



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:26 PM GMT

PDB ID : 3R1A
Title : Closed crystal structure of cytochrome P450 2B4 covalently bound to the mechanism-based inactivator tert-butylphenylacetylene
Authors : Gay, S.C.; Zhang, H.; Stout, C.D.; Hollenberg, P.F.; Halpert, J.R.
Deposited on : 2011-03-09
Resolution : 3.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

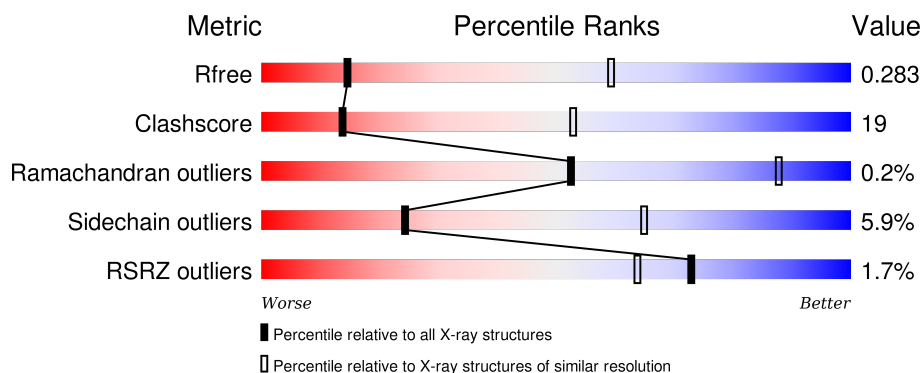
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



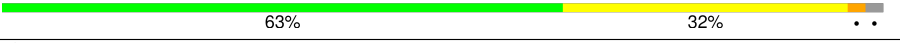


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 ≥ 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></div> <div>64% 32% ..</div> </div>
1	B	476	<div> <div></div> <div>64% 33% ..</div> </div>
1	C	476	<div> <div></div> <div>61% 33% ..</div> </div>
1	D	476	<div> <div></div> <div>63% 33% ..</div> </div>
1	E	476	<div> <div></div> <div>60% 34% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	476	
1	G	476	
1	H	476	

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	TB2	A	501	-	-	-	X
3	TB2	B	501	-	-	-	X
3	TB2	D	501	-	-	-	X
3	TB2	E	501	-	-	-	X
3	TB2	F	501	-	-	-	X
3	TB2	G	501	-	-	-	X
3	TB2	H	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28813 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3618	2332	613	663	10			
1	B	465	Total	C	N	O	S	0	0	0
			3582	2314	595	662	11			
1	C	465	Total	C	N	O	S	0	0	0
			3637	2346	618	662	11			
1	D	465	Total	C	N	O	S	0	0	0
			3608	2327	604	666	11			
1	E	465	Total	C	N	O	S	0	0	0
			3588	2319	592	666	11			
1	F	465	Total	C	N	O	S	0	0	0
			3540	2292	581	656	11			
1	G	465	Total	C	N	O	S	0	0	0
			3545	2293	583	659	10			
1	H	464	Total	C	N	O	S	0	0	0
			3239	2079	539	612	9			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	SER	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	GLY	DELETION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	ARG	DELETION	UNP P00178
A	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
A	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
A	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
A	221	SER	PRO	CONFLICT	UNP P00178
A	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
A	492	HIS	-	EXPRESSION TAG	UNP P00178
A	493	HIS	-	EXPRESSION TAG	UNP P00178
A	494	HIS	-	EXPRESSION TAG	UNP P00178
A	495	HIS	-	EXPRESSION TAG	UNP P00178
B	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	SER	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	GLY	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	ARG	DELETION	UNP P00178
B	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
B	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
B	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
B	221	SER	PRO	CONFLICT	UNP P00178
B	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
B	492	HIS	-	EXPRESSION TAG	UNP P00178
B	493	HIS	-	EXPRESSION TAG	UNP P00178
B	494	HIS	-	EXPRESSION TAG	UNP P00178
B	495	HIS	-	EXPRESSION TAG	UNP P00178
C	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	SER	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	GLY	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	ARG	DELETION	UNP P00178
C	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
C	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
C	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
C	221	SER	PRO	CONFLICT	UNP P00178
C	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
C	492	HIS	-	EXPRESSION TAG	UNP P00178
C	493	HIS	-	EXPRESSION TAG	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	EXPRESSION TAG	UNP P00178
C	495	HIS	-	EXPRESSION TAG	UNP P00178
D	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	SER	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	GLY	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	ARG	DELETION	UNP P00178
D	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
D	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
D	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
D	221	SER	PRO	CONFLICT	UNP P00178
D	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
D	492	HIS	-	EXPRESSION TAG	UNP P00178
D	493	HIS	-	EXPRESSION TAG	UNP P00178
D	494	HIS	-	EXPRESSION TAG	UNP P00178
D	495	HIS	-	EXPRESSION TAG	UNP P00178
E	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
E	?	-	PHE	DELETION	UNP P00178
E	?	-	SER	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	DELETION	UNP P00178
E	?	-	ALA	DELETION	UNP P00178
E	?	-	PHE	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	ALA	DELETION	UNP P00178
E	?	-	GLY	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	LEU	DELETION	UNP P00178
E	?	-	PHE	DELETION	UNP P00178
E	?	-	ARG	DELETION	UNP P00178
E	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
E	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
E	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
E	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
E	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
E	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
E	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
E	221	SER	PRO	CONFLICT	UNP P00178
E	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
E	492	HIS	-	EXPRESSION TAG	UNP P00178
E	493	HIS	-	EXPRESSION TAG	UNP P00178
E	494	HIS	-	EXPRESSION TAG	UNP P00178
E	495	HIS	-	EXPRESSION TAG	UNP P00178
F	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
F	?	-	PHE	DELETION	UNP P00178
F	?	-	SER	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	ALA	DELETION	UNP P00178
F	?	-	PHE	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	ALA	DELETION	UNP P00178
F	?	-	GLY	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	LEU	DELETION	UNP P00178
F	?	-	LEU	DELETION	UNP P00178
F	?	-	PHE	DELETION	UNP P00178
F	?	-	ARG	DELETION	UNP P00178
F	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
F	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
F	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
F	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
F	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
F	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
F	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
F	221	SER	PRO	CONFLICT	UNP P00178
F	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
F	492	HIS	-	EXPRESSION TAG	UNP P00178
F	493	HIS	-	EXPRESSION TAG	UNP P00178
F	494	HIS	-	EXPRESSION TAG	UNP P00178
F	495	HIS	-	EXPRESSION TAG	UNP P00178
G	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
G	?	-	PHE	DELETION	UNP P00178
G	?	-	SER	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	ALA	DELETION	UNP P00178
G	?	-	PHE	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	ALA	DELETION	UNP P00178
G	?	-	GLY	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	LEU	DELETION	UNP P00178
G	?	-	PHE	DELETION	UNP P00178
G	?	-	ARG	DELETION	UNP P00178
G	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
G	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
G	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
G	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
G	26	SER	ALA	ENGINEERED MUTATION	UNP P00178

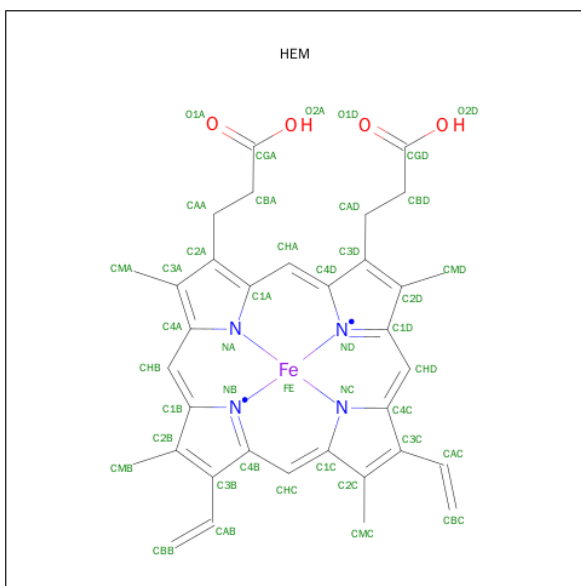
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Chain	Residue	Modelled	Actual	Comment	Reference
G	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
G	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
G	221	SER	PRO	CONFLICT	UNP P00178
G	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
G	492	HIS	-	EXPRESSION TAG	UNP P00178
G	493	HIS	-	EXPRESSION TAG	UNP P00178
G	494	HIS	-	EXPRESSION TAG	UNP P00178
G	495	HIS	-	EXPRESSION TAG	UNP P00178
H	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
H	?	-	PHE	DELETION	UNP P00178
H	?	-	SER	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	ALA	DELETION	UNP P00178
H	?	-	PHE	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	ALA	DELETION	UNP P00178
H	?	-	GLY	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	LEU	DELETION	UNP P00178
H	?	-	PHE	DELETION	UNP P00178
H	?	-	ARG	DELETION	UNP P00178
H	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
H	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
H	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
H	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
H	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
H	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
H	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
H	221	SER	PRO	CONFLICT	UNP P00178
H	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
H	492	HIS	-	EXPRESSION TAG	UNP P00178
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H	494	HIS	-	EXPRESSION TAG	UNP P00178
H	495	HIS	-	EXPRESSION TAG	UNP P00178

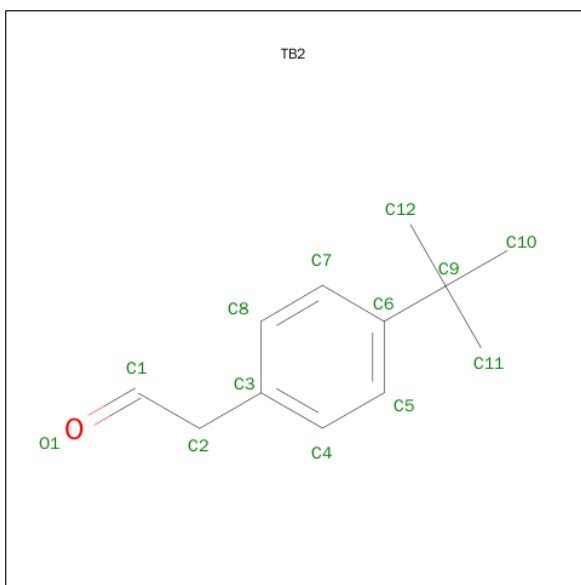
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



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
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (4-TERT-BUTYLPHENYL)ACETALDEHYDE (three-letter code: TB2) (formula: $C_{12}H_{16}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			13	12	1		
3	C	1	Total	C	O	0	0
			13	12	1		
3	D	1	Total	C	O	0	0
			13	12	1		
3	E	1	Total	C	O	0	0
			13	12	1		
3	F	1	Total	C	O	0	0
			13	12	1		
3	G	1	Total	C	O	0	0
			13	12	1		
3	H	1	Total	C	O	0	0
			13	12	1		

- Molecule 4 is water.

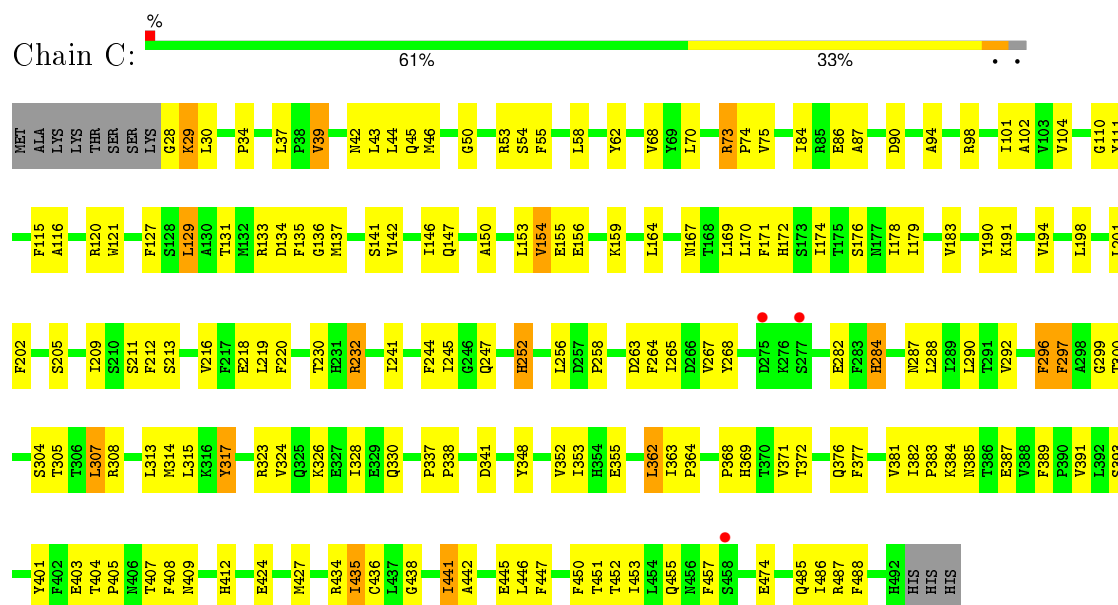
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

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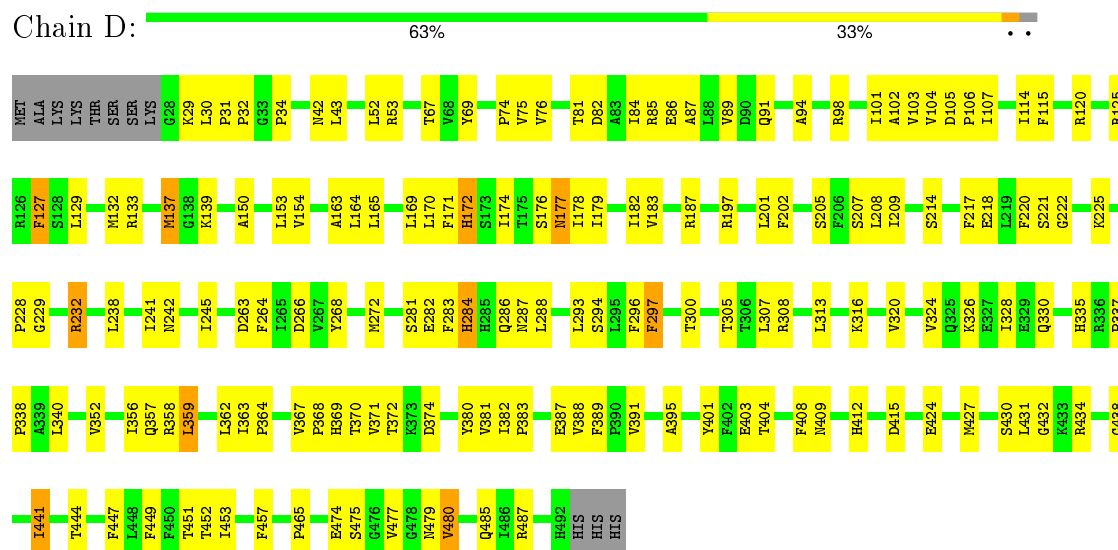
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0
4	H	1	Total 1	O 1	0	0

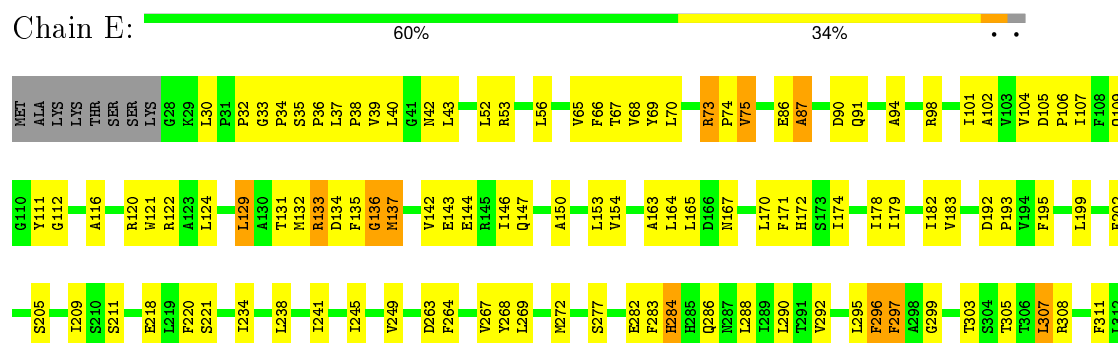
- Molecule 1: Cytochrome P450 2B4

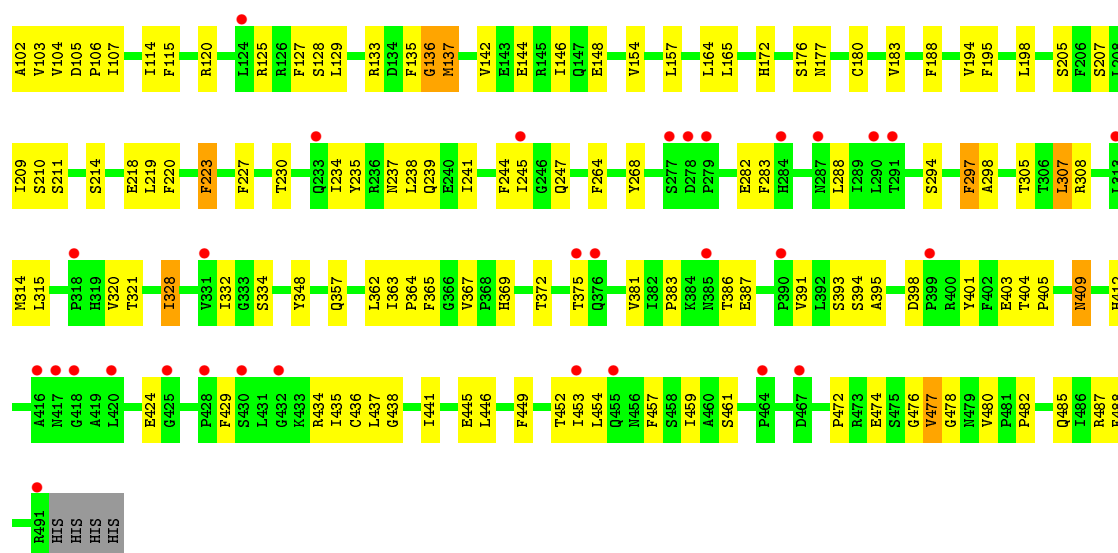


- Molecule 1: Cytochrome P450 2B4



- Molecule 1: Cytochrome P450 2B4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.38Å 144.55Å 229.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.93 – 3.50 115.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	85.5 (115.93-3.50) 89.8 (115.93-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.206 , 0.285 0.214 , 0.283	Depositor DCC
R_{free} test set	2603 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	80.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 51289 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28813	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, TB2

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	0.23	0/3711	0.48	1/5052 (0.0%)
1	B	0.23	0/3675	0.45	0/5010
1	C	0.23	0/3730	0.46	1/5072 (0.0%)
1	D	0.23	0/3701	0.49	2/5041 (0.0%)
1	E	0.23	0/3681	0.48	3/5017 (0.1%)
1	F	0.23	0/3633	0.46	0/4960
1	G	0.22	0/3638	0.49	0/4968
1	H	0.29	1/3313 (0.0%)	0.50	3/4554 (0.1%)
All	All	0.24	1/29082 (0.0%)	0.48	10/39674 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	135	PHE	CA-C	-5.95	1.37	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	136	GLY	CA-C-N	5.99	130.38	117.20
1	D	281	SER	CB-CA-C	5.89	121.28	110.10
1	E	137	MET	N-CA-C	-5.65	95.75	111.00
1	H	334	SER	N-CA-CB	-5.64	102.04	110.50
1	E	87	ALA	N-CA-C	5.51	125.87	111.00
1	H	137	MET	N-CA-CB	-5.39	100.89	110.60
1	C	134	ASP	CB-CA-C	5.31	121.03	110.40
1	E	277	SER	CB-CA-C	-5.24	100.14	110.10
1	D	335	HIS	CB-CA-C	-5.17	100.05	110.40
1	A	301	GLU	N-CA-C	5.11	124.80	111.00

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	3618	0	3491	120	0
1	B	3582	0	3425	122	0
1	C	3637	0	3538	129	0
1	D	3608	0	3466	118	0
1	E	3588	0	3434	136	0
1	F	3540	0	3353	122	0
1	G	3545	0	3353	113	0
1	H	3239	0	2900	129	0
2	A	43	0	30	8	0
2	B	43	0	30	9	0
2	C	43	0	30	11	0
2	D	43	0	30	11	0
2	E	43	0	30	9	0
2	F	43	0	30	8	0
2	G	43	0	30	13	0
2	H	43	0	30	13	0
3	A	13	0	15	5	0
3	B	13	0	15	2	0
3	C	13	0	15	0	0
3	D	13	0	15	5	0
3	E	13	0	15	1	0
3	F	13	0	15	3	0
3	G	13	0	15	3	0
3	H	13	0	15	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
All	All	28813	0	27320	1039	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 19.

All (1039) 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:B:232:ARG:HH11	1:B:232:ARG:HG2	1.00	1.15
2:H:500:HEM:HHA	2:H:500:HEM:HBD2	1.30	1.09
1:H:136:GLY:O	1:H:142:VAL:HB	1.58	1.03
1:F:136:GLY:O	1:F:142:VAL:HB	1.63	0.97
1:G:138:GLY:O	1:G:142:VAL:HG11	1.66	0.94
2:E:500:HEM:HBC2	2:E:500:HEM:HHH	1.50	0.90
2:B:500:HEM:HHH	2:B:500:HEM:HBC2	1.53	0.89
1:F:143:GLU:OE2	1:F:340:LEU:CB	2.21	0.89
1:F:305:THR:HG22	1:F:308:ARG:HH21	1.38	0.88
3:F:501:TB2:H4	3:F:501:TB2:O1	1.72	0.88
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.53	0.87
1:B:232:ARG:HG2	1:B:232:ARG:NH1	1.79	0.86
2:E:500:HEM:HBB2	2:E:500:HEM:HHC	1.57	0.86
1:E:150:ALA:HB1	1:E:452:THR:HG21	1.56	0.85
2:G:500:HEM:HBB2	2:G:500:HEM:HMB2	1.58	0.85
1:D:52:LEU:HD22	1:D:364:PRO:HB3	1.58	0.84
2:H:500:HEM:HBC2	2:H:500:HEM:HMC2	1.59	0.84
2:G:500:HEM:HBD1	2:G:500:HEM:HMD1	1.57	0.84
2:A:500:HEM:HBB2	2:A:500:HEM:HMB1	1.58	0.84
2:G:500:HEM:HMC2	2:G:500:HEM:HBC2	1.59	0.84
2:H:500:HEM:HBB2	2:H:500:HEM:HMB2	1.59	0.83
2:D:500:HEM:HBC2	2:D:500:HEM:HMC1	1.58	0.83
2:F:500:HEM:HMB2	2:F:500:HEM:HBB2	1.61	0.83
2:F:500:HEM:HMC2	2:F:500:HEM:HBC2	1.62	0.82
1:C:136:GLY:O	1:C:142:VAL:HG13	1.79	0.82
1:H:435:ILE:HG12	1:H:436:CYS:H	1.42	0.82
2:A:500:HEM:HBC2	2:A:500:HEM:HMC2	1.61	0.81
1:F:143:GLU:OE2	1:F:340:LEU:HB3	1.81	0.80
1:G:362:LEU:HD22	1:G:362:LEU:H	1.45	0.80
1:F:75:VAL:HG12	1:F:387:GLU:HB2	1.62	0.80
2:C:500:HEM:HMC2	2:C:500:HEM:HBC2	1.62	0.80
1:H:42:ASN:HD22	1:H:69:TYR:H	1.28	0.79
2:D:500:HEM:HBB2	2:D:500:HEM:HMB2	1.63	0.79
1:G:362:LEU:O	1:G:364:PRO:HD3	1.81	0.79
2:C:500:HEM:HBB2	2:C:500:HEM:HMB1	1.64	0.79
1:D:222:GLY:HA2	1:D:225:LYS:HE3	1.64	0.78
1:C:153:LEU:HD21	1:C:453:ILE:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:LEU:HD21	1:H:383:PRO:HD3	1.65	0.78
1:H:305:THR:HG22	1:H:308:ARG:HE	1.49	0.78
1:G:52:LEU:HD22	1:G:364:PRO:HB3	1.65	0.77
1:C:435:ILE:HG12	1:C:436:CYS:H	1.48	0.76
1:E:86:GLU:O	1:E:90:ASP:HB2	1.84	0.75
1:G:136:GLY:O	1:G:142:VAL:HB	1.85	0.75
1:C:232:ARG:CG	1:C:232:ARG:HH11	2.00	0.75
1:A:75:VAL:HG12	1:A:387:GLU:HB2	1.68	0.74
1:H:435:ILE:HG12	1:H:436:CYS:N	2.02	0.74
2:H:500:HEM:HHA	2:H:500:HEM:CBD	2.15	0.74
1:A:102:ALA:HB2	1:A:218:GLU:HA	1.68	0.74
1:F:320:VAL:HG21	1:F:408:PHE:HE2	1.52	0.74
1:D:133:ARG:HA	1:D:137:MET:HB3	1.70	0.73
1:F:143:GLU:OE2	1:F:340:LEU:N	2.21	0.73
1:E:102:ALA:HB2	1:E:218:GLU:HA	1.69	0.73
1:D:316:LYS:HG3	1:D:465:PRO:O	1.89	0.73
1:D:150:ALA:HB1	1:D:452:THR:HG21	1.71	0.73
1:F:278:ASP:OD1	1:F:279:PRO:N	2.22	0.72
1:D:153:LEU:HD21	1:D:453:ILE:HD11	1.71	0.72
3:F:501:TB2:C4	3:F:501:TB2:O1	2.36	0.72
1:C:135:PHE:HE2	1:C:267:VAL:HG21	1.54	0.72
1:C:136:GLY:O	1:C:142:VAL:CG1	2.38	0.72
1:G:111:TYR:HB2	1:G:290:LEU:HD12	1.71	0.72
1:F:306:THR:HG21	1:F:446:LEU:HD11	1.72	0.72
1:E:292:VAL:O	1:E:296:PHE:HB2	1.90	0.72
1:H:328:ILE:HG12	1:H:332:ILE:HD12	1.72	0.71
1:B:98:ARG:HG2	1:B:115:PHE:HA	1.72	0.71
1:B:75:VAL:HG12	1:B:387:GLU:HB2	1.70	0.71
1:A:305:THR:HG22	1:A:308:ARG:HH21	1.56	0.71
1:H:441:ILE:H	1:H:441:ILE:HD12	1.56	0.71
1:D:153:LEU:HD22	1:D:174:ILE:HG21	1.71	0.70
1:A:202:PHE:CE1	1:A:241:ILE:HD13	2.25	0.70
1:C:102:ALA:HB2	1:C:218:GLU:HA	1.73	0.70
1:F:245:ILE:HG22	1:F:289:ILE:HD13	1.73	0.70
1:F:98:ARG:HG2	1:F:115:PHE:HA	1.72	0.70
1:E:136:GLY:O	1:E:142:VAL:HB	1.91	0.70
1:E:98:ARG:NH1	1:E:367:VAL:HB	2.07	0.69
1:A:320:VAL:HG21	1:A:408:PHE:HE2	1.56	0.69
1:E:328:ILE:HG23	1:E:332:ILE:HD12	1.73	0.69
1:B:232:ARG:CG	1:B:232:ARG:HH11	1.91	0.69
1:E:101:ILE:HB	1:E:104:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LEU:HG	1:E:75:VAL:HG21	1.74	0.68
1:E:32:PRO:HD3	1:E:380:TYR:CZ	2.29	0.68
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.29	0.68
1:E:153:LEU:HD22	1:E:174:ILE:HG21	1.76	0.68
1:B:368:PRO:HG3	1:B:389:PHE:CE2	2.29	0.68
1:F:102:ALA:HB2	1:F:218:GLU:HA	1.76	0.68
1:A:132:MET:HE1	1:A:441:ILE:HD11	1.75	0.68
1:G:303:THR:HA	2:G:500:HEM:HBB1	1.76	0.67
1:F:34:PRO:HB2	1:F:42:ASN:ND2	2.08	0.67
1:G:135:PHE:HE2	1:G:267:VAL:HG21	1.58	0.67
1:G:73:ARG:HH12	1:G:218:GLU:HG3	1.60	0.67
1:B:485:GLN:HE21	1:B:485:GLN:HA	1.57	0.67
1:B:111:TYR:HB2	1:B:290:LEU:HD12	1.75	0.67
1:F:441:ILE:HD12	1:F:441:ILE:H	1.60	0.67
1:G:133:ARG:HA	1:G:137:MET:HB3	1.77	0.67
2:D:500:HEM:HMA1	2:D:500:HEM:HBA1	1.77	0.66
1:H:98:ARG:NH2	2:H:500:HEM:HBD1	2.10	0.66
1:F:143:GLU:O	1:F:147:GLN:HB2	1.96	0.66
1:G:153:LEU:HD22	1:G:174:ILE:HG21	1.77	0.66
1:F:108:PHE:HA	1:F:290:LEU:HD13	1.76	0.66
1:B:435:ILE:HG12	1:B:436:CYS:H	1.59	0.66
1:E:368:PRO:HG3	1:E:389:PHE:HE2	1.61	0.66
1:C:352:VAL:HG13	1:C:408:PHE:HZ	1.62	0.65
1:B:101:ILE:HB	1:B:104:VAL:HG22	1.77	0.65
1:B:153:LEU:HD22	1:B:174:ILE:HG21	1.77	0.65
1:D:98:ARG:HG2	1:D:115:PHE:HA	1.79	0.65
1:C:30:LEU:HD21	1:C:383:PRO:HD3	1.79	0.65
2:G:500:HEM:HBB2	2:G:500:HEM:CMB	2.27	0.65
1:H:30:LEU:CD2	1:H:383:PRO:HD3	2.26	0.65
1:H:103:VAL:HG23	1:H:104:VAL:HG13	1.79	0.65
1:C:98:ARG:HG2	1:C:115:PHE:HA	1.78	0.64
1:H:183:VAL:HA	1:H:264:PHE:HB3	1.78	0.64
1:H:98:ARG:HG2	1:H:115:PHE:HA	1.79	0.64
1:H:314:MET:HB2	1:H:459:ILE:HD11	1.79	0.64
1:A:314:MET:HB3	1:A:459:ILE:HD11	1.78	0.64
1:E:142:VAL:HG13	1:E:143:GLU:N	2.13	0.64
1:H:98:ARG:HH21	2:H:500:HEM:HBD1	1.62	0.64
1:D:284:HIS:CD2	1:D:286:GLN:HB2	2.32	0.64
1:F:147:GLN:HE21	1:F:339:ALA:HA	1.63	0.64
2:G:500:HEM:HBD1	2:G:500:HEM:CMD	2.24	0.63
1:D:202:PHE:CE1	1:D:241:ILE:HD13	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HD13	1:B:170:LEU:HD11	1.79	0.63
1:G:315:LEU:HD13	1:G:461:SER:HB2	1.81	0.63
1:B:43:LEU:HD22	1:B:220:PHE:HZ	1.62	0.63
1:H:154:VAL:HG13	1:H:457:PHE:HE2	1.64	0.63
1:H:154:VAL:HG21	1:H:452:THR:HG22	1.79	0.63
1:E:305:THR:HG22	1:E:308:ARG:HH21	1.63	0.63
1:G:404:THR:OG1	1:G:404:THR:O	2.11	0.63
1:D:284:HIS:N	1:D:284:HIS:ND1	2.47	0.63
2:H:500:HEM:HBD2	2:H:500:HEM:CHA	2.06	0.63
1:G:75:VAL:HG12	1:G:387:GLU:HB2	1.81	0.63
1:F:68:VAL:HG13	1:F:75:VAL:HG23	1.80	0.62
1:C:435:ILE:HG12	1:C:436:CYS:N	2.14	0.62
1:D:221:SER:O	1:D:225:LYS:HB3	1.98	0.62
1:D:32:PRO:HD3	1:D:380:TYR:CE1	2.34	0.62
1:G:124:LEU:HD11	1:G:287:ASN:OD1	1.98	0.62
1:C:164:LEU:HD22	1:C:485:GLN:HB3	1.81	0.62
1:E:426:PHE:CZ	1:E:428:PRO:HG3	2.35	0.62
1:G:150:ALA:O	1:G:154:VAL:HG23	1.99	0.62
1:C:403:GLU:O	1:C:412:HIS:NE2	2.32	0.62
1:F:310:GLY:O	1:F:314:MET:HG2	2.00	0.62
1:G:282:GLU:HA	1:G:284:HIS:CE1	2.35	0.62
1:B:164:LEU:HG	1:B:487:ARG:NH2	2.15	0.62
2:G:500:HEM:CMC	2:G:500:HEM:HBC2	2.29	0.62
1:H:154:VAL:HG13	1:H:457:PHE:CE2	2.35	0.62
1:B:227:PHE:HB3	1:B:228:PRO:HD2	1.82	0.62
1:D:102:ALA:HB2	1:D:218:GLU:HA	1.81	0.61
1:G:103:VAL:HG23	1:G:104:VAL:HG13	1.82	0.61
1:C:317:TYR:CE2	1:C:408:PHE:HB3	2.36	0.61
1:A:438:GLY:HA2	1:A:441:ILE:CD1	2.30	0.61
1:E:316:LYS:HE3	1:E:317:TYR:HE1	1.65	0.61
1:E:144:GLU:HA	1:E:147:GLN:HB2	1.81	0.61
1:B:303:THR:HA	2:B:500:HEM:HBB1	1.81	0.61
1:B:209:ILE:HG12	1:B:234:ILE:HD13	1.82	0.61
1:G:114:ILE:HA	2:G:500:HEM:HBD2	1.81	0.61
1:F:268:TYR:CE1	1:F:288:LEU:HB2	2.35	0.61
1:A:34:PRO:HB2	1:A:42:ASN:ND2	2.15	0.61
2:C:500:HEM:HBB2	2:C:500:HEM:CMB	2.31	0.61
1:F:245:ILE:O	1:F:249:VAL:HG23	2.00	0.61
1:D:115:PHE:CE2	3:D:501:TB2:H10	2.35	0.61
2:H:500:HEM:HBC2	2:H:500:HEM:CMC	2.30	0.61
2:A:500:HEM:CMB	2:A:500:HEM:HBB2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:HEM:HBC2	2:D:500:HEM:CMC	2.31	0.61
1:E:368:PRO:HG3	1:E:389:PHE:CE2	2.36	0.61
1:F:53:ARG:HH11	1:F:53:ARG:HB2	1.65	0.61
1:F:164:LEU:HG	1:F:487:ARG:NH2	2.16	0.61
1:C:176:SER:HB2	1:C:300:THR:HG23	1.82	0.61
1:H:128:SER:HA	1:H:264:PHE:HE2	1.67	0.60
1:C:137:MET:O	1:C:137:MET:HG3	2.00	0.60
1:B:53:ARG:HH11	1:B:53:ARG:HB2	1.65	0.60
1:H:70:LEU:HD12	1:H:75:VAL:HG11	1.83	0.60
1:F:430:SER:HB2	2:F:500:HEM:HBA2	1.83	0.60
1:G:153:LEU:HD22	1:G:174:ILE:HD13	1.84	0.60
1:E:34:PRO:HB2	1:E:42:ASN:ND2	2.15	0.60
1:A:320:VAL:O	1:A:324:VAL:HG23	2.01	0.60
1:B:282:GLU:O	1:B:287:ASN:ND2	2.35	0.60
1:F:103:VAL:HG23	1:F:104:VAL:HG13	1.83	0.60
1:E:205:SER:O	1:E:209:ILE:HG13	2.01	0.60
1:F:409:ASN:HB3	1:F:412:HIS:NE2	2.16	0.60
1:E:202:PHE:CE1	1:E:241:ILE:HD13	2.37	0.60
1:B:43:LEU:HD22	1:B:220:PHE:CZ	2.37	0.60
1:H:268:TYR:CD1	1:H:288:LEU:HD13	2.37	0.60
1:C:268:TYR:CE1	1:C:288:LEU:HB2	2.37	0.60
1:B:316:LYS:HG3	1:B:465:PRO:O	2.02	0.60
1:B:37:LEU:HD12	1:B:37:LEU:H	1.67	0.60
2:C:500:HEM:HHA	2:C:500:HEM:HBD1	1.82	0.59
1:E:146:ILE:HG12	1:E:178:ILE:HD12	1.83	0.59
1:E:299:GLY:HA2	2:E:500:HEM:HMC2	1.84	0.59
2:F:500:HEM:CMC	2:F:500:HEM:HBC2	2.31	0.59
1:D:362:LEU:O	1:D:364:PRO:HD3	2.02	0.59
1:H:157:LEU:HD12	1:H:488:PHE:HD2	1.66	0.59
1:D:125:ARG:O	1:D:129:LEU:HB2	2.02	0.59
1:G:146:ILE:HG12	1:G:178:ILE:HD12	1.83	0.59
1:G:312:LEU:HB2	1:G:484:TYR:CE1	2.37	0.59
1:F:125:ARG:O	1:F:129:LEU:HB2	2.03	0.59
1:H:205:SER:O	1:H:209:ILE:HG13	2.02	0.59
1:C:127:PHE:C	1:C:127:PHE:CD1	2.75	0.59
1:F:102:ALA:CB	1:F:218:GLU:HA	2.33	0.59
1:G:303:THR:OG1	2:G:500:HEM:HAB	2.02	0.59
2:F:500:HEM:HBB2	2:F:500:HEM:CMB	2.32	0.59
1:E:142:VAL:HG22	1:E:146:ILE:CD1	2.33	0.59
1:A:311:PHE:HD1	1:A:459:ILE:HD13	1.67	0.59
1:E:107:ILE:HG13	1:E:238:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:487:ARG:HD2	1:G:489:LEU:HD21	1.85	0.58
1:D:340:LEU:HD13	1:D:444:THR:HG23	1.86	0.58
1:C:305:THR:HG22	1:C:308:ARG:HH21	1.68	0.58
1:D:284:HIS:CE1	1:D:287:ASN:HD22	2.21	0.58
1:H:235:TYR:O	1:H:239:GLN:HB2	2.04	0.58
1:G:84:ILE:HD11	1:G:391:VAL:O	2.03	0.58
1:E:102:ALA:CB	1:E:218:GLU:HA	2.34	0.58
1:G:282:GLU:HA	1:G:284:HIS:HE1	1.68	0.58
2:D:500:HEM:CMB	2:D:500:HEM:HBB2	2.31	0.58
1:E:268:TYR:CE1	1:E:288:LEU:HB2	2.38	0.58
1:B:182:ILE:O	1:B:263:ASP:HB2	2.04	0.58
1:B:30:LEU:HD21	1:B:383:PRO:HD3	1.85	0.58
1:C:136:GLY:C	1:C:142:VAL:HG13	2.23	0.58
1:D:82:ASP:O	1:D:86:GLU:HG3	2.04	0.58
1:B:277:SER:O	1:B:279:PRO:HD3	2.03	0.58
1:C:438:GLY:HA2	1:C:441:ILE:CD1	2.34	0.57
1:E:313:LEU:HG	1:E:470:LEU:HD11	1.86	0.57
1:B:367:VAL:O	1:B:369:HIS:HD2	1.87	0.57
1:C:299:GLY:HA2	2:C:500:HEM:HMC2	1.86	0.57
1:F:82:ASP:O	1:F:86:GLU:HG3	2.04	0.57
2:H:500:HEM:CMB	2:H:500:HEM:HBB2	2.31	0.57
1:B:183:VAL:HA	1:B:264:PHE:HB3	1.86	0.57
1:E:314:MET:SD	1:E:450:PHE:HZ	2.27	0.57
2:B:500:HEM:HBD1	2:B:500:HEM:HHA	1.86	0.57
1:F:278:ASP:OD1	1:F:278:ASP:C	2.42	0.57
1:F:201:LEU:HB3	1:F:241:ILE:HD11	1.86	0.57
1:E:70:LEU:HD11	1:E:389:PHE:HE1	1.69	0.57
1:H:157:LEU:HD12	1:H:488:PHE:CD2	2.40	0.57
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.33	0.57
1:E:30:LEU:HD21	1:E:383:PRO:HD3	1.86	0.57
1:D:177:ASN:HD22	1:D:187:ARG:HE	1.52	0.57
1:G:238:LEU:HD23	1:G:241:ILE:HD12	1.87	0.57
1:C:299:GLY:HA2	2:C:500:HEM:CMC	2.34	0.57
1:C:135:PHE:CE2	1:C:267:VAL:HG21	2.37	0.57
1:D:305:THR:HG22	1:D:308:ARG:HH21	1.70	0.57
1:H:157:LEU:HD12	1:H:165:LEU:HD21	1.87	0.57
1:H:357:GLN:HE22	1:H:429:PHE:HE2	1.52	0.57
1:C:252:HIS:HD2	1:C:265:ILE:HB	1.70	0.57
1:H:314:MET:HB3	1:H:321:THR:OG1	2.05	0.57
1:C:292:VAL:O	1:C:296:PHE:HB2	2.05	0.57
1:F:153:LEU:HD21	1:F:453:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:VAL:O	1:G:265:ILE:HG13	2.05	0.56
1:F:85:ARG:O	1:F:89:VAL:HB	2.05	0.56
1:D:438:GLY:HA2	1:D:441:ILE:HD12	1.87	0.56
1:F:268:TYR:CD1	1:F:288:LEU:HD13	2.40	0.56
1:E:165:LEU:HD23	1:E:486:ILE:O	2.04	0.56
1:C:136:GLY:O	1:C:142:VAL:HG22	2.04	0.56
2:C:500:HEM:CMC	2:C:500:HEM:HBC2	2.32	0.56
1:C:232:ARG:CG	1:C:232:ARG:NH1	2.65	0.56
1:B:205:SER:O	1:B:209:ILE:HG13	2.05	0.56
1:B:438:GLY:HA2	1:B:441:ILE:HD12	1.85	0.56
1:B:225:LYS:HG2	1:B:226:TYR:CD1	2.40	0.56
1:G:471:THR:O	1:G:482:PRO:HG3	2.05	0.56
1:G:130:ALA:HA	1:G:133:ARG:HB2	1.88	0.56
1:B:168:THR:HA	1:B:308:ARG:HD3	1.87	0.56
1:H:125:ARG:O	1:H:129:LEU:HB2	2.04	0.56
1:H:42:ASN:O	1:H:46:MET:HG2	2.05	0.56
1:G:137:MET:SD	1:G:441:ILE:HD11	2.45	0.56
1:H:297:PHE:CD1	3:H:501:TB2:H10A	2.40	0.56
1:A:94:ALA:O	1:A:371:VAL:HA	2.06	0.56
1:G:111:TYR:N	1:G:111:TYR:CD1	2.74	0.56
1:A:42:ASN:O	1:A:46:MET:HG2	2.06	0.56
1:G:268:TYR:CE1	1:G:288:LEU:HB2	2.41	0.56
1:E:372:THR:O	1:E:384:LYS:HG3	2.04	0.56
1:E:111:TYR:HB2	1:E:290:LEU:HD12	1.86	0.56
1:H:164:LEU:HG	1:H:487:ARG:NH2	2.20	0.56
1:G:309:TYR:HD1	1:G:481:PRO:HB3	1.70	0.56
1:A:441:ILE:HD12	1:A:441:ILE:H	1.71	0.56
1:D:430:SER:O	1:D:431:LEU:HD23	2.05	0.56
1:D:115:PHE:HE2	3:D:501:TB2:H10	1.70	0.56
1:D:409:ASN:HB3	1:D:412:HIS:NE2	2.19	0.56
1:B:449:PHE:O	1:B:453:ILE:HG13	2.06	0.56
1:E:245:ILE:O	1:E:249:VAL:HG23	2.06	0.56
1:G:409:ASN:HB3	1:G:412:HIS:CE1	2.41	0.56
1:B:237:ASN:O	1:B:241:ILE:HG13	2.06	0.55
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.41	0.55
1:E:362:LEU:HD22	1:E:362:LEU:H	1.71	0.55
1:F:292:VAL:O	1:F:296:PHE:HB2	2.06	0.55
1:H:365:PHE:HA	1:H:391:VAL:HA	1.88	0.55
1:C:75:VAL:HG12	1:C:387:GLU:HB2	1.89	0.55
1:D:176:SER:HB2	1:D:300:THR:HG23	1.88	0.55
1:C:171:PHE:O	1:C:174:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:HIS:HE1	1:C:434:ARG:HB2	1.72	0.55
1:E:142:VAL:HG22	1:E:146:ILE:HD11	1.88	0.55
1:B:102:ALA:HB2	1:B:218:GLU:HA	1.88	0.55
1:G:195:PHE:CE2	1:G:199:LEU:HD11	2.42	0.55
1:D:264:PHE:CD1	1:D:264:PHE:O	2.60	0.55
1:C:198:LEU:HD11	1:C:244:PHE:CD1	2.41	0.55
1:G:108:PHE:HA	1:G:290:LEU:HD13	1.88	0.55
1:E:171:PHE:O	1:E:174:ILE:HG12	2.07	0.55
1:H:70:LEU:HG	1:H:75:VAL:HG21	1.88	0.55
1:H:241:ILE:O	1:H:245:ILE:HG13	2.07	0.55
1:C:323:ARG:HD3	1:C:348:TYR:CZ	2.42	0.55
1:A:301:GLU:CG	3:A:501:TB2:H2	2.37	0.55
1:D:84:ILE:HD11	1:D:391:VAL:O	2.05	0.55
1:F:103:VAL:HG12	1:F:217:PHE:CD2	2.41	0.55
1:A:121:TRP:CZ2	1:A:434:ARG:HD3	2.42	0.55
1:E:427:MET:HE2	1:E:431:LEU:HD11	1.89	0.55
1:H:314:MET:CB	1:H:459:ILE:HD11	2.36	0.55
1:A:112:GLY:O	1:A:116:ALA:HB2	2.07	0.55
1:H:157:LEU:CD1	1:H:165:LEU:HD21	2.37	0.54
1:E:65:VAL:HG21	1:E:377:PHE:HE2	1.72	0.54
1:E:142:VAL:CG1	1:E:143:GLU:N	2.70	0.54
1:B:202:PHE:CE1	1:B:241:ILE:HD13	2.42	0.54
1:H:38:PRO:O	1:H:39:VAL:HB	2.07	0.54
1:C:315:LEU:HD11	1:C:486:ILE:HG13	1.90	0.54
1:E:394:SER:O	1:E:398:ASP:HB2	2.07	0.54
1:E:87:ALA:O	1:E:91:GLN:O	2.24	0.54
1:F:127:PHE:CD1	1:F:127:PHE:C	2.81	0.54
1:E:317:TYR:CD1	1:E:317:TYR:N	2.76	0.54
1:D:69:TYR:CE2	1:D:74:PRO:HB3	2.42	0.54
1:E:317:TYR:HD1	1:E:317:TYR:N	2.05	0.54
1:E:362:LEU:O	1:E:364:PRO:HD3	2.07	0.54
1:B:154:VAL:HG13	1:B:457:PHE:CE2	2.43	0.54
1:B:299:GLY:HA2	2:B:500:HEM:HMC3	1.90	0.54
1:G:114:ILE:HG13	1:G:294:SER:HB3	1.88	0.54
1:G:358:ARG:HG3	1:G:396:LEU:HB3	1.89	0.54
1:C:150:ALA:O	1:C:154:VAL:HG23	2.07	0.54
1:F:105:ASP:HB3	1:F:106:PRO:HD3	1.88	0.54
1:E:133:ARG:HA	1:E:137:MET:HB3	1.90	0.54
1:C:34:PRO:HB2	1:C:42:ASN:ND2	2.23	0.54
1:B:206:PHE:CD2	1:B:480:VAL:HG13	2.43	0.54
1:E:164:LEU:HD21	1:E:462:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLY:O	1:C:142:VAL:CG2	2.56	0.54
1:B:245:ILE:O	1:B:249:VAL:HG23	2.08	0.54
1:E:179:ILE:HG21	1:E:295:LEU:O	2.07	0.54
1:G:316:LYS:HA	1:G:465:PRO:HB3	1.89	0.54
1:E:209:ILE:HG12	1:E:234:ILE:HD13	1.90	0.53
1:A:55:PHE:HE1	1:A:68:VAL:HG11	1.71	0.53
1:A:438:GLY:HA3	2:A:500:HEM:C2C	2.43	0.53
1:H:383:PRO:HD2	1:H:386:THR:OG1	2.08	0.53
1:A:284:HIS:N	1:A:284:HIS:ND1	2.56	0.53
1:H:438:GLY:HA3	2:H:500:HEM:C2C	2.43	0.53
1:C:232:ARG:HG2	1:C:232:ARG:NH1	2.23	0.53
1:H:101:ILE:O	1:H:105:ASP:HB2	2.09	0.53
1:B:105:ASP:HB3	1:B:106:PRO:HD3	1.90	0.53
1:E:134:ASP:OD2	1:E:135:PHE:CD2	2.61	0.53
1:C:232:ARG:HG3	1:C:232:ARG:HH11	1.73	0.53
1:E:167:ASN:ND2	1:E:171:PHE:HE2	2.07	0.53
1:C:404:THR:N	1:C:405:PRO:HD3	2.24	0.53
1:B:268:TYR:O	1:B:272:MET:HB2	2.08	0.53
1:F:278:ASP:OD1	1:F:280:SER:N	2.42	0.53
1:H:314:MET:HB2	1:H:459:ILE:CD1	2.39	0.53
1:F:172:HIS:HB3	1:F:199:LEU:HD22	1.91	0.53
1:F:209:ILE:HG22	1:F:477:VAL:HG11	1.91	0.53
1:B:98:ARG:HH22	2:B:500:HEM:HBA2	1.74	0.53
1:D:171:PHE:O	1:D:174:ILE:HG12	2.09	0.53
1:E:52:LEU:O	1:E:56:LEU:HG	2.09	0.53
1:B:195:PHE:O	1:B:199:LEU:HG	2.09	0.53
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.30	0.53
1:B:241:ILE:O	1:B:245:ILE:HG13	2.09	0.53
1:A:43:LEU:HD22	1:A:220:PHE:CZ	2.43	0.53
1:C:183:VAL:HA	1:C:264:PHE:HB3	1.89	0.53
1:D:172:HIS:HE1	1:D:305:THR:HG23	1.73	0.52
1:G:449:PHE:O	1:G:453:ILE:HG13	2.09	0.52
1:G:76:VAL:HB	1:G:388:VAL:HG13	1.90	0.52
1:H:472:PRO:HA	1:H:482:PRO:HD3	1.90	0.52
2:H:500:HEM:HHA	2:H:500:HEM:HBA2	1.91	0.52
1:C:232:ARG:HG2	1:C:232:ARG:HH11	1.73	0.52
1:C:102:ALA:CB	1:C:218:GLU:HA	2.38	0.52
1:B:51:LEU:HD22	1:B:55:PHE:CZ	2.44	0.52
1:A:222:GLY:HA2	1:A:225:LYS:HE2	1.90	0.52
1:D:75:VAL:HG12	1:D:387:GLU:HB2	1.91	0.52
1:C:120:ARG:HA	1:C:282:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLN:HG2	1:C:381:VAL:HG22	1.91	0.52
1:D:326:LYS:O	1:D:330:GLN:HG3	2.10	0.52
1:D:164:LEU:HD23	1:D:487:ARG:HB3	1.92	0.52
1:E:135:PHE:CE2	1:E:267:VAL:HG21	2.45	0.52
1:A:176:SER:HB2	1:A:300:THR:HG23	1.92	0.52
1:E:409:ASN:HB3	1:E:412:HIS:CD2	2.44	0.52
1:H:369:HIS:O	1:H:387:GLU:HA	2.10	0.52
1:H:230:THR:O	1:H:234:ILE:HG13	2.10	0.52
1:E:284:HIS:HB2	1:E:286:GLN:HB2	1.91	0.52
1:E:164:LEU:HD22	1:E:485:GLN:HB3	1.92	0.52
1:B:82:ASP:O	1:B:86:GLU:HG3	2.10	0.52
1:C:136:GLY:HA2	1:C:141:SER:OG	2.09	0.52
1:H:320:VAL:HG13	1:H:348:TYR:OH	2.10	0.52
1:G:413:PHE:O	1:G:414:LEU:HD23	2.10	0.52
1:G:111:TYR:HD1	1:G:111:TYR:N	2.07	0.51
1:A:139:LYS:HA	1:A:142:VAL:HG12	1.91	0.51
1:F:487:ARG:HD2	1:F:489:LEU:HD21	1.91	0.51
1:H:114:ILE:HG13	1:H:294:SER:HB3	1.92	0.51
1:D:430:SER:CB	2:D:500:HEM:HBA2	2.39	0.51
1:F:52:LEU:HD22	1:F:364:PRO:HB3	1.92	0.51
1:F:368:PRO:HG3	1:F:389:PHE:HE2	1.76	0.51
1:H:176:SER:HB3	1:H:195:PHE:HZ	1.75	0.51
1:A:358:ARG:HH12	1:A:397:HIS:HD2	1.58	0.51
1:B:364:PRO:HG3	1:B:479:ASN:ND2	2.25	0.51
1:C:147:GLN:O	1:C:150:ALA:HB3	2.10	0.51
1:B:195:PHE:CZ	1:B:199:LEU:HD11	2.46	0.51
1:F:103:VAL:HG12	1:F:217:PHE:HD2	1.74	0.51
1:G:135:PHE:CE2	1:G:267:VAL:HG21	2.44	0.51
1:D:102:ALA:HB1	1:D:217:PHE:HD2	1.75	0.51
1:D:163:ALA:HA	1:D:487:ARG:NH1	2.25	0.51
1:D:205:SER:O	1:D:209:ILE:HG13	2.10	0.51
1:C:87:ALA:HB2	1:C:377:PHE:CZ	2.46	0.51
1:G:363:ILE:N	1:G:363:ILE:HD12	2.26	0.51
1:C:252:HIS:CD2	1:C:265:ILE:HB	2.46	0.51
1:F:114:ILE:HG13	1:F:294:SER:HB3	1.92	0.51
1:F:242:ASN:HD21	1:F:293:LEU:HD22	1.75	0.51
1:H:244:PHE:HA	1:H:247:GLN:HG2	1.93	0.51
1:A:128:SER:HA	1:A:264:PHE:HE2	1.75	0.51
1:A:441:ILE:O	1:A:445:GLU:HG3	2.11	0.50
1:D:174:ILE:O	1:D:178:ILE:HG12	2.11	0.50
1:H:157:LEU:CD1	1:H:488:PHE:CD2	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HD11	1:B:235:TYR:HD1	1.76	0.50
1:C:326:LYS:O	1:C:330:GLN:HG3	2.11	0.50
1:A:98:ARG:NH1	1:A:367:VAL:HB	2.25	0.50
1:H:211:SER:HA	1:H:474:GLU:CG	2.42	0.50
1:H:268:TYR:CE1	1:H:288:LEU:HB2	2.46	0.50
1:A:98:ARG:HE	1:A:434:ARG:NH1	2.10	0.50
1:E:109:GLN:O	1:E:111:TYR:CD1	2.65	0.50
1:H:409:ASN:HB3	1:H:412:HIS:CD2	2.46	0.50
1:B:65:VAL:HG21	1:B:377:PHE:HE2	1.75	0.50
1:E:299:GLY:HA2	2:E:500:HEM:CMC	2.42	0.50
1:F:268:TYR:HE1	1:F:288:LEU:HB2	1.74	0.50
2:D:500:HEM:HBD1	2:D:500:HEM:HHA	1.94	0.50
1:C:438:GLY:O	1:C:442:ALA:HB3	2.12	0.50
1:B:268:TYR:CD1	1:B:288:LEU:HD13	2.47	0.50
1:A:139:LYS:HA	1:A:142:VAL:CG1	2.42	0.50
1:E:94:ALA:O	1:E:371:VAL:HA	2.12	0.50
1:A:102:ALA:CB	1:A:218:GLU:HA	2.38	0.50
1:A:438:GLY:O	1:A:442:ALA:CB	2.60	0.49
1:F:409:ASN:HB3	1:F:412:HIS:CD2	2.46	0.49
1:B:268:TYR:CE2	1:B:283:PHE:HD1	2.30	0.49
1:C:129:LEU:HD22	1:C:133:ARG:NH1	2.27	0.49
1:G:39:VAL:HG12	1:G:40:LEU:N	2.27	0.49
1:F:404:THR:OG1	1:F:407:THR:HB	2.11	0.49
1:H:102:ALA:HB2	1:H:218:GLU:HA	1.94	0.49
1:H:43:LEU:HD22	1:H:220:PHE:CZ	2.47	0.49
1:H:30:LEU:HD21	1:H:383:PRO:CD	2.39	0.49
1:H:362:LEU:HD22	1:H:362:LEU:H	1.77	0.49
1:A:114:ILE:HG12	2:A:500:HEM:HAD1	1.94	0.49
1:F:202:PHE:CE1	1:F:241:ILE:HD13	2.47	0.49
1:A:314:MET:SD	1:A:450:PHE:HZ	2.35	0.49
1:D:403:GLU:O	1:D:404:THR:CG2	2.59	0.49
1:E:321:THR:O	1:E:325:GLN:HG3	2.12	0.49
1:A:34:PRO:HG3	1:A:62:TYR:CZ	2.48	0.49
1:D:164:LEU:HD13	1:D:485:GLN:HB3	1.93	0.49
1:A:413:PHE:O	1:A:414:LEU:HD23	2.13	0.49
1:A:438:GLY:HA2	1:A:441:ILE:HD12	1.94	0.49
1:D:438:GLY:HA2	1:D:441:ILE:CD1	2.43	0.49
1:B:435:ILE:HG12	1:B:436:CYS:N	2.26	0.49
1:F:311:PHE:O	1:F:315:LEU:HG	2.13	0.49
1:B:345:LYS:O	1:B:347:PRO:HD3	2.13	0.49
1:G:102:ALA:HB2	1:G:218:GLU:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:LEU:HD22	1:H:220:PHE:HZ	1.78	0.49
1:F:342:ASP:HA	1:F:345:LYS:HE3	1.94	0.49
1:C:205:SER:O	1:C:209:ILE:HG13	2.12	0.49
1:F:252:HIS:CD2	1:F:262:ARG:HH21	2.30	0.49
1:H:194:VAL:O	1:H:198:LEU:HD23	2.13	0.49
1:A:84:ILE:HD12	1:A:395:ALA:HB2	1.94	0.49
1:A:316:LYS:C	1:A:318:PRO:HD3	2.32	0.49
1:E:352:VAL:O	1:E:356:ILE:HG13	2.12	0.49
1:E:316:LYS:C	1:E:317:TYR:HD1	2.15	0.49
1:A:80:GLY:O	1:A:84:ILE:HG13	2.12	0.49
1:H:395:ALA:HA	1:H:398:ASP:HB2	1.94	0.49
1:C:146:ILE:HG12	1:C:178:ILE:HD12	1.95	0.49
1:F:143:GLU:OE2	1:F:340:LEU:HB2	2.06	0.49
1:E:34:PRO:O	1:E:36:PRO:HD3	2.11	0.49
1:G:307:LEU:HD23	1:G:446:LEU:HD23	1.95	0.49
1:A:174:ILE:HG13	1:A:175:THR:N	2.28	0.49
1:G:36:PRO:HG3	1:G:69:TYR:CD1	2.48	0.49
1:C:70:LEU:HD22	1:C:219:LEU:HD11	1.93	0.49
1:E:112:GLY:O	1:E:116:ALA:HB2	2.13	0.49
1:B:352:VAL:O	1:B:356:ILE:HG13	2.13	0.49
1:A:194:VAL:O	1:A:198:LEU:HD23	2.12	0.49
1:D:127:PHE:CD1	1:D:127:PHE:C	2.85	0.49
1:H:157:LEU:CD1	1:H:165:LEU:CD2	2.91	0.49
1:G:268:TYR:CD1	1:G:288:LEU:HD13	2.48	0.49
1:D:132:MET:HG2	1:D:182:ILE:HG21	1.95	0.49
1:C:44:LEU:HB2	1:C:45:GLN:NE2	2.27	0.49
1:H:445:GLU:O	1:H:449:PHE:HB2	2.13	0.48
1:B:295:LEU:HD23	2:B:500:HEM:HBC1	1.95	0.48
1:B:111:TYR:HB2	1:B:290:LEU:CD1	2.42	0.48
1:D:114:ILE:HG13	1:D:294:SER:HB3	1.95	0.48
1:D:352:VAL:O	1:D:356:ILE:HG13	2.13	0.48
1:F:153:LEU:HD22	1:F:174:ILE:HG21	1.93	0.48
1:H:404:THR:N	1:H:405:PRO:HD3	2.28	0.48
1:D:324:VAL:O	1:D:328:ILE:HG13	2.13	0.48
1:E:122:ARG:CZ	1:E:122:ARG:HB2	2.42	0.48
1:H:441:ILE:O	1:H:445:GLU:HG3	2.13	0.48
1:E:68:VAL:HG22	1:E:69:TYR:N	2.28	0.48
1:E:129:LEU:O	1:E:133:ARG:HB2	2.13	0.48
1:F:143:GLU:HG3	1:F:448:LEU:HD11	1.96	0.48
1:F:98:ARG:HB2	1:F:434:ARG:NH1	2.28	0.48
1:F:311:PHE:HA	1:F:314:MET:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:SER:O	1:E:431:LEU:HD23	2.14	0.48
1:H:85:ARG:O	1:H:89:VAL:HB	2.14	0.48
1:A:150:ALA:O	1:A:154:VAL:HG23	2.13	0.48
1:B:297:PHE:CE1	3:B:501:TB2:H7	2.48	0.48
1:H:210:SER:HB3	1:H:478:GLY:O	2.12	0.48
1:C:427:MET:O	1:C:427:MET:HG3	2.14	0.48
1:C:183:VAL:HA	1:C:264:PHE:CB	2.44	0.48
1:B:297:PHE:CD1	3:B:501:TB2:H7	2.48	0.48
1:F:316:LYS:C	1:F:318:PRO:HD3	2.34	0.48
1:A:315:LEU:HD11	1:A:486:ILE:HG13	1.95	0.48
1:H:357:GLN:NE2	1:H:429:PHE:HE2	2.11	0.48
1:E:52:LEU:HD13	1:E:365:PHE:HD2	1.78	0.48
1:H:401:TYR:CD2	1:H:424:GLU:HB2	2.49	0.48
1:B:398:ASP:OD2	1:B:401:TYR:HD1	1.95	0.48
2:F:500:HEM:CBA	2:F:500:HEM:HMA1	2.42	0.48
1:B:284:HIS:HB2	1:B:287:ASN:H	1.79	0.48
1:H:107:ILE:HD11	1:H:235:TYR:HA	1.95	0.48
1:E:134:ASP:OD2	1:E:135:PHE:CE2	2.67	0.48
1:H:144:GLU:O	1:H:148:GLU:HB3	2.14	0.48
1:D:85:ARG:HA	1:D:89:VAL:HG23	1.96	0.48
1:D:313:LEU:HD22	1:D:408:PHE:CD1	2.49	0.48
1:B:163:ALA:HA	1:B:487:ARG:NH1	2.29	0.48
1:G:315:LEU:HD21	1:G:459:ILE:HB	1.96	0.48
1:H:364:PRO:HD2	1:H:477:VAL:O	2.14	0.48
1:E:297:PHE:CD1	3:E:501:TB2:H5	2.49	0.48
1:D:369:HIS:NE2	2:D:500:HEM:O2A	2.46	0.48
1:C:438:GLY:HA2	1:C:441:ILE:HD12	1.96	0.48
1:C:30:LEU:HD21	1:C:383:PRO:CD	2.42	0.48
1:G:107:ILE:HG21	1:G:238:LEU:HD13	1.96	0.48
1:D:228:PRO:HG3	1:G:213:SER:HB3	1.95	0.48
1:D:87:ALA:O	1:D:91:GLN:O	2.32	0.48
1:B:370:THR:HA	1:B:386:THR:O	2.13	0.48
1:C:30:LEU:CD2	1:C:383:PRO:HD3	2.43	0.48
1:D:30:LEU:HD22	1:D:383:PRO:HD3	1.95	0.48
1:H:364:PRO:HA	1:H:393:SER:HB2	1.94	0.48
1:H:43:LEU:HD13	1:H:219:LEU:HD23	1.96	0.48
1:E:163:ALA:HA	1:E:487:ARG:NH1	2.28	0.48
1:C:190:TYR:O	1:C:191:LYS:HD2	2.14	0.48
1:G:66:PHE:CE2	1:G:77:VAL:HG21	2.49	0.48
1:F:98:ARG:HB2	1:F:434:ARG:HH12	1.78	0.47
1:E:32:PRO:O	1:E:66:PHE:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:LEU:HG	1:H:487:ARG:CZ	2.44	0.47
1:A:384:LYS:O	1:A:385:ASN:HB2	2.14	0.47
1:A:353:ILE:HD11	1:A:447:PHE:HA	1.96	0.47
1:H:120:ARG:HG3	1:H:282:GLU:OE1	2.14	0.47
1:D:120:ARG:HA	1:D:282:GLU:HG3	1.96	0.47
1:C:362:LEU:C	1:C:363:ILE:HD12	2.34	0.47
1:E:349:THR:O	1:E:353:ILE:HG13	2.14	0.47
1:H:146:ILE:HG23	1:H:449:PHE:CZ	2.49	0.47
1:F:121:TRP:CZ2	1:F:434:ARG:HD3	2.49	0.47
1:G:69:TYR:CE2	1:G:74:PRO:HB3	2.49	0.47
1:H:127:PHE:CE1	1:H:268:TYR:HD2	2.32	0.47
1:G:34:PRO:HB2	1:G:42:ASN:ND2	2.29	0.47
1:C:457:PHE:CD1	1:C:488:PHE:HB3	2.50	0.47
1:D:177:ASN:ND2	1:D:187:ARG:HB2	2.30	0.47
1:E:120:ARG:O	1:E:124:LEU:HG	2.14	0.47
1:F:305:THR:HG22	1:F:308:ARG:NH2	2.19	0.47
1:D:30:LEU:HB3	1:D:31:PRO:HD2	1.96	0.47
1:G:32:PRO:HD3	1:G:380:TYR:CZ	2.50	0.47
1:F:404:THR:HG1	1:F:407:THR:HB	1.80	0.47
1:E:195:PHE:CE2	1:E:199:LEU:HD11	2.50	0.47
1:G:263:ASP:O	1:G:266:ASP:HB2	2.14	0.47
1:F:150:ALA:O	1:F:154:VAL:HG23	2.13	0.47
1:E:307:LEU:HD12	1:E:311:PHE:HE2	1.79	0.47
1:E:384:LYS:HG2	1:E:385:ASN:CG	2.35	0.47
1:A:43:LEU:HD22	1:A:220:PHE:HZ	1.78	0.47
1:H:211:SER:HA	1:H:474:GLU:HG3	1.96	0.47
1:C:307:LEU:HD23	1:C:446:LEU:HD23	1.97	0.47
1:B:321:THR:HG23	1:B:454:LEU:HD21	1.96	0.47
1:E:457:PHE:HA	1:E:491:ARG:HG3	1.97	0.47
1:F:429:PHE:HB3	1:F:436:CYS:HB3	1.97	0.47
1:E:317:TYR:CE2	1:E:408:PHE:HB3	2.50	0.47
1:B:37:LEU:HD12	1:B:37:LEU:N	2.30	0.47
1:G:316:LYS:HG3	1:G:465:PRO:O	2.15	0.47
1:E:263:ASP:O	1:E:267:VAL:HG23	2.15	0.47
1:A:150:ALA:HB1	1:A:452:THR:HG21	1.97	0.47
1:B:125:ARG:O	1:B:129:LEU:HB2	2.15	0.47
1:D:174:ILE:HB	1:D:449:PHE:CZ	2.50	0.47
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.50	0.47
1:B:316:LYS:HD3	1:B:317:TYR:HE1	1.80	0.47
1:H:107:ILE:HG13	1:H:238:LEU:HD12	1.97	0.47
1:G:265:ILE:HG23	1:G:288:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:PHE:O	1:F:199:LEU:HG	2.15	0.47
1:H:188:PHE:HB2	1:H:195:PHE:CD2	2.50	0.47
1:A:323:ARG:HD3	1:A:348:TYR:CZ	2.50	0.47
1:C:43:LEU:HD22	1:C:220:PHE:HZ	1.80	0.47
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.49	0.47
1:B:479:ASN:O	1:B:481:PRO:HD3	2.14	0.47
1:H:404:THR:O	1:H:404:THR:HG23	2.15	0.47
1:H:307:LEU:HD23	1:H:446:LEU:HD23	1.96	0.47
1:G:206:PHE:CE1	3:G:501:TB2:H2	2.50	0.47
1:G:295:LEU:HD23	2:G:500:HEM:HAC	1.96	0.46
1:C:434:ARG:HD2	2:C:500:HEM:O2D	2.14	0.46
1:F:34:PRO:HG3	1:F:62:TYR:CZ	2.50	0.46
1:B:102:ALA:CB	1:B:218:GLU:HA	2.44	0.46
1:D:107:ILE:HG13	1:D:238:LEU:HD12	1.97	0.46
1:F:40:LEU:O	1:F:43:LEU:HB2	2.15	0.46
1:E:43:LEU:HD22	1:E:220:PHE:CZ	2.49	0.46
1:H:66:PHE:HE1	1:H:79:CYS:SG	2.37	0.46
1:G:31:PRO:HA	1:G:380:TYR:CD1	2.51	0.46
1:G:413:PHE:O	1:G:420:LEU:HA	2.16	0.46
1:F:248:SER:HA	1:F:251:LYS:HB2	1.98	0.46
1:B:327:GLU:HG2	1:B:346:MET:HG2	1.97	0.46
1:D:241:ILE:O	1:D:245:ILE:HG13	2.15	0.46
1:F:314:MET:HA	1:F:314:MET:CE	2.44	0.46
1:D:268:TYR:CG	1:D:288:LEU:HD13	2.51	0.46
1:E:52:LEU:HD22	1:E:364:PRO:HB3	1.96	0.46
1:B:232:ARG:CG	1:B:232:ARG:NH1	2.60	0.46
1:H:237:ASN:O	1:H:241:ILE:HG13	2.14	0.46
1:E:30:LEU:CD2	1:E:383:PRO:HD3	2.45	0.46
1:E:154:VAL:HG13	1:E:457:PHE:CE2	2.51	0.46
1:A:76:VAL:HG21	1:A:382:ILE:HD13	1.97	0.46
1:A:464:PRO:HB2	1:A:466:GLU:HG2	1.98	0.46
1:E:307:LEU:HD21	1:E:449:PHE:HB2	1.97	0.46
1:C:268:TYR:CG	1:C:288:LEU:HD13	2.51	0.46
1:B:135:PHE:CZ	1:B:263:ASP:HA	2.50	0.46
1:H:364:PRO:HG2	1:H:476:GLY:O	2.15	0.46
1:A:301:GLU:HG3	3:A:501:TB2:H2	1.96	0.46
1:F:196:LEU:HD23	1:F:199:LEU:HD12	1.98	0.46
1:C:43:LEU:HD22	1:C:220:PHE:CZ	2.51	0.46
1:H:223:PHE:HE2	1:H:227:PHE:CE2	2.33	0.46
1:H:177:ASN:HA	1:H:180:CYS:HB2	1.96	0.46
1:B:384:LYS:O	1:B:385:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:PRO:HG3	1:B:69:TYR:CD1	2.51	0.46
1:H:363:ILE:N	1:H:363:ILE:HD12	2.31	0.46
1:H:328:ILE:O	1:H:332:ILE:HB	2.16	0.46
1:E:167:ASN:ND2	1:E:171:PHE:CE2	2.83	0.46
1:H:369:HIS:HE1	1:H:434:ARG:HB2	1.81	0.46
1:D:357:GLN:HE21	2:D:500:HEM:CBB	2.28	0.46
1:G:362:LEU:H	1:G:362:LEU:CD2	2.21	0.46
1:A:42:ASN:OD1	1:A:69:TYR:HB2	2.15	0.46
1:F:409:ASN:HD22	1:F:411:GLY:H	1.62	0.46
1:C:150:ALA:HB1	1:C:452:THR:HG21	1.96	0.46
1:H:66:PHE:HE1	1:H:79:CYS:HG	1.63	0.46
1:D:263:ASP:O	1:D:266:ASP:HB2	2.15	0.46
1:F:147:GLN:O	1:F:150:ALA:HB3	2.15	0.46
2:D:500:HEM:CMA	2:D:500:HEM:HBA1	2.46	0.46
1:F:438:GLY:O	1:F:439:GLU:C	2.53	0.46
1:C:127:PHE:O	1:C:131:THR:OG1	2.31	0.46
1:G:316:LYS:C	1:G:318:PRO:HD3	2.35	0.46
1:C:404:THR:OG1	1:C:407:THR:HB	2.15	0.46
1:A:358:ARG:NH1	1:A:397:HIS:HD2	2.14	0.46
1:D:137:MET:SD	1:D:441:ILE:HD11	2.56	0.46
1:F:43:LEU:HD22	1:F:220:PHE:HZ	1.81	0.46
1:G:305:THR:CG2	1:G:308:ARG:HH21	2.29	0.46
1:A:362:LEU:H	1:A:362:LEU:HD22	1.80	0.46
1:H:298:ALA:CB	4:H:8:HOH:O	2.64	0.46
1:H:165:LEU:HD21	1:H:488:PHE:HD2	1.80	0.46
1:A:94:ALA:HB1	1:A:375:THR:OG1	2.15	0.46
1:E:461:SER:OG	1:E:462:PRO:HD2	2.15	0.46
1:E:403:GLU:O	1:E:412:HIS:NE2	2.49	0.46
1:G:332:ILE:HD13	1:G:338:PRO:HB3	1.96	0.46
1:C:324:VAL:O	1:C:328:ILE:HG13	2.16	0.46
1:A:205:SER:O	1:A:209:ILE:HG13	2.16	0.46
1:C:73:ARG:HA	1:C:74:PRO:HD3	1.77	0.45
1:D:104:VAL:HG21	3:D:501:TB2:H11	1.99	0.45
1:F:164:LEU:HD11	1:F:462:PRO:HG3	1.97	0.45
1:H:125:ARG:NH1	1:H:437:LEU:HD11	2.31	0.45
1:B:150:ALA:HB1	1:B:452:THR:HG21	1.98	0.45
1:F:204:GLN:O	1:F:208:LEU:HG	2.15	0.45
1:G:205:SER:O	1:G:209:ILE:HG13	2.16	0.45
1:F:143:GLU:OE2	1:F:340:LEU:CA	2.64	0.45
1:D:297:PHE:CD1	3:D:501:TB2:H12B	2.51	0.45
1:H:103:VAL:HB	1:H:234:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD21	1:A:459:ILE:HB	1.98	0.45
1:H:154:VAL:HG12	1:H:154:VAL:O	2.16	0.45
1:G:183:VAL:HA	1:G:264:PHE:HB3	1.98	0.45
1:C:486:ILE:HG12	1:C:487:ARG:N	2.31	0.45
1:E:463:VAL:HA	1:E:464:PRO:HD3	1.84	0.45
1:F:367:VAL:O	1:F:369:HIS:HD2	2.00	0.45
1:C:384:LYS:O	1:C:385:ASN:HB2	2.17	0.45
1:G:98:ARG:NH1	1:G:367:VAL:HB	2.31	0.45
1:A:445:GLU:O	1:A:449:PHE:HB2	2.15	0.45
1:C:438:GLY:HA3	2:C:500:HEM:C2C	2.51	0.45
1:A:459:ILE:HB	1:A:486:ILE:HD11	1.98	0.45
1:H:268:TYR:OH	1:H:283:PHE:HA	2.17	0.45
1:F:105:ASP:O	1:F:109:GLN:N	2.49	0.45
1:C:364:PRO:HA	1:C:393:SER:HB2	1.97	0.45
1:C:314:MET:SD	1:C:450:PHE:HZ	2.40	0.45
1:C:284:HIS:HB2	1:C:287:ASN:H	1.81	0.45
1:E:351:ALA:HB2	1:E:414:LEU:HD21	1.99	0.45
1:A:217:PHE:O	1:A:221:SER:HB3	2.16	0.45
1:B:125:ARG:NH1	2:B:500:HEM:O1D	2.49	0.45
1:C:441:ILE:H	1:C:441:ILE:HD12	1.81	0.45
1:G:137:MET:HG3	1:G:137:MET:O	2.15	0.45
1:D:103:VAL:HG23	1:D:104:VAL:HG13	1.98	0.45
1:D:264:PHE:CD1	1:D:264:PHE:C	2.89	0.45
1:B:427:MET:HE2	1:B:431:LEU:HD11	1.99	0.45
1:F:103:VAL:HG23	1:F:104:VAL:N	2.32	0.45
1:E:32:PRO:HD3	1:E:380:TYR:OH	2.17	0.45
1:G:164:LEU:HD23	1:G:487:ARG:HB3	1.98	0.45
1:D:31:PRO:HA	1:D:380:TYR:CD1	2.51	0.45
1:E:131:THR:O	1:E:135:PHE:HD2	2.00	0.45
3:G:501:TB2:C8	3:G:501:TB2:O1	2.60	0.45
1:C:201:LEU:HB3	1:C:241:ILE:HD11	1.99	0.45
1:A:309:TYR:CE2	1:A:313:LEU:HD11	2.52	0.45
1:G:237:ASN:O	1:G:241:ILE:HG13	2.17	0.45
1:D:43:LEU:HD22	1:D:220:PHE:HZ	1.82	0.45
1:G:87:ALA:HB2	1:G:377:PHE:CE1	2.52	0.45
1:F:363:ILE:HD12	1:F:363:ILE:N	2.32	0.45
1:A:312:LEU:HD13	1:A:484:TYR:CD1	2.52	0.45
1:H:449:PHE:O	1:H:453:ILE:HG13	2.17	0.45
1:H:30:LEU:HD23	1:H:381:VAL:O	2.17	0.45
1:E:120:ARG:HA	1:E:282:GLU:HG3	1.99	0.45
1:D:401:TYR:CD2	1:D:424:GLU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:ILE:H	1:D:441:ILE:HD12	1.81	0.45
1:D:102:ALA:HB1	1:D:217:PHE:CD2	2.51	0.45
1:B:263:ASP:H	1:B:266:ASP:HB2	1.82	0.45
1:B:206:PHE:CZ	1:B:478:GLY:HA3	2.52	0.45
1:C:156:GLU:HG2	1:C:190:TYR:HD2	1.81	0.45
2:E:500:HEM:HHA	2:E:500:HEM:HBD1	1.99	0.45
1:A:299:GLY:HA2	2:A:500:HEM:CMC	2.47	0.45
1:E:174:ILE:HD12	1:E:449:PHE:CD1	2.51	0.45
1:F:164:LEU:HD22	1:F:485:GLN:HB3	1.98	0.45
1:A:353:ILE:CD1	1:A:447:PHE:HA	2.47	0.45
1:A:103:VAL:O	1:A:106:PRO:HD2	2.17	0.45
1:F:104:VAL:HG21	3:F:501:TB2:H10	1.98	0.44
1:F:112:GLY:O	1:F:116:ALA:HB2	2.15	0.44
1:A:324:VAL:O	1:A:328:ILE:HG13	2.17	0.44
1:E:392:LEU:HD22	1:E:427:MET:HG3	1.99	0.44
1:A:105:ASP:N	1:A:106:PRO:CD	2.80	0.44
1:C:213:SER:HB2	1:C:230:THR:OG1	2.17	0.44
1:A:438:GLY:O	1:A:442:ALA:HB3	2.17	0.44
1:C:441:ILE:O	1:C:445:GLU:HG3	2.17	0.44
1:D:154:VAL:HG13	1:D:457:PHE:CE2	2.52	0.44
1:D:150:ALA:O	1:D:154:VAL:HG23	2.17	0.44
1:G:460:ALA:HB3	1:G:487:ARG:HG2	1.98	0.44
1:D:30:LEU:CD2	1:D:383:PRO:HD3	2.48	0.44
1:H:238:LEU:HD23	1:H:241:ILE:HD12	1.99	0.44
1:B:107:ILE:HD11	1:B:235:TYR:CD1	2.52	0.44
1:F:146:ILE:HG12	1:F:178:ILE:HD12	1.99	0.44
1:A:120:ARG:HA	1:A:282:GLU:HG3	1.99	0.44
1:D:242:ASN:OD1	1:D:293:LEU:HD22	2.16	0.44
1:H:37:LEU:N	1:H:37:LEU:HD12	2.32	0.44
1:F:299:GLY:HA2	2:F:500:HEM:CMC	2.47	0.44
1:H:362:LEU:O	1:H:364:PRO:HD3	2.17	0.44
1:E:43:LEU:HD22	1:E:220:PHE:HZ	1.83	0.44
1:A:30:LEU:HD21	1:A:383:PRO:HD2	1.99	0.44
1:C:110:GLY:O	1:C:116:ALA:HA	2.17	0.44
1:D:207:SER:HA	1:D:480:VAL:HG21	1.99	0.44
1:A:153:LEU:HD13	1:A:170:LEU:HD11	1.99	0.44
1:B:192:ASP:HB3	1:B:195:PHE:HB3	1.97	0.44
1:A:457:PHE:CD1	1:A:488:PHE:HB3	2.52	0.44
1:B:312:LEU:HB2	1:B:484:TYR:CE1	2.53	0.44
1:C:94:ALA:O	1:C:371:VAL:HA	2.18	0.44
1:A:190:TYR:O	1:A:191:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:VAL:O	1:G:324:VAL:HG23	2.18	0.44
1:D:101:ILE:CG2	1:D:104:VAL:HG22	2.48	0.44
1:D:183:VAL:HA	1:D:264:PHE:HB3	1.99	0.44
1:G:42:ASN:O	1:G:46:MET:HG2	2.17	0.44
1:C:202:PHE:CE1	1:C:241:ILE:HD13	2.52	0.44
1:C:241:ILE:O	1:C:245:ILE:HG13	2.18	0.44
1:G:331:VAL:HG21	1:G:346:MET:HG2	1.99	0.44
1:D:208:LEU:O	1:D:214:SER:HB2	2.17	0.44
1:D:34:PRO:HB2	1:D:42:ASN:ND2	2.31	0.44
1:G:284:HIS:ND1	1:G:284:HIS:N	2.66	0.44
1:F:223:PHE:CD2	1:F:223:PHE:C	2.90	0.44
1:C:101:ILE:CG2	1:C:104:VAL:HG22	2.47	0.44
1:A:441:ILE:CD1	1:A:441:ILE:H	2.29	0.44
1:F:179:ILE:HG13	1:F:299:GLY:HA3	2.00	0.44
1:D:133:ARG:HG2	1:D:137:MET:HG2	1.99	0.44
1:H:52:LEU:HD13	1:H:364:PRO:HB3	1.99	0.44
1:E:129:LEU:HD22	1:E:133:ARG:HD3	1.98	0.44
1:A:183:VAL:HA	1:A:264:PHE:HB3	2.00	0.44
1:G:301:GLU:O	1:G:305:THR:OG1	2.35	0.44
1:E:183:VAL:HA	1:E:264:PHE:HB3	2.00	0.44
1:C:111:TYR:HB2	1:C:290:LEU:HD12	1.99	0.44
1:E:401:TYR:CE2	1:E:424:GLU:HB2	2.53	0.44
1:A:142:VAL:HG13	1:A:143:GLU:N	2.33	0.44
1:C:363:ILE:N	1:C:363:ILE:HD12	2.33	0.44
1:C:37:LEU:N	1:C:37:LEU:HD12	2.33	0.44
1:C:263:ASP:O	1:C:267:VAL:HG23	2.18	0.44
1:A:362:LEU:N	1:A:362:LEU:HD22	2.32	0.44
1:C:155:GLU:O	1:C:159:LYS:HG3	2.18	0.44
1:C:317:TYR:N	1:C:317:TYR:CD1	2.86	0.43
1:B:51:LEU:HB2	1:B:215:GLN:OE1	2.18	0.43
1:C:84:ILE:HD11	1:C:391:VAL:O	2.17	0.43
1:B:223:PHE:CD2	1:B:223:PHE:C	2.90	0.43
1:F:355:GLU:OE1	1:F:355:GLU:HA	2.18	0.43
1:A:367:VAL:CG2	2:A:500:HEM:HAA2	2.49	0.43
1:B:363:ILE:N	1:B:363:ILE:HD12	2.33	0.43
2:E:500:HEM:HBB2	2:E:500:HEM:CHC	2.36	0.43
1:F:320:VAL:HG21	1:F:408:PHE:CE2	2.42	0.43
1:F:223:PHE:HD2	1:F:223:PHE:C	2.22	0.43
1:G:401:TYR:CE2	1:G:424:GLU:HB2	2.54	0.43
1:D:105:ASP:N	1:D:106:PRO:CD	2.81	0.43
1:C:256:LEU:O	1:C:258:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LYS:HB3	1:B:421:LYS:HE2	1.75	0.43
1:G:485:GLN:HE21	1:G:485:GLN:HA	1.83	0.43
1:H:367:VAL:CG2	2:H:500:HEM:HAA1	2.48	0.43
1:F:75:VAL:HG12	1:F:387:GLU:CB	2.42	0.43
1:D:370:THR:HG22	1:D:387:GLU:HG2	2.00	0.43
1:D:432:GLY:C	1:D:434:ARG:H	2.22	0.43
1:G:73:ARG:NH1	1:G:218:GLU:HG3	2.32	0.43
1:B:164:LEU:HD13	1:B:485:GLN:HB3	1.99	0.43
1:H:457:PHE:HB3	1:H:488:PHE:HB3	2.01	0.43
1:G:287:ASN:O	1:G:291:THR:HB	2.19	0.43
1:D:409:ASN:HB3	1:D:412:HIS:CD2	2.53	0.43
1:F:368:PRO:HG3	1:F:389:PHE:CE2	2.53	0.43
1:E:447:PHE:O	1:E:451:THR:HG23	2.18	0.43
1:C:337:PRO:HA	1:C:338:PRO:HD3	1.93	0.43
1:A:287:ASN:O	1:A:291:THR:HB	2.18	0.43
1:D:447:PHE:O	1:D:451:THR:HG23	2.18	0.43
1:H:268:TYR:CG	1:H:288:LEU:HD13	2.54	0.43
1:B:36:PRO:HG3	1:B:69:TYR:CE1	2.54	0.43
1:A:352:VAL:O	1:A:356:ILE:HG13	2.18	0.43
1:C:247:GLN:HE21	1:C:247:GLN:HB3	1.64	0.43
1:A:314:MET:CB	1:A:459:ILE:HD11	2.48	0.43
1:D:284:HIS:HD2	1:D:286:GLN:HB2	1.83	0.43
1:B:53:ARG:NH1	1:B:53:ARG:HB2	2.31	0.43
3:A:501:TB2:C8	3:A:501:TB2:O1	2.61	0.43
1:A:170:LEU:HD13	1:A:170:LEU:O	2.18	0.43
1:F:321:THR:HG23	1:F:454:LEU:HD21	2.00	0.43
1:E:153:LEU:HD21	1:E:453:ILE:HD11	2.01	0.43
1:B:183:VAL:HG11	1:B:292:VAL:HG13	2.01	0.43
1:F:404:THR:N	1:F:405:PRO:HD3	2.33	0.43
1:C:37:LEU:HD12	1:C:37:LEU:H	1.84	0.43
1:E:211:SER:HA	1:E:474:GLU:OE2	2.18	0.43
1:G:384:LYS:O	1:G:385:ASN:HB2	2.19	0.43
1:F:230:THR:O	1:F:234:ILE:HG13	2.19	0.43
2:E:500:HEM:CBC	2:E:500:HEM:HHD	2.36	0.43
1:H:103:VAL:HG11	1:H:214:SER:OG	2.19	0.43
1:E:316:LYS:HE3	1:E:317:TYR:CE1	2.51	0.43
1:G:472:PRO:HA	1:G:482:PRO:HD3	1.99	0.43
1:A:105:ASP:N	1:A:106:PRO:HD2	2.33	0.43
1:F:256:LEU:O	1:F:258:PRO:HD3	2.19	0.43
1:F:353:ILE:HD13	1:F:447:PHE:HA	2.00	0.43
1:B:73:ARG:HA	1:B:74:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ALA:HB2	1:C:218:GLU:CD	2.39	0.43
1:F:241:ILE:O	1:F:245:ILE:HG13	2.19	0.43
1:G:69:TYR:HA	1:G:73:ARG:O	2.18	0.43
1:G:68:VAL:O	1:G:75:VAL:HG22	2.19	0.43
1:G:101:ILE:CG2	1:G:104:VAL:HG22	2.48	0.43
1:C:42:ASN:O	1:C:46:MET:HG2	2.19	0.43
1:D:229:GLY:O	1:D:232:ARG:HB2	2.19	0.43
1:F:79:CYS:O	1:F:83:ALA:HB3	2.18	0.43
1:C:211:SER:HA	1:C:474:GLU:HG2	2.01	0.43
1:A:402:PHE:O	1:A:405:PRO:HG3	2.18	0.43
1:E:311:PHE:O	1:E:315:LEU:HG	2.19	0.42
1:B:362:LEU:O	1:B:478:GLY:HA2	2.19	0.42
1:B:404:THR:N	1:B:405:PRO:HD3	2.34	0.42
1:E:192:ASP:HA	1:E:193:PRO:HD3	1.89	0.42
1:C:50:GLY:O	1:C:54:SER:HB2	2.19	0.42
2:G:500:HEM:CBB	2:G:500:HEM:HMB2	2.41	0.42
1:E:135:PHE:HE2	1:E:267:VAL:HG21	1.84	0.42
1:H:315:LEU:HD22	1:H:461:SER:HB2	2.01	0.42
1:G:37:LEU:N	1:G:37:LEU:HD12	2.34	0.42
1:B:157:LEU:HD22	1:B:488:PHE:CD2	2.54	0.42
1:G:154:VAL:HG13	1:G:457:PHE:HE2	1.83	0.42
1:D:475:SER:HA	1:D:479:ASN:OD1	2.19	0.42
1:B:376:GLN:HA	1:B:380:TYR:O	2.19	0.42
1:A:129:LEU:C	1:A:129:LEU:HD23	2.40	0.42
1:A:427:MET:O	1:A:427:MET:HG3	2.20	0.42
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.88	0.42
1:C:368:PRO:HG3	1:C:389:PHE:CE2	2.54	0.42
1:F:442:ALA:O	1:F:446:LEU:HB2	2.18	0.42
1:C:73:ARG:HH12	1:C:218:GLU:HG3	1.84	0.42
1:F:116:ALA:C	1:F:121:TRP:HB2	2.39	0.42
1:B:163:ALA:HA	1:B:487:ARG:HH12	1.84	0.42
1:B:153:LEU:O	1:B:153:LEU:HD12	2.18	0.42
1:H:164:LEU:HD22	1:H:485:GLN:HB3	2.01	0.42
1:B:457:PHE:HA	1:B:489:LEU:O	2.19	0.42
1:D:75:VAL:HG11	1:D:389:PHE:HE1	1.84	0.42
1:A:154:VAL:HG13	1:A:457:PHE:HE2	1.84	0.42
1:A:76:VAL:HB	1:A:388:VAL:HG13	2.02	0.42
1:C:284:HIS:ND1	1:C:284:HIS:N	2.67	0.42
1:B:32:PRO:HD3	1:B:380:TYR:CZ	2.55	0.42
1:D:197:ARG:NH2	1:D:201:LEU:HD21	2.34	0.42
1:H:438:GLY:HA2	1:H:441:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:PHE:O	1:F:430:SER:HB3	2.20	0.42
1:E:98:ARG:HE	1:E:434:ARG:NH1	2.17	0.42
1:G:315:LEU:HD11	1:G:486:ILE:HG13	2.01	0.42
1:D:382:ILE:HA	1:D:383:PRO:HD3	1.86	0.42
1:F:195:PHE:CE2	1:F:199:LEU:HD11	2.55	0.42
1:H:223:PHE:C	1:H:223:PHE:CD2	2.93	0.42
1:C:202:PHE:CZ	1:C:297:PHE:HA	2.54	0.42
1:E:38:PRO:O	1:E:39:VAL:HB	2.19	0.42
1:C:86:GLU:O	1:C:90:ASP:HB2	2.19	0.42
1:A:98:ARG:HH21	1:A:434:ARG:HH11	1.66	0.42
1:G:362:LEU:O	1:G:479:ASN:N	2.52	0.42
1:E:284:HIS:N	1:E:284:HIS:ND1	2.68	0.42
1:E:353:ILE:HD13	1:E:447:PHE:HA	2.01	0.42
1:F:480:VAL:HA	1:F:481:PRO:HD3	1.80	0.42
1:B:194:VAL:O	1:B:198:LEU:HD23	2.19	0.42
1:A:404:THR:HG23	1:A:412:HIS:HE2	1.84	0.42
1:A:409:ASN:HB3	1:A:412:HIS:CE1	2.55	0.42
1:G:370:THR:HG22	1:G:387:GLU:HG2	2.02	0.42
1:H:365:PHE:CE1	1:H:477:VAL:HA	2.54	0.42
1:H:133:ARG:HA	1:H:137:MET:HB3	2.01	0.42
1:F:73:ARG:HA	1:F:74:PRO:HD3	1.79	0.42
1:A:303:THR:HG21	1:A:445:GLU:OE1	2.20	0.42
1:E:316:LYS:HD2	1:E:468:ILE:O	2.20	0.42
1:E:39:VAL:HG12	1:E:40:LEU:N	2.34	0.42
1:A:403:GLU:O	1:A:412:HIS:NE2	2.52	0.42
1:G:194:VAL:O	1:G:198:LEU:HD23	2.20	0.42
1:E:68:VAL:O	1:E:75:VAL:HG23	2.19	0.42
1:E:487:ARG:HG3	1:E:487:ARG:O	2.20	0.42
1:H:223:PHE:CE2	1:H:227:PHE:CE2	3.07	0.42
1:B:40:LEU:HD12	1:H:227:PHE:CZ	2.55	0.42
1:C:353:ILE:HD11	1:C:447:PHE:HA	2.02	0.42
1:H:95:PHE:CE2	1:H:375:THR:HG21	2.55	0.42
1:C:28:GLY:O	1:C:29:LYS:CB	2.67	0.42
1:F:338:PRO:HD3	1:F:455:GLN:OE1	2.19	0.42
1:D:284:HIS:CE1	1:D:287:ASN:ND2	2.88	0.42
1:D:337:PRO:HA	1:D:338:PRO:HD3	1.92	0.42
1:H:207:SER:OG	1:H:480:VAL:HG21	2.20	0.42
1:E:142:VAL:O	1:E:146:ILE:HG13	2.20	0.41
1:H:75:VAL:HG23	1:H:75:VAL:O	2.19	0.41
1:H:297:PHE:HB3	3:H:501:TB2:H11B	2.02	0.41
1:G:31:PRO:HG2	1:G:76:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:436:CYS:SG	1:G:438:GLY:N	2.93	0.41
1:E:37:LEU:N	1:E:37:LEU:HD12	2.35	0.41
1:C:167:ASN:N	1:C:167:ASN:OD1	2.53	0.41
1:D:359:LEU:HD12	1:D:359:LEU:HA	1.88	0.41
2:H:500:HEM:HBD2	2:H:500:HEM:HBA2	2.02	0.41
1:D:363:ILE:HG22	1:D:363:ILE:O	2.19	0.41
1:B:316:LYS:O	1:B:465:PRO:HB3	2.19	0.41
1:E:109:GLN:O	1:E:111:TYR:HD1	2.02	0.41
1:A:171:PHE:O	1:A:174:ILE:HG12	2.20	0.41
1:D:43:LEU:HD22	1:D:220:PHE:CZ	2.55	0.41
1:G:401:TYR:CD2	1:G:424:GLU:HB2	2.55	0.41
1:A:403:GLU:O	1:A:404:THR:CG2	2.68	0.41
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.86	0.41
1:A:461:SER:OG	1:A:462:PRO:HD2	2.21	0.41
1:F:183:VAL:HG12	1:F:183:VAL:O	2.21	0.41
1:A:79:CYS:O	1:A:83:ALA:HB3	2.20	0.41
1:A:179:ILE:HG13	1:A:299:GLY:HA3	2.03	0.41
1:D:137:MET:C	1:D:139:LYS:H	2.23	0.41
1:C:304:SER:O	1:C:308:ARG:N	2.54	0.41
1:B:183:VAL:O	1:B:183:VAL:HG12	2.21	0.41
1:E:33:GLY:HA3	1:E:67:THR:O	2.19	0.41
1:F:362:LEU:HD22	1:F:362:LEU:N	2.35	0.41
1:C:436:CYS:HB2	2:C:500:HEM:NA	2.35	0.41
1:A:101:ILE:O	1:A:102:ALA:C	2.59	0.41
1:E:174:ILE:HB	1:E:449:PHE:CE1	2.55	0.41
1:D:363:ILE:HD11	3:D:501:TB2:H2A	2.01	0.41
1:C:382:ILE:HA	1:C:383:PRO:HD3	1.90	0.41
1:F:457:PHE:HA	1:F:489:LEU:O	2.20	0.41
1:B:30:LEU:CD2	1:B:383:PRO:HD3	2.49	0.41
1:E:362:LEU:N	1:E:362:LEU:HD22	2.35	0.41
1:H:114:ILE:CG1	1:H:294:SER:HB3	2.50	0.41
1:E:474:GLU:HB3	1:E:480:VAL:HG22	2.02	0.41
1:G:188:PHE:N	1:G:188:PHE:CD1	2.88	0.41
1:A:363:ILE:HD12	1:A:363:ILE:N	2.36	0.41
1:C:58:LEU:O	1:C:62:TYR:HB2	2.21	0.41
1:C:369:HIS:NE2	2:C:500:HEM:O2A	2.53	0.41
1:A:202:PHE:CD1	1:A:297:PHE:CD2	3.09	0.41
1:B:99:GLY:N	1:B:368:PRO:O	2.52	0.41
1:E:316:LYS:HG2	1:E:317:TYR:CE1	2.55	0.41
1:C:176:SER:HB2	1:C:300:THR:CG2	2.47	0.41
1:D:320:VAL:O	1:D:324:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:501:TB2:H11B	3:G:501:TB2:H5	1.88	0.41
1:A:362:LEU:O	1:A:478:GLY:HA2	2.21	0.41
1:H:98:ARG:HB2	1:H:434:ARG:CZ	2.51	0.41
2:D:500:HEM:HMB2	2:D:500:HEM:CBB	2.44	0.41
1:C:121:TRP:CZ2	1:C:434:ARG:HD3	2.56	0.41
1:B:153:LEU:CD1	1:B:170:LEU:HD11	2.47	0.41
1:G:486:ILE:HG12	1:G:487:ARG:H	1.86	0.41
1:G:365:PHE:HA	1:G:391:VAL:HA	2.03	0.41
1:G:202:PHE:CE1	1:G:241:ILE:HD13	2.56	0.41
1:H:105:ASP:N	1:H:106:PRO:CD	2.83	0.41
1:G:32:PRO:HD3	1:G:380:TYR:CE1	2.56	0.41
1:B:312:LEU:HD13	1:B:484:TYR:CD1	2.55	0.41
1:C:212:PHE:CE2	1:C:216:VAL:HG21	2.56	0.41
1:D:94:ALA:O	1:D:371:VAL:HA	2.21	0.41
1:E:111:TYR:HB2	1:E:290:LEU:CD1	2.49	0.41
1:D:485:GLN:HE21	1:D:485:GLN:HA	1.85	0.41
1:H:223:PHE:C	1:H:223:PHE:HD2	2.24	0.41
1:F:206:PHE:CD2	1:F:480:VAL:HG13	2.55	0.41
1:E:132:MET:HG2	1:E:182:ILE:HG21	2.02	0.41
1:C:451:THR:O	1:C:455:GLN:N	2.50	0.41
1:B:355:GLU:HA	1:B:355:GLU:OE1	2.21	0.41
1:H:78:LEU:HD13	1:H:84:ILE:HA	2.02	0.41
1:G:121:TRP:NE1	2:G:500:HEM:O1D	2.52	0.41
1:B:111:TYR:N	1:B:111:TYR:CD1	2.88	0.41
1:C:409:ASN:HB3	1:C:412:HIS:CE1	2.56	0.41
1:D:404:THR:HG23	1:D:412:HIS:NE2	2.35	0.41
1:A:104:VAL:HG21	3:A:501:TB2:H10	2.03	0.41
1:D:84:ILE:HG21	1:D:427:MET:SD	2.61	0.41
1:B:362:LEU:H	1:B:362:LEU:HD22	1.85	0.41
1:G:76:VAL:HB	1:G:388:VAL:CG1	2.51	0.41
1:A:382:ILE:HA	1:A:383:PRO:HD3	1.96	0.41
1:F:463:VAL:HA	1:F:464:PRO:HD3	1.83	0.41
1:C:355:GLU:HA	1:C:355:GLU:OE1	2.19	0.41
1:C:55:PHE:HE1	1:C:68:VAL:HG11	1.86	0.41
1:G:369:HIS:HE2	2:G:500:HEM:CGA	2.34	0.41
1:G:364:PRO:O	1:G:393:SER:N	2.53	0.41
1:D:174:ILE:HD12	1:D:449:PHE:CG	2.56	0.41
1:E:288:LEU:O	1:E:292:VAL:HG23	2.21	0.41
1:D:363:ILE:N	1:D:363:ILE:HD12	2.36	0.41
1:D:98:ARG:NH1	1:D:367:VAL:HB	2.36	0.41
1:H:321:THR:HG23	1:H:454:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:PRO:HG2	1:D:76:VAL:HG13	2.03	0.41
1:C:194:VAL:O	1:C:198:LEU:HD23	2.20	0.41
1:G:316:LYS:HB2	1:G:468:ILE:HG21	2.02	0.41
1:A:174:ILE:O	1:A:178:ILE:HG12	2.21	0.41
1:H:177:ASN:N	1:H:177:ASN:HD22	2.19	0.41
1:D:81:THR:HB	1:D:401:TYR:CE1	2.56	0.41
1:A:38:PRO:O	1:A:39:VAL:HB	2.21	0.41
1:C:401:TYR:CD2	1:C:424:GLU:HB2	2.55	0.41
1:H:28:GLY:O	1:H:29:LYS:CB	2.69	0.41
1:A:365:PHE:CE1	1:A:477:VAL:HA	2.56	0.41
1:B:31:PRO:HG2	1:B:76:VAL:HG13	2.02	0.41
1:E:269:LEU:O	1:E:272:MET:HB3	2.20	0.41
1:H:73:ARG:HA	1:H:74:PRO:HD3	1.86	0.41
1:B:175:THR:OG1	1:B:304:SER:HB2	2.21	0.41
1:E:438:GLY:HA3	2:E:500:HEM:C2C	2.56	0.41
1:C:317:TYR:HD1	1:C:317:TYR:N	2.19	0.41
1:A:413:PHE:N	1:A:413:PHE:CD2	2.89	0.41
1:E:105:ASP:N	1:E:106:PRO:CD	2.84	0.41
1:E:73:ARG:HA	1:E:74:PRO:HD3	1.98	0.41
1:A:486:ILE:HG12	1:A:487:ARG:N	2.36	0.40
1:G:307:LEU:HA	1:G:307:LEU:HD22	1.87	0.40
1:A:73:ARG:HA	1:A:74:PRO:HD3	1.88	0.40
1:A:327:GLU:HG2	1:A:346:MET:HG2	2.02	0.40
1:B:444:THR:CG2	1:B:448:LEU:HD12	2.51	0.40
1:F:70:LEU:HB3	1:F:219:LEU:HG	2.04	0.40
1:F:81:THR:HB	1:F:401:TYR:CE1	2.56	0.40
1:A:355:GLU:OE1	1:A:355:GLU:HA	2.22	0.40
1:D:272:MET:HG3	1:D:283:PHE:O	2.21	0.40
1:F:438:GLY:HA3	2:F:500:HEM:C2C	2.56	0.40
1:C:313:LEU:HD13	1:C:408:PHE:CD1	2.56	0.40
1:B:153:LEU:HD12	1:B:157:LEU:HG	2.04	0.40
1:F:53:ARG:HB2	1:F:53:ARG:NH1	2.34	0.40
1:B:183:VAL:HA	1:B:264:PHE:CB	2.52	0.40
1:D:358:ARG:NH2	1:D:359:LEU:HD13	2.36	0.40
1:A:338:PRO:O	1:A:448:LEU:HD22	2.20	0.40
1:G:269:LEU:HD23	1:G:269:LEU:HA	1.86	0.40
1:F:91:GLN:NE2	1:F:377:PHE:HD1	2.20	0.40
1:F:142:VAL:HG21	1:F:441:ILE:HG23	2.02	0.40
1:E:442:ALA:HB1	2:E:500:HEM:CBB	2.51	0.40
1:B:268:TYR:HE1	1:B:288:LEU:HB2	1.86	0.40
1:B:152:CYS:O	1:B:155:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:LEU:CD2	1:H:394:SER:HB3	2.52	0.40
1:E:268:TYR:OH	1:E:283:PHE:HA	2.22	0.40
1:E:121:TRP:CZ2	1:E:434:ARG:HD3	2.56	0.40
1:E:307:LEU:HD12	1:E:311:PHE:CE2	2.57	0.40
1:G:164:LEU:HA	1:G:164:LEU:HD23	1.87	0.40
1:D:176:SER:HB2	1:D:300:THR:CG2	2.51	0.40
1:A:301:GLU:HG2	3:A:501:TB2:H2	2.03	0.40
1:B:310:GLY:O	1:B:314:MET:HG2	2.21	0.40
1:B:413:PHE:O	1:B:414:LEU:HD23	2.22	0.40
1:D:362:LEU:HD22	1:D:362:LEU:N	2.36	0.40
1:A:98:ARG:HH21	1:A:434:ARG:HD2	1.87	0.40
1:B:68:VAL:O	1:B:75:VAL:HG22	2.21	0.40
1:D:202:PHE:CD1	1:D:241:ILE:HD13	2.57	0.40
1:F:314:MET:HB3	1:F:459:ILE:CD1	2.51	0.40
1:F:164:LEU:HA	1:F:164:LEU:HD23	1.80	0.40
1:D:84:ILE:HD12	1:D:395:ALA:HB2	2.03	0.40
1:E:105:ASP:N	1:E:106:PRO:HD2	2.36	0.40
1:A:454:LEU:O	1:A:491:ARG:NH1	2.55	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	463/476 (97%)	435 (94%)	28 (6%)	0	100	100
1	B	463/476 (97%)	433 (94%)	28 (6%)	2 (0%)	39	81
1	C	463/476 (97%)	435 (94%)	26 (6%)	2 (0%)	39	81
1	D	463/476 (97%)	433 (94%)	29 (6%)	1 (0%)	52	88
1	E	463/476 (97%)	432 (93%)	29 (6%)	2 (0%)	39	81
1	F	463/476 (97%)	429 (93%)	34 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	463/476 (97%)	434 (94%)	29 (6%)	0	100	100
1	H	462/476 (97%)	432 (94%)	30 (6%)	0	100	100
All	All	3703/3808 (97%)	3463 (94%)	233 (6%)	7 (0%)	52	88

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	366	GLY
1	B	39	VAL
1	B	29	LYS
1	D	29	LYS
1	C	29	LYS
1	C	39	VAL
1	E	136	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	385/421 (91%)	363 (94%)	22 (6%)	25	66
1	B	379/421 (90%)	362 (96%)	17 (4%)	34	73
1	C	389/421 (92%)	368 (95%)	21 (5%)	27	67
1	D	384/421 (91%)	358 (93%)	26 (7%)	20	60
1	E	381/421 (90%)	358 (94%)	23 (6%)	24	64
1	F	370/421 (88%)	344 (93%)	26 (7%)	19	59
1	G	371/421 (88%)	342 (92%)	29 (8%)	16	53
1	H	304/421 (72%)	294 (97%)	10 (3%)	45	79
All	All	2963/3368 (88%)	2789 (94%)	174 (6%)	24	65

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	104	VAL
1	A	168	THR
1	A	172	HIS
1	A	179	ILE
1	A	186	LYS
1	A	243	THR
1	A	249	VAL
1	A	284	HIS
1	A	296	PHE
1	A	297	PHE
1	A	307	LEU
1	A	368	PRO
1	A	372	THR
1	A	381	VAL
1	A	388	VAL
1	A	389	PHE
1	A	441	ILE
1	A	458	SER
1	A	466	GLU
1	A	480	VAL
1	A	487	ARG
1	B	35	SER
1	B	51	LEU
1	B	53	ARG
1	B	172	HIS
1	B	174	ILE
1	B	179	ILE
1	B	232	ARG
1	B	247	GLN
1	B	252	HIS
1	B	303	THR
1	B	307	LEU
1	B	372	THR
1	B	374	ASP
1	B	388	VAL
1	B	466	GLU
1	B	480	VAL
1	B	485	GLN
1	C	39	VAL
1	C	53	ARG
1	C	73	ARG
1	C	129	LEU

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Mol	Chain	Res	Type
1	C	154	VAL
1	C	169	LEU
1	C	170	LEU
1	C	172	HIS
1	C	179	ILE
1	C	232	ARG
1	C	252	HIS
1	C	284	HIS
1	C	296	PHE
1	C	297	PHE
1	C	307	LEU
1	C	317	TYR
1	C	341	ASP
1	C	362	LEU
1	C	372	THR
1	C	435	ILE
1	C	441	ILE
1	D	53	ARG
1	D	67	THR
1	D	127	PHE
1	D	137	MET
1	D	165	LEU
1	D	169	LEU
1	D	170	LEU
1	D	172	HIS
1	D	177	ASN
1	D	179	ILE
1	D	232	ARG
1	D	284	HIS
1	D	296	PHE
1	D	297	PHE
1	D	307	LEU
1	D	359	LEU
1	D	368	PRO
1	D	372	THR
1	D	374	ASP
1	D	381	VAL
1	D	388	VAL
1	D	415	ASP
1	D	441	ILE
1	D	474	GLU
1	D	477	VAL

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Mol	Chain	Res	Type
1	D	480	VAL
1	E	35	SER
1	E	53	ARG
1	E	73	ARG
1	E	75	VAL
1	E	129	LEU
1	E	133	ARG
1	E	170	LEU
1	E	172	HIS
1	E	221	SER
1	E	284	HIS
1	E	296	PHE
1	E	297	PHE
1	E	303	THR
1	E	307	LEU
1	E	314	MET
1	E	317	TYR
1	E	318	PRO
1	E	359	LEU
1	E	368	PRO
1	E	430	SER
1	E	441	ILE
1	E	470	LEU
1	E	477	VAL
1	F	39	VAL
1	F	53	ARG
1	F	129	LEU
1	F	154	VAL
1	F	165	LEU
1	F	170	LEU
1	F	172	HIS
1	F	176	SER
1	F	213	SER
1	F	223	PHE
1	F	232	ARG
1	F	251	LYS
1	F	266	ASP
1	F	284	HIS
1	F	286	GLN
1	F	296	PHE
1	F	297	PHE
1	F	307	LEU

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Mol	Chain	Res	Type
1	F	334	SER
1	F	341	ASP
1	F	372	THR
1	F	403	GLU
1	F	409	ASN
1	F	439	GLU
1	F	441	ILE
1	F	446	LEU
1	G	35	SER
1	G	39	VAL
1	G	76	VAL
1	G	111	TYR
1	G	141	SER
1	G	142	VAL
1	G	168	THR
1	G	172	HIS
1	G	179	ILE
1	G	198	LEU
1	G	207	SER
1	G	221	SER
1	G	223	PHE
1	G	249	VAL
1	G	284	HIS
1	G	296	PHE
1	G	297	PHE
1	G	305	THR
1	G	307	LEU
1	G	334	SER
1	G	341	ASP
1	G	372	THR
1	G	376	GLN
1	G	388	VAL
1	G	404	THR
1	G	441	ILE
1	G	477	VAL
1	G	480	VAL
1	G	485	GLN
1	H	76	VAL
1	H	172	HIS
1	H	223	PHE
1	H	297	PHE
1	H	307	LEU

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Mol	Chain	Res	Type
1	H	328	ILE
1	H	372	THR
1	H	403	GLU
1	H	409	ASN
1	H	477	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	HIS
1	B	485	GLN
1	C	147	GLN
1	C	247	GLN
1	D	91	GLN
1	D	177	ASN
1	D	287	ASN
1	D	357	GLN
1	D	485	GLN
1	F	147	GLN
1	F	397	HIS
1	F	409	ASN
1	G	147	GLN
1	G	455	GLN
1	G	456	ASN
1	G	485	GLN
1	H	42	ASN
1	H	45	GLN
1	H	177	ASN
1	H	357	GLN
1	H	369	HIS

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 ⓘ

16 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	30,50,50	2.20	10 (33%)	24,82,82	2.37	9 (37%)
3	TB2	A	501	1	13,13,13	0.59	0	17,18,18	0.95	1 (5%)
2	HEM	B	500	1	30,50,50	2.13	9 (30%)	24,82,82	2.22	9 (37%)
3	TB2	B	501	1	13,13,13	0.59	0	17,18,18	0.92	0
2	HEM	C	500	1	30,50,50	2.20	11 (36%)	24,82,82	2.27	7 (29%)
3	TB2	C	501	1	13,13,13	0.63	0	17,18,18	1.00	1 (5%)
2	HEM	D	500	1	30,50,50	2.16	8 (26%)	24,82,82	2.42	9 (37%)
3	TB2	D	501	1	13,13,13	0.64	0	17,18,18	0.91	0
2	HEM	E	500	1,4	30,50,50	2.11	11 (36%)	24,82,82	2.25	8 (33%)
3	TB2	E	501	1	13,13,13	0.57	0	17,18,18	0.95	1 (5%)
2	HEM	F	500	1	30,50,50	2.22	10 (33%)	24,82,82	2.52	9 (37%)
3	TB2	F	501	1	13,13,13	0.53	0	17,18,18	0.81	0
2	HEM	G	500	1	30,50,50	2.19	9 (30%)	24,82,82	2.34	8 (33%)
3	TB2	G	501	1	13,13,13	0.70	0	17,18,18	1.05	1 (5%)
2	HEM	H	500	-	30,50,50	2.16	10 (33%)	24,82,82	2.25	7 (29%)
3	TB2	H	501	1	13,13,13	0.62	0	17,18,18	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TB2	A	501	1	-	0/9/9/9	0/1/1/1
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
3	TB2	B	501	1	-	0/9/9/9	0/1/1/1
2	HEM	C	500	1	-	0/10/54/54	0/0/8/8
3	TB2	C	501	1	-	0/9/9/9	0/1/1/1
2	HEM	D	500	1	-	0/10/54/54	0/0/8/8
3	TB2	D	501	1	-	0/9/9/9	0/1/1/1
2	HEM	E	500	1,4	-	0/10/54/54	0/0/8/8
3	TB2	E	501	1	-	0/9/9/9	0/1/1/1
2	HEM	F	500	1	-	2/10/54/54	0/0/8/8
3	TB2	F	501	1	-	0/9/9/9	0/1/1/1
2	HEM	G	500	1	-	0/10/54/54	0/0/8/8
3	TB2	G	501	1	-	0/9/9/9	0/1/1/1
2	HEM	H	500	-	-	0/10/54/54	0/0/8/8
3	TB2	H	501	1	-	0/9/9/9	0/1/1/1

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	HEM	C3B-C4B	-7.25	1.45	1.51
2	D	500	HEM	C3B-C4B	-7.22	1.45	1.51
2	B	500	HEM	C3B-C4B	-7.15	1.45	1.51
2	C	500	HEM	C3B-C4B	-7.10	1.45	1.51
2	H	500	HEM	C3B-C4B	-7.06	1.45	1.51
2	G	500	HEM	C3B-C4B	-6.94	1.45	1.51
2	A	500	HEM	C3B-C4B	-6.81	1.45	1.51
2	E	500	HEM	C3B-C4B	-6.52	1.46	1.51
2	A	500	HEM	C3D-C4D	-5.28	1.44	1.51
2	G	500	HEM	C3D-C4D	-5.13	1.45	1.51
2	F	500	HEM	C3D-C4D	-5.12	1.45	1.51
2	D	500	HEM	C3D-C4D	-5.02	1.45	1.51
2	C	500	HEM	C3D-C4D	-4.94	1.45	1.51
2	E	500	HEM	C3D-C4D	-4.90	1.45	1.51
2	H	500	HEM	C3D-C4D	-4.47	1.45	1.51
2	B	500	HEM	C3D-C4D	-4.46	1.45	1.51
2	B	500	HEM	C2C-C1C	-3.84	1.45	1.52
2	F	500	HEM	C2C-C1C	-3.80	1.45	1.52
2	H	500	HEM	C2C-C1C	-3.77	1.45	1.52
2	G	500	HEM	C2C-C1C	-3.75	1.45	1.52
2	C	500	HEM	C2C-C1C	-3.72	1.45	1.52
2	D	500	HEM	C2C-C1C	-3.72	1.45	1.52
2	E	500	HEM	C2C-C1C	-3.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C2C-C1C	-3.61	1.45	1.52
2	B	500	HEM	C2D-C1D	-2.17	1.44	1.51
2	C	500	HEM	C2D-C1D	-2.14	1.44	1.51
2	H	500	HEM	C2D-C1D	-2.14	1.44	1.51
2	G	500	HEM	C2B-C1B	-2.11	1.44	1.51
2	E	500	HEM	C2D-C1D	-2.09	1.45	1.51
2	G	500	HEM	C2D-C1D	-2.07	1.45	1.51
2	F	500	HEM	C2D-C1D	-2.07	1.45	1.51
2	D	500	HEM	C2D-C1D	-2.05	1.45	1.51
2	A	500	HEM	C2D-C1D	-2.04	1.45	1.51
2	E	500	HEM	C2B-C1B	-2.02	1.45	1.51
2	B	500	HEM	C2B-C1B	-2.01	1.45	1.51
2	C	500	HEM	C2B-C1B	-2.01	1.45	1.51
2	E	500	HEM	FE-ND	2.01	2.08	1.97
2	E	500	HEM	C3C-CAC	2.01	1.55	1.51
2	F	500	HEM	C4C-NC	2.02	1.38	1.36
2	H	500	HEM	C3B-CAB	2.04	1.55	1.51
2	G	500	HEM	C4C-NC	2.05	1.38	1.36
2	D	500	HEM	C3C-CAC	2.06	1.55	1.51
2	B	500	HEM	C4C-NC	2.06	1.38	1.36
2	B	500	HEM	C1C-NC	2.07	1.38	1.36
2	D	500	HEM	C1C-NC	2.07	1.38	1.36
2	F	500	HEM	C3C-CAC	2.07	1.55	1.51
2	A	500	HEM	C3B-CAB	2.08	1.55	1.51
2	C	500	HEM	C3C-CAC	2.09	1.55	1.51
2	F	500	HEM	C1C-NC	2.10	1.38	1.36
2	D	500	HEM	C3B-CAB	2.10	1.55	1.51
2	H	500	HEM	C3C-CAC	2.11	1.55	1.51
2	C	500	HEM	FE-ND	2.11	2.08	1.97
2	E	500	HEM	FE-NB	2.12	2.08	1.97
2	C	500	HEM	C3B-CAB	2.13	1.55	1.51
2	D	500	HEM	FE-NC	2.13	2.04	1.95
2	B	500	HEM	FE-NC	2.14	2.04	1.95
2	F	500	HEM	C3B-CAB	2.14	1.55	1.51
2	H	500	HEM	C4C-NC	2.15	1.38	1.36
2	A	500	HEM	C3C-CAC	2.15	1.55	1.51
2	C	500	HEM	C4C-NC	2.16	1.38	1.36
2	C	500	HEM	C1C-NC	2.19	1.38	1.36
2	H	500	HEM	C1C-NC	2.20	1.38	1.36
2	A	500	HEM	C4C-NC	2.20	1.38	1.36
2	E	500	HEM	C1C-NC	2.21	1.38	1.36
2	E	500	HEM	C4C-NC	2.22	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	FE-ND	2.23	2.09	1.97
2	F	500	HEM	FE-NB	2.24	2.09	1.97
2	G	500	HEM	C1C-NC	2.25	1.38	1.36
2	A	500	HEM	C1C-NC	2.27	1.38	1.36
2	G	500	HEM	FE-NB	2.30	2.09	1.97
2	H	500	HEM	FE-NB	2.31	2.09	1.97
2	B	500	HEM	FE-ND	2.48	2.10	1.97
2	E	500	HEM	FE-NC	2.62	2.06	1.95
2	G	500	HEM	FE-NC	2.82	2.06	1.95
2	F	500	HEM	FE-NC	2.82	2.06	1.95
2	H	500	HEM	FE-NC	2.89	2.07	1.95
2	A	500	HEM	FE-NC	3.11	2.08	1.95
2	C	500	HEM	FE-NC	3.13	2.08	1.95

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	HEM	CAA-C2A-C1A	-4.83	121.76	127.01
2	D	500	HEM	CAA-C2A-C1A	-4.46	122.16	127.01
2	A	500	HEM	CAA-C2A-C1A	-3.37	123.35	127.01
2	C	500	HEM	CBA-CAA-C2A	-2.87	107.39	112.53
2	F	500	HEM	CAA-CBA-CGA	-2.72	107.75	112.75
2	F	500	HEM	CMA-C3A-C4A	-2.69	123.91	128.36
3	G	501	TB2	C3-C2-C1	-2.65	108.36	113.86
2	D	500	HEM	CMA-C3A-C4A	-2.63	124.01	128.36
3	C	501	TB2	C3-C2-C1	-2.56	108.55	113.86
2	E	500	HEM	CAA-CBA-CGA	-2.55	108.08	112.75
2	A	500	HEM	CAA-CBA-CGA	-2.52	108.12	112.75
2	B	500	HEM	C3B-CAB-CBB	-2.34	120.87	124.46
2	H	500	HEM	CAA-CBA-CGA	-2.24	108.64	112.75
2	D	500	HEM	CAA-CBA-CGA	-2.18	108.75	112.75
3	A	501	TB2	C3-C2-C1	-2.09	109.52	113.86
3	E	501	TB2	C3-C2-C1	-2.08	109.56	113.86
2	B	500	HEM	CAA-CBA-CGA	-2.01	109.06	112.75
2	G	500	HEM	CAA-CBA-CGA	-2.00	109.08	112.75
2	G	500	HEM	C2D-C3D-C4D	2.11	105.07	101.50
2	D	500	HEM	C2D-C3D-C4D	2.14	105.12	101.50
2	F	500	HEM	C2D-C3D-C4D	2.17	105.19	101.50
2	B	500	HEM	C2D-C3D-C4D	2.22	105.26	101.50
2	E	500	HEM	C2D-C3D-C4D	2.24	105.30	101.50
2	A	500	HEM	C3B-C4B-CHC	2.30	126.40	123.16
2	A	500	HEM	C2D-C3D-C4D	2.30	105.40	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500	HEM	C3B-C4B-CHC	2.31	126.42	123.16
2	H	500	HEM	C2D-C3D-C4D	2.37	105.52	101.50
2	C	500	HEM	C2D-C3D-C4D	2.41	105.58	101.50
2	B	500	HEM	C3B-C4B-CHC	2.46	126.62	123.16
2	E	500	HEM	C3B-C4B-CHC	2.57	126.79	123.16
2	D	500	HEM	CMD-C2D-C3D	2.82	126.83	114.35
2	F	500	HEM	CMD-C2D-C3D	2.87	127.03	114.35
2	E	500	HEM	CMD-C2D-C3D	2.88	127.07	114.35
2	C	500	HEM	CMD-C2D-C3D	2.89	127.11	114.35
2	B	500	HEM	CMD-C2D-C3D	2.91	127.20	114.35
2	H	500	HEM	CMD-C2D-C3D	2.92	127.27	114.35
2	A	500	HEM	CMD-C2D-C3D	2.92	127.28	114.35
2	G	500	HEM	CMD-C2D-C3D	3.33	129.07	114.35
2	G	500	HEM	CAD-C3D-C4D	3.53	124.93	112.47
2	B	500	HEM	CMB-C2B-C3B	3.62	125.56	116.53
2	B	500	HEM	CMC-C2C-C3C	3.68	125.72	116.53
2	E	500	HEM	CMC-C2C-C3C	3.68	125.72	116.53
2	E	500	HEM	CMB-C2B-C3B	3.85	126.14	116.53
2	B	500	HEM	CAD-C3D-C2D	3.96	124.59	113.22
2	A	500	HEM	CAD-C3D-C4D	4.07	126.82	112.47
2	D	500	HEM	CMC-C2C-C3C	4.10	126.76	116.53
2	F	500	HEM	CAD-C3D-C4D	4.21	127.32	112.47
2	H	500	HEM	CAD-C3D-C2D	4.23	125.36	113.22
2	A	500	HEM	CMC-C2C-C3C	4.25	127.13	116.53
2	F	500	HEM	CMB-C2B-C3B	4.25	127.14	116.53
2	D	500	HEM	CMB-C2B-C3B	4.25	127.14	116.53
2	G	500	HEM	CMC-C2C-C3C	4.27	127.19	116.53
2	F	500	HEM	CMC-C2C-C3C	4.27	127.20	116.53
2	C	500	HEM	CMB-C2B-C3B	4.29	127.24	116.53
2	D	500	HEM	CAD-C3D-C4D	4.32	127.70	112.47
2	H	500	HEM	CMC-C2C-C3C	4.36	127.42	116.53
2	C	500	HEM	CMC-C2C-C3C	4.38	127.47	116.53
2	A	500	HEM	CMB-C2B-C3B	4.39	127.49	116.53
2	C	500	HEM	CAD-C3D-C2D	4.40	125.87	113.22
2	H	500	HEM	CMB-C2B-C3B	4.43	127.59	116.53
2	G	500	HEM	CMB-C2B-C3B	4.48	127.71	116.53
2	E	500	HEM	CAD-C3D-C4D	4.49	128.31	112.47
2	C	500	HEM	CAD-C3D-C4D	4.56	128.55	112.47
2	E	500	HEM	CAD-C3D-C2D	4.58	126.39	113.22
2	H	500	HEM	CAD-C3D-C4D	4.72	129.12	112.47
2	D	500	HEM	CAD-C3D-C2D	4.86	127.18	113.22
2	F	500	HEM	CAD-C3D-C2D	4.97	127.50	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CAD-C3D-C4D	5.01	130.14	112.47
2	A	500	HEM	CAD-C3D-C2D	5.07	127.78	113.22
2	G	500	HEM	CAD-C3D-C2D	5.84	130.00	113.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	500	HEM	C1A-C2A-CAA-CBA
2	F	500	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

15 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	8	0
3	A	501	TB2	5	0
2	B	500	HEM	9	0
3	B	501	TB2	2	0
2	C	500	HEM	11	0
2	D	500	HEM	11	0
3	D	501	TB2	5	0
2	E	500	HEM	9	0
3	E	501	TB2	1	0
2	F	500	HEM	8	0
3	F	501	TB2	3	0
2	G	500	HEM	13	0
3	G	501	TB2	3	0
2	H	500	HEM	13	0
3	H	501	TB2	2	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, 95th 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 ²)	Q<0.9
1	A	465/476 (97%)	-0.18	3 (0%) 90 85	40, 59, 81, 119	0
1	B	465/476 (97%)	-0.17	3 (0%) 90 85	41, 67, 94, 143	0
1	C	465/476 (97%)	-0.05	3 (0%) 90 85	43, 67, 103, 147	0
1	D	465/476 (97%)	-0.27	0 100 100	41, 58, 82, 101	0
1	E	465/476 (97%)	-0.12	0 100 100	49, 65, 87, 108	0
1	F	465/476 (97%)	-0.13	1 (0%) 95 93	40, 68, 96, 114	0
1	G	465/476 (97%)	-0.04	4 (0%) 85 78	49, 75, 115, 133	0
1	H	464/476 (97%)	0.73	49 (10%) 8 7	93, 121, 143, 156	0
All	All	3719/3808 (97%)	-0.03	63 (1%) 73 64	40, 68, 126, 156	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	72	SER	4.8
1	H	425	GLY	4.4
1	H	430	SER	4.3
1	C	277	SER	4.1
1	H	80	GLY	3.8
1	H	81	THR	3.7
1	H	375	THR	3.7
1	H	92	ALA	3.7
1	H	455	GLN	3.6
1	H	73	ARG	3.6
1	A	138	GLY	3.5
1	H	287	ASN	3.4
1	H	78	LEU	3.1
1	H	91	GLN	3.1
1	H	278	ASP	3.1
1	H	467	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	64	ASP	2.9
1	H	67	THR	2.8
1	H	428	PRO	2.8
1	H	65	VAL	2.8
1	H	491	ARG	2.7
1	H	74	PRO	2.7
1	H	284	HIS	2.7
1	G	261	PRO	2.6
1	H	291	THR	2.6
1	H	417	ASN	2.6
1	A	139	LYS	2.6
1	G	260	ASN	2.5
1	H	233	GLN	2.5
1	H	101	ILE	2.5
1	H	290	LEU	2.4
1	H	277	SER	2.4
1	H	453	ILE	2.4
1	F	279	PRO	2.4
1	H	420	LEU	2.4
1	H	32	PRO	2.4
1	A	277	SER	2.4
1	H	418	GLY	2.3
1	H	245	ILE	2.3
1	B	282	GLU	2.3
1	H	279	PRO	2.3
1	H	313	LEU	2.3
1	H	124	LEU	2.3
1	H	28	GLY	2.3
1	C	275	ASP	2.2
1	H	399	PRO	2.2
1	H	432	GLY	2.2
1	H	68	VAL	2.2
1	H	464	PRO	2.2
1	H	331	VAL	2.2
1	H	84	ILE	2.2
1	H	42	ASN	2.2
1	H	88	LEU	2.1
1	B	279	PRO	2.1
1	H	390	PRO	2.1
1	G	419	ALA	2.1
1	H	376	GLN	2.1
1	H	416	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	385	ASN	2.1
1	B	281	SER	2.0
1	G	277	SER	2.0
1	H	318	PRO	2.0
1	C	458	SER	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, 95th 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 ²)	Q<0.9
3	TB2	D	501	13/13	0.95	0.41	5.22	48,56,60,60	0
3	TB2	B	501	13/13	0.95	0.48	4.39	54,60,67,69	0
3	TB2	G	501	13/13	0.96	0.42	2.99	57,62,73,77	0
3	TB2	E	501	13/13	0.93	0.45	2.63	48,53,58,59	0
3	TB2	A	501	13/13	0.97	0.42	2.60	42,49,57,57	0
3	TB2	F	501	13/13	0.94	0.47	2.18	46,51,63,66	0
3	TB2	C	501	13/13	0.97	0.38	1.30	40,51,55,57	0
2	HEM	B	500	43/43	0.98	0.32	0.93	41,59,68,72	0
2	HEM	A	500	43/43	0.98	0.31	0.77	39,49,54,57	0
2	HEM	F	500	43/43	0.97	0.34	0.76	43,53,62,72	0
2	HEM	C	500	43/43	0.97	0.33	0.55	45,56,66,72	0
2	HEM	D	500	43/43	0.98	0.30	0.54	36,44,53,55	0
2	HEM	G	500	43/43	0.97	0.34	0.47	59,70,89,98	0
3	TB2	H	501	13/13	0.93	0.40	0.42	96,103,107,110	0
2	HEM	E	500	43/43	0.98	0.28	0.02	48,55,60,62	0
2	HEM	H	500	43/43	0.94	0.38	-0.03	92,106,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.