



# Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 03:54 PM EDT

PDB ID : 2E77 / pdb\_00002e77  
Title : Crystal structure of L-lactate oxidase with pyruvate complex  
Authors : Morimoto, Y.  
Deposited on : 2007-01-06  
Resolution : 1.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

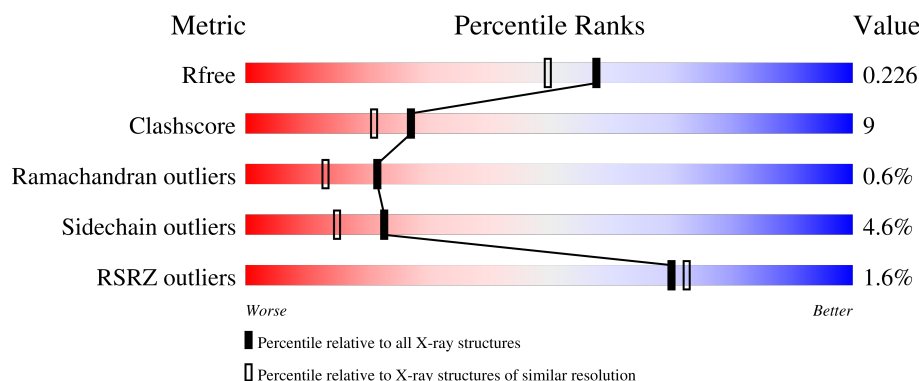
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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  $\geq 3$ , 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	374	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	B	374	<div> <div>0%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• • •</div> </div> </div>
1	C	374	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	D	374	<div> <div>0%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

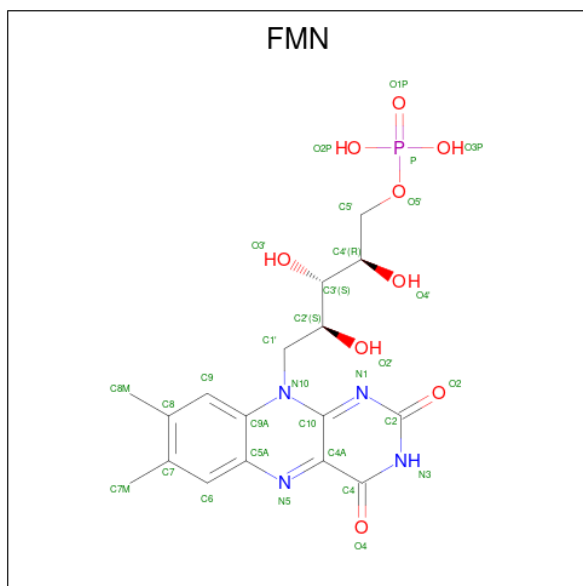
There are 4 unique types of molecules in this entry. The entry contains 12571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2738	1732	475	525	6			
1	B	368	Total	C	N	O	S	0	0	0
			2840	1794	494	545	7			
1	C	350	Total	C	N	O	S	0	0	0
			2700	1708	467	519	6			
1	D	368	Total	C	N	O	S	0	0	0
			2840	1794	494	545	7			

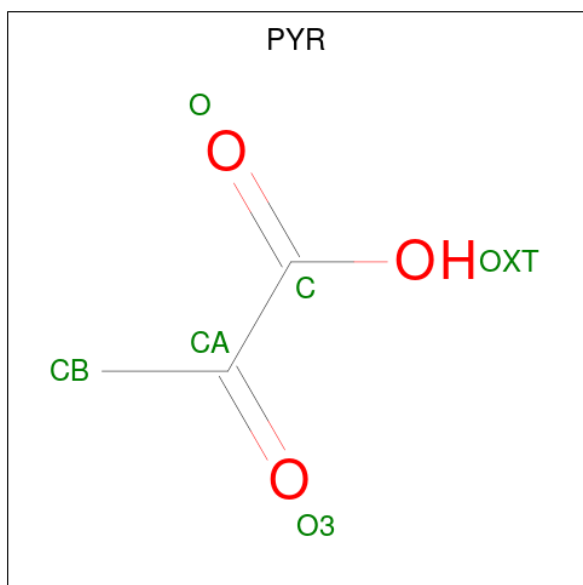
- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 3 is PYRUVIC ACID (CCD ID: 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		
3	D	1	Total	C	O	0	0
			6	3	3		

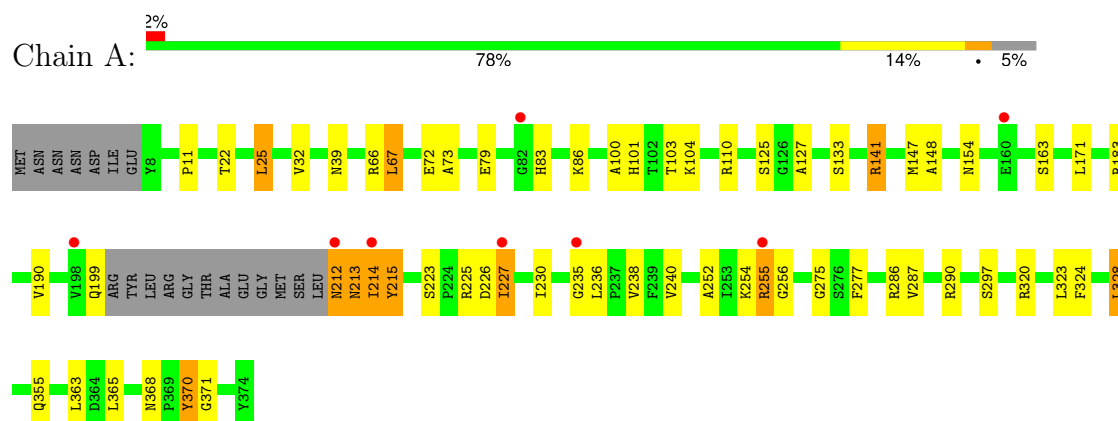
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total	O	0	0
			292	292		
4	B	370	Total	O	0	0
			370	370		
4	C	289	Total	O	0	0
			289	289		
4	D	360	Total	O	0	0
			360	360		

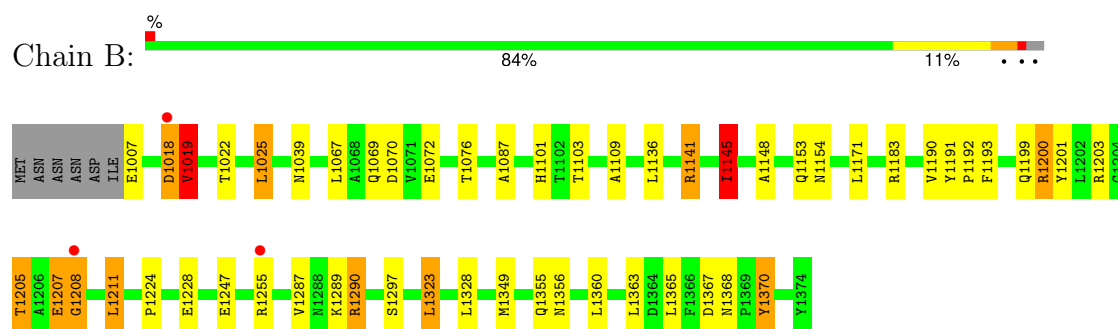
### 3 Residue-property plots

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.

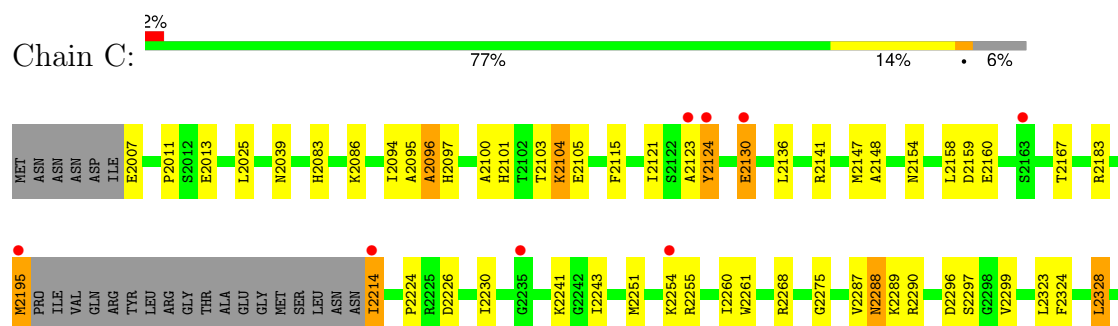
#### • Molecule 1: Lactate oxidase

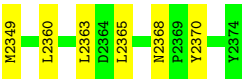


#### • Molecule 1: Lactate oxidase

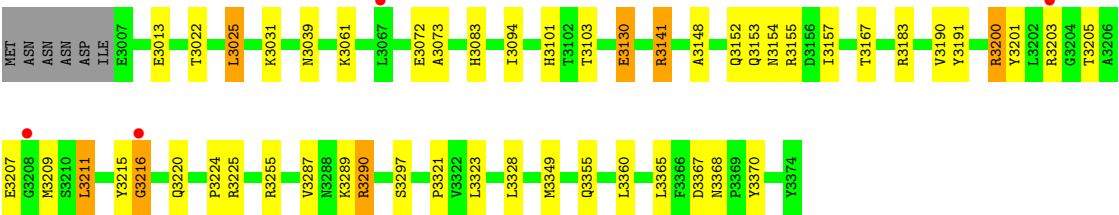
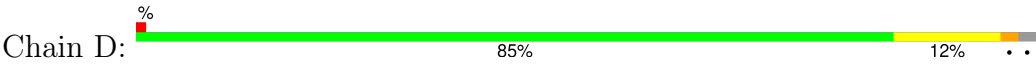


#### • Molecule 1: Lactate oxidase





● Molecule 1: Lactate oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.84Å 118.57Å 107.24Å 90.00° 121.07° 90.00°	Depositor
Resolution (Å)	37.40 – 1.90 37.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.40-1.90) 99.5 (37.40-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.227 0.176 , 0.226	Depositor DCC
$R_{free}$ test set	5657 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PYR

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	0.87	1/2800 (0.0%)	1.04	9/3795 (0.2%)
1	B	1.11	2/2904 (0.1%)	1.21	17/3935 (0.4%)
1	C	0.91	0/2761	1.00	3/3740 (0.1%)
1	D	1.06	1/2904 (0.0%)	1.08	6/3935 (0.2%)
All	All	0.99	4/11369 (0.0%)	1.09	35/15405 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1070	ASP	N-CA	7.88	1.57	1.46
1	D	3073	ALA	CA-CB	5.88	1.56	1.52
1	B	1069	GLN	C-N	-5.75	1.26	1.33
1	A	73	ALA	CA-CB	5.36	1.56	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1069	GLN	CA-C-N	-18.43	95.11	123.12
1	B	1069	GLN	C-N-CA	-18.43	95.11	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3215	TYR	CA-C-N	-11.14	104.81	122.86
1	D	3215	TYR	C-N-CA	-11.14	104.81	122.86
1	B	1069	GLN	O-C-N	-9.83	111.17	122.68
1	B	1145	ILE	CB-CA-C	-9.57	97.49	110.98
1	B	1370	TYR	CA-C-N	-9.28	103.23	121.41
1	B	1370	TYR	C-N-CA	-9.28	103.23	121.41
1	B	1018	ASP	N-CA-C	9.21	121.09	111.14
1	D	3290	ARG	NE-CZ-NH2	-9.20	110.92	119.20
1	B	1370	TYR	O-C-N	-6.31	115.66	122.85
1	D	3290	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	B	1141	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	C	2104	LYS	CB-CA-C	-6.11	108.52	115.79
1	B	1323	LEU	CA-CB-CG	-6.11	94.93	116.30
1	B	1069	GLN	N-CA-C	-6.03	101.85	110.59
1	D	3141	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	A	223	SER	CA-C-N	-5.81	113.64	119.56
1	A	223	SER	C-N-CA	-5.81	113.64	119.56
1	B	1070	ASP	CB-CA-C	5.79	120.70	111.73
1	B	1290	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	C	2275	GLY	N-CA-C	-5.71	104.68	111.36
1	A	236	LEU	N-CA-C	5.69	117.86	110.40
1	B	1290	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	B	1141	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	A	110	ARG	N-CA-C	5.33	116.77	111.07
1	A	370	TYR	CA-C-N	-5.19	111.24	121.41
1	A	370	TYR	C-N-CA	-5.19	111.24	121.41
1	A	275	GLY	N-CA-C	-5.17	105.31	111.36
1	D	3141	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	C	2299	VAL	N-CA-C	5.14	115.63	108.84
1	B	1207	GLU	O-C-N	-5.09	116.83	122.07
1	B	1207	GLU	N-CA-C	5.07	116.50	111.07
1	A	277	PHE	N-CA-C	5.01	116.74	111.28
1	A	320	ARG	N-CA-C	5.00	120.38	113.77

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	GLY	Peptide
1	B	1208	GLY	Peptide
1	D	3216	GLY	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	2738	0	2668	52	0
1	B	2840	0	2770	47	0
1	C	2700	0	2627	57	0
1	D	2840	0	2770	44	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	D	6	0	0	0	0
4	A	292	0	0	10	0
4	B	370	0	0	13	0
4	C	289	0	0	23	0
4	D	360	0	0	12	0
All	All	12571	0	10911	200	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 9.

All (200) 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:2123:ALA:HB2	4:C:2716:HOH:O	1.31	1.25
1:B:1356:ASN:HB3	4:B:1826:HOH:O	1.35	1.20
1:A:227:ILE:HB	1:A:255:ARG:NE	1.62	1.14
1:B:1228:GLU:OE2	1:B:1255:ARG:HD2	1.52	1.06
1:D:3287:VAL:O	1:D:3290:ARG:HD3	1.52	1.06
1:D:3216:GLY:HA2	1:D:3220:GLN:NE2	1.74	1.03
1:C:2195:MET:C	4:C:2744:HOH:O	2.02	1.02
1:B:1367:ASP:HB2	4:B:1830:HOH:O	1.59	1.00
1:B:1289:LYS:HD3	4:B:1876:HOH:O	1.60	0.99
1:D:3130:GLU:HG3	4:D:3712:HOH:O	1.63	0.98
1:B:1287:VAL:O	1:B:1290:ARG:HD3	1.63	0.97
1:A:286:ARG:HD2	4:A:4731:HOH:O	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2007:GLU:N	4:C:2797:HOH:O	2.00	0.95
1:A:148:ALA:H	1:A:154:ASN:HD21	0.96	0.95
1:C:2083:HIS:HE1	4:C:2775:HOH:O	1.49	0.94
1:D:3224:PRO:HB3	1:D:3255:ARG:HG3	1.52	0.91
1:C:2123:ALA:O	1:C:2124:TYR:HD1	1.53	0.91
1:C:2214:ILE:HG12	4:C:2769:HOH:O	1.68	0.91
1:B:1148:ALA:H	1:B:1154:ASN:HD21	1.17	0.91
1:D:3287:VAL:O	1:D:3290:ARG:CD	2.19	0.90
1:D:3205:THR:HG22	1:D:3207:GLU:H	1.35	0.90
1:C:2083:HIS:CE1	4:C:2775:HOH:O	2.21	0.88
1:D:3216:GLY:HA2	1:D:3220:GLN:HE22	1.39	0.86
1:A:225:ARG:HD2	4:A:4752:HOH:O	1.75	0.86
1:C:2148:ALA:H	1:C:2154:ASN:HD21	1.23	0.84
1:C:2039:ASN:HD22	1:C:2183:ARG:HH11	1.22	0.83
1:C:2095:ALA:O	1:C:2096:ALA:CB	2.26	0.83
1:B:1255:ARG:HG2	4:B:1542:HOH:O	1.77	0.83
1:D:3148:ALA:H	1:D:3154:ASN:HD21	1.27	0.82
1:C:2254:LYS:HD2	4:C:2736:HOH:O	1.79	0.82
1:B:1007:GLU:HA	4:B:1739:HOH:O	1.78	0.81
1:C:2104:LYS:HD3	4:C:2752:HOH:O	1.80	0.80
1:A:212:ASN:ND2	4:A:4803:HOH:O	2.13	0.80
1:B:1205:THR:HG22	1:B:1207:GLU:H	1.45	0.79
1:A:227:ILE:CB	1:A:255:ARG:NE	2.46	0.79
1:D:3255:ARG:HG2	4:D:3559:HOH:O	1.82	0.78
1:C:2123:ALA:O	1:C:2124:TYR:CD1	2.36	0.78
1:D:3039:ASN:HD22	1:D:3183:ARG:HH11	1.29	0.78
1:C:2159:ASP:HB3	4:C:2767:HOH:O	1.84	0.76
1:C:2243:ILE:HD12	1:C:2260:ILE:HG23	1.66	0.76
1:C:2214:ILE:CD1	4:C:2793:HOH:O	2.33	0.75
1:B:1039:ASN:HD22	1:B:1183:ARG:HH11	1.34	0.75
1:C:2254:LYS:CD	4:C:2736:HOH:O	2.32	0.75
1:C:2287:VAL:O	1:C:2290:ARG:HD3	1.87	0.74
1:D:3061:LYS:HE2	4:D:3805:HOH:O	1.87	0.73
1:A:287:VAL:O	1:A:290:ARG:HD3	1.89	0.73
1:A:148:ALA:N	1:A:154:ASN:HD21	1.79	0.72
1:B:1205:THR:CG2	1:B:1207:GLU:H	2.02	0.71
1:D:3323:LEU:HB2	4:D:3804:HOH:O	1.91	0.70
1:C:2214:ILE:HD11	4:C:2793:HOH:O	1.91	0.70
1:A:39:ASN:HD22	1:A:183:ARG:HH11	1.38	0.69
1:D:3224:PRO:CB	1:D:3255:ARG:HG3	2.21	0.69
1:A:226:ASP:O	1:A:230:ILE:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1191:TYR:OH	1:B:1211:LEU:HG	1.93	0.69
1:A:148:ALA:H	1:A:154:ASN:ND2	1.81	0.68
1:B:1148:ALA:N	1:B:1154:ASN:HD21	1.89	0.68
1:B:1200:ARG:HD2	4:B:1598:HOH:O	1.93	0.68
1:D:3323:LEU:HD13	4:D:3804:HOH:O	1.94	0.68
1:D:3224:PRO:HB3	1:D:3255:ARG:CG	2.24	0.68
1:A:147:MET:HE3	1:A:230:ILE:HD11	1.77	0.66
1:A:227:ILE:HG22	1:A:255:ARG:HH11	1.61	0.66
1:D:3148:ALA:N	1:D:3154:ASN:HD21	1.94	0.66
1:B:1228:GLU:OE2	1:B:1255:ARG:CD	2.39	0.65
1:C:2158:LEU:HD11	1:C:2230:ILE:HD12	1.78	0.65
1:C:2039:ASN:ND2	1:C:2183:ARG:HH11	1.95	0.65
1:A:227:ILE:HB	1:A:255:ARG:CD	2.25	0.65
1:D:3205:THR:HG21	4:D:3627:HOH:O	1.96	0.64
1:D:3216:GLY:CA	1:D:3220:GLN:HE22	2.10	0.64
1:C:2254:LYS:HG2	4:C:2649:HOH:O	1.97	0.64
1:A:227:ILE:HB	1:A:255:ARG:HE	1.57	0.64
1:C:2095:ALA:O	1:C:2096:ALA:HB3	1.97	0.63
1:B:1287:VAL:O	1:B:1290:ARG:CD	2.42	0.63
1:D:3072:GLU:H	1:D:3355:GLN:HE22	1.44	0.62
1:A:324:PHE:O	1:A:328:LEU:HD22	2.01	0.61
1:C:2104:LYS:CD	4:C:2752:HOH:O	2.42	0.61
1:A:227:ILE:HG21	1:A:240:VAL:HG22	1.82	0.61
1:B:1247:GLU:HB2	4:B:1879:HOH:O	2.00	0.61
1:C:2324:PHE:O	1:C:2328:LEU:HD22	2.02	0.60
1:A:171:LEU:CD2	1:A:227:ILE:HG23	2.31	0.60
1:A:104:LYS:HD2	1:A:127:ALA:HB2	1.82	0.59
1:C:2368:ASN:HD21	1:C:2370:TYR:HB2	1.67	0.59
1:A:171:LEU:HD23	1:A:227:ILE:HG23	1.84	0.59
1:A:199:GLN:HA	4:A:4801:HOH:O	2.01	0.59
1:C:2289:LYS:HD2	4:C:2683:HOH:O	2.03	0.59
1:B:1019:VAL:N	4:B:1878:HOH:O	1.72	0.58
1:A:213:ASN:HA	4:A:4725:HOH:O	2.03	0.58
1:B:1205:THR:HG22	1:B:1207:GLU:N	2.15	0.58
1:D:3191:TYR:O	1:D:3207:GLU:O	2.21	0.58
1:D:3022:THR:HA	1:D:3025:LEU:HD22	1.84	0.58
1:D:3083:HIS:HD2	4:D:3664:HOH:O	1.86	0.56
1:D:3039:ASN:ND2	1:D:3183:ARG:HH11	2.02	0.56
1:C:2095:ALA:O	1:C:2096:ALA:HB2	2.03	0.56
1:B:1148:ALA:H	1:B:1154:ASN:ND2	1.97	0.56
1:C:2214:ILE:HD12	4:C:2799:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HB	1:A:255:ARG:CZ	2.33	0.56
1:D:3216:GLY:CA	1:D:3220:GLN:NE2	2.61	0.56
1:A:227:ILE:CB	1:A:255:ARG:HE	2.14	0.55
1:B:1072:GLU:H	1:B:1355:GLN:HE22	1.53	0.55
1:A:227:ILE:CG2	1:A:255:ARG:HE	2.20	0.55
1:B:1153:GLN:HE22	1:B:1201:TYR:HB3	1.71	0.55
1:B:1101:HIS:CD2	1:B:1103:THR:H	2.25	0.54
1:B:1224:PRO:HB3	1:B:1255:ARG:HG3	1.89	0.54
1:A:214:ILE:O	1:A:215:TYR:HB2	2.08	0.54
1:D:3094:ILE:HG21	1:D:3323:LEU:HD22	1.90	0.54
1:D:3157:ILE:HD11	1:D:3200:ARG:HD3	1.90	0.54
1:A:11:PRO:HG3	1:A:32:VAL:O	2.07	0.53
1:B:1101:HIS:HD2	1:B:1103:THR:H	1.56	0.53
1:C:2094:ILE:O	1:C:2097:HIS:CD2	2.61	0.53
1:D:3153:GLN:HE22	1:D:3201:TYR:HB3	1.74	0.53
1:A:368:ASN:HD21	1:A:370:TYR:HB2	1.74	0.53
1:B:1228:GLU:OE2	1:B:1255:ARG:NH2	2.28	0.53
1:C:2086:LYS:HD3	1:C:2115:PHE:O	2.09	0.53
1:D:3152:GLN:NE2	1:D:3155:ARG:HH11	2.06	0.52
1:C:2101:HIS:HD2	1:C:2103:THR:H	1.58	0.52
1:A:252:ALA:O	1:A:255:ARG:HD3	2.09	0.52
1:C:2097:HIS:CD2	1:C:2105:GLU:HG3	2.44	0.52
1:A:101:HIS:HD2	1:A:103:THR:H	1.59	0.51
1:B:1145:ILE:HD12	1:B:1171:LEU:HA	1.92	0.51
1:C:2104:LYS:CE	4:C:2752:HOH:O	2.58	0.51
1:A:199:GLN:HB2	4:A:4624:HOH:O	2.11	0.51
1:A:255:ARG:C	1:A:255:ARG:HH21	2.20	0.50
1:B:1247:GLU:OE2	4:B:1879:HOH:O	2.19	0.50
1:C:2241:LYS:HA	1:C:2261:TRP:HB3	1.94	0.50
1:C:2121:ILE:HD11	1:C:2136:LEU:HD11	1.93	0.50
1:D:3013:GLU:O	1:D:3101:HIS:HE1	1.94	0.49
1:B:1109:ALA:HB1	1:B:1136:LEU:HG	1.93	0.49
1:C:2130:GLU:H	1:C:2130:GLU:CD	2.18	0.49
1:B:1224:PRO:CB	1:B:1255:ARG:HG3	2.43	0.49
1:A:227:ILE:HD12	1:A:255:ARG:HD2	1.95	0.49
1:A:255:ARG:NH2	1:A:256:GLY:C	2.71	0.48
1:B:1368:ASN:HD21	1:B:1370:TYR:HB2	1.78	0.48
1:B:1039:ASN:ND2	1:B:1183:ARG:HH11	2.08	0.48
1:D:3224:PRO:HB2	1:D:3255:ARG:NH2	2.28	0.48
1:D:3368:ASN:HD21	1:D:3370:TYR:HB2	1.79	0.47
1:A:101:HIS:CD2	1:A:103:THR:H	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1067:LEU:HD23	4:D:3609:HOH:O	2.14	0.47
1:C:2268:ARG:NH2	4:C:2637:HOH:O	2.47	0.47
1:D:3349:MET:HG2	1:D:3360:LEU:HD21	1.96	0.47
1:B:1076:THR:O	1:B:1087:ALA:HA	2.15	0.47
1:D:3148:ALA:H	1:D:3154:ASN:ND2	2.03	0.47
1:B:1224:PRO:HB3	1:B:1255:ARG:CG	2.45	0.47
1:A:66:ARG:C	1:A:67:LEU:HD23	2.40	0.47
1:D:3209:MET:HE3	4:D:3825:HOH:O	2.14	0.46
1:A:227:ILE:HG21	1:A:240:VAL:CG2	2.45	0.46
1:C:2086:LYS:CG	4:C:2684:HOH:O	2.61	0.46
1:D:3153:GLN:NE2	1:D:3201:TYR:HB3	2.31	0.46
1:A:39:ASN:ND2	1:A:183:ARG:HH11	2.09	0.45
1:A:227:ILE:HB	1:A:255:ARG:CG	2.45	0.45
1:B:1022:THR:HA	1:B:1025:LEU:HD22	1.98	0.45
1:D:3101:HIS:HD2	1:D:3103:THR:H	1.65	0.45
1:B:1208:GLY:HA3	4:B:1785:HOH:O	2.17	0.45
1:A:371:GLY:HA3	4:A:4587:HOH:O	2.15	0.44
1:C:2224:PRO:CB	1:C:2255:ARG:HD2	2.46	0.44
1:A:227:ILE:HG22	1:A:255:ARG:NH1	2.29	0.44
1:C:2013:GLU:O	1:C:2101:HIS:HE1	2.01	0.44
1:C:2254:LYS:HD3	4:C:2736:HOH:O	2.07	0.44
1:A:225:ARG:HG3	4:A:4787:HOH:O	2.18	0.44
1:B:1191:TYR:O	1:B:1207:GLU:O	2.35	0.44
1:B:1367:ASP:CB	4:B:1830:HOH:O	2.38	0.44
1:A:11:PRO:HD2	1:A:100:ALA:O	2.18	0.44
1:A:290:ARG:NH2	4:A:4784:HOH:O	2.50	0.44
1:C:2226:ASP:O	1:C:2230:ILE:HG12	2.18	0.44
1:A:79:GLU:HA	1:A:83:HIS:O	2.17	0.44
1:C:2101:HIS:CD2	1:C:2103:THR:H	2.34	0.44
1:C:2296:ASP:OD1	1:C:2296:ASP:C	2.61	0.44
1:D:3101:HIS:CD2	1:D:3103:THR:H	2.36	0.44
1:B:1153:GLN:NE2	1:B:1201:TYR:HB3	2.32	0.43
1:C:2251:MET:O	1:C:2255:ARG:HG2	2.17	0.43
1:C:2094:ILE:O	1:C:2097:HIS:NE2	2.51	0.43
1:C:2147:MET:HE1	1:C:2230:ILE:HD11	2.00	0.43
1:D:3130:GLU:CG	4:D:3712:HOH:O	2.40	0.43
1:B:1018:ASP:CA	4:B:1878:HOH:O	2.65	0.43
1:C:2224:PRO:HB3	1:C:2255:ARG:HG3	2.00	0.43
1:A:238:VAL:HG11	1:A:255:ARG:HH11	1.83	0.43
1:C:2011:PRO:HD2	1:C:2100:ALA:O	2.18	0.43
1:A:199:GLN:CB	4:A:4624:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3022:THR:HB	1:D:3321:PRO:HB3	2.01	0.42
1:C:2160:GLU:HG3	4:C:2734:HOH:O	2.20	0.42
1:A:133:SER:OG	1:A:141:ARG:NH1	2.53	0.42
1:B:1022:THR:O	1:B:1025:LEU:HB2	2.20	0.42
1:C:2349:MET:HG2	1:C:2360:LEU:HD21	2.01	0.42
1:D:3083:HIS:CE1	1:D:3167:THR:OG1	2.73	0.42
1:D:3148:ALA:HB2	1:D:3201:TYR:CD1	2.54	0.42
1:B:1192:PRO:HG2	1:B:1193:PHE:CD2	2.55	0.41
1:C:2101:HIS:HD2	1:C:2103:THR:OG1	2.03	0.41
1:B:1368:ASN:ND2	1:B:1368:ASN:C	2.76	0.41
1:A:22:THR:HA	1:A:25:LEU:HD22	2.01	0.41
1:C:2214:ILE:HD12	4:C:2793:HOH:O	2.07	0.41
1:A:171:LEU:HD22	1:A:227:ILE:HG23	2.01	0.41
1:B:1205:THR:CG2	1:B:1207:GLU:HB3	2.50	0.41
1:B:1349:MET:HG2	1:B:1360:LEU:HD21	2.03	0.41
1:A:72:GLU:H	1:A:355:GLN:HE22	1.68	0.41
1:C:2288:ASN:HD22	1:C:2288:ASN:HA	1.55	0.41
1:C:2101:HIS:CD2	1:C:2103:THR:OG1	2.75	0.40
1:D:3191:TYR:OH	1:D:3211:LEU:HG	2.21	0.40
1:A:101:HIS:HD2	1:A:103:THR:OG1	2.04	0.40
1:D:3323:LEU:CB	4:D:3804:HOH:O	2.56	0.40
1:C:2104:LYS:HE2	4:C:2752:HOH:O	2.19	0.40
1:D:3367:ASP:OD1	4:D:3849:HOH:O	2.22	0.40
1:B:1153:GLN:NE2	4:B:1659:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	351/374 (94%)	339 (97%)	9 (3%)	3 (1%)	14 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	366/374 (98%)	355 (97%)	9 (2%)	2 (0%)	25	17
1	C	346/374 (92%)	333 (96%)	10 (3%)	3 (1%)	14	7
1	D	366/374 (98%)	355 (97%)	10 (3%)	1 (0%)	37	29
All	All	1429/1496 (96%)	1382 (97%)	38 (3%)	9 (1%)	22	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	215	TYR
1	A	297	SER
1	B	1297	SER
1	C	2096	ALA
1	C	2124	TYR
1	D	3297	SER
1	C	2297	SER
1	B	1019	VAL

### 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	282/298 (95%)	266 (94%)	16 (6%)	17	9
1	B	292/298 (98%)	278 (95%)	14 (5%)	21	14
1	C	277/298 (93%)	266 (96%)	11 (4%)	27	19
1	D	292/298 (98%)	280 (96%)	12 (4%)	26	19
All	All	1143/1192 (96%)	1090 (95%)	53 (5%)	23	15

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	67	LEU

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Mol	Chain	Res	Type
1	A	86	LYS
1	A	125	SER
1	A	141	ARG
1	A	163	SER
1	A	190	VAL
1	A	212	ASN
1	A	214	ILE
1	A	227	ILE
1	A	254	LYS
1	A	255	ARG
1	A	323	LEU
1	A	328	LEU
1	A	363	LEU
1	A	365	LEU
1	B	1019	VAL
1	B	1025	LEU
1	B	1141	ARG
1	B	1145	ILE
1	B	1190	VAL
1	B	1199	GLN
1	B	1200	ARG
1	B	1203	ARG
1	B	1205	THR
1	B	1211	LEU
1	B	1323	LEU
1	B	1328	LEU
1	B	1363	LEU
1	B	1365	LEU
1	C	2025	LEU
1	C	2130	GLU
1	C	2141	ARG
1	C	2167	THR
1	C	2195	MET
1	C	2214	ILE
1	C	2288	ASN
1	C	2323	LEU
1	C	2328	LEU
1	C	2363	LEU
1	C	2365	LEU
1	D	3025	LEU
1	D	3031	LYS
1	D	3130	GLU

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Mol	Chain	Res	Type
1	D	3141	ARG
1	D	3190	VAL
1	D	3200	ARG
1	D	3203	ARG
1	D	3211	LEU
1	D	3225	ARG
1	D	3289	LYS
1	D	3328	LEU
1	D	3365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	ASN
1	A	83	HIS
1	A	101	HIS
1	A	137	ASN
1	A	154	ASN
1	A	187	ASN
1	A	212	ASN
1	A	288	ASN
1	A	350	GLN
1	A	355	GLN
1	A	368	ASN
1	B	1039	ASN
1	B	1069	GLN
1	B	1083	HIS
1	B	1101	HIS
1	B	1137	ASN
1	B	1153	GLN
1	B	1154	ASN
1	B	1187	ASN
1	B	1342	GLN
1	B	1355	GLN
1	B	1368	ASN
1	C	2039	ASN
1	C	2083	HIS
1	C	2101	HIS
1	C	2137	ASN
1	C	2154	ASN
1	C	2187	ASN

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Mol	Chain	Res	Type
1	C	2288	ASN
1	C	2350	GLN
1	C	2355	GLN
1	C	2368	ASN
1	D	3009	ASN
1	D	3035	HIS
1	D	3039	ASN
1	D	3083	HIS
1	D	3101	HIS
1	D	3137	ASN
1	D	3152	GLN
1	D	3153	GLN
1	D	3154	ASN
1	D	3187	ASN
1	D	3199	GLN
1	D	3288	ASN
1	D	3355	GLN
1	D	3368	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	PYR	A	4442	-	5,5,5	3.04	3 (60%)	3,6,6	1.70	1 (33%)
2	FMN	C	2512	-	33,33,33	1.13	2 (6%)	48,50,50	1.33	8 (16%)
2	FMN	D	3512	-	33,33,33	1.21	3 (9%)	48,50,50	1.35	8 (16%)
3	PYR	D	3442	-	5,5,5	2.85	3 (60%)	3,6,6	1.82	2 (66%)
2	FMN	A	4512	-	33,33,33	1.05	2 (6%)	48,50,50	1.23	6 (12%)
2	FMN	B	1512	-	33,33,33	1.41	3 (9%)	48,50,50	1.24	6 (12%)
3	PYR	B	1442	-	5,5,5	2.87	3 (60%)	3,6,6	2.11	2 (66%)

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	PYR	A	4442	-	-	0/4/4/4	-
2	FMN	C	2512	-	-	1/18/18/18	0/3/3/3
2	FMN	D	3512	-	-	1/18/18/18	0/3/3/3
3	PYR	D	3442	-	-	0/4/4/4	-
2	FMN	A	4512	-	-	1/18/18/18	0/3/3/3
2	FMN	B	1512	-	-	1/18/18/18	0/3/3/3
3	PYR	B	1442	-	-	0/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1512	FMN	C4A-N5	4.41	1.40	1.30
3	A	4442	PYR	CA-C	-4.40	1.39	1.54
3	B	1442	PYR	CA-C	-4.38	1.39	1.54
3	D	3442	PYR	CA-C	-4.32	1.40	1.54
2	C	2512	FMN	C4A-N5	4.15	1.39	1.30
2	A	4512	FMN	C4A-N5	3.71	1.38	1.30
3	A	4442	PYR	O-C	3.65	1.31	1.22
3	A	4442	PYR	O3-CA	3.58	1.31	1.23
3	B	1442	PYR	O3-CA	3.43	1.31	1.23
3	D	3442	PYR	O3-CA	3.40	1.31	1.23
2	C	2512	FMN	C10-N1	3.35	1.40	1.33
2	D	3512	FMN	C4A-N5	3.14	1.37	1.30
3	B	1442	PYR	O-C	3.12	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3442	PYR	O-C	3.10	1.30	1.22
2	B	1512	FMN	C10-N1	2.97	1.39	1.33
2	A	4512	FMN	C10-N1	2.93	1.39	1.33
2	D	3512	FMN	C10-N1	2.65	1.38	1.33
2	B	1512	FMN	C5'-C4'	2.56	1.55	1.51
2	D	3512	FMN	C5'-C4'	2.35	1.55	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2512	FMN	O4-C4-C4A	-3.10	118.34	126.53
2	D	3512	FMN	C4-C4A-N5	3.03	122.39	118.21
3	B	1442	PYR	OXT-C-CA	2.79	121.33	113.59
2	A	4512	FMN	O4'-C4'-C5'	-2.71	104.01	109.99
2	C	2512	FMN	C4A-C10-N10	2.63	120.25	116.48
2	D	3512	FMN	C4A-C4-N3	2.61	119.90	113.25
2	D	3512	FMN	C10-C4A-N5	-2.60	119.49	124.81
2	B	1512	FMN	C8M-C8-C9	-2.57	115.04	119.57
2	A	4512	FMN	C10-C4A-N5	-2.57	119.55	124.81
2	B	1512	FMN	C4A-C10-N10	2.51	120.08	116.48
2	A	4512	FMN	C4-N3-C2	-2.49	121.23	125.64
2	C	2512	FMN	C10-C4A-N5	-2.46	119.78	124.81
3	A	4442	PYR	OXT-C-CA	2.45	120.39	113.59
2	A	4512	FMN	C4A-C10-N10	2.41	119.94	116.48
3	B	1442	PYR	OXT-C-O	-2.31	118.41	123.90
2	C	2512	FMN	C9A-C5A-N5	-2.30	120.01	122.45
2	D	3512	FMN	C9A-C5A-N5	-2.29	120.03	122.45
2	D	3512	FMN	C4-N3-C2	-2.27	121.61	125.64
2	D	3512	FMN	C4A-C10-N10	2.26	119.72	116.48
2	C	2512	FMN	O3P-P-O5'	2.22	112.47	106.67
3	D	3442	PYR	OXT-C-O	-2.22	118.61	123.90
2	B	1512	FMN	C9A-C5A-N5	-2.22	120.10	122.45
2	A	4512	FMN	C9A-C5A-N5	-2.22	120.10	122.45
2	B	1512	FMN	C4-N3-C2	-2.16	121.81	125.64
2	C	2512	FMN	C4-C4A-C10	2.14	120.60	116.93
2	B	1512	FMN	C10-C4A-N5	-2.13	120.45	124.81
2	B	1512	FMN	C4A-C4-N3	2.13	118.68	113.25
3	D	3442	PYR	OXT-C-CA	2.10	119.42	113.59
2	C	2512	FMN	C4-N3-C2	-2.09	121.92	125.64
2	D	3512	FMN	O4-C4-C4A	-2.08	121.03	126.53
2	A	4512	FMN	C4A-C4-N3	2.08	118.54	113.25
2	D	3512	FMN	C10-N1-C2	2.03	121.25	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2512	FMN	C4A-C10-N1	-2.02	119.63	124.59

There are no chirality outliers.

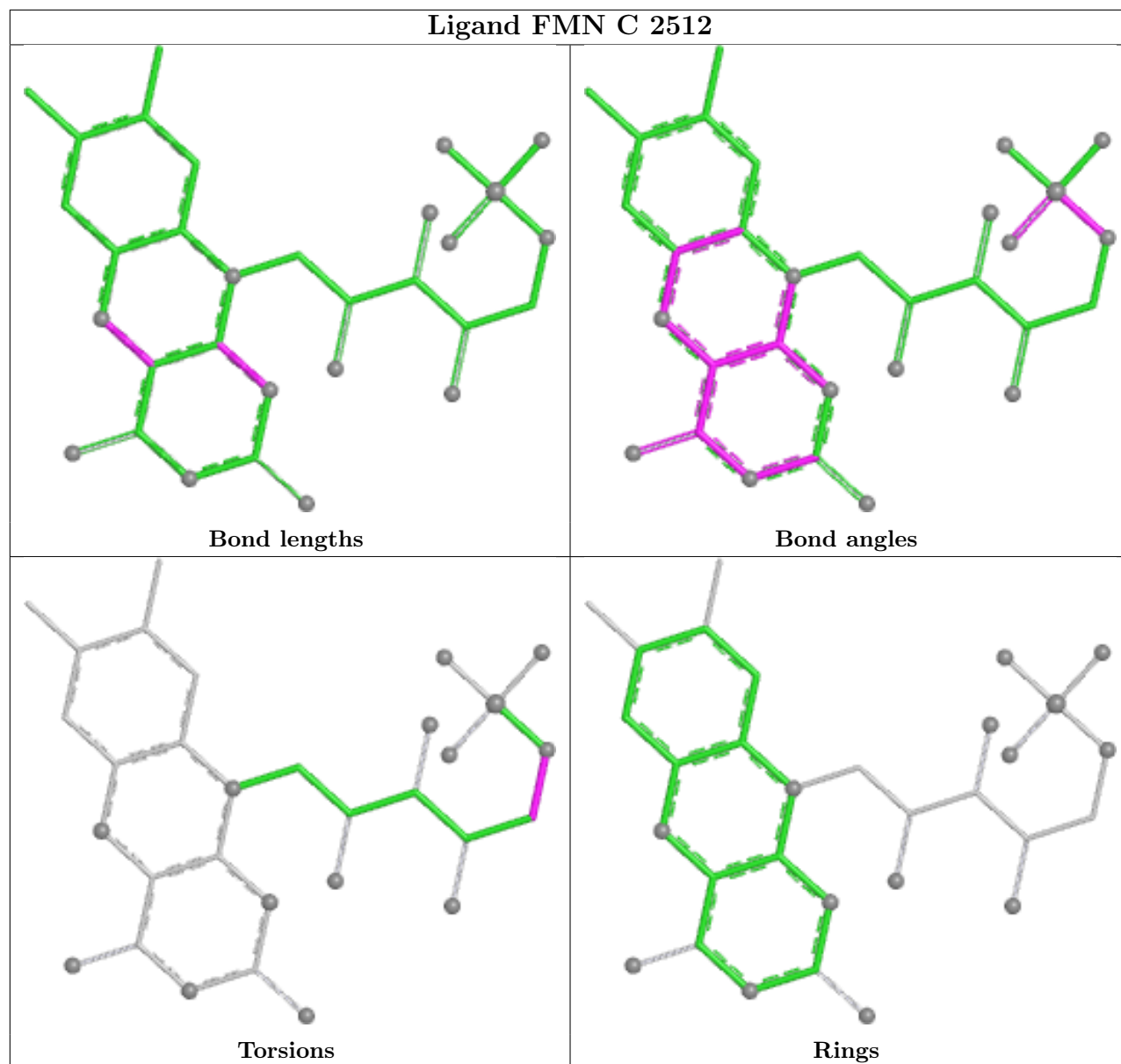
All (4) torsion outliers are listed below:

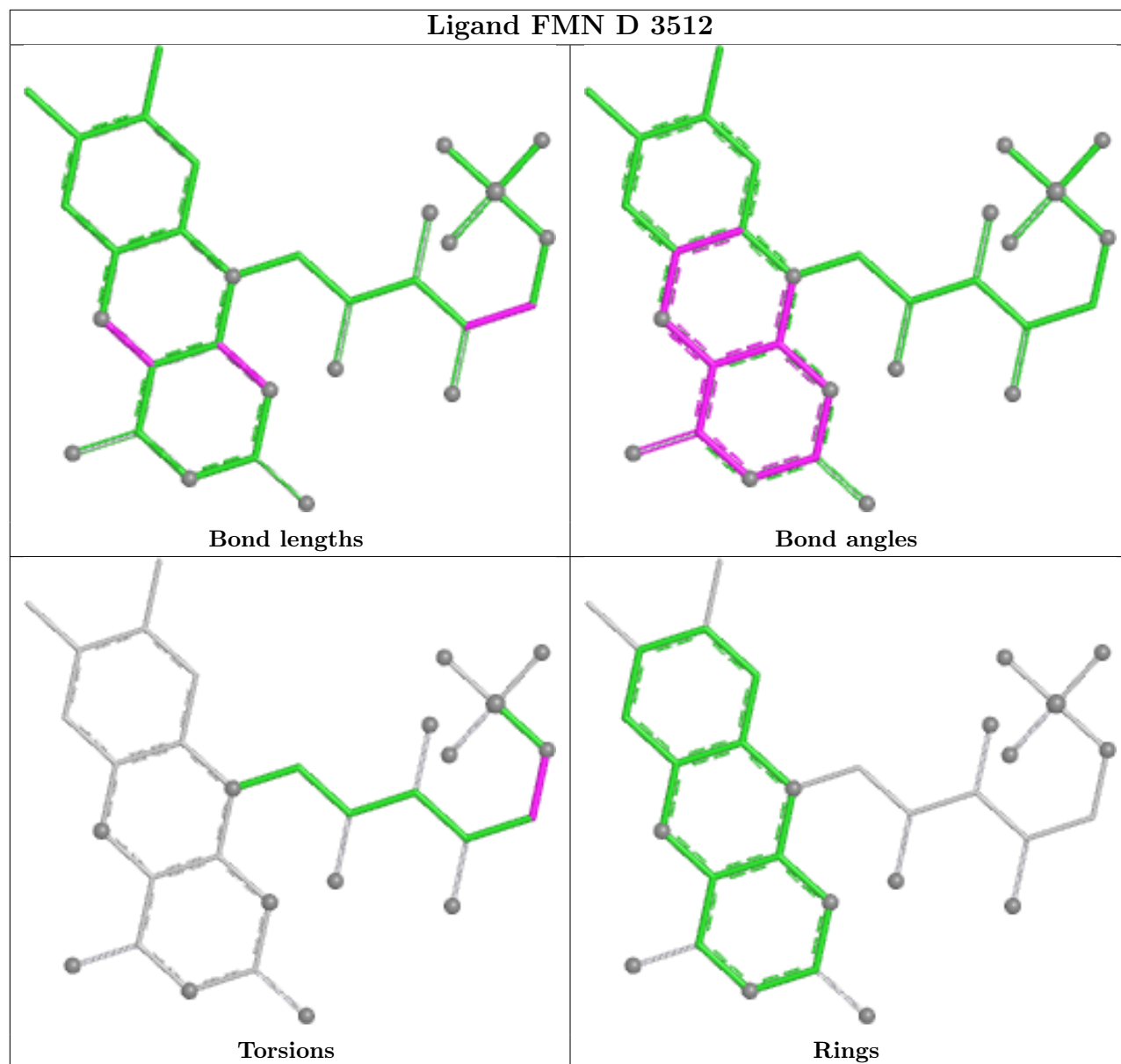
Mol	Chain	Res	Type	Atoms
2	D	3512	FMN	C4'-C5'-O5'-P
2	B	1512	FMN	C4'-C5'-O5'-P
2	C	2512	FMN	C4'-C5'-O5'-P
2	A	4512	FMN	C4'-C5'-O5'-P

There are no ring outliers.

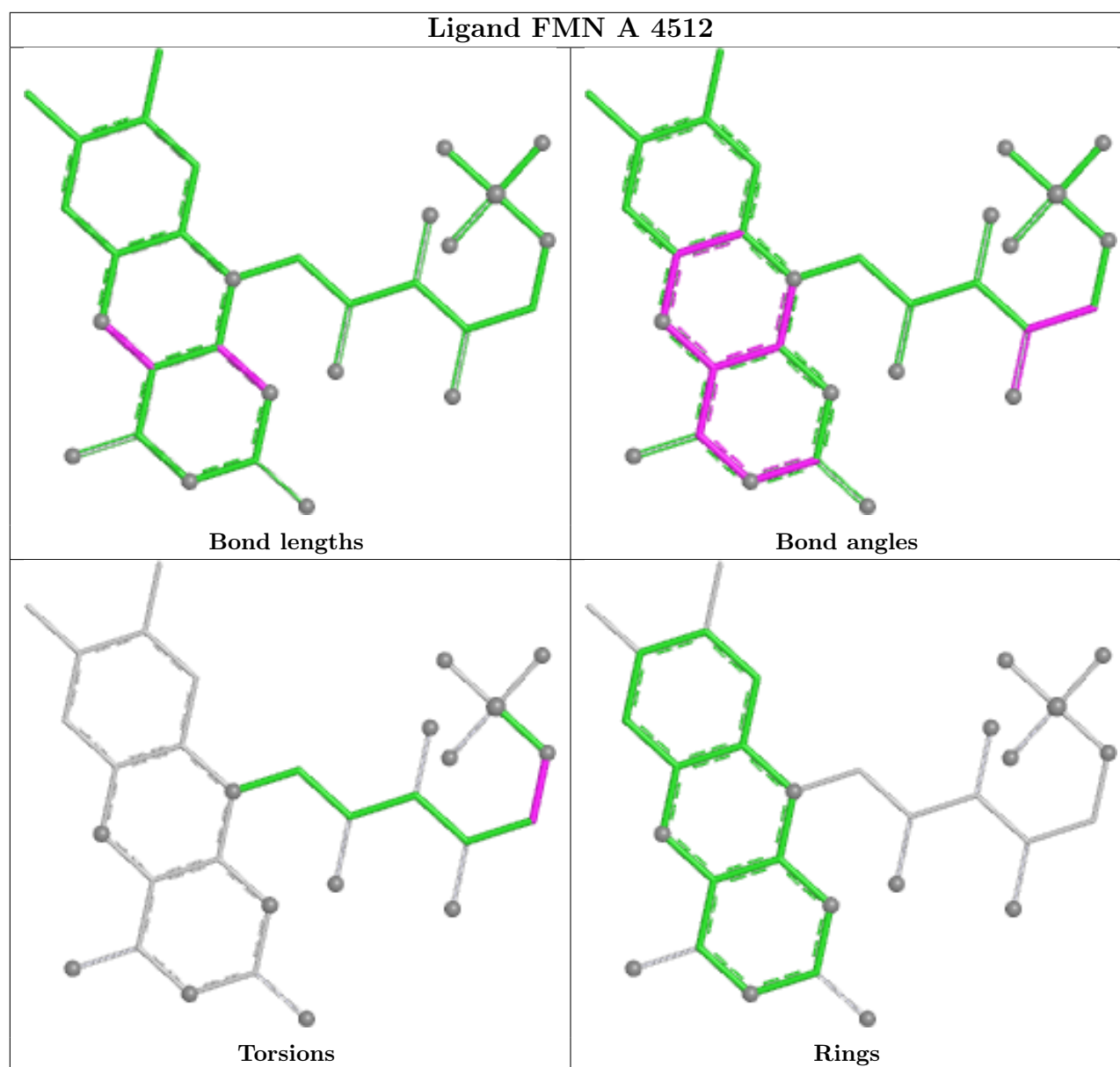
No monomer is involved in short contacts.

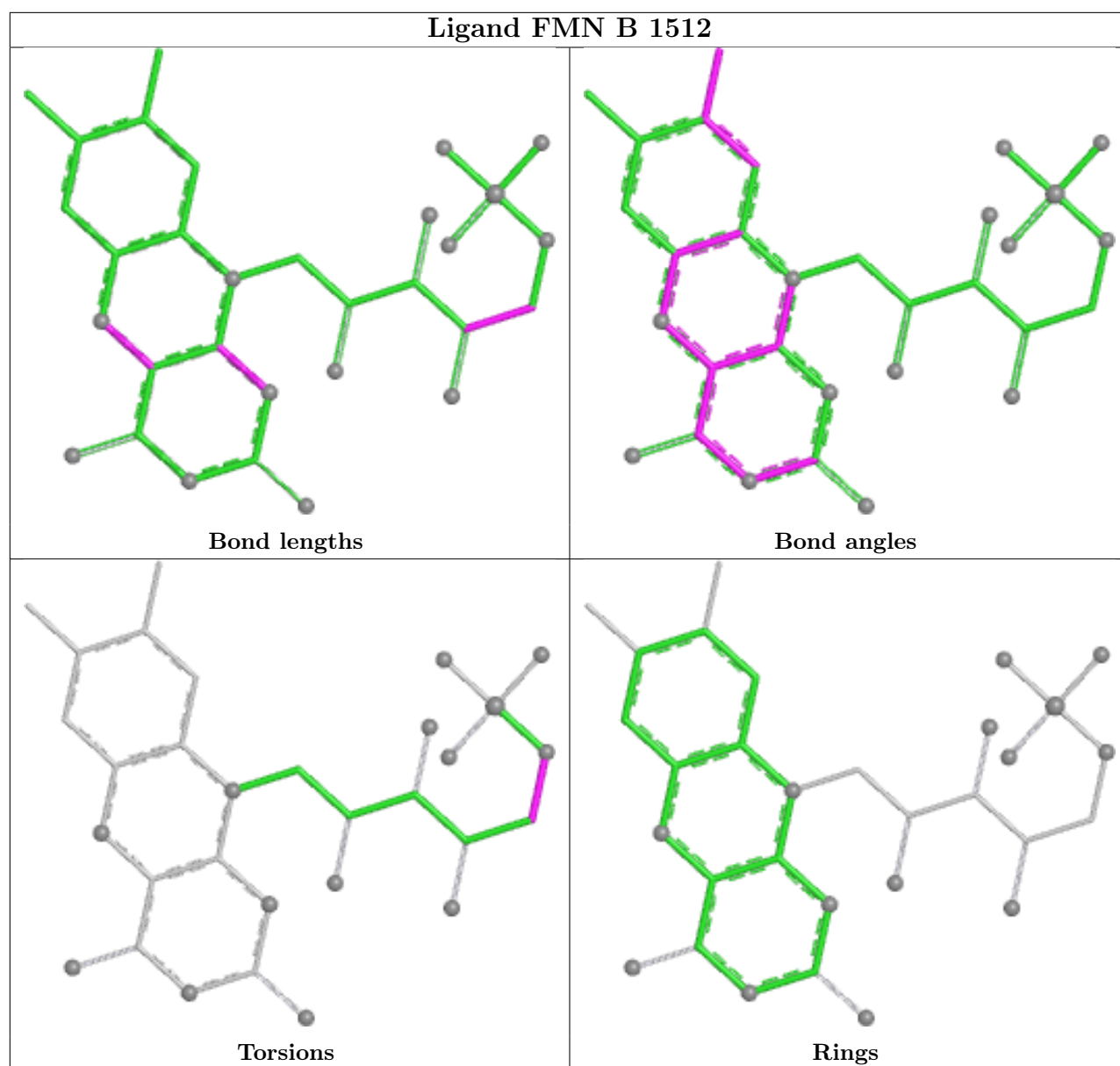
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	355/374 (94%)	0.08	8 (2%) 61 63	16, 29, 43, 51	0
1	B	368/374 (98%)	-0.38	3 (0%) 82 84	11, 19, 30, 46	0
1	C	350/374 (93%)	0.14	8 (2%) 61 63	14, 27, 43, 49	0
1	D	368/374 (98%)	-0.46	4 (1%) 77 79	11, 19, 30, 46	0
All	All	1441/1496 (96%)	-0.16	23 (1%) 70 72	11, 23, 40, 51	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	5.8
1	C	2124	TYR	4.9
1	C	2123	ALA	4.8
1	B	1208	GLY	3.5
1	C	2235	GLY	3.3
1	A	212	ASN	3.2
1	D	3216	GLY	3.1
1	C	2214	ILE	3.1
1	D	3208	GLY	3.1
1	A	235	GLY	2.8
1	C	2130	GLU	2.8
1	A	227	ILE	2.7
1	B	1255	ARG	2.6
1	A	214	ILE	2.5
1	B	1018	ASP	2.5
1	D	3203	ARG	2.3
1	D	3067	LEU	2.3
1	A	82	GLY	2.2
1	C	2195	MET	2.2
1	A	198	VAL	2.2
1	C	2163	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	2254	LYS	2.1
1	A	160	GLU	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

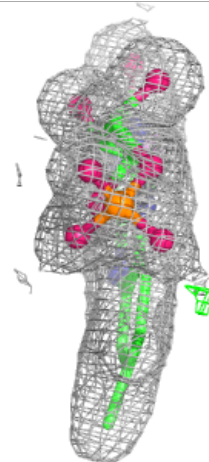
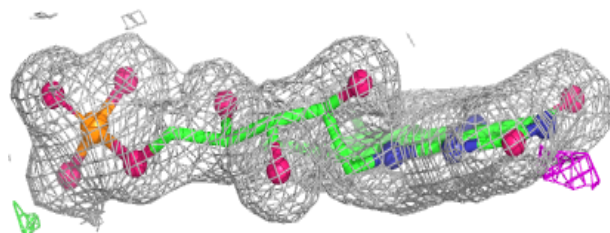
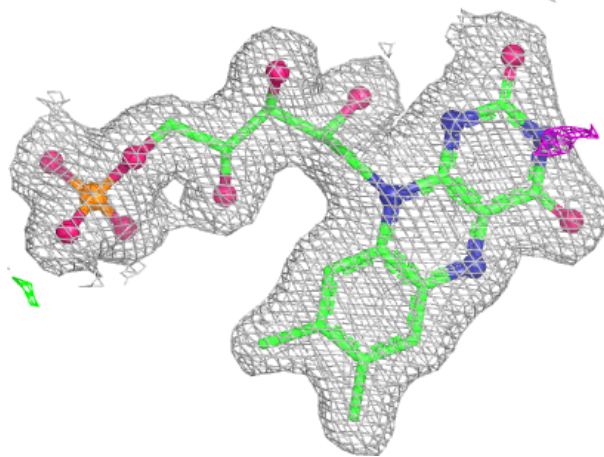
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PYR	A	4442	6/6	0.91	0.10	34,35,36,37	0
3	PYR	B	1442	6/6	0.94	0.09	25,29,33,33	0
2	FMN	A	4512	31/31	0.96	0.07	17,23,25,27	0
2	FMN	C	2512	31/31	0.96	0.07	19,25,28,28	0
3	PYR	D	3442	6/6	0.96	0.08	19,23,26,27	0
2	FMN	B	1512	31/31	0.97	0.06	9,16,19,19	0
2	FMN	D	3512	31/31	0.98	0.05	9,14,16,16	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.

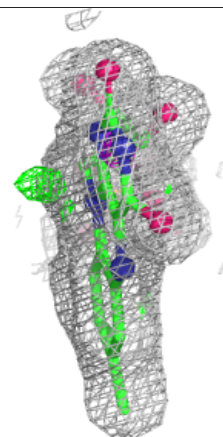
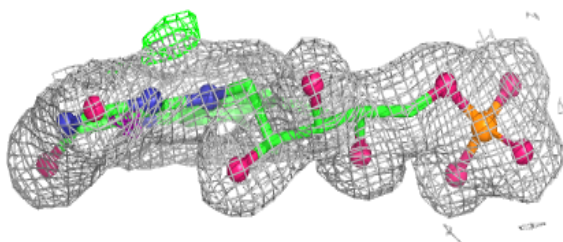
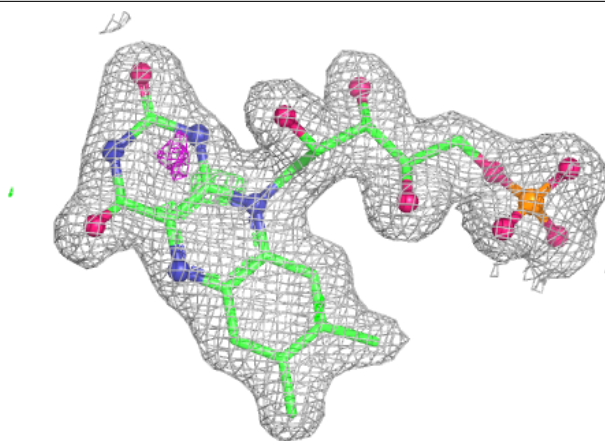
**Electron density around FMN A 4512:**

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



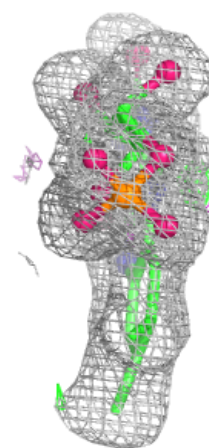
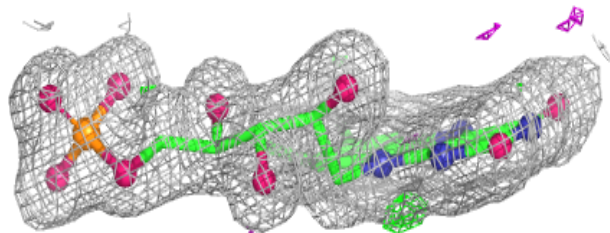
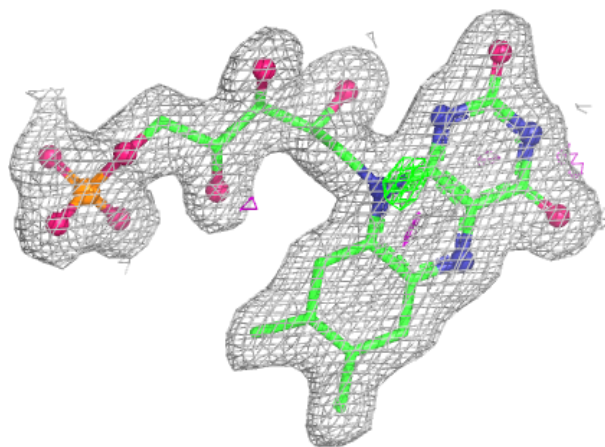
**Electron density around FMN C 2512:**

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



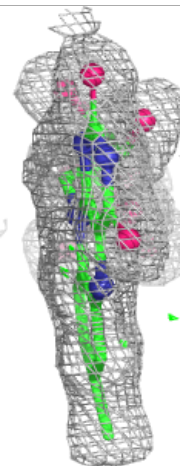
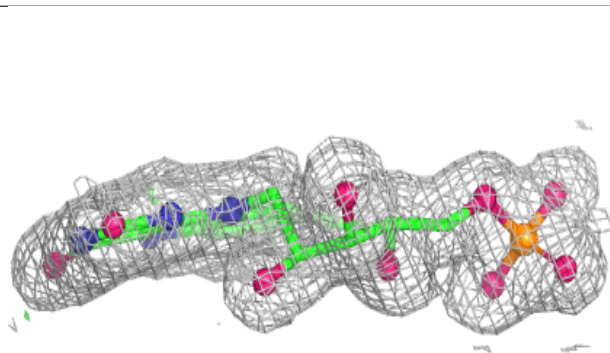
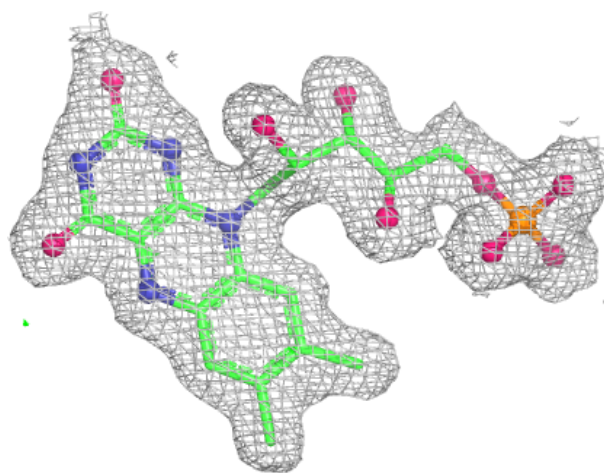
**Electron density around FMN B 1512:**

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



**Electron density around FMN D 3512:**

$2mF_o-DF_c$  (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.