



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:18 PM UTC

PDB ID : 7Q5Y / pdb_00007q5y
Title : Structure of NADH:ubichinon oxidoreductase (complex I) of the hyperthermophilic eubacterium Aquifex aeolicus
Authors : Warkentin, E.; Ermler, U.; Peng, G.
Deposited on : 2021-11-05
Resolution : 2.70 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

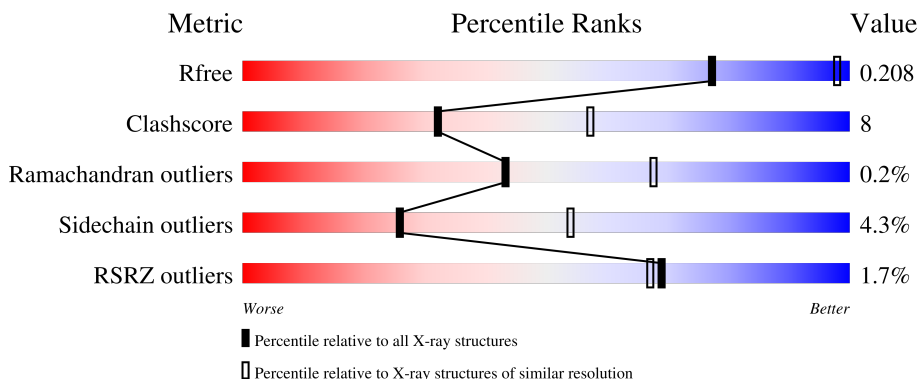
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



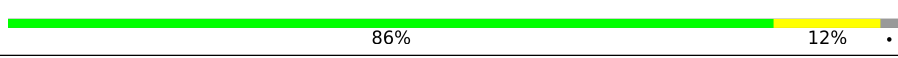
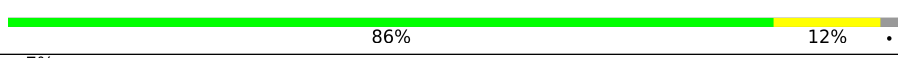
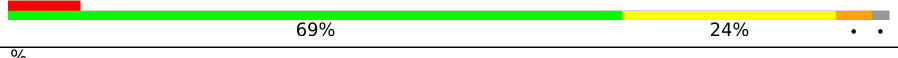
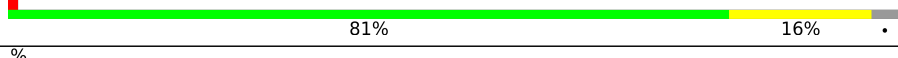
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	632	
1	G	632	
1	M	632	
1	S	632	
2	B	586	

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Mol	Chain	Length	Quality of chain
2	H	586	
2	N	586	
2	T	586	
3	C	426	
3	I	426	
3	O	426	
3	U	426	
4	D	201	
4	J	201	
4	P	201	
4	V	201	
5	E	160	
5	K	160	
5	Q	160	
5	W	160	
6	F	179	
6	L	179	
6	R	179	
6	X	179	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 69025 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 dehydrogenase I chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	626	Total	C	N	O	S	0	0	0
			5071	3250	846	946	29			
1	G	626	Total	C	N	O	S	0	0	0
			5071	3250	846	946	29			
1	M	626	Total	C	N	O	S	0	0	0
			5071	3250	846	946	29			
1	S	626	Total	C	N	O	S	0	0	0
			5071	3250	846	946	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	585	Total	C	N	O	S	0	0	0
			4789	3089	819	865	16			
2	H	585	Total	C	N	O	S	0	0	0
			4789	3089	819	865	16			
2	N	585	Total	C	N	O	S	0	0	0
			4789	3089	819	865	16			
2	T	585	Total	C	N	O	S	0	0	0
			4789	3089	819	865	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	419	Total	C	N	O	S	0	0	0
			3301	2122	550	615	14			
3	I	419	Total	C	N	O	S	0	0	0
			3301	2122	550	615	14			
3	O	419	Total	C	N	O	S	0	0	0
			3301	2122	550	615	14			
3	U	419	Total	C	N	O	S	0	0	0
			3301	2122	550	615	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1610	1029	280	286	15			
4	J	197	Total	C	N	O	S	0	0	0
			1610	1029	280	286	15			
4	P	197	Total	C	N	O	S	0	0	0
			1610	1029	280	286	15			
4	V	197	Total	C	N	O	S	0	0	0
			1610	1029	280	286	15			

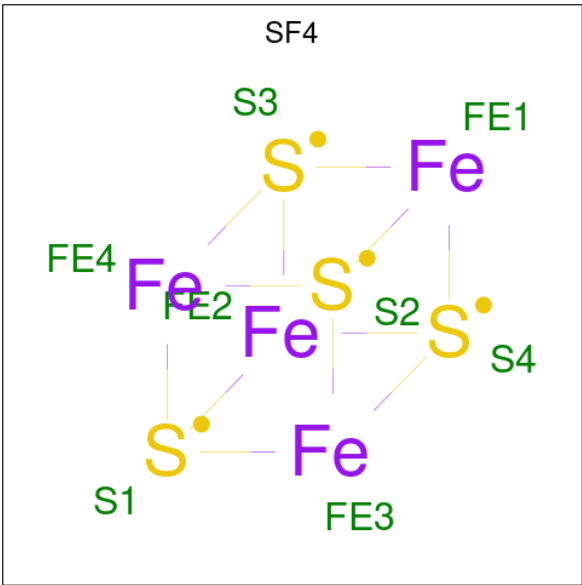
- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	155	Total	C	N	O	S	0	0	0
			1259	816	203	231	9			
5	K	155	Total	C	N	O	S	0	0	0
			1259	816	203	231	9			
5	Q	155	Total	C	N	O	S	0	0	0
			1259	816	203	231	9			
5	W	155	Total	C	N	O	S	0	0	0
			1259	816	203	231	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	135	Total	C	N	O	S	0	0	0
			1033	665	180	178	10			
6	L	135	Total	C	N	O	S	0	0	0
			1033	665	180	178	10			
6	R	135	Total	C	N	O	S	0	0	0
			1033	665	180	178	10			
6	X	135	Total	C	N	O	S	0	0	0
			1033	665	180	178	10			

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



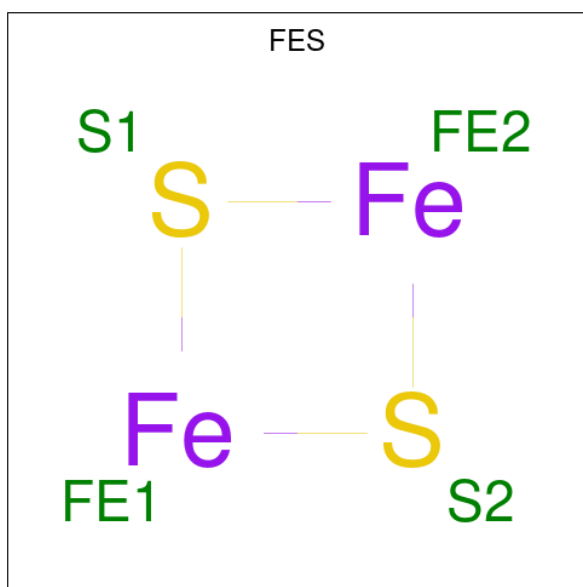
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	C	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	F	1	Total	Fe	S	0	0
			8	4	4		
7	G	1	Total	Fe	S	0	0
			8	4	4		
7	G	1	Total	Fe	S	0	0
			8	4	4		
7	G	1	Total	Fe	S	0	0
			8	4	4		
7	I	1	Total	Fe	S	0	0
			8	4	4		
7	J	1	Total	Fe	S	0	0
			8	4	4		

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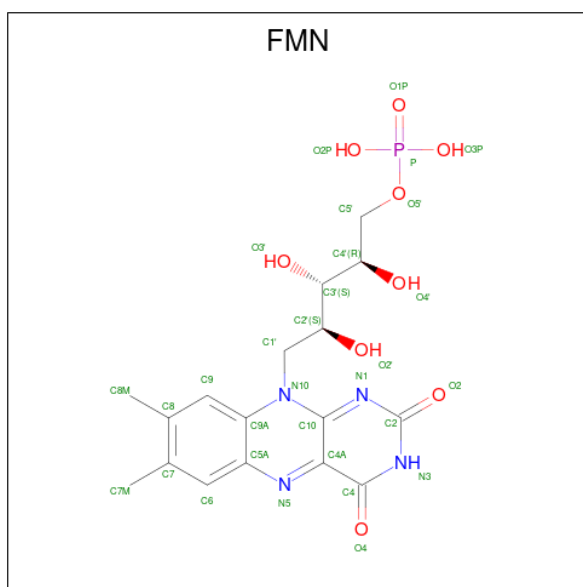
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	M	1	Total 8	Fe 4	S 4	0	0
7	M	1	Total 8	Fe 4	S 4	0	0
7	M	1	Total 8	Fe 4	S 4	0	0
7	M	1	Total 8	Fe 4	S 4	0	0
7	O	1	Total 8	Fe 4	S 4	0	0
7	P	1	Total 8	Fe 4	S 4	0	0
7	P	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	S	1	Total 8	Fe 4	S 4	0	0
7	S	1	Total 8	Fe 4	S 4	0	0
7	S	1	Total 8	Fe 4	S 4	0	0
7	S	1	Total 8	Fe 4	S 4	0	0
7	U	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	0
			4	2	2		
8	E	1	Total	Fe	S	0	0
			4	2	2		
8	G	1	Total	Fe	S	0	0
			4	2	2		
8	K	1	Total	Fe	S	0	0
			4	2	2		
8	M	1	Total	Fe	S	0	0
			4	2	2		
8	Q	1	Total	Fe	S	0	0
			4	2	2		
8	S	1	Total	Fe	S	0	0
			4	2	2		
8	W	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	79	Total	O	0	0
			79	79		
10	B	5	Total	O	0	0
			5	5		
10	C	24	Total	O	0	0
			24	24		
10	D	5	Total	O	0	0
			5	5		
10	E	14	Total	O	0	0
			14	14		
10	G	38	Total	O	0	0
			38	38		
10	H	2	Total	O	0	0
			2	2		
10	I	41	Total	O	0	0
			41	41		

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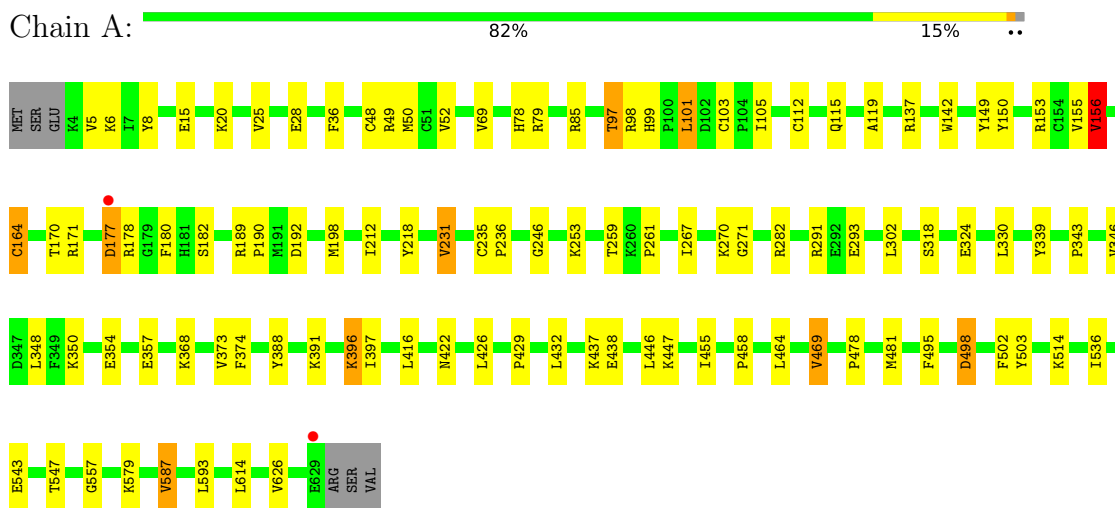
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	J	4	Total 4	O 4	0	0
10	K	14	Total 14	O 14	0	0
10	M	51	Total 51	O 51	0	0
10	N	8	Total 8	O 8	0	0
10	O	11	Total 11	O 11	0	0
10	P	3	Total 3	O 3	0	0
10	Q	10	Total 10	O 10	0	0
10	S	32	Total 32	O 32	0	0
10	T	4	Total 4	O 4	0	0
10	U	10	Total 10	O 10	0	0
10	V	2	Total 2	O 2	0	0
10	W	4	Total 4	O 4	0	0

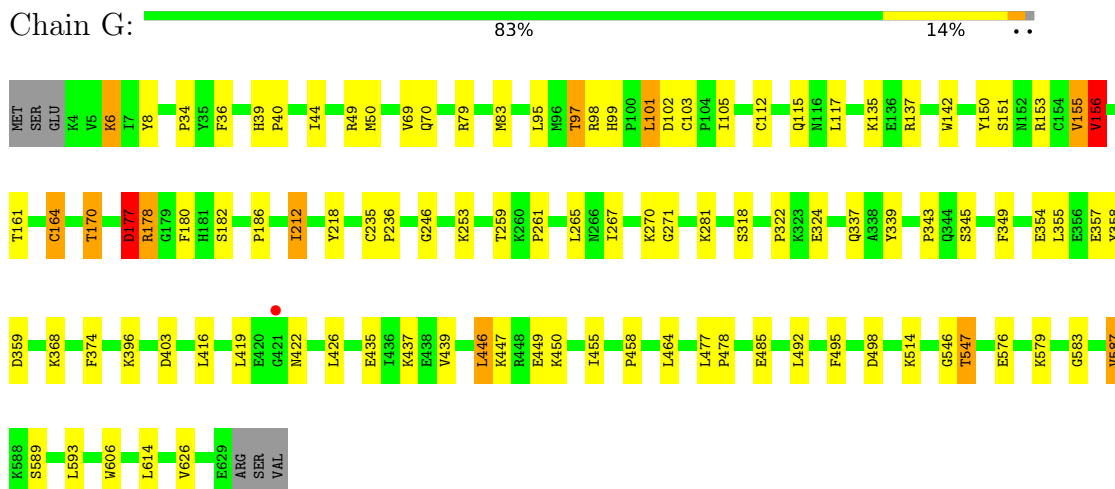
3 Residue-property plots [i](#)

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

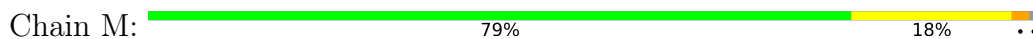
• Molecule 1: NADH dehydrogenase I chain G

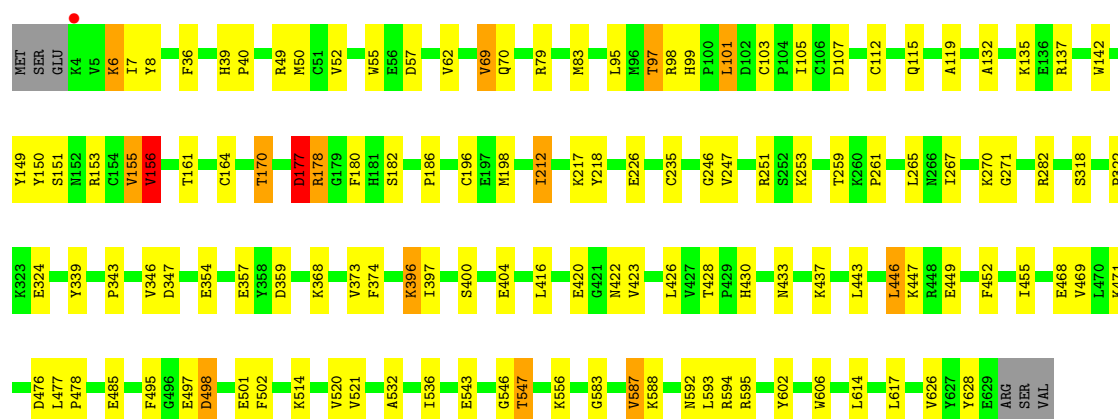


• Molecule 1: NADH dehydrogenase I chain G



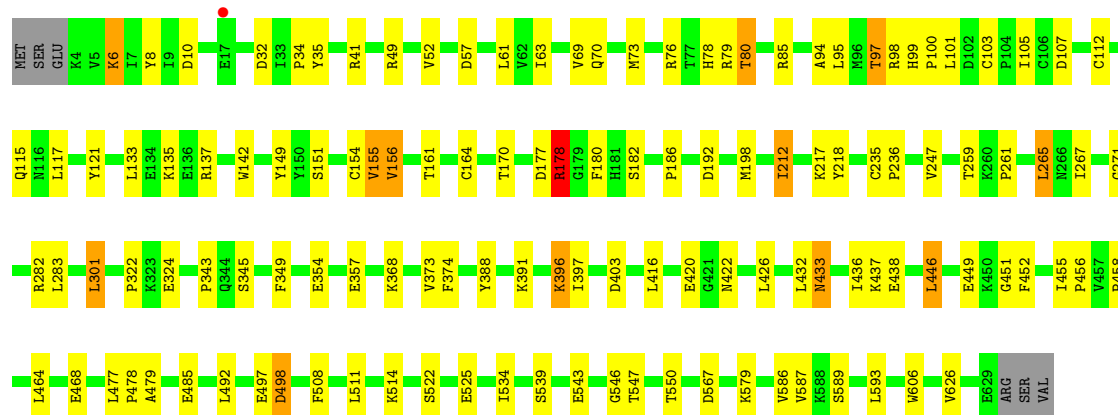
• Molecule 1: NADH dehydrogenase I chain G





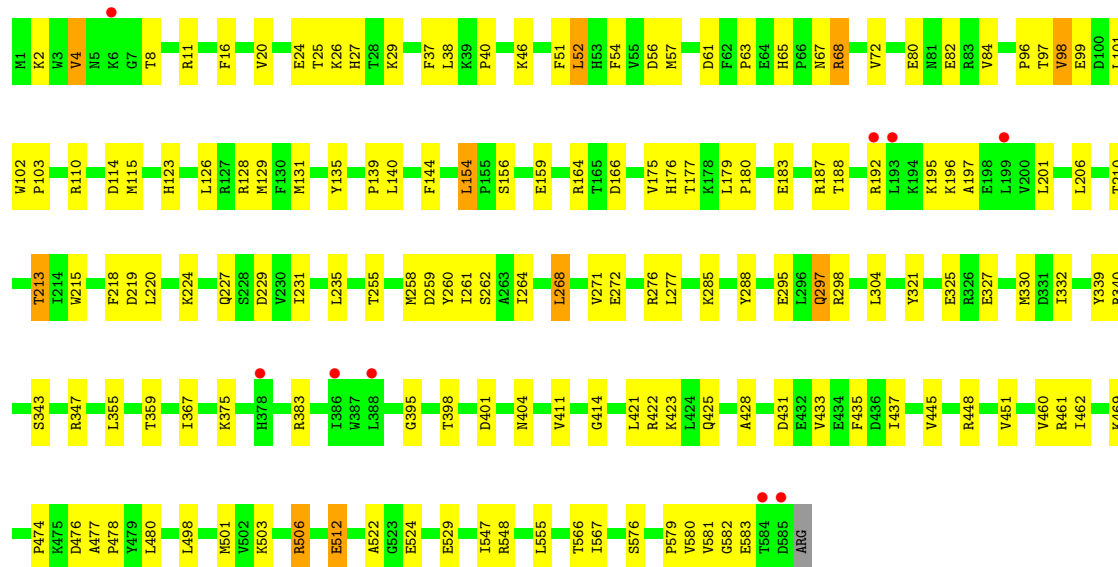
• Molecule 1: NADH dehydrogenase I chain G

Chain S: 79% 18%

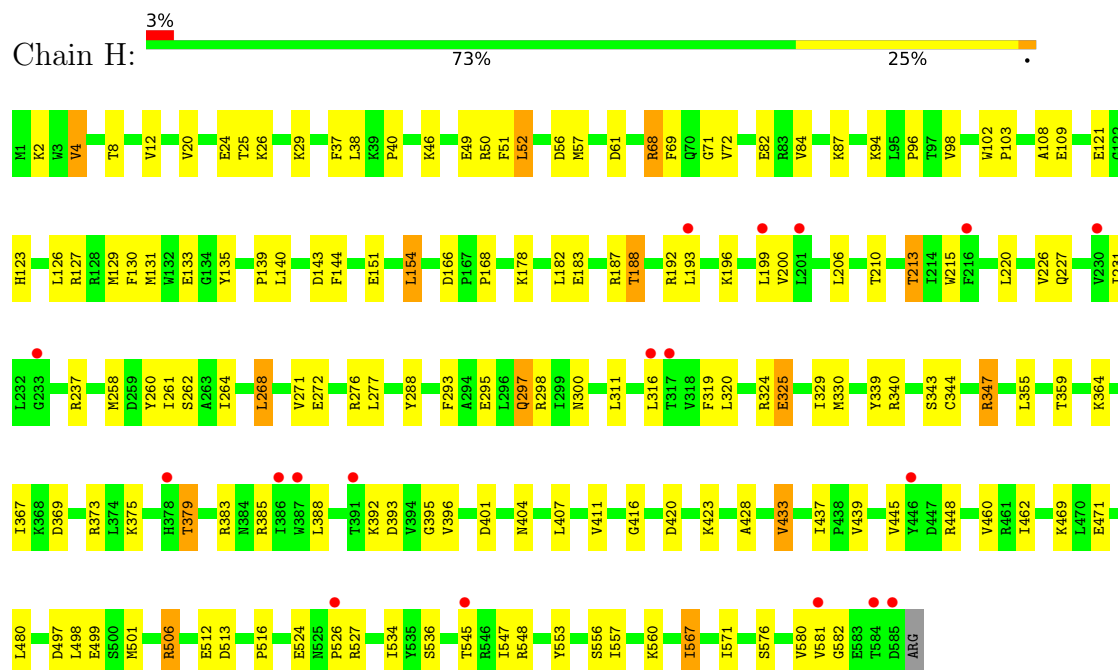


• Molecule 2: NADH-quinone oxidoreductase subunit C/D 2

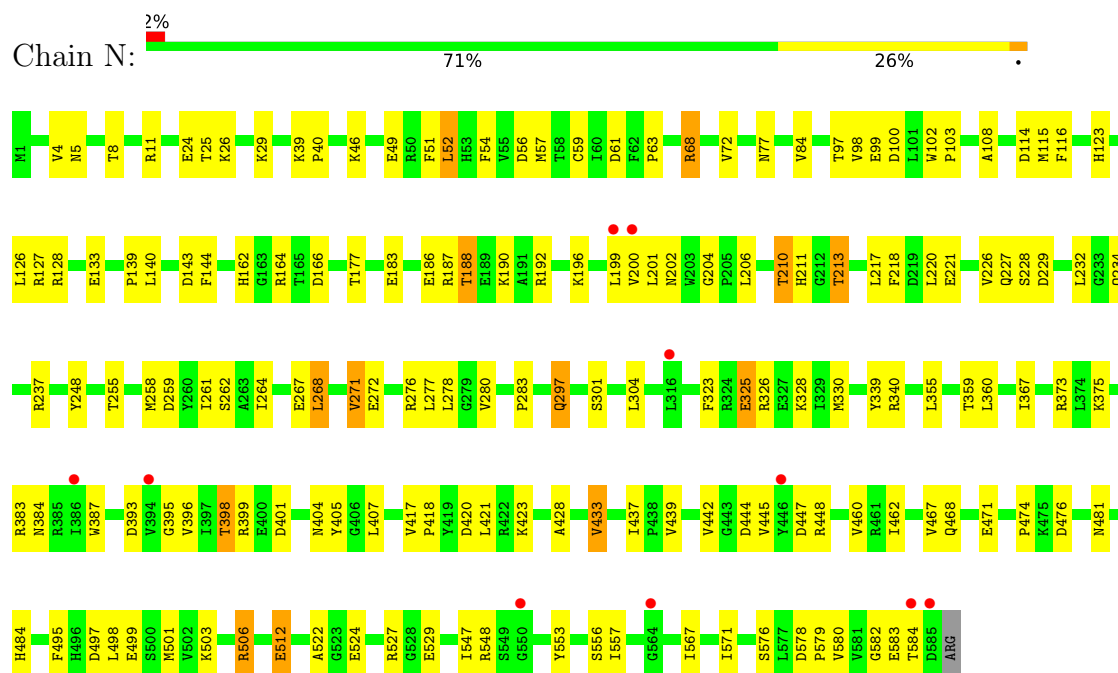
Chain B: 73% 25%



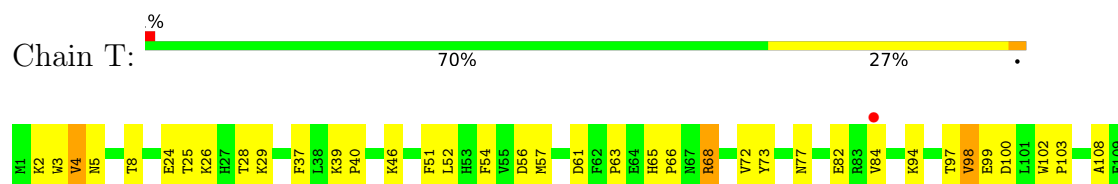
• Molecule 2: NADH-quinone oxidoreductase subunit C/D 2

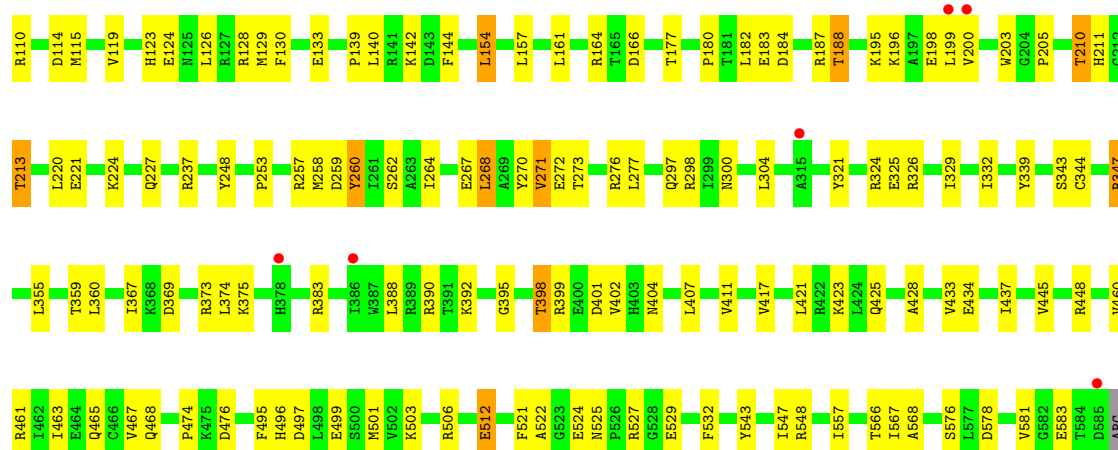


• Molecule 2: NADH-quinone oxidoreductase subunit C/D 2



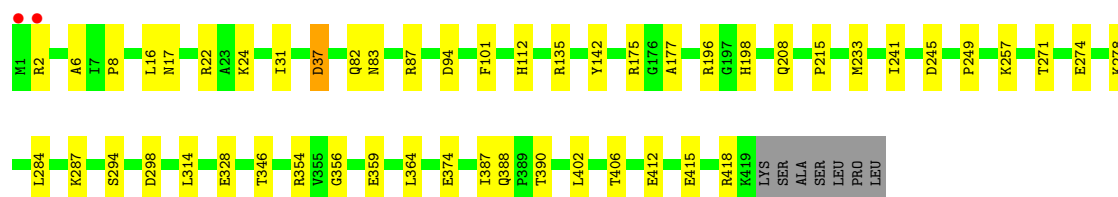
• Molecule 2: NADH-quinone oxidoreductase subunit C/D 2





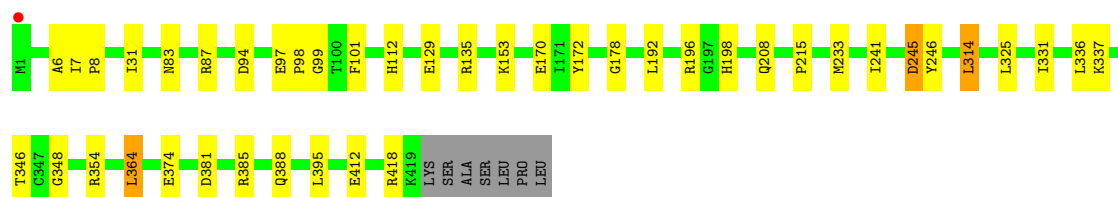
• Molecule 3: NADH-quinone oxidoreductase subunit F

Chain C: 86% 12%



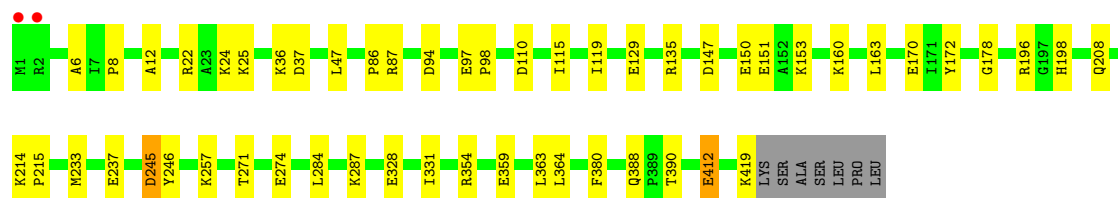
• Molecule 3: NADH-quinone oxidoreductase subunit F

Chain I: 88% 9%



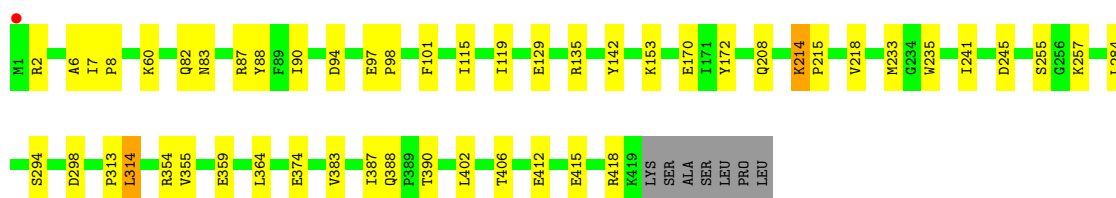
• Molecule 3: NADH-quinone oxidoreductase subunit F

Chain O: 86% 12%

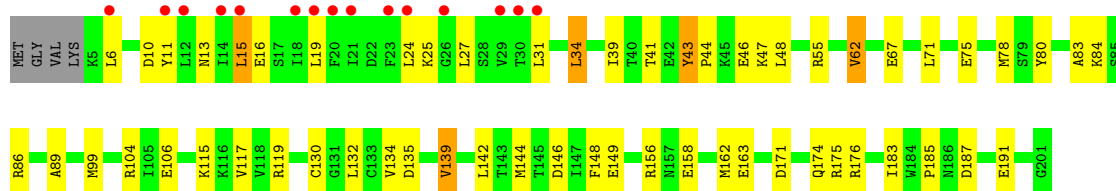


• Molecule 3: NADH-quinone oxidoreductase subunit F

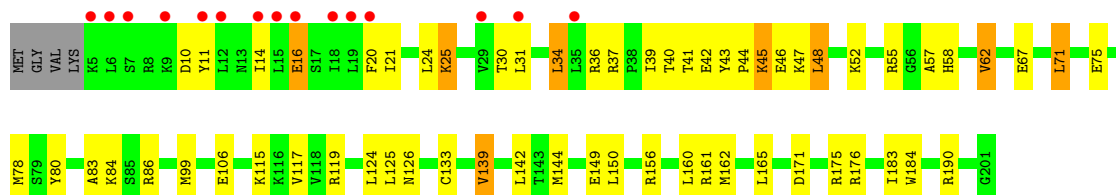
Chain U: 86% 12%



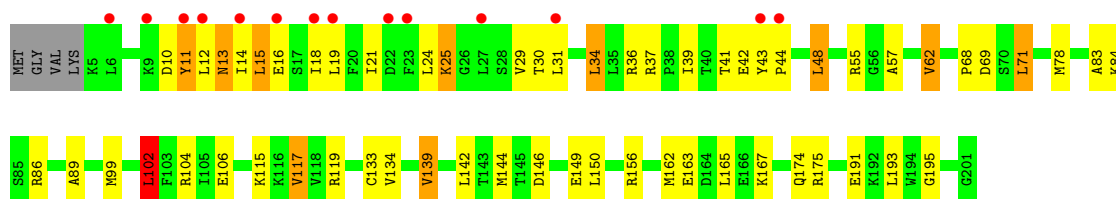
• Molecule 4: NADH-quinone oxidoreductase subunit I



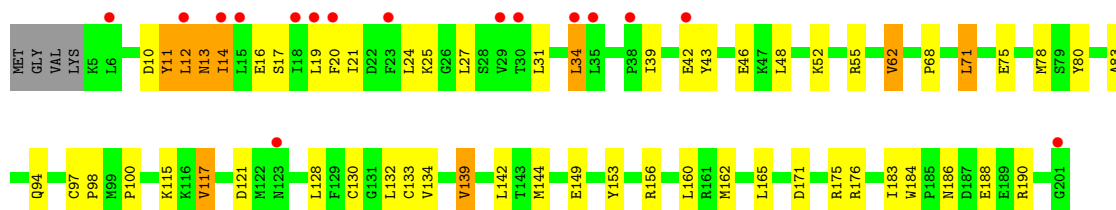
• Molecule 4: NADH-quinone oxidoreductase subunit I



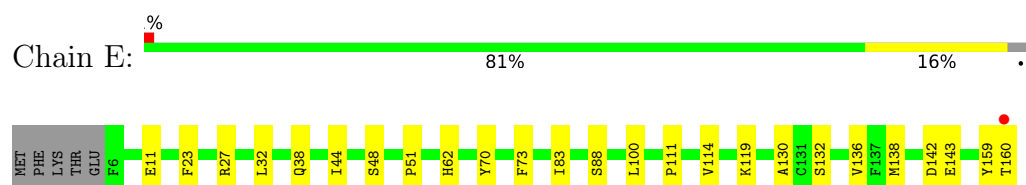
• Molecule 4: NADH-quinone oxidoreductase subunit I



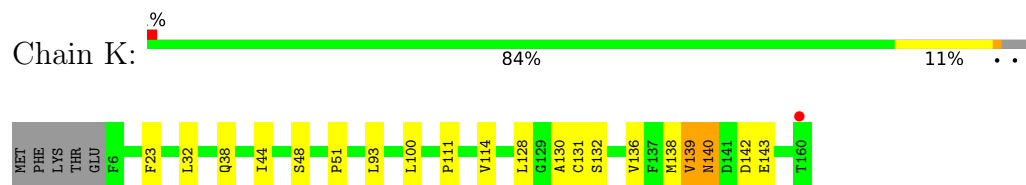
• Molecule 4: NADH-quinone oxidoreductase subunit I



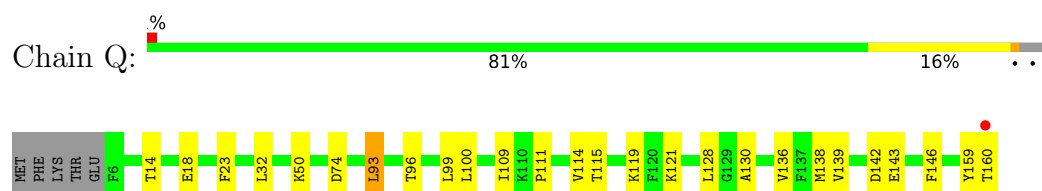
• Molecule 5: NADH-quinone oxidoreductase subunit E



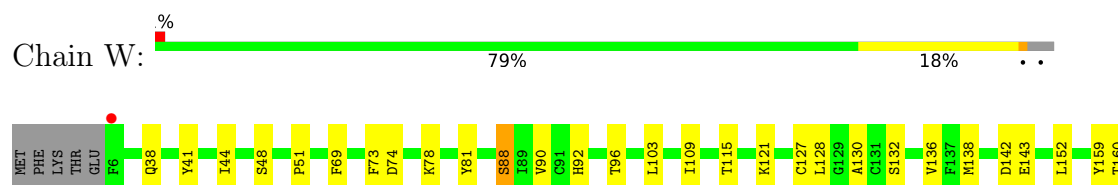
- Molecule 5: NADH-quinone oxidoreductase subunit E



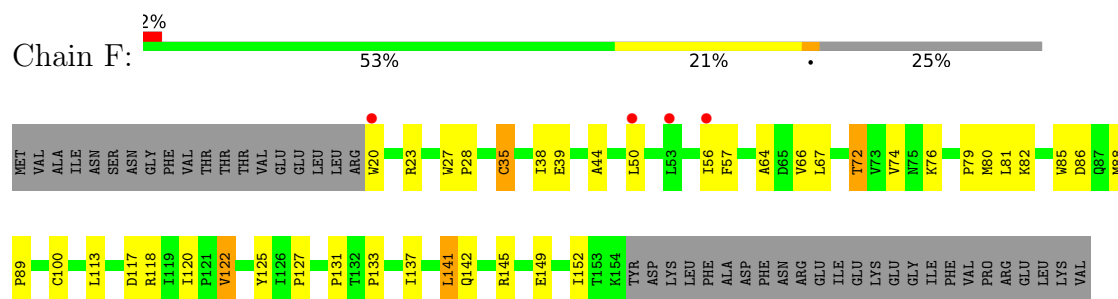
- Molecule 5: NADH-quinone oxidoreductase subunit E



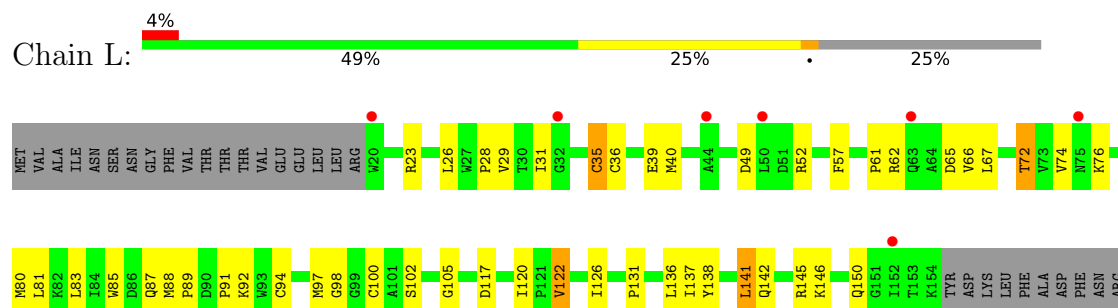
- Molecule 5: NADH-quinone oxidoreductase subunit E



- Molecule 6: NADH-quinone oxidoreductase subunit B



- Molecule 6: NADH-quinone oxidoreductase subunit B



GLU
ILE
GLU
LYS
GLU
GLY
ILE
PHE
VAL
PRO
ARG
GLU
LEU
LYS
VAL

● Molecule 6: NADH-quinone oxidoreductase subunit B



MET VAL ILE GLU LYS GLU GLY ILE PHE VAL PRO ARG GLU LEU LYS VAL
W20 W21 R22 R23 W27 P28 V29 T30 C35 E39 S46 I56 F57 S60 P61 R62 V66 L67 T72 V73 V74 N75 K76 M80 L81 W85 D86 Q87 M88 P89 D90

P91 R92 W93 C94 T95 S96 S97 C100 D117 I120 P121 V122 D123 V124 P131 T132 P133 I137 L141 Q142 R145 I31 K146 I147 K148 I152 T153 K154 TYR ASP LYS LEU PHE LEU ALA ASP PHE ASN ARG GLU ILE PHE VAL PRO ARG GLU LEU LYS VAL

● Molecule 6: NADH-quinone oxidoreductase subunit B



MET VAL ILE GLU LYS GLY ILE PHE VAL THR THR VAL GLU LEU LEU ARG W20 W21 R22 R23 W27 P28 V29 T30 C35 E39 A44 R47 L50 I56 F57 R58 R62 V66 L67 T72 V73 V74 N75 K76 P79 M80 L81 K82

L83 I84 W85 D86 Q87 M88 W93 M97 C100 P106 D117 I120 P121 V122 I126 P131 L141 Q142 R145 K146 I147 K148 I152 T153 K154 TYR ASP LYS LEU PHE LEU ALA ASP PHE ASN ARG GLU ILE GLU LYS GLU ILE PHE VAL PRO ARG GLU LEU LYS

VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.88Å 240.24Å 230.92Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	29.95 – 2.70 29.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.95-2.70) 98.4 (29.95-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.169 , 0.209 0.171 , 0.208	Depositor DCC
R_{free} test set	19447 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.5	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	0.96	EDS
Total number of atoms	69025	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, 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	A	0.48	0/5182	0.82	2/7004 (0.0%)
1	G	0.45	0/5182	0.81	0/7004
1	M	0.44	0/5182	0.79	0/7004
1	S	0.42	0/5182	0.79	1/7004 (0.0%)
2	B	0.33	0/4917	0.67	0/6657
2	H	0.28	0/4917	0.63	0/6657
2	N	0.29	0/4917	0.64	0/6657
2	T	0.31	0/4917	0.66	0/6657
3	C	0.42	0/3382	0.72	0/4574
3	I	0.46	0/3382	0.76	0/4574
3	O	0.38	0/3382	0.70	0/4574
3	U	0.35	0/3382	0.67	0/4574
4	D	0.36	0/1646	0.79	3/2216 (0.1%)
4	J	0.34	0/1646	0.72	0/2216
4	P	0.33	0/1646	0.81	4/2216 (0.2%)
4	V	0.31	0/1646	0.77	3/2216 (0.1%)
5	E	0.43	0/1288	0.76	0/1740
5	K	0.44	0/1288	0.76	1/1740 (0.1%)
5	Q	0.37	0/1288	0.72	2/1740 (0.1%)
5	W	0.32	0/1288	0.67	0/1740
6	F	0.35	0/1059	0.76	0/1442
6	L	0.27	0/1059	0.66	0/1442
6	R	0.30	0/1059	0.68	0/1442
6	X	0.30	0/1059	0.68	0/1442
All	All	0.38	0/69896	0.73	16/94532 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	139	VAL	N-CA-C	-7.07	94.64	109.34
4	P	102	LEU	CA-CB-CG	6.38	138.63	116.30
1	A	177	ASP	CA-C-N	6.21	133.39	121.54
1	A	177	ASP	C-N-CA	6.21	133.39	121.54
4	V	11	TYR	CA-C-N	-5.52	110.99	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5071	0	5048	68	0
1	G	5071	0	5048	66	0
1	M	5071	0	5049	83	0
1	S	5071	0	5048	82	0
2	B	4789	0	4743	110	0
2	H	4789	0	4743	109	0
2	N	4789	0	4743	109	0
2	T	4789	0	4743	114	0
3	C	3301	0	3282	27	0
3	I	3301	0	3282	29	0
3	O	3301	0	3282	31	0
3	U	3301	0	3282	31	0
4	D	1610	0	1623	38	0
4	J	1610	0	1623	44	0
4	P	1610	0	1623	45	0
4	V	1610	0	1623	40	0
5	E	1259	0	1263	17	0
5	K	1259	0	1263	16	0
5	Q	1259	0	1263	17	0
5	W	1259	0	1263	20	0
6	F	1033	0	1062	31	0
6	L	1033	0	1062	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	1033	0	1062	25	0
6	X	1033	0	1062	28	0
7	A	32	0	0	1	0
7	C	8	0	0	0	0
7	D	16	0	0	0	0
7	F	8	0	0	0	0
7	G	32	0	0	1	0
7	I	8	0	0	0	0
7	J	16	0	0	0	0
7	L	8	0	0	0	0
7	M	32	0	0	0	0
7	O	8	0	0	0	0
7	P	16	0	0	0	0
7	R	8	0	0	0	0
7	S	32	0	0	1	0
7	U	8	0	0	0	0
7	V	16	0	0	0	0
7	X	8	0	0	0	0
8	A	4	0	0	0	0
8	E	4	0	0	0	0
8	G	4	0	0	0	0
8	K	4	0	0	0	0
8	M	4	0	0	0	0
8	Q	4	0	0	0	0
8	S	4	0	0	1	0
8	W	4	0	0	1	0
9	C	31	0	19	1	0
9	I	31	0	19	1	0
9	O	31	0	19	0	0
9	U	31	0	19	0	0
10	A	79	0	0	2	0
10	B	5	0	0	0	0
10	C	24	0	0	0	0
10	D	5	0	0	0	0
10	E	14	0	0	1	0
10	G	38	0	0	0	0
10	H	2	0	0	0	0
10	I	41	0	0	1	0
10	J	4	0	0	0	0
10	K	14	0	0	0	0
10	M	51	0	0	0	0
10	N	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	O	11	0	0	2	0
10	P	3	0	0	0	0
10	Q	10	0	0	0	0
10	S	32	0	0	2	0
10	T	4	0	0	0	0
10	U	10	0	0	1	0
10	V	2	0	0	0	0
10	W	4	0	0	0	0
All	All	69025	0	68161	1098	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 8.

The worst 5 of 1098 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)
2:T:423:LYS:HG3	2:T:437:ILE:HD11	1.54	0.90
2:H:355:LEU:HB3	2:H:359:THR:HG21	1.54	0.89
2:B:355:LEU:HB3	2:B:359:THR:HG21	1.57	0.84
1:M:354:GLU:HG3	1:M:437:LYS:HG3	1.58	0.83
2:B:103:PRO:HD2	2:B:404:ASN:HB3	1.59	0.83

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	624/632 (99%)	592 (95%)	29 (5%)	3 (0%)	24	48
1	G	624/632 (99%)	593 (95%)	29 (5%)	2 (0%)	36	60
1	M	624/632 (99%)	589 (94%)	33 (5%)	2 (0%)	36	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	624/632 (99%)	595 (95%)	25 (4%)	4 (1%)	21	44
2	B	583/586 (100%)	556 (95%)	26 (4%)	1 (0%)	43	68
2	H	583/586 (100%)	554 (95%)	28 (5%)	1 (0%)	43	68
2	N	583/586 (100%)	557 (96%)	25 (4%)	1 (0%)	43	68
2	T	583/586 (100%)	556 (95%)	26 (4%)	1 (0%)	43	68
3	C	417/426 (98%)	405 (97%)	12 (3%)	0	100	100
3	I	417/426 (98%)	407 (98%)	10 (2%)	0	100	100
3	O	417/426 (98%)	404 (97%)	13 (3%)	0	100	100
3	U	417/426 (98%)	406 (97%)	11 (3%)	0	100	100
4	D	195/201 (97%)	187 (96%)	7 (4%)	1 (0%)	24	48
4	J	195/201 (97%)	183 (94%)	11 (6%)	1 (0%)	24	48
4	P	195/201 (97%)	183 (94%)	11 (6%)	1 (0%)	24	48
4	V	195/201 (97%)	182 (93%)	11 (6%)	2 (1%)	12	32
5	E	153/160 (96%)	146 (95%)	7 (5%)	0	100	100
5	K	153/160 (96%)	146 (95%)	6 (4%)	1 (1%)	18	41
5	Q	153/160 (96%)	147 (96%)	6 (4%)	0	100	100
5	W	153/160 (96%)	147 (96%)	6 (4%)	0	100	100
6	F	133/179 (74%)	122 (92%)	11 (8%)	0	100	100
6	L	133/179 (74%)	120 (90%)	13 (10%)	0	100	100
6	R	133/179 (74%)	119 (90%)	14 (10%)	0	100	100
6	X	133/179 (74%)	121 (91%)	12 (9%)	0	100	100
All	All	8420/8736 (96%)	8017 (95%)	382 (4%)	21 (0%)	43	68

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	VAL
1	A	177	ASP
1	G	156	VAL
1	M	156	VAL
4	P	13	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/565 (99%)	542 (97%)	17 (3%)	36	66
1	G	559/565 (99%)	531 (95%)	28 (5%)	22	48
1	M	559/565 (99%)	530 (95%)	29 (5%)	21	47
1	S	559/565 (99%)	535 (96%)	24 (4%)	26	54
2	B	513/514 (100%)	488 (95%)	25 (5%)	22	49
2	H	513/514 (100%)	489 (95%)	24 (5%)	23	51
2	N	513/514 (100%)	492 (96%)	21 (4%)	27	56
2	T	513/514 (100%)	486 (95%)	27 (5%)	20	46
3	C	345/351 (98%)	336 (97%)	9 (3%)	40	70
3	I	345/351 (98%)	338 (98%)	7 (2%)	48	76
3	O	345/351 (98%)	337 (98%)	8 (2%)	44	73
3	U	345/351 (98%)	337 (98%)	8 (2%)	44	73
4	D	178/181 (98%)	165 (93%)	13 (7%)	13	32
4	J	178/181 (98%)	164 (92%)	14 (8%)	11	28
4	P	178/181 (98%)	161 (90%)	17 (10%)	8	20
4	V	178/181 (98%)	167 (94%)	11 (6%)	16	39
5	E	141/146 (97%)	138 (98%)	3 (2%)	47	75
5	K	141/146 (97%)	140 (99%)	1 (1%)	76	90
5	Q	141/146 (97%)	137 (97%)	4 (3%)	38	68
5	W	141/146 (97%)	140 (99%)	1 (1%)	76	90
6	F	112/152 (74%)	106 (95%)	6 (5%)	20	45
6	L	112/152 (74%)	106 (95%)	6 (5%)	20	45
6	R	112/152 (74%)	105 (94%)	7 (6%)	16	39
6	X	112/152 (74%)	105 (94%)	7 (6%)	16	39
All	All	7392/7636 (97%)	7075 (96%)	317 (4%)	26	54

5 of 317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Q	114	VAL
2	T	512	GLU
6	R	141	LEU
1	S	522	SER
4	V	16	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	35	HIS
6	X	75	ASN
4	P	109	GLN
6	X	42	HIS
3	U	208	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

44 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
7	SF4	S	703	1	0,12,12	-	-	-		
7	SF4	V	302	4	0,12,12	-	-	-		
8	FES	G	705	1	0,4,4	-	-	-		
7	SF4	C	502	3	0,12,12	-	-	-		
7	SF4	P	301	4	0,12,12	-	-	-		
7	SF4	G	703	1	0,12,12	-	-	-		
8	FES	A	705	1	0,4,4	-	-	-		
7	SF4	M	702	1	0,12,12	-	-	-		
7	SF4	F	701	6	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
8	FES	Q	201	5	0,4,4	-	-	-		
7	SF4	J	301	4	0,12,12	-	-	-		
7	SF4	O	502	3	0,12,12	-	-	-		
7	SF4	R	701	6	0,12,12	-	-	-		
7	SF4	S	701	1	0,12,12	-	-	-		
8	FES	E	201	5	0,4,4	-	-	-		
8	FES	W	201	5	0,4,4	-	-	-		
7	SF4	I	502	3	0,12,12	-	-	-		
7	SF4	G	704	1	0,12,12	-	-	-		
7	SF4	D	301	4	0,12,12	-	-	-		
7	SF4	M	703	1	0,12,12	-	-	-		
7	SF4	P	302	4	0,12,12	-	-	-		
8	FES	S	705	1	0,4,4	-	-	-		
7	SF4	G	701	1	0,12,12	-	-	-		
9	FMN	C	501	-	33,33,33	1.03	2 (6%)	48,50,50	1.31	7 (14%)
8	FES	K	201	5	0,4,4	-	-	-		
8	FES	M	705	1	0,4,4	-	-	-		
7	SF4	M	701	1	0,12,12	-	-	-		
9	FMN	O	501	-	33,33,33	0.97	1 (3%)	48,50,50	1.36	8 (16%)
7	SF4	S	704	1	0,12,12	-	-	-		
7	SF4	A	702	1	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
7	SF4	D	302	4	0,12,12	-	-	-		
7	SF4	X	701	6	0,12,12	-	-	-		
7	SF4	G	702	1	0,12,12	-	-	-		
7	SF4	U	502	3	0,12,12	-	-	-		
7	SF4	M	704	1	0,12,12	-	-	-		
9	FMN	U	501	-	33,33,33	1.04	2 (6%)	48,50,50	1.34	7 (14%)
7	SF4	J	302	4	0,12,12	-	-	-		
7	SF4	V	301	4	0,12,12	-	-	-		
9	FMN	I	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.45	9 (18%)
7	SF4	A	703	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SF4	L	701	6	0,12,12	-	-	-		
7	SF4	S	702	1	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
7	SF4	S	703	1	-	-	0/6/5/5
7	SF4	V	302	4	-	-	0/6/5/5
8	FES	G	705	1	-	-	0/1/1/1
7	SF4	C	502	3	-	-	0/6/5/5
7	SF4	P	301	4	-	-	0/6/5/5
7	SF4	G	703	1	-	-	0/6/5/5
8	FES	A	705	1	-	-	0/1/1/1
7	SF4	M	702	1	-	-	0/6/5/5
7	SF4	F	701	6	-	-	0/6/5/5
7	SF4	A	701	1	-	-	0/6/5/5
8	FES	Q	201	5	-	-	0/1/1/1
7	SF4	J	301	4	-	-	0/6/5/5
7	SF4	O	502	3	-	-	0/6/5/5
7	SF4	R	701	6	-	-	0/6/5/5
7	SF4	S	701	1	-	-	0/6/5/5
8	FES	E	201	5	-	-	0/1/1/1
8	FES	W	201	5	-	-	0/1/1/1
7	SF4	I	502	3	-	-	0/6/5/5
7	SF4	G	704	1	-	-	0/6/5/5
7	SF4	D	301	4	-	-	0/6/5/5
7	SF4	M	703	1	-	-	0/6/5/5
7	SF4	P	302	4	-	-	0/6/5/5
8	FES	S	705	1	-	-	0/1/1/1
7	SF4	G	701	1	-	-	0/6/5/5
9	FMN	C	501	-	-	2/18/18/18	0/3/3/3
8	FES	K	201	5	-	-	0/1/1/1
8	FES	M	705	1	-	-	0/1/1/1
7	SF4	M	701	1	-	-	0/6/5/5
9	FMN	O	501	-	-	2/18/18/18	0/3/3/3
7	SF4	S	704	1	-	-	0/6/5/5
7	SF4	A	702	1	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5
7	SF4	D	302	4	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	X	701	6	-	-	0/6/5/5
7	SF4	G	702	1	-	-	0/6/5/5
7	SF4	U	502	3	-	-	0/6/5/5
9	FMN	U	501	-	-	2/18/18/18	0/3/3/3
7	SF4	M	704	1	-	-	0/6/5/5
7	SF4	J	302	4	-	-	0/6/5/5
7	SF4	V	301	4	-	-	0/6/5/5
9	FMN	I	501	-	-	2/18/18/18	0/3/3/3
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	L	701	6	-	-	0/6/5/5
7	SF4	S	702	1	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	501	FMN	C4A-N5	3.58	1.38	1.30
9	I	501	FMN	C4A-N5	3.48	1.38	1.30
9	O	501	FMN	C4A-N5	2.98	1.37	1.30
9	C	501	FMN	C4A-N5	2.73	1.36	1.30
9	C	501	FMN	C10-N1	2.49	1.38	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	501	FMN	C5'-C4'-C3'	-3.55	105.52	112.22
9	U	501	FMN	C4-N3-C2	-3.52	119.39	125.64
9	I	501	FMN	C5'-C4'-C3'	-3.39	105.82	112.22
9	O	501	FMN	C4-N3-C2	-3.23	119.91	125.64
9	U	501	FMN	C4A-C10-N10	3.13	120.97	116.48

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

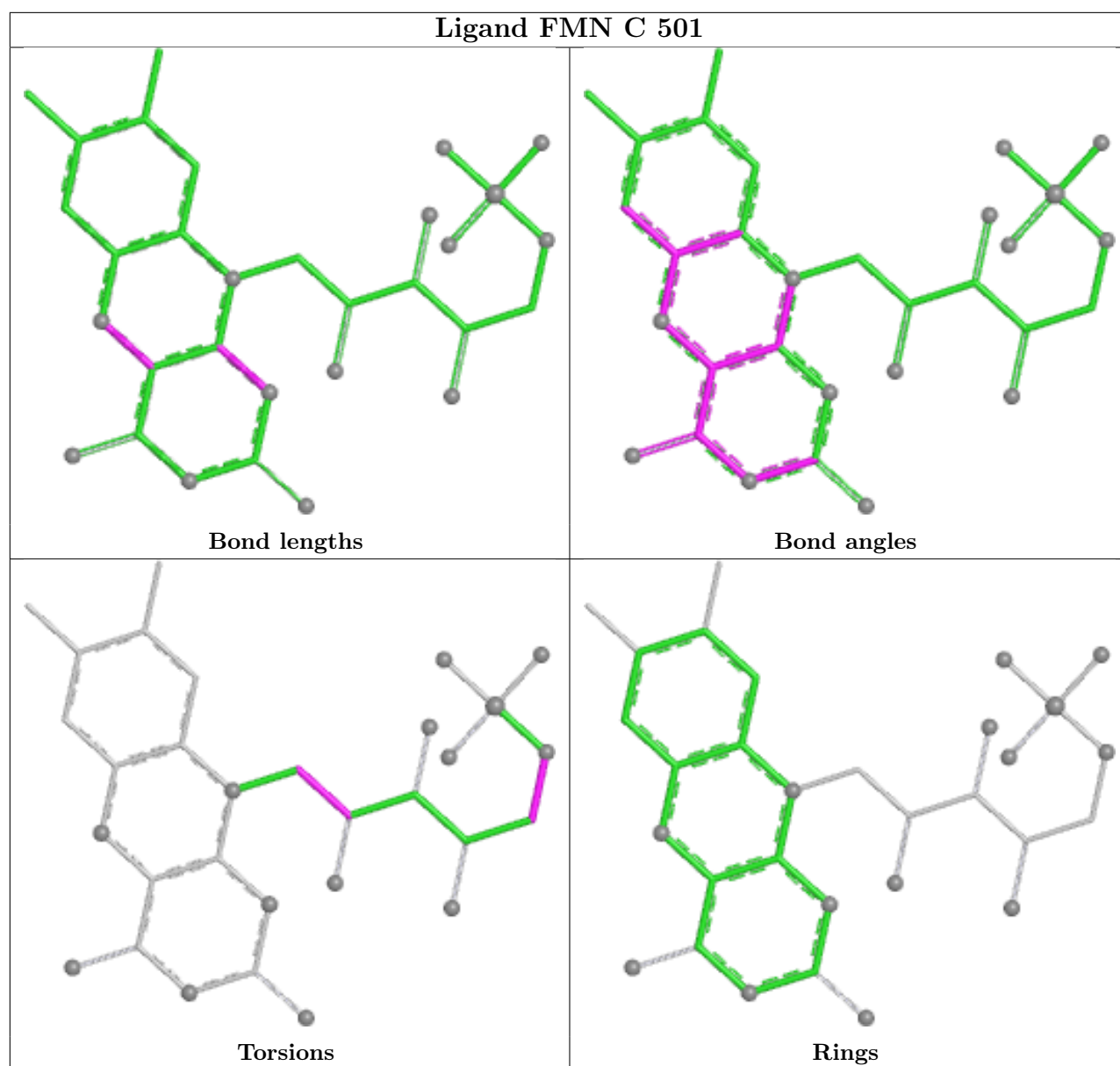
Mol	Chain	Res	Type	Atoms
9	C	501	FMN	N10-C1'-C2'-O2'
9	U	501	FMN	N10-C1'-C2'-O2'
9	C	501	FMN	C4'-C5'-O5'-P
9	O	501	FMN	C4'-C5'-O5'-P
9	I	501	FMN	C4'-C5'-O5'-P

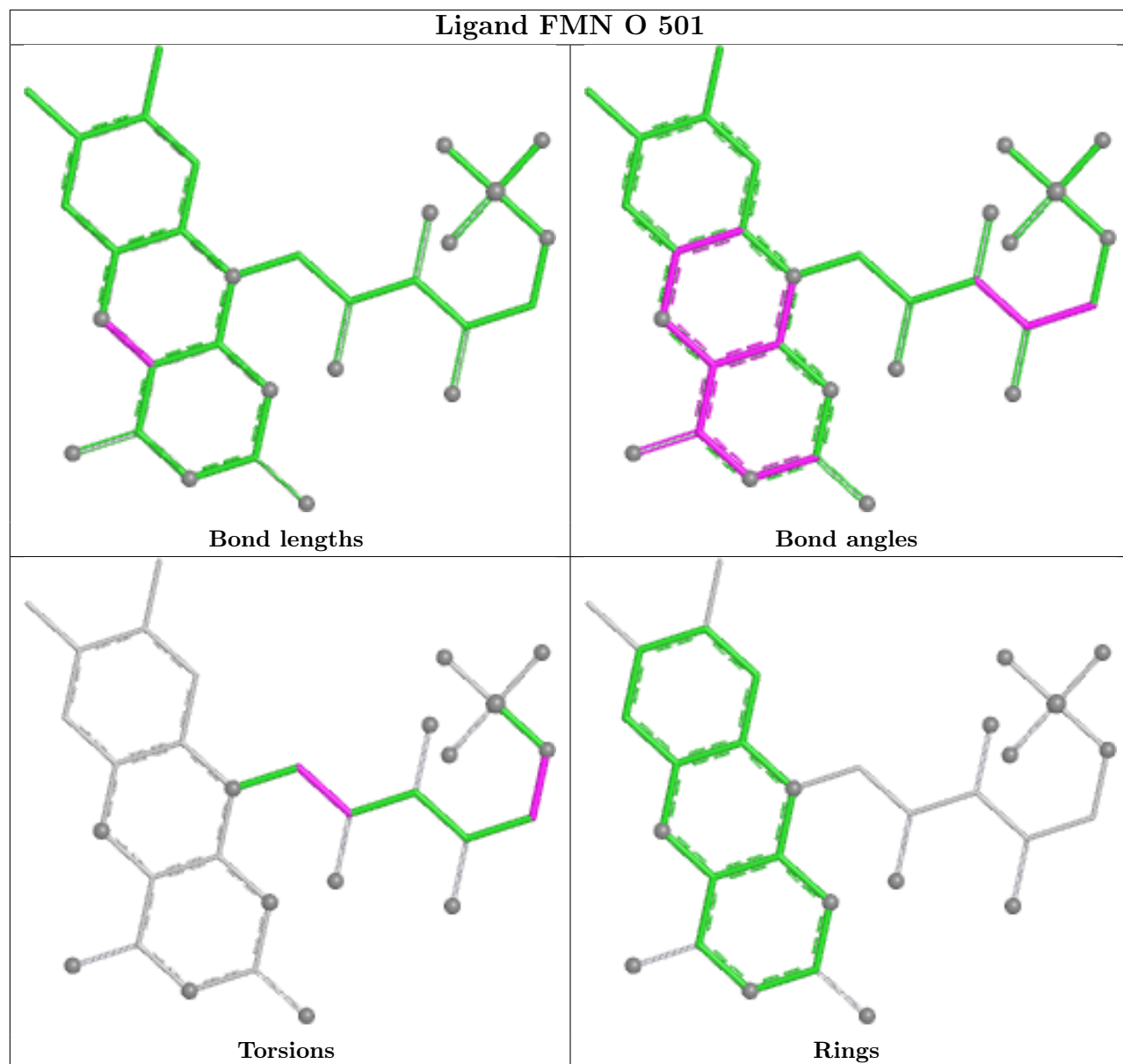
There are no ring outliers.

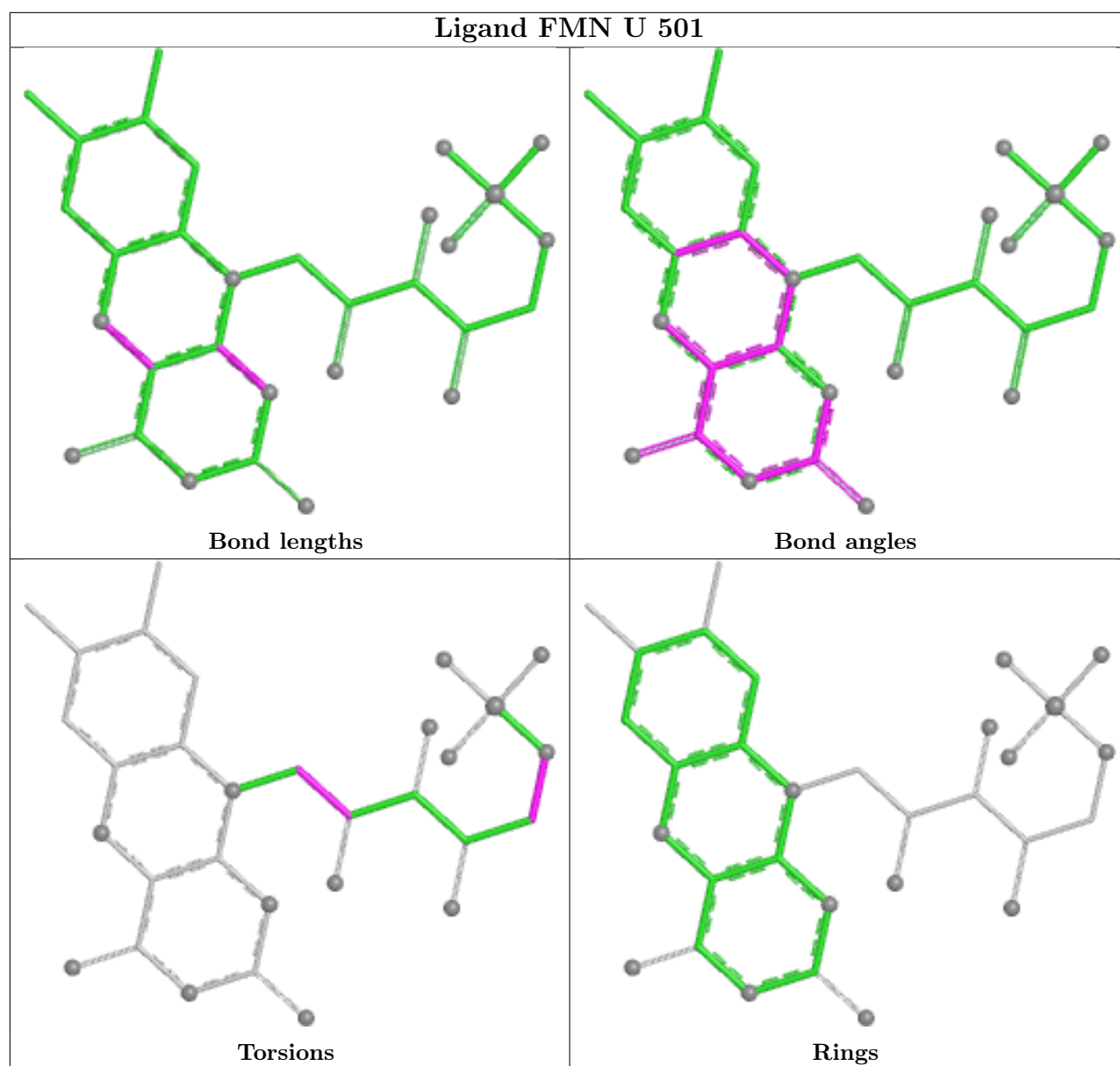
7 monomers are involved in 7 short contacts:

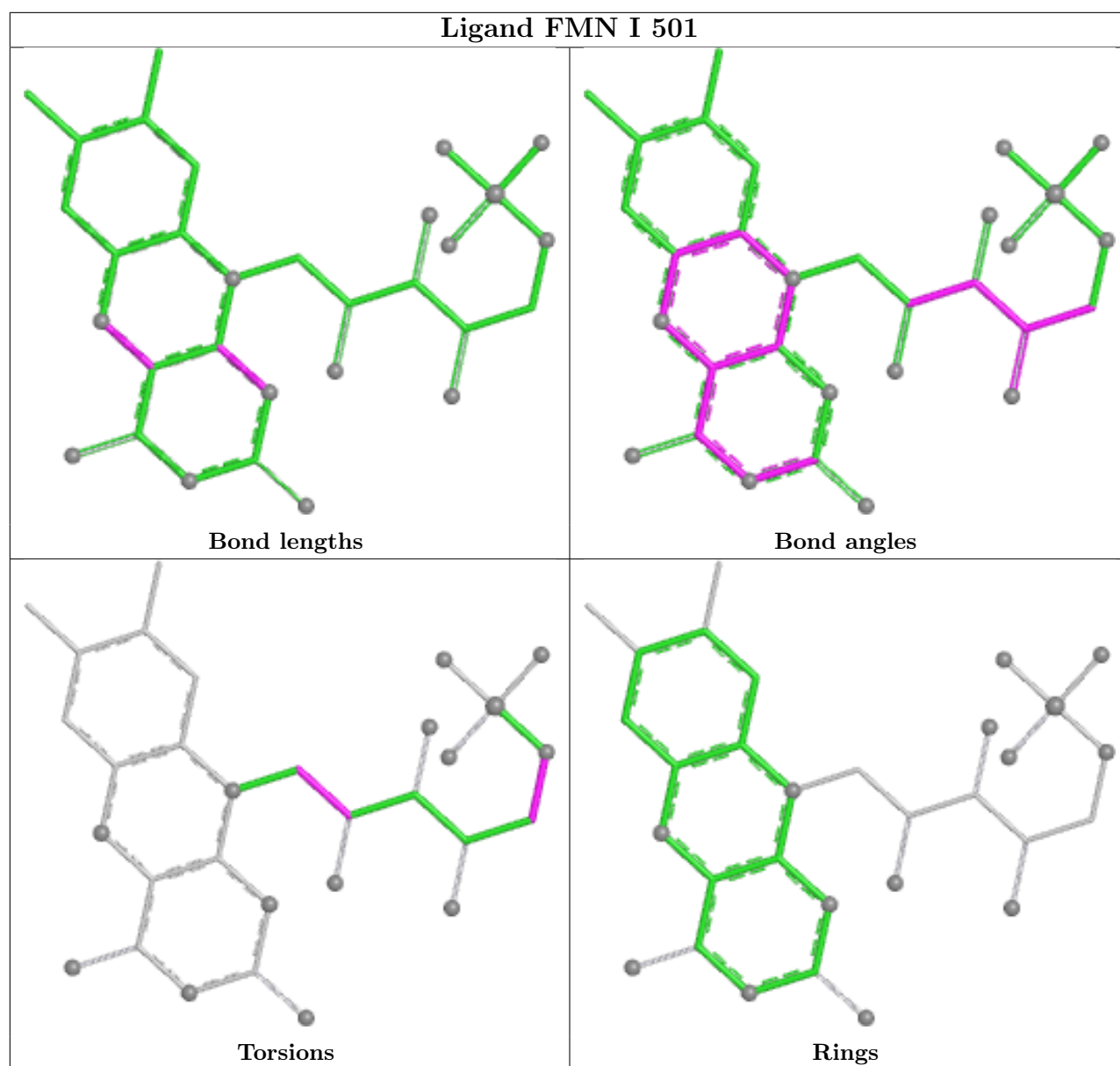
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	201	FES	1	0
7	G	704	SF4	1	0
8	S	705	FES	1	0
9	C	501	FMN	1	0
7	S	704	SF4	1	0
7	A	704	SF4	1	0
9	I	501	FMN	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	626/632 (99%)	-0.63	2 (0%) 90 89	37, 53, 90, 132	0
1	G	626/632 (99%)	-0.53	1 (0%) 91 90	38, 60, 93, 150	0
1	M	626/632 (99%)	-0.55	1 (0%) 91 90	42, 60, 93, 148	0
1	S	626/632 (99%)	-0.42	1 (0%) 91 90	50, 69, 99, 138	0
2	B	585/586 (99%)	0.11	9 (1%) 72 70	51, 104, 155, 231	0
2	H	585/586 (99%)	0.34	18 (3%) 51 48	58, 130, 188, 250	0
2	N	585/586 (99%)	0.03	10 (1%) 69 67	57, 108, 164, 237	0
2	T	585/586 (99%)	0.14	7 (1%) 76 75	73, 115, 165, 236	0
3	C	419/426 (98%)	-0.61	2 (0%) 87 86	41, 62, 94, 127	0
3	I	419/426 (98%)	-0.71	1 (0%) 91 90	35, 52, 85, 129	0
3	O	419/426 (98%)	-0.48	2 (0%) 87 86	48, 74, 105, 172	0
3	U	419/426 (98%)	-0.29	1 (0%) 91 90	59, 80, 114, 165	0
4	D	197/201 (98%)	0.05	15 (7%) 20 17	48, 79, 198, 217	0
4	J	197/201 (98%)	0.33	15 (7%) 20 17	62, 105, 223, 267	0
4	P	197/201 (98%)	0.21	14 (7%) 22 19	59, 94, 206, 254	0
4	V	197/201 (98%)	0.37	16 (8%) 18 15	76, 111, 204, 224	0
5	E	155/160 (96%)	-0.69	1 (0%) 85 85	35, 59, 83, 116	0
5	K	155/160 (96%)	-0.66	1 (0%) 85 85	40, 59, 90, 119	0
5	Q	155/160 (96%)	-0.40	1 (0%) 85 85	50, 80, 110, 145	0
5	W	155/160 (96%)	-0.17	1 (0%) 85 85	61, 90, 127, 152	0
6	F	135/179 (75%)	0.17	4 (2%) 52 49	68, 95, 159, 180	0
6	L	135/179 (75%)	0.54	7 (5%) 33 29	99, 135, 191, 241	0
6	R	135/179 (75%)	0.36	6 (4%) 39 35	76, 113, 181, 245	0
6	X	135/179 (75%)	0.46	8 (5%) 28 25	90, 123, 183, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	8468/8736 (96%)	-0.21	144 (1%) 69 67	35, 80, 159, 267	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	P	44	PRO	6.5
4	J	6	LEU	5.9
2	N	585	ASP	5.0
2	B	584	THR	4.8
4	J	18	ILE	4.7

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 oligosaccharides 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
7	SF4	G	704	8/8	0.92	0.11	99,123,183,232	8
7	SF4	M	704	8/8	0.92	0.11	100,154,218,234	8
7	SF4	A	704	8/8	0.93	0.09	78,96,170,191	8
7	SF4	S	704	8/8	0.93	0.09	84,136,176,213	8
9	FMN	C	501	31/31	0.97	0.08	41,55,65,67	0
9	FMN	U	501	31/31	0.97	0.07	61,69,74,82	0
9	FMN	I	501	31/31	0.98	0.06	32,44,54,60	0
9	FMN	O	501	31/31	0.98	0.05	48,54,65,78	0
7	SF4	L	701	8/8	0.98	0.04	99,106,113,122	0
7	SF4	J	301	8/8	0.99	0.04	77,81,83,83	0
7	SF4	J	302	8/8	0.99	0.04	69,74,78,79	0
7	SF4	D	301	8/8	0.99	0.03	60,62,65,67	0
7	SF4	D	302	8/8	0.99	0.04	54,57,59,60	0

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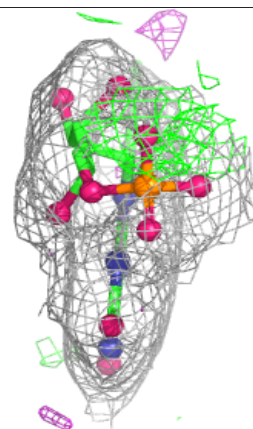
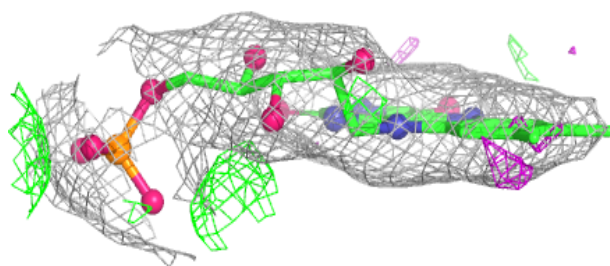
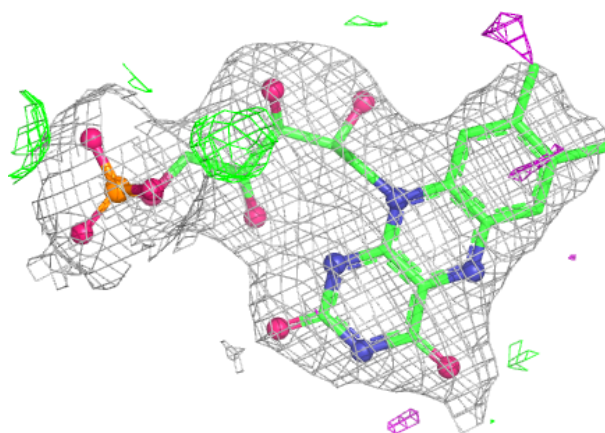
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SF4	P	302	8/8	0.99	0.04	58,65,69,72	0
7	SF4	R	701	8/8	0.99	0.03	78,83,92,97	0
7	SF4	S	701	8/8	0.99	0.03	67,69,74,79	0
7	SF4	S	702	8/8	0.99	0.04	58,62,65,66	0
7	SF4	F	701	8/8	0.99	0.03	70,72,74,75	0
7	SF4	U	502	8/8	0.99	0.04	62,65,69,70	0
7	SF4	V	301	8/8	0.99	0.03	85,87,89,90	0
7	SF4	V	302	8/8	0.99	0.03	80,82,85,90	0
7	SF4	X	701	8/8	0.99	0.04	96,99,101,101	0
8	FES	A	705	4/4	0.99	0.04	51,52,54,57	0
8	FES	M	705	4/4	0.99	0.04	52,53,54,54	0
8	FES	Q	201	4/4	0.99	0.04	66,72,77,79	0
8	FES	W	201	4/4	0.99	0.03	74,78,81,91	0
7	SF4	G	701	8/8	0.99	0.04	46,54,57,57	0
7	SF4	G	702	8/8	0.99	0.05	44,47,50,50	0
7	SF4	G	703	8/8	0.99	0.05	42,44,46,46	0
7	SF4	A	702	8/8	0.99	0.04	39,41,46,49	0
7	SF4	O	502	8/8	1.00	0.03	52,55,58,60	0
7	SF4	P	301	8/8	1.00	0.03	66,71,74,74	0
7	SF4	A	701	8/8	1.00	0.04	45,50,53,53	0
8	FES	E	201	4/4	1.00	0.03	53,56,57,59	0
8	FES	G	705	4/4	1.00	0.04	50,50,52,52	0
8	FES	K	201	4/4	1.00	0.02	52,52,53,53	0
7	SF4	C	502	8/8	1.00	0.03	45,50,52,52	0
7	SF4	A	703	8/8	1.00	0.03	37,42,46,47	0
8	FES	S	705	4/4	1.00	0.02	65,66,69,71	0
7	SF4	M	701	8/8	1.00	0.03	50,54,56,58	0
7	SF4	S	703	8/8	1.00	0.04	51,54,57,59	0
7	SF4	M	702	8/8	1.00	0.04	47,51,53,55	0
7	SF4	M	703	8/8	1.00	0.04	48,50,54,67	0
7	SF4	I	502	8/8	1.00	0.05	43,47,49,53	0

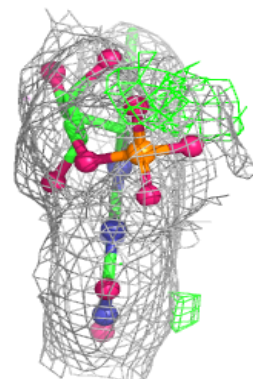
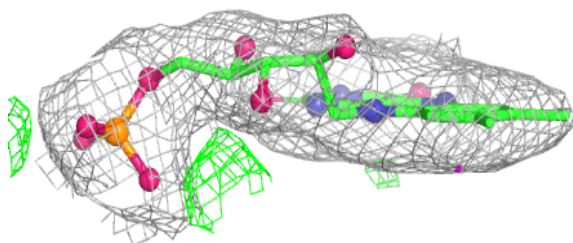
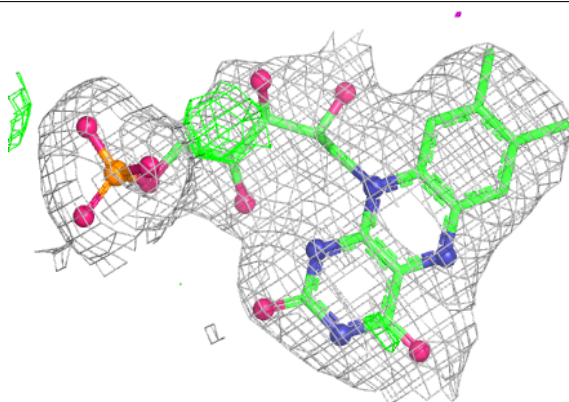
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN C 501:

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

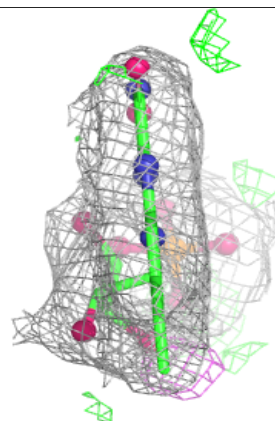
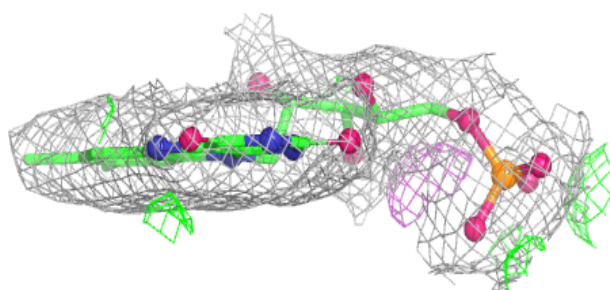
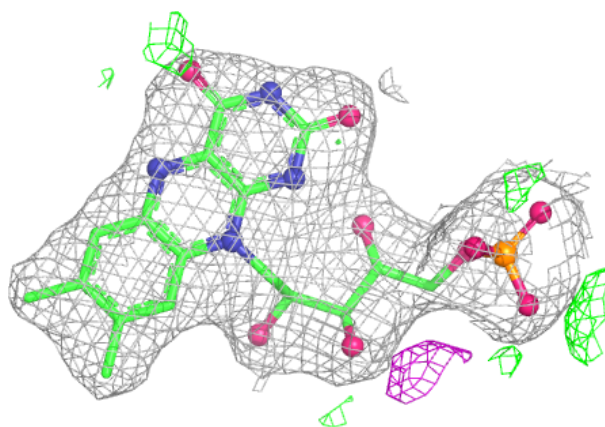
**Electron density around FMN U 501:**

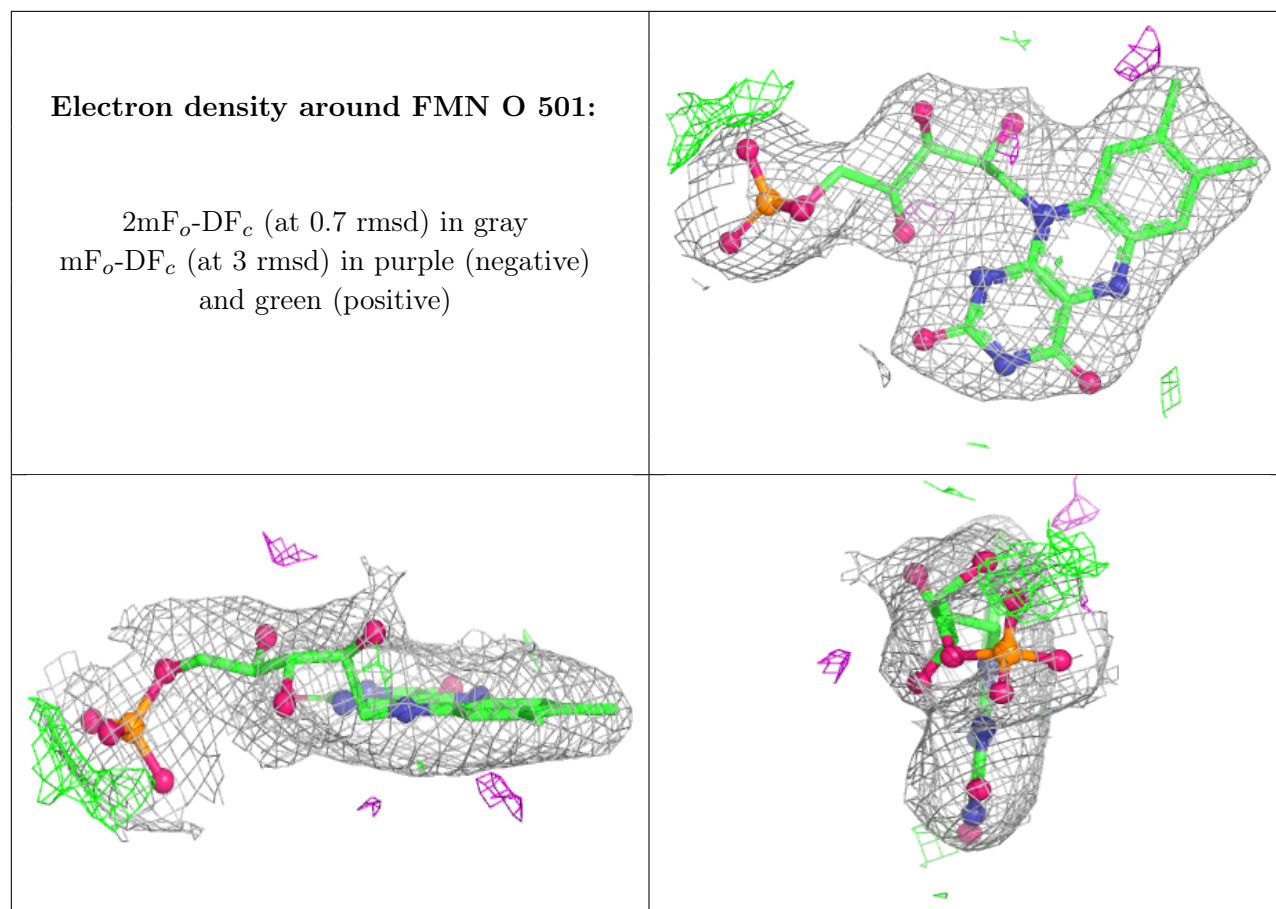
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN I 501:

$2mF_o - DF_c$ (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.