



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 07:17 pm BST

PDB ID : 3I9V
Title : Crystal structure of the hydrophilic domain of respiratory complex I from *Thermus thermophilus*, oxidized, 2 mol/ASU
Authors : Sazanov, L.A.; Berrisford, J.M.
Deposited on : 2009-07-13
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

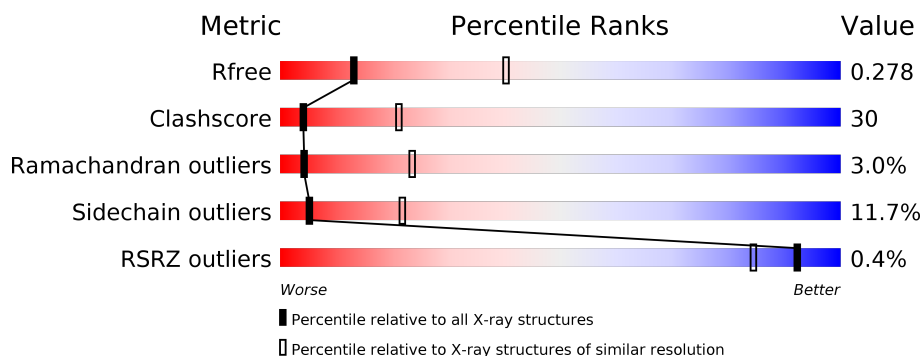
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.




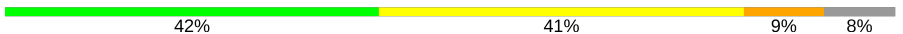
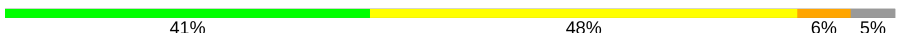

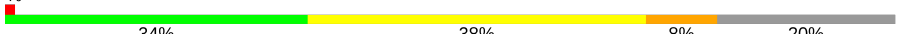




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	1	438	<div> <div>51%</div> <div>41%</div> <div>8%</div> </div>
1	A	438	<div> <div>51%</div> <div>42%</div> <div>7%</div> </div>
2	2	181	<div> <div>%</div> <div>58%</div> <div>29%</div> <div>11%</div> <div>••</div> </div>
2	B	181	<div> <div>57%</div> <div>30%</div> <div>11%</div> <div>••</div> </div>
3	3	783	<div> <div>46%</div> <div>43%</div> <div>7%</div> <div>•</div> </div>
3	C	783	<div> <div>%</div> <div>44%</div> <div>45%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
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	1	439	-	-	X	-
9	SF4	3	784	-	-	X	-
9	SF4	3	786	-	-	X	-
9	SF4	6	182	-	-	X	-
9	SF4	C	784	-	-	X	-
9	SF4	C	786	-	-	X	-
9	SF4	F	182	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 37520 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	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	B	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	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	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	D	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	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	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	F	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			

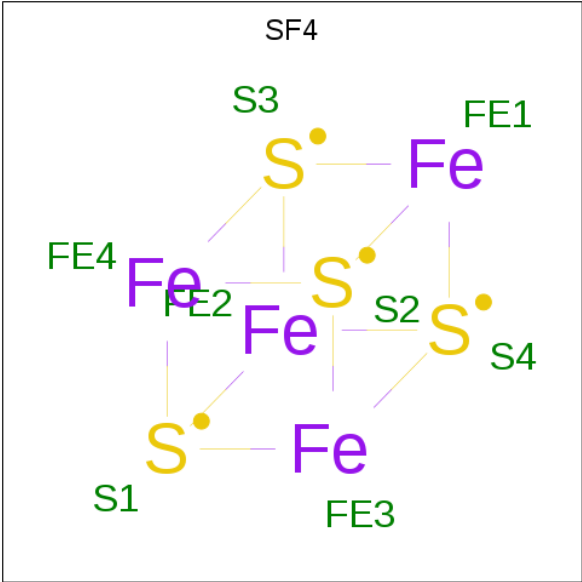
- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

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 (three-letter code: 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		

-
- The diagram illustrates the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system (rings C4A, C5A, C8A, C9A) with nitrogen atoms N1, N3, N5, and N10. The ring is substituted with a ribitol chain at N10 (C1', C2', C3', C4', C5') and a phosphate group at C5'. The ribitol chain has hydroxyl groups at C2' (O2'), C3' (O3'), and C4' (O4'). The phosphate group is represented by a phosphorus atom (P) double-bonded to an oxygen (O1P) and single-bonded to three hydroxyl groups (O2P, O3P, O5'). The ribitol chain is shown with stereochemistry: C2' and C4' are on wedges, C3' is on a dash, and C5' is on a wedge. The ribitol chain is connected to the isoalloxazine ring at N10 (C1'). The isoalloxazine ring is substituted with a ribitol chain at N10 (C1', C2', C3', C4', C5') and a phosphate group at C5'. The ribitol chain has hydroxyl groups at C2' (O2'), C3' (O3'), and C4' (O4'). The phosphate group is represented by a phosphorus atom (P) double-bonded to an oxygen (O1P) and single-bonded to three hydroxyl groups (O2P, O3P, O5'). The ribitol chain is shown with stereochemistry: C2' and C4' are on wedges, C3' is on a dash, and C5' is on a wedge. The ribitol chain is connected to the isoalloxazine ring at N10 (C1').

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

-
- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square arrangement of two iron (Fe) and two sulfur (S) atoms. The atoms are labeled S1, FE2, FE1, and S2. The connections are as follows:
- S1 (top-left, yellow) is connected to FE2 (top-right, purple) by a horizontal line.
 - FE2 (top-right, purple) is connected to S2 (bottom-right, yellow) by a vertical line.
 - S2 (bottom-right, yellow) is connected to FE1 (bottom-left, purple) by a horizontal line.
 - FE1 (bottom-left, purple) is connected to S1 (top-left, yellow) by a vertical line.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	2	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	3	1	Total 4	Fe 2	S 2	0	0
11	B	1	Total 4	Fe 2	S 2	0	0
11	C	1	Total 4	Fe 2	S 2	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	1	Total 1	Mn 1	0	0
12	E	1	Total 1	Mn 1	0	0
12	H	1	Total 1	Mn 1	0	0
12	C	2	Total 2	Mn 2	0	0
12	7	1	Total 1	Mn 1	0	0
12	4	2	Total 2	Mn 2	0	0
12	5	1	Total 1	Mn 1	0	0
12	2	1	Total 1	Mn 1	0	0
12	3	2	Total 2	Mn 2	0	0

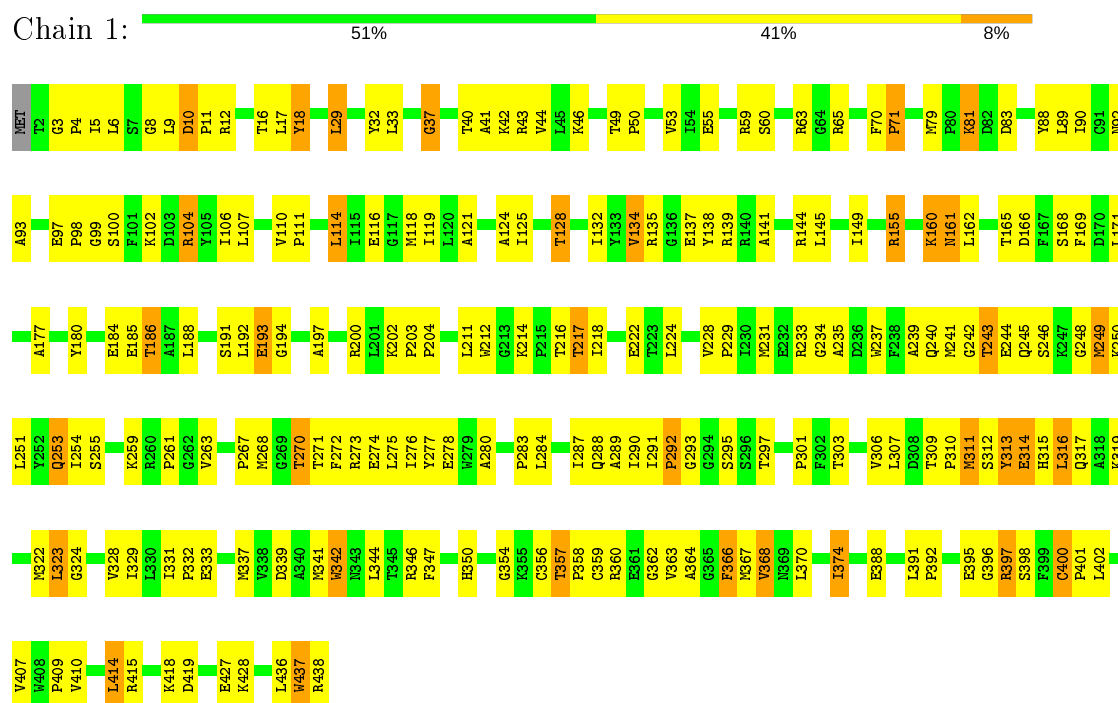
- Molecule 13 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	3	1	Total 1	Ca 1	0	0
13	C	1	Total 1	Ca 1	0	0

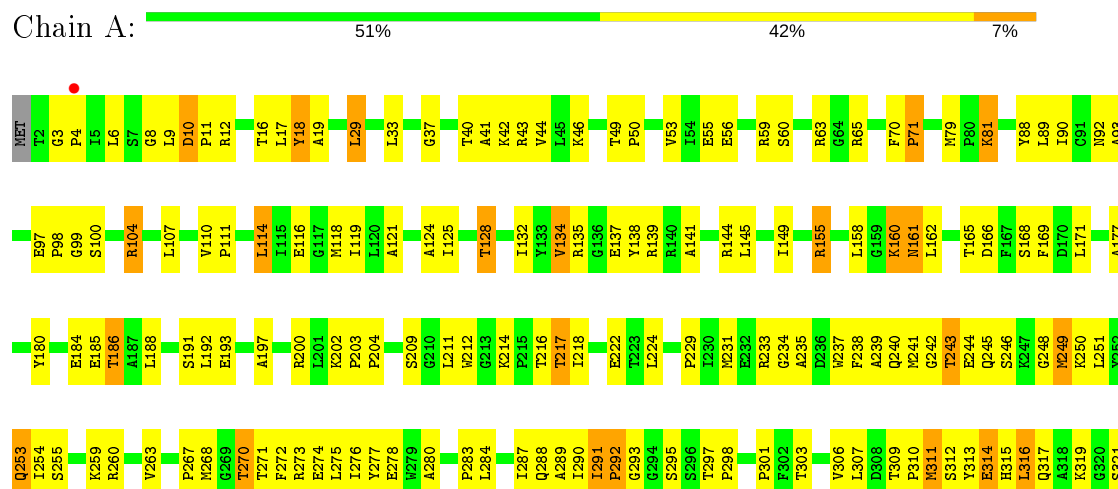
3 Residue-property plots

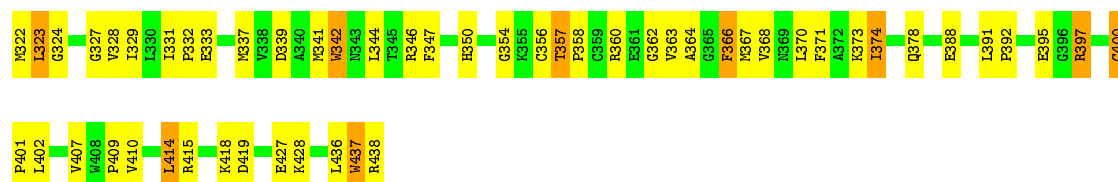
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADH-quinone oxidoreductase subunit 1

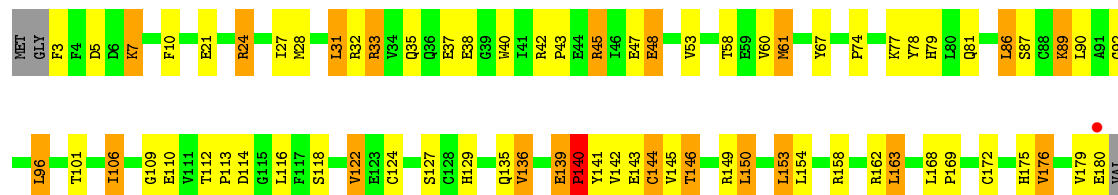


- Molecule 1: NADH-quinone oxidoreductase subunit 1

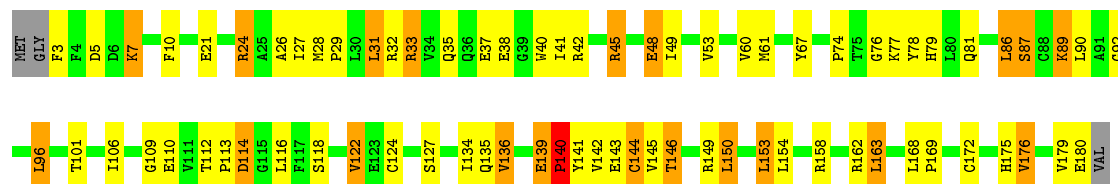




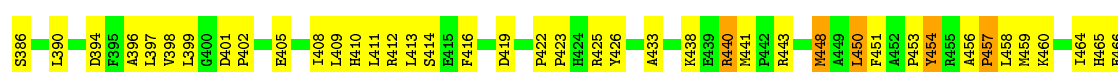
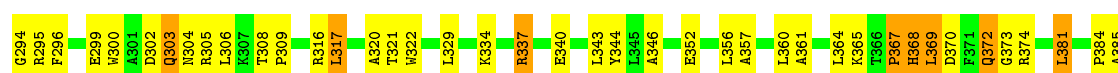
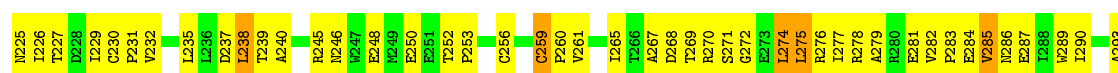
• Molecule 2: NADH-quinone oxidoreductase subunit 2

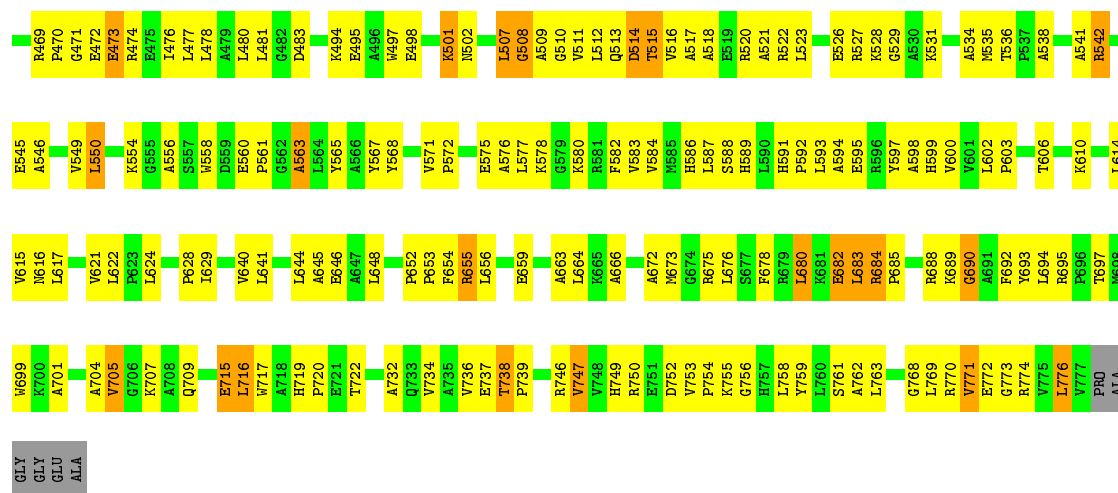


• Molecule 2: NADH-quinone oxidoreductase subunit 2

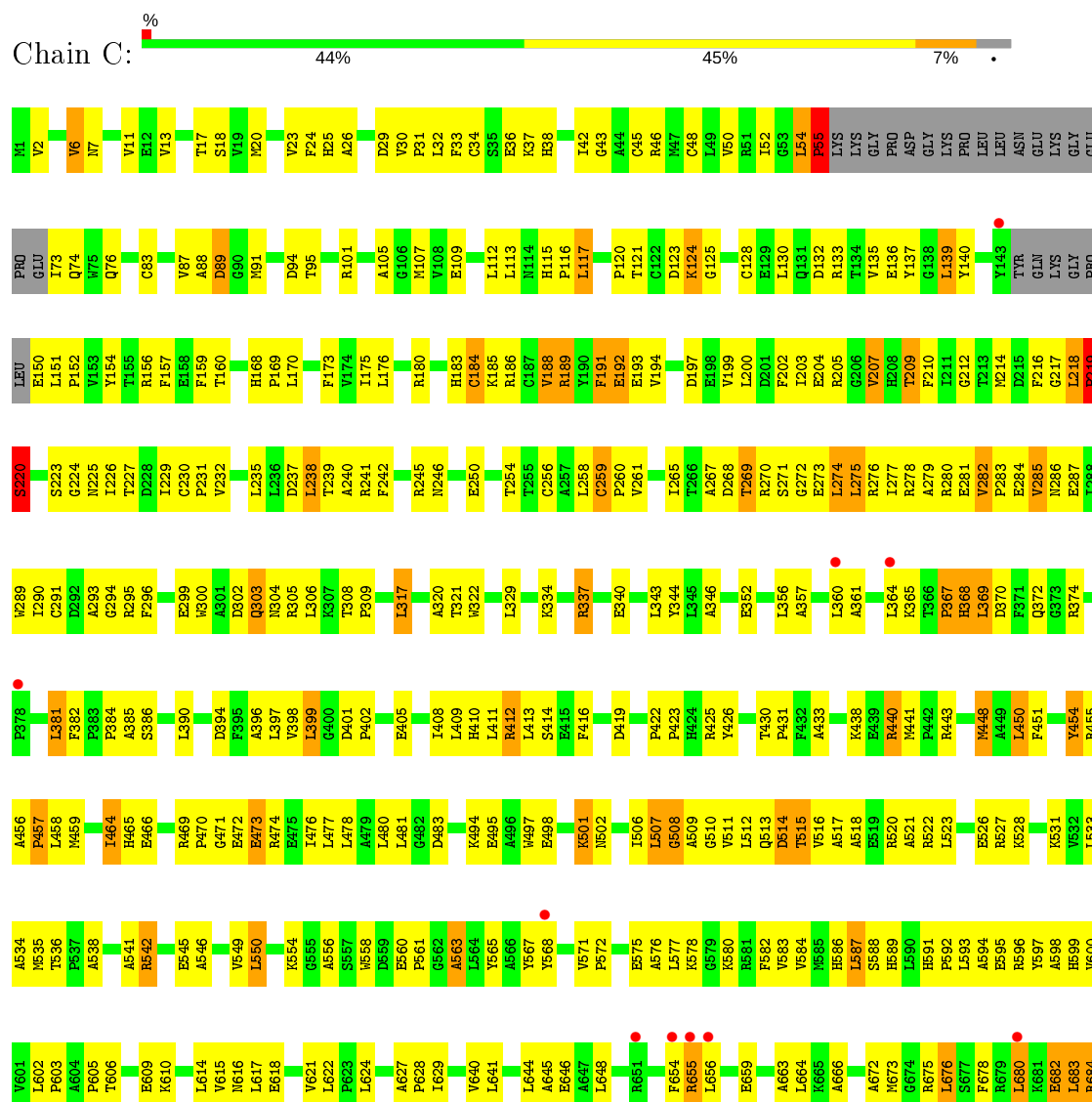


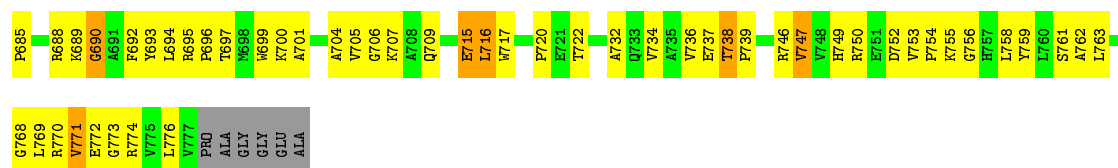
• Molecule 3: NADH-quinone oxidoreductase subunit 3



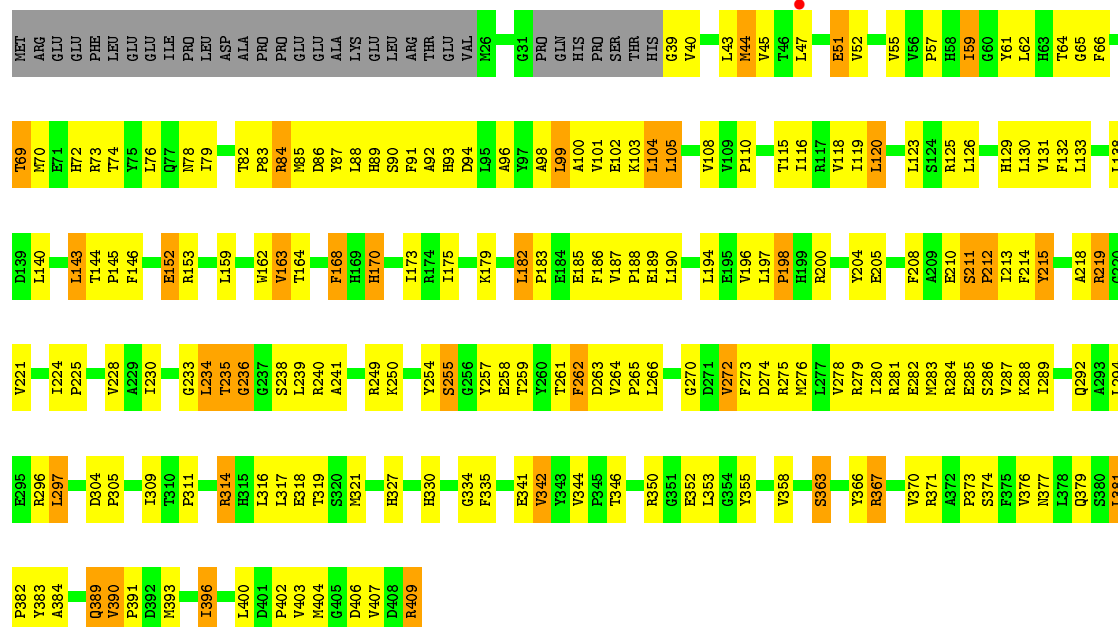


• Molecule 3: NADH-quinone oxidoreductase subunit 3

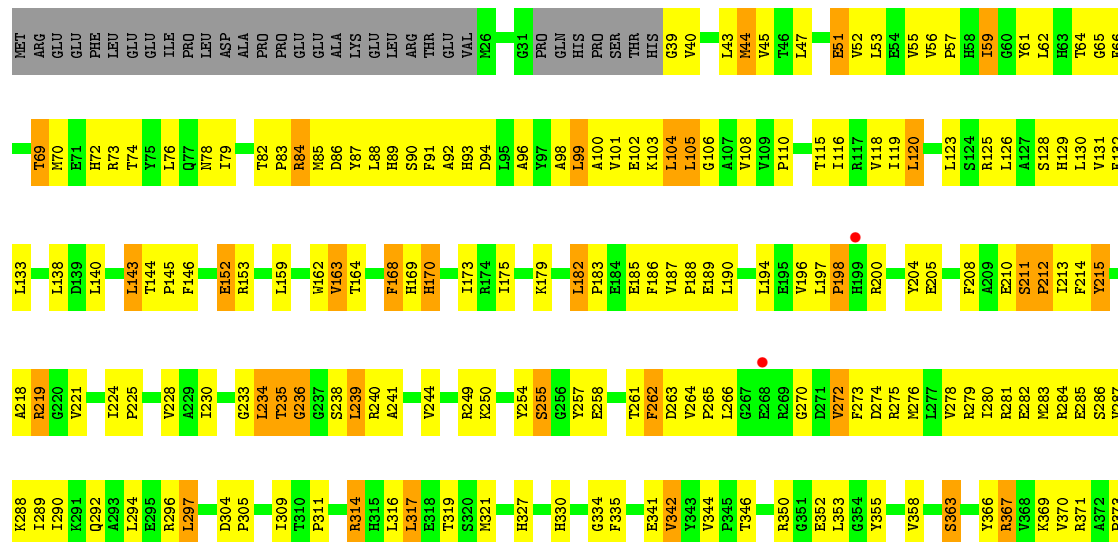




• Molecule 4: NADH-quinone oxidoreductase subunit 4



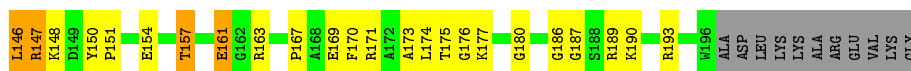
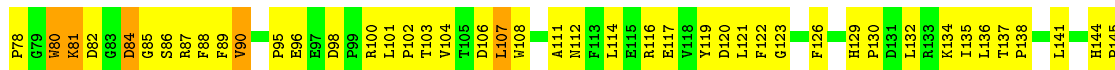
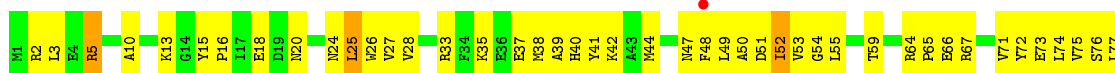
• Molecule 4: NADH-quinone oxidoreductase subunit 4





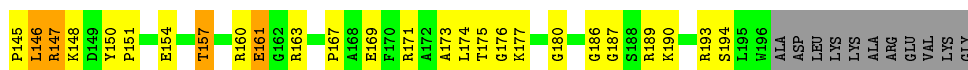
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 41% 48% 6% 5%



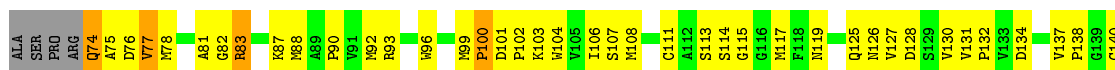
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain E: 40% 49% 6% 5%



• Molecule 6: NADH-quinone oxidoreductase subunit 6

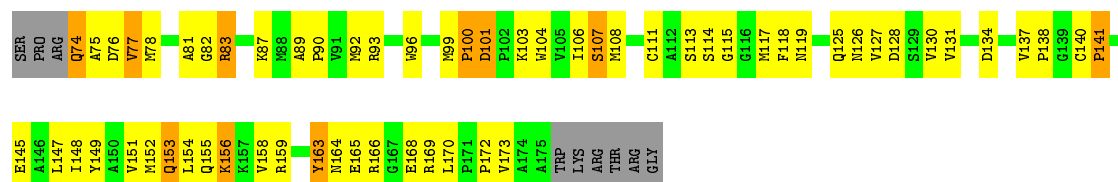
Chain 6: 34% 38% 8% 20%



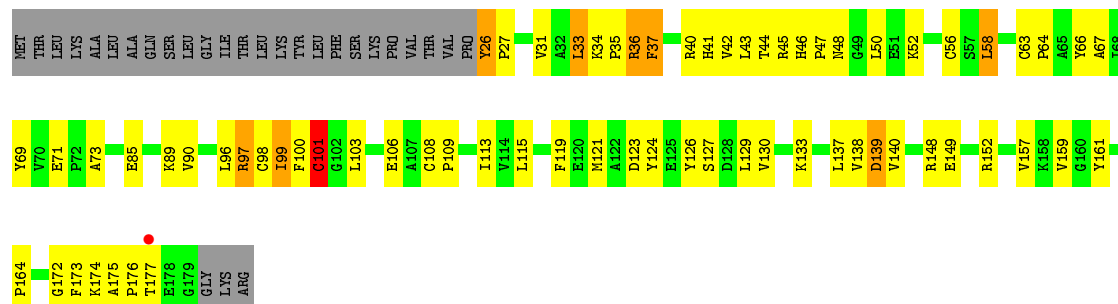
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain F: 35% 37% 8% 20%

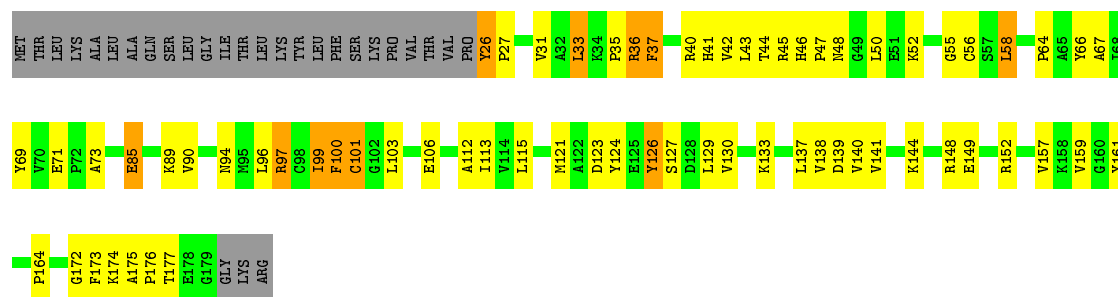




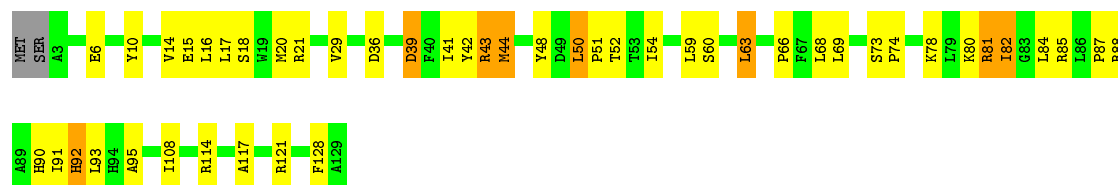
• Molecule 7: NADH-quinone oxidoreductase subunit 9



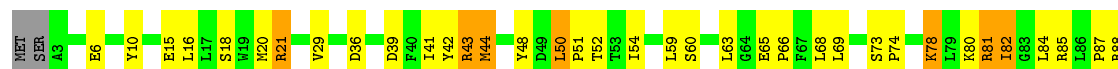
• Molecule 7: NADH-quinone oxidoreductase subunit 9



• 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	108.96Å 150.51Å 216.73Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	29.93 – 3.10 29.93 – 3.08	Depositor EDS
% Data completeness (in resolution range)	81.0 (29.93-3.10) 81.0 (29.93-3.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.06Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, R_{free}	0.235 , 0.283 0.232 , 0.278	Depositor DCC
R_{free} test set	2215 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	37520	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.56% 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: FMN, SF4, MN, CA, FES

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	0.48	1/3506 (0.0%)	0.68	1/4745 (0.0%)
1	A	0.48	1/3506 (0.0%)	0.67	0/4745
2	2	0.49	0/1439	0.66	0/1953
2	B	0.46	0/1439	0.65	0/1953
3	3	0.45	0/6019	0.67	2/8163 (0.0%)
3	C	0.44	0/6019	0.66	2/8163 (0.0%)
4	4	0.43	0/3089	0.64	1/4197 (0.0%)
4	D	0.42	0/3089	0.64	1/4197 (0.0%)
5	5	0.42	0/1656	0.64	0/2246
5	E	0.42	0/1656	0.63	0/2246
6	6	0.47	0/1137	0.67	0/1542
6	F	0.50	0/1137	0.67	0/1542
7	9	0.52	1/1224 (0.1%)	0.65	0/1663
7	G	0.48	0/1224	0.65	0/1663
8	7	0.45	0/1059	0.61	0/1429
8	H	0.47	0/1059	0.61	0/1429
All	All	0.46	3/38258 (0.0%)	0.65	7/51876 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	CYS	CB-SG	-6.45	1.71	1.82
1	1	356	CYS	CB-SG	-6.07	1.72	1.82
7	9	101	CYS	CB-SG	-5.46	1.73	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	55	PRO	CB-CA-C	-5.97	97.08	112.00
3	3	55	PRO	CB-CA-C	-5.78	97.54	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	39	GLY	N-CA-C	-5.46	99.44	113.10
4	4	39	GLY	N-CA-C	-5.40	99.61	113.10
3	3	680	LEU	CA-CB-CG	5.38	127.69	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	206	1
1	A	3417	0	3388	204	0
2	2	1406	0	1373	73	0
2	B	1406	0	1373	72	0
3	3	5880	0	5911	387	1
3	C	5880	0	5911	403	0
4	4	3011	0	3000	206	0
4	D	3011	0	3000	216	0
5	5	1607	0	1574	103	0
5	E	1607	0	1574	111	0
6	6	1113	0	1121	97	0
6	F	1113	0	1121	99	0
7	9	1193	0	1160	68	0
7	G	1193	0	1160	68	0
8	7	1031	0	1029	43	0
8	H	1031	0	1029	44	0
9	1	8	0	0	2	0
9	3	24	0	0	7	0
9	6	8	0	0	4	0
9	9	16	0	0	0	0
9	A	8	0	0	1	0
9	C	24	0	0	5	0
9	F	8	0	0	4	0
9	G	16	0	0	2	0
10	1	31	0	19	8	0
10	A	31	0	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	2	4	0	0	0	0
11	3	4	0	0	1	0
11	B	4	0	0	1	0
11	C	4	0	0	1	0
12	2	1	0	0	0	0
12	3	2	0	0	0	0
12	4	2	0	0	0	0
12	5	1	0	0	0	0
12	7	1	0	0	0	0
12	C	2	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	H	1	0	0	0	0
13	3	1	0	0	0	0
13	C	1	0	0	0	0
All	All	37520	0	37150	2215	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 30.

The worst 5 of 2215 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:C:561:PRO:HB3	3:C:576:ALA:HA	1.28	1.15
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.60	1.15
3:C:474:ARG:NH2	3:C:516:VAL:HG21	1.65	1.10
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.30	1.10
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.10	1.09

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]	2.17	0.03

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	1	435/438 (99%)	362 (83%)	58 (13%)	15 (3%)	3	21
1	A	435/438 (99%)	358 (82%)	64 (15%)	13 (3%)	4	23
2	2	176/181 (97%)	156 (89%)	16 (9%)	4 (2%)	6	28
2	B	176/181 (97%)	155 (88%)	17 (10%)	4 (2%)	6	28
3	3	748/783 (96%)	633 (85%)	92 (12%)	23 (3%)	4	23
3	C	748/783 (96%)	625 (84%)	103 (14%)	20 (3%)	5	25
4	4	373/409 (91%)	322 (86%)	37 (10%)	14 (4%)	3	19
4	D	373/409 (91%)	322 (86%)	37 (10%)	14 (4%)	3	19
5	5	194/207 (94%)	165 (85%)	23 (12%)	6 (3%)	4	23
5	E	194/207 (94%)	165 (85%)	24 (12%)	5 (3%)	5	26
6	6	141/181 (78%)	114 (81%)	22 (16%)	5 (4%)	3	20
6	F	141/181 (78%)	117 (83%)	19 (14%)	5 (4%)	3	20
7	9	152/182 (84%)	131 (86%)	17 (11%)	4 (3%)	5	26
7	G	152/182 (84%)	130 (86%)	17 (11%)	5 (3%)	4	21
8	7	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	19	54
8	H	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	19	54
All	All	4688/5020 (93%)	3978 (85%)	571 (12%)	139 (3%)	4	23

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
1	1	81	LYS
2	2	86	LEU
2	2	136	VAL
2	2	140	PRO

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%)	318 (90%)	37 (10%)	7	27
1	A	355/356 (100%)	317 (89%)	38 (11%)	6	26
2	2	150/152 (99%)	123 (82%)	27 (18%)	1	7
2	B	150/152 (99%)	124 (83%)	26 (17%)	2	9
3	3	607/628 (97%)	537 (88%)	70 (12%)	5	22
3	C	607/628 (97%)	535 (88%)	72 (12%)	5	20
4	4	325/355 (92%)	291 (90%)	34 (10%)	7	26
4	D	325/355 (92%)	290 (89%)	35 (11%)	6	25
5	5	167/175 (95%)	151 (90%)	16 (10%)	8	31
5	E	167/175 (95%)	151 (90%)	16 (10%)	8	31
6	6	118/149 (79%)	104 (88%)	14 (12%)	5	20
6	F	118/149 (79%)	103 (87%)	15 (13%)	4	18
7	9	126/150 (84%)	111 (88%)	15 (12%)	5	20
7	G	126/150 (84%)	110 (87%)	16 (13%)	4	18
8	7	104/106 (98%)	91 (88%)	13 (12%)	4	18
8	H	104/106 (98%)	92 (88%)	12 (12%)	5	22
All	All	3904/4142 (94%)	3448 (88%)	456 (12%)	5	22

5 of 456 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	9	99	ILE
1	A	363	VAL
6	F	83	ARG
7	9	159	VAL
1	A	128	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
5	5	129	HIS
3	C	38	HIS
4	D	377	ASN
8	7	92	HIS
3	3	368	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 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	$\# Z > 2$
11	FES	3	787	3	0,4,4	0.00	-	-		
11	FES	2	182	2	0,4,4	0.00	-	-		
9	SF4	G	183	7	0,12,12	0.00	-	-		
10	FMN	A	440	-	31,33,33	1.43	4 (12%)	40,50,50	1.97	7 (17%)
9	SF4	C	785	3	0,12,12	0.00	-	-		
9	SF4	9	183	7	0,12,12	0.00	-	-		
9	SF4	3	784	3	0,12,12	0.00	-	-		
9	SF4	F	182	6	0,12,12	0.00	-	-		
9	SF4	C	786	3	0,12,12	0.00	-	-		
9	SF4	3	786	3	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FES	C	787	3	0,4,4	0.00	-	-		
11	FES	B	182	2	0,4,4	0.00	-	-		
9	SF4	A	439	1	0,12,12	0.00	-	-		
10	FMN	1	440	-	31,33,33	1.43	7 (22%)	40,50,50	1.91	12 (30%)
9	SF4	3	785	3	0,12,12	0.00	-	-		
9	SF4	1	439	1	0,12,12	0.00	-	-		
9	SF4	C	784	3	0,12,12	0.00	-	-		
9	SF4	6	182	6	0,12,12	0.00	-	-		
9	SF4	G	184	7	0,12,12	0.00	-	-		
9	SF4	9	184	7	0,12,12	0.00	-	-		

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
11	FES	3	787	3	-	-	0/1/1/1
11	FES	2	182	2	-	-	0/1/1/1
9	SF4	G	183	7	-	-	0/6/5/5
10	FMN	A	440	-	-	4/18/18/18	0/3/3/3
9	SF4	C	785	3	-	-	0/6/5/5
9	SF4	9	183	7	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
9	SF4	3	786	3	-	-	0/6/5/5
11	FES	C	787	3	-	-	0/1/1/1
11	FES	B	182	2	-	-	0/1/1/1
9	SF4	A	439	1	-	-	0/6/5/5
10	FMN	1	440	-	-	10/18/18/18	0/3/3/3
9	SF4	3	785	3	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5
9	SF4	6	182	6	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
9	SF4	9	184	7	-	-	0/6/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	440	FMN	C4A-N5	4.02	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	440	FMN	C10-N1	3.71	1.38	1.33
10	1	440	FMN	C4A-N5	3.60	1.38	1.33
10	A	440	FMN	C4-N3	2.77	1.37	1.33
10	1	440	FMN	C10-N1	2.64	1.36	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	440	FMN	C1'-N10-C9A	6.69	123.56	118.29
10	1	440	FMN	C4-N3-C2	6.16	120.34	115.14
10	A	440	FMN	C4-N3-C2	5.97	120.18	115.14
10	A	440	FMN	C4A-N5-C5A	3.91	120.67	116.77
10	1	440	FMN	C5A-C9A-N10	3.44	120.21	117.72

There are no chirality outliers.

5 of 14 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	C3'-C4'-C5'-O5'
10	1	440	FMN	O4'-C4'-C5'-O5'
10	A	440	FMN	N10-C1'-C2'-O2'

There are no ring outliers.

17 monomers are involved in 40 short contacts:

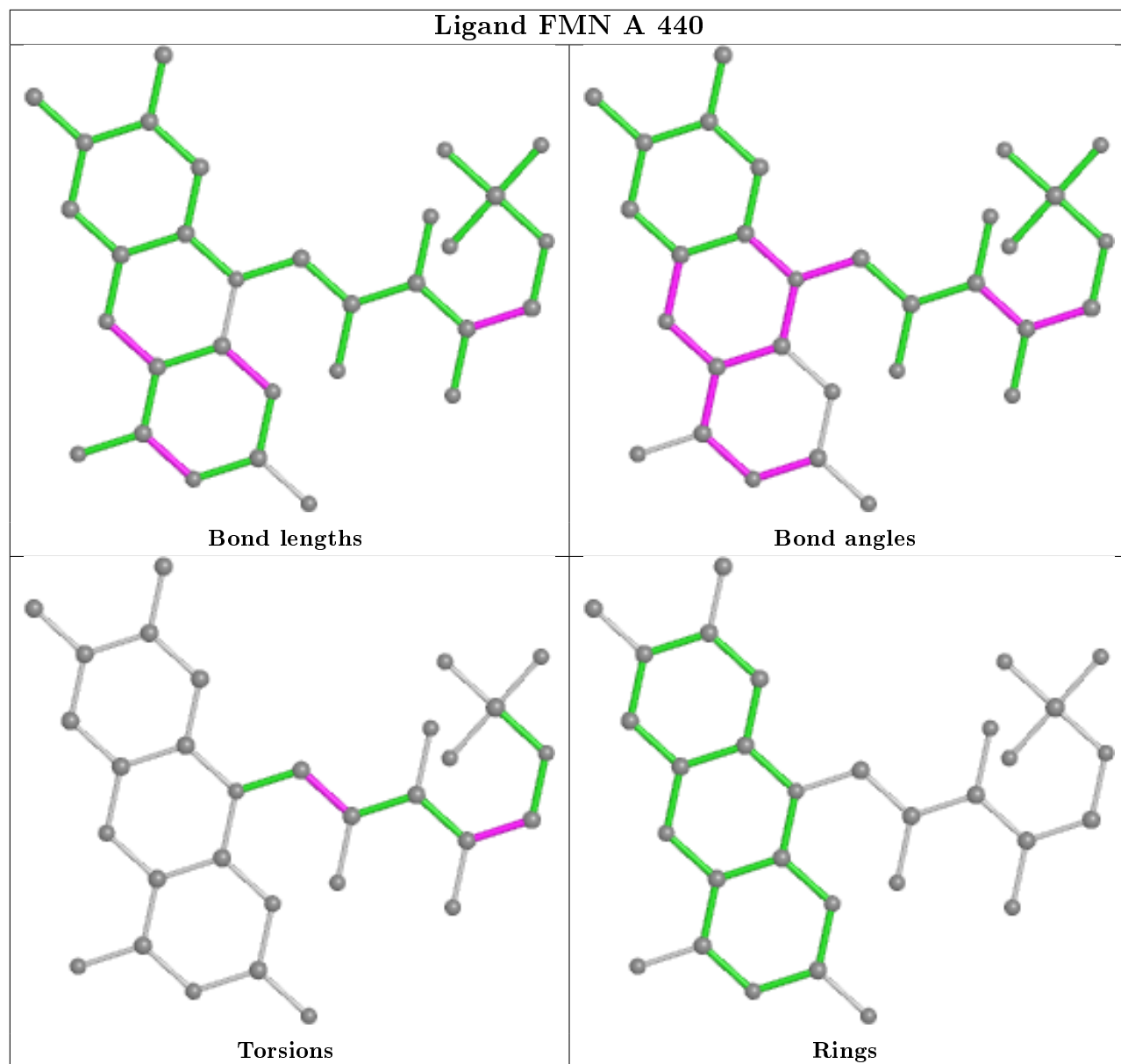
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	3	787	FES	1	0
9	G	183	SF4	1	0
10	A	440	FMN	4	0
9	C	785	SF4	1	0
9	3	784	SF4	3	0
9	F	182	SF4	4	0
9	C	786	SF4	2	0
9	3	786	SF4	3	0
11	C	787	FES	1	0
11	B	182	FES	1	0
9	A	439	SF4	1	0
10	1	440	FMN	8	0
9	3	785	SF4	1	0

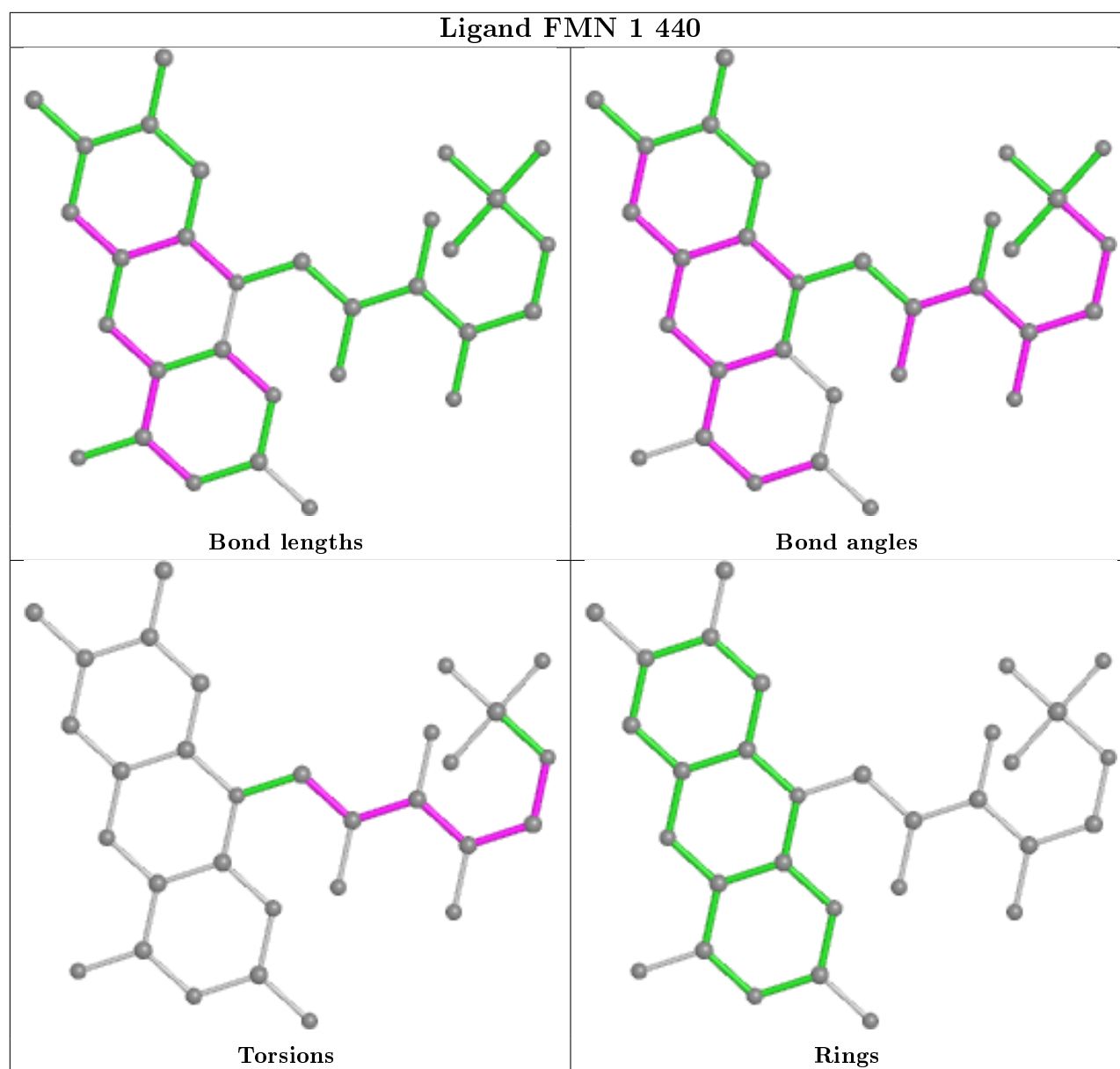
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	1	439	SF4	2	0
9	C	784	SF4	2	0
9	6	182	SF4	4	0
9	G	184	SF4	1	0

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%)	-0.31	0 100 100	26, 49, 76, 109	0
1	A	437/438 (99%)	-0.39	1 (0%) 95 90	29, 49, 77, 111	0
2	2	178/181 (98%)	-0.31	1 (0%) 89 78	28, 51, 84, 125	0
2	B	178/181 (98%)	-0.39	0 100 100	30, 51, 84, 125	0
3	3	754/783 (96%)	-0.16	0 100 100	26, 69, 107, 130	0
3	C	754/783 (96%)	-0.15	10 (1%) 77 59	28, 70, 108, 130	0
4	4	377/409 (92%)	-0.14	1 (0%) 94 88	34, 68, 103, 124	0
4	D	377/409 (92%)	-0.18	2 (0%) 91 81	35, 69, 106, 124	0
5	5	196/207 (94%)	-0.16	1 (0%) 91 81	40, 74, 106, 122	0
5	E	196/207 (94%)	-0.14	0 100 100	42, 76, 107, 122	0
6	6	145/181 (80%)	-0.16	1 (0%) 87 75	39, 64, 91, 122	0
6	F	145/181 (80%)	-0.18	0 100 100	40, 66, 92, 122	0
7	9	154/182 (84%)	-0.24	1 (0%) 89 78	31, 51, 94, 128	0
7	G	154/182 (84%)	-0.31	0 100 100	34, 52, 94, 130	0
8	7	127/129 (98%)	-0.28	0 100 100	43, 57, 93, 117	0
8	H	127/129 (98%)	-0.37	1 (0%) 86 72	43, 58, 94, 115	0
All	All	4736/5020 (94%)	-0.22	19 (0%) 92 84	26, 61, 103, 130	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	654	PHE	3.8
3	C	143	TYR	3.7
1	A	4	PRO	2.9
4	4	47	LEU	2.9
2	2	180	GLU	2.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

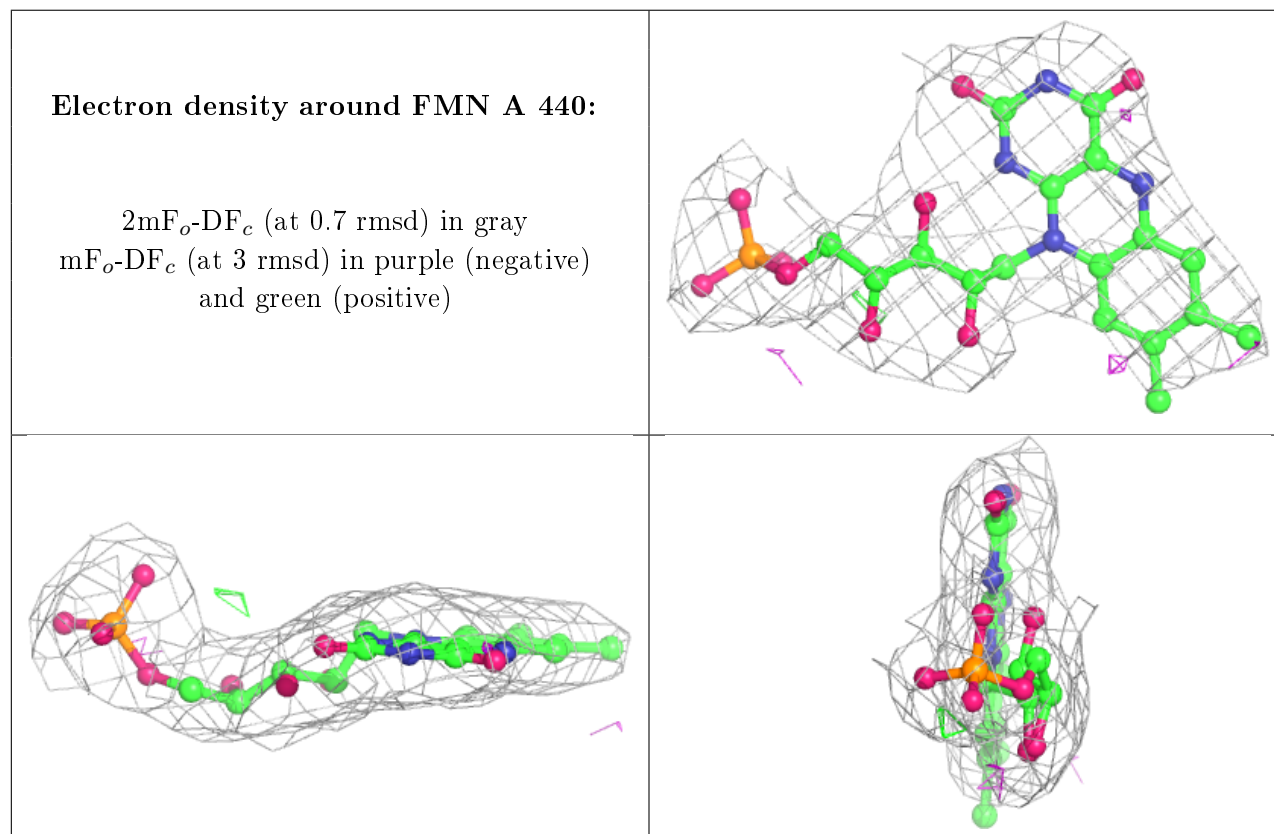
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	MN	H	202	1/1	0.94	0.20	68,68,68,68	0
12	MN	2	206	1/1	0.95	0.07	64,64,64,64	0
12	MN	5	208	1/1	0.96	0.17	67,67,67,67	0
12	MN	D	410	1/1	0.97	0.18	63,63,63,63	0
10	FMN	A	440	31/31	0.97	0.19	35,47,59,63	0
12	MN	4	411	1/1	0.98	0.16	61,61,61,61	0
12	MN	3	789	1/1	0.98	0.20	61,61,61,61	0
12	MN	7	202	1/1	0.98	0.18	63,63,63,63	0
12	MN	4	410	1/1	0.98	0.14	65,65,65,65	0
10	FMN	1	440	31/31	0.98	0.21	28,37,46,59	0
9	SF4	C	786	8/8	0.99	0.17	37,50,59,64	0
11	FES	B	182	4/4	0.99	0.17	38,41,49,51	0
12	MN	C	788	1/1	0.99	0.17	47,47,47,47	0
9	SF4	A	439	8/8	0.99	0.19	29,32,37,42	0
12	MN	E	208	1/1	0.99	0.19	93,93,93,93	0
13	CA	3	790	1/1	0.99	0.22	30,30,30,30	0
13	CA	C	790	1/1	0.99	0.25	39,39,39,39	0
12	MN	C	789	1/1	0.99	0.18	61,61,61,61	0
9	SF4	F	182	8/8	0.99	0.19	40,50,61,73	0
12	MN	3	788	1/1	0.99	0.23	32,32,32,32	0
11	FES	C	787	4/4	0.99	0.17	33,39,42,42	0
9	SF4	6	182	8/8	0.99	0.19	23,34,48,49	0
11	FES	3	787	4/4	1.00	0.18	35,36,37,38	0
9	SF4	C	785	8/8	1.00	0.18	30,32,39,46	0
9	SF4	1	439	8/8	1.00	0.20	21,24,37,40	0
11	FES	2	182	4/4	1.00	0.19	29,34,35,36	0
9	SF4	G	183	8/8	1.00	0.19	32,39,44,47	0

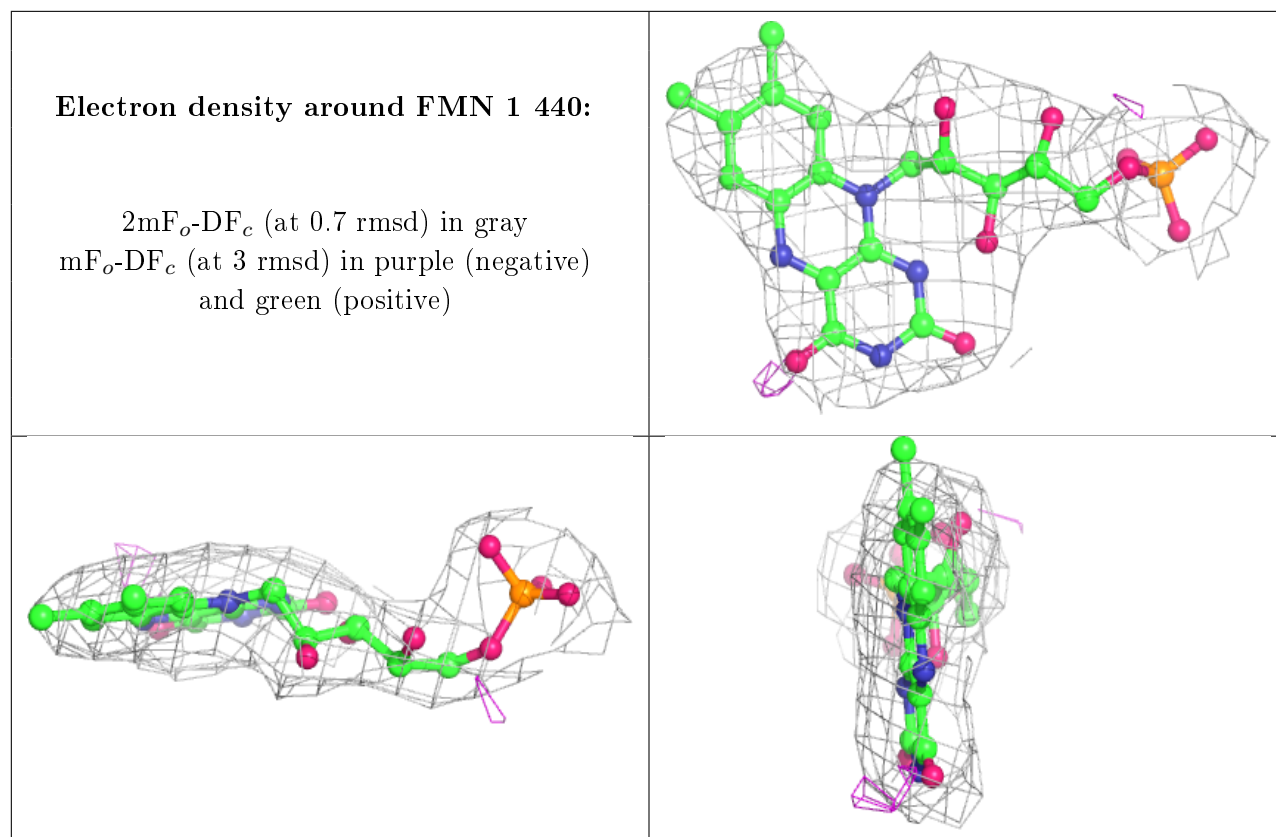
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SF4	3	784	8/8	1.00	0.20	25,27,32,34	0
9	SF4	9	183	8/8	1.00	0.20	18,28,30,33	0
9	SF4	3	785	8/8	1.00	0.18	22,23,28,34	0
9	SF4	C	784	8/8	1.00	0.18	30,35,41,42	0
9	SF4	3	786	8/8	1.00	0.18	27,34,37,39	0
9	SF4	G	184	8/8	1.00	0.18	36,43,45,48	0
9	SF4	9	184	8/8	1.00	0.19	23,26,28,32	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.