



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:21 PM UTC

PDB ID : 6JXS / pdb_00006jxs
Title : Crystal Structure of Indigo reductase (Y151F) from *Bacillus smithii* type strain DSM 4216
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.
Deposited on : 2019-04-24
Resolution : 1.95 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

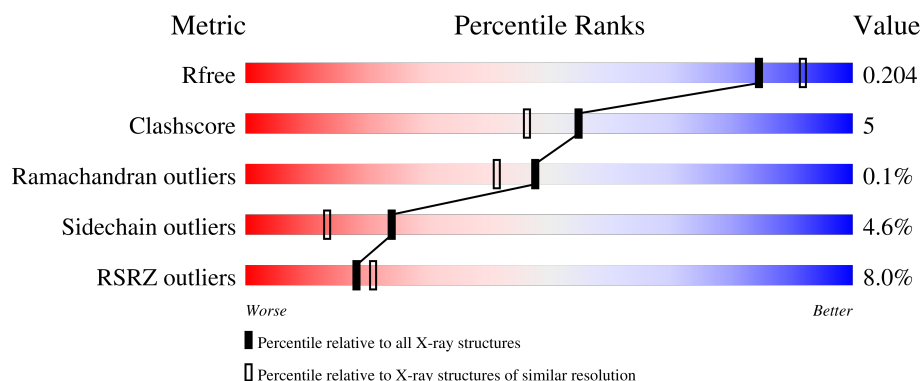
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	6% 77% 12% • 10%
1	B	231	6% 78% 11% • 9%
1	C	231	7% 78% 11% • 9%
1	D	231	10% 81% 9% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7104 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	209	Total	C	N	O	S	0	0	0
			1629	1051	262	308	8			
1	B	210	Total	C	N	O	S	0	0	0
			1638	1056	263	311	8			
1	C	211	Total	C	N	O	S	0	0	0
			1648	1062	266	312	8			
1	D	210	Total	C	N	O	S	0	0	0
			1638	1056	263	311	8			

There are 84 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
A	151	PHE	TYR	engineered mutation	UNP G9QLG5

Continued on next page...

Continued from previous page...

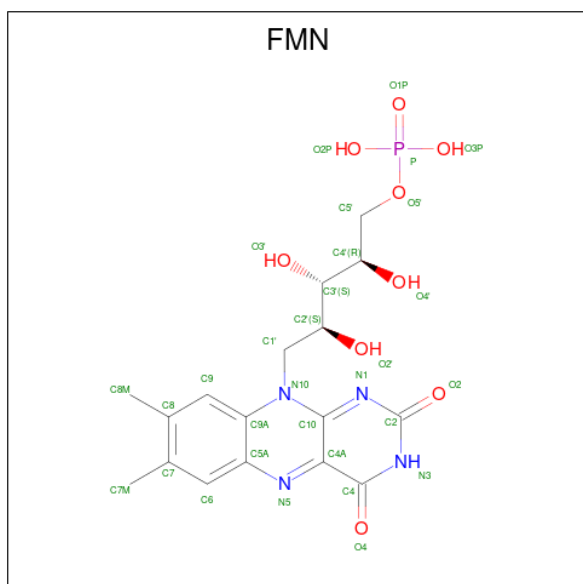
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP G9QLG5
B	-18	GLY	-	expression tag	UNP G9QLG5
B	-17	SER	-	expression tag	UNP G9QLG5
B	-16	SER	-	expression tag	UNP G9QLG5
B	-15	HIS	-	expression tag	UNP G9QLG5
B	-14	HIS	-	expression tag	UNP G9QLG5
B	-13	HIS	-	expression tag	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
B	151	PHE	TYR	engineered mutation	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
C	151	PHE	TYR	engineered mutation	UNP G9QLG5

Continued on next page...

Continued from previous page...

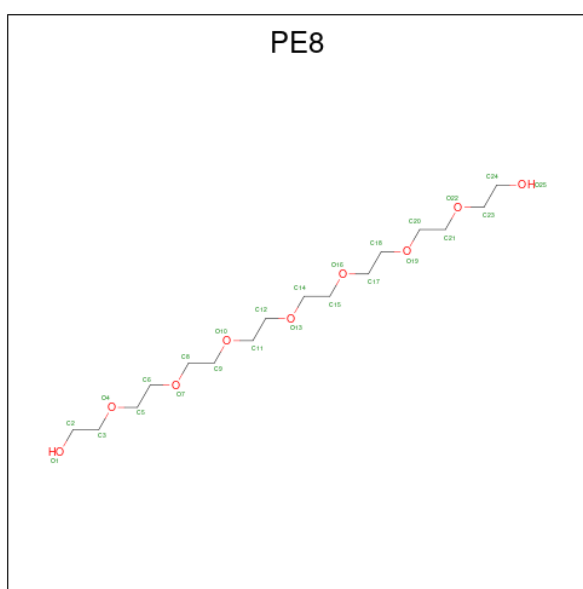
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP G9QLG5
D	-18	GLY	-	expression tag	UNP G9QLG5
D	-17	SER	-	expression tag	UNP G9QLG5
D	-16	SER	-	expression tag	UNP G9QLG5
D	-15	HIS	-	expression tag	UNP G9QLG5
D	-14	HIS	-	expression tag	UNP G9QLG5
D	-13	HIS	-	expression tag	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
D	151	PHE	TYR	engineered mutation	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).



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

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	108	Total	O	0	0
			108	108		
4	C	101	Total	O	0	0
			101	101		

Continued on next page...

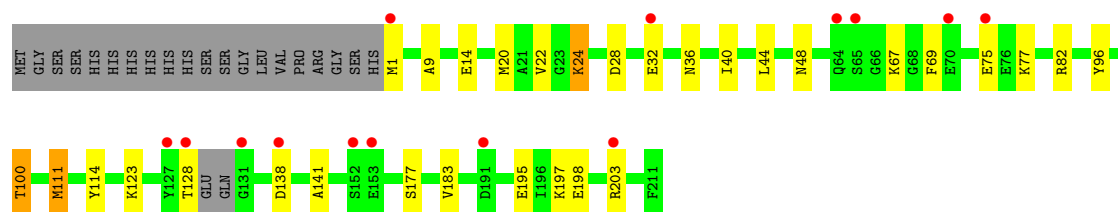
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	60	Total	O	0	0
			60	60		

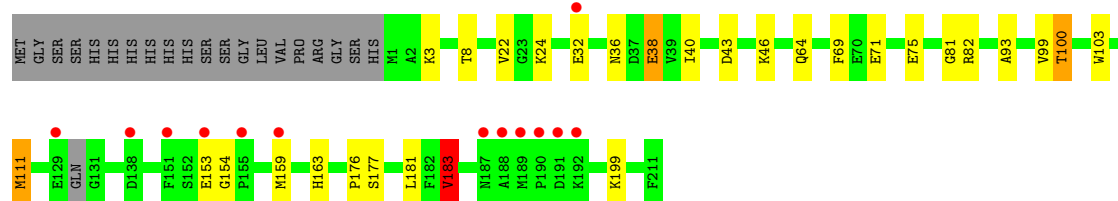
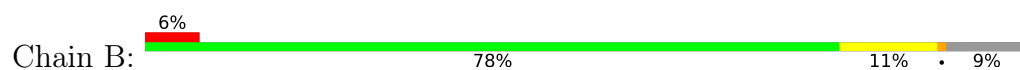
3 Residue-property plots [i](#)

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.

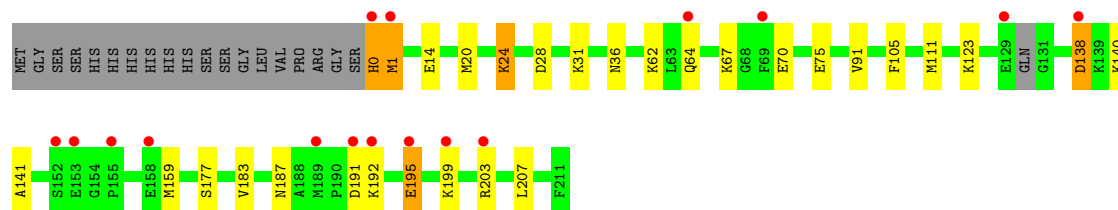
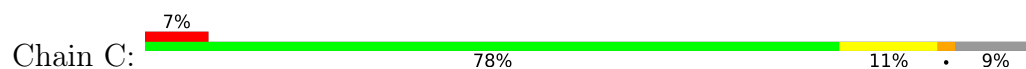
- Molecule 1: FMN-dependent NADH-azoreductase



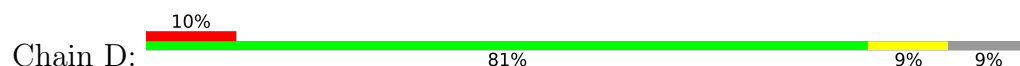
- Molecule 1: FMN-dependent NADH-azoreductase

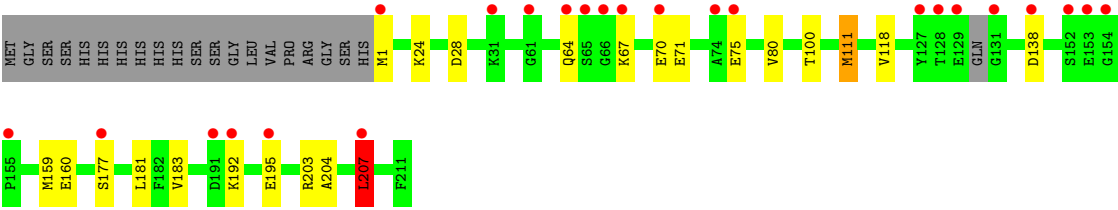


- Molecule 1: FMN-dependent NADH-azoreductase



- 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	48.27Å 104.21Å 87.72Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	33.14 – 1.95 33.14 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.14-1.95) 98.9 (33.14-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	23.72 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.197 , 0.207 0.194 , 0.204	Depositor DCC
R_{free} test set	3148 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7104	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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: PE8, 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	1.33	9/1667 (0.5%)	1.12	0/2248
1	B	1.35	10/1676 (0.6%)	1.11	2/2260 (0.1%)
1	C	1.22	3/1687 (0.2%)	1.15	3/2275 (0.1%)
1	D	1.22	6/1676 (0.4%)	1.11	3/2260 (0.1%)
All	All	1.28	28/6706 (0.4%)	1.13	8/9043 (0.1%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	207	LEU	CB-CG	-6.77	1.40	1.53
1	C	111	MET	C-O	-6.68	1.16	1.24
1	B	82	ARG	C-O	-6.63	1.16	1.24
1	A	100	THR	C-O	-6.10	1.17	1.24
1	A	48	ASN	C-O	-6.06	1.16	1.24
1	A	195	GLU	C-O	-5.97	1.17	1.24
1	D	111	MET	C-O	-5.90	1.17	1.24
1	B	111	MET	SD-CE	-5.80	1.65	1.79
1	B	81	GLY	C-O	-5.67	1.17	1.23
1	B	176	PRO	C-O	-5.66	1.17	1.24
1	A	111	MET	SD-CE	-5.58	1.65	1.79
1	B	69	PHE	C-O	-5.51	1.17	1.24
1	B	71	GLU	C-O	-5.50	1.16	1.24
1	D	160	GLU	C-O	5.48	1.30	1.24
1	D	118	VAL	C-O	-5.47	1.18	1.24
1	C	207	LEU	C-O	-5.45	1.17	1.24
1	B	100	THR	C-O	-5.44	1.18	1.24
1	B	64	GLN	C-O	-5.37	1.17	1.24
1	B	177	SER	C-O	-5.30	1.18	1.24
1	A	123	LYS	CA-C	5.29	1.57	1.52
1	B	163	HIS	N-CA	-5.28	1.40	1.46
1	A	177	SER	C-O	-5.16	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ILE	C-O	-5.12	1.18	1.24
1	D	181	LEU	N-CA	-5.11	1.39	1.46
1	C	177	SER	C-O	-5.05	1.18	1.24
1	D	100	THR	C-O	-5.03	1.18	1.24
1	A	36	ASN	C-O	-5.02	1.17	1.24
1	A	114	TYR	C-O	5.00	1.29	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	VAL	CB-CA-C	-7.25	102.54	111.32
1	D	80	VAL	CA-C-N	6.28	126.91	119.94
1	D	80	VAL	C-N-CA	6.28	126.91	119.94
1	B	183	VAL	CB-CA-C	-6.26	103.39	111.53
1	C	14	GLU	N-CA-C	5.34	119.28	112.87
1	C	1	MET	N-CA-C	5.29	122.07	110.80
1	B	38	GLU	CA-CB-CG	5.29	124.67	114.10
1	D	203	ARG	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1629	0	1602	12	0
1	B	1638	0	1608	16	0
1	C	1648	0	1615	21	0
1	D	1638	0	1608	6	0
2	A	31	0	19	1	0
2	B	31	0	19	3	0
2	C	31	0	19	2	0
2	D	31	0	19	5	0
3	A	25	0	34	3	0
3	D	25	0	34	0	0
4	A	108	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	108	0	0	7	0
4	C	101	0	0	10	0
4	D	60	0	0	1	0
All	All	7104	0	6577	64	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 (64) 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:C:31:LYS:HB2	4:C:487:HOH:O	1.37	1.24
2:B:301:FMN:H2'	4:B:461:HOH:O	1.45	1.15
1:B:38:GLU:OE2	1:B:40:ILE:HD11	1.54	1.07
1:C:0:HIS:HB2	1:C:36:ASN:O	1.62	0.97
1:A:203:ARG:HG3	4:A:442:HOH:O	1.67	0.94
4:A:439:HOH:O	1:C:159:MET:SD	2.44	0.76
1:C:20:MET:HE2	4:C:445:HOH:O	1.85	0.75
1:B:32:GLU:HG2	4:C:418:HOH:O	1.88	0.73
1:B:199:LYS:HE2	4:B:501:HOH:O	1.89	0.72
4:B:443:HOH:O	2:D:301:FMN:HM72	1.90	0.70
1:C:0:HIS:CB	1:C:36:ASN:O	2.39	0.69
1:A:22:VAL:HG21	1:A:183:VAL:HG21	1.75	0.68
1:C:192:LYS:O	1:C:195:GLU:HG2	1.97	0.65
2:D:301:FMN:N1	2:D:301:FMN:O2'	2.30	0.62
1:B:43:ASP:OD2	1:B:46:LYS:HD2	2.00	0.61
1:D:138:ASP:CG	1:D:138:ASP:O	2.43	0.58
1:B:3:LYS:HD2	1:B:93:ALA:HA	1.85	0.58
2:D:301:FMN:C4	4:D:408:HOH:O	2.52	0.57
1:A:198:GLU:OE2	3:A:302:PE8:O25	2.23	0.57
1:A:69:PHE:CE2	1:A:77:LYS:HD2	2.41	0.56
1:D:207:LEU:C	1:D:207:LEU:HD13	2.31	0.55
1:D:24:LYS:HD3	1:D:28:ASP:OD2	2.06	0.55
1:B:38:GLU:CD	1:B:40:ILE:HD11	2.29	0.54
2:D:301:FMN:HO2'	2:D:301:FMN:C10	2.20	0.52
1:B:46:LYS:HD2	4:B:452:HOH:O	2.10	0.52
1:C:24:LYS:HD3	4:C:410:HOH:O	2.09	0.52
1:C:138:ASP:HB2	4:C:403:HOH:O	2.10	0.51
1:C:199:LYS:O	1:C:203:ARG:HG2	2.11	0.51
1:C:24:LYS:HD3	1:C:28:ASP:OD2	2.09	0.51
1:A:197:LYS:HZ2	3:A:302:PE8:H151	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:FMN:C4	4:B:403:HOH:O	2.59	0.49
1:B:46:LYS:HD3	4:B:490:HOH:O	2.11	0.49
1:C:31:LYS:HD2	4:C:435:HOH:O	2.11	0.49
1:C:140:LYS:HG3	4:C:422:HOH:O	2.12	0.49
1:C:31:LYS:CE	4:C:435:HOH:O	2.61	0.48
1:A:20:MET:O	1:A:24:LYS:HB2	2.11	0.48
1:A:22:VAL:HG21	1:A:183:VAL:CG2	2.42	0.48
1:C:105:PHE:CE1	1:C:159:MET:HG2	2.49	0.47
2:A:301:FMN:C4	4:A:435:HOH:O	2.62	0.47
1:C:0:HIS:CG	1:C:36:ASN:O	2.67	0.47
1:D:159:MET:HE2	1:D:159:MET:HB2	1.74	0.46
1:B:22:VAL:HG21	1:B:183:VAL:CG2	2.45	0.46
1:B:32:GLU:HG3	4:B:430:HOH:O	2.15	0.46
1:B:103:TRP:HA	2:B:301:FMN:C5A	2.47	0.45
1:C:187:ASN:ND2	2:C:301:FMN:H3'	2.32	0.45
1:A:100:THR:CG2	1:A:111:MET:HE3	2.46	0.45
1:B:159:MET:HE2	1:B:159:MET:HB2	1.85	0.45
1:A:14:GLU:O	3:A:302:PE8:H172	2.17	0.44
1:C:24:LYS:CD	4:C:410:HOH:O	2.66	0.44
1:C:31:LYS:CD	4:C:435:HOH:O	2.66	0.44
2:D:301:FMN:O2'	2:D:301:FMN:C10	2.65	0.44
1:B:22:VAL:HG21	1:B:183:VAL:HG22	2.01	0.43
1:A:28:ASP:O	1:A:32:GLU:HG3	2.19	0.43
1:B:100:THR:CG2	1:B:111:MET:HE3	2.48	0.43
1:B:153:GLU:HG2	1:B:154:GLY:N	2.34	0.42
1:C:62:LYS:O	1:C:67:LYS:HB2	2.19	0.42
1:D:111:MET:HE3	1:D:111:MET:O	2.19	0.42
1:C:91:VAL:HG11	1:C:123:LYS:HB3	2.02	0.42
1:A:96:TYR:O	1:A:141:ALA:HA	2.19	0.41
1:D:204:ALA:O	1:D:207:LEU:HD12	2.19	0.41
1:C:140:LYS:HG3	1:C:141:ALA:N	2.35	0.40
1:A:9:ALA:HB2	1:A:44:LEU:HD12	2.04	0.40
1:B:8:THR:HG22	1:B:99:VAL:HB	2.03	0.40
2:C:301:FMN:HM81	2:C:301:FMN:HM71	1.72	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	205/231 (89%)	202 (98%)	3 (2%)	0	100	100
1	B	206/231 (89%)	202 (98%)	4 (2%)	0	100	100
1	C	207/231 (90%)	201 (97%)	5 (2%)	1 (0%)	24	16
1	D	206/231 (89%)	199 (97%)	7 (3%)	0	100	100
All	All	824/924 (89%)	804 (98%)	19 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1	MET

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	169/188 (90%)	162 (96%)	7 (4%)	27	17
1	B	170/188 (90%)	165 (97%)	5 (3%)	37	29
1	C	171/188 (91%)	163 (95%)	8 (5%)	23	12
1	D	170/188 (90%)	159 (94%)	11 (6%)	15	6
All	All	680/752 (90%)	649 (95%)	31 (5%)	24	13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	LYS
1	A	67	LYS
1	A	75	GLU
1	A	82	ARG
1	A	128	THR
1	A	138	ASP
1	B	24	LYS
1	B	36	ASN
1	B	75	GLU
1	B	181	LEU
1	B	183	VAL
1	C	0	HIS
1	C	24	LYS
1	C	64	GLN
1	C	70	GLU
1	C	75	GLU
1	C	138	ASP
1	C	191	ASP
1	C	195	GLU
1	D	1	MET
1	D	64	GLN
1	D	67	LYS
1	D	70	GLU
1	D	71	GLU
1	D	75	GLU
1	D	177	SER
1	D	183	VAL
1	D	192	LYS
1	D	195	GLU
1	D	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	145	GLN
1	A	167	GLN
1	A	194	GLN
1	B	36	ASN
1	B	64	GLN
1	B	145	GLN
1	B	194	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	48	ASN
1	C	89	GLN
1	C	145	GLN
1	D	48	ASN
1	D	167	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 ⓘ

6 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	PE8	D	302	-	24,24,24	0.66	0	23,23,23	0.72	0
2	FMN	D	301	-	33,33,33	1.98	13 (39%)	48,50,50	2.29	17 (35%)
2	FMN	B	301	-	33,33,33	1.98	12 (36%)	48,50,50	2.27	15 (31%)
2	FMN	C	301	-	33,33,33	2.02	12 (36%)	48,50,50	2.53	17 (35%)
3	PE8	A	302	-	24,24,24	0.58	0	23,23,23	0.85	1 (4%)
2	FMN	A	301	-	33,33,33	2.12	7 (21%)	48,50,50	1.90	16 (33%)

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	PE8	D	302	-	-	13/22/22/22	-
2	FMN	D	301	-	-	6/18/18/18	0/3/3/3
2	FMN	B	301	-	-	4/18/18/18	0/3/3/3
2	FMN	C	301	-	-	4/18/18/18	0/3/3/3
3	PE8	A	302	-	-	9/22/22/22	-
2	FMN	A	301	-	-	3/18/18/18	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FMN	C9A-C5A	7.23	1.52	1.41
2	C	301	FMN	C9A-C5A	5.89	1.50	1.41
2	B	301	FMN	C9A-C5A	5.87	1.50	1.41
2	A	301	FMN	C5A-N5	-4.53	1.31	1.39
2	D	301	FMN	C10-N10	3.55	1.45	1.37
2	D	301	FMN	C6-C7	-3.54	1.34	1.39
2	D	301	FMN	C10-N1	3.45	1.40	1.33
2	C	301	FMN	P-O2P	-3.24	1.42	1.54
2	B	301	FMN	C10-N10	3.17	1.44	1.37
2	A	301	FMN	C10-N10	3.16	1.44	1.37
2	D	301	FMN	C6-C5A	-3.13	1.35	1.40
2	D	301	FMN	C4'-C3'	-3.09	1.48	1.53
2	C	301	FMN	C10-N10	3.06	1.43	1.37
2	B	301	FMN	C9-C8	3.04	1.43	1.39
2	D	301	FMN	C9A-C5A	2.84	1.45	1.41
2	B	301	FMN	C6-C7	-2.76	1.35	1.39
2	D	301	FMN	C4-N3	-2.76	1.33	1.38
2	C	301	FMN	O4'-C4'	2.60	1.48	1.43
2	C	301	FMN	C4-N3	-2.57	1.34	1.38
2	C	301	FMN	P-O3P	-2.57	1.45	1.54
2	D	301	FMN	C5'-C4'	2.51	1.55	1.51
2	D	301	FMN	P-O2P	-2.49	1.45	1.54
2	D	301	FMN	C4A-C4	2.43	1.53	1.44
2	D	301	FMN	P-O3P	-2.30	1.46	1.54
2	C	301	FMN	P-O5'	-2.29	1.53	1.60
2	A	301	FMN	C6-C7	-2.24	1.36	1.39
2	A	301	FMN	C8-C7	2.22	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FMN	C8-C7	2.21	1.46	1.40
2	C	301	FMN	C2-N3	-2.21	1.34	1.39
2	B	301	FMN	C4A-N5	2.19	1.35	1.30
2	B	301	FMN	P-O5'	-2.18	1.53	1.60
2	B	301	FMN	C9-C9A	2.18	1.43	1.39
2	A	301	FMN	P-O2P	-2.15	1.46	1.54
2	A	301	FMN	P-O3P	-2.15	1.46	1.54
2	C	301	FMN	C6-C7	-2.14	1.36	1.39
2	C	301	FMN	C10-N1	2.13	1.37	1.33
2	B	301	FMN	C7M-C7	-2.13	1.47	1.51
2	C	301	FMN	C9-C8	2.11	1.42	1.39
2	B	301	FMN	C5'-C4'	2.09	1.54	1.51
2	D	301	FMN	C2'-C3'	-2.08	1.49	1.53
2	B	301	FMN	P-O2P	-2.06	1.47	1.54
2	B	301	FMN	P-O3P	-2.04	1.47	1.54
2	B	301	FMN	C1'-C2'	2.04	1.55	1.52
2	D	301	FMN	C7M-C7	-2.04	1.47	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FMN	C4-C4A-N5	8.44	129.87	118.21
2	D	301	FMN	C5'-C4'-C3'	-6.53	99.90	112.22
2	B	301	FMN	C4-C4A-N5	6.21	126.79	118.21
2	C	301	FMN	C8M-C8-C9	5.12	128.59	119.57
2	B	301	FMN	C8M-C8-C9	5.12	128.59	119.57
2	D	301	FMN	C4-C4A-N5	5.11	125.27	118.21
2	D	301	FMN	O4'-C4'-C5'	4.68	120.32	109.99
2	A	301	FMN	C8M-C8-C9	4.52	127.54	119.57
2	C	301	FMN	C5A-C9A-N10	-4.51	113.89	117.97
2	A	301	FMN	C8M-C8-C7	-4.30	111.97	120.76
2	D	301	FMN	C5A-N5-C4A	4.02	124.59	118.09
2	B	301	FMN	O4'-C4'-C5'	3.97	118.75	109.99
2	B	301	FMN	C10-C4A-N5	-3.96	116.73	124.81
2	B	301	FMN	C8M-C8-C7	-3.94	112.72	120.76
2	A	301	FMN	C4-C4A-N5	3.94	123.64	118.21
2	C	301	FMN	C10-C4A-N5	-3.93	116.79	124.81
2	C	301	FMN	C5A-N5-C4A	3.88	124.37	118.09
2	D	301	FMN	O5'-C5'-C4'	3.84	119.61	109.36
2	B	301	FMN	C5A-N5-C4A	3.80	124.24	118.09
2	C	301	FMN	C8M-C8-C7	-3.79	113.03	120.76
2	B	301	FMN	C10-N1-C2	3.74	124.95	116.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FMN	O3'-C3'-C4'	3.72	117.39	108.93
2	B	301	FMN	O2-C2-N1	-3.72	115.62	121.80
2	C	301	FMN	O4-C4-N3	-3.71	113.14	120.11
2	B	301	FMN	C4A-C10-N10	3.59	121.62	116.48
2	C	301	FMN	O4'-C4'-C5'	3.56	117.84	109.99
2	C	301	FMN	C7M-C7-C8	-3.56	113.50	120.76
2	B	301	FMN	O3'-C3'-C4'	3.42	116.69	108.93
2	C	301	FMN	O3P-P-O5'	-3.40	97.81	106.67
2	C	301	FMN	O5'-C5'-C4'	3.38	118.38	109.36
2	C	301	FMN	C10-N1-C2	3.36	124.11	116.85
2	A	301	FMN	O5'-C5'-C4'	3.35	118.30	109.36
2	D	301	FMN	C10-C4A-N5	-3.33	118.00	124.81
2	B	301	FMN	O2-C2-N3	3.29	124.90	118.58
2	B	301	FMN	C5A-C9A-N10	-3.27	115.01	117.97
2	D	301	FMN	C8M-C8-C9	3.21	125.22	119.57
2	C	301	FMN	C4A-C10-N10	3.18	121.04	116.48
2	D	301	FMN	C9-C9A-N10	3.04	125.95	121.85
2	D	301	FMN	C4A-C10-N1	-2.94	117.38	124.59
3	A	302	PE8	O13-C12-C11	2.90	123.58	110.35
2	D	301	FMN	O3'-C3'-C4'	-2.88	102.38	108.93
2	D	301	FMN	C4'-C3'-C2'	-2.82	108.87	113.57
2	A	301	FMN	C7M-C7-C8	-2.82	115.00	120.76
2	B	301	FMN	C9-C9A-N10	2.81	125.63	121.85
2	C	301	FMN	C6-C7-C8	2.78	123.77	119.69
2	D	301	FMN	O2P-P-O5'	-2.74	99.52	106.67
2	B	301	FMN	C4A-C10-N1	-2.67	118.04	124.59
2	A	301	FMN	C4A-C10-N10	2.66	120.29	116.48
2	A	301	FMN	O4'-C4'-C5'	2.64	115.80	109.99
2	A	301	FMN	C5A-C9A-N10	-2.56	115.65	117.97
2	A	301	FMN	C10-C4A-N5	-2.40	119.91	124.81
2	A	301	FMN	C5'-C4'-C3'	-2.39	107.71	112.22
2	C	301	FMN	O3'-C3'-C4'	2.34	114.24	108.93
2	A	301	FMN	C5A-N5-C4A	2.32	121.85	118.09
2	B	301	FMN	C7M-C7-C8	-2.32	116.02	120.76
2	D	301	FMN	O4-C4-N3	-2.31	115.78	120.11
2	C	301	FMN	C4A-C4-N3	2.27	119.03	113.25
2	D	301	FMN	C10-N1-C2	2.25	121.73	116.85
2	A	301	FMN	O2-C2-N1	-2.18	118.18	121.80
2	A	301	FMN	C10-N1-C2	2.17	121.54	116.85
2	A	301	FMN	C4A-C10-N1	-2.16	119.29	124.59
2	C	301	FMN	C4-C4A-C10	-2.10	113.33	116.93
2	D	301	FMN	C9-C8-C7	-2.09	116.62	119.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	FMN	C4A-C4-N3	2.05	118.48	113.25
2	D	301	FMN	C5A-C6-C7	2.02	124.57	120.83
2	A	301	FMN	C6-C7-C8	2.02	122.65	119.69

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

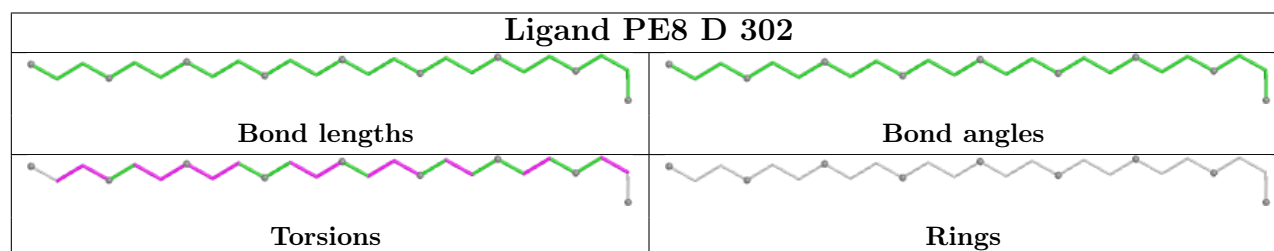
Mol	Chain	Res	Type	Atoms
2	D	301	FMN	O2'-C2'-C3'-C4'
2	C	301	FMN	O3'-C3'-C4'-C5'
3	A	302	PE8	O10-C11-C12-O13
3	D	302	PE8	C15-C14-O13-C12
3	A	302	PE8	O13-C14-C15-O16

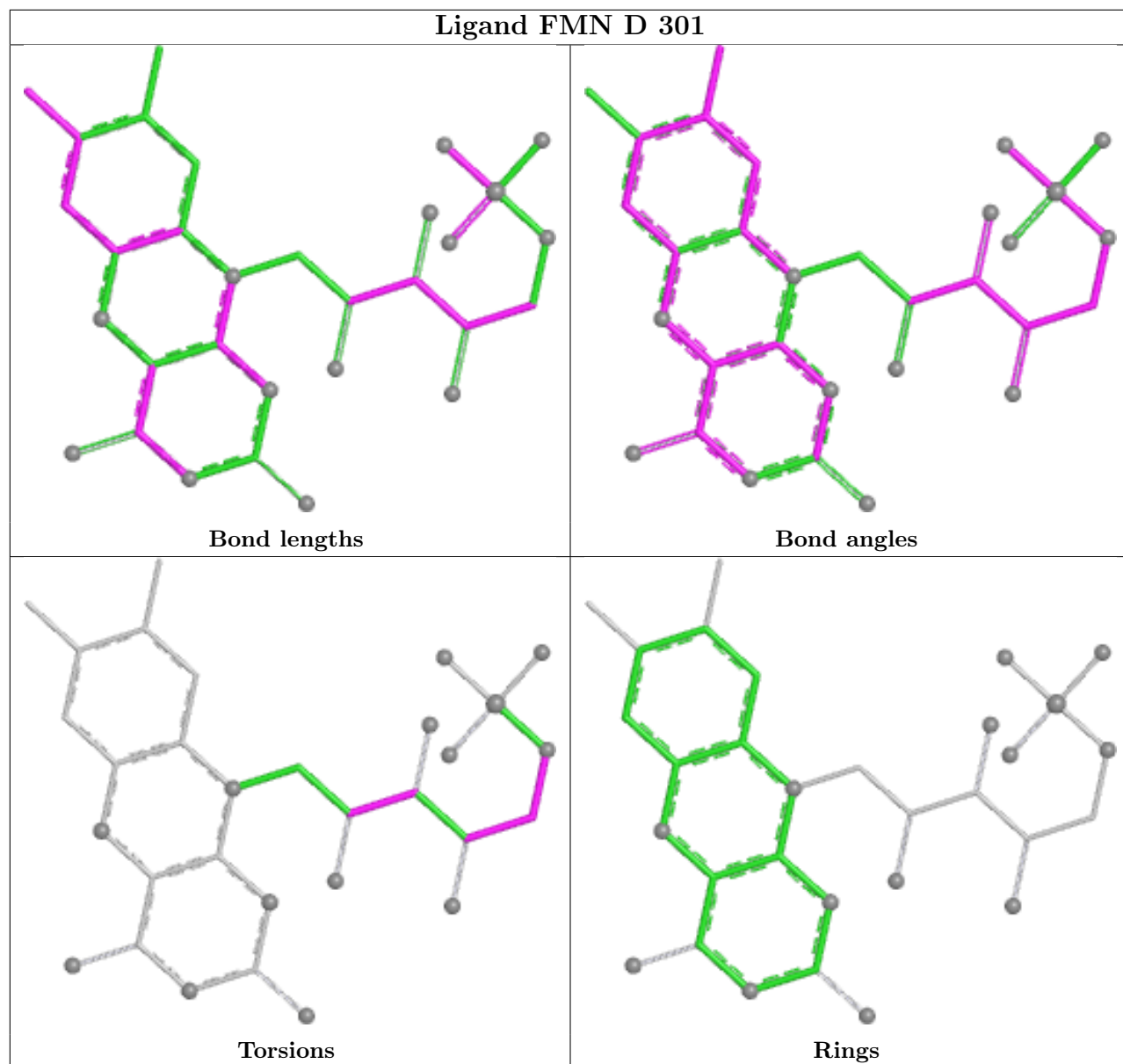
There are no ring outliers.

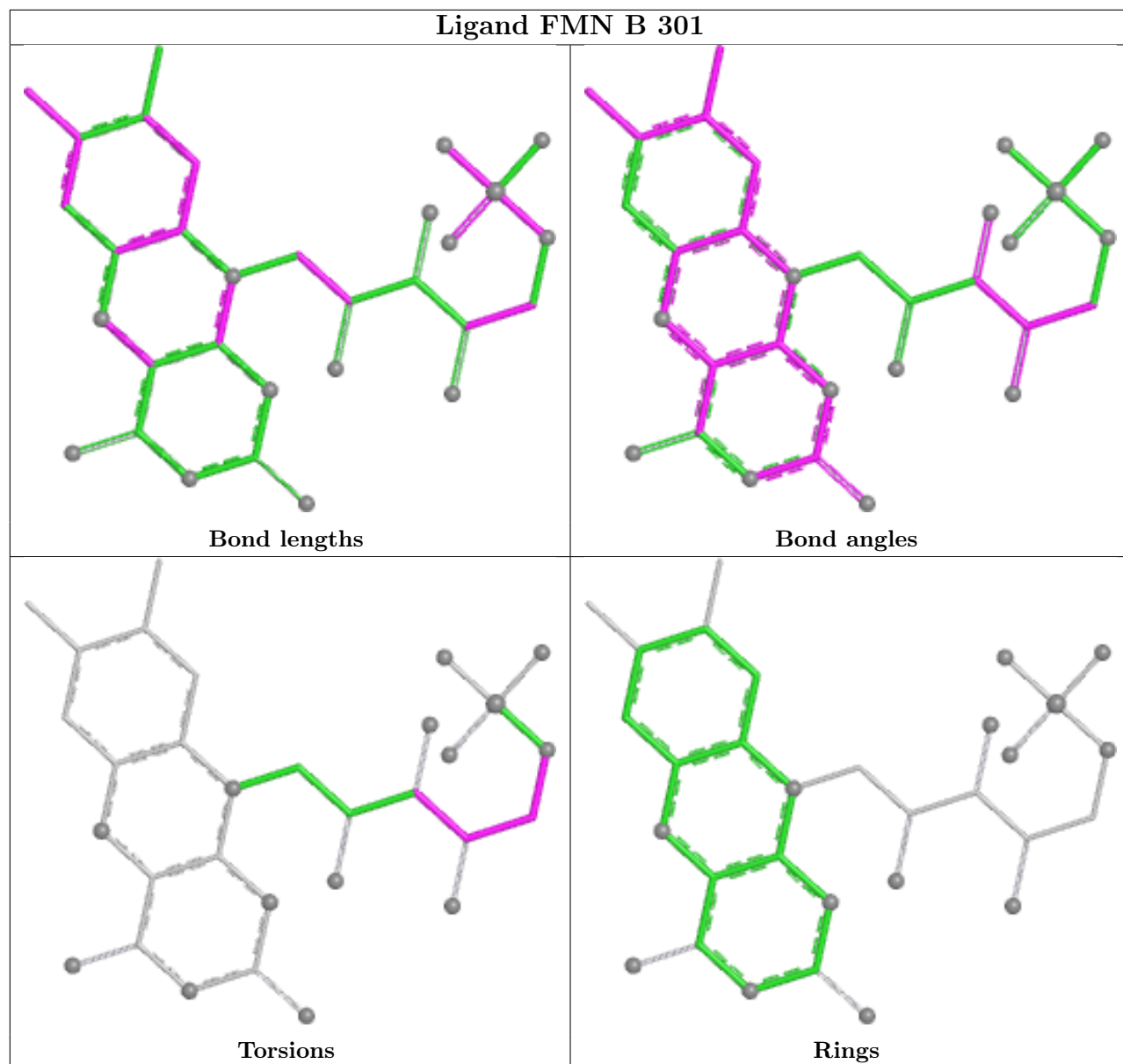
5 monomers are involved in 14 short contacts:

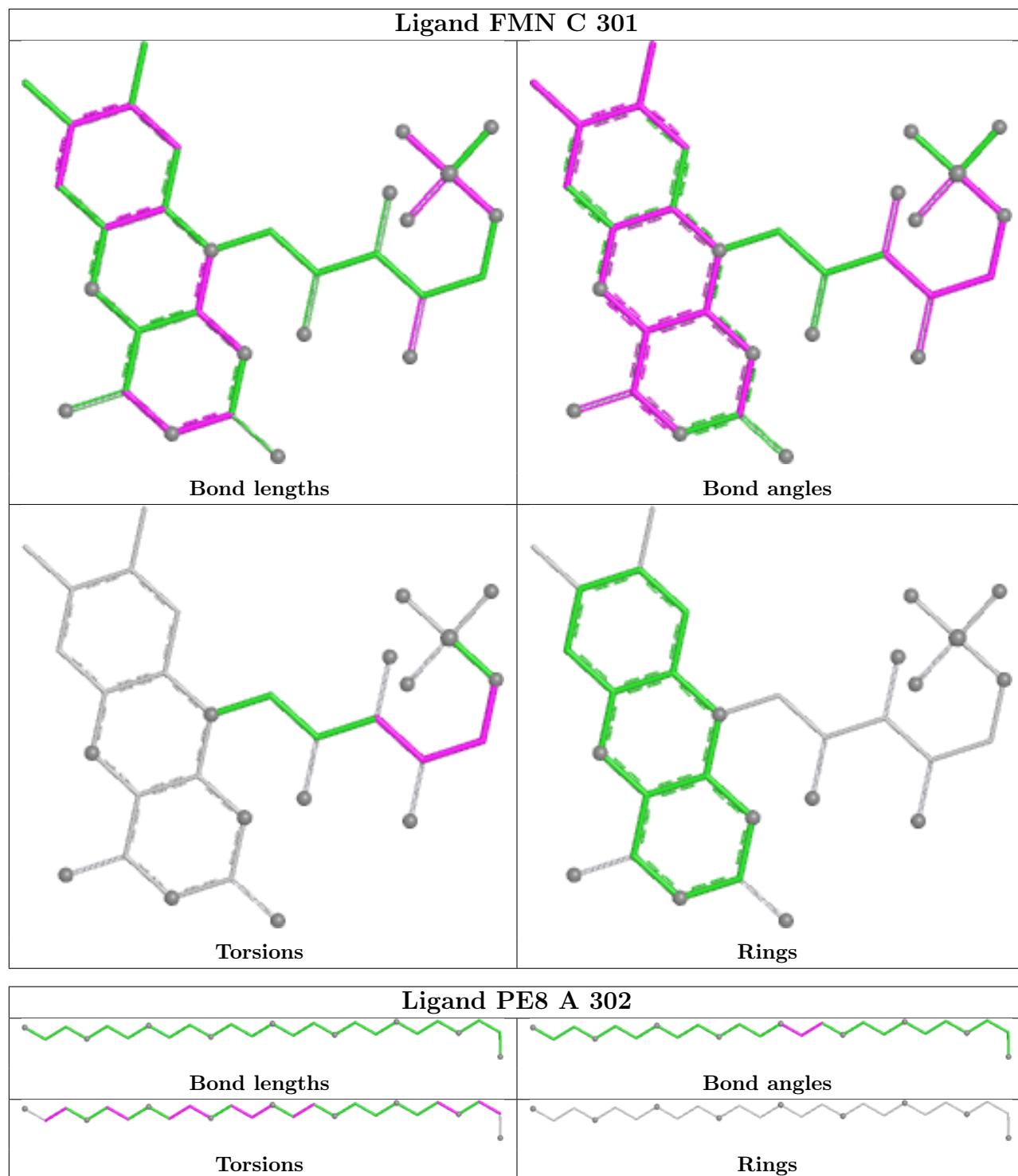
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	FMN	5	0
2	B	301	FMN	3	0
2	C	301	FMN	2	0
3	A	302	PE8	3	0
2	A	301	FMN	1	0

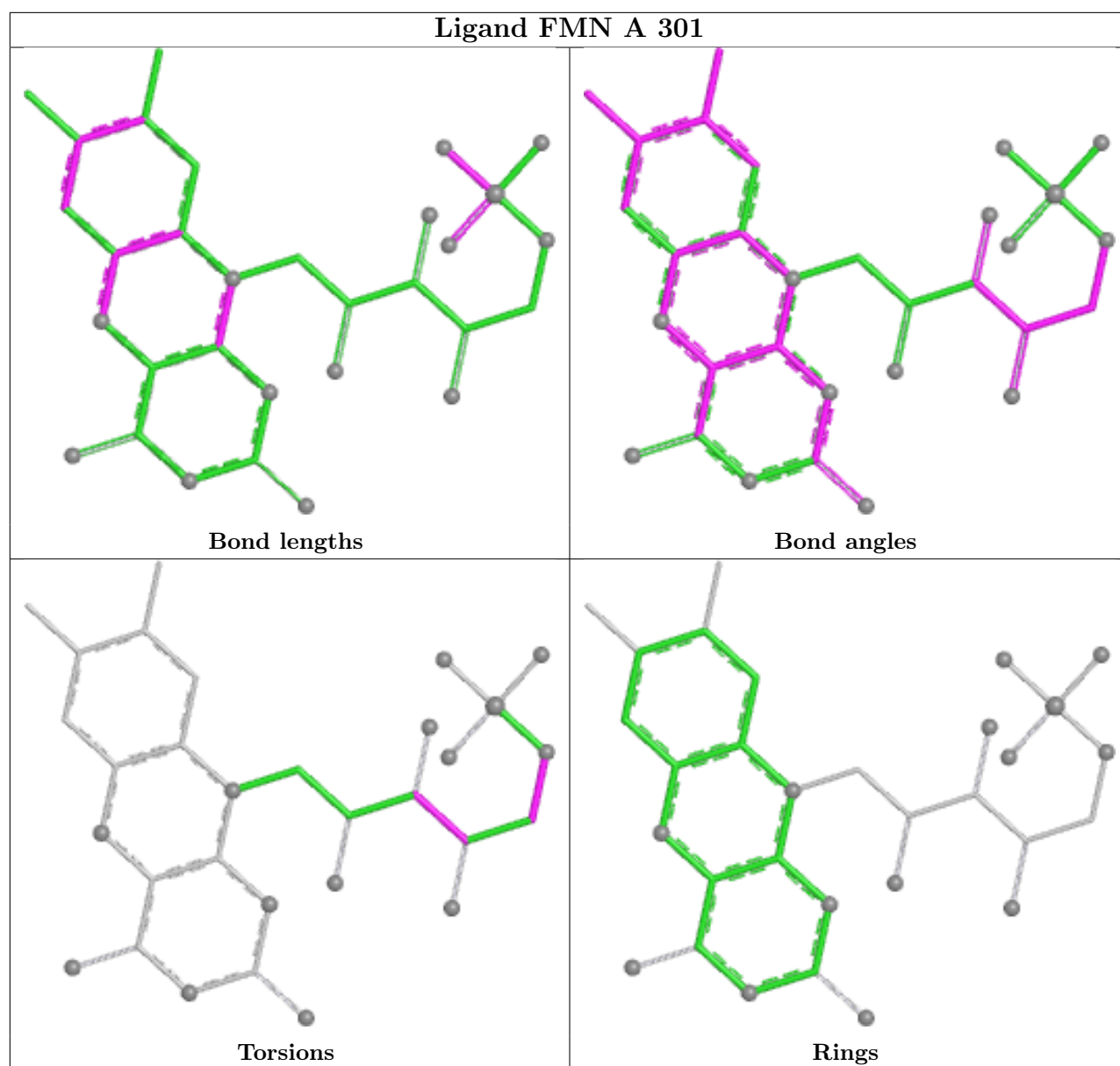
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	209/231 (90%)	0.16	14 (6%) 24 27	8, 14, 37, 63	0
1	B	210/231 (90%)	0.17	13 (6%) 26 31	8, 14, 35, 51	0
1	C	211/231 (91%)	0.26	16 (7%) 20 22	9, 17, 33, 41	0
1	D	210/231 (90%)	0.47	24 (11%) 10 11	10, 18, 47, 66	0
All	All	840/924 (90%)	0.27	67 (7%) 18 21	8, 16, 39, 66	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	HIS	6.5
1	D	155	PRO	6.4
1	A	131	GLY	5.7
1	A	191	ASP	5.1
1	D	153	GLU	5.0
1	D	131	GLY	4.9
1	D	154	GLY	4.4
1	D	152	SER	4.4
1	B	191	ASP	4.4
1	A	127	TYR	4.2
1	D	138	ASP	4.2
1	C	155	PRO	4.0
1	D	66	GLY	3.9
1	D	61	GLY	3.7
1	A	153	GLU	3.6
1	D	70	GLU	3.5
1	A	1	MET	3.5
1	D	129	GLU	3.5
1	C	1	MET	3.5
1	D	127	TYR	3.3
1	A	32	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	158	GLU	3.2
1	A	64	GLN	3.1
1	C	69	PHE	3.1
1	A	70	GLU	3.1
1	D	128	THR	3.1
1	B	155	PRO	3.1
1	B	153	GLU	3.1
1	D	177	SER	3.1
1	A	128	THR	3.0
1	D	195	GLU	3.0
1	B	190	PRO	2.9
1	B	32	GLU	2.9
1	C	195	GLU	2.8
1	B	189	MET	2.8
1	D	1	MET	2.8
1	C	129	GLU	2.8
1	C	191	ASP	2.8
1	C	203	ARG	2.7
1	C	138	ASP	2.6
1	D	192	LYS	2.6
1	D	64	GLN	2.5
1	D	65	SER	2.5
1	C	199	LYS	2.4
1	A	75	GLU	2.4
1	C	152	SER	2.4
1	C	153	GLU	2.3
1	B	188	ALA	2.3
1	D	191	ASP	2.3
1	C	189	MET	2.3
1	B	129	GLU	2.3
1	D	207	LEU	2.3
1	C	192	LYS	2.2
1	C	64	GLN	2.2
1	D	75	GLU	2.2
1	A	65	SER	2.2
1	D	31	LYS	2.2
1	B	151	PHE	2.1
1	A	203	ARG	2.1
1	B	192	LYS	2.1
1	D	67	LYS	2.1
1	B	159	MET	2.1
1	B	187	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	74	ALA	2.1
1	B	138	ASP	2.1
1	A	138	ASP	2.1
1	A	152	SER	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](#)

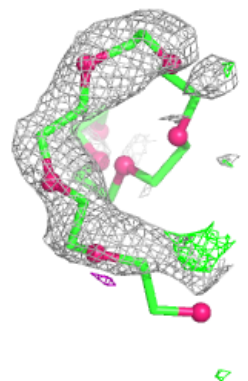
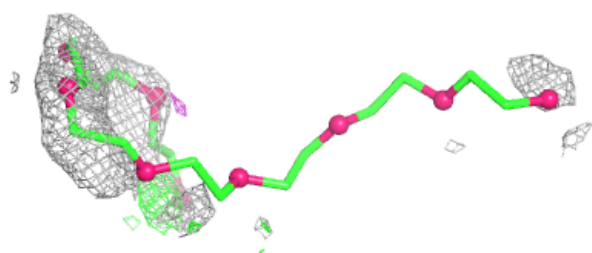
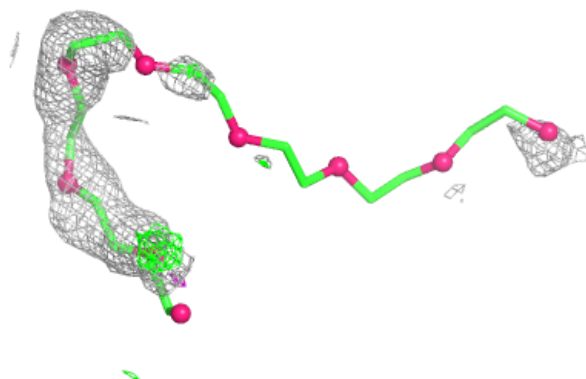
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PE8	D	302	25/25	0.62	0.31	58,71,83,85	0
3	PE8	A	302	25/25	0.81	0.22	29,54,73,73	0
2	FMN	C	301	31/31	0.82	0.20	20,45,53,54	0
2	FMN	D	301	31/31	0.84	0.20	14,48,56,56	0
2	FMN	B	301	31/31	0.86	0.18	16,41,48,49	0
2	FMN	A	301	31/31	0.87	0.17	13,31,39,44	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.

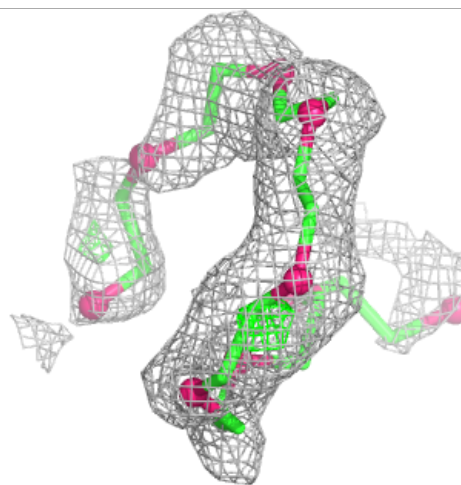
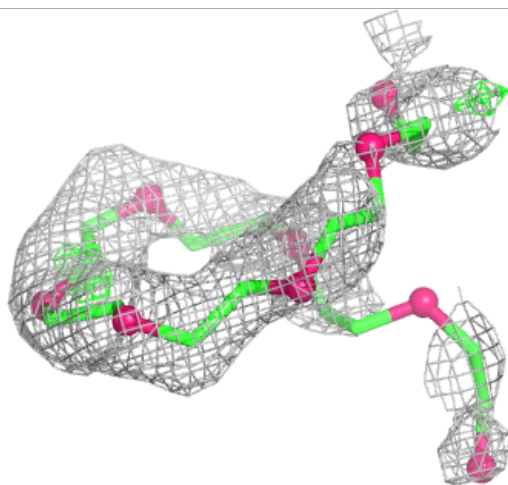
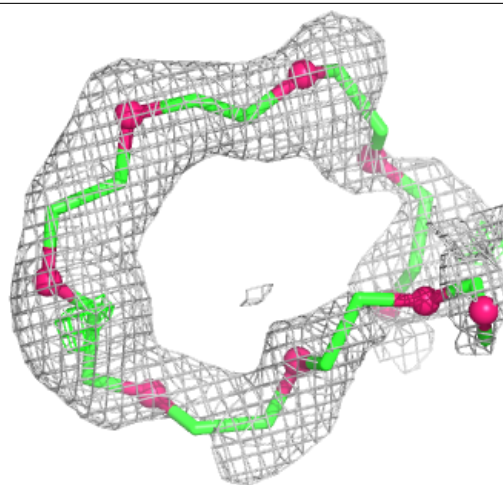
Electron density around PE8 D 302:

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



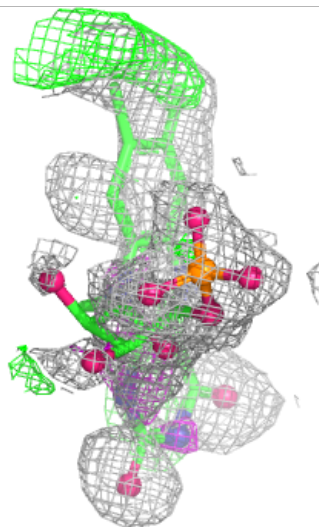
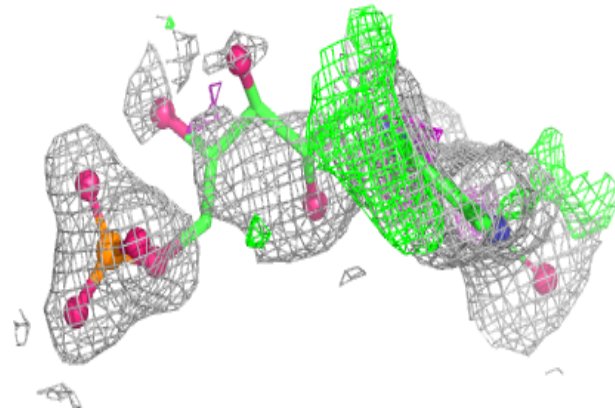
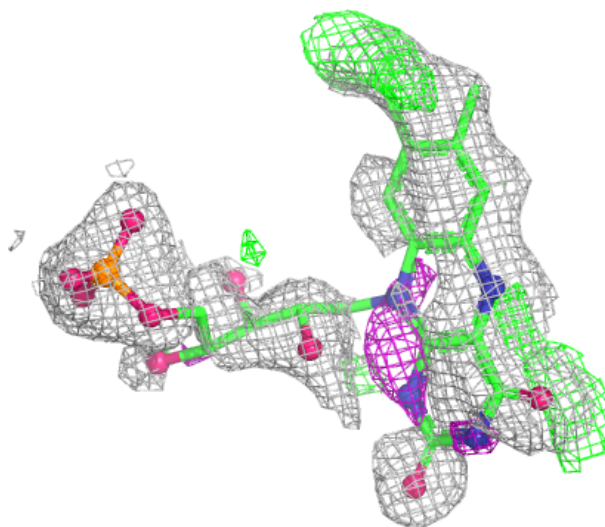
Electron density around PE8 A 302:

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



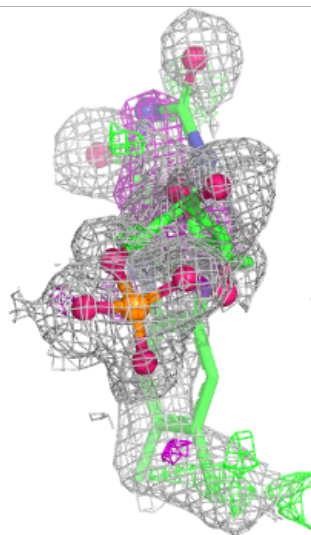
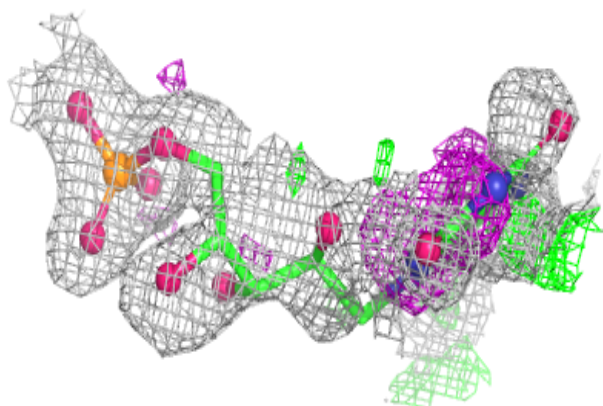
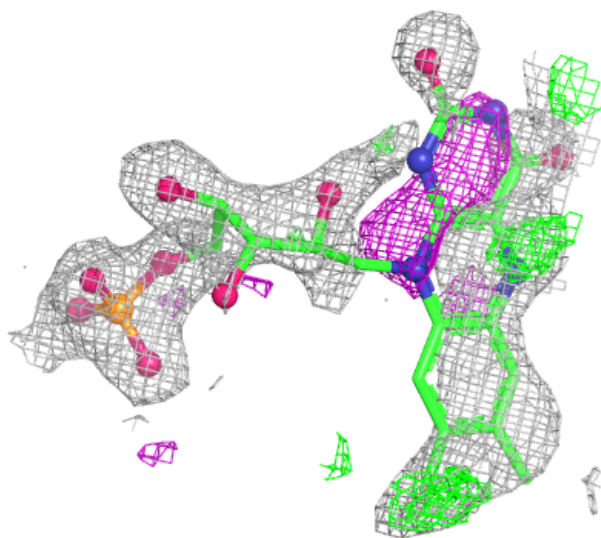
Electron density around FMN C 301:

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



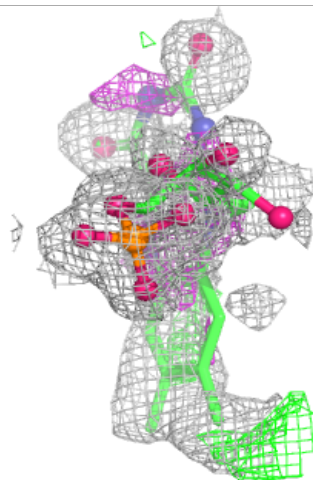
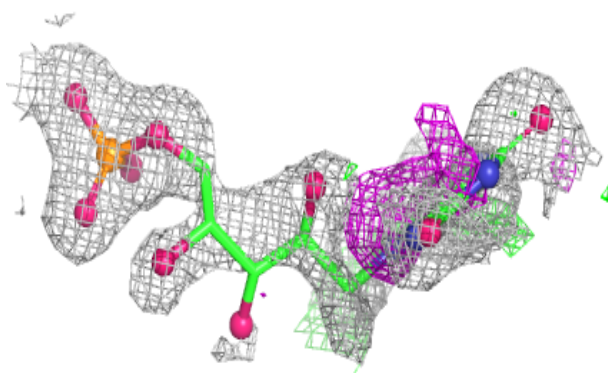
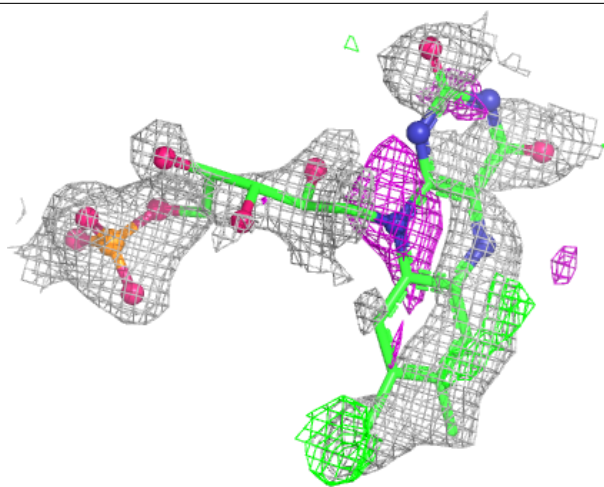
Electron density around FMN D 301:

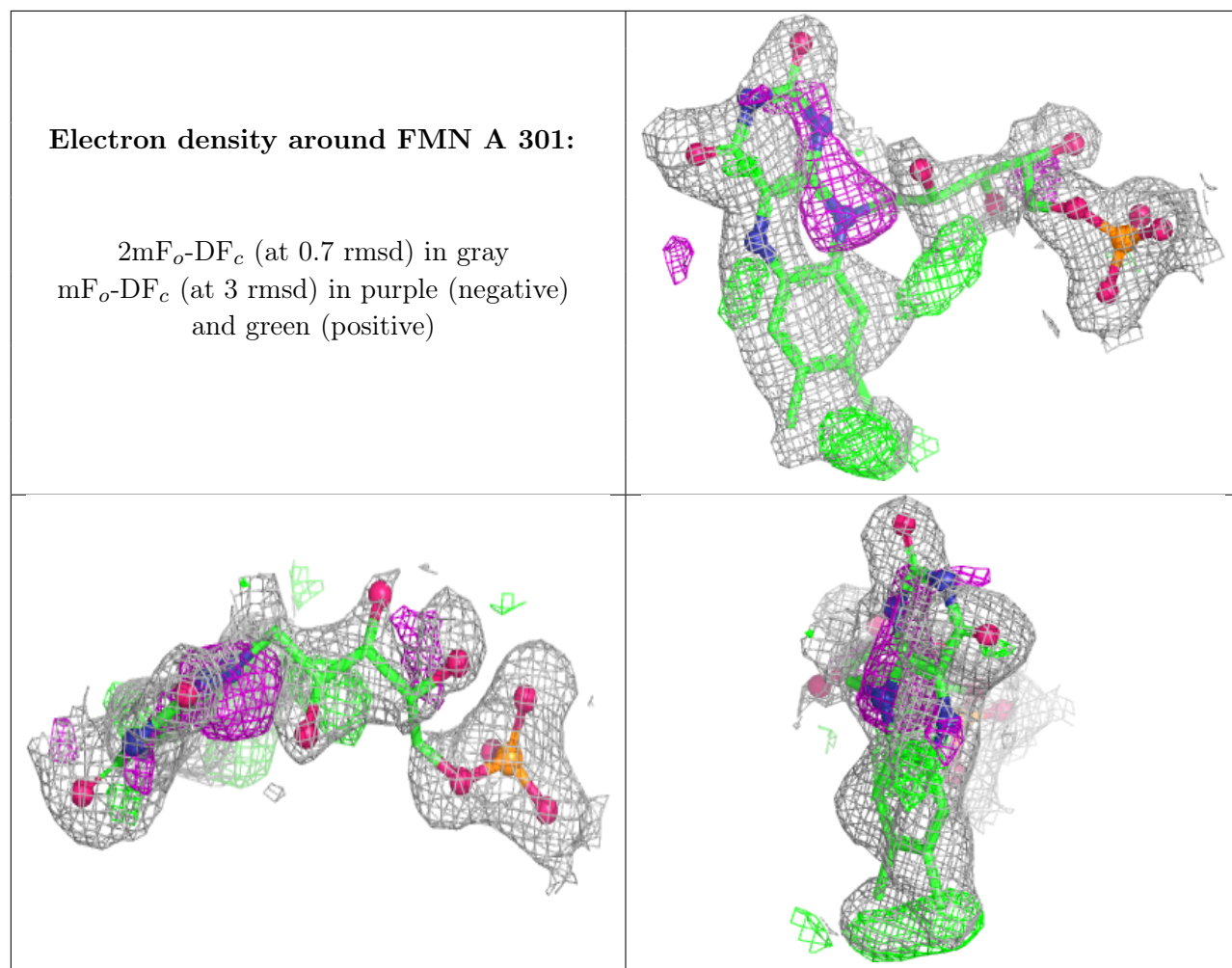
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.