



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:59 am BST

PDB ID : 1F76  
Title : ESCHERICHIA COLI DIHYDROOROTATE DEHYDROGENASE  
Authors : Norager, S.; Jensen, K.F.; Bjornberg, O.; Larsen, S.  
Deposited on : 2000-06-26  
Resolution : 2.50 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 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 : 2.11  
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) : 2.11

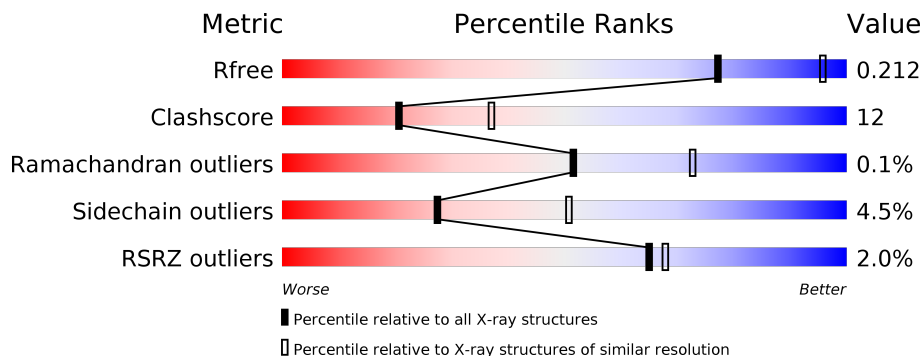
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	336	76% 22% •
1	B	336	75% 23% •
1	D	336	71% 27% •
1	E	336	73% 25% •

## 2 Entry composition [i](#)

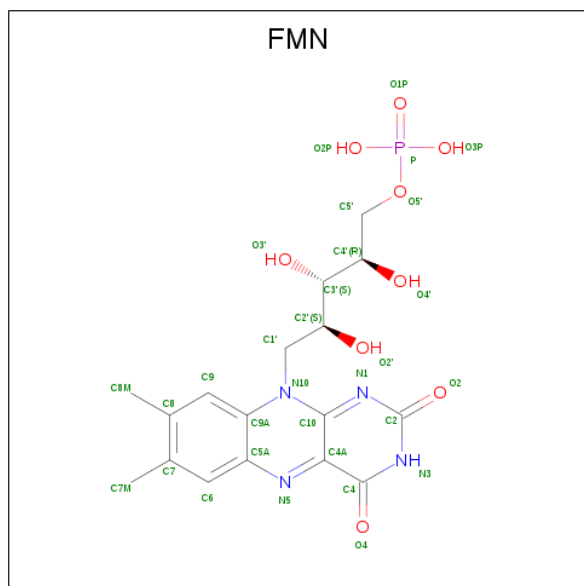
There are 5 unique types of molecules in this entry. The entry contains 11612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydroorotate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	336	Total	C	N	O	S	Se	0	2	0
			2595	1647	453	484	4	7			
1	B	336	Total	C	N	O	S	Se	0	2	0
			2595	1648	453	482	4	8			
1	D	336	Total	C	N	O	S	Se	0	0	0
			2586	1642	452	481	4	7			
1	E	336	Total	C	N	O	S	Se	0	3	0
			2601	1650	457	483	4	7			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



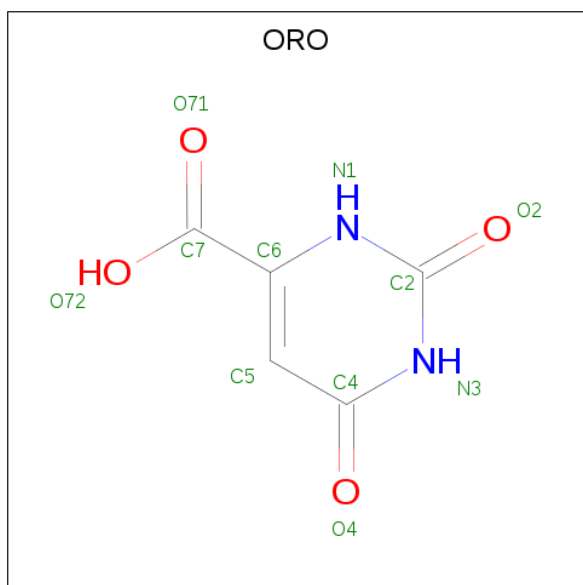
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula:  $C_5H_4N_2O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		
3	A	1	Total	C	N	O	0	1
			22	10	4	8		
3	D	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0

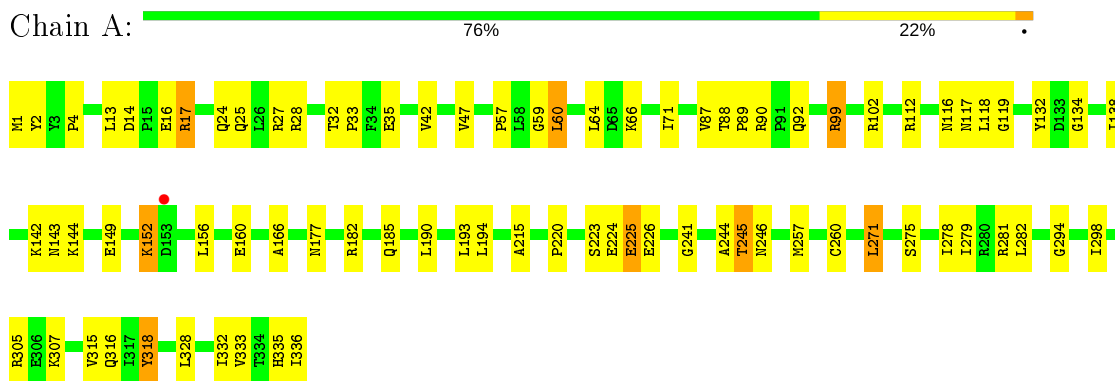
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	340	Total O 340 340	0	0
5	B	231	Total O 231 231	0	0
5	D	180	Total O 180 180	0	0
5	E	292	Total O 292 292	0	0

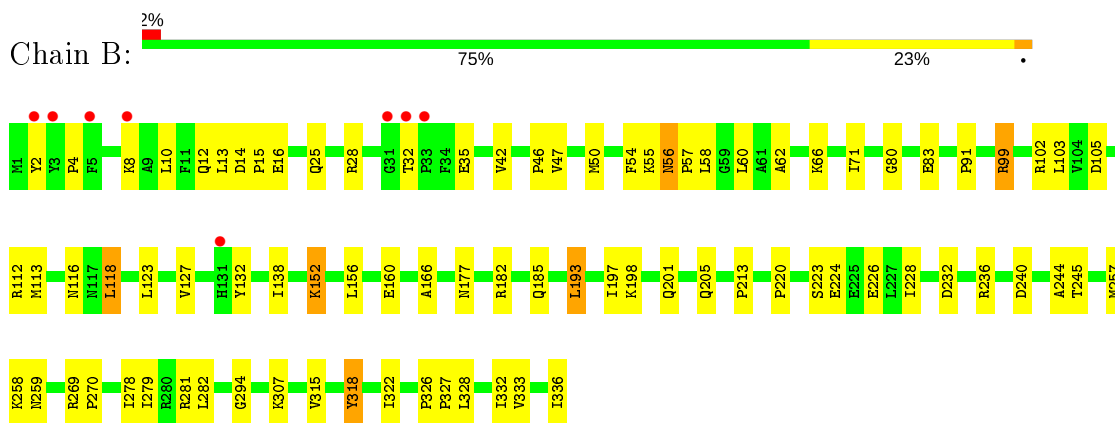
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

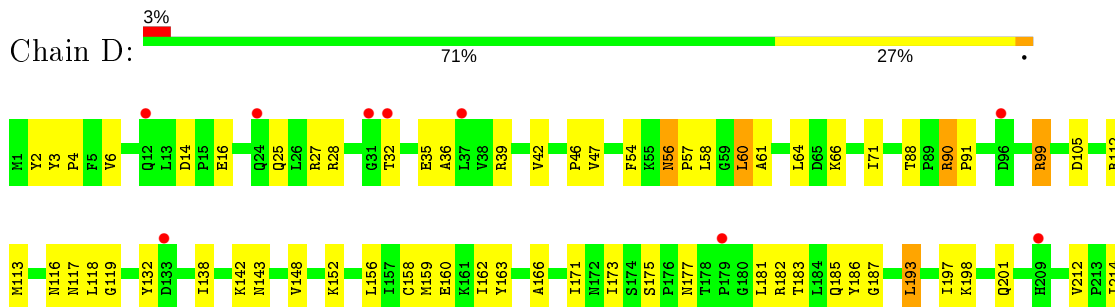
- Molecule 1: Dihydroorotate dehydrogenase (quinone)



- Molecule 1: Dihydroorotate dehydrogenase (quinone)

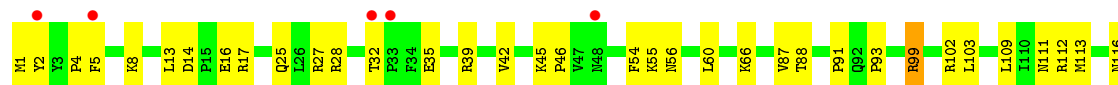
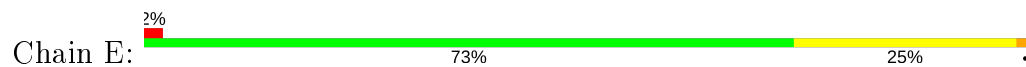


- Molecule 1: Dihydroorotate dehydrogenase (quinone)





- Molecule 1: Dihydroorotate dehydrogenase (quinone)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.70Å 119.70Å 295.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-2.50) 98.5 (19.95-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.50Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.177 , 0.217 0.172 , 0.212	Depositor DCC
$R_{free}$ test set	7460 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.280	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/2642	0.63	0/3564
1	B	0.30	0/2642	0.61	0/3563
1	D	0.30	0/2625	0.60	0/3541
1	E	0.32	0/2652	0.61	0/3577
All	All	0.32	0/10561	0.61	0/14245

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2595	0	2657	60	0
1	B	2595	0	2662	69	0
1	D	2586	0	2653	68	0
1	E	2601	0	2666	73	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
3	A	33	0	9	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11	0	3	0	0
4	B	9	0	3	1	0
4	D	6	0	2	1	0
4	E	9	0	3	2	0
5	A	340	0	0	7	0
5	B	231	0	0	4	0
5	D	180	0	0	3	0
5	E	292	0	0	7	0
All	All	11612	0	10734	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (260) 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:50[B]:MSE:HE2	1:B:213:PRO:HB2	1.32	1.08
1:A:220:PRO:HB3	1:A:245:THR:HG21	1.36	1.03
1:A:90:ARG:H	1:A:143:ASN:HD21	1.17	0.93
1:A:92:GLN:HE22	1:A:144:LYS:H	1.16	0.89
1:B:56:ASN:HD22	1:B:58:LEU:H	1.33	0.77
1:A:13:LEU:HD22	1:A:17:ARG:NH1	2.01	0.75
1:D:56:ASN:HD22	1:D:58:LEU:H	1.35	0.74
1:A:13:LEU:HD22	1:A:17:ARG:HH12	1.53	0.74
1:A:220:PRO:HB3	1:A:245:THR:CG2	2.17	0.74
1:E:198:LYS:NZ	1:E:201:GLN:HE22	1.85	0.73
1:E:66:LYS:HE2	1:E:116:ASN:OD1	1.89	0.73
1:A:149:GLU:HG3	5:A:1676:HOH:O	1.88	0.72
1:B:50[B]:MSE:HE3	1:B:240:ASP:HB2	1.75	0.69
1:D:223:SER:OG	1:D:226:GLU:HG3	1.93	0.68
1:D:182:ARG:O	1:D:185:GLN:HG2	1.94	0.68
1:E:42:VAL:CG1	1:E:333:VAL:HG11	2.23	0.68
1:E:198:LYS:HZ2	1:E:201:GLN:HE22	1.41	0.67
1:D:66:LYS:HE3	5:D:1545:HOH:O	1.95	0.67
1:E:66:LYS:HE3	5:E:1721:HOH:O	1.95	0.67
1:B:42:VAL:CG1	1:B:333:VAL:HG11	2.26	0.66
1:B:28:ARG:HH12	1:E:8:LYS:HE3	1.59	0.65
1:D:327:PRO:O	1:D:331:GLU:HG3	1.98	0.64
1:B:182:ARG:O	1:B:185:GLN:HG2	1.98	0.63
1:B:66:LYS:HE2	1:B:116:ASN:OD1	1.99	0.63
1:E:55:LYS:HG3	5:E:1720:HOH:O	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:THR:O	1:E:35:GLU:HB2	1.98	0.63
1:A:66:LYS:HE2	1:A:116:ASN:OD1	1.97	0.62
1:E:16:GLU:OE1	1:E:99:ARG:HD2	2.00	0.62
1:D:156:LEU:O	1:D:160:GLU:HG3	2.00	0.61
1:D:112:ARG:HA	1:D:177:ASN:CG	2.20	0.61
1:E:117:ASN:ND2	1:E:119:GLY:H	1.98	0.61
1:B:156:LEU:O	1:B:160:GLU:HG3	2.01	0.61
1:D:66:LYS:HE2	1:D:116:ASN:OD1	2.00	0.61
1:A:245:THR:HG23	1:A:246:ASN:O	2.02	0.60
1:A:42:VAL:CG1	1:A:333:VAL:HG11	2.31	0.60
1:E:182:ARG:O	1:E:185:GLN:HG2	2.02	0.59
1:D:56:ASN:ND2	1:D:58:LEU:H	1.98	0.59
1:A:138:ILE:HD12	1:A:166:ALA:HB2	1.83	0.59
1:A:24:GLN:OE1	1:A:27:ARG:NH2	2.35	0.59
1:B:56:ASN:ND2	1:B:58:LEU:H	1.98	0.59
1:D:42:VAL:CG1	1:D:333:VAL:HG11	2.33	0.59
1:D:232:ASP:HB3	5:D:1687:HOH:O	2.03	0.58
1:B:42:VAL:HG13	1:B:333:VAL:HG11	1.85	0.58
1:D:298:ILE:HD11	1:D:307:LYS:HG3	1.85	0.58
1:E:39[B]:ARG:NH1	1:E:39[B]:ARG:HB2	2.19	0.58
1:A:271:LEU:HD22	1:A:275:SER:HB2	1.84	0.58
1:E:111:ASN:HD21	4:E:1639:FMT:C	2.16	0.58
1:A:47:VAL:HG21	1:A:57:PRO:HG3	1.86	0.58
1:D:198:LYS:NZ	1:D:201:GLN:HE22	2.01	0.57
1:A:17:ARG:NH1	5:A:1556:HOH:O	2.37	0.57
1:A:66:LYS:HE3	5:A:1423:HOH:O	2.04	0.57
1:E:152:LYS:O	1:E:156:LEU:HG	2.03	0.57
1:B:223:SER:OG	1:B:226:GLU:HG3	2.05	0.57
1:B:16:GLU:OE1	1:B:99:ARG:HD2	2.04	0.57
1:B:66:LYS:HE3	5:B:1583:HOH:O	2.04	0.56
1:D:262:GLN:HE21	1:D:262:GLN:HA	1.71	0.56
1:B:8:LYS:NZ	1:E:28:ARG:NH1	2.53	0.56
1:E:13:LEU:HD22	1:E:17:ARG:HD3	1.87	0.56
1:A:112:ARG:HA	1:A:177:ASN:CG	2.26	0.56
1:B:198:LYS:NZ	1:B:201:GLN:HE22	2.03	0.56
1:A:281:ARG:NH1	5:A:1666:HOH:O	2.38	0.55
1:B:8:LYS:HZ3	1:E:28:ARG:NH1	2.04	0.55
1:B:13:LEU:HD23	1:E:13:LEU:HD23	1.88	0.55
1:D:46:PRO:HA	1:D:54:PHE:O	2.06	0.55
1:A:156:LEU:O	1:A:160:GLU:HG3	2.07	0.55
1:B:152:LYS:O	1:B:156:LEU:HG	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:THR:H	1:D:117:ASN:HD21	1.54	0.55
1:B:112:ARG:HA	1:B:177:ASN:CG	2.27	0.55
1:A:16:GLU:OE1	1:A:99:ARG:HD2	2.07	0.54
1:D:16:GLU:OE1	1:D:99:ARG:HD2	2.08	0.54
1:A:245:THR:HG23	1:A:246:ASN:N	2.23	0.53
1:B:138:ILE:HD12	1:B:166:ALA:HB2	1.90	0.53
1:D:175:SER:HB3	1:D:181:LEU:HD23	1.91	0.53
1:E:244:ALA:HB1	1:E:245:THR:HG22	1.91	0.53
1:E:280:ARG:NH2	5:E:1683:HOH:O	2.39	0.53
1:D:231:ALA:O	1:D:235:VAL:HG23	2.10	0.52
1:B:56:ASN:HD22	1:B:56:ASN:C	2.12	0.52
1:B:32:THR:O	1:B:35:GLU:HB2	2.09	0.52
1:B:55:LYS:HG3	1:B:80:GLY:HA2	1.92	0.52
1:E:138:ILE:HD12	1:E:166:ALA:HB2	1.90	0.52
1:B:294:GLY:O	1:B:315:VAL:HA	2.10	0.51
1:D:262:GLN:NE2	1:D:262:GLN:HA	2.25	0.51
1:D:56:ASN:HD22	1:D:56:ASN:C	2.13	0.51
1:E:117:ASN:HD22	1:E:119:GLY:H	1.59	0.51
1:A:220:PRO:O	1:A:278:ILE:HD11	2.10	0.51
1:D:294:GLY:O	1:D:315:VAL:HA	2.09	0.51
1:B:258:LYS:O	1:B:259:ASN:HB2	2.11	0.50
1:D:60:LEU:HD11	1:D:64:LEU:HD23	1.93	0.50
1:B:244:ALA:HB1	1:B:245:THR:HG22	1.94	0.50
1:D:88:THR:H	1:D:117:ASN:ND2	2.10	0.50
1:D:227:LEU:O	1:D:227:LEU:HD13	2.12	0.50
1:B:318:TYR:HE1	1:B:322:ILE:HD11	1.76	0.50
1:D:220:PRO:O	1:D:278:ILE:HD11	2.11	0.50
1:D:99:ARG:HD3	1:D:113:MSE:SE	2.61	0.50
1:E:27:ARG:HD3	5:E:1882:HOH:O	2.11	0.49
1:B:113:MSE:HB2	4:B:1440:FMT:C	2.42	0.49
1:D:255:GLN:HA	1:D:255:GLN:OE1	2.13	0.49
1:A:102:ARG:NH1	5:A:1354:HOH:O	2.43	0.49
1:D:138:ILE:HD12	1:D:166:ALA:HB2	1.93	0.49
1:D:112:ARG:HA	1:D:177:ASN:ND2	2.28	0.49
1:E:1:MSE:HG2	5:E:1899:HOH:O	2.12	0.49
1:D:318:TYR:C	1:D:318:TYR:HD1	2.15	0.49
1:E:321:PHE:CE1	1:E:329:ILE:HD11	2.47	0.49
1:A:27:ARG:HG2	5:A:1383:HOH:O	2.13	0.49
1:A:89:PRO:HD2	1:A:143:ASN:ND2	2.27	0.48
1:B:46:PRO:HA	1:B:54:PHE:O	2.13	0.48
1:D:262:GLN:HE21	1:D:262:GLN:CA	2.26	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASN:ND2	1:A:119:GLY:H	2.12	0.48
1:D:117:ASN:ND2	1:D:119:GLY:H	2.11	0.48
1:E:112:ARG:HA	1:E:177:ASN:CG	2.34	0.48
1:A:25:GLN:O	1:A:28:ARG:HB3	2.13	0.48
1:A:42:VAL:HG13	1:A:333:VAL:HG11	1.96	0.48
1:D:258:LYS:O	1:D:259:ASN:HB2	2.13	0.48
1:B:99:ARG:HG3	5:B:1481:HOH:O	2.14	0.48
1:D:224:GLU:O	1:D:228:ILE:HG13	2.14	0.48
1:D:60:LEU:HD22	1:D:61:ALA:O	2.14	0.48
1:E:25:GLN:O	1:E:28:ARG:HB3	2.13	0.48
1:B:152:LYS:HB3	1:B:152:LYS:NZ	2.29	0.47
1:D:56:ASN:ND2	1:D:56:ASN:C	2.68	0.47
1:E:102:ARG:C	1:E:103:LEU:HD12	2.35	0.47
1:E:42:VAL:HG11	1:E:333:VAL:HG11	1.96	0.47
1:B:102:ARG:C	1:B:103:LEU:HD12	2.35	0.47
1:E:318:TYR:HE1	1:E:322:ILE:HD11	1.79	0.47
1:B:8:LYS:HZ1	1:E:28:ARG:HH11	1.62	0.47
1:D:113:MSE:HB2	4:D:1539:FMT:C	2.44	0.47
1:E:280:ARG:O	1:E:284:LEU:HD22	2.15	0.47
1:D:318:TYR:C	1:D:318:TYR:CD1	2.87	0.47
1:B:28:ARG:NH1	1:E:8:LYS:HE3	2.29	0.47
1:E:223:SER:OG	1:E:226:GLU:HG3	2.15	0.47
1:D:230:VAL:O	1:D:234:LEU:HG	2.14	0.46
1:E:5:PHE:O	1:E:8:LYS:HB3	2.16	0.46
1:B:62:ALA:HB2	1:B:83:GLU:HG2	1.97	0.46
1:D:152:LYS:O	1:D:156:LEU:HG	2.15	0.46
1:E:220:PRO:O	1:E:278:ILE:HD11	2.15	0.46
1:D:105:ASP:HB2	1:D:257:MSE:HE2	1.97	0.46
1:B:15:PRO:HG3	1:B:102:ARG:HG3	1.96	0.46
1:D:244:ALA:O	1:D:294:GLY:HA2	2.15	0.46
1:B:318:TYR:HD1	1:B:318:TYR:C	2.19	0.46
1:E:193:LEU:HD22	1:E:197:ILE:CD1	2.46	0.46
1:E:46:PRO:HA	1:E:54:PHE:O	2.16	0.46
1:A:142:LYS:HG2	1:A:143:ASN:O	2.15	0.46
1:E:190:LEU:O	1:E:194:LEU:HG	2.16	0.46
1:A:32:THR:HB	1:A:33:PRO:HD2	1.98	0.46
1:B:42:VAL:HG11	1:B:333:VAL:HG11	1.96	0.46
1:D:47:VAL:HG21	1:D:57:PRO:HG3	1.97	0.46
1:B:318:TYR:CD1	1:B:318:TYR:C	2.89	0.45
1:E:258:LYS:O	1:E:259:ASN:HB2	2.16	0.45
1:E:318:TYR:CD1	1:E:318:TYR:C	2.90	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ILE:HG22	1:D:132:TYR:HB2	1.98	0.45
1:D:159:MSE:HE3	1:D:214:ILE:HD11	1.98	0.45
1:D:271:LEU:HD22	1:D:275:SER:HB2	1.98	0.45
1:B:279:ILE:HD12	1:B:307:LYS:HD2	1.97	0.45
1:E:332:ILE:O	1:E:336:ILE:HB	2.16	0.45
1:A:220:PRO:HA	1:A:278:ILE:HD13	1.99	0.45
1:A:298:ILE:HD11	1:A:307:LYS:HG3	1.99	0.45
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.17	0.45
1:A:60:LEU:HD11	1:A:64:LEU:HD23	1.98	0.45
1:E:91:PRO:HG3	1:E:118:LEU:O	2.17	0.45
1:E:93:PRO:O	1:E:99:ARG:NH2	2.49	0.45
1:A:220:PRO:HA	1:A:278:ILE:CD1	2.46	0.45
1:E:156:LEU:HB3	1:E:200:LYS:HD2	1.99	0.45
1:E:42:VAL:HG13	1:E:333:VAL:HG11	1.99	0.45
1:A:279:ILE:HD12	1:A:307:LYS:HD2	1.98	0.45
1:A:318:TYR:CD1	1:A:318:TYR:C	2.91	0.45
1:E:318:TYR:HD1	1:E:318:TYR:C	2.20	0.45
1:B:8:LYS:NZ	1:E:25:GLN:OE1	2.47	0.45
1:B:8:LYS:NZ	1:E:28:ARG:HH11	2.15	0.45
1:A:279:ILE:CD1	1:A:307:LYS:HD2	2.46	0.44
1:A:71:ILE:HG22	1:A:132:TYR:HB2	1.99	0.44
1:A:244:ALA:HA	1:A:245:THR:HA	1.68	0.44
1:B:205[A]:GLN:NE2	5:B:1586:HOH:O	2.42	0.44
1:D:193:LEU:HD22	1:D:197:ILE:CD1	2.47	0.44
1:D:198:LYS:HZ2	1:D:201:GLN:HE22	1.64	0.44
1:E:175:SER:HB3	1:E:181:LEU:HD23	1.99	0.44
1:E:113:MSE:HB2	4:E:1638:FMT:C	2.47	0.44
1:E:245:THR:O	1:E:295:VAL:HG13	2.17	0.44
1:A:182:ARG:O	1:A:185:GLN:HG2	2.17	0.44
1:D:279:ILE:HD12	1:D:307:LYS:HD2	1.99	0.44
1:A:294:GLY:O	1:A:315:VAL:HA	2.18	0.44
1:D:90:ARG:HB3	1:D:91:PRO:HD2	2.00	0.44
1:A:152:LYS:O	1:A:156:LEU:HG	2.17	0.44
1:D:163:TYR:CE1	1:D:212:VAL:HB	2.53	0.44
1:B:71:ILE:HG22	1:B:132:TYR:HB2	1.99	0.43
1:B:112:ARG:HA	1:B:177:ASN:OD1	2.18	0.43
1:A:88:THR:H	1:A:117:ASN:HD21	1.64	0.43
1:B:232:ASP:O	1:B:236:ARG:HG3	2.18	0.43
1:E:99:ARG:HG3	5:E:1695:HOH:O	2.16	0.43
1:A:32:THR:O	1:A:35:GLU:HB2	2.18	0.43
1:B:47:VAL:HG21	1:B:57:PRO:HG3	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:H	1:B:55:LYS:HG2	1.62	0.43
1:E:271:LEU:HD22	1:E:275:SER:HB2	2.00	0.43
1:B:8:LYS:HZ3	1:E:28:ARG:HH12	1.64	0.43
1:E:286:LEU:HD12	1:E:292:ILE:HD11	2.01	0.43
1:A:13:LEU:O	1:A:102:ARG:NH2	2.50	0.43
1:A:318:TYR:HD1	1:A:318:TYR:C	2.21	0.43
1:B:123:LEU:O	1:B:127:VAL:HG23	2.18	0.43
1:B:269:ARG:HB3	1:B:270:PRO:HD3	2.01	0.43
1:B:56:ASN:C	1:B:56:ASN:ND2	2.72	0.43
1:B:279:ILE:CD1	1:B:307:LYS:HD2	2.49	0.43
1:E:2:TYR:CG	1:E:4:PRO:HD2	2.54	0.43
1:E:45:LYS:O	1:E:56:ASN:HA	2.19	0.43
1:B:2:TYR:CG	1:B:4:PRO:HD2	2.53	0.42
1:D:183:THR:HA	1:D:186:TYR:CD1	2.53	0.42
1:A:332:ILE:O	1:A:336:ILE:HB	2.19	0.42
1:D:224:GLU:HG2	1:D:281:ARG:HH11	1.83	0.42
1:E:27:ARG:NH2	5:E:1929:HOH:O	2.51	0.42
1:D:36:ALA:HA	1:D:39:ARG:NH1	2.34	0.42
1:E:294:GLY:O	1:E:315:VAL:HA	2.19	0.42
1:A:90:ARG:HG2	5:A:1608:HOH:O	2.18	0.42
1:B:193:LEU:HD22	1:B:197:ILE:CD1	2.50	0.42
1:B:12:GLN:O	1:E:17:ARG:NH2	2.51	0.42
1:D:27:ARG:NH1	5:D:1604:HOH:O	2.52	0.42
1:B:91:PRO:HB3	1:B:118:LEU:C	2.39	0.42
1:E:88:THR:H	1:E:117:ASN:HD21	1.68	0.42
1:A:215:ALA:HA	1:A:241:GLY:O	2.20	0.42
1:B:220:PRO:O	1:B:278:ILE:HD11	2.19	0.42
1:D:3:TYR:O	1:D:6:VAL:N	2.53	0.42
1:E:329:ILE:O	1:E:333:VAL:HG23	2.20	0.42
1:B:224:GLU:O	1:B:228:ILE:HG13	2.20	0.41
1:E:132:TYR:CZ	1:E:134:GLY:HA3	2.55	0.41
1:E:198:LYS:NZ	1:E:201:GLN:NE2	2.62	0.41
1:A:152:LYS:NZ	1:A:152:LYS:HB3	2.36	0.41
1:B:326:PRO:N	1:B:327:PRO:CD	2.84	0.41
1:B:42:VAL:HG13	1:B:333:VAL:CG1	2.48	0.41
1:D:158:CYS:O	1:D:162:ILE:HG12	2.20	0.41
1:E:159:MSE:SE	1:E:197:ILE:HG23	2.70	0.41
1:A:190:LEU:O	1:A:194:LEU:HG	2.21	0.41
1:A:257:MSE:O	1:A:260:CYS:HB3	2.21	0.41
1:D:244:ALA:HA	1:D:245:THR:HA	1.59	0.41
1:B:332:ILE:O	1:B:336:ILE:HB	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HG22	1:D:173:ILE:HG23	2.03	0.41
1:D:2:TYR:CG	1:D:4:PRO:HD2	2.56	0.41
1:D:142:LYS:HG2	1:D:143:ASN:O	2.20	0.41
1:D:32:THR:O	1:D:35:GLU:HB2	2.20	0.41
1:E:42:VAL:HG13	1:E:333:VAL:CG1	2.50	0.41
1:A:305:ARG:NH2	1:A:335:HIS:O	2.54	0.41
1:D:42:VAL:HG11	1:D:333:VAL:HG11	2.02	0.41
1:B:10:LEU:C	1:B:12:GLN:H	2.23	0.41
1:A:2:TYR:CG	1:A:4:PRO:HD2	2.56	0.41
1:E:88:THR:H	1:E:117:ASN:ND2	2.18	0.41
1:A:59:GLY:O	1:A:316:GLN:HA	2.21	0.41
1:B:224:GLU:HG2	1:B:281:ARG:HH11	1.86	0.41
1:B:25:GLN:O	1:B:28:ARG:HB3	2.21	0.41
1:D:220:PRO:HA	1:D:278:ILE:CD1	2.51	0.41
1:E:153:ASP:O	1:E:157:ILE:HG13	2.21	0.41
1:A:223:SER:OG	1:A:226:GLU:HG3	2.20	0.40
1:A:87:VAL:HG23	1:A:117:ASN:HD22	1.86	0.40
1:A:132:TYR:CZ	1:A:134:GLY:HA3	2.56	0.40
1:B:279:ILE:HD12	1:B:307:LYS:CD	2.51	0.40
1:D:25:GLN:O	1:D:28:ARG:HB3	2.21	0.40
1:E:220:PRO:HA	1:E:278:ILE:CD1	2.51	0.40
1:E:109:LEU:O	1:E:266:LEU:HD12	2.21	0.40
1:A:13:LEU:HD13	1:A:17:ARG:HH11	1.86	0.40
1:B:105:ASP:HB2	1:B:257:MSE:HE2	2.02	0.40
1:B:257:MSE:HE2	5:B:1636:HOH:O	2.21	0.40
1:D:117:ASN:HD22	1:D:119:GLY:H	1.70	0.40
1:E:87:VAL:HG21	1:E:120:VAL:HA	2.03	0.40
1:B:220:PRO:HB3	1:B:245:THR:OG1	2.22	0.40
1:D:175:SER:HB3	1:D:181:LEU:CD2	2.50	0.40
1:E:279:ILE:CD1	1:E:307:LYS:HD2	2.52	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	336/336 (100%)	327 (97%)	9 (3%)	0	100	100
1	B	336/336 (100%)	326 (97%)	10 (3%)	0	100	100
1	D	334/336 (99%)	320 (96%)	13 (4%)	1 (0%)	41	61
1	E	337/336 (100%)	329 (98%)	8 (2%)	0	100	100
All	All	1343/1344 (100%)	1302 (97%)	40 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	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	281/272 (103%)	266 (95%)	15 (5%)	22	43
1	B	281/272 (103%)	271 (96%)	10 (4%)	35	61
1	D	279/272 (103%)	266 (95%)	13 (5%)	26	49
1	E	282/272 (104%)	270 (96%)	12 (4%)	29	53
All	All	1123/1088 (103%)	1073 (96%)	50 (4%)	27	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	14	ASP
1	A	17	ARG
1	A	60	LEU
1	A	99	ARG
1	A	118	LEU
1	A	152	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	193	LEU
1	A	224	GLU
1	A	225	GLU
1	A	245	THR
1	A	271	LEU
1	A	282	LEU
1	A	318	TYR
1	A	328	LEU
1	B	14	ASP
1	B	56	ASN
1	B	60	LEU
1	B	99	ARG
1	B	118	LEU
1	B	152	LYS
1	B	193	LEU
1	B	282	LEU
1	B	318	TYR
1	B	328	LEU
1	D	14	ASP
1	D	56	ASN
1	D	60	LEU
1	D	90	ARG
1	D	99	ARG
1	D	118	LEU
1	D	148	VAL
1	D	193	LEU
1	D	271	LEU
1	D	282	LEU
1	D	301	VAL
1	D	318	TYR
1	D	328	LEU
1	E	14	ASP
1	E	60	LEU
1	E	99	ARG
1	E	118	LEU
1	E	152	LYS
1	E	193	LEU
1	E	271	LEU
1	E	282	LEU
1	E	284	LEU
1	E	287	ASN
1	E	318	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	92	GLN
1	A	117	ASN
1	A	143	ASN
1	A	185	GLN
1	A	229	GLN
1	A	237	HIS
1	B	40	GLN
1	B	56	ASN
1	B	126	ASN
1	B	150	GLN
1	B	201	GLN
1	B	209	HIS
1	B	259	ASN
1	D	12	GLN
1	D	40	GLN
1	D	56	ASN
1	D	117	ASN
1	D	126	ASN
1	D	185	GLN
1	D	201	GLN
1	D	262	GLN
1	E	12	GLN
1	E	19	HIS
1	E	24	GLN
1	E	40	GLN
1	E	95	ASN
1	E	117	ASN
1	E	126	ASN
1	E	150	GLN
1	E	185	GLN
1	E	201	GLN
1	E	205	GLN
1	E	259	ASN
1	E	287	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMT	E	1638	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMN	B	1437	-	31,33,33	3.42	13 (41%)	40,50,50	3.19	15 (37%)
4	FMT	E	1640	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	1438	-	0,2,2	0.00	-	0,1,1	0.00	-
3	ORO	A	1338	-	6,11,11	2.76	2 (33%)	3,15,15	4.88	2 (66%)
2	FMN	D	1537	-	31,33,33	3.49	13 (41%)	40,50,50	3.16	15 (37%)
4	FMT	D	1538	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMN	A	1337	-	31,33,33	3.77	14 (45%)	40,50,50	2.99	13 (32%)
3	ORO	A	1339[A]	1	6,11,11	2.58	2 (33%)	3,15,15	4.51	2 (66%)
4	FMT	E	1639	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	1440	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	1439	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	1539	-	0,2,2	0.00	-	0,1,1	0.00	-
3	ORO	A	1339[B]	-	6,11,11	2.90	2 (33%)	3,15,15	4.59	2 (66%)
3	ORO	D	1540	-	6,11,11	2.87	2 (33%)	3,15,15	4.88	2 (66%)
2	FMN	E	1637	-	31,33,33	3.50	13 (41%)	40,50,50	3.09	12 (30%)

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	1437	-	-	5/18/18/18	0/3/3/3
3	ORO	A	1338	-	-	0/0/4/4	0/1/1/1
2	FMN	D	1537	-	-	5/18/18/18	0/3/3/3
2	FMN	A	1337	-	-	5/18/18/18	0/3/3/3
3	ORO	A	1339[A]	1	-	0/0/4/4	0/1/1/1
3	ORO	A	1339[B]	-	-	0/0/4/4	0/1/1/1
3	ORO	D	1540	-	-	0/0/4/4	0/1/1/1
2	FMN	E	1637	-	-	5/18/18/18	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1637	FMN	C1'-N10	-10.81	1.37	1.48
2	A	1337	FMN	C1'-N10	-10.76	1.37	1.48
2	D	1537	FMN	C1'-N10	-10.13	1.37	1.48
2	B	1437	FMN	C1'-N10	-9.69	1.38	1.48
2	A	1337	FMN	C4A-N5	9.41	1.46	1.33
2	D	1537	FMN	C4A-N5	7.72	1.44	1.33
2	E	1637	FMN	C4A-N5	7.57	1.44	1.33
2	B	1437	FMN	C4A-C10	6.84	1.45	1.38
2	A	1337	FMN	C4A-C10	6.24	1.45	1.38
2	B	1437	FMN	C9A-N10	6.21	1.46	1.38
2	D	1537	FMN	C4A-C10	6.16	1.45	1.38
2	A	1337	FMN	C9A-N10	6.09	1.46	1.38
2	B	1437	FMN	C4'-C3'	5.92	1.64	1.53
3	A	1339[B]	ORO	C4-N3	5.82	1.43	1.33
2	E	1637	FMN	C9A-N10	5.81	1.46	1.38
2	D	1537	FMN	C9A-N10	5.70	1.46	1.38
2	E	1637	FMN	C4A-C10	5.56	1.44	1.38
2	B	1437	FMN	C4-N3	5.56	1.42	1.33
2	E	1637	FMN	C4'-C3'	5.51	1.63	1.53
2	E	1637	FMN	C4-N3	5.48	1.42	1.33
2	D	1537	FMN	C4'-C3'	5.46	1.63	1.53
2	D	1537	FMN	C4-N3	5.42	1.42	1.33
2	A	1337	FMN	C4'-C3'	5.34	1.63	1.53
2	A	1337	FMN	C4-N3	5.31	1.42	1.33
3	A	1339[A]	ORO	C4-N3	5.21	1.42	1.33
2	B	1437	FMN	C4A-N5	5.19	1.40	1.33

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1540	ORO	C4-N3	4.93	1.41	1.33
3	A	1338	ORO	C4-N3	4.62	1.41	1.33
3	D	1540	ORO	C6-N1	4.51	1.41	1.34
3	A	1338	ORO	C6-N1	4.34	1.41	1.34
2	A	1337	FMN	C5A-N5	-4.24	1.28	1.35
2	B	1437	FMN	C4-C4A	3.88	1.48	1.41
2	D	1537	FMN	C9A-C5A	3.82	1.50	1.42
2	D	1537	FMN	C4-C4A	3.73	1.47	1.41
2	B	1437	FMN	C9A-C5A	3.69	1.50	1.42
2	A	1337	FMN	C9A-C5A	3.66	1.49	1.42
2	E	1637	FMN	C4-C4A	3.62	1.47	1.41
2	A	1337	FMN	C4-C4A	3.52	1.47	1.41
2	A	1337	FMN	C7M-C7	3.51	1.58	1.51
2	B	1437	FMN	C10-N1	3.47	1.37	1.33
2	D	1537	FMN	C7M-C7	3.45	1.57	1.51
2	E	1637	FMN	C7M-C7	3.40	1.57	1.51
2	B	1437	FMN	C7M-C7	3.30	1.57	1.51
2	E	1637	FMN	C9A-C5A	3.29	1.49	1.42
2	A	1337	FMN	C5'-C4'	-3.04	1.47	1.51
3	A	1339[B]	ORO	C6-N1	2.99	1.39	1.34
2	A	1337	FMN	C10-N1	2.90	1.37	1.33
2	D	1537	FMN	C10-N1	2.83	1.36	1.33
2	E	1637	FMN	C10-N1	2.72	1.36	1.33
3	A	1339[A]	ORO	C6-N1	2.68	1.39	1.34
2	A	1337	FMN	P-O2P	-2.59	1.44	1.54
2	B	1437	FMN	C2-N3	2.54	1.43	1.38
2	D	1537	FMN	P-O2P	-2.49	1.45	1.54
2	B	1437	FMN	P-O2P	-2.47	1.45	1.54
2	E	1637	FMN	P-O2P	-2.43	1.45	1.54
2	A	1337	FMN	C2-N3	2.39	1.42	1.38
2	E	1637	FMN	C2-N3	2.33	1.42	1.38
2	D	1537	FMN	C2-N3	2.32	1.42	1.38
2	D	1537	FMN	C5'-C4'	-2.21	1.48	1.51
2	B	1437	FMN	C5'-C4'	-2.17	1.48	1.51
2	E	1637	FMN	C5'-C4'	-2.10	1.48	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1537	FMN	C1'-N10-C9A	9.64	125.88	118.29
2	B	1437	FMN	C1'-N10-C9A	9.35	125.65	118.29
2	A	1337	FMN	C1'-N10-C9A	9.20	125.53	118.29

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1637	FMN	C1'-N10-C9A	8.88	125.28	118.29
2	B	1437	FMN	C4-N3-C2	8.11	121.99	115.14
2	A	1337	FMN	C4-N3-C2	8.00	121.89	115.14
2	D	1537	FMN	C4-N3-C2	7.98	121.88	115.14
2	E	1637	FMN	C4-N3-C2	7.93	121.84	115.14
2	D	1537	FMN	C5A-C9A-N10	7.57	123.20	117.72
3	D	1540	ORO	C5-C4-N3	-7.50	115.33	124.08
3	A	1338	ORO	C5-C4-N3	-7.37	115.47	124.08
3	A	1339[A]	ORO	C5-C4-N3	-7.25	115.62	124.08
2	E	1637	FMN	C5A-C9A-N10	7.14	122.89	117.72
3	A	1339[B]	ORO	C5-C4-N3	-7.04	115.86	124.08
2	B	1437	FMN	C5A-C9A-N10	7.01	122.80	117.72
2	B	1437	FMN	C9A-N10-C10	-6.29	113.67	121.91
2	E	1637	FMN	C9A-N10-C10	-6.11	113.90	121.91
2	D	1537	FMN	C9A-N10-C10	-6.05	113.98	121.91
2	A	1337	FMN	C9A-N10-C10	-6.01	114.04	121.91
2	E	1637	FMN	C4A-C4-N3	-5.64	115.71	123.43
2	A	1337	FMN	C4A-C4-N3	-5.60	115.77	123.43
2	D	1537	FMN	C4A-C4-N3	-5.50	115.91	123.43
2	B	1437	FMN	C4A-C4-N3	-5.44	115.99	123.43
2	A	1337	FMN	C5A-C9A-N10	5.42	121.65	117.72
2	A	1337	FMN	C4-C4A-C10	5.40	123.52	119.95
2	E	1637	FMN	C4-C4A-C10	5.19	123.39	119.95
2	B	1437	FMN	C4-C4A-C10	4.86	123.17	119.95
2	D	1537	FMN	C4-C4A-C10	4.78	123.12	119.95
2	B	1437	FMN	C4-C4A-N5	-4.32	113.66	118.60
3	A	1338	ORO	C4-C5-C6	4.08	119.36	116.73
2	E	1637	FMN	C4-C4A-N5	-3.98	114.05	118.60
3	D	1540	ORO	C4-C5-C6	3.84	119.21	116.73
3	A	1339[B]	ORO	C4-C5-C6	3.66	119.09	116.73
2	A	1337	FMN	C4-C4A-N5	-3.59	114.49	118.60
2	D	1537	FMN	C4-C4A-N5	-3.57	114.51	118.60
2	B	1437	FMN	C6-C5A-N5	3.09	122.46	119.05
2	B	1437	FMN	O5'-C5'-C4'	2.96	117.28	109.36
2	E	1637	FMN	O5'-C5'-C4'	2.88	117.04	109.36
3	A	1339[A]	ORO	C4-C5-C6	2.85	118.57	116.73
2	D	1537	FMN	O5'-C5'-C4'	2.75	116.69	109.36
2	A	1337	FMN	O5'-C5'-C4'	2.57	116.21	109.36
2	B	1437	FMN	O2P-P-O1P	2.57	120.72	110.68
2	E	1637	FMN	O2P-P-O1P	2.55	120.65	110.68
2	A	1337	FMN	O2P-P-O1P	2.54	120.62	110.68
2	E	1637	FMN	C1'-N10-C10	2.53	120.67	118.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1537	FMN	O2P-P-O1P	2.45	120.27	110.68
2	D	1537	FMN	C5'-C4'-C3'	-2.44	107.49	112.20
2	B	1437	FMN	C1'-N10-C10	2.39	120.55	118.41
2	A	1337	FMN	C5'-C4'-C3'	-2.38	107.61	112.20
2	D	1537	FMN	C6-C5A-N5	2.32	121.60	119.05
2	B	1437	FMN	P-O5'-C5'	2.28	124.57	118.30
2	B	1437	FMN	C10-C4A-N5	2.26	122.82	121.26
2	B	1437	FMN	C9A-C5A-N5	-2.25	118.84	122.36
2	D	1537	FMN	C9A-C5A-N5	-2.22	118.89	122.36
2	B	1437	FMN	C5'-C4'-C3'	-2.20	107.96	112.20
2	E	1637	FMN	C5'-C4'-C3'	-2.19	107.97	112.20
2	A	1337	FMN	C1'-N10-C10	2.18	120.36	118.41
2	D	1537	FMN	P-O5'-C5'	2.18	124.30	118.30
2	E	1637	FMN	O4'-C4'-C5'	2.15	114.74	109.92
2	A	1337	FMN	O4'-C4'-C5'	2.12	114.68	109.92
2	D	1537	FMN	O3'-C3'-C4'	2.02	113.69	108.81
2	D	1537	FMN	O4'-C4'-C5'	2.01	114.43	109.92
2	A	1337	FMN	P-O5'-C5'	2.01	123.82	118.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1437	FMN	O3'-C3'-C4'-O4'
2	D	1537	FMN	O3'-C3'-C4'-O4'
2	E	1637	FMN	O3'-C3'-C4'-O4'
2	B	1437	FMN	C2'-C3'-C4'-O4'
2	D	1537	FMN	C2'-C3'-C4'-O4'
2	E	1637	FMN	C2'-C3'-C4'-O4'
2	B	1437	FMN	O3'-C3'-C4'-C5'
2	D	1537	FMN	O3'-C3'-C4'-C5'
2	E	1637	FMN	O3'-C3'-C4'-C5'
2	B	1437	FMN	C2'-C3'-C4'-C5'
2	D	1537	FMN	C2'-C3'-C4'-C5'
2	A	1337	FMN	O3'-C3'-C4'-O4'
2	A	1337	FMN	C2'-C3'-C4'-O4'
2	E	1637	FMN	C4'-C5'-O5'-P
2	E	1637	FMN	C2'-C3'-C4'-C5'
2	B	1437	FMN	C4'-C5'-O5'-P
2	D	1537	FMN	C4'-C5'-O5'-P
2	A	1337	FMN	C4'-C5'-O5'-P
2	A	1337	FMN	O3'-C3'-C4'-C5'

*Continued on next page...*



*Continued from previous page...*

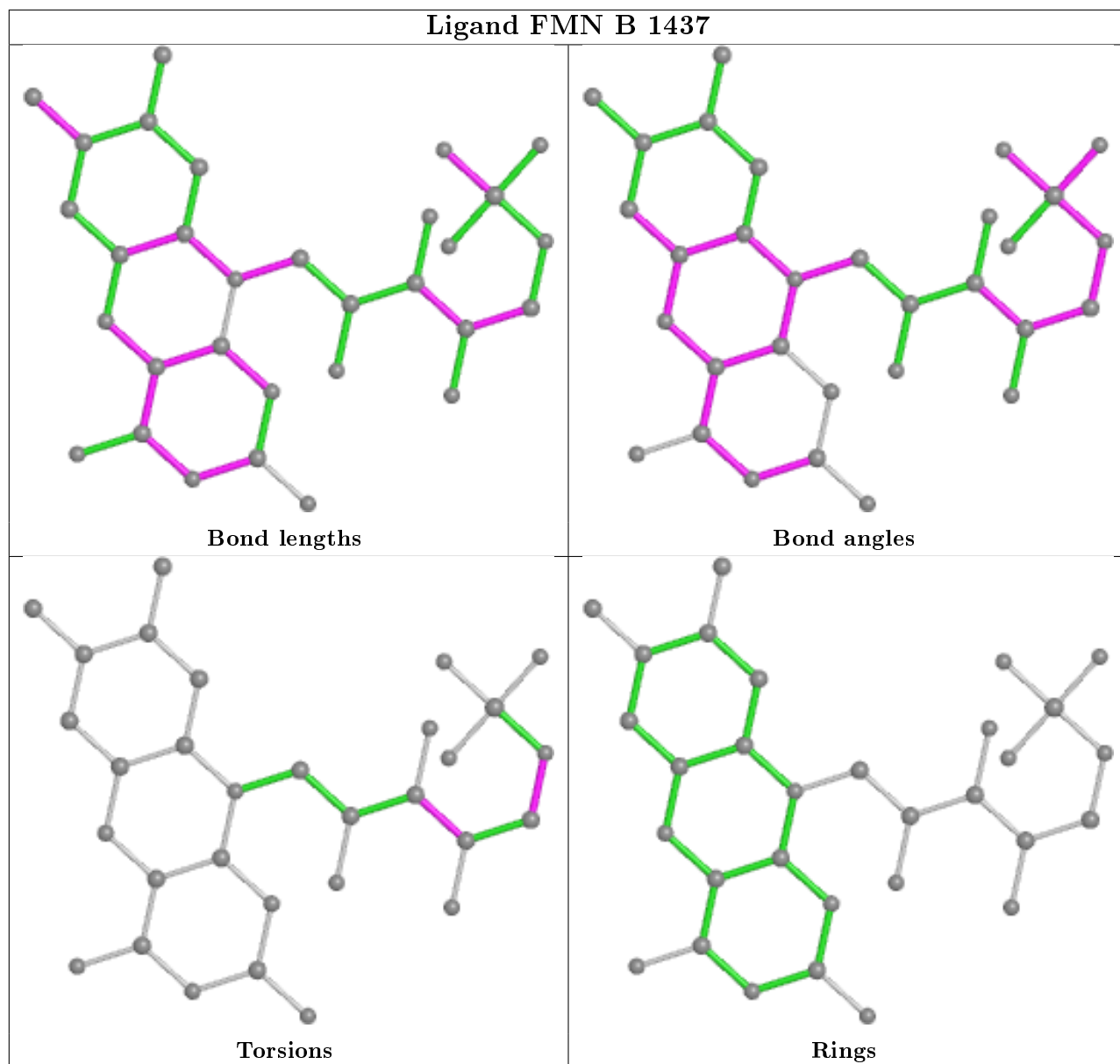
Mol	Chain	Res	Type	Atoms
2	A	1337	FMN	C2'-C3'-C4'-C5'

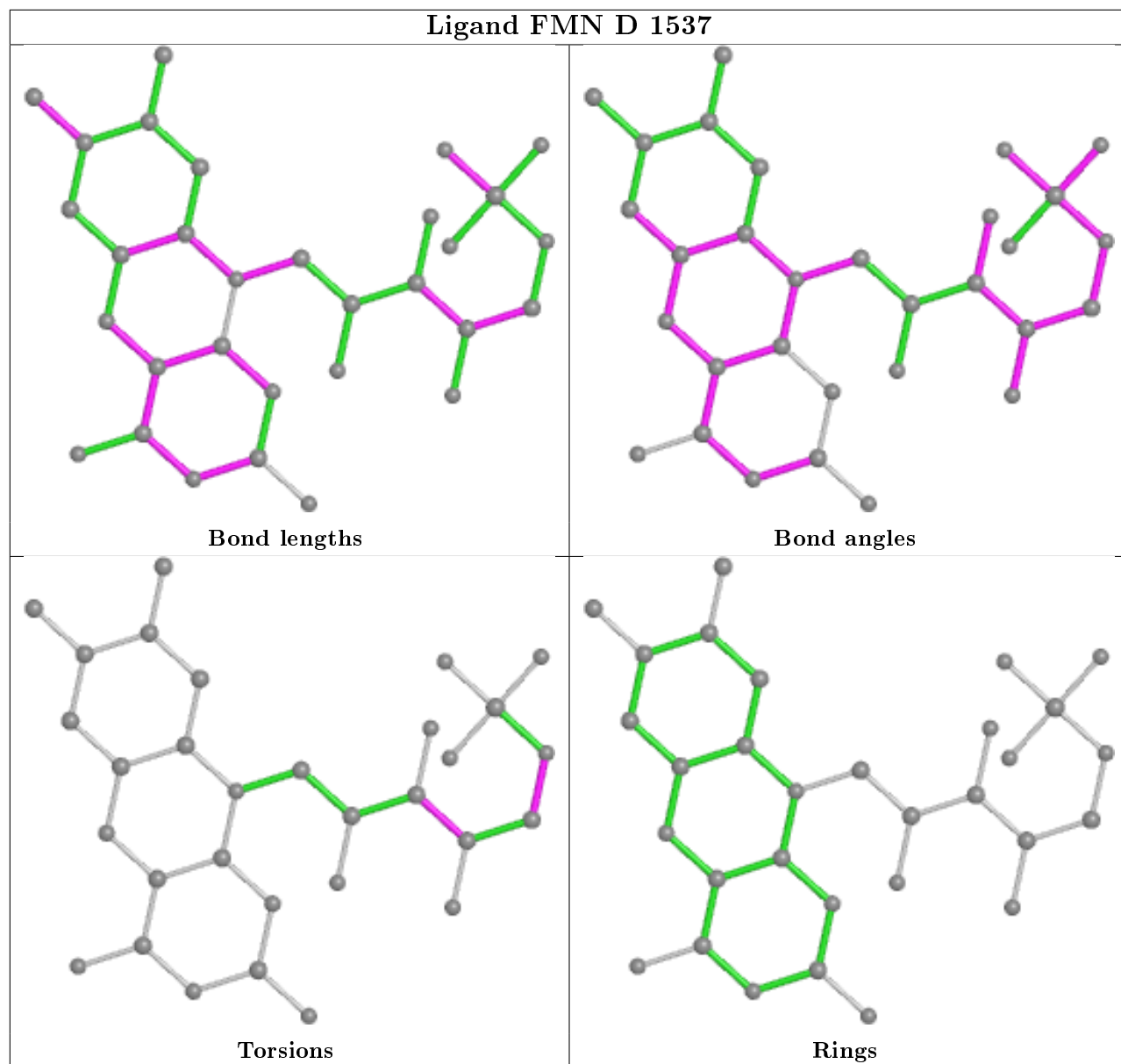
There are no ring outliers.

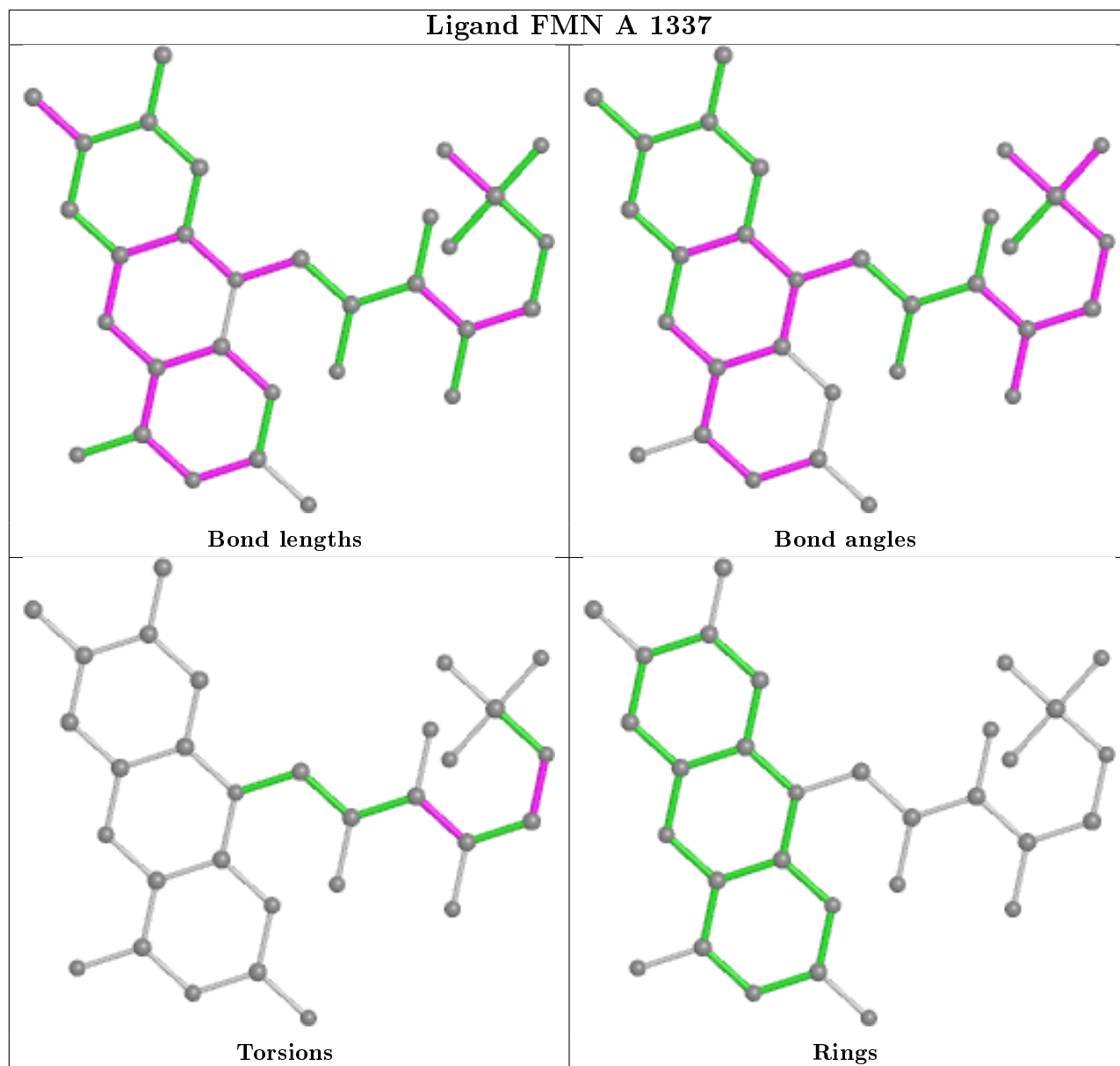
4 monomers are involved in 4 short contacts:

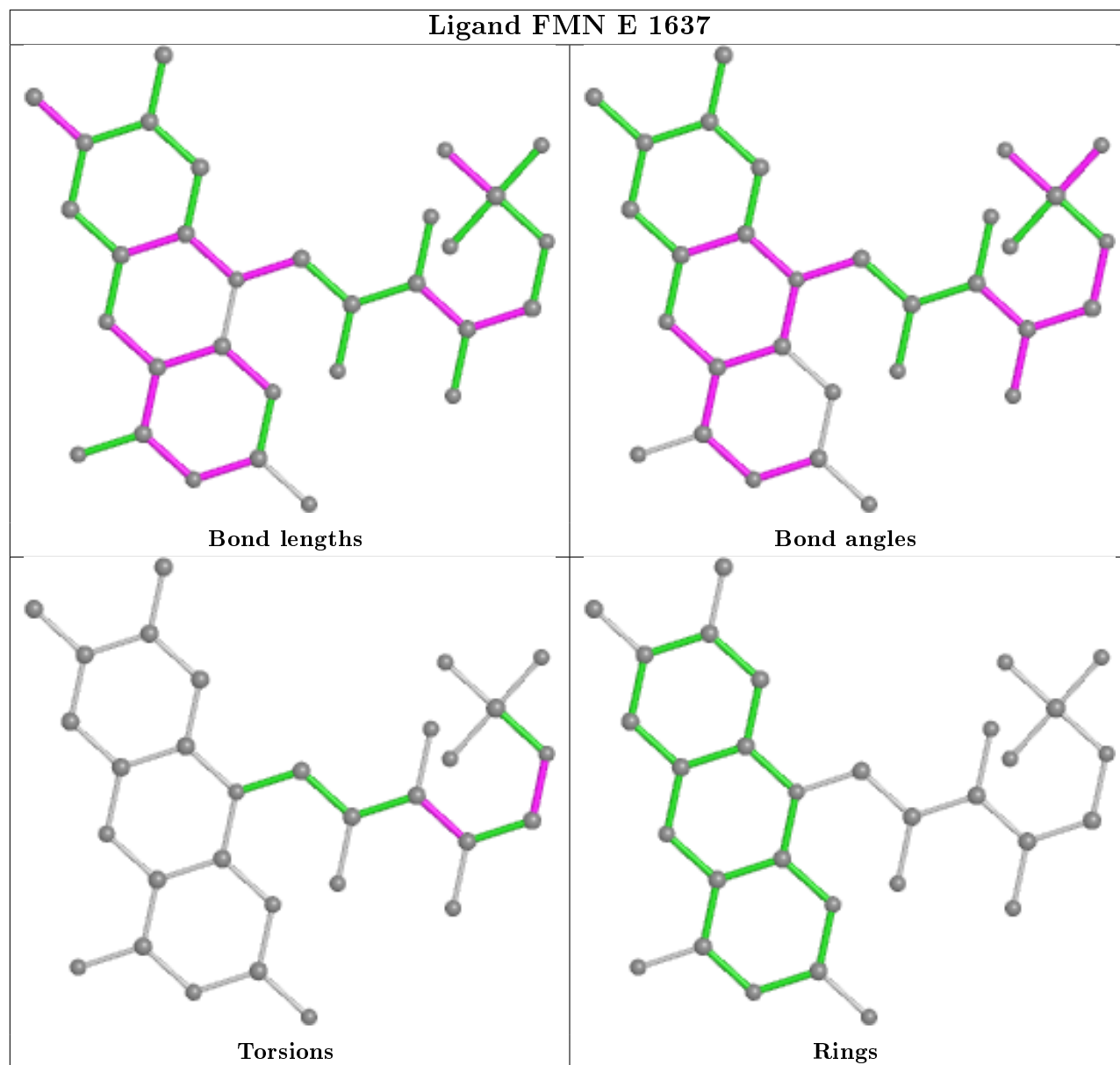
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1638	FMT	1	0
4	E	1639	FMT	1	0
4	B	1440	FMT	1	0
4	D	1539	FMT	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	329/336 (97%)	-0.70	1 (0%) 94 94	10, 20, 35, 49	11 (3%)
1	B	329/336 (97%)	-0.43	8 (2%) 59 62	12, 27, 51, 68	17 (5%)
1	D	329/336 (97%)	-0.20	10 (3%) 50 53	20, 34, 60, 67	22 (6%)
1	E	329/336 (97%)	-0.50	7 (2%) 63 66	12, 24, 46, 70	18 (5%)
All	All	1316/1344 (97%)	-0.46	26 (1%) 65 68	10, 26, 52, 70	68 (5%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	TYR	4.0
1	B	5	PHE	3.5
1	B	33	PRO	3.4
1	A	153[A]	ASP	3.1
1	E	33	PRO	2.9
1	B	2	TYR	2.9
1	E	199[A]	ASN	2.8
1	B	131	HIS	2.8
1	E	48[A]	ASN	2.8
1	D	37	LEU	2.8
1	B	3	TYR	2.7
1	B	8	LYS	2.7
1	D	31	GLY	2.6
1	B	32	THR	2.4
1	D	12	GLN	2.4
1	D	24	GLN	2.3
1	D	32	THR	2.3
1	E	131	HIS	2.3
1	D	96	ASP	2.2
1	D	209	HIS	2.2
1	B	31	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	133	ASP	2.2
1	D	284	LEU	2.2
1	E	32	THR	2.2
1	D	179	PRO	2.1
1	E	5	PHE	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 carbohydrates in this entry.

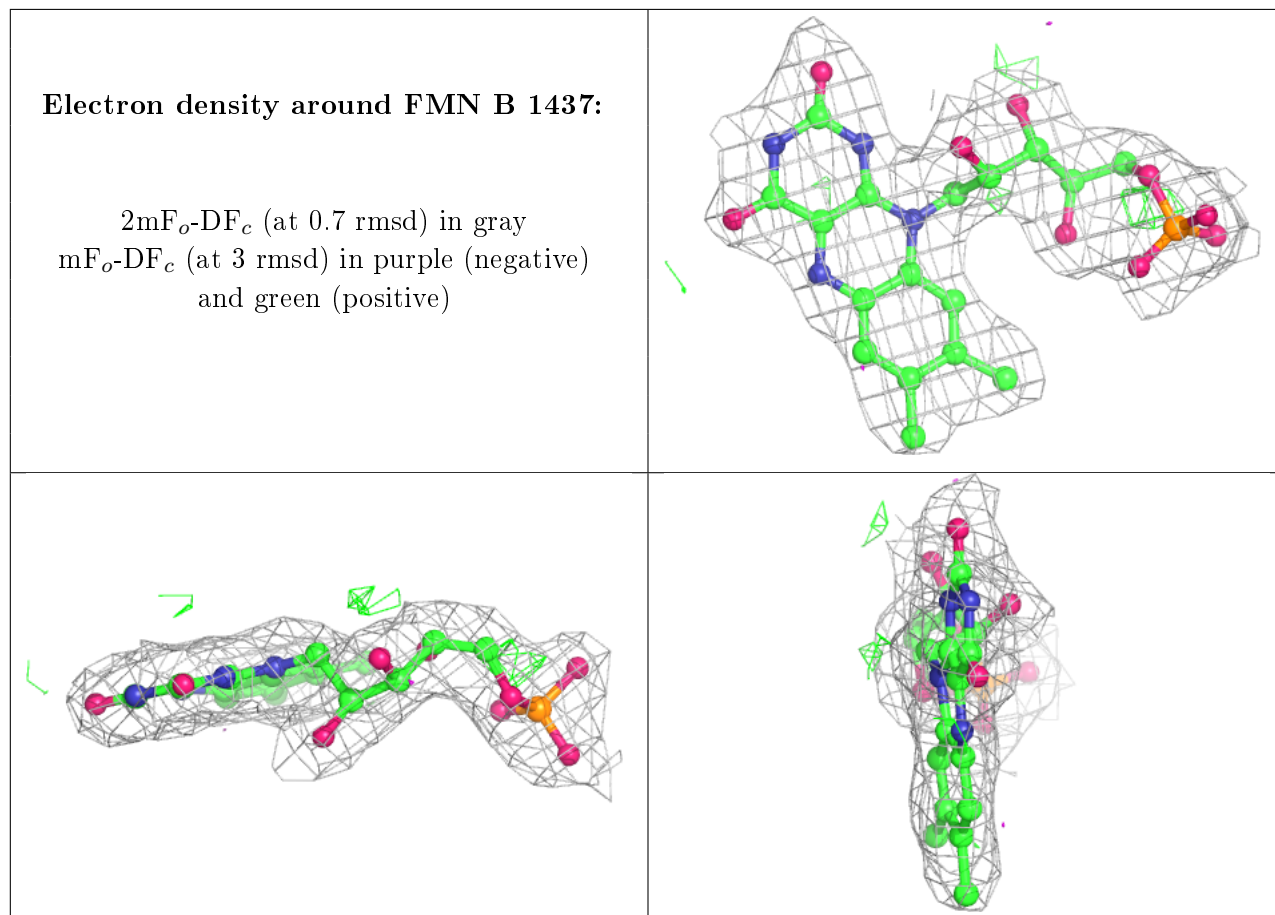
## 6.4 Ligands [i](#)

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	ORO	A	1339[A]	11/11	0.78	0.22	68,68,69,69	11
3	ORO	A	1339[B]	11/11	0.78	0.22	66,67,68,68	11
3	ORO	D	1540	11/11	0.83	0.28	75,76,77,78	0
4	FMT	B	1439	3/3	0.85	0.34	43,43,47,52	0
4	FMT	B	1438	3/3	0.87	0.31	63,63,64,64	0
4	FMT	D	1538	3/3	0.89	0.29	53,53,57,58	0
4	FMT	E	1639	3/3	0.91	0.32	59,59,61,63	0
4	FMT	E	1640	3/3	0.94	0.20	33,33,35,37	0
4	FMT	E	1638	3/3	0.96	0.15	23,23,26,27	0
4	FMT	D	1539	3/3	0.96	0.17	34,34,34,37	0
4	FMT	B	1440	3/3	0.97	0.21	40,40,40,40	0
2	FMN	B	1437	31/31	0.97	0.10	15,19,23,25	0
2	FMN	A	1337	31/31	0.97	0.09	11,15,19,20	0
3	ORO	A	1338	11/11	0.97	0.13	17,21,23,23	0
2	FMN	D	1537	31/31	0.97	0.10	23,29,33,34	0
2	FMN	E	1637	31/31	0.97	0.11	12,19,22,23	0

The following is a graphical depiction of the model fit to experimental electron density of all

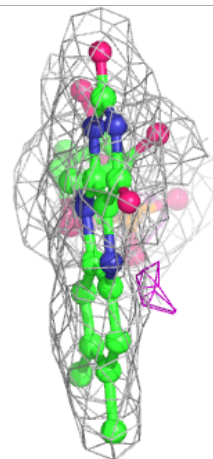
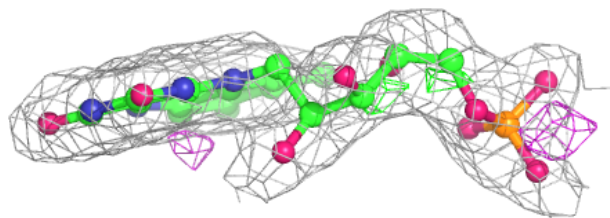
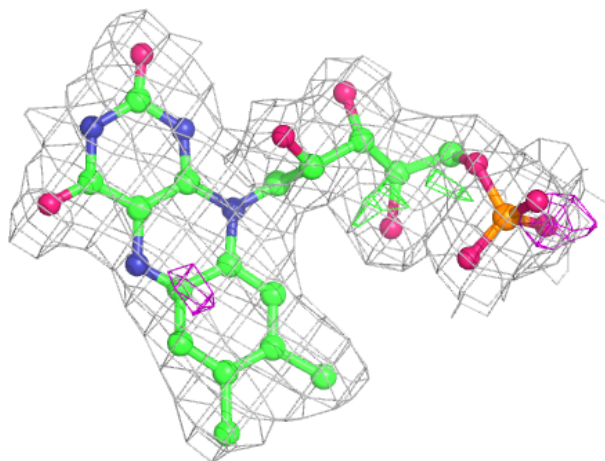
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





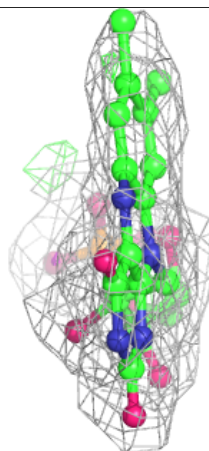
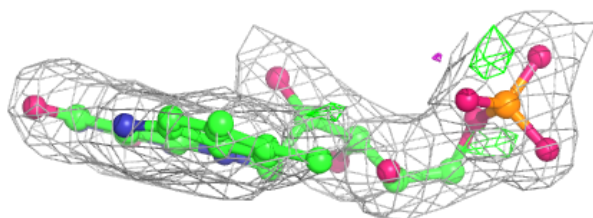
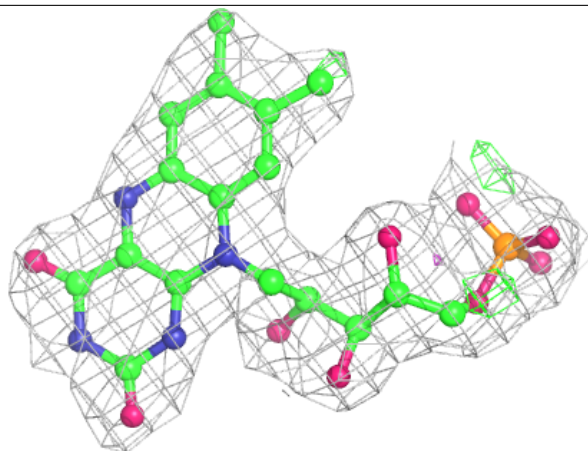
**Electron density around FMN A 1337:**

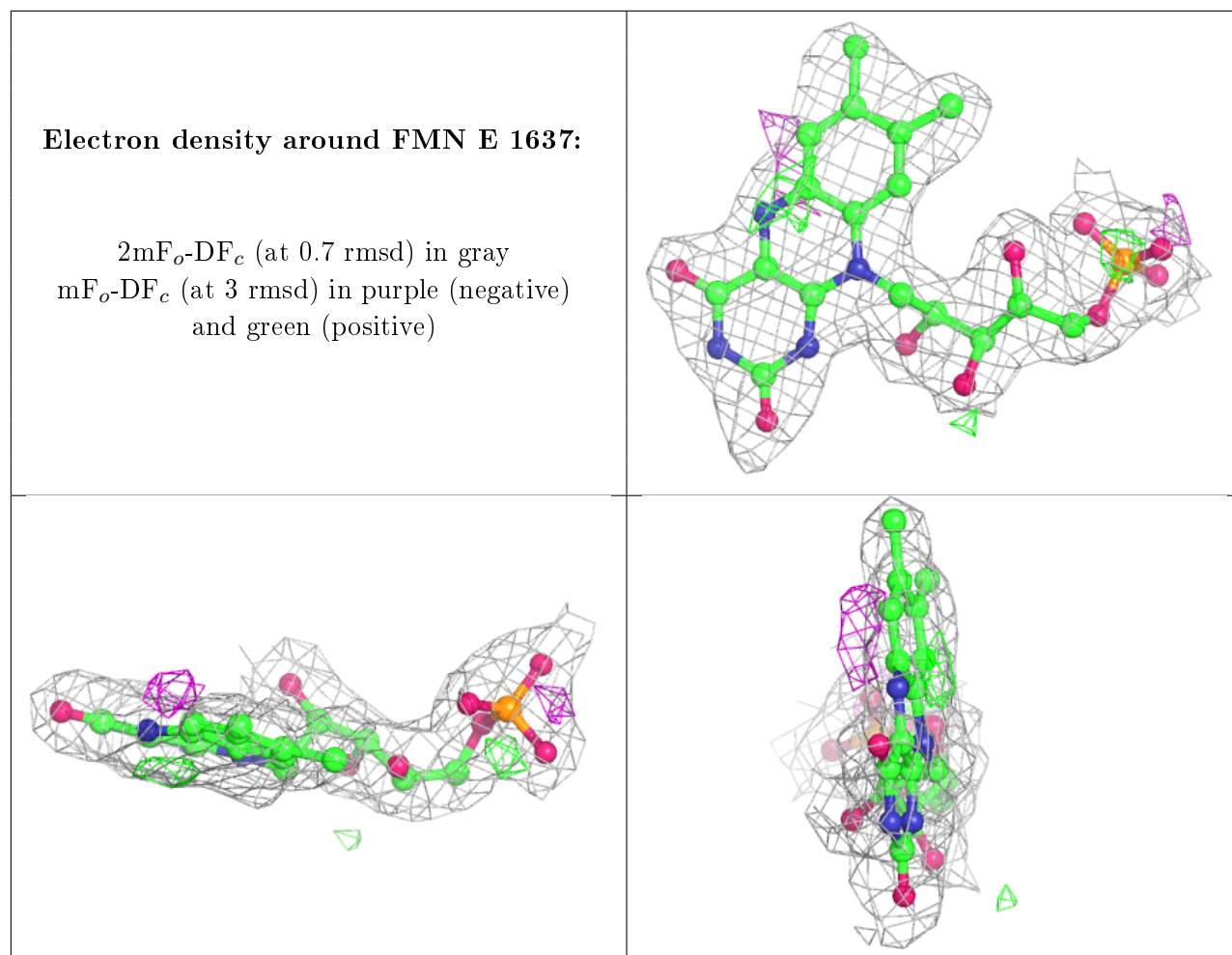
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN D 1537:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.