



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 3W1X / pdb_00003w1x
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-121
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 : 2012-11-22
Resolution : 1.45 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

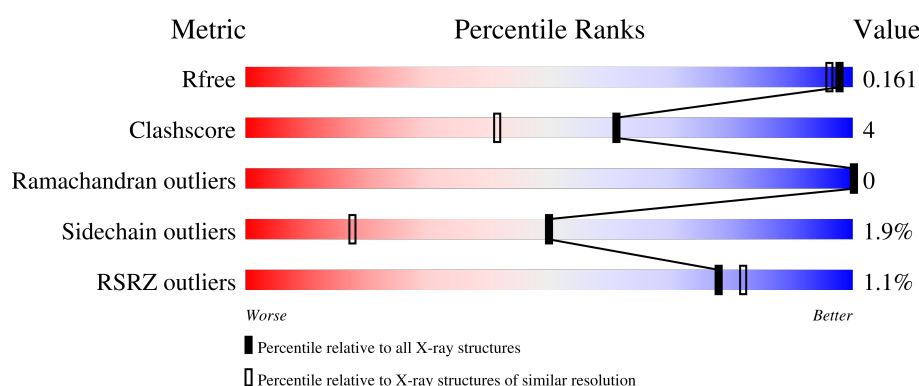
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	2% 74% 23% ..
1	B	313	% 76% 22% .

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:

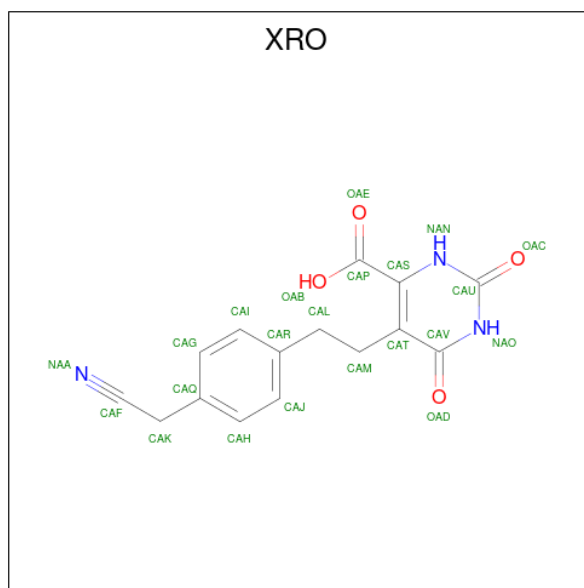
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	405	-	X	-	-

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).

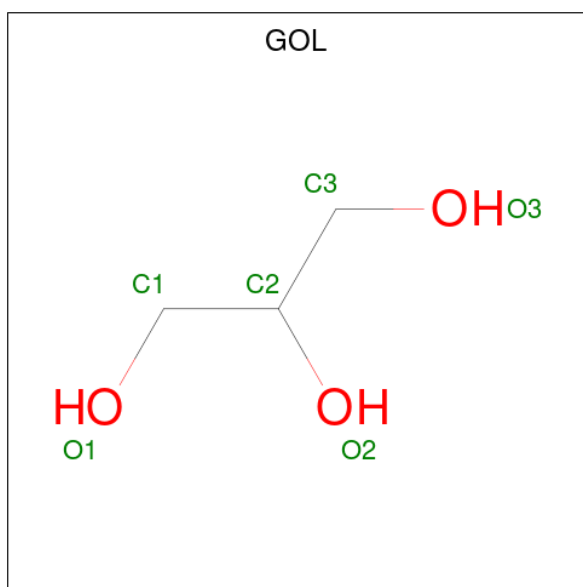
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total 2388	C 1530	N 396	O 444	S 18	0	0	0
1	B	313	Total 2388	C 1530	N 396	O 444	S 18	0	0	0

- Molecule 2 is 5-{2-[4-(cyanomethyl)phenyl]ethyl}-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (CCD ID: XRO) (formula: C₁₅H₁₃N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 22	C 15	N 3	O 4	0	0
2	B	1	Total 22	C 15	N 3	O 4	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



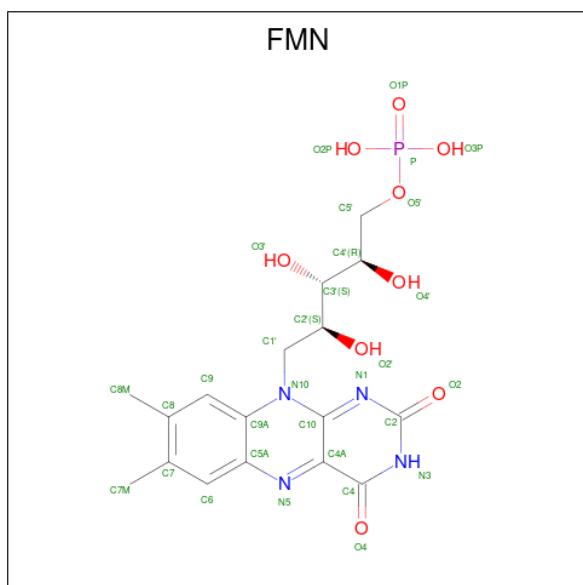
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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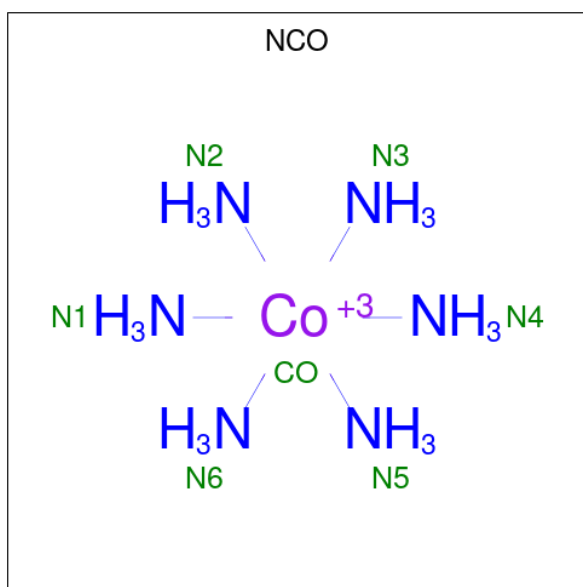
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 5 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



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

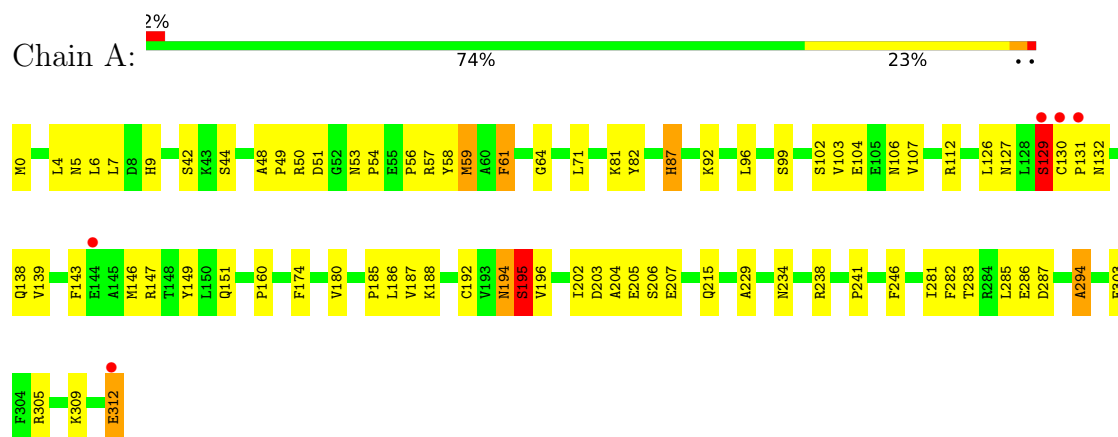
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	386	Total	O	0	0
			386	386		
6	B	384	Total	O	0	0
			384	384		

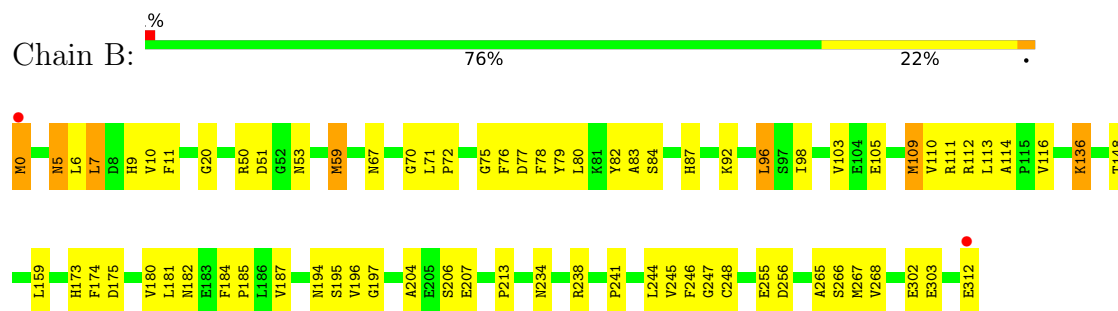
3 Residue-property plots

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	67.95Å 71.85Å 129.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.44 – 1.45 32.44 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.5 (32.44-1.45) 97.5 (32.44-1.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.139 , 0.161 0.141 , 0.161	Depositor DCC
R_{free} test set	5623 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5755	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 28.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9415e-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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.80	57/2440 (2.3%)	1.33	9/3305 (0.3%)
1	B	1.83	55/2440 (2.3%)	1.27	2/3305 (0.1%)
All	All	1.82	112/4880 (2.3%)	1.30	11/6610 (0.2%)

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	SER	C-O	-9.89	1.13	1.24
1	B	184	PHE	C-O	-9.76	1.15	1.24
1	B	112	ARG	C-O	-9.14	1.13	1.24
1	B	78	PHE	C-O	-9.04	1.13	1.24
1	B	5	ASN	CA-C	-8.87	1.42	1.52
1	B	76	PHE	C-O	-8.71	1.14	1.24
1	A	129	SER	CA-C	-8.39	1.44	1.53
1	B	75	GLY	C-O	-8.34	1.14	1.24
1	A	59	MET	C-O	-8.09	1.14	1.23
1	B	246	PHE	C-O	-7.97	1.14	1.24
1	B	50	ARG	C-O	-7.79	1.14	1.23
1	B	59	MET	SD-CE	-7.78	1.60	1.79
1	A	203	ASP	C-O	-7.75	1.14	1.24
1	A	107	VAL	C-O	-7.73	1.15	1.24
1	B	51	ASP	C-O	-7.57	1.14	1.24
1	B	247	GLY	C-O	-7.56	1.13	1.23
1	A	192	CYS	C-O	-7.53	1.15	1.24
1	A	202	ILE	C-O	-7.46	1.16	1.24
1	B	80	LEU	C-O	-7.44	1.15	1.24
1	B	79	TYR	C-O	-7.42	1.15	1.24
1	B	265	ALA	C-O	-7.33	1.15	1.23
1	B	77	ASP	C-O	-7.29	1.15	1.24
1	B	245	VAL	C-O	-7.27	1.16	1.24
1	B	113	LEU	C-O	-7.14	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	N-CD	7.11	1.57	1.47
1	A	104	GLU	C-O	-7.09	1.15	1.24
1	A	48	ALA	C-O	-7.04	1.15	1.24
1	B	256	ASP	C-O	-7.03	1.16	1.24
1	B	255	GLU	C-O	-6.99	1.16	1.24
1	A	205	GLU	C-O	-6.99	1.16	1.24
1	A	127	ASN	C-O	-6.88	1.15	1.24
1	A	61	PHE	C-O	-6.86	1.17	1.24
1	A	132	ASN	C-O	-6.78	1.18	1.23
1	B	181	LEU	C-O	-6.77	1.16	1.24
1	B	96	LEU	CB-CG	-6.77	1.40	1.53
1	A	49	PRO	N-CD	6.76	1.57	1.47
1	B	109	MET	C-O	-6.70	1.16	1.24
1	B	196	VAL	C-O	-6.61	1.17	1.24
1	B	72	PRO	N-CD	6.60	1.56	1.47
1	B	197	GLY	C-O	-6.60	1.16	1.23
1	B	268	VAL	C-O	-6.51	1.17	1.24
1	A	282	PHE	C-O	-6.50	1.16	1.24
1	B	248	CYS	C-O	-6.47	1.16	1.23
1	B	267	MET	C-O	-6.43	1.15	1.23
1	B	185	PRO	N-CD	6.35	1.56	1.47
1	A	106	ASN	C-O	-6.30	1.16	1.24
1	A	206	SER	C-O	-6.30	1.15	1.24
1	B	180	VAL	C-O	-6.29	1.17	1.24
1	A	207	GLU	C-O	-6.27	1.14	1.23
1	B	175	ASP	C-O	-6.27	1.16	1.24
1	A	42	SER	CA-C	-6.26	1.44	1.53
1	A	303	GLU	C-O	-6.25	1.16	1.24
1	A	54	PRO	C-O	-6.23	1.16	1.23
1	A	51	ASP	C-O	-6.20	1.16	1.24
1	A	204	ALA	C-O	-6.20	1.16	1.24
1	A	143	PHE	C-O	-6.19	1.16	1.24
1	B	204	ALA	C-O	-6.18	1.16	1.24
1	B	187	VAL	CA-C	-6.16	1.47	1.53
1	B	110	VAL	C-O	-6.09	1.16	1.24
1	B	103	VAL	N-CA	-6.09	1.39	1.46
1	A	283	THR	C-O	-6.08	1.17	1.24
1	B	148	THR	N-CA	6.05	1.53	1.46
1	A	64	GLY	CA-C	-6.00	1.44	1.52
1	B	194	ASN	C-O	-6.00	1.15	1.23
1	A	187	VAL	C-O	-6.00	1.15	1.23
1	A	131	PRO	C-O	-6.00	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	PRO	N-CD	5.99	1.56	1.47
1	B	244	LEU	C-O	-5.95	1.16	1.23
1	B	182	ASN	C-O	-5.94	1.16	1.24
1	A	286	GLU	C-O	-5.91	1.17	1.24
1	B	6	LEU	CA-CB	5.86	1.64	1.53
1	A	281	ILE	C-O	-5.86	1.17	1.24
1	B	114	ALA	C-O	-5.83	1.19	1.24
1	A	57	ARG	C-O	-5.75	1.17	1.24
1	B	207	GLU	C-O	-5.72	1.15	1.23
1	A	195	SER	C-O	-5.66	1.16	1.23
1	A	102	SER	C-O	-5.65	1.17	1.23
1	A	185	PRO	N-CD	5.64	1.55	1.47
1	A	186	LEU	C-O	-5.64	1.16	1.24
1	B	174	PHE	C-O	-5.63	1.17	1.24
1	A	53	ASN	C-O	-5.62	1.16	1.23
1	B	84	SER	C-O	-5.62	1.17	1.24
1	A	126	LEU	C-O	-5.61	1.17	1.24
1	A	196	VAL	C-O	-5.58	1.18	1.24
1	B	7	LEU	CA-C	5.58	1.60	1.53
1	A	147	ARG	C-O	-5.56	1.17	1.24
1	A	149	TYR	C-O	-5.54	1.17	1.24
1	B	159	LEU	CA-C	5.53	1.57	1.52
1	B	303	GLU	CD-OE2	-5.50	1.15	1.25
1	A	103	VAL	C-O	-5.45	1.17	1.24
1	A	195	SER	CB-OG	-5.44	1.31	1.42
1	A	287	ASP	C-O	-5.43	1.17	1.24
1	A	50	ARG	C-O	-5.41	1.17	1.23
1	B	255	GLU	CD-OE1	-5.38	1.15	1.25
1	B	83	ALA	C-O	-5.36	1.17	1.24
1	B	173	HIS	C-O	-5.34	1.17	1.24
1	A	294	ALA	C-O	5.31	1.30	1.24
1	A	71	LEU	CB-CG	-5.26	1.43	1.53
1	B	111	ARG	C-O	-5.24	1.18	1.24
1	A	96	LEU	CB-CG	-5.20	1.43	1.53
1	A	285	LEU	C-O	-5.16	1.18	1.24
1	A	130	CYS	C-N	5.14	1.40	1.33
1	A	6	LEU	CB-CG	-5.11	1.43	1.53
1	A	194	ASN	C-O	-5.07	1.16	1.23
1	A	146	MET	SD-CE	-5.06	1.66	1.79
1	B	72	PRO	C-O	-5.06	1.18	1.23
1	A	305	ARG	C-O	-5.05	1.17	1.23
1	B	11	PHE	CA-C	5.05	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	GLY	C-O	-5.04	1.16	1.24
1	A	58	TYR	C-O	-5.04	1.18	1.23
1	A	215	GLN	CD-NE2	-5.01	1.22	1.33
1	A	229	ALA	CA-CB	-5.01	1.45	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ASN	N-CA-CB	-6.70	105.36	111.59
1	A	139	VAL	N-CA-C	5.71	116.36	110.36
1	B	116	VAL	N-CA-C	5.30	116.08	110.72
1	A	180	VAL	O-C-N	-5.30	116.71	121.91
1	A	87	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	246	PHE	CA-C-N	-5.27	117.25	122.36
1	A	246	PHE	C-N-CA	-5.27	117.25	122.36
1	A	174	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	67	ASN	CA-C-O	5.09	126.80	120.54
1	A	48	ALA	CA-C-N	-5.01	114.62	119.78
1	A	48	ALA	C-N-CA	-5.01	114.62	119.78

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	20	0
1	B	2388	0	2391	19	0
2	A	22	0	12	0	0
2	B	22	0	12	2	0
3	A	54	0	72	4	0
3	B	42	0	56	4	0
4	A	31	0	19	0	0
4	B	31	0	19	1	0
5	A	7	0	0	0	0
6	A	386	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	384	0	0	5	0
All	All	5755	0	4972	42	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 4.

All (42) 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)
3:A:405:GOL:H12	6:A:820:HOH:O	1.69	0.93
1:B:195:SER:HB3	6:B:824:HOH:O	1.84	0.78
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.21	0.70
1:B:59:MET:HE3	6:B:625:HOH:O	1.91	0.70
1:A:61:PHE:CE1	3:A:407:GOL:H32	2.28	0.69
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.38	0.69
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.41	0.68
1:A:160:PRO:HB3	1:A:188:LYS:HG3	1.80	0.63
1:A:312:GLU:CD	1:A:312:GLU:C	2.67	0.62
1:A:7:LEU:O	1:A:9:HIS:HD2	1.85	0.60
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.84	0.59
1:A:151:GLN:HB3	6:A:731:HOH:O	2.01	0.59
1:A:241:PRO:HA	3:A:404:GOL:H32	1.82	0.59
1:A:129:SER:HA	1:A:138:GLN:OE1	2.02	0.58
1:A:194:ASN:HB3	3:A:405:GOL:H32	1.88	0.55
1:A:5:ASN:HB3	6:A:771:HOH:O	2.07	0.55
1:A:87:HIS:HE1	1:A:92:LYS:O	1.91	0.53
2:B:401:XRO:H12	3:B:403:GOL:H31	1.91	0.53
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.87	0.53
1:B:96:LEU:HD22	1:B:98:ILE:HD11	1.91	0.52
1:B:87:HIS:HE1	1:B:92:LYS:O	1.91	0.52
2:B:401:XRO:H13	3:B:403:GOL:H32	1.92	0.52
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.07	0.52
1:B:206:SER:OG	3:B:407:GOL:H2	2.09	0.51
1:B:241:PRO:HA	3:B:404:GOL:H12	1.92	0.51
1:B:105:GLU:HG2	1:B:109:MET:HE2	1.92	0.51
1:A:112:ARG:NH2	6:A:832:HOH:O	2.35	0.50
1:B:59:MET:CE	6:B:625:HOH:O	2.55	0.50
1:A:59:MET:HE3	6:A:631:HOH:O	2.12	0.49
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.95	0.48
1:B:0:MET:N	6:B:619:HOH:O	2.46	0.48
1:B:5:ASN:OD1	1:B:10:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HB3	6:A:815:HOH:O	2.13	0.47
1:B:7:LEU:O	1:B:9:HIS:HD2	1.98	0.47
1:A:309:LYS:NZ	6:A:775:HOH:O	2.49	0.45
1:B:53:ASN:HB3	1:B:213:PRO:HG3	1.99	0.44
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.11	0.44
1:A:44:SER:HB3	1:A:99:SER:HB3	2.00	0.42
1:A:9:HIS:HE1	6:A:526:HOH:O	2.02	0.42
1:A:0:MET:HE1	1:A:294:ALA:HB2	2.02	0.41
1:B:20:GLY:HA3	4:B:409:FMN:N5	2.36	0.40
1:B:136:LYS:HE2	6:B:872:HOH:O	2.21	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	311/313 (99%)	303 (97%)	8 (3%)	0	100	100
1	B	311/313 (99%)	303 (97%)	8 (3%)	0	100	100
All	All	622/626 (99%)	606 (97%)	16 (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	258/258 (100%)	253 (98%)	5 (2%)	50	17
1	B	258/258 (100%)	253 (98%)	5 (2%)	50	17
All	All	516/516 (100%)	506 (98%)	10 (2%)	50	17

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	81	LYS
1	A	129	SER
1	A	195	SER
1	A	312	GLU
1	B	0	MET
1	B	71	LEU
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	132	ASN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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	410	-	5,5,5	0.85	0	5,5,5	1.87	2 (40%)
3	GOL	B	406	-	5,5,5	0.86	0	5,5,5	1.09	0
3	GOL	B	408	-	5,5,5	1.40	1 (20%)	5,5,5	1.41	1 (20%)
3	GOL	A	403	-	5,5,5	0.82	0	5,5,5	1.02	0
3	GOL	A	405	-	5,5,5	0.63	0	5,5,5	1.60	2 (40%)
3	GOL	A	409	-	5,5,5	1.02	1 (20%)	5,5,5	0.44	0
4	FMN	A	411	-	33,33,33	1.31	6 (18%)	48,50,50	1.45	9 (18%)
3	GOL	A	406	-	5,5,5	0.66	0	5,5,5	0.94	0
3	GOL	A	404	-	5,5,5	0.63	0	5,5,5	0.71	0
2	XRO	A	401	-	23,23,23	2.25	7 (30%)	29,31,31	1.33	4 (13%)
3	GOL	A	407	-	5,5,5	1.18	1 (20%)	5,5,5	1.26	0
3	GOL	B	405	-	5,5,5	0.77	0	5,5,5	1.20	0
3	GOL	B	407	-	5,5,5	0.82	0	5,5,5	0.69	0
3	GOL	A	402	-	5,5,5	0.64	0	5,5,5	2.94	3 (60%)
3	GOL	B	404	-	5,5,5	1.08	1 (20%)	5,5,5	1.03	0
3	GOL	B	403	-	5,5,5	0.93	0	5,5,5	1.28	0
2	XRO	B	401	-	23,23,23	1.47	5 (21%)	29,31,31	1.13	3 (10%)
4	FMN	B	409	-	33,33,33	1.43	6 (18%)	48,50,50	1.19	6 (12%)
3	GOL	A	408	-	5,5,5	0.90	0	5,5,5	1.16	0
3	GOL	B	402	-	5,5,5	0.54	0	5,5,5	1.09	0
5	NCO	A	412	-	6,6,6	3.16	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	410	-	-	2/4/4/4	-
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
3	GOL	A	409	-	-	3/4/4/4	-
4	FMN	A	411	-	-	1/18/18/18	0/3/3/3
3	GOL	A	406	-	-	4/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
2	XRO	A	401	-	-	2/11/12/12	0/2/2/2
3	GOL	A	407	-	-	2/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-
3	GOL	B	407	-	-	4/4/4/4	-
3	GOL	A	402	-	-	1/4/4/4	-
3	GOL	B	404	-	-	4/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
2	XRO	B	401	-	-	4/11/12/12	0/2/2/2
4	FMN	B	409	-	-	3/18/18/18	0/3/3/3
3	GOL	A	408	-	-	0/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	XRO	CAK-CAF	4.86	1.54	1.46
2	A	401	XRO	CAG-CAI	4.81	1.46	1.38
2	A	401	XRO	CAS-CAP	4.75	1.55	1.48
5	A	412	NCO	CO-N3	4.07	2.09	1.96
5	A	412	NCO	CO-N6	3.57	2.08	1.96
4	B	409	FMN	C5A-N5	-3.41	1.33	1.39
4	B	409	FMN	C4-N3	-3.35	1.32	1.38
5	A	412	NCO	CO-N4	3.35	2.07	1.96
2	A	401	XRO	CAL-CAR	-3.11	1.42	1.51
3	B	408	GOL	O2-C2	3.04	1.52	1.43
4	A	411	FMN	C4-N3	-3.03	1.33	1.38
5	A	412	NCO	CO-N5	2.71	2.05	1.96
2	B	401	XRO	CAL-CAR	-2.66	1.44	1.51
4	B	409	FMN	C9-C8	-2.65	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	411	FMN	C2'-C3'	-2.64	1.48	1.53
2	A	401	XRO	OAB-CAP	-2.62	1.23	1.30
5	A	412	NCO	CO-N2	2.52	2.04	1.96
2	A	401	XRO	CAM-CAT	-2.49	1.44	1.51
2	B	401	XRO	CAG-CAQ	-2.38	1.34	1.38
5	A	412	NCO	CO-N1	2.38	2.04	1.96
4	A	411	FMN	C6-C7	-2.38	1.36	1.39
2	B	401	XRO	CAG-CAI	2.28	1.42	1.38
4	A	411	FMN	C2-N3	-2.23	1.34	1.39
2	A	401	XRO	CAV-NAO	2.23	1.43	1.38
3	B	404	GOL	C3-C2	2.20	1.60	1.51
3	A	407	GOL	O2-C2	-2.18	1.37	1.43
4	A	411	FMN	C8-C7	2.13	1.46	1.40
4	A	411	FMN	C1'-C2'	-2.13	1.49	1.52
4	B	409	FMN	O4-C4	2.12	1.27	1.23
4	B	409	FMN	C1'-C2'	-2.10	1.49	1.52
2	B	401	XRO	CAV-NAO	2.09	1.42	1.38
2	B	401	XRO	OAB-CAP	-2.03	1.25	1.30
4	B	409	FMN	C8M-C8	-2.00	1.47	1.51
3	A	409	GOL	O3-C3	2.00	1.50	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	XRO	CAQ-CAK-CAF	-3.97	105.43	113.33
4	A	411	FMN	C9A-C5A-N5	-3.81	118.41	122.45
3	A	402	GOL	O2-C2-C1	-3.77	93.55	109.18
3	A	402	GOL	O2-C2-C3	-3.75	93.67	109.18
4	A	411	FMN	O2-C2-N1	-3.72	115.62	121.80
3	A	402	GOL	C3-C2-C1	3.41	124.31	111.80
4	B	409	FMN	C4A-C4-N3	3.07	121.07	113.25
4	B	409	FMN	C4-N3-C2	-3.02	120.28	125.64
4	B	409	FMN	C4-C4A-N5	2.71	121.95	118.21
4	A	411	FMN	C4-C4A-N5	2.69	121.92	118.21
3	A	410	GOL	C3-C2-C1	-2.59	102.31	111.80
4	B	409	FMN	O4-C4-C4A	-2.56	119.77	126.53
3	A	410	GOL	O2-C2-C3	2.50	119.52	109.18
4	B	409	FMN	O2-C2-N1	-2.48	117.68	121.80
2	A	401	XRO	OAE-CAP-CAS	-2.46	115.91	120.20
2	B	401	XRO	CAQ-CAK-CAF	-2.46	108.43	113.33
4	A	411	FMN	C7M-C7-C6	2.44	123.88	119.57
4	A	411	FMN	C4A-C4-N3	2.40	119.36	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	XRO	CAV-NAO-CAU	-2.36	123.12	126.37
3	A	405	GOL	C3-C2-C1	-2.34	103.20	111.80
3	B	408	GOL	O2-C2-C3	2.34	118.87	109.18
4	A	411	FMN	O4-C4-C4A	-2.28	120.53	126.53
3	A	405	GOL	O2-C2-C1	2.27	118.59	109.18
4	B	409	FMN	C9A-C9-C8	2.27	123.79	119.22
2	A	401	XRO	CAM-CAT-CAS	2.26	124.06	119.56
4	A	411	FMN	C5A-C9A-N10	2.18	119.94	117.97
4	A	411	FMN	C4-N3-C2	-2.12	121.88	125.64
4	A	411	FMN	C4A-C10-N10	2.07	119.45	116.48
2	A	401	XRO	CAH-CAJ-CAR	2.07	123.71	121.00
2	B	401	XRO	CAP-CAS-CAT	2.05	126.99	123.88

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	XRO	OAB-CAP-CAS-NAN
2	B	401	XRO	OAB-CAP-CAS-NAN
3	A	404	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-C3
3	A	406	GOL	O1-C1-C2-C3
3	A	407	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
3	B	405	GOL	O1-C1-C2-C3
3	B	407	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
3	A	405	GOL	O1-C1-C2-O2
3	A	405	GOL	C1-C2-C3-O3
3	A	406	GOL	C1-C2-C3-O3
3	A	409	GOL	O1-C1-C2-C3
3	A	410	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	A	407	GOL	O2-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	B	407	GOL	O2-C2-C3-O3
3	A	406	GOL	O1-C1-C2-O2
3	A	405	GOL	O2-C2-C3-O3
3	A	409	GOL	O1-C1-C2-O2
3	A	410	GOL	O1-C1-C2-O2

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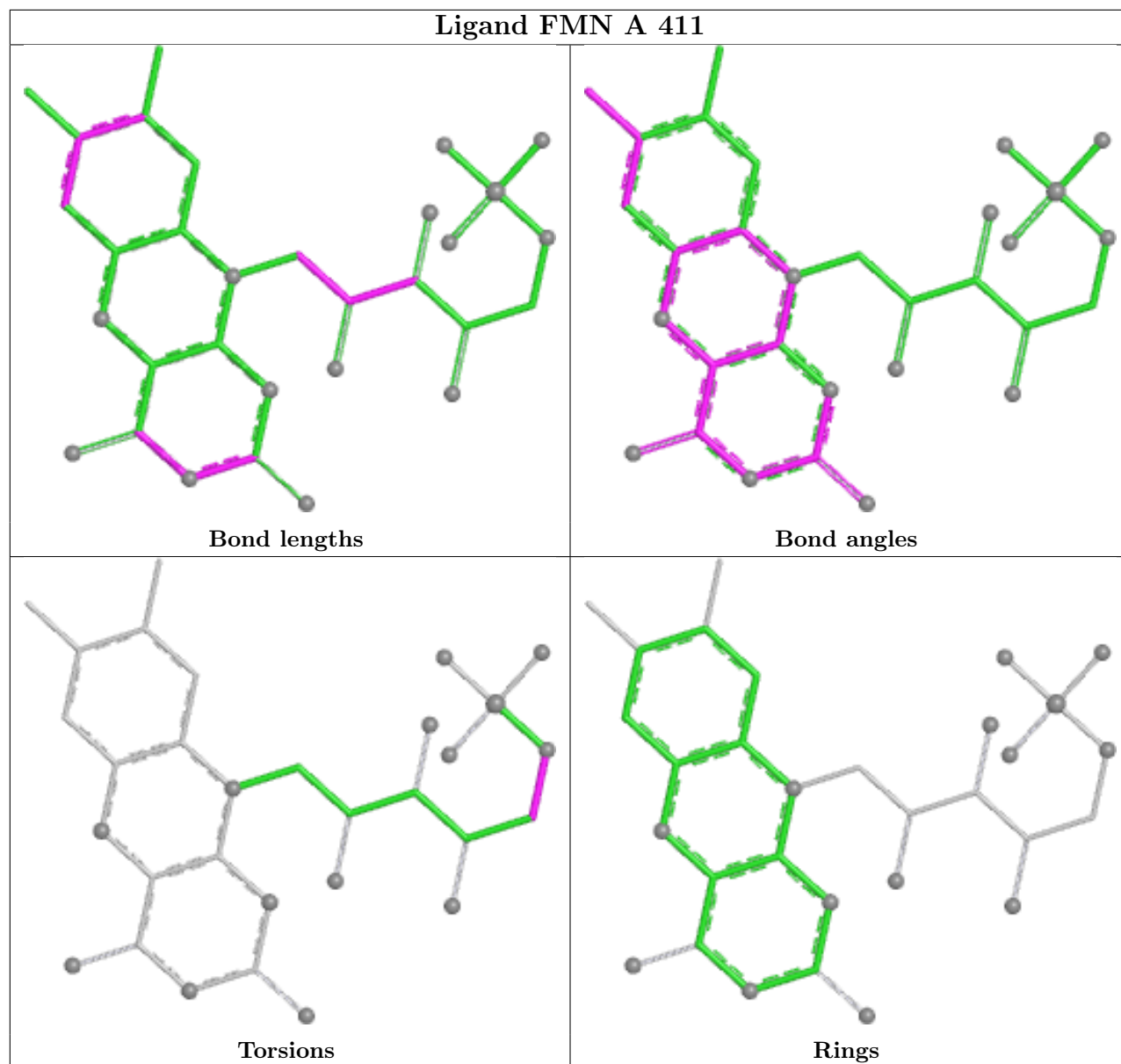
Mol	Chain	Res	Type	Atoms
3	A	406	GOL	O2-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
4	B	409	FMN	C4'-C5'-O5'-P
4	A	411	FMN	C4'-C5'-O5'-P
3	B	403	GOL	O2-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
4	B	409	FMN	C2'-C3'-C4'-O4'
3	A	409	GOL	O2-C2-C3-O3
4	B	409	FMN	O3'-C3'-C4'-O4'
3	B	407	GOL	O1-C1-C2-O2
2	B	401	XRO	OAB-CAP-CAS-CAT
2	B	401	XRO	OAE-CAP-CAS-CAT
2	A	401	XRO	OAE-CAP-CAS-NAN
2	B	401	XRO	OAE-CAP-CAS-NAN
3	B	405	GOL	O1-C1-C2-O2

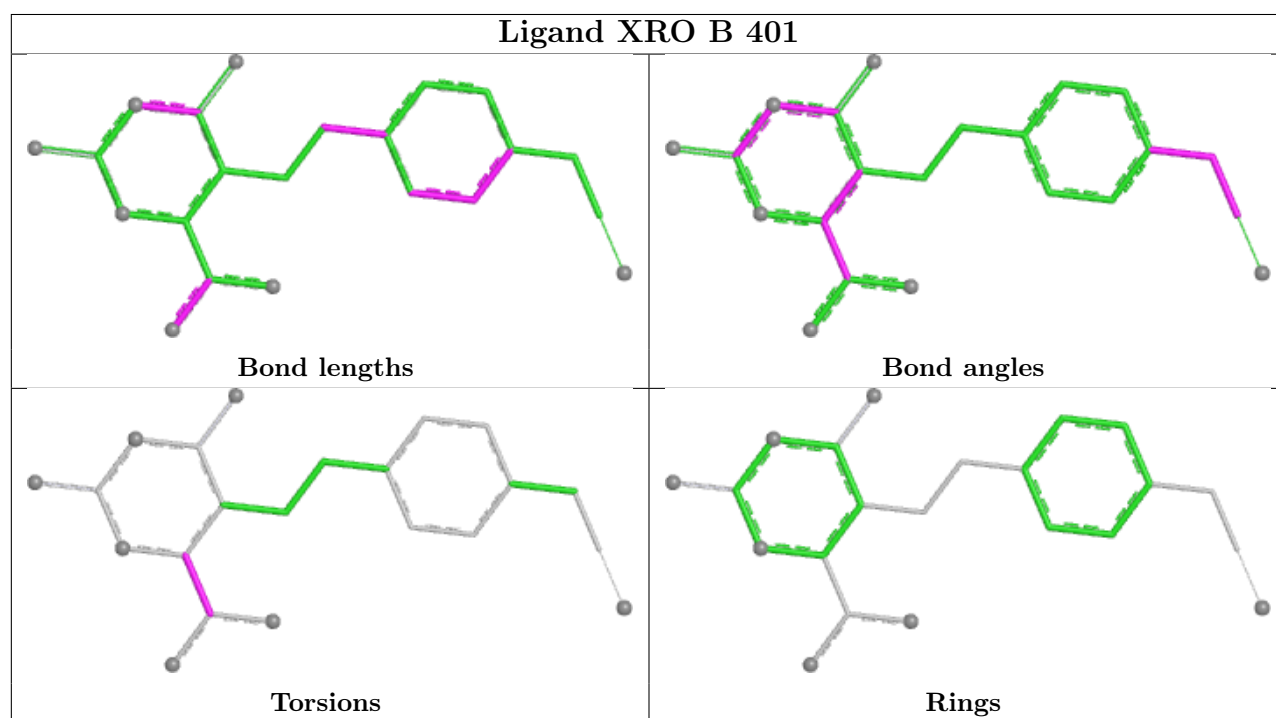
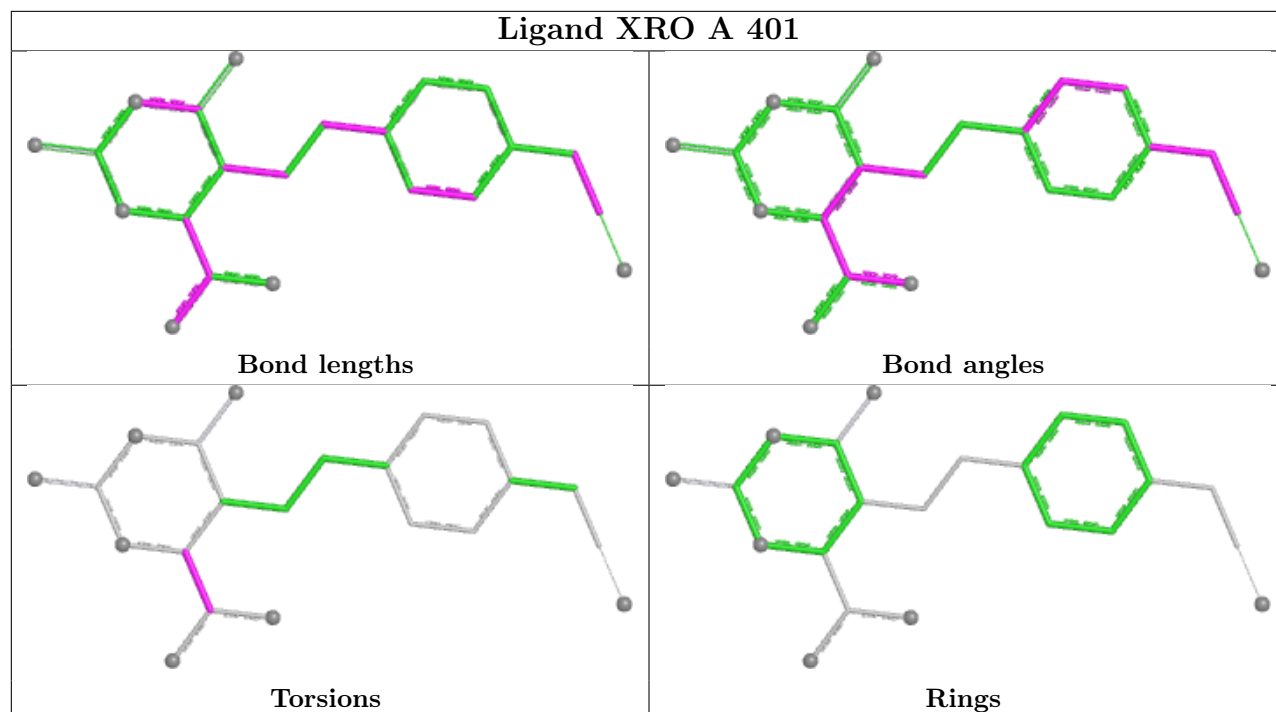
There are no ring outliers.

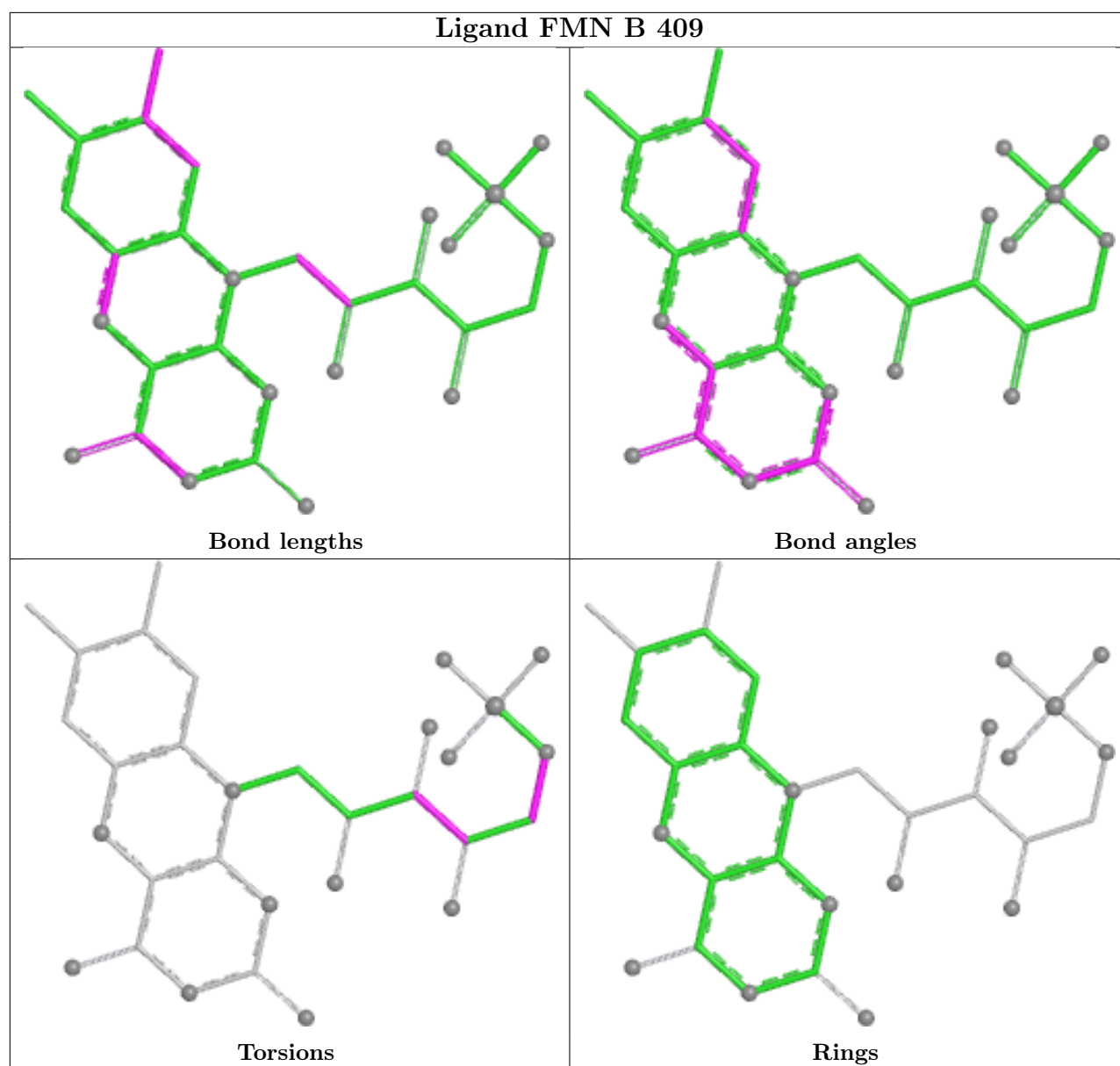
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	GOL	2	0
3	A	404	GOL	1	0
3	A	407	GOL	1	0
3	B	407	GOL	1	0
3	B	404	GOL	1	0
3	B	403	GOL	2	0
2	B	401	XRO	2	0
4	B	409	FMN	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.41	5 (1%) 70 73	5, 9, 20, 42	0
1	B	313/313 (100%)	-0.32	2 (0%) 85 89	5, 10, 21, 50	0
All	All	626/626 (100%)	-0.37	7 (1%) 78 82	5, 9, 21, 50	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	CYS	3.7
1	B	312	GLU	3.3
1	A	312	GLU	3.1
1	A	131	PRO	3.1
1	B	0	MET	2.8
1	A	129	SER	2.3
1	A	144	GLU	2.1

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](#)

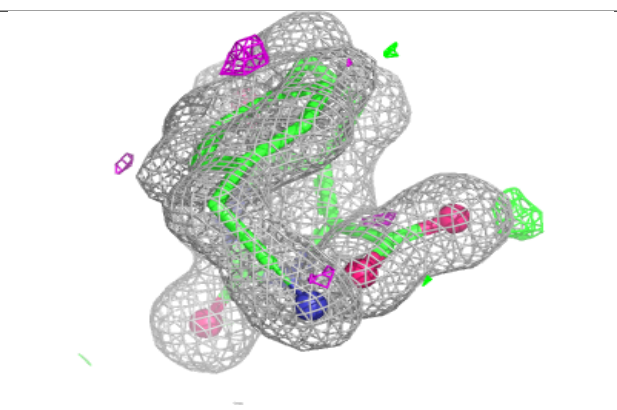
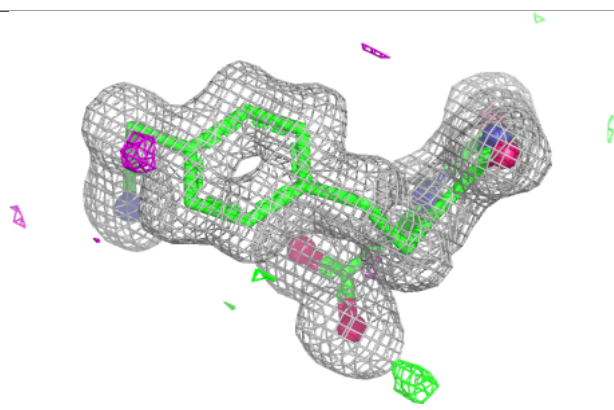
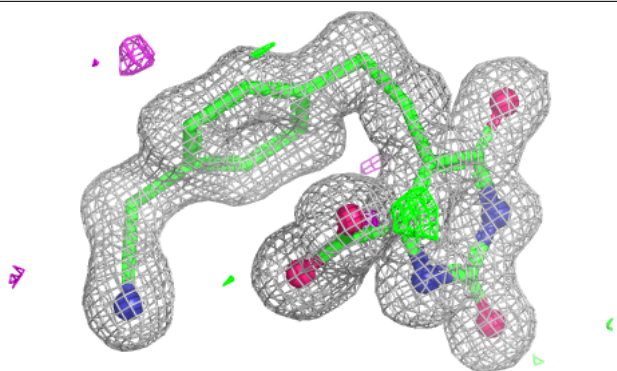
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	B	405	6/6	0.72	0.18	36,37,47,52	0
3	GOL	A	410	6/6	0.79	0.15	28,33,37,42	0
3	GOL	B	404	6/6	0.79	0.14	28,32,35,44	0
3	GOL	A	408	6/6	0.79	0.15	30,34,37,40	0
3	GOL	A	409	6/6	0.81	0.16	23,42,43,43	0
3	GOL	B	407	6/6	0.82	0.14	31,40,42,50	0
3	GOL	A	405	6/6	0.84	0.17	17,30,38,42	0
3	GOL	A	404	6/6	0.85	0.14	36,42,44,50	0
3	GOL	B	403	6/6	0.88	0.12	16,22,23,24	0
3	GOL	A	406	6/6	0.89	0.12	22,30,33,38	0
3	GOL	B	406	6/6	0.90	0.11	23,27,29,33	0
3	GOL	B	408	6/6	0.90	0.11	22,26,30,35	0
3	GOL	A	407	6/6	0.92	0.10	24,27,28,28	0
3	GOL	A	402	6/6	0.92	0.09	14,16,18,20	0
3	GOL	A	403	6/6	0.96	0.06	13,15,17,19	0
3	GOL	B	402	6/6	0.96	0.06	15,16,19,22	0
2	XRO	A	401	22/22	0.98	0.04	5,7,9,10	0
2	XRO	B	401	22/22	0.98	0.04	6,7,11,12	0
4	FMN	A	411	31/31	0.99	0.04	4,5,7,8	0
4	FMN	B	409	31/31	0.99	0.03	4,5,7,8	0
5	NCO	A	412	7/7	1.00	0.05	8,8,9,9	0

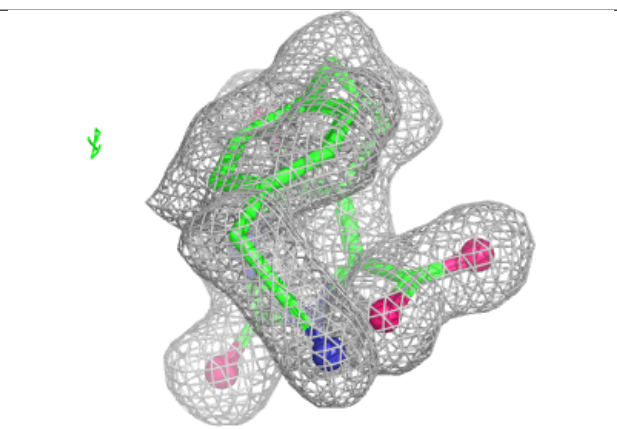
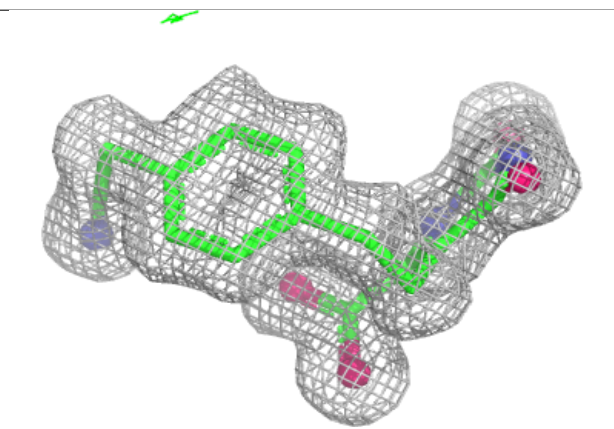
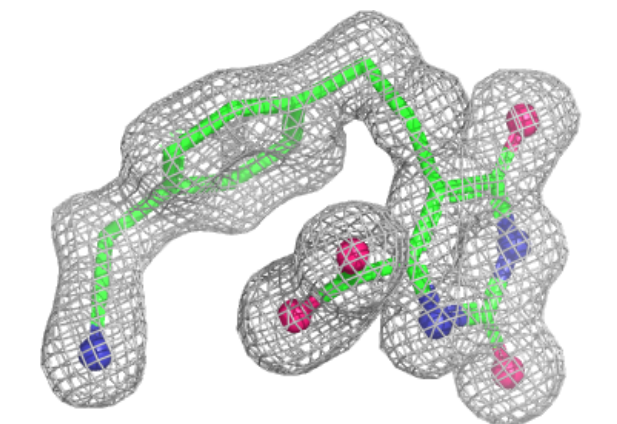
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XRO 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)

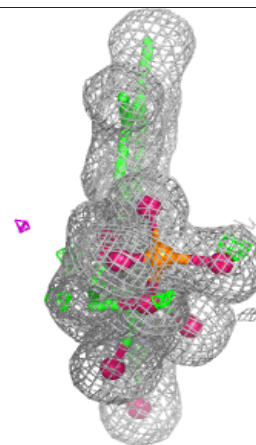
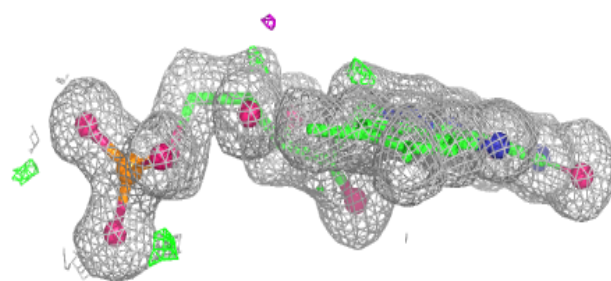
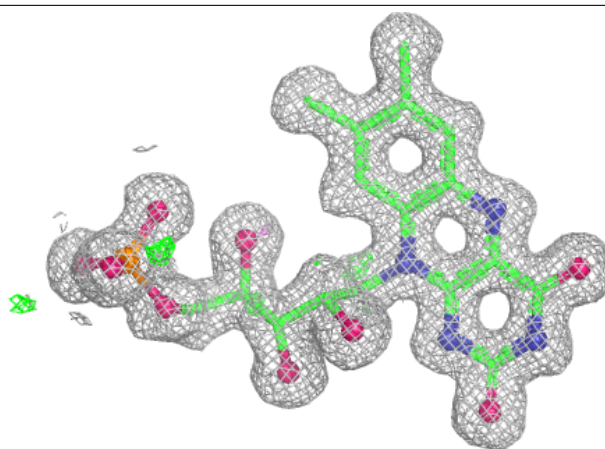
**Electron density around XRO B 401:**

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



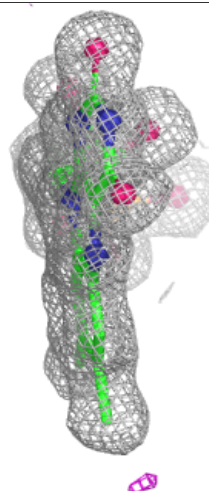
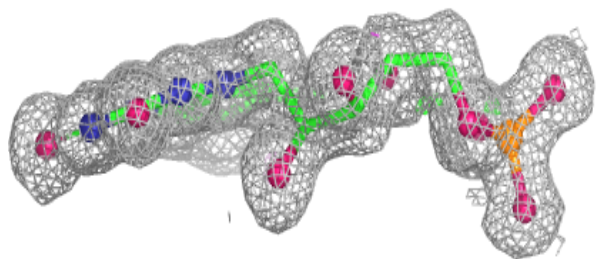
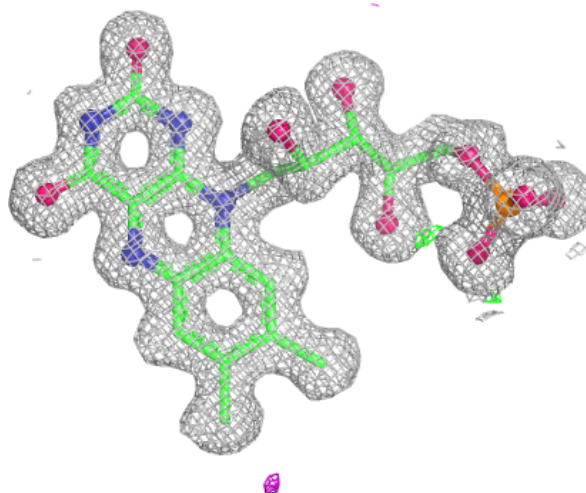
Electron density around FMN A 411:

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



Electron density around FMN B 409:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.