



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:14 PM UTC

PDB ID : 7R2S / pdb_00007r2s
Title : Crystal structure of a flavodiiron protein D52K mutant from Escherichia coli
pressurized with krypton gas
Authors : Borges, P.T.; Teixeira, M.; Romao, C.V.; Frazao, C.
Deposited on : 2022-02-05
Resolution : 2.19 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

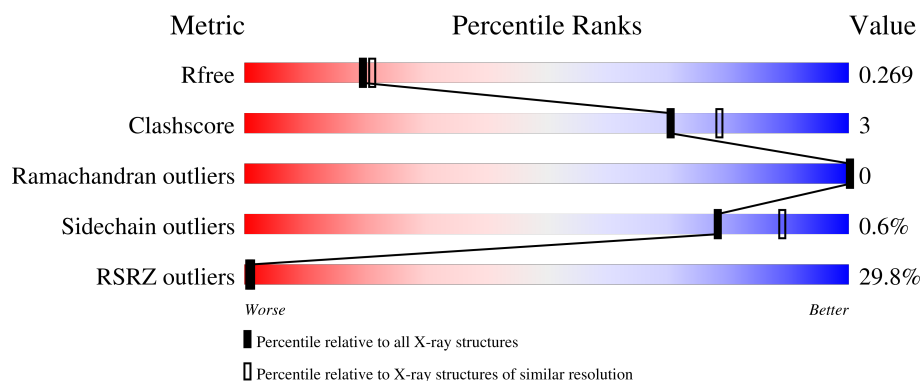
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
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	479	22% 76% 8% 16%
1	B	479	28% 76% 8% 16%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6887 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.

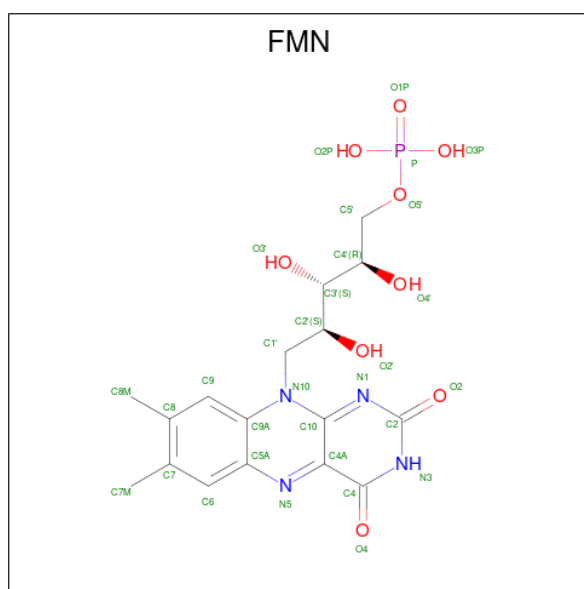
- Molecule 1 is a protein called Anaerobic nitric oxide reductase flavorubredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3215	2029	564	605	17			
1	B	400	Total	C	N	O	S	0	0	0
			3215	2029	564	605	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	LYS	ASP	engineered mutation	UNP Q46877
B	52	LYS	ASP	engineered mutation	UNP Q46877

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Fe	0	0
			2	2		
3	B	2	Total	Fe	0	0
			2	2		

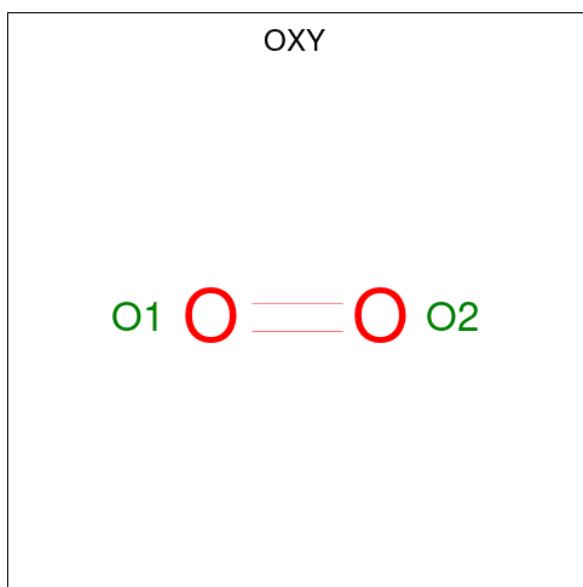
- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		

- Molecule 5 is KRYPTON (CCD ID: KR) (formula: Kr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Kr	0	0
			3	3		
5	B	3	Total	Kr	0	0
			3	3		

- Molecule 6 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

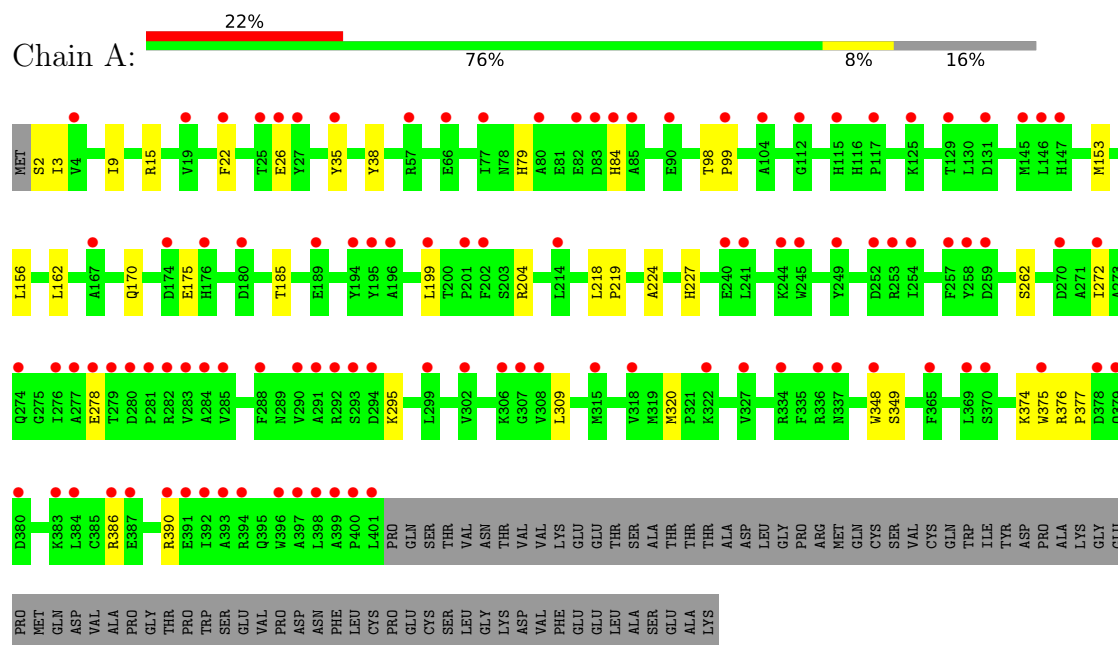
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	207	Total	O	0	0
			207	207		
7	B	174	Total	O	0	0
			174	174		

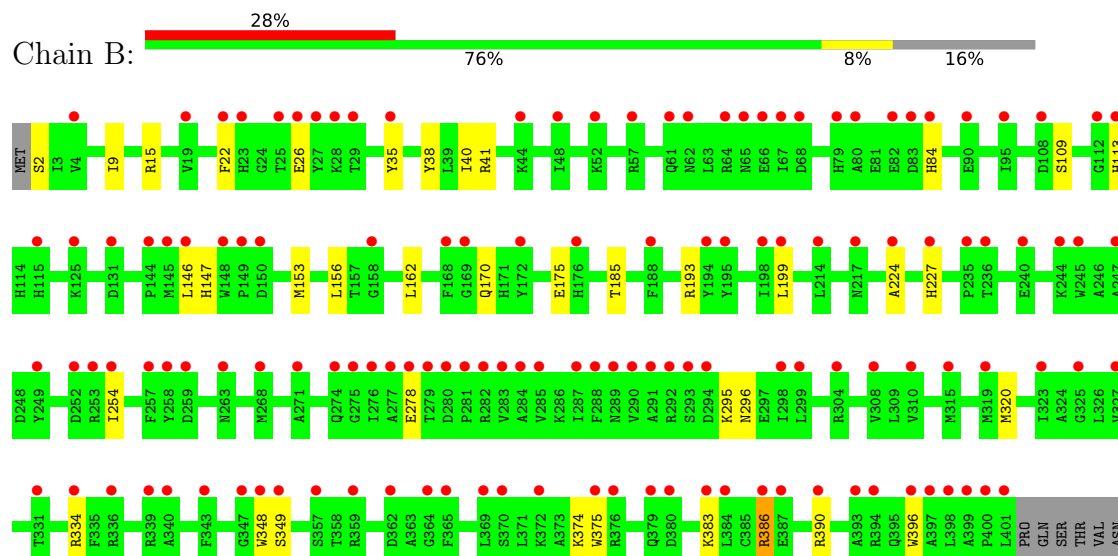
3 Residue-property plots [i](#)

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: Anaerobic nitric oxide reductase flavorubredoxin



- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.95Å 64.42Å 147.08Å 90.00° 91.46° 90.00°	Depositor
Resolution (Å)	52.34 – 2.19 52.34 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.2 (52.34-2.19) 91.3 (52.34-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 2.18Å)	Xtriage
Refinement program	PHENIX dev_1436	Depositor
R, R_{free}	0.254 , 0.295 0.269 , 0.269	Depositor DCC
R_{free} test set	637 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5915e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, O, KR, OXY, FE

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	0.26	0/3289	0.69	2/4463 (0.0%)
1	B	0.26	0/3289	0.69	2/4463 (0.0%)
All	All	0.26	0/6578	0.69	4/8926 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	MET	CA-C-N	5.62	125.73	119.32
1	A	320	MET	C-N-CA	5.62	125.73	119.32
1	B	320	MET	CA-C-N	5.59	125.70	119.32
1	B	320	MET	C-N-CA	5.59	125.70	119.32

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	3215	0	3119	21	0
1	B	3215	0	3119	23	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	1	0
5	B	3	0	0	1	0
6	A	2	0	0	0	0
7	A	207	0	0	2	0
7	B	174	0	0	5	0
All	All	6887	0	6276	43	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 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG21	1:B:185:THR:HG21	1.63	0.80
1:B:84:HIS:CE1	1:B:227:HIS:NE2	2.68	0.61
1:A:199:LEU:HD21	5:A:507:KR:KR	2.62	0.60
1:B:84:HIS:HE1	1:B:227:HIS:NE2	2.00	0.59
1:B:15:ARG:NH2	1:B:175:GLU:O	2.36	0.59
1:A:153:MET:HE3	1:A:162:LEU:HD11	1.84	0.58
1:B:41:ARG:NH2	7:B:603:HOH:O	2.38	0.55
1:A:84:HIS:HE1	1:A:227:HIS:NE2	2.05	0.55
1:B:153:MET:HE3	1:B:162:LEU:HD11	1.89	0.54
1:A:348:TRP:CD1	1:A:349:SER:H	2.25	0.54
1:A:2:SER:N	7:A:604:HOH:O	2.40	0.54
1:A:204:ARG:NH2	7:A:605:HOH:O	2.40	0.54
1:B:348:TRP:CD1	1:B:349:SER:H	2.26	0.53
1:A:272:ILE:HG21	1:A:309:LEU:HD22	1.91	0.53
1:B:109:SER:O	1:B:113:HIS:ND1	2.30	0.52
1:A:15:ARG:NH2	1:A:175:GLU:O	2.43	0.52
1:B:199:LEU:HD21	5:B:505:KR:KR	2.72	0.50
1:B:334:ARG:NH2	7:B:605:HOH:O	2.43	0.50
1:B:278:GLU:OE2	1:B:390:ARG:NH2	2.44	0.50
1:B:374:LYS:HG2	1:B:375:TRP:CD1	2.46	0.50
1:A:38:TYR:CZ	1:A:224:ALA:HB1	2.50	0.47
1:B:2:SER:N	7:B:607:HOH:O	2.47	0.46
1:B:396:TRP:HB2	7:B:678:HOH:O	2.15	0.46
1:B:38:TYR:CZ	1:B:224:ALA:HB1	2.50	0.46
1:A:374:LYS:HG2	1:A:375:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:OE1	1:B:295:LYS:NZ	2.49	0.45
1:B:146:LEU:HA	1:B:147:HIS:HA	1.85	0.44
1:A:376:ARG:HA	1:A:377:PRO:HD3	1.91	0.43
1:B:22:PHE:HZ	1:B:35:TYR:HE1	1.65	0.43
1:B:40:ILE:HD13	1:B:156:LEU:HD22	1.99	0.43
1:B:383:LYS:HG2	1:B:386:ARG:HH22	1.84	0.43
1:B:9:ILE:HD11	1:B:156:LEU:HD23	2.02	0.42
1:A:26:GLU:OE1	1:A:295:LYS:NZ	2.53	0.42
1:A:3:ILE:HD11	1:A:15:ARG:HH22	1.85	0.42
1:A:278:GLU:OE2	1:A:390:ARG:NH2	2.52	0.41
1:A:9:ILE:HD11	1:A:156:LEU:HD23	2.02	0.41
1:A:22:PHE:HZ	1:A:35:TYR:HE1	1.68	0.41
1:A:218:LEU:HA	1:A:219:PRO:HD3	1.87	0.41
1:B:254:ILE:HD11	7:B:678:HOH:O	2.20	0.41
1:A:79:HIS:HD2	1:A:84:HIS:HD2	1.68	0.41
1:A:98:THR:HA	1:A:99:PRO:HD3	1.92	0.41
1:B:193:ARG:NH2	1:B:296:ASN:HB2	2.35	0.41
1:A:262:SER:OG	2:A:501:FMN:O3P	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/479 (83%)	384 (96%)	14 (4%)	0	100	100
1	B	398/479 (83%)	384 (96%)	14 (4%)	0	100	100
All	All	796/958 (83%)	768 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	348/417 (84%)	346 (99%)	2 (1%)	78	89
1	B	348/417 (84%)	346 (99%)	2 (1%)	78	89
All	All	696/834 (84%)	692 (99%)	4 (1%)	78	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	386	ARG
1	B	170	GLN
1	B	386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	HIS
1	A	190	GLN
1	A	250	GLN
1	B	79	HIS
1	B	122	ASN
1	B	250	GLN
1	B	301	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMN	B	501	-	33,33,33	1.03	2 (6%)	48,50,50	1.18	7 (14%)
2	FMN	A	501	-	33,33,33	1.05	2 (6%)	48,50,50	1.19	8 (16%)
6	OXY	A	508	-	1,1,1	0.17	0	-		

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	501	-	-	9/18/18/18	0/3/3/3
2	FMN	A	501	-	-	9/18/18/18	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C4A-N5	3.45	1.38	1.30
2	A	501	FMN	C4A-N5	3.43	1.38	1.30
2	A	501	FMN	C10-N1	2.63	1.38	1.33
2	B	501	FMN	C10-N1	2.59	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FMN	C4-N3-C2	-3.14	120.06	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FMN	C4-N3-C2	-3.11	120.11	125.64
2	A	501	FMN	C4A-C4-N3	2.63	119.94	113.25
2	B	501	FMN	C4A-C4-N3	2.58	119.83	113.25
2	B	501	FMN	C4A-C10-N10	2.54	120.11	116.48
2	A	501	FMN	O4-C4-C4A	-2.52	119.88	126.53
2	B	501	FMN	O4-C4-C4A	-2.42	120.14	126.53
2	A	501	FMN	C5A-C9A-N10	2.41	120.14	117.97
2	A	501	FMN	C9A-C5A-N5	-2.37	119.94	122.45
2	B	501	FMN	C10-C4A-N5	-2.33	120.06	124.81
2	A	501	FMN	C4A-C10-N10	2.28	119.75	116.48
2	B	501	FMN	C9A-C5A-N5	-2.27	120.05	122.45
2	A	501	FMN	C10-C4A-N5	-2.19	120.34	124.81
2	B	501	FMN	C5A-C9A-N10	2.15	119.91	117.97
2	A	501	FMN	C4A-C10-N1	-2.04	119.58	124.59

There are no chirality outliers.

All (18) torsion outliers are listed below:

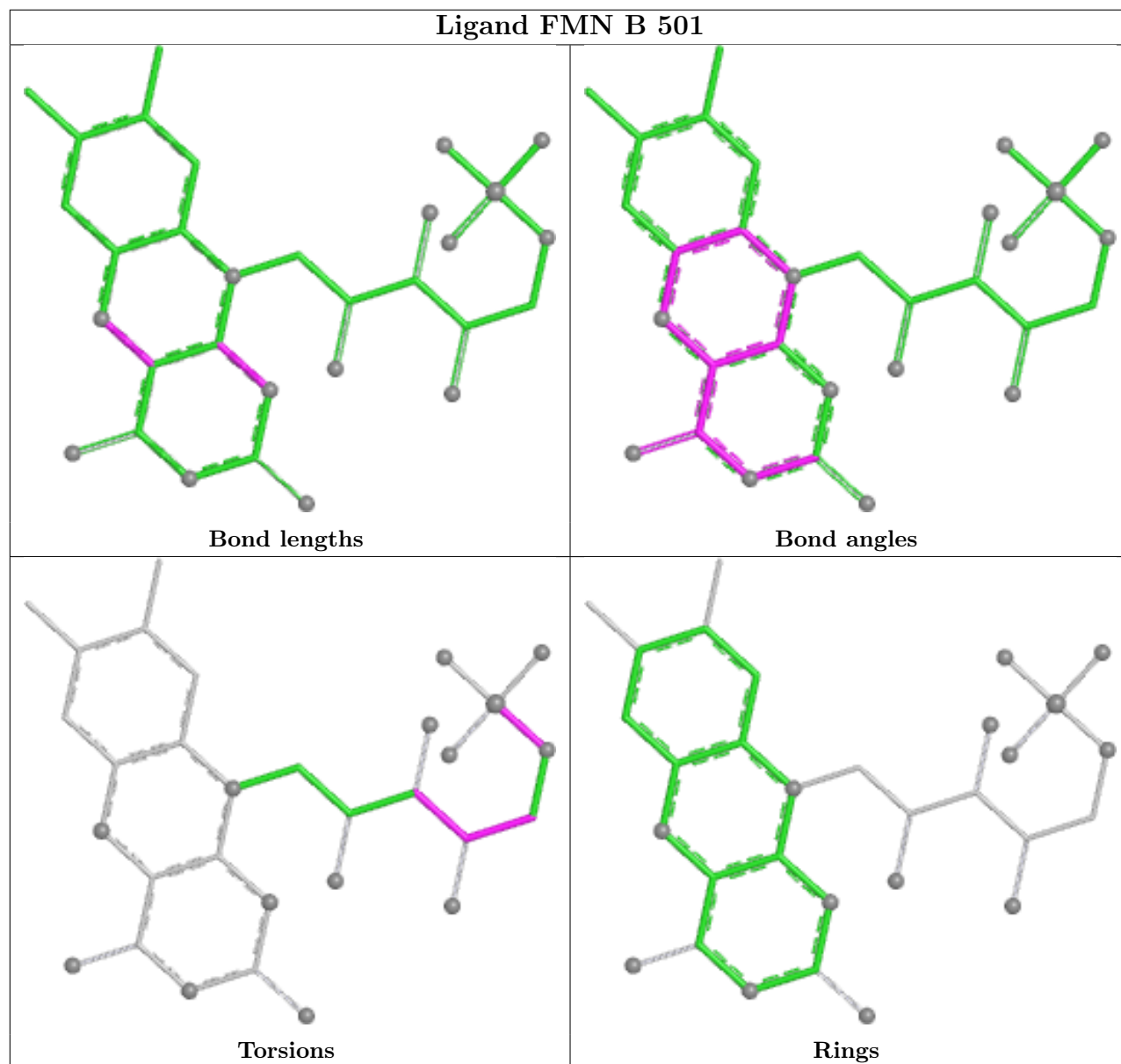
Mol	Chain	Res	Type	Atoms
2	A	501	FMN	C5'-O5'-P-O2P
2	A	501	FMN	C5'-O5'-P-O3P
2	B	501	FMN	C3'-C4'-C5'-O5'
2	B	501	FMN	O4'-C4'-C5'-O5'
2	B	501	FMN	C5'-O5'-P-O1P
2	B	501	FMN	C5'-O5'-P-O2P
2	B	501	FMN	C5'-O5'-P-O3P
2	A	501	FMN	O4'-C4'-C5'-O5'
2	A	501	FMN	O3'-C3'-C4'-C5'
2	B	501	FMN	O3'-C3'-C4'-C5'
2	A	501	FMN	O3'-C3'-C4'-O4'
2	B	501	FMN	O3'-C3'-C4'-O4'
2	A	501	FMN	C2'-C3'-C4'-C5'
2	B	501	FMN	C2'-C3'-C4'-C5'
2	A	501	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	C2'-C3'-C4'-O4'
2	A	501	FMN	C3'-C4'-C5'-O5'
2	A	501	FMN	C5'-O5'-P-O1P

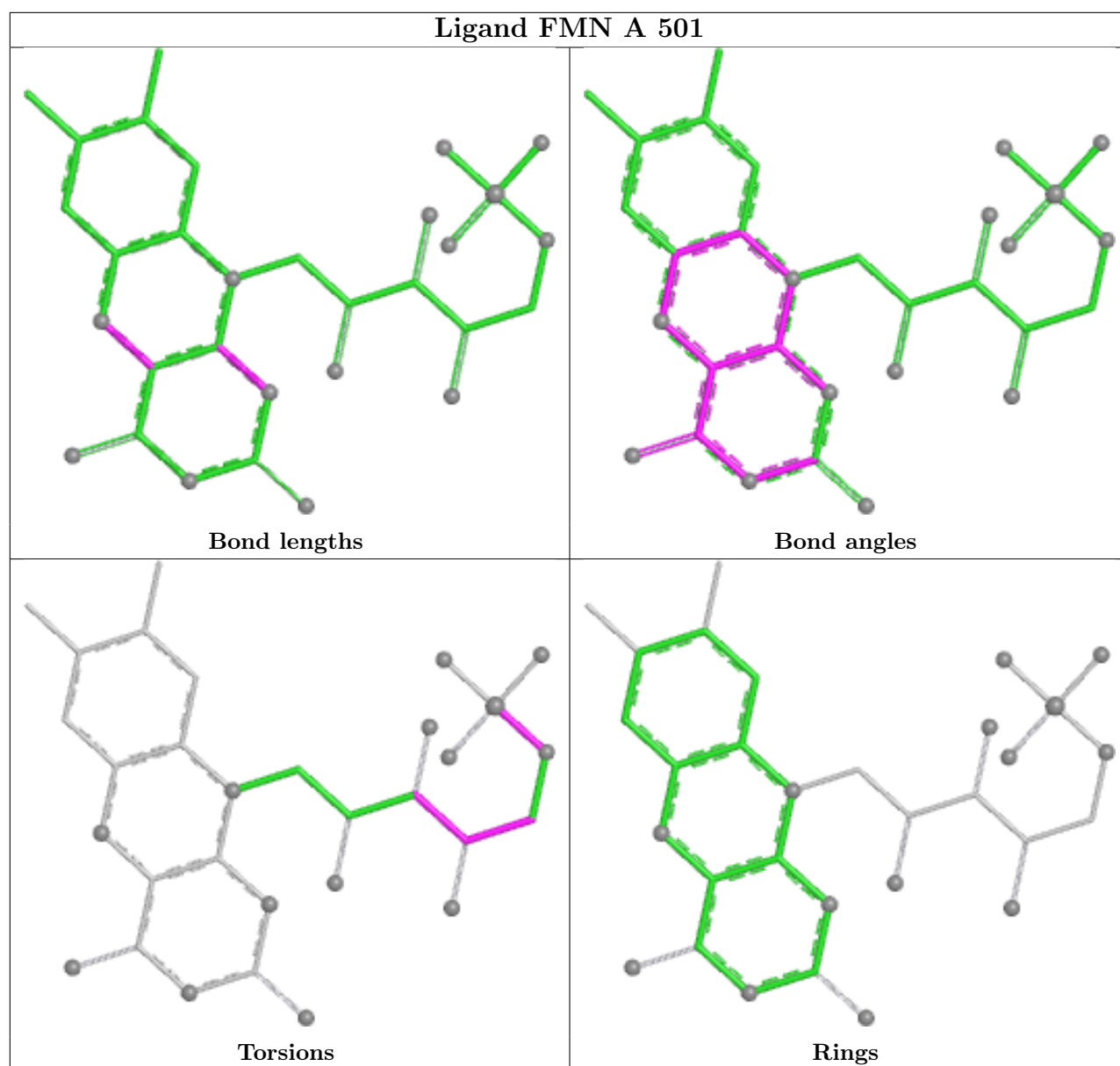
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FMN	1	0

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





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	400/479 (83%)	1.54	104 (26%)  	13, 24, 40, 77	0
1	B	400/479 (83%)	1.65	134 (33%)  	15, 26, 42, 59	0
All	All	800/958 (83%)	1.60	238 (29%)  	13, 25, 41, 77	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	8.7
1	A	400	PRO	6.2
1	B	401	LEU	6.1
1	A	278	GLU	6.0
1	B	194	TYR	4.8
1	A	57	ARG	4.8
1	B	22	PHE	4.7
1	A	380	ASP	4.7
1	B	283	VAL	4.5
1	B	334	ARG	4.3
1	B	278	GLU	4.2
1	B	400	PRO	4.2
1	A	146	LEU	4.2
1	B	380	ASP	4.1
1	B	195	TYR	4.1
1	A	283	VAL	4.0
1	B	281	PRO	3.9
1	A	392	ILE	3.9
1	A	293	SER	3.9
1	A	280	ASP	3.9
1	B	327	VAL	3.8
1	A	397	ALA	3.7
1	A	281	PRO	3.7
1	B	399	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	292	ARG	3.6
1	A	334	ARG	3.6
1	B	390	ARG	3.6
1	B	285	VAL	3.5
1	B	292	ARG	3.5
1	A	383	LYS	3.5
1	B	398	LEU	3.4
1	B	25	THR	3.4
1	B	370	SER	3.4
1	B	279	THR	3.4
1	A	394	ARG	3.4
1	A	252	ASP	3.4
1	B	364	GLY	3.4
1	B	277	ALA	3.4
1	A	390	ARG	3.3
1	B	28	LYS	3.3
1	B	252	ASP	3.3
1	A	277	ALA	3.3
1	B	274	GLN	3.3
1	A	176	HIS	3.3
1	A	196	ALA	3.3
1	A	22	PHE	3.3
1	B	26	GLU	3.3
1	B	244	LYS	3.3
1	A	194	TYR	3.3
1	A	80	ALA	3.3
1	B	57	ARG	3.2
1	B	386	ARG	3.2
1	A	384	LEU	3.2
1	A	398	LEU	3.2
1	A	131	ASP	3.2
1	B	319	MET	3.2
1	A	199	LEU	3.1
1	B	315	MET	3.1
1	A	82	GLU	3.1
1	B	394	ARG	3.1
1	B	280	ASP	3.1
1	A	84	HIS	3.0
1	B	276	ILE	3.0
1	A	315	MET	3.0
1	A	77	ILE	3.0
1	B	27	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	396	TRP	3.0
1	A	393	ALA	2.9
1	B	158	GLY	2.9
1	B	254	ILE	2.9
1	A	195	TYR	2.9
1	B	369	LEU	2.9
1	A	272	ILE	2.9
1	B	298	ILE	2.9
1	A	348	TRP	2.9
1	B	396	TRP	2.9
1	B	383	LYS	2.9
1	A	129	THR	2.9
1	B	90	GLU	2.9
1	A	83	ASP	2.8
1	B	61	GLN	2.8
1	B	131	ASP	2.8
1	B	67	ILE	2.8
1	A	27	TYR	2.8
1	B	35	TYR	2.8
1	A	308	VAL	2.8
1	B	287	ILE	2.8
1	A	284	ALA	2.8
1	B	258	TYR	2.8
1	B	290	VAL	2.8
1	B	68	ASP	2.7
1	B	288	PHE	2.7
1	A	258	TYR	2.7
1	B	249	TYR	2.7
1	B	217	ASN	2.7
1	B	82	GLU	2.7
1	B	29	THR	2.7
1	B	146	LEU	2.7
1	B	259	ASP	2.7
1	B	188	PHE	2.7
1	B	176	HIS	2.7
1	B	282	ARG	2.7
1	B	299	LEU	2.6
1	A	174	ASP	2.6
1	B	336	ARG	2.6
1	B	275	GLY	2.6
1	B	379	GLN	2.6
1	B	348	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	23	HIS	2.6
1	B	65	ASN	2.6
1	A	285	VAL	2.6
1	A	391	GLU	2.6
1	A	125	LYS	2.6
1	B	83	ASP	2.6
1	B	214	LEU	2.6
1	B	387	GLU	2.6
1	A	201	PRO	2.6
1	B	150	ASP	2.6
1	B	245	TRP	2.6
1	B	84	HIS	2.5
1	B	376	ARG	2.5
1	A	387	GLU	2.5
1	B	357	SER	2.5
1	B	375	TRP	2.5
1	B	62	ASN	2.5
1	B	172	TYR	2.5
1	A	270	ASP	2.5
1	A	104	ALA	2.5
1	A	299	LEU	2.5
1	A	369	LEU	2.5
1	A	290	VAL	2.4
1	B	95	ILE	2.5
1	A	294	ASP	2.4
1	A	214	LEU	2.4
1	B	52	LYS	2.4
1	B	199	LEU	2.4
1	A	147	HIS	2.4
1	B	347	GLY	2.4
1	B	66	GLU	2.4
1	A	318	VAL	2.4
1	A	399	ALA	2.4
1	B	393	ALA	2.4
1	B	112	GLY	2.4
1	B	64	ARG	2.4
1	B	125	LYS	2.4
1	A	99	PRO	2.4
1	B	384	LEU	2.4
1	A	66	GLU	2.3
1	A	379	GLN	2.3
1	A	202	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	244	LYS	2.3
1	A	257	PHE	2.3
1	B	359	ARG	2.3
1	A	115	HIS	2.3
1	B	144	PRO	2.3
1	A	245	TRP	2.3
1	A	35	TYR	2.3
1	A	336	ARG	2.3
1	B	44	LYS	2.3
1	A	4	VAL	2.3
1	B	4	VAL	2.3
1	A	25	THR	2.3
1	B	271	ALA	2.3
1	A	378	ASP	2.3
1	A	322	LYS	2.3
1	A	276	ILE	2.3
1	B	323	ILE	2.3
1	A	306	LYS	2.3
1	A	249	TYR	2.3
1	A	375	TRP	2.3
1	A	90	GLU	2.2
1	B	79	HIS	2.2
1	B	113	HIS	2.2
1	B	168	PHE	2.2
1	B	365	PHE	2.2
1	B	19	VAL	2.2
1	B	263	ASN	2.2
1	B	289	ASN	2.2
1	A	180	ASP	2.2
1	A	291	ALA	2.2
1	B	224	ALA	2.2
1	B	240	GLU	2.2
1	A	288	PHE	2.2
1	B	304	ARG	2.2
1	B	149	PRO	2.2
1	B	308	VAL	2.2
1	B	310	VAL	2.2
1	B	145	MET	2.2
1	B	80	ALA	2.2
1	B	284	ALA	2.2
1	B	115	HIS	2.2
1	B	148	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	253	ARG	2.2
1	B	235	PRO	2.2
1	A	259	ASP	2.2
1	A	19	VAL	2.2
1	B	349	SER	2.2
1	B	331	THR	2.2
1	A	189	GLU	2.1
1	A	254	ILE	2.1
1	B	340	ALA	2.1
1	B	362	ASP	2.1
1	A	365	PHE	2.1
1	B	257	PHE	2.1
1	A	112	GLY	2.1
1	A	253	ARG	2.1
1	A	386	ARG	2.1
1	B	291	ALA	2.1
1	B	293	SER	2.1
1	A	145	MET	2.1
1	B	268	MET	2.1
1	B	48	ILE	2.1
1	B	325	GLY	2.1
1	A	302	VAL	2.1
1	A	327	VAL	2.1
1	A	85	ALA	2.1
1	A	370	SER	2.1
1	A	274	GLN	2.1
1	B	227	HIS	2.1
1	B	236	THR	2.1
1	B	339	ARG	2.1
1	B	198	ILE	2.1
1	B	343	PHE	2.1
1	A	26	GLU	2.0
1	A	167	ALA	2.1
1	B	397	ALA	2.1
1	B	294	ASP	2.0
1	A	282	ARG	2.0
1	A	279	THR	2.0
1	A	240	GLU	2.0
1	B	247	ALA	2.0
1	A	337	ASN	2.0
1	A	241	LEU	2.0
1	B	108	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	372	LYS	2.0
1	A	117	PRO	2.0
1	A	307	GLY	2.0
1	B	169	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

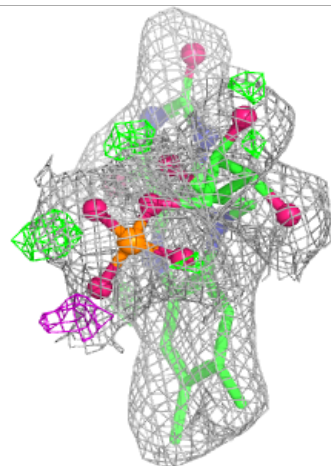
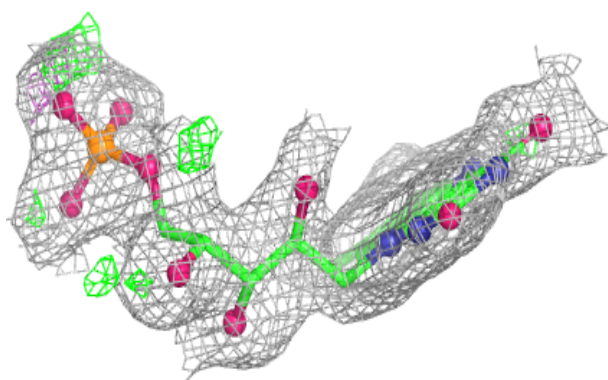
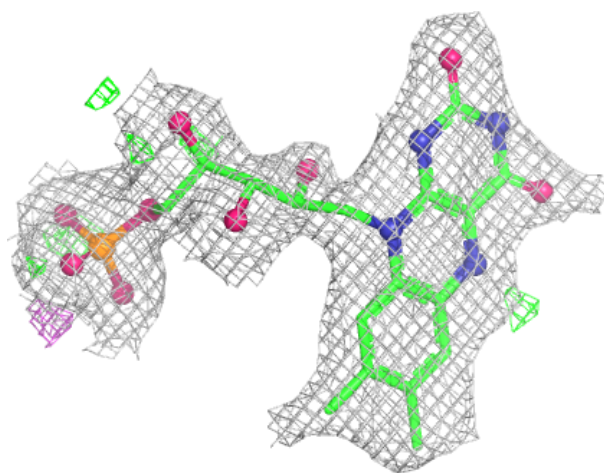
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

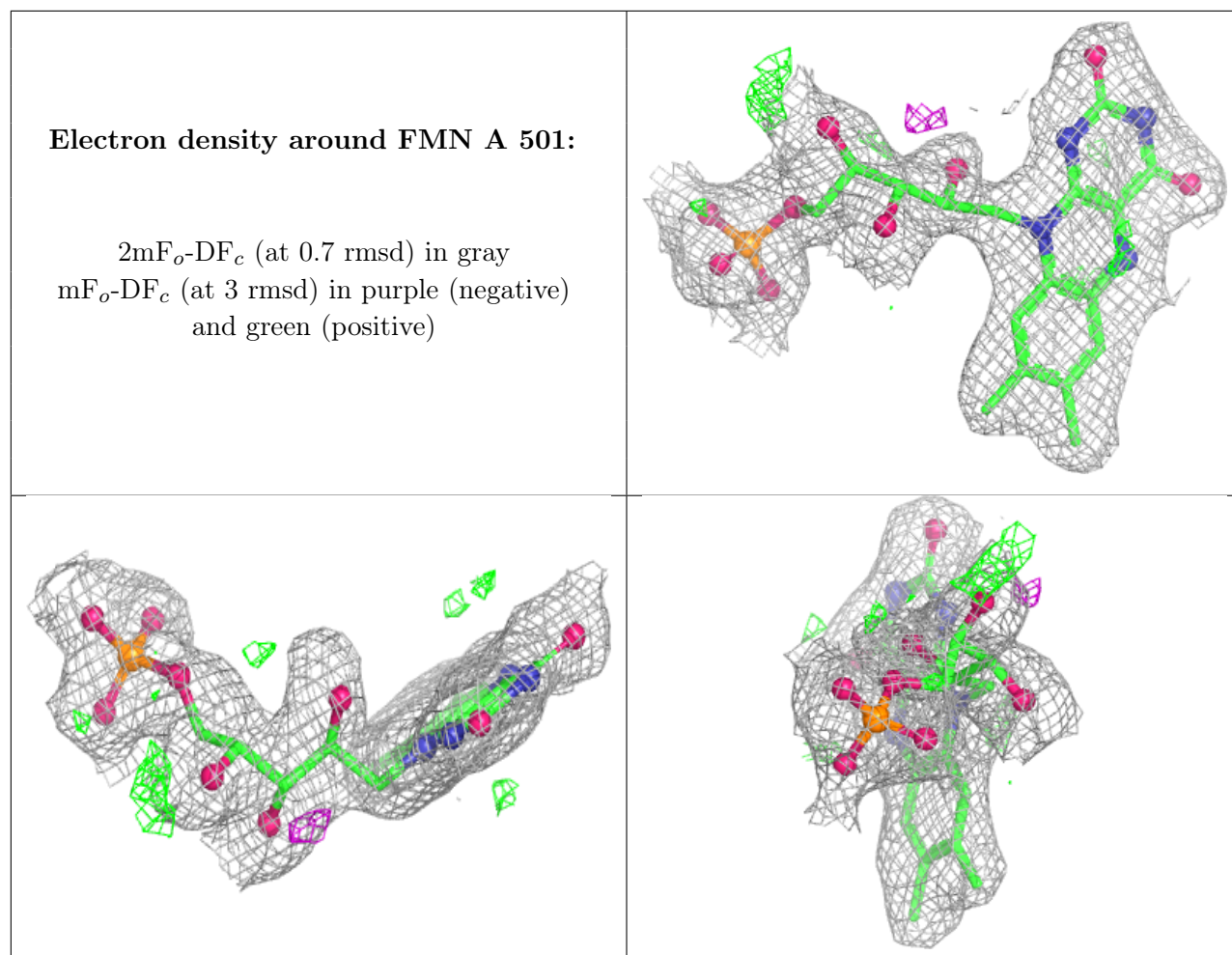
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	OXY	A	508	2/2	0.80	0.17	46,46,46,48	0
5	KR	B	507	1/1	0.85	0.09	36,36,36,36	1
5	KR	A	506	1/1	0.89	0.13	57,57,57,57	1
2	FMN	B	501	31/31	0.89	0.12	9,20,26,36	0
5	KR	A	505	1/1	0.89	0.11	38,38,38,38	1
2	FMN	A	501	31/31	0.91	0.10	4,14,19,32	0
5	KR	B	506	1/1	0.91	0.12	54,54,54,54	1
5	KR	A	507	1/1	0.93	0.10	34,34,34,34	1
3	FE	A	502	1/1	0.94	0.11	35,35,35,35	0
4	O	A	504	1/1	0.94	0.29	26,26,26,26	0
4	O	B	504	1/1	0.94	0.16	24,24,24,24	0
3	FE	B	503	1/1	0.96	0.07	34,34,34,34	0
3	FE	A	503	1/1	0.97	0.08	28,28,28,28	0
3	FE	B	502	1/1	0.97	0.08	32,32,32,32	0
5	KR	B	505	1/1	0.97	0.05	32,32,32,32	1

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 B 501:

$2mF_o-DF_c$ (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.