



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 04:25 PM EDT

PDB ID : 7UT5
Title : Acinetobacter baumannii dihydroorotate dehydrogenase bound with inhibitor DSM186
Authors : Deng, X.; Phillips, M.; Tomchick, D.
Deposited on : 2022-04-26
Resolution : 1.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

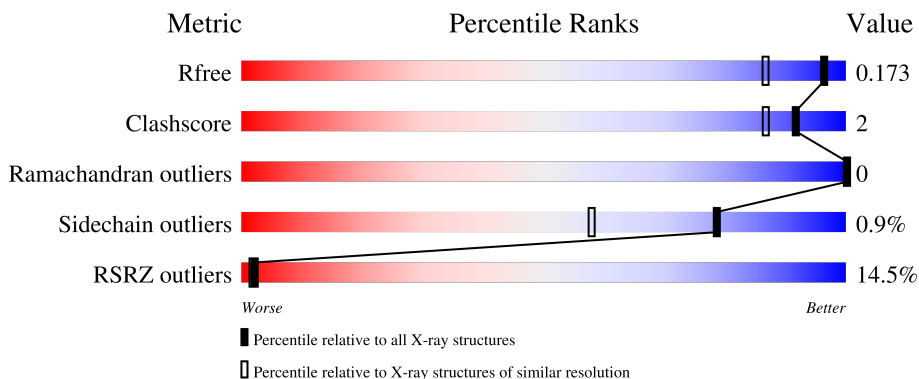
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	354	
1	B	354	

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
4	ORO	B	1003	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10742 atoms, of which 5210 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	H	N	O				S
1	A	324	5113	1605	2604	416	476	12	0	11	0
1	B	324	4984	1570	2522	417	463	12	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

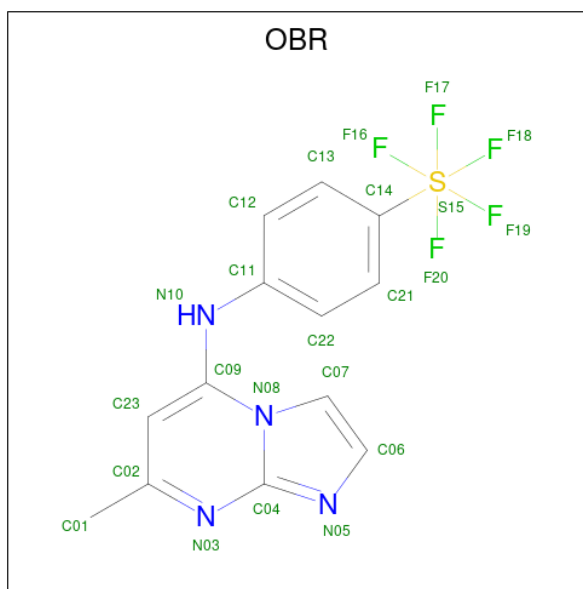
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B7GZW7
A	-18	GLY	-	expression tag	UNP B7GZW7
A	-17	SER	-	expression tag	UNP B7GZW7
A	-16	SER	-	expression tag	UNP B7GZW7
A	-15	HIS	-	expression tag	UNP B7GZW7
A	-14	HIS	-	expression tag	UNP B7GZW7
A	-13	HIS	-	expression tag	UNP B7GZW7
A	-12	HIS	-	expression tag	UNP B7GZW7
A	-11	HIS	-	expression tag	UNP B7GZW7
A	-10	HIS	-	expression tag	UNP B7GZW7
A	-9	SER	-	expression tag	UNP B7GZW7
A	-8	SER	-	expression tag	UNP B7GZW7
A	-7	GLY	-	expression tag	UNP B7GZW7
A	-6	LEU	-	expression tag	UNP B7GZW7
A	-5	VAL	-	expression tag	UNP B7GZW7
A	-4	PRO	-	expression tag	UNP B7GZW7
A	-3	ARG	-	expression tag	UNP B7GZW7
A	-2	GLY	-	expression tag	UNP B7GZW7
A	-1	SER	-	expression tag	UNP B7GZW7
A	0	HIS	-	expression tag	UNP B7GZW7
B	-19	MET	-	initiating methionine	UNP B7GZW7
B	-18	GLY	-	expression tag	UNP B7GZW7
B	-17	SER	-	expression tag	UNP B7GZW7
B	-16	SER	-	expression tag	UNP B7GZW7
B	-15	HIS	-	expression tag	UNP B7GZW7

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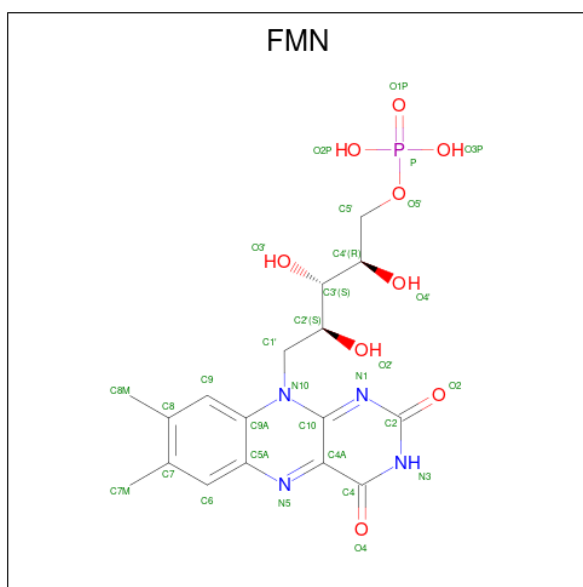
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B7GZW7
B	-13	HIS	-	expression tag	UNP B7GZW7
B	-12	HIS	-	expression tag	UNP B7GZW7
B	-11	HIS	-	expression tag	UNP B7GZW7
B	-10	HIS	-	expression tag	UNP B7GZW7
B	-9	SER	-	expression tag	UNP B7GZW7
B	-8	SER	-	expression tag	UNP B7GZW7
B	-7	GLY	-	expression tag	UNP B7GZW7
B	-6	LEU	-	expression tag	UNP B7GZW7
B	-5	VAL	-	expression tag	UNP B7GZW7
B	-4	PRO	-	expression tag	UNP B7GZW7
B	-3	ARG	-	expression tag	UNP B7GZW7
B	-2	GLY	-	expression tag	UNP B7GZW7
B	-1	SER	-	expression tag	UNP B7GZW7
B	0	HIS	-	expression tag	UNP B7GZW7

- Molecule 2 is (4R)-7-methyl-N-[4-(pentafluoro-lambda 6 -sulfanyl)phenyl]imidazo[1,2-a]pyrimidin-5-amine (three-letter code: OBR) (formula: C₁₃H₁₁F₅N₄S) (labeled as "Ligand of Interest" by depositor).



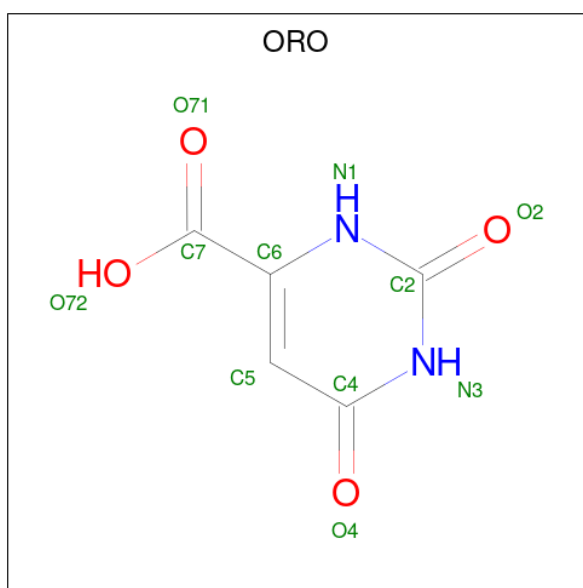
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			S
2	A	1	Total	C	F	H	N	S	0	0
			34	13	5	11	4	1		
2	B	1	Total	C	F	H	N	S	0	0
			34	13	5	11	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



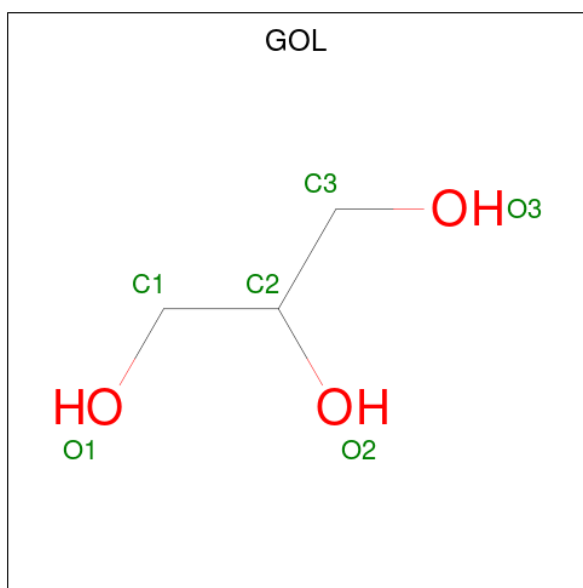
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
3	A	1	50	17	19	4	9	1	0	0
3	B	1	50	17	19	4	9	1	0	0

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	11	5	2	4	0	0
4	B	1	11	5	2	4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		

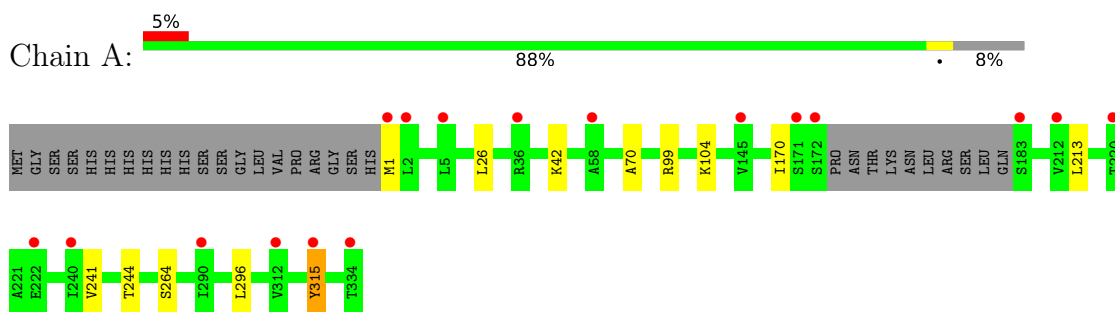
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	313	Total	O	0	0
			313	313		
6	B	100	Total	O	0	0
			100	100		

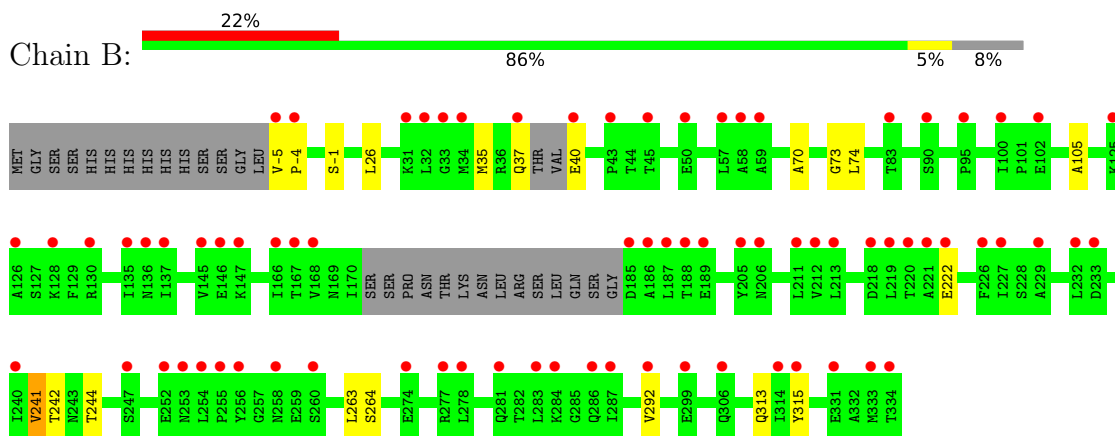
3 Residue-property plots [i](#)

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 (quinone)



- Molecule 1: Dihydroorotate dehydrogenase (quinone)



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.53Å 89.77Å 84.42Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	28.20 – 1.40 28.20 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.20-1.40) 98.1 (28.20-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.40Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.166 , 0.174 0.165 , 0.173	Depositor DCC
R_{free} test set	1981 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtrriage
Anisotropy	0.484	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10742	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/2585	0.71	2/3499 (0.1%)
1	B	0.30	0/2503	0.53	0/3388
All	All	0.43	0/5088	0.63	2/6887 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	315	TYR	CB-CG-CD1	5.12	124.07	121.00

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	2509	2604	2606	5	0
1	B	2462	2522	2524	11	0
2	A	23	11	0	0	0
2	B	23	11	0	1	0
3	A	31	19	19	0	0
3	B	31	19	19	0	0
4	A	11	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	3	0	0
5	A	18	24	24	0	0
6	A	313	0	0	1	0
6	B	100	0	0	0	0
All	All	5532	5210	5198	16	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 2.

All (16) 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:26:LEU:HG	1:B:70:ALA:HB1	1.87	0.55
1:B:105:ALA:HB1	1:B:263:LEU:HD11	1.91	0.53
1:A:42:LYS:NZ	6:A:1103:HOH:O	2.41	0.52
1:A:170:ILE:HD13	1:A:213[A]:LEU:HD13	1.90	0.52
1:A:104:LYS:HB3	1:A:296[A]:LEU:HD21	1.92	0.51
1:B:-1:SER:HB3	1:B:35:MET:HE3	1.95	0.48
1:B:37:GLN:HB2	1:B:73:GLY:O	2.14	0.47
1:B:292:VAL:HG22	1:B:313:GLN:HB2	1.99	0.44
1:A:244:THR:HG22	1:A:264:SER:HB3	2.01	0.43
1:B:74:LEU:HD11	2:B:1001:OBR:F18	2.08	0.43
1:B:40:GLU:OE1	1:B:40:GLU:HA	2.20	0.41
1:B:222:GLU:OE1	1:B:222:GLU:N	2.52	0.41
1:A:26:LEU:HG	1:A:70:ALA:HB1	2.03	0.41
1:B:-5:VAL:HB	1:B:-4:PRO:CD	2.51	0.41
1:B:241:VAL:HA	1:B:242:THR:HA	1.88	0.41
1:B:244:THR:HG22	1:B:264:SER:HB3	2.02	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	332/354 (94%)	323 (97%)	9 (3%)	0	100	100
1	B	318/354 (90%)	308 (97%)	10 (3%)	0	100	100
All	All	650/708 (92%)	631 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	276/291 (95%)	273 (99%)	3 (1%)	73	50
1	B	264/291 (91%)	262 (99%)	2 (1%)	81	62
All	All	540/582 (93%)	535 (99%)	5 (1%)	78	58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	241	VAL
1	A	315	TYR
1	B	241	VAL
1	B	315	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	ORO	A	1003	-	9,11,11	1.96	2 (22%)	8,15,15	3.15	2 (25%)
5	GOL	A	1005	-	5,5,5	1.24	1 (20%)	5,5,5	0.57	0
5	GOL	A	1004	-	5,5,5	0.99	0	5,5,5	0.89	0
3	FMN	A	1002	-	33,33,33	1.60	6 (18%)	48,50,50	1.73	13 (27%)
2	OBR	A	1001	-	21,25,25	2.40	5 (23%)	34,43,43	0.98	4 (11%)
2	OBR	B	1001	-	21,25,25	1.42	3 (14%)	34,43,43	1.14	3 (8%)
4	ORO	B	1003	-	9,11,11	2.14	5 (55%)	8,15,15	3.45	4 (50%)
5	GOL	A	1006	-	5,5,5	1.18	0	5,5,5	0.77	0
3	FMN	B	1002	-	33,33,33	1.19	2 (6%)	48,50,50	1.30	5 (10%)

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
4	ORO	A	1003	-	-	4/4/4/4	0/1/1/1
5	GOL	A	1005	-	-	0/4/4/4	-
5	GOL	A	1004	-	-	1/4/4/4	-
3	FMN	A	1002	-	-	3/18/18/18	0/3/3/3
2	OBR	A	1001	-	-	2/14/14/14	0/3/3/3
2	OBR	B	1001	-	-	1/14/14/14	0/3/3/3
4	ORO	B	1003	-	-	4/4/4/4	0/1/1/1
5	GOL	A	1006	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	B	1002	-	-	4/18/18/18	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	OBR	F17-S15	-6.80	1.50	1.58
2	A	1001	OBR	F16-S15	-5.58	1.52	1.58
3	B	1002	FMN	C4A-N5	5.03	1.40	1.30
3	A	1002	FMN	C4A-N5	4.22	1.38	1.30
4	A	1003	ORO	C4-N3	4.00	1.40	1.33
2	A	1001	OBR	C14-S15	-3.48	1.76	1.80
4	B	1003	ORO	C4-N3	3.30	1.38	1.33
4	A	1003	ORO	C6-N1	3.06	1.38	1.34
4	B	1003	ORO	O71-C7	3.04	1.31	1.22
2	A	1001	OBR	C04-N05	3.04	1.40	1.35
2	B	1001	OBR	C04-N05	3.03	1.40	1.35
2	B	1001	OBR	C14-S15	-2.99	1.77	1.80
3	A	1002	FMN	C5A-N5	2.91	1.45	1.39
3	A	1002	FMN	C10-N10	2.89	1.43	1.37
3	A	1002	FMN	C4-N3	-2.87	1.33	1.38
4	B	1003	ORO	C6-N1	2.79	1.38	1.34
2	A	1001	OBR	F20-S15	2.73	1.61	1.58
4	B	1003	ORO	O72-C7	-2.59	1.22	1.30
3	B	1002	FMN	C10-N1	2.53	1.38	1.33
3	A	1002	FMN	C10-N1	2.53	1.38	1.33
3	A	1002	FMN	C4'-C3'	2.52	1.58	1.53
4	B	1003	ORO	C6-C7	-2.18	1.47	1.50
2	B	1001	OBR	C09-N10	2.18	1.43	1.39
5	A	1005	GOL	C3-C2	2.15	1.60	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	ORO	C5-C4-N3	-6.96	115.96	124.08
4	A	1003	ORO	C5-C4-N3	-6.57	116.42	124.08
4	A	1003	ORO	C6-C5-C4	5.23	120.11	116.73
3	A	1002	FMN	C5A-C9A-N10	4.86	122.97	117.95
4	B	1003	ORO	C6-C5-C4	4.33	119.53	116.73
3	B	1002	FMN	C4A-C10-N10	3.72	121.92	116.48
4	B	1003	ORO	O71-C7-C6	-3.70	113.74	121.24
3	A	1002	FMN	O2-C2-N1	-3.28	116.39	121.83
4	B	1003	ORO	O72-C7-C6	3.27	122.13	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	FMN	C9-C8-C7	3.25	124.33	119.67
3	B	1002	FMN	C4-N3-C2	-3.25	119.65	125.64
3	A	1002	FMN	C6-C5A-C9A	2.90	123.04	118.94
3	A	1002	FMN	C7M-C7-C8	2.88	126.63	120.74
3	A	1002	FMN	O2-C2-N3	2.84	124.17	118.65
3	A	1002	FMN	C9A-C5A-N5	-2.78	119.41	122.43
3	B	1002	FMN	C10-C4A-N5	-2.66	119.22	124.86
3	A	1002	FMN	C1'-N10-C9A	2.62	124.89	120.51
3	A	1002	FMN	O4-C4-C4A	-2.54	119.87	126.60
3	A	1002	FMN	C9-C9A-N10	-2.53	118.42	121.84
2	B	1001	OBR	C09-C23-C02	2.51	118.97	117.08
3	A	1002	FMN	O4-C4-N3	2.51	124.93	120.12
3	B	1002	FMN	C4A-C4-N3	2.47	119.46	113.19
3	B	1002	FMN	C4A-C10-N1	-2.22	119.57	124.73
2	A	1001	OBR	C22-C21-C14	2.21	121.27	119.45
2	A	1001	OBR	C09-C23-C02	2.14	118.69	117.08
3	A	1002	FMN	C6-C7-C8	-2.14	116.61	119.67
2	B	1001	OBR	F17-S15-F16	2.11	179.10	106.06
2	B	1001	OBR	F20-S15-F19	2.10	178.83	106.06
2	A	1001	OBR	F20-S15-F19	2.07	177.81	106.06
2	A	1001	OBR	F17-S15-F16	2.05	176.85	106.06
3	A	1002	FMN	C9A-N10-C10	-2.02	117.62	120.77

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	OBR	C13-C14-S15-F18
2	A	1001	OBR	C21-C14-S15-F18
4	A	1003	ORO	N1-C6-C7-O72
4	A	1003	ORO	C5-C6-C7-O72
4	B	1003	ORO	N1-C6-C7-O71
4	B	1003	ORO	N1-C6-C7-O72
4	B	1003	ORO	C5-C6-C7-O71
4	B	1003	ORO	C5-C6-C7-O72
5	A	1006	GOL	O1-C1-C2-C3
4	A	1003	ORO	N1-C6-C7-O71
4	A	1003	ORO	C5-C6-C7-O71
5	A	1006	GOL	C1-C2-C3-O3
5	A	1006	GOL	O2-C2-C3-O3
3	A	1002	FMN	C2'-C3'-C4'-O4'
5	A	1006	GOL	O1-C1-C2-O2

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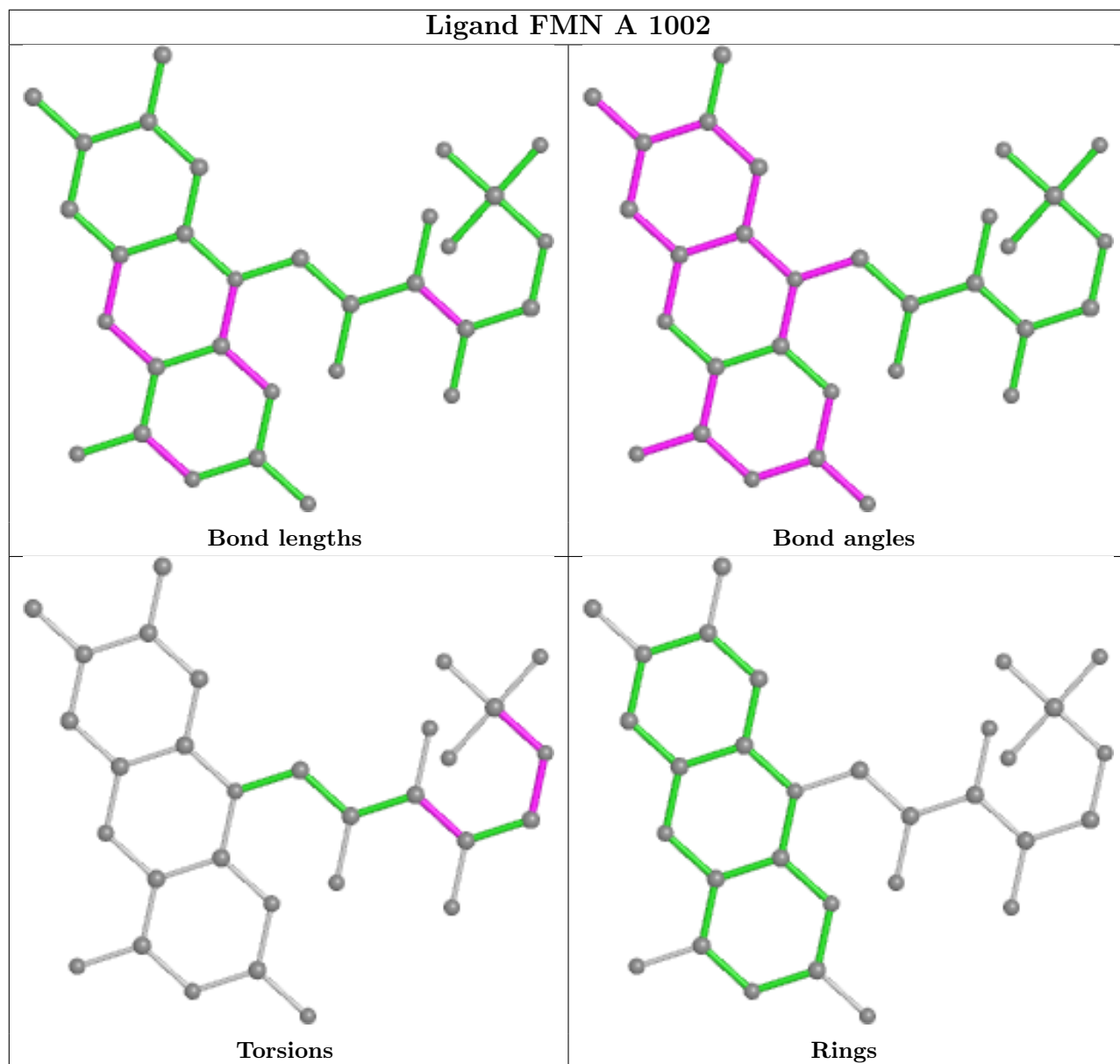
Mol	Chain	Res	Type	Atoms
3	B	1002	FMN	C4'-C5'-O5'-P
3	A	1002	FMN	C4'-C5'-O5'-P
3	B	1002	FMN	C2'-C3'-C4'-O4'
3	A	1002	FMN	C5'-O5'-P-O1P
3	B	1002	FMN	O3'-C3'-C4'-O4'
5	A	1004	GOL	O1-C1-C2-C3
2	B	1001	OBR	C21-C14-S15-F18
3	B	1002	FMN	O3'-C3'-C4'-C5'

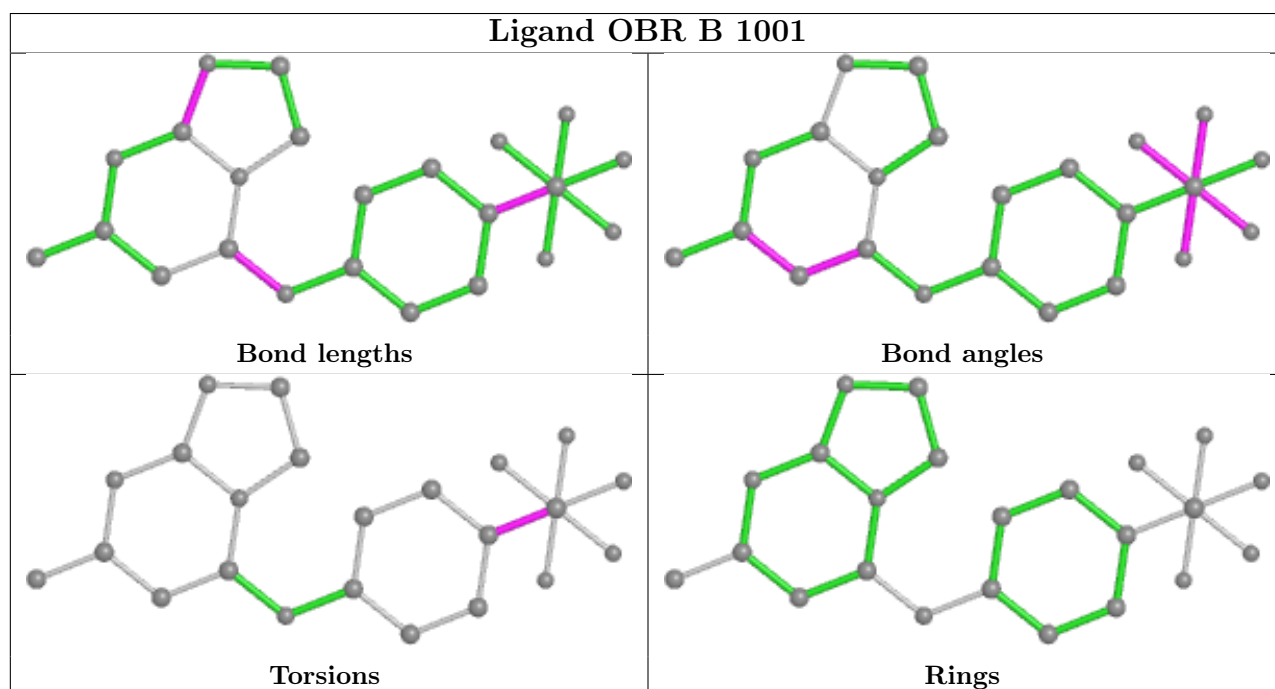
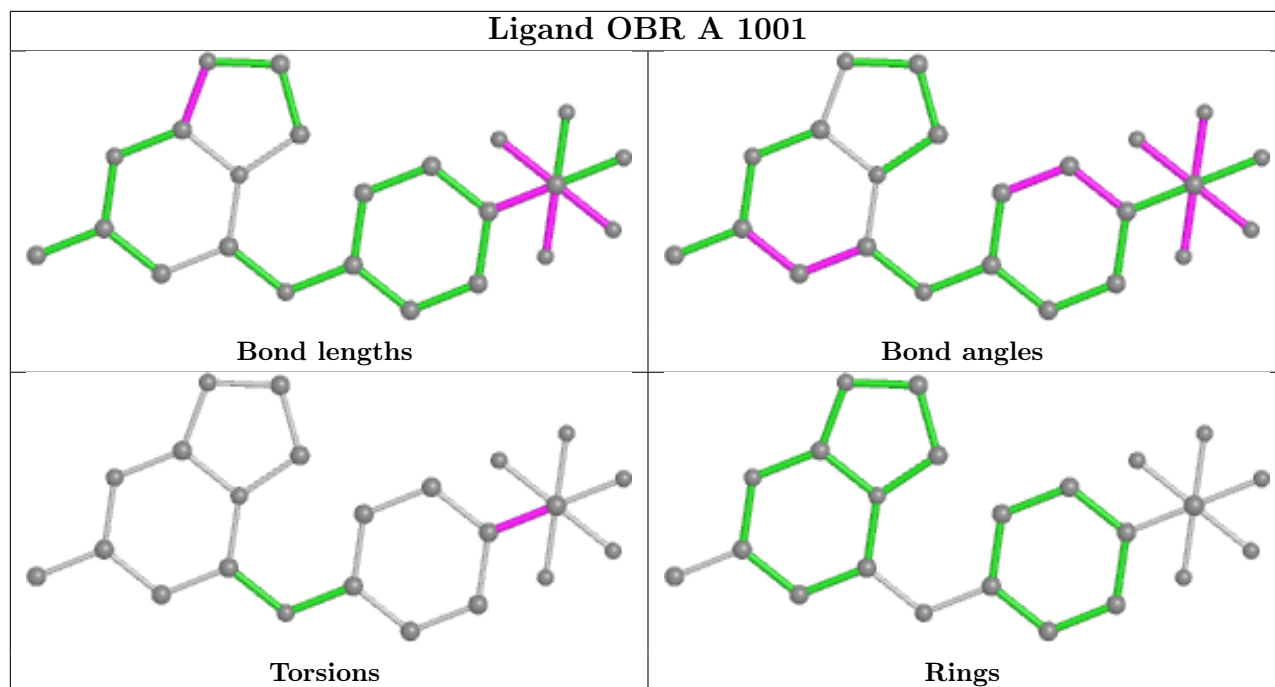
There are no ring outliers.

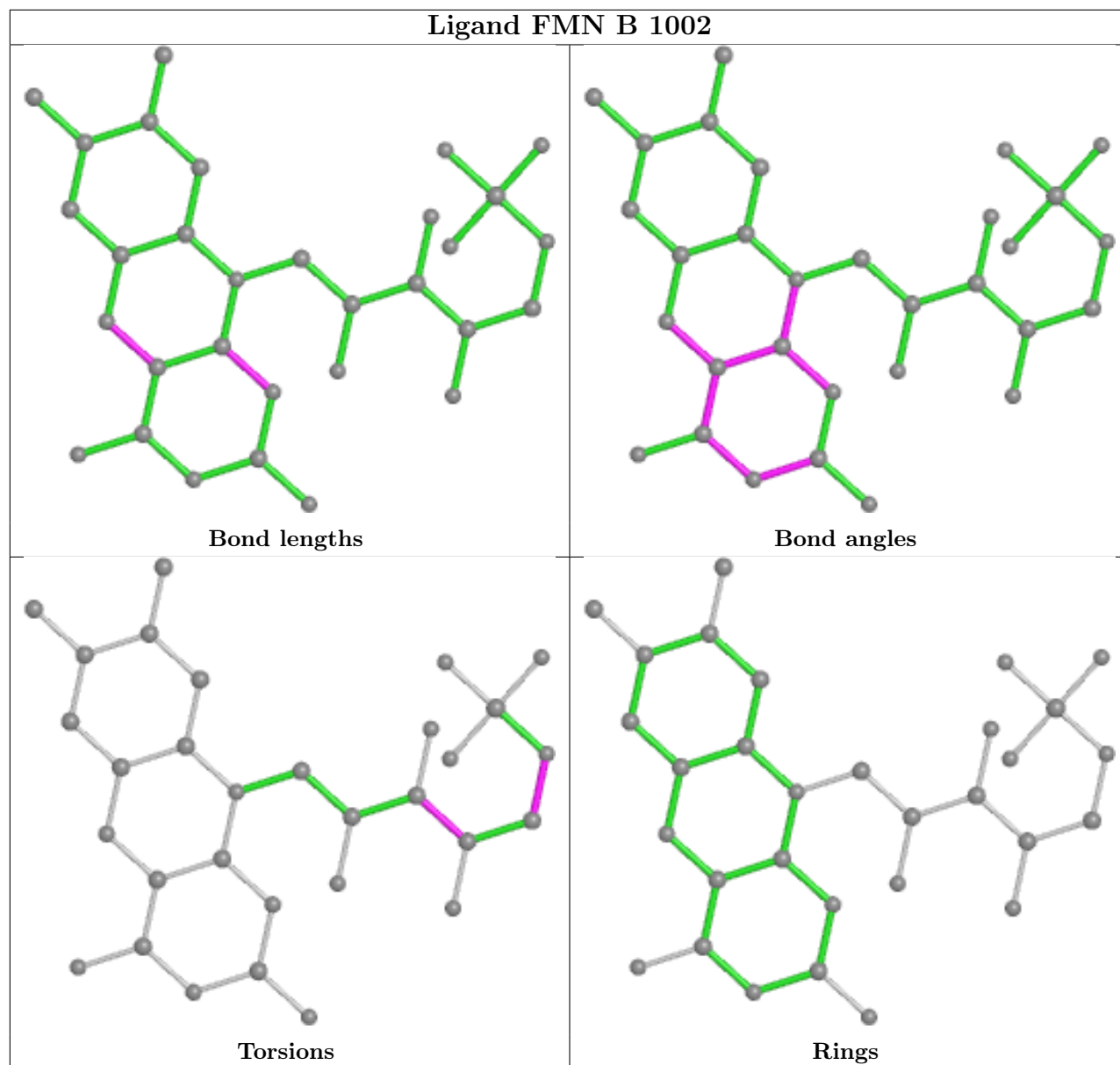
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	OBR	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	324/354 (91%)	0.19	17 (5%) 27 26	13, 23, 42, 64	0
1	B	324/354 (91%)	1.06	77 (23%) 0 0	28, 43, 69, 97	0
All	All	648/708 (91%)	0.63	94 (14%) 2 2	13, 35, 65, 97	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	VAL	7.8
1	B	226	PHE	7.3
1	B	145	VAL	6.4
1	B	220	THR	6.2
1	B	334	THR	6.1
1	B	253	ASN	5.7
1	B	32	LEU	5.4
1	B	222	GLU	5.2
1	B	306	GLN	5.2
1	B	281	GLN	5.1
1	B	283	LEU	4.9
1	B	186	ALA	4.7
1	B	185	ASP	4.7
1	B	221	ALA	4.6
1	B	258	ASN	4.6
1	A	172	SER	4.5
1	B	254	LEU	4.5
1	B	130	ARG	4.4
1	B	219	LEU	4.2
1	B	299	GLU	4.2
1	A	334	THR	4.2
1	B	212	VAL	4.2
1	B	278	LEU	4.2
1	B	58	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.0
1	B	240	ILE	3.9
1	B	45	THR	3.8
1	B	167	THR	3.8
1	B	59	ALA	3.8
1	B	187	LEU	3.6
1	A	36	ARG	3.5
1	B	90	SER	3.5
1	B	137	ILE	3.5
1	B	31	LYS	3.5
1	B	33	GLY	3.4
1	B	166	ILE	3.3
1	B	286	GLN	3.3
1	B	189	GLU	3.2
1	B	227	ILE	3.2
1	B	43	PRO	3.2
1	B	34	MET	3.2
1	B	260	SER	3.1
1	A	183	SER	3.1
1	B	50	GLU	3.1
1	B	146	GLU	3.0
1	B	274	GLU	3.0
1	B	95	PRO	3.0
1	B	256	TYR	3.0
1	A	222	GLU	3.0
1	A	5	LEU	2.9
1	B	135	ILE	2.9
1	B	229	ALA	2.9
1	B	252	GLU	2.8
1	B	284	LYS	2.8
1	A	220	THR	2.8
1	B	-4	PRO	2.7
1	B	315	TYR	2.7
1	B	206	ASN	2.7
1	B	232	LEU	2.6
1	A	2	LEU	2.6
1	A	58	ALA	2.6
1	B	233	ASP	2.6
1	B	37	GLN	2.6
1	B	213	LEU	2.5
1	B	188	THR	2.5
1	B	287	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	145	VAL	2.5
1	B	168	VAL	2.5
1	A	290	ILE	2.5
1	A	171	SER	2.3
1	B	292	VAL	2.3
1	B	102	GLU	2.3
1	A	212	VAL	2.3
1	B	40	GLU	2.3
1	B	218	ASP	2.3
1	B	331	GLU	2.3
1	B	205	TYR	2.3
1	B	125	LYS	2.2
1	B	255	PRO	2.2
1	B	126	ALA	2.2
1	B	136	ASN	2.2
1	B	211	LEU	2.2
1	A	312	VAL	2.2
1	B	128	LYS	2.2
1	B	57	LEU	2.1
1	B	333	MET	2.1
1	B	314	ILE	2.1
1	B	83	THR	2.1
1	B	277	ARG	2.1
1	A	240	ILE	2.1
1	B	100	ILE	2.1
1	A	315	TYR	2.1
1	B	247	SER	2.0
1	B	147	LYS	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 monosaccharides in this entry.

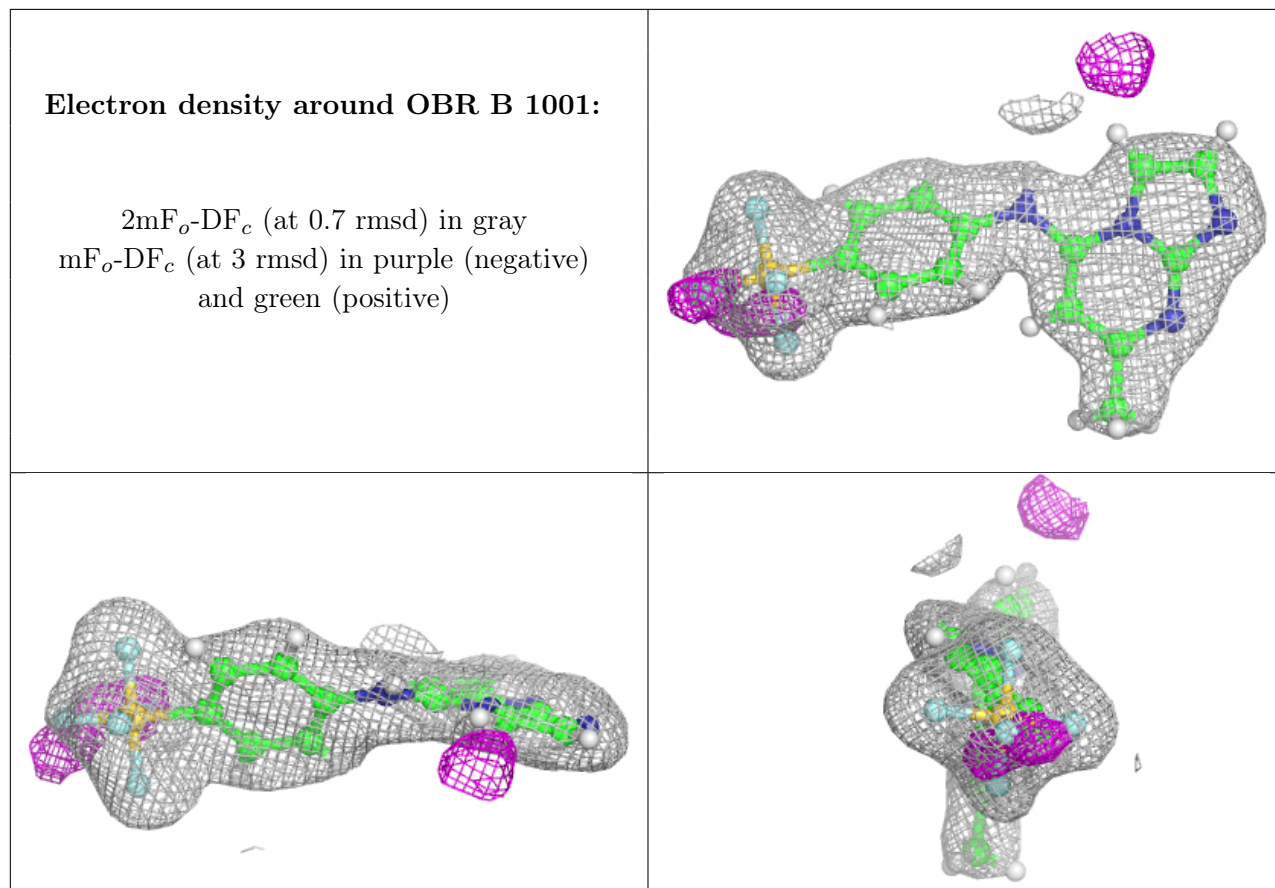
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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.

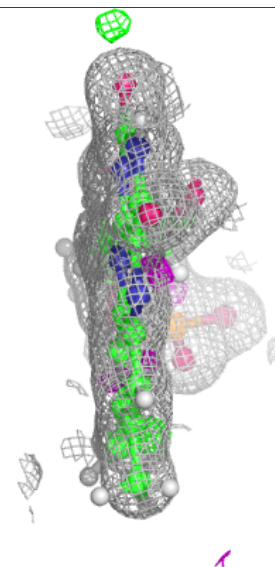
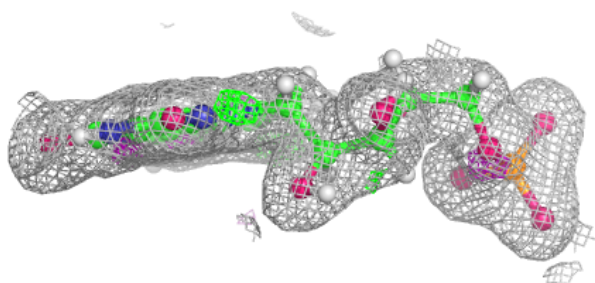
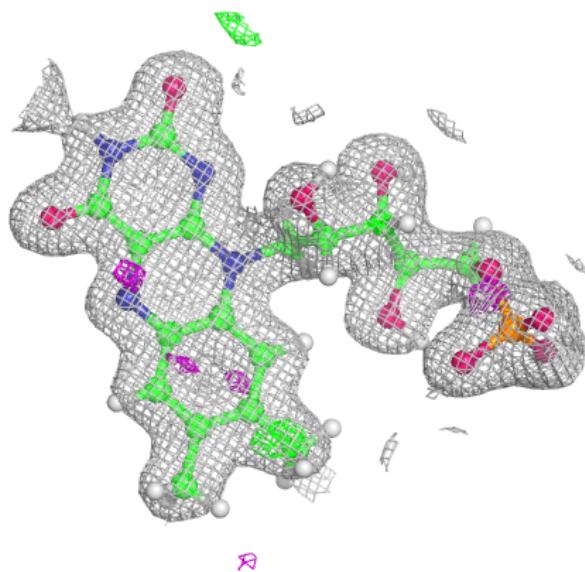
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	1006	6/6	0.78	0.21	27,42,53,54	0
5	GOL	A	1005	6/6	0.88	0.14	25,36,44,44	0
5	GOL	A	1004	6/6	0.88	0.18	28,38,47,51	0
2	OBR	B	1001	23/23	0.92	0.10	31,37,44,50	0
4	ORO	B	1003	11/11	0.93	0.12	29,30,33,34	0
3	FMN	B	1002	31/31	0.94	0.15	26,31,39,41	0
2	OBR	A	1001	23/23	0.95	0.08	16,19,23,30	0
3	FMN	A	1002	31/31	0.98	0.13	10,13,17,19	0
4	ORO	A	1003	11/11	0.99	0.11	12,13,16,16	0

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



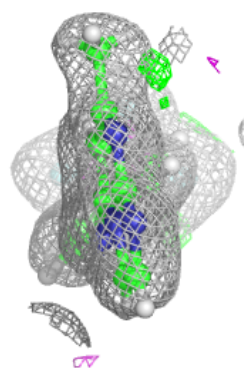
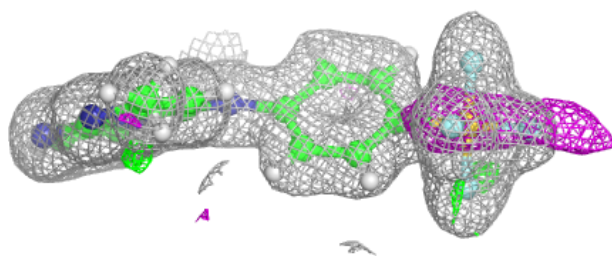
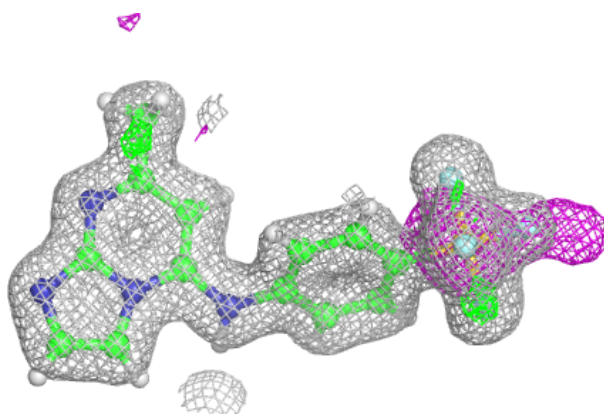
Electron density around FMN B 1002:

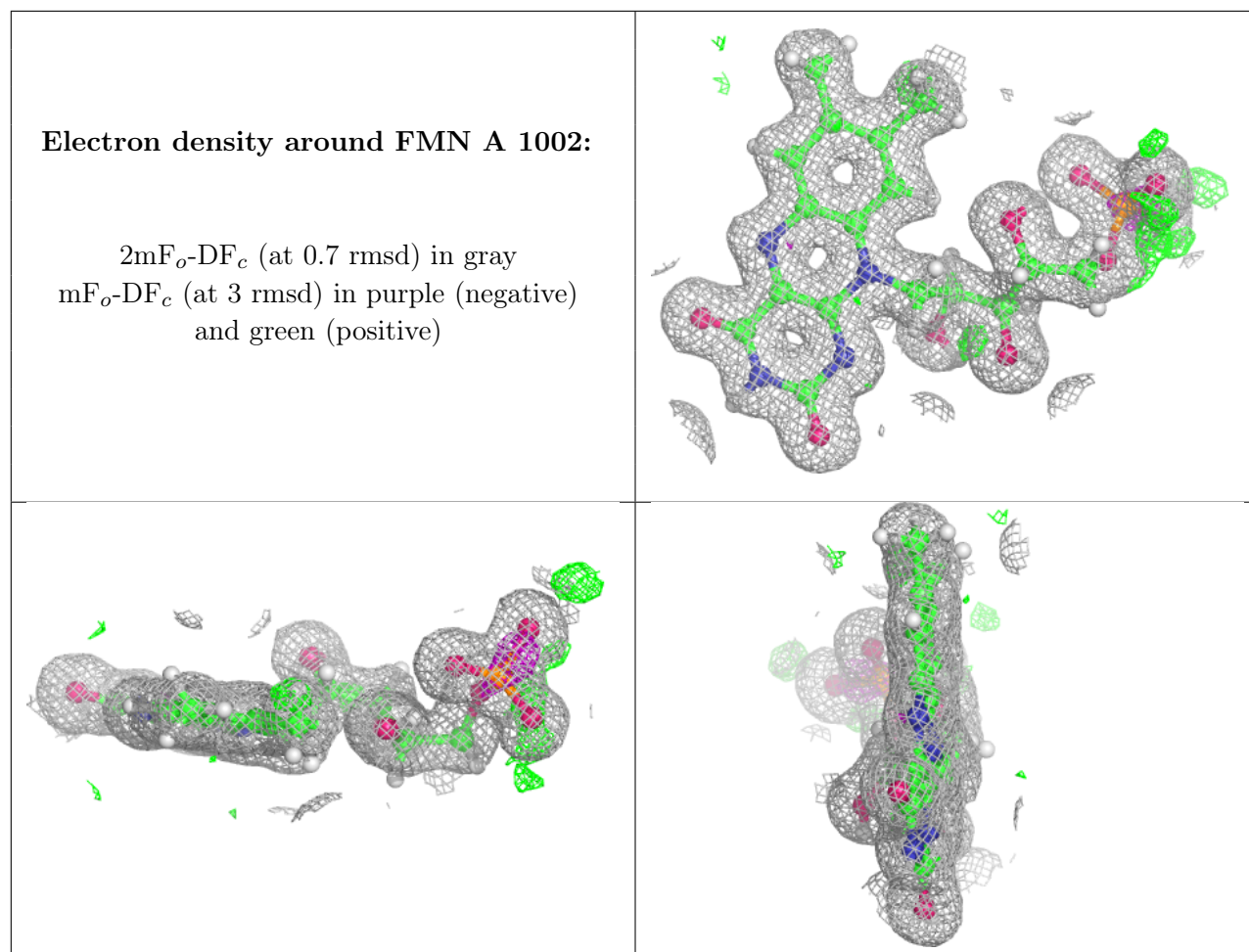
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OBR A 1001:

$2mF_o-DF_c$ (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.