



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2014 – 07:04 PM EDT

PDB ID : 4MQK  
Title : Carbonmonoxy Structure of the Human Fetal Hemoglobin Mutant HbF Toms River alphawtgammaV67M  
Authors : Soman, J.; Olson, J.S.  
Deposited on : 2013-09-16  
Resolution : 2.24 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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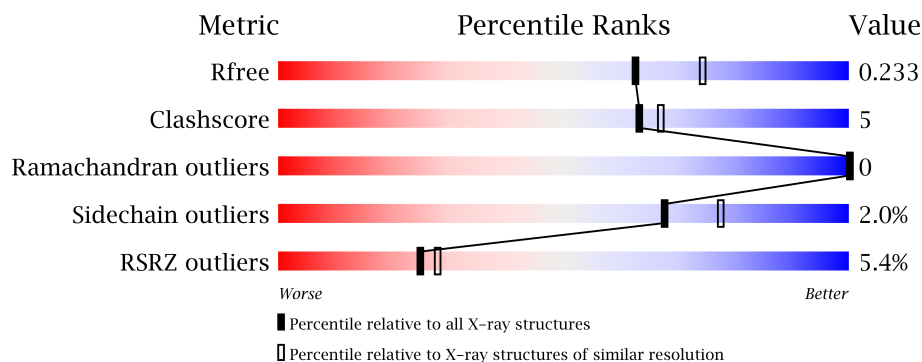
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
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) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.24 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	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	141	
1	C	141	
1	E	141	
1	G	141	
2	B	146	
2	D	146	
2	F	146	
2	H	146	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	HEM	D	201	-	X
4	CMO	A	202	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9377 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1068	685	187	193	3			
1	C	141	Total	C	N	O	S	0	0	0
			1068	685	187	193	3			
1	E	138	Total	C	N	O	S	0	0	0
			1036	664	180	189	3			
1	G	140	Total	C	N	O	S	0	0	0
			1057	679	183	192	3			

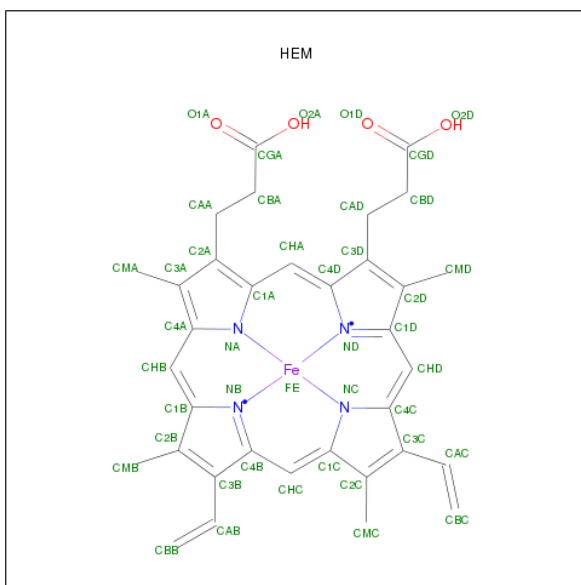
- Molecule 2 is a protein called Hemoglobin subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1126	721	192	209	4			
2	D	145	Total	C	N	O	S	0	1	0
			1134	726	194	210	4			
2	F	145	Total	C	N	O	S	0	0	0
			1127	721	192	210	4			
2	H	145	Total	C	N	O	S	0	0	0
			1121	718	190	209	4			

There are 4 discrepancies between the modelled and reference sequences:

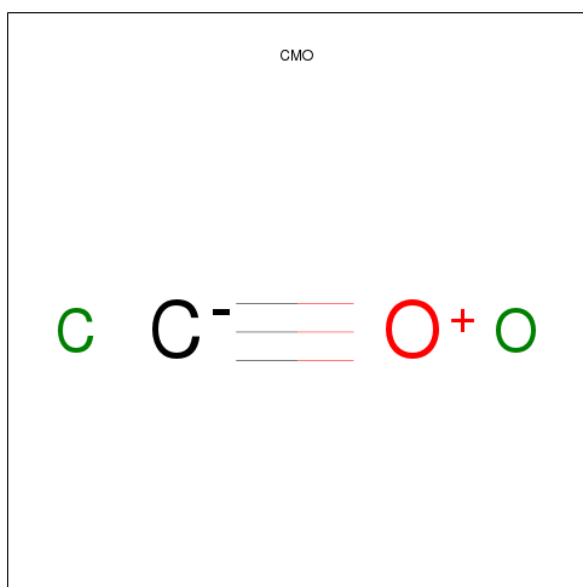
Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	VAL	ENGINEERED MUTATION	UNP P69892
D	67	MET	VAL	ENGINEERED MUTATION	UNP P69892
F	67	MET	VAL	ENGINEERED MUTATION	UNP P69892
H	67	MET	VAL	ENGINEERED MUTATION	UNP P69892

- 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	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			2	1	1		
4	B	1	Total	C	O	0	0
			2	1	1		
4	C	1	Total	C	O	0	0
			2	1	1		
4	D	1	Total	C	O	0	0
			2	1	1		
4	F	1	Total	C	O	0	0
			2	1	1		
4	H	1	Total	C	O	0	0
			2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	44	Total	O	0	0
			44	44		
5	C	56	Total	O	0	0
			56	56		
5	D	33	Total	O	0	0
			33	33		
5	E	30	Total	O	0	0
			30	30		
5	F	28	Total	O	0	0
			28	28		

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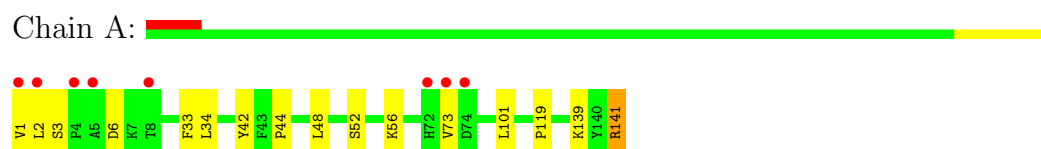
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	32	Total 32	O 32	0	0
5	H	31	Total 31	O 31	0	0

### 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.

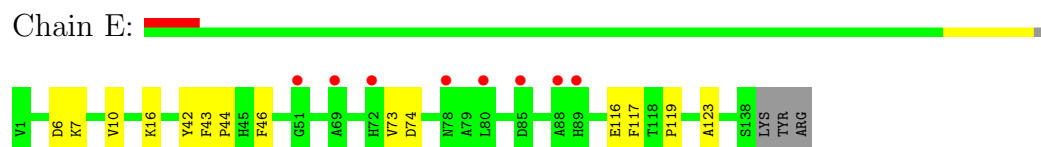
- Molecule 1: Hemoglobin subunit alpha



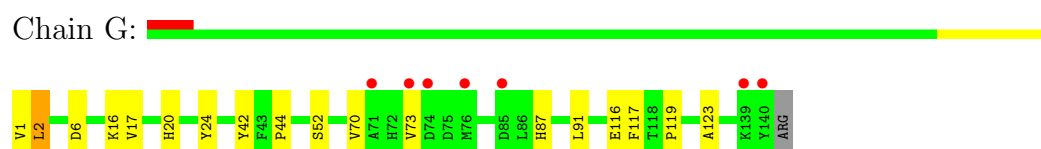
- Molecule 1: Hemoglobin subunit alpha



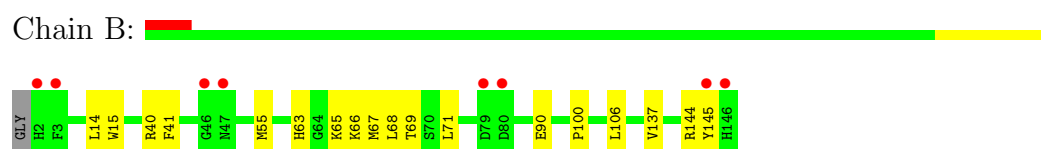
- Molecule 1: Hemoglobin subunit alpha



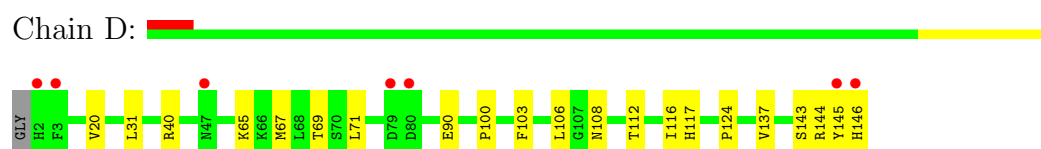
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit gamma-2

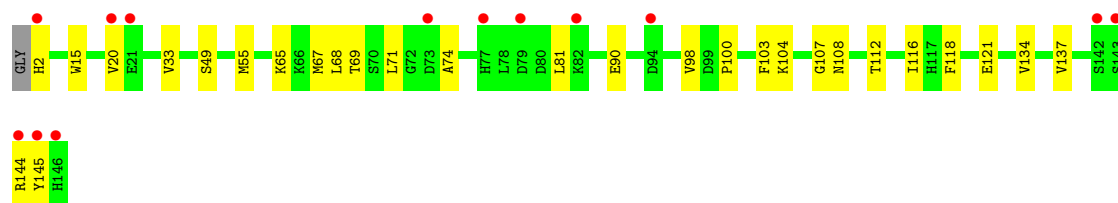


- Molecule 2: Hemoglobin subunit gamma-2





## ● Molecule 2: Hemoglobin subunit gamma-2

Chain F: 

## ● Molecule 2: Hemoglobin subunit gamma-2

Chain H: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.04Å 52.23Å 106.38Å 90.00° 114.27° 90.00°	Depositor
Resolution (Å)	45.07 – 2.24 45.07 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.07-2.24) 97.5 (45.07-2.24)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.45 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.175 , 0.232 0.175 , 0.233	Depositor DCC
$R_{free}$ test set	1977 reflections (3.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.6	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 51182 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.40 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7504e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.37	0/1096	0.53	0/1491
1	C	0.45	0/1096	0.52	0/1491
1	E	0.35	0/1063	0.48	0/1448
1	G	0.35	0/1085	0.48	0/1477
2	B	0.38	0/1152	0.49	0/1558
2	D	0.37	0/1164	0.51	0/1573
2	F	0.37	0/1153	0.51	0/1558
2	H	0.40	0/1146	0.49	0/1550
All	All	0.38	0/8955	0.50	0/12146

There are no bond length outliers.

There are no bond angle outliers.

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	1068	0	1073	8	0
1	C	1068	0	1073	7	0
1	E	1036	0	1038	9	0
1	G	1057	0	1060	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1126	0	1120	12	0
2	D	1134	0	1127	15	0
2	F	1127	0	1120	19	0
2	H	1121	0	1115	12	0
3	A	43	0	30	2	0
3	B	43	0	30	6	0
3	C	43	0	30	2	0
3	D	43	0	30	3	0
3	E	43	0	30	2	0
3	F	43	0	30	2	0
3	G	43	0	30	1	0
3	H	43	0	30	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	H	2	0	0	0	0
5	A	30	0	0	0	0
5	B	44	0	0	1	0
5	C	56	0	0	1	0
5	D	33	0	0	1	0
5	E	30	0	0	1	0
5	F	28	0	0	2	0
5	G	32	0	0	1	0
5	H	31	0	0	0	0
All	All	9377	0	8966	99	0

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 5.

All (99) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:1:VAL:N	5:G:318:HOH:O	2.16	0.79
3:C:201:HEM:HBB2	3:C:201:HEM:HHC	1.68	0.76
3:H:201:HEM:HBB2	3:H:201:HEM:HHC	1.68	0.75
1:G:16:LYS:HG3	1:G:116:GLU:HG2	1.71	0.73
2:B:63:HIS:HE1	3:B:201:HEM:HBD1	1.53	0.72
3:D:201:HEM:HHA	3:D:201:HEM:HBD1	1.72	0.71
2:H:15:TRP:HH2	2:H:68:LEU:HG	1.58	0.69
1:A:101:LEU:HD23	3:A:201:HEM:HBB2	1.76	0.68
2:D:90:GLU:HG2	2:D:144:ARG:HH11	1.58	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:98:VAL:O	2:F:145:TYR:OH	2.10	0.66
3:B:201:HEM:HHD	3:B:201:HEM:HBC2	1.77	0.66
1:E:16:LYS:HG3	1:E:116:GLU:HG2	1.80	0.64
2:F:104:LYS:NZ	5:F:322:HOH:O	2.30	0.64
2:F:15:TRP:HH2	2:F:68:LEU:HG	1.62	0.64
2:D:144:ARG:O	5:D:319:HOH:O	2.15	0.64
2:F:49:SER:OG	5:F:319:HOH:O	2.16	0.63
2:H:65:LYS:O	2:H:69:THR:HG23	1.97	0.63
2:B:63:HIS:CE1	3:B:201:HEM:HBD1	2.34	0.61
2:B:90:GLU:HG3	2:B:144:ARG:HG3	1.82	0.60
1:G:119:PRO:HG2	2:H:55:MET:HG3	1.84	0.60
2:B:15:TRP:HH2	2:B:68:LEU:HG	1.68	0.57
1:C:64:ASP:OD1	5:C:341:HOH:O	2.16	0.57
1:E:6:ASP:OD1	5:E:316:HOH:O	2.18	0.57
2:D:90:GLU:HG2	2:D:144:ARG:NH1	2.20	0.57
1:G:117:PHE:HD2	2:H:116:ILE:HD11	1.70	0.57
2:H:85:PHE:HD1	2:H:88:LEU:HD12	1.70	0.56
2:D:100:PRO:HD3	2:D:145:TYR:CE2	2.41	0.55
3:F:201:HEM:HMC2	3:F:201:HEM:HBC2	1.88	0.54
2:F:65:LYS:O	2:F:69:THR:HG23	2.07	0.54
2:H:100:PRO:HD3	2:H:145:TYR:CE2	2.43	0.54
3:H:201:HEM:HBC2	3:H:201:HEM:HMC2	1.90	0.54
2:B:41:PHE:CD2	3:B:201:HEM:HBC1	2.43	0.53
2:B:65:LYS:O	2:B:69:THR:HG23	2.09	0.53
2:B:100:PRO:HD3	2:B:145:TYR:CE2	2.44	0.53
2:D:65:LYS:O	2:D:69:THR:HG23	2.08	0.53
1:C:2:LEU:HD12	1:C:73:VAL:HG11	1.90	0.52
2:B:71:LEU:HD11	2:B:137:VAL:HG21	1.92	0.52
1:G:17:VAL:HG13	1:G:24:TYR:CD2	2.45	0.52
2:F:2:HIS:O	2:F:2:HIS:ND1	2.43	0.52
2:D:20:VAL:HG11	2:D:69:THR:HG22	1.92	0.51
3:A:201:HEM:HBB2	3:A:201:HEM:HHC	1.92	0.51
1:C:137:THR:OG1	1:C:141:ARG:NH2	2.44	0.51
3:D:201:HEM:HMC1	3:D:201:HEM:HBC2	1.93	0.50
2:H:95:LYS:NZ	3:H:201:HEM:O1D	2.44	0.50
1:E:117:PHE:HD2	2:F:116:ILE:HD11	1.76	0.49
2:D:100:PRO:HD3	2:D:145:TYR:HE2	1.77	0.49
1:G:87:HIS:HA	1:G:91:LEU:HD12	1.94	0.49
2:F:108:ASN:O	2:F:112:THR:HG23	2.13	0.48
2:F:71:LEU:HD11	2:F:137:VAL:HG21	1.95	0.48
3:H:201:HEM:HBA2	3:H:201:HEM:HHA	1.95	0.48
1:C:70:VAL:O	1:C:73:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:71:LEU:HD11	2:D:137:VAL:HG21	1.96	0.47
1:A:141:ARG:NH1	1:A:141:ARG:O	2.46	0.47
2:H:108:ASN:O	2:H:112:THR:HG23	2.15	0.47
3:G:201:HEM:HBC2	3:G:201:HEM:HMC1	1.96	0.47
1:E:42:TYR:C	1:E:44:PRO:HD3	2.34	0.47
2:D:108:ASN:O	2:D:112:THR:HG23	2.15	0.46
2:D:143:SER:O	2:D:146:HIS:HB2	2.15	0.46
1:G:123:ALA:HB2	2:H:33:VAL:HG12	1.96	0.46
1:G:70:VAL:O	1:G:73:VAL:HG23	2.16	0.46
3:E:201:HEM:HBB2	3:E:201:HEM:HMB1	1.97	0.46
2:B:66:LYS:HD2	3:B:201:HEM:HAA1	1.97	0.46
1:E:7:LYS:HG2	1:E:73:VAL:HG11	1.98	0.45
1:A:119:PRO:HG2	2:B:55:MET:HG3	1.98	0.45
1:C:21:ALA:HB1	1:C:63:ALA:HB1	1.98	0.45
1:E:43:PHE:HB3	1:E:46:PHE:HB2	1.99	0.45
2:F:90:GLU:HG3	2:F:144:ARG:HG3	1.99	0.45
2:B:144:ARG:NH2	5:B:330:HOH:O	2.35	0.45
2:B:67:MET:SD	2:B:106:LEU:HD21	2.57	0.45
2:D:100:PRO:HA	2:D:103:PHE:CD2	2.52	0.44
1:A:42:TYR:C	1:A:44:PRO:HD3	2.38	0.44
2:F:20:VAL:HG11	2:F:69:THR:HG22	2.00	0.44
2:H:71:LEU:HD11	2:H:137:VAL:HG21	1.99	0.44
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.53	0.44
1:E:119:PRO:HG2	2:F:55:MET:HG3	2.00	0.44
1:G:42:TYR:C	1:G:44:PRO:HD3	2.39	0.43
1:E:6:ASP:O	1:E:10:VAL:HG23	2.18	0.43
3:F:201:HEM:CMC	3:F:201:HEM:HBC2	2.48	0.43
1:C:86:LEU:CD2	3:C:201:HEM:HBA1	2.48	0.43
2:H:20:VAL:HG11	2:H:69:THR:HG22	1.99	0.43
1:G:20:HIS:HB3	1:G:24:TYR:CE1	2.55	0.42
2:D:31:LEU:HD22	2:D:106:LEU:HD13	2.01	0.42
2:D:112:THR:O	2:D:116:ILE:HG13	2.19	0.42
1:E:123:ALA:HB2	2:F:33:VAL:HG12	2.01	0.42
2:F:107:GLY:HA3	2:F:134:VAL:HG13	2.02	0.42
3:B:201:HEM:O1A	2:D:65:LYS:NZ	2.53	0.42
1:C:34:LEU:HD12	2:D:124:PRO:HB2	2.02	0.42
1:G:2:LEU:HG	1:G:6:ASP:HB3	2.02	0.41
3:D:201:HEM:CMC	3:D:201:HEM:HBC2	2.50	0.41
1:A:34:LEU:HA	1:A:34:LEU:HD23	1.89	0.41
1:A:139:LYS:HA	1:A:139:LYS:HD3	1.91	0.41
3:E:201:HEM:HMC1	3:E:201:HEM:HBC2	2.02	0.41
2:F:100:PRO:HA	2:F:103:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:SER:H	1:A:6:ASP:HB2	1.84	0.41
2:F:2:HIS:O	2:F:2:HIS:CG	2.74	0.40
2:F:68:LEU:HA	2:F:68:LEU:HD12	1.82	0.40
2:F:74:ALA:HB1	2:F:81:LEU:CD2	2.51	0.40
2:H:71:LEU:HA	2:H:71:LEU:HD12	1.88	0.40
2:F:118:PHE:HB3	2:F:121:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	E	136/141 (96%)	133 (98%)	3 (2%)	0	100	100
1	G	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	B	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
2	D	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
2	F	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
2	H	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
All	All	1125/1148 (98%)	1095 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	113/113 (100%)	107 (95%)	6 (5%)	32	32
1	C	113/113 (100%)	111 (98%)	2 (2%)	71	81
1	E	110/113 (97%)	109 (99%)	1 (1%)	87	93
1	G	112/113 (99%)	110 (98%)	2 (2%)	71	81
2	B	122/122 (100%)	120 (98%)	2 (2%)	75	84
2	D	123/122 (101%)	119 (97%)	4 (3%)	50	60
2	F	122/122 (100%)	121 (99%)	1 (1%)	89	94
2	H	121/122 (99%)	119 (98%)	2 (2%)	73	83
All	All	936/940 (100%)	916 (98%)	20 (2%)	68	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	2	LEU
1	A	52	SER
1	A	56	LYS
1	A	73	VAL
1	A	141	ARG
2	B	14	LEU
2	B	40	ARG
1	C	1	VAL
1	C	2	LEU
2	D	40	ARG
2	D	67	MET
2	D	117[A]	HIS
2	D	117[B]	HIS
1	E	74	ASP
2	F	67	MET
1	G	2	LEU
1	G	52	SER
2	H	67	MET
2	H	117	HIS

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

Mol	Chain	Res	Type
2	B	63	HIS



### 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 ⓘ

14 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$
3	HEM	A	201	1,4	42,50,50	3.63	16 (38%)	27,82,82	1.85	5 (18%)
4	CMO	A	202	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	B	201	2,4	42,50,50	3.98	15 (35%)	27,82,82	1.74	5 (18%)
4	CMO	B	202	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	C	201	1,4	42,50,50	3.71	13 (30%)	27,82,82	1.48	4 (14%)
4	CMO	C	202	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	D	201	2	42,50,50	3.50	15 (35%)	27,82,82	1.74	5 (18%)
4	CMO	D	202	-	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	E	201	1	42,50,50	3.55	14 (33%)	27,82,82	1.38	4 (14%)
3	HEM	F	201	2,4	42,50,50	3.53	13 (30%)	27,82,82	1.30	2 (7%)
4	CMO	F	202	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	G	201	1	42,50,50	3.52	13 (30%)	27,82,82	1.30	4 (14%)
3	HEM	H	201	2,4	42,50,50	3.69	16 (38%)	27,82,82	1.34	3 (11%)
4	CMO	H	202	3	0,1,1	0.00	-	0,0,0	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	201	1,4	-	0/14/114/114	0/0/8/8
4	CMO	A	202	3	-	0/0/0/0	0/0/0/0
3	HEM	B	201	2,4	-	0/14/114/114	0/0/8/8
4	CMO	B	202	3	-	0/0/0/0	0/0/0/0
3	HEM	C	201	1,4	-	0/14/114/114	0/0/8/8
4	CMO	C	202	3	-	0/0/0/0	0/0/0/0
3	HEM	D	201	2	-	0/14/114/114	0/0/8/8
4	CMO	D	202	-	-	0/0/0/0	0/0/0/0
3	HEM	E	201	1	-	0/14/114/114	0/0/8/8
3	HEM	F	201	2,4	-	0/14/114/114	0/0/8/8
4	CMO	F	202	3	-	0/0/0/0	0/0/0/0
3	HEM	G	201	1	-	0/14/114/114	0/0/8/8
3	HEM	H	201	2,4	-	0/14/114/114	0/0/8/8
4	CMO	H	202	3	-	0/0/0/0	0/0/0/0

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	HEM	C3C-C2C	-17.06	1.32	1.45
3	H	201	HEM	C3C-C2C	-13.70	1.34	1.45
3	E	201	HEM	C3C-C2C	-13.68	1.34	1.45
3	C	201	HEM	C3C-C2C	-13.53	1.34	1.45
3	G	201	HEM	C3C-C2C	-13.45	1.34	1.45
3	F	201	HEM	C3C-C2C	-13.43	1.34	1.45
3	D	201	HEM	C3C-C2C	-13.40	1.34	1.45
3	C	201	HEM	C3B-C2B	-12.87	1.33	1.45
3	A	201	HEM	C3B-C2B	-12.35	1.33	1.45
3	A	201	HEM	C3C-C2C	-12.26	1.35	1.45
3	H	201	HEM	C3B-C2B	-12.02	1.33	1.45
3	B	201	HEM	C3B-C2B	-11.71	1.34	1.45
3	G	201	HEM	C3B-C2B	-11.03	1.34	1.45
3	D	201	HEM	C3B-C2B	-10.86	1.35	1.45
3	E	201	HEM	C3B-C2B	-10.71	1.35	1.45
3	F	201	HEM	C3B-C2B	-10.46	1.35	1.45
3	E	201	HEM	CMB-C2B	6.32	1.55	1.45
3	A	201	HEM	CMC-C2C	6.11	1.55	1.45
3	A	201	HEM	CMB-C2B	6.08	1.55	1.45
3	E	201	HEM	CMC-C2C	6.05	1.55	1.45
3	G	201	HEM	CMB-C2B	6.04	1.55	1.45
3	H	201	HEM	CMB-C2B	5.98	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	HEM	CMC-C2C	5.89	1.55	1.45
3	C	201	HEM	CMC-C2C	5.89	1.55	1.45
3	B	201	HEM	CMB-C2B	5.88	1.55	1.45
3	F	201	HEM	CMB-C2B	5.86	1.55	1.45
3	H	201	HEM	CMC-C2C	5.84	1.55	1.45
3	D	201	HEM	CMB-C2B	5.83	1.55	1.45
3	G	201	HEM	CMC-C2C	5.83	1.55	1.45
3	D	201	HEM	CMC-C2C	5.81	1.55	1.45
3	E	201	HEM	CMD-C2D	5.80	1.55	1.45
3	C	201	HEM	CMB-C2B	5.76	1.54	1.45
3	B	201	HEM	CMD-C2D	5.65	1.54	1.45
3	B	201	HEM	CMC-C2C	5.57	1.54	1.45
3	G	201	HEM	CMD-C2D	5.51	1.54	1.45
3	A	201	HEM	CMD-C2D	5.48	1.54	1.45
3	H	201	HEM	CMD-C2D	5.34	1.54	1.45
3	F	201	HEM	CMD-C2D	5.27	1.54	1.45
3	D	201	HEM	CMD-C2D	5.26	1.54	1.45
3	C	201	HEM	CMD-C2D	4.89	1.53	1.45
3	F	201	HEM	C3B-CAB	4.75	1.55	1.40
3	D	201	HEM	C3B-CAB	4.65	1.55	1.40
3	B	201	HEM	FE-ND	4.62	2.14	1.95
3	E	201	HEM	C3B-CAB	4.58	1.55	1.40
3	E	201	HEM	C3C-CAC	4.57	1.55	1.40
3	B	201	HEM	C3B-CAB	4.57	1.55	1.40
3	H	201	HEM	C3C-CAC	4.48	1.55	1.40
3	H	201	HEM	C3B-CAB	4.48	1.55	1.40
3	C	201	HEM	C3B-CAB	4.46	1.55	1.40
3	F	201	HEM	C3C-CAC	4.44	1.54	1.40
3	A	201	HEM	C3C-CAC	4.40	1.54	1.40
3	A	201	HEM	FE-ND	4.39	2.13	1.95
3	B	201	HEM	C3C-CAC	4.37	1.54	1.40
3	A	201	HEM	C3B-CAB	4.36	1.54	1.40
3	G	201	HEM	C3B-CAB	4.36	1.54	1.40
3	G	201	HEM	C3C-CAC	4.36	1.54	1.40
3	D	201	HEM	C3C-CAC	4.33	1.54	1.40
3	C	201	HEM	FE-ND	4.32	2.12	1.95
3	C	201	HEM	C3C-CAC	4.31	1.54	1.40
3	F	201	HEM	FE-NC	4.29	2.12	1.95
3	H	201	HEM	FE-NC	4.21	2.12	1.95
3	A	201	HEM	FE-NB	4.02	2.09	1.95
3	F	201	HEM	C3D-C2D	3.93	1.53	1.43
3	H	201	HEM	FE-ND	3.93	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	HEM	C3D-C2D	3.85	1.53	1.43
3	C	201	HEM	FE-NB	3.69	2.08	1.95
3	A	201	HEM	C3D-C2D	3.69	1.53	1.43
3	E	201	HEM	C3D-C2D	3.64	1.53	1.43
3	H	201	HEM	C3D-C2D	3.58	1.52	1.43
3	D	201	HEM	C3D-C2D	3.40	1.52	1.43
3	F	201	HEM	FE-NB	3.34	2.07	1.95
3	C	201	HEM	C3D-C2D	3.31	1.52	1.43
3	G	201	HEM	C3D-C2D	3.25	1.52	1.43
3	G	201	HEM	FE-ND	3.17	2.08	1.95
3	D	201	HEM	FE-NC	3.05	2.07	1.95
3	E	201	HEM	FE-ND	2.96	2.07	1.95
3	C	201	HEM	C1C-NC	2.93	1.41	1.33
3	A	201	HEM	C1C-NC	2.88	1.40	1.33
3	A	201	HEM	C4C-NC	2.87	1.40	1.33
3	B	201	HEM	C1D-ND	2.79	1.40	1.33
3	C	201	HEM	C4C-NC	2.79	1.40	1.33
3	B	201	HEM	C4D-ND	2.79	1.40	1.33
3	A	201	HEM	FE-NC	2.77	2.06	1.95
3	D	201	HEM	C4D-ND	2.67	1.40	1.33
3	D	201	HEM	C1D-ND	2.64	1.40	1.33
3	E	201	HEM	FE-NB	2.63	2.04	1.95
3	D	201	HEM	FE-ND	2.62	2.06	1.95
3	H	201	HEM	C1D-ND	2.62	1.40	1.33
3	G	201	HEM	C1D-ND	2.61	1.40	1.33
3	D	201	HEM	FE-NB	2.61	2.04	1.95
3	G	201	HEM	FE-NC	2.57	2.06	1.95
3	H	201	HEM	FE-NB	2.54	2.04	1.95
3	A	201	HEM	C1D-ND	2.53	1.40	1.33
3	E	201	HEM	FE-NC	2.47	2.05	1.95
3	F	201	HEM	C1D-ND	2.41	1.39	1.33
3	G	201	HEM	FE-NB	2.34	2.03	1.95
3	E	201	HEM	C1D-ND	2.33	1.39	1.33
3	B	201	HEM	C4C-NC	2.28	1.39	1.33
3	F	201	HEM	FE-ND	2.28	2.04	1.95
3	F	201	HEM	C4D-ND	2.27	1.39	1.33
3	B	201	HEM	C1C-NC	2.27	1.39	1.33
3	C	201	HEM	FE-NC	2.26	2.04	1.95
3	A	201	HEM	C4D-ND	2.26	1.39	1.33
3	H	201	HEM	CAA-C2A	2.24	1.55	1.52
3	H	201	HEM	C4D-ND	2.24	1.39	1.33
3	B	201	HEM	FE-NC	2.22	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	201	HEM	C4D-ND	2.20	1.39	1.33
3	D	201	HEM	C1C-NC	2.18	1.39	1.33
3	A	201	HEM	C4A-NA	2.17	1.40	1.36
3	B	201	HEM	C4A-NA	2.15	1.39	1.36
3	G	201	HEM	C4D-ND	2.15	1.39	1.33
3	H	201	HEM	C4C-NC	2.13	1.39	1.33
3	D	201	HEM	C4C-NC	2.08	1.39	1.33
3	H	201	HEM	C1C-NC	2.02	1.38	1.33
3	E	201	HEM	C1C-NC	2.01	1.38	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	HEM	CBA-CAA-C2A	-6.21	102.29	112.63
3	B	201	HEM	CAD-C3D-C4D	4.70	132.23	125.60
3	D	201	HEM	CAD-C3D-C4D	4.61	132.11	125.60
3	D	201	HEM	CAD-CBD-CGD	-4.09	105.82	113.53
3	C	201	HEM	CAD-CBD-CGD	-3.79	106.38	113.53
3	A	201	HEM	CBD-CAD-C3D	-3.56	106.79	114.51
3	F	201	HEM	CAD-CBD-CGD	-3.47	106.99	113.53
3	B	201	HEM	C3A-C4A-NA	-3.10	107.43	109.50
3	D	201	HEM	CBA-CAA-C2A	-3.02	107.60	112.63
3	H	201	HEM	CAD-CBD-CGD	-3.01	107.86	113.53
3	G	201	HEM	CAD-CBD-CGD	-2.83	108.19	113.53
3	C	201	HEM	C3A-C4A-NA	-2.77	107.65	109.50
3	H	201	HEM	C4A-C3A-C2A	2.73	108.90	107.00
3	E	201	HEM	CBD-CAD-C3D	-2.72	108.60	114.51
3	C	201	HEM	C4A-C3A-C2A	2.66	108.85	107.00
3	H	201	HEM	C3A-C4A-NA	-2.65	107.73	109.50
3	G	201	HEM	CBA-CAA-C2A	-2.58	108.33	112.63
3	B	201	HEM	CBA-CAA-C2A	2.57	116.91	112.63
3	A	201	HEM	CAD-CBD-CGD	-2.56	108.71	113.53
3	B	201	HEM	CAA-CBA-CGA	-2.39	105.87	113.66
3	D	201	HEM	C3A-C4A-NA	-2.38	107.91	109.50
3	B	201	HEM	C4A-C3A-C2A	2.25	108.56	107.00
3	G	201	HEM	CBD-CAD-C3D	-2.23	109.67	114.51
3	F	201	HEM	C3A-C4A-NA	-2.18	108.04	109.50
3	C	201	HEM	CMC-C2C-C3C	2.17	129.39	124.26
3	A	201	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
3	D	201	HEM	C1A-C2A-C3A	2.12	109.12	106.92
3	E	201	HEM	CMC-C2C-C3C	2.12	129.27	124.26
3	E	201	HEM	CAD-CBD-CGD	-2.11	109.55	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	HEM	C1A-C2A-C3A	2.11	109.11	106.92
3	G	201	HEM	C3A-C4A-NA	-2.05	108.13	109.50
3	E	201	HEM	CAA-CBA-CGA	-2.05	106.99	113.66

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	141/141 (100%)	0.06	8 (5%)	23 26	21, 38, 69, 129	0
1	C	141/141 (100%)	-0.05	4 (2%)	50 55	18, 31, 56, 106	0
1	E	138/141 (97%)	0.13	8 (5%)	22 25	22, 45, 77, 108	0
1	G	140/141 (99%)	0.02	7 (5%)	28 31	18, 42, 73, 108	0
2	B	145/146 (99%)	0.04	8 (5%)	24 27	19, 38, 69, 115	0
2	D	145/146 (99%)	0.16	7 (4%)	29 31	21, 41, 73, 151	0
2	F	145/146 (99%)	0.21	13 (8%)	10 11	20, 42, 80, 152	0
2	H	145/146 (99%)	0.01	7 (4%)	29 31	21, 40, 69, 106	0
All	All	1140/1148 (99%)	0.07	62 (5%)	25 28	18, 39, 74, 152	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	14.4
2	F	146	HIS	10.7
2	D	146	HIS	8.0
1	C	1	VAL	8.0
2	H	146	HIS	6.1
2	B	2	HIS	5.8
1	C	74	ASP	5.2
2	F	144	ARG	4.7
1	E	78	ASN	4.6
2	B	146	HIS	4.4
2	H	79	ASP	3.9
1	A	74	ASP	3.9
2	D	145	TYR	3.9
1	A	5	ALA	3.8
1	G	73	VAL	3.8
2	F	21	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	80	ASP	3.7
2	B	145	TYR	3.7
2	D	2	HIS	3.7
2	H	143	SER	3.6
2	F	73	ASP	3.6
1	E	89	HIS	3.6
2	F	82	LYS	3.5
2	H	22	ASP	3.4
1	C	75	ASP	3.3
2	D	79	ASP	3.3
2	F	2	HIS	3.3
1	E	85	ASP	3.2
1	E	88	ALA	3.2
1	A	2	LEU	3.2
2	F	145	TYR	3.1
2	F	20	VAL	3.1
2	H	2	HIS	2.9
1	E	51	GLY	2.8
2	B	3	PHE	2.8
1	C	72	HIS	2.8
2	F	94	ASP	2.8
1	G	85	ASP	2.7
2	B	79	ASP	2.7
1	G	140	TYR	2.7
2	D	3	PHE	2.7
1	G	71	ALA	2.5
2	B	46	GLY	2.5
1	G	74	ASP	2.5
1	A	4	PRO	2.5
1	E	80	LEU	2.5
1	A	72	HIS	2.4
2	F	143	SER	2.4
1	G	139	LYS	2.3
2	F	77	HIS	2.3
2	H	87	GLN	2.3
2	B	80	ASP	2.2
1	E	72	HIS	2.1
1	E	69	ALA	2.1
1	A	73	VAL	2.1
2	F	79	ASP	2.1
2	B	47	ASN	2.1
2	F	142	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	82	LYS	2.1
1	G	76	MET	2.0
1	A	8	THR	2.0
2	D	47	ASN	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CMO	A	202	2/2	0.21	3.60	28,28,28,43	0
3	HEM	D	201	43/43	0.18	2.89	22,33,71,84	0
4	CMO	D	202	2/2	0.13	1.63	31,31,31,42	0
3	HEM	B	201	43/43	0.17	1.63	20,30,64,70	0
3	HEM	C	201	43/43	0.15	1.44	13,19,48,59	0
4	CMO	B	202	2/2	0.15	1.18	38,38,38,41	0
3	HEM	G	201	43/43	0.15	0.98	25,36,68,83	0
3	HEM	H	201	43/43	0.16	0.95	22,35,67,76	0
3	HEM	A	201	43/43	0.14	0.91	16,26,44,70	0
3	HEM	F	201	43/43	0.15	0.78	24,39,72,85	0
3	HEM	E	201	43/43	0.17	0.70	31,46,74,82	0
4	CMO	C	202	2/2	0.11	-0.44	19,19,19,28	0
4	CMO	F	202	2/2	0.11	-0.47	36,36,36,39	0
4	CMO	H	202	2/2	0.10	-0.80	34,34,34,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.