



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:55 PM GMT

PDB ID : 4DUF  
Title : cytochrome P450 BM3h-2G9 MRI sensor bound to serotonin  
Authors : Brustad, E.M.; Lelyveld, V.S.; Snow, C.D.; Crook, N.; Martinez, F.M.; Scholl, T.J.; Jasanoff, A.; Arnold, F.H.  
Deposited on : 2012-02-21  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

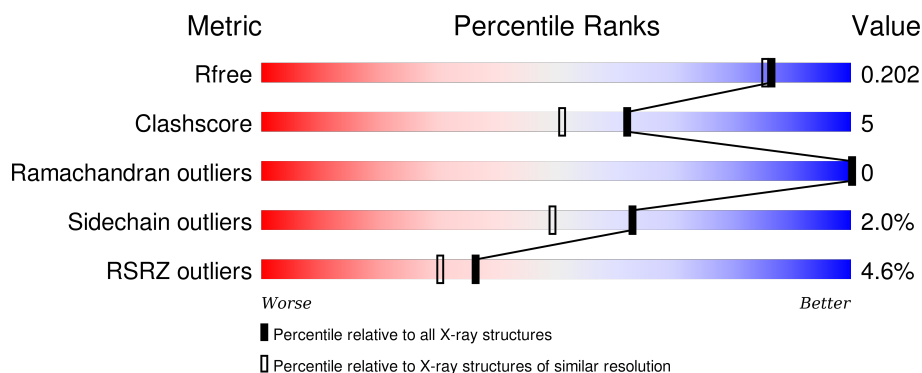
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	B	471	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	C	471	<div> <div>7%</div> <div>81%</div> <div>13%</div> <div>••</div> </div>
1	D	471	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SRO	A	501	-	-	X	X
3	SRO	B	501	-	-	X	X
3	SRO	C	501	-	-	-	X
3	SRO	D	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16229 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cytochrome P450 BM3 variant 2G9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	9	0
			3733	2380	633	700	20			
1	B	456	Total	C	N	O	S	0	10	0
			3737	2383	636	698	20			
1	C	456	Total	C	N	O	S	0	9	0
			3732	2379	632	701	20			
1	D	456	Total	C	N	O	S	0	6	0
			3704	2363	627	694	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	CYS	ARG	ENGINEERED MUTATION	UNP P14779
A	87	LEU	PHE	ENGINEERED MUTATION	UNP P14779
A	268	SER	THR	ENGINEERED MUTATION	UNP P14779
A	438	LEU	THR	ENGINEERED MUTATION	UNP P14779
A	464	LEU	-	EXPRESSION TAG	UNP P14779
A	465	GLU	-	EXPRESSION TAG	UNP P14779
A	466	HIS	-	EXPRESSION TAG	UNP P14779
A	467	HIS	-	EXPRESSION TAG	UNP P14779
A	468	HIS	-	EXPRESSION TAG	UNP P14779
A	469	HIS	-	EXPRESSION TAG	UNP P14779
A	470	HIS	-	EXPRESSION TAG	UNP P14779
A	471	HIS	-	EXPRESSION TAG	UNP P14779
B	50	CYS	ARG	ENGINEERED MUTATION	UNP P14779
B	87	LEU	PHE	ENGINEERED MUTATION	UNP P14779
B	268	SER	THR	ENGINEERED MUTATION	UNP P14779
B	438	LEU	THR	ENGINEERED MUTATION	UNP P14779
B	464	LEU	-	EXPRESSION TAG	UNP P14779
B	465	GLU	-	EXPRESSION TAG	UNP P14779
B	466	HIS	-	EXPRESSION TAG	UNP P14779
B	467	HIS	-	EXPRESSION TAG	UNP P14779
B	468	HIS	-	EXPRESSION TAG	UNP P14779

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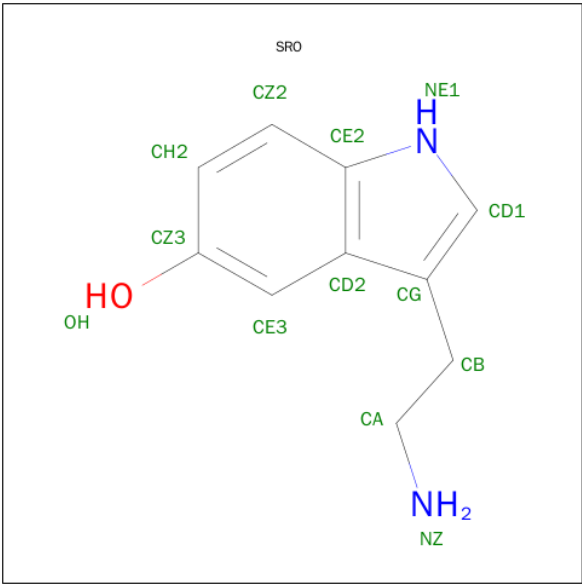
Chain	Residue	Modelled	Actual	Comment	Reference
B	469	HIS	-	EXPRESSION TAG	UNP P14779
B	470	HIS	-	EXPRESSION TAG	UNP P14779
B	471	HIS	-	EXPRESSION TAG	UNP P14779
C	50	CYS	ARG	ENGINEERED MUTATION	UNP P14779
C	87	LEU	PHE	ENGINEERED MUTATION	UNP P14779
C	268	SER	THR	ENGINEERED MUTATION	UNP P14779
C	438	LEU	THR	ENGINEERED MUTATION	UNP P14779
C	464	LEU	-	EXPRESSION TAG	UNP P14779
C	465	GLU	-	EXPRESSION TAG	UNP P14779
C	466	HIS	-	EXPRESSION TAG	UNP P14779
C	467	HIS	-	EXPRESSION TAG	UNP P14779
C	468	HIS	-	EXPRESSION TAG	UNP P14779
C	469	HIS	-	EXPRESSION TAG	UNP P14779
C	470	HIS	-	EXPRESSION TAG	UNP P14779
C	471	HIS	-	EXPRESSION TAG	UNP P14779
D	50	CYS	ARG	ENGINEERED MUTATION	UNP P14779
D	87	LEU	PHE	ENGINEERED MUTATION	UNP P14779
D	268	SER	THR	ENGINEERED MUTATION	UNP P14779
D	438	LEU	THR	ENGINEERED MUTATION	UNP P14779
D	464	LEU	-	EXPRESSION TAG	UNP P14779
D	465	GLU	-	EXPRESSION TAG	UNP P14779
D	466	HIS	-	EXPRESSION TAG	UNP P14779
D	467	HIS	-	EXPRESSION TAG	UNP P14779
D	468	HIS	-	EXPRESSION TAG	UNP P14779
D	469	HIS	-	EXPRESSION TAG	UNP P14779
D	470	HIS	-	EXPRESSION TAG	UNP P14779
D	471	HIS	-	EXPRESSION TAG	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 3 is SEROTONIN (three-letter code: SRO) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	10	2	1		
3	B	1	Total	C	N	O	0	0
			13	10	2	1		
3	C	1	Total	C	N	O	0	0
			13	10	2	1		
3	D	1	Total	C	N	O	0	0
			13	10	2	1		

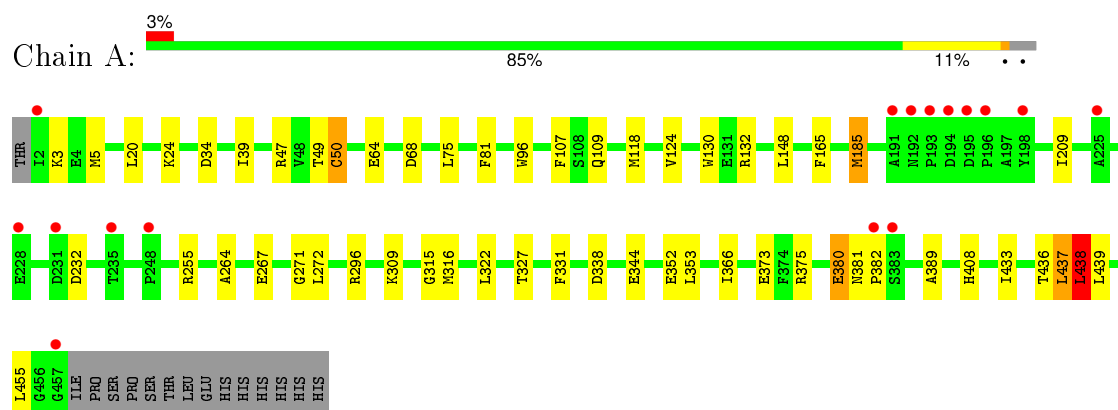
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	312	Total	O	0	0
			312	312		
4	C	242	Total	O	0	0
			242	242		
4	D	235	Total	O	0	0
			235	235		

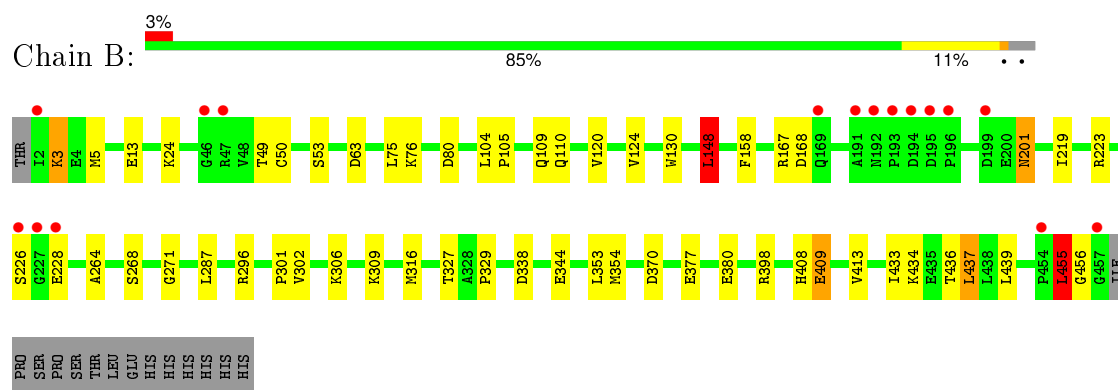
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

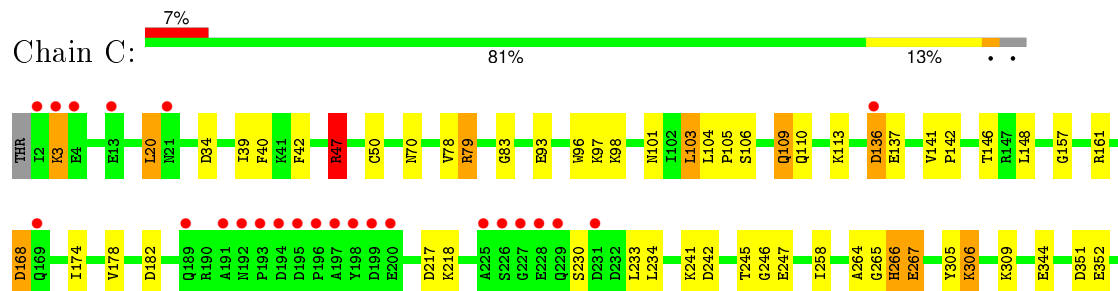
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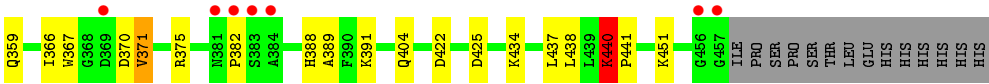
- Molecule 1: cytochrome P450 BM3 variant 2G9



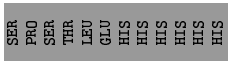
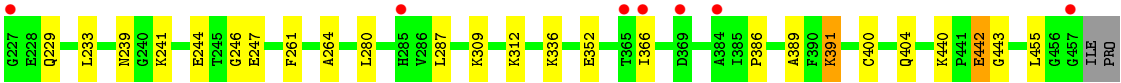
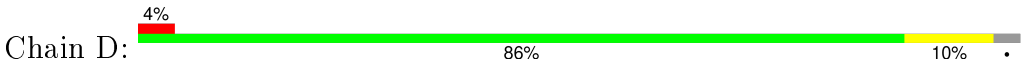
- Molecule 1: cytochrome P450 BM3 variant 2G9







● Molecule 1: cytochrome P450 BM3 variant 2G9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.69Å 150.49Å 87.71Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	29.44 – 1.80 29.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.44-1.80) 98.0 (29.44-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.163 , 0.203 0.163 , 0.202	Depositor DCC
$R_{free}$ test set	9607 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.0	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 186773 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 37.96 % 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 3.9608e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.20	9/3823 (0.2%)	1.03	13/5167 (0.3%)
1	B	1.22	4/3833 (0.1%)	1.02	11/5180 (0.2%)
1	C	1.22	7/3822 (0.2%)	1.03	12/5165 (0.2%)
1	D	1.18	4/3791 (0.1%)	1.00	7/5125 (0.1%)
All	All	1.21	24/15269 (0.2%)	1.02	43/20637 (0.2%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	GLU	CB-CG	-10.33	1.32	1.52
1	A	331	PHE	CE1-CZ	8.38	1.53	1.37
1	B	53	SER	CB-OG	-6.61	1.33	1.42
1	A	64	GLU	CD-OE2	-6.27	1.18	1.25
1	C	96	TRP	CE3-CZ3	6.22	1.49	1.38
1	C	93	GLU	CB-CG	-6.14	1.40	1.52
1	D	246	GLY	N-CA	5.68	1.54	1.46
1	B	13	GLU	CG-CD	5.58	1.60	1.51
1	A	165	PHE	CG-CD1	5.47	1.47	1.38
1	C	78	VAL	CB-CG1	5.46	1.64	1.52
1	D	352	GLU	CD-OE2	-5.41	1.19	1.25
1	C	441	PRO	C-O	5.34	1.33	1.23
1	C	40	PHE	CE2-CZ	5.30	1.47	1.37
1	A	130	TRP	CB-CG	5.24	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	440	LYS	CE-NZ	5.23	1.62	1.49
1	A	380	GLU	CB-CG	5.22	1.62	1.52
1	C	47	ARG	CG-CD	5.20	1.65	1.51
1	B	130	TRP	CE3-CZ3	5.15	1.47	1.38
1	D	216	VAL	CB-CG1	5.14	1.63	1.52
1	A	107	PHE	CD2-CE2	5.12	1.49	1.39
1	A	315	GLY	N-CA	5.09	1.53	1.46
1	D	261	PHE	CB-CG	-5.07	1.42	1.51
1	A	50[A]	CYS	CB-SG	-5.01	1.73	1.81
1	A	50[B]	CYS	CB-SG	-5.01	1.73	1.81

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	LEU	CB-CG-CD2	11.63	130.76	111.00
1	A	255	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	168	ASP	CB-CG-OD1	7.62	125.16	118.30
1	C	161	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	296	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	255	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	370	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	398	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	436	THR	N-CA-C	-6.32	93.94	111.00
1	D	68	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	C	79	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	437	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	C	161	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	103	LEU	CB-CG-CD2	-5.74	101.25	111.00
1	C	437	LEU	CB-CG-CD2	5.73	120.73	111.00
1	D	56	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	437	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	351	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	96	TRP	CA-CB-CG	-5.51	103.23	113.70
1	D	391	LYS	CD-CE-NZ	5.50	124.34	111.70
1	A	232	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	76	LYS	CD-CE-NZ	-5.40	99.29	111.70
1	B	455	LEU	CA-CB-CG	5.35	127.60	115.30
1	D	96	TRP	CA-CB-CG	-5.34	103.55	113.70
1	A	132	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	148	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	B	63	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	223	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	LEU	CB-CG-CD1	5.22	119.87	111.00
1	C	182	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	217	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	68	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	316	MET	CG-SD-CE	-5.17	91.93	100.20
1	D	68	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	34	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	68	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	84	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	96	TRP	CA-CB-CG	-5.12	103.97	113.70
1	B	338	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	223	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	436	THR	N-CA-C	-5.06	97.33	111.00
1	C	242	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	425	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	136	ASP	Peptide

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3733	0	3696	35	0
1	B	3737	0	3709	40	0
1	C	3732	0	3692	54	0
1	D	3704	0	3665	26	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	3	0
3	A	13	0	11	7	0
3	B	13	0	10	6	0
3	C	13	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	13	0	11	1	0
4	A	310	0	0	3	0
4	B	312	0	0	6	2
4	C	242	0	0	7	2
4	D	235	0	0	2	0
All	All	16229	0	14925	162	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267[A]:GLU:HG2	1:C:438:LEU:HD12	1.41	1.02
1:C:110:GLN:HE22	1:C:113:LYS:NZ	1.60	0.98
1:C:146:THR:HG23	1:C:266:HIS:CE1	2.05	0.92
1:C:146:THR:HG23	1:C:266:HIS:HE1	1.34	0.90
1:C:110:GLN:HE22	1:C:113:LYS:HZ2	0.95	0.89
1:C:39:ILE:HD11	1:C:50[B]:CYS:SG	2.13	0.88
1:D:229:GLN:HE22	1:D:239:ASN:HD21	1.20	0.87
1:A:373:GLU:OE1	1:A:375[B]:ARG:NH1	2.07	0.87
1:C:306:LYS:HD2	4:C:680:HOH:O	1.76	0.83
1:C:267[A]:GLU:CG	1:C:438:LEU:HD12	2.12	0.78
1:A:267:GLU:HB3	1:A:438:LEU:HD13	1.67	0.77
1:D:309:LYS:O	1:D:312:LYS:HE3	1.85	0.77
1:A:24:LYS:HE3	4:C:808:HOH:O	1.85	0.77
1:A:185:MET:HG3	1:A:437:LEU:HD23	1.66	0.76
1:C:20:LEU:HD22	1:C:42:PHE:CZ	2.24	0.73
1:C:110:GLN:NE2	1:C:113:LYS:HZ2	1.79	0.72
1:C:110:GLN:NE2	1:C:113:LYS:NZ	2.35	0.71
1:C:267[B]:GLU:HB3	1:C:438:LEU:HD12	1.72	0.71
1:B:201:ASN:H	1:B:201:ASN:HD22	1.39	0.71
1:C:440:LYS:N	1:C:440:LYS:HD2	2.07	0.69
1:B:49:THR:HG21	1:B:354:MET:HG2	1.76	0.68
1:B:296[B]:ARG:NH2	4:B:823:HOH:O	2.09	0.65
1:C:109:GLN:NE2	1:C:305:TYR:OH	2.25	0.65
1:D:80:ASP:OD2	4:D:795:HOH:O	2.14	0.65
1:A:338:ASP:OD2	4:A:902:HOH:O	2.15	0.65
1:A:50[A]:CYS:HB3	1:A:353:LEU:HD23	1.78	0.65
1:D:98:LYS:HE3	1:D:247:GLU:HG3	1.80	0.63
1:C:245:THR:OG1	1:C:247:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ILE:HD12	1:D:386:PRO:HG2	1.81	0.61
1:C:106:SER:HB3	1:C:233:LEU:HD23	1.80	0.61
1:A:271:GLY:HA3	1:A:327[A]:THR:HG21	1.82	0.61
1:C:39:ILE:CD1	1:C:50[B]:CYS:SG	2.89	0.61
1:D:109:GLN:HB2	1:D:404[B]:GLN:NE2	2.17	0.60
1:C:109:GLN:HE22	1:C:309:LYS:HE3	1.67	0.60
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.83	0.59
1:B:158:PHE:CE1	1:B:219:ILE:HD13	2.38	0.58
1:B:49:THR:CG2	1:B:354:MET:HG2	2.35	0.57
1:C:109:GLN:NE2	1:C:309:LYS:HE3	2.18	0.57
1:B:24:LYS:HE2	1:B:433:ILE:O	2.03	0.57
1:C:267[B]:GLU:HB2	4:C:810:HOH:O	2.04	0.57
1:D:109:GLN:HB2	1:D:404[B]:GLN:HE22	1.70	0.57
1:B:434:LYS:HE3	4:B:903:HOH:O	2.04	0.57
1:C:146:THR:CG2	1:C:266:HIS:HE1	2.13	0.57
1:A:375[B]:ARG:HB2	1:A:375[B]:ARG:CZ	2.36	0.56
1:C:34[A]:ASP:OD1	1:C:359:GLN:NE2	2.38	0.56
1:B:158:PHE:HD1	1:B:219:ILE:HG21	1.70	0.56
1:B:201:ASN:ND2	1:B:201:ASN:H	2.03	0.55
1:A:109:GLN:HE22	1:A:309:LYS:NZ	2.05	0.54
1:A:109:GLN:HE22	1:A:309:LYS:HZ2	1.55	0.54
1:C:104:LEU:HB3	1:C:105:PRO:HD3	1.90	0.54
1:D:264:ALA:HB1	3:D:501:SRO:HNZ1	1.73	0.53
1:D:366:ILE:HG21	1:D:389:ALA:HB1	1.90	0.53
1:C:97:LYS:NZ	1:C:101:ASN:HD21	2.06	0.53
1:D:62:CYS:SG	1:D:391:LYS:HE2	2.49	0.53
1:B:264:ALA:O	3:B:501:SRO:HB2	2.09	0.53
2:C:500:HEM:CMC	2:C:500:HEM:HBC2	2.39	0.52
1:A:438:LEU:HD21	3:A:501:SRO:HB1	1.91	0.52
1:B:109:GLN:HE22	1:B:309:LYS:HZ2	1.58	0.52
1:B:301:PRO:HB2	1:B:456:GLY:HA3	1.91	0.52
1:B:24:LYS:HE3	4:D:698:HOH:O	2.09	0.52
1:C:267[A]:GLU:HG2	1:C:438:LEU:CD1	2.29	0.51
1:A:437:LEU:HD12	3:A:501:SRO:HH2	1.91	0.51
1:D:97:LYS:NZ	1:D:244:GLU:HG2	2.24	0.51
1:B:377:GLU:O	1:B:380:GLU:HG2	2.11	0.51
1:A:49:THR:HB	1:A:352[B]:GLU:OE1	2.12	0.50
1:B:3:LYS:HG3	1:B:344:GLU:HB3	1.94	0.50
1:C:404[B]:GLN:OE1	4:C:614:HOH:O	2.19	0.50
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.93	0.50
1:B:168:ASP:O	4:B:858:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:500:HEM:HMC2	2:C:500:HEM:HBC2	1.94	0.49
1:C:98:LYS:HE3	1:C:247:GLU:HG3	1.95	0.49
1:B:226:SER:OG	1:B:228:GLU:HB2	2.13	0.49
1:C:157:GLY:HA2	1:C:233:LEU:HD12	1.95	0.49
1:A:118[A]:MET:HG3	4:A:627:HOH:O	2.12	0.48
1:C:382:PRO:HG3	4:C:821:HOH:O	2.13	0.48
1:C:98:LYS:NZ	1:C:247:GLU:HG3	2.29	0.48
1:B:437:LEU:HD12	3:B:501:SRO:HH2	1.94	0.48
1:D:43:GLU:HG2	1:D:48:VAL:HG22	1.96	0.48
1:B:109:GLN:HE22	1:B:309:LYS:NZ	2.11	0.48
1:B:268:SER:HB3	3:B:501:SRO:HB1	1.95	0.48
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.94	0.48
1:A:5:MET:SD	1:A:50[B]:CYS:SG	3.02	0.48
1:B:309:LYS:NZ	1:B:408:HIS:ND1	2.62	0.48
1:B:49:THR:HG21	1:B:354:MET:CG	2.44	0.47
1:B:110:GLN:HG3	4:B:638:HOH:O	2.14	0.47
1:A:124:VAL:HG13	1:A:455:LEU:HD13	1.96	0.47
3:A:501:SRO:HD1	3:A:501:SRO:HA1	1.10	0.47
1:D:280:LEU:HB3	1:D:287:LEU:HD13	1.97	0.47
1:B:80:ASP:OD2	4:B:665:HOH:O	2.20	0.47
1:C:79:ARG:HG3	1:C:83:GLY:O	2.15	0.47
1:A:24:LYS:HE2	1:A:433:ILE:O	2.14	0.47
1:C:375[B]:ARG:HB2	1:C:375[B]:ARG:CZ	2.45	0.47
1:D:192:ASN:HB3	1:D:195[A]:ASP:CG	2.36	0.46
1:C:174:ILE:O	1:C:178:VAL:HG23	2.15	0.46
1:B:50[A]:CYS:HB3	1:B:353:LEU:HD23	1.97	0.46
1:D:192:ASN:CB	1:D:195[A]:ASP:OD2	2.63	0.46
1:A:316:MET:HE1	1:A:380:GLU:HG3	1.98	0.46
1:D:106:SER:HB3	1:D:233:LEU:HD23	1.98	0.46
1:B:120:VAL:HG11	1:B:302:VAL:CG1	2.46	0.46
1:B:5:MET:SD	1:B:50[B]:CYS:SG	2.95	0.46
1:B:75:LEU:HD21	3:B:501:SRO:HZ2	1.96	0.46
1:C:264:ALA:HA	3:C:501:SRO:HB2	1.97	0.46
2:D:500:HEM:HBC2	2:D:500:HEM:HMC2	1.97	0.46
1:C:47:ARG:HA	1:C:47:ARG:HD3	1.83	0.45
1:A:39:ILE:HD11	1:A:50[A]:CYS:SG	2.56	0.45
1:C:404[A]:GLN:HG3	4:C:804:HOH:O	2.16	0.45
1:D:442:GLU:HG3	1:D:443:GLY:N	2.32	0.45
1:A:437:LEU:CD1	3:A:501:SRO:HH2	2.47	0.45
1:D:229:GLN:HE22	1:D:239:ASN:ND2	2.00	0.45
1:C:98:LYS:CE	1:C:247:GLU:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:HG13	1:B:455:LEU:CD1	2.47	0.45
1:C:70:ASN:ND2	1:C:352[A]:GLU:HG3	2.32	0.45
1:A:47:ARG:HD3	4:A:800:HOH:O	2.17	0.44
1:D:5:MET:SD	1:D:50[B]:CYS:SG	2.94	0.44
1:A:264:ALA:O	3:A:501:SRO:HB2	2.17	0.44
1:B:124:VAL:HG13	1:B:455:LEU:HD11	1.99	0.44
1:C:106:SER:HB3	1:C:233:LEU:CD2	2.44	0.44
3:B:501:SRO:HA1	3:B:501:SRO:HD1	1.02	0.44
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.99	0.44
1:D:400:CYS:HA	2:D:500:HEM:CHA	2.48	0.44
1:D:135:ALA:O	1:D:136:ASP:HB2	2.17	0.44
1:A:309:LYS:NZ	1:A:408:HIS:ND1	2.65	0.44
1:C:366:ILE:HG21	1:C:389:ALA:HB1	1.99	0.44
1:B:271:GLY:HA3	1:B:327[A]:THR:HG21	2.00	0.44
1:A:109:GLN:NE2	1:A:309:LYS:HZ2	2.15	0.43
1:C:137:GLU:OE1	4:C:833:HOH:O	2.21	0.43
1:D:192:ASN:HB2	1:D:195[A]:ASP:OD2	2.18	0.43
1:C:367:TRP:HB2	1:C:371:VAL:CG1	2.47	0.43
1:C:3:LYS:HG3	1:C:344:GLU:HB3	2.01	0.43
1:A:185:MET:CG	1:A:437:LEU:HD23	2.42	0.43
1:A:327[B]:THR:HG23	1:A:439:LEU:O	2.18	0.43
1:B:327[A]:THR:O	1:B:329:PRO:HD3	2.19	0.43
1:B:158:PHE:HE1	1:B:219:ILE:HD13	1.80	0.43
1:A:3:LYS:HG3	1:A:344:GLU:HB3	2.00	0.43
1:B:109:GLN:NE2	1:B:309:LYS:HZ2	2.17	0.42
1:C:370:ASP:OD2	1:C:375[B]:ARG:NH2	2.52	0.42
1:C:141:VAL:HB	1:C:142:PRO:HD3	2.01	0.42
1:A:185:MET:HB2	1:A:437:LEU:CD2	2.49	0.42
1:C:234:LEU:HD13	1:C:258:ILE:HD11	2.02	0.42
1:D:404[A]:GLN:H	1:D:404[A]:GLN:NE2	2.17	0.42
1:A:381:ASN:HA	1:A:382:PRO:HD3	1.74	0.42
1:D:118[A]:MET:HE3	1:D:118[A]:MET:HB2	1.93	0.42
1:C:39:ILE:CG1	1:C:50[B]:CYS:SG	3.08	0.42
2:A:500:HEM:C1B	3:A:501:SRO:HA2	2.55	0.42
1:B:264:ALA:HB1	3:B:501:SRO:HNZ1	1.83	0.42
2:C:500:HEM:CMB	2:C:500:HEM:HBB2	2.50	0.42
1:C:388:HIS:HA	1:C:391:LYS:HD3	2.01	0.42
1:C:434:LYS:HB3	1:C:440:LYS:HD3	2.01	0.42
1:A:75:LEU:HD21	3:A:501:SRO:HZ2	2.01	0.41
1:B:327[B]:THR:HG23	1:B:439:LEU:O	2.20	0.41
1:C:103:LEU:HD23	1:C:103:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD21	1:B:413:VAL:HG21	2.03	0.41
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.83	0.41
1:C:422:ASP:OD1	1:C:451:LYS:NZ	2.40	0.41
1:D:400:CYS:HA	2:D:500:HEM:C4D	2.56	0.41
1:C:265:GLY:HA2	2:C:500:HEM:C2C	2.57	0.40
1:B:306:LYS:HG3	4:B:734:HOH:O	2.21	0.40
1:C:174:ILE:N	1:C:174:ILE:HD12	2.37	0.40
1:C:241:LYS:HD3	1:C:246:GLY:O	2.22	0.40
1:B:104:LEU:HB3	1:B:105:PRO:HD3	2.04	0.40
1:A:352[B]:GLU:HG2	1:A:353:LEU:N	2.36	0.40
1:D:336:LYS:HE3	1:D:336:LYS:HB3	1.90	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:618:HOH:O	4:C:807:HOH:O[2_547]	1.15	1.05
4:B:661:HOH:O	4:C:807:HOH:O[2_547]	2.01	0.19

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/471 (98%)	451 (97%)	12 (3%)	0	100	100
1	B	464/471 (98%)	452 (97%)	12 (3%)	0	100	100
1	C	463/471 (98%)	452 (98%)	11 (2%)	0	100	100
1	D	460/471 (98%)	445 (97%)	15 (3%)	0	100	100
All	All	1850/1884 (98%)	1800 (97%)	50 (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	407/413 (98%)	404 (99%)	3 (1%)	88	86
1	B	408/413 (99%)	401 (98%)	7 (2%)	68	57
1	C	407/413 (98%)	392 (96%)	15 (4%)	41	23
1	D	403/413 (98%)	395 (98%)	8 (2%)	63	49
All	All	1625/1652 (98%)	1592 (98%)	33 (2%)	63	49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	185	MET
1	A	438	LEU
1	B	3	LYS
1	B	148	LEU
1	B	167	ARG
1	B	201	ASN
1	B	287	LEU
1	B	409	GLU
1	B	455	LEU
1	C	3	LYS
1	C	20	LEU
1	C	47	ARG
1	C	109	GLN
1	C	136	ASP
1	C	148	LEU
1	C	168	ASP
1	C	218	LYS
1	C	230	SER
1	C	266	HIS
1	C	267[A]	GLU
1	C	267[B]	GLU
1	C	306	LYS
1	C	371	VAL

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Mol	Chain	Res	Type
1	C	440	LYS
1	D	148	LEU
1	D	158	PHE
1	D	194	ASP
1	D	224	LYS
1	D	241	LYS
1	D	440	LYS
1	D	442	GLU
1	D	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	201	ASN
1	A	387	GLN
1	B	109	GLN
1	B	201	ASN
1	C	7	GLN
1	C	101	ASN
1	C	109	GLN
1	C	110	GLN
1	C	201	ASN
1	D	109	GLN
1	D	169	GLN
1	D	201	ASN
1	D	229	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 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	HEM	A	500	1,3	30,50,50	2.34	6 (20%)	24,82,82	2.80	12 (50%)
3	SRO	A	501	2	12,14,14	1.51	3 (25%)	11,19,19	5.13	6 (54%)
2	HEM	B	500	1,3	30,50,50	2.28	12 (40%)	24,82,82	2.71	14 (58%)
3	SRO	B	501	2	12,14,14	1.84	1 (8%)	11,19,19	5.87	7 (63%)
2	HEM	C	500	1,3	30,50,50	2.65	10 (33%)	24,82,82	3.00	13 (54%)
3	SRO	C	501	2	12,14,14	1.18	2 (16%)	11,19,19	3.30	6 (54%)
2	HEM	D	500	1,3	30,50,50	2.64	8 (26%)	24,82,82	2.75	11 (45%)
3	SRO	D	501	2	12,14,14	1.38	3 (25%)	11,19,19	6.11	8 (72%)

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	HEM	A	500	1,3	-	0/10/54/54	0/0/8/8
3	SRO	A	501	2	-	0/3/3/3	0/2/2/2
2	HEM	B	500	1,3	-	0/10/54/54	0/0/8/8
3	SRO	B	501	2	-	0/3/3/3	0/2/2/2
2	HEM	C	500	1,3	-	0/10/54/54	0/0/8/8
3	SRO	C	501	2	-	0/3/3/3	0/2/2/2
2	HEM	D	500	1,3	-	0/10/54/54	0/0/8/8
3	SRO	D	501	2	-	0/3/3/3	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C4B	-9.35	1.43	1.51
2	C	500	HEM	C3B-C4B	-8.87	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3B-C4B	-8.80	1.44	1.51
2	D	500	HEM	C3D-C4D	-6.68	1.43	1.51
2	B	500	HEM	C3B-C4B	-5.55	1.46	1.51
2	D	500	HEM	C2C-C1C	-5.23	1.42	1.52
2	C	500	HEM	C2C-C1C	-5.22	1.42	1.52
3	B	501	SRO	CB-CG	-5.14	1.39	1.51
2	B	500	HEM	C3D-C4D	-4.73	1.45	1.51
2	A	500	HEM	C3D-C4D	-4.69	1.45	1.51
2	B	500	HEM	C2C-C1C	-4.50	1.44	1.52
2	C	500	HEM	C3D-C4D	-4.44	1.45	1.51
2	C	500	HEM	C2D-C3D	-3.14	1.45	1.54
2	B	500	HEM	C2D-C1D	-2.97	1.42	1.51
2	D	500	HEM	C2B-C1B	-2.69	1.43	1.51
3	A	501	SRO	CB-CG	-2.64	1.45	1.51
2	B	500	HEM	C2D-C3D	-2.56	1.46	1.54
2	A	500	HEM	C2D-C1D	-2.45	1.43	1.51
2	D	500	HEM	C2D-C3D	-2.38	1.47	1.54
3	D	501	SRO	CB-CG	-2.19	1.46	1.51
2	A	500	HEM	C2B-C1B	-2.09	1.45	1.51
2	B	500	HEM	C2B-C1B	-2.03	1.45	1.51
3	C	501	SRO	CD2-CE2	2.02	1.48	1.42
2	B	500	HEM	CHC-C1C	2.02	1.41	1.36
2	D	500	HEM	CAA-C2A	2.05	1.55	1.52
2	C	500	HEM	CMB-C2B	2.08	1.58	1.53
2	B	500	HEM	CMD-C2D	2.16	1.58	1.53
3	A	501	SRO	CH2-CZ3	2.17	1.43	1.38
2	D	500	HEM	C1C-NC	2.21	1.38	1.36
3	D	501	SRO	CD2-CE2	2.22	1.48	1.42
2	B	500	HEM	CHD-C4C	2.34	1.41	1.36
3	C	501	SRO	CZ2-CH2	2.34	1.41	1.36
2	A	500	HEM	C4C-NC	2.42	1.39	1.36
3	D	501	SRO	CZ2-CH2	2.47	1.41	1.36
2	A	500	HEM	FE-ND	2.58	2.11	1.97
3	A	501	SRO	CZ2-CH2	2.79	1.42	1.36
2	B	500	HEM	FE-ND	2.80	2.12	1.97
2	C	500	HEM	C3C-CAC	2.83	1.56	1.51
2	D	500	HEM	FE-NC	2.99	2.07	1.95
2	C	500	HEM	C1C-NC	3.01	1.39	1.36
2	C	500	HEM	CMA-C3A	3.01	1.57	1.51
2	B	500	HEM	FE-NC	3.02	2.07	1.95
2	C	500	HEM	FE-NC	3.23	2.08	1.95
2	C	500	HEM	CAA-C2A	3.32	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1C-NC	3.84	1.40	1.36

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	SRO	CA-CB-CG	-10.73	85.47	113.02
3	A	501	SRO	CA-CB-CG	-9.88	87.66	113.02
3	B	501	SRO	CZ3-CE3-CD2	-7.51	115.99	120.53
3	D	501	SRO	CZ3-CE3-CD2	-7.44	116.04	120.53
3	D	501	SRO	CA-CB-CG	-5.97	97.69	113.02
2	A	500	HEM	CMA-C3A-C4A	-5.47	119.32	128.36
2	C	500	HEM	C3C-CAC-CBC	-5.31	116.31	124.46
3	A	501	SRO	CZ3-CE3-CD2	-4.95	117.54	120.53
2	D	500	HEM	CMA-C3A-C4A	-4.87	120.31	128.36
2	C	500	HEM	CBD-CAD-C3D	-4.39	100.77	113.55
2	C	500	HEM	C3B-CAB-CBB	-4.36	117.77	124.46
3	D	501	SRO	CZ2-CE2-CD2	-4.00	114.25	121.11
3	B	501	SRO	CZ2-CE2-CD2	-3.78	114.64	121.11
2	C	500	HEM	C3B-C4B-NB	-3.63	104.69	111.63
2	C	500	HEM	CBA-CAA-C2A	-3.61	106.06	112.53
3	C	501	SRO	CZ2-CE2-CD2	-3.60	114.93	121.11
2	D	500	HEM	CBD-CAD-C3D	-3.51	103.33	113.55
2	D	500	HEM	CBA-CAA-C2A	-3.50	106.25	112.53
2	A	500	HEM	C3B-CAB-CBB	-3.38	119.27	124.46
2	A	500	HEM	CBA-CAA-C2A	-3.33	106.56	112.53
2	D	500	HEM	C3B-C4B-NB	-3.33	105.26	111.63
3	A	501	SRO	CZ2-CE2-CD2	-3.32	115.42	121.11
2	A	500	HEM	CBD-CAD-C3D	-3.21	104.22	113.55
3	C	501	SRO	CZ3-CE3-CD2	-3.19	118.60	120.53
2	B	500	HEM	CBA-CAA-C2A	-3.09	106.99	112.53
2	C	500	HEM	CMA-C3A-C4A	-3.07	123.28	128.36
3	B	501	SRO	CB-CG-CD1	-2.91	122.96	127.88
2	B	500	HEM	C3B-C4B-NB	-2.79	106.30	111.63
2	B	500	HEM	C3B-CAB-CBB	-2.71	120.30	124.46
2	B	500	HEM	C1D-CHD-C4C	-2.45	121.72	125.82
2	A	500	HEM	C3B-C4B-NB	-2.33	107.17	111.63
2	B	500	HEM	CMA-C3A-C4A	-2.10	124.89	128.36
3	C	501	SRO	CA-CB-CG	-2.09	107.65	113.02
2	B	500	HEM	CBD-CAD-C3D	-2.04	107.60	113.55
3	D	501	SRO	CH2-CZ2-CE2	-2.01	118.70	120.88
3	A	501	SRO	CZ2-CH2-CZ3	2.02	122.65	120.18
2	C	500	HEM	CHC-C4B-NB	2.04	129.43	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	SRO	CZ2-CH2-CZ3	2.04	122.69	120.18
2	D	500	HEM	CMA-C3A-C2A	2.25	129.95	125.24
2	B	500	HEM	CHC-C4B-NB	2.36	130.20	124.52
2	B	500	HEM	CMD-C2D-C3D	2.40	124.98	114.35
2	A	500	HEM	CMD-C2D-C3D	2.46	125.22	114.35
3	B	501	SRO	CZ2-CE2-NE1	2.51	137.87	130.75
2	A	500	HEM	C2D-C3D-C4D	2.52	105.77	101.50
2	B	500	HEM	CHD-C1D-ND	2.54	130.63	124.52
2	B	500	HEM	C2D-C3D-C4D	2.65	105.99	101.50
2	C	500	HEM	C2D-C3D-C4D	2.68	106.04	101.50
3	D	501	SRO	CZ2-CE2-NE1	2.70	138.39	130.75
2	C	500	HEM	CMD-C2D-C3D	2.71	126.35	114.35
3	C	501	SRO	CZ2-CE2-NE1	2.73	138.47	130.75
3	A	501	SRO	CZ2-CE2-NE1	2.81	138.70	130.75
2	D	500	HEM	CMD-C2D-C3D	3.03	127.76	114.35
2	D	500	HEM	CAD-C3D-C2D	3.10	122.12	113.22
2	A	500	HEM	CMA-C3A-C2A	3.39	132.33	125.24
2	A	500	HEM	CAD-C3D-C2D	3.65	123.70	113.22
2	C	500	HEM	CAD-C3D-C2D	3.90	124.44	113.22
3	D	501	SRO	CZ2-CH2-CZ3	3.95	125.03	120.18
2	D	500	HEM	C2D-C3D-C4D	4.06	108.39	101.50
3	D	501	SRO	CB-CG-CD1	4.13	134.84	127.88
2	B	500	HEM	CAD-C3D-C2D	4.33	125.67	113.22
3	C	501	SRO	CB-CG-CD1	4.40	135.31	127.88
2	C	500	HEM	CMB-C2B-C3B	4.42	127.56	116.53
2	B	500	HEM	CAD-C3D-C4D	4.42	128.07	112.47
2	D	500	HEM	CMB-C2B-C3B	4.43	127.59	116.53
2	A	500	HEM	CMB-C2B-C3B	4.45	127.63	116.53
2	C	500	HEM	CMC-C2C-C3C	4.75	128.40	116.53
2	C	500	HEM	CAD-C3D-C4D	4.78	129.32	112.47
2	D	500	HEM	CAD-C3D-C4D	4.78	129.33	112.47
2	D	500	HEM	CMC-C2C-C3C	4.89	128.73	116.53
2	A	500	HEM	CMC-C2C-C3C	5.12	129.30	116.53
2	A	500	HEM	CAD-C3D-C4D	5.12	130.52	112.47
2	B	500	HEM	CMC-C2C-C3C	5.48	130.22	116.53
2	B	500	HEM	CMB-C2B-C3B	5.97	131.43	116.53
3	C	501	SRO	CE3-CD2-CE2	7.92	123.47	120.34
3	A	501	SRO	CE3-CD2-CE2	11.80	125.01	120.34
3	B	501	SRO	CE3-CD2-CE2	13.18	125.55	120.34
3	D	501	SRO	CE3-CD2-CE2	16.05	126.69	120.34

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	1	0
3	A	501	SRO	7	0
3	B	501	SRO	6	0
2	C	500	HEM	4	0
3	C	501	SRO	1	0
2	D	500	HEM	3	0
3	D	501	SRO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	456/471 (96%)	-0.09	16 (3%)	48 42	10, 19, 42, 58	1 (0%)
1	B	456/471 (96%)	-0.18	16 (3%)	48 42	10, 18, 37, 51	0
1	C	456/471 (96%)	0.14	31 (6%)	20 16	11, 21, 47, 66	0
1	D	456/471 (96%)	0.03	21 (4%)	36 30	11, 20, 44, 58	0
All	All	1824/1884 (96%)	-0.02	84 (4%)	36 30	10, 20, 42, 66	1 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	ALA	6.1
1	C	228	GLU	5.6
1	D	384	ALA	5.3
1	C	456	GLY	5.1
1	D	191	ALA	5.0
1	A	383	SER	4.9
1	D	21	ASN	4.9
1	A	191	ALA	4.9
1	C	227	GLY	4.9
1	C	225	ALA	4.8
1	D	197	ALA	4.5
1	B	196	PRO	4.2
1	A	196	PRO	3.9
1	A	192	ASN	3.8
1	C	2	ILE	3.8
1	C	226	SER	3.6
1	C	196	PRO	3.5
1	B	457	GLY	3.4
1	B	2	ILE	3.4
1	C	199	ASP	3.4
1	C	381	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	384	ALA	3.3
1	A	225	ALA	3.3
1	C	231	ASP	3.3
1	A	198	TYR	3.2
1	A	382	PRO	3.2
1	D	2	ILE	3.1
1	A	231	ASP	3.1
1	C	198	TYR	3.0
1	B	191	ALA	3.0
1	C	195	ASP	3.0
1	C	383	SER	3.0
1	C	136	ASP	3.0
1	A	194	ASP	3.0
1	C	192	ASN	2.9
1	D	192	ASN	2.9
1	B	227	GLY	2.9
1	C	229	GLN	2.8
1	D	189	GLN	2.8
1	D	136	ASP	2.7
1	D	369	ASP	2.7
1	C	194	ASP	2.7
1	C	191	ALA	2.7
1	C	369	ASP	2.7
1	C	457	GLY	2.7
1	D	227	GLY	2.6
1	B	192	ASN	2.6
1	D	13	GLU	2.6
1	B	46	GLY	2.6
1	D	285	HIS	2.6
1	B	193	PRO	2.5
1	C	4	GLU	2.5
1	C	13	GLU	2.5
1	D	199	ASP	2.5
1	D	198	TYR	2.4
1	B	194	ASP	2.4
1	D	195[A]	ASP	2.4
1	C	382	PRO	2.4
1	C	200	GLU	2.3
1	B	228	GLU	2.3
1	B	226	SER	2.3
1	D	457	GLY	2.3
1	C	21	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	365	THR	2.2
1	A	195	ASP	2.2
1	D	3	LYS	2.2
1	A	235	THR	2.2
1	A	248	PRO	2.1
1	C	3	LYS	2.1
1	B	199	ASP	2.1
1	A	2	ILE	2.1
1	A	228	GLU	2.1
1	C	193	PRO	2.1
1	B	195	ASP	2.1
1	A	457	GLY	2.1
1	B	454	PRO	2.1
1	C	189	GLN	2.1
1	D	194	ASP	2.1
1	A	193	PRO	2.0
1	C	169	GLN	2.0
1	B	47	ARG	2.0
1	D	366	ILE	2.0
1	D	4	GLU	2.0
1	B	169	GLN	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SRO	B	501	13/13	0.79	0.21	5.99	13,35,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SRO	A	501	13/13	0.84	0.20	3.61	14,37,41,41	0
3	SRO	C	501	13/13	0.82	0.22	3.50	17,41,43,43	0
3	SRO	D	501	13/13	0.83	0.18	2.56	15,35,39,39	0
2	HEM	D	500	43/43	0.98	0.13	0.57	9,13,16,27	0
2	HEM	A	500	43/43	0.99	0.11	0.17	7,10,14,26	0
2	HEM	B	500	43/43	0.99	0.11	0.01	6,9,13,24	0
2	HEM	C	500	43/43	0.99	0.12	-0.01	7,11,14,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.