



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:27 PM GMT

PDB ID : 1GWS
Title : HEXADECACHEME HIGH MOLECULAR WEIGHT CYTOCHROME HMC
FROM DESULFOVIBRIO VULGARIS HILDENBOROUGH
Authors : Czjzek, M.; Haser, R.; Bruschi, M.
Deposited on : 2002-03-25
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

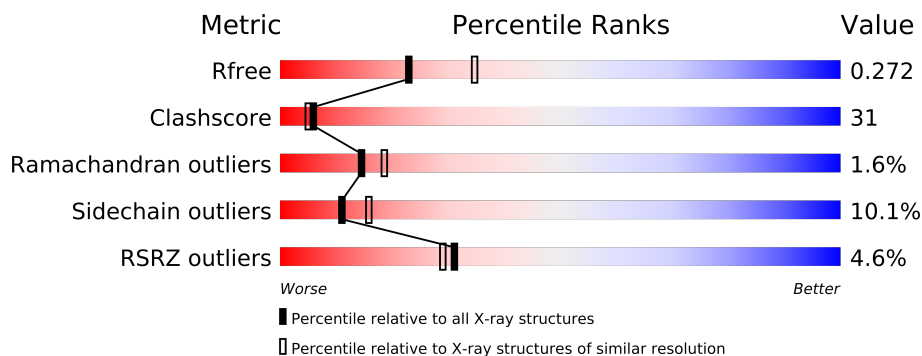
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	545	

2 Entry composition i

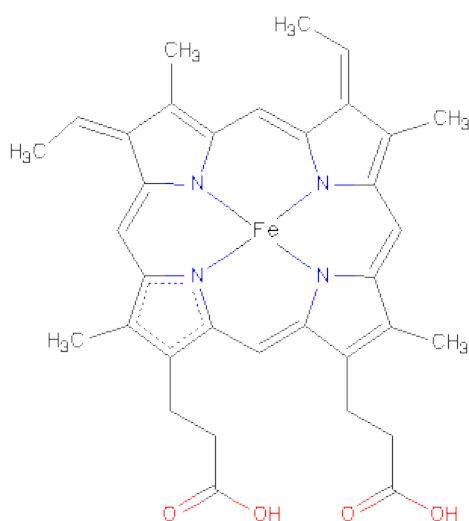
There are 4 unique types of molecules in this entry. The entry contains 4632 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HIGH-MOLECULAR-WEIGHTCYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3793	2331	715	703	44			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



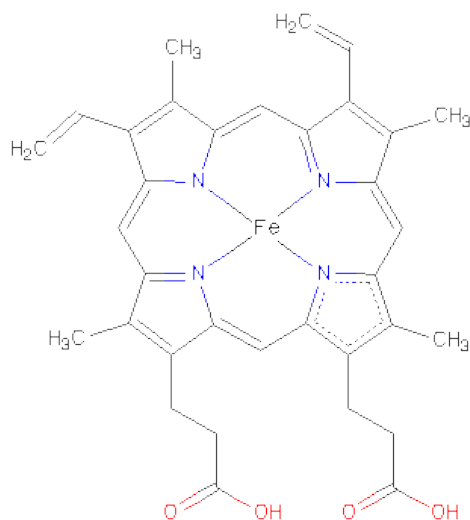
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is water.

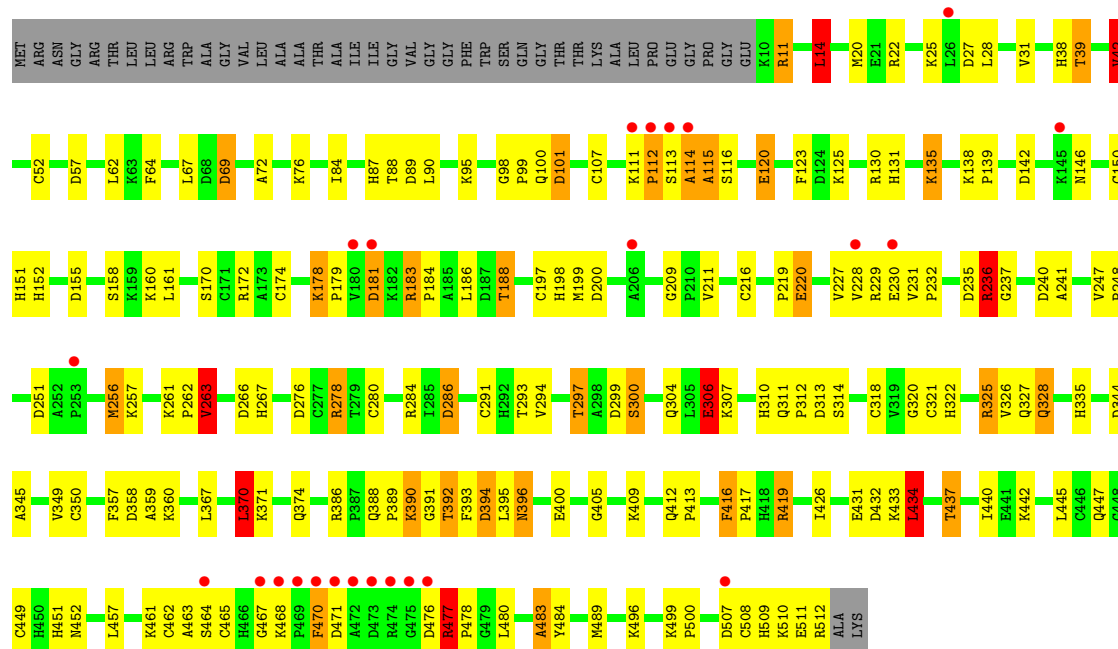
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total 151	O 151	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	108.39Å 108.39Å 102.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.52 – 2.40 33.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.52-2.40) 99.0 (33.54-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0.36	Depositor
R, R_{free}	0.201 , 0.276 0.200 , 0.272	Depositor DCC
R_{free} test set	1281 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.2	EDS
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 26599 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4632	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, 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	1.16	12/3876 (0.3%)	1.29	34/5221 (0.7%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	VAL	CB-CG1	6.94	1.67	1.52
1	A	489	MET	SD-CE	-5.97	1.44	1.77
1	A	14	LEU	CG-CD2	5.66	1.72	1.51
1	A	483	ALA	CA-CB	-5.58	1.40	1.52
1	A	306	GLU	CD-OE1	5.56	1.31	1.25
1	A	120	GLU	CG-CD	5.33	1.59	1.51
1	A	328	GLN	CG-CD	5.28	1.63	1.51
1	A	57	ASP	CB-CG	5.24	1.62	1.51
1	A	345	ALA	CA-CB	-5.20	1.41	1.52
1	A	42	VAL	CA-CB	5.12	1.65	1.54
1	A	328	GLN	CB-CG	5.06	1.66	1.52
1	A	241	ALA	CA-CB	5.03	1.63	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASP	CB-CG-OD2	9.55	126.89	118.30
1	A	240	ASP	CB-CG-OD2	9.47	126.83	118.30
1	A	394	ASP	CB-CG-OD2	9.06	126.45	118.30
1	A	236	ARG	C-N-CA	-8.73	103.97	122.30
1	A	69	ASP	CB-CG-OD2	8.61	126.05	118.30
1	A	266	ASP	CB-CG-OD2	8.38	125.84	118.30
1	A	358	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	278	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	181	ASP	CB-CG-OD2	7.61	125.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	313	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	507	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	386	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	300	SER	C-N-CA	-6.39	105.72	121.70
1	A	370	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	101	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	286	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	89	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	300	SER	N-CA-C	-5.82	95.29	111.00
1	A	142	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	199	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	57	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	276	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	263	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	A	236	ARG	N-CA-C	-5.40	96.42	111.00
1	A	419	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	130	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	A	251	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	470	PHE	N-CA-C	5.29	125.29	111.00
1	A	434	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	11	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	39	THR	N-CA-CB	-5.03	100.75	110.30
1	A	278	ARG	CA-CB-CG	5.03	124.46	113.40
1	A	344	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3793	0	3721	220	0
2	A	516	0	367	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	172	0	120	30	0
4	A	151	0	0	9	1
All	All	4632	0	4208	267	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (267) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:321:CYS:SG	2:A:610:HEC:CAC	2.10	1.39
1:A:508:CYS:SG	2:A:616:HEC:CAC	2.10	1.39
1:A:449:CYS:SG	2:A:613:HEC:CAC	2.10	1.39
1:A:280:CYS:SG	3:A:608:HEM:CAC	2.12	1.37
1:A:107:CYS:SG	2:A:603:HEC:CAC	2.18	1.31
1:A:52:CYS:SG	2:A:601:HEC:CAC	2.23	1.26
1:A:216:CYS:SG	3:A:607:HEM:CAC	2.26	1.24
1:A:150:CYS:SG	3:A:604:HEM:CAC	2.33	1.17
1:A:465:CYS:SG	2:A:614:HEC:CAC	2.33	1.16
1:A:321:CYS:SG	2:A:610:HEC:HAC	1.86	1.15
1:A:14:LEU:H	1:A:14:LEU:HD22	1.07	1.14
1:A:11:ARG:HB2	1:A:14:LEU:HD11	1.17	1.13
1:A:508:CYS:SG	2:A:616:HEC:HAC	1.87	1.11
1:A:178:LYS:HE3	1:A:179:PRO:HD3	1.33	1.09
1:A:280:CYS:SG	3:A:608:HEM:HAC	1.93	1.04
1:A:174:CYS:SG	2:A:605:HEC:HAC	1.97	1.03
2:A:609:HEC:HBC3	2:A:609:HEC:HMC1	1.40	1.03
1:A:476:ASP:O	1:A:477:ARG:O	1.76	1.02
1:A:216:CYS:SG	3:A:607:HEM:CBC	2.50	0.98
1:A:280:CYS:HG	3:A:608:HEM:CAC	1.73	0.96
1:A:449:CYS:SG	2:A:613:HEC:CBC	2.52	0.95
1:A:135:LYS:HB2	1:A:135:LYS:NZ	1.80	0.95
1:A:14:LEU:CD2	1:A:14:LEU:H	1.76	0.95
1:A:371:LYS:H	1:A:374:GLN:HE21	1.14	0.94
2:A:606:HEC:HBC3	2:A:606:HEC:HMC1	1.50	0.94
2:A:606:HEC:HMB1	2:A:606:HEC:HBB3	1.50	0.93
2:A:615:HEC:HBB3	2:A:615:HEC:HMB1	1.50	0.93
1:A:69:ASP:OD1	4:A:2016:HOH:O	1.88	0.91
1:A:476:ASP:HA	4:A:2126:HOH:O	1.70	0.90
1:A:174:CYS:SG	2:A:605:HEC:CBC	2.60	0.89
2:A:611:HEC:HMB1	2:A:611:HEC:HBB3	1.54	0.88
1:A:449:CYS:SG	2:A:613:HEC:HAC	2.12	0.87
1:A:107:CYS:SG	2:A:603:HEC:CBC	2.62	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:GLU:CD	1:A:220:GLU:H	1.76	0.87
1:A:465:CYS:SG	2:A:614:HEC:CBC	2.63	0.87
3:A:607:HEM:HMC1	3:A:607:HEM:HBC2	1.58	0.86
1:A:11:ARG:CB	1:A:14:LEU:HD11	2.05	0.86
1:A:371:LYS:H	1:A:374:GLN:NE2	1.74	0.85
1:A:20:MET:HE3	1:A:72:ALA:O	1.77	0.84
1:A:135:LYS:HB2	1:A:135:LYS:HZ3	1.41	0.84
1:A:174:CYS:O	1:A:183:ARG:HD3	1.78	0.84
1:A:350:CYS:SG	2:A:612:HEC:CBC	2.67	0.83
1:A:465:CYS:SG	2:A:614:HEC:HBC3	2.20	0.82
2:A:611:HEC:HBC3	2:A:611:HEC:HMC1	1.62	0.81
2:A:614:HEC:HBD2	2:A:614:HEC:HHA	1.61	0.81
1:A:14:LEU:N	1:A:14:LEU:HD22	1.91	0.81
1:A:111:LYS:O	1:A:113:SER:N	2.14	0.81
1:A:150:CYS:SG	3:A:604:HEM:HAC	2.22	0.80
1:A:114:ALA:O	1:A:115:ALA:HB3	1.80	0.80
1:A:107:CYS:SG	2:A:603:HEC:C3C	2.71	0.79
1:A:178:LYS:CE	1:A:179:PRO:HD3	2.14	0.78
1:A:256:MET:O	1:A:256:MET:HG2	1.82	0.78
1:A:263:VAL:HG13	2:A:612:HEC:HBD2	1.66	0.77
2:A:603:HEC:HMC1	2:A:603:HEC:HBC3	1.65	0.77
2:A:605:HEC:HBC3	2:A:605:HEC:HMC1	1.66	0.77
1:A:307:LYS:HG3	1:A:311:GLN:NE2	2.00	0.76
1:A:297:THR:HG22	1:A:299:ASP:H	1.50	0.76
1:A:172:ARG:NH1	3:A:604:HEM:O1D	2.18	0.76
2:A:613:HEC:HMB1	2:A:613:HEC:HBB3	1.68	0.76
1:A:38:HIS:O	1:A:42:VAL:HG13	1.87	0.75
2:A:606:HEC:HMC1	2:A:606:HEC:CBC	2.17	0.74
1:A:20:MET:CE	1:A:72:ALA:O	2.36	0.74
1:A:52:CYS:SG	2:A:601:HEC:HAC	2.24	0.74
3:A:608:HEM:CMB	3:A:608:HEM:HBB2	2.17	0.73
1:A:20:MET:HG3	2:A:603:HEC:O1D	1.88	0.73
1:A:280:CYS:SG	3:A:608:HEM:CBC	2.73	0.73
1:A:174:CYS:SG	2:A:605:HEC:C3C	2.76	0.73
1:A:52:CYS:SG	2:A:601:HEC:CBC	2.76	0.73
1:A:216:CYS:SG	3:A:607:HEM:C3C	2.82	0.73
1:A:27:ASP:C	1:A:28:LEU:HD12	2.09	0.73
2:A:609:HEC:HBB3	2:A:609:HEC:HMB1	1.71	0.72
1:A:508:CYS:SG	2:A:616:HEC:CBC	2.77	0.72
1:A:465:CYS:SG	2:A:614:HEC:C3C	2.77	0.72
2:A:609:HEC:CBC	2:A:609:HEC:HMC1	2.20	0.72
1:A:392:THR:HG21	1:A:426:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:ARG:HD2	1:A:278:ARG:HD3	1.71	0.71
1:A:197:CYS:SG	2:A:606:HEC:C3C	2.78	0.71
1:A:219:PRO:HD2	1:A:220:GLU:OE1	1.90	0.71
1:A:114:ALA:O	1:A:115:ALA:CB	2.39	0.70
1:A:297:THR:HG22	1:A:299:ASP:N	2.07	0.70
2:A:603:HEC:HBB3	2:A:603:HEC:HMB1	1.74	0.70
1:A:28:LEU:HD12	1:A:28:LEU:N	2.05	0.69
1:A:52:CYS:SG	2:A:601:HEC:C3C	2.81	0.69
2:A:610:HEC:O1A	2:A:610:HEC:HMA2	1.91	0.69
2:A:612:HEC:HMC1	2:A:612:HEC:HBC3	1.75	0.69
1:A:120:GLU:HG3	3:A:607:HEM:CGD	2.23	0.69
1:A:280:CYS:SG	3:A:608:HEM:C3C	2.86	0.69
1:A:476:ASP:OD1	4:A:2126:HOH:O	2.10	0.68
1:A:461:LYS:HZ2	2:A:613:HEC:CGA	2.06	0.68
1:A:449:CYS:SG	2:A:613:HEC:HBC3	2.33	0.68
1:A:350:CYS:SG	2:A:612:HEC:C3C	2.81	0.67
1:A:321:CYS:SG	2:A:610:HEC:CBC	2.82	0.67
1:A:388:GLN:HG3	1:A:389:PRO:HD2	1.75	0.67
1:A:371:LYS:N	1:A:374:GLN:HE21	1.87	0.67
3:A:607:HEM:HBC2	3:A:607:HEM:CMC	2.25	0.66
1:A:183:ARG:O	1:A:183:ARG:CG	2.44	0.66
1:A:107:CYS:SG	2:A:603:HEC:HBC3	2.34	0.65
1:A:508:CYS:SG	2:A:616:HEC:C3C	2.85	0.65
1:A:107:CYS:SG	2:A:603:HEC:HAC	2.30	0.65
2:A:611:HEC:CMB	2:A:611:HEC:HBB3	2.27	0.65
1:A:220:GLU:OE1	1:A:220:GLU:N	2.25	0.64
1:A:360:LYS:NZ	4:A:2094:HOH:O	2.29	0.64
1:A:230:GLU:HG2	1:A:230:GLU:O	1.96	0.64
1:A:321:CYS:SG	2:A:610:HEC:C3C	2.86	0.64
1:A:297:THR:CG2	1:A:299:ASP:H	2.11	0.63
1:A:150:CYS:SG	3:A:604:HEM:C3C	2.92	0.63
1:A:449:CYS:SG	2:A:613:HEC:C3C	2.86	0.63
2:A:615:HEC:HBC3	2:A:615:HEC:HMC1	1.81	0.62
1:A:14:LEU:N	1:A:14:LEU:HD13	2.16	0.61
2:A:613:HEC:HBC3	2:A:613:HEC:HMC1	1.81	0.61
1:A:113:SER:OG	1:A:114:ALA:N	2.33	0.61
1:A:367:LEU:HA	1:A:370:LEU:HD22	1.82	0.61
1:A:412:GLN:HB2	1:A:413:PRO:CD	2.31	0.60
1:A:390:LYS:NZ	1:A:440:ILE:O	2.33	0.60
1:A:88:THR:HA	1:A:100:GLN:HE22	1.65	0.59
1:A:111:LYS:O	1:A:112:PRO:C	2.41	0.59
1:A:437:THR:HG21	2:A:610:HEC:HAA2	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:612:HEC:O2A	2:A:612:HEC:HMA3	2.03	0.58
1:A:400:GLU:HA	1:A:419:ARG:HB2	1.85	0.58
1:A:135:LYS:CB	1:A:135:LYS:NZ	2.61	0.58
3:A:608:HEM:HMB2	3:A:608:HEM:CBB	2.34	0.58
1:A:412:GLN:HB2	1:A:413:PRO:HD2	1.84	0.58
1:A:178:LYS:HE3	1:A:178:LYS:HA	1.84	0.58
1:A:198:HIS:CE1	1:A:209:GLY:HA3	2.39	0.57
2:A:611:HEC:HBC3	2:A:611:HEC:CMC	2.34	0.57
1:A:52:CYS:HB3	1:A:64:PHE:CE1	2.40	0.57
1:A:465:CYS:HG	2:A:614:HEC:HBC3	1.69	0.57
3:A:602:HEM:HBB2	3:A:602:HEM:CMB	2.34	0.57
3:A:608:HEM:CMB	3:A:608:HEM:CBB	2.83	0.56
1:A:14:LEU:CD2	1:A:14:LEU:N	2.57	0.56
1:A:183:ARG:HG3	1:A:183:ARG:O	2.04	0.56
1:A:325:ARG:CG	1:A:325:ARG:HH11	2.18	0.56
1:A:123:PHE:HB2	3:A:604:HEM:CBD	2.36	0.55
1:A:112:PRO:HA	4:A:2029:HOH:O	2.05	0.55
2:A:603:HEC:HBB3	2:A:603:HEC:CMB	2.35	0.55
1:A:318:CYS:HA	2:A:610:HEC:CHC	2.36	0.55
1:A:219:PRO:CD	1:A:220:GLU:OE1	2.53	0.55
3:A:608:HEM:HMB2	3:A:608:HEM:HBB2	1.87	0.55
1:A:131:HIS:HB3	3:A:604:HEM:HBC2	1.88	0.54
2:A:606:HEC:HMB1	2:A:606:HEC:CBB	2.30	0.54
1:A:11:ARG:O	1:A:116:SER:HA	2.08	0.54
1:A:123:PHE:HB2	3:A:604:HEM:HBD2	1.89	0.54
1:A:230:GLU:O	1:A:232:PRO:HD3	2.08	0.54
1:A:220:GLU:CD	1:A:220:GLU:N	2.55	0.54
1:A:416:PHE:HB2	2:A:615:HEC:HMB2	1.89	0.53
1:A:461:LYS:NZ	2:A:613:HEC:O1A	2.39	0.53
1:A:412:GLN:HG2	1:A:510:LYS:O	2.08	0.53
1:A:310:HIS:HE1	2:A:612:HEC:C1A	2.20	0.53
3:A:602:HEM:HBC2	3:A:602:HEM:CMC	2.39	0.53
1:A:52:CYS:HB3	1:A:64:PHE:CD1	2.44	0.53
1:A:111:LYS:N	1:A:112:PRO:HD2	2.24	0.53
1:A:294:VAL:O	1:A:304:GLN:HB2	2.09	0.53
1:A:197:CYS:SG	2:A:606:HEC:CBC	2.88	0.52
1:A:335:HIS:HE1	2:A:611:HEC:C1A	2.22	0.52
2:A:605:HEC:CBC	2:A:605:HEC:HMC1	2.38	0.52
1:A:392:THR:OG1	1:A:393:PHE:N	2.42	0.52
2:A:606:HEC:HMA3	2:A:606:HEC:HBA2	1.92	0.52
1:A:28:LEU:N	1:A:28:LEU:CD1	2.72	0.52
1:A:87:HIS:CE1	1:A:98:GLY:HA3	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:LYS:HE2	4:A:2036:HOH:O	2.10	0.52
1:A:20:MET:HG3	2:A:603:HEC:CGD	2.40	0.51
2:A:613:HEC:HBB3	2:A:613:HEC:CMB	2.38	0.51
1:A:511:GLU:O	1:A:512:ARG:CB	2.58	0.51
2:A:614:HEC:HBD2	2:A:614:HEC:CHA	2.33	0.51
1:A:123:PHE:O	1:A:278:ARG:NH2	2.42	0.51
1:A:357:PHE:O	4:A:2092:HOH:O	2.19	0.51
1:A:230:GLU:O	1:A:230:GLU:CG	2.59	0.51
1:A:509:HIS:HE1	2:A:616:HEC:NB	2.08	0.51
1:A:178:LYS:CE	1:A:178:LYS:HA	2.41	0.50
1:A:433:LYS:O	1:A:437:THR:CG2	2.59	0.50
2:A:615:HEC:HHA	2:A:615:HEC:CBA	2.40	0.50
1:A:150:CYS:SG	3:A:604:HEM:CBC	2.95	0.50
1:A:467:GLY:C	1:A:468:LYS:O	2.47	0.50
2:A:612:HEC:HBB3	2:A:612:HEC:HMB1	1.93	0.50
1:A:395:LEU:HD11	1:A:426:ILE:HD12	1.92	0.50
1:A:499:LYS:HA	1:A:500:PRO:C	2.31	0.49
1:A:314:SER:O	1:A:320:GLY:HA3	2.12	0.49
1:A:84:ILE:HG21	1:A:101:ASP:HB3	1.95	0.49
1:A:174:CYS:SG	2:A:605:HEC:HBC3	2.49	0.49
2:A:606:HEC:CMA	2:A:606:HEC:HBA2	2.43	0.49
1:A:480:LEU:HG	1:A:484:TYR:CE2	2.48	0.49
1:A:120:GLU:HG3	3:A:607:HEM:O2D	2.13	0.49
1:A:325:ARG:HB3	1:A:325:ARG:HH11	1.77	0.48
1:A:322:HIS:CG	1:A:434:LEU:HD11	2.47	0.48
2:A:609:HEC:HMD1	2:A:609:HEC:HBD1	1.94	0.48
1:A:27:ASP:HB3	1:A:28:LEU:HD12	1.96	0.48
1:A:135:LYS:CB	4:A:2035:HOH:O	2.61	0.48
1:A:27:ASP:CB	1:A:28:LEU:HD12	2.43	0.48
1:A:135:LYS:HB2	1:A:135:LYS:HZ2	1.76	0.48
1:A:235:ASP:C	1:A:235:ASP:OD2	2.53	0.48
1:A:11:ARG:O	1:A:14:LEU:HD21	2.14	0.47
1:A:371:LYS:HB2	1:A:374:GLN:HE21	1.79	0.47
1:A:437:THR:CG2	2:A:610:HEC:HAA2	2.44	0.47
1:A:52:CYS:SG	2:A:601:HEC:HBC3	2.55	0.47
1:A:158:SER:O	1:A:160:LYS:HG2	2.14	0.47
1:A:247:VAL:O	1:A:293:THR:HB	2.15	0.47
1:A:248:PRO:HB3	1:A:256:MET:CE	2.44	0.47
1:A:311:GLN:HA	1:A:312:PRO:HD3	1.64	0.47
1:A:388:GLN:HG3	1:A:389:PRO:CD	2.43	0.47
1:A:307:LYS:HG3	1:A:311:GLN:HE21	1.74	0.47
1:A:158:SER:HB2	1:A:160:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ASP:OD2	1:A:236:ARG:O	2.34	0.46
1:A:463:ALA:O	1:A:464:SER:C	2.51	0.46
1:A:388:GLN:CG	1:A:389:PRO:CD	2.93	0.46
1:A:367:LEU:HD23	1:A:370:LEU:HD22	1.97	0.46
1:A:227:VAL:HG12	1:A:228:VAL:N	2.30	0.46
1:A:391:GLY:O	1:A:442:LYS:HA	2.15	0.46
1:A:452:ASN:HD22	2:A:614:HEC:CHD	2.30	0.45
2:A:609:HEC:HBD1	2:A:609:HEC:CMD	2.47	0.45
1:A:463:ALA:C	1:A:465:CYS:N	2.67	0.45
1:A:219:PRO:N	1:A:220:GLU:OE1	2.50	0.45
2:A:606:HEC:CMC	2:A:606:HEC:CBC	2.90	0.45
1:A:462:CYS:N	2:A:613:HEC:O2D	2.44	0.45
1:A:267:HIS:CE1	3:A:608:HEM:C4B	3.04	0.45
1:A:464:SER:O	1:A:465:CYS:HB3	2.17	0.44
1:A:405:GLY:HA2	2:A:616:HEC:O1D	2.17	0.44
1:A:170:SER:OG	1:A:172:ARG:HG3	2.18	0.44
1:A:138:LYS:HA	1:A:139:PRO:HD3	1.89	0.44
1:A:307:LYS:HD2	1:A:307:LYS:HA	1.65	0.44
2:A:609:HEC:HBB3	2:A:609:HEC:CMB	2.44	0.44
1:A:262:PRO:HD3	1:A:359:ALA:HB3	1.99	0.44
1:A:267:HIS:HE1	3:A:608:HEM:C4B	2.36	0.44
1:A:90:LEU:HD13	3:A:602:HEM:HMD3	2.00	0.44
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.83	0.43
2:A:614:HEC:HMC1	2:A:614:HEC:HBC3	2.00	0.43
1:A:291:CYS:O	1:A:297:THR:HB	2.19	0.43
1:A:151:HIS:CD2	3:A:604:HEM:NB	2.87	0.43
1:A:483:ALA:HB1	2:A:614:HEC:CHB	2.48	0.43
1:A:477:ARG:HB2	1:A:478:PRO:HD3	1.98	0.43
1:A:349:VAL:O	1:A:349:VAL:HG12	2.18	0.43
1:A:62:LEU:HD12	1:A:188:THR:HB	2.01	0.43
1:A:198:HIS:NE2	1:A:209:GLY:HA3	2.34	0.43
1:A:125:LYS:HE3	1:A:229:ARG:NH1	2.35	0.42
1:A:299:ASP:C	1:A:300:SER:O	2.54	0.42
1:A:183:ARG:HA	1:A:184:PRO:HD3	1.87	0.42
1:A:304:GLN:HG3	1:A:306:GLU:HG2	2.02	0.42
1:A:227:VAL:CG1	1:A:228:VAL:N	2.82	0.42
1:A:318:CYS:HB3	2:A:610:HEC:C4B	2.46	0.42
1:A:477:ARG:CB	1:A:478:PRO:CD	2.97	0.42
1:A:87:HIS:CE1	1:A:99:PRO:HD2	2.55	0.42
1:A:447:GLN:NE2	4:A:2118:HOH:O	2.52	0.42
1:A:467:GLY:O	1:A:468:LYS:C	2.58	0.42
2:A:610:HEC:HBC3	2:A:610:HEC:HMC1	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:GLN:HB2	1:A:311:GLN:HE21	1.52	0.42
1:A:20:MET:HE1	1:A:72:ALA:O	2.20	0.42
1:A:135:LYS:HG3	1:A:135:LYS:O	2.19	0.42
1:A:183:ARG:HG2	1:A:183:ARG:O	2.17	0.42
2:A:616:HEC:HMC1	2:A:616:HEC:HBC3	2.02	0.41
2:A:615:HEC:CBB	2:A:615:HEC:HMB1	2.30	0.41
1:A:477:ARG:HB2	1:A:478:PRO:CD	2.50	0.41
1:A:248:PRO:HB3	1:A:256:MET:HE2	2.02	0.41
1:A:236:ARG:HB2	1:A:237:GLY:H	1.69	0.41
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.81	0.41
1:A:367:LEU:HD23	1:A:370:LEU:CD2	2.51	0.41
1:A:433:LYS:O	1:A:437:THR:HG22	2.21	0.41
1:A:416:PHE:HA	1:A:417:PRO:HD3	1.87	0.41
1:A:432:ASP:OD2	1:A:434:LEU:N	2.54	0.41
1:A:228:VAL:O	1:A:231:VAL:CG2	2.69	0.41
1:A:261:LYS:HB3	1:A:262:PRO:HD2	2.02	0.41
1:A:325:ARG:HH11	1:A:325:ARG:CB	2.33	0.40
1:A:433:LYS:O	1:A:437:THR:HG23	2.22	0.40
2:A:613:HEC:HBC1	2:A:615:HEC:C2C	2.51	0.40
1:A:452:ASN:HD22	2:A:614:HEC:C1D	2.33	0.40
1:A:152:HIS:CD2	1:A:161:LEU:HD22	2.57	0.40
1:A:299:ASP:O	2:A:609:HEC:HMD3	2.22	0.40
1:A:335:HIS:CE1	2:A:611:HEC:C1A	3.04	0.40
1:A:394:ASP:OD2	1:A:396:ASN:HB2	2.21	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	Distance(Å)	Clash(Å)
4:A:2028:HOH:O	4:A:2136:HOH:O[4_675]	0.64	1.56

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	501/545 (92%)	460 (92%)	33 (7%)	8 (2%)	14 18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	A	181	ASP
1	A	257	LYS
1	A	477	ARG
1	A	115	ALA
1	A	114	ALA
1	A	409	LYS
1	A	286	ASP

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	405/435 (93%)	364 (90%)	41 (10%)	11 16

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	22	ARG
1	A	25	LYS
1	A	39	THR
1	A	42	VAL
1	A	67	LEU
1	A	76	LYS
1	A	95	LYS
1	A	135	LYS
1	A	146	ASN
1	A	178	LYS
1	A	183	ARG
1	A	186	LEU
1	A	188	THR
1	A	211	VAL

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Mol	Chain	Res	Type
1	A	220	GLU
1	A	236	ARG
1	A	256	MET
1	A	263	VAL
1	A	284	ARG
1	A	297	THR
1	A	306	GLU
1	A	325	ARG
1	A	326	VAL
1	A	327	GLN
1	A	328	GLN
1	A	370	LEU
1	A	390	LYS
1	A	392	THR
1	A	396	ASN
1	A	416	PHE
1	A	431	GLU
1	A	434	LEU
1	A	437	THR
1	A	445	LEU
1	A	451	HIS
1	A	457	LEU
1	A	470	PHE
1	A	471	ASP
1	A	477	ARG
1	A	496	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	100	GLN
1	A	146	ASN
1	A	222	GLN
1	A	282	HIS
1	A	311	GLN
1	A	323	ASN
1	A	346	GLN
1	A	374	GLN
1	A	447	GLN
1	A	452	ASN
1	A	486	GLN

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Mol	Chain	Res	Type
1	A	487	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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	HEC	A	601	1	50,50,50	2.95	12 (24%)	56,82,82	1.91	12 (21%)
3	HEM	A	602	1	49,50,50	2.67	14 (28%)	46,82,82	2.14	13 (28%)
2	HEC	A	603	1	50,50,50	2.75	15 (30%)	56,82,82	2.36	20 (35%)
3	HEM	A	604	1	49,50,50	2.79	14 (28%)	46,82,82	1.83	6 (13%)
2	HEC	A	605	1	50,50,50	3.27	17 (34%)	56,82,82	1.98	12 (21%)
2	HEC	A	606	1	50,50,50	2.68	14 (28%)	56,82,82	2.17	16 (28%)
3	HEM	A	607	1	49,50,50	2.69	14 (28%)	46,82,82	2.24	19 (41%)
3	HEM	A	608	1	49,50,50	3.02	14 (28%)	46,82,82	2.01	14 (30%)
2	HEC	A	609	1	50,50,50	2.99	14 (28%)	56,82,82	2.38	19 (33%)
2	HEC	A	610	1	50,50,50	3.23	19 (38%)	56,82,82	2.76	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	611	1	50,50,50	2.95	17 (34%)	56,82,82	2.70	21 (37%)
2	HEC	A	612	1	50,50,50	2.82	17 (34%)	56,82,82	2.10	15 (26%)
2	HEC	A	613	1	50,50,50	2.65	14 (28%)	56,82,82	2.34	17 (30%)
2	HEC	A	614	1	50,50,50	3.12	18 (36%)	56,82,82	2.21	18 (32%)
2	HEC	A	615	1	50,50,50	2.96	19 (38%)	56,82,82	2.48	25 (44%)
2	HEC	A	616	1	50,50,50	2.95	17 (34%)	56,82,82	2.53	23 (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	HEC	A	601	1	-	0/10/54/54	0/0/8/8
3	HEM	A	602	1	-	0/14/114/114	0/0/8/8
2	HEC	A	603	1	-	0/10/54/54	0/0/8/8
3	HEM	A	604	1	-	0/14/114/114	0/0/8/8
2	HEC	A	605	1	-	0/10/54/54	0/0/8/8
2	HEC	A	606	1	-	0/10/54/54	0/0/8/8
3	HEM	A	607	1	-	0/14/114/114	0/0/8/8
3	HEM	A	608	1	-	0/14/114/114	0/0/8/8
2	HEC	A	609	1	-	0/10/54/54	0/0/8/8
2	HEC	A	610	1	-	0/10/54/54	0/0/8/8
2	HEC	A	611	1	-	0/10/54/54	0/0/8/8
2	HEC	A	612	1	-	0/10/54/54	0/0/8/8
2	HEC	A	613	1	-	0/10/54/54	0/0/8/8
2	HEC	A	614	1	-	0/10/54/54	0/0/8/8
2	HEC	A	615	1	-	0/10/54/54	0/0/8/8
2	HEC	A	616	1	-	0/10/54/54	0/0/8/8

All (249) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	608	HEM	C3D-C4D	13.04	1.47	1.44
3	A	604	HEM	C2B-C1B	11.87	1.47	1.44
2	A	605	HEC	C3C-CAC	11.87	1.59	1.35
3	A	607	HEM	C3D-C4D	11.32	1.47	1.44
2	A	601	HEC	C3B-CAB	11.22	1.58	1.35
2	A	601	HEC	C3C-CAC	10.91	1.57	1.35
2	A	614	HEC	C3C-CAC	10.81	1.57	1.35
2	A	609	HEC	C3B-CAB	10.79	1.57	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	610	HEC	C3C-CAC	10.67	1.57	1.35
2	A	616	HEC	C3B-CAB	10.58	1.57	1.35
2	A	616	HEC	C3C-CAC	10.48	1.57	1.35
2	A	606	HEC	C3C-CAC	10.20	1.56	1.35
2	A	613	HEC	C3B-CAB	10.15	1.56	1.35
2	A	612	HEC	C3C-CAC	10.09	1.56	1.35
2	A	609	HEC	C3C-CAC	10.03	1.56	1.35
2	A	611	HEC	C3C-CAC	9.90	1.55	1.35
2	A	615	HEC	C3B-CAB	9.85	1.55	1.35
2	A	610	HEC	C3B-CAB	9.69	1.55	1.35
3	A	602	HEM	C2B-C1B	-9.65	1.42	1.44
2	A	605	HEC	C3B-CAB	9.65	1.55	1.35
2	A	612	HEC	C3B-CAB	9.54	1.55	1.35
2	A	614	HEC	C3B-CAB	9.53	1.55	1.35
2	A	603	HEC	C3C-CAC	9.38	1.54	1.35
2	A	611	HEC	C3B-CAB	9.37	1.54	1.35
2	A	615	HEC	C3C-CAC	9.01	1.54	1.35
2	A	613	HEC	C3C-CAC	9.00	1.54	1.35
2	A	603	HEC	C3B-CAB	8.93	1.53	1.35
2	A	606	HEC	C3B-CAB	8.74	1.53	1.35
3	A	608	HEM	C3B-C2B	-7.60	1.30	1.43
2	A	614	HEC	C1C-C2C	7.30	1.49	1.40
3	A	602	HEM	C3B-C2B	-7.14	1.31	1.43
2	A	610	HEC	C1B-C2B	7.06	1.49	1.40
2	A	605	HEC	C1C-C2C	6.93	1.48	1.40
2	A	614	HEC	C1B-C2B	6.85	1.48	1.40
2	A	610	HEC	C3C-C4C	6.78	1.50	1.41
3	A	604	HEM	C3B-C2B	-6.70	1.32	1.43
3	A	608	HEM	C3B-CAB	6.29	1.60	1.40
2	A	615	HEC	C1C-C2C	6.29	1.48	1.40
2	A	601	HEC	C1B-C2B	6.23	1.47	1.40
2	A	605	HEC	C1D-C2D	6.15	1.47	1.40
3	A	607	HEM	C3C-C2C	-6.05	1.33	1.43
2	A	609	HEC	C3C-C2C	-5.96	1.28	1.41
3	A	608	HEM	C3C-C2C	-5.95	1.33	1.43
2	A	610	HEC	FE-ND	5.90	2.17	1.92
3	A	602	HEM	C3C-C2C	-5.84	1.33	1.43
2	A	611	HEC	C1C-C2C	5.75	1.47	1.40
2	A	616	HEC	C3D-C2D	5.68	1.54	1.37
2	A	605	HEC	C3C-C4C	5.66	1.48	1.41
3	A	604	HEM	C3B-CAB	5.39	1.57	1.40
2	A	610	HEC	C1C-C2C	5.33	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	611	HEC	C3B-C2B	-5.23	1.30	1.41
3	A	608	HEM	C3C-CAC	5.18	1.56	1.40
2	A	601	HEC	C3D-C2D	5.01	1.52	1.37
2	A	609	HEC	C1C-C2C	4.99	1.46	1.40
3	A	602	HEM	C3C-CAC	4.98	1.56	1.40
2	A	606	HEC	C3B-C2B	-4.90	1.30	1.41
2	A	610	HEC	C3D-C2D	4.90	1.52	1.37
2	A	616	HEC	C3C-C2C	-4.86	1.31	1.41
2	A	615	HEC	C1D-C2D	4.83	1.46	1.40
2	A	605	HEC	FE-ND	4.81	2.13	1.92
3	A	607	HEM	C3C-CAC	4.76	1.55	1.40
3	A	604	HEM	C3C-C2C	-4.75	1.35	1.43
2	A	609	HEC	C3D-C2D	4.75	1.51	1.37
3	A	602	HEM	C3D-C2D	4.75	1.52	1.43
2	A	612	HEC	C1C-C2C	4.73	1.46	1.40
3	A	604	HEM	C2D-C1D	-4.73	1.43	1.44
2	A	609	HEC	FE-NB	4.72	2.12	1.92
2	A	603	HEC	C3C-C2C	-4.68	1.31	1.41
2	A	615	HEC	FE-NA	4.64	2.12	1.92
2	A	614	HEC	C3D-C2D	4.62	1.51	1.37
3	A	607	HEM	C3B-C2B	-4.60	1.35	1.43
2	A	603	HEC	C1C-C2C	4.57	1.45	1.40
2	A	613	HEC	C3D-C2D	4.55	1.51	1.37
3	A	604	HEM	C3C-CAC	4.54	1.54	1.40
2	A	611	HEC	C3C-C2C	-4.54	1.31	1.41
2	A	613	HEC	C3B-C2B	-4.53	1.31	1.41
3	A	607	HEM	CAA-C2A	4.53	1.59	1.52
2	A	609	HEC	C1B-C2B	4.50	1.45	1.40
3	A	607	HEM	C3B-CAB	4.50	1.54	1.40
2	A	605	HEC	C3D-C2D	4.42	1.50	1.37
2	A	612	HEC	C3D-C2D	4.39	1.50	1.37
3	A	607	HEM	C4A-C3A	4.36	1.45	1.40
2	A	605	HEC	CBB-CAB	-4.34	1.30	1.49
2	A	601	HEC	FE-ND	4.33	2.11	1.92
2	A	613	HEC	C3B-C4B	4.33	1.47	1.41
2	A	613	HEC	C1B-C2B	4.30	1.45	1.40
2	A	606	HEC	C3C-C2C	-4.31	1.32	1.41
2	A	603	HEC	C3D-C2D	4.30	1.50	1.37
2	A	615	HEC	C3D-C2D	4.28	1.50	1.37
2	A	615	HEC	C1B-C2B	4.25	1.45	1.40
2	A	605	HEC	C3C-C2C	-4.21	1.32	1.41
2	A	606	HEC	C3D-C2D	4.21	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	HEC	C3B-C2B	-4.19	1.32	1.41
2	A	610	HEC	C1D-C2D	4.17	1.45	1.40
2	A	611	HEC	C3D-C2D	4.16	1.50	1.37
3	A	602	HEM	C4A-C3A	4.15	1.45	1.40
3	A	608	HEM	C2D-C1D	4.11	1.45	1.44
2	A	601	HEC	C3B-C2B	-4.07	1.32	1.41
2	A	612	HEC	C1B-C2B	4.07	1.45	1.40
2	A	611	HEC	C3B-C4B	4.04	1.46	1.41
2	A	612	HEC	C3C-C2C	-4.04	1.32	1.41
3	A	604	HEM	C4A-C3A	3.99	1.45	1.40
2	A	603	HEC	CBC-CAC	-3.99	1.32	1.49
2	A	615	HEC	C4B-NB	3.99	1.42	1.37
2	A	616	HEC	C1B-C2B	3.98	1.45	1.40
2	A	614	HEC	CBB-CAB	-3.93	1.32	1.49
2	A	603	HEC	FE-NC	3.93	2.09	1.92
2	A	612	HEC	C1D-C2D	3.92	1.45	1.40
2	A	614	HEC	FE-ND	3.92	2.09	1.92
2	A	615	HEC	C3B-C2B	-3.91	1.33	1.41
2	A	611	HEC	C3C-C4C	3.87	1.46	1.41
2	A	609	HEC	C3C-C4C	3.86	1.46	1.41
2	A	606	HEC	C3C-C4C	3.86	1.46	1.41
2	A	603	HEC	FE-NA	3.83	2.08	1.92
2	A	603	HEC	C3B-C4B	3.82	1.46	1.41
2	A	610	HEC	C3B-C2B	-3.82	1.33	1.41
2	A	616	HEC	C1C-C2C	3.80	1.44	1.40
2	A	614	HEC	C3B-C2B	-3.73	1.33	1.41
3	A	607	HEM	C3D-C2D	3.68	1.50	1.43
2	A	616	HEC	CBC-CAC	-3.63	1.33	1.49
3	A	608	HEM	C3D-C2D	3.62	1.50	1.43
2	A	606	HEC	C1D-C2D	3.62	1.44	1.40
2	A	605	HEC	C4C-NC	3.60	1.42	1.37
2	A	614	HEC	FE-NA	3.60	2.07	1.92
2	A	609	HEC	CBC-CAC	-3.58	1.34	1.49
3	A	602	HEM	C4D-ND	-3.57	1.32	1.39
2	A	601	HEC	C1C-C2C	3.56	1.44	1.40
2	A	611	HEC	CBC-CAC	-3.54	1.34	1.49
2	A	612	HEC	CBB-CAB	-3.49	1.34	1.49
2	A	612	HEC	C3C-C4C	3.48	1.46	1.41
2	A	610	HEC	FE-NC	3.46	2.07	1.92
3	A	602	HEM	C3B-CAB	3.42	1.51	1.40
2	A	610	HEC	CBB-CAB	-3.42	1.34	1.49
2	A	613	HEC	CBC-CAC	-3.42	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	611	HEC	CBB-CAB	-3.40	1.34	1.49
2	A	603	HEC	CBB-CAB	-3.36	1.35	1.49
3	A	607	HEM	C2B-C1B	3.34	1.45	1.44
2	A	612	HEC	FE-NA	3.34	2.06	1.92
2	A	606	HEC	CBB-CAB	-3.34	1.35	1.49
3	A	604	HEM	FE-NA	3.33	2.06	1.92
2	A	605	HEC	FE-NB	3.31	2.06	1.92
2	A	614	HEC	O1D-CGD	3.29	1.34	1.22
2	A	611	HEC	C1D-C2D	3.29	1.44	1.40
2	A	616	HEC	CBB-CAB	-3.29	1.35	1.49
2	A	614	HEC	CBC-CAC	-3.26	1.35	1.49
2	A	615	HEC	C3C-C2C	-3.25	1.34	1.41
2	A	614	HEC	C4C-NC	3.23	1.41	1.37
2	A	611	HEC	C1B-C2B	3.22	1.44	1.40
3	A	608	HEM	C2B-C1B	3.20	1.45	1.44
2	A	615	HEC	C3C-C4C	3.16	1.45	1.41
2	A	601	HEC	C3C-C2C	-3.15	1.34	1.41
2	A	616	HEC	C3B-C2B	-3.15	1.34	1.41
2	A	606	HEC	C1C-C2C	3.14	1.44	1.40
2	A	616	HEC	C4A-NA	3.12	1.41	1.37
2	A	615	HEC	FE-NC	3.12	2.05	1.92
2	A	613	HEC	C3C-C2C	-3.11	1.34	1.41
2	A	613	HEC	C4A-NA	3.09	1.41	1.37
2	A	615	HEC	C4D-C3D	3.08	1.48	1.43
2	A	605	HEC	CBC-CAC	-3.04	1.36	1.49
2	A	609	HEC	C1D-C2D	3.03	1.43	1.40
2	A	603	HEC	C1D-C2D	3.03	1.43	1.40
2	A	616	HEC	FE-NC	-2.99	1.79	1.92
2	A	605	HEC	C3B-C4B	2.99	1.45	1.41
2	A	610	HEC	CBC-CAC	-2.98	1.36	1.49
2	A	615	HEC	C3B-C4B	2.95	1.45	1.41
2	A	614	HEC	C1D-C2D	2.94	1.43	1.40
2	A	609	HEC	CAA-C2A	2.93	1.58	1.52
2	A	612	HEC	FE-NC	2.93	2.05	1.92
3	A	604	HEM	C3D-C2D	2.93	1.48	1.43
2	A	611	HEC	C4B-NB	2.92	1.41	1.37
2	A	605	HEC	O1D-CGD	2.92	1.32	1.22
2	A	611	HEC	FE-ND	2.92	2.04	1.92
2	A	601	HEC	CBC-CAC	-2.91	1.36	1.49
2	A	605	HEC	C1B-C2B	2.90	1.43	1.40
2	A	612	HEC	CBC-CAC	-2.89	1.37	1.49
2	A	603	HEC	CAA-C2A	2.89	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	615	HEC	CBC-CAC	-2.88	1.37	1.49
3	A	608	HEM	CHD-C4C	-2.87	1.30	1.36
2	A	605	HEC	C3B-C2B	-2.84	1.35	1.41
3	A	607	HEM	CMA-C3A	2.84	1.57	1.51
2	A	606	HEC	CBC-CAC	-2.84	1.37	1.49
3	A	604	HEM	CMB-C2B	2.83	1.56	1.47
2	A	614	HEC	C3C-C4C	2.83	1.45	1.41
2	A	616	HEC	FE-ND	2.82	2.04	1.92
3	A	608	HEM	CHA-C4D	2.82	1.39	1.35
3	A	607	HEM	CMB-C2B	2.78	1.56	1.47
2	A	615	HEC	CBB-CAB	-2.77	1.37	1.49
3	A	604	HEM	CMC-C2C	2.77	1.56	1.47
3	A	602	HEM	CMC-C2C	2.76	1.56	1.47
2	A	614	HEC	C3C-C2C	-2.74	1.35	1.41
3	A	602	HEM	CAA-C2A	2.74	1.56	1.52
2	A	614	HEC	O1A-CGA	2.71	1.31	1.22
3	A	602	HEM	C3D-C4D	2.71	1.45	1.44
3	A	608	HEM	CHD-C1D	-2.70	1.32	1.39
2	A	612	HEC	C3B-C2B	-2.69	1.35	1.41
3	A	608	HEM	CMD-C2D	2.62	1.55	1.47
2	A	613	HEC	C1C-C2C	2.61	1.43	1.40
2	A	606	HEC	C2A-C3A	-2.61	1.30	1.37
2	A	610	HEC	C4C-NC	2.61	1.40	1.37
2	A	610	HEC	FE-NB	2.56	2.03	1.92
3	A	602	HEM	C4A-NA	2.55	1.41	1.36
2	A	611	HEC	CMD-C2D	2.55	1.57	1.51
3	A	602	HEM	C1B-NB	-2.52	1.34	1.39
3	A	607	HEM	CMC-C2C	2.51	1.55	1.47
3	A	608	HEM	C2A-C3A	-2.50	1.30	1.37
2	A	616	HEC	C1B-NB	2.48	1.41	1.36
2	A	615	HEC	C4D-ND	2.48	1.41	1.36
2	A	601	HEC	CBB-CAB	-2.46	1.38	1.49
2	A	609	HEC	C3B-C2B	-2.45	1.36	1.41
2	A	603	HEC	C1B-C2B	2.42	1.43	1.40
2	A	605	HEC	FE-NC	2.40	2.02	1.92
2	A	614	HEC	C3B-C4B	2.36	1.44	1.41
2	A	616	HEC	C1A-NA	2.37	1.40	1.37
2	A	616	HEC	C1D-CHD	-2.36	1.33	1.39
2	A	601	HEC	C3B-C4B	2.35	1.44	1.41
2	A	611	HEC	C4A-NA	2.33	1.40	1.37
2	A	610	HEC	C4A-NA	2.32	1.40	1.37
2	A	612	HEC	C4A-NA	-2.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	616	HEC	FE-NB	2.31	2.02	1.92
2	A	610	HEC	CAA-C2A	2.31	1.57	1.52
2	A	606	HEC	FE-ND	2.29	2.02	1.92
2	A	609	HEC	O1A-CGA	2.27	1.30	1.22
2	A	613	HEC	CAD-C3D	2.26	1.56	1.52
2	A	613	HEC	FE-NB	2.26	2.02	1.92
2	A	601	HEC	CAA-C2A	2.24	1.56	1.52
3	A	602	HEM	CMD-C2D	2.22	1.54	1.47
2	A	610	HEC	O1D-CGD	2.21	1.30	1.22
2	A	610	HEC	C3C-C2C	-2.21	1.37	1.41
3	A	607	HEM	C1D-ND	2.20	1.43	1.37
2	A	611	HEC	C4C-NC	2.17	1.40	1.37
2	A	615	HEC	FE-NB	2.17	2.01	1.92
2	A	612	HEC	C1D-ND	2.16	1.40	1.36
2	A	614	HEC	CAA-C2A	2.16	1.56	1.52
2	A	612	HEC	FE-ND	2.16	2.01	1.92
3	A	604	HEM	O1D-CGD	2.14	1.29	1.22
2	A	615	HEC	C1A-NA	-2.14	1.34	1.37
2	A	609	HEC	C1C-NC	2.13	1.40	1.36
3	A	604	HEM	CHA-C4D	2.13	1.38	1.35
2	A	603	HEC	FE-ND	2.12	2.01	1.92
3	A	608	HEM	CMC-C2C	2.12	1.54	1.47
2	A	616	HEC	C3C-C4C	2.10	1.44	1.41
3	A	607	HEM	FE-NC	-2.08	1.89	1.97
2	A	613	HEC	FE-ND	2.07	2.01	1.92
2	A	606	HEC	C1B-C2B	2.06	1.42	1.40
2	A	612	HEC	C1C-CHC	-2.05	1.34	1.39
3	A	604	HEM	CHB-C1B	2.03	1.38	1.35
2	A	610	HEC	C4B-NB	2.02	1.39	1.37
2	A	606	HEC	O1D-CGD	2.01	1.29	1.22
2	A	613	HEC	CBB-CAB	-2.01	1.40	1.49

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	614	HEC	CBB-CAB-C3B	-9.24	102.41	128.44
2	A	603	HEC	CBB-CAB-C3B	-8.61	104.21	128.44
2	A	611	HEC	C4A-CHB-C1B	-8.46	116.34	127.47
3	A	608	HEM	C4A-CHB-C1B	-8.16	116.73	127.47
3	A	604	HEM	CBA-CAA-C2A	-7.53	99.42	112.69
2	A	611	HEC	CBB-CAB-C3B	-6.91	108.98	128.44
2	A	615	HEC	CMC-C2C-C1C	-6.67	118.35	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEC	CBB-CAB-C3B	-6.67	109.67	128.44
2	A	616	HEC	CBB-CAB-C3B	-6.43	110.34	128.44
2	A	609	HEC	C4B-CHC-C1C	-6.36	119.11	127.47
2	A	610	HEC	C3B-C2B-C1B	6.21	111.20	107.07
2	A	606	HEC	C4A-CHB-C1B	-6.08	119.47	127.47
2	A	612	HEC	CBD-CAD-C3D	-5.99	102.13	112.69
2	A	613	HEC	CBB-CAB-C3B	-5.98	111.61	128.44
3	A	602	HEM	C4A-CHB-C1B	-5.96	119.63	127.47
2	A	609	HEC	CBB-CAB-C3B	-5.95	111.69	128.44
2	A	616	HEC	C4B-CHC-C1C	-5.91	119.69	127.47
2	A	601	HEC	CBB-CAB-C3B	-5.88	111.88	128.44
2	A	612	HEC	C1D-C2D-C3D	-5.70	103.03	107.00
2	A	610	HEC	C4D-ND-C1D	5.65	114.20	106.76
2	A	616	HEC	CMB-C2B-C3B	5.52	131.81	125.72
2	A	610	HEC	CMC-C2C-C1C	-5.50	120.16	128.62
2	A	611	HEC	CAA-C2A-C1A	5.50	134.59	124.67
2	A	616	HEC	C1D-C2D-C3D	-5.46	103.19	107.00
3	A	602	HEM	C3B-C4B-NB	-5.34	110.18	114.00
2	A	613	HEC	CBA-CAA-C2A	-5.34	102.37	112.35
2	A	610	HEC	C2B-C1B-NB	-5.32	105.39	109.41
2	A	611	HEC	CBC-CAC-C3C	-5.30	113.51	128.44
2	A	610	HEC	CMC-C2C-C3C	5.30	131.57	125.72
2	A	606	HEC	C1A-CHA-C4D	-5.24	120.57	127.47
2	A	616	HEC	CBD-CAD-C3D	-5.24	103.46	112.69
2	A	613	HEC	CBC-CAC-C3C	-5.17	113.89	128.44
2	A	612	HEC	CBB-CAB-C3B	-5.15	113.94	128.44
3	A	602	HEM	C4D-ND-C1D	5.13	110.41	105.16
2	A	606	HEC	CBB-CAB-C3B	-5.09	114.12	128.44
2	A	609	HEC	CBD-CAD-C3D	-5.06	103.78	112.69
2	A	613	HEC	CMC-C2C-C3C	5.00	131.24	125.72
2	A	609	HEC	CBC-CAC-C3C	-4.98	114.41	128.44
2	A	610	HEC	CBD-CAD-C3D	-4.96	103.95	112.69
2	A	610	HEC	CBB-CAB-C3B	-4.96	114.48	128.44
2	A	611	HEC	CAA-CBA-CGA	-4.94	97.59	113.47
3	A	607	HEM	CBD-CAD-C3D	-4.92	103.63	114.37
2	A	615	HEC	C3B-C2B-C1B	4.75	110.23	107.07
2	A	609	HEC	CAD-CBD-CGD	-4.73	98.26	113.47
2	A	614	HEC	C4B-CHC-C1C	-4.73	121.25	127.47
2	A	611	HEC	C4B-C3B-C2B	4.73	109.69	106.68
2	A	601	HEC	CMC-C2C-C1C	-4.71	121.37	128.62
2	A	614	HEC	CBD-CAD-C3D	-4.71	104.40	112.69
3	A	607	HEM	C4A-CHB-C1B	-4.70	121.29	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	HEC	CBC-CAC-C3C	-4.69	115.25	128.44
2	A	605	HEC	CBD-CAD-C3D	-4.67	104.47	112.69
2	A	613	HEC	CMC-C2C-C1C	-4.62	121.52	128.62
2	A	616	HEC	C2D-C1D-ND	4.61	112.89	109.41
2	A	609	HEC	CMC-C2C-C1C	-4.61	121.53	128.62
2	A	613	HEC	C4D-C3D-C2D	-4.58	102.17	106.92
2	A	611	HEC	CMC-C2C-C3C	-4.58	120.66	125.72
2	A	601	HEC	CMC-C2C-C3C	4.55	130.75	125.72
2	A	615	HEC	CBC-CAC-C3C	-4.54	115.67	128.44
2	A	605	HEC	C4D-C3D-C2D	-4.47	102.29	106.92
2	A	610	HEC	CMB-C2B-C1B	-4.45	121.78	128.62
2	A	614	HEC	C4D-ND-C1D	4.41	112.57	106.76
2	A	606	HEC	CBD-CAD-C3D	-4.39	104.95	112.69
2	A	606	HEC	CMB-C2B-C1B	-4.38	121.88	128.62
2	A	610	HEC	C1A-CHA-C4D	-4.38	121.71	127.47
2	A	609	HEC	C3B-C2B-C1B	4.37	109.97	107.07
2	A	612	HEC	CBC-CAC-C3C	-4.36	116.17	128.44
2	A	603	HEC	C4B-C3B-C2B	4.32	109.44	106.68
2	A	603	HEC	CBD-CAD-C3D	-4.29	105.13	112.69
3	A	607	HEM	C3B-C4B-NB	-4.28	110.94	114.00
3	A	607	HEM	C1A-CHA-C4D	-4.28	121.84	127.47
2	A	613	HEC	C1A-C2A-C3A	4.26	110.05	106.69
2	A	610	HEC	C4B-CHC-C1C	-4.26	121.87	127.47
3	A	604	HEM	C4D-ND-C1D	4.21	109.47	105.16
2	A	603	HEC	C4A-CHB-C1B	-4.19	121.95	127.47
3	A	602	HEM	CBD-CAD-C3D	-4.19	105.24	114.37
2	A	615	HEC	O2D-CGD-CBD	4.18	128.99	114.22
2	A	610	HEC	CBA-CAA-C2A	-4.17	104.55	112.35
2	A	611	HEC	CAA-C2A-C3A	-4.16	117.13	129.00
2	A	610	HEC	CBC-CAC-C3C	-4.08	116.95	128.44
2	A	616	HEC	CMB-C2B-C1B	-4.07	122.37	128.62
2	A	616	HEC	C1A-CHA-C4D	-4.04	122.16	127.47
2	A	613	HEC	C4B-CHC-C1C	-4.01	122.19	127.47
2	A	615	HEC	C3A-C4A-NA	-4.01	106.39	109.41
3	A	607	HEM	CMA-C3A-C4A	-3.97	122.51	128.62
2	A	615	HEC	CAD-CBD-CGD	3.96	126.21	113.47
2	A	612	HEC	CMC-C2C-C1C	-3.95	122.55	128.62
2	A	606	HEC	CMB-C2B-C3B	3.93	130.06	125.72
2	A	615	HEC	C2A-C1A-NA	-3.89	106.72	109.64
2	A	611	HEC	C4C-CHD-C1D	-3.86	122.40	127.47
2	A	610	HEC	C4B-C3B-C2B	-3.81	104.24	106.68
2	A	616	HEC	C4A-CHB-C1B	-3.78	122.49	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	HEC	C4A-C3A-C2A	3.78	109.30	106.89
2	A	605	HEC	C1A-CHA-C4D	-3.73	122.56	127.47
2	A	611	HEC	C1A-CHA-C4D	3.70	132.34	127.47
2	A	609	HEC	C2B-C1B-NB	-3.67	106.64	109.41
3	A	604	HEM	CAD-C3D-C4D	3.63	131.06	124.53
3	A	607	HEM	CHC-C4B-NB	-3.63	121.56	124.58
2	A	615	HEC	CAD-C3D-C4D	3.63	136.46	125.50
3	A	602	HEM	C4C-NC-C1C	-3.62	101.77	105.53
3	A	608	HEM	C3A-C4A-NA	-3.61	106.69	109.41
2	A	606	HEC	CBC-CAC-C3C	-3.59	118.33	128.44
2	A	611	HEC	C1D-C2D-C3D	-3.59	104.50	107.00
2	A	605	HEC	CBC-CAC-C3C	-3.56	118.41	128.44
2	A	610	HEC	C3A-C4A-NA	-3.55	106.73	109.41
3	A	602	HEM	CHC-C4B-NB	3.54	127.53	124.58
2	A	613	HEC	C3B-C2B-C1B	3.53	109.41	107.07
2	A	609	HEC	CMB-C2B-C1B	-3.49	123.26	128.62
2	A	614	HEC	CMC-C2C-C1C	-3.47	123.28	128.62
2	A	605	HEC	C3C-C2C-C1C	3.44	109.36	107.07
2	A	612	HEC	CAA-C2A-C1A	3.43	130.85	124.67
2	A	616	HEC	C4C-NC-C1C	-3.42	102.26	106.76
2	A	612	HEC	C4C-C3C-C2C	-3.40	104.50	106.68
3	A	607	HEM	CAD-C3D-C4D	3.40	130.64	124.53
2	A	615	HEC	CBB-CAB-C3B	-3.36	118.97	128.44
2	A	609	HEC	C4D-ND-C1D	3.35	111.17	106.76
2	A	606	HEC	C4B-C3B-C2B	3.34	108.81	106.68
2	A	615	HEC	O1D-CGD-CBD	-3.34	111.55	123.03
2	A	601	HEC	C4A-C3A-C2A	3.33	109.01	106.89
2	A	606	HEC	C1D-C2D-C3D	-3.30	104.70	107.00
2	A	615	HEC	CAA-C2A-C1A	3.27	130.56	124.67
3	A	607	HEM	O1D-CGD-CBD	-3.25	111.85	123.03
2	A	615	HEC	C4D-C3D-C2D	-3.25	103.56	106.92
2	A	609	HEC	C4A-C3A-C2A	3.21	108.94	106.89
2	A	610	HEC	C2C-C1C-NC	3.21	111.83	109.41
2	A	603	HEC	C1A-C2A-C3A	-3.19	104.17	106.69
2	A	615	HEC	CAD-C3D-C2D	-3.19	119.89	129.00
2	A	615	HEC	C4A-NA-C1A	3.19	110.36	105.58
3	A	604	HEM	CHD-C1D-ND	3.17	127.22	124.58
2	A	610	HEC	C2D-C1D-ND	-3.16	107.03	109.41
2	A	616	HEC	CMD-C2D-C3D	3.11	130.80	124.94
3	A	607	HEM	CAD-CBD-CGD	-3.10	103.80	113.48
2	A	614	HEC	C1A-CHA-C4D	-3.10	123.39	127.47
2	A	601	HEC	C1D-C2D-C3D	-3.09	104.84	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEC	C3B-C2B-C1B	3.09	109.12	107.07
2	A	612	HEC	CMC-C2C-C3C	3.09	129.13	125.72
2	A	615	HEC	CBD-CAD-C3D	-3.07	107.29	112.69
3	A	608	HEM	C4D-ND-C1D	3.06	108.30	105.16
3	A	607	HEM	CHD-C1D-ND	3.06	127.12	124.58
2	A	610	HEC	C1D-C2D-C3D	-3.05	104.88	107.00
2	A	611	HEC	O1A-CGA-CBA	-3.03	112.61	123.03
2	A	611	HEC	CAD-C3D-C2D	-3.03	120.36	129.00
2	A	605	HEC	C4B-CHC-C1C	-3.02	123.50	127.47
2	A	615	HEC	C2D-C1D-CHD	-3.02	120.28	126.00
2	A	616	HEC	CBC-CAC-C3C	-3.02	119.95	128.44
2	A	616	HEC	C4A-C3A-C2A	2.98	108.79	106.89
2	A	614	HEC	CBC-CAC-C3C	-2.96	120.11	128.44
2	A	613	HEC	CMD-C2D-C1D	-2.95	124.08	128.62
3	A	607	HEM	CHB-C1B-NB	-2.94	120.27	124.31
2	A	603	HEC	C3B-C4B-NB	-2.94	107.27	111.52
2	A	609	HEC	CHB-C1B-NB	2.93	129.47	124.58
2	A	615	HEC	C4C-C3C-C2C	-2.91	104.82	106.68
2	A	601	HEC	CBD-CAD-C3D	-2.91	107.56	112.69
2	A	603	HEC	CMC-C2C-C1C	-2.91	124.15	128.62
2	A	609	HEC	C3C-C2C-C1C	2.90	109.00	107.07
3	A	604	HEM	C3B-C4B-NB	-2.88	111.94	114.00
2	A	616	HEC	C2C-C1C-NC	2.88	111.58	109.41
2	A	605	HEC	C3B-C4B-NB	-2.87	107.38	111.52
2	A	611	HEC	CAD-C3D-C4D	2.86	134.14	125.50
3	A	602	HEM	O2A-CGA-O1A	-2.86	116.02	123.30
2	A	603	HEC	CMD-C2D-C1D	2.86	133.02	128.62
2	A	603	HEC	C4D-ND-C1D	2.85	110.52	106.76
2	A	606	HEC	C4C-CHD-C1D	-2.83	123.75	127.47
2	A	615	HEC	C4A-CHB-C1B	-2.82	123.76	127.47
2	A	615	HEC	CAA-C2A-C3A	-2.81	120.98	129.00
2	A	605	HEC	C2B-C1B-NB	-2.81	107.29	109.41
2	A	614	HEC	C2B-C1B-NB	-2.80	107.30	109.41
2	A	601	HEC	CBC-CAC-C3C	-2.79	120.59	128.44
3	A	608	HEM	C4C-NC-C1C	-2.78	102.64	105.53
2	A	611	HEC	C3B-C4B-NB	-2.76	107.54	111.52
2	A	612	HEC	CAA-CBA-CGA	-2.75	104.64	113.47
2	A	610	HEC	O2A-CGA-O1A	-2.74	116.32	123.30
2	A	611	HEC	C3C-C2C-C1C	2.73	108.88	107.07
2	A	615	HEC	CAA-CBA-CGA	-2.72	104.72	113.47
2	A	615	HEC	C4B-CHC-C1C	-2.72	123.89	127.47
2	A	609	HEC	C4C-NC-C1C	-2.71	103.19	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	HEM	C2D-C1D-ND	-2.66	109.79	112.93
2	A	609	HEC	C1A-CHA-C4D	-2.65	123.98	127.47
2	A	613	HEC	C1A-CHA-C4D	-2.61	124.03	127.47
2	A	612	HEC	C4A-C3A-C2A	2.60	108.55	106.89
2	A	612	HEC	CMB-C2B-C1B	-2.60	124.63	128.62
2	A	601	HEC	C2C-C1C-NC	2.59	111.37	109.41
3	A	607	HEM	C4D-ND-C1D	2.59	107.81	105.16
2	A	614	HEC	CMD-C2D-C1D	-2.58	124.65	128.62
2	A	603	HEC	CMA-C3A-C4A	-2.58	121.06	126.16
2	A	611	HEC	C2D-C1D-ND	2.57	111.35	109.41
2	A	613	HEC	C4A-CHB-C1B	-2.56	124.11	127.47
2	A	601	HEC	C4D-ND-C1D	2.56	110.13	106.76
3	A	602	HEM	CMA-C3A-C4A	-2.55	124.70	128.62
3	A	602	HEM	CMB-C2B-C3B	2.55	132.17	126.16
2	A	610	HEC	CAA-C2A-C1A	-2.55	120.07	124.67
2	A	603	HEC	CAD-C3D-C4D	2.54	133.17	125.50
2	A	612	HEC	CMD-C2D-C1D	2.54	132.53	128.62
2	A	610	HEC	CHA-C4D-ND	2.52	128.79	124.58
2	A	603	HEC	C4D-C3D-C2D	-2.52	104.31	106.92
2	A	614	HEC	O2D-CGD-O1D	2.52	129.71	123.30
2	A	614	HEC	C3A-C4A-NA	-2.51	107.52	109.41
3	A	608	HEM	C1A-C2A-C3A	2.50	109.51	106.92
2	A	616	HEC	O2D-CGD-CBD	2.50	123.06	114.22
2	A	603	HEC	CMA-C3A-C2A	2.50	129.65	124.94
2	A	613	HEC	CMD-C2D-C3D	2.48	129.62	124.94
2	A	616	HEC	C2D-C1D-CHD	-2.48	121.31	126.00
2	A	616	HEC	C4B-NB-C1B	-2.46	103.52	106.76
3	A	608	HEM	C3B-C4B-NB	-2.46	112.24	114.00
3	A	608	HEM	CAD-C3D-C4D	2.46	128.96	124.53
2	A	603	HEC	C1D-C2D-C3D	-2.46	105.29	107.00
2	A	610	HEC	O1D-CGD-CBD	-2.45	114.59	123.03
3	A	608	HEM	C1D-CHD-C4C	-2.44	120.14	126.57
2	A	614	HEC	CAD-CBD-CGD	-2.44	105.63	113.47
3	A	608	HEM	CHA-C1A-NA	2.43	128.63	124.58
2	A	609	HEC	CHC-C1C-NC	2.41	128.61	124.58
2	A	614	HEC	C4D-C3D-C2D	-2.40	104.43	106.92
2	A	603	HEC	CAA-CBA-CGA	-2.39	105.79	113.47
2	A	606	HEC	C3B-C4B-NB	-2.37	108.10	111.52
3	A	607	HEM	CHB-C4A-NA	2.36	128.52	124.58
2	A	606	HEC	CMC-C2C-C1C	-2.36	124.99	128.62
2	A	605	HEC	C3D-C4D-ND	2.36	113.01	109.73
3	A	607	HEM	C1D-CHD-C4C	-2.35	120.37	126.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	HEM	O2D-CGD-CBD	2.35	122.53	114.22
2	A	611	HEC	C3A-C4A-NA	2.35	111.19	109.41
2	A	615	HEC	C2D-C1D-ND	2.35	111.19	109.41
3	A	608	HEM	CHD-C1D-ND	2.34	126.53	124.58
2	A	606	HEC	C2A-C1A-NA	2.32	111.37	109.64
2	A	612	HEC	CHA-C4D-ND	2.31	128.44	124.58
2	A	603	HEC	CAD-C3D-C2D	-2.31	122.42	129.00
2	A	603	HEC	CMB-C2B-C1B	-2.29	125.09	128.62
2	A	616	HEC	C3B-C2B-C1B	-2.29	105.54	107.07
2	A	615	HEC	CHD-C1D-ND	2.29	128.40	124.58
2	A	606	HEC	C3D-C4D-CHA	-2.27	121.69	126.00
2	A	613	HEC	C2D-C1D-ND	2.27	111.12	109.41
2	A	612	HEC	CMB-C2B-C3B	2.27	128.23	125.72
2	A	612	HEC	C3D-C4D-CHA	-2.27	121.69	126.00
2	A	614	HEC	CHD-C1D-ND	2.26	128.35	124.58
2	A	616	HEC	C2B-C1B-CHB	-2.26	121.71	126.00
3	A	602	HEM	C4A-NA-C1A	-2.26	103.78	106.76
2	A	603	HEC	CMB-C2B-C3B	2.25	128.20	125.72
2	A	615	HEC	CMB-C2B-C1B	-2.24	125.18	128.62
3	A	602	HEM	CHB-C1B-NB	2.23	127.37	124.31
2	A	609	HEC	C3A-C4A-NA	-2.23	107.73	109.41
2	A	613	HEC	O2D-CGD-CBD	2.22	122.08	114.22
2	A	606	HEC	C1A-C2A-C3A	2.21	108.43	106.69
2	A	611	HEC	CMD-C2D-C1D	2.20	132.01	128.62
2	A	601	HEC	C4C-NC-C1C	-2.19	103.87	106.76
2	A	606	HEC	CAA-CBA-CGA	-2.19	106.42	113.47
2	A	615	HEC	C1A-C2A-C3A	2.18	108.40	106.69
2	A	610	HEC	CHB-C1B-NB	2.18	128.21	124.58
3	A	607	HEM	O2A-CGA-CBA	2.16	121.84	114.22
2	A	616	HEC	O1D-CGD-CBD	-2.14	115.67	123.03
2	A	616	HEC	C4D-C3D-C2D	-2.13	104.72	106.92
3	A	607	HEM	CMA-C3A-C2A	2.13	128.96	124.94
2	A	616	HEC	C2B-C1B-NB	2.11	111.01	109.41
2	A	601	HEC	C4D-C3D-C2D	-2.11	104.73	106.92
3	A	608	HEM	CHB-C4A-NA	2.11	128.10	124.58
2	A	601	HEC	O2D-CGD-O1D	-2.10	117.95	123.30
2	A	614	HEC	CHB-C1B-NB	2.10	128.09	124.58
2	A	614	HEC	C3B-C2B-C1B	2.10	108.46	107.07
2	A	613	HEC	O1A-CGA-CBA	-2.09	115.85	123.03
3	A	607	HEM	C3A-C4A-CHB	-2.08	122.05	126.00
2	A	609	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
2	A	609	HEC	C2C-C1C-CHC	-2.08	122.06	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	610	HEC	O2A-CGA-CBA	2.07	121.55	114.22
3	A	608	HEM	C2A-C1A-NA	-2.06	106.87	109.73
2	A	614	HEC	C4A-C3A-C2A	2.06	108.20	106.89
2	A	605	HEC	CHB-C1B-NB	2.05	128.01	124.58
2	A	613	HEC	CBD-CAD-C3D	-2.04	109.10	112.69
3	A	608	HEM	CMA-C3A-C4A	-2.04	125.49	128.62
2	A	611	HEC	C1A-C2A-C3A	2.03	108.29	106.69
2	A	614	HEC	CMD-C2D-C3D	2.03	128.77	124.94
3	A	607	HEM	C4A-C3A-C2A	2.03	108.41	107.00
3	A	608	HEM	CAA-CBA-CGA	-2.02	106.97	113.47
3	A	602	HEM	C2A-C1A-NA	2.02	112.54	109.73
2	A	616	HEC	CMC-C2C-C1C	-2.01	125.53	128.62
3	A	602	HEM	C4A-C3A-C2A	2.01	108.39	107.00
2	A	611	HEC	CBD-CAD-C3D	-2.00	109.17	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	503/545 (92%)	0.22	24 (4%)	29 27	19, 33, 64, 91	11 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	26.1
1	A	473	ASP	10.5
1	A	471	ASP	9.2
1	A	472	ALA	8.7
1	A	469	PRO	8.4
1	A	474	ARG	7.1
1	A	113	SER	5.4
1	A	468	LYS	4.6
1	A	114	ALA	3.6
1	A	181	ASP	3.1
1	A	206	ALA	2.9
1	A	112	PRO	2.8
1	A	111	LYS	2.8
1	A	145	LYS	2.6
1	A	476	ASP	2.6
1	A	464	SER	2.5
1	A	230	GLU	2.5
1	A	475	GLY	2.3
1	A	253	PRO	2.3
1	A	507	ASP	2.3
1	A	180	VAL	2.3
1	A	228	VAL	2.2
1	A	467	GLY	2.1
1	A	26	LEU	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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HEM	A	602	43/43	0.14	0.84	15,21,31,42	0
2	HEC	A	606	43/43	0.16	0.55	16,24,34,35	0
2	HEC	A	615	43/43	0.21	0.44	16,23,42,46	0
3	HEM	A	607	43/43	0.16	0.23	20,26,40,43	0
2	HEC	A	605	43/43	0.15	-0.00	19,27,41,53	0
3	HEM	A	604	43/43	0.14	-0.02	22,27,33,37	0
2	HEC	A	611	43/43	0.13	-0.04	13,20,25,28	0
3	HEM	A	608	43/43	0.14	-0.11	9,21,27,30	0
2	HEC	A	610	43/43	0.12	-0.19	13,21,32,38	0
2	HEC	A	609	43/43	0.13	-0.28	14,27,50,58	0
2	HEC	A	612	43/43	0.14	-0.33	15,22,29,35	0
2	HEC	A	614	43/43	0.15	-0.37	17,27,40,44	0
2	HEC	A	616	43/43	0.13	-0.45	12,25,31,34	0
2	HEC	A	601	43/43	0.12	-0.47	6,22,30,42	0
2	HEC	A	613	43/43	0.15	-0.48	11,25,39,43	0
2	HEC	A	603	43/43	0.10	-0.78	16,22,25,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.