



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:59 AM UTC

PDB ID : 1EP1 / pdb_00001ep1
Title : CRYSTAL STRUCTURE OF LACTOCOCCUS LACTIS DIHYDROOROTATE DEHYDROGENASE B
Authors : Rowland, P.; Norager, S.; Jensen, K.F.; Larsen, S.
Deposited on : 2000-03-27
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

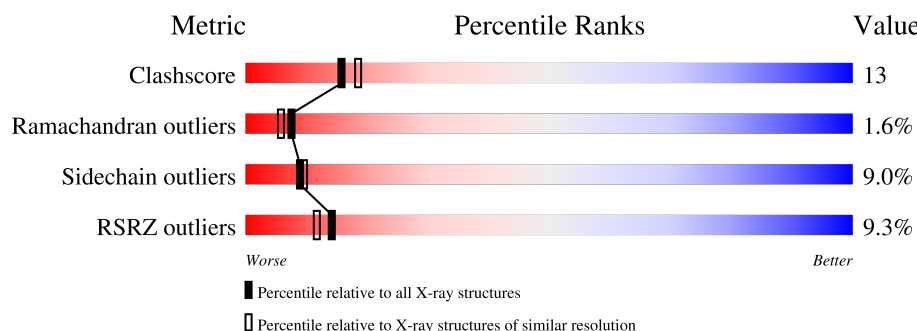
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	311	3% 77% 19% • •
2	B	261	17% 56% 36% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	A	501	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4568 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 B (PYRD SUB-UNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2294	1465	382	433	14			

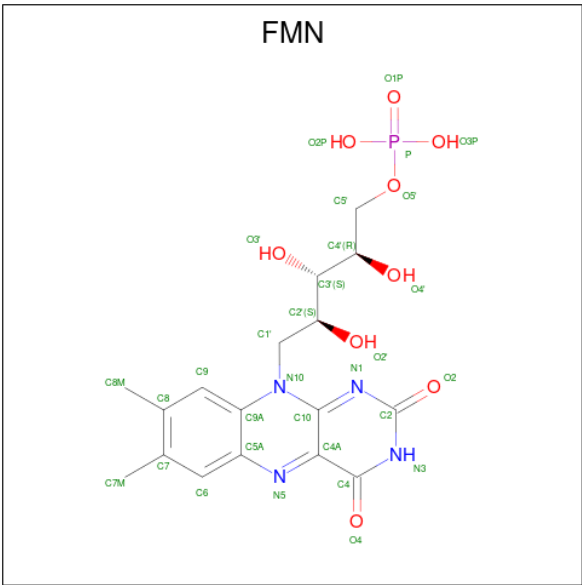
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ALA	ARG	conflict	UNP P54322
A	255	ASP	VAL	conflict	UNP P54322
A	266	ALA	ARG	conflict	UNP P54322

- Molecule 2 is a protein called DIHYDROOROTATE DEHYDROGENASE B (PYRK SUB-UNIT).

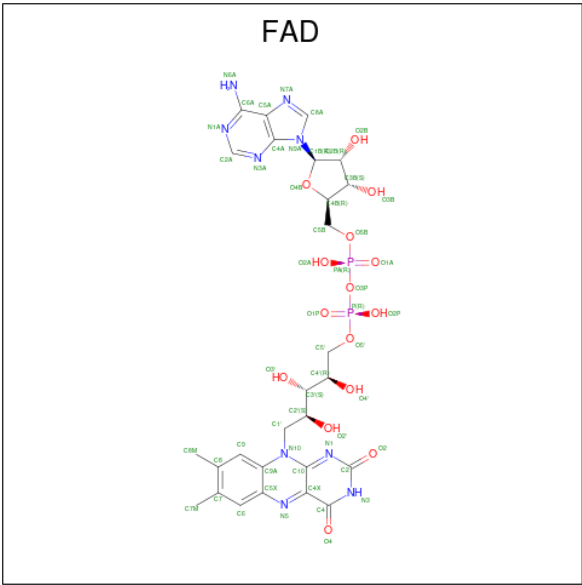
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			1991	1261	326	385	19			

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			4	2	2		

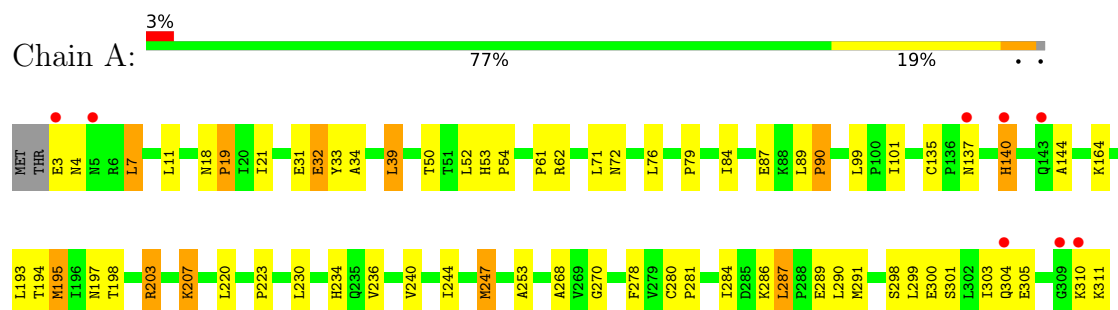
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	143	Total	O	0	0
			143	143		
6	B	52	Total	O	0	0
			52	52		

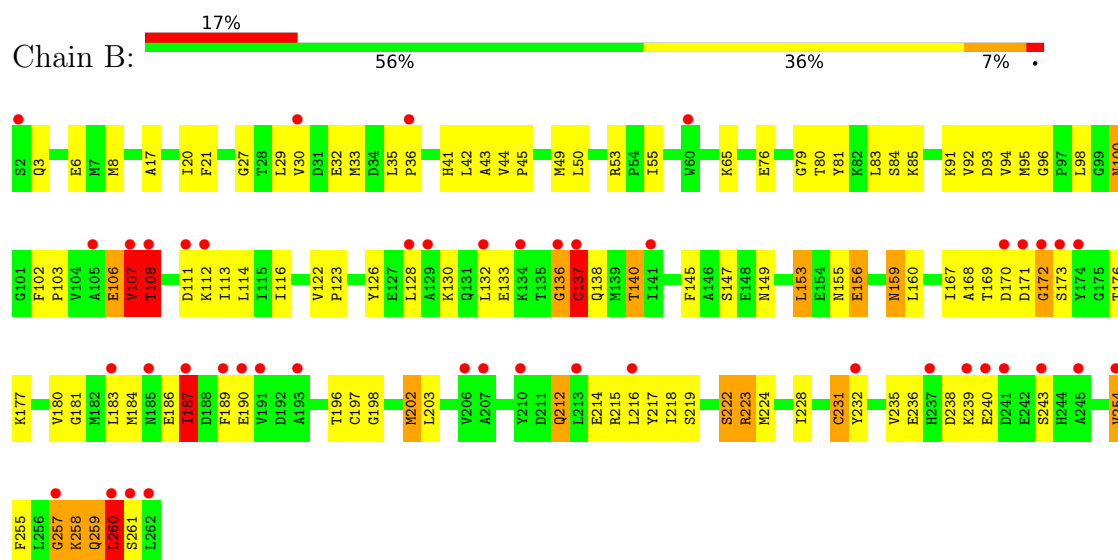
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DIHYDROOROTATE DEHYDROGENASE B (PYRD SUBUNIT)



• Molecule 2: DIHYDROOROTATE DEHYDROGENASE B (PYRK SUBUNIT)



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	202.67Å 202.67Å 81.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.70 – 2.20 30.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.70-2.20) 92.8 (30.70-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.202 , 0.256 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4568	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.68	2/2335 (0.1%)	1.03	9/3173 (0.3%)
2	B	0.51	0/2021	1.11	14/2724 (0.5%)
All	All	0.61	2/4356 (0.0%)	1.07	23/5897 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	MET	SD-CE	-10.28	1.53	1.79
1	A	195	MET	SD-CE	-6.30	1.63	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	137	CYS	N-CA-C	11.52	126.24	110.35
1	A	270	GLY	N-CA-C	9.22	118.60	110.21
2	B	235	VAL	N-CA-C	9.21	122.06	109.80
2	B	107	VAL	N-CA-C	9.09	120.42	107.88
2	B	123	PRO	N-CA-C	7.99	120.45	110.70
2	B	136	GLY	N-CA-C	7.72	131.47	113.18
2	B	257	GLY	N-CA-C	7.14	130.10	113.18
2	B	231	CYS	N-CA-C	6.99	119.93	111.82
2	B	153	LEU	N-CA-C	6.77	121.31	113.38
1	A	18	ASN	N-CA-C	-6.30	102.55	108.22
2	B	223	ARG	N-CA-C	-6.01	100.06	109.25
2	B	260	LEU	N-CA-C	5.95	123.48	110.80
1	A	289	GLU	N-CA-C	-5.91	104.75	111.07
1	A	197	ASN	N-CA-C	-5.86	100.65	109.79
2	B	3	GLN	N-CA-C	5.65	119.17	112.72
2	B	108	THR	N-CA-C	5.49	122.48	110.80
1	A	19	PRO	N-CA-C	5.43	121.13	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	VAL	N-CA-C	5.40	116.36	108.58
1	A	87	GLU	N-CA-C	5.36	119.30	112.12
1	A	198	THR	N-CA-C	5.33	117.75	110.55
2	B	186	GLU	N-CA-C	5.25	116.86	111.03
1	A	194	THR	N-CA-C	-5.18	101.31	109.50
1	A	32	GLU	N-CA-C	5.05	116.78	111.28

There are no chirality outliers.

There are no planarity outliers.

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	2294	0	2364	37	0
2	B	1991	0	2017	82	0
3	A	31	0	15	3	0
4	B	53	0	31	5	0
5	B	4	0	0	0	0
6	A	143	0	0	1	0
6	B	52	0	0	0	0
All	All	4568	0	4427	117	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 13.

All (117) 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)
2:B:107:VAL:HG21	2:B:215:ARG:HH22	1.29	0.94
2:B:107:VAL:HG21	2:B:215:ARG:NH2	1.86	0.91
2:B:53:ARG:NH2	4:B:502:FAD:H52A	1.93	0.82
2:B:30:VAL:HA	2:B:33:MET:HE3	1.62	0.82
2:B:259:GLN:O	2:B:260:LEU:HB2	1.83	0.78
2:B:112:LYS:HD3	2:B:189:PHE:HB2	1.66	0.77
2:B:181:GLY:HA2	2:B:184:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:LYS:HD2	2:B:177:LYS:H	1.51	0.74
2:B:238:ASP:HB3	2:B:243:SER:OG	1.85	0.74
2:B:116:ILE:HG23	2:B:180:VAL:HG11	1.70	0.73
2:B:42:LEU:HD13	2:B:55:ILE:HD12	1.74	0.70
2:B:140:THR:HG21	2:B:189:PHE:CZ	2.29	0.68
2:B:27:GLY:O	2:B:30:VAL:HG12	1.93	0.67
2:B:113:ILE:HD13	2:B:132:LEU:HD13	1.77	0.67
2:B:203:LEU:HD22	2:B:218:ILE:HG23	1.77	0.66
1:A:195:MET:HE1	1:A:236:VAL:HG11	1.79	0.64
2:B:258:LYS:HG3	2:B:259:GLN:H	1.63	0.63
2:B:216:LEU:HG	2:B:218:ILE:HD11	1.81	0.62
2:B:112:LYS:HG2	2:B:138:GLN:OE1	2.00	0.62
2:B:100:ASN:O	2:B:254:VAL:HG12	2.00	0.61
1:A:286:LYS:HD2	1:A:286:LYS:O	2.00	0.61
2:B:258:LYS:CG	2:B:259:GLN:H	2.14	0.61
1:A:50:THR:HG23	1:A:84:ILE:HD12	1.83	0.59
2:B:168:ALA:HA	2:B:176:THR:O	2.03	0.58
2:B:212:GLN:HE21	2:B:212:GLN:HA	1.67	0.58
1:A:21:ILE:O	1:A:268:ALA:HA	2.03	0.57
1:A:54:PRO:HB3	1:A:79:PRO:O	2.04	0.57
1:A:207:LYS:HA	1:A:207:LYS:HE2	1.87	0.57
2:B:80:THR:HG23	4:B:502:FAD:O1P	2.05	0.57
2:B:168:ALA:HB2	2:B:183:LEU:HD11	1.86	0.56
1:A:310:LYS:HG3	1:A:311:LYS:H	1.70	0.55
1:A:300:GLU:O	1:A:304:GLN:NE2	2.39	0.55
1:A:61:PRO:HB3	2:B:223:ARG:HG3	1.89	0.55
1:A:34:ALA:HA	1:A:39:LEU:HD13	1.88	0.54
2:B:96:GLY:HA2	2:B:98:LEU:HG	1.88	0.54
2:B:218:ILE:HD12	2:B:218:ILE:N	2.22	0.54
2:B:17:ALA:HB3	2:B:20:ILE:HB	1.90	0.53
1:A:291:MET:HE1	1:A:298:SER:HA	1.89	0.53
1:A:203:ARG:HH11	1:A:203:ARG:HB3	1.73	0.53
2:B:238:ASP:O	2:B:240:GLU:N	2.42	0.53
2:B:126:TYR:CZ	2:B:130:LYS:HD2	2.45	0.52
1:A:247:MET:HE2	3:A:501:FMN:C3'	2.39	0.52
2:B:222:SER:H	4:B:502:FAD:HM81	1.75	0.52
2:B:155:ASN:O	2:B:159:ASN:HB2	2.10	0.52
1:A:234:HIS:HD2	6:A:1020:HOH:O	1.93	0.52
2:B:171:ASP:O	2:B:173:SER:N	2.43	0.51
2:B:43:ALA:HB3	2:B:93:ASP:HB3	1.93	0.51
2:B:111:ASP:O	2:B:137:CYS:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LYS:C	2:B:260:LEU:H	2.19	0.51
2:B:169:THR:OG1	2:B:173:SER:HA	2.11	0.50
1:A:19:PRO:HG3	1:A:299:LEU:HD13	1.94	0.49
1:A:33:TYR:CZ	2:B:228:ILE:HD11	2.48	0.49
2:B:184:MET:O	2:B:187:ILE:HG12	2.13	0.49
2:B:92:VAL:O	2:B:94:VAL:HG23	2.13	0.48
1:A:280:CYS:HB2	1:A:281:PRO:HD3	1.94	0.48
2:B:30:VAL:HG11	2:B:65:LYS:HA	1.95	0.48
2:B:255:PHE:HB3	2:B:261:SER:O	2.14	0.48
2:B:177:LYS:H	2:B:177:LYS:CD	2.23	0.48
1:A:253:ALA:HB1	1:A:287:LEU:HD13	1.96	0.47
2:B:156:GLU:H	2:B:156:GLU:CD	2.21	0.47
2:B:167:ILE:HD12	2:B:167:ILE:N	2.29	0.47
3:A:501:FMN:H1'2	3:A:501:FMN:H9	1.73	0.47
2:B:126:TYR:CE2	2:B:130:LYS:HD2	2.49	0.47
2:B:49:MET:HE1	2:B:79:GLY:N	2.30	0.47
2:B:177:LYS:HD2	2:B:177:LYS:N	2.23	0.46
2:B:187:ILE:HB	2:B:189:PHE:CE1	2.50	0.46
1:A:3:GLU:HB3	1:A:4:ASN:H	1.65	0.46
2:B:212:GLN:HA	2:B:212:GLN:NE2	2.30	0.46
2:B:42:LEU:HD23	2:B:92:VAL:HG11	1.98	0.46
2:B:198:GLY:HA3	2:B:202:MET:CE	2.46	0.46
2:B:231:CYS:O	2:B:232:TYR:HB2	2.17	0.45
2:B:49:MET:HE2	2:B:53:ARG:HH22	1.82	0.45
2:B:153:LEU:O	2:B:156:GLU:HG2	2.16	0.45
2:B:236:GLU:HB3	2:B:260:LEU:HD23	2.00	0.44
1:A:89:LEU:HB2	1:A:90:PRO:HD3	1.98	0.44
1:A:203:ARG:HB3	1:A:203:ARG:NH1	2.33	0.44
1:A:137:ASN:OD1	1:A:140:HIS:HB2	2.18	0.43
1:A:278:PHE:O	1:A:281:PRO:HD2	2.19	0.43
1:A:299:LEU:O	1:A:303:ILE:HG13	2.18	0.43
2:B:126:TYR:CE1	2:B:156:GLU:HB2	2.52	0.43
1:A:32:GLU:H	1:A:32:GLU:CD	2.26	0.43
2:B:116:ILE:CG2	2:B:180:VAL:HG11	2.44	0.43
1:A:203:ARG:HA	1:A:203:ARG:HD2	1.81	0.43
1:A:247:MET:HE2	3:A:501:FMN:O3'	2.19	0.43
2:B:107:VAL:HG22	2:B:108:THR:N	2.34	0.42
2:B:122:VAL:HG12	2:B:153:LEU:HD12	2.00	0.42
2:B:198:GLY:HA3	2:B:202:MET:HE1	2.02	0.42
2:B:35:LEU:HA	2:B:36:PRO:HD3	1.89	0.42
2:B:197:CYS:SG	2:B:219:SER:HB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LYS:CG	2:B:259:GLN:N	2.81	0.42
1:A:193:LEU:O	1:A:244:ILE:HA	2.19	0.42
2:B:8:MET:O	2:B:91:LYS:HA	2.20	0.42
1:A:62:ARG:O	1:A:72:ASN:HA	2.19	0.42
1:A:135:CYS:O	1:A:144:ALA:HA	2.19	0.42
1:A:301:SER:O	1:A:305:GLU:HG3	2.20	0.42
2:B:6:GLU:OE1	2:B:29:LEU:HG	2.19	0.42
2:B:260:LEU:HA	2:B:260:LEU:HD12	1.79	0.42
2:B:145:PHE:O	2:B:169:THR:HA	2.19	0.41
2:B:258:LYS:HA	2:B:258:LYS:HD2	1.78	0.41
1:A:164:LYS:HA	1:A:164:LYS:HD3	1.79	0.41
2:B:53:ARG:CZ	4:B:502:FAD:H52A	2.50	0.41
2:B:21:PHE:CE2	2:B:84:SER:HB2	2.55	0.41
2:B:102:PHE:HA	2:B:103:PRO:HD3	1.89	0.41
1:A:223:PRO:HD2	2:B:50:LEU:HD11	2.03	0.41
1:A:280:CYS:O	1:A:284:ILE:HG13	2.21	0.41
2:B:81:TYR:CE1	2:B:85:LYS:HE3	2.56	0.41
2:B:44:VAL:HA	2:B:45:PRO:HD3	1.86	0.41
2:B:103:PRO:HB2	2:B:106:GLU:CD	2.44	0.41
2:B:107:VAL:HG22	2:B:108:THR:H	1.85	0.41
2:B:156:GLU:O	2:B:160:LEU:HG	2.21	0.41
2:B:217:TYR:C	2:B:218:ILE:HD12	2.46	0.41
1:A:53:HIS:HB3	1:A:54:PRO:HD2	2.02	0.41
2:B:147:SER:OG	2:B:172:GLY:HA3	2.20	0.41
2:B:224:MET:HE3	4:B:502:FAD:HM83	2.03	0.41
1:A:247:MET:HB3	1:A:268:ALA:HB3	2.04	0.40
1:A:7:LEU:O	1:A:19:PRO:HD3	2.21	0.40
2:B:94:VAL:HG12	2:B:95:MET:N	2.36	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	307/311 (99%)	299 (97%)	8 (3%)	0	100	100
2	B	259/261 (99%)	223 (86%)	27 (10%)	9 (4%)	3	1
All	All	566/572 (99%)	522 (92%)	35 (6%)	9 (2%)	7	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	187	ILE
2	B	239	LYS
2	B	257	GLY
2	B	260	LEU
2	B	172	GLY
2	B	170	ASP
2	B	108	THR
2	B	259	GLN
2	B	136	GLY

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	246/248 (99%)	228 (93%)	18 (7%)	13	15
2	B	219/219 (100%)	195 (89%)	24 (11%)	6	6
All	All	465/467 (100%)	423 (91%)	42 (9%)	9	9

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	LEU
1	A	31	GLU
1	A	39	LEU
1	A	52	LEU
1	A	71	LEU
1	A	76	LEU

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Mol	Chain	Res	Type
1	A	90	PRO
1	A	99	LEU
1	A	101	ILE
1	A	140	HIS
1	A	203	ARG
1	A	207	LYS
1	A	220	LEU
1	A	230	LEU
1	A	240	VAL
1	A	287	LEU
1	A	290	LEU
2	B	32	GLU
2	B	41	HIS
2	B	76	GLU
2	B	83	LEU
2	B	100	ASN
2	B	106	GLU
2	B	107	VAL
2	B	114	LEU
2	B	128	LEU
2	B	133	GLU
2	B	137	CYS
2	B	140	THR
2	B	149	ASN
2	B	156	GLU
2	B	159	ASN
2	B	187	ILE
2	B	190	GLU
2	B	196	THR
2	B	202	MET
2	B	212	GLN
2	B	214	GLU
2	B	222	SER
2	B	258	LYS
2	B	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	95	ASN
1	A	234	HIS

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Mol	Chain	Res	Type
2	B	5	GLN
2	B	19	ASN
2	B	41	HIS
2	B	149	ASN
2	B	159	ASN
2	B	212	GLN
2	B	237	HIS
2	B	259	GLN

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMN	A	501	-	33,33,33	2.24	8 (24%)	48,50,50	2.41	17 (35%)
4	FAD	B	502	-	58,58,58	2.37	11 (18%)	85,89,89	1.18	8 (9%)
5	FES	B	503	2	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	501	-	2/2/4/4	9/18/18/18	0/3/3/3
4	FAD	B	502	-	-	8/34/50/50	0/6/6/6
5	FES	B	503	2	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	FAD	P-O3P	-13.13	1.45	1.59
3	A	501	FMN	C1'-N10	-6.12	1.33	1.47
4	B	502	FAD	O5'-C5'	4.79	1.62	1.44
3	A	501	FMN	C4A-N5	4.77	1.41	1.30
3	A	501	FMN	C5'-C4'	-4.51	1.45	1.51
4	B	502	FAD	PA-O2A	-4.46	1.34	1.55
3	A	501	FMN	C4'-C3'	-4.42	1.45	1.53
4	B	502	FAD	P-O2P	-3.64	1.38	1.55
3	A	501	FMN	C1'-C2'	-3.60	1.47	1.52
4	B	502	FAD	C1'-C2'	3.37	1.57	1.52
3	A	501	FMN	O2'-C2'	-3.31	1.36	1.43
3	A	501	FMN	C2'-C3'	-3.23	1.47	1.53
4	B	502	FAD	O4B-C1B	2.78	1.48	1.42
4	B	502	FAD	O2-C2	-2.64	1.19	1.24
3	A	501	FMN	O4'-C4'	-2.48	1.38	1.43
4	B	502	FAD	C5A-C6A	2.40	1.47	1.41
4	B	502	FAD	O4B-C4B	2.28	1.50	1.45
4	B	502	FAD	C6-C7	-2.07	1.36	1.39
4	B	502	FAD	PA-O3P	-2.04	1.57	1.59

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	FMN	C1'-C2'-C3'	6.64	127.67	109.66
3	A	501	FMN	C10-N1-C2	5.41	128.56	116.85
3	A	501	FMN	O4'-C4'-C3'	5.19	121.39	109.25
3	A	501	FMN	C4'-C3'-C2'	5.01	121.91	113.57
3	A	501	FMN	C4A-C10-N1	-4.79	112.85	124.59
3	A	501	FMN	C5'-C4'-C3'	3.88	119.55	112.22
3	A	501	FMN	C4-C4A-C10	3.75	123.36	116.93
3	A	501	FMN	O5'-C5'-C4'	-3.27	100.63	109.36
4	B	502	FAD	C4'-C3'-C2'	-3.19	108.26	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	FMN	N10-C10-N1	2.85	126.90	118.51
3	A	501	FMN	O2-C2-N3	2.79	123.94	118.58
3	A	501	FMN	N3-C2-N1	-2.67	113.84	119.50
3	A	501	FMN	O2'-C2'-C1'	2.62	120.99	110.20
3	A	501	FMN	C9A-C5A-N5	-2.62	119.68	122.45
3	A	501	FMN	C10-C4A-N5	-2.58	119.54	124.81
4	B	502	FAD	O4B-C1B-C2B	-2.58	101.10	106.62
4	B	502	FAD	C4X-C10-N10	2.56	120.15	116.48
4	B	502	FAD	C4-N3-C2	-2.47	121.26	125.64
3	A	501	FMN	O3'-C3'-C2'	-2.39	103.50	108.93
3	A	501	FMN	C4A-C10-N10	2.37	119.87	116.48
3	A	501	FMN	O3'-C3'-C4'	2.36	114.30	108.93
4	B	502	FAD	O5B-PA-O1A	-2.27	99.92	108.94
4	B	502	FAD	O4B-C1B-N9A	-2.14	103.98	108.09
4	B	502	FAD	C5X-C9A-N10	-2.09	116.08	117.97
4	B	502	FAD	O2A-PA-O1A	2.08	122.14	112.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	FMN	C2'
3	A	501	FMN	C4'

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	FMN	N10-C1'-C2'-O2'
3	A	501	FMN	O2'-C2'-C3'-O3'
3	A	501	FMN	O2'-C2'-C3'-C4'
3	A	501	FMN	C2'-C3'-C4'-O4'
3	A	501	FMN	O3'-C3'-C4'-O4'
3	A	501	FMN	C3'-C4'-C5'-O5'
3	A	501	FMN	O4'-C4'-C5'-O5'
4	B	502	FAD	O4B-C4B-C5B-O5B
4	B	502	FAD	C5'-O5'-P-O1P
4	B	502	FAD	C5'-O5'-P-O2P
4	B	502	FAD	C5'-O5'-P-O3P
4	B	502	FAD	C3B-C4B-C5B-O5B
3	A	501	FMN	C4'-C5'-O5'-P
4	B	502	FAD	P-O3P-PA-O2A
4	B	502	FAD	P-O3P-PA-O1A
4	B	502	FAD	PA-O3P-P-O1P

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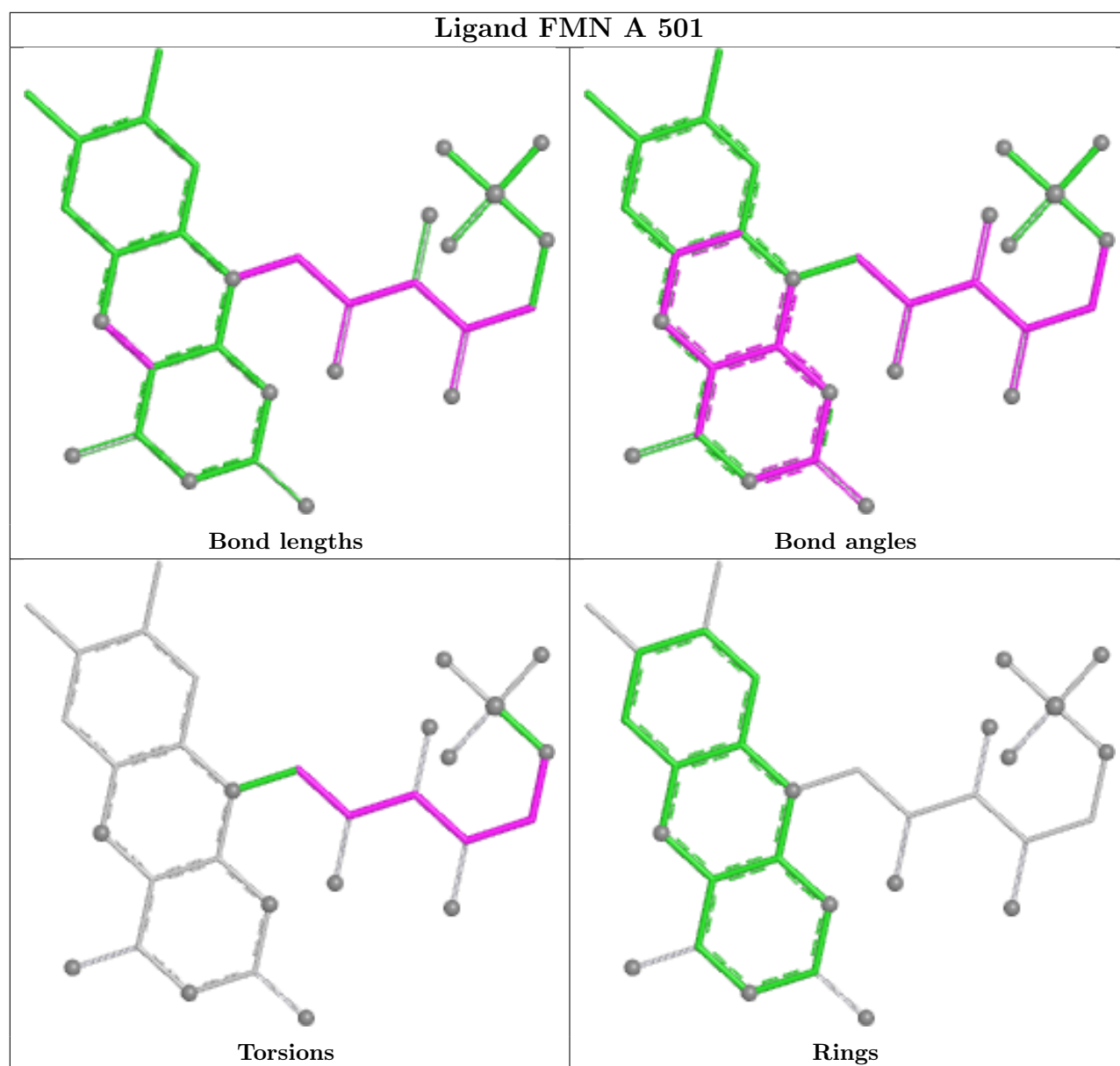
Mol	Chain	Res	Type	Atoms
3	A	501	FMN	C1'-C2'-C3'-O3'

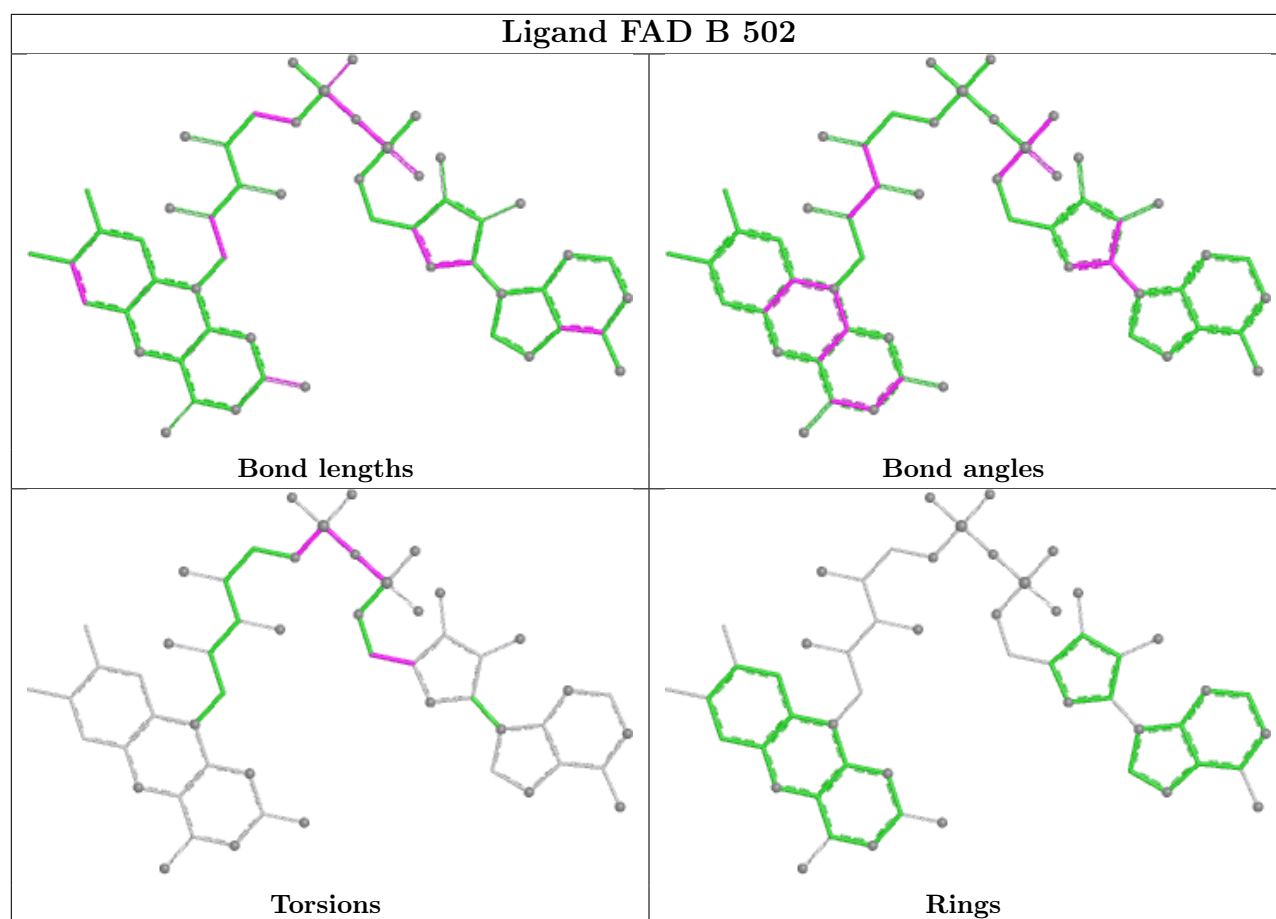
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	FMN	3	0
4	B	502	FAD	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/311 (99%)	-0.27	8 (2%) 57 54	8, 19, 45, 85	0
2	B	261/261 (100%)	1.15	45 (17%) 4 3	19, 52, 81, 96	0
All	All	570/572 (99%)	0.38	53 (9%) 14 12	8, 31, 78, 96	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	262	LEU	4.3
1	A	309	GLY	3.8
2	B	260	LEU	3.8
2	B	172	GLY	3.7
2	B	261	SER	3.7
1	A	5	ASN	3.7
2	B	107	VAL	3.7
2	B	241	ASP	3.6
2	B	136	GLY	3.5
1	A	3	GLU	3.5
2	B	171	ASP	3.4
2	B	129	ALA	3.3
1	A	304	GLN	3.2
2	B	189	PHE	3.1
2	B	216	LEU	3.0
2	B	173	SER	3.0
2	B	243	SER	3.0
2	B	207	ALA	3.0
2	B	137	CYS	2.9
2	B	105	ALA	2.8
2	B	112	LYS	2.8
1	A	143	GLN	2.7
2	B	108	THR	2.7
2	B	30	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	191	VAL	2.6
2	B	2	SER	2.6
2	B	187	ILE	2.5
2	B	213	LEU	2.5
2	B	60	TRP	2.5
2	B	240	GLU	2.5
1	A	310	LYS	2.5
2	B	210	TYR	2.4
2	B	190	GLU	2.4
2	B	36	PRO	2.4
2	B	170	ASP	2.3
2	B	174	TYR	2.3
2	B	183	LEU	2.3
2	B	239	LYS	2.3
2	B	254	VAL	2.3
2	B	245	ALA	2.2
2	B	132	LEU	2.2
2	B	111	ASP	2.2
2	B	141	ILE	2.2
2	B	206	VAL	2.1
2	B	128	LEU	2.1
2	B	193	ALA	2.0
2	B	237	HIS	2.0
2	B	232	TYR	2.0
2	B	257	GLY	2.0
1	A	140	HIS	2.0
1	A	137	ASN	2.0
2	B	185	ASN	2.0
2	B	134	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

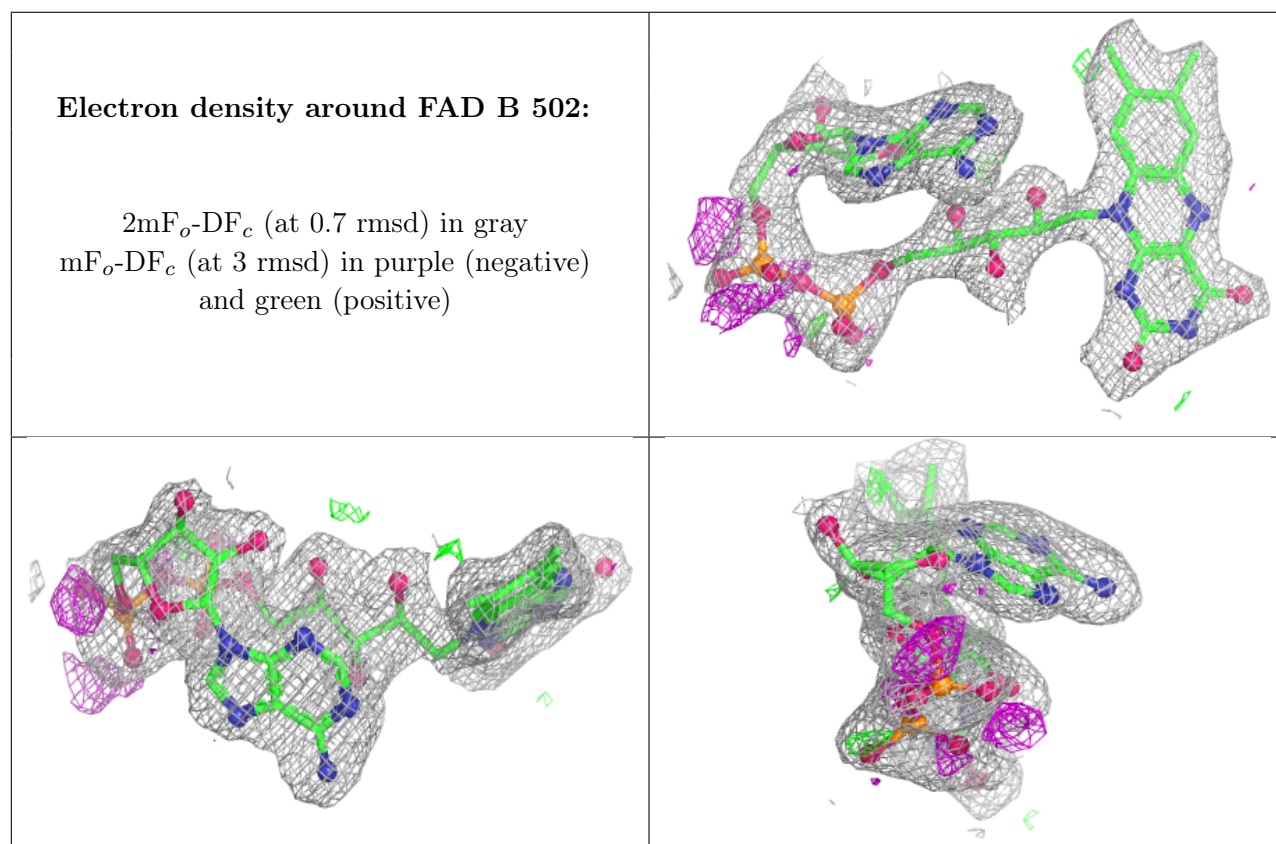
There are no oligosaccharides in this entry.

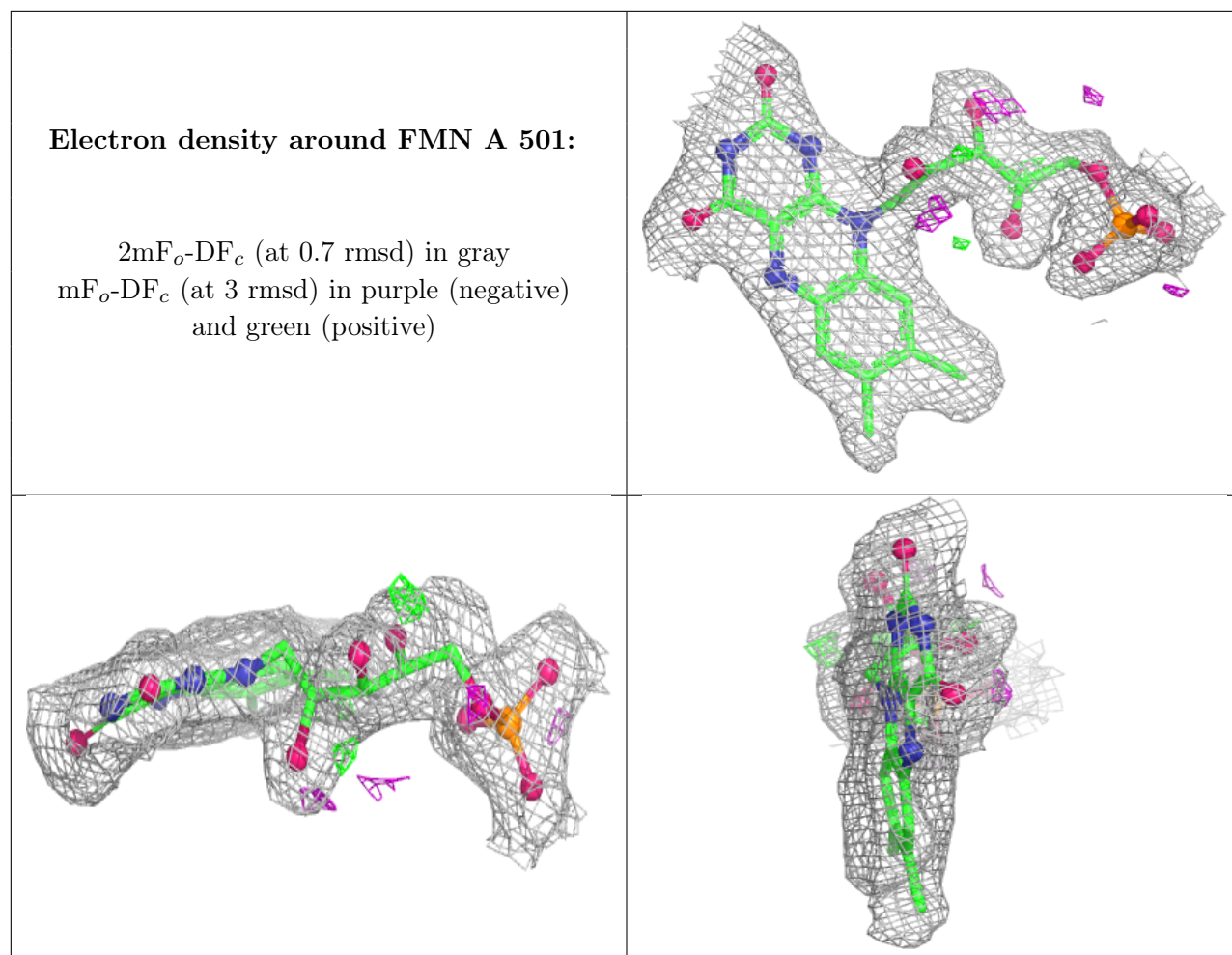
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FAD	B	502	53/53	0.92	0.10	34,41,48,48	0
5	FES	B	503	4/4	0.97	0.05	31,32,32,32	0
3	FMN	A	501	31/31	0.98	0.05	9,12,13,14	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.