



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:47 PM GMT

PDB ID : 3IAM
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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

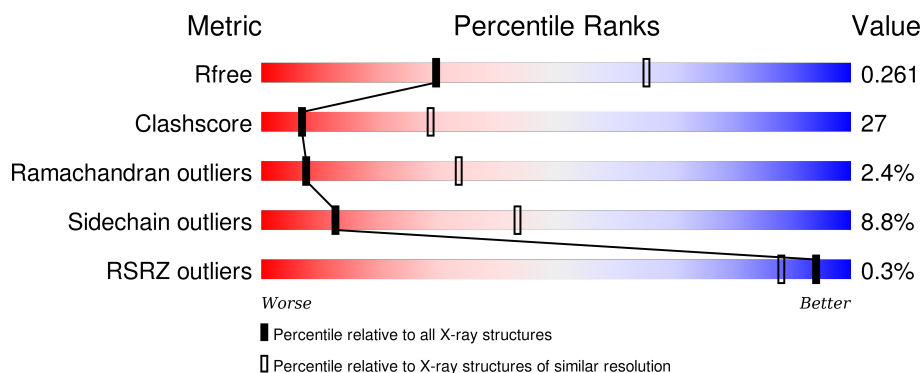
1 Overall quality at a glance

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	
1	A	438	
2	2	181	
2	B	181	
3	3	783	

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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			

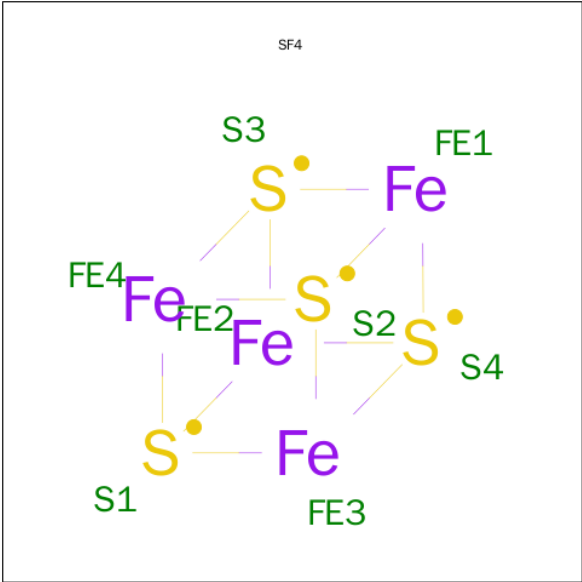
- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

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.

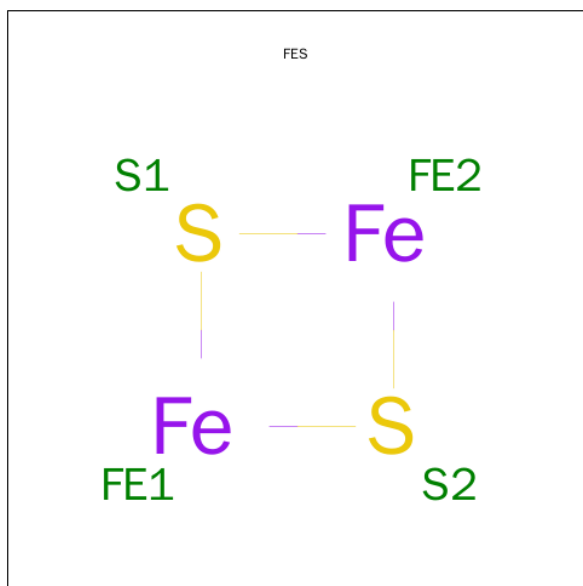
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	H	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



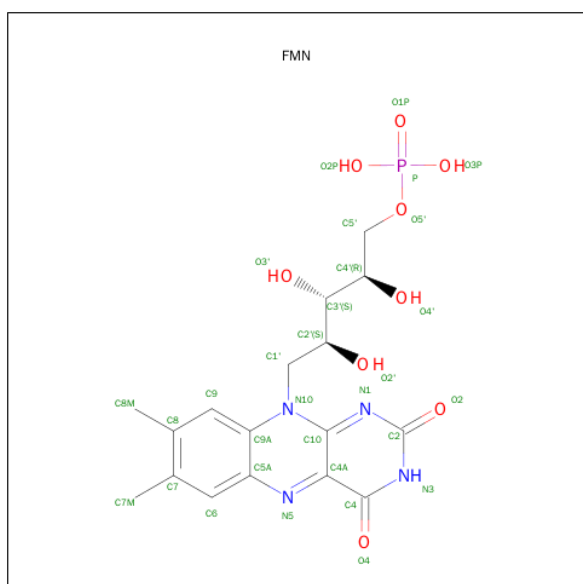
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	6	1	Total	Fe	S	0	0
			8	4	4		
9	9	1	Total	Fe	S	0	0
			8	4	4		
9	9	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	1	1	Total	Fe	S	0	0
			8	4	4		
9	F	1	Total	Fe	S	0	0
			8	4	4		
9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

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



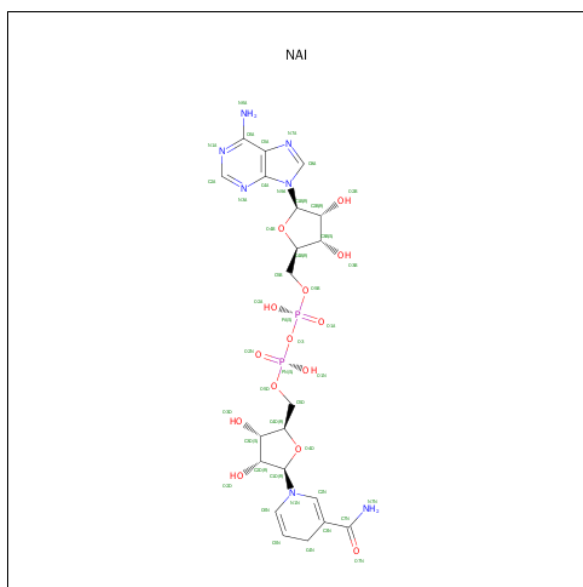
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	3	1	Total	Fe	S	0	0
			4	2	2		
10	2	1	Total	Fe	S	0	0
			4	2	2		
10	C	1	Total	Fe	S	0	0
			4	2	2		
10	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 12 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	1	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
12	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	1	1	Total	Mg	0	0
			1	1		
13	E	1	Total	Mg	0	0
			1	1		
13	C	2	Total	Mg	0	0
			2	2		
13	A	1	Total	Mg	0	0
			1	1		
13	4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	5	1	Total 1	Mg 1	0	0
13	2	1	Total 1	Mg 1	0	0
13	3	2	Total 2	Mg 2	0	0

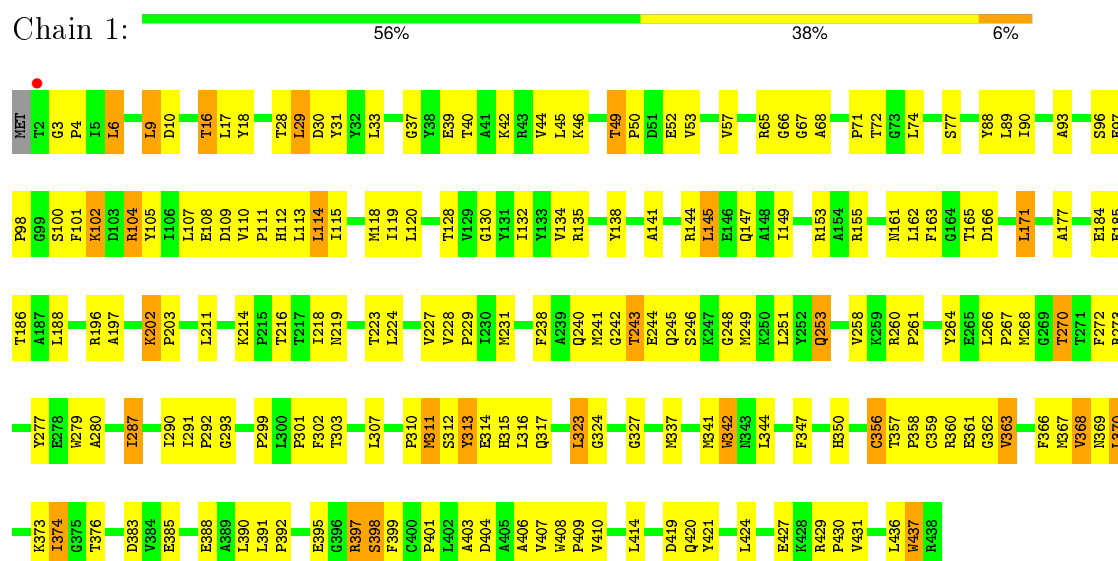
- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

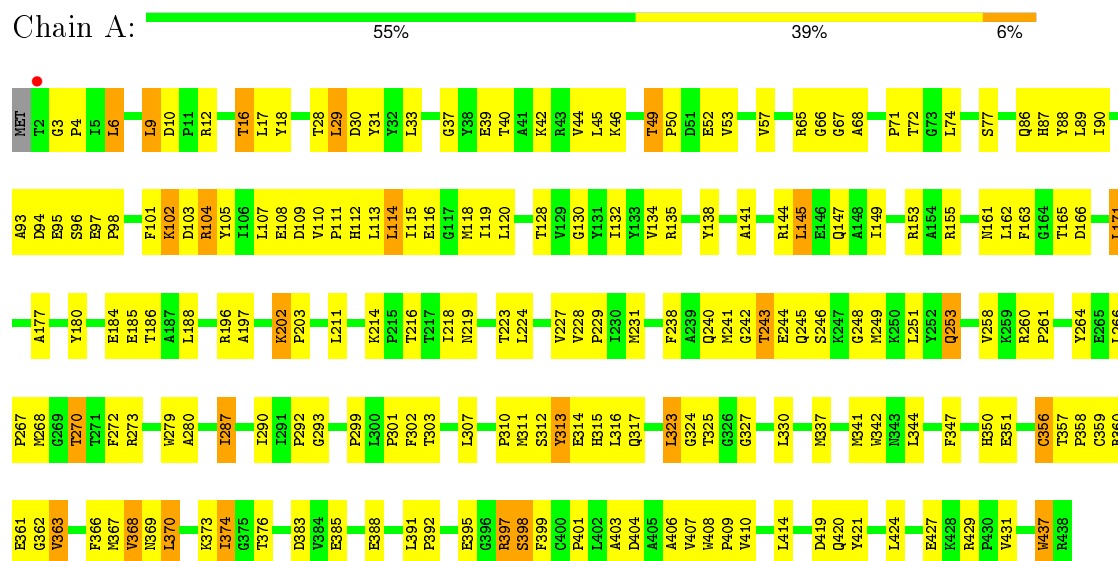
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

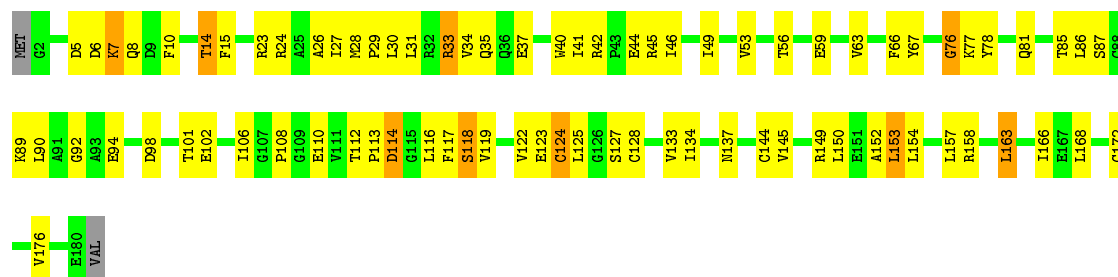


• Molecule 1: NADH-quinone oxidoreductase subunit 1



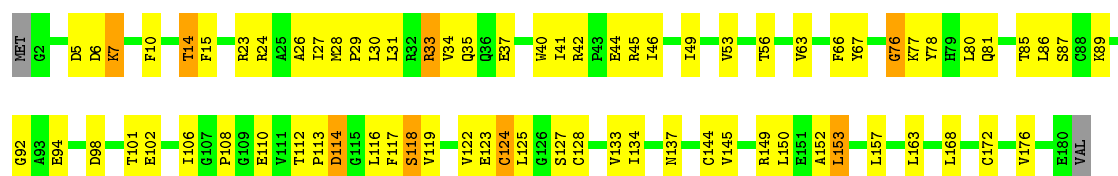
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 



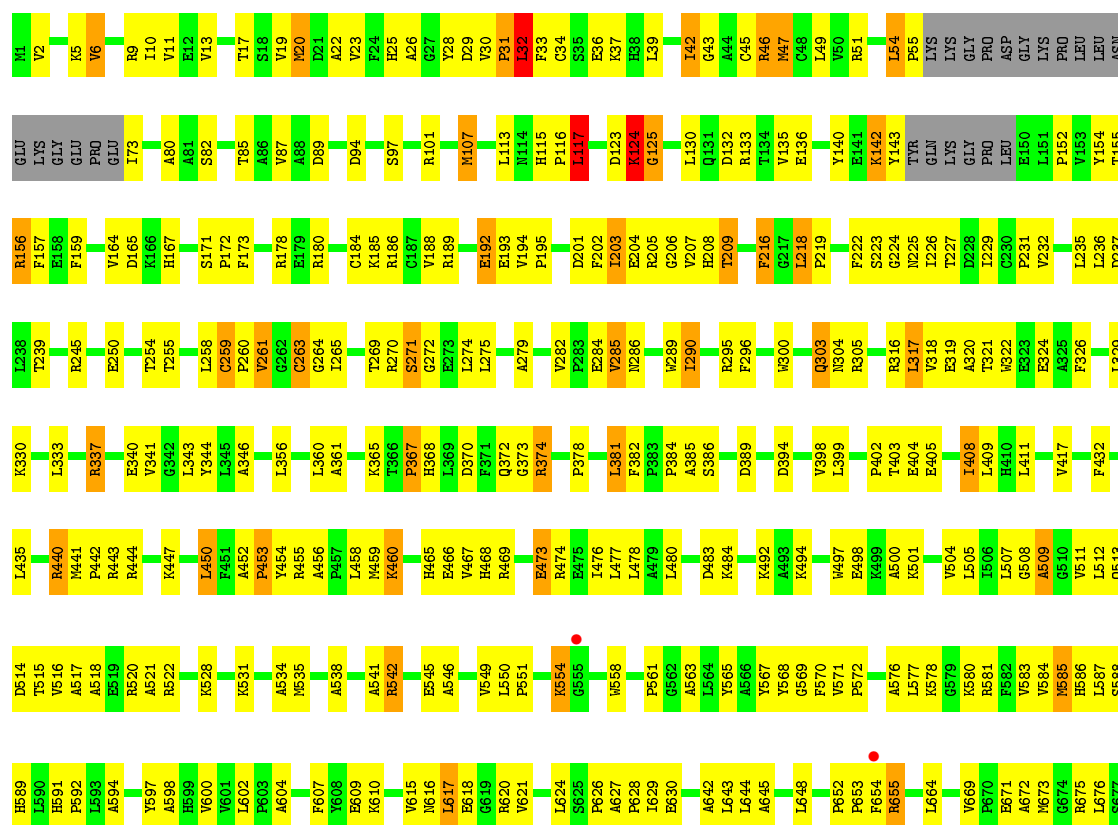
• Molecule 2: NADH-quinone oxidoreductase subunit 2

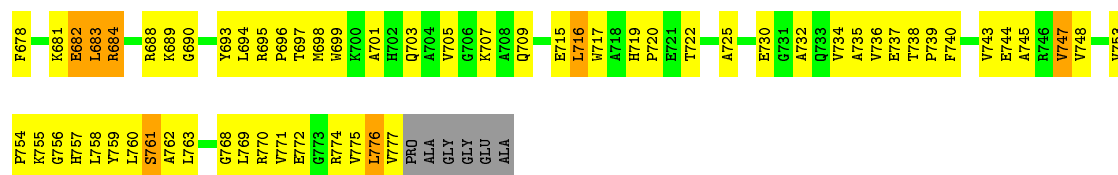
Chain B: 



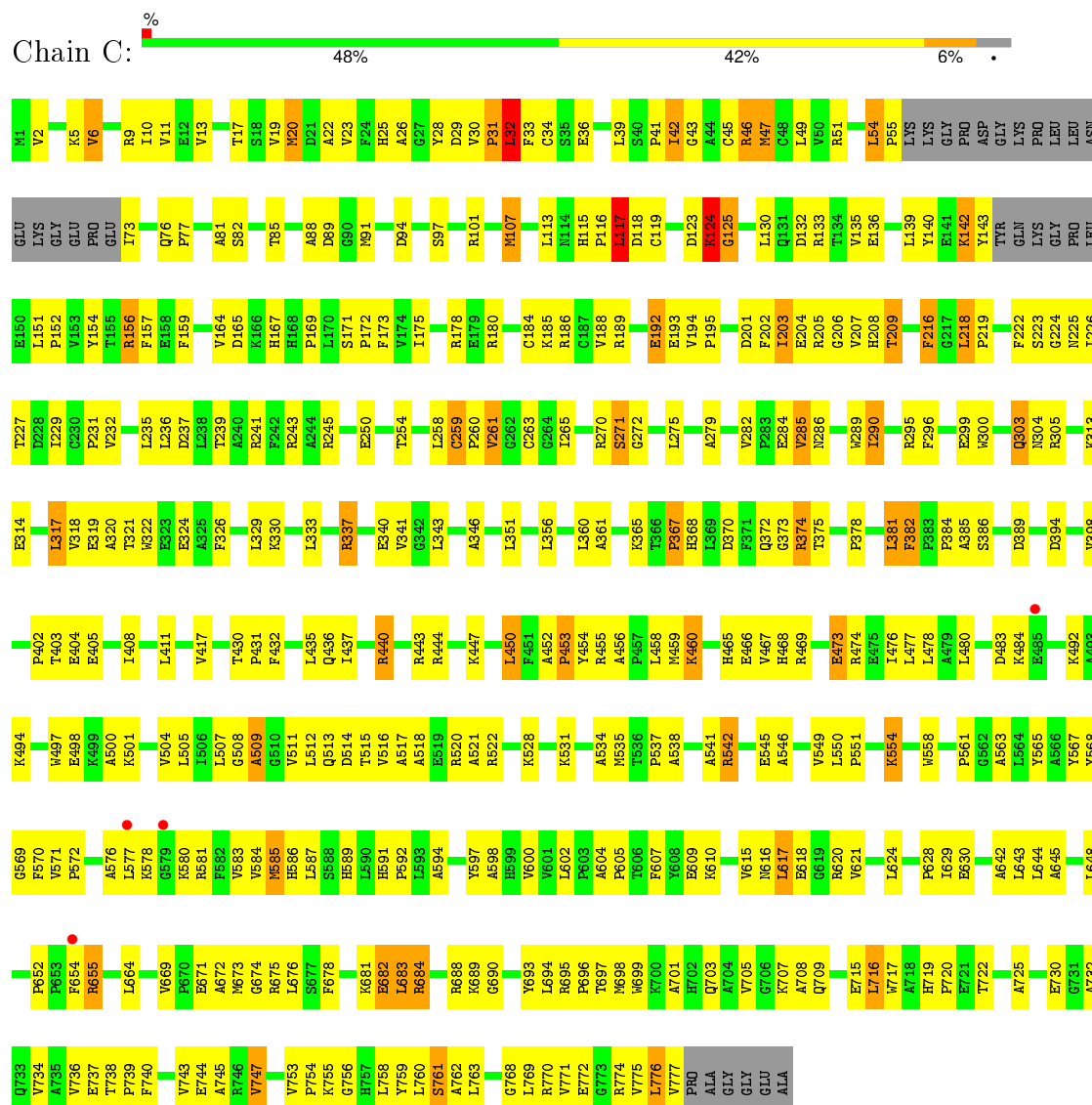
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3: 

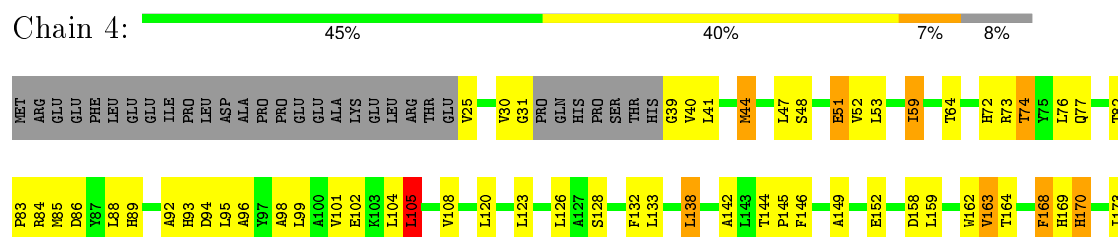


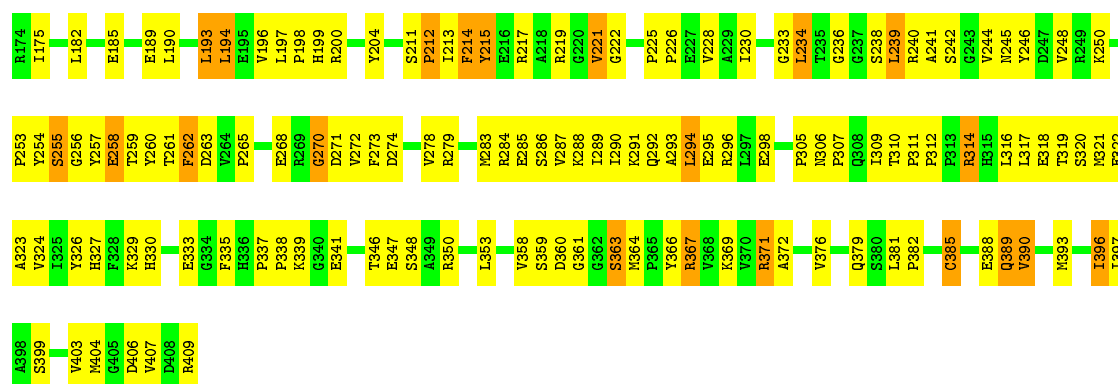


• Molecule 3: NADH-quinone oxidoreductase subunit 3

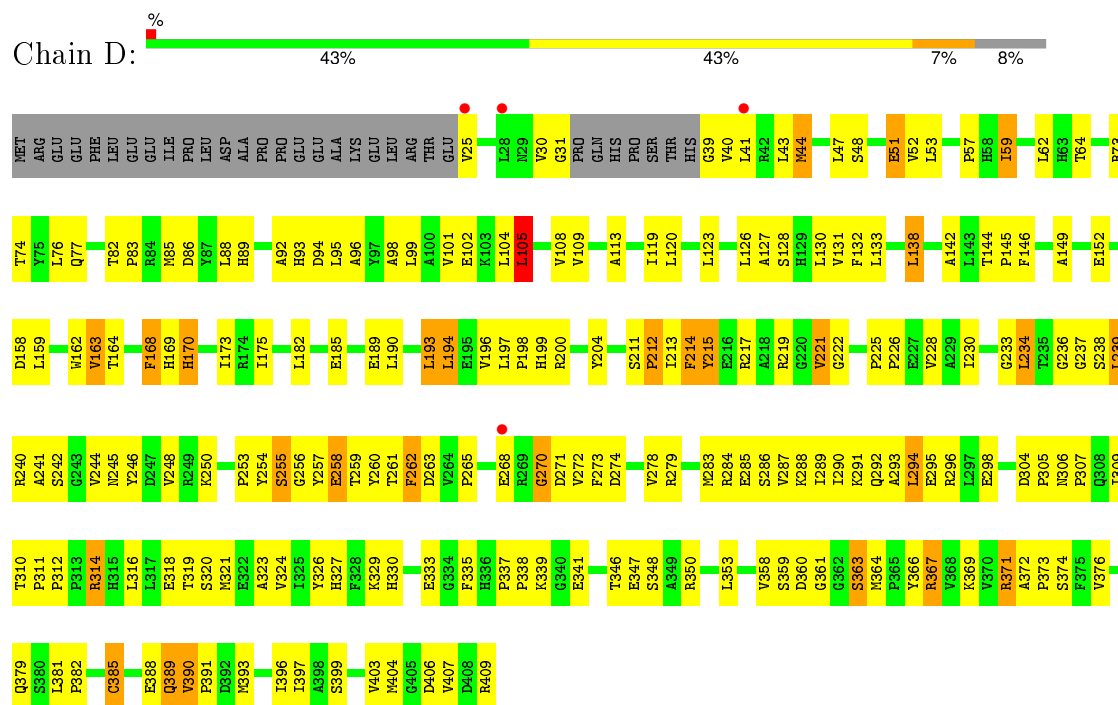


• Molecule 4: NADH-quinone oxidoreductase subunit 4

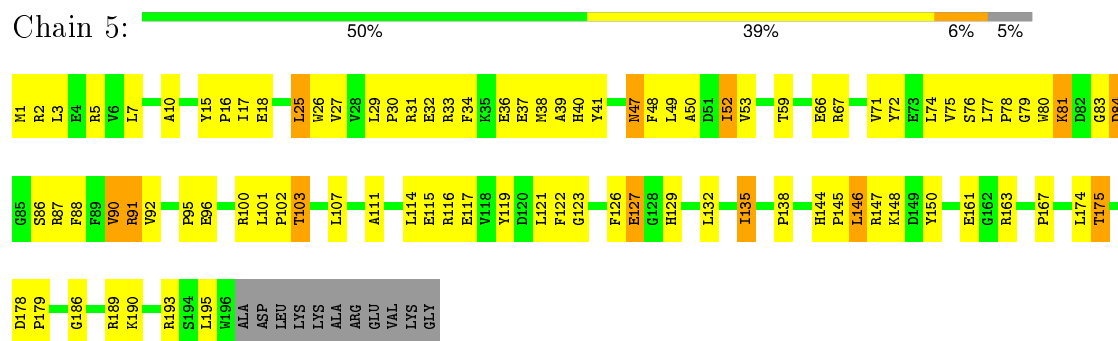




• Molecule 4: NADH-quinone oxidoreductase subunit 4

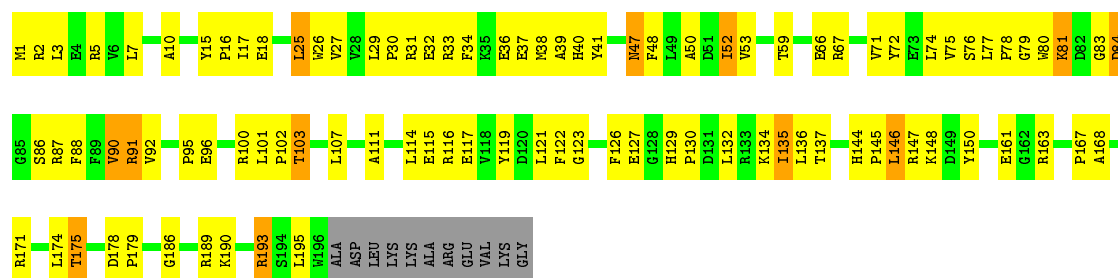


• Molecule 5: NADH-quinone oxidoreductase subunit 5

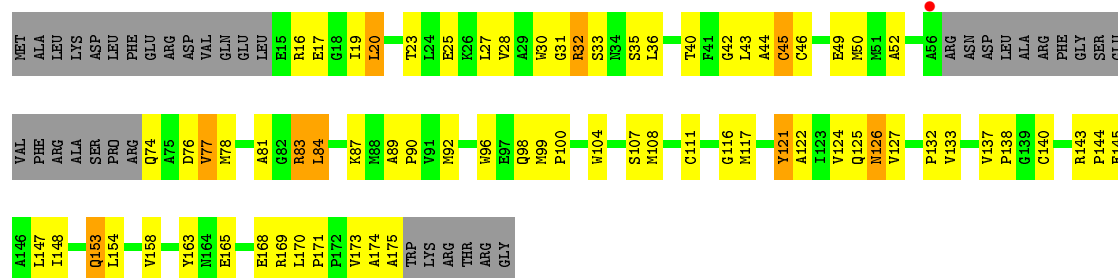


• Molecule 5: NADH-quinone oxidoreductase subunit 5

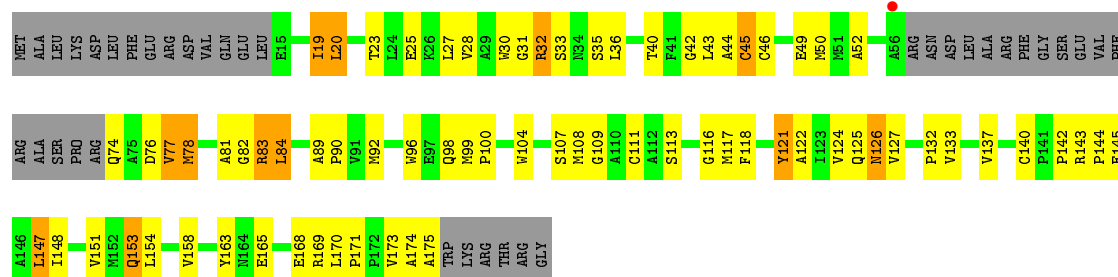




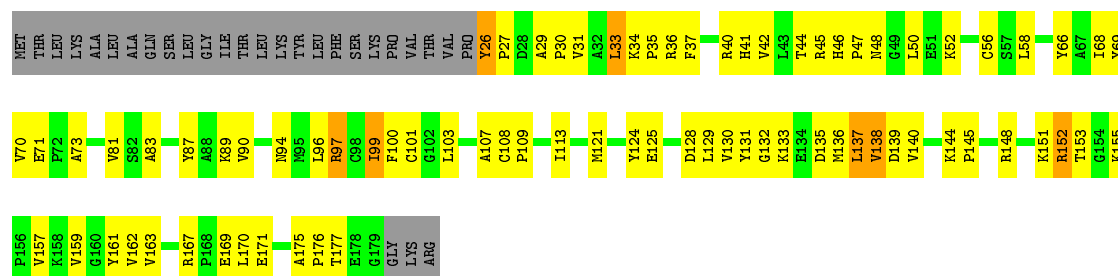
• Molecule 6: NADH-quinone oxidoreductase subunit 6



• Molecule 6: NADH-quinone oxidoreductase subunit 6

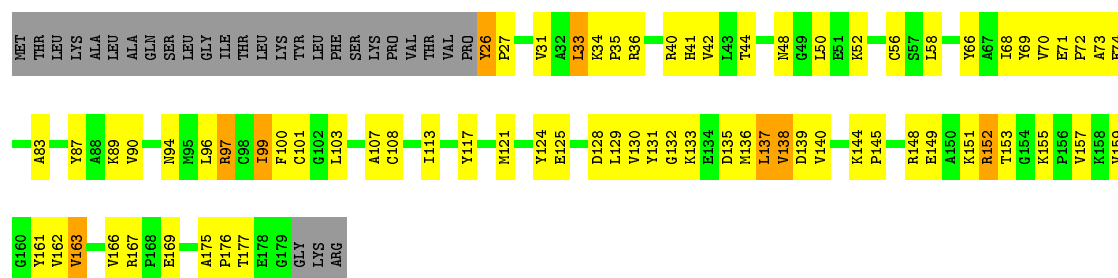


• Molecule 7: NADH-quinone oxidoreductase subunit 9



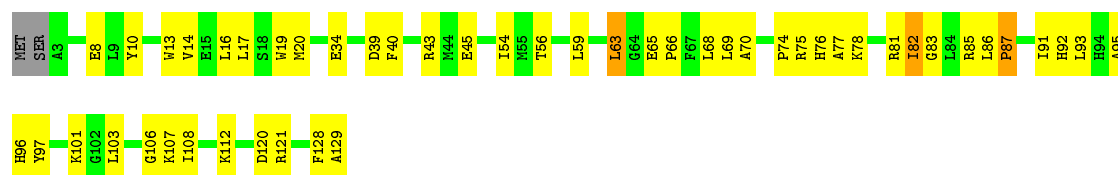
• Molecule 7: NADH-quinone oxidoreductase subunit 9





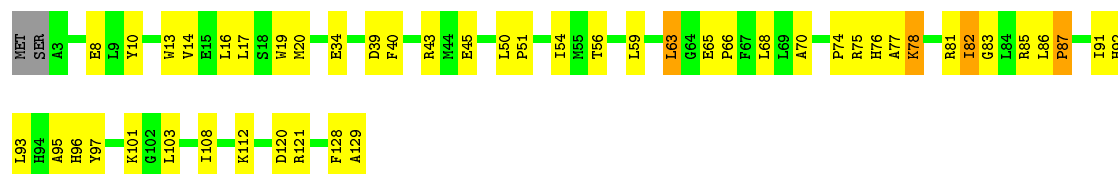
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7: 60% 36%



- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain H: 61% 34%



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 29.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.57-3.10) 89.9 (29.91-3.10)	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 (phenix.refine)	Depositor
R, R_{free}	0.231 , 0.262 0.231 , 0.261	Depositor DCC
R_{free} test set	2215 reflections (1.98%)	DCC
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 , 24.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 114091 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CA, NAI, FMN, FES, SF4

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	0.45	1/3506 (0.0%)	0.63	2/4745 (0.0%)
1	A	0.44	1/3506 (0.0%)	0.62	1/4745 (0.0%)
2	2	0.45	0/1443	0.64	0/1958
2	B	0.43	0/1443	0.63	0/1958
3	3	0.43	0/6019	0.61	1/8163 (0.0%)
3	C	0.41	0/6019	0.59	1/8163 (0.0%)
4	4	0.40	0/3096	0.59	2/4207 (0.0%)
4	D	0.39	0/3096	0.59	2/4207 (0.0%)
5	5	0.43	0/1656	0.61	0/2246
5	E	0.40	0/1656	0.61	0/2246
6	6	0.48	0/1126	0.64	0/1528
6	F	0.45	0/1126	0.63	0/1528
7	9	0.48	0/1224	0.66	0/1663
7	G	0.46	0/1224	0.65	0/1663
8	7	0.43	0/1059	0.60	0/1429
8	H	0.42	0/1059	0.60	0/1429
All	All	0.43	2/38258 (0.0%)	0.61	9/51878 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	CYS	CB-SG	-5.67	1.72	1.81
1	1	356	CYS	CB-SG	-5.08	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	39	GLY	N-CA-C	-7.74	93.76	113.10
4	D	39	GLY	N-CA-C	-7.61	94.08	113.10
4	4	105	LEU	CA-CB-CG	7.23	131.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	105	LEU	CA-CB-CG	7.19	131.84	115.30
3	3	32	LEU	CA-CB-CG	5.90	128.88	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	165	1
1	A	3417	0	3388	167	0
2	2	1410	0	1376	70	0
2	B	1410	0	1376	66	0
3	3	5880	0	5911	347	1
3	C	5880	0	5911	366	0
4	4	3018	0	3009	194	0
4	D	3018	0	3009	213	0
5	5	1607	0	1574	97	0
5	E	1607	0	1574	98	0
6	6	1102	0	1108	80	0
6	F	1102	0	1108	81	0
7	9	1193	0	1160	64	0
7	G	1193	0	1160	71	0
8	7	1031	0	1029	41	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	2	4	0	0	0	0
10	3	4	0	0	1	0
10	B	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	4	0	0	1	0
11	1	31	0	19	6	0
11	A	31	0	19	0	0
12	1	44	0	27	5	0
12	A	44	0	27	7	0
13	1	1	0	0	0	0
13	2	1	0	0	0	0
13	3	2	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	A	1	0	0	0	0
13	C	2	0	0	0	0
13	E	1	0	0	0	0
14	7	1	0	0	0	0
14	H	1	0	0	0	0
All	All	37606	0	37202	1998	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 27.

The worst 5 of 1998 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

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%)	380 (87%)	48 (11%)	7 (2%)	12	44
1	A	435/438 (99%)	379 (87%)	50 (12%)	6 (1%)	14	48
2	2	177/181 (98%)	152 (86%)	21 (12%)	4 (2%)	8	35
2	B	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	8	35
3	3	748/783 (96%)	624 (83%)	100 (13%)	24 (3%)	5	26
3	C	748/783 (96%)	626 (84%)	98 (13%)	24 (3%)	5	26
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	7	33
4	D	374/409 (91%)	332 (89%)	32 (9%)	10 (3%)	6	31
5	5	194/207 (94%)	167 (86%)	23 (12%)	4 (2%)	9	37
5	E	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	9	37
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	4	24
6	F	140/181 (77%)	113 (81%)	21 (15%)	6 (4%)	3	19
7	9	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	26	65
7	G	152/182 (84%)	132 (87%)	19 (12%)	1 (1%)	26	65
8	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	24	63
8	H	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	24	63
All	All	4690/5020 (93%)	4019 (86%)	560 (12%)	111 (2%)	7	33

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%)	321 (90%)	34 (10%)	10	37
1	A	355/356 (100%)	322 (91%)	33 (9%)	11	39
2	2	150/152 (99%)	135 (90%)	15 (10%)	9	34
2	B	150/152 (99%)	134 (89%)	16 (11%)	8	31
3	3	607/628 (97%)	560 (92%)	47 (8%)	16	50
3	C	607/628 (97%)	559 (92%)	48 (8%)	15	49
4	4	326/355 (92%)	296 (91%)	30 (9%)	11	40
4	D	326/355 (92%)	298 (91%)	28 (9%)	13	45
5	5	167/175 (95%)	155 (93%)	12 (7%)	18	53
5	E	167/175 (95%)	154 (92%)	13 (8%)	16	49
6	6	117/149 (78%)	107 (92%)	10 (8%)	13	45
6	F	117/149 (78%)	106 (91%)	11 (9%)	11	39
7	9	126/150 (84%)	111 (88%)	15 (12%)	6	25
7	G	126/150 (84%)	111 (88%)	15 (12%)	6	25
8	7	104/106 (98%)	96 (92%)	8 (8%)	16	50
8	H	104/106 (98%)	96 (92%)	8 (8%)	16	50
All	All	3904/4142 (94%)	3561 (91%)	343 (9%)	12	43

5 of 343 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	9	99	ILE
1	A	342	TRP
6	F	121	TYR
7	9	139	ASP
1	A	16	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
7	9	94	ASN
1	A	161	ASN
5	E	112	ASN
1	A	87	HIS
1	A	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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
9	SF4	1	439	1	0,12,12	0.00	-	0,24,24	0.00	-
11	FMN	1	440	-	32,33,33	1.45	4 (12%)	34,50,50	2.00	6 (17%)
12	NAI	1	441	-	41,48,48	3.70	26 (63%)	46,73,73	1.96	5 (10%)
10	FES	2	182	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	3	784	3	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	3	785	3	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	3	786	3	0,12,12	0.00	-	0,24,24	0.00	-
10	FES	3	787	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	6	182	6	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SF4	9	183	7	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	9	184	7	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	A	439	1	0,12,12	0.00	-	0,24,24	0.00	-
11	FMN	A	440	-	32,33,33	1.22	3 (9%)	34,50,50	1.84	8 (23%)
12	NAI	A	441	-	41,48,48	3.66	26 (63%)	46,73,73	2.08	7 (15%)
10	FES	B	182	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	C	784	3	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	C	785	3	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	C	786	3	0,12,12	0.00	-	0,24,24	0.00	-
10	FES	C	787	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	F	182	6	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	G	183	7	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	G	184	7	0,12,12	0.00	-	0,24,24	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
9	SF4	1	439	1	-	0/0/48/48	0/6/5/5
11	FMN	1	440	-	-	0/18/18/18	0/3/3/3
12	NAI	1	441	-	-	0/25/72/72	0/5/5/5
10	FES	2	182	2	-	0/0/4/4	0/1/1/1
9	SF4	3	784	3	-	0/0/48/48	0/6/5/5
9	SF4	3	785	3	-	0/0/48/48	0/6/5/5
9	SF4	3	786	3	-	0/0/48/48	0/6/5/5
10	FES	3	787	3	-	0/0/4/4	0/1/1/1
9	SF4	6	182	6	-	0/0/48/48	0/6/5/5
9	SF4	9	183	7	-	0/0/48/48	0/6/5/5
9	SF4	9	184	7	-	0/0/48/48	0/6/5/5
9	SF4	A	439	1	-	0/0/48/48	0/6/5/5
11	FMN	A	440	-	-	0/18/18/18	0/3/3/3
12	NAI	A	441	-	-	0/25/72/72	0/5/5/5
10	FES	B	182	2	-	0/0/4/4	0/1/1/1
9	SF4	C	784	3	-	0/0/48/48	0/6/5/5
9	SF4	C	785	3	-	0/0/48/48	0/6/5/5
9	SF4	C	786	3	-	0/0/48/48	0/6/5/5
10	FES	C	787	3	-	0/0/4/4	0/1/1/1
9	SF4	F	182	6	-	0/0/48/48	0/6/5/5
9	SF4	G	183	7	-	0/0/48/48	0/6/5/5
9	SF4	G	184	7	-	0/0/48/48	0/6/5/5

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	441	NAI	C2B-C1B	-9.32	1.38	1.53
12	A	441	NAI	C2B-C1B	-9.15	1.39	1.53
12	A	441	NAI	C3D-C4D	-6.01	1.36	1.53
12	1	441	NAI	C2B-C3B	-5.72	1.38	1.53
12	1	441	NAI	C3D-C4D	-5.52	1.38	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	441	NAI	N3A-C2A-N1A	-11.06	120.18	128.87
12	1	441	NAI	N3A-C2A-N1A	-9.79	121.18	128.87
11	A	440	FMN	N3-C2-N1	-5.01	119.25	127.69
11	1	440	FMN	N3-C2-N1	-4.46	120.18	127.69
12	1	441	NAI	C4D-O4D-C1D	-3.88	100.97	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	440	FMN	6	0
12	1	441	NAI	5	0
9	3	784	SF4	1	0
9	3	785	SF4	1	0
9	3	786	SF4	1	0
10	3	787	FES	1	0
9	6	182	SF4	1	0
9	9	183	SF4	2	0
12	A	441	NAI	7	0
10	B	182	FES	1	0
9	C	784	SF4	1	0
9	C	785	SF4	1	0
9	C	786	SF4	1	0
10	C	787	FES	1	0
9	F	182	SF4	2	0
9	G	183	SF4	1	0

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%)	-0.37	1 (0%) 95 91	28, 49, 71, 111	0
1	A	437/438 (99%)	-0.47	1 (0%) 95 91	29, 49, 72, 111	0
2	2	179/181 (98%)	-0.40	0 100 100	32, 48, 78, 118	0
2	B	179/181 (98%)	-0.48	0 100 100	33, 48, 79, 118	0
3	3	754/783 (96%)	-0.19	2 (0%) 94 88	25, 68, 106, 126	0
3	C	754/783 (96%)	-0.24	4 (0%) 91 83	26, 69, 107, 127	0
4	4	378/409 (92%)	-0.18	0 100 100	33, 66, 103, 119	0
4	D	378/409 (92%)	-0.21	4 (1%) 82 66	33, 67, 103, 119	0
5	5	196/207 (94%)	-0.18	0 100 100	34, 66, 102, 116	0
5	E	196/207 (94%)	-0.28	0 100 100	35, 68, 103, 117	0
6	6	144/181 (79%)	-0.13	1 (0%) 89 78	36, 62, 93, 135	0
6	F	144/181 (79%)	-0.24	1 (0%) 89 78	37, 63, 93, 135	0
7	9	154/182 (84%)	-0.33	0 100 100	30, 48, 86, 120	0
7	G	154/182 (84%)	-0.43	0 100 100	31, 48, 86, 120	0
8	7	127/129 (98%)	-0.32	0 100 100	43, 55, 91, 115	0
8	H	127/129 (98%)	-0.33	0 100 100	43, 56, 91, 114	0
All	All	4738/5020 (94%)	-0.28	14 (0%) 94 88	25, 58, 101, 135	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	654	PHE	4.0
6	F	56	ALA	3.0
3	C	577	LEU	2.7
3	3	654	PHE	2.7
3	3	555	GLY	2.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
14	CA	7	204	1/1	0.98	0.22	1.96	36,36,36,36	0
14	CA	H	204	1/1	1.00	0.22	1.33	32,32,32,32	0
11	FMN	1	440	31/31	0.96	0.20	0.52	34,42,46,48	0
9	SF4	F	182	8/8	0.99	0.18	0.35	22,32,48,55	0
12	NAI	A	441	44/44	0.95	0.19	0.22	45,59,68,71	0
9	SF4	9	184	8/8	0.99	0.20	0.18	8,12,33,34	0
12	NAI	1	441	44/44	0.95	0.20	0.15	39,50,62,65	0
9	SF4	1	439	8/8	0.99	0.19	0.13	0,12,24,25	0
9	SF4	C	784	8/8	0.99	0.17	0.02	6,11,31,36	0
9	SF4	G	184	8/8	0.99	0.19	0.00	13,20,37,39	0
9	SF4	A	439	8/8	0.99	0.17	-0.03	0,22,31,38	0
11	FMN	A	440	31/31	0.97	0.17	-0.10	39,44,47,51	0
9	SF4	9	183	8/8	0.99	0.19	-0.12	2,19,36,39	0
9	SF4	C	785	8/8	0.99	0.17	-0.21	10,13,29,33	0
9	SF4	G	183	8/8	1.00	0.17	-0.34	11,15,32,36	0
10	FES	B	182	4/4	0.99	0.16	-0.37	22,22,37,45	0
9	SF4	3	784	8/8	0.99	0.18	-0.39	0,9,26,36	0
13	MG	4	410	1/1	0.91	0.24	-0.40	59,59,59,59	0
9	SF4	C	786	8/8	0.99	0.16	-0.43	19,27,45,47	0
9	SF4	6	182	8/8	0.99	0.18	-0.56	0,23,42,50	0
9	SF4	3	786	8/8	0.99	0.18	-0.64	3,15,43,48	0
10	FES	2	182	4/4	0.99	0.16	-0.71	11,20,27,33	0
10	FES	C	787	4/4	0.99	0.15	-0.76	19,26,32,33	0
9	SF4	3	785	8/8	0.99	0.17	-1.02	0,11,22,22	0
10	FES	3	787	4/4	0.99	0.16	-1.57	9,14,30,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	MG	2	206	1/1	0.91	0.12	-2.99	32,32,32,32	0
13	MG	3	789	1/1	0.97	0.20	-	42,42,42,42	0
13	MG	5	208	1/1	0.97	0.18	-	26,26,26,26	0
13	MG	C	789	1/1	0.96	0.06	-	44,44,44,44	0
13	MG	3	788	1/1	0.99	0.28	-	23,23,23,23	0
13	MG	A	442	1/1	0.93	0.16	-	54,54,54,54	0
13	MG	C	788	1/1	0.99	0.27	-	35,35,35,35	0
13	MG	E	208	1/1	0.94	0.10	-	44,44,44,44	0
13	MG	1	442	1/1	0.98	0.19	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.