



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:12 am GMT

PDB ID : 1NU1
Title : Crystal Structure of Mitochondrial Cytochrome bc1 Complexed with 2-nonyl-4-hydroxyquinoline N-oxide (NQNO)
Authors : Gao, X.; Wen, X.; Esser, L.; Quinn, B.; Yu, L.; Yu, C.-A.; Xia, D.
Deposited on : 2003-01-30
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

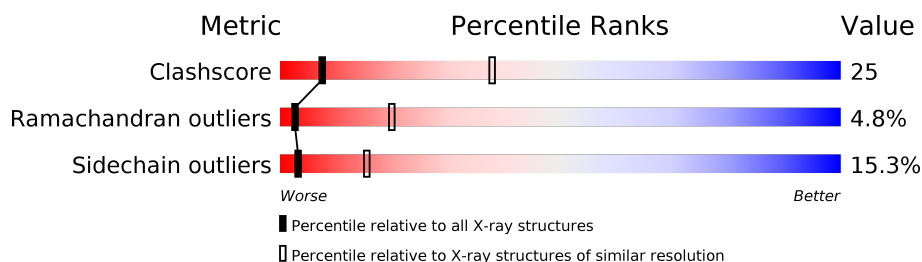
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	

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Mol	Chain	Length	Quality of chain
8	H	78	
9	I	57	
10	J	62	
11	K	56	

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
13	FES	E	200	-	-	X	-
14	QNO	C	383	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16666 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 Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	18			

- Molecule 4 is a protein called cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			575	347	102	121	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase 8 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	S	0	0	0
			483	316	82	85				

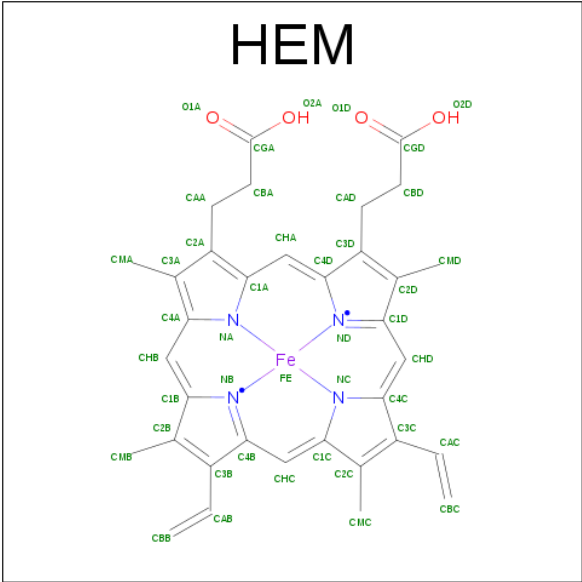
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			437	292	78	66	1			

There is a discrepancy between the modelled and reference sequences:

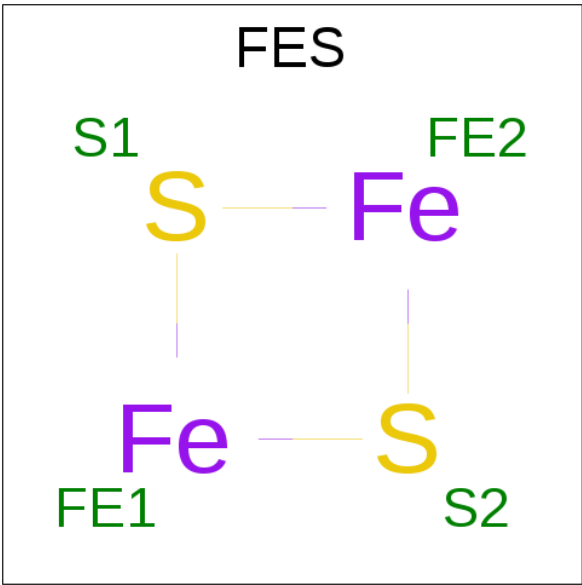
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



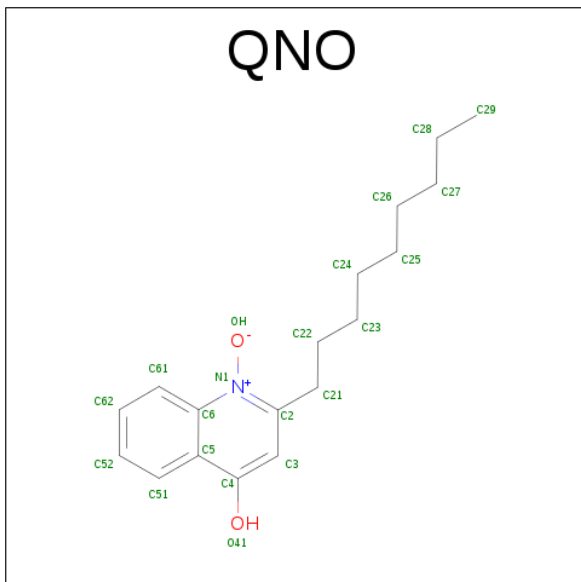
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 14 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (three-letter code: QNO) (formula: $C_{18}H_{25}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 15 is water.

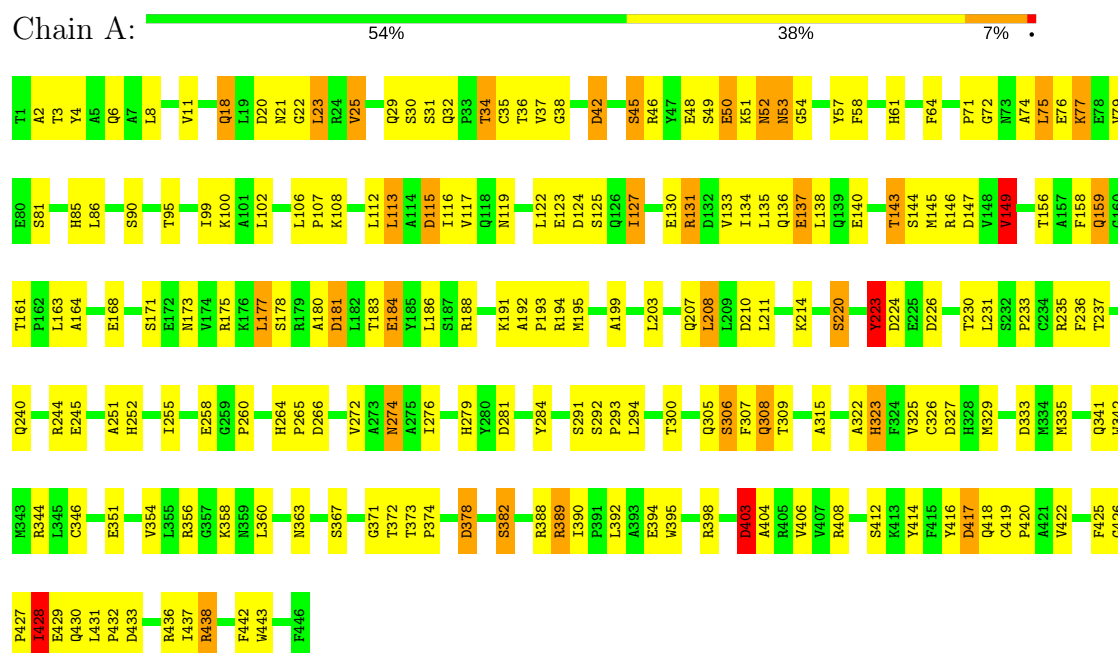
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	2	Total	O	0	0
			2	2		

3 Residue-property plots

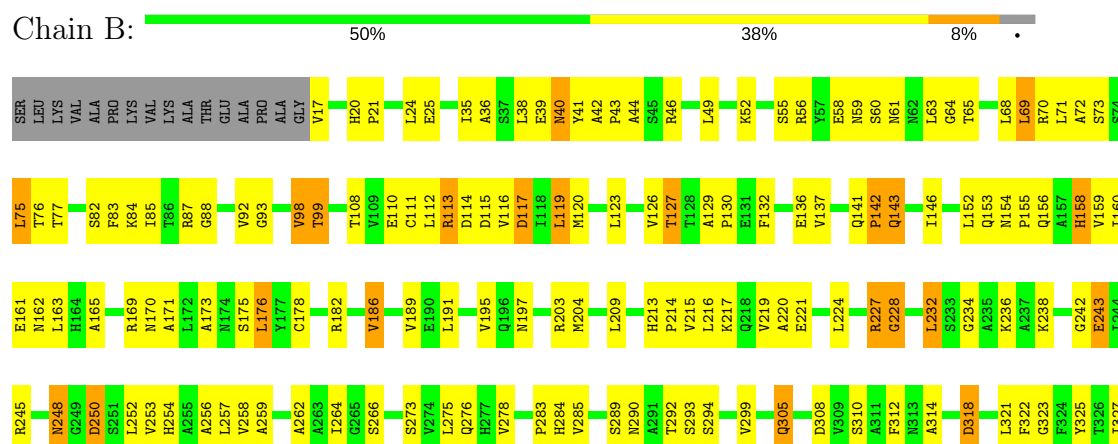
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

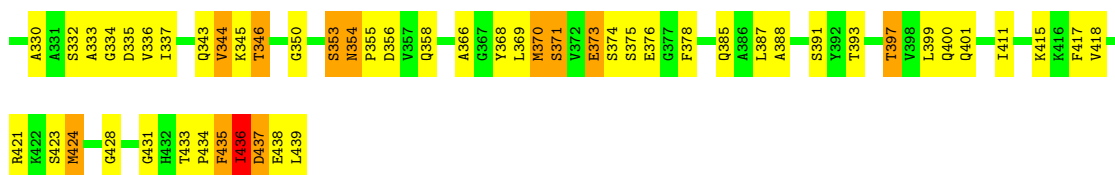
Note EDS was not executed.

- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial



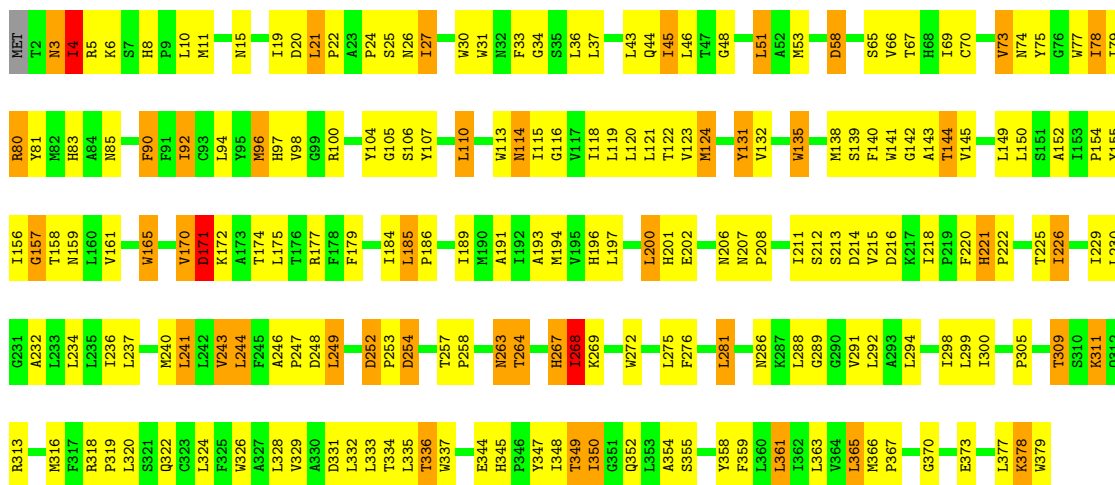
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial





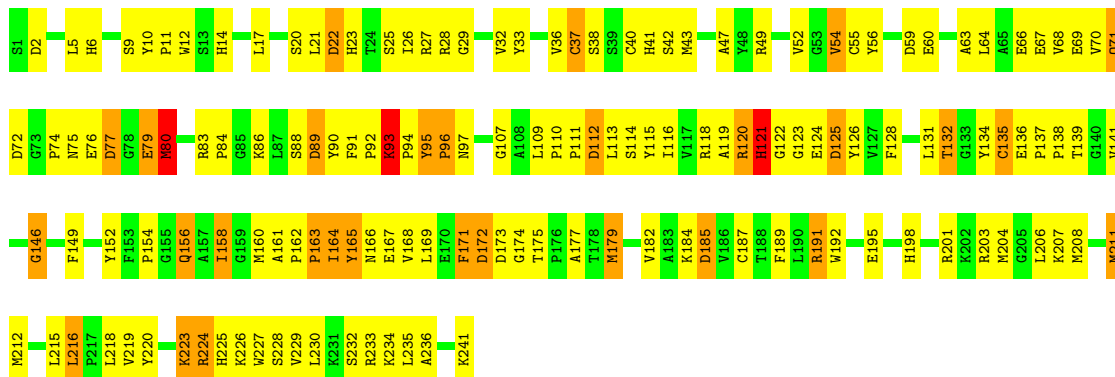
• Molecule 3: Cytochrome b

Chain C: 46% 41% 11%



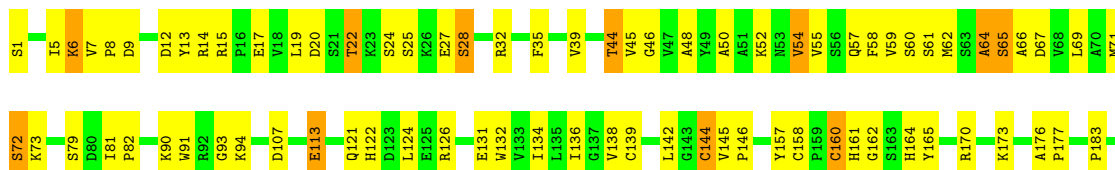
• Molecule 4: cytochrome c1

Chain D: 38% 49% 12%



• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial

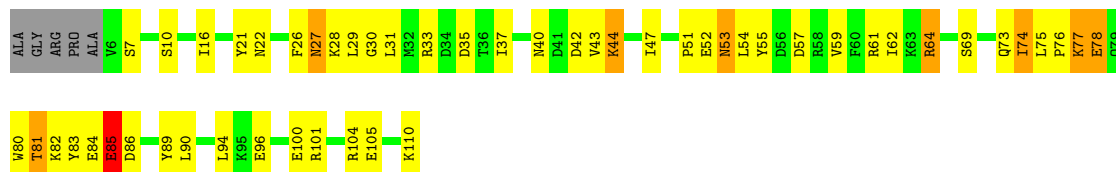
Chain E: 57% 37% 6%





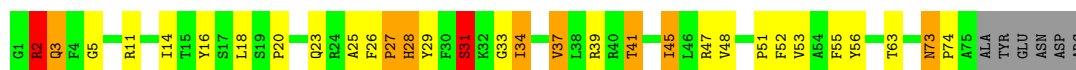
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F: 48% 39% 7% • 5%



- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G: 54% 26% 10% • 7%



- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H: 54% 29% 5% • 10%



- Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein

Chain I: 18% 39% 32% 12%



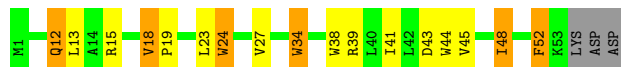
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J: 47% 42% 8% • •



- Molecule 11: Ubiquinol-cytochrome C reductase complex 6.4 kDa protein

Chain K: 64% 20% 11% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.84Å 153.84Å 590.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.9 (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.215 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16666	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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: HEM, QNO, 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	0.83	1/3531 (0.0%)	0.96	14/4792 (0.3%)
2	B	1.11	5/3232 (0.2%)	1.04	8/4386 (0.2%)
3	C	0.79	0/3100	0.92	10/4242 (0.2%)
4	D	0.66	0/1977	0.98	12/2684 (0.4%)
5	E	0.60	0/1553	0.89	5/2100 (0.2%)
6	F	0.97	0/930	1.03	2/1246 (0.2%)
7	G	0.83	0/649	0.87	0/878
8	H	0.55	0/580	0.96	6/777 (0.8%)
9	I	1.00	0/411	1.48	5/558 (0.9%)
10	J	0.67	0/495	0.86	0/672
11	K	0.67	0/453	0.87	1/621 (0.2%)
All	All	0.85	6/16911 (0.0%)	0.97	63/22956 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	2	0
3	C	2	0
4	D	2	0
7	G	1	0
8	H	1	0
9	I	2	0
All	All	10	0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	437	ASP	CB-CG	-6.05	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	VAL	CB-CG2	-5.79	1.40	1.52
2	B	159	VAL	CB-CG2	-5.26	1.41	1.52
2	B	262	ALA	CA-CB	-5.22	1.41	1.52
2	B	137	VAL	CB-CG2	-5.18	1.42	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	122	GLY	N-CA-C	-7.87	93.42	113.10
2	B	250	ASP	CB-CG-OD2	7.34	124.91	118.30
6	F	85	GLU	N-CA-C	-7.32	91.25	111.00
2	B	318	ASP	CB-CG-OD2	7.16	124.75	118.30
5	E	67	ASP	CB-CG-OD2	6.75	124.37	118.30

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	197	ASN	CA
2	B	305	GLN	CA
3	C	221	HIS	CA
3	C	345	HIS	CA
4	D	145	GLU	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	150	0
2	B	3172	0	3152	160	1
3	C	3003	0	3065	184	0
4	D	1918	0	1870	138	0
5	E	1519	0	1503	66	0
6	F	911	0	904	37	0
7	G	628	0	636	31	0
8	H	575	0	550	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	406	0	437	99	0
10	J	483	0	465	40	0
11	K	437	0	439	17	0
12	C	86	0	60	21	0
12	D	43	0	30	5	0
13	E	4	0	0	2	0
14	C	21	0	24	6	0
15	C	2	0	0	5	0
All	All	16666	0	16491	814	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 25.

The worst 5 of 814 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:11:MET:SD	3:C:11:MET:CE	2.05	1.45
10:J:18:SER:HA	11:K:24:TRP:CZ3	1.76	1.21
10:J:18:SER:HA	11:K:24:TRP:HZ3	0.94	1.11
9:I:20:ARG:HG3	9:I:51:CYS:HB2	1.28	1.08
2:B:76:THR:HG22	2:B:82:SER:H	1.19	1.05

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)
2:B:169:ARG:NH1	2:B:437:ASP:OD2[10_665]	1.98	0.22

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	444/446 (100%)	376 (85%)	53 (12%)	15 (3%)	4	28
2	B	421/439 (96%)	373 (89%)	39 (9%)	9 (2%)	8	42
3	C	376/379 (99%)	302 (80%)	56 (15%)	18 (5%)	2	20
4	D	239/241 (99%)	181 (76%)	38 (16%)	20 (8%)	1	6
5	E	194/196 (99%)	160 (82%)	29 (15%)	5 (3%)	6	36
6	F	103/110 (94%)	84 (82%)	17 (16%)	2 (2%)	9	46
7	G	73/81 (90%)	62 (85%)	5 (7%)	6 (8%)	1	6
8	H	68/78 (87%)	50 (74%)	12 (18%)	6 (9%)	1	5
9	I	55/57 (96%)	25 (46%)	16 (29%)	14 (26%)	0	0
10	J	59/62 (95%)	44 (75%)	11 (19%)	4 (7%)	1	10
11	K	51/56 (91%)	38 (74%)	11 (22%)	2 (4%)	3	25
All	All	2083/2145 (97%)	1695 (81%)	287 (14%)	101 (5%)	2	20

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
2	B	266	SER
2	B	305	GLN
2	B	353	SER
2	B	436	ILE

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	370/370 (100%)	322 (87%)	48 (13%)	5	22
2	B	332/343 (97%)	285 (86%)	47 (14%)	4	18
3	C	326/327 (100%)	272 (83%)	54 (17%)	2	12
4	D	206/206 (100%)	172 (84%)	34 (16%)	2	12
5	E	168/168 (100%)	155 (92%)	13 (8%)	15	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	96/98 (98%)	76 (79%)	20 (21%)	1	6
7	G	66/71 (93%)	57 (86%)	9 (14%)	4	20
8	H	67/74 (90%)	56 (84%)	11 (16%)	2	12
9	I	44/44 (100%)	31 (70%)	13 (30%)	0	1
10	J	46/52 (88%)	36 (78%)	10 (22%)	1	6
11	K	42/46 (91%)	32 (76%)	10 (24%)	1	3
All	All	1763/1799 (98%)	1494 (85%)	269 (15%)	3	15

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	185	LEU
4	D	17	LEU
9	I	56	ARG
3	C	225	THR
3	C	281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	ASN
2	B	342	ASN
6	F	53	ASN
2	B	170	ASN
2	B	197	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

5 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
12	HEM	C	381	3	28,50,50	3.33	17 (60%)	17,82,82	1.76	4 (23%)
12	HEM	C	382	3	28,50,50	2.92	16 (57%)	17,82,82	1.88	5 (29%)
14	QNO	C	383	-	21,22,22	1.38	2 (9%)	22,28,28	1.26	4 (18%)
12	HEM	D	242	4	28,50,50	3.31	17 (60%)	17,82,82	2.00	7 (41%)
13	FES	E	200	5	0,4,4	0.00	-	0,4,4	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
12	HEM	C	381	3	-	0/6/54/54	0/0/8/8
12	HEM	C	382	3	-	0/6/54/54	0/0/8/8
14	QNO	C	383	-	1/1/0/0	0/9/9/9	0/2/2/2
12	HEM	D	242	4	-	0/6/54/54	0/0/8/8
13	FES	E	200	5	-	0/0/4/4	0/1/1/1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	C3B-C2B	-6.84	1.31	1.40
12	C	381	HEM	C3C-C2C	-6.46	1.31	1.40
12	C	382	HEM	C3B-C2B	-6.05	1.32	1.40
12	D	242	HEM	C3C-C2C	-5.89	1.32	1.40
12	C	381	HEM	C3B-C2B	-5.26	1.33	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	CAA-CBA-CGA	-5.06	104.02	112.66
12	C	381	HEM	CBA-CAA-C2A	-3.33	106.12	112.48
12	D	242	HEM	CAA-CBA-CGA	-3.06	107.43	112.66
12	C	382	HEM	CMD-C2D-C1D	-2.80	124.15	128.46
12	D	242	HEM	C4A-C3A-C2A	-2.72	105.11	107.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	383	QNO	C2

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	7	0
12	C	382	HEM	14	0
14	C	383	QNO	6	0
12	D	242	HEM	5	0
13	E	200	FES	2	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.