



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:49 AM GMT

PDB ID : 2ISA  
Title : Crystal Structure of Vibrio salmonicida catalase  
Authors : Riise, E.K.; Lorentzen, M.S.; Helland, R.; Smalas, A.O.; Leiros, H.K.S.; Willassen, N.P.  
Deposited on : 2006-10-17  
Resolution : 1.97 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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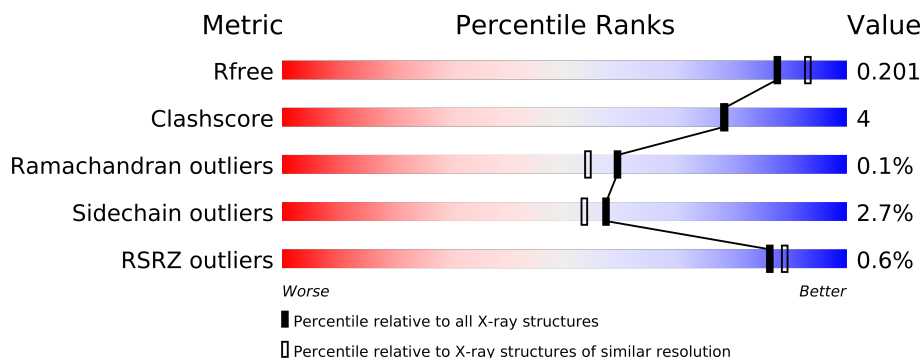
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.97 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	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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	483	
1	B	483	
1	C	483	
1	D	483	
1	E	483	
1	F	483	
1	G	483	
1	H	483	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	5489	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	B	5490	-	X
4	GOL	C	5487	-	X
4	GOL	D	5488	-	X
4	GOL	E	5493	-	X
4	GOL	G	5491	-	X
4	GOL	H	5492	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35944 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 Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	3	0
			3871	2443	688	728	12			
1	B	482	Total	C	N	O	S	3	3	0
			3869	2442	688	727	12			
1	C	482	Total	C	N	O	S	3	3	0
			3869	2442	688	727	12			
1	D	482	Total	C	N	O	S	11	3	0
			3869	2442	688	727	12			
1	E	482	Total	C	N	O	S	6	2	0
			3868	2442	688	726	12			
1	F	482	Total	C	N	O	S	11	3	0
			3869	2442	688	727	12			
1	G	482	Total	C	N	O	S	7	2	0
			3868	2442	688	726	12			
1	H	482	Total	C	N	O	S	7	3	0
			3871	2443	688	728	12			

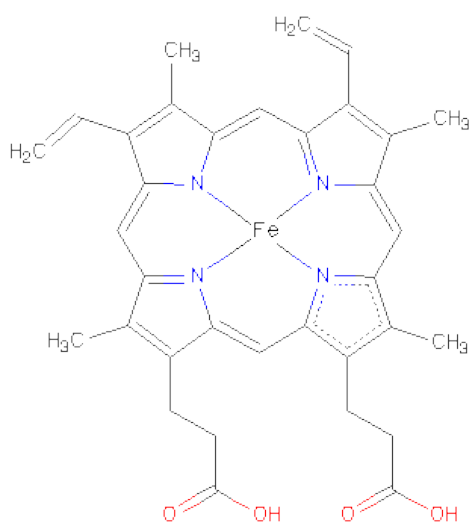
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
B	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
C	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
D	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
E	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
F	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
G	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1
H	53	OMT	MET	MODIFIED RESIDUE	UNP Q3LSM1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

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



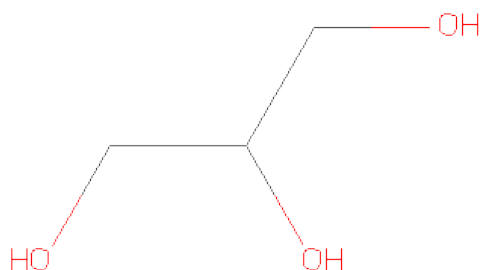
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	E	1	Total C Fe N O 43 34 1 4 4	0	0
3	F	1	Total C Fe N O 43 34 1 4 4	0	0
3	G	1	Total C Fe N O 43 34 1 4 4	0	0

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

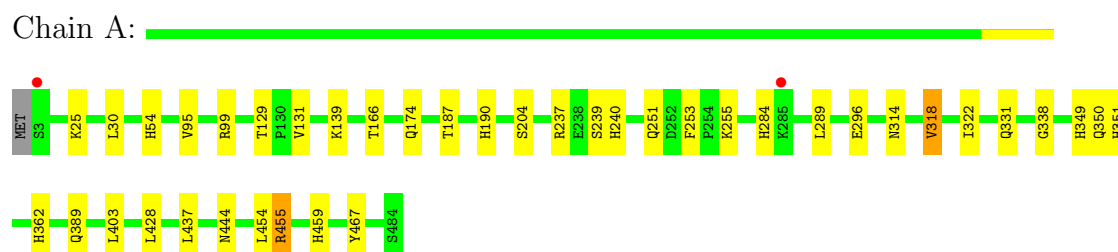
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	578	Total O 578 578	0	0
5	B	611	Total O 611 611	0	0
5	C	588	Total O 588 588	0	0
5	D	609	Total O 609 609	0	0
5	E	541	Total O 541 541	0	0
5	F	543	Total O 543 543	0	0
5	G	556	Total O 556 556	0	0
5	H	568	Total O 568 568	0	0

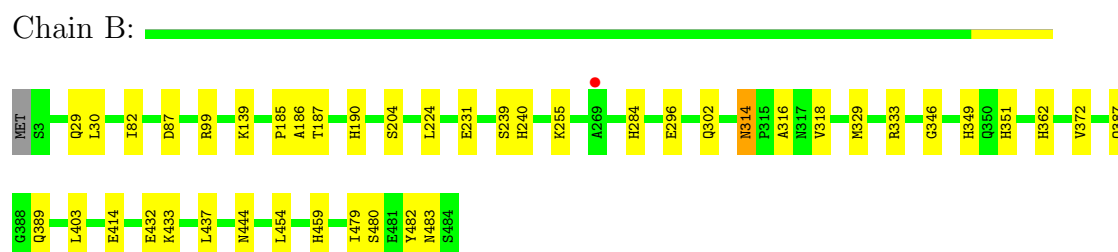
### 3 Residue-property plots

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.

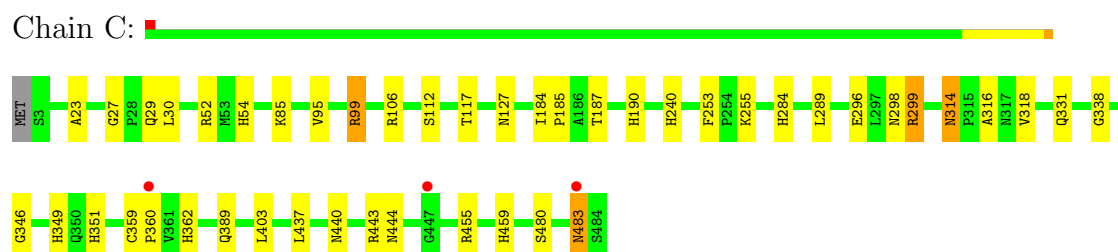
- Molecule 1: Catalase



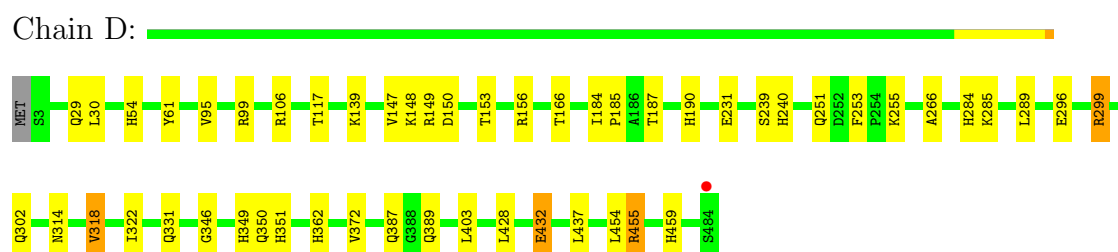
- Molecule 1: Catalase



- Molecule 1: Catalase

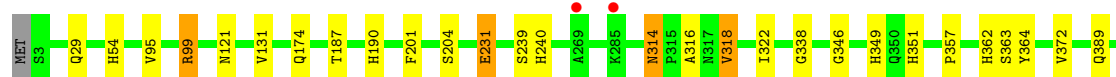


- Molecule 1: Catalase

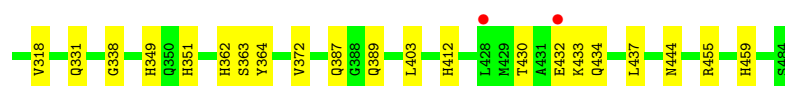
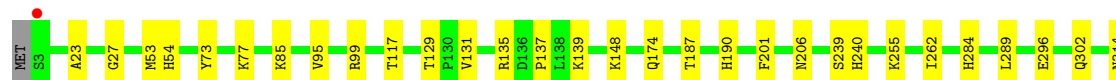


- Molecule 1: Catalase

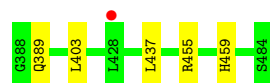
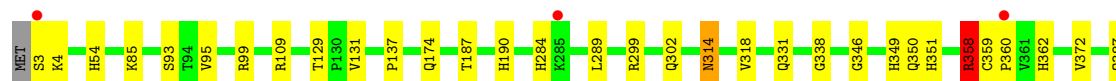


Chain E: 

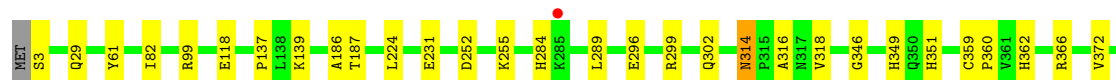
• Molecule 1: Catalase

Chain F: 

• Molecule 1: Catalase

Chain G: 

• Molecule 1: Catalase

Chain H: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.15Å 217.76Å 99.28Å 90.00° 110.48° 90.00°	Depositor
Resolution (Å)	20.00 – 1.97 19.93 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-1.97) 96.6 (19.93-1.97)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.148 , 0.200 0.148 , 0.201	Depositor DCC
$R_{free}$ test set	13407 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 52.9	EDS
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 266177 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	35944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GOL, CL, HEM, OMT

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	0.52	0/3989	0.63	2/5411 (0.0%)
1	B	0.54	1/3987 (0.0%)	0.61	0/5408
1	C	0.65	1/3987 (0.0%)	1.09	5/5408 (0.1%)
1	D	0.52	1/3987 (0.0%)	0.63	3/5408 (0.1%)
1	E	0.71	1/3981 (0.0%)	0.68	3/5400 (0.1%)
1	F	0.50	1/3987 (0.0%)	0.63	3/5408 (0.1%)
1	G	1.30	4/3981 (0.1%)	0.80	9/5400 (0.2%)
1	H	0.55	1/3989 (0.0%)	0.66	4/5411 (0.1%)
All	All	0.71	10/31888 (0.0%)	0.73	29/43254 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	358	ARG	CZ-NH1	67.58	2.21	1.33
1	E	231	GLU	CD-OE1	31.67	1.60	1.25
1	C	299	ARG	NE-CZ	-24.75	1.00	1.33
1	G	358	ARG	NE-CZ	24.29	1.64	1.33
1	G	358	ARG	CZ-NH2	21.48	1.60	1.33
1	H	231	GLU	CG-CD	11.56	1.69	1.51
1	G	302	GLN	CG-CD	-7.61	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	GLU	CG-CD	7.31	1.62	1.51
1	F	302	GLN	CG-CD	-6.54	1.35	1.51
1	D	231	GLU	CG-CD	5.42	1.60	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ARG	NE-CZ-NH1	-48.48	96.06	120.30
1	C	299	ARG	NE-CZ-NH2	41.48	141.04	120.30
1	E	231	GLU	OE1-CD-OE2	-23.53	95.07	123.30
1	G	358	ARG	NH1-CZ-NH2	-23.48	93.57	119.40
1	C	299	ARG	CD-NE-CZ	17.39	147.94	123.60
1	G	358	ARG	NE-CZ-NH1	17.04	128.82	120.30
1	G	358	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	F	302	GLN	CG-CD-OE1	-11.00	99.61	121.60
1	F	302	GLN	CB-CG-CD	10.48	138.86	111.60
1	G	302	GLN	CB-CG-CD	10.48	138.84	111.60
1	G	302	GLN	CG-CD-OE1	-10.17	101.25	121.60
1	H	99[A]	ARG	C-N-CA	-9.72	101.88	122.30
1	H	99[B]	ARG	C-N-CA	-9.72	101.88	122.30
1	F	302	GLN	CG-CD-NE2	8.76	137.72	116.70
1	G	358	ARG	CD-NE-CZ	8.46	135.45	123.60
1	G	302	GLN	CG-CD-NE2	8.20	136.39	116.70
1	H	302	GLN	CG-CD-OE1	8.15	137.91	121.60
1	H	302	GLN	CG-CD-NE2	-7.11	99.63	116.70
1	D	302	GLN	CG-CD-OE1	6.38	134.37	121.60
1	E	99[A]	ARG	N-CA-C	6.14	127.59	111.00
1	E	99[B]	ARG	N-CA-C	6.14	127.59	111.00
1	D	302	GLN	CG-CD-NE2	-5.96	102.41	116.70
1	A	99[A]	ARG	N-CA-C	5.86	126.83	111.00
1	A	99[B]	ARG	N-CA-C	5.86	126.83	111.00
1	C	99[A]	ARG	N-CA-C	5.78	126.61	111.00
1	C	99[B]	ARG	N-CA-C	5.78	126.61	111.00
1	G	99[A]	ARG	N-CA-C	5.57	126.04	111.00
1	G	99[B]	ARG	N-CA-C	5.57	126.04	111.00
1	D	299	ARG	CB-CG-CD	5.22	125.17	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	231	GLU	Sidechain
1	G	358	ARG	Sidechain

## 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	3871	0	3646	25	0
1	B	3869	0	3647	34	0
1	C	3869	0	3647	26	0
1	D	3869	0	3647	30	0
1	E	3868	0	3646	20	0
1	F	3869	0	3647	26	0
1	G	3868	0	3646	29	0
1	H	3871	0	3645	27	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
3	C	43	0	30	3	0
3	D	43	0	30	1	0
3	E	43	0	30	2	0
3	F	43	0	30	2	0
3	G	43	0	30	2	0
3	H	43	0	30	1	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	F	6	0	8	1	0
4	G	6	0	8	1	0
4	H	6	0	8	0	0
5	A	578	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	611	0	0	19	0
5	C	588	0	0	5	0
5	D	609	0	0	10	0
5	E	541	0	0	9	0
5	F	543	0	0	9	0
5	G	556	0	0	13	0
5	H	568	0	0	7	0
All	All	35944	0	29475	217	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 4.

All (217) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:387:GLN:HG2	5:F:8755:HOH:O	1.46	1.10
1:B:432:GLU:HG2	5:B:6655:HOH:O	1.73	0.88
1:B:387:GLN:HG2	5:B:6834:HOH:O	1.76	0.84
1:C:362:HIS:HE1	1:C:389:GLN:OE1	1.63	0.81
1:A:362:HIS:HE1	1:A:389:GLN:OE1	1.65	0.78
1:D:387:GLN:HG2	5:D:5647:HOH:O	1.83	0.77
1:D:387:GLN:HG2	5:D:5568:HOH:O	1.84	0.77
1:G:362:HIS:HE1	1:G:389:GLN:OE1	1.70	0.74
1:D:255:LYS:HG2	1:D:296:GLU:HB3	1.70	0.72
3:B:486:HEM:HBB2	3:B:486:HEM:HMB1	1.72	0.71
1:A:318:VAL:HG13	1:A:322:ILE:O	1.91	0.70
1:B:362:HIS:HD2	5:B:6699:HOH:O	1.75	0.68
1:F:362:HIS:HE1	1:F:389:GLN:OE1	1.77	0.68
1:A:362:HIS:HD2	5:A:5565:HOH:O	1.77	0.68
1:B:82:ILE:HD13	5:B:6929:HOH:O	1.93	0.68
1:B:349:HIS:HE1	5:B:6527:HOH:O	1.78	0.67
1:B:362:HIS:HE1	1:B:389:GLN:OE1	1.77	0.67
1:H:362:HIS:HD2	5:H:7540:HOH:O	1.78	0.66
1:A:349:HIS:HE1	5:A:5532:HOH:O	1.78	0.66
1:A:318:VAL:CG1	1:A:322:ILE:O	2.44	0.66
1:C:85:LYS:HE2	5:C:5970:HOH:O	1.96	0.66
1:E:362:HIS:HE1	1:E:389:GLN:OE1	1.80	0.65
1:E:99[A]:ARG:O	5:E:5729:HOH:O	2.15	0.65
1:C:187:THR:OG1	1:C:190:HIS:HD2	1.80	0.64
1:B:433:LYS:HE2	5:B:6634:HOH:O	1.96	0.64
1:C:480:SER:HA	1:C:483:ASN:HB2	1.79	0.64
1:H:346:GLY:O	1:H:349:HIS:HD2	1.82	0.63
1:B:255:LYS:HG2	1:B:296:GLU:HB3	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:187:THR:OG1	1:B:190:HIS:HD2	1.81	0.63
1:B:87:ASP:HB3	5:B:6999:HOH:O	2.00	0.62
1:G:459:HIS:HD2	5:G:5609:HOH:O	1.82	0.62
1:B:351:HIS:HD2	5:B:6490:HOH:O	1.81	0.62
1:F:351:HIS:HD2	5:F:8538:HOH:O	1.80	0.62
1:D:362:HIS:HE1	1:D:389:GLN:OE1	1.83	0.61
3:D:485:HEM:HBB2	3:D:485:HEM:HMB2	1.83	0.61
1:G:359:CYS:HB2	1:G:360:PRO:HD2	1.83	0.61
1:B:459:HIS:HD2	5:B:6513:HOH:O	1.84	0.61
3:C:485:HEM:HBB2	3:C:485:HEM:HMB2	1.83	0.61
1:A:351:HIS:HD2	5:A:5581:HOH:O	1.84	0.60
1:C:351:HIS:HD2	5:C:5507:HOH:O	1.85	0.59
1:H:362:HIS:HE1	1:H:389:GLN:OE1	1.85	0.59
1:G:3:SER:O	5:G:6047:HOH:O	2.17	0.59
3:B:486:HEM:HBB2	3:B:486:HEM:CMB	2.32	0.58
1:H:349:HIS:HE1	5:H:7546:HOH:O	1.85	0.58
1:E:349:HIS:HE1	5:E:5520:HOH:O	1.84	0.58
1:D:187:THR:OG1	1:D:190:HIS:HD2	1.86	0.58
1:H:139:LYS:HA	1:H:139:LYS:HE2	1.85	0.58
1:E:187:THR:OG1	1:E:190:HIS:HD2	1.86	0.58
1:F:73:TYR:CD2	1:F:262:ILE:HD13	2.39	0.58
1:G:351:HIS:HD2	5:G:5536:HOH:O	1.86	0.58
1:C:359:CYS:HB2	1:C:360:PRO:HD2	1.86	0.57
3:A:486:HEM:HMB1	3:A:486:HEM:HBB2	1.86	0.57
1:A:331:GLN:NE2	1:B:29:GLN:H	2.02	0.56
1:F:139:LYS:HA	1:F:139:LYS:HE2	1.87	0.56
1:G:349:HIS:HE1	5:G:5511:HOH:O	1.88	0.56
1:H:433:LYS:HD2	5:H:7639:HOH:O	2.05	0.56
3:E:486:HEM:HBB2	3:E:486:HEM:HMB2	1.88	0.56
1:D:139:LYS:HE2	1:D:139:LYS:HA	1.87	0.56
1:G:137:PRO:HB3	3:G:485:HEM:HBB1	1.89	0.55
1:H:255:LYS:HG2	1:H:296:GLU:HB3	1.88	0.55
1:A:331:GLN:HE21	1:B:29:GLN:H	1.55	0.55
1:C:29:GLN:H	1:D:331:GLN:NE2	2.05	0.54
5:B:6692:HOH:O	1:H:82:ILE:HD13	2.07	0.54
1:B:139:LYS:HE2	1:B:139:LYS:HA	1.90	0.54
1:C:29:GLN:H	1:D:331:GLN:HE21	1.56	0.53
1:H:255:LYS:HG2	1:H:296:GLU:CB	2.39	0.53
1:F:187:THR:OG1	1:F:190:HIS:HD2	1.91	0.53
1:E:459:HIS:HD2	5:E:5717:HOH:O	1.92	0.53
1:B:433:LYS:HD2	5:B:6602:HOH:O	2.08	0.53
1:H:137:PRO:HB3	3:H:485:HEM:HBB1	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:349:HIS:HE1	5:D:5518:HOH:O	1.93	0.52
1:E:351:HIS:HD2	5:E:5497:HOH:O	1.93	0.52
1:F:372:VAL:HG21	1:H:372:VAL:HG21	1.92	0.52
1:B:346:GLY:O	1:B:349:HIS:HD2	1.93	0.52
1:B:480:SER:HA	1:B:483:ASN:HD22	1.75	0.51
1:D:54:HIS:CE1	1:D:95:VAL:HG22	2.46	0.51
1:C:314:ASN:ND2	1:C:316:ALA:H	2.09	0.51
1:D:106:ARG:HA	1:D:184:ILE:HG12	1.93	0.51
1:F:53:OMT:CE	1:F:148:LYS:HE2	2.40	0.50
1:C:359:CYS:HB2	1:C:360:PRO:CD	2.41	0.50
1:A:338:GLY:HA3	4:A:5489:GOL:H2	1.93	0.50
1:G:131:VAL:HG23	1:G:174:GLN:HE21	1.76	0.50
1:A:239:SER:OG	1:A:240:HIS:HD2	1.95	0.50
1:G:54:HIS:CE1	1:G:95:VAL:HG22	2.47	0.50
1:A:139:LYS:HA	1:A:139:LYS:HE2	1.94	0.49
1:C:185:PRO:O	1:C:240:HIS:HE1	1.95	0.49
1:A:255:LYS:HG2	1:A:296:GLU:HB3	1.95	0.49
1:B:387:GLN:HG2	5:B:6735:HOH:O	2.11	0.49
1:A:54:HIS:CE1	1:A:95:VAL:HG22	2.48	0.49
5:E:6001:HOH:O	1:G:350:GLN:HB3	2.11	0.49
1:B:351:HIS:HE1	5:B:7022:HOH:O	1.96	0.49
5:D:5963:HOH:O	1:H:82:ILE:HD11	2.12	0.49
1:C:255:LYS:HG2	1:C:296:GLU:HB3	1.95	0.49
1:B:372:VAL:HG21	1:D:372:VAL:HG21	1.93	0.49
1:C:346:GLY:O	1:C:349:HIS:HD2	1.96	0.48
1:B:351:HIS:CD2	5:B:6490:HOH:O	2.61	0.48
1:D:346:GLY:O	1:D:349:HIS:HD2	1.96	0.48
1:E:362:HIS:HD2	5:E:5598:HOH:O	1.96	0.48
1:F:77:LYS:HE2	5:F:8884:HOH:O	2.12	0.48
1:A:131:VAL:HG23	1:A:174:GLN:HE21	1.77	0.48
1:D:185:PRO:O	1:D:240:HIS:HE1	1.96	0.48
1:G:187:THR:OG1	1:G:190:HIS:HD2	1.97	0.48
1:F:137:PRO:HB3	3:F:486:HEM:HBB1	1.96	0.48
1:G:85:LYS:HE2	5:G:5872:HOH:O	2.14	0.48
1:F:459:HIS:HD2	5:F:8594:HOH:O	1.96	0.48
1:H:346:GLY:O	1:H:349:HIS:CD2	2.66	0.48
1:F:349:HIS:HE1	5:F:8604:HOH:O	1.96	0.48
1:C:349:HIS:HE1	5:C:5647:HOH:O	1.97	0.47
1:G:331:GLN:NE2	1:H:29:GLN:H	2.12	0.47
1:D:266:ALA:HB3	5:D:6037:HOH:O	2.14	0.47
1:E:54:HIS:CE1	1:E:95:VAL:HG22	2.50	0.47
1:A:350:GLN:HG2	5:A:5892:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:5915:HOH:O	1:G:4:LYS:HE2	2.15	0.47
1:D:351:HIS:HD2	5:D:5515:HOH:O	1.97	0.47
1:G:4:LYS:HA	5:G:6047:HOH:O	2.15	0.47
1:G:351:HIS:CD2	5:G:5536:HOH:O	2.62	0.47
1:C:187:THR:OG1	1:C:190:HIS:CD2	2.65	0.47
3:A:486:HEM:CMB	3:A:486:HEM:HBB2	2.45	0.47
1:E:131:VAL:HG23	1:E:174:GLN:HE21	1.79	0.47
1:G:314:ASN:ND2	5:G:5580:HOH:O	2.48	0.47
1:F:338:GLY:HA3	4:F:5494:GOL:H2	1.97	0.47
1:F:85:LYS:NZ	5:F:8905:HOH:O	2.43	0.46
1:C:331:GLN:NE2	1:D:29:GLN:H	2.14	0.46
1:G:359:CYS:HB2	1:G:360:PRO:CD	2.45	0.46
1:F:433:LYS:HE2	5:F:8746:HOH:O	2.15	0.46
1:A:351:HIS:CD2	5:A:5581:HOH:O	2.64	0.46
1:F:255:LYS:HG2	1:F:296:GLU:HB3	1.98	0.46
1:H:351:HIS:HD2	5:H:7488:HOH:O	1.99	0.46
1:D:459:HIS:HE1	5:D:5750:HOH:O	1.99	0.46
1:C:459:HIS:HD2	5:C:5534:HOH:O	1.99	0.45
1:A:459:HIS:HD2	5:A:5578:HOH:O	1.97	0.45
1:H:359:CYS:HB2	1:H:360:PRO:HD2	1.97	0.45
1:F:430:THR:O	1:F:434:GLN:HG3	2.15	0.45
1:F:363:SER:O	1:F:364:TYR:HB3	2.16	0.45
1:B:82:ILE:CD1	5:B:6929:HOH:O	2.57	0.45
1:D:239:SER:OG	1:D:240:HIS:HD2	1.99	0.45
5:B:6717:HOH:O	1:D:350:GLN:HB3	2.16	0.45
1:A:187:THR:OG1	1:A:190:HIS:HD2	1.99	0.45
3:C:485:HEM:HBB2	3:C:485:HEM:CMB	2.46	0.45
1:C:52:ARG:HE	1:C:52:ARG:HA	1.82	0.45
1:F:239:SER:OG	1:F:240:HIS:HD2	1.99	0.45
1:B:302:GLN:NE2	5:B:6797:HOH:O	2.50	0.45
1:F:54:HIS:CE1	1:F:95:VAL:HG22	2.52	0.45
1:A:30:LEU:HD23	1:D:30:LEU:HD23	1.98	0.45
3:F:486:HEM:HMB2	3:F:486:HEM:HBB2	1.98	0.44
1:D:318:VAL:HG13	1:D:322:ILE:O	2.16	0.44
1:D:432:GLU:HB3	5:D:5571:HOH:O	2.16	0.44
1:E:29:GLN:H	1:F:331:GLN:NE2	2.15	0.44
1:C:23:ALA:O	1:C:27:GLY:HA3	2.17	0.44
1:A:25:LYS:HD3	1:B:414:GLU:OE2	2.18	0.44
1:B:479:ILE:HA	1:B:482:TYR:CZ	2.52	0.44
1:F:351:HIS:CD2	5:F:8538:HOH:O	2.61	0.44
1:E:346:GLY:O	1:E:349:HIS:HD2	2.00	0.44
1:H:314:ASN:ND2	1:H:316:ALA:H	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:387:GLN:NE2	5:H:7794:HOH:O	2.51	0.43
1:C:106:ARG:HA	1:C:184:ILE:HG12	1.98	0.43
1:G:358:ARG:NH2	5:G:5918:HOH:O	2.51	0.43
1:C:54:HIS:CE1	1:C:95:VAL:HG22	2.52	0.43
1:G:187:THR:OG1	1:G:190:HIS:CD2	2.71	0.43
1:H:480:SER:HA	1:H:483:ASN:HD22	1.84	0.43
1:A:318:VAL:HG11	1:A:322:ILE:O	2.18	0.43
1:G:346:GLY:O	1:G:349:HIS:HD2	2.01	0.43
1:G:331:GLN:HE21	1:H:29:GLN:H	1.65	0.43
1:B:239:SER:OG	1:B:240:HIS:HD2	2.02	0.43
1:B:186:ALA:HA	1:B:224:LEU:HG	2.01	0.43
1:E:372:VAL:HG21	1:G:372:VAL:HG21	2.01	0.42
1:G:362:HIS:HD2	5:G:5828:HOH:O	2.01	0.42
1:F:362:HIS:HD2	5:F:8617:HOH:O	2.03	0.42
1:D:150:ASP:HB3	1:D:153:THR:OG1	2.20	0.42
1:B:329:MET:O	1:B:333:ARG:HG3	2.20	0.42
1:C:127:ASN:CG	3:C:485:HEM:HAC	2.39	0.42
3:G:485:HEM:CMB	3:G:485:HEM:HBB2	2.50	0.42
1:H:366:ARG:HA	1:H:366:ARG:HD2	1.90	0.42
1:B:314:ASN:ND2	1:B:316:ALA:H	2.17	0.42
1:C:338:GLY:HA3	4:C:5487:GOL:H2	2.01	0.42
3:E:486:HEM:HBB2	3:E:486:HEM:CMB	2.48	0.42
1:A:251:GLN:HA	1:A:253:PHE:CE2	2.55	0.42
1:H:440:ASN:HD22	1:H:443:ARG:NH2	2.18	0.42
1:E:187:THR:OG1	1:E:190:HIS:CD2	2.69	0.42
1:G:387:GLN:NE2	5:G:5724:HOH:O	2.52	0.42
1:F:131:VAL:HG23	1:F:174:GLN:HE21	1.84	0.42
1:H:483:ASN:ND2	5:H:7874:HOH:O	2.53	0.41
1:H:118:GLU:HB2	5:H:7748:HOH:O	2.20	0.41
1:A:166:THR:HB	1:A:455:ARG:HB3	2.02	0.41
1:G:299:ARG:HD3	5:G:5873:HOH:O	2.20	0.41
1:H:61:TYR:HB2	1:H:299:ARG:HB3	2.01	0.41
1:B:30:LEU:HD23	1:C:30:LEU:HD23	2.03	0.41
1:G:93:SER:O	1:G:109:ARG:HA	2.20	0.41
1:D:61:TYR:HB2	1:D:299:ARG:HB3	2.03	0.41
1:F:23:ALA:O	1:F:27:GLY:HA3	2.21	0.41
1:C:253:PHE:CD2	1:C:298:ASN:HA	2.55	0.41
1:D:147:VAL:O	1:D:156:ARG:HD3	2.20	0.41
1:D:166:THR:HB	1:D:455:ARG:HB3	2.02	0.41
1:E:121:ASN:HD21	1:E:357:PRO:HA	1.86	0.41
1:E:314:ASN:ND2	1:E:316:ALA:H	2.19	0.41
1:H:186:ALA:HA	1:H:224:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:135:ARG:HD2	1:F:412:HIS:ND1	2.35	0.41
1:E:318:VAL:HG13	1:E:322:ILE:O	2.20	0.41
1:E:338:GLY:HA3	4:E:5493:GOL:H2	2.02	0.41
1:D:387:GLN:CG	5:D:5647:HOH:O	2.54	0.41
1:B:483:ASN:CG	5:B:6994:HOH:O	2.60	0.41
1:D:148:LYS:HB3	1:D:149:ARG:H	1.79	0.41
1:B:187:THR:OG1	1:B:190:HIS:CD2	2.67	0.40
1:E:459:HIS:HE1	5:E:5742:HOH:O	2.04	0.40
1:A:255:LYS:HG2	1:A:296:GLU:CB	2.50	0.40
1:C:440:ASN:HD22	1:C:443:ARG:NH2	2.19	0.40
5:D:5719:HOH:O	1:H:252:ASP:HB2	2.21	0.40
1:A:459:HIS:HE1	5:A:5883:HOH:O	2.03	0.40
1:G:338:GLY:HA3	4:G:5491:GOL:H2	2.03	0.40
1:E:239:SER:OG	1:E:240:HIS:HD2	2.04	0.40
1:B:185:PRO:O	1:B:240:HIS:HE1	2.05	0.40
1:E:363:SER:O	1:E:364:TYR:HB3	2.22	0.40
1:G:3:SER:HA	5:G:5810:HOH:O	2.21	0.40
1:D:251:GLN:HA	1:D:253:PHE:CE2	2.56	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	482/483 (100%)	466 (97%)	16 (3%)	0	100	100
1	B	482/483 (100%)	463 (96%)	17 (4%)	2 (0%)	43	34
1	C	482/483 (100%)	462 (96%)	20 (4%)	0	100	100
1	D	482/483 (100%)	465 (96%)	15 (3%)	2 (0%)	43	34
1	E	481/483 (100%)	463 (96%)	18 (4%)	0	100	100
1	F	482/483 (100%)	462 (96%)	18 (4%)	2 (0%)	43	34
1	G	481/483 (100%)	465 (97%)	16 (3%)	0	100	100
1	H	482/483 (100%)	465 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3854/3864 (100%)	3711 (96%)	137 (4%)	6 (0%)	59	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	99[A]	ARG
1	F	99[B]	ARG
1	B	99[A]	ARG
1	B	99[B]	ARG
1	D	99[A]	ARG
1	D	99[B]	ARG

### 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	407/406 (100%)	393 (97%)	14 (3%)	49	42
1	B	407/406 (100%)	399 (98%)	8 (2%)	68	67
1	C	407/406 (100%)	394 (97%)	13 (3%)	51	45
1	D	407/406 (100%)	395 (97%)	12 (3%)	55	50
1	E	406/406 (100%)	399 (98%)	7 (2%)	73	73
1	F	407/406 (100%)	394 (97%)	13 (3%)	51	45
1	G	406/406 (100%)	397 (98%)	9 (2%)	64	63
1	H	407/406 (100%)	396 (97%)	11 (3%)	57	53
All	All	3254/3248 (100%)	3167 (97%)	87 (3%)	57	53

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	204	SER
1	A	237	ARG
1	A	284	HIS
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	314	ASN
1	A	318	VAL
1	A	403	LEU
1	A	428	LEU
1	A	437	LEU
1	A	444	ASN
1	A	454	LEU
1	A	455	ARG
1	A	467	TYR
1	B	204	SER
1	B	284	HIS
1	B	314	ASN
1	B	318	VAL
1	B	403	LEU
1	B	437	LEU
1	B	444	ASN
1	B	454	LEU
1	C	99[A]	ARG
1	C	99[B]	ARG
1	C	112	SER
1	C	117	THR
1	C	284	HIS
1	C	289	LEU
1	C	314	ASN
1	C	318	VAL
1	C	403	LEU
1	C	437	LEU
1	C	444	ASN
1	C	455	ARG
1	C	483	ASN
1	D	117	THR
1	D	284	HIS
1	D	285	LYS
1	D	289	LEU
1	D	314	ASN
1	D	318	VAL
1	D	403	LEU
1	D	428	LEU
1	D	432	GLU
1	D	437	LEU
1	D	454	LEU
1	D	455	ARG

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Mol	Chain	Res	Type
1	E	201	PHE
1	E	204	SER
1	E	314	ASN
1	E	318	VAL
1	E	403	LEU
1	E	437	LEU
1	E	454	LEU
1	F	117	THR
1	F	129	THR
1	F	201	PHE
1	F	206	ASN
1	F	284	HIS
1	F	289	LEU
1	F	314	ASN
1	F	318	VAL
1	F	403	LEU
1	F	432	GLU
1	F	437	LEU
1	F	444	ASN
1	F	455	ARG
1	G	129	THR
1	G	284	HIS
1	G	289	LEU
1	G	314	ASN
1	G	318	VAL
1	G	358	ARG
1	G	403	LEU
1	G	437	LEU
1	G	455	ARG
1	H	3	SER
1	H	187	THR
1	H	284	HIS
1	H	289	LEU
1	H	314	ASN
1	H	318	VAL
1	H	403	LEU
1	H	432	GLU
1	H	437	LEU
1	H	454	LEU
1	H	455	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	121	ASN
1	A	160	ASN
1	A	174	GLN
1	A	190	HIS
1	A	240	HIS
1	A	250	ASN
1	A	284	HIS
1	A	300	ASN
1	A	314	ASN
1	A	317	ASN
1	A	331	GLN
1	A	349	HIS
1	A	351	HIS
1	A	362	HIS
1	A	402	ASN
1	A	440	ASN
1	A	459	HIS
1	B	32	GLN
1	B	121	ASN
1	B	160	ASN
1	B	174	GLN
1	B	190	HIS
1	B	235	ASN
1	B	240	HIS
1	B	250	ASN
1	B	300	ASN
1	B	314	ASN
1	B	317	ASN
1	B	331	GLN
1	B	349	HIS
1	B	351	HIS
1	B	362	HIS
1	B	402	ASN
1	B	440	ASN
1	B	459	HIS
1	B	483	ASN
1	C	32	GLN
1	C	121	ASN
1	C	160	ASN
1	C	174	GLN
1	C	190	HIS
1	C	240	HIS

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Mol	Chain	Res	Type
1	C	284	HIS
1	C	300	ASN
1	C	314	ASN
1	C	317	ASN
1	C	331	GLN
1	C	349	HIS
1	C	351	HIS
1	C	362	HIS
1	C	402	ASN
1	C	440	ASN
1	C	459	HIS
1	D	32	GLN
1	D	121	ASN
1	D	160	ASN
1	D	174	GLN
1	D	190	HIS
1	D	235	ASN
1	D	240	HIS
1	D	250	ASN
1	D	284	HIS
1	D	300	ASN
1	D	314	ASN
1	D	317	ASN
1	D	331	GLN
1	D	349	HIS
1	D	351	HIS
1	D	362	HIS
1	D	402	ASN
1	D	440	ASN
1	D	459	HIS
1	E	32	GLN
1	E	121	ASN
1	E	160	ASN
1	E	174	GLN
1	E	190	HIS
1	E	240	HIS
1	E	250	ASN
1	E	300	ASN
1	E	314	ASN
1	E	317	ASN
1	E	331	GLN
1	E	349	HIS

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Mol	Chain	Res	Type
1	E	351	HIS
1	E	362	HIS
1	E	402	ASN
1	E	440	ASN
1	E	459	HIS
1	F	32	GLN
1	F	121	ASN
1	F	160	ASN
1	F	174	GLN
1	F	190	HIS
1	F	235	ASN
1	F	240	HIS
1	F	250	ASN
1	F	284	HIS
1	F	300	ASN
1	F	314	ASN
1	F	317	ASN
1	F	331	GLN
1	F	349	HIS
1	F	351	HIS
1	F	362	HIS
1	F	402	ASN
1	F	440	ASN
1	F	459	HIS
1	G	32	GLN
1	G	121	ASN
1	G	174	GLN
1	G	190	HIS
1	G	240	HIS
1	G	300	ASN
1	G	314	ASN
1	G	317	ASN
1	G	331	GLN
1	G	349	HIS
1	G	350	GLN
1	G	351	HIS
1	G	362	HIS
1	G	402	ASN
1	G	440	ASN
1	G	459	HIS
1	H	32	GLN
1	H	121	ASN

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Mol	Chain	Res	Type
1	H	160	ASN
1	H	174	GLN
1	H	190	HIS
1	H	240	HIS
1	H	250	ASN
1	H	251	GLN
1	H	284	HIS
1	H	300	ASN
1	H	314	ASN
1	H	317	ASN
1	H	331	GLN
1	H	349	HIS
1	H	351	HIS
1	H	362	HIS
1	H	402	ASN
1	H	440	ASN
1	H	459	HIS
1	H	483	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	OMT	A	53	1	9,9,10	7.26	6 (66%)	10,12,14	3.10	5 (50%)
1	OMT	B	53	1	9,9,10	6.45	3 (33%)	10,12,14	2.79	3 (30%)
1	OMT	C	53	1	9,9,10	6.72	4 (44%)	10,12,14	3.27	5 (50%)
1	OMT	D	53	1	9,9,10	6.47	3 (33%)	10,12,14	3.58	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMT	E	53	1	9,9,10	7.32	3 (33%)	10,12,14	3.16	5 (50%)
1	OMT	F	53	1	9,9,10	6.59	3 (33%)	10,12,14	3.42	3 (30%)
1	OMT	G	53	1	9,9,10	7.00	3 (33%)	10,12,14	2.75	3 (30%)
1	OMT	H	53	1	9,9,10	6.32	3 (33%)	10,12,14	2.69	3 (30%)

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
1	OMT	A	53	1	-	0/6/8/10	0/0/0/0
1	OMT	B	53	1	-	0/6/8/10	0/0/0/0
1	OMT	C	53	1	-	0/6/8/10	0/0/0/0
1	OMT	D	53	1	-	0/6/8/10	0/0/0/0
1	OMT	E	53	1	-	0/6/8/10	0/0/0/0
1	OMT	F	53	1	-	0/6/8/10	0/0/0/0
1	OMT	G	53	1	-	0/6/8/10	0/0/0/0
1	OMT	H	53	1	-	0/6/8/10	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	OMT	O-C	19.21	1.24	1.11
1	A	53	OMT	O-C	18.72	1.24	1.11
1	G	53	OMT	O-C	18.47	1.24	1.11
1	C	53	OMT	O-C	17.55	1.23	1.11
1	F	53	OMT	O-C	16.84	1.23	1.11
1	D	53	OMT	O-C	16.58	1.22	1.11
1	B	53	OMT	O-C	16.32	1.22	1.11
1	H	53	OMT	O-C	16.25	1.22	1.11
1	E	53	OMT	CG-SD	-8.56	1.67	1.78
1	A	53	OMT	CG-SD	-8.29	1.67	1.78
1	G	53	OMT	CG-SD	-7.89	1.68	1.78
1	D	53	OMT	CG-SD	-7.75	1.68	1.78
1	H	53	OMT	CG-SD	-7.71	1.68	1.78
1	F	53	OMT	CG-SD	-7.49	1.68	1.78
1	C	53	OMT	CG-SD	-7.38	1.68	1.78
1	B	53	OMT	CG-SD	-7.22	1.68	1.78
1	B	53	OMT	CE-SD	-7.12	1.65	1.75
1	F	53	OMT	CE-SD	-7.00	1.65	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	OMT	CE-SD	-6.40	1.66	1.75
1	C	53	OMT	CE-SD	-5.91	1.67	1.75
1	E	53	OMT	CE-SD	-5.89	1.67	1.75
1	D	53	OMT	CE-SD	-5.86	1.67	1.75
1	G	53	OMT	CE-SD	-5.57	1.67	1.75
1	H	53	OMT	CE-SD	-5.51	1.67	1.75
1	A	53	OMT	CB-CA	2.21	1.55	1.53
1	A	53	OMT	CB-CG	2.17	1.54	1.52
1	C	53	OMT	CB-CG	2.15	1.54	1.52
1	A	53	OMT	CA-C	2.14	1.52	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	OMT	C-CA-N	-8.99	104.85	113.83
1	D	53	OMT	C-CA-N	-8.67	105.17	113.83
1	E	53	OMT	C-CA-N	-8.26	105.58	113.83
1	A	53	OMT	C-CA-N	-7.28	106.56	113.83
1	C	53	OMT	C-CA-N	-7.20	106.64	113.83
1	G	53	OMT	C-CA-N	-7.18	106.66	113.83
1	H	53	OMT	C-CA-N	-7.03	106.81	113.83
1	B	53	OMT	C-CA-N	-6.87	106.96	113.83
1	D	53	OMT	OD2-SD-CG	5.18	111.65	108.27
1	C	53	OMT	OD1-SD-CG	4.85	111.43	108.27
1	F	53	OMT	OD1-SD-CE	4.35	111.87	108.80
1	B	53	OMT	OD2-SD-CG	4.04	110.91	108.27
1	D	53	OMT	OD1-SD-CG	3.56	110.59	108.27
1	C	53	OMT	OD2-SD-CG	3.51	110.56	108.27
1	D	53	OMT	OD2-SD-OD1	-3.43	107.94	116.95
1	A	53	OMT	OD2-SD-OD1	-3.37	108.10	116.95
1	H	53	OMT	OD1-SD-CE	-3.26	106.49	108.80
1	A	53	OMT	OD1-SD-CG	3.26	110.39	108.27
1	B	53	OMT	OD2-SD-OD1	-3.22	108.51	116.95
1	G	53	OMT	OD2-SD-OD1	-3.20	108.56	116.95
1	G	53	OMT	OD1-SD-CG	3.19	110.35	108.27
1	F	53	OMT	OD2-SD-OD1	-3.14	108.72	116.95
1	A	53	OMT	OD2-SD-CG	3.13	110.31	108.27
1	E	53	OMT	OD2-SD-OD1	-3.04	108.97	116.95
1	C	53	OMT	OD2-SD-OD1	-3.03	109.01	116.95
1	C	53	OMT	OD1-SD-CE	-2.94	106.72	108.80
1	A	53	OMT	OD1-SD-CE	-2.41	107.09	108.80
1	E	53	OMT	OD1-SD-CG	2.40	109.83	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	OMT	OD2-SD-CG	2.38	109.83	108.27
1	E	53	OMT	OD1-SD-CE	-2.33	107.15	108.80
1	H	53	OMT	OD2-SD-OD1	-2.26	111.03	116.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	486	1	49,50,50	2.43	15 (30%)	46,82,82	2.23	11 (23%)
4	GOL	A	5489	-	5,5,5	0.19	0	5,5,5	0.57	0
3	HEM	B	486	1	49,50,50	2.35	18 (36%)	46,82,82	2.26	8 (17%)
4	GOL	B	5490	-	5,5,5	0.22	0	5,5,5	0.63	0
3	HEM	C	485	1	49,50,50	2.42	16 (32%)	46,82,82	2.23	12 (26%)
4	GOL	C	5487	-	5,5,5	0.18	0	5,5,5	0.43	0
3	HEM	D	485	1	49,50,50	2.47	17 (34%)	46,82,82	2.24	10 (21%)
4	GOL	D	5488	-	5,5,5	0.23	0	5,5,5	0.45	0
3	HEM	E	486	1	49,50,50	2.32	18 (36%)	46,82,82	2.18	8 (17%)
4	GOL	E	5493	-	5,5,5	0.17	0	5,5,5	0.53	0
3	HEM	F	486	1	49,50,50	2.28	14 (28%)	46,82,82	2.19	9 (19%)
4	GOL	F	5494	-	5,5,5	0.26	0	5,5,5	0.56	0
3	HEM	G	485	1	49,50,50	2.52	17 (34%)	46,82,82	2.35	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	G	5491	-	5,5,5	0.14	0	5,5,5	0.55	0
3	HEM	H	485	1	49,50,50	2.55	17 (34%)	46,82,82	2.26	12 (26%)
4	GOL	H	5492	-	5,5,5	0.22	0	5,5,5	0.47	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	486	1	-	0/14/114/114	0/0/8/8
4	GOL	A	5489	-	-	0/4/4/4	0/0/0/0
3	HEM	B	486	1	-	0/14/114/114	0/0/8/8
4	GOL	B	5490	-	-	0/4/4/4	0/0/0/0
3	HEM	C	485	1	-	0/14/114/114	0/0/8/8
4	GOL	C	5487	-	-	0/4/4/4	0/0/0/0
3	HEM	D	485	1	-	0/14/114/114	0/0/8/8
4	GOL	D	5488	-	-	0/4/4/4	0/0/0/0
3	HEM	E	486	1	-	0/14/114/114	0/0/8/8
4	GOL	E	5493	-	-	0/4/4/4	0/0/0/0
3	HEM	F	486	1	-	0/14/114/114	0/0/8/8
4	GOL	F	5494	-	-	0/4/4/4	0/0/0/0
3	HEM	G	485	1	-	0/14/114/114	0/0/8/8
4	GOL	G	5491	-	-	0/4/4/4	0/0/0/0
3	HEM	H	485	1	-	0/14/114/114	0/0/8/8
4	GOL	H	5492	-	-	0/4/4/4	0/0/0/0

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	485	HEM	C2D-C1D	6.53	1.46	1.44
3	A	486	HEM	C3D-C2D	6.44	1.55	1.43
3	A	486	HEM	C2B-C1B	6.40	1.46	1.44
3	G	485	HEM	C2B-C1B	6.14	1.46	1.44
3	H	485	HEM	C2B-C1B	5.98	1.46	1.44
3	G	485	HEM	C3D-C2D	5.74	1.53	1.43
3	C	485	HEM	C3D-C4D	5.65	1.46	1.44
3	D	485	HEM	C2B-C1B	5.65	1.46	1.44
3	E	486	HEM	C3D-C2D	5.48	1.53	1.43
3	D	485	HEM	C3D-C2D	5.39	1.53	1.43
3	C	485	HEM	C3D-C2D	5.32	1.53	1.43
3	G	485	HEM	C3C-C2C	-5.32	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	485	HEM	C3B-C2B	-5.31	1.34	1.43
3	F	486	HEM	C3D-C2D	5.29	1.53	1.43
3	B	486	HEM	C3D-C2D	5.28	1.53	1.43
3	B	486	HEM	C3C-C2C	-5.17	1.34	1.43
3	E	486	HEM	C3C-C2C	-5.08	1.34	1.43
3	C	485	HEM	C3C-C2C	-5.03	1.35	1.43
3	H	485	HEM	C3D-C2D	5.00	1.52	1.43
3	A	486	HEM	C3C-C2C	-4.95	1.35	1.43
3	H	485	HEM	C3B-CAB	4.94	1.56	1.40
3	E	486	HEM	C3C-CAC	4.92	1.55	1.40
3	C	485	HEM	C3B-CAB	4.92	1.55	1.40
3	H	485	HEM	C3C-C2C	-4.91	1.35	1.43
3	G	485	HEM	C4A-C3A	4.89	1.46	1.40
3	G	485	HEM	C3C-CAC	4.86	1.55	1.40
3	F	486	HEM	C3C-C2C	-4.86	1.35	1.43
3	H	485	HEM	C3B-C2B	-4.85	1.35	1.43
3	E	486	HEM	C3B-CAB	4.85	1.55	1.40
3	B	486	HEM	C4A-C3A	4.81	1.46	1.40
3	G	485	HEM	C3B-CAB	4.80	1.55	1.40
3	B	486	HEM	C3B-C2B	-4.80	1.35	1.43
3	B	486	HEM	C3B-CAB	4.78	1.55	1.40
3	F	486	HEM	C4A-C3A	4.75	1.46	1.40
3	D	485	HEM	C3B-CAB	4.74	1.55	1.40
3	H	485	HEM	C4A-C3A	4.73	1.46	1.40
3	D	485	HEM	C3B-C2B	-4.73	1.35	1.43
3	D	485	HEM	C3C-CAC	4.72	1.55	1.40
3	C	485	HEM	C3B-C2B	-4.72	1.35	1.43
3	A	486	HEM	C3B-CAB	4.70	1.55	1.40
3	D	485	HEM	C3C-C2C	-4.69	1.35	1.43
3	F	486	HEM	C3B-C2B	-4.69	1.35	1.43
3	C	485	HEM	C3C-CAC	4.68	1.55	1.40
3	G	485	HEM	FE-NB	4.68	2.14	1.97
3	A	486	HEM	C3B-C2B	-4.67	1.35	1.43
3	B	486	HEM	C3C-CAC	4.66	1.55	1.40
3	A	486	HEM	C3C-CAC	4.65	1.55	1.40
3	A	486	HEM	C4A-C3A	4.65	1.46	1.40
3	F	486	HEM	C3B-CAB	4.63	1.55	1.40
3	H	485	HEM	C3C-CAC	4.63	1.55	1.40
3	F	486	HEM	C3C-CAC	4.59	1.54	1.40
3	B	486	HEM	C2D-C1D	4.58	1.45	1.44
3	D	485	HEM	C4A-C3A	4.51	1.45	1.40
3	E	486	HEM	C4A-C3A	4.46	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	486	HEM	FE-NB	4.45	2.14	1.97
3	C	485	HEM	C4A-C3A	4.28	1.45	1.40
3	E	486	HEM	C3B-C2B	-4.27	1.36	1.43
3	F	486	HEM	C2D-C1D	4.27	1.45	1.44
3	B	486	HEM	C2B-C1B	4.24	1.45	1.44
3	D	485	HEM	FE-NA	4.12	2.10	1.92
3	D	485	HEM	C3D-C4D	4.12	1.45	1.44
3	C	485	HEM	FE-ND	4.06	2.12	1.97
3	F	486	HEM	FE-NB	4.06	2.12	1.97
3	E	486	HEM	C2B-C1B	3.95	1.45	1.44
3	C	485	HEM	C2B-C1B	3.94	1.45	1.44
3	B	486	HEM	FE-NA	3.87	2.09	1.92
3	D	485	HEM	FE-ND	3.82	2.11	1.97
3	F	486	HEM	FE-NC	3.71	2.11	1.97
3	H	485	HEM	FE-NA	3.67	2.08	1.92
3	D	485	HEM	C2D-C1D	3.66	1.45	1.44
3	E	486	HEM	FE-NB	3.64	2.11	1.97
3	G	485	HEM	C3D-C4D	3.50	1.45	1.44
3	C	485	HEM	FE-NB	3.47	2.10	1.97
3	H	485	HEM	FE-ND	3.40	2.10	1.97
3	F	486	HEM	FE-NA	3.35	2.06	1.92
3	E	486	HEM	FE-NA	3.30	2.06	1.92
3	A	486	HEM	FE-NA	3.24	2.06	1.92
3	G	485	HEM	FE-NC	3.20	2.09	1.97
3	D	485	HEM	FE-NC	3.18	2.09	1.97
3	E	486	HEM	FE-NC	3.14	2.09	1.97
3	H	485	HEM	C3D-C4D	3.13	1.45	1.44
3	C	485	HEM	FE-NA	3.10	2.05	1.92
3	B	486	HEM	FE-NC	3.04	2.09	1.97
3	G	485	HEM	FE-NA	2.92	2.04	1.92
3	A	486	HEM	FE-ND	2.85	2.08	1.97
3	E	486	HEM	CMC-C2C	2.82	1.56	1.47
3	G	485	HEM	CMC-C2C	2.78	1.56	1.47
3	C	485	HEM	CMC-C2C	2.76	1.56	1.47
3	E	486	HEM	C3D-C4D	2.73	1.45	1.44
3	E	486	HEM	CMB-C2B	2.65	1.55	1.47
3	A	486	HEM	CMC-C2C	2.64	1.55	1.47
3	B	486	HEM	CMB-C2B	2.63	1.55	1.47
3	D	485	HEM	FE-NB	2.55	2.07	1.97
3	F	486	HEM	CMC-C2C	2.55	1.55	1.47
3	E	486	HEM	CMD-C2D	2.55	1.55	1.47
3	B	486	HEM	FE-ND	2.53	2.07	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	486	HEM	FE-ND	2.53	2.07	1.97
3	H	485	HEM	FE-NC	2.52	2.07	1.97
3	F	486	HEM	CMB-C2B	2.51	1.55	1.47
3	A	486	HEM	CMB-C2B	2.50	1.55	1.47
3	G	485	HEM	CMB-C2B	2.44	1.55	1.47
3	C	485	HEM	CMB-C2B	2.44	1.55	1.47
3	B	486	HEM	FE-NB	2.43	2.06	1.97
3	F	486	HEM	CHA-C4D	2.42	1.39	1.35
3	G	485	HEM	CMD-C2D	2.40	1.54	1.47
3	D	485	HEM	CHA-C4D	2.40	1.39	1.35
3	E	486	HEM	CHB-C1B	2.38	1.39	1.35
3	G	485	HEM	C2D-C1D	2.37	1.45	1.44
3	H	485	HEM	CMC-C2C	2.36	1.54	1.47
3	B	486	HEM	CMC-C2C	2.36	1.54	1.47
3	H	485	HEM	CMB-C2B	2.35	1.54	1.47
3	D	485	HEM	CMC-C2C	2.35	1.54	1.47
3	D	485	HEM	CMB-C2B	2.35	1.54	1.47
3	G	485	HEM	FE-ND	2.35	2.06	1.97
3	H	485	HEM	CMD-C2D	2.34	1.54	1.47
3	B	486	HEM	CMD-C2D	2.31	1.54	1.47
3	D	485	HEM	CMD-C2D	2.24	1.54	1.47
3	A	486	HEM	C2D-C1D	-2.24	1.44	1.44
3	C	485	HEM	CMD-C2D	2.21	1.54	1.47
3	G	485	HEM	CHB-C1B	2.21	1.39	1.35
3	E	486	HEM	CHA-C4D	2.20	1.39	1.35
3	C	485	HEM	CHB-C1B	2.19	1.39	1.35
3	A	486	HEM	CMD-C2D	2.15	1.54	1.47
3	B	486	HEM	CMA-C3A	2.09	1.56	1.51
3	B	486	HEM	CHB-C1B	2.09	1.38	1.35
3	C	485	HEM	CAA-C2A	2.08	1.55	1.52
3	H	485	HEM	FE-NB	2.08	2.05	1.97
3	F	486	HEM	CMD-C2D	2.08	1.53	1.47
3	H	485	HEM	CHB-C1B	2.06	1.38	1.35
3	E	486	HEM	C2D-C1D	2.04	1.45	1.44
3	B	486	HEM	CHA-C4D	2.01	1.38	1.35
3	A	486	HEM	CHA-C4D	2.00	1.38	1.35

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	485	HEM	C3B-C4B-NB	-8.68	107.79	114.00
3	B	486	HEM	C3B-C4B-NB	-8.47	107.94	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	485	HEM	C3B-C4B-NB	-8.41	107.98	114.00
3	E	486	HEM	C3B-C4B-NB	-8.25	108.10	114.00
3	H	485	HEM	C3B-C4B-NB	-7.96	108.31	114.00
3	F	486	HEM	C3B-C4B-NB	-7.85	108.38	114.00
3	C	485	HEM	C3B-C4B-NB	-7.83	108.40	114.00
3	A	486	HEM	C3B-C4B-NB	-7.62	108.55	114.00
3	A	486	HEM	C4D-ND-C1D	7.31	112.64	105.16
3	G	485	HEM	C4D-ND-C1D	6.92	112.25	105.16
3	C	485	HEM	C4D-ND-C1D	6.86	112.18	105.16
3	B	486	HEM	C4D-ND-C1D	6.79	112.11	105.16
3	F	486	HEM	C4D-ND-C1D	6.69	112.01	105.16
3	E	486	HEM	C4D-ND-C1D	6.67	111.99	105.16
3	D	485	HEM	C4D-ND-C1D	6.49	111.80	105.16
3	H	485	HEM	C4D-ND-C1D	6.18	111.48	105.16
3	H	485	HEM	CBA-CAA-C2A	-5.99	102.13	112.69
3	G	485	HEM	CBA-CAA-C2A	-5.90	102.30	112.69
3	B	486	HEM	CBA-CAA-C2A	-5.78	102.52	112.69
3	A	486	HEM	CBA-CAA-C2A	-5.35	103.27	112.69
3	E	486	HEM	CBA-CAA-C2A	-5.34	103.28	112.69
3	D	485	HEM	CBA-CAA-C2A	-5.12	103.67	112.69
3	C	485	HEM	CBA-CAA-C2A	-5.08	103.74	112.69
3	F	486	HEM	CBA-CAA-C2A	-4.72	104.38	112.69
3	F	486	HEM	C2D-C1D-ND	-4.01	108.20	112.93
3	B	486	HEM	C2D-C1D-ND	-3.99	108.21	112.93
3	H	485	HEM	C2D-C1D-ND	-3.94	108.27	112.93
3	A	486	HEM	C2D-C1D-ND	-3.93	108.29	112.93
3	G	485	HEM	C2D-C1D-ND	-3.86	108.37	112.93
3	D	485	HEM	C2D-C1D-ND	-3.80	108.45	112.93
3	C	485	HEM	C2D-C1D-ND	-3.56	108.72	112.93
3	G	485	HEM	C1B-NB-C4B	3.40	108.64	105.16
3	E	486	HEM	C2D-C1D-ND	-3.34	108.99	112.93
3	D	485	HEM	C4C-NC-C1C	3.25	108.92	105.53
3	D	485	HEM	C1B-NB-C4B	3.24	108.47	105.16
3	F	486	HEM	CMA-C3A-C4A	-3.11	123.84	128.62
3	H	485	HEM	C1B-NB-C4B	3.04	108.28	105.16
3	F	486	HEM	C4C-NC-C1C	3.04	108.69	105.53
3	A	486	HEM	CBD-CAD-C3D	-2.96	107.92	114.37
3	E	486	HEM	C1B-NB-C4B	2.93	108.16	105.16
3	B	486	HEM	C1B-NB-C4B	2.86	108.09	105.16
3	C	485	HEM	CMA-C3A-C4A	-2.85	124.23	128.62
3	H	485	HEM	CBD-CAD-C3D	-2.84	108.18	114.37
3	H	485	HEM	CMA-C3A-C4A	-2.83	124.27	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	485	HEM	C4C-NC-C1C	2.82	108.47	105.53
3	C	485	HEM	C1B-NB-C4B	2.74	107.96	105.16
3	F	486	HEM	CAD-CBD-CGD	-2.73	104.98	113.48
3	A	486	HEM	CMA-C3A-C4A	-2.69	124.48	128.62
3	G	485	HEM	C3A-C4A-NA	-2.69	107.38	109.41
3	B	486	HEM	C4C-NC-C1C	2.63	108.27	105.53
3	G	485	HEM	CBD-CAD-C3D	-2.60	108.70	114.37
3	E	486	HEM	CAD-CBD-CGD	-2.55	105.53	113.48
3	C	485	HEM	CAD-CBD-CGD	-2.54	105.57	113.48
3	H	485	HEM	CAD-CBD-CGD	-2.53	105.59	113.48
3	A	486	HEM	C1B-NB-C4B	2.49	107.71	105.16
3	F	486	HEM	C1B-NB-C4B	2.40	107.62	105.16
3	G	485	HEM	CHD-C4C-NC	2.39	126.81	124.73
3	G	485	HEM	CMA-C3A-C4A	-2.31	125.07	128.62
3	D	485	HEM	C3A-C4A-NA	-2.23	107.72	109.41
3	G	485	HEM	CAD-C3D-C4D	2.21	128.50	124.53
3	C	485	HEM	CBD-CAD-C3D	-2.19	109.59	114.37
3	B	486	HEM	CHC-C4B-NB	2.18	126.40	124.58
3	A	486	HEM	O1A-CGA-CBA	-2.17	115.56	123.03
3	E	486	HEM	C3A-C4A-NA	-2.16	107.78	109.41
3	H	485	HEM	CHA-C4D-ND	2.14	127.25	124.31
3	G	485	HEM	C4C-NC-C1C	2.14	107.76	105.53
3	E	486	HEM	CBD-CAD-C3D	-2.13	109.73	114.37
3	C	485	HEM	C4C-NC-C1C	2.11	107.73	105.53
3	H	485	HEM	C3A-C4A-NA	-2.10	107.82	109.41
3	C	485	HEM	CAD-C3D-C4D	2.09	128.29	124.53
3	A	486	HEM	CAD-CBD-CGD	-2.09	106.96	113.48
3	B	486	HEM	CBD-CAD-C3D	-2.09	109.81	114.37
3	G	485	HEM	CHD-C1D-ND	2.08	126.31	124.58
3	F	486	HEM	CMA-C3A-C2A	2.07	128.85	124.94
3	C	485	HEM	CHD-C4C-NC	2.06	126.53	124.73
3	D	485	HEM	CHD-C1D-ND	2.06	126.30	124.58
3	A	486	HEM	C3A-C4A-NA	-2.05	107.87	109.41
3	D	485	HEM	CAD-CBD-CGD	-2.04	107.12	113.48
3	H	485	HEM	CHD-C1D-ND	2.04	126.28	124.58
3	D	485	HEM	CBD-CAD-C3D	-2.01	109.99	114.37
3	C	485	HEM	C4A-CHB-C1B	-2.01	124.83	127.47
3	A	486	HEM	C4C-NC-C1C	2.01	107.62	105.53

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(Å <sup>2</sup> )	Q<0.9
1	A	482/483 (99%)	-0.54	2 (0%) 90 92	5, 10, 20, 29	0
1	B	482/483 (99%)	-0.50	1 (0%) 93 94	5, 11, 19, 30	1 (0%)
1	C	482/483 (99%)	-0.57	3 (0%) 86 89	4, 9, 20, 32	1 (0%)
1	D	482/483 (99%)	-0.48	1 (0%) 93 94	4, 11, 21, 28	3 (0%)
1	E	482/483 (99%)	-0.40	6 (1%) 75 78	5, 13, 26, 36	2 (0%)
1	F	482/483 (99%)	-0.36	3 (0%) 86 89	8, 14, 24, 32	3 (0%)
1	G	482/483 (99%)	-0.45	4 (0%) 83 85	6, 11, 24, 31	2 (0%)
1	H	482/483 (99%)	-0.44	2 (0%) 90 92	6, 12, 22, 32	3 (0%)
All	All	3856/3864 (99%)	-0.47	22 (0%) 86 89	4, 11, 22, 36	15 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	SER	5.5
1	G	360	PRO	3.3
1	F	428	LEU	2.9
1	H	285	LYS	2.7
1	E	269	ALA	2.7
1	H	428	LEU	2.6
1	E	428	LEU	2.6
1	E	478	ASP	2.6
1	E	432	GLU	2.5
1	A	285	LYS	2.4
1	B	269	ALA	2.3
1	C	360	PRO	2.3
1	C	483	ASN	2.2
1	G	285	LYS	2.3
1	D	484	SER	2.2
1	F	432	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	428	LEU	2.1
1	F	3	SER	2.1
1	E	285	LYS	2.1
1	C	447	GLY	2.1
1	E	484	SER	2.0
1	A	3	SER	2.0

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

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
1	OMT	F	53	10/11	0.07	0.72	10,11,18,20	0
1	OMT	C	53	10/11	0.06	-0.21	6,7,14,14	0
1	OMT	A	53	10/11	0.06	-0.30	5,6,12,12	0
1	OMT	G	53	10/11	0.07	-0.32	8,9,13,15	0
1	OMT	B	53	10/11	0.06	-0.55	6,7,16,17	0
1	OMT	H	53	10/11	0.05	-1.15	8,8,12,12	0
1	OMT	D	53	10/11	0.06	-1.36	6,6,12,13	0
1	OMT	E	53	10/11	0.05	-1.76	8,8,16,18	0

## 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	GOL	E	5493	6/6	0.14	14.43	18,21,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	G	5491	6/6	0.14	7.39	15,20,21,22	0
4	GOL	A	5489	6/6	0.12	6.86	10,17,18,18	0
4	GOL	H	5492	6/6	0.11	6.74	18,21,22,25	0
4	GOL	C	5487	6/6	0.10	5.11	7,11,12,13	0
4	GOL	B	5490	6/6	0.10	3.95	13,17,17,20	0
4	GOL	D	5488	6/6	0.10	3.75	12,16,17,18	0
4	GOL	F	5494	6/6	0.08	0.99	12,16,17,18	0
3	HEM	F	486	43/43	0.07	0.82	8,11,13,13	0
3	HEM	A	486	43/43	0.07	0.38	5,7,9,10	0
3	HEM	G	485	43/43	0.07	0.24	7,10,12,14	0
3	HEM	H	485	43/43	0.07	0.21	6,10,12,13	0
3	HEM	E	486	43/43	0.07	0.18	8,10,12,13	0
3	HEM	C	485	43/43	0.06	0.03	4,7,9,10	0
3	HEM	B	486	43/43	0.07	-0.18	6,7,8,10	0
3	HEM	D	485	43/43	0.07	-0.46	3,10,11,12	0
2	CL	H	7485	1/1	0.04	-2.36	17,17,17,17	0
2	CL	F	8485	1/1	0.04	-4.57	16,16,16,16	0
2	CL	D	5485	1/1	0.03	-4.94	14,14,14,14	0
2	CL	B	6485	1/1	0.03	-6.28	13,13,13,13	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.