



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:48 AM GMT

PDB ID : 3G1Q  
Title : Crystal structure of sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei in ligand free state  
Authors : Lepesheva, G.I.; Hargrove, T.Y.; Harp, J.; Wawrzak, Z.; Waterman, M.R.; Park, H.  
Deposited on : 2009-01-30  
Resolution : 1.89 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

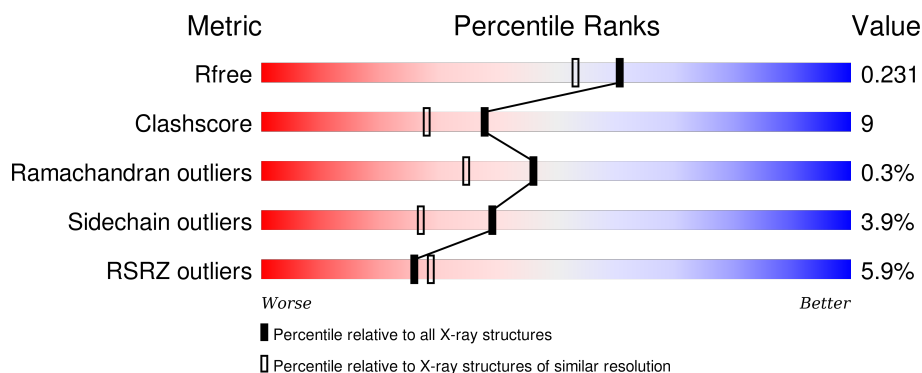
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	450	<div> <div>5%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	B	450	<div> <div>5%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	C	450	<div> <div>8%</div> <div>84%</div> <div>14%</div> <div>...</div> </div>
1	D	450	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14858 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 Sterol 14-alpha-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	B	444	Total	C	N	O	S	0	0	0
			3526	2254	615	630	27			
1	C	447	Total	C	N	O	S	0	0	0
			3552	2270	621	634	27			
1	D	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	THR	ENGINEERED	UNP Q385E8
A	28	LYS	ARG	ENGINEERED	UNP Q385E8
A	29	GLY	PRO	ENGINEERED	UNP Q385E8
A	30	LYS	THR	ENGINEERED	UNP Q385E8
A	31	LEU	ASP	ENGINEERED	UNP Q385E8
B	27	SER	THR	ENGINEERED	UNP Q385E8
B	28	LYS	ARG	ENGINEERED	UNP Q385E8
B	29	GLY	PRO	ENGINEERED	UNP Q385E8
B	30	LYS	THR	ENGINEERED	UNP Q385E8
B	31	LEU	ASP	ENGINEERED	UNP Q385E8
C	27	SER	THR	ENGINEERED	UNP Q385E8
C	28	LYS	ARG	ENGINEERED	UNP Q385E8
C	29	GLY	PRO	ENGINEERED	UNP Q385E8
C	30	LYS	THR	ENGINEERED	UNP Q385E8
C	31	LEU	ASP	ENGINEERED	UNP Q385E8
D	27	SER	THR	ENGINEERED	UNP Q385E8
D	28	LYS	ARG	ENGINEERED	UNP Q385E8
D	29	GLY	PRO	ENGINEERED	UNP Q385E8
D	30	LYS	THR	ENGINEERED	UNP Q385E8
D	31	LEU	ASP	ENGINEERED	UNP Q385E8

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

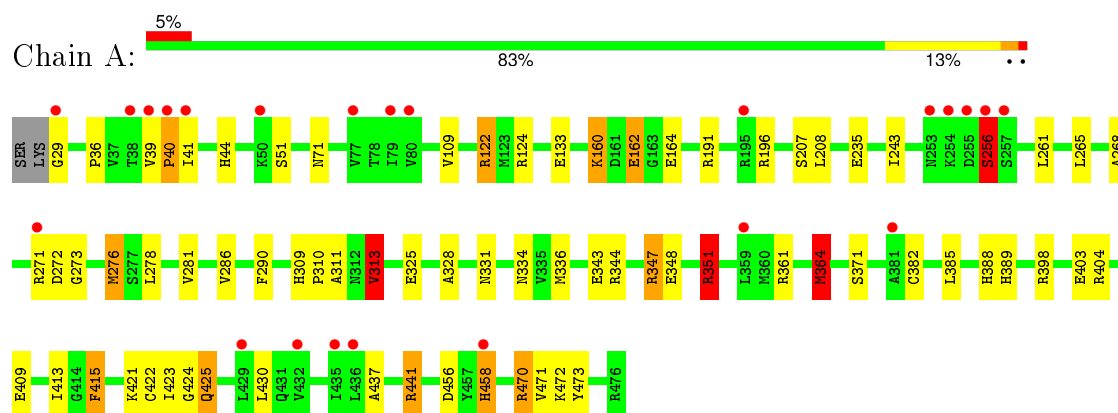
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	132	Total	O	0	0
			132	132		
3	C	102	Total	O	0	0
			102	102		
3	D	98	Total	O	0	0
			98	98		

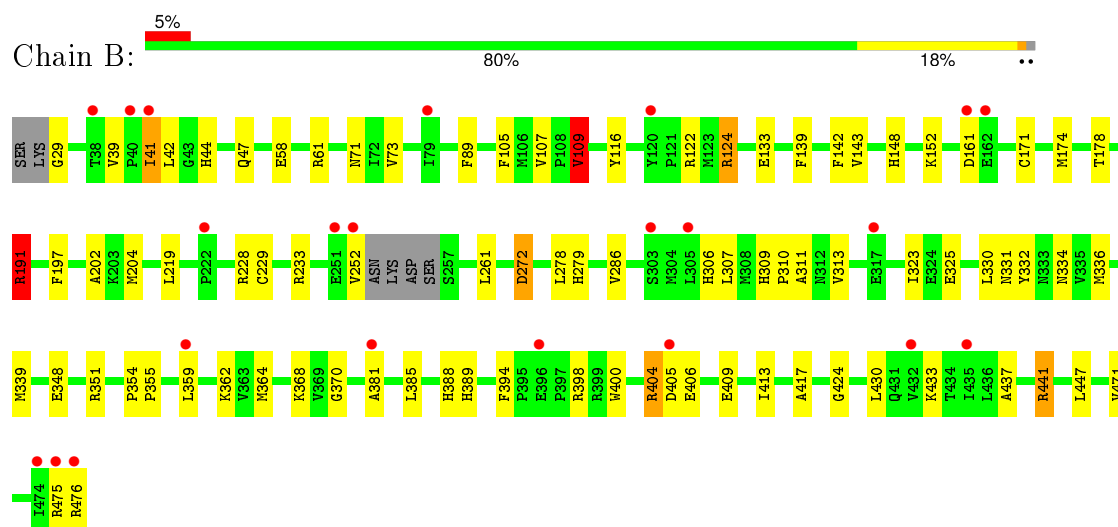
### 3 Residue-property plots

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.

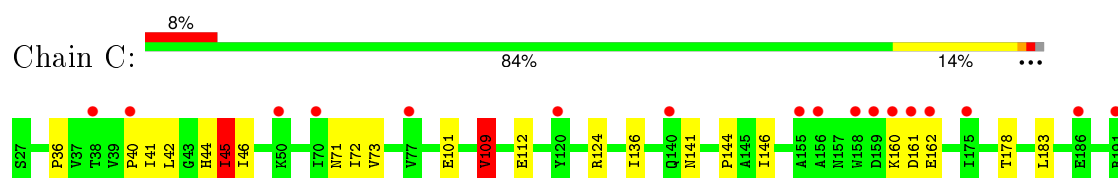
#### • Molecule 1: Sterol 14-alpha-demethylase

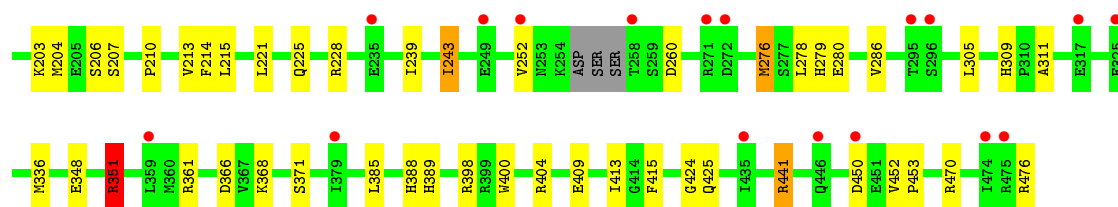


#### • Molecule 1: Sterol 14-alpha-demethylase

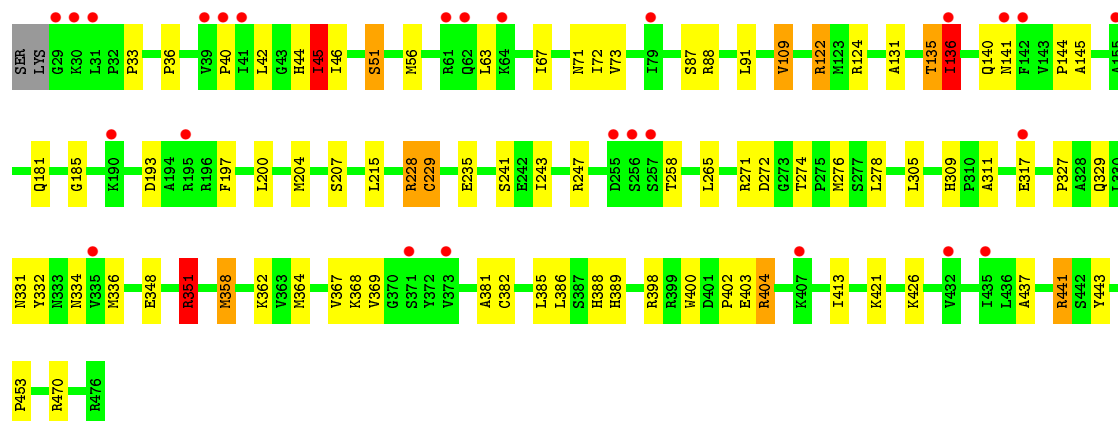
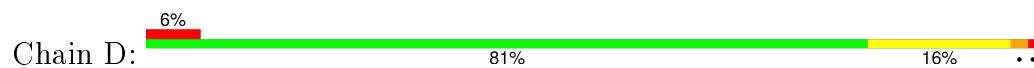


#### • Molecule 1: Sterol 14-alpha-demethylase





• Molecule 1: Sterol 14-alpha-demethylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.82Å 79.87Å 117.15Å 74.21° 81.56° 68.49°	Depositor
Resolution (Å)	28.62 – 1.89 27.99 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.62-1.89) 89.9 (27.99-1.89)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.195 , 0.234 0.193 , 0.231	Depositor DCC
$R_{free}$ test set	7519 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 150245 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

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	1.29	8/3639 (0.2%)	1.07	16/4922 (0.3%)
1	B	1.29	10/3607 (0.3%)	0.98	9/4878 (0.2%)
1	C	1.15	5/3633 (0.1%)	0.96	8/4911 (0.2%)
1	D	1.07	4/3639 (0.1%)	0.92	10/4922 (0.2%)
All	All	1.21	27/14518 (0.2%)	0.98	43/19633 (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	D	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	VAL	CB-CG1	-7.94	1.36	1.52
1	A	351	ARG	CD-NE	-7.52	1.33	1.46
1	B	116	TYR	CD1-CE1	6.41	1.49	1.39
1	A	281	VAL	CB-CG2	6.32	1.66	1.52
1	C	101	GLU	CG-CD	6.18	1.61	1.51
1	D	229	CYS	CB-SG	-6.17	1.71	1.82
1	C	351	ARG	CD-NE	-5.88	1.36	1.46
1	A	382	CYS	CB-SG	-5.83	1.72	1.81
1	A	29	GLY	N-CA	5.81	1.54	1.46
1	A	415	PHE	CE2-CZ	5.81	1.48	1.37
1	B	89	PHE	CD2-CE2	5.72	1.50	1.39
1	D	235	GLU	CG-CD	5.70	1.60	1.51
1	D	382	CYS	CB-SG	-5.69	1.72	1.81
1	B	417	ALA	CA-CB	5.62	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	VAL	CA-CB	5.51	1.66	1.54
1	C	361	ARG	CZ-NH1	5.48	1.40	1.33
1	A	290	PHE	CD1-CE1	5.42	1.50	1.39
1	B	197	PHE	CD2-CE2	5.38	1.50	1.39
1	A	235	GLU	CG-CD	5.36	1.59	1.51
1	C	206	SER	CA-CB	5.35	1.60	1.52
1	B	107	VAL	CB-CG2	5.31	1.64	1.52
1	A	425	GLN	CB-CG	-5.26	1.38	1.52
1	B	286	VAL	CB-CG2	5.26	1.63	1.52
1	B	202	ALA	CA-CB	5.19	1.63	1.52
1	B	197	PHE	CE1-CZ	5.14	1.47	1.37
1	B	171	CYS	CB-SG	5.13	1.91	1.82
1	D	443	TYR	CD2-CE2	-5.02	1.31	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ARG	NE-CZ-NH2	-18.76	110.92	120.30
1	A	351	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	C	351	ARG	NE-CZ-NH2	-14.07	113.26	120.30
1	C	404	ARG	NE-CZ-NH2	-12.89	113.86	120.30
1	B	404	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	D	404	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	B	404	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	C	404	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	D	404	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	351	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	351	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	361	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	228	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	D	351	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	347	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	471	VAL	CG1-CB-CG2	7.15	122.34	110.90
1	B	124	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	351	ARG	CD-NE-CZ	6.97	133.36	123.60
1	A	344	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	124	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	109	VAL	CG1-CB-CG2	6.53	121.34	110.90
1	B	109	VAL	CA-CB-CG1	6.35	120.42	110.90
1	C	45	ILE	CB-CA-C	-6.32	98.96	111.60
1	B	228	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	228	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	D	136	ILE	CB-CA-C	-6.00	99.60	111.60
1	A	344	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	122	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	364	MET	CG-SD-CE	5.78	109.44	100.20
1	A	313	VAL	CB-CA-C	-5.75	100.47	111.40
1	C	361	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	124	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	124	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	361	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	247	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	366	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	221	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	D	45	ILE	CB-CA-C	-5.23	101.14	111.60
1	A	347	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	136	ILE	N-CA-C	5.21	125.08	111.00
1	D	229	CYS	CA-CB-SG	-5.19	104.66	114.00
1	A	122	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	135	THR	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3557	0	3594	64	0
1	B	3526	0	3565	77	0
1	C	3552	0	3597	55	0
1	D	3557	0	3594	69	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	162	0	0	7	0
3	B	132	0	0	22	0
3	C	102	0	0	8	0
3	D	98	0	0	15	0
All	All	14858	0	14470	265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (265) 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:A:423:ILE:CG1	1:A:423:ILE:CD1	1.75	1.64
1:A:328:ALA:HA	1:A:441:ARG:HH22	1.08	1.12
1:D:135:THR:HB	1:D:136:ILE:HG13	1.37	1.06
1:C:228:ARG:HD2	3:C:514:HOH:O	1.57	1.03
1:A:348:GLU:OE1	1:A:351:ARG:HD3	1.61	0.99
1:A:44:HIS:HD2	1:A:71:ASN:H	1.13	0.94
1:B:229:CYS:CB	3:B:603:HOH:O	2.14	0.94
1:A:328:ALA:HA	1:A:441:ARG:NH2	1.82	0.94
1:A:388:HIS:HE1	1:A:413:ILE:H	1.16	0.92
1:B:362:LYS:HG3	1:B:364:MET:CE	2.02	0.90
1:D:388:HIS:HE1	1:D:413:ILE:H	1.08	0.90
1:A:364:MET:HA	1:A:364:MET:CE	2.02	0.90
1:B:406:GLU:HG3	3:D:535:HOH:O	1.75	0.87
1:B:388:HIS:HE1	1:B:413:ILE:H	1.19	0.86
1:C:388:HIS:HE1	1:C:413:ILE:H	1.20	0.85
1:B:336:MET:CE	1:B:430:LEU:CD1	2.55	0.85
1:B:44:HIS:HD2	1:B:71:ASN:H	1.23	0.85
1:A:336:MET:CE	1:A:430:LEU:HD13	2.05	0.85
1:B:336:MET:HE3	1:B:430:LEU:CD1	2.05	0.85
1:A:409:GLU:OE2	1:C:368:LYS:HD2	1.75	0.85
1:B:229:CYS:HB3	3:B:603:HOH:O	1.71	0.84
1:B:362:LYS:HG3	1:B:364:MET:HE3	1.58	0.84
1:B:336:MET:CE	1:B:430:LEU:HD13	2.08	0.83
1:C:210:PRO:O	1:C:213:VAL:HG12	1.78	0.83
1:B:406:GLU:HB2	3:B:516:HOH:O	1.77	0.83
1:B:252:VAL:HA	3:B:543:HOH:O	1.76	0.83
1:D:73:VAL:O	1:D:73:VAL:HG12	1.76	0.83
1:B:309:HIS:HD2	1:B:311:ALA:H	1.26	0.82
1:A:336:MET:HE1	1:A:430:LEU:HD13	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:HD3	3:D:498:HOH:O	1.80	0.81
1:C:44:HIS:HD2	1:C:71:ASN:H	1.26	0.81
1:C:228:ARG:NH2	3:C:488:HOH:O	2.13	0.81
1:B:229:CYS:SG	3:B:603:HOH:O	2.39	0.80
1:D:388:HIS:CE1	1:D:413:ILE:H	1.97	0.80
1:A:309:HIS:HD2	1:A:311:ALA:H	1.29	0.80
1:C:389:HIS:HE1	1:C:398:ARG:HH11	1.28	0.79
1:D:207:SER:HB2	3:D:528:HOH:O	1.83	0.79
1:B:61:ARG:HD2	3:B:582:HOH:O	1.83	0.77
1:B:336:MET:HE1	1:B:430:LEU:HD13	1.66	0.77
1:A:403:GLU:HG2	3:A:578:HOH:O	1.83	0.76
1:A:364:MET:HA	1:A:364:MET:HE2	1.67	0.76
1:D:336:MET:HA	1:D:336:MET:CE	2.17	0.75
1:A:191:ARG:HE	1:A:196:ARG:HH12	1.33	0.74
1:B:336:MET:HE2	3:B:538:HOH:O	1.86	0.74
1:B:41:ILE:HG13	3:B:514:HOH:O	1.87	0.73
1:D:348:GLU:OE1	1:D:351:ARG:HD3	1.89	0.73
1:B:388:HIS:CE1	1:B:413:ILE:H	2.06	0.73
1:D:136:ILE:HA	3:D:547:HOH:O	1.88	0.72
1:A:389:HIS:HE1	1:A:398:ARG:HH11	1.35	0.72
1:D:389:HIS:HE1	1:D:398:ARG:HH11	1.37	0.71
1:D:229:CYS:SG	3:D:528:HOH:O	2.48	0.71
1:D:44:HIS:HD2	1:D:71:ASN:H	1.39	0.71
1:C:45:ILE:HG23	1:C:72:ILE:HG23	1.70	0.71
1:A:423:ILE:CD1	1:A:423:ILE:CB	2.66	0.71
1:D:336:MET:HE1	3:D:499:HOH:O	1.91	0.71
1:A:389:HIS:CE1	1:A:398:ARG:HH11	2.10	0.70
1:B:441:ARG:HG3	3:B:502:HOH:O	1.91	0.70
1:A:388:HIS:CE1	1:A:413:ILE:H	2.07	0.70
1:A:39:VAL:HG12	3:A:582:HOH:O	1.92	0.69
1:A:310:PRO:O	1:A:313:VAL:HG22	1.92	0.68
1:D:122:ARG:HD3	3:D:492:HOH:O	1.94	0.68
1:B:409:GLU:HB2	1:D:136:ILE:HG23	1.75	0.68
1:B:336:MET:CE	1:B:430:LEU:HD12	2.25	0.67
1:C:336:MET:HA	1:C:336:MET:CE	2.24	0.67
1:B:362:LYS:HG3	1:B:364:MET:HE1	1.76	0.67
1:B:336:MET:HE1	1:B:430:LEU:CD1	2.24	0.66
1:B:139:PHE:HA	1:B:142:PHE:HB2	1.78	0.66
1:D:331:ASN:H	1:D:334:ASN:HD22	1.42	0.66
1:B:364:MET:HE2	3:B:599:HOH:O	1.96	0.65
1:D:437:ALA:O	1:D:441:ARG:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:HG3	1:B:261:LEU:HD12	1.77	0.65
1:B:385:LEU:O	1:B:389:HIS:HD2	1.79	0.65
1:A:309:HIS:CD2	1:A:311:ALA:H	2.12	0.65
1:C:389:HIS:CE1	1:C:398:ARG:HH11	2.11	0.65
1:D:229:CYS:HB2	3:D:528:HOH:O	1.97	0.65
1:D:332:TYR:CE1	1:D:336:MET:HG3	2.32	0.65
1:D:73:VAL:O	1:D:73:VAL:CG1	2.45	0.64
1:D:389:HIS:CE1	1:D:398:ARG:HH11	2.15	0.64
1:D:185:GLY:HA3	1:D:258:THR:HG21	1.79	0.64
1:A:364:MET:HA	1:A:364:MET:HE3	1.78	0.64
1:B:310:PRO:O	1:B:313:VAL:HG23	1.98	0.63
1:A:336:MET:HE2	1:A:430:LEU:HD13	1.80	0.63
1:A:328:ALA:CA	1:A:441:ARG:HH22	1.99	0.62
1:C:441:ARG:HD3	3:C:574:HOH:O	1.99	0.61
1:C:348:GLU:OE1	1:C:351:ARG:HD3	2.01	0.61
1:D:336:MET:HA	1:D:336:MET:HE2	1.81	0.61
1:A:456:ASP:OD2	1:A:458:HIS:CE1	2.53	0.61
1:D:358:MET:CE	1:D:381:ALA:HB1	2.30	0.61
1:B:475:ARG:HD3	3:B:560:HOH:O	2.00	0.61
2:D:480:HEM:HMC2	2:D:480:HEM:HBC2	1.83	0.61
1:B:400:TRP:CZ3	3:B:602:HOH:O	2.52	0.60
1:C:309:HIS:CD2	1:C:311:ALA:H	2.19	0.60
1:A:351:ARG:HD2	1:A:404:ARG:HD2	1.83	0.60
1:D:44:HIS:CD2	1:D:71:ASN:H	2.20	0.60
1:B:362:LYS:CG	1:B:364:MET:HE1	2.33	0.59
1:B:331:ASN:H	1:B:334:ASN:ND2	1.99	0.59
1:C:252:VAL:HG12	1:C:252:VAL:O	2.03	0.59
1:B:279:HIS:HD2	3:B:519:HOH:O	1.86	0.59
1:D:358:MET:HE2	1:D:381:ALA:HB1	1.84	0.59
1:A:256:SER:O	1:A:256:SER:OG	2.17	0.59
1:D:141:ASN:HB3	3:D:540:HOH:O	2.02	0.58
1:D:362:LYS:HG2	1:D:364:MET:HE1	1.85	0.58
1:A:348:GLU:OE1	1:A:351:ARG:CD	2.43	0.57
1:D:228:ARG:HD2	3:D:518:HOH:O	2.03	0.57
1:A:265:LEU:O	1:A:276:MET:HE3	2.04	0.57
1:A:44:HIS:HD2	1:A:71:ASN:N	1.95	0.57
1:B:44:HIS:CD2	1:B:71:ASN:H	2.14	0.57
1:B:309:HIS:CD2	1:B:311:ALA:H	2.14	0.57
1:C:441:ARG:O	1:C:476:ARG:HD3	2.04	0.56
1:C:309:HIS:HD2	1:C:311:ALA:H	1.52	0.56
1:B:389:HIS:HE1	1:B:398:ARG:HH11	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:HG3	3:B:556:HOH:O	2.05	0.56
1:B:44:HIS:HD2	1:B:71:ASN:N	1.99	0.56
2:C:480:HEM:HMC2	2:C:480:HEM:HBC2	1.86	0.56
1:C:388:HIS:CE1	1:C:413:ILE:H	2.12	0.56
1:A:44:HIS:CD2	1:A:71:ASN:H	2.06	0.56
1:B:306:HIS:C	3:B:602:HOH:O	2.43	0.56
1:B:331:ASN:H	1:B:334:ASN:HD22	1.54	0.56
1:C:160:LYS:HE2	3:C:556:HOH:O	2.06	0.56
1:C:44:HIS:CD2	1:C:71:ASN:H	2.16	0.55
1:A:325:GLU:OE1	1:C:136:ILE:HG12	2.07	0.55
1:C:336:MET:HE2	1:C:336:MET:HA	1.89	0.55
1:A:331:ASN:H	1:A:334:ASN:ND2	2.04	0.55
1:D:145:ALA:HB1	1:D:181:GLN:HG3	1.88	0.55
1:B:339:MET:HE1	1:B:437:ALA:HB2	1.89	0.55
1:A:336:MET:CG	1:C:409:GLU:HG3	2.37	0.55
1:D:229:CYS:CB	3:D:528:HOH:O	2.55	0.54
1:D:265:LEU:O	1:D:276:MET:HE3	2.08	0.54
1:B:73:VAL:O	1:B:73:VAL:HG12	2.07	0.54
1:B:336:MET:HE3	1:B:430:LEU:HD12	1.83	0.54
1:D:331:ASN:H	1:D:334:ASN:ND2	2.05	0.54
1:D:140:GLN:HG2	3:D:537:HOH:O	2.08	0.53
1:C:44:HIS:HD2	1:C:71:ASN:N	2.00	0.53
1:A:162:GLU:OE1	1:A:472:LYS:HE3	2.08	0.53
1:A:191:ARG:NE	1:A:196:ARG:HH12	2.04	0.53
1:A:385:LEU:O	1:A:389:HIS:HD2	1.92	0.53
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.44	0.53
1:C:73:VAL:HG12	1:C:73:VAL:O	2.10	0.52
1:D:364:MET:HE2	1:D:364:MET:HA	1.92	0.52
1:B:330:LEU:HA	1:B:334:ASN:HD22	1.75	0.52
1:A:41:ILE:HG22	1:A:41:ILE:O	2.09	0.52
1:A:424:GLY:HA3	2:A:480:HEM:C3C	2.45	0.52
2:B:480:HEM:HBC2	2:B:480:HEM:HMC2	1.91	0.52
1:A:364:MET:CE	1:A:364:MET:CA	2.82	0.51
1:C:470:ARG:NE	3:C:571:HOH:O	2.39	0.51
1:B:105:PHE:HA	1:B:219:LEU:HD21	1.92	0.51
1:B:309:HIS:HD2	1:B:311:ALA:N	2.02	0.51
1:D:87:SER:HB2	1:D:91:LEU:HD12	1.93	0.51
1:A:336:MET:HG3	1:C:409:GLU:HG3	1.93	0.51
1:C:42:LEU:HD13	1:C:46:ILE:HD13	1.92	0.51
1:B:364:MET:HA	1:B:364:MET:HE2	1.92	0.50
1:D:358:MET:HA	1:D:358:MET:HE3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:VAL:HG22	1:C:204:MET:HB3	1.93	0.50
1:B:348:GLU:OE1	1:B:404:ARG:HD3	2.11	0.50
1:A:347:ARG:HD3	3:A:482:HOH:O	2.11	0.50
1:A:109:VAL:HG13	1:A:286:VAL:HG11	1.92	0.50
1:D:400:TRP:CH2	1:D:402:PRO:HG3	2.47	0.50
1:C:425:GLN:NE2	3:C:518:HOH:O	2.17	0.50
1:B:351:ARG:HD3	1:B:394:PHE:CD2	2.46	0.50
1:C:213:VAL:HG13	1:C:214:PHE:CD1	2.48	0.49
1:C:42:LEU:HD22	1:C:45:ILE:HD11	1.94	0.49
1:C:228:ARG:CD	3:C:514:HOH:O	2.33	0.49
1:C:415:PHE:CE1	1:C:425:GLN:HG3	2.48	0.49
1:C:305:LEU:HD13	1:C:453:PRO:HD2	1.93	0.49
1:A:331:ASN:H	1:A:334:ASN:HD22	1.59	0.49
1:D:135:THR:HB	1:D:136:ILE:CG1	2.25	0.49
1:D:426:LYS:HD2	3:D:546:HOH:O	2.12	0.49
1:A:164:GLU:HG2	1:A:470:ARG:NH2	2.28	0.48
1:B:323:ILE:HD12	1:B:441:ARG:HG2	1.96	0.48
1:C:160:LYS:HG3	1:C:162:GLU:O	2.13	0.48
1:B:389:HIS:CE1	1:B:398:ARG:HH11	2.30	0.48
1:B:109:VAL:HG23	3:B:603:HOH:O	2.13	0.47
1:D:348:GLU:OE1	1:D:404:ARG:HD3	2.14	0.47
2:C:480:HEM:CMC	2:C:480:HEM:HBC2	2.43	0.47
1:B:424:GLY:HA3	2:B:480:HEM:C3C	2.48	0.47
1:A:39:VAL:HA	1:A:40:PRO:HD2	1.70	0.47
1:C:146:ILE:HG23	1:C:178:THR:HG21	1.96	0.47
1:A:422:CYS:HB3	1:A:425:GLN:HG3	1.95	0.47
1:C:424:GLY:HA3	2:C:480:HEM:C3C	2.50	0.47
2:C:480:HEM:HBB2	2:C:480:HEM:HHC	1.97	0.47
1:B:279:HIS:CD2	3:B:519:HOH:O	2.65	0.47
1:D:305:LEU:HD13	1:D:453:PRO:HD2	1.97	0.47
1:B:58:GLU:OE1	1:B:61:ARG:NH1	2.49	0.46
1:B:161:ASP:HA	1:B:475:ARG:HB3	1.97	0.46
1:B:143:VAL:CG2	1:B:430:LEU:HD11	2.45	0.46
1:B:433:LYS:CE	3:B:538:HOH:O	2.64	0.46
1:D:336:MET:CE	1:D:336:MET:CA	2.93	0.46
1:C:183:LEU:O	1:C:260:ASP:HB2	2.15	0.46
1:A:41:ILE:N	3:A:582:HOH:O	2.48	0.46
2:A:480:HEM:HBC2	2:A:480:HEM:HMC2	1.98	0.46
1:D:36:PRO:O	1:D:44:HIS:HE1	1.98	0.46
1:D:272:ASP:HB3	1:D:274:THR:H	1.81	0.46
1:D:88:ARG:HH21	1:D:368:LYS:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ALA:HB1	1:D:181:GLN:CG	2.46	0.45
1:C:36:PRO:O	1:C:44:HIS:HE1	1.99	0.45
1:A:415:PHE:CD2	1:A:425:GLN:HG2	2.51	0.45
1:A:133:GLU:HG3	1:A:261:LEU:HD12	1.99	0.45
1:B:362:LYS:CG	1:B:364:MET:CE	2.82	0.45
1:D:332:TYR:CZ	1:D:336:MET:HG3	2.52	0.45
1:C:213:VAL:HG11	3:C:522:HOH:O	2.17	0.45
1:B:389:HIS:HE1	1:B:398:ARG:HD2	1.82	0.45
1:A:268:ALA:HB3	1:A:276:MET:HE2	1.99	0.44
1:D:271:ARG:NH2	3:D:491:HOH:O	2.50	0.44
1:D:56:MET:HE1	1:D:386:LEU:HB2	1.99	0.44
1:B:29:GLY:N	3:B:590:HOH:O	2.50	0.44
1:C:112:GLU:O	1:C:279:HIS:HE1	2.01	0.44
1:B:41:ILE:HD12	1:B:42:LEU:HG	2.00	0.44
1:B:307:LEU:HA	3:B:602:HOH:O	2.17	0.44
1:D:131:ALA:O	1:D:135:THR:HG23	2.17	0.44
1:B:325:GLU:OE1	1:B:325:GLU:HA	2.17	0.43
1:D:45:ILE:HG13	1:D:45:ILE:H	1.63	0.43
1:B:354:PRO:HA	1:B:355:PRO:HD3	1.88	0.43
1:A:313:VAL:HG22	3:A:558:HOH:O	2.18	0.43
1:D:364:MET:CE	1:D:364:MET:HA	2.48	0.43
1:A:160:LYS:HG2	1:A:473:TYR:OH	2.19	0.43
1:B:368:LYS:HE2	1:B:370:GLY:O	2.18	0.43
1:A:313:VAL:CG2	3:A:558:HOH:O	2.66	0.43
1:B:409:GLU:HB2	1:D:136:ILE:CG2	2.47	0.43
1:D:73:VAL:HG11	1:D:215:LEU:HD21	2.01	0.43
1:A:271:ARG:C	1:A:273:GLY:H	2.20	0.43
1:C:141:ASN:O	1:C:144:PRO:HD2	2.18	0.42
1:D:336:MET:CE	3:D:499:HOH:O	2.60	0.42
1:B:41:ILE:N	3:B:514:HOH:O	2.51	0.42
1:D:348:GLU:HG3	1:D:400:TRP:CD1	2.54	0.42
1:B:174:MET:O	1:B:178:THR:HG23	2.19	0.42
1:C:40:PRO:HB2	1:C:41:ILE:HG13	2.02	0.42
1:D:109:VAL:HG22	1:D:204:MET:HB3	2.02	0.42
1:A:470:ARG:HD2	3:A:598:HOH:O	2.20	0.42
1:D:45:ILE:HG23	1:D:72:ILE:HG23	1.99	0.42
1:C:348:GLU:HG3	1:C:400:TRP:CD1	2.54	0.42
1:A:109:VAL:HG13	1:A:286:VAL:CG1	2.49	0.42
1:D:309:HIS:CD2	1:D:311:ALA:H	2.38	0.42
1:A:437:ALA:O	1:A:441:ARG:HB2	2.20	0.42
1:A:36:PRO:O	1:A:44:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:HE2	1:A:430:LEU:CD1	2.49	0.42
1:C:207:SER:HA	1:C:225:GLN:HB3	2.02	0.42
1:C:276:MET:HG2	1:C:280:GLU:HB2	2.00	0.42
1:D:327:PRO:HG2	1:D:329:GLN:O	2.20	0.41
1:D:51:SER:OG	1:D:51:SER:O	2.37	0.41
1:B:204:MET:CE	1:B:233:ARG:HA	2.50	0.41
1:B:364:MET:CE	3:B:599:HOH:O	2.63	0.41
1:B:385:LEU:O	1:B:389:HIS:CD2	2.67	0.41
1:D:141:ASN:O	1:D:144:PRO:HD2	2.20	0.41
1:D:67:ILE:HD13	1:D:369:VAL:HG12	2.02	0.41
1:C:73:VAL:HG11	1:C:215:LEU:HG	2.01	0.41
1:D:33:PRO:HB2	1:D:63:LEU:HD22	2.02	0.41
1:C:415:PHE:CZ	1:C:425:GLN:HG3	2.55	0.41
1:B:368:LYS:HA	1:B:368:LYS:HD2	1.96	0.41
1:D:385:LEU:O	1:D:389:HIS:HD2	2.04	0.41
1:C:252:VAL:CG1	1:C:252:VAL:O	2.67	0.41
1:C:203:LYS:HE2	1:C:228:ARG:HB3	2.03	0.41
1:C:385:LEU:O	1:C:389:HIS:HD2	2.04	0.41
1:A:456:ASP:OD1	1:A:458:HIS:ND1	2.54	0.41
1:C:146:ILE:HG23	1:C:178:THR:CG2	2.51	0.41
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.88	0.41
1:C:239:ILE:O	1:C:243:ILE:HD12	2.20	0.41
1:C:109:VAL:HG13	1:C:286:VAL:CG1	2.52	0.40
1:B:148:HIS:O	1:B:152:LYS:HG3	2.21	0.40
1:A:404:ARG:HD3	1:A:404:ARG:HH11	1.79	0.40
1:A:41:ILE:CG2	1:A:41:ILE:O	2.69	0.40
1:D:185:GLY:CA	1:D:258:THR:HG21	2.48	0.40
1:D:200:LEU:O	1:D:204:MET:HG3	2.21	0.40
1:B:359:LEU:O	1:B:381:ALA:HA	2.21	0.40
1:C:309:HIS:HD2	1:C:311:ALA:HB3	1.85	0.40
1:D:42:LEU:HD13	1:D:46:ILE:HD12	2.02	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	446/450 (99%)	432 (97%)	11 (2%)	3 (1%)	26	14
1	B	440/450 (98%)	426 (97%)	13 (3%)	1 (0%)	52	42
1	C	443/450 (98%)	429 (97%)	14 (3%)	0	100	100
1	D	446/450 (99%)	424 (95%)	20 (4%)	2 (0%)	39	27
All	All	1775/1800 (99%)	1711 (96%)	58 (3%)	6 (0%)	46	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	256	SER
1	B	272	ASP
1	D	136	ILE
1	A	272	ASP
1	D	40	PRO

### 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	390/392 (100%)	372 (95%)	18 (5%)	33	21
1	B	386/392 (98%)	373 (97%)	13 (3%)	44	33
1	C	389/392 (99%)	377 (97%)	12 (3%)	47	37
1	D	390/392 (100%)	372 (95%)	18 (5%)	33	21
All	All	1555/1568 (99%)	1494 (96%)	61 (4%)	39	27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	122	ARG

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Mol	Chain	Res	Type
1	A	160	LYS
1	A	162	GLU
1	A	207	SER
1	A	243	ILE
1	A	256	SER
1	A	276	MET
1	A	278	LEU
1	A	313	VAL
1	A	343	GLU
1	A	351	ARG
1	A	364	MET
1	A	371	SER
1	A	421	LYS
1	A	441	ARG
1	A	458	HIS
1	A	470	ARG
1	B	39	VAL
1	B	41	ILE
1	B	47	GLN
1	B	109	VAL
1	B	122	ARG
1	B	124	ARG
1	B	191	ARG
1	B	272	ASP
1	B	278	LEU
1	B	405	ASP
1	B	441	ARG
1	B	447	LEU
1	B	476	ARG
1	C	45	ILE
1	C	109	VAL
1	C	124	ARG
1	C	161	ASP
1	C	243	ILE
1	C	276	MET
1	C	278	LEU
1	C	351	ARG
1	C	371	SER
1	C	441	ARG
1	C	450	ASP
1	C	452	VAL
1	D	45	ILE

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Mol	Chain	Res	Type
1	D	51	SER
1	D	109	VAL
1	D	122	ARG
1	D	124	ARG
1	D	136	ILE
1	D	193	ASP
1	D	197	PHE
1	D	241	SER
1	D	243	ILE
1	D	278	LEU
1	D	317	GLU
1	D	351	ARG
1	D	358	MET
1	D	367	VAL
1	D	403	GLU
1	D	421	LYS
1	D	441	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	62	GLN
1	A	309	HIS
1	A	334	ASN
1	A	388	HIS
1	A	389	HIS
1	B	44	HIS
1	B	47	GLN
1	B	62	GLN
1	B	177	ASN
1	B	181	GLN
1	B	279	HIS
1	B	309	HIS
1	B	329	GLN
1	B	333	ASN
1	B	334	ASN
1	B	388	HIS
1	B	389	HIS
1	B	425	GLN
1	C	44	HIS
1	C	62	GLN

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Mol	Chain	Res	Type
1	C	279	HIS
1	C	309	HIS
1	C	333	ASN
1	C	334	ASN
1	C	388	HIS
1	C	389	HIS
1	D	44	HIS
1	D	253	ASN
1	D	279	HIS
1	D	309	HIS
1	D	334	ASN
1	D	388	HIS
1	D	389	HIS
1	D	425	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	480	1	30,50,50	2.72	11 (36%)	24,82,82	2.62	7 (29%)
2	HEM	B	480	1	30,50,50	2.58	10 (33%)	24,82,82	2.60	12 (50%)
2	HEM	C	480	1	30,50,50	2.53	14 (46%)	24,82,82	2.59	12 (50%)
2	HEM	D	480	1	30,50,50	2.92	11 (36%)	24,82,82	2.41	11 (45%)

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	480	1	-	0/10/54/54	0/0/8/8
2	HEM	B	480	1	-	0/10/54/54	0/0/8/8
2	HEM	C	480	1	-	0/10/54/54	0/0/8/8
2	HEM	D	480	1	-	0/10/54/54	0/0/8/8

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	480	HEM	C3B-C4B	-10.25	1.42	1.51
2	A	480	HEM	C3B-C4B	-8.34	1.44	1.51
2	C	480	HEM	C3B-C4B	-7.99	1.44	1.51
2	B	480	HEM	C3D-C4D	-6.56	1.43	1.51
2	B	480	HEM	C3B-C4B	-6.37	1.46	1.51
2	D	480	HEM	C3D-C4D	-5.93	1.44	1.51
2	B	480	HEM	C2C-C1C	-5.18	1.42	1.52
2	C	480	HEM	C3D-C4D	-4.97	1.45	1.51
2	A	480	HEM	C3D-C4D	-4.91	1.45	1.51
2	A	480	HEM	C2C-C1C	-4.08	1.44	1.52
2	A	480	HEM	C2D-C1D	-3.91	1.39	1.51
2	B	480	HEM	C2D-C1D	-3.22	1.41	1.51
2	C	480	HEM	C2C-C1C	-3.10	1.46	1.52
2	A	480	HEM	C2B-C1B	-3.01	1.42	1.51
2	D	480	HEM	C2C-C1C	-2.88	1.47	1.52
2	C	480	HEM	C2B-C1B	-2.51	1.43	1.51
2	A	480	HEM	C2D-C3D	-2.47	1.47	1.54
2	C	480	HEM	C2D-C1D	-2.45	1.43	1.51
2	D	480	HEM	C2D-C1D	-2.41	1.44	1.51
2	C	480	HEM	C2D-C3D	-2.04	1.48	1.54
2	B	480	HEM	C2B-C1B	-2.00	1.45	1.51
2	C	480	HEM	CMD-C2D	2.10	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	480	HEM	C4C-NC	2.10	1.38	1.36
2	B	480	HEM	CMD-C2D	2.12	1.58	1.53
2	C	480	HEM	CMB-C2B	2.19	1.58	1.53
2	D	480	HEM	FE-NB	2.22	2.09	1.97
2	D	480	HEM	C3B-CAB	2.59	1.56	1.51
2	A	480	HEM	CMB-C2B	2.77	1.59	1.53
2	D	480	HEM	C4C-NC	2.78	1.39	1.36
2	C	480	HEM	CMC-C2C	2.88	1.59	1.53
2	C	480	HEM	CMA-C3A	2.89	1.57	1.51
2	A	480	HEM	CMD-C2D	2.96	1.60	1.53
2	B	480	HEM	C1C-NC	3.02	1.39	1.36
2	C	480	HEM	C3B-CAB	3.13	1.57	1.51
2	B	480	HEM	C3B-CAB	3.20	1.57	1.51
2	D	480	HEM	CMB-C2B	3.35	1.60	1.53
2	D	480	HEM	FE-NC	3.40	2.09	1.95
2	C	480	HEM	FE-NC	3.41	2.09	1.95
2	B	480	HEM	CAA-C2A	3.56	1.58	1.52
2	A	480	HEM	FE-NC	3.77	2.10	1.95
2	B	480	HEM	FE-NC	3.78	2.10	1.95
2	A	480	HEM	CMA-C3A	3.82	1.59	1.51
2	C	480	HEM	CAA-C2A	3.90	1.58	1.52
2	D	480	HEM	CAA-C2A	4.10	1.59	1.52
2	A	480	HEM	C3C-CAC	4.21	1.59	1.51
2	D	480	HEM	C1C-NC	4.55	1.41	1.36

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	HEM	C3C-CAC-CBC	-4.85	117.01	124.46
2	C	480	HEM	C3B-CAB-CBB	-3.81	118.61	124.46
2	B	480	HEM	C3B-CAB-CBB	-3.20	119.54	124.46
2	C	480	HEM	C3C-CAC-CBC	-3.14	119.64	124.46
2	C	480	HEM	CMA-C3A-C4A	-2.76	123.80	128.36
2	D	480	HEM	CBD-CAD-C3D	-2.53	106.19	113.55
2	B	480	HEM	CBA-CAA-C2A	-2.39	108.25	112.53
2	B	480	HEM	CAA-C2A-C1A	-2.29	124.53	127.01
2	D	480	HEM	CAA-C2A-C1A	-2.25	124.57	127.01
2	B	480	HEM	CBD-CAD-C3D	-2.21	107.11	113.55
2	C	480	HEM	C3B-C4B-NB	-2.15	107.52	111.63
2	A	480	HEM	C3B-C4B-NB	-2.03	107.75	111.63
2	D	480	HEM	CAD-CBD-CGD	-2.02	104.78	113.02
2	C	480	HEM	C3B-C4B-CHC	2.22	126.29	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	HEM	C1D-CHD-C4C	2.23	129.56	125.82
2	D	480	HEM	C2C-C1C-CHC	2.45	127.41	123.68
2	C	480	HEM	CMD-C2D-C3D	2.46	125.23	114.35
2	C	480	HEM	C2D-C3D-C4D	2.49	105.73	101.50
2	D	480	HEM	C2D-C3D-C4D	2.55	105.83	101.50
2	D	480	HEM	C1D-CHD-C4C	2.59	130.15	125.82
2	A	480	HEM	C1D-CHD-C4C	2.61	130.18	125.82
2	B	480	HEM	C3B-C4B-CHC	2.83	127.15	123.16
2	C	480	HEM	C2C-C1C-CHC	2.87	128.05	123.68
2	B	480	HEM	CMD-C2D-C3D	2.92	127.26	114.35
2	B	480	HEM	C2D-C3D-C4D	2.94	106.48	101.50
2	D	480	HEM	CMD-C2D-C3D	3.09	128.00	114.35
2	D	480	HEM	CMB-C2B-C3B	3.10	124.27	116.53
2	A	480	HEM	CMB-C2B-C3B	3.51	125.29	116.53
2	C	480	HEM	CMB-C2B-C3B	3.56	125.42	116.53
2	A	480	HEM	CAD-C3D-C4D	3.56	125.03	112.47
2	B	480	HEM	CAD-C3D-C4D	3.58	125.10	112.47
2	D	480	HEM	CAD-C3D-C4D	3.97	126.49	112.47
2	B	480	HEM	CMB-C2B-C3B	4.13	126.83	116.53
2	C	480	HEM	CAD-C3D-C4D	4.23	127.39	112.47
2	C	480	HEM	CAD-C3D-C2D	4.75	126.87	113.22
2	D	480	HEM	CAD-C3D-C2D	5.01	127.62	113.22
2	B	480	HEM	CAD-C3D-C2D	5.28	128.40	113.22
2	D	480	HEM	CMC-C2C-C3C	5.32	129.80	116.53
2	C	480	HEM	CMC-C2C-C3C	5.35	129.89	116.53
2	B	480	HEM	CMC-C2C-C3C	5.89	131.24	116.53
2	A	480	HEM	CAD-C3D-C2D	6.08	130.69	113.22
2	A	480	HEM	CMC-C2C-C3C	6.57	132.93	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	HEM	2	0
2	B	480	HEM	2	0
2	C	480	HEM	4	0
2	D	480	HEM	1	0



## 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	448/450 (99%)	0.23	23 (5%)	32	35	16, 30, 47, 70	0
1	B	444/450 (98%)	0.29	22 (4%)	32	35	19, 33, 49, 61	0
1	C	447/450 (99%)	0.41	34 (7%)	17	18	21, 37, 58, 70	0
1	D	448/450 (99%)	0.38	26 (5%)	26	29	25, 39, 57, 69	0
All	All	1787/1800 (99%)	0.33	105 (5%)	26	29	16, 35, 55, 70	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	8.6
1	A	256	SER	8.2
1	A	257	SER	5.0
1	A	40	PRO	4.8
1	A	38	THR	4.4
1	A	29	GLY	4.1
1	A	41	ILE	4.1
1	C	159	ASP	4.0
1	D	41	ILE	4.0
1	C	155	ALA	3.9
1	D	195	ARG	3.8
1	D	255	ASP	3.7
1	B	40	PRO	3.7
1	D	40	PRO	3.6
1	B	251	GLU	3.4
1	C	249	GLU	3.4
1	A	254	LYS	3.4
1	A	195	ARG	3.4
1	D	29	GLY	3.4
1	D	64	LYS	3.4
1	D	30	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	435	ILE	3.3
1	B	162	GLU	3.3
1	B	405	ASP	3.3
1	C	161	ASP	3.2
1	C	435	ILE	3.2
1	D	39	VAL	3.2
1	D	373	VAL	3.2
1	A	253	ASN	3.2
1	D	31	LEU	3.1
1	A	432	VAL	3.1
1	A	381	ALA	3.1
1	C	175	ILE	2.9
1	C	450	ASP	2.9
1	C	120	TYR	2.9
1	C	252	VAL	2.9
1	A	255	ASP	2.8
1	B	38	THR	2.8
1	B	161	ASP	2.8
1	C	475	ARG	2.7
1	A	39	VAL	2.7
1	C	160	LYS	2.7
1	C	50	LYS	2.7
1	D	432	VAL	2.6
1	D	371	SER	2.6
1	B	359	LEU	2.6
1	A	436	LEU	2.6
1	C	140	GLN	2.6
1	D	136	ILE	2.5
1	A	359	LEU	2.5
1	C	446	GLN	2.5
1	B	432	VAL	2.5
1	C	38	THR	2.5
1	C	40	PRO	2.5
1	C	271	ARG	2.5
1	C	258	THR	2.5
1	C	235	GLU	2.4
1	D	256	SER	2.4
1	C	191	ARG	2.4
1	C	186	GLU	2.4
1	D	335	VAL	2.4
1	B	396	GLU	2.3
1	C	317	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	2.3
1	C	272	ASP	2.3
1	C	162	GLU	2.3
1	C	296	SER	2.3
1	D	435	ILE	2.3
1	C	77	VAL	2.3
1	D	62	GLN	2.3
1	A	271	ARG	2.2
1	B	435	ILE	2.2
1	D	141	ASN	2.2
1	C	156	ALA	2.2
1	A	79	ILE	2.2
1	A	458	HIS	2.2
1	B	303	SER	2.2
1	B	120	TYR	2.2
1	C	359	LEU	2.2
1	A	77	VAL	2.2
1	C	70	ILE	2.1
1	C	474	ILE	2.1
1	B	475	ARG	2.1
1	C	158	TRP	2.1
1	B	79	ILE	2.1
1	C	295	THR	2.1
1	B	305	LEU	2.1
1	D	317	GLU	2.1
1	A	50	LYS	2.1
1	B	222	PRO	2.1
1	B	317	GLU	2.1
1	D	257	SER	2.1
1	B	474	ILE	2.0
1	B	476	ARG	2.0
1	C	379	ILE	2.0
1	A	429	LEU	2.0
1	A	80	VAL	2.0
1	D	190	LYS	2.0
1	D	407	LYS	2.0
1	B	381	ALA	2.0
1	B	41	ILE	2.0
1	D	142	PHE	2.0
1	C	325	GLU	2.0
1	D	61	ARG	2.0
1	D	79	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	480	43/43	0.99	0.14	0.12	14,18,26,34	0
2	HEM	C	480	43/43	0.98	0.13	-0.02	17,21,26,34	0
2	HEM	B	480	43/43	0.99	0.13	-0.16	18,21,27,35	0
2	HEM	D	480	43/43	0.98	0.12	-0.38	22,28,35,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.