



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:41 PM UTC

PDB ID : 1KBI / pdb_00001kbi
Title : Crystallographic Study of the Recombinant Flavin-binding Domain of Baker's Yeast Flavocytochrome b2: Comparison with the Intact Wild-type Enzyme
Authors : Cunane, L.M.; Barton, J.D.; Chen, Z.-W.; Welsh, F.E.; Chapman, S.K.; Reid, G.A.; Mathews, F.S.
Deposited on : 2001-11-06
Resolution : 2.30 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

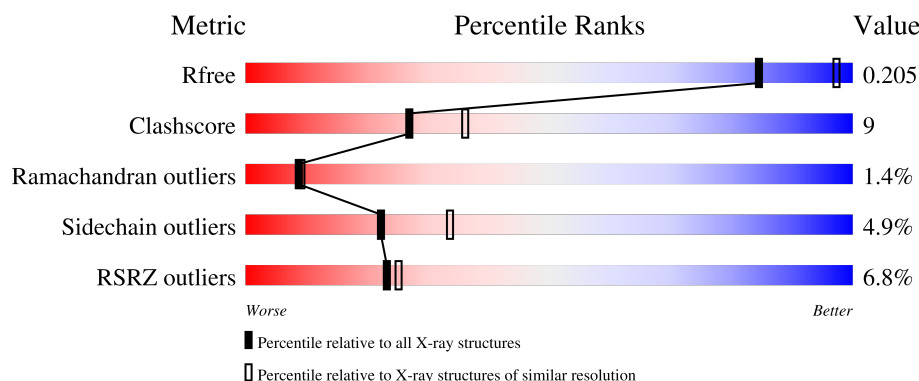
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	511	
1	B	511	

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
5	PO4	B	900	-	-	X	-
6	PYR	B	800	-	X	-	-

2 Entry composition [i](#)

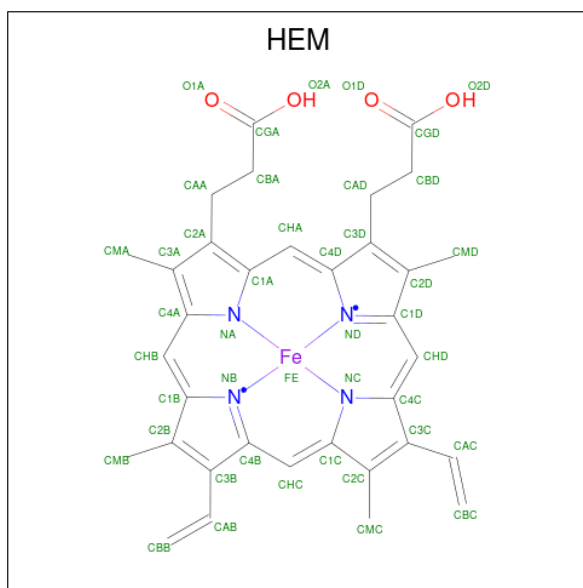
There are 7 unique types of molecules in this entry. The entry contains 7863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYTOCHROME B2.

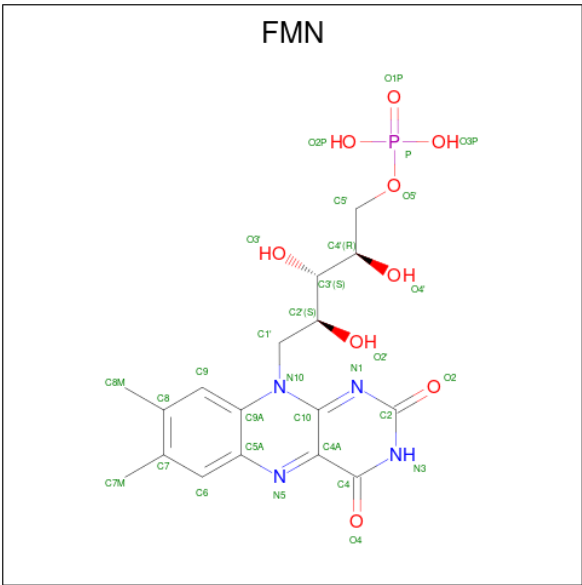
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	4	0
			3939	2498	668	758	15			
1	B	405	Total	C	N	O	S	0	0	0
			3152	1994	538	609	11			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



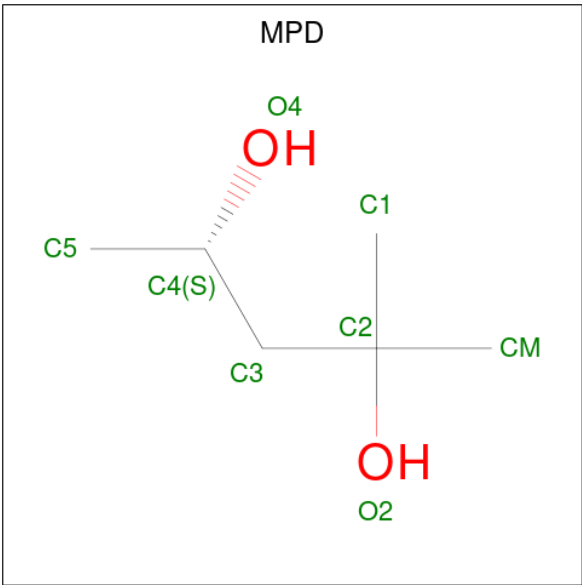
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



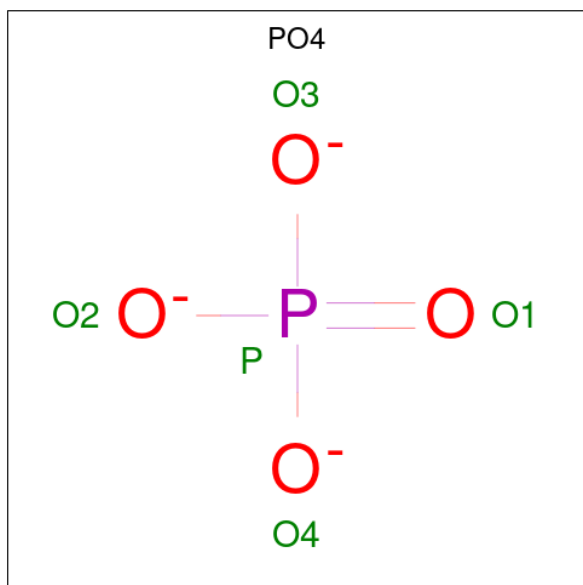
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

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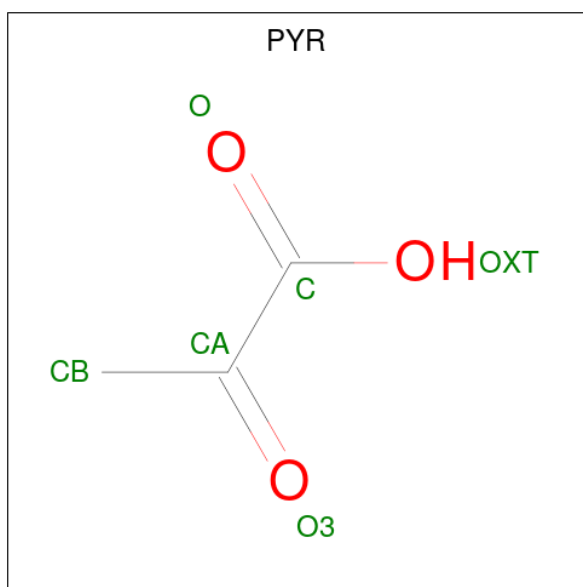
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			3	2	1		

- Molecule 6 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

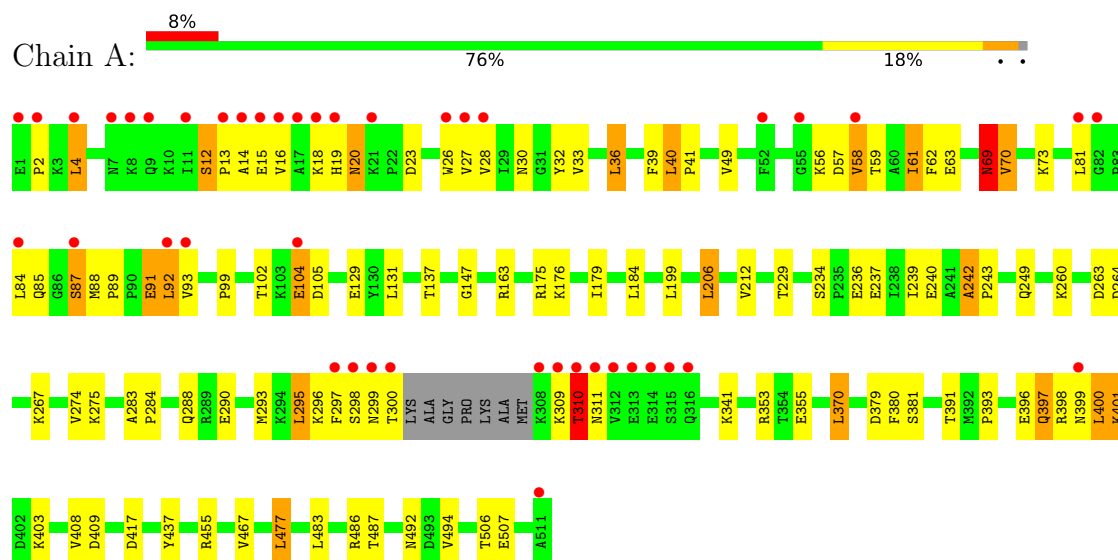
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	371	Total	O	0	0
			371	371		
7	B	247	Total	O	0	0
			247	247		

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: CYTOCHROME B2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.16Å 164.16Å 111.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	80.5 (30.00-2.30) 80.5 (30.00-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.29 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.170 , 0.211 0.163 , 0.205	Depositor DCC
R_{free} test set	6657 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7863	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MPD, FMN, PYR, PO4, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/4014 (0.0%)	1.22	35/5439 (0.6%)
1	B	0.74	6/3202 (0.2%)	1.22	32/4326 (0.7%)
All	All	0.68	7/7216 (0.1%)	1.22	67/9765 (0.7%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	GLU	C-N	9.84	1.46	1.33
1	B	311	ASN	C-N	-8.25	1.22	1.33
1	B	314	GLU	N-CA	8.14	1.56	1.46
1	B	313	GLU	C-N	-7.53	1.23	1.33
1	B	310	THR	C-N	-5.33	1.26	1.33
1	B	313	GLU	N-CA	-5.29	1.39	1.46
1	A	311	ASN	CA-C	5.13	1.58	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	THR	CA-C-O	-33.55	72.54	120.51
1	B	313	GLU	O-C-N	-28.54	84.63	122.59
1	A	310	THR	O-C-N	-20.09	95.87	122.59
1	B	310	THR	O-C-N	-11.74	106.98	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	LEU	N-CA-C	-10.37	100.65	113.20
1	B	100	GLY	N-CA-C	-9.61	100.25	116.01
1	A	381	SER	N-CA-C	-9.35	96.64	110.48
1	B	381	SER	N-CA-C	-8.86	97.36	110.48
1	B	312	VAL	O-C-N	8.86	133.65	122.57
1	A	70	VAL	N-CA-C	8.03	118.83	110.72
1	A	310	THR	N-CA-C	7.86	127.54	110.80
1	A	73	LYS	N-CA-C	7.75	120.62	111.71
1	B	314	GLU	O-C-N	7.43	132.48	122.59
1	A	391	THR	N-CA-C	7.32	119.04	111.14
1	A	370	LEU	N-CA-C	-7.20	99.01	109.59
1	A	487	THR	N-CA-C	7.09	121.05	109.85
1	B	242	ALA	CA-C-N	7.03	126.73	119.56
1	B	242	ALA	C-N-CA	7.03	126.73	119.56
1	A	87	SER	N-CA-C	6.87	115.34	108.75
1	A	62	PHE	N-CA-C	6.73	118.31	110.97
1	B	494	VAL	N-CA-C	6.62	117.11	110.23
1	B	490	VAL	N-CA-C	-6.54	102.94	109.02
1	A	12	SER	N-CA-C	6.46	119.64	110.40
1	B	486	ARG	N-CA-C	-6.30	98.27	108.41
1	B	391	THR	N-CA-C	6.26	117.90	111.14
1	B	311	ASN	O-C-N	-6.24	114.29	122.59
1	A	39	PHE	N-CA-C	6.21	117.85	111.14
1	B	199	LEU	N-CA-C	6.17	120.16	111.52
1	A	403	LYS	N-CA-C	-6.09	105.97	113.41
1	B	370	LEU	N-CA-C	-6.04	100.45	109.15
1	A	87	SER	CA-C-O	6.02	122.12	118.33
1	B	312	VAL	N-CA-C	6.01	121.84	109.34
1	B	313	GLU	CA-C-N	5.93	132.87	121.54
1	B	313	GLU	C-N-CA	5.93	132.87	121.54
1	A	69	ASN	N-CA-C	5.88	120.16	112.92
1	A	58	VAL	N-CA-C	5.86	117.74	112.17
1	A	290	GLU	N-CA-C	5.84	118.43	111.71
1	B	487	THR	N-CA-C	5.80	119.01	109.85
1	B	357	VAL	N-CA-C	-5.76	104.73	111.00
1	A	494	VAL	N-CA-C	5.64	115.77	110.30
1	A	87	SER	CB-CA-C	-5.58	108.33	116.53
1	A	61	ILE	N-CA-C	-5.53	106.31	111.45
1	A	147	GLY	N-CA-C	-5.49	103.63	111.42
1	A	417	ASP	N-CA-C	-5.46	105.41	111.36
1	B	229	THR	N-CA-C	-5.38	105.52	111.71
1	B	364	GLY	N-CA-C	5.38	123.45	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	LYS	N-CA-C	-5.37	103.05	110.35
1	A	12	SER	CA-C-N	5.36	126.54	119.84
1	A	12	SER	C-N-CA	5.36	126.54	119.84
1	B	290	GLU	N-CA-C	5.31	117.82	111.71
1	B	100	GLY	CA-C-O	5.30	123.75	118.77
1	B	123	ILE	N-CA-C	5.26	117.16	111.58
1	A	212	VAL	N-CA-C	-5.25	105.59	110.53
1	A	242	ALA	CA-C-N	5.25	124.86	119.56
1	A	242	ALA	C-N-CA	5.25	124.86	119.56
1	A	137	THR	N-CA-C	-5.24	103.61	110.53
1	A	199	LEU	N-CA-C	5.20	118.76	111.74
1	A	40	LEU	CA-C-N	-5.18	114.75	119.82
1	A	40	LEU	C-N-CA	-5.18	114.75	119.82
1	B	312	VAL	CB-CA-C	-5.15	102.85	111.29
1	B	481	SER	N-CA-C	5.11	118.61	112.38
1	A	274	VAL	N-CA-C	-5.09	104.46	110.21
1	B	479	ASP	N-CA-C	-5.06	99.03	107.99
1	A	105	ASP	N-CA-C	-5.05	105.69	111.14
1	B	204	ASN	CA-C-N	5.04	125.06	119.32
1	B	204	ASN	C-N-CA	5.04	125.06	119.32
1	B	218	GLN	N-CA-C	5.02	119.11	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	THR	Mainchain

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	3939	0	3956	84	1
1	B	3152	0	3206	49	1
2	A	43	0	30	8	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	56	3	0
4	B	8	0	14	0	0
5	B	3	0	0	0	2
6	B	6	0	0	0	0
7	A	371	0	0	6	0
7	B	247	0	0	4	0
All	All	7863	0	7300	134	3

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 9.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:THR:HB	7:B:1098:HOH:O	1.75	0.85
1:B:270:GLU:OE2	1:B:343:LYS:HG2	1.76	0.84
1:B:317:GLY:O	1:B:320:ARG:HG2	1.82	0.80
1:A:20:ASN:HD22	1:A:20:ASN:H	1.29	0.78
1:B:186:SER:HB3	1:B:248:ILE:HD11	1.66	0.77
1:B:399:ASN:C	1:B:401:LYS:H	1.92	0.76
1:A:28:VAL:CG2	1:A:57:ASP:HA	2.16	0.76
1:B:343:LYS:N	1:B:343:LYS:HD3	2.02	0.75
1:B:313:GLU:O	1:B:314:GLU:CB	2.33	0.74
1:A:355:GLU:HG2	4:A:702:MPD:H51	1.69	0.73
1:A:396:GLU:C	1:A:398:ARG:H	1.95	0.73
1:A:58:VAL:HG21	2:A:760:HEM:HBC1	1.71	0.73
1:B:235:PRO:HG2	1:B:236:GLU:OE1	1.90	0.71
1:A:28:VAL:HG22	1:A:57:ASP:HA	1.75	0.68
1:A:49:VAL:HG21	2:A:760:HEM:HMD3	1.76	0.67
1:A:16:VAL:HB	1:A:88:MET:HE1	1.77	0.66
1:B:136:LEU:HD21	1:B:440:SER:HB3	1.75	0.66
1:A:399:ASN:O	1:A:401:LYS:N	2.29	0.65
1:A:19:HIS:HB2	1:A:26:TRP:HB2	1.77	0.65
1:B:399:ASN:C	1:B:401:LYS:N	2.55	0.64
1:A:58:VAL:CG2	1:A:61:ILE:HD12	2.29	0.62
1:B:396:GLU:C	1:B:398:ARG:H	2.07	0.61
1:A:263:ASP:OD1	4:A:701:MPD:H51	2.00	0.61
1:B:99:PRO:HA	7:B:1073:HOH:O	1.98	0.61
1:A:58:VAL:HG23	1:A:61:ILE:HD12	1.81	0.61
1:A:89:PRO:HB3	1:A:91:GLU:OE2	2.01	0.60
1:B:396:GLU:HG2	1:B:401:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:CB	1:B:248:ILE:HD11	2.31	0.59
1:B:379:ASP:O	1:B:380:PHE:HB2	2.01	0.59
1:A:40:LEU:HG	1:A:41:PRO:HD3	1.84	0.58
1:A:396:GLU:C	1:A:398:ARG:N	2.62	0.58
1:A:56:LYS:HE3	7:A:1132:HOH:O	2.04	0.57
1:A:93:VAL:O	1:A:93:VAL:HG23	2.05	0.57
1:A:28:VAL:HG23	1:A:57:ASP:HA	1.87	0.57
1:B:343:LYS:N	1:B:343:LYS:CD	2.65	0.57
1:A:63:GLU:HG3	7:A:1086:HOH:O	2.03	0.56
1:A:36:LEU:O	1:A:40:LEU:HD23	2.05	0.56
1:A:102:THR:OG1	1:A:104[B]:GLU:HG2	2.05	0.56
1:B:129:GLU:HG3	1:B:437:TYR:CE2	2.41	0.55
1:B:230:LEU:HD21	1:B:325:PHE:CE2	2.41	0.55
1:A:2:PRO:HB2	1:A:4:LEU:CD2	2.37	0.55
1:A:26:TRP:CE2	1:A:81:LEU:HD11	2.42	0.54
1:A:20:ASN:HD22	1:A:20:ASN:N	1.96	0.53
1:B:405:GLU:HG2	1:B:427:LYS:HD3	1.90	0.53
1:B:310:THR:O	1:B:311:ASN:CG	2.51	0.53
1:A:129:GLU:HG3	1:A:437:TYR:CE2	2.44	0.53
1:B:370:LEU:HB2	1:B:408:VAL:HG12	1.90	0.53
1:A:89:PRO:HB2	1:A:92:LEU:HB2	1.91	0.52
1:B:400:LEU:HA	1:B:403:LYS:HG2	1.90	0.52
1:A:234:SER:OG	1:A:237:GLU:HG2	2.10	0.52
1:A:33:VAL:HG12	1:A:81:LEU:HD12	1.92	0.51
1:A:260:LYS:HE2	1:A:264:ASP:OD1	2.10	0.51
1:A:16:VAL:C	1:A:18:LYS:N	2.69	0.51
1:A:239:ILE:HA	1:A:249:GLN:HE22	1.76	0.51
1:B:310:THR:O	1:B:311:ASN:ND2	2.44	0.51
1:A:396:GLU:O	1:A:398:ARG:N	2.44	0.50
1:B:329:SER:O	1:B:331:THR:HG23	2.12	0.50
1:B:234:SER:OG	1:B:237:GLU:HG2	2.12	0.50
1:A:296:LYS:HE2	7:A:1081:HOH:O	2.12	0.49
1:A:370:LEU:HB2	1:A:408:VAL:HG12	1.92	0.49
1:B:467:VAL:HG11	1:B:477:LEU:HD21	1.94	0.49
1:A:20:ASN:H	1:A:20:ASN:ND2	2.04	0.49
1:A:398:ARG:C	1:A:400:LEU:H	2.21	0.49
1:B:506:THR:CB	7:B:1098:HOH:O	2.46	0.49
1:A:49:VAL:HG21	2:A:760:HEM:CMD	2.42	0.49
1:A:58:VAL:HG21	2:A:760:HEM:CBC	2.42	0.49
1:A:299:ASN:O	1:A:300:THR:C	2.56	0.48
1:A:206:LEU:HB2	7:A:1033:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASP:O	1:A:380:PHE:HB2	2.13	0.48
1:A:2:PRO:HB2	1:A:4:LEU:HD21	1.94	0.48
1:A:20:ASN:N	1:A:20:ASN:ND2	2.62	0.48
1:A:12:SER:C	1:A:14:ALA:H	2.22	0.48
7:A:847:HOH:O	1:B:491:PRO:HD3	2.13	0.47
1:B:433:ARG:HG3	3:B:870:FMN:O1P	2.14	0.47
1:A:19:HIS:CD2	1:A:19:HIS:N	2.82	0.47
1:A:70:VAL:HB	2:A:760:HEM:HMB2	1.96	0.47
1:A:288[A]:GLN:HG3	1:A:293:MET:SD	2.55	0.47
1:A:33:VAL:CG1	1:A:81:LEU:HD12	2.43	0.47
1:A:275:LYS:NZ	7:A:1063:HOH:O	2.45	0.47
1:A:297:PHE:C	1:A:299:ASN:N	2.73	0.47
1:A:399:ASN:C	1:A:401:LYS:N	2.71	0.47
1:A:263:ASP:OD2	1:A:267:LYS:HE2	2.14	0.47
1:A:30:ASN:ND2	1:A:59:THR:HG21	2.30	0.47
1:A:399:ASN:C	1:A:401:LYS:H	2.23	0.47
1:B:283:ALA:HA	1:B:377:GLN:NE2	2.30	0.46
1:B:179:ILE:HD11	1:B:455:ARG:HG3	1.98	0.46
1:B:342:THR:C	1:B:343:LYS:HD3	2.41	0.46
1:B:347:VAL:HG13	1:B:367:GLY:C	2.41	0.46
1:B:454:LEU:O	1:B:458:ILE:HG13	2.16	0.46
1:A:16:VAL:C	1:A:18:LYS:H	2.24	0.45
1:A:70:VAL:HB	2:A:760:HEM:CMB	2.46	0.45
1:A:297:PHE:C	1:A:299:ASN:H	2.24	0.45
1:A:467:VAL:HG11	1:A:477:LEU:HD21	1.99	0.45
1:B:256:ASN:O	1:B:259:ARG:HD3	2.17	0.45
1:A:57:ASP:HB3	1:A:93:VAL:HG12	1.98	0.45
1:A:4:LEU:HB3	1:A:32:TYR:CZ	2.52	0.44
1:A:99:PRO:HB2	1:A:295:LEU:HD13	1.98	0.44
1:A:40:LEU:HG	1:A:41:PRO:CD	2.47	0.44
1:B:397:GLN:C	1:B:398:ARG:HG3	2.43	0.44
1:A:393:PRO:O	1:A:397:GLN:HG3	2.17	0.44
1:B:396:GLU:C	1:B:398:ARG:N	2.73	0.44
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.99	0.44
1:A:16:VAL:O	1:A:18:LYS:N	2.51	0.43
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.81	0.43
1:A:23:ASP:OD1	1:A:23:ASP:N	2.51	0.43
1:A:88:MET:O	1:A:89:PRO:C	2.61	0.43
1:B:116:LEU:CD2	1:B:131:LEU:HG	2.48	0.43
1:A:27:VAL:CG1	1:A:36:LEU:HD22	2.48	0.43
1:A:353:ARG:HH22	4:A:702:MPD:HM1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:HA	1:B:243:PRO:HD3	1.81	0.43
1:A:506:THR:HB	7:B:1099:HOH:O	2.19	0.42
1:B:102:THR:HG23	1:B:105:ASP:OD2	2.19	0.42
1:A:58:VAL:HG22	1:A:61:ILE:HB	2.02	0.42
1:A:179:ILE:HD11	1:A:455:ARG:HG3	2.01	0.42
1:A:93:VAL:O	1:A:93:VAL:CG2	2.68	0.42
1:B:111:GLN:HE21	1:B:111:GLN:HB3	1.56	0.42
1:B:510:ASP:O	1:B:511:ALA:OXT	2.37	0.42
1:A:163:ARG:NH2	1:A:486:ARG:HG3	2.35	0.41
1:A:283:ALA:N	1:A:284:PRO:CD	2.84	0.41
1:A:27:VAL:HG12	1:A:36:LEU:HD22	2.02	0.41
1:A:297:PHE:O	1:A:299:ASN:N	2.54	0.41
1:A:409:ASP:OD1	1:A:409:ASP:C	2.64	0.41
1:A:58:VAL:CG2	2:A:760:HEM:HBC1	2.47	0.41
1:A:84:LEU:HG	1:A:85:GLN:N	2.35	0.41
1:A:87:SER:O	1:A:88:MET:HG2	2.19	0.41
1:A:242:ALA:HA	1:A:243:PRO:HD3	1.89	0.41
1:B:286:LEU:HD22	1:B:286:LEU:HA	1.89	0.41
1:B:492:ASN:OD1	1:B:497:ASN:ND2	2.54	0.41
1:B:392:MET:HB2	1:B:393:PRO:HD3	2.02	0.40
1:A:69:ASN:N	1:A:69:ASN:HD22	2.19	0.40
1:B:119:LEU:HD13	1:B:442:TYR:CG	2.57	0.40
1:B:399:ASN:O	1:B:399:ASN:CG	2.64	0.40
2:A:760:HEM:HBC2	2:A:760:HEM:HHD	2.02	0.40
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.87	0.40

All (3) 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)
5:B:900:PO4:P	5:B:900:PO4:O1[4_555]	1.53	0.67
5:B:900:PO4:P	5:B:900:PO4:O2[4_555]	1.57	0.63
1:A:341:LYS:O	1:B:312:VAL:CG1[3_665]	1.92	0.28

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	504/511 (99%)	465 (92%)	33 (6%)	6 (1%)	10	12
1	B	401/511 (78%)	378 (94%)	16 (4%)	7 (2%)	7	7
All	All	905/1022 (89%)	843 (93%)	49 (5%)	13 (1%)	9	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	THR
1	A	400	LEU
1	B	312	VAL
1	B	313	GLU
1	B	314	GLU
1	A	397	GLN
1	B	310	THR
1	B	311	ASN
1	A	309	LYS
1	B	397	GLN
1	B	399	ASN
1	A	298	SER
1	A	13	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/440 (98%)	411 (95%)	22 (5%)	21	32
1	B	348/440 (79%)	330 (95%)	18 (5%)	21	31
All	All	781/880 (89%)	741 (95%)	40 (5%)	22	32

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	15	GLU
1	A	20	ASN
1	A	36	LEU
1	A	69	ASN
1	A	91	GLU
1	A	92	LEU
1	A	104[A]	GLU
1	A	104[B]	GLU
1	A	131	LEU
1	A	175	ARG
1	A	184	LEU
1	A	206	LEU
1	A	229	THR
1	A	236	GLU
1	A	240	GLU
1	A	295	LEU
1	A	477	LEU
1	A	483	LEU
1	A	492[A]	ASN
1	A	492[B]	ASN
1	A	507	GLU
1	B	105	ASP
1	B	111	GLN
1	B	131	LEU
1	B	184	LEU
1	B	206	LEU
1	B	229	THR
1	B	236	GLU
1	B	240	GLU
1	B	260	LYS
1	B	286	LEU
1	B	295	LEU
1	B	312	VAL
1	B	316	GLN
1	B	343	LYS
1	B	402	ASP
1	B	477	LEU
1	B	483	LEU
1	B	507	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	30	ASN
1	A	47	GLN
1	A	53	ASN
1	A	69	ASN
1	A	85	GLN
1	A	111	GLN
1	A	159	ASN
1	A	225	GLN
1	A	249	GLN
1	A	316	GLN
1	A	397	GLN
1	B	111	GLN
1	B	149	ASN
1	B	159	ASN
1	B	225	GLN
1	B	311	ASN
1	B	316	GLN
1	B	397	GLN
1	B	399	ASN

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 ⓘ

10 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	FMN	B	870	-	33,33,33	1.44	8 (24%)	48,50,50	1.07	3 (6%)
4	MPD	A	703	-	7,7,7	0.47	0	9,10,10	0.58	0
4	MPD	A	704	-	7,7,7	0.55	0	9,10,10	0.56	0
3	FMN	A	770	-	33,33,33	1.49	5 (15%)	48,50,50	0.99	2 (4%)
5	PO4	B	900	-	0,2,4	-	-	0,1,6	-	-
4	MPD	B	801	-	7,7,7	0.60	0	9,10,10	0.44	0
4	MPD	A	701	-	7,7,7	0.50	0	9,10,10	0.58	0
4	MPD	A	702	-	7,7,7	0.45	0	9,10,10	0.52	0
6	PYR	B	800	-	5,5,5	3.04	1 (20%)	3,6,6	1.60	1 (33%)
2	HEM	A	760	1	50,50,50	1.59	10 (20%)	67,82,82	1.43	9 (13%)

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	FMN	B	870	-	-	6/18/18/18	0/3/3/3
4	MPD	A	703	-	-	1/5/5/5	-
4	MPD	A	704	-	-	2/5/5/5	-
3	FMN	A	770	-	-	7/18/18/18	0/3/3/3
4	MPD	B	801	-	-	2/5/5/5	-
4	MPD	A	701	-	-	0/5/5/5	-
4	MPD	A	702	-	-	2/5/5/5	-
6	PYR	B	800	-	-	4/4/4/4	-
2	HEM	A	760	1	-	7/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	PYR	CA-C	-6.25	1.33	1.54
3	A	770	FMN	C4A-N5	3.76	1.38	1.30
3	A	770	FMN	C9A-C5A	3.54	1.46	1.41
2	A	760	HEM	CBC-CAC	3.42	1.46	1.30
2	A	760	HEM	C3C-C4C	3.25	1.51	1.46
2	A	760	HEM	FE-NA	3.04	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	870	FMN	C4A-N5	2.86	1.36	1.30
2	A	760	HEM	CHA-C4D	2.82	1.44	1.38
3	B	870	FMN	C9A-C5A	2.70	1.45	1.41
3	B	870	FMN	C1'-C2'	2.69	1.56	1.52
3	B	870	FMN	C10-N1	2.58	1.38	1.33
3	A	770	FMN	C6-C5A	2.54	1.43	1.40
2	A	760	HEM	C4A-NA	2.41	1.44	1.39
2	A	760	HEM	CBB-CAB	2.39	1.41	1.30
2	A	760	HEM	FE-NC	2.35	2.02	1.95
2	A	760	HEM	C1D-ND	2.28	1.43	1.38
3	A	770	FMN	C9-C9A	2.16	1.43	1.39
3	A	770	FMN	C9A-N10	2.15	1.44	1.41
2	A	760	HEM	C4A-C3A	2.13	1.48	1.43
3	B	870	FMN	C6-C5A	2.07	1.43	1.40
2	A	760	HEM	CMC-C2C	2.07	1.55	1.50
3	B	870	FMN	C8-C7	2.06	1.45	1.40
3	B	870	FMN	C2-N3	2.01	1.43	1.39
3	B	870	FMN	C10-N10	2.00	1.41	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CAC-C3C-C4C	3.37	132.85	124.82
2	A	760	HEM	CMD-C2D-C1D	3.25	130.11	125.03
2	A	760	HEM	CAD-C3D-C2D	-3.07	122.11	127.87
2	A	760	HEM	C4C-C3C-C2C	-3.03	104.19	106.81
2	A	760	HEM	C3B-C4B-NB	2.89	111.55	109.47
2	A	760	HEM	CHD-C4C-NC	-2.87	121.32	124.45
3	A	770	FMN	C10-N1-C2	2.85	123.02	116.85
2	A	760	HEM	C4D-C3D-C2D	2.70	110.83	106.89
3	B	870	FMN	C10-N1-C2	2.68	122.65	116.85
2	A	760	HEM	C1D-C2D-C3D	-2.41	104.45	106.98
2	A	760	HEM	C2D-C1D-ND	2.37	112.64	109.90
6	B	800	PYR	OXT-C-CA	2.32	120.02	113.59
3	B	870	FMN	C5A-N5-C4A	2.28	121.78	118.09
3	B	870	FMN	C9A-C5A-N5	-2.21	120.11	122.45
3	A	770	FMN	C9A-C5A-N5	-2.03	120.31	122.45

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	760	HEM	C2B-C3B-CAB-CBB
3	A	770	FMN	C5'-O5'-P-O1P
6	B	800	PYR	O-C-CA-O3
6	B	800	PYR	O-C-CA-CB
6	B	800	PYR	OXT-C-CA-O3
3	A	770	FMN	C2'-C3'-C4'-O4'
3	B	870	FMN	C2'-C3'-C4'-O4'
3	A	770	FMN	O3'-C3'-C4'-O4'
3	B	870	FMN	C5'-O5'-P-O1P
3	B	870	FMN	C4'-C5'-O5'-P
2	A	760	HEM	C4B-C3B-CAB-CBB
2	A	760	HEM	C4C-C3C-CAC-CBC
3	A	770	FMN	O3'-C3'-C4'-C5'
3	A	770	FMN	C2'-C3'-C4'-C5'
6	B	800	PYR	OXT-C-CA-CB
3	A	770	FMN	C4'-C5'-O5'-P
3	B	870	FMN	O3'-C3'-C4'-O4'
2	A	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAD-CBD-CGD-O2D
2	A	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAD-CBD-CGD-O1D
3	A	770	FMN	C5'-O5'-P-O3P
4	A	704	MPD	O2-C2-C3-C4
3	B	870	FMN	O3'-C3'-C4'-C5'
4	A	702	MPD	C1-C2-C3-C4
4	A	702	MPD	CM-C2-C3-C4
4	A	703	MPD	C1-C2-C3-C4
4	A	704	MPD	C1-C2-C3-C4
4	B	801	MPD	C1-C2-C3-C4
4	B	801	MPD	CM-C2-C3-C4
3	B	870	FMN	C2'-C3'-C4'-C5'

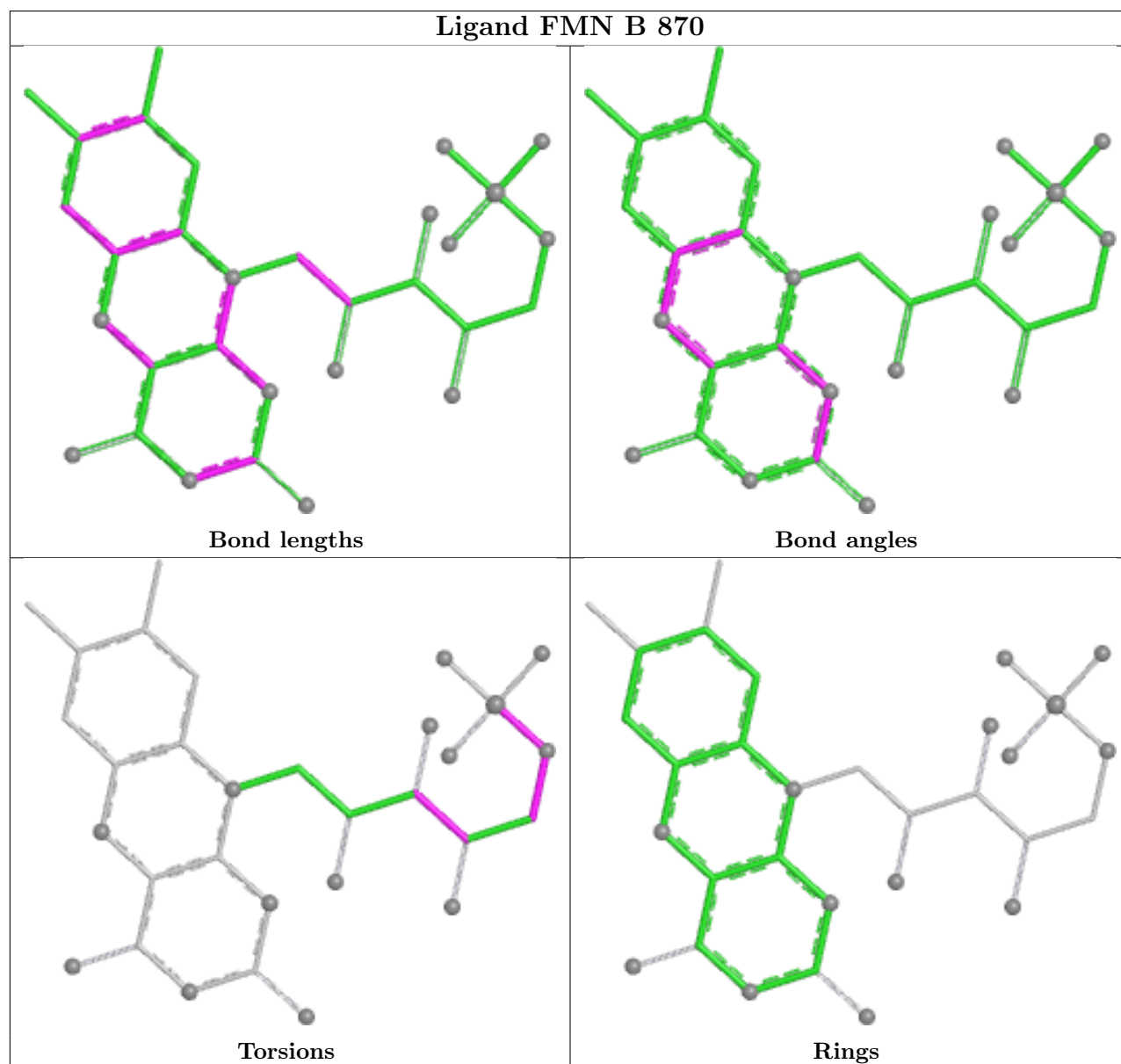
There are no ring outliers.

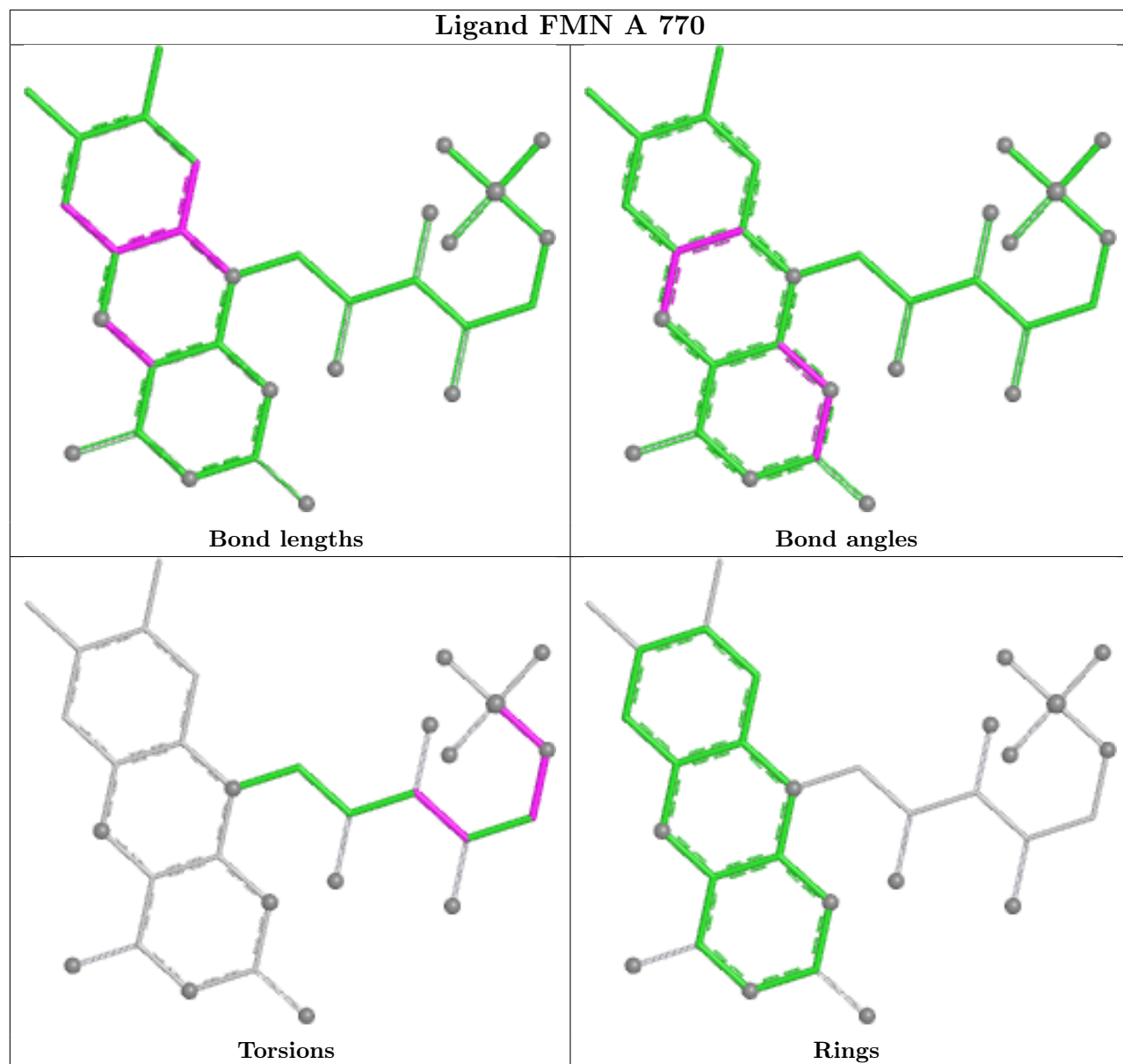
5 monomers are involved in 14 short contacts:

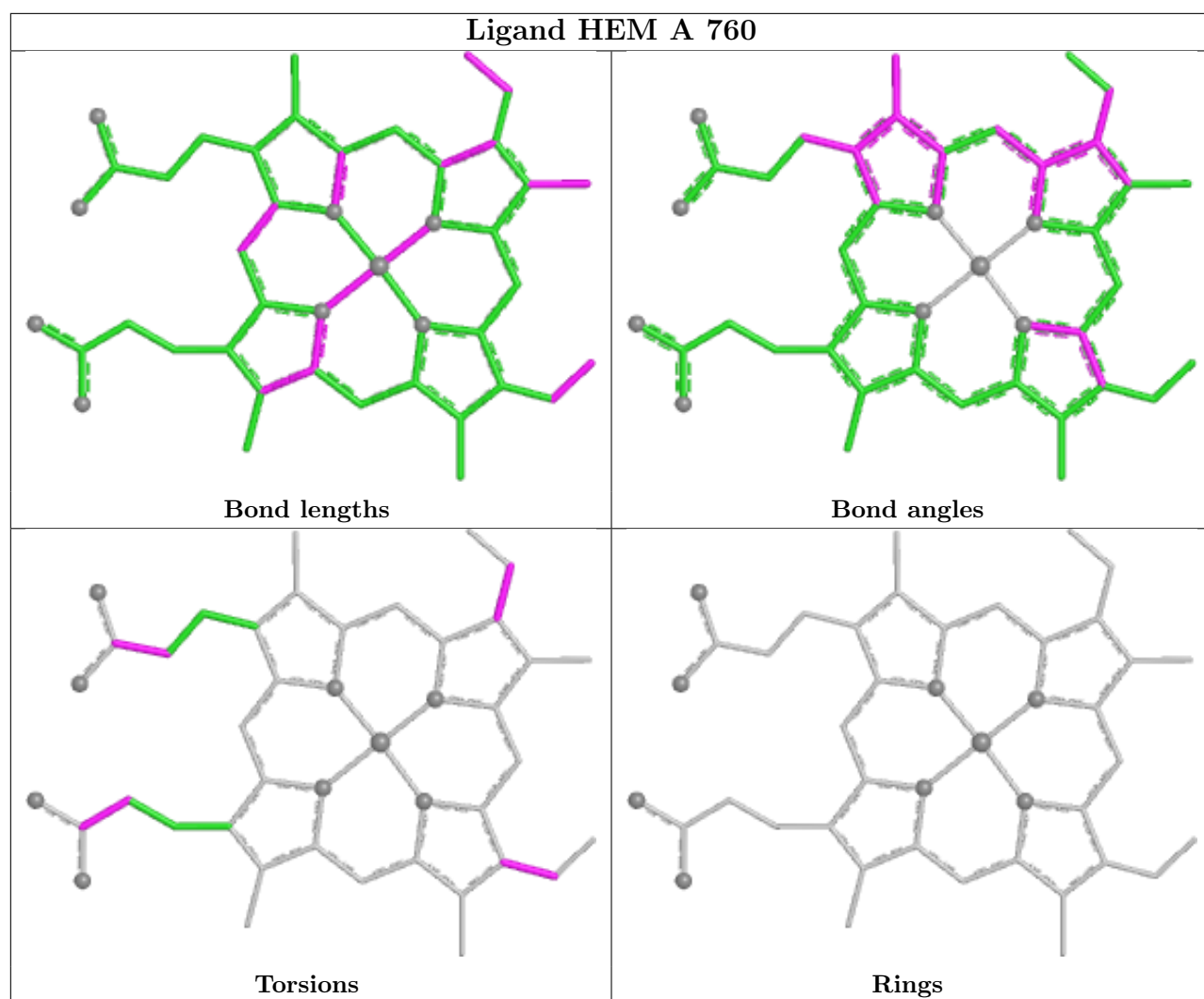
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	870	FMN	1	0
5	B	900	PO4	0	2
4	A	701	MPD	1	0
4	A	702	MPD	2	0
2	A	760	HEM	8	0

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	504/511 (98%)	-0.12	43 (8%)	16 18	11, 29, 83, 99	4 (0%)
1	B	405/511 (79%)	-0.20	19 (4%)	36 38	17, 29, 70, 99	0
All	All	909/1022 (88%)	-0.16	62 (6%)	23 25	11, 29, 80, 99	4 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	THR	9.3
1	A	310	THR	7.6
1	B	311	ASN	6.1
1	B	300	THR	5.2
1	A	315	SER	4.9
1	B	325	PHE	4.7
1	A	312	VAL	4.7
1	B	312	VAL	4.7
1	A	309	LYS	4.5
1	B	99	PRO	4.4
1	A	311	ASN	4.2
1	B	314	GLU	4.0
1	A	308	LYS	3.9
1	A	17	ALA	3.7
1	A	511	ALA	3.5
1	A	16	VAL	3.4
1	A	8	LYS	3.3
1	A	15	GLU	3.2
1	B	313	GLU	3.2
1	A	313	GLU	3.2
1	A	11	ILE	3.2
1	A	104[A]	GLU	3.1
1	B	299	ASN	3.1
1	A	298	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	3.0
1	A	300	THR	3.0
1	A	52	PHE	3.0
1	B	309	LYS	2.9
1	A	9	GLN	2.9
1	A	87	SER	2.8
1	A	297	PHE	2.8
1	A	314	GLU	2.8
1	A	26	TRP	2.7
1	B	315	SER	2.7
1	A	13	PRO	2.7
1	A	18	LYS	2.7
1	A	14	ALA	2.6
1	B	399	ASN	2.6
1	A	299	ASN	2.6
1	A	55	GLY	2.6
1	A	19	HIS	2.6
1	A	21	LYS	2.6
1	B	511	ALA	2.5
1	A	92	LEU	2.4
1	B	103	LYS	2.4
1	B	246	LYS	2.4
1	A	58	VAL	2.4
1	A	399	ASN	2.3
1	B	100	GLY	2.3
1	A	93	VAL	2.3
1	A	316	GLN	2.2
1	A	82	GLY	2.2
1	B	316	GLN	2.2
1	B	298	SER	2.2
1	A	7	ASN	2.1
1	A	27	VAL	2.1
1	A	28	VAL	2.1
1	A	1	GLU	2.1
1	B	297	PHE	2.1
1	A	4	LEU	2.1
1	A	84	LEU	2.1
1	A	2	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

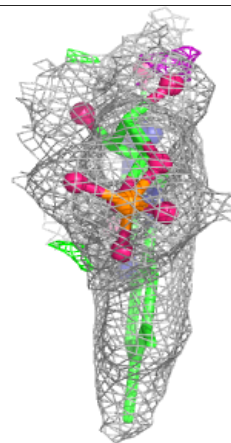
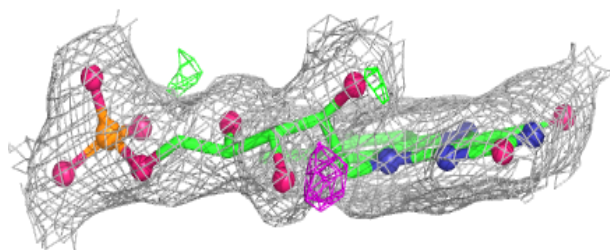
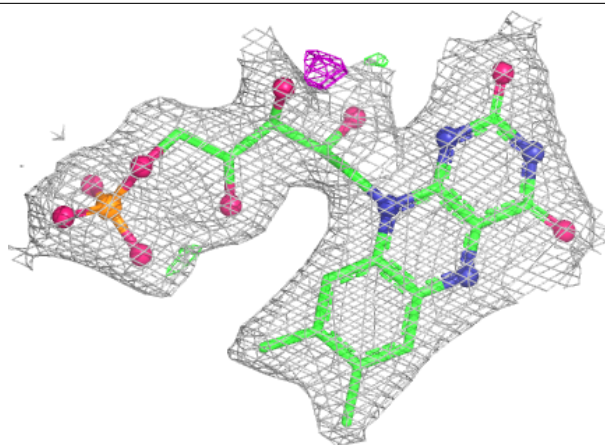
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MPD	A	702	8/8	0.76	0.28	80,82,84,84	0
4	MPD	A	704	8/8	0.81	0.28	96,96,99,99	0
4	MPD	A	703	8/8	0.82	0.23	91,91,92,92	0
5	PO4	B	900	3/5	0.92	0.14	65,65,68,72	1
4	MPD	B	801	8/8	0.93	0.15	70,72,72,73	0
4	MPD	A	701	8/8	0.93	0.12	39,43,52,54	0
6	PYR	B	800	6/6	0.94	0.13	41,45,51,52	0
3	FMN	A	770	31/31	0.98	0.05	15,19,24,26	0
2	HEM	A	760	43/43	0.98	0.06	21,28,34,39	0
3	FMN	B	870	31/31	0.99	0.04	18,23,27,29	0

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

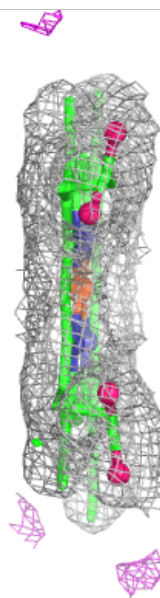
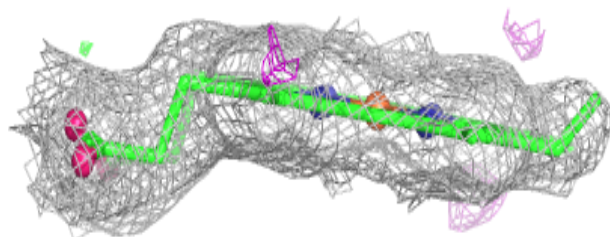
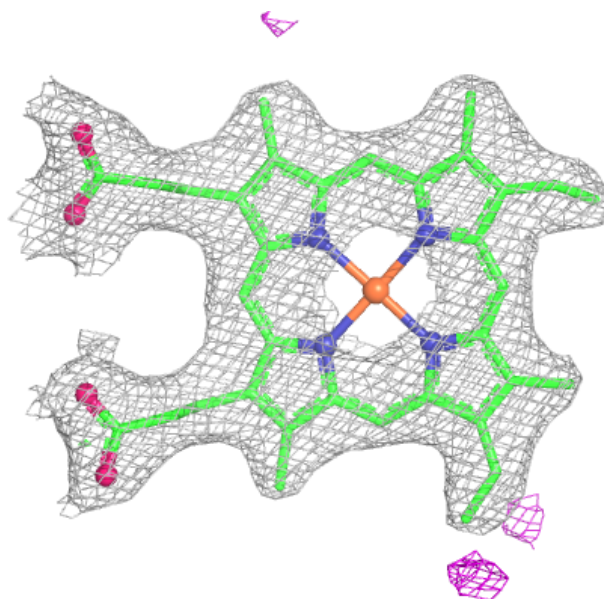
Electron density around FMN A 770:

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



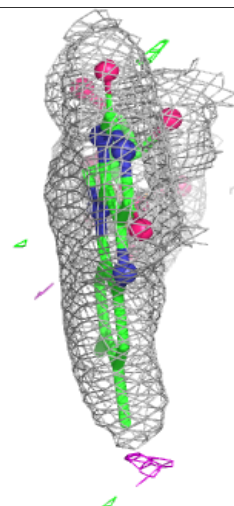
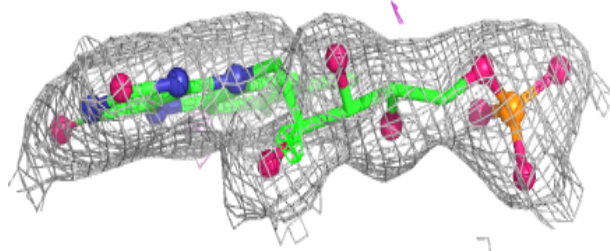
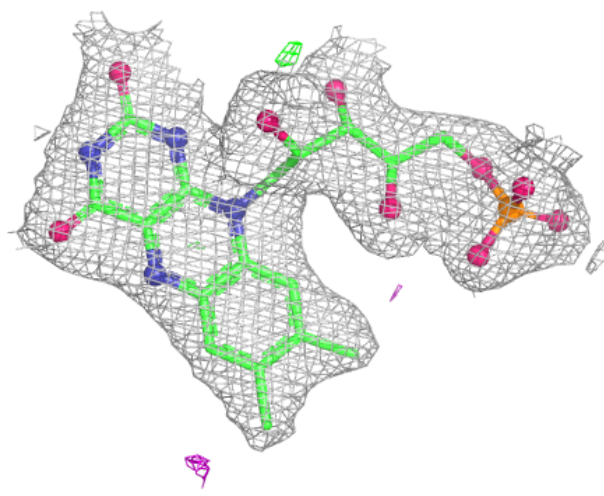
Electron density around HEM A 760:

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



Electron density around FMN B 870:

$2mF_o-DF_c$ (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.