



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KQG
Title : FORMATE DEHYDROGENASE N FROM E. COLI
Authors : Jormakka, M.; Tornroth, S.; Byrne, B.; Iwata, S.
Deposited on : 2002-01-05
Resolution : 2.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

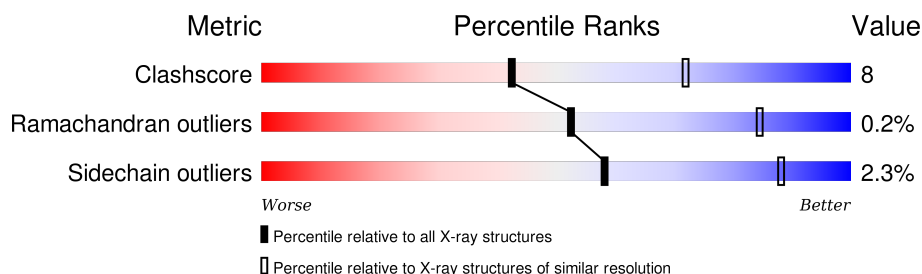
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	1015	 73% 21% • •
2	B	294	 78% 17% • •
3	C	217	 61% 32% 6% •

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14003 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 FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	982	Total	C	N	O	S	Se	0	0	0
			7719	4872	1352	1457	37	1			

- Molecule 2 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2207	1383	381	421	22			

- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

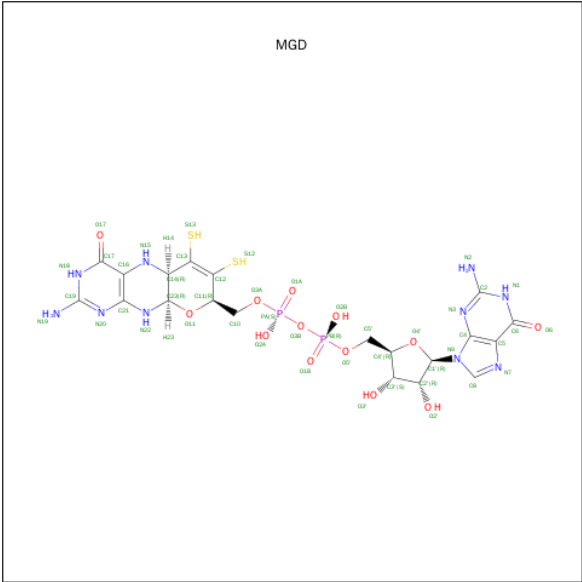
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1783	1192	301	276	14			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

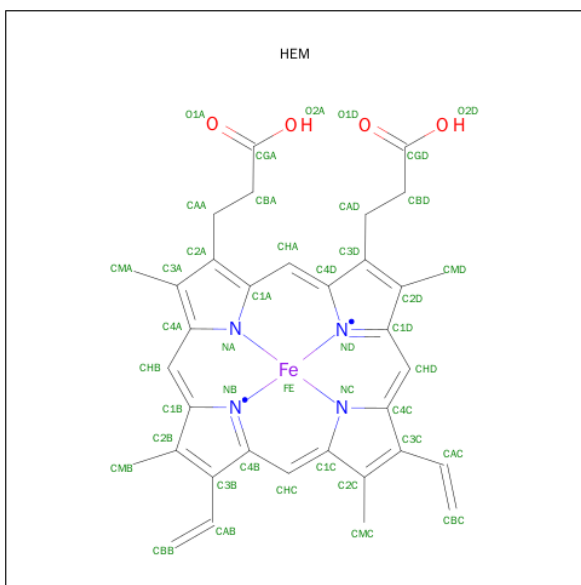


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

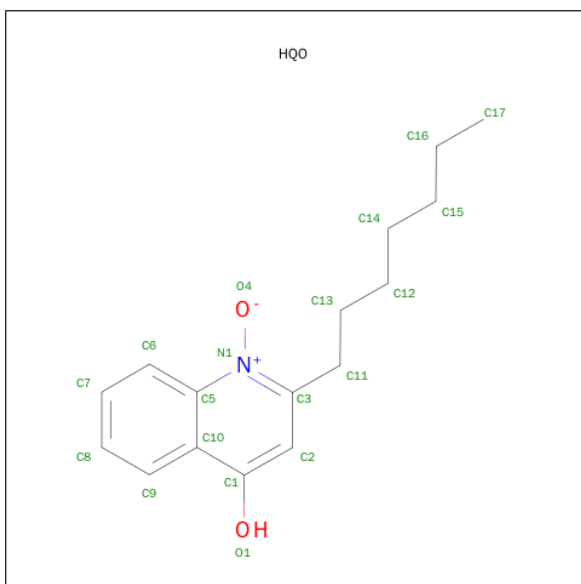
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



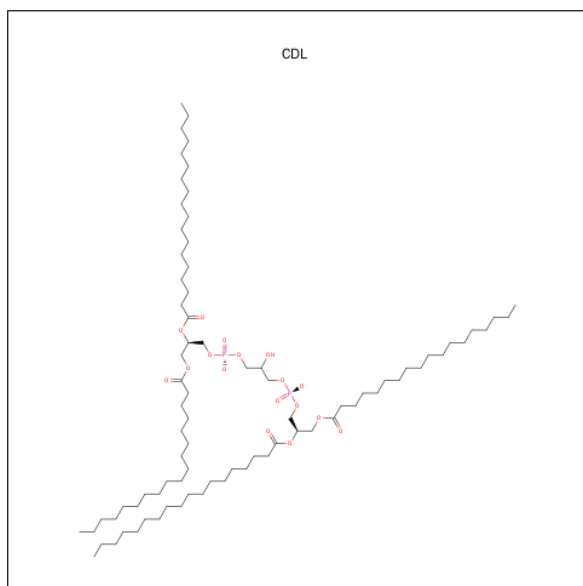
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	P	0	0
			70	51	17	2		

- Molecule 10 is water.

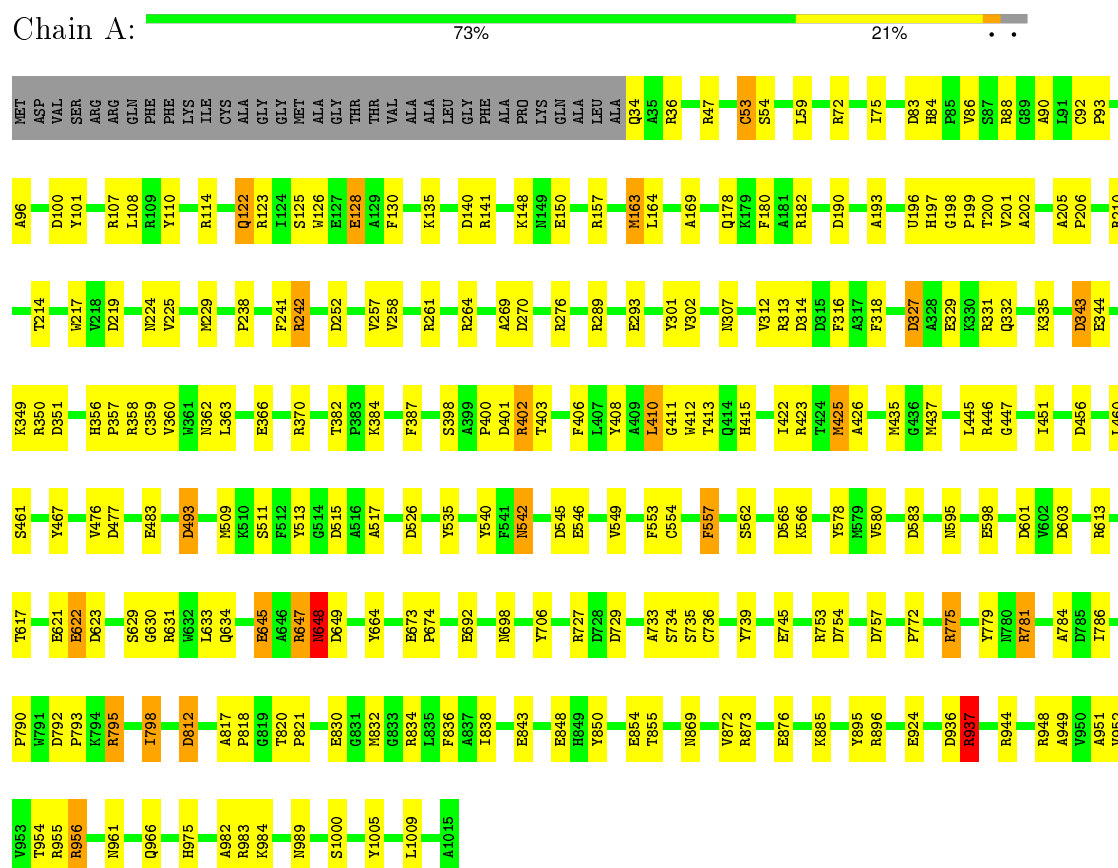
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1493	Total	O	0	0
			1493	1493		
10	B	410	Total	O	0	0
			410	410		
10	C	81	Total	O	0	0
			81	81		

3 Residue-property plots

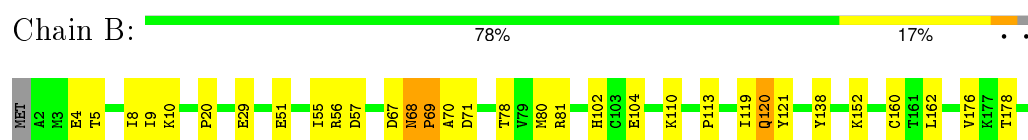
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT

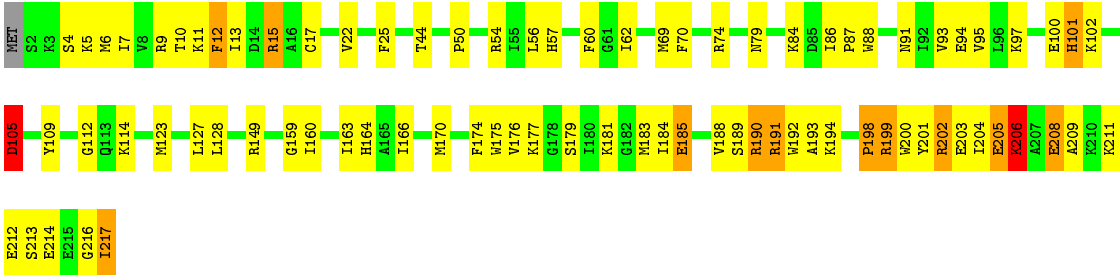


- Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT





● Molecule 3: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	203.00 Å 203.00 Å 203.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.8 (40.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14003	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, MGD, CDL, SF4, SEC, HQO, HEM

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	0.75	1/7910 (0.0%)	1.88	205/10749 (1.9%)
2	B	0.76	0/2255	1.66	39/3056 (1.3%)
3	C	0.67	0/1840	1.65	28/2483 (1.1%)
All	All	0.74	1/12005 (0.0%)	1.81	272/16288 (1.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	GLU	CD-OE1	5.14	1.31	1.25

The worst 5 of 272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	NE-CZ-NH2	-36.10	102.25	120.30
1	A	937	ARG	NE-CZ-NH2	-21.45	109.57	120.30
1	A	873	ARG	NE-CZ-NH1	18.68	129.64	120.30
1	A	157	ARG	NE-CZ-NH2	16.52	128.56	120.30
3	C	74	ARG	NE-CZ-NH2	-16.10	112.25	120.30

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	A	7719	0	7457	102	0
2	B	2207	0	2140	30	0
3	C	1783	0	1836	67	0
4	A	8	0	0	0	0
4	B	32	0	0	0	0
5	A	94	0	43	5	0
6	A	1	0	0	0	0
7	C	86	0	60	3	0
8	C	19	0	21	1	0
9	B	70	0	83	4	0
10	A	1493	0	0	27	0
10	B	410	0	0	11	0
10	C	81	0	0	9	0
All	All	14003	0	11640	196	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 196 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:830:GLU:HG3	1:A:832:MET:HE2	1.40	0.98
1:A:356:HIS:HD2	1:A:358:ARG:H	1.11	0.89
1:A:869:ASN:HB3	1:A:872:VAL:HG23	1.58	0.85
1:A:224:ASN:HD22	1:A:403:THR:H	1.21	0.84
3:C:101:HIS:HD2	3:C:102:LYS:H	1.25	0.84

There are no symmetry-related clashes.

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	A	979/1015 (96%)	949 (97%)	29 (3%)	1 (0%)	56	87
2	B	287/294 (98%)	280 (98%)	7 (2%)	0	100	100
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	21	55
All	All	1480/1526 (97%)	1435 (97%)	42 (3%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	208	GLU
1	A	838	ILE
3	C	198	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	815/837 (97%)	805 (99%)	10 (1%)	78	95
2	B	238/243 (98%)	225 (94%)	13 (6%)	27	59
3	C	188/189 (100%)	183 (97%)	5 (3%)	52	85
All	All	1241/1269 (98%)	1213 (98%)	28 (2%)	58	88

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	68	ASN
2	B	160	CYS
3	C	189	SER
2	B	69	PRO
2	B	113	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	GLN
1	A	689	GLN
3	C	79	ASN
1	A	362	ASN
1	A	415	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
4	SF4	A	1016	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	A	1017	6	38,52,52	2.09	7 (18%)	43,81,81	3.30	22 (51%)
5	MGD	A	1018	6	38,52,52	2.35	9 (23%)	43,81,81	2.68	19 (44%)
4	SF4	B	805	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	806	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	807	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	808	2	0,12,12	0.00	-	0,24,24	0.00	-
9	CDL	B	812	-	69,69,99	2.86	20 (28%)	71,81,111	2.77	17 (23%)
7	HEM	C	809	3	30,50,50	2.43	5 (16%)	24,82,82	2.72	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEM	C	810	3	30,50,50	2.50	9 (30%)	24,82,82	3.00	12 (50%)
8	HQO	C	811	-	20,20,20	2.91	8 (40%)	21,26,26	2.36	6 (28%)

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
4	SF4	A	1016	1	-	0/0/48/48	0/6/5/5
5	MGD	A	1017	6	-	0/18/66/66	0/6/6/6
5	MGD	A	1018	6	-	0/18/66/66	0/6/6/6
4	SF4	B	805	2	-	0/0/48/48	0/6/5/5
4	SF4	B	806	2	-	0/0/48/48	0/6/5/5
4	SF4	B	807	2	-	0/0/48/48	0/6/5/5
4	SF4	B	808	2	-	0/0/48/48	0/6/5/5
9	CDL	B	812	-	-	0/80/80/110	0/0/0/0
7	HEM	C	809	3	-	0/10/54/54	0/0/8/8
7	HEM	C	810	3	-	0/10/54/54	0/0/8/8
8	HQO	C	811	-	-	0/7/7/7	0/2/2/2

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	812	CDL	OB8-CB6	-15.51	1.10	1.45
5	A	1018	MGD	O3A-C10	-9.80	1.04	1.44
5	A	1017	MGD	O3A-C10	-9.41	1.06	1.44
7	C	810	HEM	C3B-C4B	-7.60	1.45	1.51
7	C	809	HEM	C3B-C4B	-7.05	1.45	1.51

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	812	CDL	CB6-OB8-CB7	-8.87	92.04	116.85
5	A	1017	MGD	C5-C6-N1	-8.20	112.38	123.59
5	A	1018	MGD	C4'-O4'-C1'	-7.16	101.86	109.72
9	B	812	CDL	CA6-CA4-CA3	-7.09	95.49	112.07
9	B	812	CDL	C52-C51-CB5	-6.66	87.41	113.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1017	MGD	3	0
5	A	1018	MGD	2	0
9	B	812	CDL	4	0
7	C	810	HEM	3	0
8	C	811	HQO	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.