



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 09:23 am GMT

PDB ID : 4N4N
Title : Nitrosomonas europea HAO
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 : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

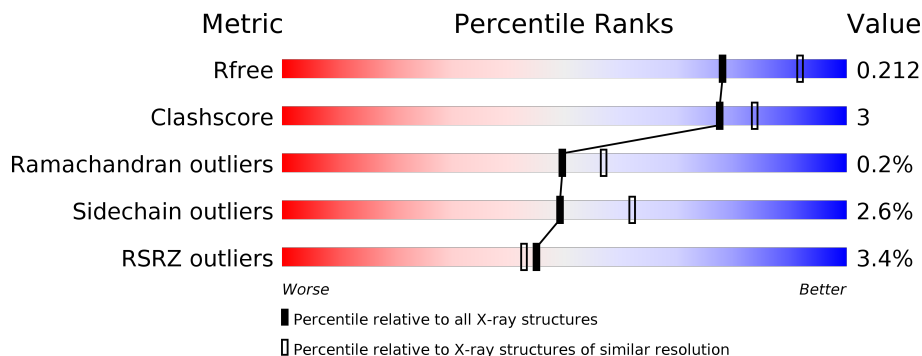
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	546	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 86%, yellow 86%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 86% 5% 8% </div> </div>
1	C	546	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 85%, yellow 85%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 85% 6% 8% </div> </div>
1	E	546	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 82%, yellow 82%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 82% 9% 8% </div> </div>
2	B	57	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 26%, green 26%, green 93%, yellow 93%, yellow 98%, grey 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 26% 93% 5% . </div> </div>
2	D	57	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 19%, green 19%, green 89%, yellow 89%, yellow 98%, grey 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 19% 89% 9% . </div> </div>
2	F	57	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 25%, green 25%, green 89%, yellow 89%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 25% 89% 7% . </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15450 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	56	Total	C	N	O	S	0	0	0
			423	263	75	82	3			
2	D	57	Total	C	N	O	S	0	0	0
			429	266	76	84	3			
2	F	56	Total	C	N	O	S	0	0	0
			425	264	75	83	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



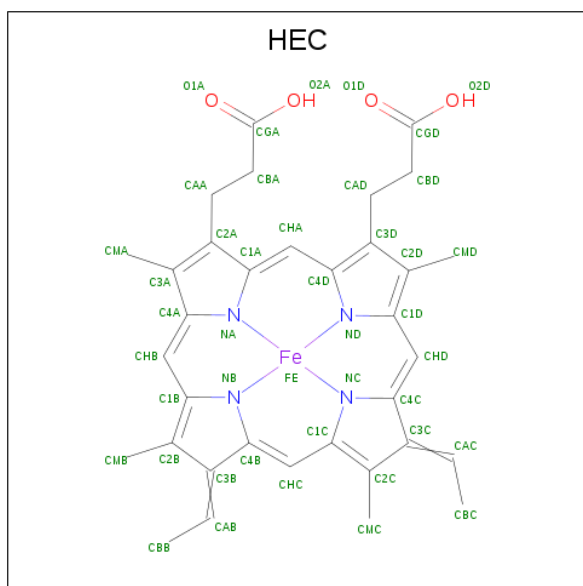
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
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	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

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

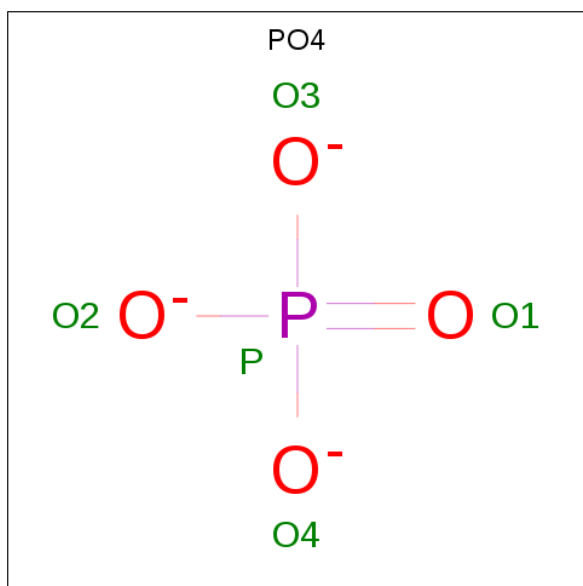


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

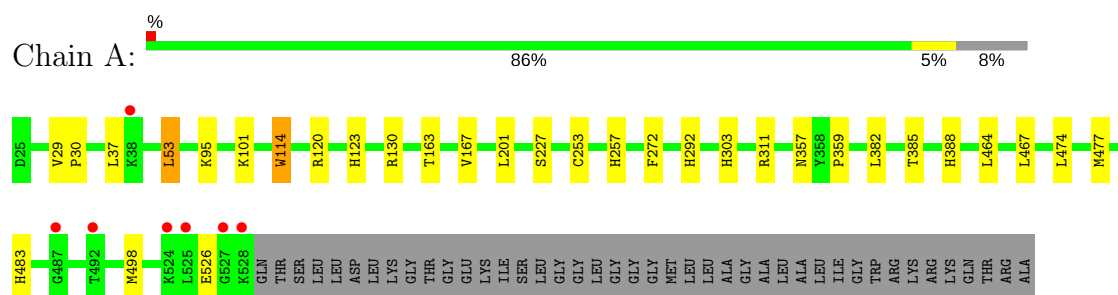
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	330	Total O 330 330	0	0
7	B	42	Total O 42 42	0	0
7	C	328	Total O 328 328	0	0
7	D	37	Total O 37 37	0	0
7	E	314	Total O 314 314	0	0
7	F	43	Total O 43 43	0	0

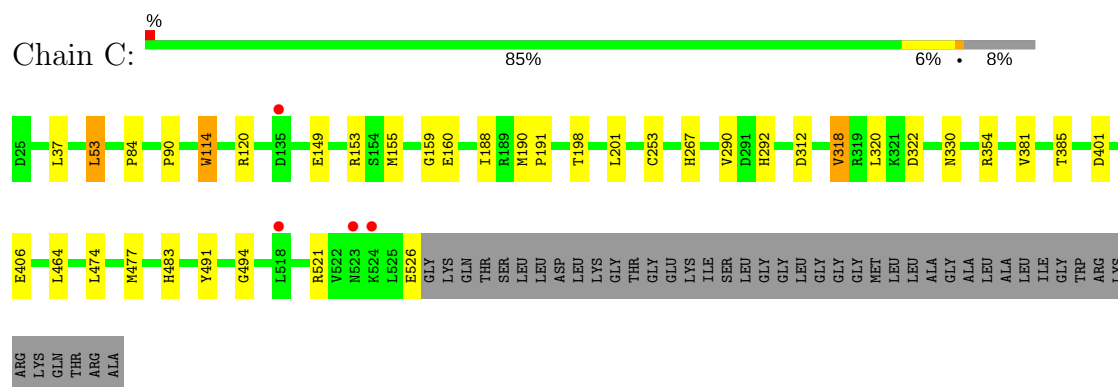
3 Residue-property plots [i](#)

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.

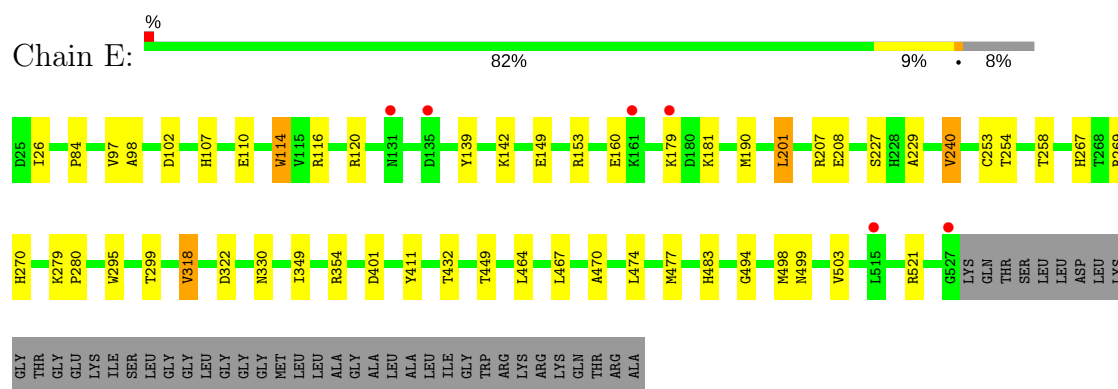
- Molecule 1: Hydroxylamine oxidoreductase



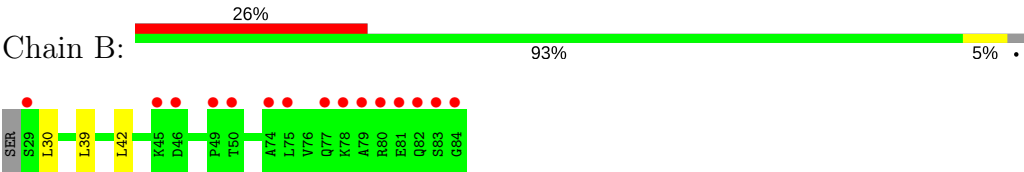
- Molecule 1: Hydroxylamine oxidoreductase



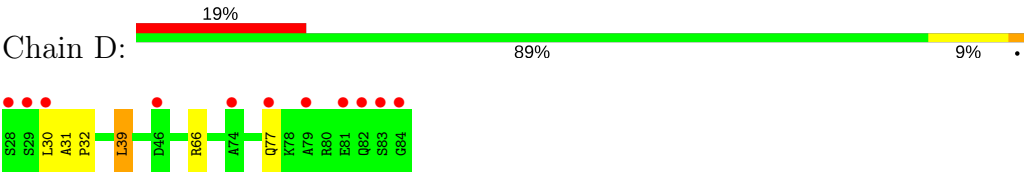
- Molecule 1: Hydroxylamine oxidoreductase



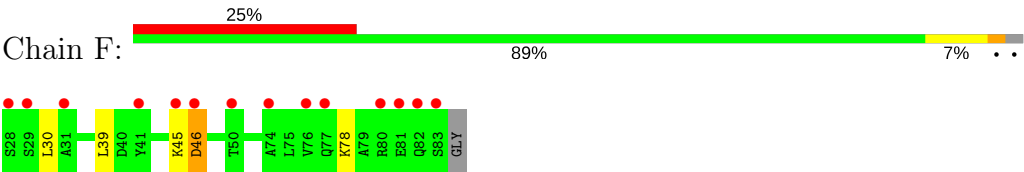
- Molecule 2: hydroxylamine oxidoreductase



● 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, α , β , γ	140.72Å 141.97Å 106.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.40 – 2.20 47.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.40-2.20) 99.6 (47.07-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.179 , 0.213 0.179 , 0.212	Depositor DCC
R_{free} test set	10263 reflections (9.47%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15450	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.333 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: HEM, K, PO4, 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	0/4121	0.50	0/5583
1	C	0.35	0/4108	0.51	0/5567
1	E	0.35	0/4121	0.51	0/5583
2	B	0.33	0/426	0.53	0/571
2	D	0.33	0/432	0.57	0/579
2	F	0.32	0/428	0.53	0/574
All	All	0.35	0/13636	0.51	0/18457

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	20	0
1	C	4005	0	3805	22	0
1	E	4018	0	3820	38	0
2	B	423	0	444	0	0
2	D	429	0	449	2	0
2	F	425	0	446	1	0
3	A	301	0	210	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	301	0	210	5	0
3	E	301	0	210	7	0
4	A	43	0	29	2	0
4	C	43	0	29	3	0
4	E	43	0	29	2	0
5	A	1	0	0	0	0
6	E	5	0	0	0	0
7	A	330	0	0	1	0
7	B	42	0	0	0	0
7	C	328	0	0	0	0
7	D	37	0	0	0	0
7	E	314	0	0	1	0
7	F	43	0	0	0	0
All	All	15450	0	13502	90	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 3.

All (90) 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:E:179[B]:LYS:HD3	1:E:179[B]:LYS:N	1.62	1.10
1:E:179[B]:LYS:CD	1:E:179[B]:LYS:H	1.69	1.03
1:E:179[B]:LYS:HD3	1:E:179[B]:LYS:H	0.81	0.94
2:F:45:LYS:O	2:F:46:ASP:HB2	1.82	0.78
1:C:37:LEU:HD11	1:C:53:LEU:HD13	1.66	0.78
1:A:477:MET:SD	1:A:498:MET:CE	2.76	0.72
1:C:153:ARG:HD2	1:C:160:GLU:HA	1.70	0.72
1:C:149:GLU:O	1:C:153:ARG:HG3	1.91	0.70
1:E:207:ARG:HH11	1:E:229:ALA:HA	1.55	0.70
1:A:477:MET:SD	1:A:498:MET:HE2	2.33	0.69
1:A:37:LEU:HD11	1:A:53:LEU:HD13	1.75	0.69
4:A:608:HEC:HMB1	4:A:608:HEC:HBB3	1.76	0.68
1:E:207:ARG:NH1	1:E:229:ALA:HA	2.13	0.63
1:E:318:VAL:HG13	1:E:322:ASP:HB2	1.80	0.62
1:C:253:CYS:HA	4:E:601:HEC:HMC3	1.81	0.61
1:C:120:ARG:HH21	1:E:330:ASN:HB3	1.66	0.60
4:C:601:HEC:HMB1	4:C:601:HEC:HBB3	1.83	0.59
1:E:240:VAL:HG13	1:E:449:THR:HG23	1.84	0.59
4:E:601:HEC:HMB1	4:E:601:HEC:HBB3	1.86	0.58
1:A:477:MET:SD	1:A:498:MET:HE1	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ARG:NH1	1:E:208:GLU:OE2	2.37	0.58
1:E:97:VAL:HG12	1:E:181:LYS:HE2	1.86	0.57
1:E:477:MET:SD	1:E:498:MET:HE1	2.45	0.57
1:A:311:ARG:NH2	7:A:924:HOH:O	2.35	0.56
1:E:179[B]:LYS:CD	1:E:179[B]:LYS:N	2.42	0.56
1:A:526:GLU:OE2	1:C:521:ARG:HD2	2.06	0.56
4:A:608:HEC:HMC3	1:E:253:CYS:HA	1.87	0.55
1:C:153:ARG:HD3	1:C:159:GLY:O	2.06	0.55
1:E:116:ARG:O	1:E:120:ARG:HG3	2.07	0.54
1:E:477:MET:SD	1:E:498:MET:CE	2.96	0.54
1:A:357:ASN:O	1:A:359:PRO:HD3	2.09	0.53
1:A:120:ARG:HH21	1:C:330:ASN:HB3	1.74	0.52
3:A:605:HEM:HMA1	3:A:606:HEM:HBA2	1.91	0.51
1:C:114:TRP:CE3	1:C:114:TRP:HA	2.46	0.51
1:A:114:TRP:HA	1:A:114:TRP:CE3	2.47	0.50
1:E:477:MET:HB2	1:E:494:GLY:HA2	1.92	0.50
1:A:385:THR:HA	1:A:388:HIS:O	2.12	0.49
1:E:483:HIS:HD2	3:E:606:HEM:C1C	2.30	0.49
3:E:606:HEM:HMA1	3:E:607:HEM:HBA2	1.94	0.49
1:E:354:ARG:NH2	1:E:401:ASP:OD1	2.45	0.49
1:A:253:CYS:HA	4:C:601:HEC:HMC3	1.93	0.49
1:E:240:VAL:HG22	7:E:802:HOH:O	2.12	0.49
1:E:26:ILE:HD11	1:E:201:LEU:HD13	1.96	0.48
1:C:318:VAL:HG13	1:C:322:ASP:HB2	1.95	0.48
1:E:114:TRP:HA	1:E:114:TRP:CE3	2.49	0.48
1:C:114:TRP:HE3	1:C:114:TRP:HA	1.79	0.47
1:C:491:TYR:HD2	4:C:601:HEC:HMC2	1.79	0.47
1:E:107:HIS:HA	1:E:110:GLU:HB3	1.96	0.47
1:A:483:HIS:HD2	3:A:605:HEM:C1C	2.33	0.47
1:A:114:TRP:HE3	1:A:114:TRP:HA	1.79	0.46
3:E:603:HEM:CHC	3:E:605:HEM:HBC1	2.45	0.46
1:E:411:TYR:CE1	1:E:470:ALA:HB2	2.50	0.46
1:E:153:ARG:HD3	1:E:160:GLU:HA	1.98	0.46
1:A:227:SER:O	3:A:606:HEM:HBD1	2.16	0.46
1:C:354:ARG:NH2	1:C:401:ASP:OD1	2.47	0.46
1:C:477:MET:HB2	1:C:494:GLY:HA2	1.99	0.45
3:A:601:HEM:HBC1	3:A:606:HEM:C4B	2.53	0.44
1:A:123:HIS:HB3	1:A:167:VAL:HB	1.99	0.44
1:C:381:VAL:O	1:C:385:THR:HG23	2.17	0.44
1:E:227:SER:O	3:E:607:HEM:HBD1	2.18	0.44
1:A:303:HIS:CD2	3:A:607:HEM:ND	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PHE:O	3:A:602:HEM:HBA1	2.18	0.43
1:E:114:TRP:HA	1:E:114:TRP:HE3	1.84	0.43
1:E:269:ARG:HA	1:E:270:HIS:HA	1.80	0.43
1:A:29:VAL:HA	1:A:30:PRO:HD3	1.91	0.43
1:E:254:THR:O	1:E:258:THR:HG23	2.18	0.42
1:A:130:ARG:NH2	1:A:163:THR:HB	2.34	0.42
1:E:483:HIS:CD2	3:E:606:HEM:C1C	3.06	0.42
1:C:90:PRO:HB3	1:C:188:ILE:HB	2.01	0.42
3:C:606:HEM:HMA1	3:C:607:HEM:HBA2	2.00	0.42
1:E:499:ASN:O	1:E:503:VAL:HG23	2.19	0.42
1:C:526:GLU:OE2	1:E:521:ARG:HD2	2.19	0.42
1:E:84:PRO:HB3	1:E:190:MET:HB2	2.00	0.42
1:E:139:TYR:CE1	1:E:142:LYS:HD3	2.55	0.42
1:C:155:MET:CE	1:C:198:THR:HG23	2.50	0.42
1:C:406:GLU:HG3	2:D:39:LEU:HD21	2.02	0.42
1:E:98:ALA:HB1	1:E:102:ASP:HB2	2.01	0.42
1:E:295:TRP:CZ2	1:E:299:THR:HG21	2.55	0.42
1:C:84:PRO:HB3	1:C:190:MET:HB2	2.01	0.42
1:C:190:MET:HA	1:C:191:PRO:HD3	1.92	0.41
3:C:604:HEM:HAA1	3:C:605:HEM:HMA1	2.02	0.41
3:E:602:HEM:HBC1	3:E:607:HEM:C4B	2.56	0.41
1:A:257:HIS:CE1	3:A:606:HEM:HMD2	2.55	0.41
1:C:483:HIS:HD2	3:C:606:HEM:C1C	2.39	0.41
3:C:602:HEM:HBC1	3:C:607:HEM:C4B	2.56	0.41
2:D:31:ALA:HA	2:D:32:PRO:HD3	1.95	0.41
1:E:349:ILE:HD13	3:E:607:HEM:C2A	2.56	0.40
1:E:279:LYS:HA	1:E:280:PRO:HD3	1.97	0.40
1:E:149:GLU:O	1:E:153:ARG:HG3	2.21	0.40
3:C:603:HEM:CHC	3:C:605:HEM:HBC1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/546 (92%)	487 (97%)	14 (3%)	1 (0%)	49	57
1	C	500/546 (92%)	485 (97%)	14 (3%)	1 (0%)	49	57
1	E	502/546 (92%)	488 (97%)	14 (3%)	0	100	100
2	B	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	D	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
2	F	54/57 (95%)	52 (96%)	1 (2%)	1 (2%)	9	5
All	All	1667/1809 (92%)	1619 (97%)	45 (3%)	3 (0%)	49	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	46	ASP
1	C	292	HIS
1	A	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%)	421 (98%)	9 (2%)	56	70
1	C	429/459 (94%)	419 (98%)	10 (2%)	53	67
1	E	430/459 (94%)	421 (98%)	9 (2%)	56	70
2	B	48/49 (98%)	45 (94%)	3 (6%)	20	22
2	D	49/49 (100%)	45 (92%)	4 (8%)	12	12
2	F	49/49 (100%)	46 (94%)	3 (6%)	20	23
All	All	1435/1524 (94%)	1397 (97%)	38 (3%)	49	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	95	LYS

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Mol	Chain	Res	Type
1	A	101	LYS
1	A	114	TRP
1	A	201	LEU
1	A	382	LEU
1	A	464	LEU
1	A	467	LEU
1	A	474	LEU
2	B	30	LEU
2	B	39	LEU
2	B	42	LEU
1	C	53	LEU
1	C	114	TRP
1	C	201	LEU
1	C	267	HIS
1	C	290	VAL
1	C	312	ASP
1	C	318	VAL
1	C	320	LEU
1	C	464	LEU
1	C	474	LEU
2	D	30	LEU
2	D	39	LEU
2	D	66	ARG
2	D	77	GLN
1	E	114	TRP
1	E	201	LEU
1	E	240	VAL
1	E	267	HIS
1	E	318	VAL
1	E	432	THR
1	E	464	LEU
1	E	467	LEU
1	E	474	LEU
2	F	30	LEU
2	F	39	LEU
2	F	78	LYS

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

Mol	Chain	Res	Type
1	A	386	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 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	27,50,50	2.13	5 (18%)	17,82,82	1.79	4 (23%)
3	HEM	A	602	1	27,50,50	2.16	6 (22%)	17,82,82	1.34	1 (5%)
3	HEM	A	603	1	27,50,50	2.11	5 (18%)	17,82,82	1.46	4 (23%)
3	HEM	A	604	1	27,50,50	2.25	6 (22%)	17,82,82	1.44	3 (17%)
3	HEM	A	605	1	27,50,50	2.16	6 (22%)	17,82,82	1.57	3 (17%)
3	HEM	A	606	1	27,50,50	2.15	6 (22%)	17,82,82	1.49	1 (5%)
3	HEM	A	607	1	27,50,50	2.12	5 (18%)	17,82,82	1.64	3 (17%)
4	HEC	A	608	1,7	26,50,50	2.64	9 (34%)	18,82,82	2.09	9 (50%)
4	HEC	C	601	1	26,50,50	2.68	9 (34%)	18,82,82	2.03	6 (33%)
3	HEM	C	602	1	27,50,50	2.15	6 (22%)	17,82,82	1.75	4 (23%)
3	HEM	C	603	1	27,50,50	2.12	5 (18%)	17,82,82	1.43	1 (5%)
3	HEM	C	604	1	27,50,50	2.13	6 (22%)	17,82,82	1.45	3 (17%)
3	HEM	C	605	1	27,50,50	2.17	6 (22%)	17,82,82	1.64	4 (23%)
3	HEM	C	606	1	27,50,50	2.13	6 (22%)	17,82,82	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	C	607	1	27,50,50	2.20	6 (22%)	17,82,82	1.54	3 (17%)
3	HEM	C	608	1	27,50,50	2.13	7 (25%)	17,82,82	1.50	2 (11%)
4	HEC	E	601	1,7	26,50,50	2.65	10 (38%)	18,82,82	2.25	10 (55%)
3	HEM	E	602	1	27,50,50	2.11	6 (22%)	17,82,82	1.63	5 (29%)
3	HEM	E	603	1	27,50,50	2.14	6 (22%)	17,82,82	1.47	2 (11%)
3	HEM	E	604	1	27,50,50	2.16	5 (18%)	17,82,82	1.46	3 (17%)
3	HEM	E	605	1	27,50,50	2.19	6 (22%)	17,82,82	1.46	4 (23%)
3	HEM	E	606	1	27,50,50	2.14	6 (22%)	17,82,82	1.63	4 (23%)
3	HEM	E	607	1	27,50,50	2.14	5 (18%)	17,82,82	1.68	4 (23%)
3	HEM	E	608	1	27,50,50	2.14	5 (18%)	17,82,82	1.69	4 (23%)
6	PO4	E	609	-	4,4,4	0.79	0	6,6,6	0.41	0

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
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	1,7	-	0/6/54/54	0/0/8/8
4	HEC	C	601	1	-	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
4	HEC	E	601	1,7	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
6	PO4	E	609	-	-	0/0/0/0	0/0/0/0

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	605	HEM	C3B-C2B	-4.80	1.33	1.40
3	A	604	HEM	C3B-C2B	-4.64	1.33	1.40
4	C	601	HEC	C3C-C2C	-4.58	1.35	1.40
3	C	605	HEM	C3B-C2B	-4.54	1.34	1.40
3	C	602	HEM	C3C-C2C	-4.43	1.34	1.40
3	E	607	HEM	C3C-C2C	-4.43	1.34	1.40
3	A	604	HEM	C3C-C2C	-4.43	1.34	1.40
3	E	602	HEM	C3C-C2C	-4.41	1.34	1.40
4	A	608	HEC	C3C-C2C	-4.40	1.36	1.40
3	A	602	HEM	C3C-C2C	-4.39	1.34	1.40
3	C	603	HEM	C3B-C2B	-4.36	1.34	1.40
3	E	606	HEM	C3B-C2B	-4.36	1.34	1.40
3	A	601	HEM	C3C-C2C	-4.35	1.34	1.40
3	C	607	HEM	C3C-C2C	-4.33	1.34	1.40
3	C	602	HEM	C3B-C2B	-4.32	1.34	1.40
3	A	605	HEM	C3C-C2C	-4.28	1.34	1.40
3	E	604	HEM	C3B-C2B	-4.27	1.34	1.40
3	C	606	HEM	C3B-C2B	-4.26	1.34	1.40
3	C	605	HEM	C3C-C2C	-4.26	1.34	1.40
3	E	605	HEM	C3C-C2C	-4.26	1.34	1.40
3	A	601	HEM	C3B-C2B	-4.22	1.34	1.40
3	C	608	HEM	C3B-C2B	-4.22	1.34	1.40
3	A	607	HEM	C3B-C2B	-4.21	1.34	1.40
3	C	604	HEM	C3B-C2B	-4.18	1.34	1.40
3	A	605	HEM	C3B-C2B	-4.18	1.34	1.40
3	E	608	HEM	C3C-C2C	-4.17	1.34	1.40
3	C	607	HEM	C3B-C2B	-4.17	1.34	1.40
3	E	608	HEM	C3B-C2B	-4.16	1.34	1.40
3	A	606	HEM	C3C-C2C	-4.12	1.34	1.40
3	A	606	HEM	C3B-C2B	-4.12	1.34	1.40
3	A	602	HEM	C3B-C2B	-4.11	1.34	1.40
3	C	606	HEM	C3C-C2C	-4.11	1.34	1.40
3	E	603	HEM	C3B-C2B	-4.09	1.34	1.40
3	E	602	HEM	C3B-C2B	-4.08	1.34	1.40
3	A	607	HEM	C3C-C2C	-4.08	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	HEM	C3C-C2C	-4.05	1.34	1.40
3	A	603	HEM	C3B-C2B	-4.05	1.34	1.40
3	E	604	HEM	C3C-C2C	-4.01	1.34	1.40
4	E	601	HEC	C3C-C2C	-3.99	1.36	1.40
3	E	606	HEM	C3C-C2C	-3.98	1.34	1.40
3	C	603	HEM	C3C-C2C	-3.95	1.34	1.40
3	E	607	HEM	C3B-C2B	-3.89	1.35	1.40
3	C	608	HEM	C3C-C2C	-3.85	1.35	1.40
3	C	604	HEM	C3C-C2C	-3.78	1.35	1.40
3	A	603	HEM	C3C-C2C	-3.77	1.35	1.40
4	E	601	HEC	C3B-C2B	-3.13	1.37	1.40
4	C	601	HEC	C3B-C2B	-3.13	1.37	1.40
4	A	608	HEC	C3B-C2B	-3.03	1.37	1.40
4	E	601	HEC	CAD-C3D	-2.10	1.48	1.52
3	E	603	HEM	CAA-C2A	2.03	1.55	1.52
3	E	606	HEM	CAA-C2A	2.05	1.55	1.52
3	C	608	HEM	C1D-ND	2.05	1.40	1.36
3	C	606	HEM	CAA-C2A	2.08	1.55	1.52
3	A	602	HEM	CAA-C2A	2.08	1.55	1.52
3	C	604	HEM	CAA-C2A	2.09	1.55	1.52
3	C	602	HEM	CAA-C2A	2.10	1.55	1.52
3	A	606	HEM	CAA-C2A	2.15	1.55	1.52
3	C	608	HEM	CAA-C2A	2.17	1.55	1.52
3	A	605	HEM	CAA-C2A	2.18	1.55	1.52
3	E	602	HEM	CAA-C2A	2.21	1.55	1.52
3	C	605	HEM	CAA-C2A	2.25	1.55	1.52
3	C	607	HEM	CAA-C2A	2.35	1.55	1.52
4	A	608	HEC	C4A-C3A	2.37	1.48	1.42
3	E	605	HEM	CAA-C2A	2.37	1.56	1.52
4	C	601	HEC	C4A-C3A	2.43	1.48	1.42
3	A	604	HEM	CAA-C2A	2.56	1.56	1.52
4	E	601	HEC	C4A-C3A	2.57	1.48	1.42
4	E	601	HEC	C1D-ND	2.92	1.42	1.36
4	C	601	HEC	C1D-ND	2.93	1.42	1.36
4	A	608	HEC	C1D-ND	2.94	1.42	1.36
4	E	601	HEC	C4D-ND	2.95	1.42	1.36
4	C	601	HEC	C4D-ND	3.13	1.42	1.36
4	A	608	HEC	C4D-ND	3.14	1.42	1.36
4	C	601	HEC	C1C-CHC	3.26	1.48	1.40
4	A	608	HEC	C1C-CHC	3.34	1.49	1.40
4	E	601	HEC	C1C-CHC	3.42	1.49	1.40
3	E	602	HEM	C3C-CAC	3.43	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	HEM	C3B-CAB	3.45	1.54	1.47
3	C	608	HEM	C3B-CAB	3.47	1.54	1.47
3	C	606	HEM	C3B-CAB	3.47	1.54	1.47
3	E	608	HEM	C3B-CAB	3.48	1.54	1.47
3	E	605	HEM	C3B-CAB	3.48	1.54	1.47
3	C	604	HEM	C3B-CAB	3.51	1.54	1.47
3	E	606	HEM	C3B-CAB	3.52	1.54	1.47
3	C	605	HEM	C3B-CAB	3.57	1.55	1.47
3	A	607	HEM	C3B-CAB	3.60	1.55	1.47
3	A	603	HEM	C3B-CAB	3.60	1.55	1.47
3	A	602	HEM	C3B-CAB	3.62	1.55	1.47
3	A	604	HEM	C3B-CAB	3.64	1.55	1.47
3	A	601	HEM	C3C-CAC	3.65	1.55	1.47
3	E	603	HEM	C3B-CAB	3.67	1.55	1.47
3	C	602	HEM	C3C-CAC	3.68	1.55	1.47
3	A	605	HEM	C3B-CAB	3.69	1.55	1.47
3	E	604	HEM	C3B-CAB	3.71	1.55	1.47
3	A	607	HEM	C3C-CAC	3.78	1.55	1.47
3	A	606	HEM	C3B-CAB	3.79	1.55	1.47
3	E	602	HEM	C3B-CAB	3.79	1.55	1.47
3	C	602	HEM	C3B-CAB	3.79	1.55	1.47
3	E	607	HEM	C3B-CAB	3.80	1.55	1.47
3	E	605	HEM	C3C-CAC	3.81	1.55	1.47
3	C	607	HEM	C3B-CAB	3.81	1.55	1.47
3	E	604	HEM	C3C-CAC	3.82	1.55	1.47
3	E	606	HEM	C3C-CAC	3.84	1.55	1.47
3	A	602	HEM	C3C-CAC	3.87	1.55	1.47
3	A	606	HEM	C3C-CAC	3.89	1.55	1.47
3	A	601	HEM	C3B-CAB	3.91	1.55	1.47
3	E	608	HEM	C3C-CAC	3.91	1.55	1.47
3	E	607	HEM	C3C-CAC	3.92	1.55	1.47
3	E	603	HEM	C3C-CAC	3.93	1.55	1.47
3	C	603	HEM	C3C-CAC	3.93	1.55	1.47
3	C	605	HEM	C3C-CAC	3.97	1.55	1.47
3	C	608	HEM	C3C-CAC	3.99	1.55	1.47
3	A	605	HEM	C3C-CAC	4.02	1.55	1.47
3	C	606	HEM	C3C-CAC	4.06	1.55	1.47
3	A	603	HEM	C3C-CAC	4.08	1.55	1.47
3	C	604	HEM	C3C-CAC	4.18	1.56	1.47
3	A	604	HEM	C3C-CAC	4.20	1.56	1.47
3	C	607	HEM	C3C-CAC	4.21	1.56	1.47
4	E	601	HEC	C1A-C2A	5.08	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	HEC	C3C-C4C	5.10	1.52	1.43
4	C	601	HEC	C1A-C2A	5.14	1.54	1.42
4	A	608	HEC	C1A-C2A	5.20	1.54	1.42
4	E	601	HEC	C3C-C4C	5.20	1.52	1.43
3	C	602	HEM	C3D-C2D	5.22	1.53	1.37
4	C	601	HEC	C3C-C4C	5.23	1.52	1.43
3	C	605	HEM	C3D-C2D	5.27	1.53	1.37
3	A	601	HEM	C3D-C2D	5.28	1.53	1.37
3	E	605	HEM	C3D-C2D	5.30	1.53	1.37
3	C	603	HEM	C3D-C2D	5.31	1.53	1.37
3	A	604	HEM	C3D-C2D	5.36	1.53	1.37
3	E	602	HEM	C3D-C2D	5.36	1.53	1.37
3	A	603	HEM	C3D-C2D	5.36	1.53	1.37
3	A	607	HEM	C3D-C2D	5.39	1.53	1.37
3	E	607	HEM	C3D-C2D	5.40	1.53	1.37
3	C	608	HEM	C3D-C2D	5.41	1.53	1.37
3	C	604	HEM	C3D-C2D	5.42	1.53	1.37
3	E	603	HEM	C3D-C2D	5.42	1.53	1.37
3	A	606	HEM	C3D-C2D	5.46	1.53	1.37
3	C	607	HEM	C3D-C2D	5.47	1.53	1.37
3	C	606	HEM	C3D-C2D	5.47	1.53	1.37
3	E	608	HEM	C3D-C2D	5.49	1.53	1.37
3	A	602	HEM	C3D-C2D	5.50	1.54	1.37
3	E	606	HEM	C3D-C2D	5.50	1.54	1.37
3	A	605	HEM	C3D-C2D	5.51	1.54	1.37
3	E	604	HEM	C3D-C2D	5.60	1.54	1.37
4	A	608	HEC	C3B-C4B	6.31	1.54	1.43
4	C	601	HEC	C3B-C4B	6.39	1.54	1.43
4	E	601	HEC	C3B-C4B	6.45	1.54	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	CBD-CAD-C3D	-4.68	103.54	112.47
3	C	602	HEM	CBD-CAD-C3D	-4.43	104.02	112.47
3	E	602	HEM	CBD-CAD-C3D	-3.96	104.91	112.47
4	A	608	HEC	C3B-C4B-NB	-3.96	103.47	110.94
4	C	601	HEC	C3B-C4B-NB	-3.95	103.48	110.94
4	E	601	HEC	C3B-C4B-NB	-3.75	103.86	110.94
3	E	608	HEM	CBD-CAD-C3D	-3.54	105.72	112.47
4	A	608	HEC	C3C-C4C-NC	-3.40	104.53	110.94
3	C	608	HEM	CBD-CAD-C3D	-3.39	105.99	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	607	HEM	CBD-CAD-C3D	-3.37	106.05	112.47
3	E	606	HEM	CBD-CAD-C3D	-3.36	106.06	112.47
3	A	607	HEM	CBD-CAD-C3D	-3.34	106.09	112.47
3	E	607	HEM	CBD-CAD-C3D	-3.29	106.19	112.47
3	A	605	HEM	CBD-CAD-C3D	-3.22	106.33	112.47
4	E	601	HEC	C3C-C4C-NC	-3.21	104.89	110.94
4	E	601	HEC	CMB-C2B-C1B	-3.16	123.60	128.46
3	A	606	HEM	CBD-CAD-C3D	-3.14	106.47	112.47
4	E	601	HEC	CMC-C2C-C1C	-3.08	123.72	128.46
3	E	608	HEM	C1D-C2D-C3D	-3.08	104.85	107.00
3	C	605	HEM	CBD-CAD-C3D	-2.95	106.83	112.47
4	C	601	HEC	C3C-C4C-NC	-2.94	105.40	110.94
4	C	601	HEC	CMB-C2B-C1B	-2.93	123.97	128.46
4	C	601	HEC	CMC-C2C-C1C	-2.89	124.03	128.46
4	A	608	HEC	CMB-C2B-C1B	-2.87	124.05	128.46
3	C	603	HEM	CAA-CBA-CGA	-2.87	107.75	112.66
3	A	601	HEM	C1D-C2D-C3D	-2.74	105.09	107.00
3	C	608	HEM	C1D-C2D-C3D	-2.74	105.09	107.00
3	C	605	HEM	CMA-C3A-C4A	-2.72	124.28	128.46
3	A	605	HEM	CMA-C3A-C4A	-2.71	124.31	128.46
3	E	605	HEM	CMA-C3A-C4A	-2.65	124.39	128.46
3	C	605	HEM	C1D-C2D-C3D	-2.64	105.16	107.00
3	A	607	HEM	C1D-C2D-C3D	-2.63	105.17	107.00
4	E	601	HEC	CAD-CBD-CGD	-2.61	108.20	112.66
3	A	604	HEM	C1D-C2D-C3D	-2.60	105.19	107.00
3	E	606	HEM	CMA-C3A-C4A	-2.55	124.54	128.46
3	E	607	HEM	C1D-C2D-C3D	-2.54	105.23	107.00
3	E	605	HEM	CBD-CAD-C3D	-2.54	107.63	112.47
3	A	603	HEM	CAD-CBD-CGD	-2.52	108.35	112.66
3	E	603	HEM	CAA-CBA-CGA	-2.51	108.37	112.66
3	C	606	HEM	CBD-CAD-C3D	-2.51	107.67	112.47
3	A	607	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
3	E	606	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
3	C	604	HEM	CMA-C3A-C4A	-2.48	124.65	128.46
3	E	607	HEM	CBA-CAA-C2A	-2.48	107.75	112.48
4	A	608	HEC	CMC-C2C-C1C	-2.45	124.69	128.46
3	A	603	HEM	C1D-C2D-C3D	-2.45	105.29	107.00
3	C	606	HEM	CMA-C3A-C4A	-2.44	124.72	128.46
3	E	607	HEM	CMA-C3A-C4A	-2.42	124.74	128.46
3	E	606	HEM	CBA-CAA-C2A	-2.42	107.86	112.48
3	A	605	HEM	C1D-C2D-C3D	-2.39	105.33	107.00
3	E	605	HEM	C1D-C2D-C3D	-2.38	105.34	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	HEC	CMD-C2D-C1D	-2.37	124.82	128.46
3	C	602	HEM	C1D-C2D-C3D	-2.35	105.36	107.00
3	A	604	HEM	CMA-C3A-C4A	-2.33	124.88	128.46
3	E	604	HEM	CAD-CBD-CGD	-2.32	108.69	112.66
3	A	602	HEM	CMA-C3A-C4A	-2.32	124.91	128.46
3	E	608	HEM	CMA-C3A-C4A	-2.31	124.91	128.46
3	E	603	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
4	E	601	HEC	C4C-C3C-C2C	-2.27	103.90	106.35
3	E	602	HEM	C1D-C2D-C3D	-2.24	105.44	107.00
4	A	608	HEC	CAA-C2A-C3A	-2.24	122.61	129.00
4	A	608	HEC	CAD-CBD-CGD	-2.22	108.87	112.66
3	A	603	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
4	A	608	HEC	CMD-C2D-C1D	-2.19	125.10	128.46
3	E	604	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
3	C	604	HEM	C1D-C2D-C3D	-2.18	105.48	107.00
3	C	607	HEM	CBA-CAA-C2A	-2.17	108.34	112.48
3	A	603	HEM	CBA-CAA-C2A	-2.17	108.34	112.48
4	C	601	HEC	CAD-CBD-CGD	-2.14	109.00	112.66
3	C	602	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
3	E	608	HEM	CBA-CAA-C2A	-2.10	108.47	112.48
3	A	601	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
3	C	607	HEM	CMA-C3A-C4A	-2.06	125.30	128.46
3	E	602	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
4	E	601	HEC	CMC-C2C-C3C	2.01	128.19	125.82
3	E	604	HEM	C4A-C3A-C2A	2.10	108.45	107.00
4	A	608	HEC	CAA-CBA-CGA	2.11	116.27	112.66
3	E	602	HEM	C4C-C3C-C2C	2.15	108.40	106.90
3	E	605	HEM	C4A-C3A-C2A	2.16	108.50	107.00
3	C	605	HEM	C4A-C3A-C2A	2.20	108.53	107.00
4	C	601	HEC	CMC-C2C-C3C	2.30	128.53	125.82
3	C	604	HEM	C4A-C3A-C2A	2.35	108.63	107.00
3	E	602	HEM	C4A-C3A-C2A	2.45	108.70	107.00
4	A	608	HEC	CMC-C2C-C3C	2.46	128.71	125.82
3	A	601	HEM	C4A-C3A-C2A	2.46	108.71	107.00
3	A	604	HEM	C4A-C3A-C2A	2.50	108.73	107.00
3	C	602	HEM	C4A-C3A-C2A	2.57	108.78	107.00
4	E	601	HEC	CBA-CAA-C2A	2.59	117.42	112.47
4	E	601	HEC	CAA-CBA-CGA	3.25	118.21	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	1	0
3	A	602	HEM	1	0
3	A	605	HEM	2	0
3	A	606	HEM	4	0
3	A	607	HEM	1	0
4	A	608	HEC	2	0
4	C	601	HEC	3	0
3	C	602	HEM	1	0
3	C	603	HEM	1	0
3	C	604	HEM	1	0
3	C	605	HEM	2	0
3	C	606	HEM	2	0
3	C	607	HEM	2	0
4	E	601	HEC	2	0
3	E	602	HEM	1	0
3	E	603	HEM	1	0
3	E	605	HEM	1	0
3	E	606	HEM	3	0
3	E	607	HEM	4	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

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	504/546 (92%)	-0.35	7 (1%) 75 73	18, 26, 38, 61	0
1	C	502/546 (91%)	-0.33	4 (0%) 86 85	18, 26, 40, 56	0
1	E	503/546 (92%)	-0.38	6 (1%) 79 77	18, 26, 39, 54	0
2	B	56/57 (98%)	0.89	15 (26%) 0 0	28, 40, 67, 68	0
2	D	57/57 (100%)	0.44	11 (19%) 1 1	26, 32, 63, 65	0
2	F	56/57 (98%)	0.96	14 (25%) 0 0	29, 41, 69, 70	0
All	All	1678/1809 (92%)	-0.24	57 (3%) 45 43	18, 27, 44, 70	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	84	GLY	7.1
2	D	83	SER	5.7
2	B	79	ALA	5.3
2	F	81	GLU	4.9
2	F	28	SER	4.7
2	D	82	GLN	4.3
2	B	77	GLN	4.2
2	B	81	GLU	4.0
1	A	527	GLY	4.0
2	D	84	GLY	4.0
2	D	81	GLU	3.9
1	C	524	LYS	3.9
1	E	527	GLY	3.8
2	D	28	SER	3.8
2	F	31	ALA	3.8
2	B	46	ASP	3.7
2	B	83	SER	3.7
2	D	46	ASP	3.5
1	C	523	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	46	ASP	3.2
2	F	45	LYS	3.2
2	D	77	GLN	3.2
2	B	29	SER	3.1
2	F	83	SER	2.9
2	D	30	LEU	2.9
2	B	82	GLN	2.8
2	F	82	GLN	2.8
1	A	38	LYS	2.7
2	B	78	LYS	2.7
1	A	525	LEU	2.7
2	F	50	THR	2.6
2	B	75	LEU	2.6
2	B	45	LYS	2.6
1	A	524	LYS	2.6
2	F	76	VAL	2.5
2	B	74	ALA	2.5
2	D	29	SER	2.5
2	F	80	ARG	2.4
2	F	77	GLN	2.4
1	E	135	ASP	2.4
2	B	49	PRO	2.3
1	C	518	LEU	2.3
2	F	41	TYR	2.3
2	B	80	ARG	2.2
2	F	29	SER	2.2
1	E	161	LYS	2.2
1	E	131	ASN	2.2
2	F	74	ALA	2.1
1	A	492	THR	2.1
2	B	50	THR	2.1
2	D	79	ALA	2.1
1	A	528	LYS	2.0
1	E	179[A]	LYS	2.0
1	E	515	LEU	2.0
1	C	135	ASP	2.0
1	A	487	GLY	2.0
2	D	74	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

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. 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	B-factors(\AA^2)	Q<0.9
5	K	A	609	1/1	0.88	0.15	38,38,38,38	0
4	HEC	C	601	43/43	0.96	0.14	21,22,24,25	0
4	HEC	E	601	43/43	0.97	0.12	21,23,25,26	0
3	HEM	E	605	43/43	0.97	0.10	22,24,26,27	0
3	HEM	C	606	43/43	0.97	0.14	17,19,22,24	0
4	HEC	A	608	43/43	0.97	0.12	20,22,23,24	0
3	HEM	E	604	43/43	0.97	0.10	26,31,34,34	0
3	HEM	C	605	43/43	0.97	0.10	21,22,24,24	0
3	HEM	A	601	43/43	0.97	0.11	19,21,23,23	0
3	HEM	E	603	43/43	0.97	0.10	22,24,24,25	0
3	HEM	E	602	43/43	0.97	0.11	19,21,22,23	0
3	HEM	A	603	43/43	0.97	0.10	22,24,25,26	0
3	HEM	A	606	43/43	0.98	0.13	18,19,23,24	0
3	HEM	E	608	43/43	0.98	0.10	19,21,22,23	0
3	HEM	E	607	43/43	0.98	0.11	18,19,22,24	0
3	HEM	C	607	43/43	0.98	0.13	17,20,24,26	0
3	HEM	A	605	43/43	0.98	0.12	17,19,22,23	0
3	HEM	C	602	43/43	0.98	0.10	19,21,23,23	0
3	HEM	C	604	43/43	0.98	0.09	23,28,29,31	0
3	HEM	A	607	43/43	0.98	0.11	19,21,22,24	0
3	HEM	C	603	43/43	0.98	0.09	19,22,24,24	0
3	HEM	E	606	43/43	0.98	0.12	17,18,19,20	0
6	PO4	E	609	5/5	0.98	0.19	53,53,53,54	0
3	HEM	C	608	43/43	0.98	0.12	18,19,22,25	0
3	HEM	A	602	43/43	0.98	0.09	22,23,24,24	0
3	HEM	A	604	43/43	0.98	0.10	16,21,22,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.