



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:29 PM EDT

PDB ID : 1SZF
Title : A198G:L230A mutant flavocytochrome b2 with pyruvate bound
Authors : Mowat, C.G.; Wehenkel, A.; Green, A.J.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2004-04-05
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

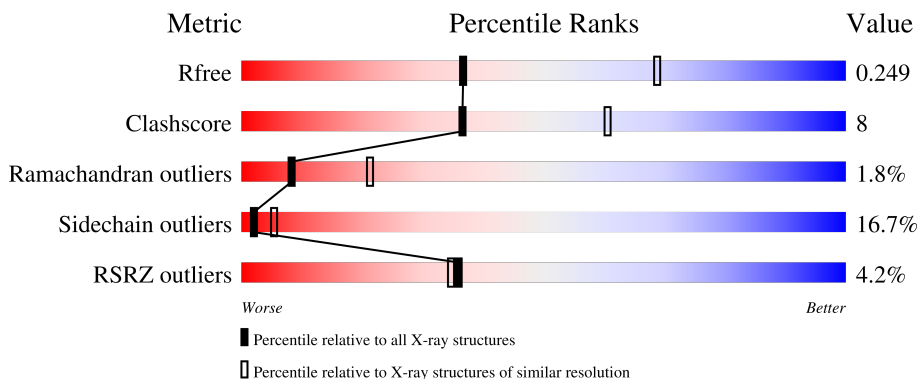
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>16%</div> <div>• •</div> <div>23%</div> </div> </div>
1	B	511	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>21%</div> <div>•</div> <div>24%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6334 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.

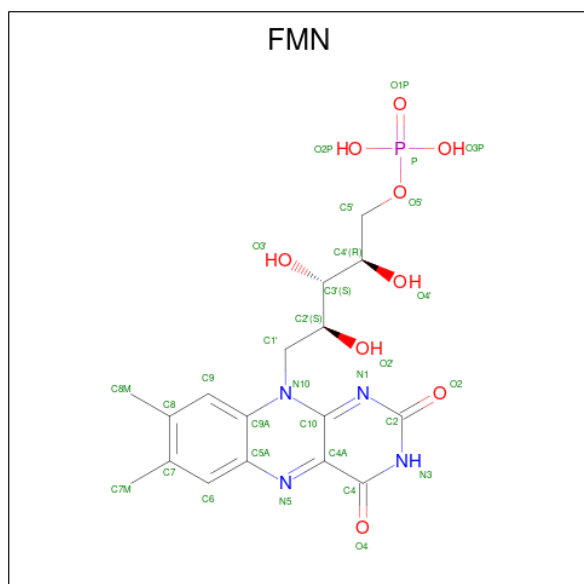
- Molecule 1 is a protein called Cytochrome b2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3061	1939	523	588	11			
1	B	389	Total	C	N	O	S	0	0	0
			3029	1923	514	581	11			

There are 4 discrepancies between the modelled and reference sequences:

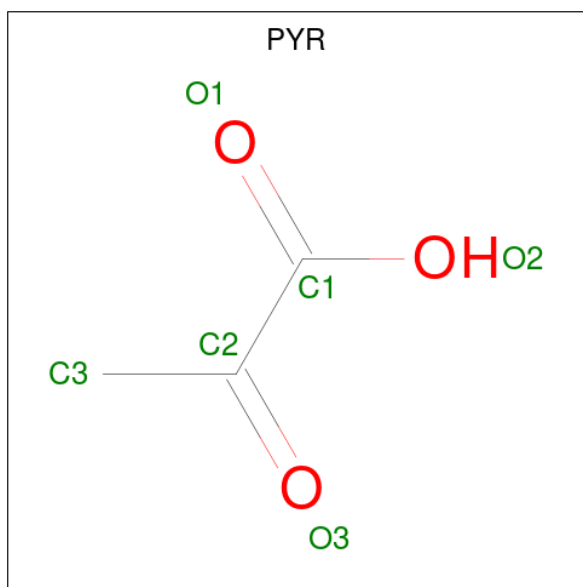
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	GLY	ALA	engineered mutation	UNP P00175
A	230	ALA	LEU	engineered mutation	UNP P00175
B	198	GLY	ALA	engineered mutation	UNP P00175
B	230	ALA	LEU	engineered mutation	UNP P00175

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).

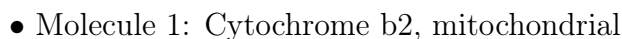


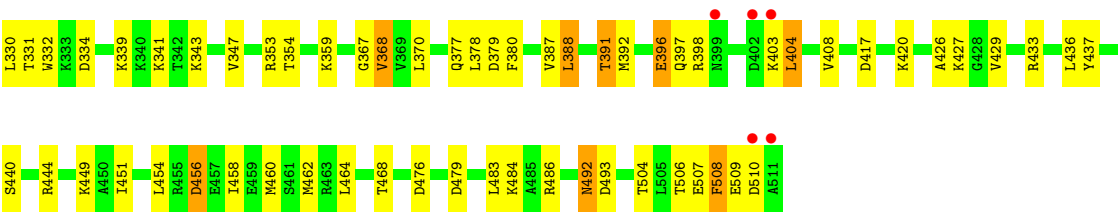
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	77	Total	O	0	0
			77	77		

- Molecule 1: Cytochrome b2, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.41Å 163.41Å 112.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.00 – 2.70 23.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.00-2.70) 99.6 (23.83-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.220 , 0.253 0.219 , 0.249	Depositor DCC
R_{free} test set	2407 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6334	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: PYR, 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	0.52	1/3110 (0.0%)	0.85	9/4201 (0.2%)
1	B	0.57	3/3078 (0.1%)	0.83	13/4159 (0.3%)
All	All	0.54	4/6188 (0.1%)	0.84	22/8360 (0.3%)

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	1	3
1	B	0	1
All	All	1	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	GLU	CD-OE1	12.45	1.39	1.25
1	B	240	GLU	CD-OE2	5.81	1.32	1.25
1	B	103	LYS	CE-NZ	5.67	1.63	1.49
1	A	103	LYS	CE-NZ	5.22	1.62	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	112	LEU	CA-CB-CG	7.02	131.45	115.30
1	A	334	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	327	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	379	ASP	CB-CG-OD2	6.21	123.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	127	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	211	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	104	GLU	N-CA-C	-5.69	95.63	111.00
1	A	263	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	456	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	292	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	334	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	476	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	263	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	479	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	211	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	417	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	189	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	245	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	178	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	379	ASP	CB-CG-OD2	5.02	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	492	ASN	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	LYS	Peptide
1	A	104	GLU	Peptide
1	A	114	SER	Peptide
1	B	506	THR	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	3061	0	3107	43	0
1	B	3029	0	3086	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	19	0	0
2	B	31	0	18	1	0
3	A	6	0	3	0	0
3	B	6	0	3	0	0
4	A	93	0	0	0	0
4	B	77	0	0	0	0
All	All	6334	0	6236	98	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 8.

All (98) 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:113:LYS:O	1:A:115:LEU:N	1.83	1.09
1:A:197:THR:HG21	1:A:436:LEU:HD21	1.46	0.97
1:A:256:ASN:HD22	1:A:258:ASP:H	1.20	0.87
1:B:100:GLY:O	1:B:101:GLU:HG2	1.78	0.84
1:B:507:GLU:O	1:B:508:PHE:HB2	1.77	0.84
1:B:492:ASN:HD22	1:B:493:ASP:H	1.27	0.80
1:B:113:LYS:O	1:B:115:LEU:N	2.19	0.76
1:B:108:ARG:HH11	1:B:108:ARG:HG2	1.52	0.74
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.17	0.73
1:A:507:GLU:O	1:A:508:PHE:HB2	1.90	0.72
1:B:256:ASN:HD22	1:B:258:ASP:H	1.36	0.71
1:B:108:ARG:O	1:B:112:LEU:HD23	1.91	0.70
1:B:456:ASP:O	1:B:460:MET:HG3	1.92	0.69
1:A:197:THR:HG21	1:A:436:LEU:CD2	2.22	0.69
1:B:387:VAL:O	1:B:391:THR:HG23	1.93	0.68
1:B:197:THR:O	1:B:197:THR:HG23	1.94	0.67
1:A:113:LYS:C	1:A:115:LEU:H	1.92	0.66
1:B:197:THR:O	1:B:197:THR:CG2	2.44	0.65
1:A:188:VAL:HG12	1:A:190:VAL:H	1.64	0.63
1:B:110:GLU:O	1:B:113:LYS:HB3	1.99	0.62
1:A:248:ILE:HD11	1:A:250:TRP:CE2	2.36	0.61
1:B:102:THR:C	1:B:104:GLU:H	2.03	0.60
1:A:351:VAL:HG21	1:A:368:VAL:HG22	1.82	0.60
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.65	0.60
1:B:112:LEU:HD22	1:B:135:THR:HB	1.84	0.60
1:B:354:THR:HG23	1:B:391:THR:HB	1.84	0.59
1:A:211:ASP:HB3	1:A:439:ASN:HD21	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLY:H	1:B:377:GLN:HE22	1.50	0.59
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.18	0.58
1:A:243:PRO:HD2	1:A:247:GLN:OE1	2.04	0.57
1:B:255:VAL:HG13	1:B:330:LEU:HD11	1.87	0.57
1:A:467:VAL:HG11	1:A:477:LEU:HD21	1.87	0.57
1:A:218:GLN:HE22	1:A:444:ARG:HD2	1.70	0.56
1:B:454:LEU:O	1:B:458:ILE:HG13	2.06	0.56
1:B:108:ARG:HH12	1:B:137:THR:HA	1.71	0.56
1:B:177:VAL:HG22	1:B:468:THR:HA	1.88	0.55
1:A:104:GLU:H	1:A:106:ILE:H	1.53	0.55
1:A:190:VAL:HG13	1:A:192:PHE:H	1.72	0.55
1:B:287:GLY:H	1:B:377:GLN:NE2	2.05	0.54
1:B:113:LYS:C	1:B:115:LEU:N	2.61	0.54
1:B:102:THR:O	1:B:104:GLU:N	2.35	0.54
1:A:372:ASN:ND2	1:A:375:GLY:H	2.07	0.53
1:B:347:VAL:HG13	1:B:368:VAL:N	2.24	0.53
1:B:100:GLY:O	1:B:101:GLU:CG	2.52	0.53
1:A:388:LEU:HD22	1:A:392:MET:HG2	1.91	0.52
1:A:256:ASN:ND2	1:A:258:ASP:H	1.97	0.52
1:B:331:THR:HG22	1:B:332:TRP:N	2.25	0.52
1:B:388:LEU:HD11	1:B:426:ALA:HB2	1.92	0.52
1:B:113:LYS:C	1:B:115:LEU:H	2.12	0.52
1:B:119:LEU:HD22	1:B:449:LYS:HG2	1.92	0.52
1:B:102:THR:C	1:B:104:GLU:N	2.63	0.51
1:B:113:LYS:HG2	1:B:114:SER:N	2.26	0.50
1:B:218:GLN:HE22	1:B:444:ARG:HH11	1.57	0.50
1:A:339:LYS:HE3	1:A:364:GLY:O	2.11	0.50
1:B:136:LEU:HD21	1:B:440:SER:HB3	1.94	0.49
1:A:124:ASN:ND2	1:A:126:TYR:HB2	2.28	0.49
1:B:223:VAL:HG21	1:B:451:ILE:HG12	1.94	0.49
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.95	0.49
1:A:136:LEU:HD21	1:A:440:SER:HB3	1.93	0.48
1:A:102:THR:O	1:A:102:THR:HG22	2.13	0.48
1:A:190:VAL:HG11	1:A:223:VAL:HG22	1.94	0.48
1:A:137:THR:HG22	1:A:140:ALA:H	1.78	0.48
1:A:188:VAL:HG12	1:A:190:VAL:O	2.14	0.48
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.28	0.47
1:A:283:ALA:N	1:A:284:PRO:CD	2.78	0.47
1:B:396:GLU:C	1:B:398:ARG:H	2.17	0.47
1:B:107:ALA:O	1:B:111:GLN:HG2	2.13	0.47
1:A:124:ASN:HD21	1:A:126:TYR:HB2	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:HG3	1:A:437:TYR:CE2	2.51	0.46
1:A:102:THR:O	1:A:102:THR:CG2	2.63	0.45
1:A:103:LYS:HE2	1:A:103:LYS:HB2	1.80	0.45
1:A:151:GLU:O	1:A:155:ARG:HD3	2.17	0.45
1:A:317:GLY:O	1:A:318:ALA:HB3	2.17	0.45
1:A:372:ASN:HD22	1:A:375:GLY:H	1.62	0.45
1:B:507:GLU:O	1:B:508:PHE:CB	2.56	0.45
1:B:367:GLY:HA2	1:B:404:LEU:HD22	1.98	0.45
1:A:137:THR:HG22	1:A:139:GLN:H	1.82	0.44
1:A:392:MET:HG3	1:A:424:LEU:O	2.17	0.44
1:B:152:VAL:HG21	1:B:380:PHE:CE1	2.53	0.44
1:B:197:THR:HG21	1:B:436:LEU:HG	2.00	0.43
1:B:228:SER:HA	1:B:252:GLN:HG3	2.01	0.43
1:B:112:LEU:HA	1:B:116:LEU:HG	2.01	0.43
1:A:179:ILE:HD11	1:A:455:ARG:HG3	2.00	0.42
1:A:248:ILE:CD1	1:A:250:TRP:NE1	2.83	0.42
1:B:121:ASN:N	1:B:121:ASN:HD22	2.18	0.42
1:A:112:LEU:O	1:A:113:LYS:C	2.57	0.42
1:B:209:GLU:OE2	1:B:232:SER:HB2	2.20	0.42
1:B:331:THR:CG2	1:B:332:TRP:N	2.82	0.42
1:A:372:ASN:HD22	1:A:372:ASN:C	2.23	0.42
1:A:197:THR:HG21	1:A:436:LEU:CG	2.49	0.42
1:B:327:ASP:HA	1:B:328:PRO:HD2	1.93	0.42
2:B:9570:FMN:H1'2	2:B:9570:FMN:H9	1.74	0.41
1:B:354:THR:OG1	1:B:391:THR:HG22	2.20	0.41
1:B:433:ARG:HB3	1:B:437:TYR:CE2	2.54	0.41
1:A:124:ASN:HD22	1:A:126:TYR:N	2.20	0.40
1:B:164:ILE:O	1:B:420:LYS:HE2	2.21	0.40
1:B:242:ALA:HA	1:B:243:PRO:HD3	1.84	0.40
1:A:408:VAL:HG12	1:A:429:VAL:HB	2.03	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	391/511 (76%)	370 (95%)	15 (4%)	6 (2%)	10	26
1	B	385/511 (75%)	360 (94%)	17 (4%)	8 (2%)	7	18
All	All	776/1022 (76%)	730 (94%)	32 (4%)	14 (2%)	8	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	SER
1	B	101	GLU
1	B	114	SER
1	B	510	ASP
1	A	104	GLU
1	B	105	ASP
1	B	397	GLN
1	A	318	ALA
1	B	103	LYS
1	A	510	ASP
1	B	508	PHE
1	A	508	PHE
1	A	105	ASP
1	B	198	GLY

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	335/439 (76%)	279 (83%)	56 (17%)	2	5
1	B	334/439 (76%)	278 (83%)	56 (17%)	2	5
All	All	669/878 (76%)	557 (83%)	112 (17%)	2	5

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	105	ASP
1	A	109	LYS
1	A	110	GLU
1	A	111	GLN
1	A	112	LEU
1	A	113	LYS
1	A	114	SER
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	139	GLN
1	A	175	ARG
1	A	184	LEU
1	A	190	VAL
1	A	197	THR
1	A	206	LEU
1	A	222	LYS
1	A	246	LYS
1	A	248	ILE
1	A	255	VAL
1	A	256	ASN
1	A	257	SER
1	A	260	LYS
1	A	265	LEU
1	A	270	GLU
1	A	271	LYS
1	A	286	LEU
1	A	292	ASP
1	A	294	LYS
1	A	320	ARG
1	A	324	LYS
1	A	330	LEU
1	A	331	THR
1	A	333	LYS
1	A	338	LEU
1	A	341	LYS
1	A	353	ARG
1	A	365	VAL
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	397	GLN
1	A	398	ARG
1	A	401	LYS
1	A	408	VAL
1	A	429	VAL
1	A	460	MET
1	A	464	LEU
1	A	476	ASP
1	A	477	LEU
1	A	483	LEU
1	A	492	ASN
1	A	504	THR
1	A	509	GLU
1	B	103	LYS
1	B	104	GLU
1	B	108	ARG
1	B	112	LEU
1	B	119	LEU
1	B	124	ASN
1	B	125	LEU
1	B	131	LEU
1	B	139	GLN
1	B	146	SER
1	B	152	VAL
1	B	167	LYS
1	B	176	LYS
1	B	184	LEU
1	B	186	SER
1	B	197	THR
1	B	222	LYS
1	B	246	LYS
1	B	248	ILE
1	B	252	GLN
1	B	256	ASN
1	B	257	SER
1	B	260	LYS
1	B	263	ASP
1	B	271	LYS
1	B	275	LYS
1	B	277	LEU
1	B	286	LEU
1	B	292	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	294	LYS
1	B	295	LEU
1	B	323	SER
1	B	324	LYS
1	B	339	LYS
1	B	341	LYS
1	B	343	LYS
1	B	353	ARG
1	B	359	LYS
1	B	368	VAL
1	B	370	LEU
1	B	378	LEU
1	B	388	LEU
1	B	391	THR
1	B	396	GLU
1	B	403	LYS
1	B	404	LEU
1	B	408	VAL
1	B	427	LYS
1	B	429	VAL
1	B	462	MET
1	B	464	LEU
1	B	483	LEU
1	B	484	LYS
1	B	492	ASN
1	B	504	THR
1	B	509	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	124	ASN
1	A	157	ASN
1	A	159	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	268	ASN
1	A	372	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	377	GLN
1	A	439	ASN
1	A	497	ASN
1	B	121	ASN
1	B	124	ASN
1	B	139	GLN
1	B	159	ASN
1	B	218	GLN
1	B	225	GLN
1	B	247	GLN
1	B	256	ASN
1	B	377	GLN
1	B	492	ASN
1	B	497	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	9570	-	31,33,33	1.39	2 (6%)	40,50,50	3.91	18 (45%)
3	PYR	A	5580	-	2,5,5	5.92	2 (100%)	2,6,6	0.86	0
3	PYR	B	9580	-	2,5,5	5.88	2 (100%)	2,6,6	0.64	0
2	FMN	A	5570	-	31,33,33	1.43	2 (6%)	40,50,50	3.86	19 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	9570	-	-	4/18/18/18	0/3/3/3
3	PYR	A	5580	-	-	0/0/4/4	-
3	PYR	B	9580	-	-	0/0/4/4	-
2	FMN	A	5570	-	-	5/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9580	PYR	C3-C2	6.40	1.68	1.49
3	A	5580	PYR	C3-C2	6.37	1.68	1.49
3	A	5580	PYR	O3-C2	5.43	1.39	1.22
3	B	9580	PYR	O3-C2	5.31	1.39	1.22
2	A	5570	FMN	C4A-C10	5.04	1.43	1.38
2	B	9570	FMN	C4A-C10	4.87	1.43	1.38
2	A	5570	FMN	C4-C4A	3.84	1.48	1.41
2	B	9570	FMN	C4-C4A	3.67	1.47	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9570	FMN	C4-N3-C2	15.11	127.89	115.14
2	A	5570	FMN	C4-N3-C2	14.85	127.68	115.14
2	B	9570	FMN	C4-C4A-C10	-6.82	115.43	119.95
2	A	5570	FMN	C4-C4A-C10	-6.81	115.45	119.95
2	B	9570	FMN	P-O5'-C5'	6.56	136.36	118.30
2	A	5570	FMN	P-O5'-C5'	6.44	136.03	118.30
2	B	9570	FMN	C4A-C10-N10	-6.23	113.90	120.30
2	A	5570	FMN	C4A-C4-N3	-6.19	114.97	123.43
2	A	5570	FMN	C4A-C10-N10	-6.14	113.99	120.30
2	B	9570	FMN	C4A-C4-N3	-6.12	115.07	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5570	FMN	O2'-C2'-C3'	5.22	121.79	109.10
2	B	9570	FMN	O2'-C2'-C1'	5.22	122.15	109.59
2	B	9570	FMN	O3'-C3'-C2'	-5.13	96.43	108.81
2	A	5570	FMN	C4'-C3'-C2'	4.58	122.88	113.36
2	A	5570	FMN	C4A-N5-C5A	4.49	121.26	116.77
2	A	5570	FMN	O2'-C2'-C1'	4.48	120.38	109.59
2	A	5570	FMN	O4'-C4'-C5'	4.44	119.90	109.92
2	B	9570	FMN	C4A-N5-C5A	4.37	121.14	116.77
2	B	9570	FMN	O2'-C2'-C3'	4.23	119.38	109.10
2	A	5570	FMN	O3'-C3'-C2'	-3.97	99.22	108.81
2	B	9570	FMN	C6-C5A-N5	3.94	123.39	119.05
2	A	5570	FMN	C6-C5A-N5	3.87	123.32	119.05
2	B	9570	FMN	C4'-C3'-C2'	3.86	121.38	113.36
2	A	5570	FMN	C5'-C4'-C3'	-3.85	104.77	112.20
2	B	9570	FMN	O3'-C3'-C4'	3.83	118.07	108.81
2	B	9570	FMN	O4'-C4'-C5'	3.79	118.44	109.92
2	B	9570	FMN	C10-C4A-N5	3.64	123.77	121.26
2	A	5570	FMN	C10-C4A-N5	3.31	123.55	121.26
2	B	9570	FMN	C5'-C4'-C3'	-3.23	105.97	112.20
2	A	5570	FMN	O3'-C3'-C4'	2.50	114.85	108.81
2	B	9570	FMN	O5'-C5'-C4'	-2.41	102.93	109.36
2	B	9570	FMN	C9A-C5A-N5	-2.32	118.73	122.36
2	A	5570	FMN	C9A-C5A-N5	-2.21	118.90	122.36
2	A	5570	FMN	C9A-N10-C10	2.12	124.68	121.91
2	A	5570	FMN	C4-C4A-N5	2.10	121.00	118.60
2	A	5570	FMN	O5'-C5'-C4'	-2.05	103.88	109.36
2	B	9570	FMN	C7-C6-C5A	2.04	124.11	121.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5570	FMN	O2'-C2'-C3'-C4'
2	A	5570	FMN	O2'-C2'-C3'-O3'
2	B	9570	FMN	O2'-C2'-C3'-C4'
2	A	5570	FMN	C4'-C5'-O5'-P
2	B	9570	FMN	C4'-C5'-O5'-P
2	A	5570	FMN	C2'-C3'-C4'-O4'
2	B	9570	FMN	C5'-O5'-P-O3P
2	A	5570	FMN	O3'-C3'-C4'-O4'
2	B	9570	FMN	O2'-C2'-C3'-O3'

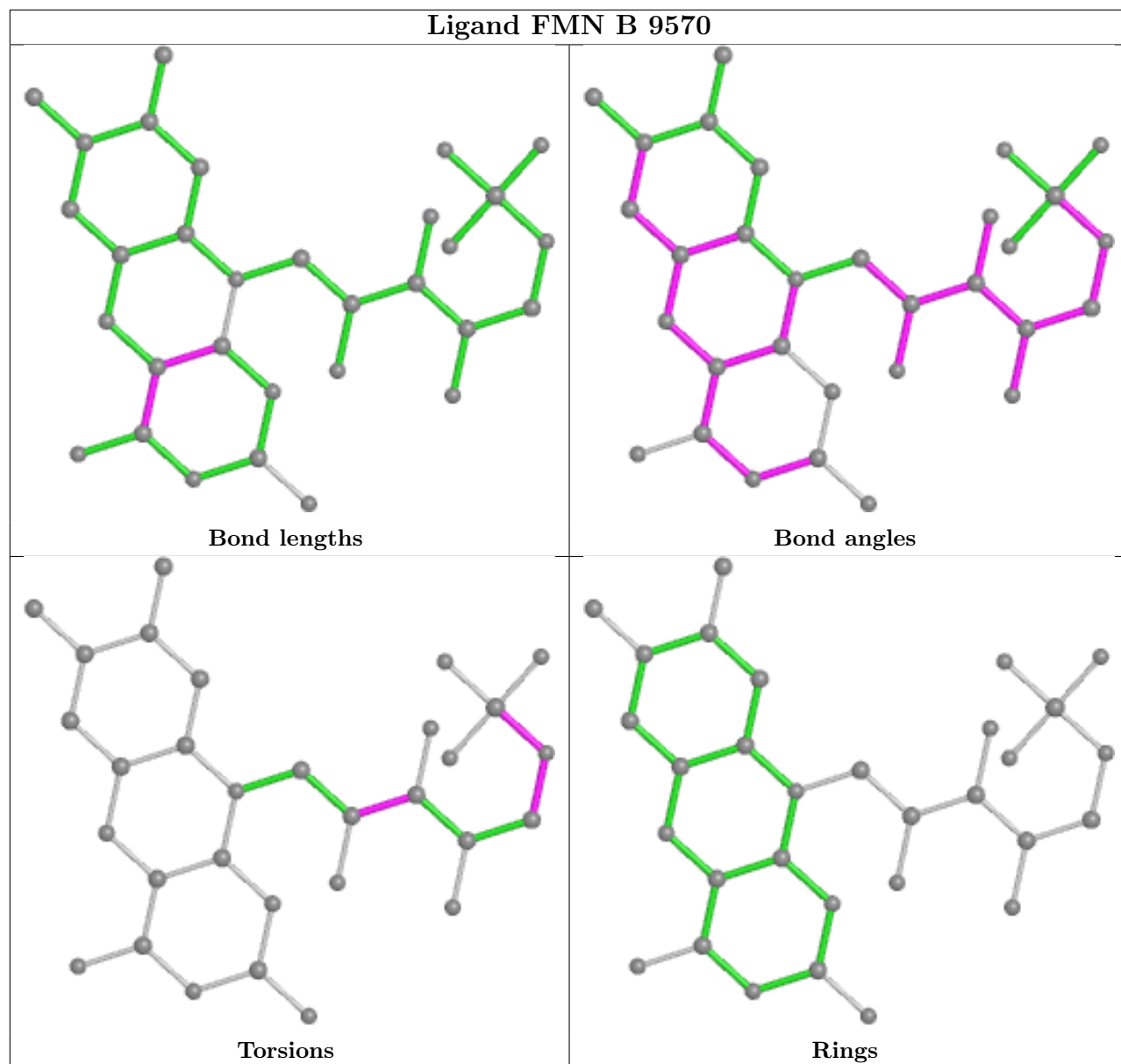
There are no ring outliers.

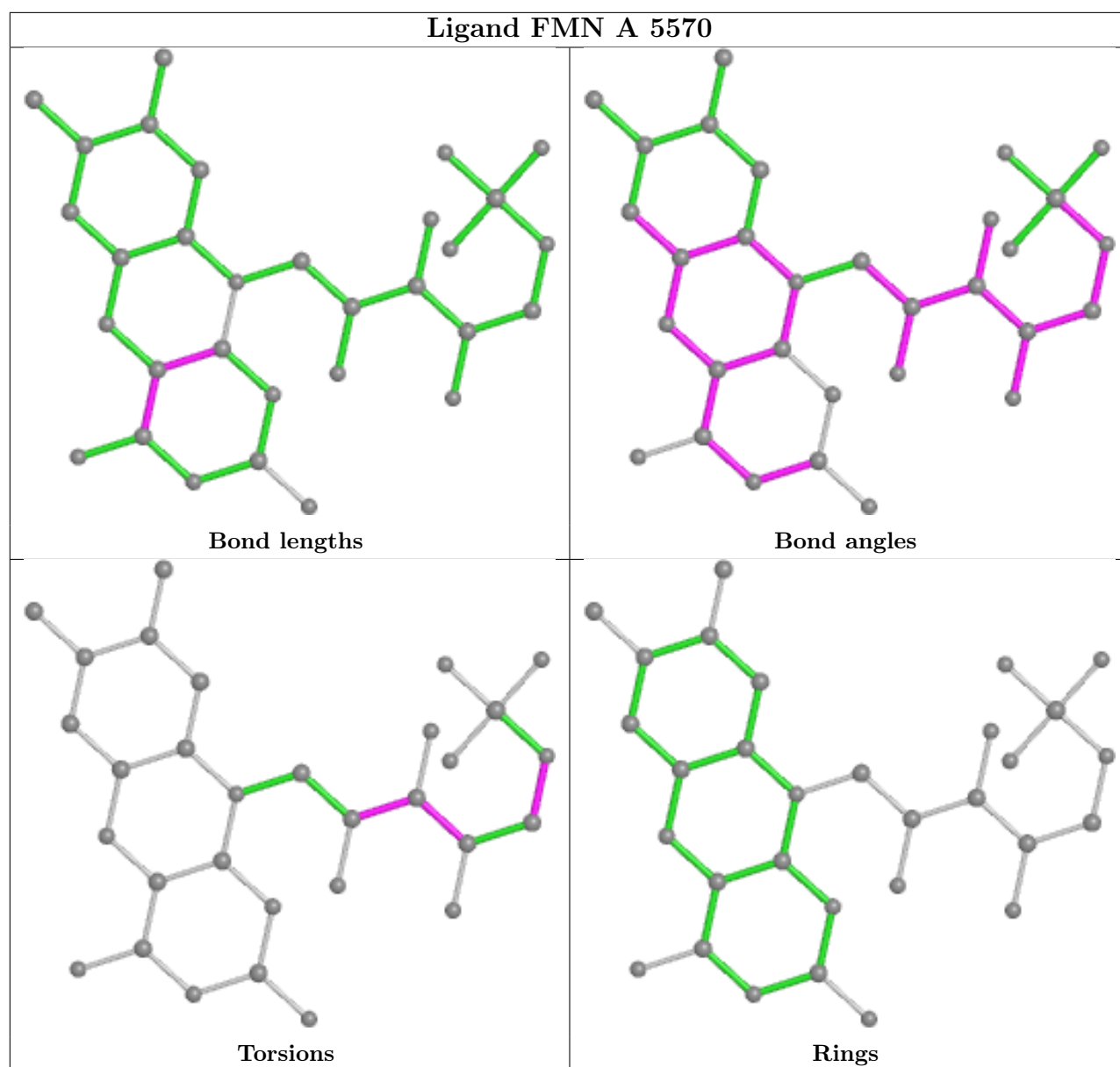
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9570	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.

Ligand FMN B 9570





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	395/511 (77%)	-0.33	10 (2%) 57 59	30, 44, 74, 85	0
1	B	389/511 (76%)	-0.09	23 (5%) 22 21	34, 53, 81, 87	0
All	All	784/1022 (76%)	-0.21	33 (4%) 36 35	30, 47, 78, 87	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	SER	7.4
1	A	114	SER	6.2
1	B	322	LEU	4.5
1	A	511	ALA	4.1
1	B	321	ALA	4.0
1	B	399	ASN	3.9
1	B	236	GLU	3.7
1	B	106	ILE	3.6
1	A	399	ASN	3.4
1	A	106	ILE	3.4
1	B	240	GLU	3.4
1	A	319	SER	3.3
1	B	102	THR	3.2
1	B	324	LYS	3.1
1	A	297	PHE	3.1
1	B	246	LYS	2.9
1	A	320	ARG	2.8
1	B	402	ASP	2.7
1	B	245	ASP	2.7
1	A	102	THR	2.6
1	A	103	LYS	2.5
1	A	402	ASP	2.4
1	B	113	LYS	2.4
1	B	271	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	237	GLU	2.2
1	B	206	LEU	2.1
1	B	100	GLY	2.1
1	B	511	ALA	2.1
1	B	185	GLY	2.1
1	B	510	ASP	2.0
1	B	297	PHE	2.0
1	B	403	LYS	2.0
1	B	103	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

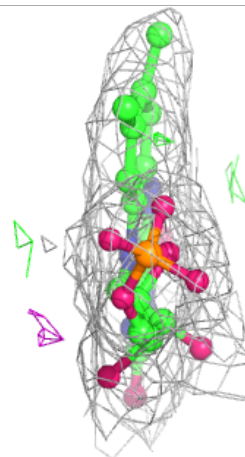
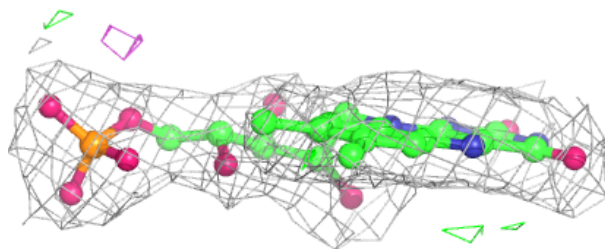
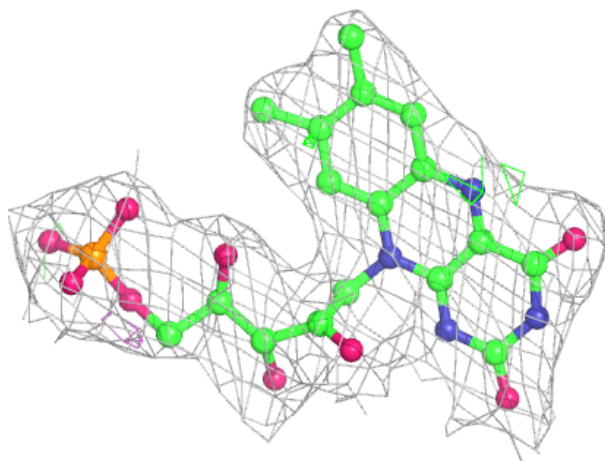
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PYR	B	9580	6/6	0.76	0.24	69,71,71,72	0
3	PYR	A	5580	6/6	0.89	0.20	59,62,62,63	0
2	FMN	A	5570	31/31	0.98	0.11	31,36,40,42	0
2	FMN	B	9570	31/31	0.98	0.09	39,43,47,51	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.

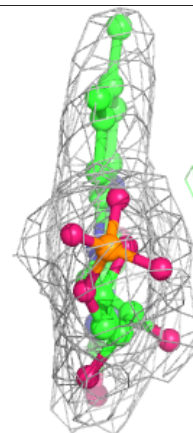
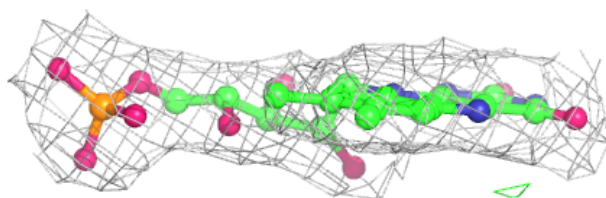
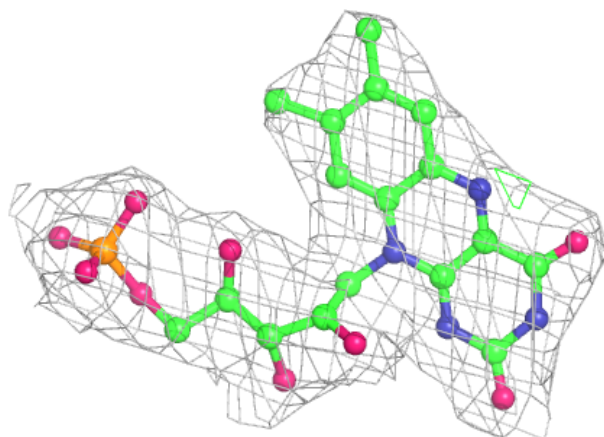
Electron density around FMN A 5570:

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



Electron density around FMN B 9570:

$2mF_o - DF_c$ (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.