



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VR0
Title : CRYSTAL STRUCTURE OF CYTOCHROME C NITRITE REDUCTASE
NRFHA COMPLEX BOUND TO THE HQNO INHIBITOR
Authors : Rodrigues, M.L.; Archer, M.
Deposited on : 2008-03-24
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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

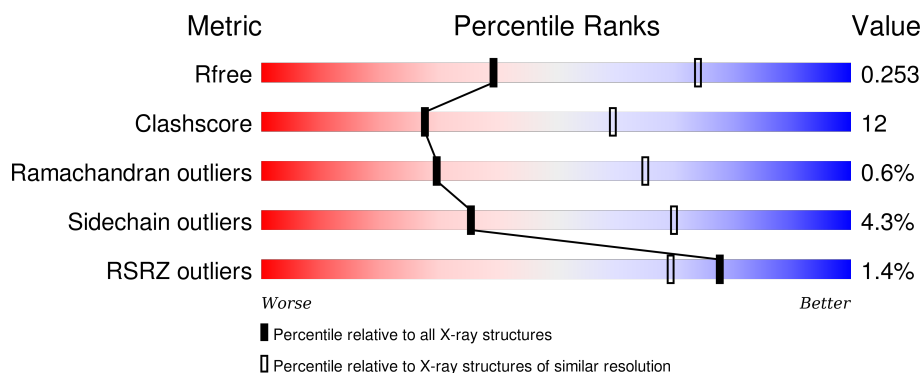
1 Overall quality at a glance

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))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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.

Mol	Chain	Length	Quality of chain
1	A	524	<div> <div>0%</div> <div>78%</div> <div>14%</div> <div>6%</div> </div>
1	B	524	<div> <div>0%</div> <div>78%</div> <div>14%</div> <div>5%</div> </div>
1	D	524	<div> <div>2%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
1	E	524	<div> <div>2%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
2	C	159	<div> <div>3%</div> <div>75%</div> <div>15%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	159	 % 72% 20% 8%

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
5	HQO	F	1005	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19601 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 CYTOCHROME C NITRITE REDUCTASE, CATALYTIC SUBUNIT NFRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			4009	2546	692	742	29			
1	B	498	Total	C	N	O	S	0	1	0
			4035	2561	698	747	29			
1	D	494	Total	C	N	O	S	0	0	0
			4002	2541	691	741	29			
1	E	495	Total	C	N	O	S	0	0	0
			4007	2544	692	742	29			

- Molecule 2 is a protein called NAPC/NIRT CYTOCHROME C FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	144	Total	C	N	O	S	0	1	0
			1088	675	200	197	16			
2	F	146	Total	C	N	O	S	0	0	0
			1096	680	200	200	16			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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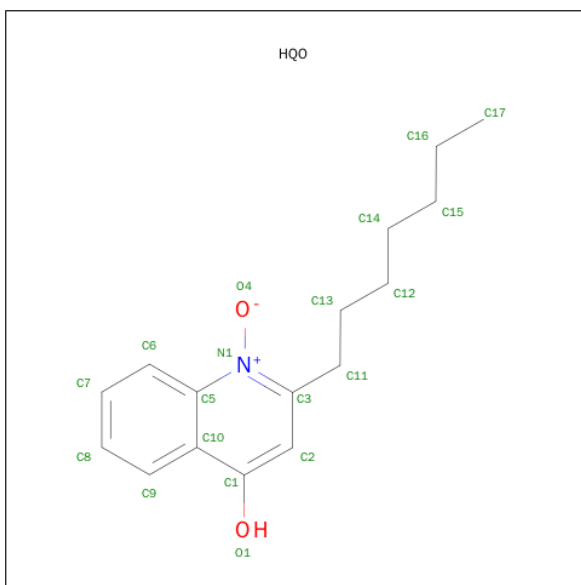
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ca 2	0	0
4	A	2	Total 2	Ca 2	0	0
4	D	2	Total 2	Ca 2	0	0
4	E	2	Total 2	Ca 2	0	0

- Molecule 5 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: C₁₆H₂₁NO₂).



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

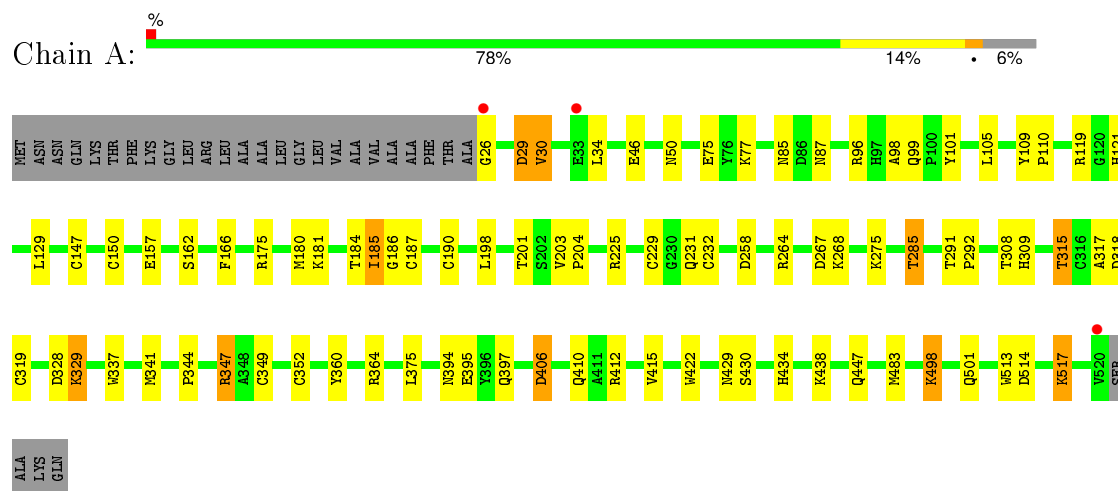
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	41	Total	O	0	0
			41	41		
6	C	5	Total	O	0	0
			5	5		
6	D	21	Total	O	0	0
			21	21		
6	E	14	Total	O	0	0
			14	14		
6	F	10	Total	O	0	0
			10	10		

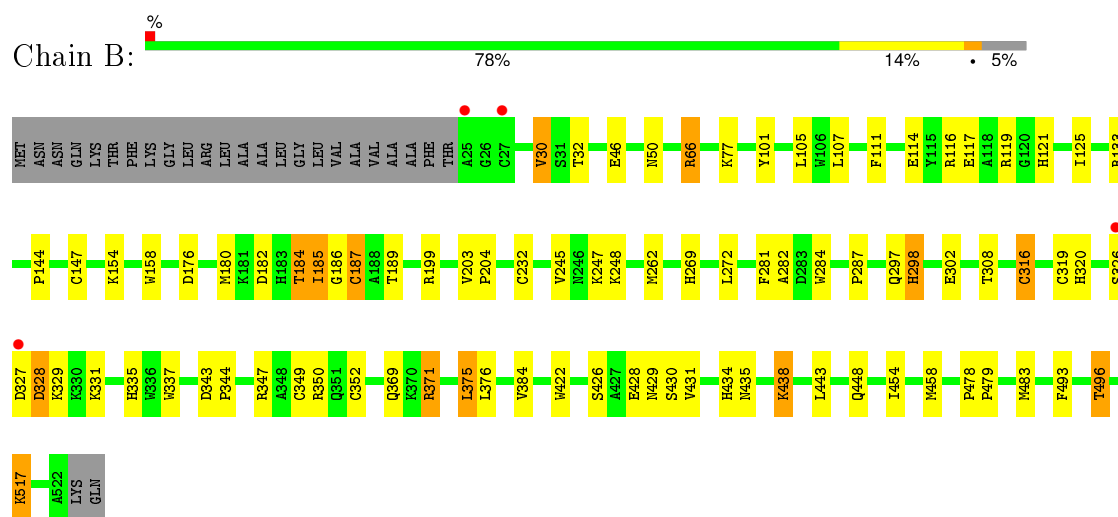
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: CYTOCHROME C NITRITE REDUCTASE, CATALYTIC SUBUNIT NFRA

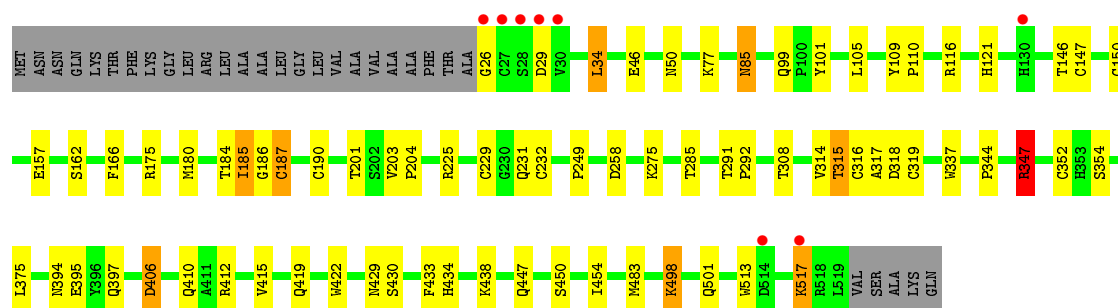


• Molecule 1: CYTOCHROME C NITRITE REDUCTASE, CATALYTIC SUBUNIT NFRA

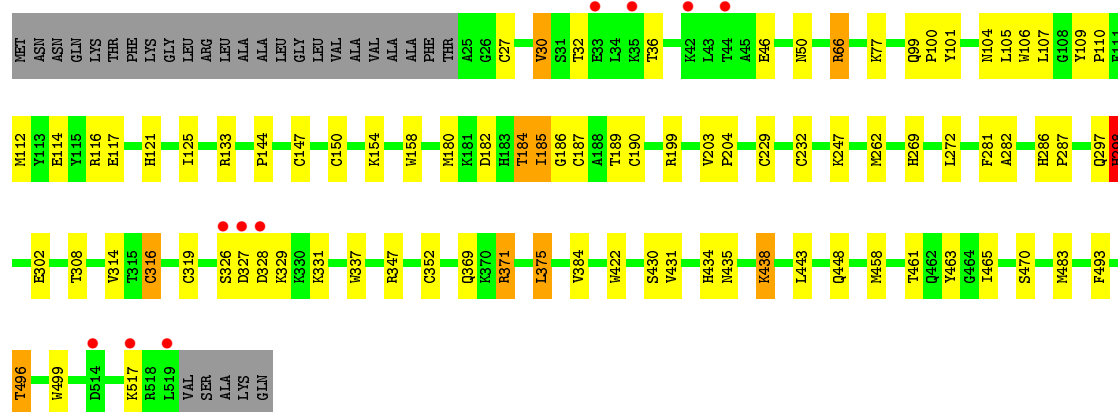
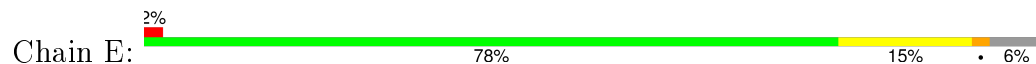


• Molecule 1: CYTOCHROME C NITRITE REDUCTASE, CATALYTIC SUBUNIT NFRA

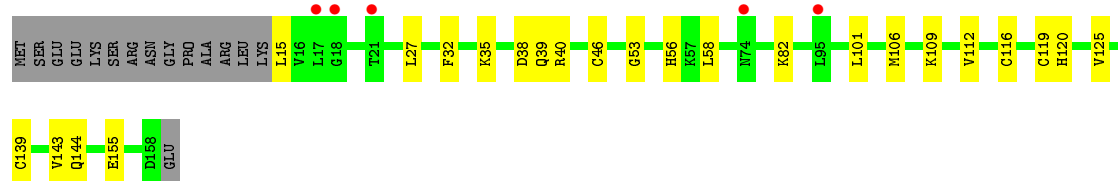
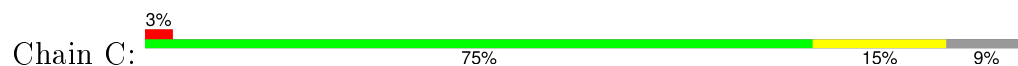




- Molecule 1: CYTOCHROME C NITRITE REDUCTASE, CATALYTIC SUBUNIT NFRA



- Molecule 2: NAPC/NIRT CYTOCHROME C FAMILY PROTEIN



- Molecule 2: NAPC/NIRT CYTOCHROME C FAMILY PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.10Å 189.12Å 263.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.30 – 2.80 29.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.0 (154.30-2.80) 87.1 (29.77-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.3.0013	Depositor
R, R_{free}	0.220 , 0.261 0.215 , 0.253	Depositor DCC
R_{free} test set	2592 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 86568 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19601	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CA, HQO

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	0.59	0/4123	0.64	0/5579
1	B	0.60	0/4150	0.67	0/5616
1	D	0.56	0/4116	0.64	2/5569 (0.0%)
1	E	0.54	0/4121	0.62	0/5576
2	C	0.56	0/1109	0.66	0/1502
2	F	0.55	0/1116	0.64	0/1509
All	All	0.57	0/18735	0.64	2/25351 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	347	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	D	347	ARG	NE-CZ-NH2	-6.47	117.06	120.30

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	4009	0	3876	86	0
1	B	4035	0	3898	80	0
1	D	4002	0	3869	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4007	0	3875	89	0
2	C	1088	0	1084	38	0
2	F	1096	0	1099	52	0
3	A	215	0	150	34	0
3	B	215	0	150	36	0
3	C	172	0	120	32	0
3	D	215	0	150	41	0
3	E	215	0	150	45	0
3	F	172	0	120	47	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	C	19	0	21	1	0
5	F	19	0	21	2	0
6	A	23	0	0	0	0
6	B	41	0	0	2	0
6	C	5	0	0	0	0
6	D	21	0	0	1	0
6	E	14	0	0	1	0
6	F	10	0	0	1	0
All	All	19601	0	18583	429	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 12.

The worst 5 of 429 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:B:316:CYS:SG	3:B:1004:HEM:HAB	1.18	1.71
1:D:316:CYS:SG	3:D:1004:HEM:HAB	1.19	1.70
2:F:66:CYS:SG	3:F:1002:HEM:HAB	1.32	1.67
1:B:187:CYS:SG	3:B:1002:HEM:HAB	1.34	1.66
1:D:352:CYS:SG	3:D:1005:HEM:HAC	1.28	1.64

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	493/524 (94%)	473 (96%)	18 (4%)	2 (0%)	39	74
1	B	497/524 (95%)	474 (95%)	18 (4%)	5 (1%)	19	52
1	D	492/524 (94%)	469 (95%)	22 (4%)	1 (0%)	52	84
1	E	493/524 (94%)	470 (95%)	18 (4%)	5 (1%)	19	52
2	C	143/159 (90%)	138 (96%)	5 (4%)	0	100	100
2	F	144/159 (91%)	139 (96%)	4 (3%)	1 (1%)	26	62
All	All	2262/2414 (94%)	2163 (96%)	85 (4%)	14 (1%)	30	65

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	ILE
1	B	329	LYS
1	E	185	ILE
1	E	329	LYS
1	A	185	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	429/449 (96%)	411 (96%)	18 (4%)	36	71
1	B	431/449 (96%)	410 (95%)	21 (5%)	31	65
1	D	428/449 (95%)	412 (96%)	16 (4%)	41	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	428/449 (95%)	407 (95%)	21 (5%)	31	65
2	C	119/131 (91%)	116 (98%)	3 (2%)	55	86
2	F	120/131 (92%)	115 (96%)	5 (4%)	36	71
All	All	1955/2058 (95%)	1871 (96%)	84 (4%)	35	70

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	496	THR
1	D	157	GLU
1	E	496	THR
2	C	58	LEU
1	D	29	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	56	HIS
1	D	97	HIS
1	E	269	HIS
2	C	50	ASN
1	D	447	GLN

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 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 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$
3	HEM	A	1001	1	30,50,50	2.20	9 (30%)	24,82,82	2.58	11 (45%)
3	HEM	A	1002	1	30,50,50	2.17	5 (16%)	24,82,82	2.24	7 (29%)
3	HEM	A	1003	1,4	30,50,50	2.36	10 (33%)	24,82,82	2.66	9 (37%)
3	HEM	A	1004	1,4	30,50,50	2.14	4 (13%)	24,82,82	2.42	8 (33%)
3	HEM	A	1005	1	30,50,50	2.26	9 (30%)	24,82,82	2.56	8 (33%)
3	HEM	B	1001	1,6	30,50,50	2.40	7 (23%)	24,82,82	2.29	9 (37%)
3	HEM	B	1002	1	30,50,50	2.12	8 (26%)	24,82,82	2.44	11 (45%)
3	HEM	B	1003	1,4	30,50,50	2.31	7 (23%)	24,82,82	2.72	11 (45%)
3	HEM	B	1004	1,4	30,50,50	2.20	11 (36%)	24,82,82	2.96	13 (54%)
3	HEM	B	1005	1	30,50,50	2.16	9 (30%)	24,82,82	2.43	9 (37%)
3	HEM	C	1001	2	30,50,50	2.41	9 (30%)	24,82,82	2.39	9 (37%)
3	HEM	C	1002	2	30,50,50	2.27	11 (36%)	24,82,82	2.48	10 (41%)
3	HEM	C	1003	2	30,50,50	1.93	6 (20%)	24,82,82	2.65	13 (54%)
3	HEM	C	1004	1,2	30,50,50	2.33	8 (26%)	24,82,82	2.76	8 (33%)
5	HQO	C	1005	-	20,20,20	1.37	3 (15%)	21,26,26	1.16	3 (14%)
3	HEM	D	1001	1,6	30,50,50	2.22	9 (30%)	24,82,82	2.37	10 (41%)
3	HEM	D	1002	1	30,50,50	2.01	6 (20%)	24,82,82	2.32	7 (29%)
3	HEM	D	1003	1,4	30,50,50	2.06	10 (33%)	24,82,82	2.37	11 (45%)
3	HEM	D	1004	1,4	30,50,50	2.21	6 (20%)	24,82,82	2.66	10 (41%)
3	HEM	D	1005	1	30,50,50	2.33	7 (23%)	24,82,82	2.36	9 (37%)
3	HEM	E	1001	1,6	30,50,50	2.09	8 (26%)	24,82,82	2.23	8 (33%)
3	HEM	E	1002	1	30,50,50	2.39	5 (16%)	24,82,82	2.36	8 (33%)
3	HEM	E	1003	1,4	30,50,50	2.13	8 (26%)	24,82,82	2.24	7 (29%)
3	HEM	E	1004	1,4	30,50,50	1.93	6 (20%)	24,82,82	2.15	8 (33%)
3	HEM	E	1005	1	30,50,50	2.16	7 (23%)	24,82,82	2.56	11 (45%)
3	HEM	F	1001	2	30,50,50	2.32	11 (36%)	24,82,82	2.23	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	F	1002	2	30,50,50	2.18	6 (20%)	24,82,82	2.33	9 (37%)
3	HEM	F	1003	2	30,50,50	2.25	4 (13%)	24,82,82	2.73	10 (41%)
3	HEM	F	1004	1,2	30,50,50	2.14	8 (26%)	24,82,82	2.49	9 (37%)
5	HQO	F	1005	-	20,20,20	1.34	3 (15%)	21,26,26	1.19	2 (9%)

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
3	HEM	A	1001	1	-	0/10/54/54	0/0/8/8
3	HEM	A	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	A	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	A	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	A	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	B	1001	1,6	-	0/10/54/54	0/0/8/8
3	HEM	B	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	B	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	B	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	B	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	C	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	C	1002	2	-	2/10/54/54	0/0/8/8
3	HEM	C	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	C	1004	1,2	-	0/10/54/54	0/0/8/8
5	HQO	C	1005	-	-	0/7/7/7	0/2/2/2
3	HEM	D	1001	1,6	-	0/10/54/54	0/0/8/8
3	HEM	D	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	D	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	D	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	D	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	E	1001	1,6	-	0/10/54/54	0/0/8/8
3	HEM	E	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	E	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	E	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	E	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	F	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	F	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	F	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	F	1004	1,2	-	0/10/54/54	0/0/8/8
5	HQO	F	1005	-	-	0/7/7/7	0/2/2/2

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1005	HEM	C3B-C4B	-8.90	1.43	1.51
3	E	1002	HEM	C3B-C4B	-8.89	1.43	1.51
3	C	1004	HEM	C3B-C4B	-8.82	1.44	1.51
3	A	1003	HEM	C3B-C4B	-8.58	1.44	1.51
3	B	1001	HEM	C3B-C4B	-8.51	1.44	1.51

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	HEM	CBA-CAA-C2A	-6.95	100.07	112.53
3	C	1004	HEM	CBA-CAA-C2A	-6.44	100.98	112.53
3	C	1004	HEM	C3B-CAB-CBB	-5.71	115.70	124.46
3	A	1005	HEM	CBA-CAA-C2A	-5.45	102.76	112.53
3	D	1004	HEM	C3B-CAB-CBB	-5.31	116.31	124.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1002	HEM	C3A-C2A-CAA-CBA
3	C	1002	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

30 monomers are involved in 238 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	HEM	4	0
3	A	1002	HEM	7	0
3	A	1003	HEM	9	0
3	A	1004	HEM	6	0
3	A	1005	HEM	8	0
3	B	1001	HEM	4	0
3	B	1002	HEM	3	0
3	B	1003	HEM	6	0
3	B	1004	HEM	12	0
3	B	1005	HEM	11	0
3	C	1001	HEM	4	0
3	C	1002	HEM	10	0
3	C	1003	HEM	11	0
3	C	1004	HEM	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1005	HQO	1	0
3	D	1001	HEM	12	0
3	D	1002	HEM	9	0
3	D	1003	HEM	9	0
3	D	1004	HEM	7	0
3	D	1005	HEM	4	0
3	E	1001	HEM	14	0
3	E	1002	HEM	9	0
3	E	1003	HEM	10	0
3	E	1004	HEM	9	0
3	E	1005	HEM	4	0
3	F	1001	HEM	5	0
3	F	1002	HEM	14	0
3	F	1003	HEM	12	0
3	F	1004	HEM	16	0
5	F	1005	HQO	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	495/524 (94%)	-0.23	3 (0%) 90 86	22, 25, 27, 32	0
1	B	498/524 (95%)	-0.31	4 (0%) 87 81	20, 25, 27, 32	0
1	D	494/524 (94%)	-0.19	8 (1%) 74 66	22, 25, 27, 32	0
1	E	495/524 (94%)	-0.08	10 (2%) 68 58	20, 24, 27, 32	0
2	C	144/159 (90%)	-0.03	5 (3%) 48 35	21, 24, 27, 29	0
2	F	146/159 (91%)	-0.03	2 (1%) 78 69	21, 24, 27, 29	0
All	All	2272/2414 (94%)	-0.18	32 (1%) 78 69	20, 25, 27, 32	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	CYS	3.9
1	E	328	ASP	3.7
1	A	26	GLY	3.6
1	B	326	SER	3.5
1	D	28	SER	3.4

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 ⓘ

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
5	HQO	F	1005	19/19	0.85	0.31	3.84	66,67,68,68	0
5	HQO	C	1005	19/19	0.88	0.22	1.09	55,55,61,62	0
3	HEM	F	1001	43/43	0.93	0.17	-0.28	38,41,48,52	0
3	HEM	A	1003	43/43	0.96	0.15	-0.64	10,13,21,25	0
3	HEM	E	1001	43/43	0.95	0.14	-0.75	29,31,33,36	0
3	HEM	C	1002	43/43	0.95	0.14	-0.86	20,23,26,27	0
3	HEM	E	1005	43/43	0.96	0.14	-0.86	23,25,29,34	0
3	HEM	D	1003	43/43	0.96	0.12	-0.91	14,19,26,27	0
3	HEM	A	1001	43/43	0.96	0.14	-0.92	17,21,25,30	0
3	HEM	C	1001	43/43	0.96	0.13	-1.00	22,25,33,37	0
3	HEM	E	1003	43/43	0.97	0.13	-1.02	26,35,36,38	0
3	HEM	A	1004	43/43	0.97	0.12	-1.09	3,7,17,21	0
3	HEM	E	1004	43/43	0.97	0.12	-1.16	25,29,31,32	0
3	HEM	A	1005	43/43	0.97	0.13	-1.28	9,15,18,24	0
3	HEM	F	1002	43/43	0.96	0.12	-1.29	23,27,32,34	0
3	HEM	F	1004	43/43	0.97	0.12	-1.33	11,15,28,36	0
3	HEM	F	1003	43/43	0.97	0.11	-1.42	13,18,25,28	0
3	HEM	C	1004	43/43	0.97	0.11	-1.50	16,20,28,32	0
3	HEM	D	1002	43/43	0.96	0.13	-1.55	16,18,23,28	0
3	HEM	E	1002	43/43	0.96	0.13	-1.56	27,30,33,37	0
3	HEM	B	1003	43/43	0.97	0.12	-1.56	4,7,18,18	0
3	HEM	A	1002	43/43	0.97	0.12	-1.57	21,22,28,31	0
3	HEM	B	1001	43/43	0.96	0.13	-1.58	9,13,17,21	0
3	HEM	D	1005	43/43	0.97	0.12	-1.60	15,17,24,26	0
3	HEM	C	1003	43/43	0.97	0.12	-1.65	19,22,26,29	0
3	HEM	B	1004	43/43	0.98	0.10	-1.67	2,3,11,15	0
3	HEM	D	1004	43/43	0.98	0.10	-1.81	11,13,20,22	0
3	HEM	B	1005	43/43	0.97	0.12	-1.85	15,17,25,27	0
3	HEM	D	1001	43/43	0.98	0.10	-1.89	22,27,32,34	0
3	HEM	B	1002	43/43	0.97	0.11	-1.95	17,21,25,27	0
4	CA	D	1006	1/1	0.96	0.12	-1.99	30,30,30,30	0
4	CA	A	1007	1/1	0.96	0.06	-2.87	36,36,36,36	0
4	CA	E	1007	1/1	0.99	0.05	-3.27	25,25,25,25	0
4	CA	E	1006	1/1	0.96	0.10	-3.91	24,24,24,24	0
4	CA	D	1007	1/1	0.97	0.04	-4.62	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	B	1007	1/1	0.99	0.03	-4.63	19,19,19,19	0
4	CA	B	1006	1/1	0.95	0.05	-5.76	20,20,20,20	0
4	CA	A	1006	1/1	0.97	0.06	-6.21	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.