



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:32 am GMT

PDB ID : 3QU8  
Title : Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with the inhibitor 4-(4-Nitrobenzyl)pyridine.  
Authors : Shah, M.B.; Pascual, J.; Stout, C.D.; Halpert, J.R.  
Deposited on : 2011-02-23  
Resolution : 2.80 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

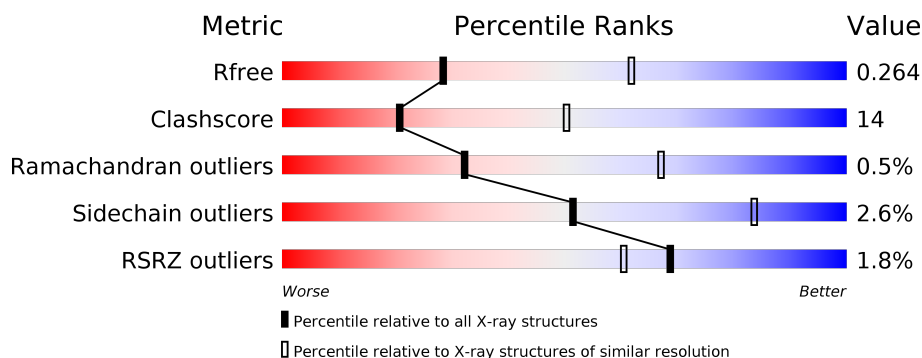
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	476	<div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	B	476	<div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	C	476	<div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
1	D	476	<div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
1	E	476	<div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
1	F	476	<div> <div>7%</div> <div>71%</div> <div>22%</div> <div>• 5%</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	3QU	A	501	-	-	-	X
3	3QU	B	501	-	-	-	X
3	3QU	D	501	-	-	-	X
3	3QU	E	501	-	-	-	X
4	CM5	B	602	-	-	-	X
4	CM5	B	608	-	-	-	X
4	CM5	C	603	-	-	-	X
4	CM5	D	604	X	-	-	-
4	CM5	D	607	-	-	-	X
4	CM5	F	606	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22964 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3732	2416	641	658	17			
1	B	459	Total	C	N	O	S	0	0	0
			3713	2403	639	655	16			
1	C	462	Total	C	N	O	S	0	0	0
			3724	2408	642	658	16			
1	D	458	Total	C	N	O	S	0	0	0
			3693	2389	635	653	16			
1	E	459	Total	C	N	O	S	0	0	0
			3717	2406	640	655	16			
1	F	453	Total	C	N	O	S	0	0	0
			3649	2359	625	649	16			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813

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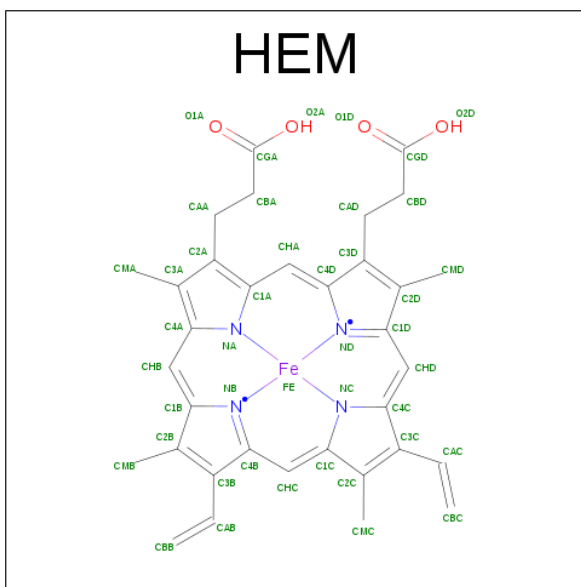
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813
C	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
C	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
C	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
C	26	SER	THR	ENGINEERED MUTATION	UNP P20813
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
C	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
C	492	HIS	-	EXPRESSION TAG	UNP P20813
C	493	HIS	-	EXPRESSION TAG	UNP P20813
C	494	HIS	-	EXPRESSION TAG	UNP P20813
C	495	HIS	-	EXPRESSION TAG	UNP P20813
D	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
D	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
D	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
D	26	SER	THR	ENGINEERED MUTATION	UNP P20813
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
D	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
D	492	HIS	-	EXPRESSION TAG	UNP P20813
D	493	HIS	-	EXPRESSION TAG	UNP P20813
D	494	HIS	-	EXPRESSION TAG	UNP P20813

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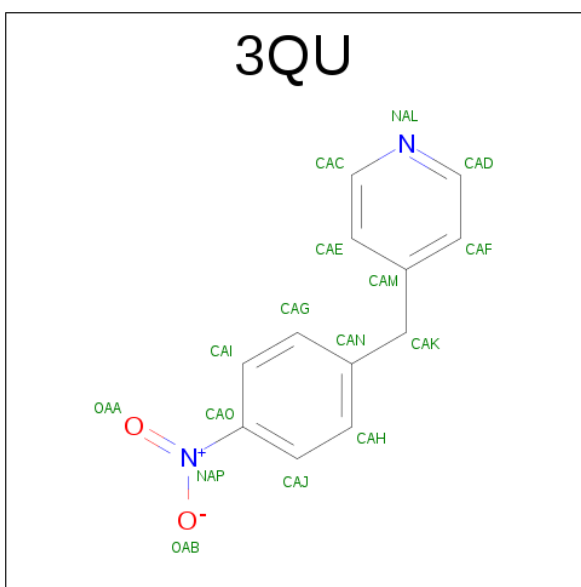
Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	EXPRESSION TAG	UNP P20813
E	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
E	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
E	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
E	26	SER	THR	ENGINEERED MUTATION	UNP P20813
E	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
E	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
E	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
E	492	HIS	-	EXPRESSION TAG	UNP P20813
E	493	HIS	-	EXPRESSION TAG	UNP P20813
E	494	HIS	-	EXPRESSION TAG	UNP P20813
E	495	HIS	-	EXPRESSION TAG	UNP P20813
F	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
F	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
F	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
F	26	SER	THR	ENGINEERED MUTATION	UNP P20813
F	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
F	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
F	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
F	492	HIS	-	EXPRESSION TAG	UNP P20813
F	493	HIS	-	EXPRESSION TAG	UNP P20813
F	494	HIS	-	EXPRESSION TAG	UNP P20813
F	495	HIS	-	EXPRESSION TAG	UNP P20813

- 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
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

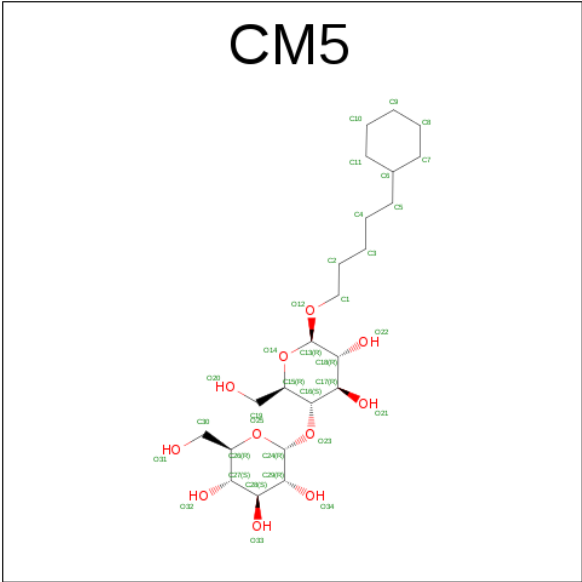
- Molecule 3 is 4-(4-NITROBENZYL)PYRIDINE (three-letter code: 3QU) (formula:  $C_{12}H_{10}N_2O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			7	6	1		
3	B	1	Total	C	N	0	0
			16	12	2		
3	C	1	Total	C	N	0	0
			7	6	1		
3	D	1	Total	C	N	0	0
			13	12	1		
3	E	1	Total	C	N	0	0
			13	12	1		

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: C<sub>23</sub>H<sub>42</sub>O<sub>11</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			34	23	11		
4	B	1	Total	C	O	0	0
			34	23	11		
4	B	1	Total	C	O	0	0
			34	23	11		
4	C	1	Total	C	O	0	0
			34	23	11		
4	D	1	Total	C	O	0	0
			34	23	11		
4	D	1	Total	C	O	0	0
			34	23	11		
4	E	1	Total	C	O	0	0
			34	23	11		
4	F	1	Total	C	O	0	0
			34	23	11		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	23	Total	O	0	0
			23	23		
5	C	29	Total	O	0	0
			29	29		
5	D	38	Total	O	0	0
			38	38		

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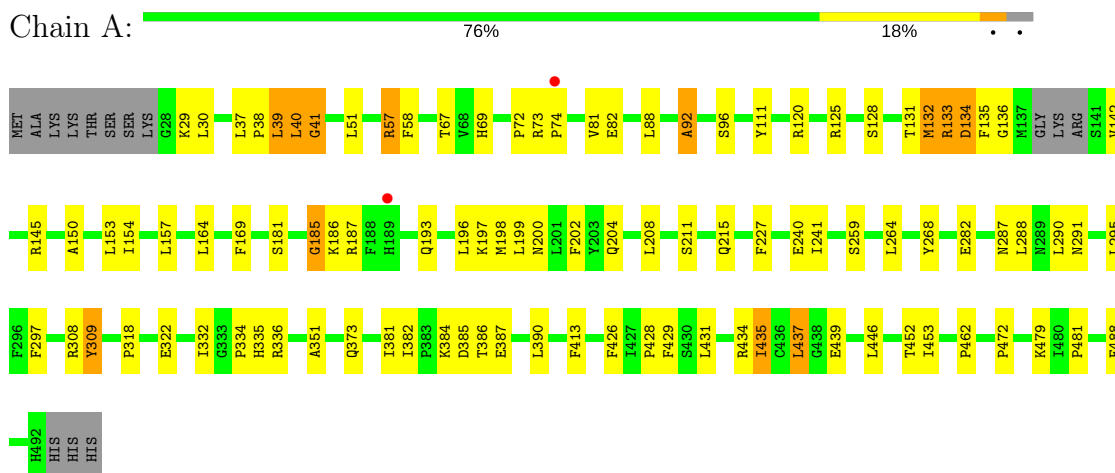
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	23	Total	O	0	0
			23	23		
5	F	12	Total	O	0	0
			12	12		

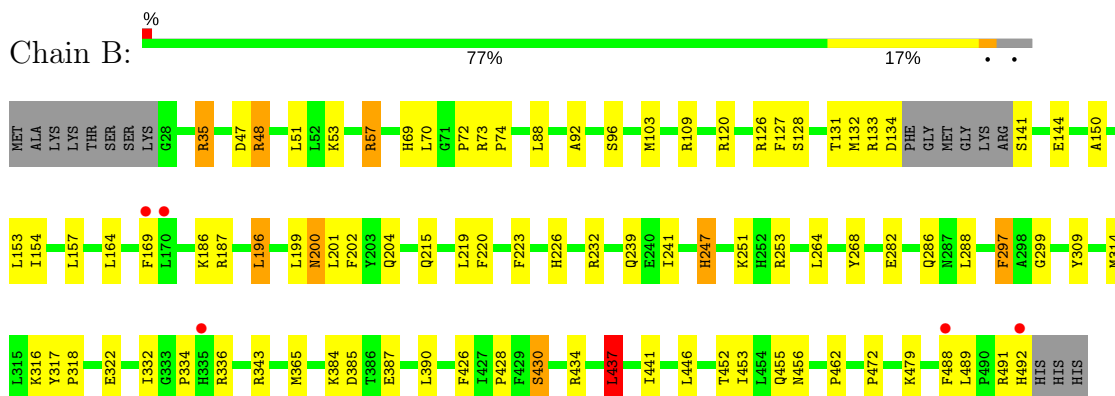
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

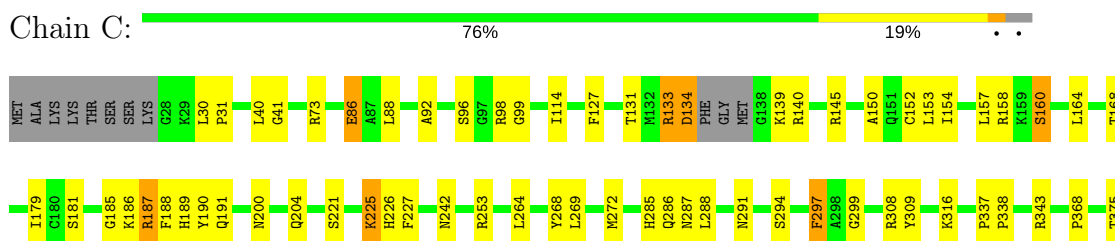
#### • Molecule 1: Cytochrome P450 2B6

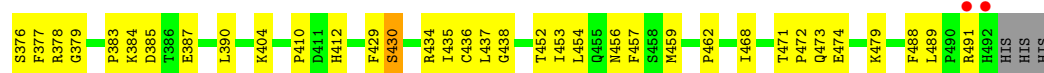


#### • Molecule 1: Cytochrome P450 2B6

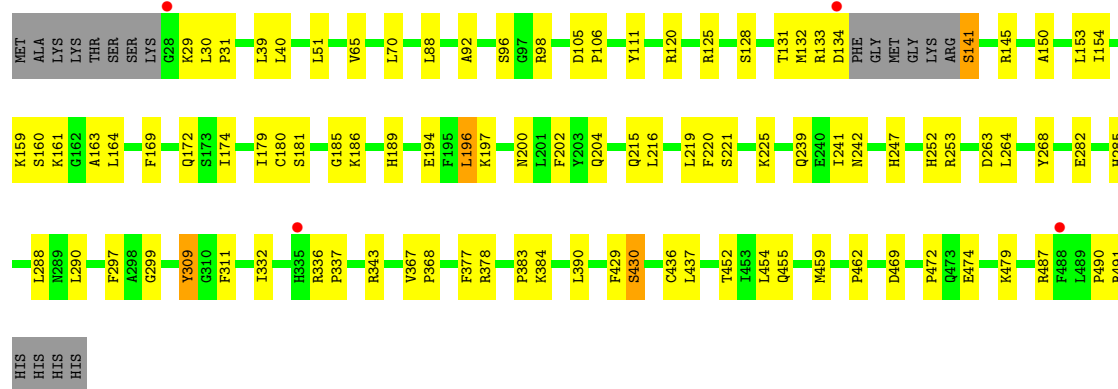
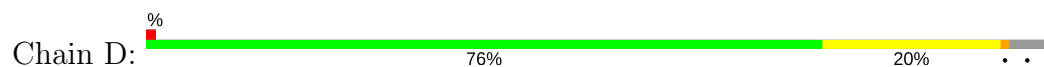


#### • Molecule 1: Cytochrome P450 2B6

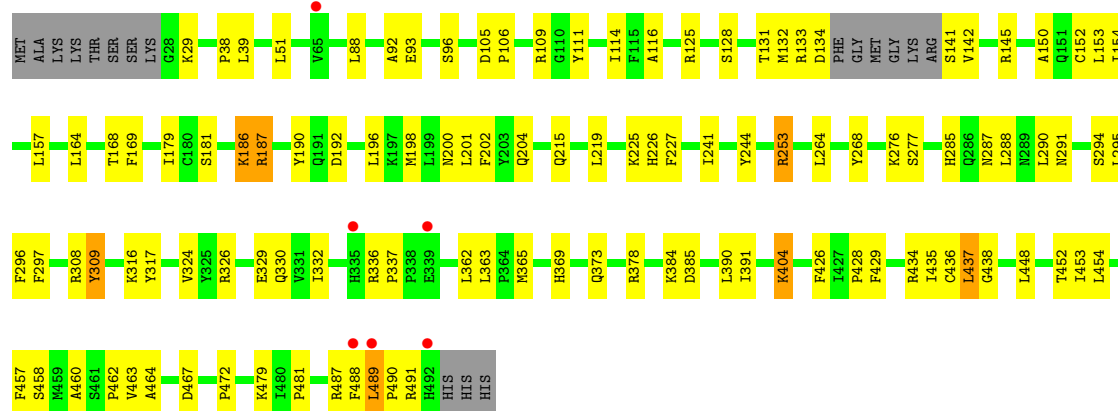


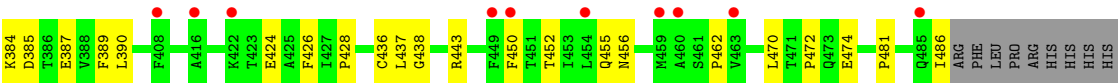


• Molecule 1: Cytochrome P450 2B6



• Molecule 1: Cytochrome P450 2B6





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.88Å 101.88Å 299.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.51 – 2.80 50.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.51-2.80) 88.9 (50.22-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.218 , 0.259 0.226 , 0.264	Depositor DCC
$R_{free}$ test set	3810 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 23.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l 0.149 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, CM5, 3QU

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	0.84	0/3833	0.75	1/5185 (0.0%)
1	B	0.83	0/3813	0.78	4/5158 (0.1%)
1	C	0.90	2/3822 (0.1%)	0.76	1/5167 (0.0%)
1	D	0.83	0/3791	0.78	2/5129 (0.0%)
1	E	0.82	0/3817	0.75	0/5162
1	F	0.95	1/3745 (0.0%)	0.78	0/5067
All	All	0.86	3/22821 (0.0%)	0.77	8/30868 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	450	PHE	CE2-CZ	5.42	1.47	1.37
1	C	152	CYS	CB-SG	-5.35	1.73	1.81
1	C	86	GLU	CG-CD	5.07	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	474	GLU	CB-CA-C	-5.88	98.64	110.40
1	A	185	GLY	N-CA-C	5.46	126.76	113.10
1	C	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	103	MET	CG-SD-CE	-5.40	91.57	100.20
1	B	35	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	437	LEU	CA-CB-CG	5.28	127.43	115.30
1	D	343	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3732	0	3712	103	0
1	B	3713	0	3702	93	0
1	C	3724	0	3711	83	0
1	D	3693	0	3682	97	0
1	E	3717	0	3713	117	0
1	F	3649	0	3635	100	0
2	A	43	0	30	10	0
2	B	43	0	30	4	0
2	C	43	0	30	9	0
2	D	43	0	30	12	0
2	E	43	0	30	9	0
2	F	43	0	30	18	0
3	A	7	0	4	0	0
3	B	16	0	10	0	0
3	C	7	0	4	0	0
3	D	13	0	10	0	0
3	E	13	0	10	1	0
4	A	34	0	35	1	0
4	B	68	0	77	34	0
4	C	34	0	40	5	0
4	D	68	0	78	12	0
4	E	34	0	40	3	0
4	F	34	0	38	5	0
5	A	25	0	0	1	0
5	B	23	0	0	12	0
5	C	29	0	0	2	0
5	D	38	0	0	5	0
5	E	23	0	0	5	0
5	F	12	0	0	5	0
All	All	22964	0	22681	629	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 14.

All (629) 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)
4:B:608:CM5:C16	4:B:608:CM5:O23	1.64	1.42
4:B:608:CM5:H17	4:B:608:CM5:C24	1.61	1.28
1:A:381:ILE:HG21	1:B:239:GLN:CG	1.65	1.25
1:A:136:GLY:HA2	1:A:142:VAL:CG2	1.65	1.24
1:B:232:ARG:HH12	4:B:602:CM5:C19	1.48	1.24
1:F:148:GLU:HG2	5:F:506:HOH:O	1.36	1.21
1:B:232:ARG:NH1	4:B:602:CM5:H191	1.54	1.19
1:A:381:ILE:HG21	1:B:239:GLN:HG2	1.24	1.16
1:E:384:LYS:O	1:E:385:ASP:HB2	1.46	1.15
1:E:362:LEU:O	1:E:363:LEU:HD23	1.48	1.10
1:E:253:ARG:HH11	1:E:253:ARG:CG	1.65	1.09
1:E:253:ARG:HG3	1:E:253:ARG:NH1	1.50	1.08
4:B:608:CM5:C24	4:B:608:CM5:C17	2.31	1.06
1:F:437:LEU:HD21	2:F:500:HEM:HMD1	1.36	1.03
4:B:608:CM5:O23	4:B:608:CM5:C17	2.06	1.02
4:B:608:CM5:H191	4:B:608:CM5:H12	1.41	1.01
4:B:602:CM5:H11	4:B:602:CM5:O22	1.60	1.00
1:E:198:MET:HE2	1:E:244:TYR:CD2	1.97	1.00
1:A:136:GLY:CA	1:A:142:VAL:CG2	2.41	0.98
2:A:500:HEM:HBC2	2:A:500:HEM:HHD	1.46	0.97
1:D:454:LEU:HD23	1:D:459:MET:CE	1.95	0.96
1:E:225:LYS:HE2	1:E:226:HIS:CE1	2.00	0.96
1:F:437:LEU:HD21	2:F:500:HEM:CMD	1.96	0.95
1:B:437:LEU:O	1:B:437:LEU:HD23	1.65	0.94
1:B:226:HIS:HB3	4:B:602:CM5:H32A	1.45	0.94
4:C:603:CM5:H301	4:C:603:CM5:H191	1.47	0.94
1:C:375:THR:C	1:C:376:SER:CA	2.37	0.93
1:B:232:ARG:HH12	4:B:602:CM5:H191	0.76	0.92
2:E:500:HEM:HHD	2:E:500:HEM:HBC2	1.53	0.91
1:D:253:ARG:HH12	1:D:285:HIS:CE1	1.88	0.91
1:E:437:LEU:C	1:E:437:LEU:HD23	1.92	0.90
1:F:437:LEU:CD2	2:F:500:HEM:HMD1	2.02	0.89
1:D:40:LEU:CD2	4:D:607:CM5:H102	2.02	0.88
1:A:136:GLY:HA2	1:A:142:VAL:HG22	1.54	0.88
1:E:128:SER:O	1:E:132:MET:HG2	1.74	0.87
1:A:437:LEU:O	1:A:437:LEU:HD12	1.74	0.87
1:A:381:ILE:HG12	1:B:239:GLN:HG3	1.55	0.87
1:A:88:LEU:HD11	1:A:390:LEU:HD13	1.54	0.87
1:A:88:LEU:HD21	1:A:390:LEU:HD11	1.56	0.87
1:A:88:LEU:HD11	1:A:390:LEU:CD1	2.05	0.86
1:D:39:LEU:CD2	4:F:606:CM5:H111	2.06	0.86
1:F:141:SER:O	1:F:145:ARG:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:C	1:A:437:LEU:HD12	1.96	0.85
1:D:454:LEU:CD2	1:D:459:MET:CE	2.55	0.85
1:A:134:ASP:OD2	1:A:134:ASP:C	2.14	0.85
1:A:336:ARG:HG2	1:A:336:ARG:HH11	1.42	0.85
1:A:381:ILE:HG21	1:B:239:GLN:HG3	1.58	0.84
4:B:608:CM5:H191	4:B:608:CM5:C1	2.05	0.84
1:A:136:GLY:O	1:A:142:VAL:HG23	1.78	0.84
1:A:384:LYS:O	1:A:385:ASP:HB2	1.77	0.83
1:D:454:LEU:HD23	1:D:459:MET:HE3	1.57	0.83
1:C:473:GLN:O	1:C:474:GLU:HG2	1.78	0.82
1:E:326:ARG:O	1:E:330:GLN:HG2	1.80	0.82
1:C:437:LEU:O	1:C:437:LEU:HD12	1.81	0.81
1:E:198:MET:CE	1:E:244:TYR:CD2	2.63	0.81
4:E:605:CM5:O20	4:E:605:CM5:O25	1.99	0.81
1:B:437:LEU:HD23	1:B:437:LEU:C	2.01	0.80
1:D:454:LEU:CD2	1:D:459:MET:HE1	2.11	0.80
1:D:454:LEU:HD23	1:D:459:MET:HE1	1.63	0.80
1:A:198:MET:HE1	1:A:241:ILE:HA	1.61	0.80
1:A:136:GLY:HA2	1:A:142:VAL:HG21	1.62	0.79
1:B:384:LYS:O	1:B:385:ASP:HB2	1.80	0.79
1:D:436:CYS:HB2	2:D:500:HEM:NA	1.95	0.79
1:F:128:SER:O	1:F:132:MET:HG2	1.82	0.79
1:F:384:LYS:O	1:F:385:ASP:HB2	1.83	0.79
1:E:157:LEU:HD22	1:E:488:PHE:CD2	2.18	0.78
1:A:437:LEU:CD1	1:A:437:LEU:O	2.31	0.78
1:F:88:LEU:HD11	1:F:390:LEU:CD1	2.14	0.78
1:E:436:CYS:HB2	2:E:500:HEM:NA	1.97	0.78
1:B:141:SER:HB3	1:B:144:GLU:HB2	1.65	0.77
1:E:152:CYS:HB3	5:E:508:HOH:O	1.83	0.77
1:A:136:GLY:C	1:A:142:VAL:HG23	2.04	0.77
1:A:136:GLY:C	1:A:142:VAL:CG2	2.53	0.77
1:D:253:ARG:NH1	1:D:285:HIS:NE2	2.32	0.77
4:B:608:CM5:C16	4:B:608:CM5:C24	2.63	0.76
1:F:299:GLY:N	2:F:500:HEM:HBC2	2.00	0.76
1:F:88:LEU:HD21	1:F:390:LEU:HD11	1.67	0.76
4:B:602:CM5:C1	4:B:602:CM5:O22	2.30	0.76
1:B:365:MET:HB2	5:B:506:HOH:O	1.84	0.76
1:A:136:GLY:CA	1:A:142:VAL:HG23	2.15	0.76
1:E:253:ARG:HH22	1:E:285:HIS:CE1	2.03	0.76
2:F:500:HEM:HMB1	2:F:500:HEM:HBB2	1.67	0.75
1:E:436:CYS:HB2	2:E:500:HEM:C1A	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:LEU:HD11	1:F:390:LEU:HD12	1.69	0.74
1:D:164:LEU:HD23	1:D:487:ARG:HG3	1.68	0.74
4:C:603:CM5:O25	4:C:603:CM5:C19	2.35	0.74
1:A:133:ARG:O	1:A:136:GLY:N	2.21	0.73
1:E:489:LEU:N	1:E:489:LEU:HD23	2.02	0.73
1:B:169:PHE:CE1	1:B:196:LEU:HG	2.24	0.72
2:F:500:HEM:HBB2	2:F:500:HEM:CMB	2.18	0.72
1:F:242:ASN:HB3	5:F:499:HOH:O	1.88	0.72
1:C:299:GLY:HA2	2:C:500:HEM:HBC2	1.72	0.72
1:F:131:THR:HG21	1:F:267:THR:HG21	1.72	0.72
1:D:39:LEU:HA	5:D:509:HOH:O	1.89	0.72
1:F:154:ILE:HD11	1:F:452:THR:HG22	1.71	0.72
1:A:336:ARG:HG2	1:A:336:ARG:NH1	2.03	0.71
4:C:603:CM5:O25	4:C:603:CM5:H191	1.91	0.71
4:B:608:CM5:H17	4:B:608:CM5:O25	1.90	0.71
1:D:39:LEU:HD21	4:F:606:CM5:H111	1.71	0.71
1:F:125:ARG:NH1	2:F:500:HEM:O1D	2.24	0.70
1:B:223:PHE:HA	4:B:602:CM5:H102	1.72	0.70
1:C:437:LEU:HD21	2:C:500:HEM:HMD1	1.74	0.70
1:A:136:GLY:CA	1:A:142:VAL:HG21	2.19	0.70
1:C:437:LEU:CD2	2:C:500:HEM:HMD1	2.21	0.69
1:B:128:SER:O	1:B:132:MET:HG2	1.92	0.69
1:F:437:LEU:CD2	2:F:500:HEM:CMD	2.68	0.69
1:B:491:ARG:O	1:B:492:HIS:CB	2.41	0.69
1:C:73:ARG:HD2	1:C:387:GLU:OE1	1.93	0.69
1:D:40:LEU:CD2	4:D:607:CM5:C10	2.70	0.69
1:E:253:ARG:HH11	1:E:253:ARG:HG3	0.70	0.69
1:E:488:PHE:O	1:E:490:PRO:HD3	1.93	0.69
1:F:437:LEU:O	1:F:437:LEU:HD12	1.93	0.69
1:D:252:HIS:NE2	1:D:263:ASP:OD2	2.26	0.68
1:C:179:ILE:HD11	2:C:500:HEM:HBC1	1.73	0.68
1:C:253:ARG:NH1	5:C:521:HOH:O	2.26	0.68
1:E:226:HIS:O	1:E:227:PHE:CG	2.47	0.68
1:C:456:ASN:O	1:C:491:ARG:N	2.20	0.67
1:E:384:LYS:O	1:E:385:ASP:CB	2.31	0.67
4:B:608:CM5:C19	4:B:608:CM5:C1	2.64	0.67
2:A:500:HEM:HBA1	2:A:500:HEM:HMA1	1.76	0.66
1:D:437:LEU:HD12	1:D:437:LEU:C	2.16	0.66
1:D:299:GLY:CA	2:D:500:HEM:HBC2	2.26	0.66
1:A:136:GLY:HA2	1:A:142:VAL:HG23	1.67	0.66
4:B:608:CM5:H191	4:B:608:CM5:H31A	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ILE:HG21	1:F:296:PHE:HA	1.77	0.66
1:B:200:ASN:O	1:B:204:GLN:HG2	1.94	0.66
2:C:500:HEM:HBB2	2:C:500:HEM:HMB2	1.75	0.66
1:E:332:ILE:HA	1:E:336:ARG:HH21	1.60	0.66
1:B:72:PRO:HB3	5:B:517:HOH:O	1.94	0.66
4:B:602:CM5:O20	4:B:602:CM5:O25	2.13	0.65
1:E:454:LEU:O	1:E:491:ARG:NH1	2.28	0.65
1:B:92:ALA:O	1:B:96:SER:HB3	1.97	0.65
1:F:181:SER:OG	1:F:182:ILE:N	2.30	0.65
1:D:128:SER:O	1:D:132:MET:HG2	1.96	0.65
1:E:458:SER:HB3	1:E:489:LEU:HB2	1.78	0.65
1:F:227:PHE:HA	4:F:606:CM5:O22	1.96	0.65
1:E:154:ILE:HD11	1:E:452:THR:HG22	1.78	0.65
1:D:437:LEU:O	1:D:437:LEU:HD12	1.97	0.65
1:F:377:PHE:O	1:F:378:ARG:C	2.32	0.64
1:F:299:GLY:CA	2:F:500:HEM:HBC2	2.27	0.64
1:A:198:MET:CE	1:A:241:ILE:HA	2.26	0.64
1:B:316:LYS:HG2	1:B:317:TYR:CE1	2.32	0.64
1:C:227:PHE:HA	4:C:603:CM5:O22	1.97	0.64
1:F:178:ILE:O	1:F:182:ILE:HG13	1.97	0.64
1:C:377:PHE:O	1:C:378:ARG:C	2.35	0.64
4:B:608:CM5:O12	4:B:608:CM5:H192	1.97	0.64
1:C:200:ASN:O	1:C:204:GLN:HG2	1.98	0.64
1:A:73:ARG:HD2	1:A:387:GLU:OE1	1.97	0.63
1:B:35:ARG:HB2	5:B:508:HOH:O	1.98	0.63
4:B:608:CM5:O22	4:B:608:CM5:H301	1.98	0.63
1:A:334:PRO:HD2	1:A:335:HIS:CD2	2.33	0.63
1:A:88:LEU:CD1	1:A:390:LEU:HD13	2.25	0.63
1:A:128:SER:O	1:A:132:MET:CG	2.47	0.63
1:E:169:PHE:CE2	1:E:196:LEU:HG	2.34	0.63
1:C:73:ARG:NE	1:C:387:GLU:OE1	2.32	0.63
1:E:316:LYS:HG2	1:E:316:LYS:O	1.99	0.62
1:F:47:ASP:CG	1:F:49:ARG:HH21	2.03	0.62
1:A:92:ALA:O	1:A:96:SER:HB3	1.98	0.62
1:B:133:ARG:O	1:B:134:ASP:C	2.38	0.62
1:E:164:LEU:HD21	1:E:462:PRO:HD3	1.80	0.62
1:E:88:LEU:HD21	1:E:390:LEU:HD11	1.79	0.62
1:F:141:SER:O	1:F:145:ARG:CG	2.46	0.62
1:C:384:LYS:O	1:C:385:ASP:HB2	1.99	0.62
1:D:181:SER:HA	1:D:186:LYS:H	1.64	0.62
1:E:198:MET:HE2	1:E:244:TYR:CG	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HD22	4:F:606:CM5:H52	1.82	0.61
1:C:133:ARG:HG2	1:C:134:ASP:N	2.14	0.61
1:A:136:GLY:C	1:A:142:VAL:HG21	2.21	0.61
1:A:437:LEU:C	1:A:437:LEU:CD1	2.68	0.61
1:C:154:ILE:HD11	1:C:452:THR:HG22	1.83	0.61
2:D:500:HEM:HBB2	2:D:500:HEM:CMB	2.31	0.61
1:E:198:MET:CE	1:E:244:TYR:HD2	2.10	0.61
1:B:154:ILE:HD11	1:B:452:THR:HG22	1.83	0.61
1:D:88:LEU:HD21	1:D:390:LEU:HD11	1.82	0.61
4:B:608:CM5:C18	4:B:608:CM5:H192	2.31	0.61
1:C:134:ASP:O	1:C:134:ASP:CG	2.40	0.60
1:B:232:ARG:NH1	4:B:602:CM5:C19	2.31	0.60
1:E:464:ALA:HB3	1:E:467:ASP:HB2	1.82	0.60
1:E:157:LEU:HD22	1:E:488:PHE:CE2	2.37	0.60
1:A:164:LEU:HD21	1:A:462:PRO:HD3	1.84	0.60
1:C:73:ARG:CD	1:C:387:GLU:OE1	2.50	0.60
1:E:192:ASP:O	1:E:196:LEU:HD13	2.01	0.60
1:F:299:GLY:HA2	2:F:500:HEM:HMC3	1.82	0.60
1:E:150:ALA:O	1:E:154:ILE:HG12	2.02	0.60
1:A:308:ARG:HH11	1:A:481:PRO:HG2	1.66	0.60
1:B:472:PRO:HG3	1:B:479:LYS:HE3	1.84	0.60
1:B:132:MET:HB3	5:B:503:HOH:O	2.01	0.59
1:F:316:LYS:HG2	1:F:317:TYR:CE1	2.37	0.59
2:A:500:HEM:CBA	2:A:500:HEM:CMA	2.80	0.59
1:B:491:ARG:O	1:B:492:HIS:HB3	2.02	0.59
1:C:133:ARG:O	1:C:134:ASP:C	2.41	0.59
1:D:141:SER:O	1:D:145:ARG:HD2	2.03	0.59
1:E:268:TYR:CE1	1:E:288:LEU:HB2	2.37	0.59
1:F:247:HIS:NE2	1:F:251:LYS:HE3	2.18	0.59
1:F:73:ARG:HD2	1:F:387:GLU:OE1	2.02	0.59
1:A:309:TYR:CD1	1:A:481:PRO:HB3	2.38	0.59
1:C:131:THR:HB	1:C:264:LEU:HD12	1.84	0.59
1:B:332:ILE:HA	1:B:336:ARG:NH2	2.16	0.59
1:C:473:GLN:HG3	1:C:474:GLU:HG2	1.84	0.59
1:D:454:LEU:CD2	1:D:459:MET:HE3	2.29	0.59
1:E:437:LEU:C	1:E:437:LEU:CD2	2.66	0.59
4:B:608:CM5:H191	4:B:608:CM5:C3	2.33	0.58
1:C:140:ARG:NH1	1:C:145:ARG:HG2	2.19	0.58
1:D:332:ILE:HA	1:D:336:ARG:HH21	1.69	0.58
1:D:40:LEU:HD23	4:D:607:CM5:H102	1.82	0.58
1:F:332:ILE:HA	1:F:336:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:PHE:O	1:F:379:GLY:N	2.36	0.58
1:F:164:LEU:HD21	1:F:462:PRO:HD3	1.85	0.58
1:B:226:HIS:CB	4:B:602:CM5:H32A	2.27	0.58
1:E:186:LYS:HG2	1:E:187:ARG:N	2.17	0.58
1:A:381:ILE:CG2	1:B:239:GLN:HG2	2.16	0.58
1:E:253:ARG:NH2	1:E:285:HIS:CE1	2.71	0.57
1:B:437:LEU:CD2	1:B:437:LEU:C	2.73	0.57
4:B:602:CM5:O20	4:B:602:CM5:C24	2.52	0.57
1:D:454:LEU:HD21	1:D:459:MET:HE1	1.85	0.57
1:D:164:LEU:HD21	1:D:462:PRO:HD3	1.87	0.57
1:A:69:HIS:NE2	1:A:74:PRO:HG3	2.18	0.57
1:F:73:ARG:NE	1:F:387:GLU:OE1	2.37	0.57
1:F:299:GLY:H	2:F:500:HEM:HBC2	1.70	0.57
1:B:69:HIS:HA	1:B:73:ARG:O	2.04	0.57
1:D:154:ILE:HD11	1:D:452:THR:HG22	1.85	0.57
1:C:436:CYS:HB2	2:C:500:HEM:NA	2.18	0.57
1:E:88:LEU:HD21	1:E:390:LEU:CD1	2.35	0.57
1:B:247:HIS:C	1:B:247:HIS:CD2	2.77	0.57
1:B:316:LYS:O	1:B:316:LYS:HG3	2.04	0.57
1:C:383:PRO:O	1:C:384:LYS:C	2.43	0.57
1:D:40:LEU:HD23	4:D:607:CM5:C11	2.35	0.56
4:B:608:CM5:H17	4:B:608:CM5:C26	2.35	0.56
1:F:47:ASP:OD2	1:F:49:ARG:NH2	2.36	0.56
1:A:202:PHE:CE2	1:A:241:ILE:HD13	2.40	0.56
1:E:141:SER:O	1:E:145:ARG:HG3	2.06	0.56
1:D:164:LEU:HG	1:D:487:ARG:CZ	2.35	0.56
1:A:198:MET:HE1	1:A:241:ILE:HG12	1.87	0.56
1:B:247:HIS:NE2	1:B:251:LYS:HE3	2.20	0.56
1:D:299:GLY:N	2:D:500:HEM:HBC2	2.21	0.56
1:A:198:MET:CE	1:A:241:ILE:HG23	2.35	0.56
1:A:128:SER:O	1:A:132:MET:HG2	2.06	0.56
1:A:38:PRO:O	1:A:39:LEU:HB2	2.06	0.55
1:B:430:SER:CB	2:B:500:HEM:HBA1	2.35	0.55
1:D:88:LEU:HD11	1:D:390:LEU:CD1	2.36	0.55
1:F:268:TYR:CG	1:F:288:LEU:HD13	2.41	0.55
1:F:287:ASN:O	1:F:291:ASN:HB2	2.06	0.55
1:A:40:LEU:O	1:A:41:GLY:C	2.45	0.55
1:B:223:PHE:CD1	4:B:608:CM5:H112	2.42	0.55
1:B:164:LEU:HD21	1:B:462:PRO:HD3	1.87	0.55
1:D:31:PRO:HB3	1:D:65:VAL:HG12	1.89	0.55
1:E:488:PHE:C	1:E:489:LEU:HD23	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ILE:HG22	1:F:182:ILE:O	2.06	0.55
1:B:126:ARG:CD	5:B:515:HOH:O	2.54	0.55
1:E:133:ARG:O	1:E:134:ASP:C	2.45	0.55
1:F:133:ARG:O	1:F:134:ASP:C	2.45	0.55
1:A:227:PHE:CE1	4:A:601:CM5:H22A	2.42	0.55
2:A:500:HEM:CBA	2:A:500:HEM:HMA1	2.37	0.55
1:F:275:GLU:O	1:F:277:SER:N	2.40	0.54
1:A:131:THR:HB	1:A:264:LEU:HD12	1.88	0.54
1:E:169:PHE:HZ	1:E:190:TYR:O	1.90	0.54
1:A:135:PHE:HB3	1:A:145:ARG:HH12	1.71	0.54
1:A:154:ILE:HD11	1:A:452:THR:HG22	1.89	0.54
1:A:382:ILE:HG22	1:A:386:THR:HB	1.89	0.54
1:D:179:ILE:HD11	2:D:500:HEM:HBC1	1.89	0.54
1:A:373:GLN:HA	1:A:384:LYS:HG3	1.88	0.54
1:C:86:GLU:OE2	1:C:378:ARG:NH2	2.25	0.54
1:C:88:LEU:HD11	1:C:390:LEU:HD13	1.89	0.54
1:A:197:LYS:HE2	1:A:240:GLU:OE1	2.07	0.54
1:E:435:ILE:HG12	1:E:436:CYS:N	2.22	0.54
1:A:381:ILE:CG2	1:B:239:GLN:CG	2.61	0.53
1:D:92:ALA:O	1:D:96:SER:HB3	2.09	0.53
1:E:253:ARG:NH1	1:E:253:ARG:CG	2.37	0.53
1:F:150:ALA:HB1	1:F:452:THR:HG21	1.90	0.53
1:E:92:ALA:O	1:E:96:SER:HB3	2.08	0.53
1:C:164:LEU:HD21	1:C:462:PRO:HD3	1.91	0.53
1:E:114:ILE:HG13	1:E:294:SER:HB3	1.89	0.53
1:E:404:LYS:HA	1:E:404:LYS:HE3	1.90	0.53
1:C:473:GLN:C	1:C:474:GLU:HG2	2.26	0.53
1:D:40:LEU:HD23	4:D:607:CM5:C10	2.38	0.53
1:A:429:PHE:CD1	1:A:439:GLU:HB2	2.44	0.53
1:C:473:GLN:O	1:C:474:GLU:CG	2.54	0.53
1:B:202:PHE:CE2	1:B:241:ILE:HD13	2.43	0.53
1:C:472:PRO:HG3	1:C:479:LYS:HE3	1.91	0.53
1:F:168:THR:OG1	1:F:308:ARG:HD3	2.07	0.53
2:F:500:HEM:HMB1	2:F:500:HEM:CBB	2.36	0.53
1:A:133:ARG:O	1:A:136:GLY:CA	2.56	0.53
1:C:92:ALA:O	1:C:96:SER:HB3	2.09	0.53
1:C:140:ARG:NH1	1:C:145:ARG:CG	2.72	0.52
1:E:332:ILE:HA	1:E:336:ARG:NH2	2.23	0.52
1:F:275:GLU:C	1:F:277:SER:H	2.12	0.52
1:E:472:PRO:HG3	1:E:479:LYS:HE3	1.91	0.52
1:A:37:LEU:HD12	5:A:508:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:HG21	1:A:74:PRO:HB3	1.91	0.52
1:B:126:ARG:HD2	5:B:515:HOH:O	2.08	0.52
1:E:88:LEU:HD11	1:E:390:LEU:CD1	2.39	0.52
1:A:434:ARG:O	1:A:435:ILE:C	2.47	0.52
1:D:311:PHE:HE1	1:D:459:MET:HE1	1.75	0.52
1:D:332:ILE:HA	1:D:336:ARG:NH2	2.25	0.52
1:C:158:ARG:C	1:C:160:SER:H	2.12	0.52
1:C:434:ARG:O	1:C:435:ILE:C	2.46	0.51
1:D:133:ARG:O	1:D:134:ASP:C	2.47	0.51
1:E:116:ALA:O	1:E:434:ARG:NH2	2.30	0.51
1:D:120:ARG:HA	1:D:282:GLU:HG3	1.91	0.51
1:F:257:ASP:O	1:F:260:ALA:N	2.36	0.51
1:E:463:VAL:HG12	1:E:464:ALA:N	2.25	0.51
1:A:381:ILE:CG2	1:B:239:GLN:HG3	2.37	0.51
2:D:500:HEM:HBB2	2:D:500:HEM:HMB2	1.91	0.51
1:E:437:LEU:HD23	1:E:438:GLY:N	2.26	0.51
1:F:437:LEU:HD21	2:F:500:HEM:HMD2	1.87	0.51
1:E:51:LEU:HG	1:E:215:GLN:HB3	1.92	0.51
1:F:73:ARG:CD	1:F:387:GLU:OE1	2.58	0.51
1:B:318:PRO:O	1:B:322:GLU:HG2	2.11	0.51
1:E:326:ARG:O	1:E:330:GLN:CG	2.55	0.51
1:B:70:LEU:HB3	1:B:219:LEU:HD12	1.93	0.51
1:F:437:LEU:C	1:F:437:LEU:HD12	2.31	0.51
1:D:472:PRO:HG3	1:D:479:LYS:HE3	1.93	0.50
1:D:220:PHE:CE1	4:D:607:CM5:H112	2.46	0.50
1:E:168:THR:OG1	1:E:308:ARG:HD3	2.11	0.50
1:F:180:CYS:HA	1:F:184:PHE:HD2	1.77	0.50
1:C:225:LYS:CG	1:C:225:LYS:O	2.58	0.50
1:C:429:PHE:O	1:C:430:SER:CB	2.59	0.50
1:F:299:GLY:CA	2:F:500:HEM:CBC	2.89	0.50
1:D:430:SER:CB	2:D:500:HEM:HBA1	2.42	0.50
1:F:179:ILE:HG12	1:F:299:GLY:HA3	1.93	0.50
1:C:410:PRO:C	1:C:412:HIS:H	2.13	0.50
1:E:457:PHE:HA	1:E:490:PRO:HA	1.93	0.50
1:F:38:PRO:O	1:F:39:LEU:HB2	2.10	0.50
1:C:299:GLY:CA	2:C:500:HEM:HBC2	2.40	0.50
1:D:181:SER:O	1:D:185:GLY:HA2	2.11	0.50
1:D:70:LEU:HB3	1:D:219:LEU:HD12	1.93	0.50
1:B:247:HIS:O	1:B:247:HIS:CD2	2.64	0.50
1:C:134:ASP:OD2	1:C:134:ASP:O	2.30	0.50
1:D:125:ARG:NH1	2:D:500:HEM:O1D	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:PHE:CE2	1:E:241:ILE:HD13	2.46	0.50
1:F:47:ASP:OD2	1:F:49:ARG:NE	2.45	0.50
1:C:286:GLN:HG3	1:E:384:LYS:HD2	1.93	0.50
1:E:131:THR:HB	1:E:264:LEU:HD12	1.93	0.50
1:E:125:ARG:NH1	1:E:435:ILE:O	2.43	0.50
1:E:472:PRO:CG	1:E:479:LYS:HE3	2.42	0.49
1:E:227:PHE:HA	4:E:605:CM5:O22	2.12	0.49
2:A:500:HEM:CHD	2:A:500:HEM:HBC2	2.25	0.49
1:C:40:LEU:O	1:C:41:GLY:C	2.50	0.49
1:B:169:PHE:CD1	1:B:196:LEU:HG	2.47	0.49
1:B:268:TYR:CG	1:B:288:LEU:HD13	2.47	0.49
1:D:150:ALA:O	1:D:154:ILE:HG12	2.12	0.49
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.94	0.49
1:B:169:PHE:CD1	1:B:199:LEU:HD12	2.48	0.49
1:D:185:GLY:O	1:D:186:LYS:HB3	2.12	0.49
1:D:88:LEU:HD21	1:D:390:LEU:CD1	2.42	0.49
1:C:268:TYR:CE1	1:C:288:LEU:HB2	2.48	0.49
1:C:287:ASN:O	1:C:291:ASN:CB	2.61	0.49
1:D:469:ASP:HB3	5:D:527:HOH:O	2.13	0.49
1:F:120:ARG:HA	1:F:282:GLU:HG3	1.95	0.49
1:A:373:GLN:CA	1:A:384:LYS:HG3	2.42	0.49
1:C:150:ALA:O	1:C:154:ILE:HG12	2.12	0.49
1:F:149:GLU:OE2	1:F:177:ASN:ND2	2.45	0.49
1:F:310:GLY:O	1:F:313:LEU:HB2	2.13	0.49
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.48	0.49
1:D:429:PHE:O	1:D:430:SER:HB3	2.13	0.49
1:A:384:LYS:HD2	1:B:286:GLN:HG3	1.95	0.48
1:B:150:ALA:O	1:B:154:ILE:HG12	2.14	0.48
1:C:133:ARG:CG	1:C:134:ASP:N	2.76	0.48
2:F:500:HEM:HBD1	2:F:500:HEM:HHA	1.94	0.48
1:A:318:PRO:O	1:A:322:GLU:HG2	2.13	0.48
1:C:436:CYS:HB2	2:C:500:HEM:C4A	2.48	0.48
1:F:486:ILE:C	5:F:497:HOH:O	2.52	0.48
1:B:297:PHE:C	1:B:297:PHE:HD2	2.17	0.48
1:B:47:ASP:OD1	1:B:48:ARG:N	2.46	0.48
1:C:189:HIS:CD2	1:C:191:GLN:OE1	2.66	0.48
1:F:150:ALA:O	1:F:154:ILE:HG12	2.12	0.48
1:C:153:LEU:HD21	1:C:453:ILE:HD11	1.95	0.48
4:D:604:CM5:O32	4:D:604:CM5:O31	2.19	0.48
1:F:114:ILE:HG13	1:F:294:SER:HB3	1.95	0.48
1:B:430:SER:HB2	2:B:500:HEM:HBA1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:LEU:O	1:F:472:PRO:HD3	2.14	0.48
1:A:309:TYR:OH	1:A:472:PRO:HG3	2.13	0.48
1:D:472:PRO:CG	1:D:479:LYS:HE3	2.44	0.48
1:D:88:LEU:HD11	1:D:390:LEU:HD12	1.94	0.48
1:D:309:TYR:OH	1:D:472:PRO:HG3	2.14	0.48
1:B:120:ARG:HA	1:B:282:GLU:HG3	1.96	0.47
1:E:38:PRO:O	1:E:39:LEU:HB2	2.14	0.47
1:B:297:PHE:C	1:B:297:PHE:CD2	2.87	0.47
1:E:226:HIS:C	1:E:227:PHE:CG	2.88	0.47
1:E:435:ILE:CG1	1:E:436:CYS:H	2.27	0.47
1:E:458:SER:O	1:E:489:LEU:N	2.38	0.47
1:F:332:ILE:HA	1:F:336:ARG:NH2	2.29	0.47
1:F:443:ARG:HB3	5:F:508:HOH:O	2.14	0.47
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.95	0.47
1:A:150:ALA:O	1:A:154:ILE:HG12	2.14	0.47
1:E:219:LEU:N	1:E:219:LEU:CD1	2.78	0.47
1:F:436:CYS:HB2	2:F:500:HEM:NA	2.29	0.47
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.50	0.47
1:D:163:ALA:HA	1:D:487:ARG:NH1	2.28	0.47
1:D:40:LEU:HD22	4:D:607:CM5:H102	1.95	0.47
1:A:431:LEU:HA	1:A:435:ILE:HD12	1.96	0.47
1:A:169:PHE:CE1	1:A:199:LEU:HD12	2.49	0.47
1:B:365:MET:N	5:B:506:HOH:O	2.33	0.47
1:D:153:LEU:HD22	1:D:174:ILE:HD13	1.96	0.47
2:E:500:HEM:CBC	2:E:500:HEM:HHD	2.35	0.47
1:F:88:LEU:CD1	1:F:390:LEU:CD1	2.90	0.47
2:A:500:HEM:CBC	2:A:500:HEM:HHD	2.33	0.47
1:F:257:ASP:HB3	1:F:260:ALA:HB3	1.96	0.47
1:A:134:ASP:OD2	1:A:135:PHE:N	2.48	0.47
1:E:309:TYR:OH	1:E:472:PRO:HG3	2.15	0.47
1:A:434:ARG:NH1	2:A:500:HEM:O2D	2.47	0.47
1:E:462:PRO:HB2	5:E:520:HOH:O	2.15	0.47
1:E:287:ASN:O	1:E:291:ASN:CB	2.64	0.47
1:E:316:LYS:HD3	1:E:317:TYR:CE1	2.50	0.47
1:E:435:ILE:CG1	1:E:436:CYS:N	2.78	0.47
1:F:86:GLU:O	1:F:90:ASP:HB2	2.14	0.47
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.50	0.46
1:E:429:PHE:HB2	5:E:511:HOH:O	2.15	0.46
1:F:200:ASN:O	1:F:204:GLN:HG2	2.15	0.46
1:C:242:ASN:HB3	5:C:508:HOH:O	2.15	0.46
1:D:437:LEU:O	1:D:437:LEU:CD1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:ASN:O	1:F:291:ASN:CB	2.64	0.46
1:F:51:LEU:HG	1:F:215:GLN:HB3	1.97	0.46
1:B:57:ARG:HB3	1:B:57:ARG:HE	1.37	0.46
1:D:454:LEU:HD21	1:D:459:MET:CE	2.43	0.46
1:D:200:ASN:O	1:D:204:GLN:HG2	2.15	0.46
1:D:383:PRO:O	1:D:384:LYS:C	2.54	0.46
1:C:158:ARG:C	1:C:160:SER:N	2.69	0.46
1:F:183:VAL:HG12	1:F:184:PHE:N	2.28	0.46
1:A:429:PHE:CE1	1:A:439:GLU:HA	2.50	0.46
1:B:314:MET:O	5:B:513:HOH:O	2.21	0.46
1:D:40:LEU:HD21	4:D:607:CM5:C10	2.45	0.46
1:A:208:LEU:O	1:A:211:SER:OG	2.25	0.46
2:D:500:HEM:HMB2	2:D:500:HEM:CBB	2.46	0.46
1:E:200:ASN:O	1:E:204:GLN:HG2	2.15	0.46
1:E:111:TYR:HB2	1:E:290:LEU:HD12	1.98	0.46
1:B:150:ALA:HB1	1:B:452:THR:HG21	1.97	0.46
1:C:437:LEU:HD21	2:C:500:HEM:CMD	2.44	0.46
1:C:286:GLN:HG2	1:E:373:GLN:CB	2.45	0.46
1:B:299:GLY:HA2	2:B:500:HEM:HMC3	1.97	0.45
1:F:212:VAL:O	1:F:213:PHE:C	2.50	0.45
1:A:128:SER:O	1:A:132:MET:HG3	2.16	0.45
1:C:316:LYS:HD2	1:C:468:ILE:HB	1.98	0.45
1:F:309:TYR:OH	1:F:472:PRO:HG3	2.16	0.45
1:D:39:LEU:N	5:D:509:HOH:O	2.49	0.45
1:E:436:CYS:CB	2:E:500:HEM:NA	2.69	0.45
1:B:73:ARG:HD2	1:B:387:GLU:OE1	2.17	0.45
1:D:131:THR:HB	1:D:264:LEU:HD12	1.99	0.45
1:E:169:PHE:CZ	1:E:190:TYR:O	2.68	0.45
1:E:226:HIS:O	1:E:227:PHE:CD1	2.70	0.45
1:E:437:LEU:O	1:E:437:LEU:HG	2.17	0.45
1:F:318:PRO:O	1:F:322:GLU:HG2	2.16	0.45
1:A:287:ASN:O	1:A:291:ASN:CB	2.65	0.45
1:E:105:ASP:O	1:E:109:ARG:HG2	2.17	0.45
4:D:604:CM5:C30	4:D:604:CM5:O21	2.65	0.45
1:F:443:ARG:C	5:F:508:HOH:O	2.55	0.45
4:B:608:CM5:H18	4:B:608:CM5:H192	1.98	0.45
1:A:135:PHE:O	1:A:145:ARG:NH1	2.49	0.45
1:D:164:LEU:H	1:D:487:ARG:NH1	2.15	0.45
1:E:308:ARG:NH1	1:E:481:PRO:HG2	2.32	0.45
1:F:182:ILE:CG2	1:F:182:ILE:O	2.64	0.45
1:F:275:GLU:C	1:F:277:SER:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.81	0.44
1:B:220:PHE:HD1	4:B:608:CM5:H22A	1.82	0.44
1:E:458:SER:CB	1:E:489:LEU:O	2.64	0.44
1:F:299:GLY:HA2	2:F:500:HEM:CMC	2.46	0.44
1:B:51:LEU:HG	1:B:215:GLN:HB3	1.98	0.44
1:C:189:HIS:O	1:C:191:GLN:N	2.51	0.44
1:D:436:CYS:HB2	2:D:500:HEM:C1A	2.52	0.44
1:E:153:LEU:HD21	1:E:453:ILE:HD11	2.00	0.44
1:A:200:ASN:O	1:A:204:GLN:HG2	2.18	0.44
1:E:219:LEU:N	1:E:219:LEU:HD12	2.32	0.44
1:E:268:TYR:CG	1:E:288:LEU:HD13	2.53	0.44
1:C:221:SER:O	1:C:225:LYS:HB3	2.17	0.44
1:D:196:LEU:O	1:D:197:LYS:C	2.54	0.44
1:D:164:LEU:N	1:D:487:ARG:HG2	2.32	0.44
1:F:257:ASP:HA	1:F:258:PRO:HD2	1.86	0.44
1:B:88:LEU:HD11	1:B:390:LEU:HD13	1.99	0.44
1:A:332:ILE:HA	1:A:336:ARG:NH2	2.33	0.44
1:A:426:PHE:CZ	1:A:428:PRO:HG3	2.53	0.44
1:D:29:LYS:HB3	1:D:30:LEU:H	1.58	0.44
1:E:201:LEU:HA	1:E:201:LEU:HD23	1.69	0.44
1:F:47:ASP:OD2	1:F:49:ARG:HB2	2.18	0.44
1:B:127:PHE:O	1:B:131:THR:HG22	2.17	0.44
1:C:436:CYS:C	1:C:438:GLY:H	2.21	0.44
1:C:98:ARG:HD3	1:C:368:PRO:O	2.18	0.44
1:E:227:PHE:CZ	4:E:605:CM5:H52	2.53	0.44
1:B:365:MET:CA	5:B:506:HOH:O	2.65	0.44
1:E:157:LEU:CD2	1:E:488:PHE:CE2	3.01	0.44
1:A:132:MET:HE2	1:A:132:MET:HB3	1.72	0.43
1:B:437:LEU:HD13	2:B:500:HEM:HMD1	1.99	0.43
1:B:223:PHE:HD2	4:B:602:CM5:H92	1.83	0.43
1:E:181:SER:HA	1:E:186:LYS:H	1.83	0.43
1:E:436:CYS:HA	2:E:500:HEM:CHA	2.48	0.43
1:F:231:HIS:H	1:F:231:HIS:CD2	2.36	0.43
2:D:500:HEM:CBB	2:D:500:HEM:CMB	2.97	0.43
1:F:437:LEU:HG	2:F:500:HEM:C2D	2.52	0.43
1:D:436:CYS:HB2	2:D:500:HEM:C4A	2.53	0.43
1:A:51:LEU:HG	1:A:215:GLN:HB3	2.00	0.43
1:B:169:PHE:CE1	1:B:196:LEU:CD1	3.01	0.43
1:D:39:LEU:HD22	4:F:606:CM5:H111	1.93	0.43
1:A:309:TYR:CG	1:A:481:PRO:HB3	2.53	0.43
1:B:53:LYS:HA	1:B:53:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:PHE:CZ	1:E:428:PRO:HG3	2.54	0.43
1:C:285:HIS:CE1	1:E:93:GLU:HG2	2.53	0.43
1:A:153:LEU:HD21	1:A:453:ILE:HD11	2.00	0.43
1:B:441:ILE:HD11	5:B:503:HOH:O	2.18	0.43
1:C:168:THR:OG1	1:C:308:ARG:HD3	2.18	0.43
1:C:287:ASN:O	1:C:291:ASN:HB2	2.19	0.43
1:A:446:LEU:HD23	1:A:446:LEU:HA	1.87	0.43
1:C:457:PHE:HA	1:C:489:LEU:O	2.18	0.43
2:E:500:HEM:C1A	3:E:501:3QU:HAC	2.54	0.43
1:F:178:ILE:O	1:F:181:SER:OG	2.36	0.43
1:C:253:ARG:HG2	1:C:253:ARG:NH1	2.33	0.43
1:D:98:ARG:HD3	1:D:368:PRO:O	2.19	0.43
1:E:460:ALA:O	1:E:487:ARG:HB2	2.19	0.43
1:F:98:ARG:HG3	1:F:99:GLY:O	2.19	0.43
1:E:296:PHE:O	1:E:296:PHE:CD1	2.72	0.43
1:E:437:LEU:O	1:E:437:LEU:CG	2.66	0.43
1:F:119:ASN:O	1:F:120:ARG:C	2.56	0.43
1:F:276:LYS:O	1:F:276:LYS:HG3	2.18	0.43
1:A:67:THR:CG2	1:A:74:PRO:HB3	2.47	0.43
1:B:127:PHE:HE1	1:B:264:LEU:HD21	1.83	0.43
1:C:454:LEU:HD21	1:C:459:MET:HE1	2.01	0.43
1:E:226:HIS:C	1:E:227:PHE:CD2	2.93	0.43
1:F:202:PHE:CE2	1:F:241:ILE:HD13	2.53	0.43
1:B:226:HIS:CE1	4:B:602:CM5:H101	2.53	0.42
1:D:202:PHE:CE2	1:D:241:ILE:HD13	2.54	0.42
4:D:604:CM5:O20	4:D:604:CM5:O23	2.24	0.42
1:B:297:PHE:O	1:B:297:PHE:HD2	2.02	0.42
1:B:73:ARG:NE	1:B:387:GLU:OE1	2.51	0.42
1:D:39:LEU:CA	5:D:509:HOH:O	2.57	0.42
1:E:463:VAL:CG1	1:E:464:ALA:N	2.82	0.42
1:F:455:GLN:HB3	1:F:456:ASN:HD22	1.85	0.42
1:A:132:MET:SD	1:A:295:LEU:HD22	2.59	0.42
1:F:88:LEU:HG	1:F:390:LEU:HD13	2.01	0.42
1:A:57:ARG:O	1:A:58:PHE:C	2.56	0.42
1:C:127:PHE:CZ	1:C:131:THR:HG21	2.55	0.42
1:D:247:HIS:CD2	1:D:247:HIS:C	2.92	0.42
1:E:142:VAL:HG21	5:E:517:HOH:O	2.19	0.42
1:E:225:LYS:HE2	1:E:226:HIS:NE2	2.32	0.42
1:E:324:VAL:HG11	1:E:454:LEU:HD12	2.01	0.42
1:F:309:TYR:CE2	1:F:481:PRO:HB3	2.55	0.42
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:LEU:HD22	1:C:488:PHE:CD2	2.55	0.42
1:D:437:LEU:CD1	1:D:437:LEU:C	2.87	0.42
1:D:98:ARG:NH1	1:D:367:VAL:HG12	2.34	0.42
1:E:365:MET:HG2	1:E:391:ILE:HD12	2.02	0.42
1:F:474:GLU:HA	1:F:474:GLU:OE1	2.19	0.42
1:A:429:PHE:CG	1:A:439:GLU:HB2	2.55	0.42
1:C:297:PHE:C	1:C:297:PHE:CD2	2.93	0.42
1:E:179:ILE:HG21	1:E:296:PHE:HA	2.02	0.42
1:A:308:ARG:HH12	1:A:481:PRO:HD2	1.85	0.42
1:C:268:TYR:CG	1:C:288:LEU:HD13	2.54	0.42
1:C:114:ILE:HG13	1:C:294:SER:HB3	2.02	0.42
1:C:337:PRO:O	1:C:338:PRO:C	2.57	0.42
1:D:429:PHE:O	1:D:430:SER:CB	2.68	0.42
1:A:181:SER:O	1:A:185:GLY:HA2	2.20	0.42
1:B:220:PHE:CD1	4:B:608:CM5:H22A	2.54	0.42
1:C:410:PRO:C	1:C:412:HIS:N	2.73	0.42
1:D:169:PHE:O	1:D:172:GLN:HB2	2.19	0.42
1:D:51:LEU:HG	1:D:215:GLN:HB3	2.02	0.42
1:F:268:TYR:CE1	1:F:288:LEU:HB2	2.54	0.42
1:A:193:GLN:H	1:A:193:GLN:HG3	1.65	0.42
1:A:120:ARG:HA	1:A:282:GLU:HG3	2.02	0.42
1:B:126:ARG:NE	5:B:515:HOH:O	2.53	0.42
2:A:500:HEM:HBA1	2:A:500:HEM:CMA	2.45	0.41
1:A:125:ARG:NH1	2:A:500:HEM:O1D	2.53	0.41
1:B:153:LEU:HD21	1:B:453:ILE:HD11	2.02	0.41
1:A:373:GLN:HA	1:B:286:GLN:HG2	2.02	0.41
1:C:185:GLY:O	1:C:186:LYS:HB3	2.20	0.41
1:D:159:LYS:O	1:D:161:LYS:HG3	2.19	0.41
1:A:157:LEU:HD22	1:A:488:PHE:CD2	2.55	0.41
1:C:131:THR:CB	1:C:264:LEU:HD12	2.48	0.41
1:D:216:LEU:HA	1:D:216:LEU:HD12	1.89	0.41
1:D:239:GLN:OE1	1:D:239:GLN:HA	2.20	0.41
1:F:297:PHE:CD2	1:F:297:PHE:C	2.93	0.41
1:F:436:CYS:C	1:F:438:GLY:H	2.23	0.41
1:B:434:ARG:HB2	5:B:505:HOH:O	2.20	0.41
1:B:446:LEU:HA	1:B:446:LEU:HD23	1.91	0.41
1:C:187:ARG:HG3	1:C:188:PHE:N	2.35	0.41
1:C:269:LEU:O	1:C:272:MET:HB3	2.21	0.41
1:E:435:ILE:HG12	1:E:436:CYS:H	1.83	0.41
1:B:455:GLN:HB3	1:B:456:ASN:HD22	1.85	0.41
1:C:471:THR:HA	1:C:472:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:HIS:HE2	2:E:500:HEM:CGA	2.33	0.41
1:E:436:CYS:HB2	2:E:500:HEM:C4A	2.54	0.41
1:A:181:SER:HA	1:A:186:LYS:O	2.21	0.41
1:B:157:LEU:HD22	1:B:488:PHE:CD2	2.55	0.41
1:D:179:ILE:CG2	1:D:180:CYS:N	2.82	0.41
1:E:226:HIS:O	1:E:227:PHE:CD2	2.73	0.41
1:E:362:LEU:C	1:E:363:LEU:HD23	2.34	0.41
1:E:448:LEU:HA	1:E:448:LEU:HD23	1.90	0.41
1:E:458:SER:N	1:E:489:LEU:O	2.53	0.41
1:F:188:PHE:HZ	1:F:244:TYR:HH	1.67	0.41
1:F:196:LEU:O	1:F:197:LYS:C	2.58	0.41
1:B:47:ASP:C	1:B:47:ASP:OD1	2.59	0.41
1:C:377:PHE:O	1:C:379:GLY:N	2.52	0.41
1:F:309:TYR:CD2	1:F:481:PRO:HB3	2.55	0.41
1:B:426:PHE:CZ	1:B:428:PRO:HG3	2.56	0.41
1:C:99:GLY:HA3	1:C:368:PRO:HB2	2.02	0.41
1:C:226:HIS:CG	4:C:603:CM5:H71	2.55	0.41
1:E:105:ASP:N	1:E:106:PRO:CD	2.84	0.41
1:E:336:ARG:HA	1:E:337:PRO:HD2	1.93	0.41
1:E:88:LEU:HD11	1:E:390:LEU:HD12	2.02	0.41
1:F:194:GLU:O	1:F:198:MET:HG2	2.21	0.41
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.88	0.41
4:B:608:CM5:O22	4:B:608:CM5:C30	2.67	0.41
1:D:160:SER:O	1:D:161:LYS:C	2.58	0.41
1:D:221:SER:O	1:D:225:LYS:HB3	2.21	0.41
1:D:455:GLN:O	1:D:491:ARG:HD2	2.21	0.41
4:D:604:CM5:H301	4:D:604:CM5:O21	2.21	0.41
1:F:77:MET:SD	1:F:389:PHE:HB2	2.61	0.41
1:D:247:HIS:CD2	1:D:247:HIS:O	2.74	0.41
1:F:426:PHE:CZ	1:F:428:PRO:HG3	2.56	0.41
1:D:336:ARG:HA	1:D:337:PRO:HD2	1.85	0.41
1:F:126:ARG:O	1:F:127:PHE:C	2.58	0.41
1:A:29:LYS:O	1:A:30:LEU:C	2.59	0.40
1:A:332:ILE:HG23	1:A:336:ARG:NH1	2.36	0.40
1:A:351:ALA:HB1	1:A:413:PHE:HB2	2.02	0.40
1:A:88:LEU:HD21	1:A:390:LEU:CD1	2.40	0.40
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.85	0.40
1:D:105:ASP:N	1:D:106:PRO:CD	2.84	0.40
1:C:181:SER:HA	1:C:186:LYS:H	1.85	0.40
1:D:111:TYR:HB2	1:D:290:LEU:HD12	2.03	0.40
1:D:242:ASN:HB3	5:D:523:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:PHE:O	1:D:378:ARG:C	2.60	0.40
1:E:190:TYR:HB2	5:E:518:HOH:O	2.21	0.40
1:C:286:GLN:HG2	1:E:373:GLN:HA	2.03	0.40
1:F:334:PRO:C	1:F:335:HIS:HD1	2.25	0.40
1:A:81:VAL:O	1:A:82:GLU:C	2.60	0.40
1:D:179:ILE:HG22	1:D:180:CYS:N	2.36	0.40
1:D:263:ASP:OD1	1:D:263:ASP:C	2.59	0.40
1:A:308:ARG:NH1	1:A:481:PRO:HD2	2.37	0.40
2:A:500:HEM:HBB2	2:A:500:HEM:CMB	2.51	0.40
1:B:226:HIS:ND1	4:B:602:CM5:H101	2.36	0.40
1:A:472:PRO:HG3	1:A:479:LYS:HE3	2.04	0.40
1:B:131:THR:HG23	1:B:264:LEU:CD1	2.52	0.40
1:B:316:LYS:HG2	1:B:317:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

## 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	458/476 (96%)	436 (95%)	18 (4%)	4 (1%)	20	52
1	B	455/476 (96%)	431 (95%)	21 (5%)	3 (1%)	25	59
1	C	456/476 (96%)	424 (93%)	30 (7%)	2 (0%)	38	72
1	D	454/476 (95%)	424 (93%)	28 (6%)	2 (0%)	38	72
1	E	455/476 (96%)	433 (95%)	22 (5%)	0	100	100
1	F	449/476 (94%)	417 (93%)	29 (6%)	3 (1%)	25	59
All	All	2727/2856 (96%)	2565 (94%)	148 (5%)	14 (0%)	32	67

All (14) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	C	430	SER
1	F	276	LYS
1	F	378	ARG
1	B	430	SER
1	C	190	TYR
1	F	424	GLU
1	A	92	ALA
1	D	430	SER
1	B	334	PRO
1	B	74	PRO
1	A	72	PRO
1	A	435	ILE
1	D	490	PRO
1	A	41	GLY

### 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	404/418 (97%)	392 (97%)	12 (3%)	46	80
1	B	403/418 (96%)	391 (97%)	12 (3%)	46	80
1	C	402/418 (96%)	393 (98%)	9 (2%)	57	87
1	D	400/418 (96%)	394 (98%)	6 (2%)	70	92
1	E	404/418 (97%)	390 (96%)	14 (4%)	41	75
1	F	396/418 (95%)	387 (98%)	9 (2%)	56	86
All	All	2409/2508 (96%)	2347 (97%)	62 (3%)	51	83

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	40	LEU
1	A	57	ARG
1	A	132	MET
1	A	133	ARG

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Mol	Chain	Res	Type
1	A	134	ASP
1	A	187	ARG
1	A	196	LEU
1	A	259	SER
1	A	297	PHE
1	A	309	TYR
1	A	437	LEU
1	B	48	ARG
1	B	57	ARG
1	B	109	ARG
1	B	186	LYS
1	B	187	ARG
1	B	196	LEU
1	B	200	ASN
1	B	247	HIS
1	B	297	PHE
1	B	309	TYR
1	B	437	LEU
1	B	489	LEU
1	C	133	ARG
1	C	134	ASP
1	C	139	LYS
1	C	160	SER
1	C	187	ARG
1	C	225	LYS
1	C	297	PHE
1	C	309	TYR
1	C	404	LYS
1	D	141	SER
1	D	189	HIS
1	D	194	GLU
1	D	196	LEU
1	D	297	PHE
1	D	309	TYR
1	E	29	LYS
1	E	186	LYS
1	E	187	ARG
1	E	253	ARG
1	E	276	LYS
1	E	277	SER
1	E	295	LEU
1	E	297	PHE

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Mol	Chain	Res	Type
1	E	309	TYR
1	E	329	GLU
1	E	378	ARG
1	E	404	LYS
1	E	437	LEU
1	E	489	LEU
1	F	48	ARG
1	F	145	ARG
1	F	151	GLN
1	F	182	ILE
1	F	186	LYS
1	F	259	SER
1	F	297	PHE
1	F	309	TYR
1	F	335	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	GLN
1	B	455	GLN
1	B	456	ASN
1	C	231	HIS
1	C	285	HIS
1	E	226	HIS
1	E	286	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

19 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	28,50,50	2.26	6 (21%)	17,82,82	1.39	1 (5%)
3	3QU	A	501	2	7,7,17	0.25	0	8,8,22	1.21	0
4	CM5	A	601	-	36,36,36	4.28	16 (44%)	49,49,49	5.81	26 (53%)
2	HEM	B	500	1,3	28,50,50	2.12	8 (28%)	17,82,82	2.67	6 (35%)
3	3QU	B	501	2	16,17,17	0.85	1 (6%)	20,22,22	1.76	5 (25%)
4	CM5	B	602	-	36,36,36	2.91	10 (27%)	49,49,49	5.09	24 (48%)
4	CM5	B	608	-	36,36,36	3.27	15 (41%)	49,49,49	6.21	26 (53%)
2	HEM	C	500	1,3	28,50,50	2.83	10 (35%)	17,82,82	1.89	3 (17%)
3	3QU	C	501	2	7,7,17	0.26	0	8,8,22	1.20	0
4	CM5	C	603	-	36,36,36	3.48	13 (36%)	49,49,49	5.64	23 (46%)
2	HEM	D	500	1,3	28,50,50	2.27	6 (21%)	17,82,82	1.40	1 (5%)
3	3QU	D	501	2	14,14,17	0.33	0	17,17,22	0.87	0
4	CM5	D	604	-	36,36,36	4.22	16 (44%)	49,49,49	6.52	25 (51%)
4	CM5	D	607	-	36,36,36	3.65	13 (36%)	49,49,49	5.26	26 (53%)
2	HEM	E	500	1,3	28,50,50	2.26	6 (21%)	17,82,82	1.40	1 (5%)
3	3QU	E	501	2	14,14,17	0.82	0	17,17,22	0.91	1 (5%)
4	CM5	E	605	-	36,36,36	3.60	14 (38%)	49,49,49	3.28	23 (46%)
2	HEM	F	500	1	28,50,50	2.26	6 (21%)	17,82,82	1.39	1 (5%)
4	CM5	F	606	-	36,36,36	3.09	13 (36%)	49,49,49	4.45	25 (51%)

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	-	0/6/54/54	0/0/8/8
3	3QU	A	501	2	-	0/0/0/8	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CM5	A	601	-	-	0/17/65/65	0/3/3/3
2	HEM	B	500	1,3	-	0/6/54/54	0/0/8/8
3	3QU	B	501	2	-	0/6/8/8	0/2/2/2
4	CM5	B	602	-	-	0/17/65/65	0/3/3/3
4	CM5	B	608	-	-	0/17/65/65	0/3/3/3
2	HEM	C	500	1,3	-	0/6/54/54	0/0/8/8
3	3QU	C	501	2	-	0/0/0/8	0/1/1/2
4	CM5	C	603	-	-	0/17/65/65	0/3/3/3
2	HEM	D	500	1,3	-	0/6/54/54	0/0/8/8
3	3QU	D	501	2	-	0/4/4/8	0/2/2/2
4	CM5	D	604	-	1/1/11/11	0/17/65/65	0/3/3/3
4	CM5	D	607	-	-	0/17/65/65	0/3/3/3
2	HEM	E	500	1,3	-	0/6/54/54	0/0/8/8
3	3QU	E	501	2	-	0/4/4/8	0/2/2/2
4	CM5	E	605	-	-	0/17/65/65	0/3/3/3
2	HEM	F	500	1	-	0/6/54/54	0/0/8/8
4	CM5	F	606	-	-	0/17/65/65	0/3/3/3

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	CM5	O23-C24	-14.16	1.04	1.41
4	A	601	CM5	O21-C17	-13.88	1.11	1.43
4	E	605	CM5	O23-C24	-11.73	1.10	1.41
4	D	604	CM5	C29-C28	-11.27	1.23	1.52
4	D	604	CM5	O25-C26	-10.81	1.18	1.44
4	F	606	CM5	C28-C27	-10.77	1.24	1.52
4	B	602	CM5	O25-C26	-9.76	1.20	1.44
4	A	601	CM5	C28-C27	-9.46	1.28	1.52
4	A	601	CM5	C27-C26	-9.39	1.33	1.53
4	D	607	CM5	C30-C26	-9.00	1.21	1.51
2	C	500	HEM	C3C-C2C	-8.84	1.28	1.40
4	E	605	CM5	O33-C28	-8.60	1.23	1.43
2	C	500	HEM	C3B-C2B	-8.42	1.29	1.40
4	D	604	CM5	C28-C27	-8.26	1.31	1.52
4	F	606	CM5	C17-C18	-8.17	1.31	1.52
4	A	601	CM5	C16-C15	-7.75	1.32	1.52
4	E	605	CM5	O14-C13	-7.39	1.23	1.41
4	D	607	CM5	O34-C29	-6.49	1.28	1.43
4	F	606	CM5	O32-C27	-6.36	1.28	1.43
4	D	604	CM5	C16-C15	-6.31	1.36	1.52
4	B	602	CM5	C27-C26	-6.01	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	CM5	C17-C18	-5.98	1.37	1.52
4	D	607	CM5	C28-C27	-5.94	1.37	1.52
4	C	603	CM5	C30-C26	-5.79	1.32	1.51
4	B	608	CM5	C13-C18	-5.56	1.36	1.52
4	A	601	CM5	O23-C16	-5.54	1.30	1.43
4	A	601	CM5	C17-C18	-5.45	1.38	1.52
4	B	608	CM5	C30-C26	-5.29	1.33	1.51
2	B	500	HEM	C3C-C2C	-5.28	1.33	1.40
4	D	604	CM5	C19-C15	-5.18	1.34	1.51
4	E	605	CM5	O12-C13	-5.00	1.31	1.40
2	D	500	HEM	C3C-C2C	-4.91	1.33	1.40
2	E	500	HEM	C3C-C2C	-4.88	1.33	1.40
2	F	500	HEM	C3B-C2B	-4.86	1.33	1.40
2	F	500	HEM	C3C-C2C	-4.85	1.33	1.40
2	A	500	HEM	C3C-C2C	-4.83	1.34	1.40
2	A	500	HEM	C3B-C2B	-4.82	1.34	1.40
2	E	500	HEM	C3B-C2B	-4.80	1.34	1.40
2	D	500	HEM	C3B-C2B	-4.78	1.34	1.40
4	E	605	CM5	C28-C27	-4.71	1.40	1.52
4	A	601	CM5	O25-C24	-4.68	1.30	1.41
4	F	606	CM5	O25-C24	-4.33	1.31	1.41
4	A	601	CM5	O23-C24	-4.31	1.30	1.41
4	E	605	CM5	C17-C18	-4.09	1.41	1.52
4	A	601	CM5	O14-C15	-4.00	1.34	1.44
4	C	603	CM5	C16-C15	-3.75	1.42	1.52
4	B	602	CM5	C29-C28	-3.70	1.42	1.52
4	B	602	CM5	C17-C18	-3.65	1.43	1.52
4	A	601	CM5	C24-C29	-3.64	1.42	1.52
4	B	608	CM5	C27-C26	-3.60	1.45	1.53
4	B	602	CM5	C24-C29	-3.56	1.42	1.52
4	B	602	CM5	O34-C29	-3.56	1.34	1.43
4	A	601	CM5	C29-C28	-3.28	1.44	1.52
2	B	500	HEM	C3B-C2B	-3.19	1.36	1.40
4	D	604	CM5	O14-C15	-3.17	1.36	1.44
2	C	500	HEM	C1D-CHD	-3.13	1.31	1.40
2	C	500	HEM	C2A-C3A	-3.04	1.28	1.37
3	B	501	3QU	CAO-NAP	-2.92	1.39	1.45
4	A	601	CM5	O14-C13	-2.86	1.34	1.41
4	B	608	CM5	O34-C29	-2.82	1.36	1.43
2	C	500	HEM	C4B-CHC	-2.79	1.32	1.40
4	D	604	CM5	O14-C13	-2.78	1.34	1.41
4	D	604	CM5	O25-C24	-2.73	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	CM5	C30-C26	-2.55	1.43	1.51
2	C	500	HEM	C4A-CHB	-2.45	1.33	1.40
4	F	606	CM5	C19-C15	-2.32	1.44	1.51
2	C	500	HEM	C1A-CHA	-2.29	1.34	1.40
4	D	607	CM5	C17-C18	-2.28	1.46	1.52
2	B	500	HEM	C1D-CHD	-2.24	1.34	1.40
4	B	602	CM5	O23-C16	-2.05	1.38	1.43
4	B	608	CM5	C19-C15	2.04	1.58	1.51
4	E	605	CM5	O25-C26	2.08	1.49	1.44
4	F	606	CM5	C13-C18	2.15	1.58	1.52
4	F	606	CM5	O12-C13	2.16	1.44	1.40
4	C	603	CM5	O12-C13	2.16	1.44	1.40
4	F	606	CM5	O23-C24	2.16	1.47	1.41
4	B	608	CM5	O22-C18	2.21	1.48	1.43
2	B	500	HEM	CMA-C3A	2.25	1.56	1.51
4	E	605	CM5	C29-C28	2.31	1.58	1.52
4	C	603	CM5	C13-C18	2.38	1.59	1.52
4	A	601	CM5	O22-C18	2.39	1.48	1.43
4	F	606	CM5	C16-C15	2.40	1.59	1.52
4	E	605	CM5	O31-C30	2.42	1.52	1.42
2	B	500	HEM	C1B-NB	2.44	1.39	1.36
2	E	500	HEM	C4D-ND	2.50	1.39	1.36
2	A	500	HEM	C4D-ND	2.50	1.39	1.36
4	C	603	CM5	O25-C24	2.51	1.48	1.41
4	C	603	CM5	O14-C15	2.51	1.50	1.44
2	D	500	HEM	C4D-ND	2.52	1.39	1.36
4	D	604	CM5	C13-C18	2.52	1.59	1.52
4	F	606	CM5	O21-C17	2.54	1.48	1.43
2	F	500	HEM	C4D-ND	2.58	1.39	1.36
4	D	607	CM5	C16-C15	2.59	1.59	1.52
4	D	604	CM5	O20-C19	2.61	1.53	1.42
4	B	608	CM5	C17-C18	2.61	1.59	1.52
4	A	601	CM5	O34-C29	2.71	1.49	1.43
4	B	608	CM5	O12-C13	2.79	1.45	1.40
2	C	500	HEM	C3B-CAB	2.81	1.53	1.47
2	C	500	HEM	C3C-CAC	2.85	1.53	1.47
4	C	603	CM5	C28-C27	2.92	1.59	1.52
4	B	608	CM5	C16-C15	2.98	1.60	1.52
4	D	607	CM5	O31-C30	3.03	1.55	1.42
4	E	605	CM5	O21-C17	3.13	1.50	1.43
4	F	606	CM5	O23-C16	3.14	1.51	1.43
4	D	607	CM5	C13-C18	3.20	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-CAB	3.25	1.54	1.47
4	C	603	CM5	C17-C18	3.32	1.60	1.52
2	D	500	HEM	C3B-CAB	3.49	1.54	1.47
2	F	500	HEM	C3B-CAB	3.51	1.54	1.47
2	A	500	HEM	C3B-CAB	3.52	1.54	1.47
2	C	500	HEM	C3D-C2D	3.52	1.48	1.37
2	E	500	HEM	C3B-CAB	3.53	1.54	1.47
2	F	500	HEM	C3C-CAC	3.56	1.54	1.47
2	A	500	HEM	C3C-CAC	3.58	1.54	1.47
2	E	500	HEM	C3C-CAC	3.58	1.54	1.47
4	D	607	CM5	C24-C29	3.59	1.62	1.52
2	D	500	HEM	C3C-CAC	3.61	1.54	1.47
4	A	601	CM5	C17-C16	3.71	1.62	1.52
4	D	604	CM5	C27-C26	3.88	1.61	1.53
4	C	603	CM5	C17-C16	3.91	1.63	1.52
2	B	500	HEM	C3C-CAC	3.92	1.55	1.47
4	D	607	CM5	C17-C16	4.02	1.63	1.52
4	E	605	CM5	O32-C27	4.05	1.52	1.43
4	B	602	CM5	O22-C18	4.21	1.52	1.43
4	B	608	CM5	C17-C16	4.22	1.63	1.52
4	B	608	CM5	O25-C24	4.23	1.52	1.41
4	E	605	CM5	O25-C24	4.23	1.52	1.41
4	F	606	CM5	O34-C29	4.60	1.53	1.43
4	B	602	CM5	O31-C30	4.71	1.62	1.42
4	F	606	CM5	O14-C13	4.72	1.53	1.41
2	B	500	HEM	C3D-C2D	4.78	1.51	1.37
4	C	603	CM5	O31-C30	4.94	1.63	1.42
4	E	605	CM5	O22-C18	5.19	1.54	1.43
2	D	500	HEM	C3D-C2D	5.46	1.53	1.37
2	F	500	HEM	C3D-C2D	5.48	1.53	1.37
2	A	500	HEM	C3D-C2D	5.49	1.53	1.37
2	E	500	HEM	C3D-C2D	5.50	1.54	1.37
4	B	608	CM5	O14-C15	5.89	1.58	1.44
4	A	601	CM5	O32-C27	6.06	1.56	1.43
4	D	604	CM5	O32-C27	6.16	1.57	1.43
4	E	605	CM5	O34-C29	6.58	1.58	1.43
4	C	603	CM5	O21-C17	6.72	1.58	1.43
4	D	607	CM5	O23-C16	6.98	1.60	1.43
4	B	608	CM5	O23-C24	7.04	1.60	1.41
4	D	607	CM5	O23-C24	7.17	1.60	1.41
4	C	603	CM5	O32-C27	7.31	1.59	1.43
4	D	604	CM5	O23-C24	7.42	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	CM5	O32-C27	7.47	1.60	1.43
4	D	604	CM5	O23-C16	7.84	1.62	1.43
4	D	607	CM5	O33-C28	8.25	1.61	1.43
4	B	608	CM5	O21-C17	8.31	1.62	1.43
4	B	608	CM5	O23-C16	8.36	1.64	1.43
4	D	607	CM5	O25-C24	8.67	1.63	1.41

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	CM5	O33-C28-C27	-18.70	69.67	110.36
4	A	601	CM5	O33-C28-C29	-18.10	70.97	110.36
4	B	608	CM5	O14-C15-C19	-17.96	63.38	106.41
4	B	608	CM5	O14-C13-O12	-16.63	70.54	110.02
4	F	606	CM5	O12-C13-C18	-16.43	81.43	108.23
4	C	603	CM5	O23-C16-C15	-15.57	71.04	109.34
4	B	602	CM5	O33-C28-C27	-14.84	78.07	110.36
4	D	604	CM5	O33-C28-C29	-14.81	78.13	110.36
4	C	603	CM5	C24-O23-C16	-13.75	84.50	118.00
4	D	604	CM5	C30-C26-C27	-13.73	80.87	113.00
4	D	607	CM5	O21-C17-C16	-13.47	79.21	109.87
4	C	603	CM5	O32-C27-C26	-12.68	77.33	109.28
4	B	608	CM5	O25-C24-C29	-12.24	86.68	110.30
4	B	608	CM5	O23-C16-C17	-12.12	78.02	107.19
4	B	602	CM5	O23-C16-C17	-11.99	78.35	107.19
4	C	603	CM5	O21-C17-C18	-11.89	84.48	110.36
4	D	604	CM5	O12-C13-C18	-11.78	89.01	108.23
4	A	601	CM5	O23-C24-C29	-11.62	81.94	108.11
4	B	602	CM5	O12-C13-C18	-11.29	89.82	108.23
4	D	604	CM5	C24-O23-C16	-11.00	91.19	118.00
4	F	606	CM5	O22-C18-C13	-10.95	87.13	110.03
4	D	607	CM5	O25-C24-C29	-10.84	89.39	110.30
4	B	602	CM5	C17-C16-C15	-10.55	88.49	110.88
4	A	601	CM5	O32-C27-C28	-10.16	88.25	110.36
4	D	607	CM5	C17-C16-C15	-10.06	89.52	110.88
4	D	607	CM5	O14-C13-C18	-9.93	91.14	110.30
4	D	604	CM5	O14-C13-C18	-9.92	91.16	110.30
4	D	604	CM5	O32-C27-C26	-9.80	84.59	109.28
4	A	601	CM5	O34-C29-C28	-9.70	89.25	110.36
4	A	601	CM5	O22-C18-C17	-9.69	89.26	110.36
4	B	608	CM5	C17-C16-C15	-9.52	90.68	110.88
4	B	602	CM5	O22-C18-C13	-9.46	90.24	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	CM5	O32-C27-C26	-9.46	85.46	109.28
4	E	605	CM5	O32-C27-C26	-9.35	85.73	109.28
4	A	601	CM5	O14-C13-C18	-8.89	93.15	110.30
4	C	603	CM5	O23-C24-O25	-8.66	89.67	110.70
4	A	601	CM5	C18-C17-C16	-8.66	91.65	109.61
4	D	607	CM5	O23-C24-C29	-8.62	88.69	108.11
4	B	608	CM5	O21-C17-C18	-8.27	92.37	110.36
4	C	603	CM5	O32-C27-C28	-8.12	92.69	110.36
4	F	606	CM5	O23-C16-C15	-7.94	89.82	109.34
4	D	607	CM5	O23-C16-C17	-7.90	88.19	107.19
4	D	607	CM5	C30-C26-C27	-7.79	94.76	113.00
4	B	602	CM5	O14-C13-C18	-7.68	95.48	110.30
4	A	601	CM5	O23-C16-C15	-7.25	91.51	109.34
4	B	602	CM5	C28-C27-C26	-7.18	97.56	110.22
4	B	608	CM5	C19-C15-C16	-7.16	93.69	113.24
4	B	608	CM5	O21-C17-C16	-7.16	93.57	109.87
4	D	607	CM5	O12-C13-C18	-7.14	96.59	108.23
4	D	607	CM5	O32-C27-C26	-6.84	92.04	109.28
4	D	604	CM5	C28-C27-C26	-6.53	98.72	110.22
4	A	601	CM5	O32-C27-C26	-6.48	92.96	109.28
4	F	606	CM5	O14-C13-C18	-6.21	98.32	110.30
4	F	606	CM5	O32-C27-C28	-6.09	97.11	110.36
4	A	601	CM5	C13-O14-C15	-5.88	102.64	113.72
4	B	608	CM5	O12-C13-C18	-5.72	98.90	108.23
2	B	500	HEM	C1D-C2D-C3D	-5.68	103.05	107.00
4	B	602	CM5	O32-C27-C28	-5.59	98.19	110.36
4	E	605	CM5	O22-C18-C17	-5.55	98.29	110.36
4	F	606	CM5	C17-C16-C15	-5.52	99.17	110.88
4	D	607	CM5	O31-C30-C26	-5.48	92.91	111.34
4	C	603	CM5	O22-C18-C13	-5.44	98.65	110.03
2	B	500	HEM	CAA-CBA-CGA	-5.42	103.40	112.66
4	D	607	CM5	O32-C27-C28	-5.38	98.65	110.36
4	B	602	CM5	O21-C17-C18	-5.34	98.74	110.36
4	B	602	CM5	C13-O14-C15	-4.98	104.33	113.72
4	E	605	CM5	O25-C24-C29	-4.94	100.77	110.30
4	B	608	CM5	C13-O14-C15	-4.60	105.04	113.72
4	D	604	CM5	C24-C29-C28	-4.59	101.44	109.98
4	C	603	CM5	O25-C26-C30	-4.53	95.56	106.41
4	B	608	CM5	C28-C27-C26	-4.26	102.71	110.22
4	D	604	CM5	C17-C16-C15	-4.22	101.92	110.88
4	D	604	CM5	C1-O12-C13	-4.07	106.87	113.87
3	B	501	3QU	CAJ-CAO-NAP	-4.00	116.36	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	607	CM5	O21-C17-C18	-3.98	101.70	110.36
4	A	601	CM5	O12-C13-C18	-3.78	102.08	108.23
4	B	608	CM5	C24-O23-C16	-3.77	108.82	118.00
4	D	607	CM5	C19-C15-C16	-3.76	102.98	113.24
4	F	606	CM5	O22-C18-C17	-3.71	102.29	110.36
4	E	605	CM5	O22-C18-C13	-3.70	102.28	110.03
4	E	605	CM5	O12-C13-C18	-3.70	102.20	108.23
4	B	602	CM5	C18-C17-C16	-3.69	101.96	109.61
4	A	601	CM5	O25-C24-C29	-3.63	103.29	110.30
4	D	604	CM5	O23-C16-C15	-3.62	100.45	109.34
4	A	601	CM5	C17-C16-C15	-3.59	103.25	110.88
4	C	603	CM5	C24-O25-C26	-3.59	106.96	113.72
4	C	603	CM5	C17-C16-C15	-3.56	103.32	110.88
4	D	604	CM5	O14-C13-O12	-3.46	101.80	110.02
4	C	603	CM5	O12-C13-C18	-3.46	102.59	108.23
4	A	601	CM5	O14-C15-C16	-3.46	102.68	109.75
2	C	500	HEM	CAA-CBA-CGA	-3.41	106.84	112.66
2	B	500	HEM	CMA-C3A-C4A	-3.23	123.50	128.46
4	E	605	CM5	O23-C24-C29	-3.18	100.95	108.11
4	A	601	CM5	C1-O12-C13	-3.14	108.47	113.87
4	C	603	CM5	C24-C29-C28	-3.12	104.18	109.98
4	E	605	CM5	O31-C30-C26	-3.10	100.92	111.34
4	F	606	CM5	C24-O23-C16	-3.08	110.50	118.00
4	B	602	CM5	O25-C24-C29	-3.01	104.49	110.30
4	D	607	CM5	O22-C18-C13	-2.97	103.82	110.03
4	D	607	CM5	C8-C7-C6	-2.97	106.75	112.19
4	A	601	CM5	C24-O25-C26	-2.97	108.13	113.72
4	B	602	CM5	C1-O12-C13	-2.89	108.91	113.87
4	C	603	CM5	O14-C13-C18	-2.89	104.73	110.30
4	C	603	CM5	C13-O14-C15	-2.88	108.29	113.72
4	F	606	CM5	O34-C29-C28	-2.84	104.17	110.36
4	A	601	CM5	C29-C28-C27	-2.79	105.92	110.84
4	B	608	CM5	O32-C27-C28	-2.79	104.30	110.36
4	A	601	CM5	O25-C26-C30	-2.72	99.90	106.41
4	B	608	CM5	C13-C18-C17	-2.71	104.95	109.98
4	E	605	CM5	O23-C16-C17	-2.67	100.76	107.19
4	D	607	CM5	C29-C28-C27	-2.66	106.14	110.84
4	E	605	CM5	C17-C16-C15	-2.64	105.27	110.88
4	E	605	CM5	O21-C17-C18	-2.62	104.65	110.36
4	B	608	CM5	C24-O25-C26	-2.60	108.81	113.72
4	F	606	CM5	C1-O12-C13	-2.56	109.48	113.87
4	F	606	CM5	O21-C17-C16	-2.55	104.07	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	CM5	C1-O12-C13	-2.53	109.52	113.87
4	D	607	CM5	C13-O14-C15	-2.53	108.95	113.72
2	B	500	HEM	CAD-CBD-CGD	-2.49	108.40	112.66
4	B	608	CM5	O22-C18-C17	-2.45	105.02	110.36
3	B	501	3QU	CAJ-CAH-CAN	-2.43	117.66	121.02
4	E	605	CM5	C30-C26-C27	-2.43	107.32	113.00
3	B	501	3QU	CAG-CAI-CAO	-2.41	116.63	120.10
4	F	606	CM5	O23-C16-C17	-2.41	101.41	107.19
4	B	602	CM5	O22-C18-C17	-2.33	105.28	110.36
3	E	501	3QU	CAF-CAD-NAL	-2.33	119.57	123.63
4	F	606	CM5	O25-C26-C30	-2.32	100.86	106.41
4	D	604	CM5	O34-C29-C24	-2.32	105.19	110.03
4	E	605	CM5	C13-C18-C17	-2.31	105.68	109.98
4	E	605	CM5	O32-C27-C28	-2.27	105.41	110.36
2	E	500	HEM	C1D-C2D-C3D	-2.24	105.44	107.00
2	A	500	HEM	C1D-C2D-C3D	-2.23	105.45	107.00
4	D	607	CM5	C11-C6-C7	-2.21	103.81	109.27
2	F	500	HEM	C1D-C2D-C3D	-2.21	105.46	107.00
2	D	500	HEM	C1D-C2D-C3D	-2.19	105.47	107.00
4	D	604	CM5	O22-C18-C13	-2.19	105.46	110.03
4	C	603	CM5	O22-C18-C17	-2.13	105.73	110.36
4	B	602	CM5	O20-C19-C15	-2.09	104.31	111.34
2	C	500	HEM	C1D-C2D-C3D	-2.04	105.58	107.00
4	E	605	CM5	O21-C17-C16	2.02	114.48	109.87
2	B	500	HEM	CBA-CAA-C2A	2.18	116.64	112.48
4	B	602	CM5	C13-C18-C17	2.21	114.09	109.98
4	E	605	CM5	O33-C28-C27	2.24	115.23	110.36
4	B	608	CM5	O22-C18-C13	2.36	114.97	110.03
4	C	603	CM5	O25-C26-C27	2.39	114.07	109.66
4	A	601	CM5	O22-C18-C13	2.42	115.09	110.03
3	B	501	3QU	CAG-CAN-CAH	2.49	122.11	118.16
4	B	602	CM5	O23-C16-C15	2.54	115.60	109.34
3	B	501	3QU	CAI-CAO-NAP	2.63	121.41	119.41
4	D	607	CM5	O25-C26-C30	2.65	112.75	106.41
4	F	606	CM5	C28-C27-C26	2.81	115.17	110.22
4	F	606	CM5	O21-C17-C18	2.84	116.55	110.36
4	D	604	CM5	C24-O25-C26	3.09	119.53	113.72
4	F	606	CM5	O25-C26-C27	3.20	115.55	109.66
4	D	604	CM5	C18-C17-C16	3.20	116.25	109.61
4	B	608	CM5	O31-C30-C26	3.21	122.14	111.34
4	A	601	CM5	O21-C17-C16	3.25	117.27	109.87
4	B	602	CM5	C29-C28-C27	3.27	116.61	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	CM5	O34-C29-C24	3.34	117.01	110.03
4	A	601	CM5	O23-C16-C17	3.34	115.24	107.19
4	F	606	CM5	O23-C24-O25	3.43	119.01	110.70
4	B	608	CM5	O25-C26-C30	3.50	114.79	106.41
4	D	607	CM5	C1-O12-C13	3.52	119.91	113.87
4	E	605	CM5	C18-C17-C16	3.53	116.92	109.61
4	D	607	CM5	O14-C15-C16	3.57	117.05	109.75
4	F	606	CM5	O31-C30-C26	3.76	124.00	111.34
4	B	602	CM5	O23-C24-C29	3.78	116.62	108.11
4	B	602	CM5	O34-C29-C24	3.88	118.14	110.03
4	E	605	CM5	O25-C26-C30	3.98	115.94	106.41
4	F	606	CM5	O32-C27-C26	4.02	119.42	109.28
2	C	500	HEM	C3B-C4B-NB	4.08	114.49	109.21
4	D	604	CM5	O31-C30-C26	4.13	125.23	111.34
4	E	605	CM5	C28-C27-C26	4.17	117.57	110.22
4	F	606	CM5	C24-C29-C28	4.18	117.74	109.98
4	E	605	CM5	O34-C29-C28	4.22	119.54	110.36
4	E	605	CM5	C13-O14-C15	4.34	121.90	113.72
4	D	607	CM5	C28-C27-C26	4.50	118.15	110.22
2	B	500	HEM	CMB-C2B-C3B	4.53	133.30	124.89
4	D	604	CM5	O23-C24-C29	4.73	118.77	108.11
4	D	607	CM5	O22-C18-C17	4.73	120.66	110.36
4	C	603	CM5	C30-C26-C27	4.96	124.61	113.00
4	D	604	CM5	O20-C19-C15	5.30	129.16	111.34
4	A	601	CM5	O21-C17-C18	5.46	122.23	110.36
4	F	606	CM5	C30-C26-C27	5.64	126.19	113.00
4	D	607	CM5	C24-C29-C28	5.68	120.54	109.98
4	F	606	CM5	O20-C19-C15	5.70	130.51	111.34
4	E	605	CM5	C24-O23-C16	5.75	132.00	118.00
4	B	602	CM5	O33-C28-C29	5.77	122.92	110.36
4	B	608	CM5	O14-C13-C18	5.79	121.45	110.30
4	F	606	CM5	O14-C15-C16	6.07	122.18	109.75
4	D	604	CM5	O33-C28-C27	6.22	123.89	110.36
4	B	608	CM5	C30-C26-C27	6.34	127.85	113.00
4	E	605	CM5	O33-C28-C29	6.55	124.61	110.36
4	C	603	CM5	O23-C24-C29	6.58	122.94	108.11
4	B	602	CM5	O25-C26-C27	6.84	122.26	109.66
4	B	608	CM5	O23-C24-O25	6.98	127.64	110.70
4	C	603	CM5	O21-C17-C16	7.27	126.42	109.87
4	A	601	CM5	O25-C26-C27	7.53	123.53	109.66
4	F	606	CM5	O23-C24-C29	7.59	125.22	108.11
4	C	603	CM5	O14-C15-C16	7.64	125.38	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	CM5	C13-C18-C17	7.77	124.41	109.98
4	B	608	CM5	C18-C17-C16	8.17	126.55	109.61
4	D	604	CM5	O23-C24-O25	8.37	131.01	110.70
4	A	601	CM5	C24-C29-C28	8.42	125.64	109.98
4	D	607	CM5	C24-O23-C16	8.75	139.32	118.00
4	B	602	CM5	O23-C24-O25	9.66	134.16	110.70
4	F	606	CM5	C18-C17-C16	9.81	129.96	109.61
4	D	604	CM5	O25-C26-C30	10.17	130.77	106.41
4	E	605	CM5	O14-C13-O12	10.41	134.73	110.02
4	B	608	CM5	O14-C15-C16	10.49	131.21	109.75
4	B	608	CM5	O23-C24-C29	11.06	133.03	108.11
4	B	608	CM5	O23-C16-C15	11.98	138.81	109.34
4	D	604	CM5	C29-C28-C27	12.45	132.81	110.84
4	D	604	CM5	O34-C29-C28	12.69	137.97	110.36
4	D	607	CM5	O23-C16-C15	15.10	146.50	109.34
4	A	601	CM5	O23-C24-O25	15.97	149.48	110.70
4	D	604	CM5	O23-C16-C17	20.94	157.57	107.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	CM5	C16

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	10	0
4	A	601	CM5	1	0
2	B	500	HEM	4	0
4	B	602	CM5	14	0
4	B	608	CM5	20	0
2	C	500	HEM	9	0
4	C	603	CM5	5	0
2	D	500	HEM	12	0
4	D	604	CM5	4	0
4	D	607	CM5	8	0
2	E	500	HEM	9	0
3	E	501	3QU	1	0
4	E	605	CM5	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	HEM	18	0
4	F	606	CM5	5	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	462/476 (97%)	0.09	2 (0%) 92 90	26, 51, 74, 82	0
1	B	459/476 (96%)	0.12	5 (1%) 80 74	28, 51, 74, 82	0
1	C	462/476 (97%)	0.14	2 (0%) 92 90	24, 50, 74, 79	0
1	D	458/476 (96%)	0.07	4 (0%) 84 79	24, 51, 74, 82	0
1	E	459/476 (96%)	0.01	6 (1%) 77 71	26, 51, 74, 87	0
1	F	453/476 (95%)	0.39	31 (6%) 18 10	24, 51, 74, 79	0
All	All	2753/2856 (96%)	0.14	50 (1%) 69 60	24, 51, 74, 87	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	463	VAL	5.7
1	F	153	LEU	4.3
1	F	450	PHE	3.6
1	F	459	MET	3.5
1	F	280	HIS	3.5
1	F	422	LYS	3.5
1	F	460	ALA	3.4
1	F	345	LYS	3.4
1	C	491	ARG	3.4
1	F	416	ALA	3.2
1	B	335	HIS	3.1
1	F	164	LEU	3.1
1	C	492	HIS	3.0
1	D	335	HIS	3.0
1	F	408	PHE	3.0
1	E	488	PHE	2.9
1	B	492	HIS	2.8
1	F	324	VAL	2.7
1	B	169	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	329	GLU	2.6
1	F	326	ARG	2.6
1	E	65	VAL	2.6
1	E	335	HIS	2.6
1	B	488	PHE	2.6
1	F	334	PRO	2.5
1	F	278	ASN	2.5
1	F	279	ALA	2.5
1	F	309	TYR	2.4
1	F	165	MET	2.4
1	F	454	LEU	2.3
1	A	74	PRO	2.3
1	D	488	PHE	2.3
1	F	319	HIS	2.3
1	E	492	HIS	2.3
1	E	489	LEU	2.3
1	F	150	ALA	2.2
1	F	485	GLN	2.2
1	B	170	LEU	2.2
1	F	449	PHE	2.2
1	F	162	GLY	2.2
1	D	28	GLY	2.2
1	F	315	LEU	2.2
1	D	134	ASP	2.1
1	F	335	HIS	2.1
1	F	191	GLN	2.1
1	F	192	ASP	2.1
1	A	189	HIS	2.1
1	E	339	GLU	2.1
1	F	195	PHE	2.0
1	F	157	LEU	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(Å <sup>2</sup> )	Q<0.9
4	CM5	F	606	34/34	0.69	0.37	4.67	45,62,74,76	0
3	3QU	B	501	16/16	0.89	0.41	4.67	47,51,60,66	0
3	3QU	A	501	7/16	0.90	0.30	4.30	47,50,51,52	0
4	CM5	B	602	34/34	0.69	0.32	3.95	61,72,84,85	0
3	3QU	D	501	13/16	0.90	0.30	3.46	47,49,54,54	0
4	CM5	D	607	34/34	0.75	0.25	2.85	72,97,101,103	0
4	CM5	C	603	34/34	0.76	0.30	2.76	54,63,70,71	0
4	CM5	B	608	34/34	0.74	0.26	2.20	46,84,100,100	0
3	3QU	E	501	13/16	0.95	0.27	2.14	55,57,60,63	0
4	CM5	A	601	34/34	0.87	0.26	1.82	53,60,73,74	0
3	3QU	C	501	7/16	0.94	0.26	1.43	47,50,51,52	0
4	CM5	E	605	34/34	0.77	0.28	1.43	66,73,91,92	0
2	HEM	D	500	43/43	0.96	0.22	0.69	23,33,38,39	0
2	HEM	A	500	43/43	0.97	0.23	0.55	25,31,39,43	0
4	CM5	D	604	34/34	0.88	0.21	0.45	58,67,77,79	0
2	HEM	E	500	43/43	0.97	0.20	0.18	17,28,36,40	0
2	HEM	B	500	43/43	0.98	0.19	-0.14	15,20,29,31	0
2	HEM	F	500	43/43	0.95	0.22	-0.24	53,65,66,67	0
2	HEM	C	500	43/43	0.98	0.16	-0.91	21,27,36,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.