



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 PM GMT

PDB ID : 4N4M
Title : Kuenenia stuttgartiensis hydroxylamine oxidoreductase soaked in phenyl hydrazine
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 : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

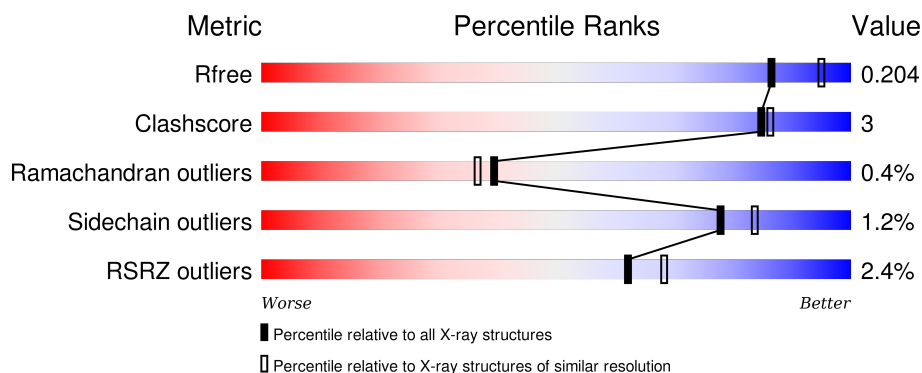
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	500	<div> <div>2%</div> <div>94%</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
2	PO4	A	602	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	610	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4596 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	494	Total	C	N	O	S	0	1	0
			3930	2471	700	728	31			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



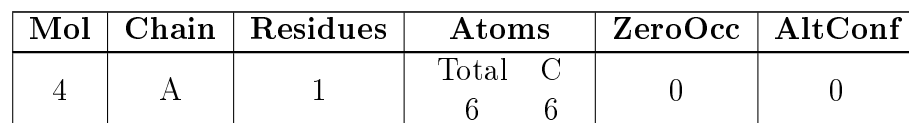
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1-PHENYLHYDRAZINE (three-letter code: PHZ) (formula: C₆H₈N₂).



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- The diagram illustrates the chemical structure of Heme (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (C=C), methyl groups (CH₃), and a long phytol chain (C₂₀H₄₁). The structure is labeled with various atoms and bonds, including O_{1A}, O_{2A}, O_{1D}, O_{2D}, C_{1A}, C_{2A}, C_{3A}, C_{4A}, C_{1B}, C_{2B}, C_{3B}, C_{4B}, C_{1C}, C_{2C}, C_{3C}, C_{4C}, C_{1D}, C_{2D}, C_{3D}, C_{4D}, C_{1E}, C_{2E}, C_{3E}, C_{4E}, C_{1F}, C_{2F}, C_{3F}, C_{4F}, C_{1G}, C_{2G}, C_{3G}, C_{4G}, C_{1H}, C_{2H}, C_{3H}, C_{4H}, C_{1I}, C_{2I}, C_{3I}, C_{4I}, C_{1J}, C_{2J}, C_{3J}, C_{4J}, C_{1K}, C_{2K}, C_{3K}, C_{4K}, C_{1L}, C_{2L}, C_{3L}, C_{4L}, C_{1M}, C_{2M}, C_{3M}, C_{4M}, C_{1N}, C_{2N}, C_{3N}, C_{4N}, C_{1O}, C_{2O}, C_{3O}, C_{4O}, C_{1P}, C_{2P}, C_{3P}, C_{4P}, C_{1Q}, C_{2Q}, C_{3Q}, C_{4Q}, C_{1R}, C_{2R}, C_{3R}, C_{4R}, C_{1S}, C_{2S}, C_{3S}, C_{4S}, C_{1T}, C_{2T}, C_{3T}, C_{4T}, C_{1U}, C_{2U}, C_{3U}, C_{4U}, C_{1V}, C_{2V}, C_{3V}, C_{4V}, C_{1W}, C_{2W}, C_{3W}, C_{4W}, C_{1X}, C_{2X}, C_{3X}, C_{4X}, C_{1Y}, C_{2Y}, C_{3Y}, C_{4Y}, C_{1Z}, C_{2Z}, C_{3Z}, C_{4Z}, C_{1AA}, C_{2AA}, C_{3AA}, C_{4AA}, C_{1AB}, C_{2AB}, C_{3AB}, C_{4AB}, C_{1AC}, C_{2AC}, C_{3AC}, C_{4AC}, C_{1AD}, C_{2AD}, C_{3AD}, C_{4AD}, C_{1AE}, C_{2AE}, C_{3AE}, C_{4AE}, C_{1AF}, C_{2AF}, C_{3AF}, C_{4AF}, C_{1AG}, C_{2AG}, C_{3AG}, C_{4AG}, C_{1AH}, C_{2AH}, C_{3AH}, C_{4AH}, C_{1AI}, C_{2AI}, C_{3AI}, C_{4AI}, C_{1AJ}, C_{2AJ}, C_{3AJ}, C_{4AJ}, C_{1AK}, C_{2AK}, C_{3AK}, C_{4AK}, C_{1AL}, C_{2AL}, C_{3AL}, C_{4AL}, C_{1AM}, C_{2AM}, C_{3AM}, C_{4AM}, C_{1AN}, C_{2AN}, C_{3AN}, C_{4AN}, C_{1AO}, C_{2AO}, C_{3AO}, C_{4AO}, C_{1AP}, C_{2AP}, C_{3AP}, C_{4AP}, C_{1AQ}, C_{2AQ}, C_{3AQ}, C_{4AQ}, C_{1AR}, C_{2AR}, C_{3AR}, C_{4AR}, C_{1AS}, C_{2AS}, C_{3AS}, C_{4AS}, C_{1AT}, C_{2AT}, C_{3AT}, C_{4AT}, C_{1AU}, C_{2AU}, C_{3AU}, C_{4AU}, C_{1AV}, C_{2AV}, C_{3AV}, C_{4AV}, C_{1AW}, C_{2AW}, C_{3AW}, C_{4AW}, C_{1AX}, C_{2AX}, C_{3AX}, C_{4AX}, C_{1AY}, C_{2AY}, C_{3AY}, C_{4AY}, C_{1AZ}, C_{2AZ}, C_{3AZ}, C_{4AZ}, C_{1BA}, C_{2BA}, C_{3BA}, C_{4BA}, C_{1BB}, C_{2BB}, C_{3BB}, C_{4BB}, C_{1BC}, C_{2BC}, C_{3BC}, C_{4BC}, C_{1BD}, C_{2BD}, C_{3BD}, C_{4BD}, C_{1BE}, C_{2BE}, C_{3BE}, C_{4BE}, C_{1BF}, C_{2BF}, C_{3BF}, C_{4BF}, C_{1BG}, C_{2BG}, C_{3BG}, C_{4BG}, C_{1BH}, C_{2BH}, C_{3BH}, C_{4BH}, C_{1BI}, C_{2BI}, C_{3BI}, C_{4BI}, C_{1BJ}, C_{2BJ}, C_{3BJ}, C_{4BJ}, C_{1BK}, C_{2BK}, C_{3BK}, C_{4BK}, C_{1BL}, C_{2BL}, C_{3BL}, C_{4BL}, C_{1BM}, C_{2BM}, C_{3BM}, C_{4BM}, C_{1BN}, C_{2BN}, C_{3BN}, C_{4BN}, C_{1BO}, C_{2BO}, C_{3BO}, C_{4BO}, C_{1BP}, C_{2BP}, C_{3BP}, C_{4BP}, C_{1BQ}, C_{2BQ}, C_{3BQ}, C_{4BQ}, C_{1BR}, C_{2BR}, C_{3BR}, C_{4BR}, C_{1BS}, C_{2BS}, C_{3BS}, C_{4BS}, C_{1BT}, C_{2BT}, C_{3BT}, C_{4BT}, C_{1BU}, C_{2BU}, C_{3BU}, C_{4BU}, C_{1BV}, C_{2BV}, C_{3BV}, C_{4BV}, C_{1BW}, C_{2BW}, C_{3BW}, C_{4BW}, C_{1BX}, C_{2BX}, C_{3BX}, C_{4BX}, C_{1BY}, C_{2BY}, C_{3BY}, C_{4BY}, C_{1BZ}, C_{2BZ}, C_{3BZ}, C_{4BZ}, C_{1CA}, C_{2CA}, C_{3CA}, C_{4CA}, C_{1CB}, C_{2CB}, C_{3CB}, C_{4CB}, C_{1CC}, C_{2CC}, C_{3CC}, C_{4CC}, C_{1CD}, C_{2CD}, C_{3CD}, C_{4CD}, C_{1CE}, C_{2CE}, C_{3CE}, C_{4CE}, C_{1CF}, C_{2CF}, C_{3CF}, C_{4CF}, C_{1CG}, C_{2CG}, C_{3CG}, C_{4CG}, C_{1CH}, C_{2CH}, C_{3CH}, C_{4CH}, C_{1CI}, C_{2CI}, C_{3CI}, C_{4CI}, C_{1CJ}, C_{2CJ}, C_{3CJ}, C_{4CJ}, C_{1CK}, C_{2CK}, C_{3CK}, C_{4CK}, C_{1CL}, C_{2CL}, C_{3CL}, C_{4CL}, C_{1CM}, C_{2CM}, C_{3CM}, C_{4CM}, C_{1CN}, C_{2CN}, C_{3CN}, C_{4CN}, C_{1CO}, C_{2CO}, C_{3CO}, C_{4CO}, C_{1CP}, C_{2CP}, C_{3CP}, C_{4CP}, C_{1CQ}, C_{2CQ}, C_{3CQ}, C_{4CQ}, C_{1CR}, C_{2CR}, C_{3CR}, C_{4CR}, C_{1CS}, C_{2CS}, C_{3CS}, C_{4CS}, C_{1CT}, C_{2CT}, C_{3CT}, C_{4CT}, C_{1CU}, C_{2CU}, C_{3CU}, C_{4CU}, C_{1CV}, C_{2CV}, C_{3CV}, C_{4CV}, C_{1CW}, C_{2CW}, C_{3CW}, C_{4CW}, C_{1CX}, C_{2CX}, C_{3CX}, C_{4CX}, C_{1CY}, C_{2CY}, C_{3CY}, C_{4CY}, C_{1CZ}, C_{2CZ}, C_{3CZ}, C_{4CZ}, C_{1DA}, C_{2DA}, C_{3DA}, C_{4DA}, C_{1DB}, C_{2DB}, C_{3DB}, C_{4DB}, C_{1DC}, C_{2DC}, C_{3DC}, C_{4DC}, C_{1DD}, C_{2DD}, C_{3DD}, C_{4DD}, C

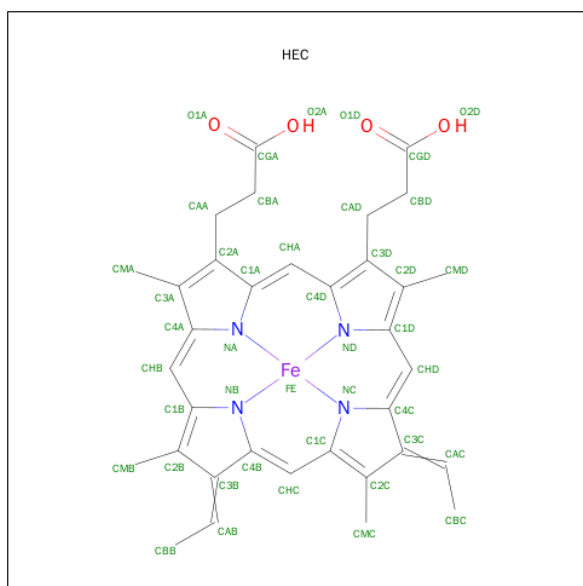
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



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

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

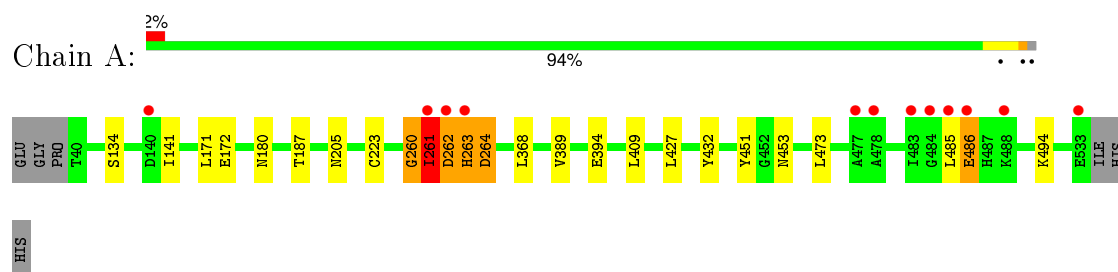
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	268	Total	O	0	0
			268	268		

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 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.

- Molecule 1: hydroxylamine oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	130.26 Å 130.26 Å 130.26 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.05 – 2.10 43.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.05-2.10) 100.0 (43.42-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.197 0.182 , 0.204	Depositor DCC
R_{free} test set	2068 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.8	EDS
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43163 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4596	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: PHZ, PO4, EDO, HEM, HEC

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	0.35	0/4044	0.52	0/5472

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	GLY	Peptide

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	3930	0	3718	18	1
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	42	0	0
4	A	6	0	4	0	0
5	A	301	0	210	5	0
6	A	43	0	30	5	1
7	A	268	0	0	0	0
All	All	4596	0	4004	24	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 3.

All (24) 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)
6:A:616:HEC:HBB3	6:A:616:HEC:HMB1	1.62	0.79
6:A:616:HEC:HBC3	6:A:616:HEC:HMC1	1.63	0.79
1:A:172[B]:GLU:HA	1:A:172[B]:GLU:OE2	1.84	0.75
1:A:263:HIS:ND1	1:A:453:ASN:HB3	2.03	0.73
1:A:260:GLY:N	1:A:264:ASP:HB2	2.14	0.61
1:A:260:GLY:C	1:A:262:ASP:N	2.58	0.57
1:A:171:LEU:HD13	5:A:613:HEM:C3A	2.46	0.50
1:A:261:ILE:HG22	1:A:432:TYR:CD1	2.47	0.50
1:A:389:VAL:HA	1:A:473:LEU:HD13	1.95	0.49
6:A:616:HEC:HMD3	5:A:618:HEM:C1D	2.49	0.48
5:A:613:HEM:HBC2	5:A:613:HEM:HMC2	1.98	0.46
1:A:427:LEU:C	1:A:427:LEU:HD13	2.38	0.45
1:A:223:CYS:HA	6:A:616:HEC:HMC3	2.00	0.44
1:A:180:ASN:HB2	1:A:187:THR:HG21	2.00	0.43
1:A:394:GLU:O	1:A:494:LYS:NZ	2.51	0.43
1:A:368:LEU:HD13	1:A:368:LEU:C	2.40	0.42
1:A:485:LEU:HD23	1:A:486:GLU:N	2.35	0.42
5:A:617:HEM:CMB	5:A:617:HEM:HBB2	2.51	0.41
1:A:205:ASN:O	6:A:616:HEC:HHB	2.21	0.41
1:A:134:SER:C	1:A:141:ILE:HD11	2.42	0.41
1:A:486:GLU:O	1:A:486:GLU:HG2	2.20	0.40
1:A:261:ILE:O	1:A:262:ASP:CB	2.70	0.40
1:A:368:LEU:HD13	1:A:368:LEU:O	2.21	0.40
5:A:613:HEM:HBC2	5:A:613:HEM:CMC	2.51	0.40

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)
1:A:451:TYR:OH	6:A:616:HEC:C3B[7_454]	2.12	0.08

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	493/500 (99%)	478 (97%)	13 (3%)	2 (0%)	39 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ASP
1	A	261	ILE

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	412/416 (99%)	407 (99%)	5 (1%)	78 84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	ILE
1	A	263	HIS
1	A	264	ASP
1	A	409	LEU

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Mol	Chain	Res	Type
1	A	486	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

20 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	$\# Z > 2$
2	PO4	A	601	-	4,4,4	0.58	0	6,6,6	0.28	0
2	PO4	A	602	-	4,4,4	0.69	0	6,6,6	0.26	0
2	PO4	A	603	-	4,4,4	0.39	0	6,6,6	0.27	0
2	PO4	A	604	-	4,4,4	0.60	0	6,6,6	0.27	0
3	EDO	A	605	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	A	606	-	3,3,3	0.43	0	2,2,2	0.49	0
3	EDO	A	607	-	3,3,3	0.49	0	2,2,2	0.43	0
3	EDO	A	608	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	A	609	-	3,3,3	0.59	0	2,2,2	0.10	0
3	EDO	A	610	-	3,3,3	0.53	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	611	-	3,3,3	0.56	0	2,2,2	0.10	0
4	PHZ	A	612	-	6,6,8	0.85	0	6,6,9	0.72	0
5	HEM	A	613	1	30,50,50	2.17	9 (30%)	24,82,82	2.32	11 (45%)
5	HEM	A	614	1	30,50,50	2.17	5 (16%)	24,82,82	2.30	10 (41%)
5	HEM	A	615	1	30,50,50	2.20	8 (26%)	24,82,82	2.35	9 (37%)
6	HEC	A	616	1	24,50,50	2.24	3 (12%)	19,82,82	2.90	8 (42%)
5	HEM	A	617	1	30,50,50	2.34	7 (23%)	24,82,82	2.33	8 (33%)
5	HEM	A	618	1	30,50,50	2.18	7 (23%)	24,82,82	2.27	11 (45%)
5	HEM	A	619	1	30,50,50	2.22	8 (26%)	24,82,82	2.45	11 (45%)
5	HEM	A	620	1	30,50,50	2.19	5 (16%)	24,82,82	2.37	10 (41%)

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
2	PO4	A	601	-	-	0/0/0/0	0/0/0/0
2	PO4	A	602	-	-	0/0/0/0	0/0/0/0
2	PO4	A	603	-	-	0/0/0/0	0/0/0/0
2	PO4	A	604	-	-	0/0/0/0	0/0/0/0
3	EDO	A	605	-	-	0/1/1/1	0/0/0/0
3	EDO	A	606	-	-	0/1/1/1	0/0/0/0
3	EDO	A	607	-	-	0/1/1/1	0/0/0/0
3	EDO	A	608	-	-	0/1/1/1	0/0/0/0
3	EDO	A	609	-	-	0/1/1/1	0/0/0/0
3	EDO	A	610	-	-	0/1/1/1	0/0/0/0
3	EDO	A	611	-	-	0/1/1/1	0/0/0/0
4	PHZ	A	612	-	-	0/0/0/2	0/1/1/1
5	HEM	A	613	1	-	0/10/54/54	0/0/8/8
5	HEM	A	614	1	-	0/10/54/54	0/0/8/8
5	HEM	A	615	1	-	0/10/54/54	0/0/8/8
6	HEC	A	616	1	-	0/6/54/54	0/0/8/8
5	HEM	A	617	1	-	0/10/54/54	0/0/8/8
5	HEM	A	618	1	-	0/10/54/54	0/0/8/8
5	HEM	A	619	1	-	0/10/54/54	0/0/8/8
5	HEM	A	620	1	-	0/10/54/54	0/0/8/8

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	617	HEM	C3B-C4B	-8.75	1.44	1.51
5	A	619	HEM	C3B-C4B	-8.02	1.44	1.51
5	A	614	HEM	C3B-C4B	-7.59	1.45	1.51
5	A	615	HEM	C3B-C4B	-7.48	1.45	1.51
5	A	613	HEM	C3B-C4B	-7.42	1.45	1.51
5	A	620	HEM	C3B-C4B	-7.34	1.45	1.51
5	A	618	HEM	C3B-C4B	-7.27	1.45	1.51
6	A	616	HEC	C3B-C2B	-5.78	1.34	1.40
6	A	616	HEC	C3C-C2C	-5.57	1.34	1.40
5	A	617	HEM	C3D-C4D	-5.30	1.44	1.51
5	A	615	HEM	C3D-C4D	-5.20	1.44	1.51
5	A	614	HEM	C3D-C4D	-5.15	1.45	1.51
5	A	620	HEM	C3D-C4D	-5.12	1.45	1.51
5	A	618	HEM	C3D-C4D	-5.11	1.45	1.51
5	A	613	HEM	C3D-C4D	-4.77	1.45	1.51
5	A	619	HEM	C3D-C4D	-4.56	1.45	1.51
5	A	617	HEM	C2C-C1C	-4.07	1.44	1.52
5	A	614	HEM	C2C-C1C	-4.03	1.44	1.52
5	A	620	HEM	C2C-C1C	-3.97	1.45	1.52
5	A	618	HEM	C2C-C1C	-3.87	1.45	1.52
5	A	613	HEM	C2C-C1C	-3.82	1.45	1.52
5	A	615	HEM	C2C-C1C	-3.73	1.45	1.52
5	A	619	HEM	C2C-C1C	-3.65	1.45	1.52
5	A	618	HEM	C2D-C1D	-2.34	1.44	1.51
5	A	614	HEM	C2D-C1D	-2.31	1.44	1.51
5	A	617	HEM	C2B-C1B	-2.13	1.44	1.51
5	A	615	HEM	C2B-C1B	-2.09	1.45	1.51
5	A	615	HEM	C2D-C1D	-2.08	1.45	1.51
5	A	617	HEM	C2D-C1D	-2.07	1.45	1.51
5	A	620	HEM	C2B-C1B	-2.07	1.45	1.51
5	A	618	HEM	C2B-C1B	-2.06	1.45	1.51
5	A	613	HEM	C2D-C1D	-2.05	1.45	1.51
5	A	619	HEM	C2D-C1D	-2.00	1.45	1.51
5	A	615	HEM	C3B-CAB	2.00	1.55	1.51
5	A	617	HEM	C3C-CAC	2.01	1.55	1.51
5	A	613	HEM	C1C-NC	2.02	1.38	1.36
5	A	619	HEM	C3C-CAC	2.02	1.55	1.51
5	A	619	HEM	C1C-NC	2.03	1.38	1.36
5	A	614	HEM	FE-NC	2.10	2.04	1.95
5	A	619	HEM	FE-ND	2.11	2.08	1.97
5	A	613	HEM	C4C-NC	2.18	1.38	1.36
5	A	618	HEM	FE-NC	2.18	2.04	1.95
5	A	613	HEM	C3C-CAC	2.24	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	613	HEM	FE-NC	2.26	2.04	1.95
5	A	613	HEM	FE-ND	2.37	2.10	1.97
5	A	615	HEM	C3C-CAC	2.39	1.55	1.51
5	A	620	HEM	C1C-NC	2.53	1.39	1.36
5	A	619	HEM	FE-NC	2.61	2.06	1.95
5	A	618	HEM	C1C-NC	2.62	1.39	1.36
5	A	615	HEM	FE-NC	2.72	2.06	1.95
5	A	617	HEM	FE-NC	3.12	2.08	1.95
6	A	616	HEC	C3D-C2D	5.37	1.53	1.37

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	616	HEC	CBC-CAC-C3C	-7.29	111.14	127.35
6	A	616	HEC	CBB-CAB-C3B	-6.81	112.23	127.35
5	A	617	HEM	C3C-CAC-CBC	-4.31	117.85	124.46
5	A	615	HEM	C3B-CAB-CBB	-3.80	118.63	124.46
5	A	619	HEM	C3C-CAC-CBC	-3.78	118.66	124.46
5	A	619	HEM	C3B-CAB-CBB	-3.65	118.85	124.46
5	A	618	HEM	C3C-CAC-CBC	-3.52	119.06	124.46
5	A	614	HEM	C3B-CAB-CBB	-3.46	119.15	124.46
5	A	614	HEM	C3C-CAC-CBC	-3.30	119.40	124.46
6	A	616	HEC	C3B-C4B-NB	-3.26	104.78	110.94
5	A	620	HEM	C3C-CAC-CBC	-3.19	119.56	124.46
5	A	620	HEM	C3B-CAB-CBB	-3.16	119.61	124.46
6	A	616	HEC	CMB-C2B-C1B	-3.07	123.29	128.36
5	A	613	HEM	C3B-CAB-CBB	-2.91	119.99	124.46
5	A	618	HEM	C3B-CAB-CBB	-2.80	120.15	124.46
5	A	615	HEM	CBA-CAA-C2A	-2.76	107.58	112.53
5	A	613	HEM	CMA-C3A-C4A	-2.63	124.01	128.36
5	A	613	HEM	CBA-CAA-C2A	-2.51	108.03	112.53
5	A	613	HEM	C3C-CAC-CBC	-2.45	120.70	124.46
5	A	615	HEM	C3C-CAC-CBC	-2.44	120.72	124.46
5	A	614	HEM	CMA-C3A-C4A	-2.35	124.48	128.36
5	A	618	HEM	CBD-CAD-C3D	-2.28	106.93	113.55
6	A	616	HEC	CAA-CBA-CGA	-2.24	108.64	112.75
5	A	613	HEM	C3B-C4B-NB	-2.23	107.37	111.63
6	A	616	HEC	CMC-C2C-C1C	-2.22	124.69	128.36
6	A	616	HEC	C3C-C4C-NC	-2.18	106.83	110.94
5	A	618	HEM	CMA-C3A-C4A	-2.12	124.86	128.36
5	A	617	HEM	C3B-C4B-NB	-2.07	107.67	111.63
5	A	619	HEM	CAA-C2A-C1A	-2.04	124.79	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	620	HEM	CAA-C2A-C1A	-2.02	124.81	127.01
5	A	615	HEM	C2D-C3D-C4D	2.03	104.95	101.50
5	A	618	HEM	C3B-C4B-CHC	2.08	126.10	123.16
5	A	620	HEM	C2D-C3D-C4D	2.11	105.07	101.50
5	A	614	HEM	C3B-C4B-CHC	2.16	126.20	123.16
5	A	618	HEM	C2D-C3D-C4D	2.24	105.31	101.50
5	A	619	HEM	C2D-C3D-C4D	2.25	105.31	101.50
5	A	614	HEM	C2D-C3D-C4D	2.25	105.32	101.50
5	A	617	HEM	C2D-C3D-C4D	2.27	105.35	101.50
5	A	619	HEM	C3B-C4B-CHC	2.30	126.41	123.16
5	A	619	HEM	C2C-C1C-CHC	2.35	127.25	123.68
5	A	620	HEM	C3B-C4B-CHC	2.39	126.53	123.16
6	A	616	HEC	C4B-C3B-C2B	2.41	108.95	106.35
5	A	613	HEM	CMD-C2D-C3D	2.47	125.29	114.35
5	A	613	HEM	C2D-C3D-C4D	2.49	105.72	101.50
5	A	614	HEM	CMD-C2D-C3D	2.51	125.46	114.35
5	A	620	HEM	CMD-C2D-C3D	2.71	126.32	114.35
5	A	615	HEM	CMD-C2D-C3D	2.74	126.46	114.35
5	A	617	HEM	CMD-C2D-C3D	2.76	126.58	114.35
5	A	619	HEM	CMD-C2D-C3D	2.81	126.78	114.35
5	A	618	HEM	CMD-C2D-C3D	2.85	126.95	114.35
5	A	614	HEM	CMB-C2B-C3B	3.51	125.29	116.53
5	A	618	HEM	CAD-C3D-C2D	3.62	123.62	113.22
5	A	615	HEM	CMB-C2B-C3B	3.84	126.11	116.53
5	A	618	HEM	CMB-C2B-C3B	3.87	126.18	116.53
5	A	619	HEM	CMC-C2C-C3C	3.93	126.35	116.53
5	A	618	HEM	CAD-C3D-C4D	3.97	126.47	112.47
5	A	613	HEM	CMB-C2B-C3B	3.98	126.45	116.53
5	A	614	HEM	CMC-C2C-C3C	3.98	126.47	116.53
5	A	617	HEM	CAD-C3D-C4D	4.08	126.86	112.47
5	A	615	HEM	CMC-C2C-C3C	4.08	126.72	116.53
5	A	617	HEM	CMC-C2C-C3C	4.16	126.90	116.53
5	A	615	HEM	CAD-C3D-C4D	4.21	127.33	112.47
5	A	619	HEM	CAD-C3D-C4D	4.23	127.39	112.47
5	A	620	HEM	CMC-C2C-C3C	4.26	127.16	116.53
5	A	620	HEM	CMB-C2B-C3B	4.26	127.16	116.53
5	A	617	HEM	CMB-C2B-C3B	4.26	127.17	116.53
5	A	619	HEM	CMB-C2B-C3B	4.28	127.21	116.53
5	A	613	HEM	CAD-C3D-C2D	4.28	125.53	113.22
5	A	620	HEM	CAD-C3D-C4D	4.28	127.58	112.47
5	A	613	HEM	CMC-C2C-C3C	4.33	127.35	116.53
5	A	618	HEM	CMC-C2C-C3C	4.34	127.36	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	613	HEM	CAD-C3D-C4D	4.36	127.84	112.47
5	A	614	HEM	CAD-C3D-C4D	4.37	127.89	112.47
5	A	619	HEM	CAD-C3D-C2D	4.41	125.91	113.22
5	A	614	HEM	CAD-C3D-C2D	4.44	125.98	113.22
5	A	617	HEM	CAD-C3D-C2D	4.60	126.44	113.22
5	A	615	HEM	CAD-C3D-C2D	4.71	126.76	113.22
5	A	620	HEM	CAD-C3D-C2D	4.92	127.35	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	613	HEM	3	0
6	A	616	HEC	5	1
5	A	617	HEM	1	0
5	A	618	HEM	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 [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	494/500 (98%)	-0.16	12 (2%) 62 68	17, 27, 42, 52	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	HIS	5.0
1	A	485	LEU	3.7
1	A	533	GLU	3.2
1	A	486	GLU	3.2
1	A	262	ASP	3.1
1	A	261	ILE	3.1
1	A	483	ILE	2.7
1	A	488	LYS	2.6
1	A	477	ALA	2.3
1	A	484	GLY	2.2
1	A	478	ALA	2.1
1	A	140	ASP	2.0

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 [i](#)

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
3	EDO	A	610	4/4	0.72	0.24	11.93	51,52,52,52	0
2	PO4	A	602	5/5	0.97	0.13	3.33	33,33,34,35	0
3	EDO	A	605	4/4	0.90	0.22	1.19	42,42,42,42	0
3	EDO	A	611	4/4	0.70	0.19	1.15	42,43,43,43	0
2	PO4	A	601	5/5	0.99	0.10	0.89	32,32,33,34	0
3	EDO	A	609	4/4	0.97	0.10	0.66	24,25,25,26	0
4	PHZ	A	612	6/8	0.88	0.17	0.63	28,30,31,31	0
3	EDO	A	608	4/4	0.95	0.12	0.59	29,30,30,32	0
5	HEM	A	617	43/43	0.98	0.10	0.25	17,19,21,24	0
5	HEM	A	618	43/43	0.98	0.10	0.06	16,19,24,24	0
5	HEM	A	620	43/43	0.99	0.10	-0.20	17,19,20,21	0
6	HEC	A	616	43/43	0.97	0.12	-0.22	24,25,29,32	0
5	HEM	A	615	43/43	0.98	0.09	-0.26	19,21,25,26	0
5	HEM	A	619	43/43	0.98	0.10	-0.39	16,18,22,24	0
5	HEM	A	613	43/43	0.98	0.09	-0.48	23,25,29,30	0
5	HEM	A	614	43/43	0.99	0.08	-0.72	19,20,22,22	0
2	PO4	A	603	5/5	0.99	0.10	-	35,35,35,36	5
3	EDO	A	607	4/4	0.86	0.13	-	40,42,42,42	0
3	EDO	A	606	4/4	0.82	0.15	-	41,42,42,42	0
2	PO4	A	604	5/5	0.91	0.31	-	16,16,17,18	5

6.5 Other polymers

There are no such residues in this entry.