



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:01 PM UTC

PDB ID : 3IAM / pdb_00003iam
Title : Crystal structure of the hydrophilic domain of respiratory complex I from
Thermus thermophilus, reduced, 2 mol/ASU, with bound NADH
Authors : Sazanov, L.A.; Berrisford, J.M.
Deposited on : 2009-07-14
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

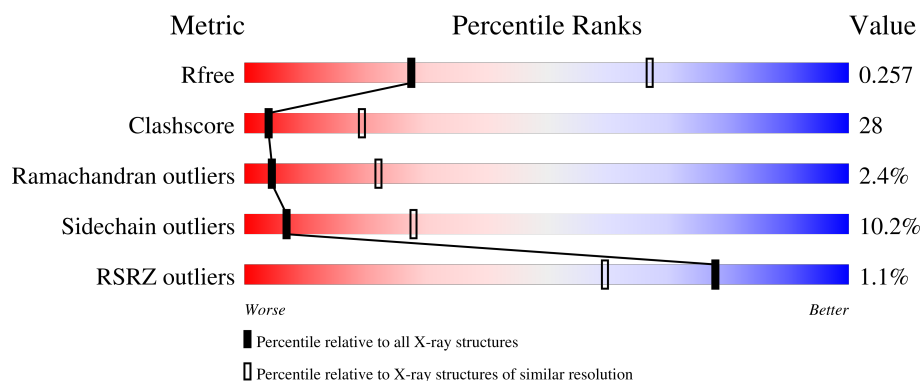
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1	438	53% 38% 8%
1	A	438	53% 40% 7%
2	2	181	51% 40% 7% .
2	B	181	55% 38% 6% .
3	3	783	2% 47% 41% 8% . .

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Mol	Chain	Length	Quality of chain
3	C	783	
4	4	409	
4	D	409	
5	5	207	
5	E	207	
6	6	181	
6	F	181	
7	9	182	
7	G	182	
8	7	129	
8	H	129	

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
9	SF4	9	183	-	-	X	-
9	SF4	F	182	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 37606 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 NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	A	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	179	Total	C	N	O	S	0	0	0
			1410	897	239	266	8			
2	B	179	Total	C	N	O	S	0	0	0
			1410	897	239	266	8			

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	C	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	378	Total	C	N	O	S	0	0	0
			3018	1946	511	550	11			
4	D	378	Total	C	N	O	S	0	0	0
			3018	1946	511	550	11			

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	E	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	F	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			

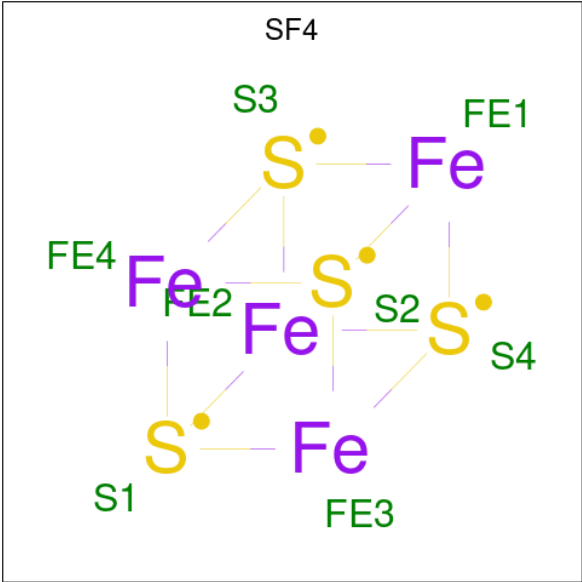
- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	G	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

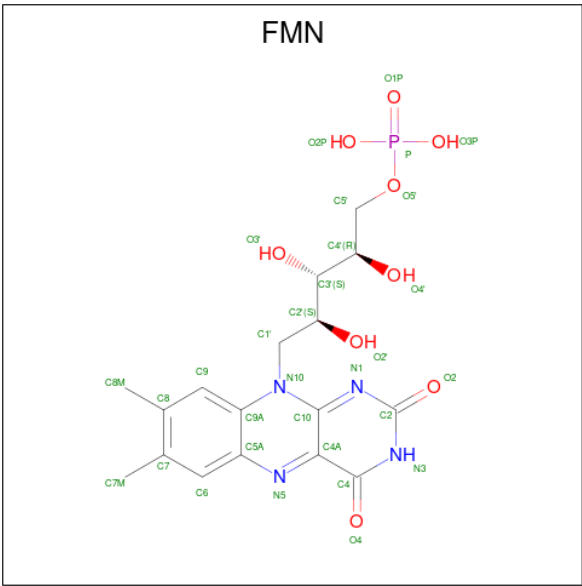
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	H	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



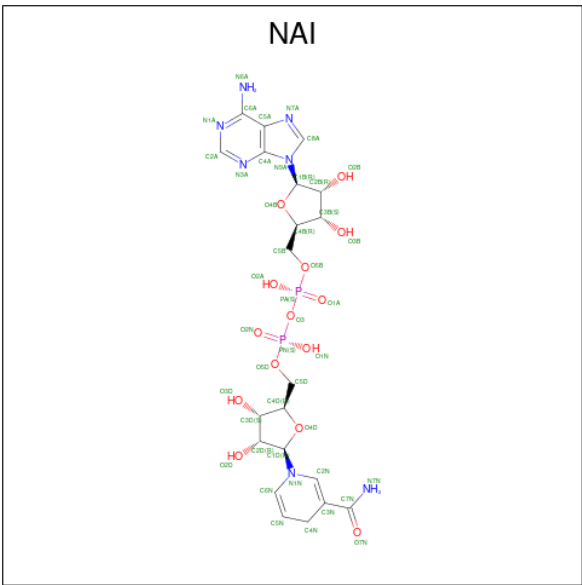
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	1	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	6	1	Total	Fe	S	0	0
			8	4	4		
9	9	1	Total	Fe	S	0	0
			8	4	4		
9	9	1	Total	Fe	S	0	0
			8	4	4		
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	G	1	Total	Fe	S	0	0
			8	4	4		
9	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 11 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

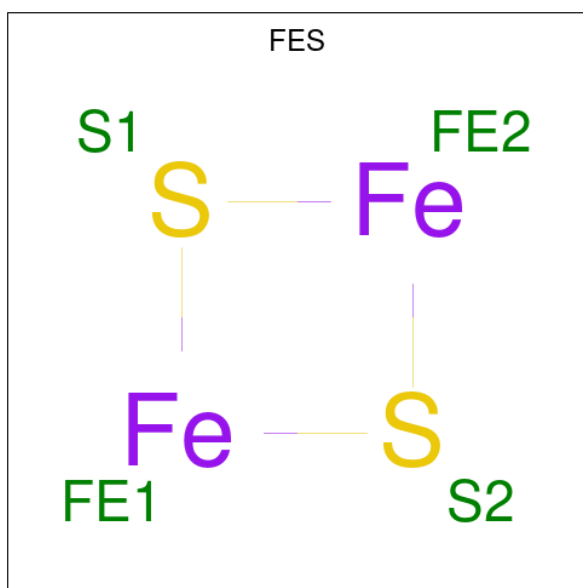


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
11	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	1	1	Total	Mg	0	0
			1	1		
12	2	1	Total	Mg	0	0
			1	1		
12	3	2	Total	Mg	0	0
			2	2		
12	4	1	Total	Mg	0	0
			1	1		
12	5	1	Total	Mg	0	0
			1	1		
12	A	1	Total	Mg	0	0
			1	1		
12	C	2	Total	Mg	0	0
			2	2		
12	E	1	Total	Mg	0	0
			1	1		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	2	1	Total 4	Fe 2	S 2	0	0
13	3	1	Total 4	Fe 2	S 2	0	0
13	B	1	Total 4	Fe 2	S 2	0	0
13	C	1	Total 4	Fe 2	S 2	0	0

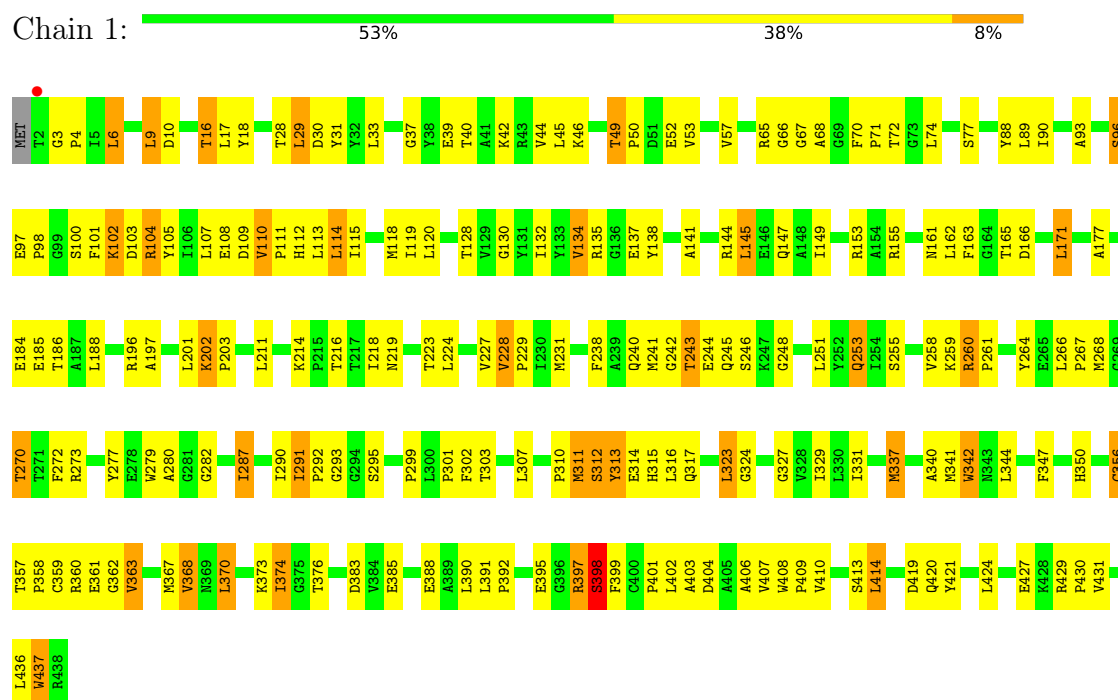
- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	7	1	Total 1	Ca 1	0	0
14	H	1	Total 1	Ca 1	0	0

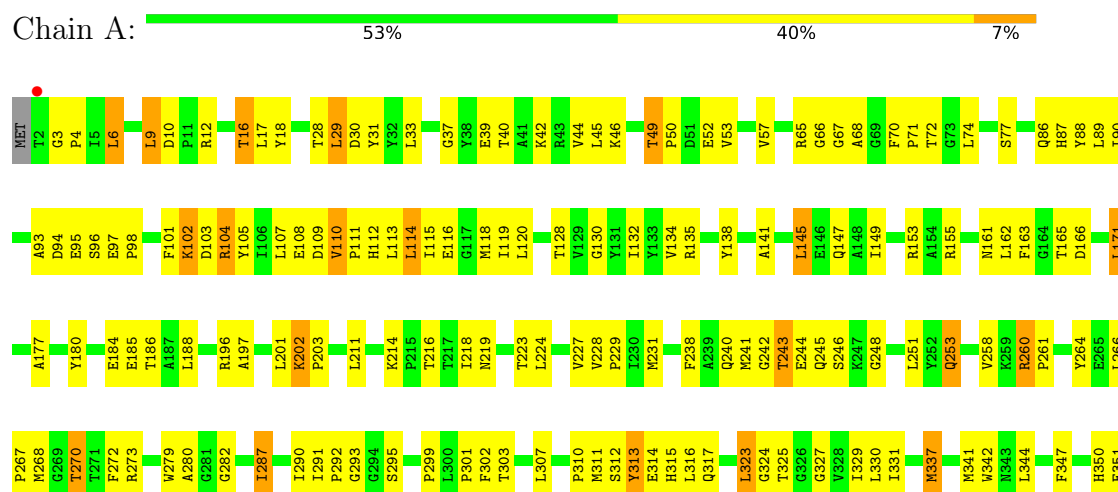
3 Residue-property plots

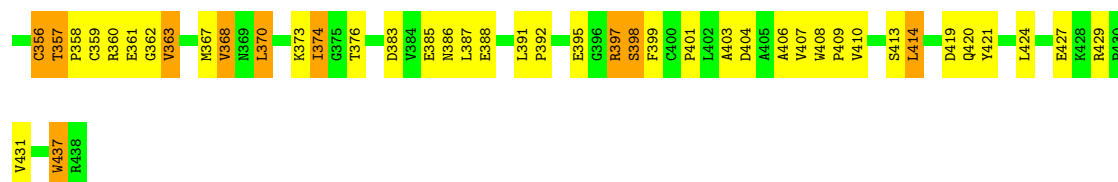
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADH-quinone oxidoreductase subunit 1



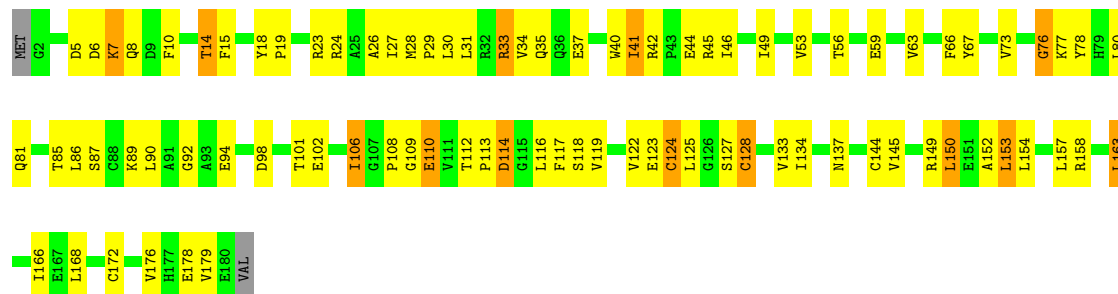
• Molecule 1: NADH-quinone oxidoreductase subunit 1





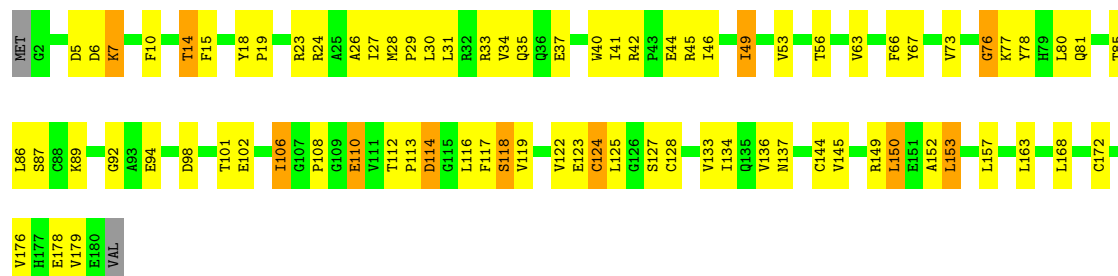
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 51% 40% 7%



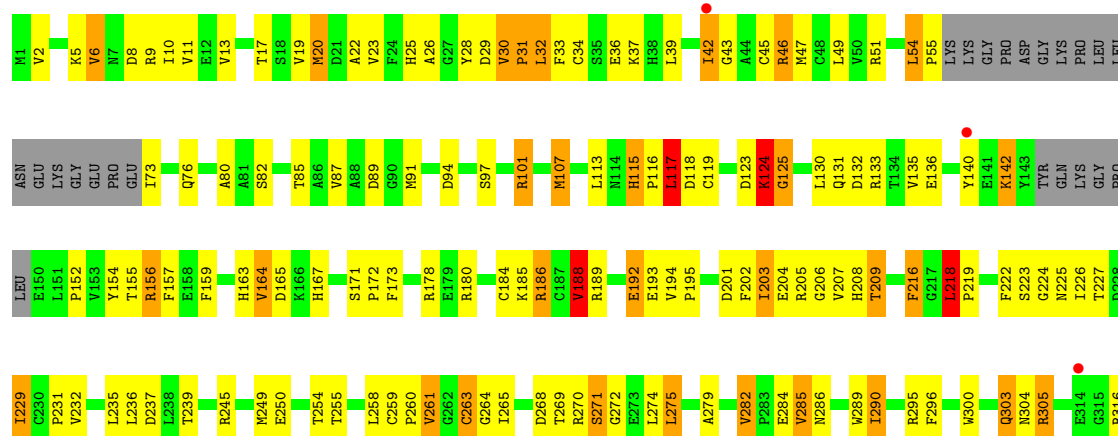
• Molecule 2: NADH-quinone oxidoreductase subunit 2

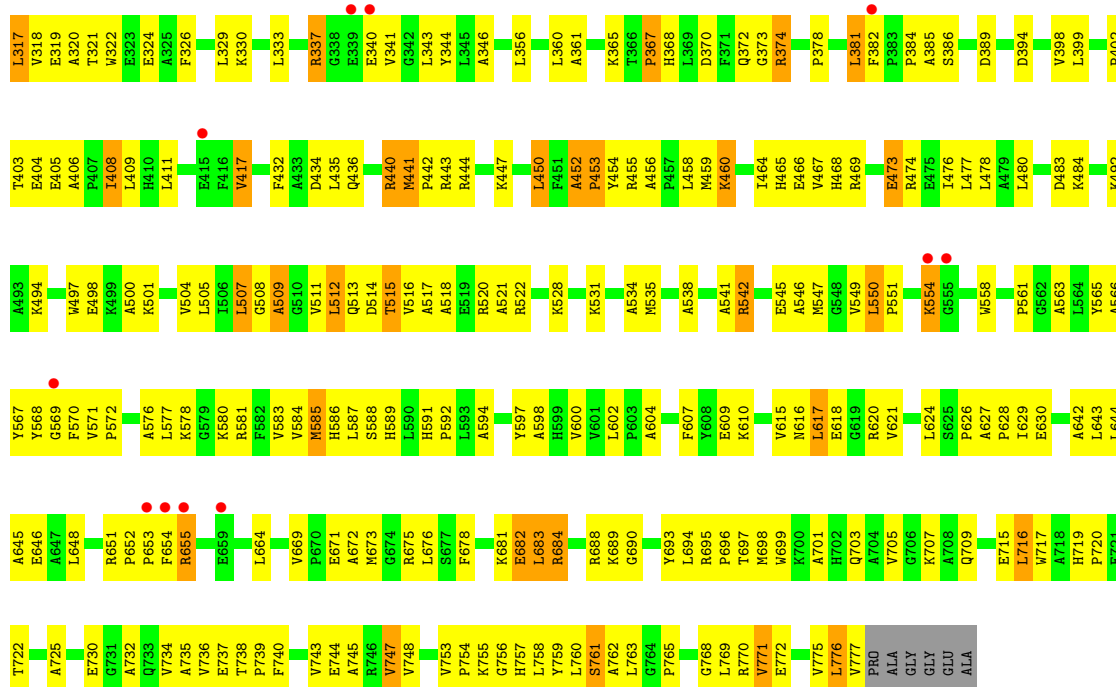
Chain B: 55% 38% 6%



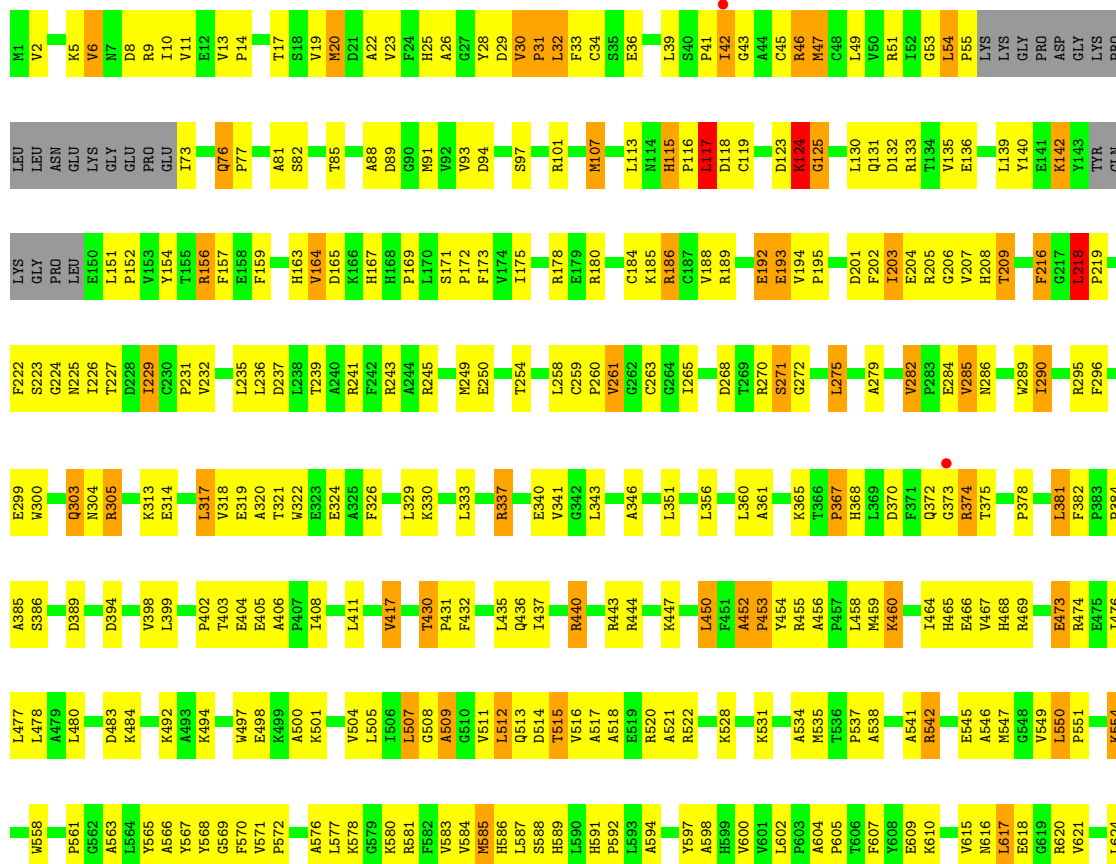
• Molecule 3: NADH-quinone oxidoreductase subunit 3

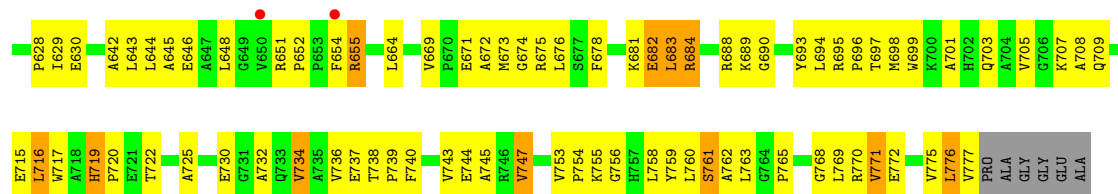
Chain 3: 47% 41% 8%



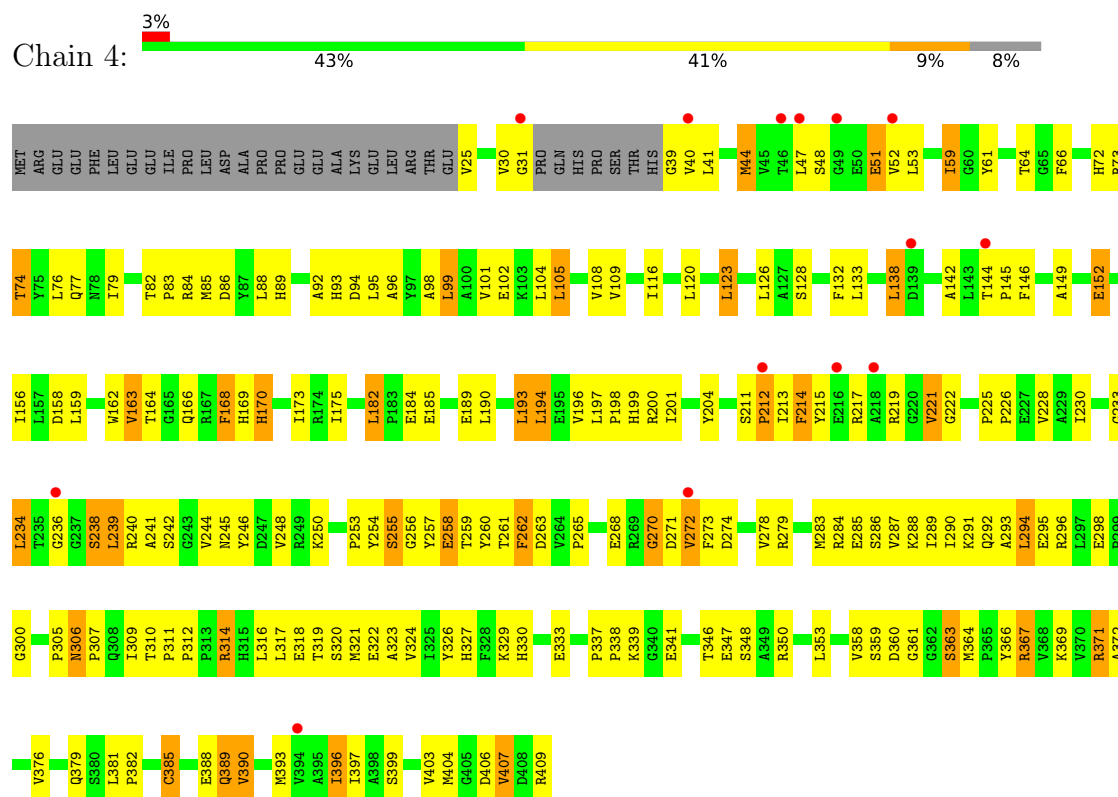


• Molecule 3: NADH-quinone oxidoreductase subunit 3

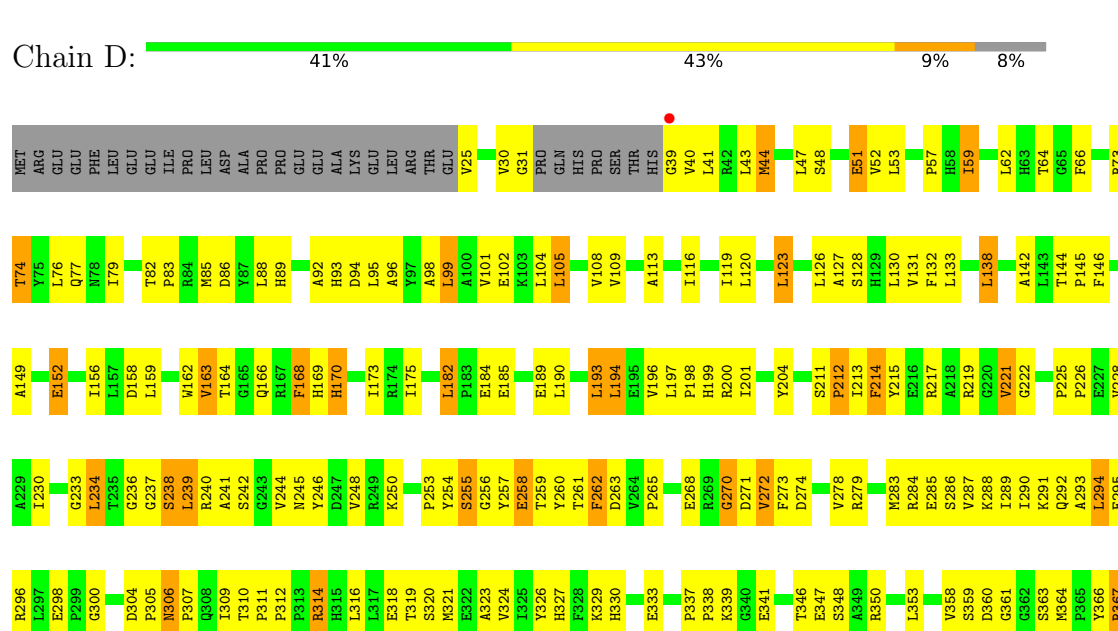




• Molecule 4: NADH-quinone oxidoreductase subunit 4

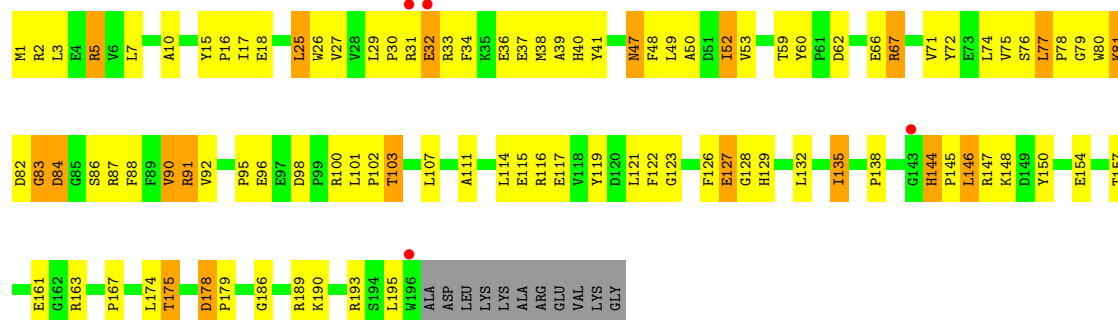


• Molecule 4: NADH-quinone oxidoreductase subunit 4

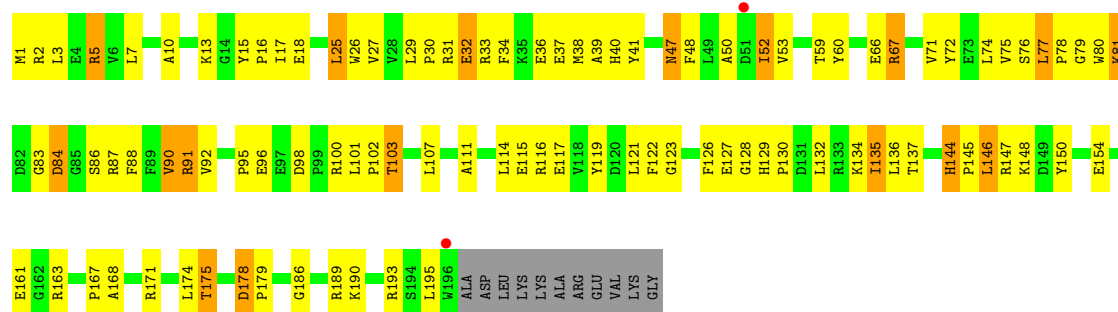




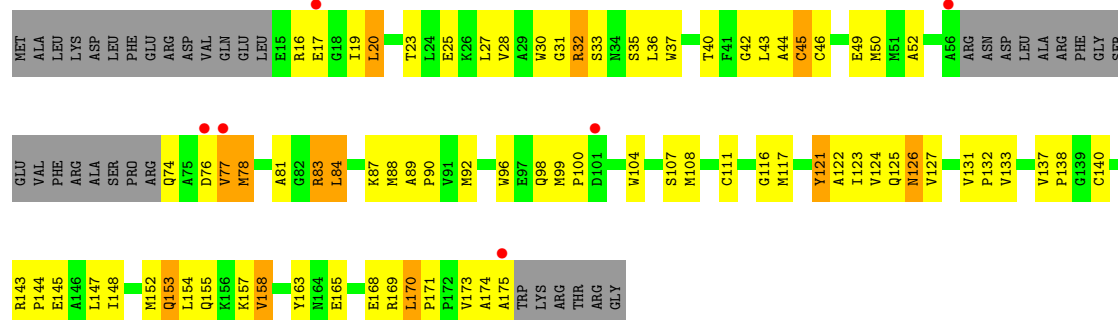
• Molecule 5: NADH-quinone oxidoreductase subunit 5



• Molecule 5: NADH-quinone oxidoreductase subunit 5

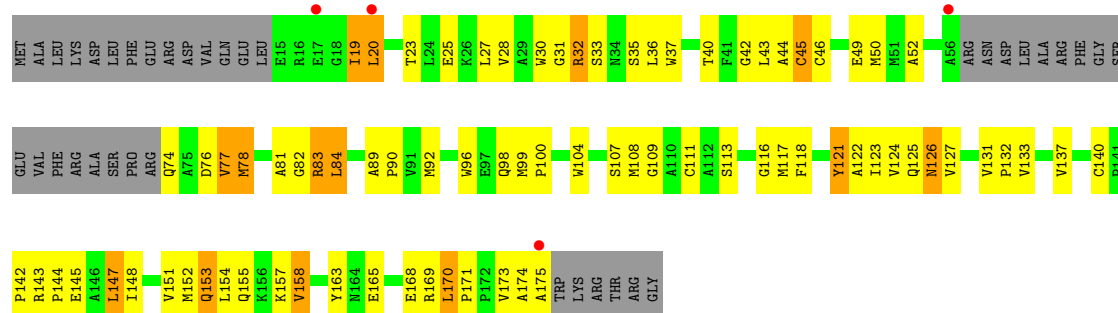


• Molecule 6: NADH-quinone oxidoreductase subunit 6

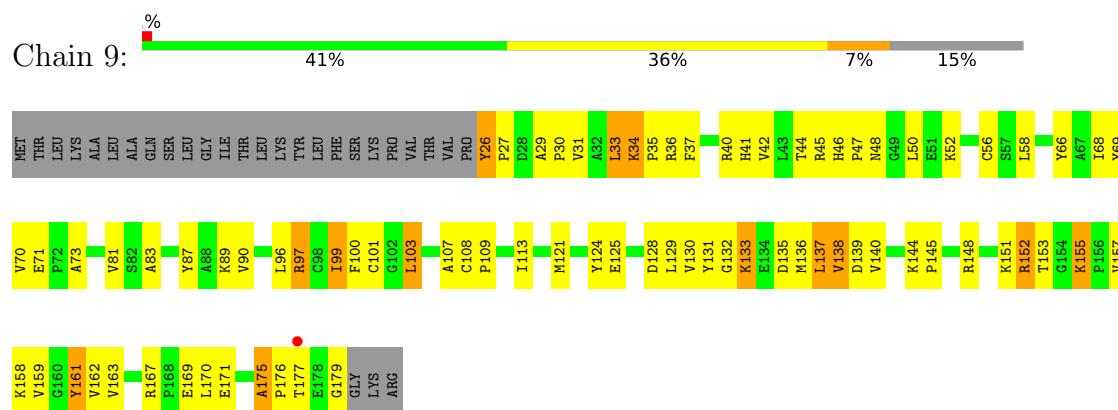


• Molecule 6: NADH-quinone oxidoreductase subunit 6

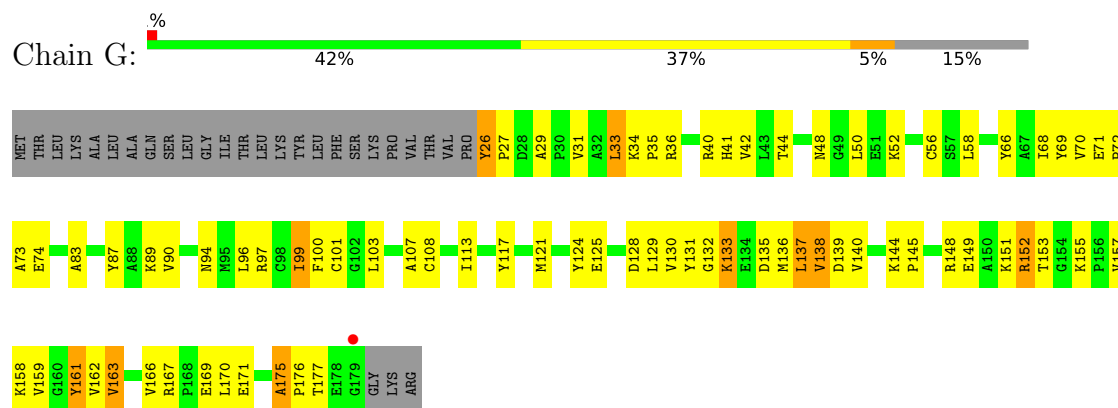




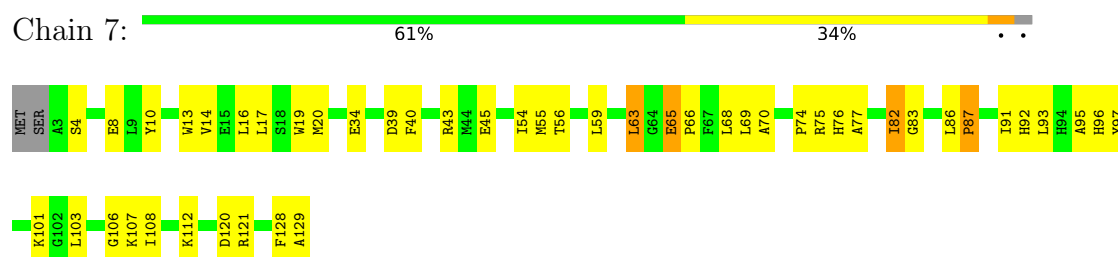
- Molecule 7: NADH-quinone oxidoreductase subunit 9



- Molecule 7: NADH-quinone oxidoreductase subunit 9



- Molecule 8: NADH-quinone oxidoreductase subunit 15



- Molecule 8: NADH-quinone oxidoreductase subunit 15



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.00Å 151.01Å 216.62Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	29.57 – 3.10 29.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.57-3.10) 89.8 (29.57-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.11Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.262 0.226 , 0.257	Depositor DCC
R_{free} test set	2215 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	37606	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, FES, SF4, CA, FMN, MG

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	1	0.58	0/3506	1.00	17/4745 (0.4%)
1	A	0.54	0/3506	0.99	14/4745 (0.3%)
2	2	0.55	0/1443	1.03	8/1958 (0.4%)
2	B	0.50	0/1443	1.06	9/1958 (0.5%)
3	3	0.57	1/6019 (0.0%)	0.99	19/8163 (0.2%)
3	C	0.50	0/6019	0.96	24/8163 (0.3%)
4	4	0.55	0/3096	0.93	8/4207 (0.2%)
4	D	0.49	0/3096	0.92	8/4207 (0.2%)
5	5	0.56	0/1656	1.03	13/2246 (0.6%)
5	E	0.48	0/1656	1.04	12/2246 (0.5%)
6	6	0.61	0/1126	1.05	5/1528 (0.3%)
6	F	0.55	0/1126	1.03	5/1528 (0.3%)
7	9	0.59	0/1224	1.10	8/1663 (0.5%)
7	G	0.54	0/1224	1.08	5/1663 (0.3%)
8	7	0.55	0/1059	0.99	3/1429 (0.2%)
8	H	0.53	0/1059	1.00	4/1429 (0.3%)
All	All	0.54	1/38258 (0.0%)	0.99	162/51878 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	188	VAL	CA-CB	5.53	1.60	1.54

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	115	HIS	CA-C-N	11.55	130.99	118.97
3	3	115	HIS	C-N-CA	11.55	130.99	118.97
3	3	218	LEU	CA-C-N	11.52	131.95	119.28
3	3	218	LEU	C-N-CA	11.52	131.95	119.28
3	C	218	LEU	CA-C-N	11.31	131.72	119.28

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	1	3417	0	3388	180	1
1	A	3417	0	3388	177	0
2	2	1410	0	1376	74	0
2	B	1410	0	1376	68	0
3	3	5880	0	5911	366	1
3	C	5880	0	5911	383	0
4	4	3018	0	3009	203	0
4	D	3018	0	3009	220	0
5	5	1607	0	1574	99	0
5	E	1607	0	1574	99	0
6	6	1102	0	1108	87	0
6	F	1102	0	1108	85	0
7	9	1193	0	1160	66	0
7	G	1193	0	1160	74	0
8	7	1031	0	1029	42	0
8	H	1031	0	1029	42	0
9	1	8	0	0	0	0
9	3	24	0	0	3	0
9	6	8	0	0	1	0
9	9	16	0	0	2	0
9	A	8	0	0	0	0
9	C	24	0	0	3	0
9	F	8	0	0	2	0
9	G	16	0	0	1	0
10	1	31	0	19	6	0
10	A	31	0	19	0	0
11	1	44	0	27	4	0
11	A	44	0	27	7	0
12	1	1	0	0	0	0
12	2	1	0	0	0	0
12	3	2	0	0	0	0
12	4	1	0	0	0	0
12	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	1	0	0	0	0
12	C	2	0	0	0	0
12	E	1	0	0	0	0
13	2	4	0	0	0	0
13	3	4	0	0	1	0
13	B	4	0	0	1	0
13	C	4	0	0	1	0
14	7	1	0	0	0	0
14	H	1	0	0	0	0
All	All	37606	0	37202	2093	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 2093 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:104:ARG:HH21	2:B:127:SER:HB3	1.09	1.17
3:3:474:ARG:HH21	3:3:516:VAL:HG21	1.03	1.17
6:6:83:ARG:HH11	6:6:83:ARG:HG3	1.13	1.13
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.04	1.12
3:3:11:VAL:HG11	3:3:25:HIS:HD2	1.16	1.11

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:427:GLU:O	3:3:316:ARG:NH1[2_545]	2.12	0.08

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	1	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	7	30
1	A	435/438 (99%)	379 (87%)	50 (12%)	6 (1%)	9	34
2	2	177/181 (98%)	152 (86%)	21 (12%)	4 (2%)	5	23
2	B	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	5	23
3	3	748/783 (96%)	624 (83%)	100 (13%)	24 (3%)	3	18
3	C	748/783 (96%)	626 (84%)	98 (13%)	24 (3%)	3	18
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	4	22
4	D	374/409 (91%)	332 (89%)	32 (9%)	10 (3%)	4	20
5	5	194/207 (94%)	167 (86%)	23 (12%)	4 (2%)	5	25
5	E	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	5	25
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	2	16
6	F	140/181 (77%)	113 (81%)	21 (15%)	6 (4%)	2	12
7	9	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	18	49
7	G	152/182 (84%)	132 (87%)	19 (12%)	1 (1%)	18	49
8	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	16	47
8	H	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	16	47
All	All	4690/5020 (93%)	4019 (86%)	560 (12%)	111 (2%)	4	22

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE

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	1	355/356 (100%)	316 (89%)	39 (11%)	6	24
1	A	355/356 (100%)	321 (90%)	34 (10%)	8	30
2	2	150/152 (99%)	129 (86%)	21 (14%)	3	15
2	B	150/152 (99%)	129 (86%)	21 (14%)	3	15
3	3	607/628 (97%)	553 (91%)	54 (9%)	9	33
3	C	607/628 (97%)	553 (91%)	54 (9%)	9	33
4	4	326/355 (92%)	287 (88%)	39 (12%)	5	21
4	D	326/355 (92%)	289 (89%)	37 (11%)	5	23
5	5	167/175 (95%)	151 (90%)	16 (10%)	8	30
5	E	167/175 (95%)	152 (91%)	15 (9%)	9	33
6	6	117/149 (78%)	104 (89%)	13 (11%)	6	24
6	F	117/149 (78%)	104 (89%)	13 (11%)	6	24
7	9	126/150 (84%)	110 (87%)	16 (13%)	4	18
7	G	126/150 (84%)	111 (88%)	15 (12%)	5	21
8	7	104/106 (98%)	99 (95%)	5 (5%)	23	54
8	H	104/106 (98%)	99 (95%)	5 (5%)	23	54
All	All	3904/4142 (94%)	3507 (90%)	397 (10%)	7	28

5 of 397 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	ARG
3	C	408	ILE
2	B	7	LYS
3	C	42	ILE
3	C	617	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	ASN
4	D	292	GLN
3	C	38	HIS
3	C	757	HIS
4	D	330	HIS

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 ⓘ

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	FMN	1	440	-	33,33,33	1.24	2 (6%)	48,50,50	1.88	12 (25%)
9	SF4	9	184	7	0,12,12	-	-	-		
9	SF4	A	439	1	0,12,12	-	-	-		
9	SF4	C	785	3	0,12,12	-	-	-		
13	FES	B	182	2	0,4,4	-	-	-		
13	FES	C	787	3	0,4,4	-	-	-		
13	FES	2	182	2	0,4,4	-	-	-		
13	FES	3	787	3	0,4,4	-	-	-		
9	SF4	6	182	6	0,12,12	-	-	-		
9	SF4	F	182	6	0,12,12	-	-	-		
9	SF4	G	184	7	0,12,12	-	-	-		
9	SF4	9	183	7	0,12,12	-	-	-		
9	SF4	3	784	3	0,12,12	-	-	-		
9	SF4	1	439	1	0,12,12	-	-	-		
9	SF4	C	786	3	0,12,12	-	-	-		
9	SF4	C	784	3	0,12,12	-	-	-		
11	NAI	1	441	-	47,48,48	3.97	32 (68%)	64,73,73	1.76	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SF4	3	786	3	0,12,12	-	-	-		
9	SF4	3	785	3	0,12,12	-	-	-		
10	FMN	A	440	-	33,33,33	1.10	3 (9%)	48,50,50	1.54	10 (20%)
11	NAI	A	441	-	47,48,48	4.08	31 (65%)	64,73,73	1.80	16 (25%)
9	SF4	G	183	7	0,12,12	-	-	-		

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
10	FMN	1	440	-	-	6/18/18/18	0/3/3/3
9	SF4	9	184	7	-	-	0/6/5/5
9	SF4	A	439	1	-	-	0/6/5/5
9	SF4	C	785	3	-	-	0/6/5/5
13	FES	B	182	2	-	-	0/1/1/1
13	FES	C	787	3	-	-	0/1/1/1
13	FES	2	182	2	-	-	0/1/1/1
13	FES	3	787	3	-	-	0/1/1/1
9	SF4	6	182	6	-	-	0/6/5/5
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
9	SF4	9	183	7	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5
11	NAI	1	441	-	-	7/29/72/72	0/5/5/5
9	SF4	3	786	3	-	-	0/6/5/5
10	FMN	A	440	-	-	8/18/18/18	0/3/3/3
9	SF4	3	785	3	-	-	0/6/5/5
11	NAI	A	441	-	-	10/29/72/72	0/5/5/5
9	SF4	G	183	7	-	-	0/6/5/5

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	441	NAI	C2A-N1A	11.91	1.55	1.33
11	A	441	NAI	C2A-N1A	11.78	1.54	1.33
11	A	441	NAI	PA-O3	8.55	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	441	NAI	C5A-N7A	7.92	1.53	1.39
11	1	441	NAI	PA-O3	7.67	1.67	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	441	NAI	N3A-C2A-N1A	-5.55	120.18	128.58
10	1	440	FMN	O2'-C2'-C3'	5.24	121.52	109.25
10	1	440	FMN	C5'-C4'-C3'	-5.23	102.34	112.22
11	1	441	NAI	N3A-C2A-N1A	-4.89	121.18	128.58
11	A	441	NAI	C5A-C4A-N3A	-4.83	120.06	126.72

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1	440	FMN	N10-C1'-C2'-O2'
10	1	440	FMN	N10-C1'-C2'-C3'
10	1	440	FMN	C1'-C2'-C3'-O3'
10	1	440	FMN	C1'-C2'-C3'-C4'
10	A	440	FMN	N10-C1'-C2'-O2'

There are no ring outliers.

16 monomers are involved in 32 short contacts:

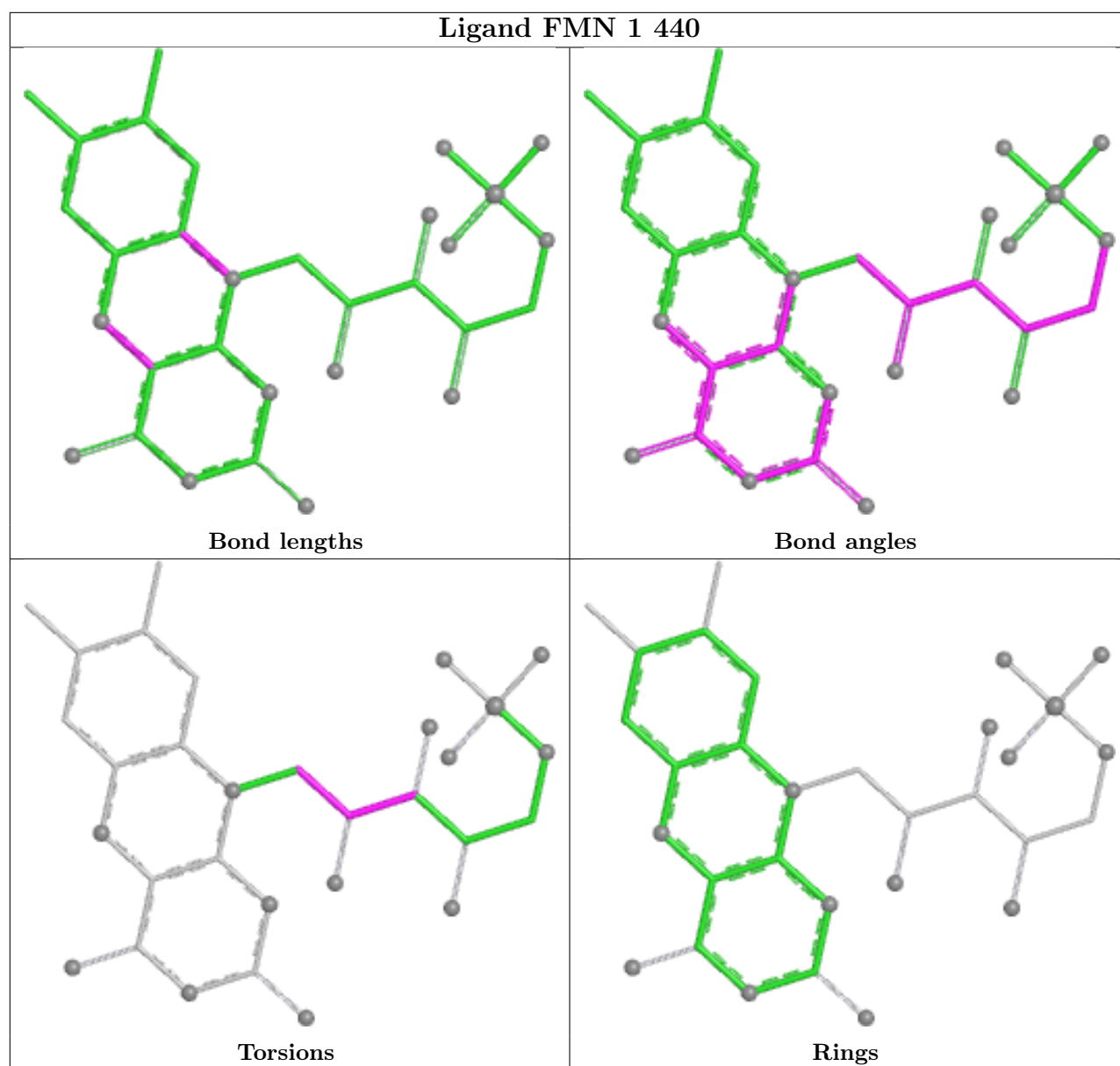
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	1	440	FMN	6	0
9	C	785	SF4	1	0
13	B	182	FES	1	0
13	C	787	FES	1	0
13	3	787	FES	1	0
9	6	182	SF4	1	0
9	F	182	SF4	2	0
9	9	183	SF4	2	0
9	3	784	SF4	1	0
9	C	786	SF4	1	0
9	C	784	SF4	1	0
11	1	441	NAI	4	0
9	3	786	SF4	1	0
9	3	785	SF4	1	0
11	A	441	NAI	7	0

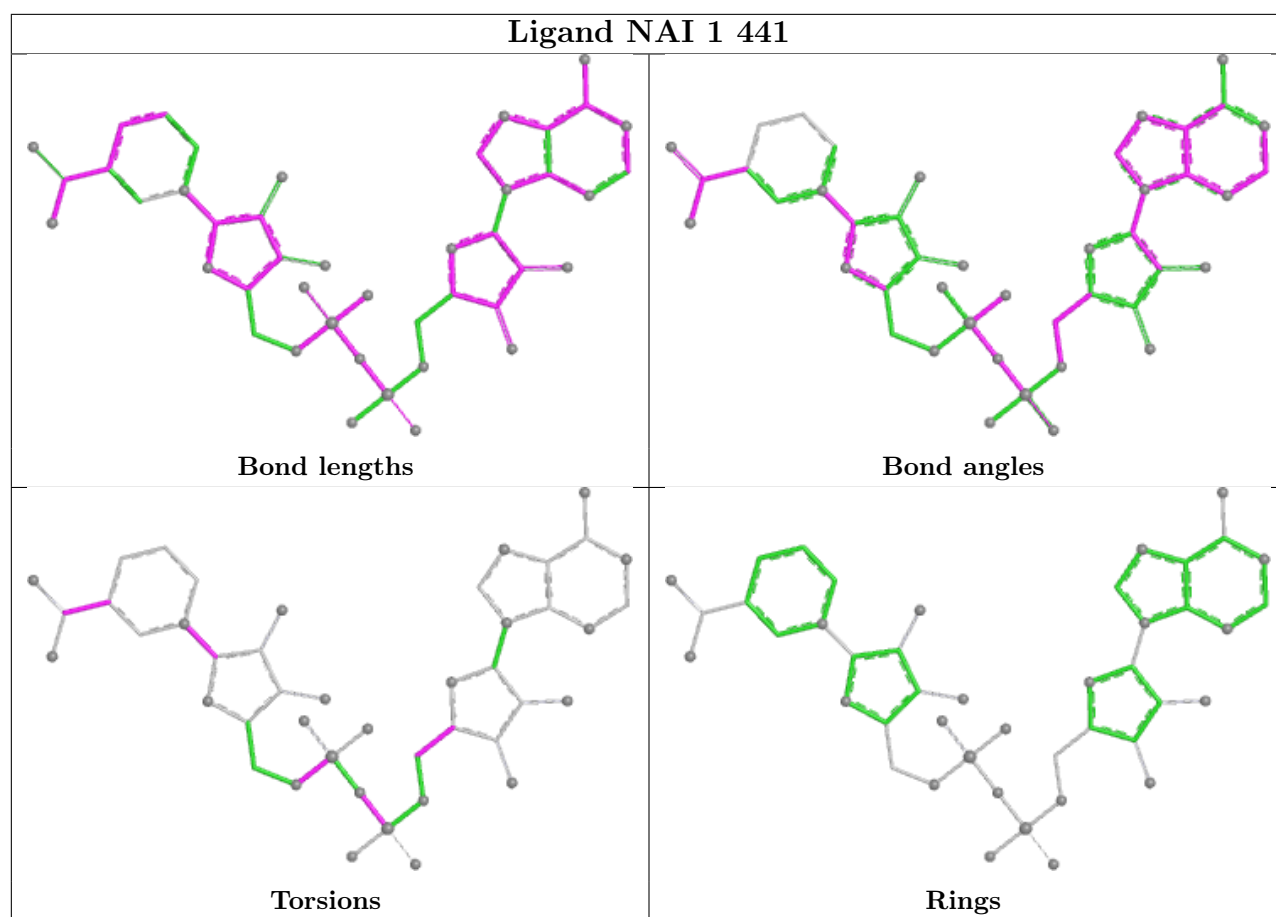
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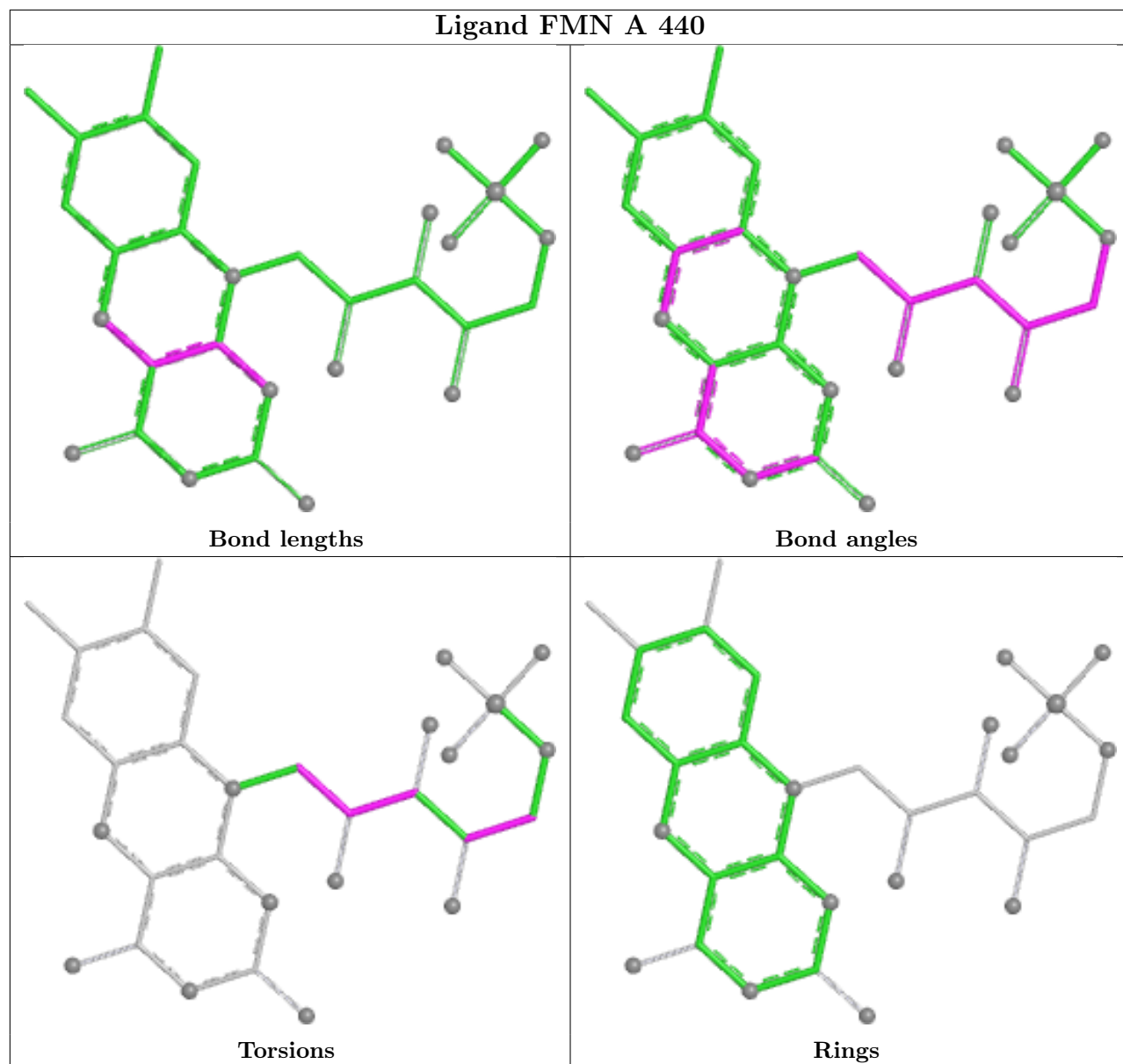
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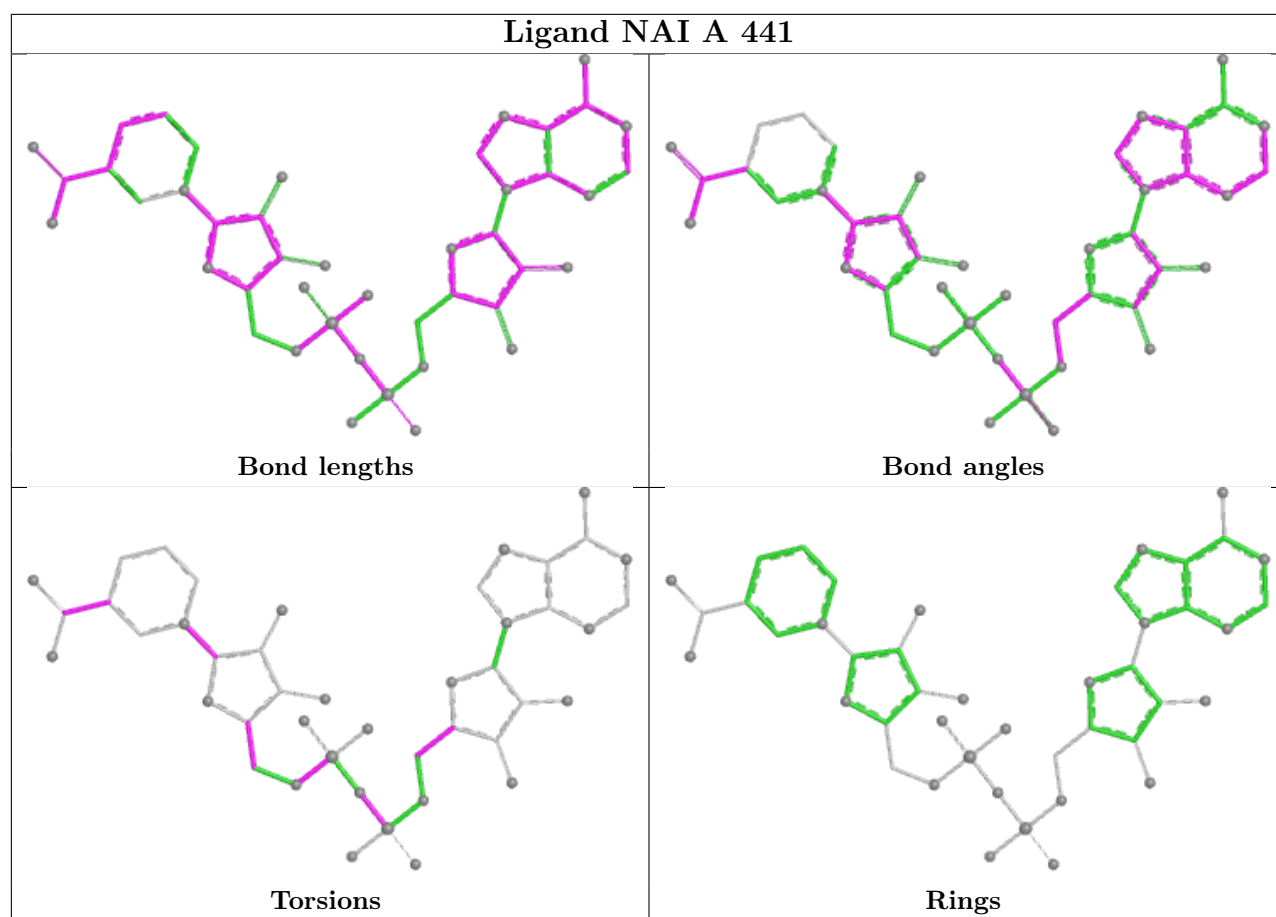
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	183	SF4	1	0

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	1	437/438 (99%)	-0.22	1 (0%) 91 83	28, 49, 71, 111	0
1	A	437/438 (99%)	-0.28	1 (0%) 91 83	29, 49, 72, 111	0
2	2	179/181 (98%)	-0.19	0 100 100	32, 48, 78, 118	0
2	B	179/181 (98%)	-0.25	0 100 100	33, 48, 79, 118	0
3	3	754/783 (96%)	0.21	14 (1%) 66 45	25, 68, 106, 126	0
3	C	754/783 (96%)	0.11	4 (0%) 87 73	26, 69, 107, 127	0
4	4	378/409 (92%)	0.27	14 (3%) 45 25	33, 66, 103, 119	0
4	D	378/409 (92%)	0.08	1 (0%) 90 80	33, 67, 103, 119	0
5	5	196/207 (94%)	0.55	4 (2%) 65 44	34, 66, 102, 116	0
5	E	196/207 (94%)	0.12	2 (1%) 79 61	35, 68, 103, 117	0
6	6	144/181 (79%)	0.38	6 (4%) 40 22	36, 62, 93, 135	0
6	F	144/181 (79%)	0.22	4 (2%) 55 34	37, 63, 93, 135	0
7	9	154/182 (84%)	-0.05	1 (0%) 85 70	30, 48, 86, 120	0
7	G	154/182 (84%)	-0.09	1 (0%) 85 70	31, 48, 86, 120	0
8	7	127/129 (98%)	-0.08	0 100 100	43, 55, 91, 115	0
8	H	127/129 (98%)	-0.13	1 (0%) 82 65	43, 56, 91, 114	0
All	All	4738/5020 (94%)	0.05	54 (1%) 78 59	25, 58, 101, 135	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	236	GLY	3.5
6	6	175	ALA	3.4
6	6	76	ASP	3.2
3	3	654	PHE	3.1
3	3	554	LYS	3.0

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
12	MG	C	789	1/1	0.88	0.09	44,44,44,44	0
12	MG	A	442	1/1	0.90	0.12	54,54,54,54	0
12	MG	E	208	1/1	0.90	0.14	44,44,44,44	0
12	MG	3	789	1/1	0.91	0.17	42,42,42,42	0
11	NAI	A	441	44/44	0.91	0.10	45,59,68,71	0
10	FMN	A	440	31/31	0.93	0.10	39,44,47,51	0
10	FMN	1	440	31/31	0.93	0.11	34,42,46,48	0
12	MG	2	206	1/1	0.94	0.06	32,32,32,32	0
11	NAI	1	441	44/44	0.94	0.09	39,50,62,65	0
12	MG	4	410	1/1	0.94	0.23	59,59,59,59	0
12	MG	5	208	1/1	0.96	0.13	26,26,26,26	0
12	MG	1	442	1/1	0.97	0.18	40,40,40,40	0
12	MG	3	788	1/1	0.98	0.17	23,23,23,23	0
12	MG	C	788	1/1	0.98	0.19	35,35,35,35	0
14	CA	H	204	1/1	0.98	0.12	32,32,32,32	0
9	SF4	6	182	8/8	0.99	0.04	0,23,42,50	0
9	SF4	9	183	8/8	0.99	0.04	2,19,36,39	0
9	SF4	9	184	8/8	0.99	0.04	8,12,33,34	0
9	SF4	A	439	8/8	0.99	0.04	0,22,31,38	0
9	SF4	C	785	8/8	0.99	0.03	10,13,29,33	0
9	SF4	C	786	8/8	0.99	0.05	19,27,45,47	0
9	SF4	F	182	8/8	0.99	0.05	22,32,48,55	0
9	SF4	G	183	8/8	0.99	0.04	11,15,32,36	0
9	SF4	G	184	8/8	0.99	0.05	13,20,37,39	0
9	SF4	1	439	8/8	0.99	0.04	0,12,24,25	0
9	SF4	3	784	8/8	0.99	0.03	0,9,26,36	0
13	FES	2	182	4/4	0.99	0.05	11,20,27,33	0

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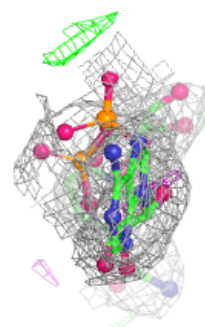
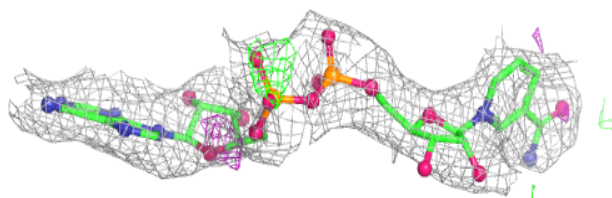
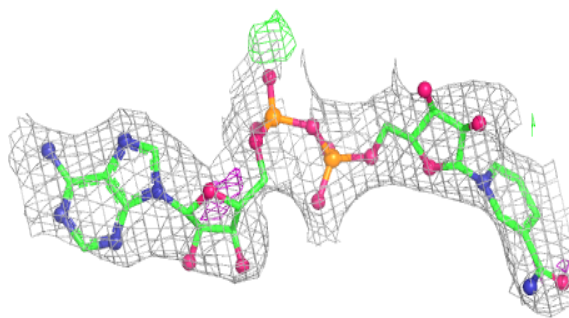
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	FES	3	787	4/4	0.99	0.05	9,14,30,34	0
13	FES	B	182	4/4	0.99	0.04	22,22,37,45	0
13	FES	C	787	4/4	0.99	0.05	19,26,32,33	0
14	CA	7	204	1/1	0.99	0.11	36,36,36,36	0
9	SF4	3	786	8/8	0.99	0.04	3,15,43,48	0
9	SF4	C	784	8/8	1.00	0.03	6,11,31,36	0
9	SF4	3	785	8/8	1.00	0.02	0,11,22,22	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.

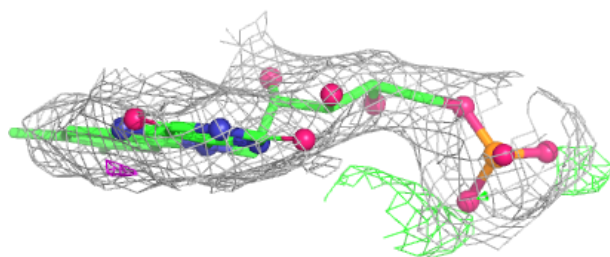
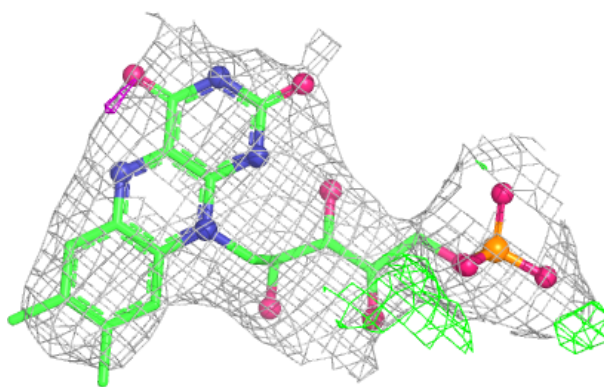
Electron density around NAI A 441:

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

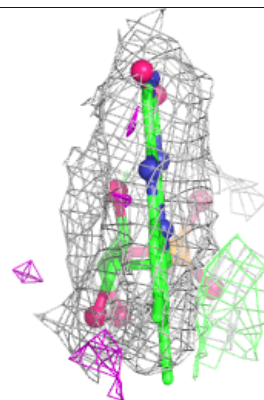
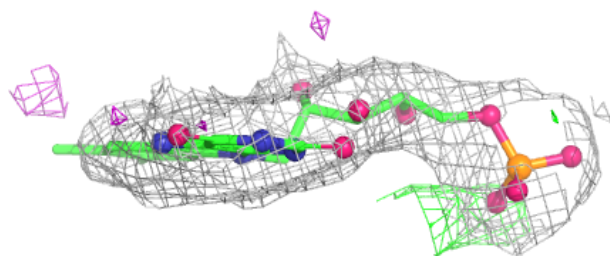
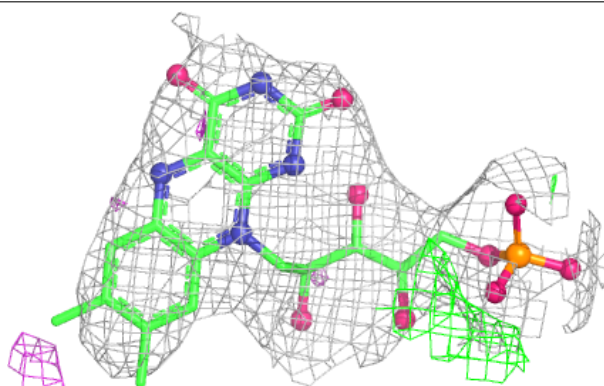


Electron density around FMN A 440:

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

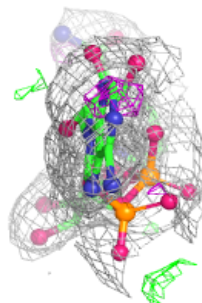
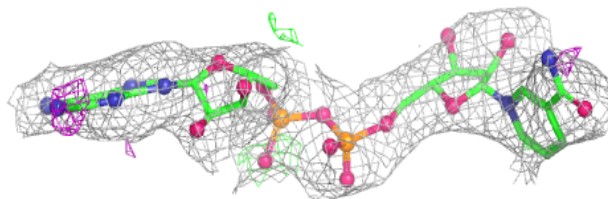
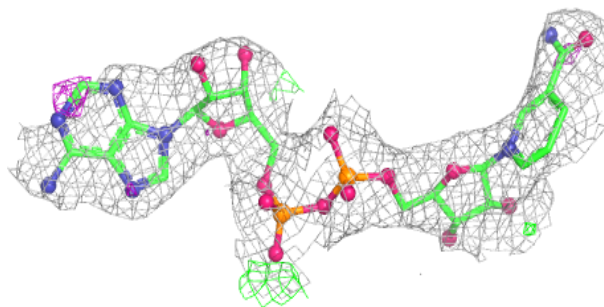
**Electron density around FMN 1 440:**

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



Electron density around NAI 1 441:

$2mF_o-DF_c$ (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.