



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 06:54 am BST

PDB ID : 4RJE
Title : Aerococcus viridans L-lactate oxidase mutant
Authors : Rainer, D.; Nidetzky, B.; Wilson, D.K.
Deposited on : 2014-10-08
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

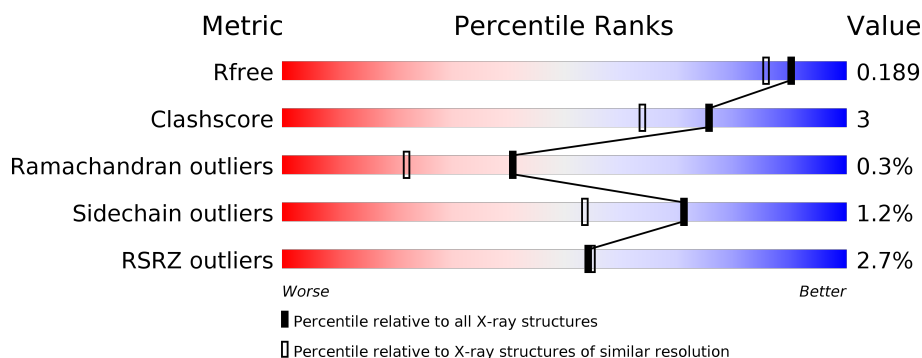
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>•</div> </div> </div>
1	B	374	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	374	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>• •</div> </div> </div>
1	D	374	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

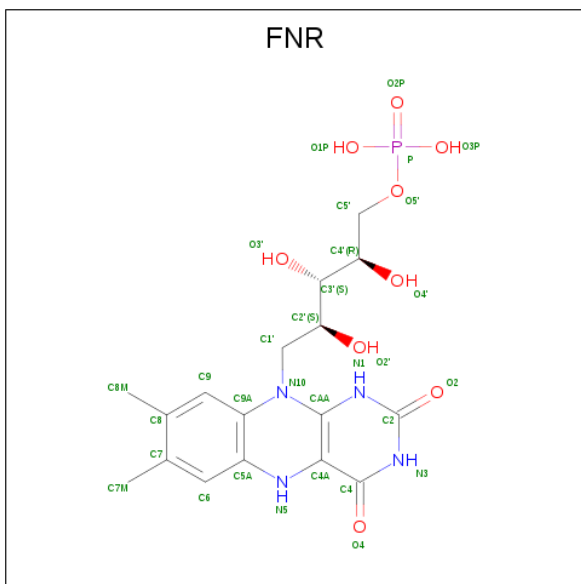
- Molecule 1 is a protein called Lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2824	1787	487	543	7			
1	B	362	Total	C	N	O	S	0	0	0
			2776	1755	478	536	7			
1	C	361	Total	C	N	O	S	0	0	0
			2778	1756	481	534	7			
1	D	365	Total	C	N	O	S	0	0	0
			2807	1776	485	539	7			

There are 20 discrepancies between the modelled and reference sequences:

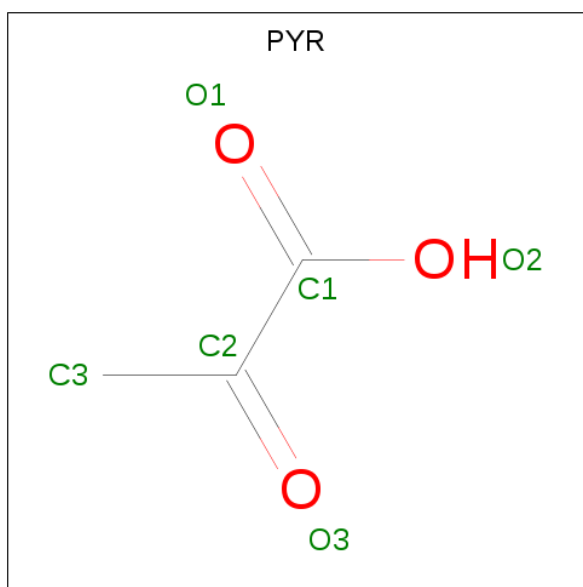
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	ALA	ENGINEERED MUTATION	UNP Q44467
A	102	ALA	THR	ENGINEERED MUTATION	UNP Q44467
A	163	GLY	SER	ENGINEERED MUTATION	UNP Q44467
A	232	ALA	GLY	ENGINEERED MUTATION	UNP Q44467
A	255	ALA	ARG	ENGINEERED MUTATION	UNP Q44467
B	95	GLY	ALA	ENGINEERED MUTATION	UNP Q44467
B	102	ALA	THR	ENGINEERED MUTATION	UNP Q44467
B	163	GLY	SER	ENGINEERED MUTATION	UNP Q44467
B	232	ALA	GLY	ENGINEERED MUTATION	UNP Q44467
B	255	ALA	ARG	ENGINEERED MUTATION	UNP Q44467
C	95	GLY	ALA	ENGINEERED MUTATION	UNP Q44467
C	102	ALA	THR	ENGINEERED MUTATION	UNP Q44467
C	163	GLY	SER	ENGINEERED MUTATION	UNP Q44467
C	232	ALA	GLY	ENGINEERED MUTATION	UNP Q44467
C	255	ALA	ARG	ENGINEERED MUTATION	UNP Q44467
D	95	GLY	ALA	ENGINEERED MUTATION	UNP Q44467
D	102	ALA	THR	ENGINEERED MUTATION	UNP Q44467
D	163	GLY	SER	ENGINEERED MUTATION	UNP Q44467
D	232	ALA	GLY	ENGINEERED MUTATION	UNP Q44467
D	255	ALA	ARG	ENGINEERED MUTATION	UNP Q44467

- Molecule 2 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]P TERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR) (formula: $C_{17}H_{23}N_4O_9P$).



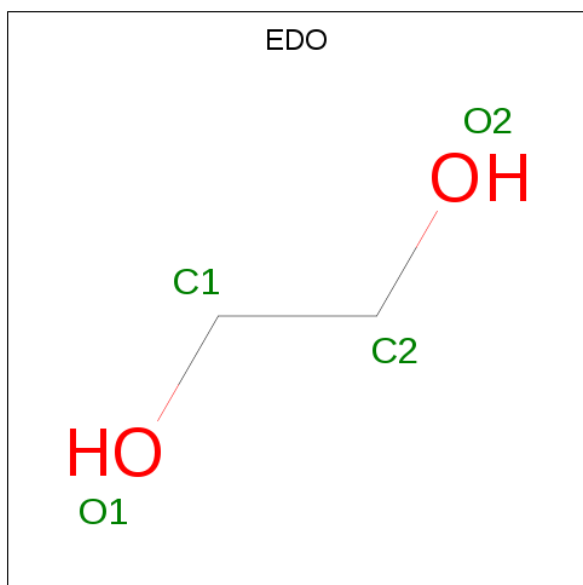
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

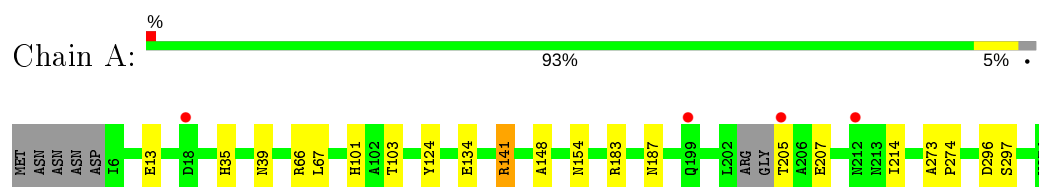
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	229	Total O 229 229	0	0
5	B	211	Total O 211 211	0	0
5	C	236	Total O 236 236	0	0
5	D	244	Total O 244 244	0	0

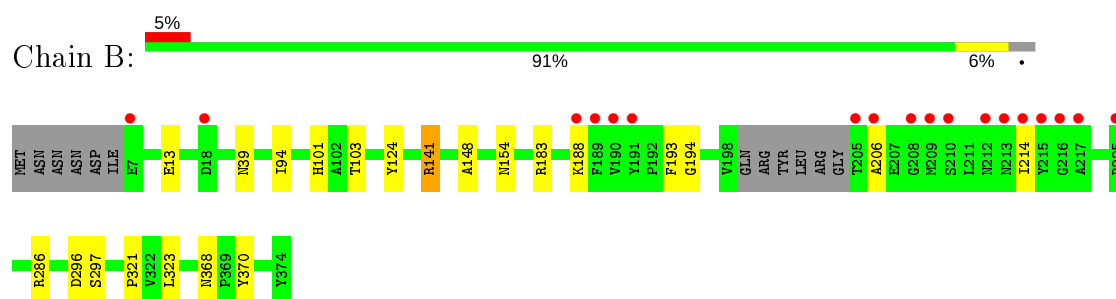
3 Residue-property plots [i](#)

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.

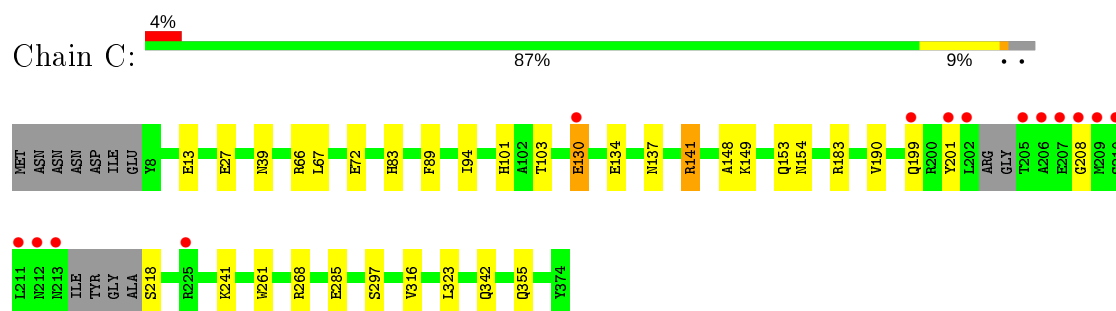
• Molecule 1: Lactate oxidase



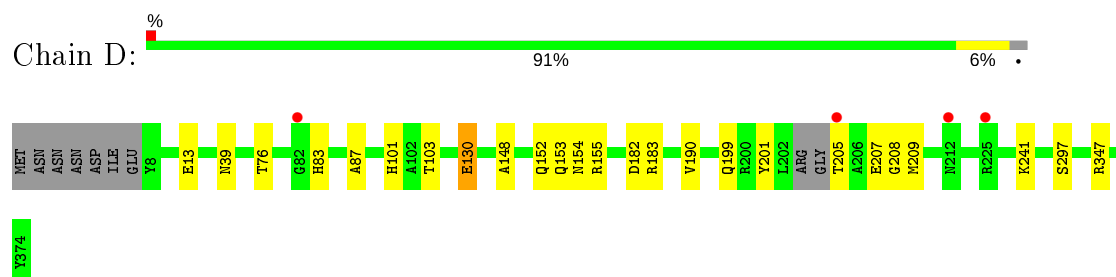
• Molecule 1: Lactate oxidase



• Molecule 1: Lactate oxidase



• Molecule 1: Lactate oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.59Å 124.36Å 106.89Å 90.00° 124.29° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65 10.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-1.65) 98.2 (10.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.152 , 0.180 0.166 , 0.189	Depositor DCC
R_{free} test set	7791 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-1/2*h-1/2*k-l 0.018 for -k,-h,-1/2*h+1/2*k-l 0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12265	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.65	0/2887	0.81	2/3911 (0.1%)
1	B	0.65	0/2838	0.82	3/3845 (0.1%)
1	C	0.65	0/2839	0.78	1/3844 (0.0%)
1	D	0.65	0/2870	0.77	2/3888 (0.1%)
All	All	0.65	0/11434	0.79	8/15488 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ARG	NE-CZ-NH1	-14.27	113.16	120.30
1	A	141	ARG	NE-CZ-NH1	-12.14	114.23	120.30
1	B	141	ARG	NE-CZ-NH2	9.07	124.83	120.30
1	B	286	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	A	141	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	D	182	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	141	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	D	347	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	2824	0	2752	15	0
1	B	2776	0	2700	12	0
1	C	2778	0	2706	18	1
1	D	2807	0	2735	21	0
2	A	31	0	22	0	0
2	B	31	0	22	0	0
2	C	31	0	22	2	0
2	D	31	0	22	1	0
3	A	6	0	3	1	0
3	B	6	0	3	1	0
3	C	6	0	3	1	0
3	D	6	0	3	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
5	A	229	0	0	1	0
5	B	211	0	0	1	0
5	C	236	0	0	3	0
5	D	244	0	0	2	0
All	All	12265	0	11011	70	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ALA:H	1:C:154:ASN:HD21	1.13	0.91
1:B:148:ALA:H	1:B:154:ASN:HD21	1.23	0.87
3:A:402:PYR:H32	5:A:695:HOH:O	1.74	0.87
3:D:402:PYR:H32	5:D:634:HOH:O	1.81	0.81
1:D:148:ALA:H	1:D:154:ASN:HD21	1.31	0.74
3:B:402:PYR:H32	5:B:693:HOH:O	1.87	0.74
1:B:94:ILE:HG21	1:B:323:LEU:HD11	1.71	0.73
1:A:148:ALA:H	1:A:154:ASN:HD21	1.35	0.73
1:C:39:ASN:HD22	1:C:183:ARG:HH11	1.35	0.71
1:D:190:VAL:HG21	1:D:208:GLY:O	1.91	0.70
1:B:39:ASN:HD22	1:B:183:ARG:HH11	1.40	0.70
1:A:39:ASN:HD22	1:A:183:ARG:HH11	1.40	0.69
1:D:190:VAL:CG2	1:D:208:GLY:C	2.64	0.66
1:C:101:HIS:HD2	1:C:103:THR:H	1.45	0.65
1:A:148:ALA:N	1:A:154:ASN:HD21	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASN:HD22	1:D:183:ARG:HH11	1.45	0.62
1:D:148:ALA:N	1:D:154:ASN:HD21	1.98	0.61
1:C:94:ILE:HG21	1:C:323:LEU:HD11	1.85	0.59
3:C:402:PYR:H32	5:C:735:HOH:O	2.03	0.58
1:C:13:GLU:O	1:C:101:HIS:HE1	1.87	0.57
1:D:101:HIS:HD2	1:D:103:THR:H	1.54	0.55
1:D:13:GLU:O	1:D:101:HIS:HE1	1.91	0.54
1:B:101:HIS:HD2	1:B:103:THR:H	1.56	0.54
1:D:190:VAL:CG2	1:D:208:GLY:O	2.56	0.54
1:A:101:HIS:HD2	1:A:103:THR:H	1.57	0.52
1:C:83:HIS:HD2	5:C:626:HOH:O	1.92	0.52
1:A:35:HIS:HE1	1:A:187:ASN:HD21	1.59	0.51
1:B:148:ALA:N	1:B:154:ASN:HD21	2.00	0.51
1:D:190:VAL:HG23	1:D:209:MET:C	2.31	0.51
1:D:190:VAL:HG21	1:D:208:GLY:C	2.29	0.50
1:A:205:THR:HG23	1:A:207:GLU:H	1.77	0.49
1:C:101:HIS:CD2	1:C:103:THR:H	2.28	0.49
1:C:72:GLU:H	1:C:355:GLN:HE22	1.60	0.49
1:D:130:GLU:H	1:D:130:GLU:CD	2.17	0.49
1:D:83:HIS:HD2	5:D:657:HOH:O	1.96	0.48
1:B:368:ASN:HD21	1:B:370:TYR:HB2	1.79	0.48
1:B:124:TYR:CE2	1:B:214:ILE:HG22	2.49	0.48
1:D:205:THR:HG23	1:D:207:GLU:H	1.79	0.47
1:A:148:ALA:H	1:A:154:ASN:ND2	2.09	0.47
1:D:101:HIS:CD2	1:D:103:THR:H	2.33	0.47
1:A:39:ASN:ND2	1:A:183:ARG:HH11	2.10	0.46
1:A:101:HIS:CD2	1:A:103:THR:H	2.34	0.46
1:C:66:ARG:C	1:C:67:LEU:HD23	2.37	0.45
1:D:153:GLN:NE2	1:D:201:TYR:HB3	2.32	0.45
1:B:101:HIS:CD2	1:B:103:THR:H	2.34	0.44
1:D:39:ASN:ND2	1:D:183:ARG:HH11	2.15	0.44
1:A:124:TYR:CZ	1:A:214:ILE:HG22	2.53	0.44
1:D:190:VAL:HG23	1:D:209:MET:O	2.17	0.44
1:A:35:HIS:HE1	1:A:187:ASN:ND2	2.16	0.42
1:B:124:TYR:CE2	1:B:214:ILE:CG2	3.03	0.42
1:C:268:ARG:NH1	2:C:401:FNR:H7M2	2.34	0.42
1:A:273:ALA:HB1	1:A:274:PRO:HD2	2.02	0.42
1:C:89:PHE:HA	1:C:316:VAL:O	2.20	0.42
1:D:76:THR:O	1:D:87:ALA:HA	2.20	0.42
1:D:130:GLU:CD	1:D:130:GLU:N	2.74	0.41
1:C:241:LYS:HA	1:C:261:TRP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:C	1:A:67:LEU:HD12	2.41	0.41
1:B:296:ASP:OD1	1:B:296:ASP:C	2.59	0.41
1:C:94:ILE:HG23	2:C:401:FNR:C6	2.50	0.41
1:D:152:GLN:OE1	1:D:155:ARG:NH1	2.54	0.41
1:B:13:GLU:O	1:B:101:HIS:HE1	2.04	0.41
1:A:13:GLU:O	1:A:101:HIS:HE1	2.04	0.41
1:C:134:GLU:CG	5:C:632:HOH:O	2.69	0.41
1:A:296:ASP:C	1:A:296:ASP:OD1	2.59	0.40
1:C:130:GLU:CD	1:C:130:GLU:H	2.24	0.40
1:B:194:GLY:HA2	1:B:206:ALA:HB3	2.04	0.40
1:C:149:LYS:NZ	1:C:218:SER:O	2.48	0.40
1:D:241:LYS:HZ1	2:D:401:FNR:HN1	1.70	0.40
1:C:153:GLN:NE2	1:C:201:TYR:HB3	2.37	0.40
1:C:190:VAL:HG13	1:C:208:GLY:C	2.41	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLU:OE1	1:C:285:GLU:OE1[2_454]	1.24	0.96

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	363/374 (97%)	355 (98%)	7 (2%)	1 (0%)	41 22
1	B	358/374 (96%)	351 (98%)	6 (2%)	1 (0%)	41 22
1	C	355/374 (95%)	347 (98%)	7 (2%)	1 (0%)	41 22
1	D	361/374 (96%)	352 (98%)	8 (2%)	1 (0%)	41 22
All	All	1437/1496 (96%)	1405 (98%)	28 (2%)	4 (0%)	41 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	297	SER
1	C	297	SER
1	D	297	SER

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	289/295 (98%)	287 (99%)	2 (1%)	84	73
1	B	284/295 (96%)	280 (99%)	4 (1%)	67	46
1	C	285/295 (97%)	279 (98%)	6 (2%)	53	29
1	D	287/295 (97%)	285 (99%)	2 (1%)	84	73
All	All	1145/1180 (97%)	1131 (99%)	14 (1%)	71	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	141	ARG
1	B	141	ARG
1	B	188	LYS
1	B	193	PHE
1	B	321	PRO
1	C	27	GLU
1	C	130	GLU
1	C	137	ASN
1	C	141	ARG
1	C	199	GLN
1	C	342	GLN
1	D	130	GLU
1	D	199	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	ASN
1	A	83	HIS
1	A	101	HIS
1	A	137	ASN
1	A	154	ASN
1	A	187	ASN
1	A	355	GLN
1	A	368	ASN
1	B	35	HIS
1	B	39	ASN
1	B	83	HIS
1	B	101	HIS
1	B	137	ASN
1	B	153	GLN
1	B	154	ASN
1	B	187	ASN
1	B	288	ASN
1	B	368	ASN
1	C	35	HIS
1	C	39	ASN
1	C	83	HIS
1	C	101	HIS
1	C	153	GLN
1	C	154	ASN
1	C	187	ASN
1	C	199	GLN
1	C	288	ASN
1	C	355	GLN
1	C	368	ASN
1	D	9	ASN
1	D	39	ASN
1	D	83	HIS
1	D	101	HIS
1	D	153	GLN
1	D	154	ASN
1	D	187	ASN
1	D	368	ASN

5.3.3 RNA ⓘ

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](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PYR	B	402	-	2,5,5	0.27	0	2,6,6	1.40	0
4	EDO	A	403	-	3,3,3	0.86	0	2,2,2	0.16	0
4	EDO	C	403	-	3,3,3	0.64	0	2,2,2	0.41	0
3	PYR	D	402	-	2,5,5	0.70	0	2,6,6	0.67	0
2	FNR	C	401	-	31,33,33	2.02	6 (19%)	40,50,50	1.93	9 (22%)
2	FNR	A	401	-	31,33,33	1.66	5 (16%)	40,50,50	1.76	7 (17%)
2	FNR	B	401	-	31,33,33	1.85	6 (19%)	40,50,50	1.96	7 (17%)
3	PYR	A	402	-	2,5,5	0.57	0	2,6,6	1.15	0
4	EDO	B	403	-	3,3,3	0.78	0	2,2,2	0.13	0
2	FNR	D	401	-	31,33,33	1.82	9 (29%)	40,50,50	2.40	7 (17%)
3	PYR	C	402	-	2,5,5	0.28	0	2,6,6	1.57	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
3	PYR	B	402	-	-	0/0/4/4	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYR	D	402	-	-	0/0/4/4	-
2	FNR	C	401	-	-	1/18/18/18	0/3/3/3
2	FNR	A	401	-	-	1/18/18/18	0/3/3/3
2	FNR	B	401	-	-	1/18/18/18	0/3/3/3
3	PYR	A	402	-	-	0/0/4/4	-
4	EDO	B	403	-	-	0/1/1/1	-
2	FNR	D	401	-	-	1/18/18/18	0/3/3/3
3	PYR	C	402	-	-	0/0/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FNR	CAA-N1	5.44	1.40	1.33
2	B	401	FNR	CAA-N1	5.04	1.39	1.33
2	C	401	FNR	C1'-N10	4.53	1.52	1.48
2	A	401	FNR	C4-N3	4.34	1.40	1.33
2	D	401	FNR	C7M-C7	-4.31	1.42	1.51
2	C	401	FNR	C4-N3	4.14	1.40	1.33
2	D	401	FNR	CAA-N1	3.77	1.38	1.33
2	A	401	FNR	C8M-C8	-3.73	1.43	1.51
2	B	401	FNR	C1'-N10	3.70	1.52	1.48
2	C	401	FNR	C8M-C8	-3.69	1.43	1.51
2	C	401	FNR	C7M-C7	-3.66	1.43	1.51
2	B	401	FNR	C4-N3	3.46	1.39	1.33
2	D	401	FNR	C4A-N5	3.43	1.38	1.33
2	A	401	FNR	CAA-N1	3.27	1.37	1.33
2	B	401	FNR	C7M-C7	-3.21	1.44	1.51
2	B	401	FNR	C8M-C8	-3.12	1.44	1.51
2	A	401	FNR	C7M-C7	-3.05	1.44	1.51
2	D	401	FNR	C8M-C8	-2.98	1.45	1.51
2	B	401	FNR	C4A-N5	2.82	1.37	1.33
2	C	401	FNR	C4A-N5	2.75	1.37	1.33
2	D	401	FNR	C5'-C4'	2.73	1.55	1.51
2	D	401	FNR	C4-N3	2.56	1.37	1.33
2	A	401	FNR	C1'-N10	2.49	1.50	1.48
2	D	401	FNR	C4A-CAA	2.33	1.41	1.38
2	D	401	FNR	C2'-C3'	2.12	1.57	1.53
2	D	401	FNR	C1'-N10	2.01	1.50	1.48

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FNR	C4-N3-C2	11.63	124.96	115.14
2	B	401	FNR	C4-N3-C2	7.97	121.87	115.14
2	A	401	FNR	C4-N3-C2	7.92	121.83	115.14
2	C	401	FNR	C4-N3-C2	7.45	121.44	115.14
2	C	401	FNR	C1'-N10-C9A	4.69	121.98	118.29
2	D	401	FNR	C4A-C4-N3	-4.50	117.28	123.43
2	B	401	FNR	C1'-N10-C9A	4.25	121.64	118.29
2	D	401	FNR	C9A-N10-CAA	-3.99	116.68	121.91
2	D	401	FNR	C5A-C9A-N10	3.61	120.33	117.72
2	C	401	FNR	C9A-N10-CAA	-3.60	117.19	121.91
2	B	401	FNR	C4A-C4-N3	-3.52	118.61	123.43
2	B	401	FNR	C5A-C9A-N10	3.52	120.26	117.72
2	B	401	FNR	C9A-N10-CAA	-3.36	117.51	121.91
2	C	401	FNR	C4A-C4-N3	-3.23	119.02	123.43
2	D	401	FNR	C1'-N10-C9A	3.14	120.76	118.29
2	C	401	FNR	CAA-C4A-N5	-3.11	119.11	121.26
2	D	401	FNR	CAA-C4A-N5	-3.11	119.11	121.26
2	A	401	FNR	C4A-C4-N3	-2.99	119.35	123.43
2	A	401	FNR	C1'-N10-C9A	2.92	120.59	118.29
2	C	401	FNR	C4-C4A-N5	2.72	121.70	118.60
2	B	401	FNR	CAA-C4A-N5	-2.46	119.56	121.26
2	A	401	FNR	C4-C4A-N5	2.45	121.39	118.60
2	A	401	FNR	C9A-N10-CAA	-2.38	118.79	121.91
2	A	401	FNR	CAA-C4A-N5	-2.26	119.70	121.26
2	D	401	FNR	C4-C4A-N5	2.20	121.11	118.60
2	B	401	FNR	O3P-P-O1P	2.19	116.01	107.64
2	A	401	FNR	O3P-P-O1P	2.17	115.93	107.64
2	C	401	FNR	C5A-C9A-N10	2.16	119.28	117.72
2	C	401	FNR	C4A-CAA-N10	2.10	122.46	120.30
2	C	401	FNR	C6-C5A-N5	-2.04	116.80	119.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

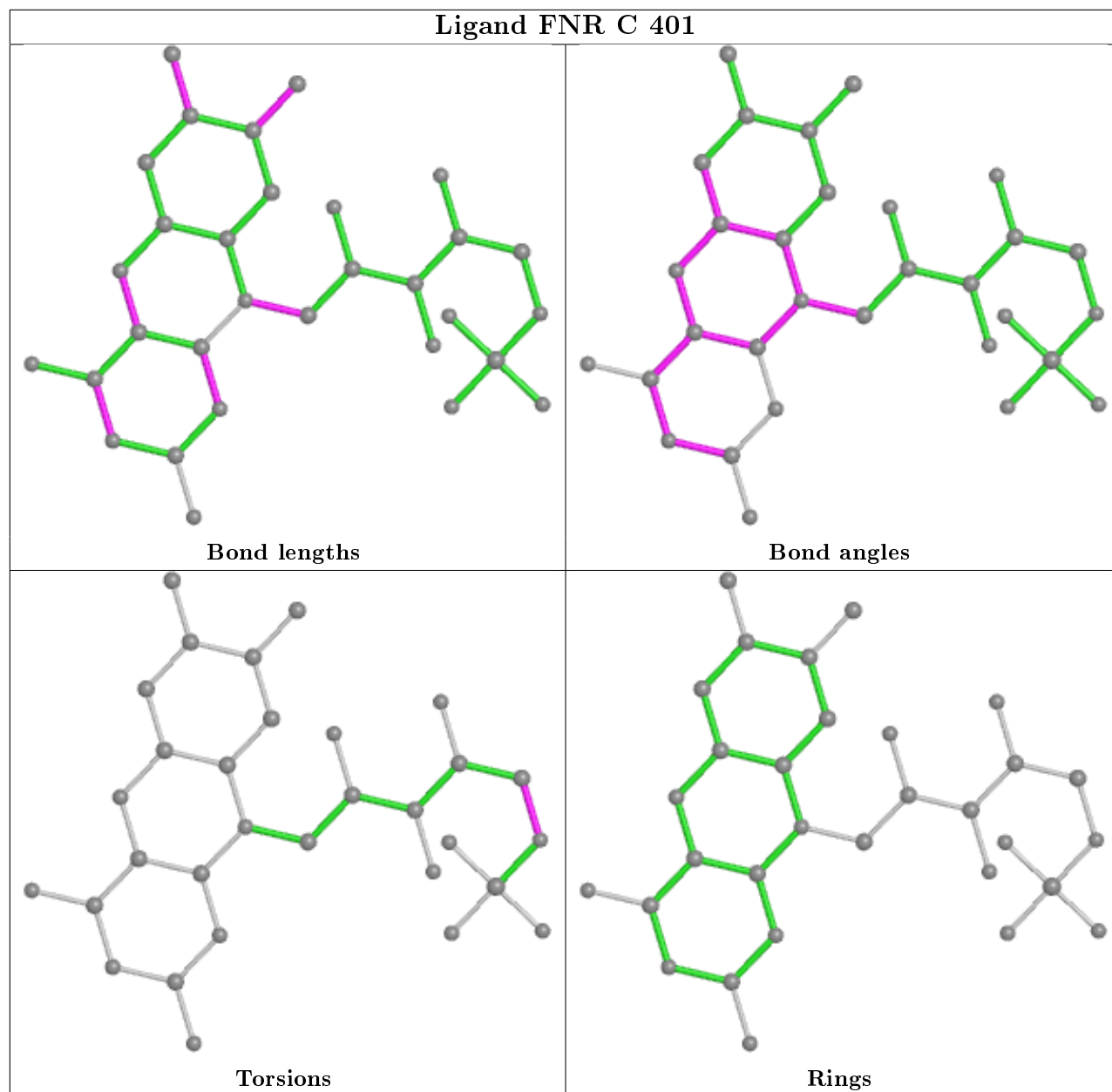
Mol	Chain	Res	Type	Atoms
2	A	401	FNR	C4'-C5'-O5'-P
2	B	401	FNR	C4'-C5'-O5'-P
2	D	401	FNR	C4'-C5'-O5'-P
2	C	401	FNR	C4'-C5'-O5'-P

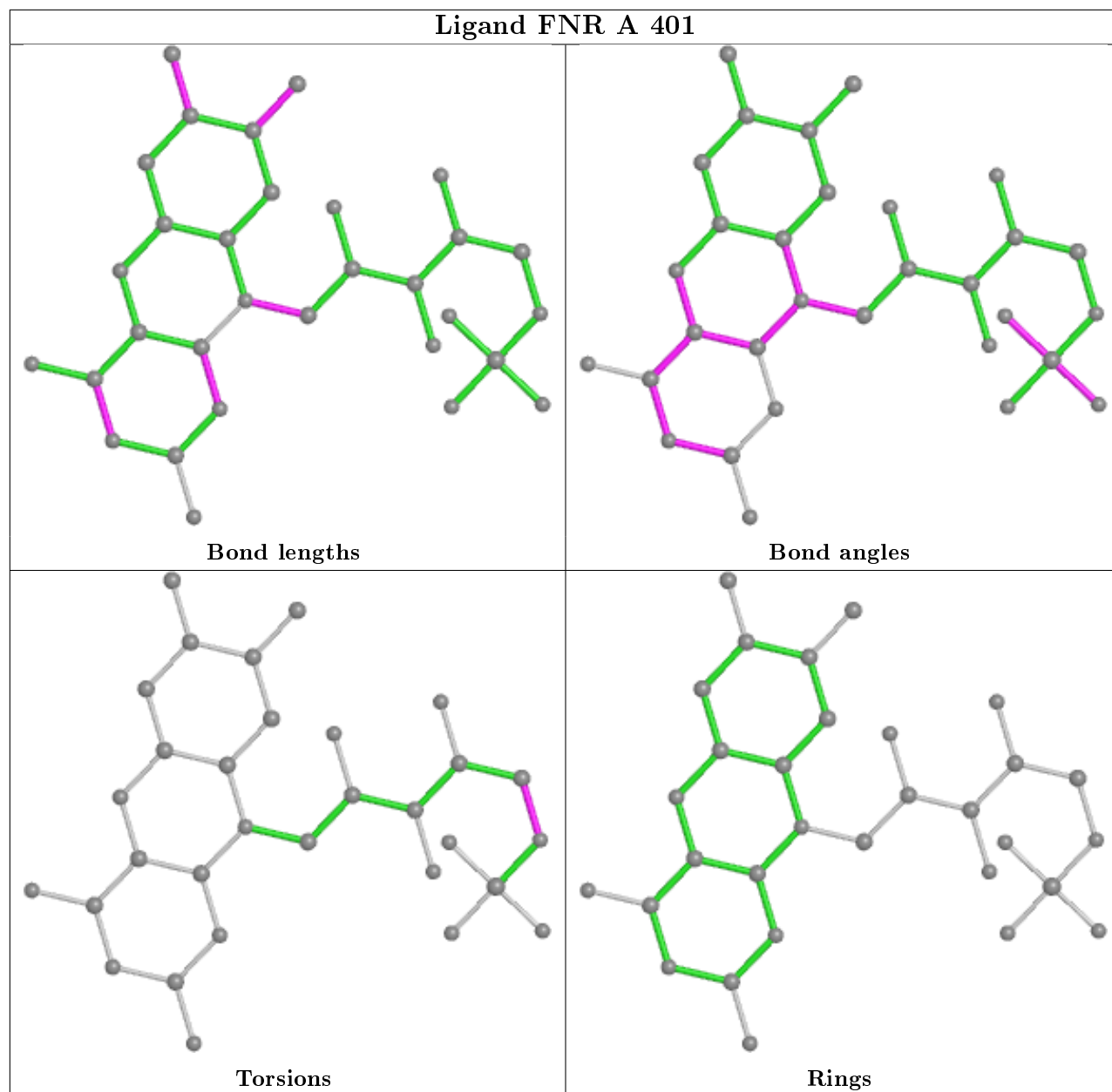
There are no ring outliers.

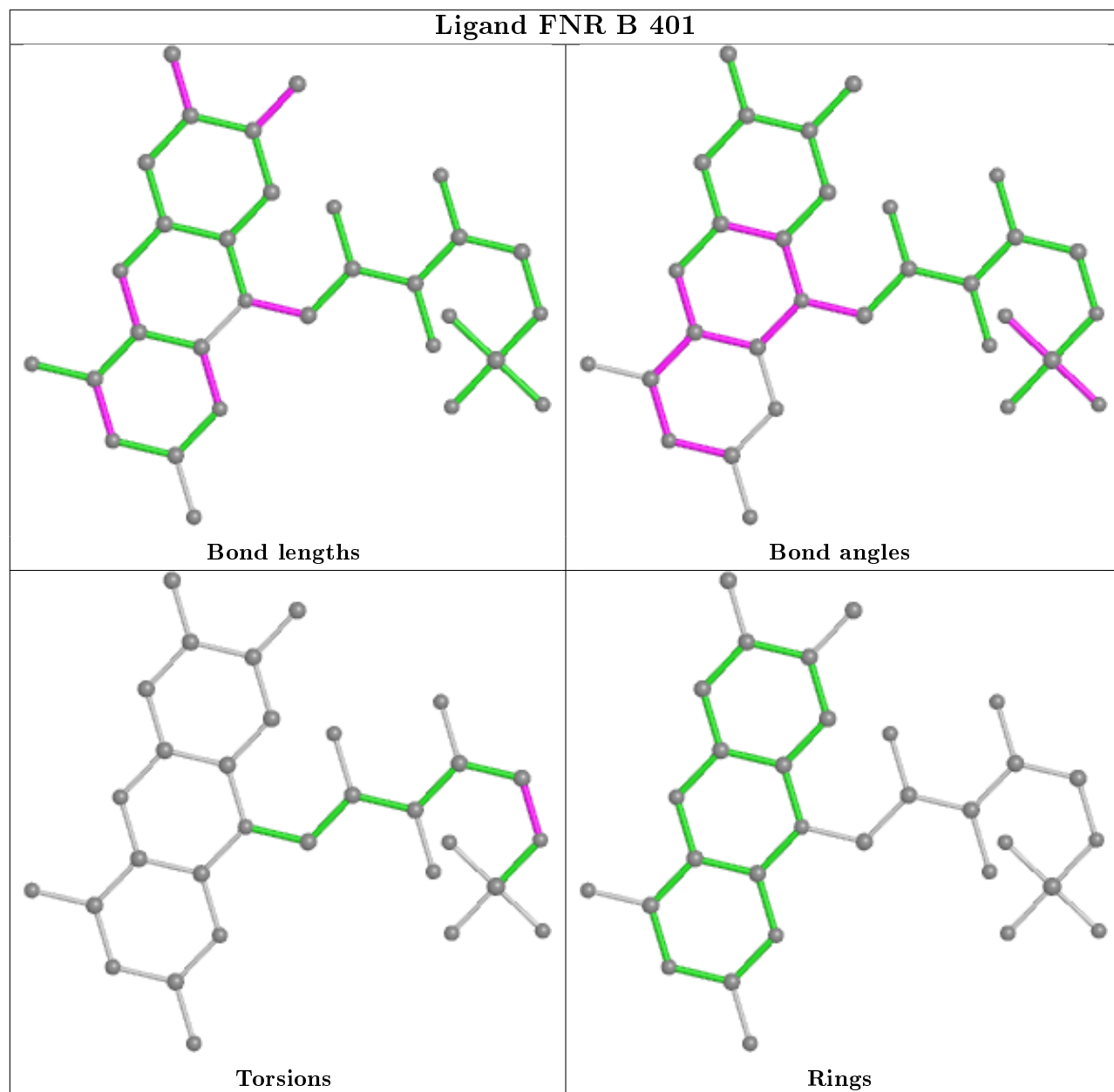
6 monomers are involved in 7 short contacts:

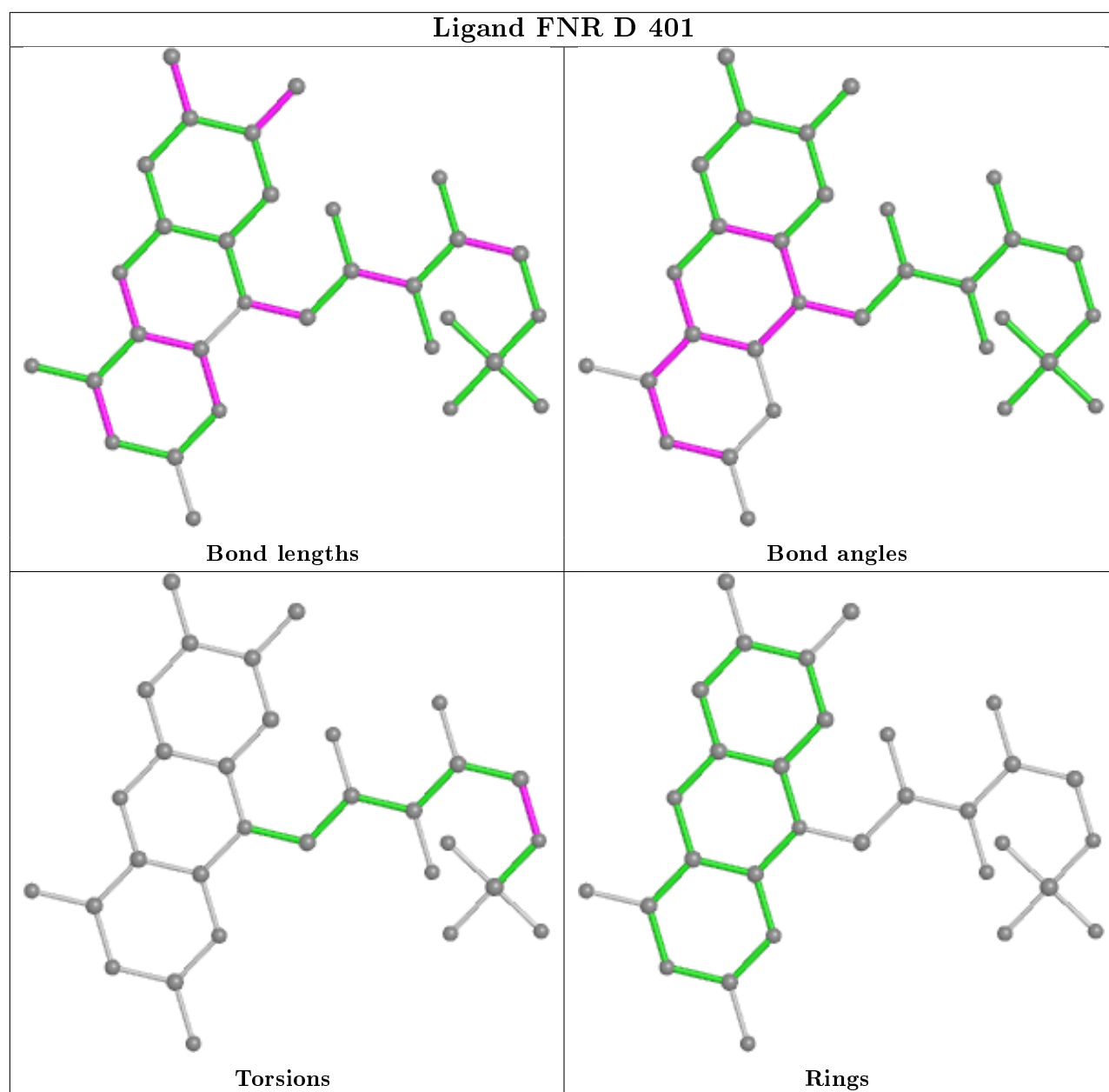
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	PYR	1	0
3	D	402	PYR	1	0
2	C	401	FNR	2	0
3	A	402	PYR	1	0
2	D	401	FNR	1	0
3	C	402	PYR	1	0

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	367/374 (98%)	-0.46	4 (1%) 80 83	7, 12, 23, 34	0
1	B	362/374 (96%)	-0.27	18 (4%) 28 27	8, 12, 31, 52	0
1	C	361/374 (96%)	-0.34	14 (3%) 39 39	7, 12, 26, 75	0
1	D	365/374 (97%)	-0.45	4 (1%) 80 83	8, 12, 23, 36	0
All	All	1455/1496 (97%)	-0.38	40 (2%) 54 55	7, 12, 25, 75	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	THR	9.2
1	C	212	ASN	7.5
1	B	205	THR	6.9
1	B	212	ASN	6.5
1	C	202	LEU	6.4
1	B	208	GLY	5.4
1	C	213	ASN	5.3
1	B	210	SER	4.9
1	C	211	LEU	4.7
1	B	206	ALA	4.5
1	A	205	THR	4.4
1	C	208	GLY	4.4
1	B	213	ASN	4.4
1	B	7	GLU	4.3
1	D	205	THR	4.3
1	C	206	ALA	3.8
1	C	209	MET	3.7
1	C	199	GLN	3.7
1	A	199	GLN	3.5
1	B	188	LYS	3.5
1	B	209	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	217	ALA	3.3
1	B	225	ARG	3.2
1	C	201	TYR	3.2
1	B	216	GLY	3.1
1	B	215	TYR	3.1
1	B	191	TYR	3.0
1	B	190	VAL	2.9
1	B	214	ILE	2.9
1	A	18	ASP	2.8
1	C	210	SER	2.8
1	D	225	ARG	2.7
1	C	225	ARG	2.6
1	A	212	ASN	2.5
1	D	82	GLY	2.4
1	C	207	GLU	2.4
1	C	130	GLU	2.3
1	B	18	ASP	2.3
1	D	212	ASN	2.2
1	B	189	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

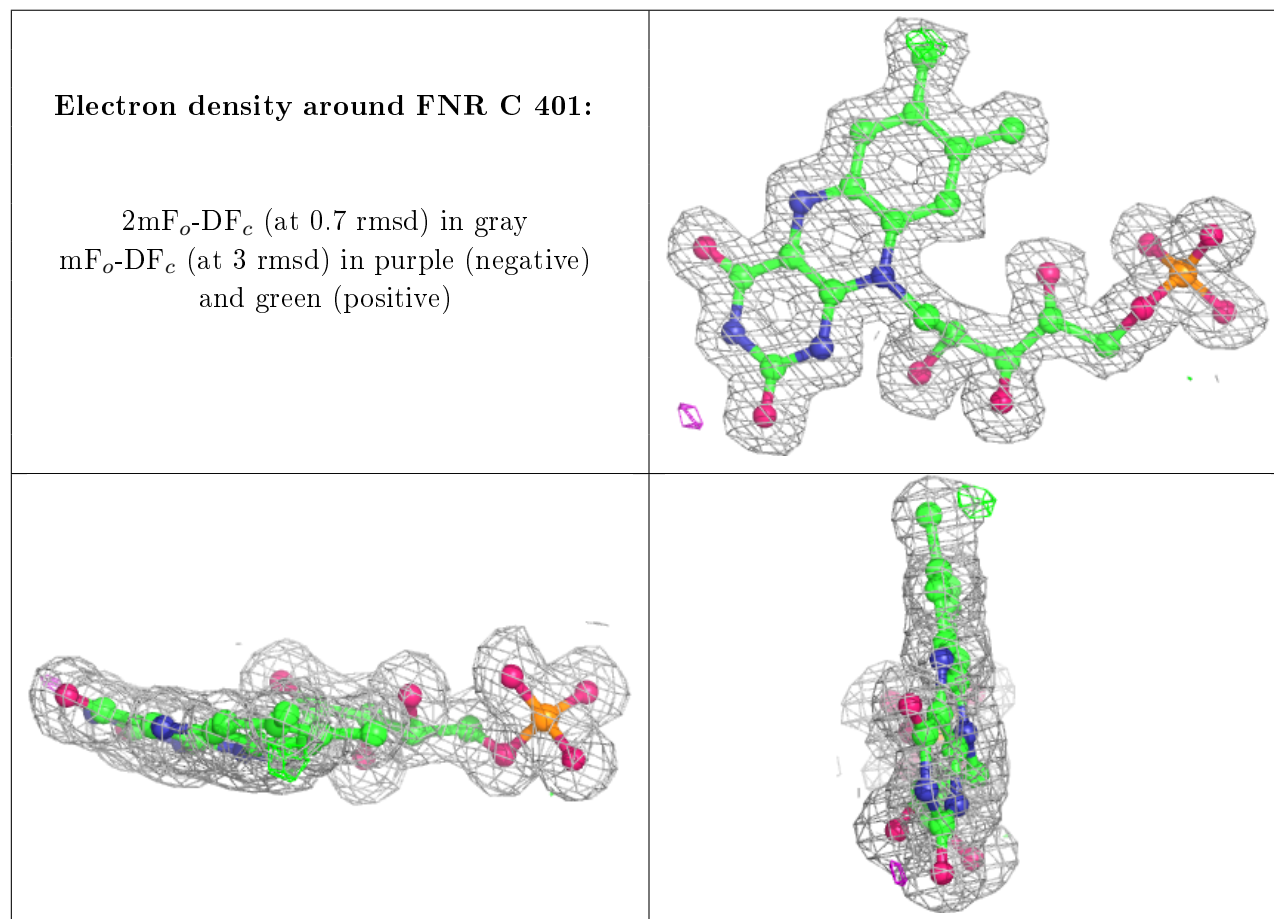
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PYR	C	402	6/6	0.79	0.21	30,32,32,33	0
3	PYR	B	402	6/6	0.80	0.18	20,23,23,27	0
3	PYR	A	402	6/6	0.89	0.15	18,20,20,23	0
4	EDO	A	403	4/4	0.92	0.09	14,17,17,18	0

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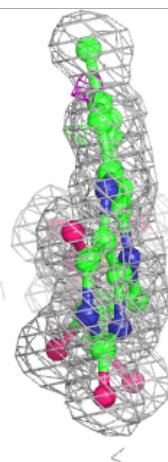
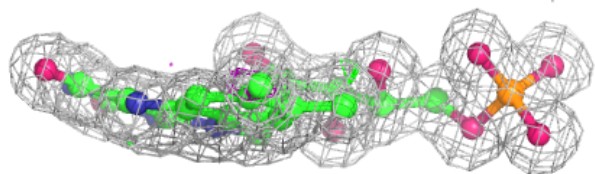
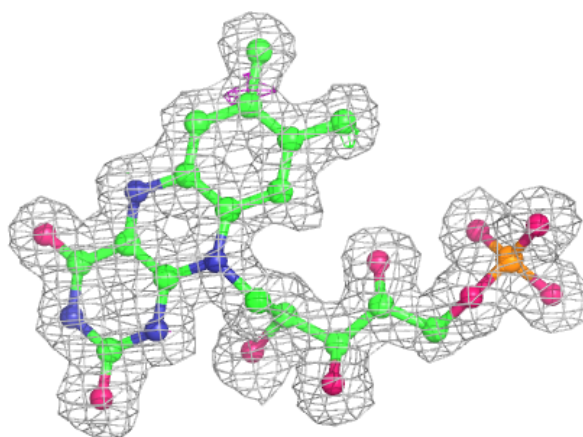
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PYR	D	402	6/6	0.93	0.09	17,18,18,19	0
4	EDO	B	403	4/4	0.95	0.09	14,16,16,17	0
4	EDO	C	403	4/4	0.96	0.07	16,19,19,19	0
2	FNR	C	401	31/31	0.98	0.05	7,9,13,15	0
2	FNR	A	401	31/31	0.98	0.06	7,9,12,12	0
2	FNR	D	401	31/31	0.98	0.06	7,9,12,13	0
2	FNR	B	401	31/31	0.98	0.05	8,9,12,13	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.



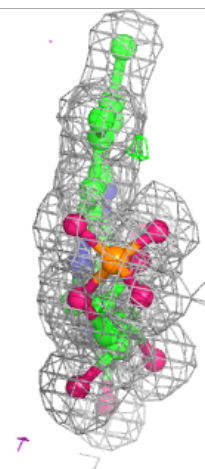
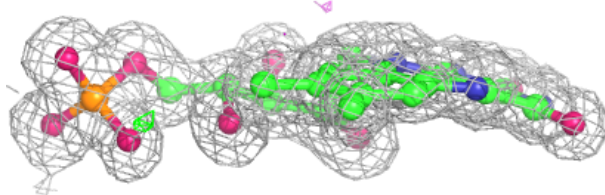
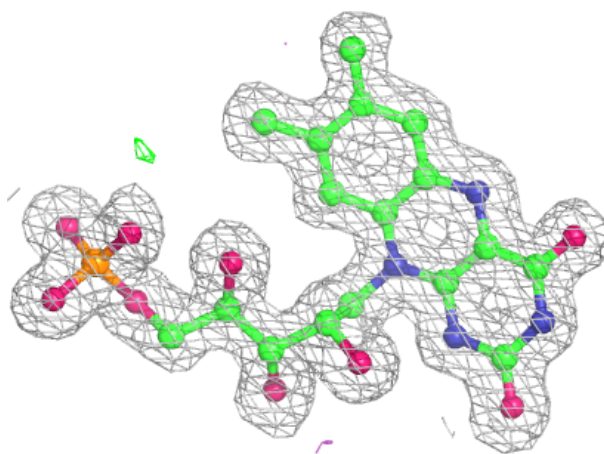
Electron density around FNR A 401:

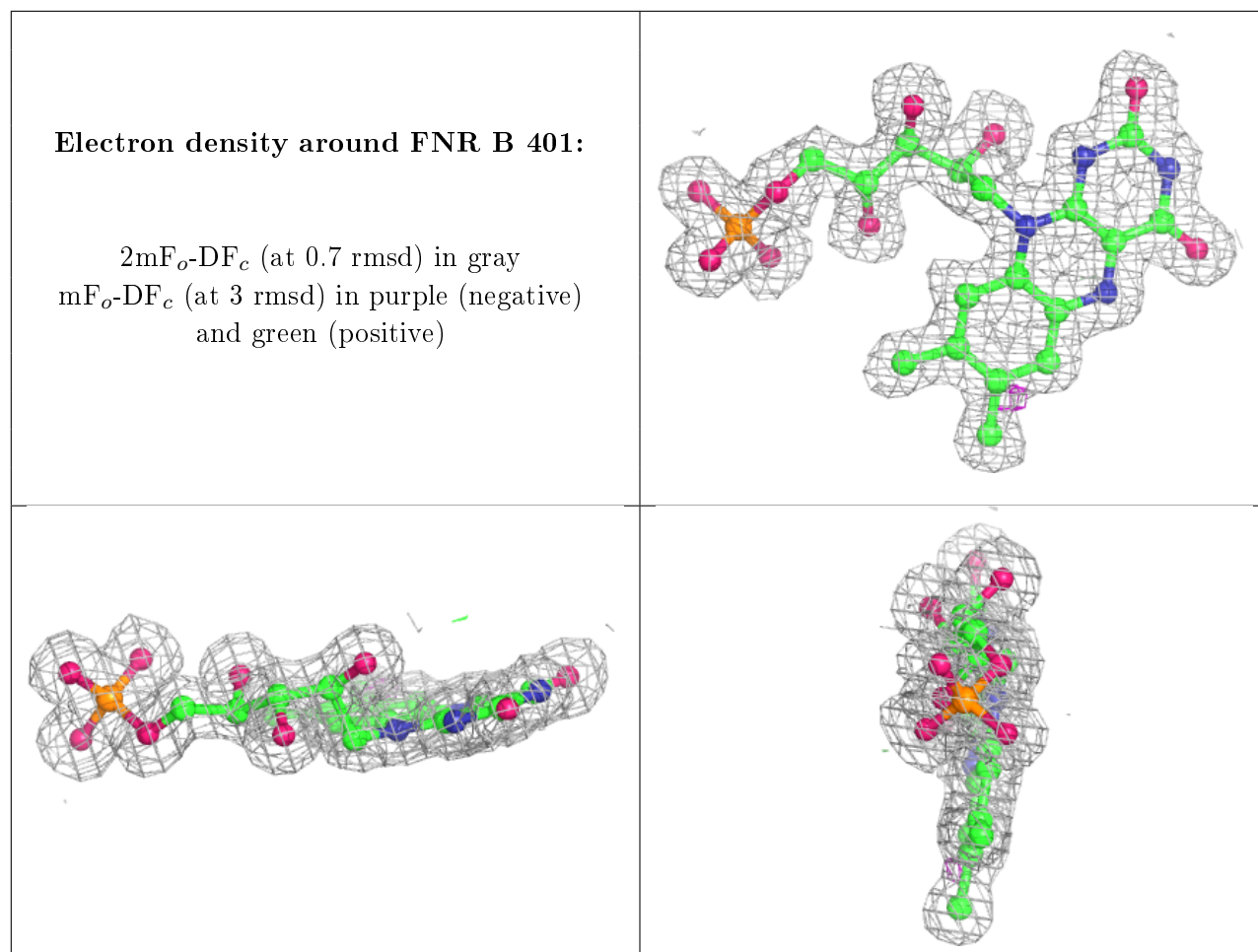
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FNR D 401:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.