



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 02:47 pm GMT

PDB ID : 1NEN
Title : Complex II (Succinate Dehydrogenase) From E. Coli with Dinitrophenol-17 inhibitor co-crystallized at the ubiquinone binding site
Authors : Yankovskaya, V.; Horsefield, R.; Tornroth, S.; Luna-Chavez, C.; Miyoshi, H.; Leger, C.; Byrne, B.; Cecchini, G.; Iwata, S.
Deposited on : 2002-12-11
Resolution : 2.90 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)
Xtrriage (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

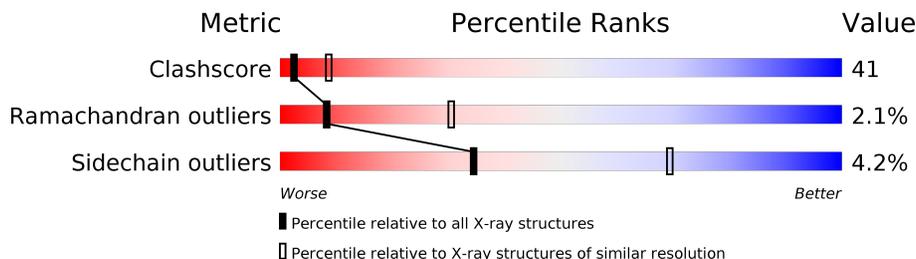
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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	588	
2	B	238	
3	C	129	
4	D	115	

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
10	F3S	B	304	-	-	X	-
12	DNT	C	306	X	-	-	-
13	CDN	C	308	X	-	-	-
5	OAA	A	589	-	-	X	-
8	FES	B	302	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 8695 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4522	2812	821	861	28	88	0	0

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	1869	1172	329	348	20	0	0	0

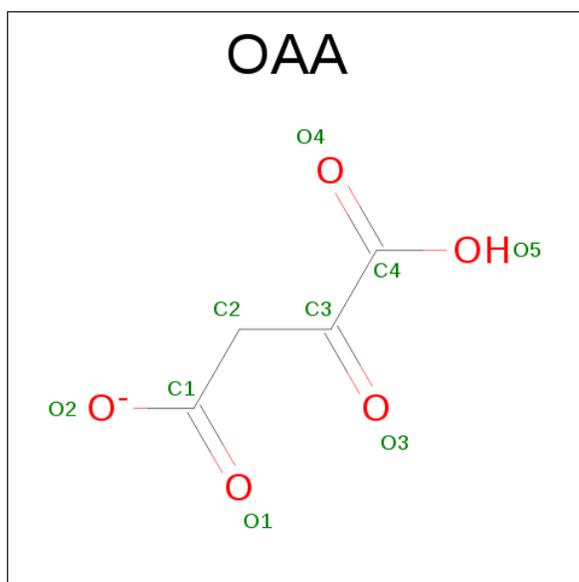
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b-556 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	129	1008	668	166	168	6	0	0	0

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	113	898	615	136	144	3	0	0	0

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: C₄H₃O₅).

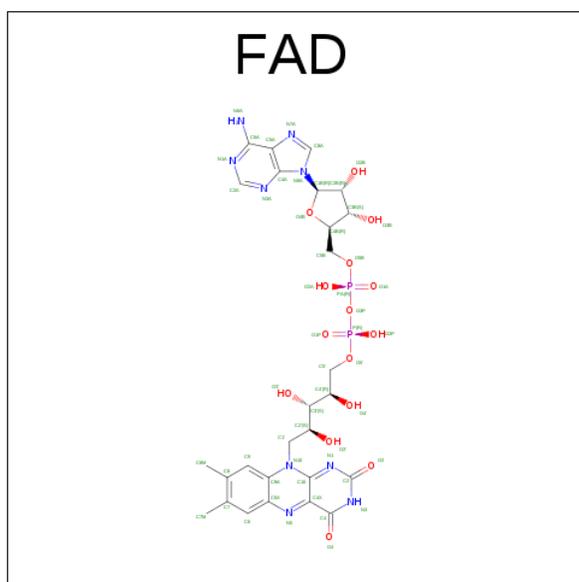


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

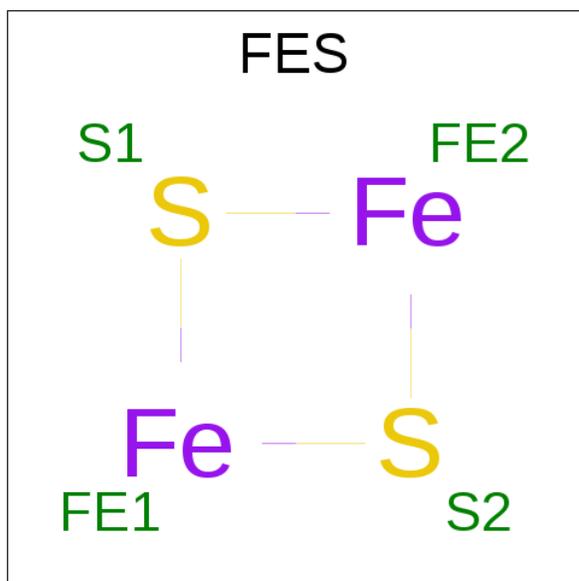
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



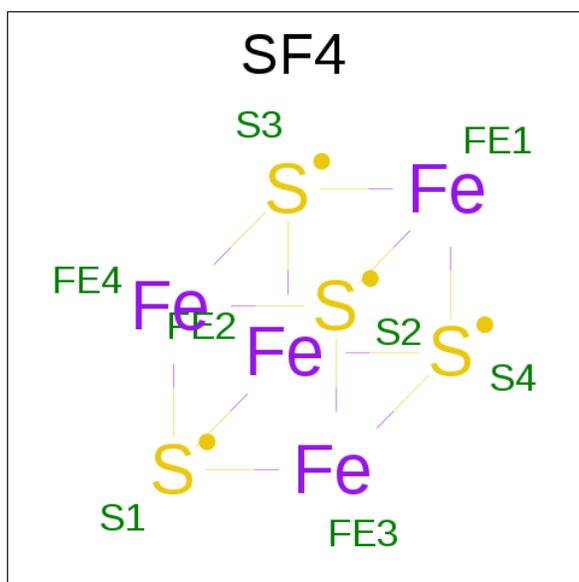
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	53	27	9	15	2	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



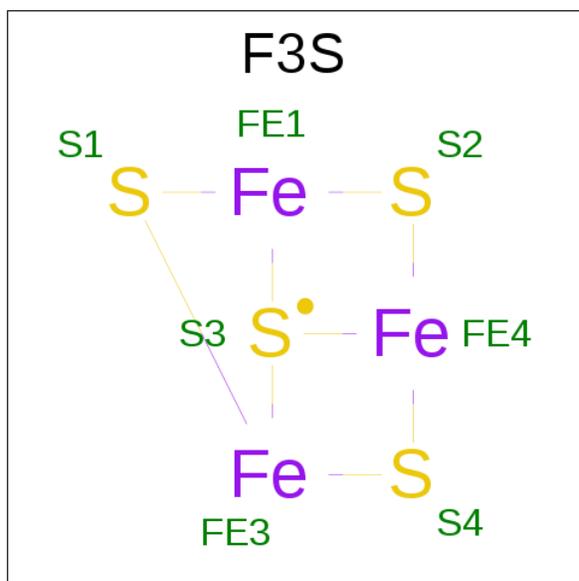
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	4	2	2	0	0

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



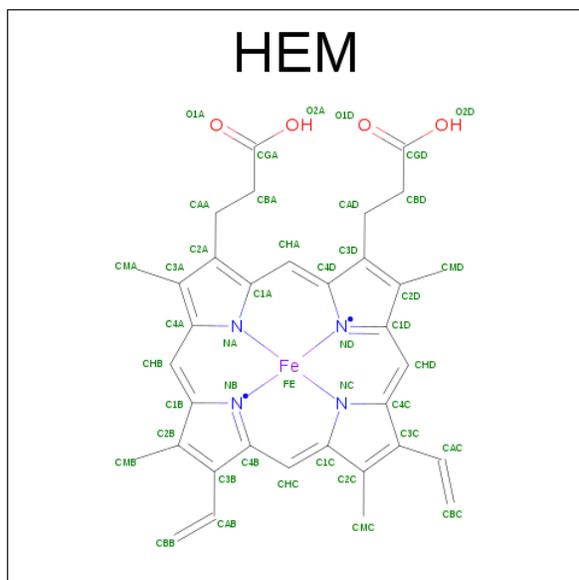
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



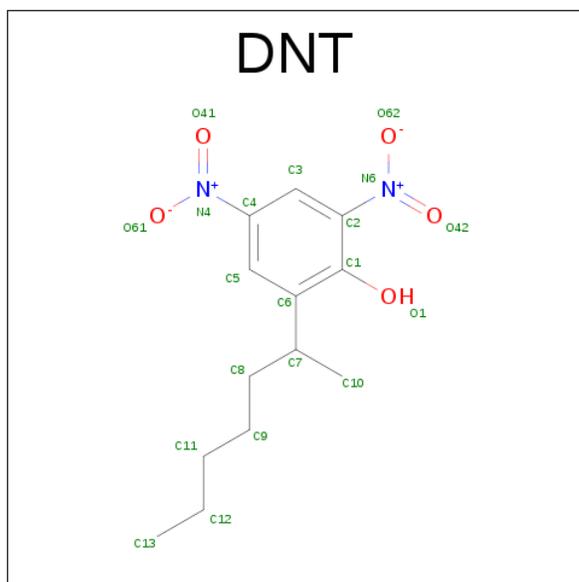
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



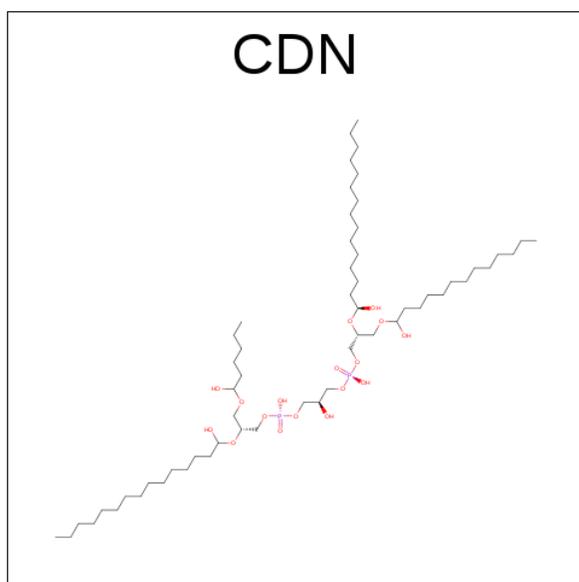
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is 2-[1-METHYLHEXYL]-4,6-DINITROPHENOL (three-letter code: DNT) (formula: $C_{13}H_{18}N_2O_5$).



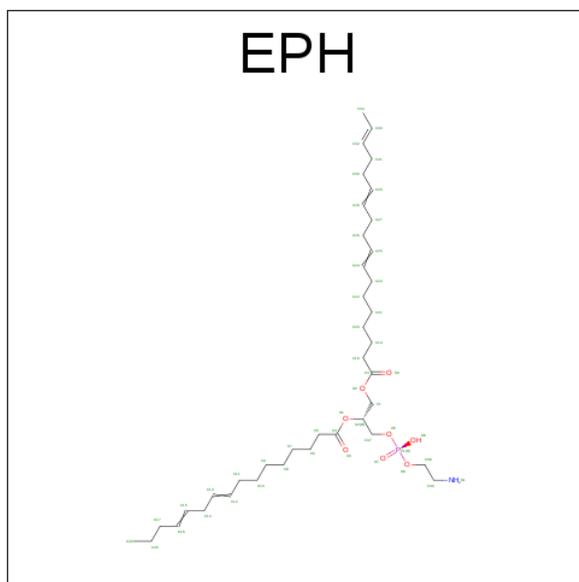
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	N	O	0	0
			20	13	2	5		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
13	C	1	77	58	17	2	0	0

- Molecule 14 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	C	1	35	25	1	8	1	0	0

- Molecule 15 is water.

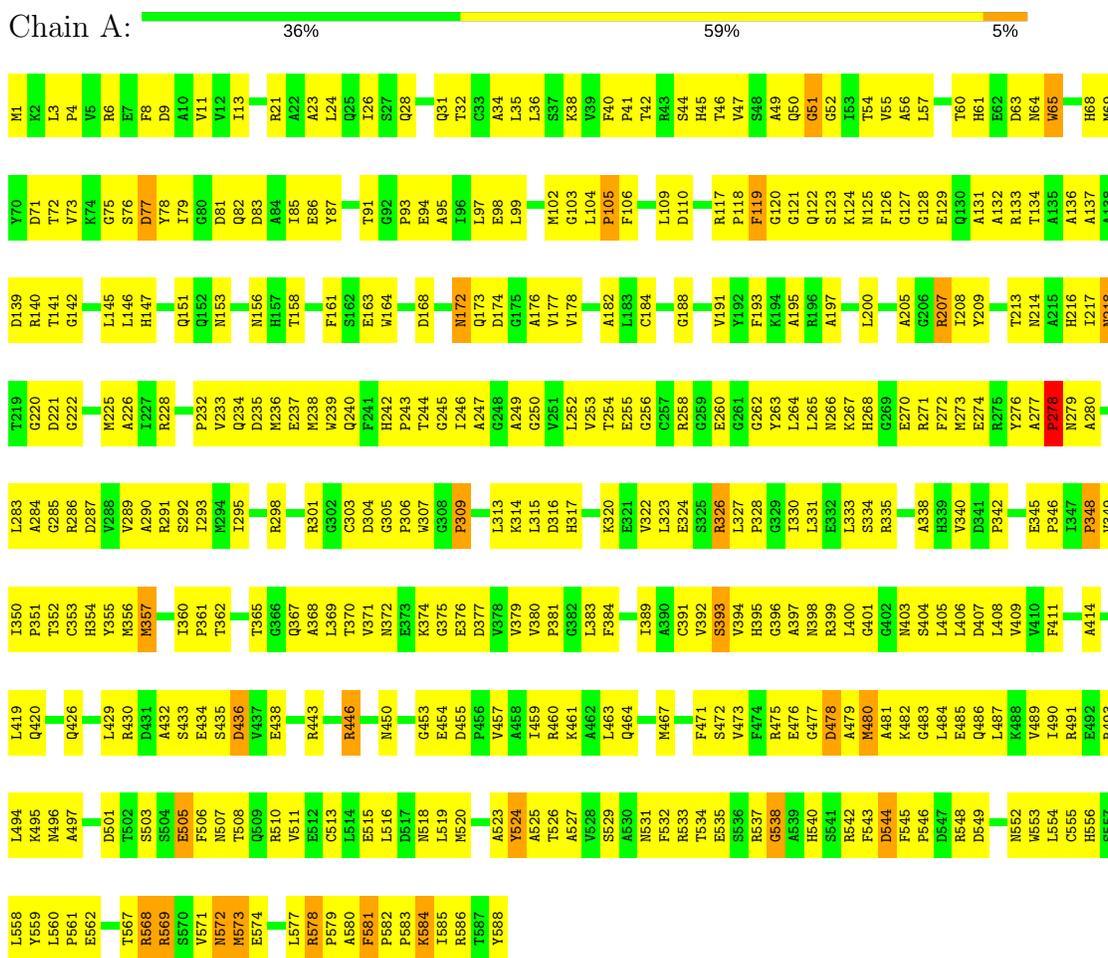
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	61	Total O 61 61	0	0
15	B	51	Total O 51 51	0	0
15	C	13	Total O 13 13	0	0
15	D	15	Total O 15 15	0	0

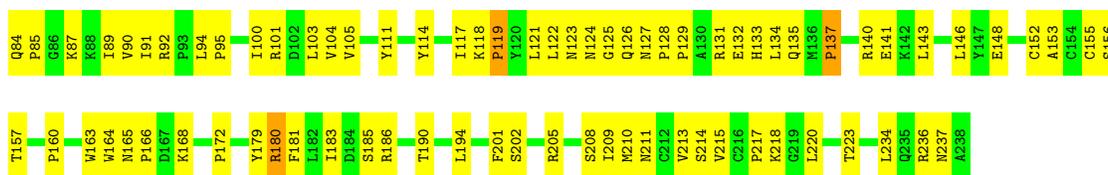
3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Succinate dehydrogenase flavoprotein subunit





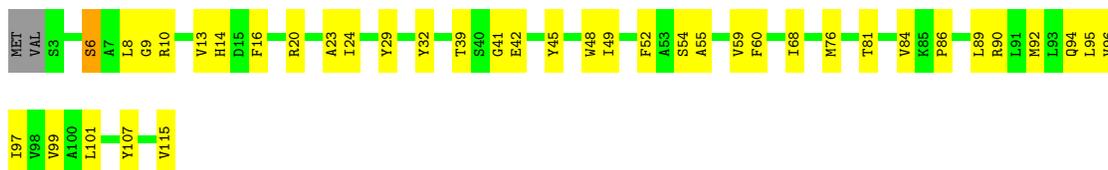
- Molecule 3: Succinate dehydrogenase cytochrome b-556 subunit

Chain C: 59% 37%



- Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor protein

Chain D: 64% 33%



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.80Å 138.80Å 521.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8695	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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: SF4, OAA, CDN, DNT, F3S, FES, EPH, HEM, CA, FAD

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	0.45	0/4611	0.71	1/6237 (0.0%)
2	B	0.44	0/1908	0.69	0/2578
3	C	0.48	0/1030	0.67	0/1394
4	D	0.53	0/923	0.65	0/1262
All	All	0.46	0/8472	0.69	1/11471 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLY	N-CA-C	-5.42	99.54	113.10

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	4522	0	4426	469	0
2	B	1869	0	1850	149	0
3	C	1008	0	1066	58	0
4	D	898	0	936	37	0
5	A	9	0	2	6	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	53	0	29	8	0
8	B	4	0	0	3	0
9	B	8	0	0	1	0
10	B	7	0	0	4	0
11	C	43	0	30	10	0
12	C	20	0	16	3	0
13	C	77	0	112	13	0
14	C	35	0	40	2	0
15	A	61	0	0	9	0
15	B	51	0	0	0	0
15	C	13	0	0	1	0
15	D	15	0	0	1	0
All	All	8695	0	8507	690	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 41.

The worst 5 of 690 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)
11:C:305:HEM:HBB1	13:C:308:CDN:C24	1.73	1.17
1:A:559:TYR:HB2	1:A:569:ARG:NH2	1.69	1.07
1:A:584:LYS:HG2	1:A:585:ILE:H	1.17	1.04
3:C:6:LYS:HG2	3:C:7:LYS:H	1.21	1.02
2:B:223:THR:HG22	10:B:304:F3S:S1	2.00	1.01

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	586/588 (100%)	503 (86%)	69 (12%)	14 (2%)	7	27
2	B	236/238 (99%)	209 (89%)	22 (9%)	5 (2%)	8	30
3	C	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	7	27
4	D	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
All	All	1060/1070 (99%)	936 (88%)	102 (10%)	22 (2%)	8	30

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLY
1	A	77	ASP
1	A	110	ASP
1	A	119	PHE
1	A	278	PRO

5.3.2 Protein sidechains [i](#)

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	473/473 (100%)	450 (95%)	23 (5%)	29	63
2	B	208/208 (100%)	203 (98%)	5 (2%)	54	84
3	C	109/109 (100%)	104 (95%)	5 (5%)	31	65
4	D	94/96 (98%)	90 (96%)	4 (4%)	33	68
All	All	884/886 (100%)	847 (96%)	37 (4%)	34	69

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	TYR
1	A	572	ASN
4	D	8	LEU
1	A	544	ASP
1	A	568	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	540	HIS
4	D	78	GLN
1	A	470	ASN
1	A	486	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
5	OAA	A	589	-	2,8,8	4.25	2 (100%)	2,10,10	4.33	2 (100%)
7	FAD	A	601	1	51,58,58	2.86	14 (27%)	54,89,89	2.56	10 (18%)
8	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	HEM	C	305	3,4	28,50,50	1.15	3 (10%)	17,82,82	1.69	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	DNT	C	306	-	16,20,20	4.72	10 (62%)	18,27,27	2.57	5 (27%)
13	CDN	C	308	-	76,76,76	2.39	8 (10%)	74,88,88	1.97	5 (6%)
14	EPH	C	309	-	34,34,48	1.16	3 (8%)	36,39,53	0.97	1 (2%)

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
5	OAA	A	589	-	-	0/2/8/8	0/0/0/0
7	FAD	A	601	1	-	0/28/50/50	0/6/6/6
8	FES	B	302	2	-	0/0/4/4	0/1/1/1
9	SF4	B	303	2	-	0/0/48/48	0/6/5/5
10	F3S	B	304	2	-	0/0/24/24	0/0/3/3
11	HEM	C	305	3,4	-	0/6/54/54	0/0/8/8
12	DNT	C	306	-	1/1/3/3	0/13/17/17	0/1/1/1
13	CDN	C	308	-	3/3/9/9	0/85/87/87	0/0/0/0
14	EPH	C	309	-	-	0/38/38/52	0/0/0/0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	306	DNT	C4-N4	-8.99	1.27	1.45
13	C	308	CDN	OA9-CA7	-7.98	1.21	1.39
13	C	308	CDN	OB7-CB5	-7.98	1.21	1.39
13	C	308	CDN	OB9-CB7	-7.68	1.22	1.39
13	C	308	CDN	OA6-CA5	-6.30	1.24	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	FAD	C4X-C4-N3	-6.23	114.62	123.48
7	A	601	FAD	C1'-N10-C9A	-5.91	112.93	118.35
5	A	589	OAA	C1-C2-C3	-5.16	106.13	115.52
7	A	601	FAD	N3A-C2A-N1A	-4.90	124.59	128.86
7	A	601	FAD	C5X-C9A-N10	-2.70	115.66	117.66

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	306	DNT	C7
13	C	308	CDN	CB5
13	C	308	CDN	CB7
13	C	308	CDN	CA7

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	589	OAA	6	0
7	A	601	FAD	8	0
8	B	302	FES	3	0
9	B	303	SF4	1	0
10	B	304	F3S	4	0
11	C	305	HEM	10	0
12	C	306	DNT	3	0
13	C	308	CDN	13	0
14	C	309	EPH	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.