1	A	68	GLY	3.3
1	A	138	ASP	3.0
1	A	129	GLU	2.9
1	A	128	THR	2.9
1	B	203	ARG	2.9
1	D	1	MET	2.8
1	A	155	PRO	2.8
1	A	70	GLU	2.7
1	B	129	GLU	2.7
1	A	131	GLY	2.7
1	A	127	TYR	2.6
1	D	191	ASP	2.6
1	D	129	GLU	2.6
1	C	1	MET	2.5
1	B	1	MET	2.4
1	C	127	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	154	GLY	2.2
1	D	179	GLU	2.1
1	A	195	GLU	2.1
1	A	74	ALA	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](#)

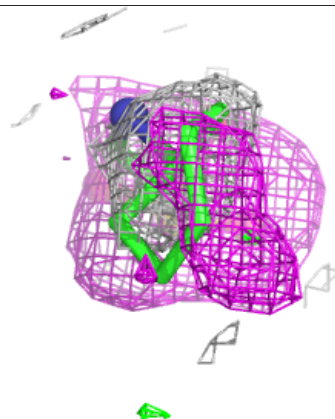
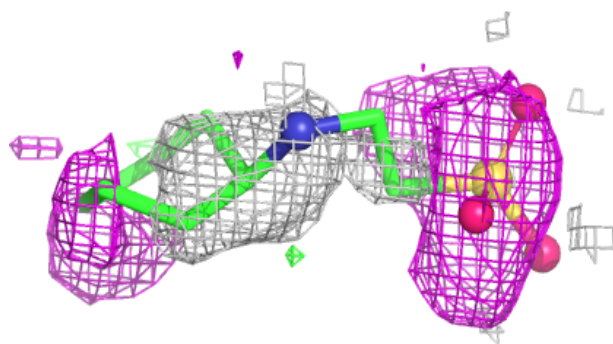
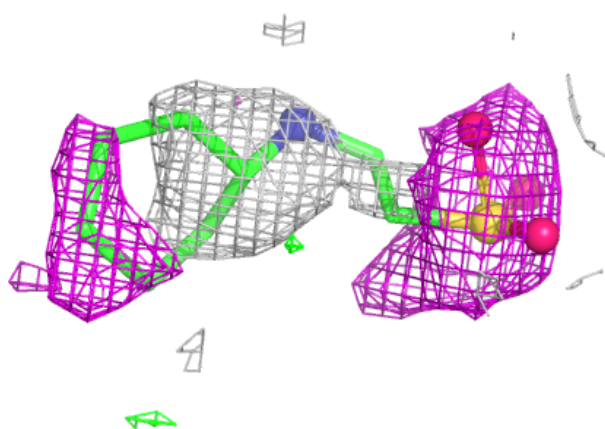
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NHE	D	302	13/13	0.65	0.32	67,69,94,94	0
4	NHE	B	302	13/13	0.68	0.23	53,55,75,76	0
4	NHE	B	303	13/13	0.74	0.24	49,53,80,81	0
3	PE8	A	302	25/25	0.83	0.14	35,52,65,66	0
3	PE8	C	302	25/25	0.84	0.15	28,54,72,73	0
2	FMN	B	301	31/31	0.94	0.08	20,23,27,29	0
2	FMN	D	301	31/31	0.95	0.07	14,21,25,26	0
2	FMN	A	301	31/31	0.95	0.07	17,23,27,28	0
2	FMN	C	301	31/31	0.97	0.06	13,16,19,21	0

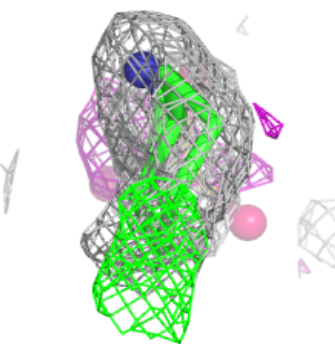
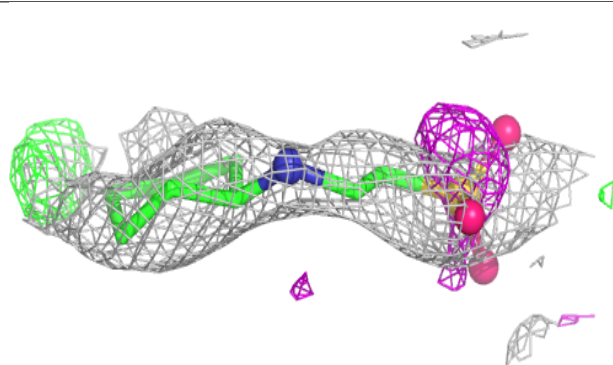
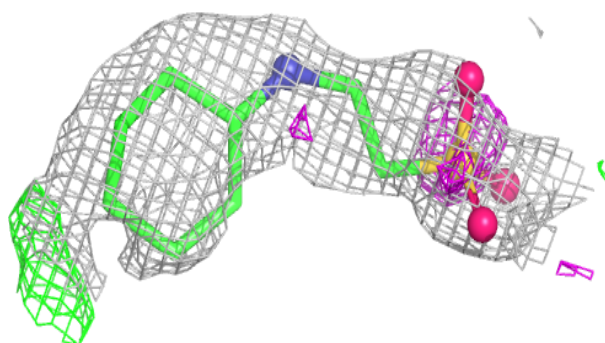
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NHE D 302:

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

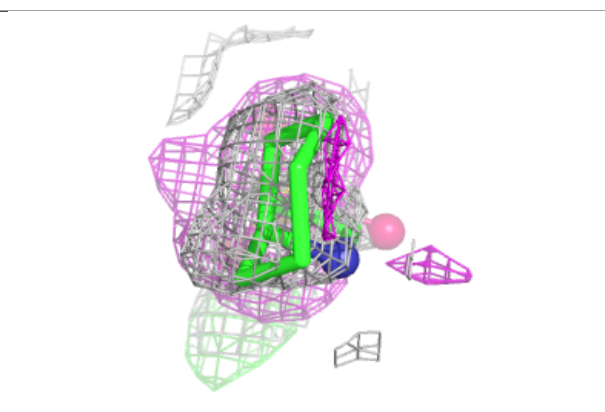
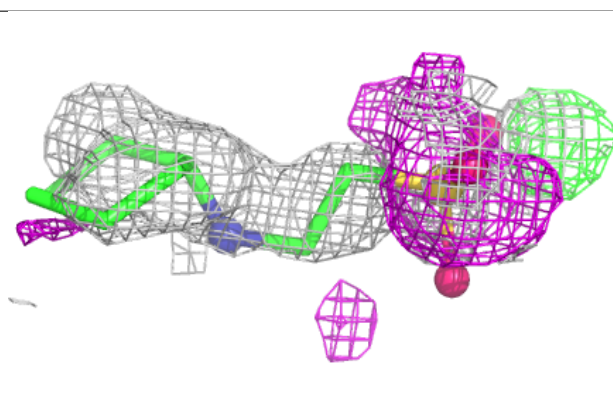
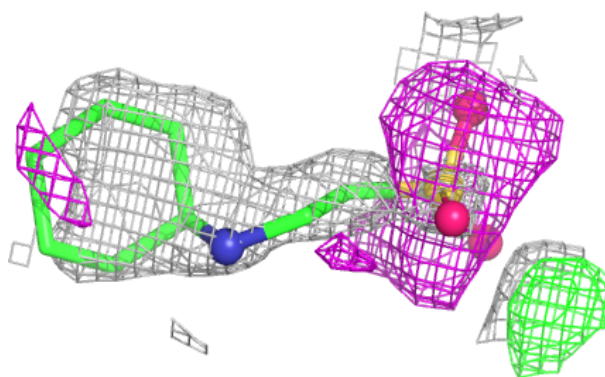
**Electron density around NHE B 302:**

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

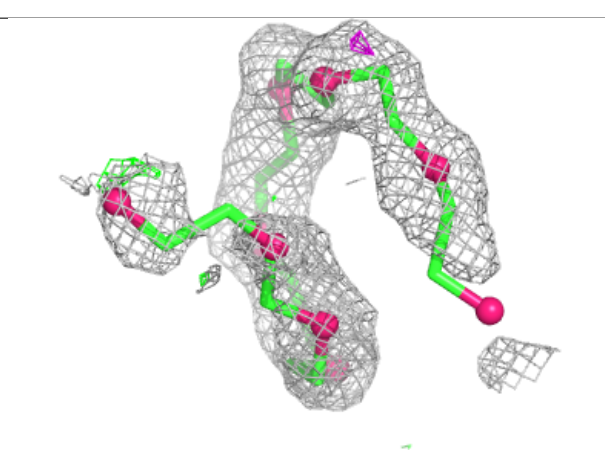
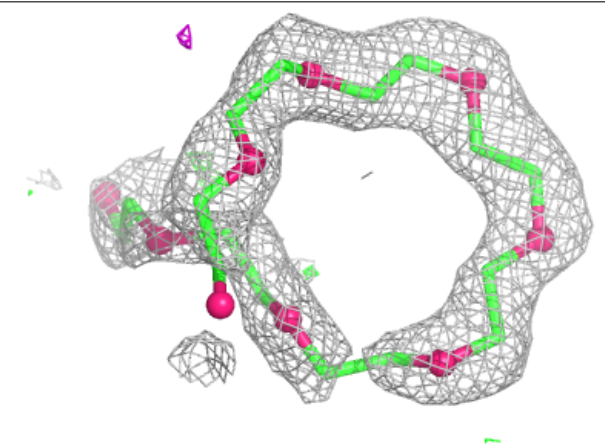


Electron density around NHE B 303:

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

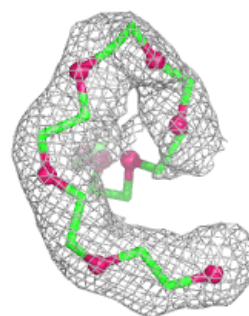
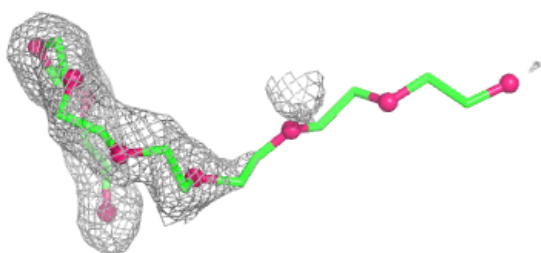
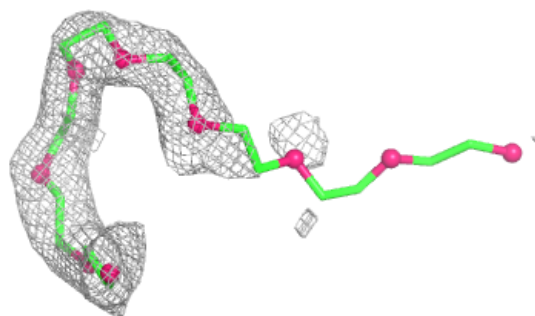
**Electron density around PE8 A 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



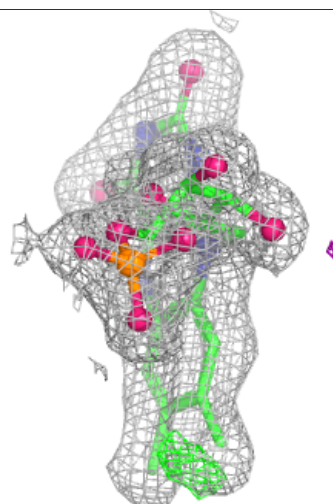
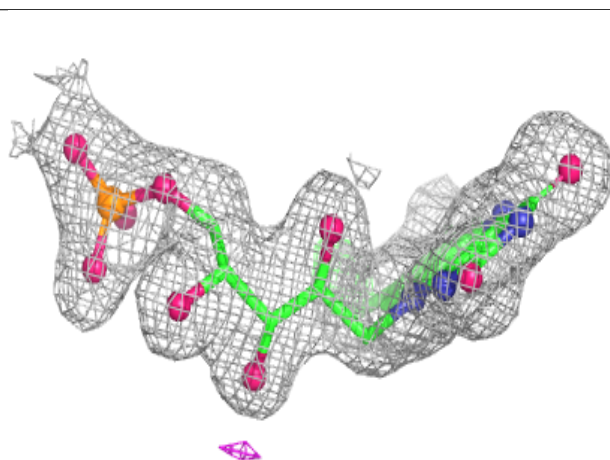
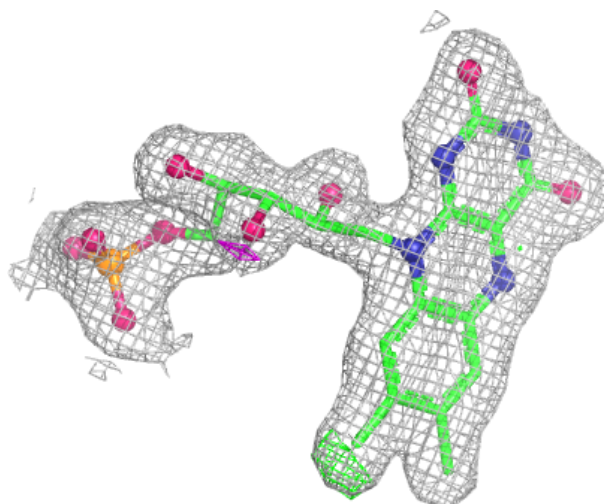
Electron density around PE8 C 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



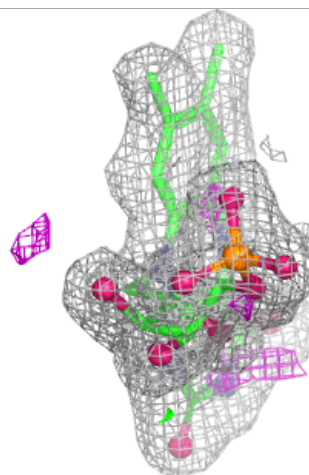
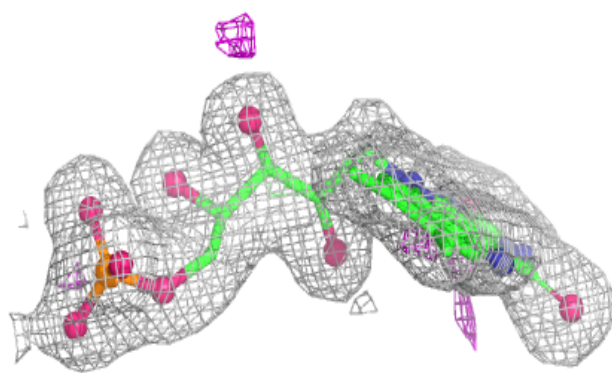
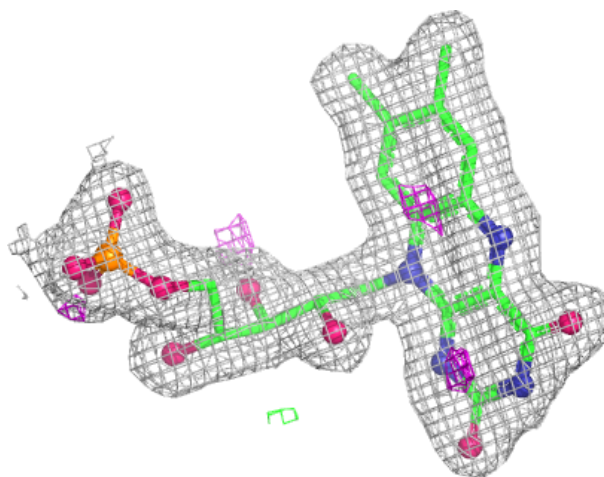
Electron density around FMN B 301:

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



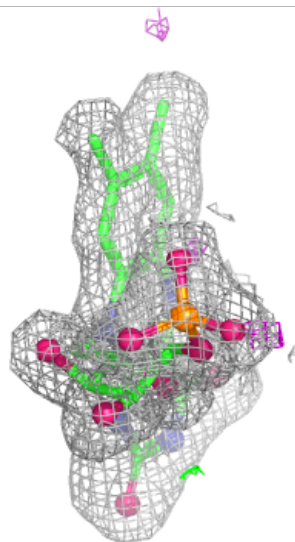
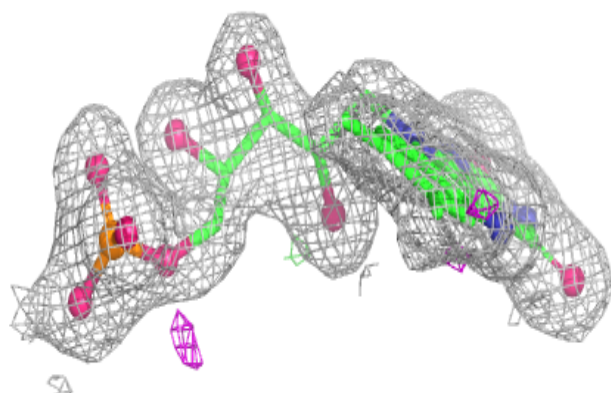
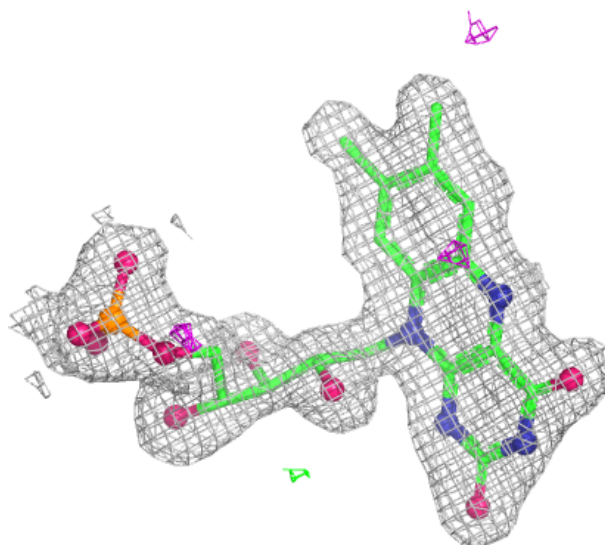
Electron density around FMN D 301:

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and green (positive)



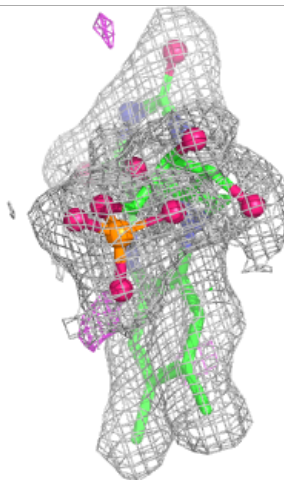
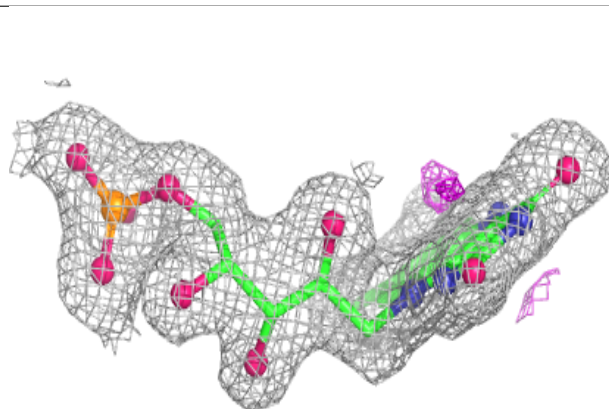
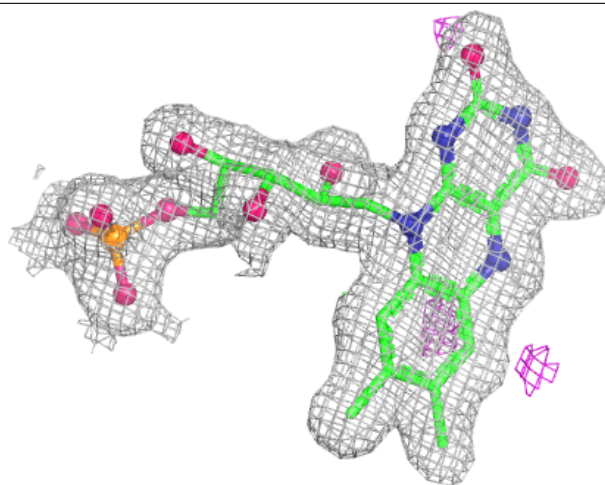
Electron density around FMN A 301:

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



Electron density around FMN C 301:

$2mF_o-DF_c$ (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.