



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:57 PM EDT

PDB ID : 3W2J / pdb_00003w2j
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-135
Authors : Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Shiba, T.; Sakamoto, K.; Suzuki, S.; Balogun, E.O.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on : 2012-11-28
Resolution : 1.42 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](#) ①) 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

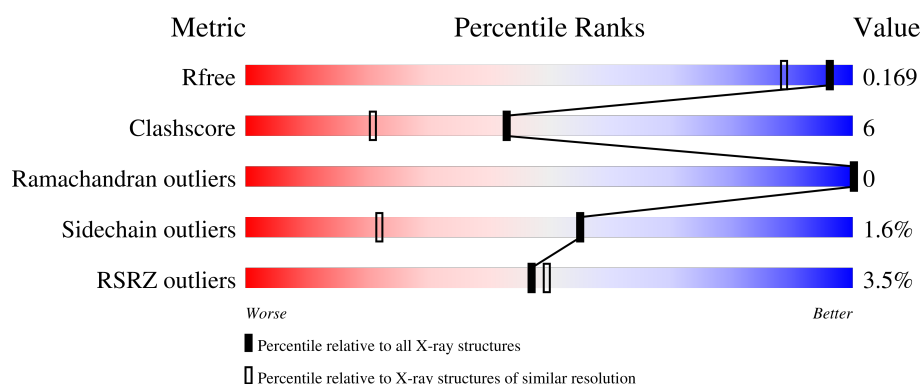
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	313	3% 73% 24% .
1	B	313	4% 64% 34% .

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	GOL	A	405	-	X	-	-
3	GOL	B	410	-	-	X	-

2 Entry composition [i](#)

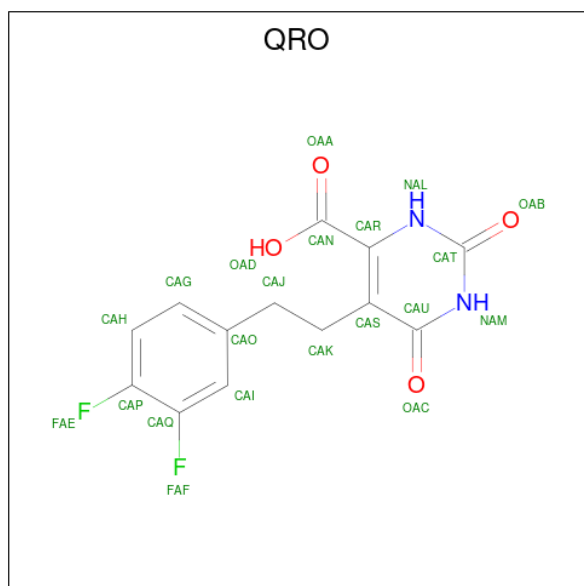
There are 6 unique types of molecules in this entry. The entry contains 5789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (fumarate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			
1	B	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			

- Molecule 2 is 5-[2-(3,4-difluorophenyl)ethyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (CCD ID: QRO) (formula: C₁₃H₁₀F₂N₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			21	13	2	2	4		
2	B	1	Total	C	F	N	O	0	0
			21	13	2	2	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

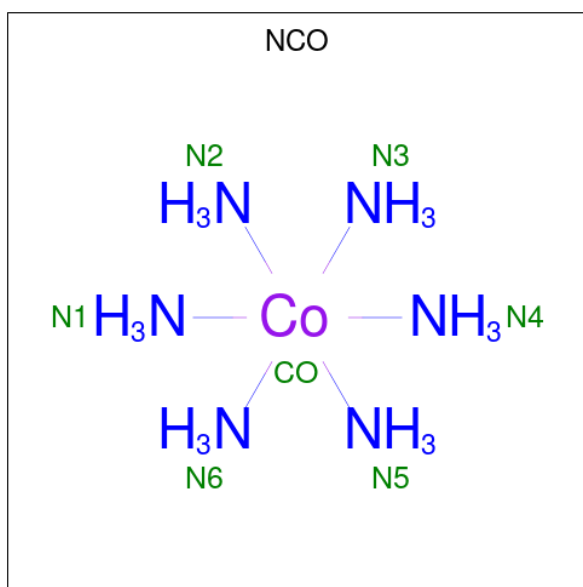
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5) attached to a ribitol chain. The ribitol chain is a five-carbon chain (C1' to C5') with hydroxyl groups at C1', C2', C3', and C4'. The C5' carbon is attached to a phosphate group (O1P, P, O2P, O3P, O4P). The ribitol chain is shown in a specific conformation with stereochemistry indicated by wedges and dashes. The isoalloxazine ring system is shown in a specific conformation with stereochemistry indicated by wedges and dashes. The atoms are labeled with their respective symbols and numbers.

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Co	N	0	0
			7	1	6		

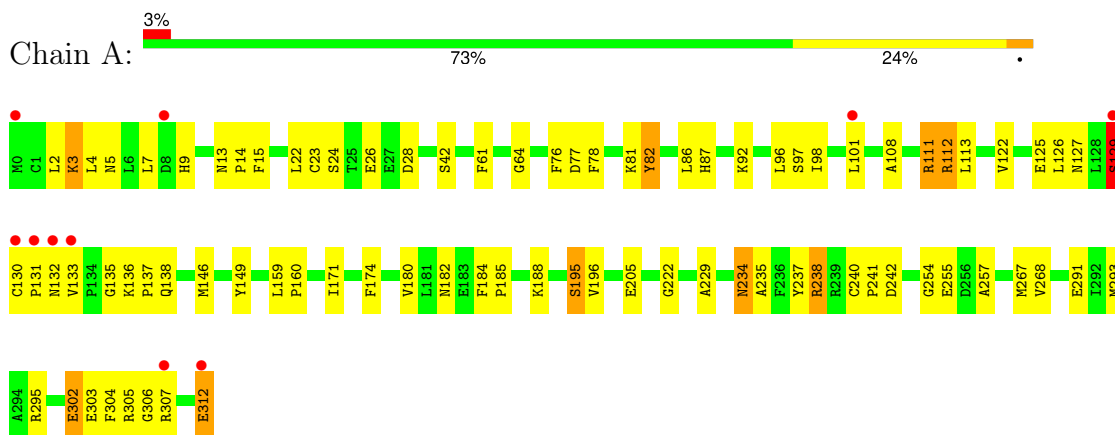
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	398	Total	O	0	0
			398	398		
6	B	390	Total	O	0	0
			390	390		

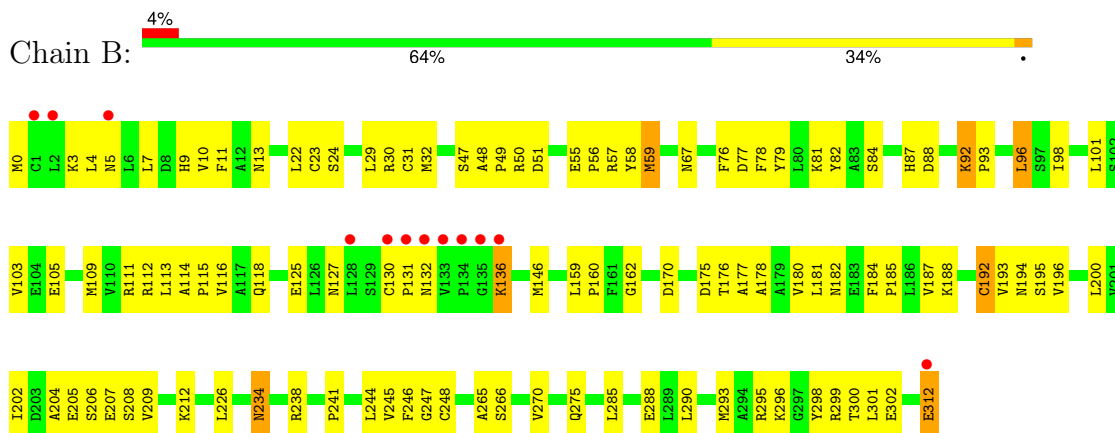
3 Residue-property plots

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 (fumarate)



- Molecule 1: Dihydroorotate dehydrogenase (fumarate)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.10Å 71.82Å 129.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.87 – 1.42 46.87 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.87-1.42) 99.7 (46.87-1.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.142 , 0.168 0.144 , 0.169	Depositor DCC
R_{free} test set	5999 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5789	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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 27.88 % 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 2.0316e-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, QRO, GOL, NCO

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	1.84	57/2440 (2.3%)	1.42	19/3305 (0.6%)
1	B	1.96	81/2440 (3.3%)	1.37	14/3305 (0.4%)
All	All	1.90	138/4880 (2.8%)	1.40	33/6610 (0.5%)

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	ALA	C-O	-10.66	1.13	1.24
1	A	23	CYS	C-O	-8.83	1.17	1.23
1	B	184	PHE	C-O	-8.51	1.14	1.24
1	B	79	TYR	C-O	-8.40	1.14	1.24
1	B	159	LEU	CA-C	8.34	1.60	1.52
1	A	127	ASN	C-O	-8.32	1.13	1.24
1	B	51	ASP	C-O	-8.02	1.14	1.24
1	B	76	PHE	C-O	-7.86	1.15	1.24
1	B	23	CYS	C-O	-7.81	1.18	1.23
1	B	162	GLY	CA-C	-7.79	1.45	1.52
1	B	78	PHE	C-O	-7.72	1.15	1.24
1	A	42	SER	CA-C	-7.69	1.42	1.53
1	A	255	GLU	C-O	-7.66	1.15	1.24
1	A	113	LEU	C-O	-7.62	1.15	1.24
1	A	24	SER	C-O	-7.53	1.14	1.24
1	B	177	ALA	C-O	-7.46	1.15	1.24
1	B	245	VAL	C-O	-7.42	1.16	1.24
1	B	31	CYS	C-O	-7.37	1.15	1.24
1	B	112	ARG	C-O	-7.36	1.14	1.24
1	A	26	GLU	C-O	-7.33	1.15	1.24
1	A	303	GLU	C-O	-7.26	1.15	1.24
1	B	127	ASN	C-O	-7.24	1.15	1.24
1	B	57	ARG	C-O	-7.23	1.15	1.24
1	B	4	LEU	C-O	-7.15	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	ASP	C-O	-7.10	1.15	1.24
1	B	170	ASP	C-O	-7.10	1.16	1.23
1	B	58	TYR	C-O	-7.01	1.16	1.23
1	B	49	PRO	N-CD	6.88	1.57	1.47
1	B	56	PRO	N-CD	6.85	1.57	1.47
1	A	129	SER	CA-C	-6.83	1.46	1.53
1	B	192	CYS	C-O	-6.77	1.16	1.24
1	B	178	ALA	C-O	-6.70	1.16	1.24
1	A	3	LYS	CE-NZ	6.67	1.69	1.49
1	A	268	VAL	C-O	-6.67	1.16	1.24
1	B	208	SER	C-O	-6.67	1.15	1.23
1	B	130	CYS	C-O	-6.64	1.17	1.24
1	A	133	VAL	C-N	6.59	1.42	1.33
1	B	300	THR	C-O	-6.57	1.15	1.23
1	A	112	ARG	C-O	-6.56	1.15	1.24
1	A	111	ARG	C-O	-6.52	1.16	1.24
1	B	270	VAL	C-N	6.48	1.38	1.33
1	B	296	LYS	C-O	-6.47	1.15	1.24
1	B	247	GLY	C-O	-6.44	1.14	1.23
1	B	298	TYR	C-O	-6.43	1.16	1.24
1	B	96	LEU	C-O	-6.43	1.16	1.24
1	B	246	PHE	C-O	-6.41	1.16	1.24
1	B	114	ALA	C-O	-6.38	1.18	1.24
1	B	196	VAL	C-O	-6.37	1.17	1.24
1	B	248	CYS	C-O	-6.37	1.16	1.23
1	B	11	PHE	C-O	-6.36	1.15	1.24
1	B	204	ALA	C-O	-6.33	1.16	1.24
1	B	125	GLU	C-O	-6.26	1.16	1.24
1	B	159	LEU	C-O	-6.22	1.17	1.24
1	B	288	GLU	C-O	-6.21	1.16	1.24
1	A	101	LEU	CB-CG	6.19	1.65	1.53
1	B	131	PRO	N-CD	6.19	1.56	1.47
1	A	267	MET	C-O	-6.19	1.16	1.23
1	B	22	LEU	C-O	-6.18	1.15	1.23
1	A	146	MET	SD-CE	-6.18	1.64	1.79
1	B	200	LEU	CA-C	-6.17	1.45	1.52
1	B	59	MET	C-O	-6.17	1.16	1.23
1	B	185	PRO	N-CD	6.14	1.56	1.47
1	B	182	ASN	C-O	-6.13	1.16	1.24
1	A	304	PHE	C-O	-6.12	1.16	1.24
1	B	202	ILE	C-O	-6.12	1.17	1.24
1	B	285	LEU	C-O	-6.12	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	MET	C-O	-6.08	1.17	1.24
1	A	129	SER	CB-OG	6.04	1.54	1.42
1	B	205	GLU	C-O	-6.04	1.17	1.24
1	A	295	ARG	C-O	6.04	1.31	1.24
1	A	182	ASN	CA-C	6.04	1.61	1.52
1	B	207	GLU	C-O	-5.99	1.15	1.23
1	B	113	LEU	C-O	-5.97	1.16	1.24
1	A	64	GLY	CA-C	-5.96	1.44	1.52
1	A	255	GLU	CD-OE1	-5.94	1.14	1.25
1	B	32	MET	C-O	-5.89	1.17	1.24
1	B	111	ARG	C-O	-5.87	1.17	1.24
1	B	175	ASP	C-O	-5.85	1.17	1.24
1	A	130	CYS	CA-C	5.84	1.59	1.52
1	A	229	ALA	CA-CB	-5.81	1.44	1.53
1	A	131	PRO	N-CD	5.79	1.55	1.47
1	A	15	PHE	N-CA	5.76	1.53	1.46
1	A	184	PHE	CA-C	-5.74	1.45	1.52
1	A	22	LEU	C-O	-5.73	1.16	1.23
1	B	92	LYS	N-CA	5.72	1.51	1.46
1	A	235	ALA	C-O	5.71	1.30	1.24
1	B	88	ASP	CA-C	5.71	1.59	1.52
1	B	181	LEU	C-O	-5.68	1.17	1.24
1	A	82	TYR	CA-CB	5.68	1.62	1.53
1	A	234	ASN	CG-ND2	-5.68	1.21	1.33
1	A	76	PHE	C-O	-5.66	1.17	1.24
1	A	2	LEU	C-O	-5.64	1.16	1.24
1	B	7	LEU	C-O	-5.64	1.15	1.23
1	B	103	VAL	N-CA	-5.63	1.39	1.46
1	B	187	VAL	C-O	5.63	1.31	1.23
1	B	234	ASN	CG-OD1	5.63	1.34	1.23
1	A	293	MET	C-O	5.62	1.30	1.24
1	B	295	ARG	CZ-NH2	-5.62	1.26	1.33
1	A	257	ALA	C-O	-5.60	1.17	1.24
1	B	24	SER	C-O	-5.59	1.16	1.24
1	A	171	ILE	CA-CB	-5.58	1.47	1.54
1	B	176	THR	C-O	-5.57	1.17	1.24
1	B	29	LEU	C-O	-5.56	1.17	1.24
1	A	234	ASN	CG-OD1	5.51	1.34	1.23
1	A	185	PRO	N-CA	-5.50	1.40	1.47
1	B	30	ARG	C-O	-5.50	1.17	1.24
1	A	149	TYR	C-O	-5.45	1.17	1.24
1	A	136	LYS	CA-C	5.43	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	ARG	C-O	-5.40	1.17	1.23
1	B	13	ASN	C-O	-5.38	1.17	1.24
1	A	306	GLY	C-O	-5.37	1.16	1.23
1	A	4	LEU	C-O	-5.37	1.17	1.23
1	A	137	PRO	C-O	5.36	1.30	1.23
1	B	3	LYS	C-O	-5.34	1.17	1.23
1	B	84	SER	N-CA	5.34	1.53	1.46
1	B	185	PRO	C-O	-5.34	1.17	1.24
1	B	226	LEU	N-CA	5.32	1.51	1.46
1	A	196	VAL	C-O	-5.30	1.18	1.23
1	A	130	CYS	C-N	5.30	1.40	1.33
1	A	195	SER	C-O	-5.30	1.17	1.23
1	B	48	ALA	C-N	5.29	1.40	1.33
1	B	244	LEU	C-O	-5.28	1.17	1.23
1	B	299	ARG	C-O	-5.27	1.17	1.24
1	B	194	ASN	C-O	-5.25	1.16	1.23
1	A	302	GLU	C-O	-5.23	1.17	1.24
1	A	195	SER	CB-OG	-5.23	1.31	1.42
1	A	98	ILE	CB-CG1	-5.21	1.43	1.53
1	A	254	GLY	C-O	-5.17	1.17	1.23
1	A	96	LEU	CB-CG	-5.15	1.43	1.53
1	A	126	LEU	C-O	-5.15	1.17	1.24
1	A	222	GLY	N-CA	-5.14	1.38	1.45
1	A	86	LEU	C-O	-5.14	1.16	1.23
1	B	265	ALA	CA-CB	-5.14	1.44	1.53
1	B	130	CYS	C-N	5.13	1.40	1.33
1	A	240	CYS	CA-CB	5.12	1.58	1.53
1	B	101	LEU	C-O	-5.08	1.17	1.24
1	A	133	VAL	C-O	-5.06	1.18	1.24
1	B	301	LEU	C-O	-5.02	1.18	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	CD-CE-NZ	9.52	142.35	111.90
1	A	205	GLU	CB-CG-CD	7.16	124.77	112.60
1	A	28	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	77	ASP	CA-C-N	-6.30	112.25	120.44
1	A	77	ASP	C-N-CA	-6.30	112.25	120.44
1	A	122	VAL	O-C-N	-6.18	116.14	122.75
1	B	266	SER	O-C-N	-6.07	115.34	122.32
1	B	48	ALA	O-C-N	5.94	126.54	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	PHE	CA-C-O	5.79	125.03	119.99
1	A	3	LYS	CG-CD-CE	5.77	124.58	111.30
1	A	159	LEU	O-C-N	5.67	125.98	121.55
1	B	116	VAL	N-CA-C	5.63	116.41	110.72
1	B	115	PRO	N-CA-C	5.61	121.22	113.65
1	A	180	VAL	O-C-N	-5.60	116.42	121.91
1	B	47	SER	O-C-N	5.56	128.02	122.12
1	A	238	ARG	CA-C-O	-5.51	114.58	120.42
1	B	159	LEU	O-C-N	5.41	125.77	121.55
1	A	133	VAL	CA-C-N	-5.32	114.28	119.76
1	A	133	VAL	C-N-CA	-5.32	114.28	119.76
1	B	81	LYS	CA-C-O	5.29	126.16	120.55
1	A	135	GLY	CA-C-O	5.26	124.84	119.10
1	A	174	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	108	ALA	CA-C-O	5.24	126.10	120.55
1	A	129	SER	N-CA-C	-5.19	102.39	109.71
1	A	131	PRO	N-CA-C	5.17	119.44	111.21
1	A	78	PHE	N-CA-C	5.16	116.59	111.07
1	B	290	LEU	CA-C-O	-5.13	114.98	120.42
1	B	130	CYS	CA-C-N	-5.11	114.52	119.78
1	B	130	CYS	C-N-CA	-5.11	114.52	119.78
1	B	55	GLU	C-N-CD	5.11	131.84	120.60
1	B	187	VAL	CB-CA-C	5.10	117.20	111.80
1	B	67	ASN	CA-C-O	5.02	126.71	120.54
1	A	242	ASP	CA-C-O	5.00	125.41	119.56

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	2388	0	2391	25	0
1	B	2388	0	2391	29	0
2	A	21	0	9	0	0
2	B	21	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	54	0	70	7	0
3	B	60	0	79	16	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
5	A	7	0	0	0	0
6	A	398	0	0	10	0
6	B	390	0	0	9	0
All	All	5789	0	4987	62	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 6.

All (62) 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:3:LYS:CE	1:A:3:LYS:NZ	1.69	1.53
1:B:9:HIS:CE1	3:B:410:GOL:H11	1.88	1.09
1:B:9:HIS:ND1	3:B:410:GOL:H11	1.76	1.00
1:B:118:GLN:HG3	6:B:879:HOH:O	1.62	0.97
1:B:9:HIS:CE1	3:B:410:GOL:C1	2.56	0.89
1:A:312:GLU:CD	1:A:312:GLU:C	2.48	0.81
1:B:136:LYS:HE2	6:B:864:HOH:O	1.84	0.76
1:B:195:SER:HB3	6:B:815:HOH:O	1.87	0.73
1:A:195:SER:HB3	6:A:812:HOH:O	1.91	0.71
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.37	0.70
3:B:407:GOL:H11	6:B:873:HOH:O	1.91	0.70
3:A:410:GOL:H32	6:A:703:HOH:O	1.94	0.67
1:B:9:HIS:HE1	3:B:410:GOL:C1	2.08	0.67
1:B:5:ASN:OD1	1:B:10:VAL:HG22	1.93	0.67
2:B:401:QRO:FAF	3:B:403:GOL:H31	1.85	0.66
3:B:410:GOL:H31	6:B:799:HOH:O	1.94	0.65
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.44	0.65
3:B:410:GOL:H12	6:B:510:HOH:O	1.97	0.64
1:B:9:HIS:ND1	3:B:410:GOL:C1	2.58	0.63
1:A:7:LEU:O	1:A:9:HIS:HD2	1.82	0.62
1:A:61:PHE:CE1	3:A:407:GOL:H32	2.34	0.62
1:B:59:MET:HE3	6:B:622:HOH:O	1.98	0.62
1:A:112:ARG:NH2	6:A:828:HOH:O	2.29	0.62
1:B:93:PRO:HG3	3:B:410:GOL:H32	1.81	0.61
1:A:129:SER:HA	1:A:138:GLN:OE1	2.00	0.61
1:B:241:PRO:HA	3:B:404:GOL:H12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.31	0.60
1:B:132:ASN:HB2	6:B:589:HOH:O	2.02	0.60
1:B:206:SER:OG	3:B:407:GOL:H2	2.01	0.60
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.87	0.57
2:B:401:QRO:CAQ	3:B:403:GOL:H31	2.36	0.56
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.89	0.56
1:A:87:HIS:HE1	1:A:92:LYS:O	1.90	0.55
1:A:307:ARG:NH2	6:A:853:HOH:O	2.41	0.53
1:B:87:HIS:HE1	1:B:92:LYS:O	1.91	0.53
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.06	0.53
1:A:312:GLU:C	1:A:312:GLU:OE1	2.52	0.52
1:B:209:VAL:O	3:B:407:GOL:H31	2.10	0.52
1:B:146:MET:HE2	1:B:180:VAL:CG1	2.40	0.51
2:B:401:QRO:CAI	3:B:403:GOL:H31	2.42	0.50
1:A:132:ASN:HB3	6:A:604:HOH:O	2.11	0.50
1:A:291:GLU:CD	6:A:804:HOH:O	2.54	0.50
1:A:111:ARG:HD3	6:A:896:HOH:O	2.13	0.47
1:B:105:GLU:HG2	1:B:109:MET:HE2	1.96	0.46
1:B:275:GLN:NE2	6:B:611:HOH:O	2.48	0.44
1:A:13:ASN:HB2	1:A:14:PRO:HD2	2.00	0.44
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.11	0.44
1:A:241:PRO:HA	3:A:404:GOL:H32	1.99	0.43
1:B:160:PRO:HB3	1:B:188:LYS:HG3	1.99	0.43
1:A:302:GLU:CG	3:A:406:GOL:O2	2.66	0.43
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.97	0.43
1:A:237:TYR:O	3:A:404:GOL:H11	2.18	0.43
1:A:312:GLU:HG3	1:B:212:LYS:NZ	2.34	0.43
3:A:405:GOL:H11	6:A:532:HOH:O	2.19	0.43
1:A:160:PRO:HB3	1:A:188:LYS:HG3	2.01	0.42
1:A:302:GLU:HG3	1:A:305:ARG:HH12	1.84	0.41
1:A:9:HIS:HE1	6:A:527:HOH:O	2.03	0.41
1:B:312:GLU:N	1:B:312:GLU:OE2	2.54	0.41
1:A:97:SER:HA	1:A:125:GLU:O	2.21	0.40
3:A:410:GOL:C3	6:A:703:HOH:O	2.61	0.40
1:B:192:CYS:HA	1:B:193:VAL:HA	1.87	0.40
1:B:9:HIS:HE1	3:B:410:GOL:O1	2.05	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	311/313 (99%)	303 (97%)	8 (3%)	0	100	100
1	B	311/313 (99%)	304 (98%)	7 (2%)	0	100	100
All	All	622/626 (99%)	607 (98%)	15 (2%)	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	258/258 (100%)	254 (98%)	4 (2%)	55	22
1	B	258/258 (100%)	254 (98%)	4 (2%)	55	22
All	All	516/516 (100%)	508 (98%)	8 (2%)	55	22

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	81	LYS
1	A	129	SER
1	A	312	GLU
1	B	0	MET
1	B	136	LYS
1	B	302	GLU
1	B	312	GLU

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	9	HIS
1	A	87	HIS
1	A	152	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	234	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	GOL	A	408	-	5,5,5	0.66	0	5,5,5	1.61	1 (20%)
3	GOL	A	410	-	5,5,5	0.76	0	5,5,5	1.86	2 (40%)
3	GOL	A	403	-	5,5,5	0.58	0	5,5,5	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	405	-	5,5,5	2.58	3 (60%)	5,5,5	2.82	3 (60%)
2	QRO	B	401	-	22,22,22	2.06	7 (31%)	29,31,31	1.66	8 (27%)
3	GOL	B	406	-	5,5,5	1.11	0	5,5,5	0.96	0
3	GOL	B	410	-	5,5,5	0.99	0	5,5,5	1.23	1 (20%)
3	GOL	B	411	-	5,5,5	0.76	0	5,5,5	0.65	0
3	GOL	B	403	-	5,5,5	1.00	0	5,5,5	2.71	3 (60%)
3	GOL	B	409	-	5,5,5	0.54	0	5,5,5	1.29	0
3	GOL	B	402	-	5,5,5	0.70	0	5,5,5	0.87	0
4	FMN	B	412	-	33,33,33	1.47	6 (18%)	48,50,50	1.39	8 (16%)
3	GOL	A	406	-	5,5,5	0.96	0	5,5,5	0.91	0
2	QRO	A	401	-	22,22,22	2.74	7 (31%)	29,31,31	2.54	8 (27%)
3	GOL	A	409	-	5,5,5	1.18	1 (20%)	5,5,5	0.56	0
3	GOL	B	407	-	5,5,5	0.84	0	5,5,5	0.88	0
3	GOL	B	408	-	5,5,5	1.27	1 (20%)	5,5,5	1.33	1 (20%)
3	GOL	A	404	-	5,5,5	0.73	0	5,5,5	0.77	0
4	FMN	A	411	-	33,33,33	1.35	5 (15%)	48,50,50	1.33	4 (8%)
3	GOL	A	402	-	5,5,5	0.52	0	5,5,5	3.01	4 (80%)
3	GOL	A	407	-	5,5,5	1.40	1 (20%)	5,5,5	1.77	2 (40%)
3	GOL	B	404	-	5,5,5	1.12	1 (20%)	5,5,5	0.86	0
3	GOL	B	405	-	5,5,5	0.75	0	5,5,5	0.95	0
5	NCO	A	412	-	6,6,6	3.92	6 (100%)	-		

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	GOL	A	408	-	-	0/4/4/4	-
3	GOL	A	410	-	-	2/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	405	-	-	3/4/4/4	-
2	QRO	B	401	-	-	4/9/9/9	0/2/2/2
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	B	410	-	-	2/4/4/4	-
3	GOL	B	411	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	409	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	402	-	-	0/4/4/4	-
4	FMN	B	412	-	-	2/18/18/18	0/3/3/3
3	GOL	A	406	-	-	0/4/4/4	-
2	QRO	A	401	-	-	4/9/9/9	0/2/2/2
3	GOL	A	409	-	-	3/4/4/4	-
3	GOL	B	407	-	-	4/4/4/4	-
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
4	FMN	A	411	-	-	2/18/18/18	0/3/3/3
3	GOL	A	402	-	-	1/4/4/4	-
3	GOL	A	407	-	-	2/4/4/4	-
3	GOL	B	404	-	-	4/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	QRO	CAR-CAN	9.00	1.62	1.48
2	B	401	QRO	CAJ-CAO	-6.46	1.33	1.51
5	A	412	NCO	CO-N3	5.71	2.14	1.96
5	A	412	NCO	CO-N5	4.62	2.11	1.96
2	A	401	QRO	CAG-CAO	4.49	1.47	1.38
2	A	401	QRO	CAJ-CAO	-4.29	1.39	1.51
4	B	412	FMN	C5A-N5	-4.14	1.31	1.39
3	A	405	GOL	O1-C1	3.85	1.58	1.42
5	A	412	NCO	CO-N6	3.62	2.08	1.96
4	B	412	FMN	C4-N3	-3.50	1.32	1.38
5	A	412	NCO	CO-N2	3.28	2.07	1.96
3	A	405	GOL	O2-C2	3.07	1.52	1.43
2	A	401	QRO	CAI-CAQ	2.83	1.42	1.37
5	A	412	NCO	CO-N1	2.74	2.05	1.96
5	A	412	NCO	CO-N4	2.67	2.05	1.96
3	A	405	GOL	C1-C2	2.65	1.61	1.51
2	B	401	QRO	CAU-CAS	-2.62	1.40	1.44
3	B	408	GOL	O2-C2	2.62	1.51	1.43
2	A	401	QRO	CAG-CAH	2.62	1.43	1.38
4	A	411	FMN	C5A-N5	-2.60	1.34	1.39
4	B	412	FMN	C6-C7	-2.50	1.36	1.39
2	B	401	QRO	OAD-CAN	-2.49	1.23	1.30
2	A	401	QRO	CAI-CAO	2.48	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	QRO	FAE-CAP	2.47	1.42	1.35
4	B	412	FMN	C9A-C5A	2.45	1.45	1.41
4	A	411	FMN	C2'-C3'	-2.44	1.49	1.53
2	B	401	QRO	CAI-CAQ	2.39	1.41	1.37
3	A	407	GOL	O2-C2	-2.32	1.36	1.43
4	A	411	FMN	C4A-N5	2.32	1.35	1.30
3	A	409	GOL	O3-C3	2.30	1.52	1.42
2	B	401	QRO	CAR-CAN	2.28	1.51	1.48
2	A	401	QRO	FAE-CAP	2.25	1.41	1.35
4	A	411	FMN	C4'-C3'	2.20	1.57	1.53
3	B	404	GOL	C3-C2	2.19	1.60	1.51
2	B	401	QRO	CAR-NAL	2.11	1.42	1.38
4	A	411	FMN	C4-N3	-2.05	1.35	1.38
4	B	412	FMN	O2'-C2'	2.03	1.47	1.43
4	B	412	FMN	O4-C4	2.02	1.27	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	QRO	OAD-CAN-OAA	7.71	142.25	123.90
2	A	401	QRO	OAA-CAN-CAR	-6.87	108.24	120.20
2	A	401	QRO	OAD-CAN-CAR	-4.76	109.20	116.73
4	A	411	FMN	C4-C4A-N5	4.10	123.88	118.21
3	B	403	GOL	O2-C2-C3	-4.00	92.60	109.18
2	A	401	QRO	CAO-CAI-CAQ	3.99	121.99	119.37
3	A	405	GOL	O2-C2-C1	3.92	125.40	109.18
3	A	405	GOL	O2-C2-C3	-3.89	93.08	109.18
3	A	402	GOL	C3-C2-C1	3.81	125.77	111.80
4	B	412	FMN	C4-C4A-N5	3.73	123.36	118.21
3	A	402	GOL	O2-C2-C3	-3.59	94.33	109.18
3	B	403	GOL	O1-C1-C2	3.57	126.47	110.38
2	B	401	QRO	OAA-CAN-CAR	-3.47	114.15	120.20
3	A	402	GOL	O2-C2-C1	-3.40	95.08	109.18
3	A	410	GOL	O1-C1-C2	-3.24	95.78	110.38
4	B	412	FMN	C4A-C4-N3	3.19	121.37	113.25
2	B	401	QRO	CAK-CAS-CAU	3.12	120.83	116.64
2	B	401	QRO	CAS-CAU-NAM	2.98	117.97	115.70
2	B	401	QRO	OAD-CAN-OAA	2.96	130.95	123.90
2	A	401	QRO	CAG-CAH-CAP	2.95	122.68	119.04
4	A	411	FMN	O2-C2-N1	-2.84	117.08	121.80
3	A	407	GOL	C3-C2-C1	2.81	122.12	111.80
4	A	411	FMN	O5'-C5'-C4'	2.77	116.77	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	GOL	C3-C2-C1	2.77	121.97	111.80
4	A	411	FMN	C4A-C4-N3	2.76	120.27	113.25
4	B	412	FMN	O4-C4-C4A	-2.71	119.38	126.53
4	B	412	FMN	C4-N3-C2	-2.69	120.86	125.64
4	B	412	FMN	C9-C8-C7	-2.58	115.90	119.69
3	B	408	GOL	O2-C2-C3	2.56	119.78	109.18
4	B	412	FMN	C6-C7-C8	2.48	123.33	119.69
2	B	401	QRO	CAU-NAM-CAT	-2.41	123.05	126.37
3	A	405	GOL	O3-C3-C2	2.35	120.97	110.38
2	A	401	QRO	CAK-CAS-CAU	2.27	119.68	116.64
4	B	412	FMN	C4-C4A-C10	-2.26	113.06	116.93
3	A	408	GOL	O2-C2-C1	-2.25	99.85	109.18
2	A	401	QRO	CAH-CAG-CAO	-2.25	118.05	121.00
2	B	401	QRO	NAM-CAT-NAL	2.24	119.27	115.74
2	B	401	QRO	CAO-CAI-CAQ	2.23	120.83	119.37
3	A	402	GOL	O3-C3-C2	2.23	120.40	110.38
3	A	407	GOL	O3-C3-C2	2.18	120.20	110.38
3	B	410	GOL	O3-C3-C2	-2.16	100.67	110.38
2	A	401	QRO	CAN-CAR-CAS	2.15	127.13	123.88
4	B	412	FMN	O2-C2-N1	-2.12	118.28	121.80
3	A	410	GOL	O3-C3-C2	-2.07	101.04	110.38
2	B	401	QRO	OAC-CAU-NAM	-2.00	116.35	120.11

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	QRO	OAD-CAN-CAR-NAL
2	B	401	QRO	OAD-CAN-CAR-NAL
3	A	405	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-C3
3	A	407	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-C3
3	B	405	GOL	C1-C2-C3-O3
3	B	405	GOL	O2-C2-C3-O3
3	B	407	GOL	C1-C2-C3-O3
3	B	410	GOL	C1-C2-C3-O3
3	B	410	GOL	O2-C2-C3-O3
3	B	411	GOL	C1-C2-C3-O3
3	A	407	GOL	O2-C2-C3-O3
3	B	411	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O1-C1-C2-C3
3	A	409	GOL	O1-C1-C2-C3
3	A	410	GOL	C1-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
3	B	409	GOL	O1-C1-C2-C3
3	A	402	GOL	O2-C2-C3-O3
3	A	410	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3
3	B	407	GOL	O2-C2-C3-O3
3	B	409	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	A	409	GOL	O1-C1-C2-O2
3	B	407	GOL	O1-C1-C2-O2
3	A	409	GOL	O2-C2-C3-O3
2	A	401	QRO	OAD-CAN-CAR-CAS
2	B	401	QRO	OAA-CAN-CAR-CAS
2	B	401	QRO	OAD-CAN-CAR-CAS
4	B	412	FMN	C4'-C5'-O5'-P
3	A	405	GOL	O2-C2-C3-O3
4	A	411	FMN	C4'-C5'-O5'-P
4	A	411	FMN	O3'-C3'-C4'-C5'
4	B	412	FMN	O3'-C3'-C4'-O4'
2	A	401	QRO	OAA-CAN-CAR-CAS
2	A	401	QRO	OAA-CAN-CAR-NAL
2	B	401	QRO	OAA-CAN-CAR-NAL

There are no ring outliers.

10 monomers are involved in 23 short contacts:

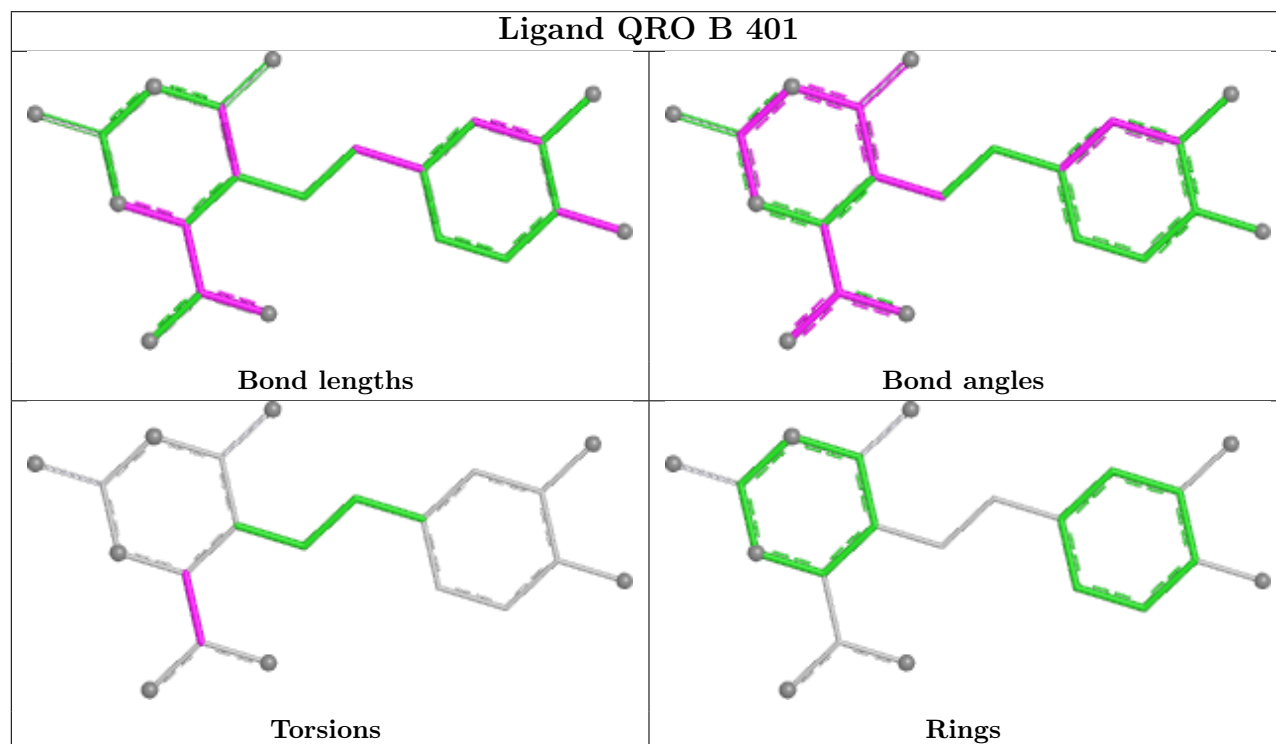
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	GOL	2	0
3	A	405	GOL	1	0
2	B	401	QRO	3	0
3	B	410	GOL	9	0
3	B	403	GOL	3	0
3	A	406	GOL	1	0
3	B	407	GOL	3	0
3	A	404	GOL	2	0
3	A	407	GOL	1	0

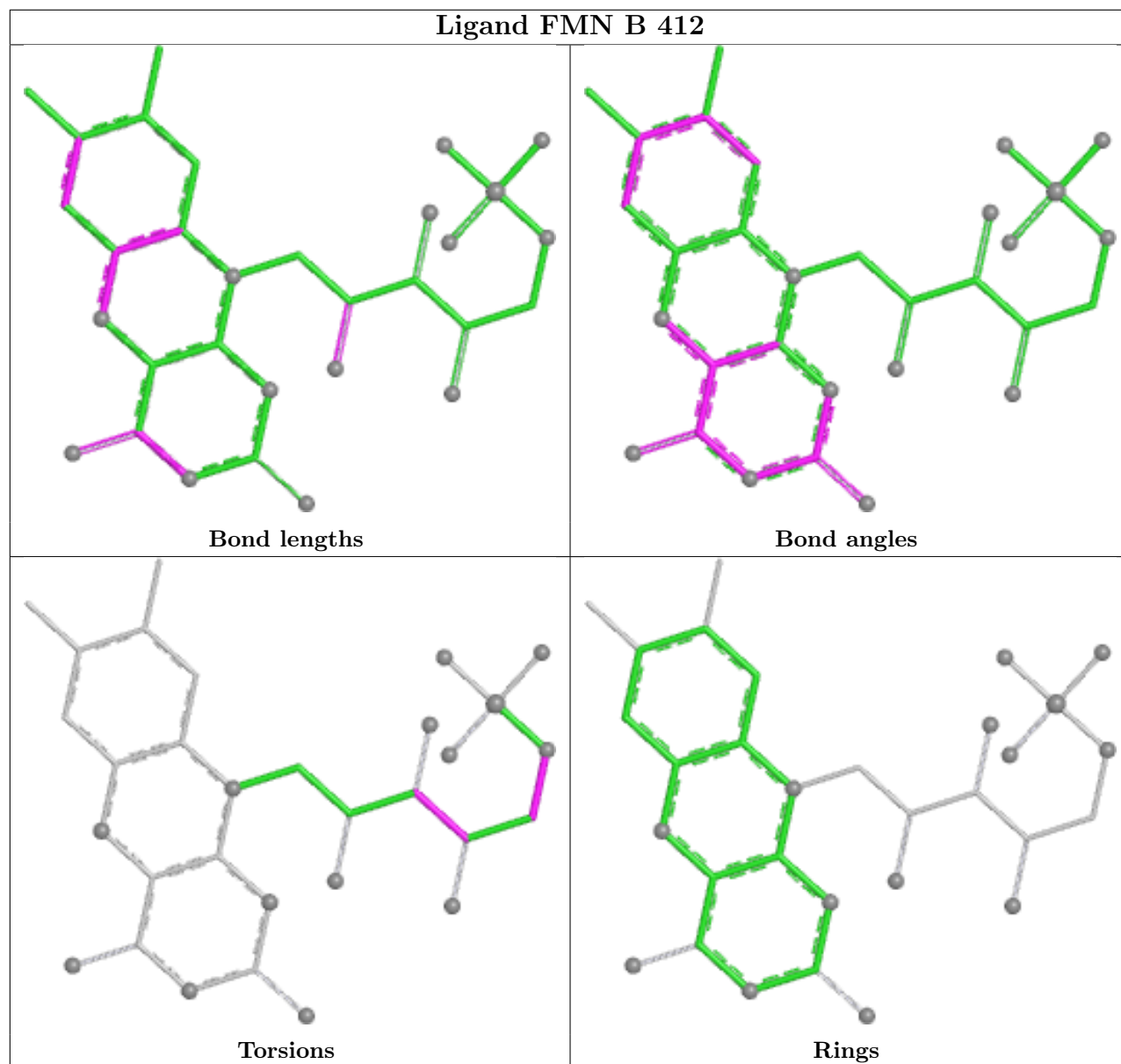
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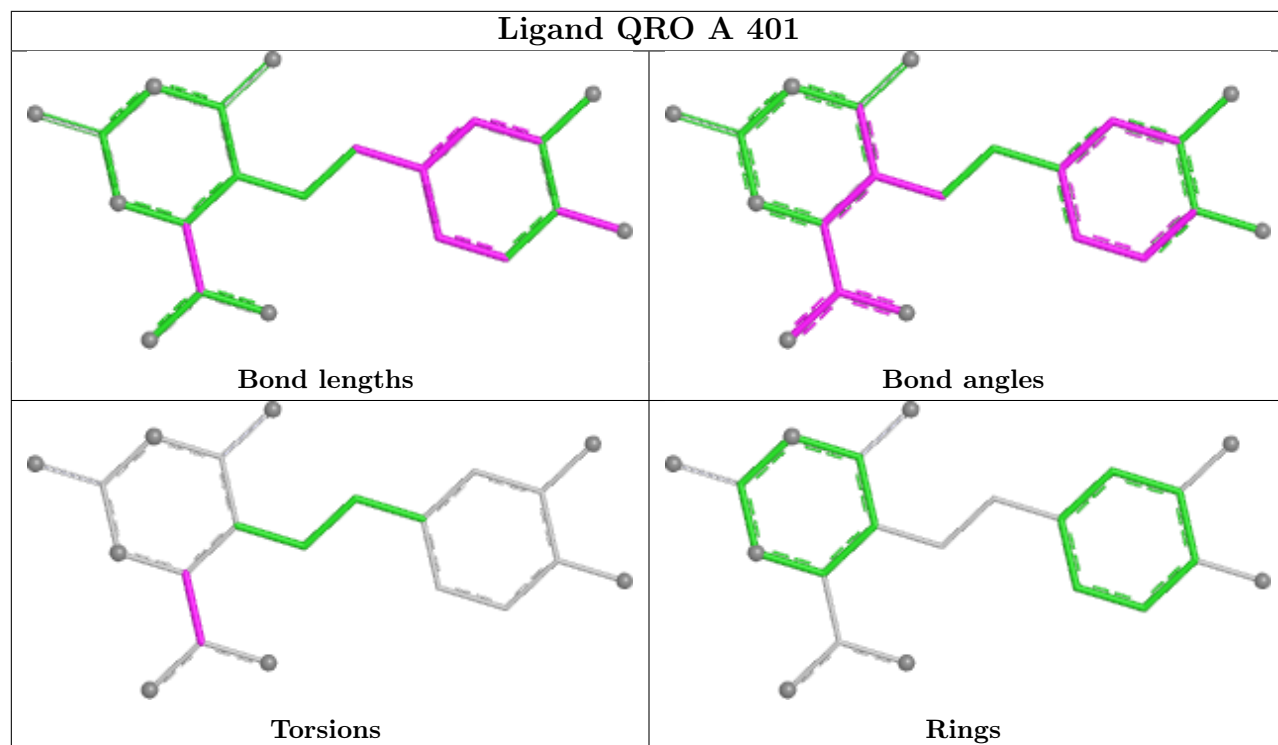
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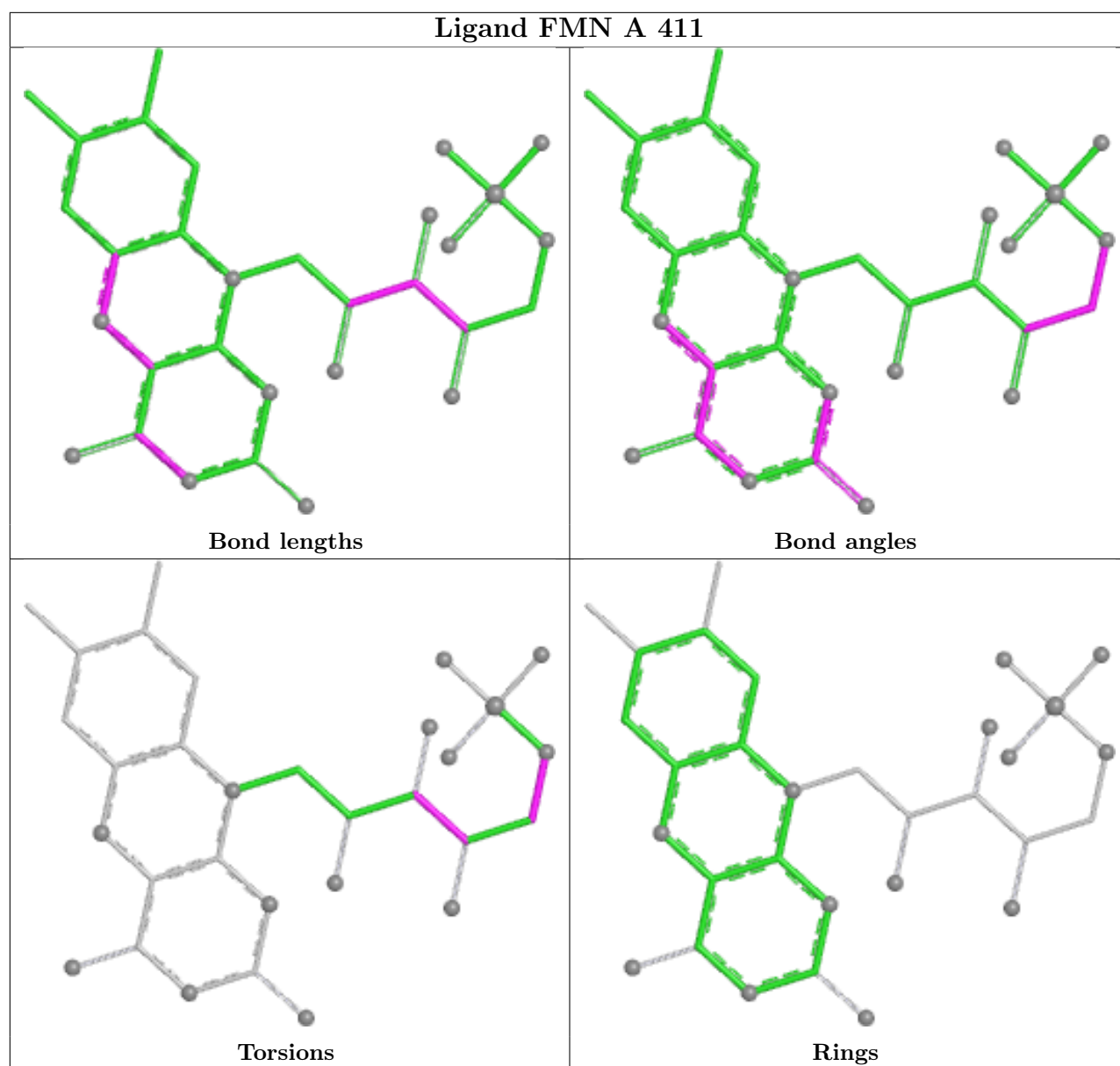
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	GOL	1	0

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	313/313 (100%)	-0.30	10 (3%)	50	53	5, 9, 21, 41	0
1	B	313/313 (100%)	-0.13	12 (3%)	44	46	5, 10, 23, 44	0
All	All	626/626 (100%)	-0.21	22 (3%)	47	49	5, 10, 22, 44	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	CYS	5.7
1	A	131	PRO	5.3
1	B	131	PRO	4.9
1	B	128	LEU	3.6
1	B	312	GLU	3.4
1	B	133	VAL	3.2
1	A	312	GLU	3.1
1	B	130	CYS	3.0
1	B	135	GLY	3.0
1	A	129	SER	3.0
1	B	5	ASN	2.6
1	B	132	ASN	2.6
1	B	1	CYS	2.6
1	A	101	LEU	2.6
1	B	134	PRO	2.4
1	B	136	LYS	2.4
1	B	2	LEU	2.4
1	A	307	ARG	2.3
1	A	132	ASN	2.2
1	A	0	MET	2.2
1	A	133	VAL	2.1
1	A	8	ASP	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.

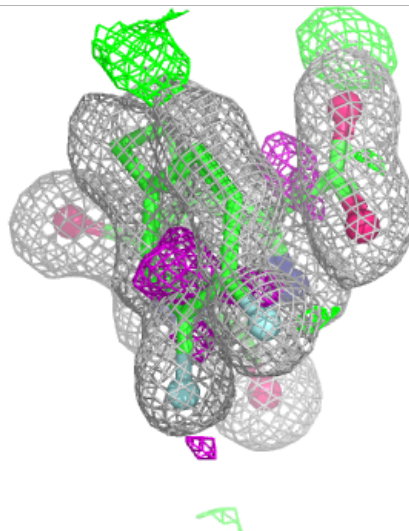
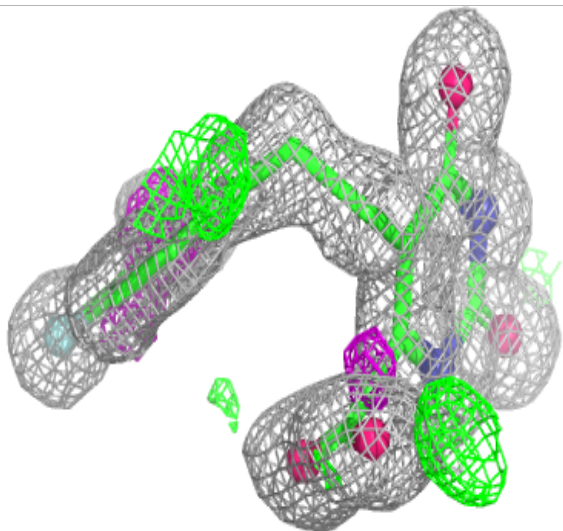
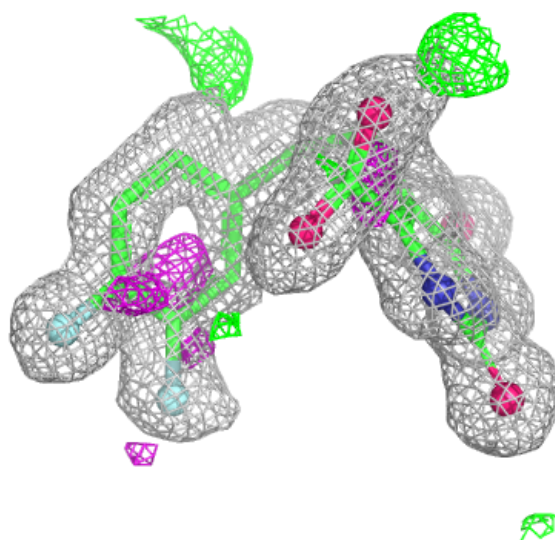
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	408	6/6	0.73	0.17	28,35,35,40	0
3	GOL	B	405	6/6	0.73	0.18	35,41,47,50	0
3	GOL	B	411	6/6	0.73	0.18	28,33,37,41	0
3	GOL	A	410	6/6	0.76	0.17	30,39,39,44	0
3	GOL	A	409	6/6	0.77	0.17	29,47,50,52	0
3	GOL	B	404	6/6	0.79	0.15	29,32,35,43	0
3	GOL	B	409	6/6	0.82	0.15	27,39,43,49	0
3	GOL	A	405	6/6	0.83	0.16	17,22,27,28	0
3	GOL	A	404	6/6	0.83	0.15	36,44,46,55	0
3	GOL	B	407	6/6	0.86	0.13	30,37,40,43	0
3	GOL	B	408	6/6	0.86	0.13	24,27,34,41	0
3	GOL	A	406	6/6	0.88	0.11	20,24,25,29	0
3	GOL	B	403	6/6	0.88	0.14	18,22,31,35	0
3	GOL	B	406	6/6	0.89	0.12	22,30,31,31	0
3	GOL	B	410	6/6	0.90	0.12	21,31,33,33	0
3	GOL	A	407	6/6	0.90	0.12	24,27,29,29	0
3	GOL	A	402	6/6	0.93	0.09	13,16,18,18	0
3	GOL	B	402	6/6	0.94	0.08	16,17,20,22	0
3	GOL	A	403	6/6	0.96	0.07	15,16,17,18	0
2	QRO	A	401	21/21	0.96	0.08	6,10,21,23	0
2	QRO	B	401	21/21	0.98	0.06	6,10,23,36	0
4	FMN	A	411	31/31	0.99	0.04	4,5,7,10	0
4	FMN	B	412	31/31	0.99	0.03	4,5,7,9	0
5	NCO	A	412	7/7	1.00	0.05	8,8,9,9	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.

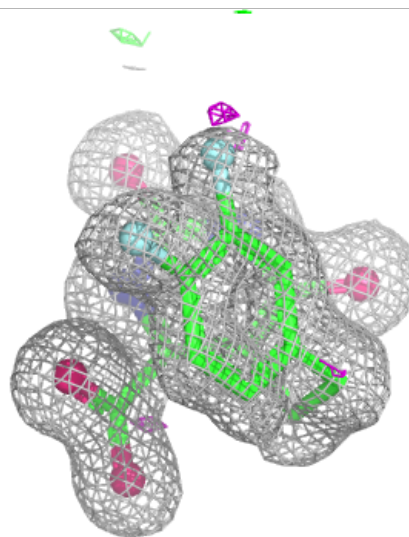
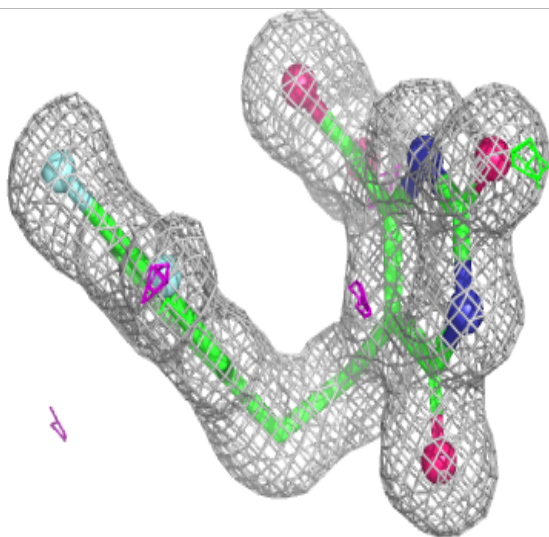
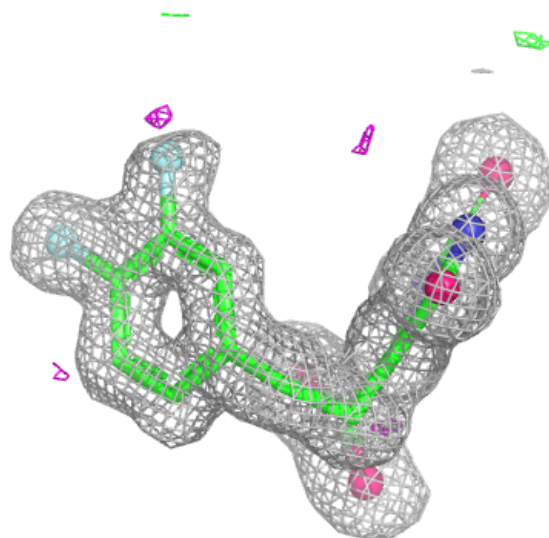
Electron density around QRO A 401:

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



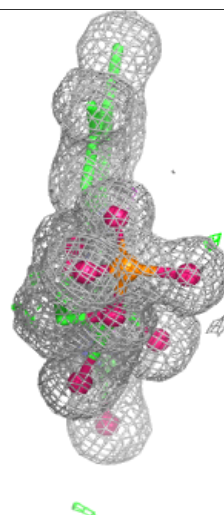
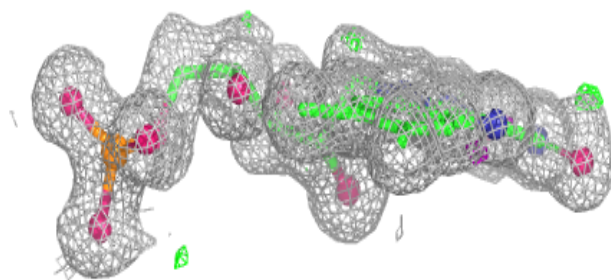
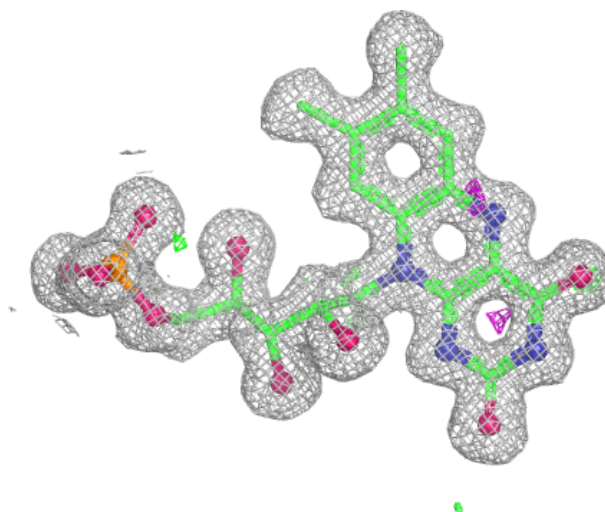
Electron density around QRO B 401:

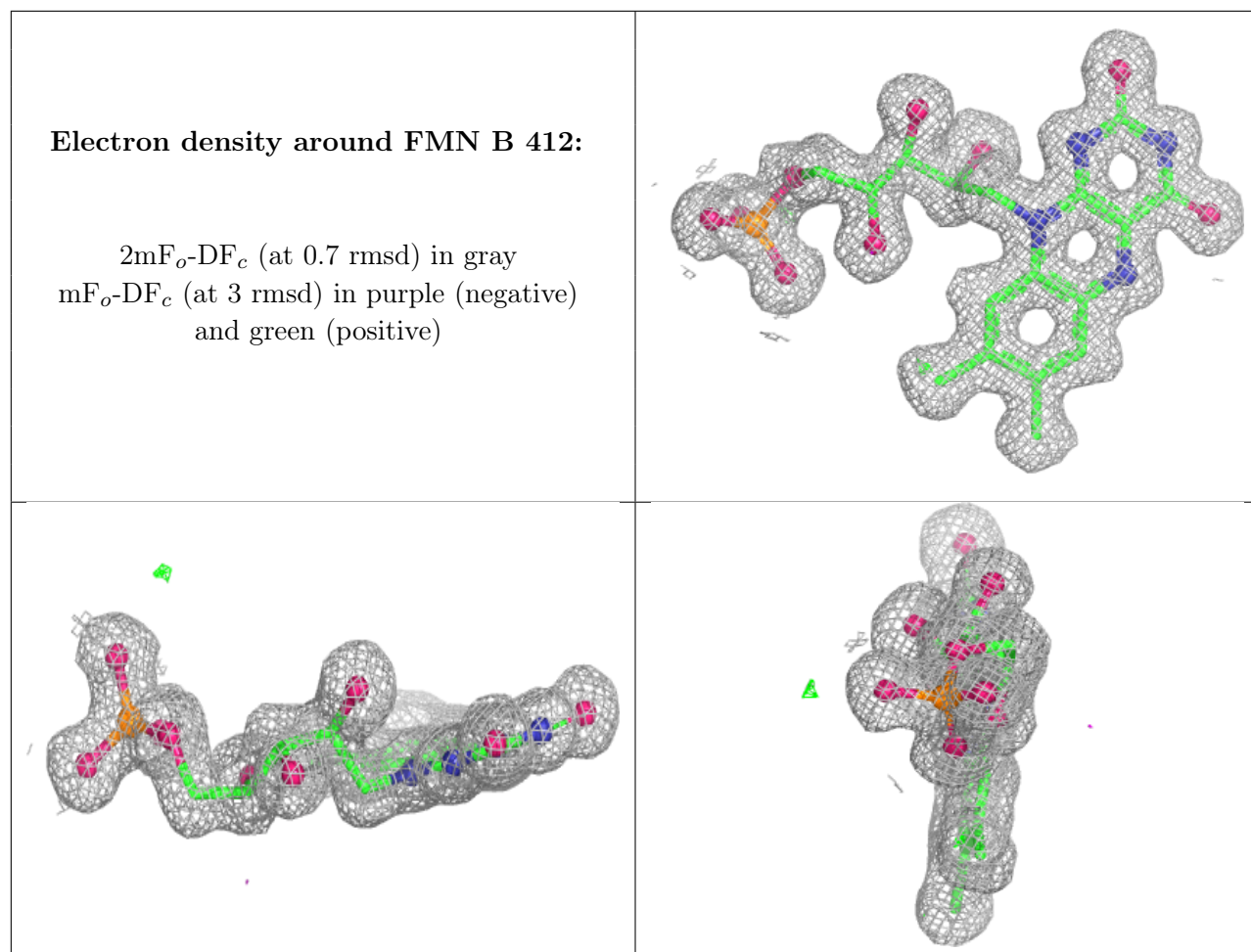
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN A 411:

$2mF_o-DF_c$ (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.