



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:45 am GMT

PDB ID : 4N4O  
Title : Nitrosomonas europea HAO soaked in NH<sub>2</sub>OH  
Authors : Maalcke, W.J.; Dietl, A.; Marritt, S.J.; Butt, J.N.; Jetten, M.S.M.; Keltjens, J.T.; Barends, T.R.M.B.; Kartal, B.  
Deposited on : 2013-10-08  
Resolution : 2.47 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](mailto: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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

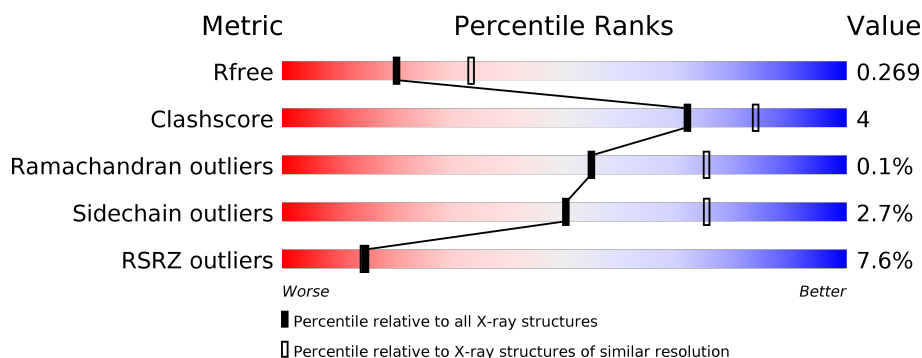
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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))
$R_{free}$	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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  $\geq 3$ , 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	546	<div> <div>4%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	C	546	<div> <div>5%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	E	546	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
2	B	57	<div> <div>37%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
2	D	57	<div> <div>23%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
2	F	57	<div> <div>42%</div> <div>86%</div> <div>9%</div> <div>.</div> <div>.</div> </div>

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
7	12P	A	611	-	-	-	X
7	12P	C	610	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15367 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 Hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	C	502	Total	C	N	O	S	0	0	0
			4005	2491	710	772	32			
1	E	503	Total	C	N	O	S	0	1	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	53	Total	C	N	O	S	0	0	0
			404	253	71	77	3			
2	D	57	Total	C	N	O	S	0	0	0
			429	266	76	84	3			
2	F	55	Total	C	N	O	S	0	0	0
			419	261	74	81	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



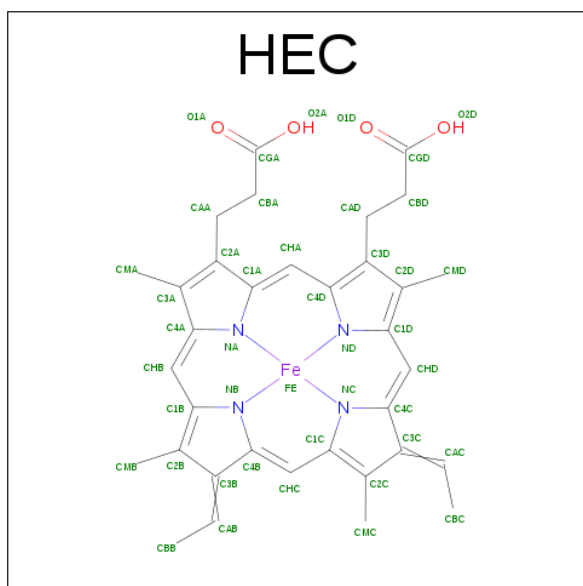
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).

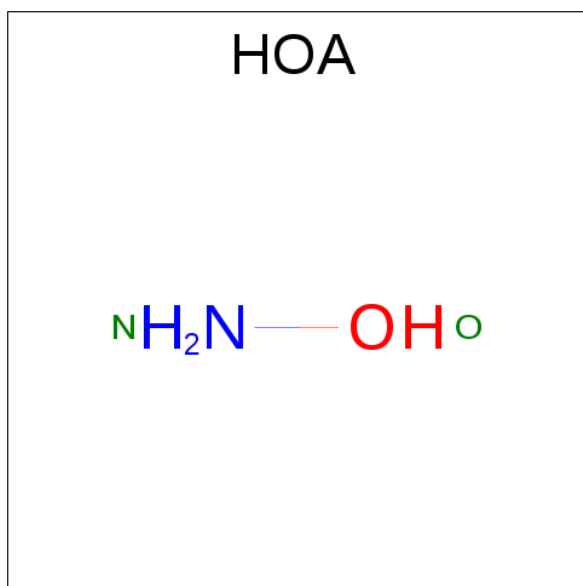


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

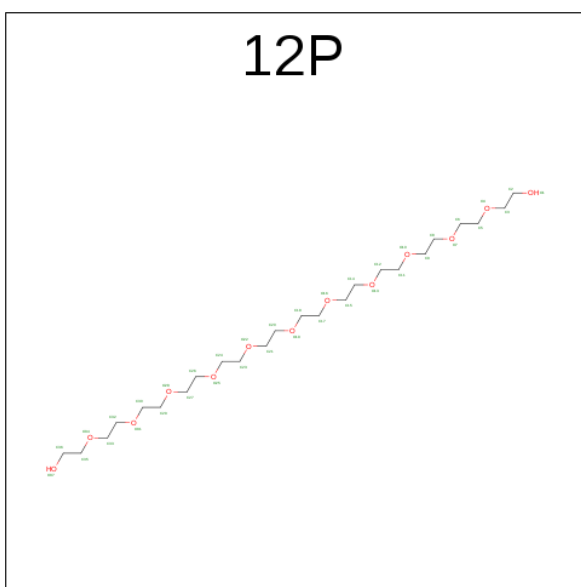
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0

- Molecule 6 is HYDROXYAMINE (three-letter code: HOA) (formula:  $\text{H}_3\text{NO}$ ).



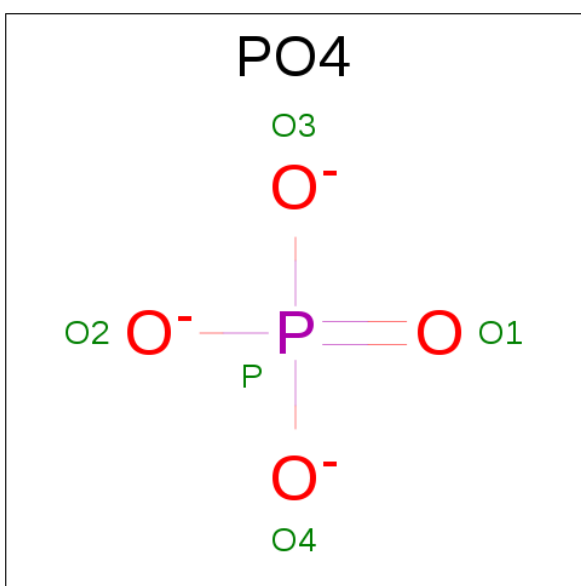
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N O 2 1 1	0	0
6	C	1	Total N O 2 1 1	0	0
6	E	1	Total N O 2 1 1	0	0

- Molecule 7 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula:  $\text{C}_{24}\text{H}_{50}\text{O}_{13}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		
7	C	1	Total	C	O	0	0
			25	16	9		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is water.

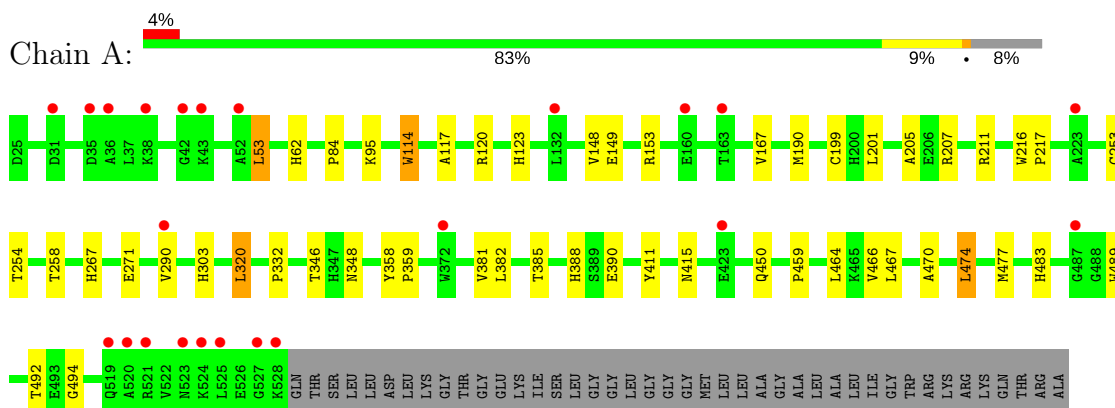


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	295	Total 295	O 295	0	0
9	B	37	Total 37	O 37	0	0
9	C	284	Total 284	O 284	0	0
9	D	41	Total 41	O 41	0	0
9	E	301	Total 301	O 301	0	0
9	F	35	Total 35	O 35	0	0

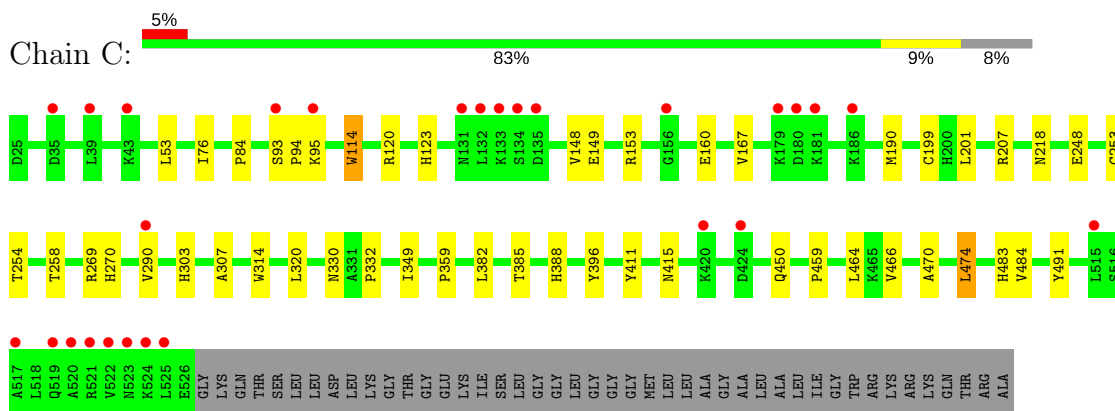
### 3 Residue-property plots [i](#)

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.

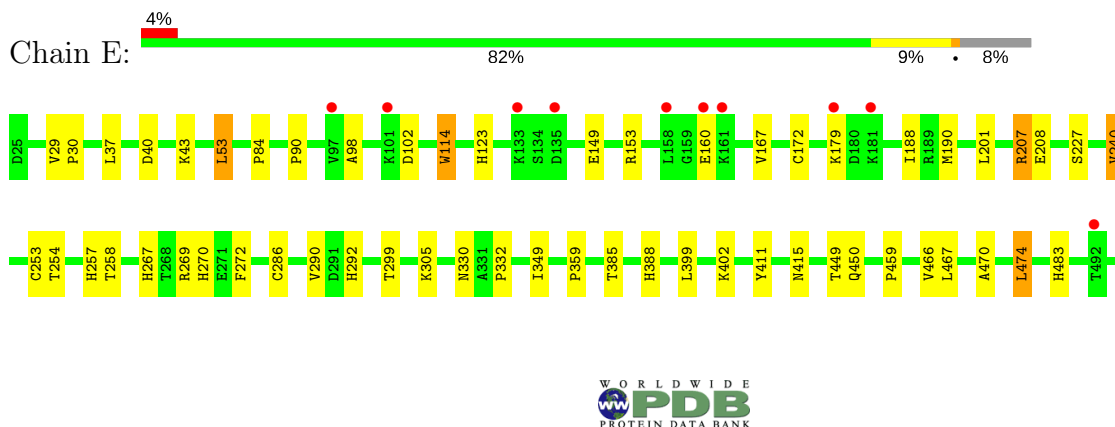
- Molecule 1: Hydroxylamine oxidoreductase

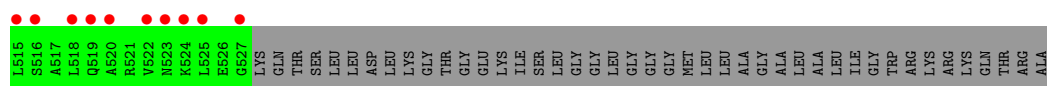


- Molecule 1: Hydroxylamine oxidoreductase

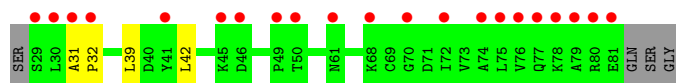
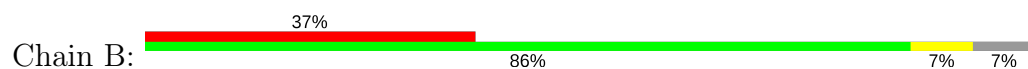


- Molecule 1: Hydroxylamine oxidoreductase

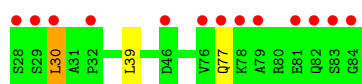
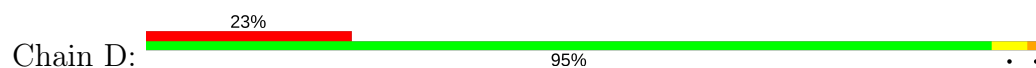




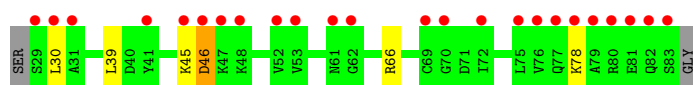
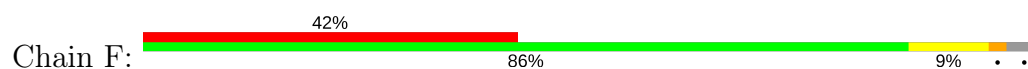
- Molecule 2: hydroxylamine oxidoreductase



- Molecule 2: hydroxylamine oxidoreductase



- Molecule 2: hydroxylamine oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.09Å 141.96Å 106.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.47 46.96 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.95-2.47) 98.2 (46.96-2.47)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.224 , 0.273 0.221 , 0.269	Depositor DCC
$R_{free}$ test set	7133 reflections (10.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: HOA, K, 12P, HEC, HEM, PO4

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	0.30	0/4121	0.46	0/5583
1	C	0.30	0/4108	0.46	0/5567
1	E	0.30	0/4121	0.47	0/5583
2	B	0.31	0/407	0.48	0/546
2	D	0.31	0/432	0.51	0/579
2	F	0.31	0/422	0.49	0/566
All	All	0.30	0/13611	0.47	0/18424

There are no bond length outliers.

There are no bond angle outliers.

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	4018	0	3821	31	0
1	C	4005	0	3806	29	0
1	E	4018	0	3823	40	0
2	B	404	0	428	1	0
2	D	429	0	449	1	0
2	F	419	0	441	1	0
3	A	301	0	210	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	301	0	210	10	0
3	E	301	0	210	13	0
4	A	43	0	30	3	0
4	C	43	0	29	3	0
4	E	43	0	29	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
7	A	12	0	15	1	0
7	C	25	0	33	0	0
8	E	5	0	0	0	0
9	A	295	0	0	0	0
9	B	37	0	0	0	0
9	C	284	0	0	0	0
9	D	41	0	0	0	0
9	E	301	0	0	0	0
9	F	35	0	0	0	0
All	All	15367	0	13534	111	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 4.

The worst 5 of 111 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:C:253:CYS:HA	4:E:601:HEC:HMC3	1.64	0.78
1:E:37:LEU:HD21	1:E:53:LEU:HD13	1.68	0.76
1:A:346:THR:HG22	1:A:348:ASN:H	1.50	0.75
1:A:253:CYS:HA	4:C:601:HEC:HMC3	1.71	0.72
1:E:179[B]:LYS:HD3	1:E:179[B]:LYS:H	1.54	0.72

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	502/546 (92%)	484 (96%)	18 (4%)	0	100	100
1	C	500/546 (92%)	482 (96%)	18 (4%)	0	100	100
1	E	502/546 (92%)	484 (96%)	17 (3%)	1 (0%)	51	71
2	B	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
2	D	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
2	F	53/57 (93%)	49 (92%)	3 (6%)	1 (2%)	9	14
All	All	1663/1809 (92%)	1602 (96%)	59 (4%)	2 (0%)	55	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	46	ASP
1	E	292	HIS

### 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	430/459 (94%)	419 (97%)	11 (3%)	51	76
1	C	429/459 (94%)	419 (98%)	10 (2%)	56	79
1	E	430/459 (94%)	422 (98%)	8 (2%)	62	83
2	B	46/49 (94%)	44 (96%)	2 (4%)	33	56
2	D	49/49 (100%)	46 (94%)	3 (6%)	22	38
2	F	48/49 (98%)	44 (92%)	4 (8%)	13	23
All	All	1432/1524 (94%)	1394 (97%)	38 (3%)	50	75

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	207	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	464	LEU
2	F	39	LEU
1	C	320	LEU
1	C	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	523	ASN

### 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 31 ligands modelled in this entry, 1 is 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	601	1	28,50,50	2.21	6 (21%)	17,82,82	1.56	4 (23%)
3	HEM	A	602	1	28,50,50	2.22	6 (21%)	17,82,82	1.42	1 (5%)
3	HEM	A	603	1	28,50,50	2.21	6 (21%)	17,82,82	1.39	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	A	604	1	28,50,50	2.26	7 (25%)	17,82,82	1.34	2 (11%)
3	HEM	A	605	1	28,50,50	2.20	6 (21%)	17,82,82	1.43	3 (17%)
3	HEM	A	606	1	28,50,50	2.21	6 (21%)	17,82,82	1.37	1 (5%)
3	HEM	A	607	1	28,50,50	2.21	6 (21%)	17,82,82	1.52	2 (11%)
4	HEC	A	608	1,6	28,50,50	4.10	11 (39%)	16,82,82	2.67	6 (37%)
6	HOA	A	610	4	0,1,1	0.00	-	0,0,0	0.00	-
7	12P	A	611	-	11,11,36	0.52	0	10,10,35	0.18	0
4	HEC	C	601	1,6	28,50,50	4.07	11 (39%)	16,82,82	2.20	6 (37%)
3	HEM	C	602	1	28,50,50	2.21	6 (21%)	17,82,82	1.48	2 (11%)
3	HEM	C	603	1	28,50,50	2.21	6 (21%)	17,82,82	1.35	1 (5%)
3	HEM	C	604	1	28,50,50	2.22	6 (21%)	17,82,82	1.30	1 (5%)
3	HEM	C	605	1	28,50,50	2.24	7 (25%)	17,82,82	1.38	3 (17%)
3	HEM	C	606	1	28,50,50	2.21	6 (21%)	17,82,82	1.46	3 (17%)
3	HEM	C	607	1	28,50,50	2.20	6 (21%)	17,82,82	1.40	3 (17%)
3	HEM	C	608	1	28,50,50	2.20	6 (21%)	17,82,82	1.36	2 (11%)
6	HOA	C	609	4	0,1,1	0.00	-	0,0,0	0.00	-
7	12P	C	610	-	24,24,36	0.51	0	23,23,35	0.22	0
4	HEC	E	601	1,6	28,50,50	4.10	11 (39%)	16,82,82	2.26	6 (37%)
3	HEM	E	602	1	28,50,50	2.22	6 (21%)	17,82,82	1.43	2 (11%)
3	HEM	E	603	1	28,50,50	2.20	6 (21%)	17,82,82	1.49	4 (23%)
3	HEM	E	604	1	28,50,50	2.21	6 (21%)	17,82,82	1.32	2 (11%)
3	HEM	E	605	1	28,50,50	2.23	7 (25%)	17,82,82	1.37	2 (11%)
3	HEM	E	606	1	28,50,50	2.21	6 (21%)	17,82,82	1.48	1 (5%)
3	HEM	E	607	1	28,50,50	2.19	6 (21%)	17,82,82	1.40	1 (5%)
3	HEM	E	608	1	28,50,50	2.22	6 (21%)	17,82,82	1.37	2 (11%)
8	PO4	E	609	-	4,4,4	0.78	0	6,6,6	0.39	0
6	HOA	E	610	4	0,1,1	0.00	-	0,0,0	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
3	HEM	A	601	1	-	0/6/54/54	0/0/8/8
3	HEM	A	602	1	-	0/6/54/54	0/0/8/8
3	HEM	A	603	1	-	0/6/54/54	0/0/8/8
3	HEM	A	604	1	-	0/6/54/54	0/0/8/8

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	605	1	-	0/6/54/54	0/0/8/8
3	HEM	A	606	1	-	0/6/54/54	0/0/8/8
3	HEM	A	607	1	-	0/6/54/54	0/0/8/8
4	HEC	A	608	1,6	-	0/6/54/54	0/0/8/8
6	HOA	A	610	4	-	0/0/0/0	0/0/0/0
7	12P	A	611	-	-	0/9/9/34	0/0/0/0
4	HEC	C	601	1,6	-	0/6/54/54	0/0/8/8
3	HEM	C	602	1	-	0/6/54/54	0/0/8/8
3	HEM	C	603	1	-	0/6/54/54	0/0/8/8
3	HEM	C	604	1	-	0/6/54/54	0/0/8/8
3	HEM	C	605	1	-	0/6/54/54	0/0/8/8
3	HEM	C	606	1	-	0/6/54/54	0/0/8/8
3	HEM	C	607	1	-	0/6/54/54	0/0/8/8
3	HEM	C	608	1	-	0/6/54/54	0/0/8/8
6	HOA	C	609	4	-	0/0/0/0	0/0/0/0
7	12P	C	610	-	-	0/22/22/34	0/0/0/0
4	HEC	E	601	1,6	-	0/6/54/54	0/0/8/8
3	HEM	E	602	1	-	0/6/54/54	0/0/8/8
3	HEM	E	603	1	-	0/6/54/54	0/0/8/8
3	HEM	E	604	1	-	0/6/54/54	0/0/8/8
3	HEM	E	605	1	-	0/6/54/54	0/0/8/8
3	HEM	E	606	1	-	0/6/54/54	0/0/8/8
3	HEM	E	607	1	-	0/6/54/54	0/0/8/8
3	HEM	E	608	1	-	0/6/54/54	0/0/8/8
8	PO4	E	609	-	-	0/0/0/0	0/0/0/0
6	HOA	E	610	4	-	0/0/0/0	0/0/0/0

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	HEM	C3B-C2B	-4.77	1.34	1.40
3	A	604	HEM	C3C-C2C	-4.73	1.34	1.40
3	A	606	HEM	C3C-C2C	-4.68	1.34	1.40
3	C	605	HEM	C3B-C2B	-4.62	1.34	1.40
3	E	602	HEM	C3C-C2C	-4.62	1.34	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	HEC	C3C-C4C-NC	-4.58	102.29	110.94
4	A	608	HEC	C3B-C4B-NB	-4.18	103.06	110.94
4	E	601	HEC	C3B-C4B-NB	-3.92	103.54	110.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	HEC	C3B-C4B-NB	-3.86	103.65	110.94
4	A	608	HEC	CMC-C2C-C1C	-3.46	123.15	128.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	2	0
3	A	602	HEM	1	0
3	A	604	HEM	1	0
3	A	605	HEM	3	0
3	A	606	HEM	2	0
3	A	607	HEM	2	0
4	A	608	HEC	3	0
7	A	611	12P	1	0
4	C	601	HEC	3	0
3	C	602	HEM	1	0
3	C	603	HEM	2	0
3	C	604	HEM	1	0
3	C	605	HEM	1	0
3	C	606	HEM	4	0
3	C	607	HEM	3	0
3	C	608	HEM	2	0
4	E	601	HEC	2	0
3	E	602	HEM	1	0
3	E	603	HEM	2	0
3	E	605	HEM	1	0
3	E	606	HEM	5	0
3	E	607	HEM	5	0
3	E	608	HEM	3	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	504/546 (92%)	0.40	23 (4%)	33 34	18, 31, 50, 60	0
1	C	502/546 (91%)	0.41	27 (5%)	26 27	18, 32, 48, 51	0
1	E	503/546 (92%)	0.24	20 (3%)	39 41	18, 29, 45, 56	0
2	B	53/57 (92%)	1.69	21 (39%)	0 0	32, 43, 62, 64	0
2	D	57/57 (100%)	1.06	13 (22%)	1 1	25, 33, 58, 59	0
2	F	55/57 (96%)	1.82	24 (43%)	0 0	40, 46, 68, 68	0
All	All	1674/1809 (92%)	0.46	128 (7%)	15 14	18, 32, 50, 68	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	28	SER	7.7
1	C	93	SER	7.3
2	D	84	GLY	6.6
2	B	29	SER	6.0
2	D	83	SER	6.0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	12P	A	611	12/37	0.71	0.30	8.09	50,51,51,51	0
7	12P	C	610	25/37	0.69	0.29	3.33	57,58,59,59	0
3	HEM	C	604	43/43	0.88	0.24	0.79	39,42,43,43	0
3	HEM	A	602	43/43	0.94	0.19	0.54	34,36,37,37	0
3	HEM	A	606	43/43	0.96	0.17	0.24	21,23,25,26	0
3	HEM	E	607	43/43	0.97	0.15	0.17	19,19,20,21	0
3	HEM	E	606	43/43	0.96	0.15	0.14	19,20,21,22	0
3	HEM	C	607	43/43	0.96	0.16	0.12	18,19,21,22	0
3	HEM	E	604	43/43	0.91	0.18	0.11	38,40,41,42	0
3	HEM	C	605	43/43	0.95	0.16	0.11	34,36,37,37	0
3	HEM	C	606	43/43	0.96	0.16	0.01	19,20,21,22	0
3	HEM	A	605	43/43	0.95	0.17	-0.06	22,23,24,25	0
3	HEM	A	603	43/43	0.95	0.15	-0.10	27,30,31,32	0
3	HEM	A	604	43/43	0.97	0.15	-0.12	25,27,30,31	0
4	HEC	C	601	43/43	0.94	0.15	-0.22	20,21,23,23	0
3	HEM	E	605	43/43	0.94	0.16	-0.25	29,30,32,34	0
3	HEM	C	608	43/43	0.96	0.15	-0.28	19,21,23,23	0
3	HEM	C	603	43/43	0.95	0.15	-0.30	31,32,33,33	0
3	HEM	E	603	43/43	0.95	0.16	-0.31	31,32,33,35	0
4	HEC	A	608	43/43	0.94	0.15	-0.43	22,24,27,28	0
4	HEC	E	601	43/43	0.94	0.15	-0.44	23,25,27,28	0
3	HEM	A	607	43/43	0.96	0.15	-0.48	26,27,27,28	0
3	HEM	E	602	43/43	0.97	0.13	-0.52	26,26,27,27	0
3	HEM	C	602	43/43	0.96	0.14	-0.57	25,26,28,29	0
3	HEM	E	608	43/43	0.97	0.14	-0.62	24,24,27,28	0
3	HEM	A	601	43/43	0.95	0.14	-0.94	27,28,29,29	0
8	PO4	E	609	5/5	0.95	0.15	-1.54	51,51,52,52	0
6	HOA	C	609	2/2	0.98	0.10	-	26,26,26,26	0
5	K	A	609	1/1	0.83	0.23	-	31,31,31,31	0
6	HOA	E	610	2/2	0.93	0.25	-	23,23,23,24	0
6	HOA	A	610	2/2	0.96	0.17	-	21,21,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.