



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:39 AM EDT

PDB ID : 2Q6N  
Title : Structure of Cytochrome P450 2B4 with Bound 1-(4-chlorophenyl)imidazole  
Authors : Zhao, Y.; Sun, L.; Muralidhara, B.K.; Kumar, S.; White, M.A.; Stout, C.D.; Halpert, J.R.  
Deposited on : 2007-06-05  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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:

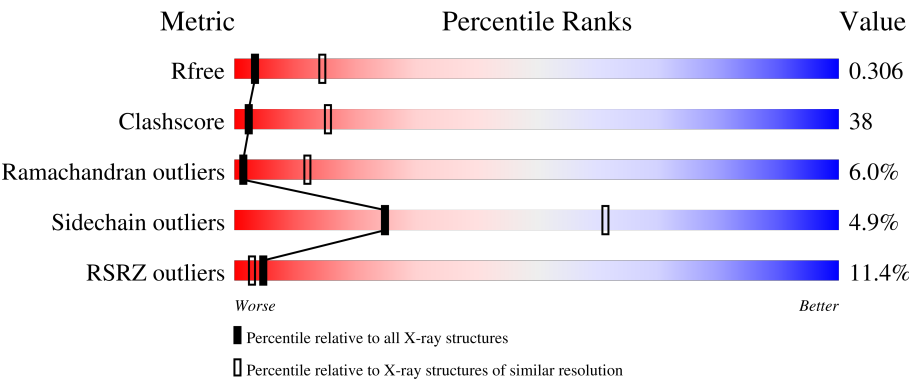
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	478	<div><div>4%</div><div>46%</div><div>45%</div><div>6%</div><div></div></div>
1	B	478	<div><div>10%</div><div>41%</div><div>51%</div><div></div><div></div></div>
1	C	478	<div><div>11%</div><div>34%</div><div>56%</div><div>7%</div><div></div></div>
1	D	478	<div><div>7%</div><div>40%</div><div>51%</div><div>7%</div><div></div></div>
1	E	478	<div><div>13%</div><div>36%</div><div>54%</div><div>8%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	478	
1	G	478	

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	1CI	A	501	-	-	-	X
3	1CI	E	501	-	-	-	X
3	1CI	G	501	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26523 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
			3734	2405	649	669	11			
1	B	465	Total	C	N	O	S	0	0	0
			3734	2405	649	669	11			
1	C	465	Total	C	N	O	S	0	0	0
			3734	2405	649	669	11			
1	D	465	Total	C	N	O	S	0	0	0
			3734	2405	649	669	11			
1	E	465	Total	C	N	O	S	0	0	0
			3734	2405	649	669	11			
1	F	465	Total	C	N	O	S	0	0	0
			3734	2405	649	669	11			
1	G	465	Total	C	N	O	S	0	0	0
			3734	2405	649	669	11			

There are 245 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
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	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	?	-	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	engineered mutation	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
A	496	HIS	-	expression tag	UNP P00178
A	497	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	engineered mutation	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
B	496	HIS	-	expression tag	UNP P00178
B	497	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	?	-	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	engineered mutation	UNP P00178
C	226	TYR	HIS	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
C	492	HIS	-	expression tag	UNP P00178
C	493	HIS	-	expression tag	UNP P00178
C	494	HIS	-	expression tag	UNP P00178
C	495	HIS	-	expression tag	UNP P00178
C	496	HIS	-	expression tag	UNP P00178
C	497	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	?	-	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	engineered mutation	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
D	496	HIS	-	expression tag	UNP P00178
D	497	HIS	-	expression tag	UNP P00178
E	21	ALA	GLU	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	engineered mutation	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
E	496	HIS	-	expression tag	UNP P00178
E	497	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

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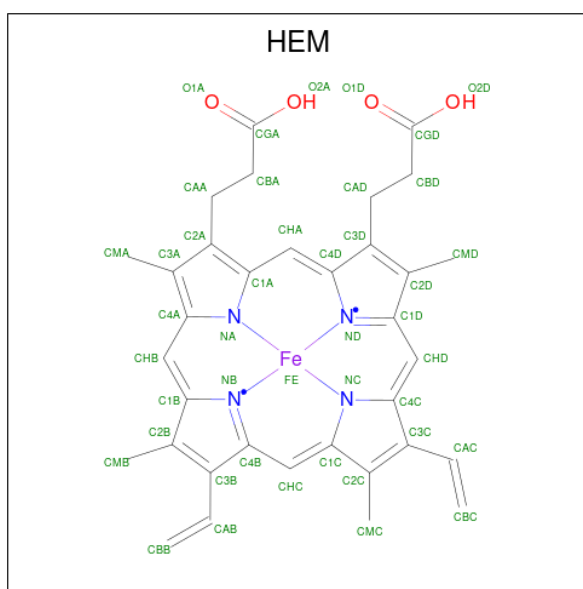
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP P00178
F	?	-	PHE	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	ALA	deletion	UNP P00178
F	?	-	GLY	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	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	engineered mutation	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
F	496	HIS	-	expression tag	UNP P00178
F	497	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
G	27	LYS	HIS	engineered mutation	UNP P00178
G	29	LYS	ARG	engineered mutation	UNP P00178
G	221	SER	PRO	engineered mutation	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
G	496	HIS	-	expression tag	UNP P00178
G	497	HIS	-	expression tag	UNP P00178

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



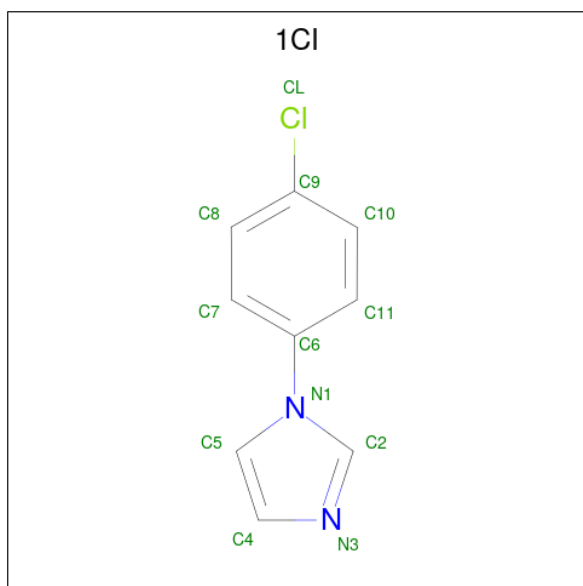
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is 1-(4-CHLOROPHENYL)-1H-IMIDAZOLE (three-letter code: 1CI) (formula:  $C_9H_7ClN_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N		
			12	9	1	2		
3	B	1	Total	C	Cl	N		
			12	9	1	2		
3	C	1	Total	C	Cl	N		
			12	9	1	2		
3	D	1	Total	C	Cl	N		
			12	9	1	2		
3	E	1	Total	C	Cl	N		
			12	9	1	2		

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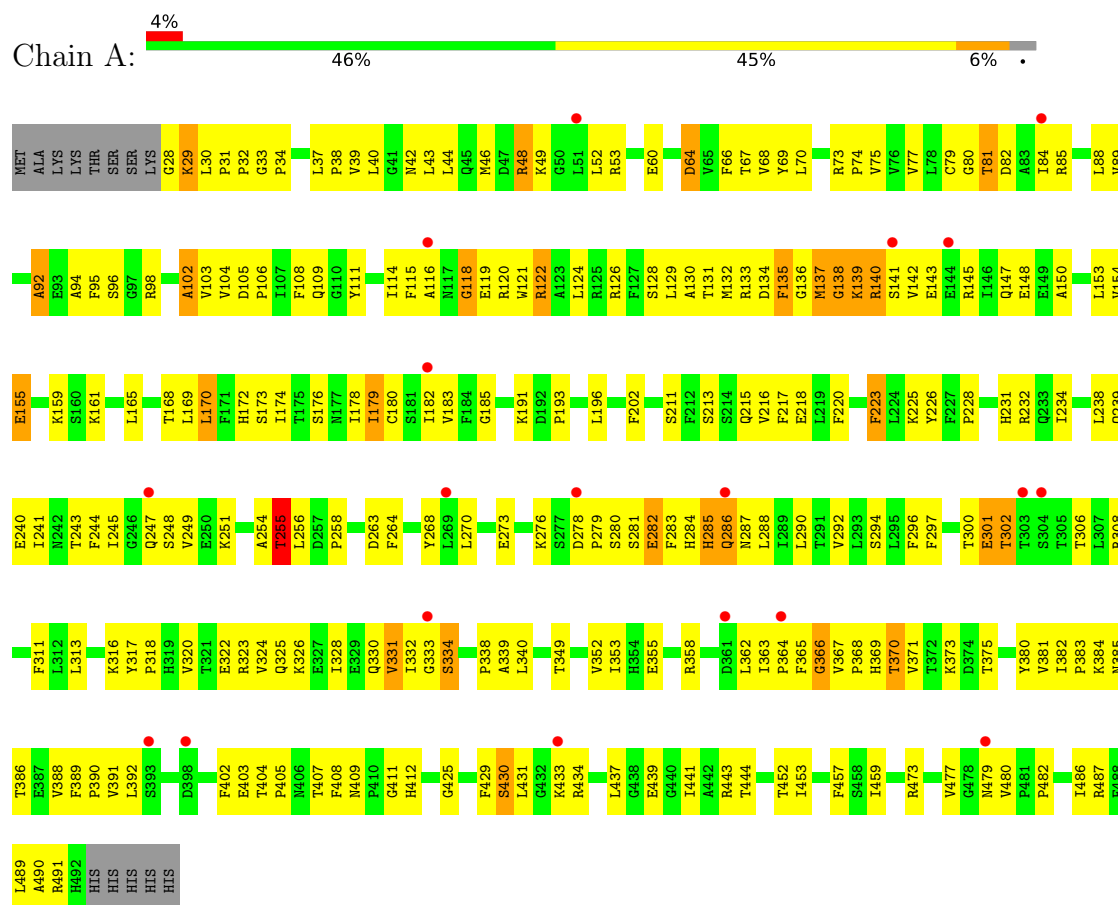
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	G	1	Total	C	Cl	N	0	0
			12	9	1	2		

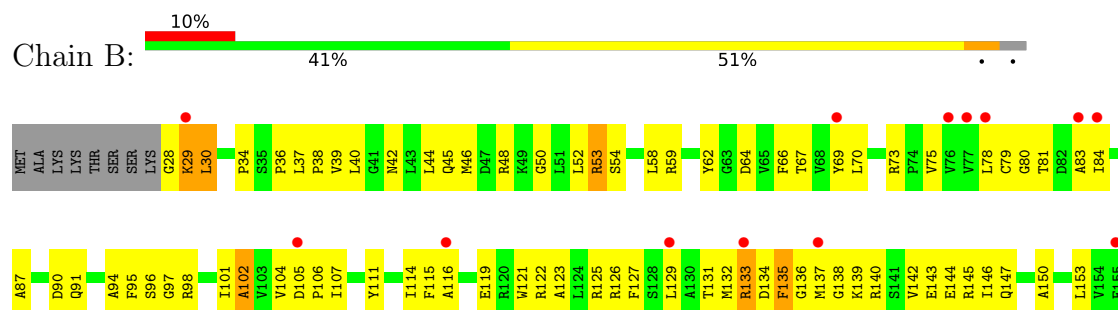
### 3 Residue-property plots

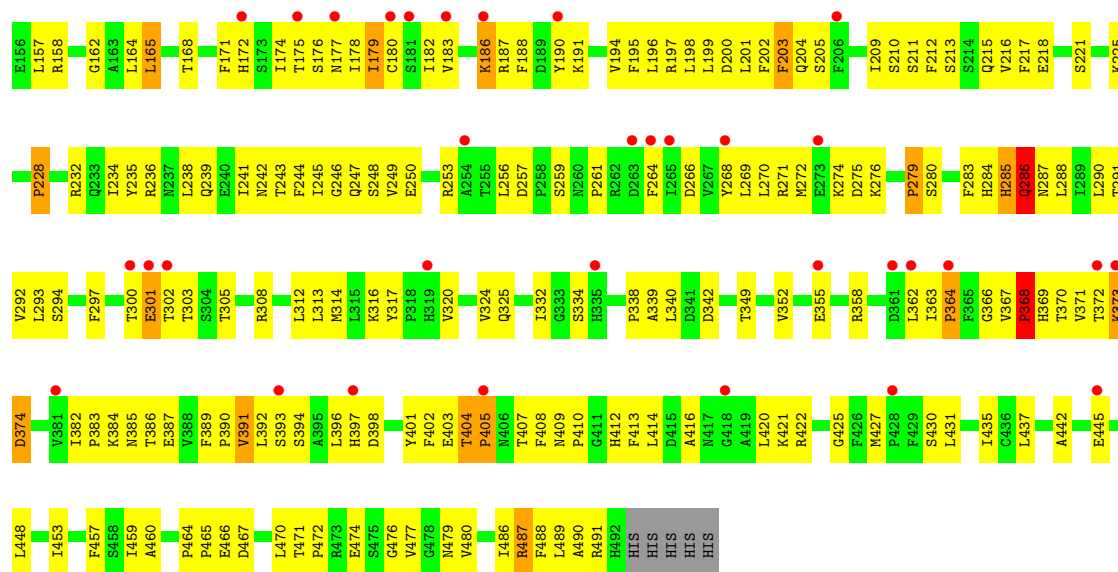
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2B4

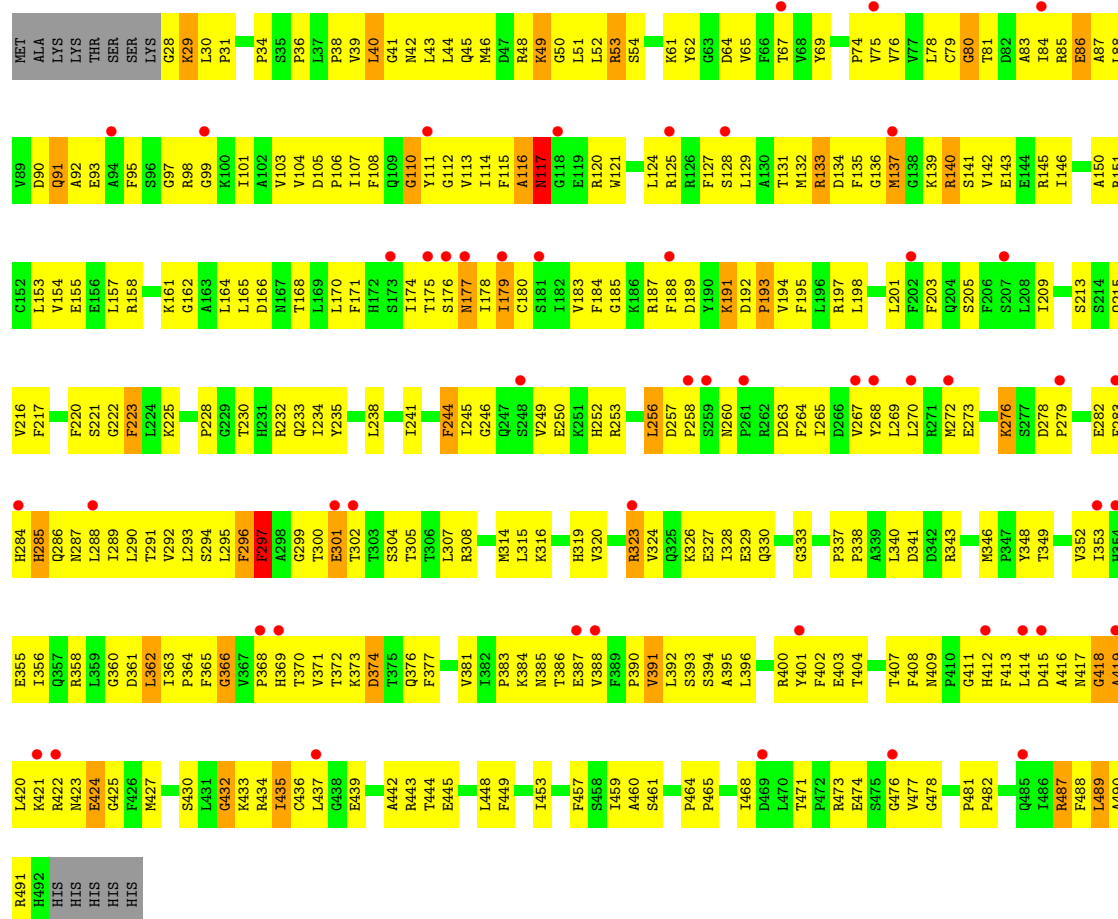


#### • Molecule 1: Cytochrome P450 2B4

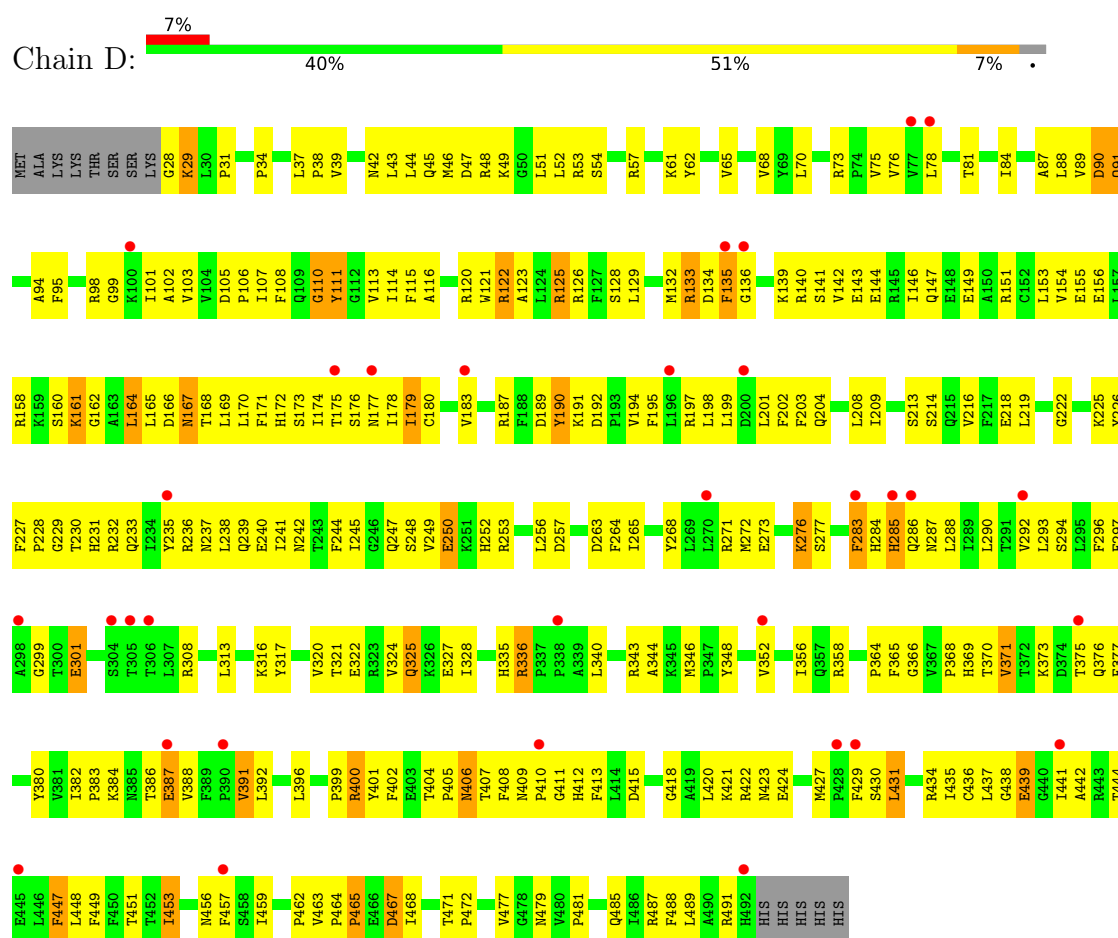




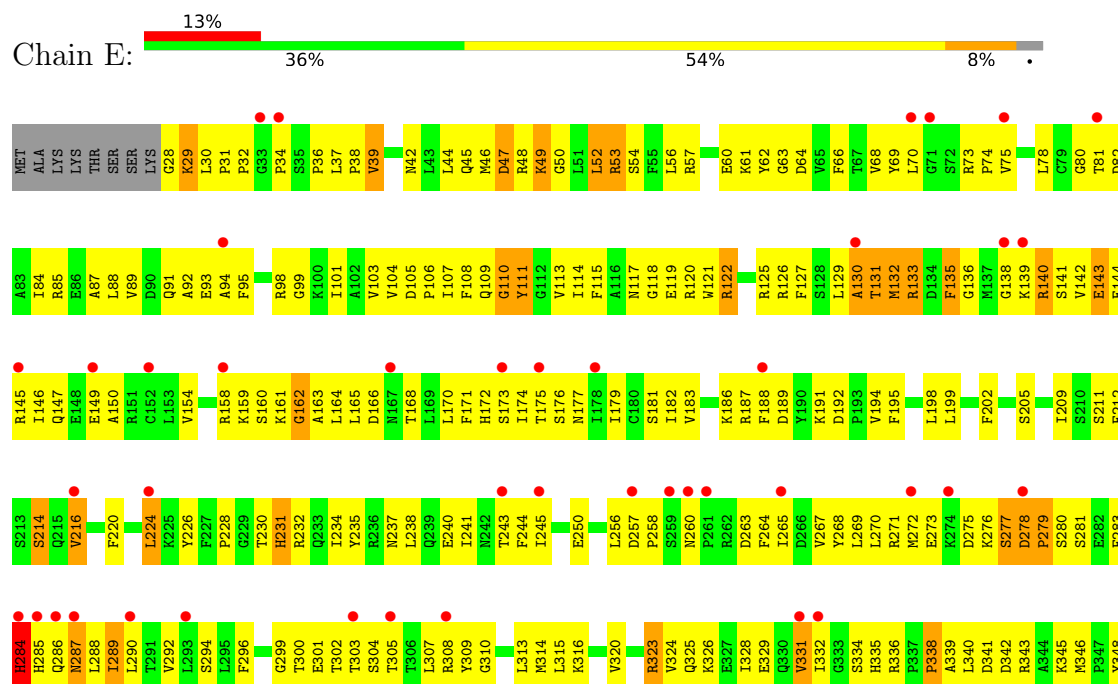
• Molecule 1: Cytochrome P450 2B4

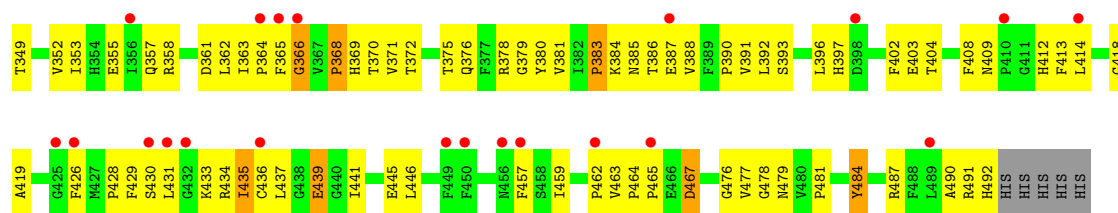


• Molecule 1: Cytochrome P450 2B4



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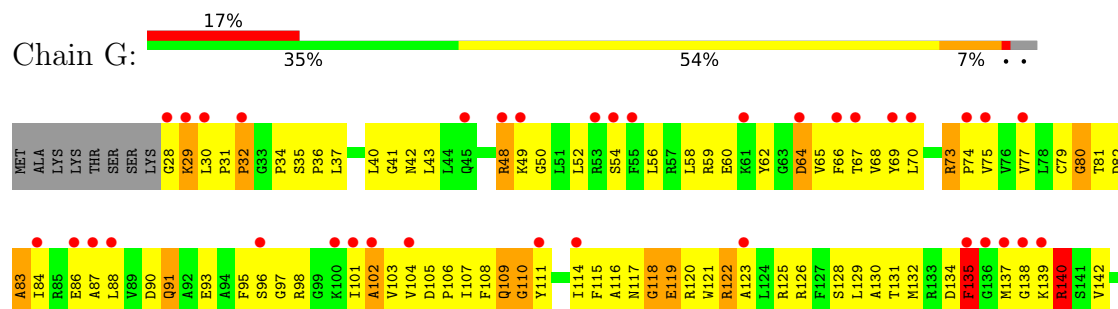


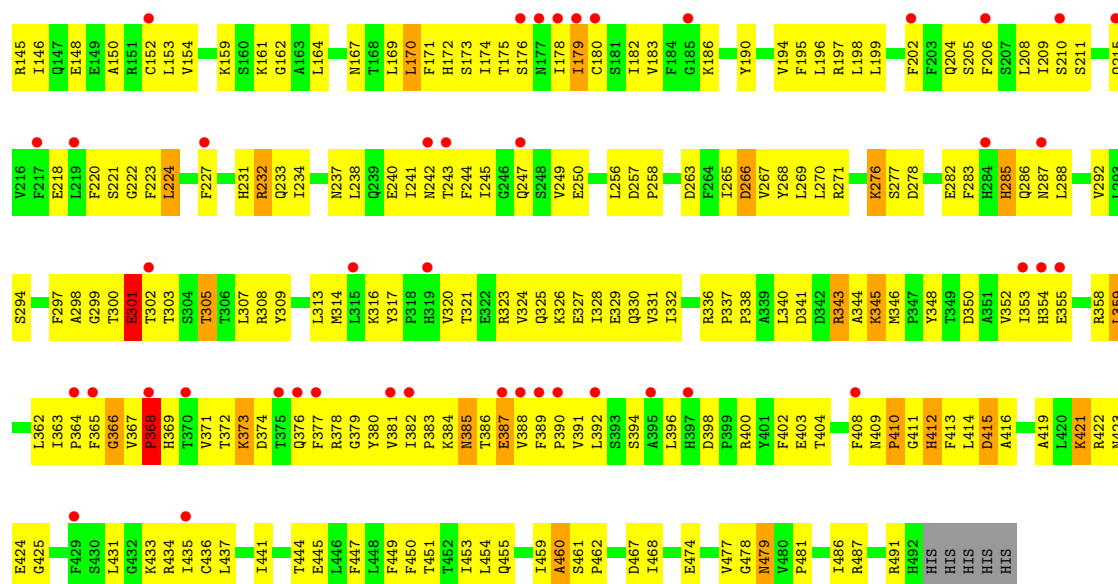


● Molecule 1: Cytochrome P450 2B4



● 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, $\alpha$ , $\beta$ , $\gamma$	140.00Å 147.31Å 238.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 147.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-3.20) 99.1 (147.31-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.27 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.311 0.232 , 0.306	Depositor DCC
$R_{free}$ test set	4077 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 88.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	26523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1CI, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/3828	0.59	0/5181
1	B	0.31	0/3828	0.56	0/5181
1	C	0.31	0/3828	0.55	0/5181
1	D	0.31	0/3828	0.58	0/5181
1	E	0.30	0/3828	0.55	0/5181
1	F	0.31	0/3828	0.55	0/5181
1	G	0.31	0/3828	0.56	0/5181
All	All	0.31	0/26796	0.56	0/36267

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3734	0	3744	240	0
1	B	3734	0	3744	260	0
1	C	3734	0	3744	313	0
1	D	3734	0	3744	278	0
1	E	3734	0	3745	326	0
1	F	3734	0	3744	328	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3734	0	3744	305	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	4	0
2	D	43	0	30	6	0
2	E	43	0	30	8	0
2	F	43	0	30	7	0
2	G	43	0	30	4	0
3	A	12	0	7	1	0
3	B	12	0	7	3	0
3	C	12	0	7	3	0
3	D	12	0	7	2	0
3	E	12	0	7	1	0
3	F	12	0	7	3	0
3	G	12	0	7	4	0
All	All	26523	0	26468	2018	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 38.

All (2018) 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:D:114:ILE:HD13	1:D:294:SER:HB3	1.38	1.05
1:E:111:TYR:HB2	1:E:290:LEU:HD12	1.35	1.03
1:E:75:VAL:HG12	1:E:387:GLU:HB2	1.44	1.00
1:E:98:ARG:HG2	1:E:115:PHE:HA	1.47	0.97
1:D:216:VAL:HG11	1:F:228:PRO:HD3	1.48	0.96
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.47	0.95
1:B:209:ILE:HD13	1:B:234:ILE:HD13	1.48	0.94
1:A:213:SER:HA	1:A:216:VAL:HG12	1.47	0.94
1:G:232:ARG:NH1	1:G:232:ARG:HA	1.84	0.92
1:D:373:LYS:HA	1:D:384:LYS:HG3	1.51	0.92
1:G:140:ARG:NH1	1:G:140:ARG:HB2	1.86	0.91
1:E:362:LEU:H	1:E:362:LEU:HD22	1.35	0.91
1:B:232:ARG:HB3	1:B:232:ARG:HH11	1.33	0.90
1:F:135:PHE:HE1	1:F:145:ARG:HH12	1.21	0.89
1:E:284:HIS:H	1:E:284:HIS:CD2	1.83	0.89
1:E:52:LEU:HD13	1:E:364:PRO:HB3	1.56	0.88
1:B:373:LYS:HA	1:B:384:LYS:HG3	1.56	0.87
1:F:141:SER:HB3	1:F:144:GLU:HG3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ASN:HD21	1:E:187:ARG:HB2	1.39	0.87
1:E:376:GLN:HE22	1:E:379:GLY:H	1.23	0.86
1:A:256:LEU:HD21	1:A:270:LEU:HD23	1.53	0.86
1:A:34:PRO:HG2	1:A:42:ASN:ND2	1.90	0.86
1:E:176:SER:HB2	1:E:300:THR:HG23	1.56	0.86
1:C:107:ILE:HG13	1:C:238:LEU:HD12	1.58	0.86
1:D:325:GLN:HA	1:D:325:GLN:HE21	1.39	0.86
1:F:37:LEU:H	1:F:37:LEU:HD12	1.38	0.86
1:E:332:ILE:HG21	1:E:338:PRO:HG3	1.56	0.85
1:A:368:PRO:HG3	1:A:389:PHE:HE2	1.41	0.85
1:A:94:ALA:O	1:A:371:VAL:HA	1.75	0.85
1:C:49:LYS:HE3	1:C:53:ARG:NH1	1.91	0.85
1:D:228:PRO:HD3	1:E:216:VAL:HG11	1.58	0.84
1:F:53:ARG:HA	1:F:53:ARG:HH11	1.42	0.84
1:D:276:LYS:HD2	1:D:277:SER:H	1.43	0.84
1:A:124:LEU:HD21	1:A:287:ASN:HD22	1.40	0.84
1:E:268:TYR:O	1:E:272:MET:HG2	1.77	0.84
1:G:232:ARG:HA	1:G:232:ARG:HH11	1.37	0.84
1:E:107:ILE:HG13	1:E:238:LEU:HD12	1.59	0.83
1:F:320:VAL:HG21	1:F:408:PHE:HE2	1.41	0.83
1:A:102:ALA:HB2	1:A:218:GLU:HA	1.59	0.82
1:G:328:ILE:HG23	1:G:332:ILE:HD12	1.59	0.82
1:B:409:ASN:HB3	1:B:412:HIS:CE1	2.15	0.82
1:D:53:ARG:HH11	1:D:53:ARG:HA	1.43	0.82
1:A:153:LEU:HD22	1:A:174:ILE:HD13	1.60	0.82
1:B:409:ASN:HB3	1:B:412:HIS:HE1	1.44	0.82
1:A:69:TYR:CE2	1:A:74:PRO:HB3	2.14	0.82
1:A:273:GLU:HA	1:A:276:LYS:HE3	1.61	0.81
1:G:140:ARG:HB2	1:G:140:ARG:HH11	1.44	0.81
1:C:52:LEU:HD22	1:C:364:PRO:HB3	1.60	0.81
1:D:232:ARG:HB3	1:D:232:ARG:HH11	1.45	0.81
1:G:422:ARG:HG2	1:G:423:ASN:H	1.45	0.81
1:A:52:LEU:HD22	1:A:364:PRO:HB3	1.63	0.81
1:E:194:VAL:O	1:E:198:LEU:HD23	1.81	0.81
1:G:164:LEU:HG	1:G:487:ARG:HH21	1.45	0.81
1:E:177:ASN:ND2	1:E:187:ARG:HB2	1.96	0.80
1:E:358:ARG:HG3	1:E:396:LEU:HD22	1.61	0.80
1:A:362:LEU:HD22	1:A:362:LEU:H	1.45	0.80
1:B:164:LEU:HD23	1:B:487:ARG:HB3	1.62	0.80
1:F:320:VAL:HA	1:F:323:ARG:HB2	1.62	0.80
1:D:164:LEU:HD22	1:D:485:GLN:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:LEU:HD22	1:G:362:LEU:H	1.46	0.80
1:G:138:GLY:HA3	1:G:145:ARG:HH21	1.46	0.80
1:G:303:THR:HG21	1:G:445:GLU:OE1	1.82	0.80
1:C:417:ASN:OD1	1:G:271:ARG:HB2	1.81	0.80
1:B:364:PRO:HG3	1:B:479:ASN:ND2	1.97	0.79
1:F:49:LYS:HE2	1:F:53:ARG:HG2	1.63	0.79
1:A:102:ALA:HB1	1:A:217:PHE:HD2	1.48	0.79
1:E:99:GLY:HA3	1:E:368:PRO:HB2	1.64	0.79
1:G:138:GLY:HA3	1:G:145:ARG:NH2	1.98	0.79
1:E:328:ILE:HG23	1:E:332:ILE:HD12	1.66	0.78
1:C:98:ARG:HG2	1:C:115:PHE:HA	1.63	0.78
1:D:222:GLY:HA2	1:D:225:LYS:HE3	1.64	0.78
1:G:224:LEU:HD23	1:G:227:PHE:HB2	1.64	0.78
1:D:352:VAL:HG13	1:D:408:PHE:HZ	1.48	0.78
1:G:245:ILE:O	1:G:249:VAL:HG23	1.84	0.78
1:E:122:ARG:HB3	1:E:126:ARG:HH11	1.48	0.78
1:C:125:ARG:HH12	1:C:437:LEU:HB2	1.49	0.78
1:B:101:ILE:HD11	1:B:368:PRO:HD2	1.66	0.77
1:B:232:ARG:HB3	1:B:232:ARG:NH1	1.98	0.77
1:F:140:ARG:HH22	1:F:148:GLU:HG2	1.48	0.77
1:D:245:ILE:O	1:D:249:VAL:HG23	1.84	0.77
1:C:179:ILE:O	1:C:179:ILE:HD13	1.83	0.77
1:G:123:ALA:HA	1:G:126:ARG:HG2	1.66	0.77
1:E:53:ARG:HA	1:E:53:ARG:HH11	1.49	0.77
1:F:194:VAL:O	1:F:198:LEU:HD23	1.84	0.77
1:C:38:PRO:O	1:C:40:LEU:HD23	1.85	0.77
1:C:232:ARG:NH1	1:C:232:ARG:HB3	2.00	0.76
1:D:52:LEU:HD22	1:D:364:PRO:HB3	1.68	0.76
1:E:147:GLN:HE22	1:E:339:ALA:HA	1.49	0.76
1:A:138:GLY:O	1:A:139:LYS:HD2	1.85	0.76
1:B:305:THR:HG22	1:B:308:ARG:HH21	1.51	0.76
1:E:125:ARG:HH12	1:E:437:LEU:HB2	1.50	0.76
1:G:79:CYS:O	1:G:83:ALA:HB3	1.86	0.76
1:G:130:ALA:O	1:G:134:ASP:HB2	1.86	0.76
1:G:101:ILE:HB	1:G:104:VAL:HG22	1.68	0.76
1:C:297:PHE:CD2	3:C:501:1CI:H8	2.20	0.76
1:E:258:PRO:HG3	1:E:270:LEU:HD21	1.68	0.75
1:B:34:PRO:HG2	1:B:42:ASN:ND2	2.02	0.75
1:A:129:LEU:HD21	1:A:133:ARG:NH2	2.01	0.75
1:D:70:LEU:HD22	1:D:219:LEU:HD11	1.67	0.75
1:D:409:ASN:HB3	1:D:412:HIS:CE1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLN:NE2	1:E:339:ALA:HA	2.01	0.75
1:E:370:THR:HA	1:E:386:THR:O	1.87	0.75
1:G:285:HIS:O	1:G:287:ASN:N	2.20	0.75
1:F:320:VAL:HG21	1:F:408:PHE:CE2	2.21	0.75
1:C:75:VAL:HG12	1:C:387:GLU:HB2	1.69	0.74
1:F:101:ILE:HB	1:F:104:VAL:HG22	1.68	0.74
1:A:95:PHE:O	1:A:369:HIS:HD2	1.70	0.74
1:B:217:PHE:O	1:B:221:SER:HB3	1.87	0.74
1:D:44:LEU:H	1:D:44:LEU:HD12	1.49	0.74
1:D:276:LYS:HD2	1:D:277:SER:N	2.01	0.74
1:C:409:ASN:HB3	1:C:412:HIS:ND1	2.02	0.74
1:G:98:ARG:HG2	1:G:115:PHE:HA	1.68	0.74
1:E:75:VAL:HG12	1:E:387:GLU:CB	2.16	0.74
1:E:98:ARG:HD3	1:E:99:GLY:H	1.51	0.74
1:F:95:PHE:CE1	1:F:371:VAL:HG12	2.22	0.74
1:G:73:ARG:HH21	1:G:387:GLU:HB2	1.51	0.74
1:G:29:LYS:HE3	1:G:379:GLY:O	1.86	0.74
1:B:133:ARG:NH2	1:B:139:LYS:HE2	2.03	0.74
1:B:53:ARG:HH11	1:B:53:ARG:HA	1.53	0.74
1:B:136:GLY:O	1:B:142:VAL:HG13	1.87	0.74
1:C:205:SER:O	1:C:209:ILE:HG13	1.87	0.74
1:E:125:ARG:NH1	1:E:437:LEU:HB2	2.03	0.74
1:F:249:VAL:HG21	1:F:288:LEU:HD21	1.69	0.74
1:F:446:LEU:O	1:F:450:PHE:HB2	1.88	0.74
1:E:256:LEU:HD11	1:E:270:LEU:HG	1.69	0.73
1:B:383:PRO:HG2	1:B:386:THR:OG1	1.89	0.73
1:D:101:ILE:HD11	1:D:368:PRO:HD2	1.70	0.73
1:D:411:GLY:O	1:D:413:PHE:N	2.20	0.73
1:G:209:ILE:HG22	1:G:477:VAL:HG11	1.70	0.73
1:C:245:ILE:O	1:C:249:VAL:HG23	1.88	0.73
1:D:158:ARG:HG2	1:D:457:PHE:HZ	1.53	0.73
1:G:409:ASN:HB3	1:G:412:HIS:CE1	2.23	0.73
1:B:297:PHE:CE2	3:B:501:1CI:H8	2.24	0.73
1:B:364:PRO:HG3	1:B:479:ASN:HD21	1.54	0.73
1:F:443:ARG:NH1	1:F:443:ARG:HB3	2.03	0.73
1:G:371:VAL:HG11	1:G:382:ILE:HG21	1.71	0.73
1:G:398:ASP:OD2	1:G:400:ARG:HB2	1.88	0.73
1:E:140:ARG:HB2	1:E:144:GLU:HG2	1.71	0.72
1:B:153:LEU:HD22	1:B:174:ILE:HD13	1.70	0.72
1:C:402:PHE:CD1	1:C:412:HIS:HD2	2.06	0.72
1:G:364:PRO:HG3	1:G:479:ASN:ND2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HB2	1:D:434:ARG:HH12	1.53	0.72
1:E:441:ILE:HD11	2:E:500:HEM:HBC2	1.70	0.72
1:D:76:VAL:HB	1:D:388:VAL:HG22	1.71	0.72
1:F:358:ARG:HG3	1:F:396:LEU:HD22	1.71	0.72
1:E:113:VAL:HG13	1:E:114:ILE:CD1	2.19	0.72
1:E:413:PHE:O	1:E:414:LEU:HD23	1.89	0.72
1:E:131:THR:HG1	1:E:135:PHE:HD1	1.38	0.72
1:F:137:MET:HG3	1:F:138:GLY:H	1.54	0.72
1:G:461:SER:HB2	1:G:462:PRO:HD2	1.69	0.72
1:F:114:ILE:HG12	2:F:500:HEM:HAD1	1.69	0.72
1:A:256:LEU:O	1:A:258:PRO:HD3	1.88	0.72
1:C:257:ASP:OD2	1:C:260:ASN:HB3	1.90	0.72
1:D:168:THR:HG22	1:D:169:LEU:HD12	1.71	0.72
1:A:368:PRO:HG3	1:A:389:PHE:CE2	2.24	0.72
1:C:340:LEU:HD11	1:C:343:ARG:NH2	2.05	0.72
1:G:305:THR:CG2	1:G:481:PRO:HD2	2.20	0.72
1:C:114:ILE:HG12	2:C:500:HEM:HAD1	1.73	0.71
1:E:284:HIS:H	1:E:284:HIS:HD2	1.36	0.71
1:D:335:HIS:O	1:D:336:ARG:HB3	1.89	0.71
1:F:388:VAL:O	1:F:390:PRO:HD3	1.90	0.71
1:B:44:LEU:HB2	1:B:45:GLN:NE2	2.05	0.71
1:C:411:GLY:HA2	1:C:414:LEU:HD12	1.73	0.71
1:F:143:GLU:O	1:F:147:GLN:HG3	1.91	0.71
1:C:253:ARG:HH22	1:C:272:MET:CE	2.03	0.70
1:G:409:ASN:HB3	1:G:412:HIS:HE1	1.56	0.70
1:C:50:GLY:O	1:C:54:SER:HB2	1.89	0.70
1:D:273:GLU:O	1:D:276:LYS:HG3	1.90	0.70
1:B:168:THR:HA	1:B:308:ARG:HD3	1.72	0.70
1:C:90:ASP:O	1:C:91:GLN:HG3	1.90	0.70
1:C:358:ARG:HA	1:C:396:LEU:HD22	1.72	0.70
1:D:174:ILE:HG13	1:D:175:THR:H	1.56	0.70
1:F:217:PHE:HA	1:F:224:LEU:HD12	1.74	0.70
1:F:241:ILE:O	1:F:245:ILE:HG13	1.91	0.70
1:B:97:GLY:HA3	1:B:370:THR:O	1.90	0.70
1:D:241:ILE:O	1:D:245:ILE:HG13	1.92	0.70
1:F:332:ILE:HG21	1:F:338:PRO:HG3	1.72	0.70
1:C:232:ARG:HB3	1:C:232:ARG:HH11	1.56	0.70
1:D:321:THR:O	1:D:325:GLN:HG2	1.92	0.70
1:E:258:PRO:HA	1:E:270:LEU:HD11	1.73	0.69
1:B:422:ARG:NH1	1:B:422:ARG:HB2	2.07	0.69
1:A:220:PHE:HB3	1:A:223:PHE:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:HH22	1:C:272:MET:HE1	1.54	0.69
1:E:32:PRO:HB2	1:E:62:TYR:HD1	1.57	0.69
1:G:305:THR:HG22	1:G:481:PRO:HD2	1.74	0.69
1:C:171:PHE:HB3	1:C:304:SER:OG	1.92	0.69
1:C:489:LEU:HD12	1:C:489:LEU:H	1.57	0.69
1:G:415:ASP:CG	1:G:416:ALA:H	1.96	0.69
1:C:128:SER:O	1:C:132:MET:HG2	1.90	0.69
1:G:139:LYS:O	1:G:140:ARG:HG3	1.91	0.69
1:A:32:PRO:O	1:A:66:PHE:HB2	1.93	0.69
1:E:273:GLU:O	1:E:276:LYS:HE2	1.92	0.69
1:F:99:GLY:HA3	1:F:368:PRO:HB2	1.75	0.69
1:C:121:TRP:HE1	1:C:125:ARG:HD2	1.58	0.69
1:D:167:ASN:HD22	1:D:171:PHE:HE2	1.41	0.69
1:A:128:SER:O	1:A:132:MET:HG2	1.92	0.69
1:A:28:GLY:O	1:A:29:LYS:HG2	1.92	0.69
1:A:216:VAL:HG11	1:B:228:PRO:HD3	1.73	0.69
1:C:155:GLU:O	1:C:158:ARG:HB2	1.92	0.69
1:C:161:LYS:NZ	1:F:485:GLN:HE22	1.91	0.68
1:E:114:ILE:HD13	1:E:294:SER:HB3	1.76	0.68
1:A:284:HIS:O	1:A:286:GLN:N	2.27	0.68
1:F:323:ARG:HB3	1:F:348:TYR:CE2	2.28	0.68
1:D:412:HIS:O	1:D:421:LYS:HE2	1.93	0.68
1:G:139:LYS:C	1:G:140:ARG:HG3	2.13	0.68
1:B:79:CYS:O	1:B:83:ALA:HB3	1.93	0.68
1:C:323:ARG:HB3	1:C:348:TYR:CE2	2.29	0.68
1:C:421:LYS:HG2	1:C:422:ARG:H	1.58	0.68
1:F:364:PRO:HG3	1:F:479:ASN:ND2	2.08	0.68
1:F:53:ARG:NH1	1:F:56:LEU:HD12	2.08	0.68
1:G:164:LEU:HG	1:G:487:ARG:NH2	2.09	0.68
1:D:114:ILE:HD13	1:D:294:SER:CB	2.20	0.68
1:E:113:VAL:HG13	1:E:114:ILE:HD12	1.75	0.68
1:F:77:VAL:HG12	1:F:78:LEU:N	2.09	0.68
1:F:369:HIS:O	1:F:387:GLU:HA	1.93	0.68
1:G:68:VAL:O	1:G:74:PRO:HA	1.93	0.68
1:B:410:PRO:O	1:B:414:LEU:HD12	1.94	0.68
1:D:441:ILE:HD12	1:D:441:ILE:H	1.58	0.68
1:F:276:LYS:HD2	1:F:276:LYS:C	2.15	0.68
1:A:126:ARG:HE	1:A:130:ALA:HB2	1.58	0.68
1:D:90:ASP:O	1:D:91:GLN:HG3	1.93	0.67
1:D:392:LEU:HD11	1:D:430:SER:HB2	1.76	0.67
1:E:176:SER:HB2	1:E:300:THR:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:NH1	1:A:367:VAL:HB	2.10	0.67
1:F:282:GLU:HB3	1:F:287:ASN:ND2	2.10	0.67
1:D:232:ARG:HB3	1:D:232:ARG:NH1	2.09	0.67
1:G:325:GLN:HE21	1:G:491:ARG:HH11	1.42	0.67
1:D:116:ALA:HB1	1:D:120:ARG:HG2	1.77	0.67
1:D:129:LEU:HB2	1:D:437:LEU:HD11	1.76	0.67
1:F:278:ASP:OD1	1:F:279:PRO:HD2	1.95	0.67
1:F:357:GLN:HE22	2:F:500:HEM:HBB2	1.60	0.67
1:D:430:SER:O	1:D:435:ILE:HG13	1.95	0.67
1:A:489:LEU:HD21	1:D:489:LEU:CD1	2.26	0.66
1:C:129:LEU:O	1:C:133:ARG:HB2	1.94	0.66
1:E:114:ILE:HD13	1:E:294:SER:CB	2.25	0.66
1:G:40:LEU:O	1:G:43:LEU:HB2	1.95	0.66
1:D:87:ALA:HB2	1:D:377:PHE:CZ	2.30	0.66
1:A:114:ILE:HG12	2:A:500:HEM:HAD1	1.78	0.66
1:E:302:THR:OG1	3:E:501:1CI:H4	1.93	0.66
1:G:32:PRO:HB2	1:G:62:TYR:HB3	1.76	0.66
1:A:137:MET:O	1:A:138:GLY:C	2.33	0.66
1:F:186:LYS:HD2	1:F:186:LYS:H	1.60	0.66
1:B:81:THR:HG21	1:B:425:GLY:HA2	1.77	0.66
1:D:364:PRO:HG3	1:D:479:ASN:ND2	2.11	0.66
1:A:98:ARG:HG2	1:A:115:PHE:HA	1.78	0.66
1:F:137:MET:HG3	1:F:138:GLY:N	2.11	0.66
1:F:320:VAL:O	1:F:324:VAL:HG23	1.96	0.66
1:C:409:ASN:HB3	1:C:412:HIS:CE1	2.31	0.66
1:B:391:VAL:HG12	1:B:394:SER:H	1.61	0.66
1:D:132:MET:C	1:D:134:ASP:H	1.99	0.66
1:F:205:SER:O	1:F:209:ILE:HG13	1.96	0.66
1:B:107:ILE:HG13	1:B:238:LEU:HD12	1.77	0.66
1:D:308:ARG:HG2	1:D:308:ARG:HH11	1.61	0.65
1:E:50:GLY:O	1:E:54:SER:HB2	1.96	0.65
1:E:94:ALA:O	1:E:371:VAL:HA	1.96	0.65
1:B:98:ARG:HG2	1:B:115:PHE:HA	1.79	0.65
1:C:272:MET:O	1:C:276:LYS:HB3	1.95	0.65
1:E:139:LYS:HE2	1:E:145:ARG:HD3	1.77	0.65
1:E:183:VAL:HG11	1:E:292:VAL:HG13	1.78	0.65
1:A:119:GLU:HA	1:A:122:ARG:HD3	1.77	0.65
1:D:42:ASN:O	1:D:46:MET:HG2	1.96	0.65
1:G:107:ILE:HG13	1:G:238:LEU:HD12	1.79	0.65
1:F:231:HIS:CE1	1:F:232:ARG:HG2	2.30	0.65
1:F:232:ARG:NH1	1:F:232:ARG:HB3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TYR:HB2	1:A:290:LEU:CD1	2.25	0.65
1:C:103:VAL:HG11	1:C:234:ILE:HD12	1.79	0.65
1:G:167:ASN:HB2	1:G:171:PHE:CE1	2.31	0.65
1:F:95:PHE:C	1:F:97:GLY:H	1.99	0.65
1:G:374:ASP:HA	1:G:382:ILE:O	1.96	0.65
1:D:105:ASP:HB3	1:D:106:PRO:HD3	1.79	0.65
1:D:348:TYR:O	1:D:352:VAL:HG23	1.97	0.65
1:C:352:VAL:HG13	1:C:408:PHE:HZ	1.62	0.65
1:D:316:LYS:HG3	1:D:465:PRO:O	1.97	0.65
1:E:258:PRO:HA	1:E:270:LEU:CD1	2.27	0.65
1:F:357:GLN:HG2	1:F:428:PRO:HG3	1.78	0.65
1:A:133:ARG:HA	1:A:137:MET:HB3	1.78	0.65
1:D:174:ILE:HG13	1:D:175:THR:N	2.12	0.65
1:G:363:ILE:HG13	2:G:500:HEM:HMA3	1.77	0.65
1:G:73:ARG:HB2	1:G:73:ARG:CZ	2.27	0.64
1:G:153:LEU:CD1	1:G:170:LEU:HD22	2.27	0.64
1:A:383:PRO:HG2	1:A:386:THR:OG1	1.97	0.64
1:B:200:ASP:O	1:B:204:GLN:HB2	1.96	0.64
1:C:105:ASP:HB3	1:C:106:PRO:HD3	1.78	0.64
1:E:305:THR:HG22	1:E:308:ARG:HE	1.62	0.64
1:F:430:SER:HB2	2:F:500:HEM:HBA1	1.79	0.64
1:G:422:ARG:HG2	1:G:423:ASN:N	2.11	0.64
1:D:164:LEU:HG	1:D:487:ARG:HG3	1.79	0.64
1:G:52:LEU:HD13	1:G:364:PRO:HB3	1.79	0.64
1:C:139:LYS:HE2	1:C:340:LEU:HB3	1.78	0.64
1:E:352:VAL:HG13	1:E:408:PHE:HZ	1.63	0.64
1:C:141:SER:O	1:C:145:ARG:HG2	1.98	0.64
1:B:178:ILE:O	1:B:182:ILE:HD13	1.97	0.64
1:C:93:GLU:OE1	1:C:433:LYS:HE3	1.97	0.64
1:C:374:ASP:OD2	1:C:384:LYS:HB2	1.98	0.64
1:G:308:ARG:HG2	1:G:308:ARG:HH11	1.63	0.64
1:E:80:GLY:O	1:E:84:ILE:HG12	1.97	0.64
1:F:390:PRO:O	1:F:392:LEU:N	2.30	0.64
1:C:44:LEU:HB2	1:C:45:GLN:NE2	2.13	0.64
1:G:40:LEU:HD22	1:G:43:LEU:HD23	1.80	0.64
1:A:147:GLN:NE2	1:A:339:ALA:HA	2.13	0.64
1:B:136:GLY:HA2	1:B:145:ARG:HH12	1.62	0.64
1:C:85:ARG:NE	1:C:424:GLU:HG3	2.13	0.64
1:D:153:LEU:HD22	1:D:174:ILE:HD13	1.80	0.64
1:F:135:PHE:HE1	1:F:145:ARG:NH1	1.92	0.64
1:G:137:MET:HG3	1:G:138:GLY:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:479:ASN:O	1:G:481:PRO:HD3	1.98	0.64
1:C:352:VAL:O	1:C:356:ILE:HG13	1.99	0.63
1:D:114:ILE:CD1	1:D:294:SER:HB3	2.23	0.63
1:A:308:ARG:HG2	1:A:308:ARG:HH11	1.64	0.63
1:C:443:ARG:HG2	1:C:443:ARG:HH11	1.62	0.63
1:B:253:ARG:HH12	1:B:272:MET:HE3	1.63	0.63
1:B:442:ALA:HB1	2:B:500:HEM:HAB	1.81	0.63
1:B:474:GLU:HB3	1:B:480:VAL:HG12	1.80	0.63
1:E:93:GLU:OE1	1:E:433:LYS:HE3	1.98	0.63
1:A:213:SER:HA	1:A:216:VAL:CG1	2.25	0.63
1:E:205:SER:O	1:E:209:ILE:HG13	1.98	0.63
1:E:328:ILE:HA	1:E:346:MET:HE3	1.81	0.63
1:F:376:GLN:HE21	1:F:381:VAL:HG22	1.64	0.63
1:C:349:THR:O	1:C:353:ILE:HG13	1.99	0.63
1:E:174:ILE:HG13	1:E:175:THR:H	1.64	0.63
1:E:224:LEU:H	1:E:224:LEU:HD23	1.64	0.63
1:A:404:THR:HG21	1:A:409:ASN:HD22	1.64	0.63
1:B:202:PHE:CE1	1:B:241:ILE:HD13	2.34	0.63
1:B:284:HIS:O	1:B:285:HIS:C	2.37	0.63
1:D:37:LEU:H	1:D:37:LEU:HD12	1.63	0.63
1:G:336:ARG:HB2	1:G:337:PRO:HD2	1.81	0.63
1:E:114:ILE:CD1	1:E:294:SER:HB3	2.29	0.63
1:E:158:ARG:HH11	1:E:158:ARG:HG3	1.64	0.63
1:E:105:ASP:HB3	1:E:106:PRO:HD3	1.80	0.62
1:F:202:PHE:CE1	1:F:241:ILE:HD13	2.34	0.62
1:C:81:THR:HG23	1:C:425:GLY:HA2	1.81	0.62
1:F:425:GLY:O	1:F:427:MET:HG2	1.99	0.62
1:A:120:ARG:HA	1:A:282:GLU:HG3	1.81	0.62
1:C:139:LYS:HD3	1:C:140:ARG:CZ	2.29	0.62
1:C:174:ILE:HD12	1:C:449:PHE:CD1	2.34	0.62
1:F:371:VAL:HG22	1:F:386:THR:H	1.64	0.62
1:B:70:LEU:O	1:B:73:ARG:HG2	1.98	0.62
1:B:129:LEU:O	1:B:129:LEU:HD23	1.99	0.62
1:C:340:LEU:HD11	1:C:343:ARG:CZ	2.28	0.62
1:F:105:ASP:HB3	1:F:106:PRO:HD3	1.81	0.62
1:F:364:PRO:O	1:F:393:SER:HB2	1.98	0.62
1:E:52:LEU:O	1:E:56:LEU:HG	2.00	0.62
1:A:268:TYR:CD1	1:A:288:LEU:HD13	2.34	0.62
1:A:363:ILE:CG2	1:A:366:GLY:HA2	2.30	0.62
1:F:118:GLY:O	1:F:122:ARG:HD3	1.99	0.62
1:A:429:PHE:HE2	1:A:443:ARG:HD3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:ASN:HB3	1:E:412:HIS:CE1	2.34	0.62
1:F:162:GLY:O	1:F:487:ARG:HB2	2.00	0.62
1:B:78:LEU:HB2	1:B:84:ILE:HD13	1.81	0.62
1:C:198:LEU:O	1:C:201:LEU:HB2	1.99	0.62
1:D:113:VAL:HG13	1:D:114:ILE:HD12	1.80	0.62
1:E:362:LEU:H	1:E:362:LEU:CD2	2.12	0.62
1:F:49:LYS:CE	1:F:53:ARG:HG2	2.30	0.62
1:A:349:THR:O	1:A:353:ILE:HG13	2.00	0.62
1:B:101:ILE:HB	1:B:104:VAL:CG2	2.30	0.62
1:G:95:PHE:O	1:G:369:HIS:HD2	1.83	0.62
1:B:98:ARG:NH1	1:B:367:VAL:HB	2.15	0.62
1:E:258:PRO:HG3	1:E:270:LEU:CD2	2.29	0.62
1:C:170:LEU:O	1:C:170:LEU:HD23	2.00	0.61
1:F:288:LEU:O	1:F:292:VAL:HG23	2.00	0.61
1:F:323:ARG:HB3	1:F:348:TYR:HE2	1.65	0.61
1:A:320:VAL:O	1:A:324:VAL:HG23	2.00	0.61
1:C:209:ILE:HG22	1:C:477:VAL:HG11	1.82	0.61
1:D:98:ARG:HB2	1:D:434:ARG:NH1	2.14	0.61
1:G:324:VAL:O	1:G:328:ILE:HG13	1.99	0.61
1:A:124:LEU:HD11	1:A:287:ASN:ND2	2.16	0.61
1:A:129:LEU:C	1:A:129:LEU:HD23	2.21	0.61
1:B:81:THR:CG2	1:B:425:GLY:HA2	2.30	0.61
1:B:297:PHE:CD2	3:B:501:1CI:H8	2.35	0.61
1:F:132:MET:CE	1:F:441:ILE:HD11	2.30	0.61
1:F:138:GLY:O	1:F:139:LYS:HG2	1.99	0.61
1:F:146:ILE:HG12	1:F:178:ILE:HD12	1.82	0.61
1:F:238:LEU:HD23	1:F:241:ILE:HD12	1.83	0.61
1:A:369:HIS:O	1:A:370:THR:HG23	1.99	0.61
1:C:125:ARG:NH1	1:C:437:LEU:HB2	2.14	0.61
1:D:31:PRO:HB3	1:D:65:VAL:HG12	1.80	0.61
1:D:324:VAL:O	1:D:328:ILE:HG13	2.00	0.61
1:E:168:THR:HA	1:E:308:ARG:CD	2.30	0.61
1:B:422:ARG:HB2	1:B:422:ARG:HH11	1.65	0.61
1:C:363:ILE:HG22	1:C:366:GLY:H	1.65	0.61
1:E:163:ALA:HA	1:E:487:ARG:HH12	1.64	0.61
1:C:121:TRP:NE1	1:C:125:ARG:HD2	2.14	0.61
1:C:154:VAL:HG12	1:C:158:ARG:NH1	2.16	0.61
1:D:204:GLN:O	1:D:208:LEU:HD23	2.00	0.61
1:A:245:ILE:O	1:A:249:VAL:HG23	2.00	0.61
1:B:253:ARG:HH12	1:B:272:MET:CE	2.14	0.61
1:E:237:ASN:O	1:E:241:ILE:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:GLY:HA3	1:F:368:PRO:CB	2.31	0.61
1:C:136:GLY:O	1:C:142:VAL:HB	2.01	0.60
1:C:308:ARG:HG2	1:C:308:ARG:HH11	1.66	0.60
1:A:137:MET:O	1:A:139:LYS:N	2.34	0.60
1:B:143:GLU:O	1:B:147:GLN:HG3	2.01	0.60
1:C:84:ILE:HG21	1:C:427:MET:SD	2.41	0.60
1:D:299:GLY:HA2	2:D:500:HEM:HMC3	1.83	0.60
1:E:168:THR:HA	1:E:308:ARG:HD2	1.82	0.60
1:B:183:VAL:HG11	1:B:292:VAL:HG13	1.83	0.60
1:D:284:HIS:O	1:D:286:GLN:N	2.34	0.60
1:D:370:THR:HA	1:D:386:THR:O	2.00	0.60
1:G:328:ILE:O	1:G:332:ILE:HB	2.01	0.60
1:F:249:VAL:CG2	1:F:288:LEU:HD21	2.31	0.60
1:B:134:ASP:O	1:B:135:PHE:HB3	2.00	0.60
1:D:125:ARG:HH11	1:D:125:ARG:HG3	1.65	0.60
1:B:127:PHE:O	1:B:131:THR:HG22	2.01	0.60
1:C:81:THR:CG2	1:C:425:GLY:HA2	2.31	0.60
1:C:376:GLN:HG2	1:C:381:VAL:HG22	1.83	0.60
1:E:136:GLY:O	1:E:141:SER:HA	2.01	0.60
1:E:145:ARG:HD2	1:E:181:SER:HB3	1.82	0.60
1:E:154:VAL:O	1:E:158:ARG:HG2	2.01	0.60
1:B:102:ALA:HB2	1:B:218:GLU:HA	1.84	0.60
1:G:316:LYS:HB2	1:G:468:ILE:HG21	1.84	0.60
1:B:369:HIS:HE1	2:B:500:HEM:O2A	1.85	0.60
1:D:73:ARG:HH21	1:D:387:GLU:CD	2.05	0.60
1:D:340:LEU:HD11	1:D:343:ARG:NH2	2.17	0.60
1:B:245:ILE:O	1:B:249:VAL:HG23	2.02	0.60
1:C:78:LEU:O	1:C:84:ILE:HD11	2.01	0.60
1:C:404:THR:HG23	1:C:412:HIS:HE1	1.67	0.60
1:F:327:GLU:OE2	1:F:347:PRO:HD2	2.02	0.60
1:G:265:ILE:O	1:G:269:LEU:HG	2.02	0.60
1:G:383:PRO:O	1:G:386:THR:HG22	2.02	0.60
1:D:442:ALA:HB2	2:D:500:HEM:HMC2	1.83	0.59
1:F:245:ILE:O	1:F:249:VAL:HB	2.02	0.59
1:G:344:ALA:C	1:G:346:MET:H	2.05	0.59
1:G:421:LYS:HG2	1:G:422:ARG:H	1.67	0.59
1:A:179:ILE:HD13	1:A:179:ILE:O	2.02	0.59
1:A:404:THR:OG1	1:A:407:THR:HB	2.01	0.59
1:C:288:LEU:O	1:C:292:VAL:HG23	2.01	0.59
1:C:363:ILE:HG21	1:C:366:GLY:HA2	1.83	0.59
1:A:69:TYR:CZ	1:A:74:PRO:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PHE:O	1:A:366:GLY:O	2.20	0.59
1:C:256:LEU:HD12	1:C:257:ASP:H	1.67	0.59
1:D:404:THR:HB	1:D:407:THR:HB	1.83	0.59
1:G:90:ASP:O	1:G:91:GLN:HB2	2.03	0.59
1:G:105:ASP:N	1:G:106:PRO:CD	2.65	0.59
1:F:167:ASN:ND2	1:F:486:ILE:HG21	2.17	0.59
1:C:390:PRO:O	1:C:392:LEU:N	2.35	0.59
1:C:457:PHE:CD1	1:C:490:ALA:HA	2.37	0.59
1:E:53:ARG:HH11	1:E:53:ARG:CA	2.15	0.59
1:A:473:ARG:HB2	1:A:482:PRO:HA	1.84	0.59
1:D:133:ARG:HD2	1:D:142:VAL:CG2	2.33	0.59
1:F:464:PRO:HB2	1:F:467:ASP:CB	2.33	0.59
1:G:54:SER:O	1:G:58:LEU:HB2	2.03	0.59
1:F:132:MET:HB2	1:F:182:ILE:HG21	1.85	0.59
1:B:91:GLN:HB3	1:B:94:ALA:HB3	1.84	0.59
1:E:303:THR:HG21	1:E:445:GLU:OE1	2.02	0.59
1:G:95:PHE:C	1:G:97:GLY:H	2.06	0.59
1:B:205:SER:O	1:B:209:ILE:HG12	2.03	0.59
1:C:191:LYS:HE3	1:C:191:LYS:HA	1.85	0.59
1:C:316:LYS:O	1:C:465:PRO:HB3	2.02	0.59
1:G:50:GLY:HA2	1:G:215:GLN:OE1	2.03	0.59
1:G:384:LYS:O	1:G:385:ASN:HB2	2.03	0.59
1:B:236:ARG:O	1:B:239:GLN:HB2	2.03	0.59
1:C:402:PHE:HD1	1:C:412:HIS:HD2	1.47	0.59
1:E:220:PHE:HB2	1:E:224:LEU:HD21	1.84	0.59
1:G:348:TYR:O	1:G:352:VAL:HG23	2.02	0.59
1:A:226:TYR:CD2	1:C:43:LEU:HG	2.37	0.58
1:A:313:LEU:O	1:A:313:LEU:HD23	2.02	0.58
1:D:101:ILE:HD11	1:D:368:PRO:CD	2.32	0.58
1:E:29:LYS:C	1:E:30:LEU:HD12	2.22	0.58
1:E:34:PRO:HG2	1:E:42:ASN:OD1	2.03	0.58
1:G:116:ALA:O	1:G:121:TRP:HB2	2.03	0.58
1:D:43:LEU:HD11	1:F:226:TYR:HD2	1.68	0.58
1:E:99:GLY:HA3	1:E:368:PRO:CB	2.30	0.58
1:G:73:ARG:HB2	1:G:73:ARG:NH1	2.19	0.58
1:G:256:LEU:HD22	1:G:269:LEU:HD12	1.86	0.58
1:G:358:ARG:HA	1:G:396:LEU:HD13	1.86	0.58
1:A:364:PRO:HG3	1:A:479:ASN:ND2	2.18	0.58
1:B:52:LEU:HD22	1:B:364:PRO:HB3	1.84	0.58
1:B:203:PHE:HA	1:B:301:GLU:OE1	2.02	0.58
1:D:325:GLN:HA	1:D:325:GLN:NE2	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:398:ASP:OD2	1:F:400:ARG:HB2	2.04	0.58
1:A:37:LEU:HD11	1:A:44:LEU:HD12	1.85	0.58
1:B:279:PRO:HG2	1:B:280:SER:H	1.67	0.58
1:B:320:VAL:HG21	1:B:408:PHE:CE2	2.38	0.58
1:D:108:PHE:O	1:D:110:GLY:N	2.32	0.58
1:D:202:PHE:CD1	1:D:297:PHE:HD1	2.21	0.58
1:D:322:GLU:HA	1:D:325:GLN:HB2	1.85	0.58
1:D:405:PRO:HG2	1:D:406:ASN:OD1	2.02	0.58
1:E:94:ALA:HB1	1:E:375:THR:OG1	2.03	0.58
1:A:70:LEU:HD12	1:A:75:VAL:HG11	1.85	0.58
1:E:111:TYR:HB2	1:E:290:LEU:CD1	2.23	0.58
1:E:173:SER:O	1:E:177:ASN:HB2	2.03	0.58
1:F:362:LEU:H	1:F:362:LEU:HD22	1.69	0.58
1:F:363:ILE:HG22	1:F:366:GLY:H	1.69	0.58
1:B:190:TYR:O	1:B:196:LEU:HD21	2.03	0.58
1:C:449:PHE:O	1:C:453:ILE:HG13	2.04	0.58
1:C:489:LEU:HD12	1:C:489:LEU:N	2.18	0.58
1:E:47:ASP:HB3	1:E:54:SER:HA	1.86	0.58
1:E:108:PHE:HA	1:E:290:LEU:HD13	1.85	0.58
1:E:305:THR:HG22	1:E:308:ARG:HH21	1.69	0.58
1:F:61:LYS:HD3	1:F:62:TYR:HE2	1.69	0.58
1:F:253:ARG:NH2	1:F:269:LEU:HD22	2.19	0.58
1:G:70:LEU:HB2	1:G:73:ARG:HG3	1.85	0.58
1:G:142:VAL:O	1:G:146:ILE:HG13	2.04	0.58
1:A:324:VAL:HG13	1:A:349:THR:OG1	2.04	0.58
1:C:319:HIS:CE1	1:C:320:VAL:HG23	2.39	0.58
1:C:327:GLU:OE1	1:C:346:MET:HB3	2.03	0.58
1:D:236:ARG:O	1:D:239:GLN:HB2	2.04	0.58
1:D:320:VAL:O	1:D:324:VAL:HG23	2.04	0.58
1:E:228:PRO:HG3	1:F:213:SER:OG	2.04	0.58
1:E:308:ARG:HH11	1:E:308:ARG:HB3	1.69	0.58
1:A:174:ILE:O	1:A:178:ILE:HG12	2.04	0.58
1:D:179:ILE:HD13	1:D:179:ILE:C	2.24	0.58
1:G:332:ILE:HD13	1:G:338:PRO:HG3	1.84	0.58
1:G:362:LEU:HD22	1:G:362:LEU:N	2.18	0.58
1:D:70:LEU:HD12	1:D:75:VAL:HG11	1.84	0.57
1:E:164:LEU:HD21	1:E:462:PRO:HD3	1.86	0.57
1:F:222:GLY:HA2	1:F:225:LYS:HE3	1.86	0.57
1:G:276:LYS:HD2	1:G:277:SER:N	2.19	0.57
1:B:75:VAL:HG12	1:B:387:GLU:HB2	1.84	0.57
1:E:372:THR:O	1:E:384:LYS:HE3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASP:C	1:G:84:ILE:H	2.06	0.57
1:B:371:VAL:HG21	1:B:382:ILE:HG22	1.85	0.57
1:D:44:LEU:HD12	1:D:44:LEU:N	2.19	0.57
1:G:28:GLY:O	1:G:380:TYR:HD1	1.87	0.57
1:B:158:ARG:HH11	1:B:158:ARG:HG3	1.67	0.57
1:C:51:LEU:O	1:C:54:SER:HB3	2.04	0.57
1:C:272:MET:HG3	1:C:283:PHE:O	2.03	0.57
1:F:48:ARG:HG3	1:F:48:ARG:HH11	1.69	0.57
1:F:404:THR:OG1	1:F:407:THR:HB	2.05	0.57
1:G:137:MET:HG3	1:G:138:GLY:N	2.19	0.57
1:G:202:PHE:CE1	1:G:241:ILE:HD13	2.39	0.57
1:C:413:PHE:O	1:C:420:LEU:HD12	2.04	0.57
1:E:174:ILE:HG13	1:E:175:THR:N	2.19	0.57
1:E:404:THR:O	1:E:404:THR:HG23	2.04	0.57
1:F:98:ARG:N	1:F:117:ASN:OD1	2.36	0.57
1:A:132:MET:HB2	1:A:182:ILE:HG21	1.86	0.57
1:B:362:LEU:H	1:B:362:LEU:HD22	1.69	0.57
1:G:150:ALA:O	1:G:154:VAL:HG23	2.05	0.57
1:G:460:ALA:O	1:G:487:ARG:HG2	2.04	0.57
1:A:324:VAL:O	1:A:328:ILE:HG13	2.05	0.57
1:C:284:HIS:O	1:C:286:GLN:N	2.37	0.57
1:D:158:ARG:HG2	1:D:457:PHE:CZ	2.37	0.57
1:E:414:LEU:HA	1:E:419:ALA:O	2.05	0.57
1:C:111:TYR:HB2	1:C:290:LEU:HD12	1.86	0.57
1:E:37:LEU:HD12	1:E:37:LEU:N	2.20	0.57
1:C:34:PRO:HD2	1:C:67:THR:O	2.04	0.57
1:E:145:ARG:HD2	1:E:181:SER:CB	2.35	0.57
1:F:315:LEU:HG	1:F:459:ILE:HD12	1.86	0.57
1:C:79:CYS:O	1:C:83:ALA:HB3	2.05	0.56
1:D:103:VAL:HG21	1:D:209:ILE:HG23	1.87	0.56
1:E:140:ARG:HB2	1:E:144:GLU:CB	2.35	0.56
1:C:108:PHE:O	1:C:110:GLY:N	2.34	0.56
1:C:372:THR:O	1:C:384:LYS:HE3	2.05	0.56
1:E:358:ARG:HG3	1:E:396:LEU:HB3	1.88	0.56
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.41	0.56
1:C:174:ILE:O	1:C:178:ILE:HG12	2.05	0.56
1:C:457:PHE:HA	1:C:491:ARG:HG3	1.88	0.56
1:D:133:ARG:HD2	1:D:142:VAL:HG21	1.87	0.56
1:D:268:TYR:O	1:D:272:MET:HB2	2.06	0.56
1:E:171:PHE:CD2	1:E:307:LEU:HB3	2.40	0.56
1:E:358:ARG:HD2	1:E:396:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:VAL:O	1:F:265:ILE:HG13	2.06	0.56
1:F:232:ARG:HB3	1:F:232:ARG:HH11	1.71	0.56
1:F:243:THR:O	1:F:243:THR:HG22	2.05	0.56
1:G:145:ARG:O	1:G:148:GLU:HB3	2.06	0.56
1:G:298:ALA:HB1	3:G:501:1CI:H4	1.87	0.56
1:A:85:ARG:HA	1:A:89:VAL:HG23	1.87	0.56
1:E:358:ARG:HG3	1:E:396:LEU:CD2	2.32	0.56
1:F:140:ARG:NH2	1:F:148:GLU:HG2	2.19	0.56
1:G:372:THR:O	1:G:373:LYS:HB3	2.05	0.56
1:C:112:GLY:O	1:C:116:ALA:HB2	2.05	0.56
1:G:210:SER:O	1:G:474:GLU:HG3	2.06	0.56
1:D:94:ALA:O	1:D:371:VAL:HA	2.05	0.56
1:D:238:LEU:HD22	1:D:293:LEU:HD21	1.86	0.56
1:F:285:HIS:O	1:F:287:ASN:N	2.38	0.56
1:A:81:THR:CG2	1:A:425:GLY:HA2	2.36	0.56
1:A:362:LEU:HD22	1:A:362:LEU:N	2.18	0.56
1:C:158:ARG:HH11	1:C:158:ARG:HG3	1.70	0.56
1:C:391:VAL:HG12	1:C:394:SER:H	1.69	0.56
1:F:242:ASN:C	1:F:244:PHE:H	2.09	0.56
1:F:250:GLU:C	1:F:252:HIS:H	2.08	0.56
1:A:137:MET:HA	1:A:142:VAL:HG21	1.88	0.56
1:B:48:ARG:HH11	1:B:48:ARG:HG3	1.70	0.56
1:B:268:TYR:CD1	1:B:288:LEU:HD13	2.40	0.56
1:B:352:VAL:HG13	1:B:408:PHE:HZ	1.71	0.56
1:E:279:PRO:HG2	1:E:280:SER:H	1.70	0.56
1:F:435:ILE:HG12	1:F:436:CYS:N	2.20	0.56
1:D:141:SER:HB2	1:D:144:GLU:HG2	1.88	0.56
1:E:332:ILE:HD13	1:E:338:PRO:HB3	1.87	0.56
1:G:423:ASN:C	1:G:425:GLY:H	2.10	0.56
1:C:421:LYS:CG	1:C:422:ARG:H	2.17	0.56
1:D:98:ARG:HG3	1:D:99:GLY:O	2.06	0.56
1:E:69:TYR:CZ	1:E:74:PRO:HB3	2.40	0.56
1:F:176:SER:HB2	1:F:300:THR:HG23	1.88	0.56
1:F:215:GLN:O	1:F:218:GLU:HB3	2.06	0.56
1:G:358:ARG:HG3	1:G:396:LEU:HB3	1.86	0.56
1:A:60:GLU:OE2	1:A:60:GLU:HA	2.06	0.55
1:C:34:PRO:HG2	1:C:42:ASN:OD1	2.06	0.55
1:E:98:ARG:HD3	1:E:99:GLY:N	2.20	0.55
1:E:132:MET:SD	1:E:133:ARG:N	2.79	0.55
1:G:320:VAL:HG21	1:G:408:PHE:HE2	1.70	0.55
1:C:183:VAL:O	1:C:265:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:H	1:C:198:LEU:HD22	1.71	0.55
1:F:167:ASN:HD22	1:F:486:ILE:HG21	1.71	0.55
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.70	0.55
1:D:308:ARG:NH2	1:D:481:PRO:O	2.39	0.55
1:E:273:GLU:OE2	1:E:276:LYS:HD3	2.06	0.55
1:F:93:GLU:HB2	1:F:433:LYS:HE3	1.88	0.55
1:C:132:MET:HG3	1:C:137:MET:HE2	1.87	0.55
1:C:244:PHE:CD1	1:C:244:PHE:C	2.80	0.55
1:E:29:LYS:HE3	1:E:380:TYR:CD1	2.41	0.55
1:E:111:TYR:CB	1:E:290:LEU:HD12	2.25	0.55
1:F:88:LEU:HD11	1:F:369:HIS:NE2	2.22	0.55
1:A:94:ALA:HB2	1:A:373:LYS:HE2	1.89	0.55
1:A:459:ILE:HB	1:A:486:ILE:HD11	1.89	0.55
1:E:70:LEU:O	1:E:73:ARG:HG2	2.06	0.55
1:E:127:PHE:CD2	1:E:283:PHE:HE2	2.25	0.55
1:F:443:ARG:HB3	1:F:443:ARG:HH11	1.69	0.55
1:A:231:HIS:CE1	1:A:232:ARG:HG2	2.41	0.55
1:B:105:ASP:N	1:B:106:PRO:CD	2.70	0.55
1:B:285:HIS:O	1:B:286:GLN:C	2.44	0.55
1:G:363:ILE:HD13	1:G:478:GLY:HA2	1.88	0.55
1:A:33:GLY:HA3	1:A:67:THR:O	2.05	0.55
1:A:102:ALA:HB1	1:A:217:PHE:CD2	2.36	0.55
1:A:308:ARG:HG2	1:A:308:ARG:NH1	2.22	0.55
1:E:140:ARG:HB2	1:E:144:GLU:CG	2.36	0.55
1:B:73:ARG:NH2	1:B:387:GLU:OE1	2.39	0.55
1:F:48:ARG:HG3	1:F:48:ARG:NH1	2.22	0.55
1:G:145:ARG:HG2	1:G:145:ARG:HH11	1.72	0.55
1:A:390:PRO:O	1:A:392:LEU:N	2.40	0.55
1:B:162:GLY:HA3	1:B:489:LEU:HD23	1.89	0.55
1:B:202:PHE:O	1:B:203:PHE:HB3	2.07	0.55
1:B:302:THR:HG21	3:B:501:1CI:H4	1.88	0.55
1:C:88:LEU:HD22	1:C:432:GLY:HA3	1.89	0.55
1:D:70:LEU:HD22	1:D:219:LEU:CD1	2.36	0.55
1:D:98:ARG:HG2	1:D:115:PHE:HA	1.87	0.55
1:E:133:ARG:CZ	1:E:141:SER:HB2	2.36	0.55
1:F:276:LYS:HD2	1:F:277:SER:N	2.22	0.55
1:G:56:LEU:C	1:G:58:LEU:H	2.10	0.55
1:G:128:SER:O	1:G:131:THR:HB	2.07	0.55
1:G:362:LEU:H	1:G:362:LEU:CD2	2.19	0.55
1:G:380:TYR:OH	1:G:383:PRO:HD3	2.07	0.55
1:A:52:LEU:CD2	1:A:364:PRO:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD23	1:A:129:LEU:O	2.07	0.55
1:C:183:VAL:HG11	1:C:292:VAL:HG13	1.88	0.55
1:G:31:PRO:HD3	1:G:380:TYR:CB	2.36	0.55
1:B:253:ARG:HH22	1:B:272:MET:HE1	1.72	0.54
1:C:187:ARG:O	1:C:187:ARG:HG3	2.07	0.54
1:E:146:ILE:HD13	1:E:445:GLU:HG2	1.89	0.54
1:E:376:GLN:NE2	1:E:379:GLY:H	1.99	0.54
1:G:101:ILE:HD11	1:G:368:PRO:HD2	1.89	0.54
1:G:331:VAL:HG21	1:G:345:LYS:O	2.06	0.54
1:C:49:LYS:HG2	1:C:53:ARG:HB2	1.88	0.54
1:C:340:LEU:O	1:C:340:LEU:HD12	2.07	0.54
1:D:167:ASN:HB2	1:D:171:PHE:CE2	2.42	0.54
1:E:316:LYS:O	1:E:465:PRO:HB3	2.07	0.54
1:G:362:LEU:O	1:G:363:ILE:HD13	2.07	0.54
1:A:39:VAL:HG12	1:A:40:LEU:HD23	1.89	0.54
1:A:355:GLU:OE2	1:A:358:ARG:NH2	2.39	0.54
1:C:241:ILE:O	1:C:245:ILE:HG13	2.07	0.54
1:D:297:PHE:CD2	3:D:501:1CI:H10	2.42	0.54
1:F:62:TYR:HD2	1:F:62:TYR:N	2.05	0.54
1:B:59:ARG:O	1:B:59:ARG:HG2	2.06	0.54
1:B:172:HIS:CE1	1:B:203:PHE:HB2	2.42	0.54
1:E:355:GLU:HG2	1:E:409:ASN:H	1.73	0.54
1:G:128:SER:O	1:G:132:MET:HG2	2.07	0.54
1:G:422:ARG:CG	1:G:423:ASN:H	2.20	0.54
1:C:168:THR:HA	1:C:308:ARG:HD2	1.89	0.54
1:C:222:GLY:HA2	1:C:225:LYS:HE3	1.89	0.54
1:G:400:ARG:HG2	1:G:400:ARG:HH11	1.71	0.54
1:C:308:ARG:NH2	1:C:481:PRO:HB2	2.23	0.54
1:D:369:HIS:HE1	2:D:500:HEM:O2A	1.90	0.54
1:E:32:PRO:HB2	1:E:62:TYR:CD1	2.41	0.54
1:A:80:GLY:O	1:A:84:ILE:HG12	2.07	0.54
1:C:268:TYR:CD1	1:C:288:LEU:HD13	2.42	0.54
1:D:198:LEU:O	1:D:201:LEU:HB2	2.08	0.54
1:F:357:GLN:CG	1:F:428:PRO:HG3	2.37	0.54
1:G:65:VAL:HG21	1:G:377:PHE:HE2	1.71	0.54
1:A:131:THR:O	1:A:135:PHE:HB2	2.08	0.54
1:C:75:VAL:HG12	1:C:387:GLU:CB	2.37	0.54
1:C:97:GLY:O	1:C:370:THR:N	2.41	0.54
1:C:150:ALA:O	1:C:154:VAL:HG23	2.07	0.54
1:C:437:LEU:O	1:C:437:LEU:HD23	2.07	0.54
1:A:429:PHE:O	1:A:430:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ILE:HB	1:B:104:VAL:HG22	1.89	0.54
1:B:179:ILE:HG22	1:B:180:CYS:N	2.22	0.54
1:D:29:LYS:HE3	1:D:380:TYR:HE1	1.72	0.54
1:E:129:LEU:HG	1:E:437:LEU:HD11	1.89	0.54
1:B:272:MET:HG3	1:B:283:PHE:O	2.07	0.54
1:C:388:VAL:O	1:C:390:PRO:HD3	2.07	0.54
1:D:202:PHE:HD1	1:D:297:PHE:HD1	1.56	0.54
1:E:163:ALA:HA	1:E:487:ARG:NH1	2.23	0.54
1:A:114:ILE:HG13	1:A:294:SER:HB3	1.91	0.53
1:A:183:VAL:HA	1:A:264:PHE:HB3	1.90	0.53
1:A:369:HIS:HE1	2:A:500:HEM:O2A	1.90	0.53
1:C:161:LYS:HZ3	1:F:485:GLN:HE22	1.56	0.53
1:D:249:VAL:HG11	1:D:288:LEU:HD21	1.91	0.53
1:E:164:LEU:HG	1:E:487:ARG:NH2	2.24	0.53
1:E:284:HIS:CD2	1:E:284:HIS:N	2.62	0.53
1:F:98:ARG:NH1	1:F:367:VAL:HB	2.23	0.53
1:F:464:PRO:HB2	1:F:467:ASP:HB2	1.90	0.53
1:G:172:HIS:CE1	1:G:301:GLU:HA	2.43	0.53
1:G:172:HIS:HE1	1:G:301:GLU:HA	1.73	0.53
1:G:376:GLN:CD	1:G:376:GLN:H	2.11	0.53
1:A:402:PHE:O	1:A:405:PRO:HD3	2.08	0.53
1:B:242:ASN:HD21	1:B:290:LEU:HD23	1.73	0.53
1:C:88:LEU:O	1:C:432:GLY:HA2	2.07	0.53
1:C:103:VAL:CG1	1:C:234:ILE:HD12	2.38	0.53
1:C:442:ALA:HB1	2:C:500:HEM:CBB	2.39	0.53
1:D:225:LYS:C	1:D:227:PHE:H	2.10	0.53
1:E:42:ASN:HB3	1:E:45:GLN:HB2	1.90	0.53
1:E:436:CYS:SG	1:E:439:GLU:N	2.81	0.53
1:F:62:TYR:N	1:F:62:TYR:CD2	2.76	0.53
1:C:61:LYS:HG2	1:C:62:TYR:CE2	2.43	0.53
1:D:228:PRO:CD	1:E:216:VAL:HG11	2.36	0.53
1:D:429:PHE:CD2	1:D:439:GLU:HG3	2.42	0.53
1:E:257:ASP:OD2	1:E:260:ASN:HB3	2.09	0.53
1:E:305:THR:HG22	1:E:308:ARG:NE	2.23	0.53
1:F:297:PHE:CD2	3:F:501:1CI:H10	2.42	0.53
1:A:43:LEU:HD22	1:A:220:PHE:CZ	2.44	0.53
1:C:153:LEU:HD13	1:C:170:LEU:HD21	1.89	0.53
1:C:370:THR:HA	1:C:386:THR:O	2.08	0.53
1:C:403:GLU:O	1:C:412:HIS:NE2	2.41	0.53
1:D:139:LYS:HD2	1:D:144:GLU:OE1	2.09	0.53
1:E:272:MET:SD	1:E:283:PHE:O	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:ILE:HD12	1:G:449:PHE:CD2	2.44	0.53
1:A:49:LYS:HE2	1:A:53:ARG:HG2	1.90	0.53
1:G:101:ILE:HB	1:G:104:VAL:CG2	2.37	0.53
1:A:64:ASP:HA	1:A:79:CYS:HB2	1.91	0.53
1:B:183:VAL:HA	1:B:264:PHE:HB3	1.90	0.53
1:E:114:ILE:HD12	1:E:114:ILE:N	2.23	0.53
1:G:88:LEU:HD13	1:G:431:LEU:O	2.08	0.53
1:G:195:PHE:O	1:G:199:LEU:HG	2.09	0.53
1:G:404:THR:HG23	1:G:404:THR:O	2.09	0.53
1:B:409:ASN:O	1:B:412:HIS:ND1	2.40	0.53
1:F:409:ASN:HB3	1:F:412:HIS:HE1	1.73	0.53
1:G:172:HIS:ND1	1:G:300:THR:HG22	2.23	0.53
1:A:138:GLY:C	1:A:139:LYS:HD2	2.28	0.53
1:A:487:ARG:CD	1:A:489:LEU:HD11	2.39	0.53
1:B:253:ARG:HH22	1:B:272:MET:CE	2.21	0.53
1:D:105:ASP:N	1:D:106:PRO:CD	2.71	0.53
1:D:142:VAL:O	1:D:146:ILE:HG13	2.08	0.53
1:D:383:PRO:HG2	1:D:386:THR:OG1	2.08	0.53
1:F:132:MET:HE3	1:F:441:ILE:HD11	1.91	0.53
1:F:449:PHE:O	1:F:453:ILE:HG13	2.09	0.53
1:G:73:ARG:NH2	1:G:387:GLU:HB2	2.21	0.53
1:G:341:ASP:C	1:G:343:ARG:H	2.10	0.53
1:D:297:PHE:CE2	3:D:501:1CI:H10	2.44	0.53
1:E:85:ARG:HG2	1:E:85:ARG:NH1	2.23	0.53
1:E:195:PHE:CE2	1:E:199:LEU:HD11	2.44	0.53
1:G:31:PRO:HD3	1:G:380:TYR:CG	2.43	0.53
1:B:140:ARG:O	1:B:144:GLU:HG3	2.09	0.53
1:C:176:SER:O	1:C:180:CYS:HB2	2.08	0.53
1:E:393:SER:O	1:E:397:HIS:HB2	2.09	0.53
1:G:326:LYS:O	1:G:329:GLU:HB3	2.09	0.53
1:E:464:PRO:HB2	1:E:467:ASP:HB2	1.92	0.52
1:F:324:VAL:HG13	1:F:349:THR:OG1	2.08	0.52
1:G:234:ILE:O	1:G:238:LEU:HG	2.09	0.52
1:G:320:VAL:O	1:G:324:VAL:HG23	2.08	0.52
1:G:421:LYS:HG2	1:G:422:ARG:N	2.23	0.52
1:B:177:ASN:OD1	1:B:187:ARG:HB2	2.09	0.52
1:C:49:LYS:HG2	1:C:53:ARG:CB	2.39	0.52
1:C:363:ILE:CG2	1:C:366:GLY:HA2	2.39	0.52
1:D:87:ALA:HB1	1:D:95:PHE:CE2	2.44	0.52
1:E:101:ILE:CG2	1:E:104:VAL:HG22	2.39	0.52
1:E:171:PHE:CE2	1:E:307:LEU:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:PHE:HB3	1:E:304:SER:OG	2.10	0.52
1:E:340:LEU:HD11	1:E:343:ARG:NH2	2.24	0.52
1:E:388:VAL:O	1:E:390:PRO:HD3	2.08	0.52
1:E:430:SER:O	1:E:431:LEU:HD23	2.08	0.52
1:F:168:THR:HA	1:F:308:ARG:HD2	1.90	0.52
1:F:213:SER:HA	1:F:216:VAL:CG1	2.38	0.52
1:A:129:LEU:HD21	1:A:133:ARG:CZ	2.39	0.52
1:D:135:PHE:HE1	1:D:263:ASP:HA	1.75	0.52
1:E:129:LEU:O	1:E:132:MET:HG3	2.10	0.52
1:F:103:VAL:HG11	1:F:214:SER:HA	1.91	0.52
1:G:31:PRO:HB2	1:G:66:PHE:HA	1.91	0.52
1:G:73:ARG:HH21	1:G:387:GLU:CB	2.21	0.52
1:A:248:SER:HA	1:A:251:LYS:HD2	1.90	0.52
1:A:489:LEU:HD21	1:D:489:LEU:HD11	1.90	0.52
1:E:375:THR:HG22	1:E:376:GLN:N	2.25	0.52
1:A:352:VAL:HG13	1:A:408:PHE:HZ	1.74	0.52
1:B:62:TYR:HB3	1:B:66:PHE:HB3	1.92	0.52
1:B:248:SER:C	1:B:250:GLU:H	2.12	0.52
1:C:43:LEU:HD22	1:C:220:PHE:HZ	1.74	0.52
1:C:120:ARG:HB2	1:C:282:GLU:OE2	2.08	0.52
1:D:34:PRO:HG2	1:D:42:ASN:OD1	2.09	0.52
1:F:229:GLY:C	1:F:231:HIS:H	2.12	0.52
1:A:153:LEU:HD21	1:A:453:ILE:HD11	1.91	0.52
1:A:369:HIS:HB2	1:A:388:VAL:O	2.10	0.52
1:D:195:PHE:CE2	1:D:199:LEU:HD11	2.44	0.52
1:E:111:TYR:HD2	1:E:287:ASN:HD22	1.58	0.52
1:G:108:PHE:O	1:G:110:GLY:N	2.43	0.52
1:A:88:LEU:O	1:A:92:ALA:HB2	2.10	0.52
1:A:105:ASP:N	1:A:106:PRO:CD	2.73	0.52
1:A:297:PHE:O	1:A:301:GLU:HB2	2.10	0.52
1:B:119:GLU:OE2	1:B:123:ALA:HB2	2.10	0.52
1:B:404:THR:HG23	1:B:412:HIS:CE1	2.43	0.52
1:C:85:ARG:HE	1:C:424:GLU:HG3	1.73	0.52
1:C:189:ASP:OD2	1:E:159:LYS:HE2	2.10	0.52
1:D:78:LEU:HB2	1:D:84:ILE:HD13	1.92	0.52
1:F:327:GLU:OE2	1:F:346:MET:HA	2.10	0.52
1:F:430:SER:CB	2:F:500:HEM:HBA1	2.38	0.52
1:G:206:PHE:CZ	1:G:478:GLY:HA3	2.45	0.52
1:A:94:ALA:HB1	1:A:375:THR:OG1	2.10	0.52
1:B:153:LEU:HD22	1:B:174:ILE:HG21	1.91	0.52
1:C:176:SER:O	1:C:180:CYS:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ARG:HH11	1:D:308:ARG:CG	2.22	0.52
1:F:31:PRO:HA	1:F:380:TYR:CE1	2.45	0.52
1:F:182:ILE:HD12	1:F:182:ILE:N	2.25	0.52
1:F:265:ILE:O	1:F:269:LEU:HG	2.10	0.52
1:B:98:ARG:HH12	1:B:367:VAL:HB	1.74	0.52
1:E:78:LEU:O	1:E:84:ILE:HD11	2.09	0.52
1:E:161:LYS:O	1:E:162:GLY:C	2.49	0.52
1:E:324:VAL:O	1:E:328:ILE:HG13	2.10	0.52
1:G:41:GLY:C	1:G:43:LEU:H	2.13	0.52
1:B:457:PHE:CD1	1:B:490:ALA:HA	2.45	0.52
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.45	0.52
1:G:32:PRO:HB2	1:G:62:TYR:CD1	2.45	0.52
1:G:171:PHE:CE2	1:G:307:LEU:HB3	2.45	0.52
1:A:202:PHE:CE1	1:A:241:ILE:HD13	2.45	0.51
1:B:271:ARG:HA	1:B:274:LYS:HB3	1.92	0.51
1:D:42:ASN:HA	1:D:45:GLN:OE1	2.10	0.51
1:G:380:TYR:CG	1:G:381:VAL:N	2.78	0.51
1:A:42:ASN:O	1:A:46:MET:HG2	2.10	0.51
1:B:202:PHE:O	1:B:204:GLN:N	2.43	0.51
1:C:372:THR:O	1:C:384:LYS:HG3	2.09	0.51
1:F:34:PRO:O	1:F:36:PRO:HD3	2.10	0.51
1:F:362:LEU:HD22	1:F:362:LEU:N	2.25	0.51
1:A:176:SER:O	1:A:179:ILE:HG22	2.10	0.51
1:B:303:THR:HG21	1:B:445:GLU:OE1	2.10	0.51
1:B:384:LYS:O	1:B:385:ASN:HB2	2.11	0.51
1:D:136:GLY:CA	1:D:140:ARG:HB3	2.40	0.51
1:E:403:GLU:O	1:E:412:HIS:NE2	2.43	0.51
1:F:178:ILE:O	1:F:182:ILE:HD13	2.10	0.51
1:G:80:GLY:O	1:G:84:ILE:HG12	2.10	0.51
1:B:134:ASP:C	1:B:136:GLY:H	2.14	0.51
1:B:242:ASN:OD1	1:B:293:LEU:HD22	2.10	0.51
1:C:140:ARG:H	1:C:143:GLU:HB3	1.76	0.51
1:C:299:GLY:HA2	2:C:500:HEM:HMC3	1.91	0.51
1:D:164:LEU:HB2	1:D:487:ARG:CZ	2.40	0.51
1:E:87:ALA:O	1:E:95:PHE:HD2	1.94	0.51
1:E:299:GLY:HA2	2:E:500:HEM:HMC3	1.91	0.51
1:G:327:GLU:OE2	1:G:346:MET:HA	2.11	0.51
1:A:430:SER:O	1:A:431:LEU:HD23	2.10	0.51
1:B:70:LEU:HB2	1:B:73:ARG:CG	2.40	0.51
1:C:103:VAL:HG22	1:C:217:PHE:HD2	1.76	0.51
1:C:460:ALA:HB3	1:C:489:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:TYR:HB2	1:D:290:LEU:HD12	1.93	0.51
1:D:114:ILE:HD11	2:D:500:HEM:HMD3	1.93	0.51
1:D:192:ASP:HB3	1:D:195:PHE:HB3	1.92	0.51
1:D:209:ILE:HG22	1:D:477:VAL:HG11	1.93	0.51
1:D:256:LEU:HD12	1:D:257:ASP:N	2.26	0.51
1:E:78:LEU:HB3	1:E:84:ILE:HD13	1.91	0.51
1:E:127:PHE:CZ	1:E:267:VAL:HG12	2.45	0.51
1:A:340:LEU:HD13	1:A:444:THR:HG23	1.92	0.51
1:B:384:LYS:HG2	1:B:385:ASN:ND2	2.25	0.51
1:C:142:VAL:O	1:C:145:ARG:HB2	2.10	0.51
1:E:113:VAL:HG22	1:E:113:VAL:O	2.10	0.51
1:F:132:MET:HE1	1:F:441:ILE:HD11	1.93	0.51
1:A:49:LYS:CE	1:A:53:ARG:HE	2.24	0.51
1:C:437:LEU:HD23	1:C:437:LEU:C	2.31	0.51
1:D:198:LEU:HD11	1:D:244:PHE:CD2	2.45	0.51
1:E:390:PRO:O	1:E:392:LEU:N	2.44	0.51
1:F:31:PRO:HB3	1:F:32:PRO:HD2	1.92	0.51
1:F:439:GLU:O	1:F:443:ARG:HG2	2.10	0.51
1:G:326:LYS:O	1:G:330:GLN:HG3	2.11	0.51
1:G:332:ILE:HA	1:G:336:ARG:NH2	2.26	0.51
1:C:107:ILE:HG22	1:C:108:PHE:N	2.26	0.51
1:E:272:MET:HE3	1:E:283:PHE:HD2	1.75	0.51
1:E:430:SER:CB	2:E:500:HEM:HBA1	2.41	0.51
1:F:37:LEU:H	1:F:37:LEU:CD1	2.17	0.51
1:F:95:PHE:HE1	1:F:371:VAL:HG12	1.72	0.51
1:F:415:ASP:CG	1:F:416:ALA:N	2.64	0.51
1:G:35:SER:O	1:G:37:LEU:HD12	2.10	0.51
1:G:95:PHE:O	1:G:97:GLY:N	2.43	0.51
1:G:403:GLU:O	1:G:412:HIS:NE2	2.44	0.51
1:A:43:LEU:HD22	1:A:220:PHE:HZ	1.75	0.51
1:D:316:LYS:O	1:D:465:PRO:HB3	2.10	0.51
1:E:170:LEU:HD23	1:E:170:LEU:O	2.11	0.51
1:F:50:GLY:O	1:F:54:SER:HB2	2.10	0.51
1:F:61:LYS:CD	1:F:62:TYR:HE2	2.23	0.51
1:F:77:VAL:HG13	1:F:391:VAL:CG2	2.41	0.51
1:A:487:ARG:HD2	1:A:489:LEU:HD11	1.92	0.51
1:C:302:THR:OG1	3:C:501:1CI:H4	2.11	0.51
1:E:48:ARG:HH11	1:E:48:ARG:HG3	1.76	0.51
1:E:53:ARG:NH1	1:E:53:ARG:HB2	2.26	0.51
1:F:84:ILE:HG13	1:F:395:ALA:HB2	1.93	0.51
1:F:246:GLY:O	1:F:249:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:459:ILE:O	1:G:460:ALA:HB2	2.10	0.51
1:B:80:GLY:O	1:B:84:ILE:HG12	2.11	0.50
1:C:404:THR:HG23	1:C:412:HIS:CE1	2.45	0.50
1:E:304:SER:O	1:E:307:LEU:HB2	2.10	0.50
1:F:77:VAL:CG1	1:F:78:LEU:N	2.72	0.50
1:G:309:TYR:HB2	1:G:481:PRO:HG2	1.93	0.50
1:B:460:ALA:HB3	1:B:487:ARG:HG3	1.94	0.50
1:E:477:VAL:O	1:E:477:VAL:HG22	2.11	0.50
1:F:140:ARG:HH12	1:F:148:GLU:CG	2.25	0.50
1:F:364:PRO:HD2	1:F:477:VAL:O	2.12	0.50
1:F:402:PHE:O	1:F:405:PRO:HD3	2.11	0.50
1:G:441:ILE:O	1:G:445:GLU:HG3	2.11	0.50
1:A:256:LEU:HD21	1:A:270:LEU:CD2	2.32	0.50
1:A:363:ILE:HG22	1:A:363:ILE:O	2.11	0.50
1:B:174:ILE:O	1:B:178:ILE:HG12	2.12	0.50
1:C:76:VAL:HB	1:C:388:VAL:HG22	1.93	0.50
1:C:151:ARG:HG2	1:C:151:ARG:HH11	1.76	0.50
1:C:195:PHE:HA	1:C:198:LEU:HD23	1.92	0.50
1:F:435:ILE:HG12	1:F:436:CYS:H	1.75	0.50
1:G:43:LEU:HD13	1:G:220:PHE:HZ	1.76	0.50
1:A:382:ILE:HG22	1:A:386:THR:HB	1.93	0.50
1:E:272:MET:SD	1:E:283:PHE:HB3	2.52	0.50
1:F:40:LEU:HD22	1:F:40:LEU:H	1.76	0.50
1:F:44:LEU:HB2	1:F:45:GLN:NE2	2.26	0.50
1:F:140:ARG:HH12	1:F:148:GLU:HG2	1.76	0.50
1:F:246:GLY:C	1:F:248:SER:H	2.14	0.50
1:F:268:TYR:CD1	1:F:288:LEU:HD13	2.46	0.50
1:G:69:TYR:CD1	1:G:74:PRO:HB3	2.46	0.50
1:B:34:PRO:HB3	1:B:62:TYR:OH	2.11	0.50
1:C:326:LYS:O	1:C:329:GLU:HB3	2.12	0.50
1:F:47:ASP:HB3	1:F:54:SER:HA	1.94	0.50
1:F:120:ARG:HA	1:F:282:GLU:HG3	1.93	0.50
1:F:359:LEU:O	1:F:359:LEU:HD13	2.11	0.50
1:A:135:PHE:CE1	1:A:263:ASP:HA	2.46	0.50
1:C:99:GLY:HA3	1:C:368:PRO:HB2	1.94	0.50
1:C:223:PHE:C	1:C:223:PHE:CD2	2.85	0.50
1:E:195:PHE:CZ	1:E:199:LEU:HD11	2.47	0.50
1:G:238:LEU:O	1:G:242:ASN:ND2	2.44	0.50
1:G:386:THR:HG23	1:G:386:THR:O	2.11	0.50
1:A:48:ARG:HG3	1:A:48:ARG:HH11	1.76	0.50
1:A:404:THR:HG1	1:A:407:THR:HB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HG11	1:C:228:PRO:HD3	1.93	0.50
1:B:268:TYR:OH	1:B:283:PHE:HA	2.11	0.50
1:C:28:GLY:O	1:C:29:LYS:HG2	2.11	0.50
1:C:46:MET:HE2	1:C:51:LEU:HD23	1.94	0.50
1:C:362:LEU:O	1:C:362:LEU:HD13	2.12	0.50
1:E:73:ARG:HG3	1:E:73:ARG:O	2.12	0.50
1:E:85:ARG:HG2	1:E:85:ARG:HH11	1.76	0.50
1:F:39:VAL:O	1:F:41:GLY:N	2.44	0.50
1:F:223:PHE:C	1:F:223:PHE:CD2	2.85	0.50
1:F:402:PHE:CE2	1:F:425:GLY:HA3	2.47	0.50
1:G:36:PRO:HA	1:G:42:ASN:ND2	2.26	0.50
1:C:363:ILE:HG22	1:C:366:GLY:N	2.27	0.50
1:C:369:HIS:HB2	1:C:388:VAL:O	2.12	0.50
1:D:402:PHE:CD1	1:D:412:HIS:HD2	2.30	0.50
1:D:415:ASP:OD1	1:D:418:GLY:N	2.39	0.50
1:E:121:TRP:HE1	1:E:125:ARG:HD2	1.75	0.50
1:E:220:PHE:HB2	1:E:224:LEU:CD2	2.42	0.50
1:G:75:VAL:HG23	1:G:77:VAL:HG23	1.94	0.50
1:A:170:LEU:O	1:A:173:SER:HB2	2.12	0.50
1:C:477:VAL:O	1:C:477:VAL:HG22	2.12	0.50
1:A:247:GLN:O	1:A:251:LYS:HE3	2.12	0.49
1:A:429:PHE:CE2	1:A:443:ARG:HD3	2.44	0.49
1:B:153:LEU:HD21	1:B:453:ILE:HD11	1.95	0.49
1:B:186:LYS:H	1:B:186:LYS:HD3	1.77	0.49
1:B:358:ARG:HG2	1:B:358:ARG:HH11	1.77	0.49
1:D:132:MET:C	1:D:134:ASP:N	2.66	0.49
1:F:75:VAL:HG12	1:F:387:GLU:HB2	1.93	0.49
1:A:362:LEU:H	1:A:362:LEU:CD2	2.19	0.49
1:A:362:LEU:C	1:A:363:ILE:HD12	2.32	0.49
1:B:165:LEU:HD12	1:B:486:ILE:O	2.11	0.49
1:C:30:LEU:HD21	1:C:383:PRO:HD2	1.94	0.49
1:C:132:MET:HG3	1:C:137:MET:CE	2.42	0.49
1:D:322:GLU:O	1:D:325:GLN:HB2	2.13	0.49
1:E:305:THR:HG22	1:E:308:ARG:NH2	2.27	0.49
1:E:403:GLU:O	1:E:404:THR:HG22	2.11	0.49
1:F:29:LYS:C	1:F:30:LEU:HD23	2.32	0.49
1:F:409:ASN:HB3	1:F:412:HIS:CE1	2.47	0.49
1:G:167:ASN:HB2	1:G:171:PHE:CD1	2.46	0.49
1:B:142:VAL:C	1:B:144:GLU:N	2.64	0.49
1:B:382:ILE:CG2	1:B:386:THR:HB	2.42	0.49
1:D:268:TYR:CD1	1:D:288:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:HG12	1:F:78:LEU:H	1.77	0.49
1:F:77:VAL:HG13	1:F:391:VAL:HG21	1.94	0.49
1:D:202:PHE:CE1	1:D:241:ILE:HD13	2.47	0.49
1:E:73:ARG:NH2	1:E:387:GLU:OE1	2.45	0.49
1:F:403:GLU:O	1:F:404:THR:C	2.51	0.49
1:B:248:SER:C	1:B:250:GLU:N	2.65	0.49
1:C:38:PRO:O	1:C:40:LEU:N	2.39	0.49
1:C:174:ILE:HG13	1:C:175:THR:N	2.28	0.49
1:D:122:ARG:HG2	1:D:122:ARG:HH11	1.78	0.49
1:D:139:LYS:HG3	1:D:139:LYS:O	2.12	0.49
1:E:230:THR:O	1:E:234:ILE:HG13	2.13	0.49
1:E:329:GLU:OE2	1:E:334:SER:HB3	2.11	0.49
1:E:457:PHE:CD1	1:E:490:ALA:HA	2.48	0.49
1:F:409:ASN:O	1:F:412:HIS:ND1	2.46	0.49
1:F:415:ASP:HA	1:F:421:LYS:HD3	1.95	0.49
1:F:443:ARG:HH11	1:F:443:ARG:CB	2.25	0.49
1:G:123:ALA:CA	1:G:126:ARG:HG2	2.40	0.49
1:G:205:SER:O	1:G:209:ILE:HG13	2.13	0.49
1:B:188:PHE:HB2	1:B:195:PHE:CG	2.47	0.49
1:B:213:SER:O	1:B:216:VAL:HG12	2.13	0.49
1:C:203:PHE:HA	1:C:301:GLU:OE1	2.13	0.49
1:C:329:GLU:O	1:C:333:GLY:N	2.46	0.49
1:F:108:PHE:HA	1:F:290:LEU:HD13	1.93	0.49
1:G:209:ILE:HG22	1:G:477:VAL:CG1	2.42	0.49
1:B:362:LEU:HD22	1:B:362:LEU:N	2.27	0.49
1:C:128:SER:HA	1:C:264:PHE:HE2	1.77	0.49
1:C:194:VAL:O	1:C:197:ARG:HB3	2.12	0.49
1:C:352:VAL:HG13	1:C:408:PHE:CZ	2.46	0.49
1:C:392:LEU:HD21	1:C:430:SER:HA	1.95	0.49
1:D:43:LEU:HD21	1:F:226:TYR:CD2	2.47	0.49
1:D:44:LEU:HB2	1:D:45:GLN:HE22	1.78	0.49
1:E:34:PRO:HG2	1:E:42:ASN:CG	2.33	0.49
1:E:263:ASP:OD1	1:E:265:ILE:HB	2.11	0.49
1:F:88:LEU:HD21	1:F:369:HIS:NE2	2.27	0.49
1:F:328:ILE:HG12	1:F:346:MET:HE1	1.95	0.49
1:G:114:ILE:HG12	2:G:500:HEM:HAD1	1.93	0.49
1:A:122:ARG:CD	1:A:122:ARG:H	2.26	0.49
1:A:136:GLY:C	1:A:142:VAL:HG23	2.33	0.49
1:B:111:TYR:CD2	1:B:286:GLN:HB3	2.48	0.49
1:B:253:ARG:HA	1:B:269:LEU:HD13	1.94	0.49
1:E:362:LEU:HD22	1:E:362:LEU:N	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:ASP:O	1:F:91:GLN:CG	2.61	0.49
1:B:234:ILE:O	1:B:238:LEU:HG	2.13	0.49
1:C:263:ASP:OD1	1:C:265:ILE:HB	2.13	0.49
1:D:413:PHE:O	1:D:420:LEU:HD12	2.13	0.49
1:D:438:GLY:O	1:D:439:GLU:C	2.51	0.49
1:E:42:ASN:ND2	1:E:69:TYR:HB2	2.28	0.49
1:G:65:VAL:HG21	1:G:377:PHE:CE2	2.47	0.49
1:G:403:GLU:O	1:G:404:THR:C	2.51	0.49
1:B:316:LYS:HD3	1:B:317:TYR:HE1	1.76	0.49
1:C:49:LYS:HE3	1:C:53:ARG:HH12	1.74	0.49
1:D:108:PHE:C	1:D:110:GLY:H	2.14	0.49
1:D:146:ILE:HG21	1:D:448:LEU:HD12	1.95	0.49
1:D:155:GLU:HA	1:D:158:ARG:HG3	1.93	0.49
1:D:409:ASN:C	1:D:411:GLY:H	2.16	0.49
1:E:121:TRP:CZ2	1:E:434:ARG:HD3	2.47	0.49
1:F:137:MET:CG	1:F:138:GLY:H	2.25	0.49
1:A:302:THR:OG1	3:A:501:1CI:H4	2.13	0.48
1:B:325:GLN:NE2	1:B:491:ARG:HH11	2.11	0.48
1:C:170:LEU:HD23	1:C:170:LEU:C	2.33	0.48
1:D:136:GLY:HA3	1:D:140:ARG:HB3	1.93	0.48
1:D:154:VAL:O	1:D:158:ARG:HG3	2.12	0.48
1:D:176:SER:O	1:D:180:CYS:HB2	2.13	0.48
1:F:118:GLY:O	1:F:122:ARG:HB2	2.13	0.48
1:F:122:ARG:HB2	1:F:122:ARG:HH11	1.78	0.48
1:F:355:GLU:HG2	1:F:408:PHE:CD1	2.46	0.48
1:B:194:VAL:O	1:B:198:LEU:HD23	2.13	0.48
1:D:202:PHE:HD1	1:D:297:PHE:CD1	2.31	0.48
1:D:449:PHE:O	1:D:453:ILE:HG13	2.14	0.48
1:E:232:ARG:HG2	1:E:232:ARG:HH11	1.78	0.48
1:E:331:VAL:HG21	1:E:345:LYS:O	2.14	0.48
1:F:464:PRO:HB2	1:F:467:ASP:HB3	1.94	0.48
1:G:305:THR:HG21	1:G:481:PRO:HD2	1.92	0.48
1:G:371:VAL:HG11	1:G:382:ILE:CG2	2.40	0.48
1:A:278:ASP:C	1:A:280:SER:H	2.16	0.48
1:B:171:PHE:O	1:B:174:ILE:HG12	2.14	0.48
1:E:81:THR:O	1:E:85:ARG:HG3	2.13	0.48
1:E:172:HIS:HB3	1:E:199:LEU:HD22	1.95	0.48
1:E:188:PHE:CD2	1:E:195:PHE:HB2	2.48	0.48
1:E:271:ARG:HG3	1:E:272:MET:HE1	1.95	0.48
1:F:268:TYR:CE1	1:F:288:LEU:HB2	2.48	0.48
1:G:325:GLN:NE2	1:G:491:ARG:HH11	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:VAL:O	1:B:480:VAL:HG13	2.13	0.48
2:C:500:HEM:NA	3:C:501:1CI:N3	2.61	0.48
1:D:324:VAL:HG12	1:D:328:ILE:HD11	1.95	0.48
1:D:399:PRO:O	1:D:401:TYR:N	2.47	0.48
1:E:31:PRO:HB3	1:E:32:PRO:HD2	1.95	0.48
1:E:42:ASN:HD22	1:E:42:ASN:N	2.12	0.48
1:E:85:ARG:HA	1:E:89:VAL:HG23	1.94	0.48
1:F:97:GLY:HA2	1:F:117:ASN:OD1	2.13	0.48
1:F:415:ASP:CG	1:F:416:ALA:H	2.16	0.48
1:G:364:PRO:HG3	1:G:479:ASN:HD22	1.77	0.48
1:G:415:ASP:CG	1:G:416:ALA:N	2.66	0.48
1:A:119:GLU:OE1	1:A:122:ARG:NH1	2.46	0.48
1:A:168:THR:HA	1:A:308:ARG:HD3	1.95	0.48
1:A:317:TYR:HB3	1:A:320:VAL:HG23	1.95	0.48
1:A:384:LYS:O	1:A:385:ASN:HB2	2.12	0.48
1:C:52:LEU:CD2	1:C:364:PRO:HB3	2.36	0.48
1:C:124:LEU:HD11	1:C:287:ASN:OD1	2.14	0.48
1:D:37:LEU:HD13	1:D:44:LEU:HD13	1.95	0.48
1:F:61:LYS:HD3	1:F:62:TYR:CE2	2.48	0.48
1:A:136:GLY:HA3	1:A:145:ARG:HH12	1.79	0.48
1:B:241:ILE:O	1:B:245:ILE:HG13	2.13	0.48
1:B:486:ILE:O	1:B:486:ILE:HG23	2.12	0.48
1:C:146:ILE:HD13	1:C:445:GLU:HG2	1.96	0.48
1:C:323:ARG:HB3	1:C:348:TYR:HE2	1.77	0.48
1:C:365:PHE:O	1:C:366:GLY:O	2.31	0.48
1:D:400:ARG:HG2	1:D:400:ARG:HH11	1.78	0.48
1:E:173:SER:HA	1:E:199:LEU:HD11	1.94	0.48
1:F:96:SER:HB2	1:F:121:TRP:CZ3	2.49	0.48
1:F:114:ILE:CD1	1:F:294:SER:HB3	2.43	0.48
1:F:122:ARG:HB2	1:F:122:ARG:NH1	2.29	0.48
1:G:373:LYS:HA	1:G:384:LYS:HD2	1.94	0.48
1:A:37:LEU:H	1:A:37:LEU:HD12	1.78	0.48
1:A:49:LYS:HE3	1:A:53:ARG:HE	1.78	0.48
1:A:128:SER:HA	1:A:264:PHE:HE2	1.79	0.48
1:C:457:PHE:CA	1:C:491:ARG:HG3	2.44	0.48
1:C:489:LEU:HD23	1:F:487:ARG:HD2	1.96	0.48
1:D:102:ALA:CB	1:D:218:GLU:HA	2.44	0.48
1:E:140:ARG:O	1:E:144:GLU:HB3	2.14	0.48
1:G:194:VAL:O	1:G:198:LEU:HD13	2.14	0.48
1:G:344:ALA:O	1:G:346:MET:N	2.47	0.48
1:G:368:PRO:HG3	1:G:389:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:GLY:O	1:G:413:PHE:N	2.46	0.48
1:A:191:LYS:O	1:A:193:PRO:HD3	2.13	0.48
1:C:129:LEU:O	1:C:133:ARG:HD3	2.13	0.48
1:C:157:LEU:HD22	1:C:488:PHE:CD2	2.48	0.48
1:D:487:ARG:HG2	1:D:487:ARG:HH11	1.78	0.48
1:F:53:ARG:HH11	1:F:53:ARG:CA	2.20	0.48
1:F:80:GLY:O	1:F:84:ILE:HG12	2.12	0.48
1:G:30:LEU:HD22	1:G:67:THR:OG1	2.14	0.48
1:G:79:CYS:O	1:G:80:GLY:O	2.31	0.48
1:G:152:CYS:HB3	1:G:190:TYR:HE2	1.78	0.48
1:G:244:PHE:CD1	1:G:244:PHE:C	2.86	0.48
1:A:155:GLU:O	1:A:159:LYS:HG3	2.14	0.48
1:B:316:LYS:HG3	1:B:465:PRO:O	2.14	0.48
1:C:174:ILE:HD12	1:C:449:PHE:CG	2.49	0.48
1:D:247:GLN:O	1:D:250:GLU:HB2	2.13	0.48
1:E:131:THR:OG1	1:E:135:PHE:HD1	1.95	0.48
1:E:284:HIS:HB2	1:E:285:HIS:H	1.56	0.48
1:F:40:LEU:H	1:F:40:LEU:CD2	2.27	0.48
1:F:88:LEU:HD11	1:F:369:HIS:CE1	2.49	0.48
1:F:90:ASP:O	1:F:91:GLN:CB	2.61	0.48
1:F:95:PHE:C	1:F:97:GLY:N	2.66	0.48
1:F:223:PHE:HD2	1:F:223:PHE:O	1.97	0.48
1:G:87:ALA:HB1	1:G:95:PHE:CE2	2.49	0.48
1:A:320:VAL:HG21	1:A:408:PHE:HE2	1.79	0.48
1:C:188:PHE:HB2	1:C:195:PHE:CG	2.48	0.48
1:D:89:VAL:C	1:D:91:GLN:H	2.18	0.48
1:D:358:ARG:HG3	1:D:396:LEU:HB3	1.94	0.48
1:F:250:GLU:C	1:F:252:HIS:N	2.66	0.48
1:G:174:ILE:HG13	1:G:175:THR:N	2.28	0.48
1:B:136:GLY:HA2	1:B:145:ARG:NH1	2.29	0.47
1:B:139:LYS:HD2	1:B:139:LYS:N	2.29	0.47
1:B:186:LYS:H	1:B:186:LYS:CD	2.27	0.47
1:B:243:THR:O	1:B:247:GLN:HG2	2.14	0.47
1:B:288:LEU:O	1:B:292:VAL:HG23	2.13	0.47
1:B:370:THR:HG22	1:B:387:GLU:HG2	1.95	0.47
1:C:107:ILE:HG21	1:C:238:LEU:HD13	1.96	0.47
1:C:113:VAL:HG22	1:C:113:VAL:O	2.13	0.47
1:D:121:TRP:CZ2	1:D:434:ARG:HD3	2.49	0.47
1:D:129:LEU:C	1:D:129:LEU:HD23	2.33	0.47
1:E:52:LEU:HD23	1:E:53:ARG:HH12	1.78	0.47
1:F:162:GLY:HA2	1:F:488:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:477:VAL:HG13	1:G:478:GLY:N	2.29	0.47
1:A:223:PHE:C	1:A:223:PHE:CD2	2.88	0.47
1:C:108:PHE:CD1	1:C:290:LEU:HD22	2.49	0.47
1:C:161:LYS:HZ1	1:F:485:GLN:HE22	1.61	0.47
1:C:285:HIS:O	1:C:288:LEU:N	2.47	0.47
1:E:125:ARG:HG3	1:E:437:LEU:CD1	2.43	0.47
1:E:129:LEU:O	1:E:132:MET:CG	2.62	0.47
1:E:240:GLU:O	1:E:243:THR:HB	2.14	0.47
1:F:312:LEU:HD13	1:F:484:TYR:CD2	2.48	0.47
1:A:153:LEU:HB2	1:A:174:ILE:HG21	1.96	0.47
1:A:213:SER:C	1:A:215:GLN:H	2.16	0.47
1:A:404:THR:HG21	1:A:409:ASN:ND2	2.27	0.47
1:B:73:ARG:HG3	1:B:73:ARG:O	2.14	0.47
1:D:153:LEU:HD22	1:D:174:ILE:HG21	1.95	0.47
1:E:139:LYS:HD3	1:E:139:LYS:N	2.29	0.47
1:E:143:GLU:OE1	1:E:340:LEU:HB3	2.15	0.47
1:E:269:LEU:O	1:E:272:MET:HB2	2.13	0.47
1:E:358:ARG:CG	1:E:396:LEU:HB3	2.44	0.47
1:F:101:ILE:CB	1:F:104:VAL:HG22	2.42	0.47
1:F:129:LEU:O	1:F:129:LEU:HD23	2.13	0.47
1:G:180:CYS:C	1:G:182:ILE:H	2.17	0.47
1:G:320:VAL:HG21	1:G:408:PHE:CE2	2.50	0.47
1:G:410:PRO:O	1:G:414:LEU:HD12	2.14	0.47
1:A:326:LYS:O	1:A:330:GLN:HG3	2.14	0.47
1:B:48:ARG:HG3	1:B:48:ARG:NH1	2.29	0.47
1:D:249:VAL:HG22	1:D:265:ILE:HD13	1.94	0.47
1:D:456:ASN:O	1:D:491:ARG:HB2	2.14	0.47
1:F:384:LYS:O	1:F:385:ASN:HB2	2.13	0.47
1:B:54:SER:O	1:B:58:LEU:HG	2.15	0.47
1:B:132:MET:O	1:B:133:ARG:C	2.53	0.47
1:B:212:PHE:CD1	1:B:212:PHE:C	2.87	0.47
1:B:257:ASP:C	1:B:259:SER:H	2.18	0.47
1:B:373:LYS:O	1:B:374:ASP:C	2.52	0.47
1:C:373:LYS:O	1:C:374:ASP:C	2.52	0.47
1:E:198:LEU:HD21	1:E:244:PHE:HD2	1.80	0.47
1:F:90:ASP:O	1:F:91:GLN:HG3	2.14	0.47
1:G:183:VAL:HG11	1:G:292:VAL:HG13	1.96	0.47
1:G:233:GLN:HG3	1:G:237:ASN:ND2	2.30	0.47
1:A:150:ALA:O	1:A:154:VAL:HG23	2.14	0.47
1:D:285:HIS:O	1:D:286:GLN:C	2.52	0.47
1:D:288:LEU:O	1:D:292:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:GLU:OE1	1:D:348:TYR:HB3	2.14	0.47
1:D:463:VAL:HB	1:D:468:ILE:HD11	1.96	0.47
1:E:336:ARG:NH2	1:E:342:ASP:OD1	2.47	0.47
1:E:484:TYR:N	1:E:484:TYR:CD1	2.82	0.47
1:F:102:ALA:HB3	1:F:218:GLU:HA	1.96	0.47
1:F:438:GLY:HA3	2:F:500:HEM:HBC2	1.96	0.47
1:G:256:LEU:HD12	1:G:257:ASP:N	2.30	0.47
1:A:34:PRO:HG2	1:A:42:ASN:CG	2.35	0.47
1:A:241:ILE:O	1:A:245:ILE:HG13	2.14	0.47
1:A:254:ALA:O	1:A:255:THR:HG23	2.15	0.47
1:B:172:HIS:HB3	1:B:199:LEU:HD22	1.97	0.47
1:B:314:MET:HB3	1:B:459:ILE:HD13	1.97	0.47
1:B:324:VAL:HG13	1:B:349:THR:OG1	2.14	0.47
1:C:48:ARG:HH11	1:C:48:ARG:HG3	1.79	0.47
1:C:116:ALA:O	1:C:117:ASN:HB2	2.15	0.47
1:C:135:PHE:CE2	1:C:263:ASP:HA	2.50	0.47
1:C:176:SER:HB2	1:C:300:THR:HG23	1.97	0.47
1:C:370:THR:CG2	1:C:385:ASN:HA	2.45	0.47
1:C:489:LEU:CD2	1:F:489:LEU:HD11	2.45	0.47
1:D:125:ARG:NH1	2:D:500:HEM:O1D	2.48	0.47
1:D:189:ASP:C	1:D:191:LYS:H	2.17	0.47
1:E:129:LEU:HG	1:E:437:LEU:CD1	2.45	0.47
1:E:310:GLY:O	1:E:314:MET:HG2	2.15	0.47
1:F:165:LEU:C	1:F:165:LEU:HD12	2.35	0.47
1:G:146:ILE:HG12	1:G:178:ILE:HD12	1.97	0.47
1:A:213:SER:C	1:A:215:GLN:N	2.68	0.47
1:A:403:GLU:O	1:A:412:HIS:NE2	2.47	0.47
1:B:157:LEU:HD13	1:B:488:PHE:CG	2.50	0.47
1:B:312:LEU:HG	1:B:470:LEU:HD23	1.97	0.47
1:B:464:PRO:HG3	1:E:492:HIS:CE1	2.50	0.47
1:C:415:ASP:OD1	1:C:418:GLY:N	2.45	0.47
1:D:95:PHE:O	1:D:369:HIS:HD2	1.98	0.47
1:D:179:ILE:HG21	1:D:299:GLY:HA3	1.96	0.47
1:D:194:VAL:O	1:D:197:ARG:HB3	2.15	0.47
1:D:316:LYS:HD3	1:D:317:TYR:HE1	1.78	0.47
1:E:42:ASN:O	1:E:46:MET:HG2	2.15	0.47
1:E:114:ILE:HG13	2:E:500:HEM:HAD1	1.96	0.47
1:F:285:HIS:O	1:F:286:GLN:C	2.53	0.47
1:F:415:ASP:O	1:F:416:ALA:HB2	2.14	0.47
1:G:36:PRO:HA	1:G:42:ASN:HD22	1.80	0.47
1:G:43:LEU:HD13	1:G:220:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ILE:HG13	1:G:238:LEU:CD1	2.42	0.47
1:G:241:ILE:O	1:G:245:ILE:HG13	2.14	0.47
1:B:162:GLY:O	1:B:487:ARG:NH1	2.47	0.47
1:B:202:PHE:CD1	1:B:297:PHE:CD1	3.03	0.47
1:C:291:THR:O	1:C:295:LEU:HG	2.14	0.47
1:D:248:SER:O	1:D:252:HIS:ND1	2.47	0.47
1:A:176:SER:HB2	1:A:300:THR:HG23	1.97	0.47
1:A:247:GLN:O	1:A:251:LYS:HG3	2.14	0.47
1:B:174:ILE:HG13	1:B:175:THR:N	2.30	0.47
1:C:323:ARG:HD3	1:C:348:TYR:CD2	2.50	0.47
1:D:44:LEU:H	1:D:44:LEU:CD1	2.22	0.47
1:D:427:MET:HE2	1:D:431:LEU:HD21	1.95	0.47
1:E:286:GLN:OE1	1:E:286:GLN:HA	2.14	0.47
1:F:101:ILE:HB	1:F:104:VAL:CG2	2.40	0.47
1:F:223:PHE:C	1:F:223:PHE:HD2	2.18	0.47
1:F:350:ASP:OD1	1:F:420:LEU:HD21	2.15	0.47
1:G:60:GLU:HA	1:G:60:GLU:OE2	2.15	0.47
1:G:101:ILE:O	1:G:103:VAL:N	2.47	0.47
1:G:305:THR:HA	1:G:308:ARG:HD3	1.96	0.47
1:C:241:ILE:HG22	1:C:245:ILE:HD11	1.97	0.46
1:C:301:GLU:OE2	1:C:305:THR:HG21	2.15	0.46
1:D:38:PRO:O	1:D:39:VAL:HB	2.15	0.46
1:D:371:VAL:HG23	1:D:386:THR:H	1.80	0.46
1:F:52:LEU:C	1:F:54:SER:H	2.17	0.46
1:F:85:ARG:O	1:F:89:VAL:HG23	2.15	0.46
1:F:253:ARG:HG3	1:F:253:ARG:HH11	1.80	0.46
1:G:233:GLN:HE21	1:G:237:ASN:ND2	2.12	0.46
1:A:278:ASP:O	1:A:280:SER:N	2.43	0.46
1:B:114:ILE:CD1	1:B:294:SER:HB3	2.45	0.46
1:B:285:HIS:HB3	1:B:286:GLN:H	1.57	0.46
1:E:182:ILE:HD12	1:E:182:ILE:N	2.30	0.46
1:F:30:LEU:HD22	1:F:383:PRO:HD2	1.97	0.46
1:F:121:TRP:O	1:F:124:LEU:N	2.48	0.46
1:A:30:LEU:HD21	1:A:383:PRO:HD2	1.98	0.46
1:A:268:TYR:OH	1:A:287:ASN:HB2	2.16	0.46
1:B:127:PHE:C	1:B:127:PHE:CD1	2.89	0.46
1:C:315:LEU:HD13	1:C:461:SER:HB3	1.97	0.46
1:E:38:PRO:O	1:E:39:VAL:HB	2.15	0.46
1:E:138:GLY:C	1:E:139:LYS:HD3	2.35	0.46
1:E:250:GLU:OE2	1:E:250:GLU:HA	2.15	0.46
1:E:435:ILE:O	1:E:436:CYS:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:ALA:CB	1:G:218:GLU:HA	2.46	0.46
1:G:182:ILE:O	1:G:263:ASP:HB2	2.14	0.46
1:G:316:LYS:HD3	1:G:317:TYR:CE1	2.50	0.46
1:G:341:ASP:C	1:G:343:ARG:N	2.69	0.46
1:B:287:ASN:O	1:B:291:THR:HB	2.15	0.46
1:E:98:ARG:HB2	1:E:434:ARG:NH2	2.30	0.46
1:E:325:GLN:NE2	1:E:491:ARG:NH1	2.63	0.46
1:F:208:LEU:HD22	1:F:230:THR:HB	1.98	0.46
1:F:336:ARG:NH2	1:F:342:ASP:OD1	2.48	0.46
1:G:90:ASP:O	1:G:91:GLN:CB	2.62	0.46
1:G:146:ILE:HD12	1:G:444:THR:HG22	1.97	0.46
1:A:70:LEU:CD1	1:A:75:VAL:HG11	2.46	0.46
1:B:466:GLU:OE1	1:B:466:GLU:N	2.37	0.46
1:D:149:GLU:CD	1:D:187:ARG:HH21	2.19	0.46
1:E:68:VAL:O	1:E:75:VAL:HG22	2.16	0.46
1:E:403:GLU:O	1:E:404:THR:CG2	2.64	0.46
1:F:36:PRO:HB3	1:F:69:TYR:CD1	2.50	0.46
1:G:116:ALA:HB1	1:G:120:ARG:HD2	1.97	0.46
1:G:316:LYS:HB2	1:G:468:ILE:CG2	2.46	0.46
1:G:435:ILE:HG12	1:G:436:CYS:N	2.31	0.46
1:G:444:THR:HG22	1:G:444:THR:O	2.15	0.46
1:A:31:PRO:HA	1:A:380:TYR:CD1	2.50	0.46
1:A:383:PRO:HG2	1:A:386:THR:HG1	1.79	0.46
1:B:73:ARG:NH2	1:B:387:GLU:CD	2.69	0.46
1:B:143:GLU:OE2	1:B:340:LEU:HB3	2.16	0.46
1:B:211:SER:HA	1:B:474:GLU:OE2	2.16	0.46
1:C:44:LEU:HB2	1:C:45:GLN:HE21	1.80	0.46
1:D:409:ASN:O	1:D:411:GLY:N	2.48	0.46
1:E:371:VAL:HG21	1:E:383:PRO:O	2.16	0.46
1:G:422:ARG:CG	1:G:423:ASN:N	2.79	0.46
1:A:285:HIS:O	1:A:286:GLN:C	2.52	0.46
1:C:43:LEU:HD22	1:C:220:PHE:CZ	2.50	0.46
1:C:192:ASP:HB3	1:C:195:PHE:HB3	1.97	0.46
1:C:443:ARG:CZ	1:C:443:ARG:HB3	2.46	0.46
1:C:457:PHE:CE1	1:C:490:ALA:HA	2.51	0.46
1:E:325:GLN:O	1:E:329:GLU:HB2	2.16	0.46
1:F:78:LEU:HD11	1:F:388:VAL:HG11	1.97	0.46
1:F:202:PHE:CD1	1:F:297:PHE:HD1	2.34	0.46
1:F:235:TYR:O	1:F:236:ARG:C	2.54	0.46
1:G:98:ARG:N	1:G:117:ASN:OD1	2.47	0.46
1:G:325:GLN:NE2	1:G:491:ARG:NH1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:O	1:A:284:HIS:CG	2.68	0.46
1:B:34:PRO:HD2	1:B:67:THR:O	2.15	0.46
1:B:37:LEU:HD12	1:B:37:LEU:N	2.31	0.46
1:B:122:ARG:O	1:B:126:ARG:HB2	2.16	0.46
1:C:370:THR:HG23	1:C:386:THR:N	2.31	0.46
1:D:441:ILE:H	1:D:441:ILE:CD1	2.28	0.46
1:E:133:ARG:NH2	1:E:141:SER:CB	2.78	0.46
1:F:153:LEU:HD21	1:F:453:ILE:HD11	1.97	0.46
1:F:202:PHE:HE1	1:F:241:ILE:HD13	1.78	0.46
1:G:179:ILE:HG13	1:G:299:GLY:HA3	1.98	0.46
1:G:380:TYR:CE2	1:G:382:ILE:HA	2.51	0.46
1:A:240:GLU:O	1:A:243:THR:HB	2.16	0.46
1:E:457:PHE:HD1	1:E:490:ALA:HA	1.79	0.46
1:F:245:ILE:O	1:F:245:ILE:HG22	2.15	0.46
1:G:164:LEU:CG	1:G:487:ARG:HH21	2.24	0.46
1:G:282:GLU:O	1:G:287:ASN:ND2	2.45	0.46
1:G:308:ARG:HG2	1:G:308:ARG:NH1	2.31	0.46
1:G:340:LEU:HD22	1:G:444:THR:HG23	1.98	0.46
1:B:474:GLU:HB3	1:B:480:VAL:CG1	2.44	0.46
1:D:29:LYS:HE3	1:D:380:TYR:CE1	2.50	0.46
1:D:151:ARG:O	1:D:154:VAL:HB	2.16	0.46
1:D:171:PHE:HA	1:D:174:ILE:HG12	1.97	0.46
1:D:213:SER:HA	1:D:216:VAL:HG12	1.98	0.46
1:E:129:LEU:O	1:E:130:ALA:C	2.55	0.46
1:E:166:ASP:OD1	1:E:168:THR:HB	2.15	0.46
1:E:355:GLU:OE1	1:E:355:GLU:HA	2.16	0.46
1:F:85:ARG:HG3	1:F:89:VAL:HG21	1.96	0.46
1:F:354:HIS:HB3	1:F:413:PHE:CD2	2.51	0.46
1:F:404:THR:HG1	1:F:407:THR:HB	1.80	0.46
1:G:114:ILE:HG22	1:G:115:PHE:CD2	2.51	0.46
1:G:268:TYR:CE1	1:G:288:LEU:HB2	2.50	0.46
1:A:234:ILE:O	1:A:238:LEU:HG	2.16	0.45
1:A:285:HIS:O	1:A:288:LEU:N	2.49	0.45
1:C:85:ARG:HG2	1:C:85:ARG:NH1	2.31	0.45
1:C:177:ASN:HA	1:C:180:CYS:HB3	1.98	0.45
1:D:47:ASP:OD1	1:D:53:ARG:HG3	2.16	0.45
1:E:111:TYR:N	1:E:111:TYR:CD1	2.85	0.45
1:E:127:PHE:C	1:E:127:PHE:CD1	2.89	0.45
1:F:186:LYS:H	1:F:186:LYS:CD	2.29	0.45
1:G:321:THR:HG23	1:G:454:LEU:HD13	1.98	0.45
1:A:69:TYR:CD2	1:A:74:PRO:HB3	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ARG:HH12	1:B:437:LEU:HB2	1.80	0.45
1:B:382:ILE:HG22	1:B:386:THR:HB	1.98	0.45
1:C:65:VAL:HG22	1:C:78:LEU:CD2	2.45	0.45
1:C:111:TYR:CD1	1:C:111:TYR:N	2.83	0.45
1:D:98:ARG:NE	1:D:434:ARG:HH12	2.14	0.45
1:D:256:LEU:HD12	1:D:257:ASP:H	1.79	0.45
1:D:409:ASN:C	1:D:411:GLY:N	2.69	0.45
1:E:119:GLU:HA	1:E:122:ARG:NH1	2.31	0.45
1:E:429:PHE:O	1:E:430:SER:HB3	2.16	0.45
1:F:113:VAL:CG1	1:F:291:THR:HG23	2.45	0.45
1:F:310:GLY:O	1:F:314:MET:HG2	2.16	0.45
1:G:411:GLY:O	1:G:414:LEU:N	2.45	0.45
1:G:435:ILE:HG12	1:G:436:CYS:H	1.81	0.45
1:A:48:ARG:NH2	1:B:235:TYR:CD2	2.84	0.45
1:C:139:LYS:HD3	1:C:140:ARG:NH1	2.31	0.45
1:D:160:SER:O	1:D:161:LYS:C	2.54	0.45
1:D:201:LEU:HD11	1:D:240:GLU:CD	2.37	0.45
1:D:373:LYS:CA	1:D:384:LYS:HG3	2.33	0.45
1:D:429:PHE:HB3	1:D:436:CYS:HB3	1.98	0.45
1:E:150:ALA:O	1:E:154:VAL:HG23	2.17	0.45
1:E:235:TYR:CG	1:F:48:ARG:NH2	2.83	0.45
1:F:210:SER:HB3	1:F:476:GLY:H	1.80	0.45
1:G:32:PRO:CB	1:G:62:TYR:HB3	2.46	0.45
1:G:131:THR:O	1:G:134:ASP:HB3	2.16	0.45
1:A:161:LYS:HE3	1:D:462:PRO:HG3	1.97	0.45
1:A:489:LEU:N	1:A:489:LEU:HD12	2.31	0.45
1:B:373:LYS:O	1:B:373:LYS:HD2	2.16	0.45
1:C:38:PRO:C	1:C:40:LEU:H	2.18	0.45
1:C:136:GLY:C	1:C:142:VAL:HB	2.36	0.45
1:D:253:ARG:HH11	1:D:253:ARG:HG3	1.80	0.45
1:E:142:VAL:O	1:E:146:ILE:HG13	2.16	0.45
1:F:77:VAL:CG1	1:F:78:LEU:H	2.30	0.45
1:F:77:VAL:O	1:F:78:LEU:HD23	2.16	0.45
1:F:195:PHE:O	1:F:199:LEU:HG	2.15	0.45
1:G:40:LEU:HB3	1:G:43:LEU:HB3	1.98	0.45
1:C:140:ARG:N	1:C:143:GLU:HB3	2.31	0.45
1:D:107:ILE:HD11	1:D:235:TYR:CD1	2.52	0.45
1:D:123:ALA:O	1:D:126:ARG:HB3	2.16	0.45
1:D:371:VAL:HG21	1:D:382:ILE:HG22	1.98	0.45
1:E:108:PHE:O	1:E:110:GLY:N	2.40	0.45
1:E:127:PHE:HZ	1:E:267:VAL:HG12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:LYS:CE	1:E:145:ARG:HD3	2.45	0.45
1:E:476:GLY:C	1:E:478:GLY:H	2.20	0.45
1:G:355:GLU:O	1:G:359:LEU:HB2	2.16	0.45
1:A:28:GLY:HA2	1:A:381:VAL:HG23	1.97	0.45
1:A:121:TRP:HH2	1:A:433:LYS:HB3	1.80	0.45
1:C:164:LEU:HD23	1:C:487:ARG:HB3	1.98	0.45
1:D:340:LEU:HD13	1:D:444:THR:HG23	1.98	0.45
1:E:29:LYS:HE3	1:E:380:TYR:HD1	1.82	0.45
1:E:320:VAL:O	1:E:324:VAL:HG23	2.17	0.45
1:F:111:TYR:HB2	1:F:290:LEU:HD12	1.99	0.45
1:F:137:MET:CG	1:F:138:GLY:N	2.80	0.45
1:G:129:LEU:HG	1:G:437:LEU:HD11	1.99	0.45
1:G:138:GLY:HA3	1:G:145:ARG:CZ	2.47	0.45
1:A:81:THR:HG23	1:A:425:GLY:HA2	1.97	0.45
1:A:318:PRO:O	1:A:322:GLU:HG2	2.16	0.45
1:B:221:SER:O	1:B:225:LYS:HD3	2.15	0.45
1:B:340:LEU:C	1:B:342:ASP:H	2.20	0.45
1:C:85:ARG:HG2	1:C:85:ARG:HH11	1.82	0.45
1:C:256:LEU:HG	1:C:258:PRO:HD3	1.99	0.45
1:C:308:ARG:NH2	1:C:481:PRO:O	2.49	0.45
1:D:81:THR:HG23	1:D:424:GLU:O	2.17	0.45
1:D:271:ARG:O	1:D:271:ARG:HG2	2.17	0.45
1:D:313:LEU:HD12	1:D:356:ILE:HG12	1.99	0.45
1:D:464:PRO:O	1:D:467:ASP:HB2	2.17	0.45
1:E:149:GLU:OE1	1:E:177:ASN:ND2	2.37	0.45
1:E:202:PHE:HZ	1:E:296:PHE:CD2	2.35	0.45
1:E:363:ILE:CG2	1:E:366:GLY:HA2	2.46	0.45
1:F:229:GLY:O	1:F:231:HIS:N	2.44	0.45
1:F:297:PHE:HD2	3:F:501:1CI:H10	1.81	0.45
1:G:314:MET:SD	1:G:450:PHE:HZ	2.39	0.45
1:G:423:ASN:O	1:G:425:GLY:N	2.50	0.45
1:A:228:PRO:HD3	1:C:216:VAL:HG11	1.99	0.45
1:A:281:SER:O	1:A:283:PHE:N	2.50	0.45
1:A:331:VAL:HG12	1:A:332:ILE:N	2.31	0.45
1:B:313:LEU:HD23	1:B:470:LEU:HD11	1.99	0.45
1:B:430:SER:O	1:B:431:LEU:HD23	2.17	0.45
1:C:90:ASP:O	1:C:91:GLN:CB	2.64	0.45
1:D:335:HIS:O	1:D:336:ARG:CB	2.62	0.45
1:F:256:LEU:HG	1:F:257:ASP:N	2.32	0.45
1:F:283:PHE:N	1:F:283:PHE:CD1	2.85	0.45
1:A:429:PHE:O	1:A:430:SER:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:PHE:C	1:B:246:GLY:N	2.70	0.45
1:C:176:SER:O	1:C:180:CYS:CB	2.65	0.45
1:E:127:PHE:HE2	1:E:271:ARG:HG2	1.82	0.45
1:E:308:ARG:NH1	1:E:308:ARG:CB	2.80	0.45
1:F:145:ARG:HH11	1:F:182:ILE:CD1	2.30	0.45
1:F:268:TYR:OH	1:F:283:PHE:HA	2.16	0.45
1:F:464:PRO:HA	1:F:465:PRO:HD3	1.88	0.45
1:G:209:ILE:CG2	1:G:477:VAL:HG11	2.43	0.45
1:A:137:MET:HE3	1:A:441:ILE:HD11	1.98	0.45
1:B:200:ASP:O	1:B:204:GLN:CB	2.65	0.45
1:C:221:SER:O	1:C:225:LYS:HG2	2.17	0.45
1:E:34:PRO:HG3	1:E:45:GLN:HG2	1.99	0.45
1:E:309:TYR:CE2	1:E:313:LEU:HD12	2.52	0.45
1:F:146:ILE:HA	1:F:178:ILE:HD11	1.98	0.45
1:F:363:ILE:HG22	1:F:366:GLY:N	2.32	0.45
1:F:390:PRO:O	1:F:391:VAL:C	2.55	0.45
1:F:447:PHE:O	1:F:451:THR:HG23	2.17	0.45
1:A:333:GLY:O	1:A:334:SER:HB3	2.17	0.44
1:A:352:VAL:HG13	1:A:408:PHE:CZ	2.52	0.44
1:B:285:HIS:O	1:B:287:ASN:N	2.51	0.44
1:B:398:ASP:OD2	1:B:401:TYR:HD1	2.00	0.44
1:C:80:GLY:O	1:C:84:ILE:HG12	2.17	0.44
1:C:125:ARG:NH2	1:C:435:ILE:O	2.50	0.44
1:C:435:ILE:HG12	1:C:436:CYS:N	2.31	0.44
1:C:464:PRO:O	1:C:468:ILE:HG12	2.17	0.44
1:D:125:ARG:HG3	1:D:125:ARG:NH1	2.30	0.44
1:D:172:HIS:CE1	1:D:301:GLU:HA	2.52	0.44
1:D:375:THR:HG22	1:D:376:GLN:N	2.32	0.44
1:E:278:ASP:HB3	1:E:281:SER:HB2	1.99	0.44
1:E:357:GLN:NE2	1:E:446:LEU:HD11	2.32	0.44
1:G:211:SER:HA	1:G:474:GLU:CG	2.46	0.44
1:A:98:ARG:HB2	1:A:434:ARG:CZ	2.47	0.44
1:C:36:PRO:HA	1:C:42:ASN:ND2	2.32	0.44
1:C:256:LEU:CD1	1:C:257:ASP:H	2.30	0.44
1:C:403:GLU:O	1:C:404:THR:CG2	2.65	0.44
1:D:170:LEU:O	1:D:173:SER:HB2	2.17	0.44
1:D:229:GLY:C	1:D:231:HIS:H	2.20	0.44
1:D:232:ARG:CZ	1:E:212:PHE:CE2	3.01	0.44
1:E:103:VAL:CG1	1:E:234:ILE:HD12	2.47	0.44
1:F:40:LEU:HD22	1:F:40:LEU:N	2.32	0.44
1:G:73:ARG:HG3	1:G:73:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:HG3	1:A:404:THR:HG22	1.99	0.44
1:B:97:GLY:CA	1:B:370:THR:O	2.63	0.44
1:C:146:ILE:CD1	1:C:445:GLU:HG2	2.47	0.44
1:D:70:LEU:CD2	1:D:219:LEU:HD11	2.44	0.44
1:D:401:TYR:O	1:D:423:ASN:ND2	2.44	0.44
1:F:189:ASP:C	1:F:191:LYS:H	2.21	0.44
1:F:276:LYS:NZ	1:F:277:SER:HB2	2.33	0.44
1:F:405:PRO:C	1:F:407:THR:H	2.20	0.44
1:G:325:GLN:HE21	1:G:491:ARG:NH1	2.13	0.44
1:D:154:VAL:HA	1:D:457:PHE:HE2	1.83	0.44
1:E:36:PRO:HB3	1:E:69:TYR:HB2	1.99	0.44
1:E:183:VAL:HA	1:E:264:PHE:HB3	1.99	0.44
1:F:102:ALA:CB	1:F:218:GLU:HA	2.47	0.44
1:G:86:GLU:HA	1:G:90:ASP:OD2	2.18	0.44
1:G:298:ALA:HB2	3:G:501:1CI:H5	1.99	0.44
1:A:37:LEU:HD12	1:A:37:LEU:N	2.32	0.44
1:B:34:PRO:HG2	1:B:42:ASN:HD21	1.79	0.44
1:C:143:GLU:OE1	1:C:340:LEU:HB3	2.18	0.44
1:C:400:ARG:HG2	1:C:400:ARG:NH1	2.32	0.44
1:C:434:ARG:O	1:C:435:ILE:C	2.55	0.44
1:D:53:ARG:HA	1:D:53:ARG:NH1	2.21	0.44
1:D:429:PHE:CE2	1:D:439:GLU:HG3	2.53	0.44
1:D:487:ARG:HG2	1:D:487:ARG:NH1	2.31	0.44
1:E:277:SER:O	1:E:278:ASP:C	2.56	0.44
1:E:363:ILE:HG21	1:E:366:GLY:HA2	1.99	0.44
1:F:98:ARG:HG2	1:F:115:PHE:HA	2.00	0.44
1:F:99:GLY:H	1:F:368:PRO:C	2.20	0.44
1:A:284:HIS:O	1:A:285:HIS:C	2.55	0.44
1:C:31:PRO:HD2	1:C:67:THR:OG1	2.18	0.44
1:C:418:GLY:O	1:C:419:ALA:O	2.36	0.44
1:D:61:LYS:HD3	1:D:62:TYR:CE2	2.53	0.44
1:E:479:ASN:O	1:E:481:PRO:HD3	2.17	0.44
1:G:34:PRO:HG2	1:G:42:ASN:OD1	2.17	0.44
1:G:98:ARG:NH2	1:G:434:ARG:HD2	2.32	0.44
1:G:355:GLU:CD	1:G:358:ARG:HH21	2.21	0.44
1:A:68:VAL:HG12	1:A:75:VAL:HG22	2.00	0.44
1:A:136:GLY:HA3	1:A:145:ARG:NH1	2.33	0.44
1:B:339:ALA:O	1:B:342:ASP:HB2	2.18	0.44
1:C:176:SER:OG	1:C:296:PHE:HE1	2.00	0.44
1:D:325:GLN:NE2	1:D:491:ARG:NH1	2.66	0.44
1:F:93:GLU:HA	1:F:433:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:TRP:O	1:F:123:ALA:N	2.51	0.44
1:F:351:ALA:O	1:F:354:HIS:HB2	2.18	0.44
1:G:140:ARG:HB2	1:G:140:ARG:CZ	2.45	0.44
1:G:363:ILE:HG22	1:G:366:GLY:N	2.32	0.44
1:G:451:THR:O	1:G:455:GLN:N	2.46	0.44
1:B:202:PHE:CD1	1:B:297:PHE:HD1	2.36	0.44
1:B:249:VAL:HG11	1:B:288:LEU:HD21	1.98	0.44
1:C:364:PRO:HA	1:C:393:SER:HB2	1.98	0.44
1:C:369:HIS:O	1:C:388:VAL:N	2.49	0.44
1:D:111:TYR:N	1:D:111:TYR:CD1	2.86	0.44
1:D:225:LYS:C	1:D:227:PHE:N	2.71	0.44
1:D:239:GLN:OE1	1:D:239:GLN:HA	2.18	0.44
1:D:287:ASN:O	1:D:288:LEU:C	2.56	0.44
1:D:344:ALA:C	1:D:346:MET:H	2.20	0.44
1:E:365:PHE:O	1:E:366:GLY:O	2.36	0.44
2:F:500:HEM:NA	3:F:501:1CI:N3	2.65	0.44
1:G:378:ARG:HG3	1:G:378:ARG:O	2.17	0.44
1:A:81:THR:HG21	1:A:425:GLY:HA2	1.99	0.44
1:A:362:LEU:O	1:A:364:PRO:HD3	2.18	0.44
1:B:390:PRO:O	1:B:392:LEU:N	2.47	0.44
1:B:403:GLU:O	1:B:404:THR:HB	2.18	0.44
1:B:413:PHE:O	1:B:420:LEU:HA	2.17	0.44
1:C:86:GLU:HB3	1:C:377:PHE:CE1	2.53	0.44
1:C:135:PHE:CG	1:C:135:PHE:O	2.70	0.44
1:C:326:LYS:HG2	1:C:330:GLN:HE21	1.82	0.44
1:D:108:PHE:C	1:D:110:GLY:N	2.71	0.44
1:E:42:ASN:ND2	1:E:42:ASN:N	2.66	0.44
1:E:164:LEU:HG	1:E:487:ARG:CZ	2.48	0.44
1:E:308:ARG:HB3	1:E:308:ARG:NH1	2.31	0.44
1:F:141:SER:HB3	1:F:144:GLU:CG	2.36	0.44
1:F:183:VAL:HA	1:F:264:PHE:HB3	2.00	0.44
1:F:370:THR:HA	1:F:386:THR:O	2.18	0.44
1:F:373:LYS:C	1:F:375:THR:H	2.21	0.44
1:F:402:PHE:HZ	1:F:426:PHE:N	2.15	0.44
1:G:111:TYR:HB3	1:G:287:ASN:OD1	2.18	0.44
1:G:459:ILE:CG2	1:G:486:ILE:HD11	2.48	0.44
1:A:28:GLY:C	1:A:29:LYS:HG2	2.38	0.43
1:A:172:HIS:O	1:A:176:SER:HB2	2.17	0.43
1:A:332:ILE:HD13	1:A:338:PRO:HB3	2.00	0.43
1:A:409:ASN:C	1:A:411:GLY:H	2.21	0.43
1:B:30:LEU:HD22	1:B:383:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:CD1	1:B:234:ILE:HD13	2.35	0.43
1:B:427:MET:HG3	1:B:427:MET:O	2.18	0.43
1:C:104:VAL:HG11	1:C:209:ILE:HD13	2.00	0.43
1:C:154:VAL:HG12	1:C:158:ARG:HH12	1.83	0.43
1:C:171:PHE:CE2	1:C:307:LEU:HB3	2.52	0.43
1:C:360:GLY:O	1:C:361:ASP:C	2.56	0.43
1:C:476:GLY:C	1:C:478:GLY:H	2.21	0.43
1:D:231:HIS:CE1	1:D:232:ARG:HG2	2.52	0.43
1:F:79:CYS:O	1:F:83:ALA:HB3	2.17	0.43
1:F:116:ALA:O	1:F:434:ARG:NH2	2.37	0.43
1:F:320:VAL:HG22	1:F:348:TYR:OH	2.17	0.43
1:G:414:LEU:HD23	1:G:419:ALA:O	2.18	0.43
1:B:36:PRO:HG3	1:B:69:TYR:CD1	2.53	0.43
1:B:116:ALA:O	1:B:121:TRP:HB2	2.18	0.43
1:B:211:SER:HA	1:B:474:GLU:CD	2.39	0.43
1:B:213:SER:HA	1:C:228:PRO:HB3	2.00	0.43
1:B:487:ARG:HB3	1:B:487:ARG:NH1	2.33	0.43
1:C:269:LEU:O	1:C:272:MET:HB3	2.18	0.43
1:C:293:LEU:O	1:C:297:PHE:HB2	2.18	0.43
1:F:32:PRO:HD3	1:F:380:TYR:OH	2.18	0.43
1:F:465:PRO:C	1:F:467:ASP:H	2.20	0.43
1:G:197:ARG:HH21	1:G:240:GLU:CD	2.20	0.43
1:G:364:PRO:CG	1:G:479:ASN:ND2	2.80	0.43
1:B:249:VAL:HG11	1:B:288:LEU:CD2	2.48	0.43
1:C:30:LEU:HB3	1:C:31:PRO:CD	2.48	0.43
1:C:213:SER:O	1:C:216:VAL:HG12	2.18	0.43
1:E:328:ILE:HG12	1:E:346:MET:CE	2.49	0.43
1:F:140:ARG:HH22	1:F:148:GLU:CG	2.24	0.43
1:F:457:PHE:HA	1:F:489:LEU:O	2.19	0.43
1:F:479:ASN:O	1:F:481:PRO:HD3	2.18	0.43
1:B:285:HIS:O	1:B:288:LEU:N	2.22	0.43
1:B:368:PRO:HG3	1:B:389:PHE:CZ	2.53	0.43
1:C:52:LEU:C	1:C:54:SER:H	2.21	0.43
1:C:90:ASP:O	1:C:91:GLN:CG	2.61	0.43
1:D:87:ALA:HB2	1:D:377:PHE:CE1	2.53	0.43
1:D:143:GLU:O	1:D:147:GLN:HG3	2.19	0.43
1:D:441:ILE:HD12	1:D:441:ILE:N	2.30	0.43
1:E:113:VAL:O	1:E:113:VAL:CG2	2.66	0.43
1:F:39:VAL:C	1:F:41:GLY:H	2.22	0.43
1:F:411:GLY:C	1:F:413:PHE:N	2.72	0.43
1:B:50:GLY:O	1:B:54:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:C	1:B:144:GLU:H	2.20	0.43
1:B:153:LEU:CD2	1:B:174:ILE:HD13	2.45	0.43
1:C:139:LYS:HZ2	1:C:140:ARG:HD3	1.83	0.43
1:C:188:PHE:HB3	1:C:195:PHE:HB2	2.00	0.43
1:C:444:THR:HG22	1:C:448:LEU:HD12	2.00	0.43
1:D:308:ARG:CG	1:D:308:ARG:NH1	2.81	0.43
1:E:139:LYS:O	1:E:140:ARG:C	2.57	0.43
1:F:77:VAL:HG12	1:F:79:CYS:H	1.82	0.43
1:F:153:LEU:HD13	1:F:170:LEU:HD22	1.99	0.43
1:F:371:VAL:HG23	1:F:385:ASN:H	1.84	0.43
1:G:202:PHE:CD1	1:G:297:PHE:HD1	2.37	0.43
1:G:344:ALA:C	1:G:346:MET:N	2.71	0.43
1:A:191:LYS:HA	1:A:196:LEU:HD11	1.99	0.43
1:A:316:LYS:HD3	1:A:317:TYR:CE1	2.54	0.43
1:B:53:ARG:HH11	1:B:53:ARG:CA	2.26	0.43
1:C:127:PHE:CZ	1:C:267:VAL:HG12	2.54	0.43
1:C:401:TYR:CE2	1:C:424:GLU:HB2	2.54	0.43
1:D:141:SER:C	1:D:143:GLU:N	2.70	0.43
1:D:427:MET:CE	1:D:431:LEU:HD21	2.48	0.43
1:E:49:LYS:HG2	1:E:49:LYS:O	2.18	0.43
1:E:114:ILE:CD1	1:E:114:ILE:N	2.81	0.43
1:E:441:ILE:O	1:E:445:GLU:HG3	2.17	0.43
1:F:68:VAL:O	1:F:75:VAL:HG22	2.19	0.43
1:F:331:VAL:HG11	1:F:345:LYS:HB2	2.01	0.43
1:G:455:GLN:O	1:G:455:GLN:HG2	2.19	0.43
1:A:338:PRO:HD2	1:A:452:THR:OG1	2.18	0.43
1:A:407:THR:O	1:A:408:PHE:C	2.55	0.43
1:C:183:VAL:HA	1:C:264:PHE:HB3	2.01	0.43
1:C:184:PHE:CD1	1:C:265:ILE:HD11	2.54	0.43
1:C:348:TYR:O	1:C:352:VAL:HG23	2.18	0.43
1:D:98:ARG:HD3	1:D:368:PRO:O	2.18	0.43
1:D:179:ILE:HD13	1:D:179:ILE:O	2.19	0.43
1:D:226:TYR:O	1:E:216:VAL:HG21	2.18	0.43
1:E:284:HIS:NE2	1:E:287:ASN:ND2	2.66	0.43
1:F:38:PRO:O	1:F:39:VAL:HB	2.19	0.43
1:F:170:LEU:O	1:F:173:SER:N	2.51	0.43
1:F:189:ASP:O	1:F:191:LYS:N	2.51	0.43
1:G:373:LYS:HA	1:G:384:LYS:HB2	2.00	0.43
1:A:108:PHE:HA	1:A:290:LEU:HD13	2.01	0.43
1:B:312:LEU:CD2	1:B:470:LEU:HD23	2.48	0.43
1:B:487:ARG:CB	1:B:487:ARG:HH11	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:THR:HG23	1:C:267:VAL:HG11	2.01	0.43
1:D:78:LEU:O	1:D:84:ILE:HD11	2.19	0.43
1:E:172:HIS:O	1:E:176:SER:HB3	2.19	0.43
1:E:268:TYR:CG	1:E:288:LEU:HD13	2.54	0.43
1:F:85:ARG:O	1:F:86:GLU:C	2.57	0.43
1:G:98:ARG:NH1	1:G:367:VAL:HB	2.34	0.43
1:G:169:LEU:HD11	1:G:196:LEU:CD2	2.49	0.43
1:G:268:TYR:CZ	1:G:288:LEU:HB2	2.54	0.43
1:A:320:VAL:HG21	1:A:408:PHE:CE2	2.54	0.43
1:B:134:ASP:O	1:B:135:PHE:CB	2.66	0.43
1:B:158:ARG:HG3	1:B:158:ARG:NH1	2.31	0.43
1:B:290:LEU:O	1:B:293:LEU:HB3	2.19	0.43
1:B:402:PHE:O	1:B:405:PRO:HD3	2.19	0.43
1:C:363:ILE:HG22	1:C:363:ILE:O	2.18	0.43
1:D:42:ASN:OD1	1:D:68:VAL:HA	2.19	0.43
1:D:111:TYR:HB2	1:D:290:LEU:CD1	2.48	0.43
1:D:365:PHE:HA	1:D:391:VAL:HA	2.00	0.43
1:E:34:PRO:CG	1:E:45:GLN:HG2	2.49	0.43
1:E:101:ILE:HG22	1:E:104:VAL:HG22	2.01	0.43
1:E:117:ASN:O	1:E:120:ARG:HB3	2.19	0.43
1:E:244:PHE:CD1	1:E:244:PHE:C	2.91	0.43
1:E:402:PHE:HZ	1:E:426:PHE:N	2.17	0.43
1:E:430:SER:HB3	2:E:500:HEM:HBA1	2.00	0.43
1:F:327:GLU:CD	1:F:346:MET:HA	2.39	0.43
1:G:305:THR:HA	1:G:308:ARG:HB2	2.01	0.43
1:A:66:PHE:CE1	1:A:77:VAL:HB	2.54	0.43
1:A:116:ALA:HB1	1:A:120:ARG:HG2	2.00	0.43
1:A:126:ARG:HH21	1:A:126:ARG:HG2	1.84	0.43
1:A:140:ARG:O	1:A:141:SER:C	2.57	0.43
1:A:178:ILE:O	1:A:182:ILE:HD13	2.19	0.43
1:B:249:VAL:O	1:B:249:VAL:HG12	2.17	0.43
1:B:370:THR:HA	1:B:386:THR:O	2.19	0.43
1:D:156:GLU:HG2	1:D:190:TYR:HD2	1.83	0.43
1:E:158:ARG:HG3	1:E:158:ARG:NH1	2.31	0.43
1:E:349:THR:O	1:E:353:ILE:HG13	2.17	0.43
1:F:311:PHE:CD1	1:F:459:ILE:HG21	2.53	0.43
1:G:31:PRO:HB3	1:G:32:PRO:HD2	2.01	0.43
1:G:34:PRO:HD3	1:G:62:TYR:CE2	2.54	0.43
1:G:93:GLU:OE1	1:G:433:LYS:HE3	2.19	0.43
1:G:174:ILE:HD12	1:G:449:PHE:CE2	2.54	0.43
1:G:250:GLU:HA	1:G:250:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:SER:O	1:G:278:ASP:C	2.57	0.43
1:G:390:PRO:O	1:G:392:LEU:N	2.51	0.43
1:A:142:VAL:O	1:A:145:ARG:HB2	2.19	0.42
1:B:53:ARG:NH1	1:B:53:ARG:HB2	2.33	0.42
1:B:147:GLN:O	1:B:150:ALA:HB3	2.19	0.42
1:B:176:SER:HB2	1:B:300:THR:HG23	2.00	0.42
1:C:188:PHE:CZ	1:C:244:PHE:HZ	2.37	0.42
1:C:217:PHE:CE1	1:C:221:SER:HA	2.54	0.42
1:C:320:VAL:HG11	1:C:408:PHE:HE2	1.84	0.42
1:D:43:LEU:HG	1:F:226:TYR:CE2	2.54	0.42
1:D:235:TYR:CD2	1:E:48:ARG:NH2	2.86	0.42
1:E:29:LYS:O	1:E:30:LEU:HD12	2.19	0.42
1:E:91:GLN:O	1:E:93:GLU:N	2.52	0.42
1:E:309:TYR:HE2	1:E:313:LEU:HD12	1.84	0.42
1:F:203:PHE:C	1:F:205:SER:H	2.23	0.42
1:F:369:HIS:HE1	2:F:500:HEM:O2A	2.02	0.42
1:B:34:PRO:O	1:B:36:PRO:HD3	2.19	0.42
1:B:102:ALA:CB	1:B:218:GLU:HA	2.47	0.42
1:B:215:GLN:NE2	1:B:476:GLY:HA3	2.34	0.42
1:B:391:VAL:HG12	1:B:391:VAL:O	2.18	0.42
1:C:151:ARG:HG2	1:C:151:ARG:NH1	2.34	0.42
1:D:48:ARG:NH2	1:F:235:TYR:CG	2.87	0.42
1:D:471:THR:HA	1:D:472:PRO:HD3	1.92	0.42
1:E:119:GLU:HA	1:E:122:ARG:HD3	2.01	0.42
1:E:271:ARG:HG3	1:E:272:MET:CE	2.49	0.42
1:F:52:LEU:C	1:F:54:SER:N	2.72	0.42
1:F:399:PRO:HA	1:F:402:PHE:O	2.20	0.42
1:G:118:GLY:O	1:G:119:GLU:C	2.58	0.42
1:G:137:MET:CG	1:G:138:GLY:H	2.25	0.42
1:G:298:ALA:C	1:G:300:THR:N	2.72	0.42
1:A:213:SER:O	1:A:215:GLN:N	2.51	0.42
1:A:325:GLN:NE2	1:A:491:ARG:NH1	2.67	0.42
1:B:275:ASP:O	1:B:276:LYS:C	2.57	0.42
1:B:407:THR:O	1:B:408:PHE:C	2.58	0.42
1:C:103:VAL:HG22	1:C:217:PHE:CD2	2.54	0.42
1:C:215:GLN:NE2	1:C:476:GLY:CA	2.82	0.42
1:D:411:GLY:O	1:D:412:HIS:HB2	2.19	0.42
1:D:459:ILE:HG22	1:D:488:PHE:CE1	2.54	0.42
1:E:111:TYR:CD2	1:E:287:ASN:ND2	2.87	0.42
1:E:119:GLU:HA	1:E:122:ARG:HH11	1.84	0.42
1:F:164:LEU:HG	1:F:487:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:ILE:HG22	1:F:386:THR:HB	2.02	0.42
1:G:176:SER:O	1:G:179:ILE:HG22	2.19	0.42
1:A:38:PRO:O	1:A:40:LEU:N	2.46	0.42
1:A:111:TYR:CB	1:A:290:LEU:HD12	2.32	0.42
1:A:223:PHE:C	1:A:223:PHE:HD2	2.23	0.42
1:B:96:SER:HB3	1:B:372:THR:CG2	2.49	0.42
1:C:407:THR:HG22	1:C:408:PHE:N	2.35	0.42
1:C:471:THR:O	1:C:482:PRO:HD3	2.20	0.42
1:D:132:MET:O	1:D:134:ASP:N	2.38	0.42
1:D:168:THR:HG22	1:D:169:LEU:N	2.33	0.42
1:D:371:VAL:C	1:D:373:LYS:H	2.22	0.42
1:E:114:ILE:HD11	2:E:500:HEM:HMD2	2.00	0.42
1:E:122:ARG:C	1:E:126:ARG:HD3	2.39	0.42
1:E:275:ASP:C	1:E:277:SER:N	2.71	0.42
1:F:30:LEU:HD23	1:F:30:LEU:N	2.35	0.42
1:F:203:PHE:O	1:F:205:SER:N	2.52	0.42
1:F:309:TYR:CZ	1:F:360:GLY:HA2	2.54	0.42
1:G:69:TYR:HA	1:G:74:PRO:HA	2.00	0.42
1:A:103:VAL:HG23	1:A:104:VAL:HG13	2.00	0.42
1:A:281:SER:C	1:A:283:PHE:H	2.23	0.42
1:B:266:ASP:O	1:B:270:LEU:HG	2.19	0.42
1:B:269:LEU:HD23	1:B:272:MET:HE1	2.01	0.42
1:C:30:LEU:HD21	1:C:383:PRO:CD	2.49	0.42
1:C:203:PHE:CZ	1:C:473:ARG:NH2	2.87	0.42
1:C:404:THR:HG23	1:C:404:THR:O	2.19	0.42
1:D:114:ILE:HG22	1:D:115:PHE:CG	2.54	0.42
1:D:176:SER:O	1:D:180:CYS:CB	2.67	0.42
1:D:233:GLN:NE2	1:D:237:ASN:OD1	2.52	0.42
1:D:244:PHE:CD1	1:D:244:PHE:C	2.93	0.42
1:E:241:ILE:C	1:E:243:THR:N	2.73	0.42
1:F:198:LEU:CD2	1:F:198:LEU:N	2.82	0.42
1:F:310:GLY:HA3	1:F:356:ILE:HD13	2.02	0.42
1:G:43:LEU:HD22	1:G:220:PHE:CZ	2.54	0.42
1:G:323:ARG:HB2	1:G:348:TYR:CE2	2.54	0.42
1:A:134:ASP:OD1	1:A:134:ASP:O	2.37	0.42
1:B:355:GLU:OE2	1:B:358:ARG:NE	2.53	0.42
1:B:398:ASP:OD2	1:B:401:TYR:CD1	2.72	0.42
1:B:471:THR:HA	1:B:472:PRO:HD3	1.89	0.42
1:C:87:ALA:O	1:C:95:PHE:HB2	2.20	0.42
1:C:443:ARG:HH11	1:C:443:ARG:CG	2.26	0.42
1:E:28:GLY:HA3	1:E:381:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:LEU:HD21	1:E:369:HIS:CE1	2.54	0.42
1:E:121:TRP:NE1	1:E:125:ARG:HD2	2.34	0.42
1:E:198:LEU:HD21	1:E:244:PHE:CD2	2.54	0.42
1:F:283:PHE:H	1:F:283:PHE:HD1	1.67	0.42
1:F:373:LYS:HG3	1:F:375:THR:OG1	2.20	0.42
1:G:365:PHE:CE1	1:G:477:VAL:HA	2.54	0.42
1:G:388:VAL:HG12	1:G:389:PHE:N	2.35	0.42
1:A:137:MET:CE	1:A:441:ILE:HD11	2.50	0.42
1:A:153:LEU:HD22	1:A:174:ILE:CD1	2.41	0.42
1:B:268:TYR:CG	1:B:288:LEU:HD13	2.55	0.42
1:C:246:GLY:HA2	1:C:289:ILE:HD11	2.01	0.42
1:C:314:MET:HB3	1:C:459:ILE:HD11	2.01	0.42
1:C:392:LEU:O	1:C:395:ALA:HB3	2.19	0.42
1:C:401:TYR:HB3	1:C:423:ASN:OD1	2.20	0.42
1:D:238:LEU:O	1:D:242:ASN:ND2	2.53	0.42
1:D:369:HIS:O	1:D:387:GLU:HA	2.19	0.42
1:E:348:TYR:O	1:E:352:VAL:HG23	2.18	0.42
1:F:53:ARG:HG3	1:F:53:ARG:O	2.20	0.42
1:G:95:PHE:C	1:G:97:GLY:N	2.72	0.42
1:G:153:LEU:HD13	1:G:170:LEU:HD22	2.02	0.42
1:G:313:LEU:O	1:G:316:LYS:N	2.53	0.42
2:G:500:HEM:NC	3:G:501:1CI:H4	2.34	0.42
1:A:38:PRO:O	1:A:39:VAL:HB	2.18	0.42
1:A:139:LYS:O	1:A:140:ARG:HB2	2.20	0.42
1:A:437:LEU:O	1:A:437:LEU:HD23	2.20	0.42
1:B:284:HIS:O	1:B:284:HIS:ND1	2.52	0.42
1:C:270:LEU:C	1:C:272:MET:H	2.23	0.42
1:C:416:ALA:HB3	1:G:267:VAL:HG11	2.01	0.42
1:E:268:TYR:CE1	1:E:272:MET:SD	3.13	0.42
1:G:402:PHE:CD1	1:G:412:HIS:HD2	2.38	0.42
1:G:454:LEU:HA	1:G:454:LEU:HD23	1.85	0.42
1:A:183:VAL:HA	1:A:264:PHE:CB	2.50	0.42
1:A:215:GLN:C	1:A:217:PHE:N	2.72	0.42
1:A:489:LEU:HD12	1:A:489:LEU:H	1.84	0.42
1:B:42:ASN:O	1:B:46:MET:HG2	2.20	0.42
1:B:90:ASP:O	1:B:91:GLN:HG3	2.20	0.42
1:C:69:TYR:CE2	1:C:74:PRO:HB3	2.55	0.42
1:C:139:LYS:HZ3	1:C:143:GLU:CD	2.22	0.42
1:C:319:HIS:ND1	1:C:320:VAL:HG23	2.34	0.42
1:C:371:VAL:HG23	1:C:371:VAL:O	2.19	0.42
1:D:44:LEU:HB2	1:D:45:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LYS:HE2	1:D:53:ARG:HG2	2.02	0.42
1:D:121:TRP:HZ2	1:D:125:ARG:HH11	1.68	0.42
1:E:82:ASP:O	1:E:85:ARG:HB2	2.20	0.42
1:E:104:VAL:O	1:E:105:ASP:C	2.58	0.42
1:E:328:ILE:HG12	1:E:346:MET:HE3	2.02	0.42
1:F:98:ARG:HD3	1:F:368:PRO:O	2.20	0.42
1:F:286:GLN:O	1:F:287:ASN:C	2.58	0.42
1:F:322:GLU:O	1:F:326:LYS:HB2	2.20	0.42
1:G:59:ARG:NH1	1:G:394:SER:HB2	2.35	0.42
1:G:204:GLN:O	1:G:208:LEU:HG	2.20	0.42
1:G:353:ILE:CD1	1:G:447:PHE:HA	2.50	0.42
1:A:143:GLU:O	1:A:147:GLN:HG3	2.19	0.42
1:A:473:ARG:NH2	1:A:480:VAL:HG11	2.34	0.42
1:B:364:PRO:HA	1:B:393:SER:HB2	2.02	0.42
1:D:272:MET:HG3	1:D:283:PHE:O	2.20	0.42
1:E:34:PRO:CB	1:E:45:GLN:HG2	2.50	0.42
1:E:168:THR:HA	1:E:308:ARG:HD3	2.00	0.42
1:E:226:TYR:CD1	1:F:43:LEU:HD21	2.55	0.42
1:F:239:GLN:HA	1:F:239:GLN:OE1	2.19	0.42
1:F:466:GLU:OE1	1:F:466:GLU:N	2.53	0.42
1:G:82:ASP:O	1:G:84:ILE:N	2.53	0.42
1:G:221:SER:O	1:G:223:PHE:N	2.53	0.42
1:A:487:ARG:HG3	1:A:489:LEU:CD1	2.49	0.41
1:C:403:GLU:O	1:C:404:THR:HG22	2.20	0.41
1:D:164:LEU:CD2	1:D:485:GLN:HB3	2.41	0.41
1:D:166:ASP:O	1:D:168:THR:N	2.53	0.41
1:D:299:GLY:HA2	2:D:500:HEM:CMC	2.49	0.41
1:D:325:GLN:NE2	1:D:491:ARG:HH12	2.18	0.41
1:E:37:LEU:HD12	1:E:37:LEU:H	1.84	0.41
1:E:158:ARG:C	1:E:160:SER:H	2.23	0.41
1:E:323:ARG:HB3	1:E:348:TYR:CE2	2.55	0.41
1:G:64:ASP:O	1:G:66:PHE:HD1	2.03	0.41
1:G:243:THR:O	1:G:247:GLN:HG2	2.19	0.41
1:G:266:ASP:O	1:G:270:LEU:HG	2.19	0.41
1:G:299:GLY:HA2	2:G:500:HEM:HMC2	2.02	0.41
1:B:362:LEU:C	1:B:363:ILE:HG13	2.40	0.41
1:C:403:GLU:O	1:C:403:GLU:HG3	2.20	0.41
1:D:141:SER:C	1:D:143:GLU:H	2.24	0.41
1:D:183:VAL:HA	1:D:264:PHE:HB3	2.02	0.41
1:F:98:ARG:O	1:F:99:GLY:O	2.39	0.41
1:F:364:PRO:HD2	1:F:477:VAL:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ASN:HD22	1:G:42:ASN:N	2.18	0.41
1:G:82:ASP:C	1:G:84:ILE:N	2.72	0.41
1:A:28:GLY:O	1:A:29:LYS:CG	2.65	0.41
1:A:118:GLY:O	1:A:122:ARG:HD2	2.20	0.41
1:A:363:ILE:HD12	1:A:363:ILE:N	2.35	0.41
1:B:125:ARG:HG3	1:B:125:ARG:HH11	1.85	0.41
1:B:305:THR:HG22	1:B:308:ARG:NH2	2.27	0.41
1:C:52:LEU:C	1:C:54:SER:N	2.72	0.41
1:C:133:ARG:HB3	1:C:134:ASP:H	1.74	0.41
1:D:51:LEU:O	1:D:54:SER:HB2	2.20	0.41
1:E:63:GLY:O	1:E:66:PHE:HD1	2.03	0.41
1:E:111:TYR:HD2	1:E:287:ASN:ND2	2.17	0.41
1:E:464:PRO:HA	1:E:465:PRO:HD3	1.88	0.41
1:F:119:GLU:C	1:F:121:TRP:N	2.73	0.41
1:F:362:LEU:H	1:F:362:LEU:CD2	2.32	0.41
1:F:430:SER:O	1:F:431:LEU:HD23	2.20	0.41
1:G:114:ILE:CD1	1:G:294:SER:HB3	2.50	0.41
1:G:134:ASP:O	1:G:135:PHE:C	2.58	0.41
1:G:138:GLY:CA	1:G:145:ARG:HE	2.32	0.41
1:G:169:LEU:HD11	1:G:196:LEU:HD23	2.02	0.41
1:A:31:PRO:HG3	1:A:380:TYR:CG	2.55	0.41
1:A:457:PHE:HD1	1:A:490:ALA:HA	1.84	0.41
1:B:62:TYR:CB	1:B:66:PHE:HB3	2.50	0.41
1:B:146:ILE:CG2	1:B:448:LEU:HD12	2.50	0.41
1:B:194:VAL:O	1:B:197:ARG:HB3	2.21	0.41
1:B:332:ILE:HD13	1:B:338:PRO:HG3	2.02	0.41
1:C:320:VAL:O	1:C:320:VAL:HG12	2.20	0.41
1:D:399:PRO:C	1:D:401:TYR:N	2.74	0.41
1:E:355:GLU:CD	1:E:358:ARG:HH21	2.23	0.41
1:E:428:PRO:HG2	1:E:429:PHE:CD2	2.54	0.41
1:F:87:ALA:O	1:F:95:PHE:CD2	2.74	0.41
1:F:344:ALA:O	1:F:346:MET:N	2.54	0.41
1:G:198:LEU:HD21	1:G:244:PHE:CD2	2.54	0.41
1:G:449:PHE:O	1:G:453:ILE:HG13	2.19	0.41
1:A:145:ARG:O	1:A:148:GLU:HB3	2.21	0.41
1:A:409:ASN:C	1:A:411:GLY:N	2.73	0.41
1:C:52:LEU:HD22	1:C:364:PRO:CB	2.42	0.41
1:E:108:PHE:O	1:E:109:GLN:HB2	2.21	0.41
1:E:212:PHE:CD1	1:E:212:PHE:C	2.93	0.41
1:E:457:PHE:O	1:E:491:ARG:HD2	2.20	0.41
1:F:78:LEU:HD11	1:F:388:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:PHE:C	1:F:205:SER:N	2.74	0.41
1:F:209:ILE:HG22	1:F:209:ILE:O	2.20	0.41
1:F:429:PHE:HB3	1:F:436:CYS:CB	2.50	0.41
1:G:171:PHE:HE2	1:G:307:LEU:HB3	1.84	0.41
1:B:28:GLY:O	1:B:29:LYS:O	2.38	0.41
1:B:121:TRP:C	1:B:123:ALA:N	2.73	0.41
1:G:102:ALA:HB2	1:G:218:GLU:HA	2.02	0.41
1:G:409:ASN:O	1:G:411:GLY:N	2.53	0.41
1:A:122:ARG:H	1:A:122:ARG:HD2	1.85	0.41
1:A:244:PHE:C	1:A:244:PHE:CD1	2.93	0.41
1:B:101:ILE:O	1:B:102:ALA:C	2.58	0.41
1:C:213:SER:HA	1:C:216:VAL:HG12	2.02	0.41
1:C:223:PHE:HD2	1:C:223:PHE:O	2.03	0.41
1:D:177:ASN:HA	1:D:180:CYS:HB3	2.02	0.41
1:D:189:ASP:C	1:D:191:LYS:N	2.74	0.41
1:E:93:GLU:O	1:E:94:ALA:C	2.58	0.41
1:E:299:GLY:HA2	2:E:500:HEM:CMC	2.50	0.41
1:E:302:THR:HB	2:E:500:HEM:HAB	2.02	0.41
1:F:154:VAL:HG13	1:F:457:PHE:CZ	2.55	0.41
1:F:432:GLY:C	1:F:434:ARG:H	2.24	0.41
1:F:460:ALA:O	1:F:487:ARG:HG2	2.20	0.41
1:G:73:ARG:NH1	1:G:73:ARG:CB	2.83	0.41
1:G:81:THR:HG23	1:G:425:GLY:HA2	2.03	0.41
1:G:125:ARG:HH12	1:G:437:LEU:HB2	1.85	0.41
1:G:162:GLY:O	1:G:487:ARG:HD3	2.21	0.41
1:G:336:ARG:HB2	1:G:337:PRO:CD	2.50	0.41
1:G:461:SER:HB2	1:G:462:PRO:CD	2.46	0.41
1:A:213:SER:O	1:A:217:PHE:HB2	2.20	0.41
1:A:439:GLU:O	1:A:443:ARG:HG3	2.21	0.41
1:B:38:PRO:C	1:B:40:LEU:H	2.24	0.41
1:B:320:VAL:O	1:B:324:VAL:HG23	2.21	0.41
1:C:34:PRO:N	1:C:62:TYR:HE1	2.19	0.41
1:C:101:ILE:CG2	1:C:104:VAL:HG22	2.50	0.41
1:C:278:ASP:OD1	1:C:279:PRO:HD2	2.20	0.41
1:C:443:ARG:CG	1:C:443:ARG:NH1	2.82	0.41
1:D:162:GLY:O	1:D:487:ARG:NH1	2.54	0.41
1:D:179:ILE:HD12	1:D:296:PHE:HA	2.02	0.41
1:D:232:ARG:NE	1:E:212:PHE:CE2	2.89	0.41
1:D:447:PHE:O	1:D:448:LEU:C	2.59	0.41
1:E:69:TYR:CE1	1:E:74:PRO:HB3	2.56	0.41
1:E:103:VAL:HG21	1:E:214:SER:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:HIS:ND1	1:E:231:HIS:C	2.73	0.41
1:F:411:GLY:O	1:F:413:PHE:N	2.54	0.41
1:G:31:PRO:CB	1:G:66:PHE:HA	2.51	0.41
1:G:111:TYR:CD1	1:G:111:TYR:N	2.89	0.41
1:A:75:VAL:HG21	1:A:389:PHE:HD1	1.85	0.41
1:A:180:CYS:O	1:A:185:GLY:N	2.54	0.41
1:A:202:PHE:CD1	1:A:297:PHE:CD1	3.09	0.41
1:A:404:THR:HG23	1:A:412:HIS:NE2	2.36	0.41
1:B:138:GLY:O	1:B:139:LYS:HB2	2.20	0.41
1:B:355:GLU:OE2	1:B:358:ARG:NH2	2.53	0.41
1:B:358:ARG:HG2	1:B:358:ARG:NH1	2.34	0.41
1:B:358:ARG:HA	1:B:396:LEU:HD22	2.02	0.41
1:B:397:HIS:HD2	1:B:405:PRO:O	2.03	0.41
1:C:252:HIS:CD2	1:C:265:ILE:HD12	2.55	0.41
1:C:324:VAL:O	1:C:328:ILE:HG13	2.20	0.41
1:D:121:TRP:HZ2	1:D:125:ARG:NH1	2.19	0.41
1:D:129:LEU:CB	1:D:437:LEU:HD11	2.48	0.41
1:D:155:GLU:CA	1:D:158:ARG:HG3	2.51	0.41
1:D:247:GLN:O	1:D:250:GLU:N	2.53	0.41
1:E:47:ASP:HB2	1:E:57:ARG:HD3	2.03	0.41
1:E:48:ARG:HG3	1:E:48:ARG:NH1	2.36	0.41
1:E:61:LYS:O	1:E:61:LYS:HG2	2.21	0.41
1:E:154:VAL:HG12	1:E:158:ARG:NH1	2.36	0.41
1:E:324:VAL:C	1:E:326:LYS:H	2.24	0.41
1:E:361:ASP:OD1	1:E:364:PRO:HA	2.21	0.41
1:F:212:PHE:O	1:F:216:VAL:HG12	2.20	0.41
1:F:220:PHE:O	1:F:224:LEU:HG	2.20	0.41
1:F:249:VAL:HG21	1:F:288:LEU:CD2	2.45	0.41
1:G:256:LEU:O	1:G:258:PRO:HD3	2.21	0.41
1:G:350:ASP:O	1:G:354:HIS:ND1	2.53	0.41
1:A:457:PHE:CD1	1:A:490:ALA:HA	2.56	0.41
1:B:111:TYR:HD2	1:B:286:GLN:HB3	1.86	0.41
1:B:131:THR:HG23	1:B:132:MET:N	2.35	0.41
1:B:256:LEU:HD21	1:B:270:LEU:HD23	2.03	0.41
1:C:355:GLU:HA	1:C:355:GLU:OE1	2.21	0.41
1:D:179:ILE:CD1	1:D:296:PHE:HA	2.51	0.41
1:E:315:LEU:HD23	1:E:459:ILE:HD12	2.02	0.41
1:F:156:GLU:HG2	1:F:190:TYR:CD2	2.56	0.41
1:F:198:LEU:N	1:F:198:LEU:HD22	2.36	0.41
1:F:308:ARG:HG2	1:F:308:ARG:HH11	1.86	0.41
1:F:477:VAL:O	1:F:477:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.21	0.40
1:B:114:ILE:HG13	1:B:294:SER:HB3	2.04	0.40
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.85	0.40
1:B:487:ARG:NH2	1:E:162:GLY:O	2.54	0.40
1:C:120:ARG:HD3	1:C:287:ASN:OD1	2.21	0.40
1:C:142:VAL:HA	1:C:145:ARG:HG3	2.03	0.40
1:C:250:GLU:HA	1:C:250:GLU:OE2	2.20	0.40
1:C:273:GLU:O	1:C:276:LYS:HE3	2.22	0.40
1:F:69:TYR:HA	1:F:74:PRO:HA	2.02	0.40
1:F:94:ALA:HA	1:F:372:THR:OG1	2.21	0.40
1:F:325:GLN:HA	1:F:328:ILE:HD12	2.02	0.40
1:G:400:ARG:CZ	1:G:400:ARG:HB3	2.51	0.40
1:A:311:PHE:HD1	1:A:459:ILE:HG21	1.86	0.40
1:B:210:SER:HA	1:B:477:VAL:HG12	2.04	0.40
1:B:257:ASP:O	1:B:259:SER:N	2.55	0.40
1:B:284:HIS:CE1	1:B:287:ASN:ND2	2.89	0.40
1:B:367:VAL:O	1:B:368:PRO:C	2.60	0.40
1:B:430:SER:HB3	2:B:500:HEM:HBA1	2.03	0.40
1:C:125:ARG:HH11	1:C:125:ARG:HG3	1.86	0.40
1:C:230:THR:O	1:C:233:GLN:N	2.54	0.40
1:D:28:GLY:O	1:D:29:LYS:O	2.39	0.40
1:D:88:LEU:HD12	1:D:431:LEU:HD12	2.02	0.40
1:D:216:VAL:HG22	1:D:216:VAL:O	2.21	0.40
1:D:316:LYS:HA	1:D:465:PRO:HA	2.03	0.40
1:E:323:ARG:O	1:E:326:LYS:HB3	2.21	0.40
1:E:463:VAL:HA	1:E:464:PRO:HD3	1.93	0.40
1:F:35:SER:O	1:F:37:LEU:HD12	2.20	0.40
1:F:216:VAL:HG22	1:F:224:LEU:CD1	2.52	0.40
1:F:317:TYR:N	1:F:317:TYR:CD1	2.88	0.40
1:G:108:PHE:O	1:G:109:GLN:HB2	2.21	0.40
1:G:170:LEU:O	1:G:173:SER:HB2	2.22	0.40
1:A:283:PHE:N	1:A:283:PHE:CD1	2.87	0.40
1:A:288:LEU:O	1:A:292:VAL:HG23	2.20	0.40
1:B:186:LYS:CD	1:B:186:LYS:N	2.84	0.40
1:B:421:LYS:HE2	1:B:421:LYS:HB3	1.92	0.40
1:C:113:VAL:HB	1:C:291:THR:HG23	2.03	0.40
1:C:114:ILE:HG13	1:C:294:SER:HB3	2.04	0.40
1:C:370:THR:HG23	1:C:386:THR:H	1.87	0.40
1:D:43:LEU:C	1:D:45:GLN:H	2.25	0.40
1:F:284:HIS:O	1:F:285:HIS:C	2.60	0.40
1:F:441:ILE:H	1:F:441:ILE:HG13	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:ARG:HG2	1:G:49:LYS:N	2.36	0.40
1:G:125:ARG:HG3	1:G:437:LEU:HD13	2.02	0.40
1:G:298:ALA:O	1:G:300:THR:N	2.55	0.40
1:G:372:THR:O	1:G:373:LYS:CB	2.69	0.40
1:G:423:ASN:C	1:G:425:GLY:N	2.74	0.40
1:B:48:ARG:NH2	1:C:235:TYR:CG	2.90	0.40
1:B:201:LEU:HB3	1:B:241:ILE:HD11	2.03	0.40
1:C:192:ASP:HA	1:C:193:PRO:HD3	1.94	0.40
1:C:337:PRO:HA	1:C:338:PRO:HD3	1.94	0.40
1:C:445:GLU:HB3	1:C:449:PHE:CE2	2.56	0.40
1:D:103:VAL:HG11	1:D:214:SER:HB3	2.03	0.40
1:E:133:ARG:NH2	1:E:141:SER:HB2	2.37	0.40
1:E:189:ASP:HB3	1:E:192:ASP:HB2	2.03	0.40
1:F:81:THR:HG23	1:F:425:GLY:HA2	2.03	0.40
1:F:96:SER:HB2	1:F:121:TRP:HZ3	1.85	0.40
1:F:215:GLN:NE2	1:F:476:GLY:HA2	2.37	0.40
1:G:298:ALA:HB1	3:G:501:1CI:C4	2.50	0.40
1:A:180:CYS:SG	1:A:296:PHE:CE1	3.15	0.40
1:B:95:PHE:O	1:B:369:HIS:HD2	2.04	0.40
1:B:403:GLU:O	1:B:404:THR:CB	2.70	0.40
1:C:140:ARG:H	1:C:143:GLU:CB	2.34	0.40
1:C:166:ASP:C	1:C:168:THR:N	2.75	0.40
1:C:223:PHE:C	1:C:223:PHE:HD2	2.25	0.40
1:D:226:TYR:OH	1:E:44:LEU:HD23	2.22	0.40
1:E:125:ARG:NH2	1:E:435:ILE:O	2.55	0.40
1:E:245:ILE:HG22	1:E:289:ILE:CD1	2.51	0.40
1:F:97:GLY:HA3	1:F:370:THR:OG1	2.22	0.40
1:F:151:ARG:HG2	1:F:151:ARG:HH11	1.87	0.40
1:G:42:ASN:H	1:G:69:TYR:HB2	1.87	0.40
1:G:87:ALA:HB1	1:G:95:PHE:CZ	2.57	0.40
1:G:116:ALA:HB1	1:G:120:ARG:CD	2.51	0.40
1:G:119:GLU:HA	1:G:122:ARG:HH11	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/478 (97%)	380 (82%)	60 (13%)	23 (5%)	2	16
1	B	463/478 (97%)	365 (79%)	76 (16%)	22 (5%)	2	17
1	C	463/478 (97%)	356 (77%)	80 (17%)	27 (6%)	1	13
1	D	463/478 (97%)	360 (78%)	82 (18%)	21 (4%)	2	18
1	E	463/478 (97%)	366 (79%)	69 (15%)	28 (6%)	1	12
1	F	463/478 (97%)	327 (71%)	97 (21%)	39 (8%)	1	5
1	G	463/478 (97%)	339 (73%)	88 (19%)	36 (8%)	1	6
All	All	3241/3346 (97%)	2493 (77%)	552 (17%)	196 (6%)	1	12

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	102	ALA
1	A	137	MET
1	A	255	THR
1	A	285	HIS
1	A	334	SER
1	A	366	GLY
1	A	391	VAL
1	B	29	LYS
1	B	133	ARG
1	B	137	MET
1	B	285	HIS
1	B	286	GLN
1	B	334	SER
1	B	404	THR
1	C	29	LYS
1	C	91	GLN
1	C	285	HIS
1	C	301	GLU
1	C	391	VAL
1	C	419	ALA
1	D	29	LYS
1	D	167	ASN
1	D	285	HIS

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Mol	Chain	Res	Type
1	D	336	ARG
1	E	301	GLU
1	E	391	VAL
1	F	79	CYS
1	F	86	GLU
1	F	91	GLN
1	F	140	ARG
1	F	286	GLN
1	F	391	VAL
1	G	48	ARG
1	G	64	ASP
1	G	102	ALA
1	G	286	GLN
1	G	373	LYS
1	G	391	VAL
1	G	415	ASP
1	A	64	ASP
1	A	92	ALA
1	A	118	GLY
1	A	138	GLY
1	A	331	VAL
1	A	430	SER
1	B	102	ALA
1	B	368	PRO
1	C	39	VAL
1	C	41	GLY
1	C	116	ALA
1	C	297	PHE
1	C	366	GLY
1	C	435	ILE
1	D	91	GLN
1	D	161	LYS
1	D	400	ARG
1	D	447	PHE
1	E	29	LYS
1	E	92	ALA
1	E	118	GLY
1	E	162	GLY
1	E	331	VAL
1	E	366	GLY
1	E	378	ARG
1	F	40	LEU

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Mol	Chain	Res	Type
1	F	122	ARG
1	F	230	THR
1	F	263	ASP
1	F	345	LYS
1	F	416	ALA
1	G	29	LYS
1	G	80	GLY
1	G	91	GLN
1	G	96	SER
1	G	118	GLY
1	G	119	GLU
1	G	140	ARG
1	G	159	LYS
1	G	283	PHE
1	G	285	HIS
1	G	343	ARG
1	G	345	LYS
1	G	366	GLY
1	G	368	PRO
1	G	387	GLU
1	G	412	HIS
1	G	424	GLU
1	G	460	ALA
1	A	96	SER
1	A	225	LYS
1	A	282	GLU
1	A	286	GLN
1	C	49	LYS
1	C	110	GLY
1	C	137	MET
1	C	432	GLY
1	D	128	SER
1	D	203	PHE
1	E	140	ARG
1	E	284	HIS
1	E	418	GLY
1	F	29	LYS
1	F	99	GLY
1	F	161	LYS
1	F	190	TYR
1	F	247	GLN
1	F	421	LYS

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Mol	Chain	Res	Type
1	G	32	PRO
1	G	83	ALA
1	G	301	GLU
1	A	140	ARG
1	A	279	PRO
1	B	39	VAL
1	B	87	ALA
1	B	228	PRO
1	B	279	PRO
1	B	374	ASP
1	C	92	ALA
1	C	133	ARG
1	C	177	ASN
1	C	193	PRO
1	D	90	ASP
1	D	110	GLY
1	D	283	PHE
1	D	422	ARG
1	D	453	ILE
1	E	60	GLU
1	E	211	SER
1	E	277	SER
1	E	278	ASP
1	E	279	PRO
1	F	49	LYS
1	F	139	LYS
1	F	331	VAL
1	F	374	ASP
1	F	422	ARG
1	G	109	GLN
1	G	410	PRO
1	G	421	LYS
1	A	109	GLN
1	A	211	SER
1	A	301	GLU
1	B	366	GLY
1	B	405	PRO
1	B	416	ALA
1	C	117	ASN
1	D	190	TYR
1	E	110	GLY
1	E	130	ALA

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Mol	Chain	Res	Type
1	E	368	PRO
1	E	385	ASN
1	E	439	GLU
1	F	203	PHE
1	F	335	HIS
1	F	378	ARG
1	F	406	ASN
1	G	135	PHE
1	B	203	PHE
1	C	80	GLY
1	C	86	GLU
1	C	256	LEU
1	D	178	ILE
1	D	439	GLU
1	E	39	VAL
1	E	49	LYS
1	F	221	SER
1	F	366	GLY
1	F	412	HIS
1	F	418	GLY
1	F	437	LEU
1	G	161	LYS
1	G	385	ASN
1	B	435	ILE
1	C	185	GLY
1	D	391	VAL
1	D	410	PRO
1	E	289	ILE
1	E	435	ILE
1	F	39	VAL
1	F	441	ILE
1	B	261	PRO
1	B	391	VAL
1	F	112	GLY
1	G	222	GLY
1	C	162	GLY
1	G	110	GLY
1	B	364	PRO
1	C	418	GLY
1	D	366	GLY
1	E	383	PRO
1	F	106	PRO

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Mol	Chain	Res	Type
1	F	162	GLY
1	F	364	PRO
1	F	465	PRO
1	E	338	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/423 (97%)	392 (95%)	19 (5%)	27	63
1	B	411/423 (97%)	398 (97%)	13 (3%)	39	71
1	C	411/423 (97%)	389 (95%)	22 (5%)	22	58
1	D	411/423 (97%)	390 (95%)	21 (5%)	24	60
1	E	411/423 (97%)	385 (94%)	26 (6%)	18	52
1	F	411/423 (97%)	389 (95%)	22 (5%)	22	58
1	G	411/423 (97%)	392 (95%)	19 (5%)	27	63
All	All	2877/2961 (97%)	2735 (95%)	142 (5%)	25	61

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	73	ARG
1	A	81	THR
1	A	82	ASP
1	A	122	ARG
1	A	135	PHE
1	A	139	LYS
1	A	155	GLU
1	A	165	LEU
1	A	169	LEU
1	A	170	LEU
1	A	179	ILE
1	A	223	PHE

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Mol	Chain	Res	Type
1	A	255	THR
1	A	302	THR
1	A	306	THR
1	A	323	ARG
1	A	370	THR
1	A	477	VAL
1	B	30	LEU
1	B	53	ARG
1	B	64	ASP
1	B	135	PHE
1	B	165	LEU
1	B	179	ILE
1	B	186	LYS
1	B	286	GLN
1	B	301	GLU
1	B	368	PRO
1	B	373	LYS
1	B	467	ASP
1	B	487	ARG
1	C	40	LEU
1	C	53	ARG
1	C	64	ASP
1	C	117	ASN
1	C	140	ARG
1	C	165	LEU
1	C	179	ILE
1	C	191	LYS
1	C	223	PHE
1	C	244	PHE
1	C	276	LYS
1	C	296	PHE
1	C	297	PHE
1	C	323	ARG
1	C	341	ASP
1	C	362	LEU
1	C	374	ASP
1	C	424	GLU
1	C	439	GLU
1	C	474	GLU
1	C	487	ARG
1	C	489	LEU
1	D	57	ARG

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Mol	Chain	Res	Type
1	D	111	TYR
1	D	122	ARG
1	D	125	ARG
1	D	133	ARG
1	D	135	PHE
1	D	164	LEU
1	D	165	LEU
1	D	179	ILE
1	D	230	THR
1	D	250	GLU
1	D	276	LYS
1	D	301	GLU
1	D	325	GLN
1	D	371	VAL
1	D	387	GLU
1	D	406	ASN
1	D	431	LEU
1	D	451	THR
1	D	465	PRO
1	D	467	ASP
1	E	47	ASP
1	E	52	LEU
1	E	53	ARG
1	E	64	ASP
1	E	111	TYR
1	E	122	ARG
1	E	131	THR
1	E	132	MET
1	E	133	ARG
1	E	135	PHE
1	E	143	GLU
1	E	165	LEU
1	E	179	ILE
1	E	186	LYS
1	E	191	LYS
1	E	214	SER
1	E	216	VAL
1	E	224	LEU
1	E	231	HIS
1	E	284	HIS
1	E	287	ASN
1	E	323	ARG

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Mol	Chain	Res	Type
1	E	335	HIS
1	E	341	ASP
1	E	467	ASP
1	E	484	TYR
1	F	30	LEU
1	F	53	ARG
1	F	62	TYR
1	F	64	ASP
1	F	76	VAL
1	F	124	LEU
1	F	135	PHE
1	F	170	LEU
1	F	172	HIS
1	F	179	ILE
1	F	186	LYS
1	F	204	GLN
1	F	216	VAL
1	F	223	PHE
1	F	276	LYS
1	F	284	HIS
1	F	301	GLU
1	F	323	ARG
1	F	335	HIS
1	F	341	ASP
1	F	359	LEU
1	F	466	GLU
1	G	73	ARG
1	G	122	ARG
1	G	135	PHE
1	G	140	ARG
1	G	170	LEU
1	G	179	ILE
1	G	186	LYS
1	G	224	LEU
1	G	231	HIS
1	G	232	ARG
1	G	266	ASP
1	G	276	LYS
1	G	301	GLU
1	G	302	THR
1	G	305	THR
1	G	359	LEU

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Mol	Chain	Res	Type
1	G	368	PRO
1	G	467	ASP
1	G	479	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	325	GLN
1	A	369	HIS
1	B	172	HIS
1	B	286	GLN
1	B	287	ASN
1	B	325	GLN
1	B	335	HIS
1	B	369	HIS
1	B	385	ASN
1	B	397	HIS
1	C	172	HIS
1	C	260	ASN
1	C	284	HIS
1	C	330	GLN
1	C	335	HIS
1	C	354	HIS
1	C	369	HIS
1	C	385	ASN
1	C	397	HIS
1	C	412	HIS
1	C	492	HIS
1	D	172	HIS
1	D	204	GLN
1	D	233	GLN
1	D	237	ASN
1	D	284	HIS
1	D	325	GLN
1	D	369	HIS
1	D	397	HIS
1	D	412	HIS
1	E	42	ASN
1	E	172	HIS
1	E	284	HIS
1	E	287	ASN

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Mol	Chain	Res	Type
1	E	330	GLN
1	E	335	HIS
1	E	357	GLN
1	E	376	GLN
1	E	417	ASN
1	F	45	GLN
1	F	172	HIS
1	F	204	GLN
1	F	233	GLN
1	F	237	ASN
1	F	319	HIS
1	F	357	GLN
1	F	376	GLN
1	F	485	GLN
1	G	42	ASN
1	G	204	GLN
1	G	233	GLN
1	G	260	ASN
1	G	325	GLN
1	G	369	HIS
1	G	479	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

14 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	C	500	1,3	27,50,50	1.91	8 (29%)	17,82,82	1.68	3 (17%)
3	1CI	E	501	-	13,13,13	2.47	3 (23%)	15,17,17	0.61	0
3	1CI	D	501	2	13,13,13	2.48	3 (23%)	15,17,17	0.62	0
2	HEM	F	500	1,3	27,50,50	1.98	9 (33%)	17,82,82	1.56	3 (17%)
3	1CI	F	501	2	13,13,13	2.48	3 (23%)	15,17,17	0.61	0
2	HEM	A	500	1,3	27,50,50	1.93	10 (37%)	17,82,82	1.67	3 (17%)
2	HEM	E	500	-	27,50,50	2.03	10 (37%)	17,82,82	1.88	5 (29%)
3	1CI	A	501	2	13,13,13	2.47	3 (23%)	15,17,17	0.63	0
3	1CI	G	501	2	13,13,13	2.46	3 (23%)	15,17,17	0.55	0
2	HEM	G	500	1,3	27,50,50	1.95	9 (33%)	17,82,82	1.90	3 (17%)
3	1CI	C	501	2	13,13,13	2.47	3 (23%)	15,17,17	0.61	0
2	HEM	D	500	1,3	27,50,50	1.96	7 (25%)	17,82,82	1.75	4 (23%)
3	1CI	B	501	-	13,13,13	2.49	3 (23%)	15,17,17	0.62	0
2	HEM	B	500	1	27,50,50	1.99	10 (37%)	17,82,82	1.80	4 (23%)

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	C	500	1,3	-	0/6/54/54	-
3	1CI	E	501	-	-	0/4/4/4	0/2/2/2
3	1CI	D	501	2	-	0/4/4/4	0/2/2/2
2	HEM	F	500	1,3	-	0/6/54/54	-
3	1CI	F	501	2	-	0/4/4/4	0/2/2/2
2	HEM	A	500	1,3	-	0/6/54/54	-
2	HEM	E	500	-	-	0/6/54/54	-
3	1CI	A	501	2	-	0/4/4/4	0/2/2/2
3	1CI	G	501	2	-	0/4/4/4	0/2/2/2
2	HEM	G	500	1,3	-	0/6/54/54	-
3	1CI	C	501	2	-	0/4/4/4	0/2/2/2
2	HEM	D	500	1,3	-	0/6/54/54	-
3	1CI	B	501	-	-	0/4/4/4	0/2/2/2
2	HEM	B	500	1	-	0/6/54/54	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	1CI	C6-N1	-7.18	1.33	1.45
3	D	501	1CI	C6-N1	-7.16	1.33	1.45
3	B	501	1CI	C6-N1	-7.12	1.33	1.45
3	E	501	1CI	C6-N1	-7.12	1.33	1.45
3	A	501	1CI	C6-N1	-7.11	1.33	1.45
3	C	501	1CI	C6-N1	-7.07	1.33	1.45
3	G	501	1CI	C6-N1	-7.04	1.33	1.45
2	D	500	HEM	C3C-CAC	-5.49	1.36	1.47
2	F	500	HEM	C3C-CAC	-5.19	1.37	1.47
2	E	500	HEM	C3C-CAC	-5.13	1.37	1.47
2	G	500	HEM	C3C-CAC	-5.13	1.37	1.47
2	A	500	HEM	C3C-CAC	-5.06	1.37	1.47
2	B	500	HEM	C3C-CAC	-4.99	1.37	1.47
2	C	500	HEM	C3C-CAC	-4.92	1.37	1.47
3	B	501	1CI	C5-N1	-4.05	1.33	1.39
3	G	501	1CI	C5-N1	-4.05	1.33	1.39
3	A	501	1CI	C5-N1	-4.01	1.33	1.39
3	D	501	1CI	C5-N1	-3.98	1.33	1.39
3	C	501	1CI	C5-N1	-3.98	1.33	1.39
3	F	501	1CI	C5-N1	-3.96	1.33	1.39
3	E	501	1CI	C5-N1	-3.94	1.33	1.39
2	F	500	HEM	CAD-C3D	3.28	1.58	1.52
2	E	500	HEM	CMA-C3A	3.28	1.58	1.51
2	A	500	HEM	CMA-C3A	3.27	1.58	1.51
2	B	500	HEM	CAD-C3D	3.27	1.58	1.52
2	E	500	HEM	CAD-C3D	3.26	1.57	1.52
2	B	500	HEM	CMA-C3A	3.19	1.58	1.51
2	D	500	HEM	CMA-C3A	3.18	1.58	1.51
2	G	500	HEM	CMA-C3A	3.17	1.58	1.51
2	E	500	HEM	C1D-ND	-3.15	1.29	1.36
2	C	500	HEM	CMA-C3A	3.13	1.58	1.51
2	F	500	HEM	CMA-C3A	3.11	1.58	1.51
3	B	501	1CI	C2-N1	-3.05	1.33	1.36
3	C	501	1CI	C2-N1	-3.05	1.33	1.36
3	D	501	1CI	C2-N1	-3.04	1.33	1.36
3	G	501	1CI	C2-N1	-3.01	1.33	1.36
2	G	500	HEM	CAD-C3D	3.01	1.57	1.52
3	F	501	1CI	C2-N1	-3.00	1.33	1.36
3	A	501	1CI	C2-N1	-2.97	1.33	1.36
3	E	501	1CI	C2-N1	-2.97	1.33	1.36
2	C	500	HEM	C3B-CAB	-2.96	1.41	1.47
2	D	500	HEM	CBB-CAB	2.96	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-CAB	-2.94	1.41	1.47
2	F	500	HEM	C1D-ND	-2.93	1.30	1.36
2	G	500	HEM	CBB-CAB	2.92	1.48	1.29
2	C	500	HEM	CBB-CAB	2.92	1.48	1.29
2	D	500	HEM	C1D-ND	-2.90	1.30	1.36
2	F	500	HEM	CBB-CAB	2.90	1.48	1.29
2	G	500	HEM	C1D-ND	-2.90	1.30	1.36
2	B	500	HEM	CBB-CAB	2.88	1.48	1.29
2	C	500	HEM	C1D-ND	-2.87	1.30	1.36
2	A	500	HEM	CBB-CAB	2.84	1.48	1.29
2	A	500	HEM	C1D-ND	-2.84	1.30	1.36
2	E	500	HEM	CBB-CAB	2.84	1.48	1.29
2	F	500	HEM	C3B-CAB	-2.81	1.42	1.47
2	D	500	HEM	CAD-C3D	2.77	1.57	1.52
2	C	500	HEM	CAD-C3D	2.76	1.57	1.52
2	B	500	HEM	C1D-ND	-2.68	1.30	1.36
2	G	500	HEM	C3B-CAB	-2.66	1.42	1.47
2	D	500	HEM	C3B-CAB	-2.65	1.42	1.47
2	E	500	HEM	C4A-NA	-2.65	1.30	1.36
2	E	500	HEM	C3B-CAB	-2.55	1.42	1.47
2	B	500	HEM	CAA-C2A	2.43	1.55	1.52
2	A	500	HEM	CAD-C3D	2.42	1.56	1.52
2	B	500	HEM	C4A-NA	-2.40	1.31	1.36
2	B	500	HEM	C3B-CAB	-2.39	1.43	1.47
2	F	500	HEM	CMC-C2C	2.26	1.56	1.51
2	B	500	HEM	CMC-C2C	2.20	1.56	1.51
2	A	500	HEM	CMC-C2C	2.17	1.56	1.51
2	G	500	HEM	CMC-C2C	2.16	1.56	1.51
2	E	500	HEM	CAA-C2A	2.14	1.55	1.52
2	A	500	HEM	C4B-NB	-2.12	1.31	1.36
2	D	500	HEM	CMC-C2C	2.12	1.56	1.51
2	C	500	HEM	CMC-C2C	2.11	1.56	1.51
2	A	500	HEM	C4A-NA	-2.10	1.31	1.36
2	B	500	HEM	CBC-CAC	2.06	1.42	1.29
2	G	500	HEM	C4A-NA	-2.05	1.31	1.36
2	E	500	HEM	C1C-C2C	-2.05	1.37	1.42
2	F	500	HEM	C4A-NA	-2.04	1.32	1.36
2	F	500	HEM	C4B-NB	-2.03	1.32	1.36
2	A	500	HEM	C1D-CHD	-2.01	1.35	1.41
2	C	500	HEM	C1D-CHD	-2.01	1.35	1.41
2	E	500	HEM	CBC-CAC	2.00	1.42	1.29
2	G	500	HEM	C4B-NB	-2.00	1.32	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500	HEM	CAD-CBD-CGD	4.73	120.60	112.67
2	E	500	HEM	CAD-CBD-CGD	4.31	119.91	112.67
2	B	500	HEM	CAD-CBD-CGD	4.10	119.55	112.67
2	C	500	HEM	CAD-CBD-CGD	3.75	118.95	112.67
2	A	500	HEM	CAD-CBD-CGD	3.59	118.70	112.67
2	D	500	HEM	CAD-CBD-CGD	3.59	118.69	112.67
2	F	500	HEM	CAD-CBD-CGD	3.54	118.61	112.67
2	G	500	HEM	C4C-C3C-C2C	-3.48	104.47	106.90
2	B	500	HEM	C4C-C3C-C2C	-3.46	104.48	106.90
2	A	500	HEM	C4C-C3C-C2C	-3.35	104.56	106.90
2	E	500	HEM	C4C-C3C-C2C	-3.21	104.66	106.90
2	C	500	HEM	C4C-C3C-C2C	-3.12	104.72	106.90
2	D	500	HEM	C4C-C3C-C2C	-3.06	104.76	106.90
2	D	500	HEM	CMB-C2B-C3B	3.03	130.35	124.68
2	C	500	HEM	CMB-C2B-C3B	2.98	130.25	124.68
2	B	500	HEM	CMB-C2B-C3B	2.90	130.11	124.68
2	A	500	HEM	CMB-C2B-C3B	2.83	129.97	124.68
2	G	500	HEM	CMB-C2B-C3B	2.82	129.96	124.68
2	F	500	HEM	C4C-C3C-C2C	-2.76	104.97	106.90
2	E	500	HEM	CMB-C2B-C3B	2.68	129.70	124.68
2	F	500	HEM	CMB-C2B-C3B	2.64	129.61	124.68
2	E	500	HEM	CBA-CAA-C2A	2.45	117.01	112.49
2	D	500	HEM	CBA-CAA-C2A	2.23	116.59	112.49
2	B	500	HEM	CAA-CBA-CGA	2.12	116.23	112.67
2	E	500	HEM	CMA-C3A-C4A	-2.02	125.36	128.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 48 short contacts:

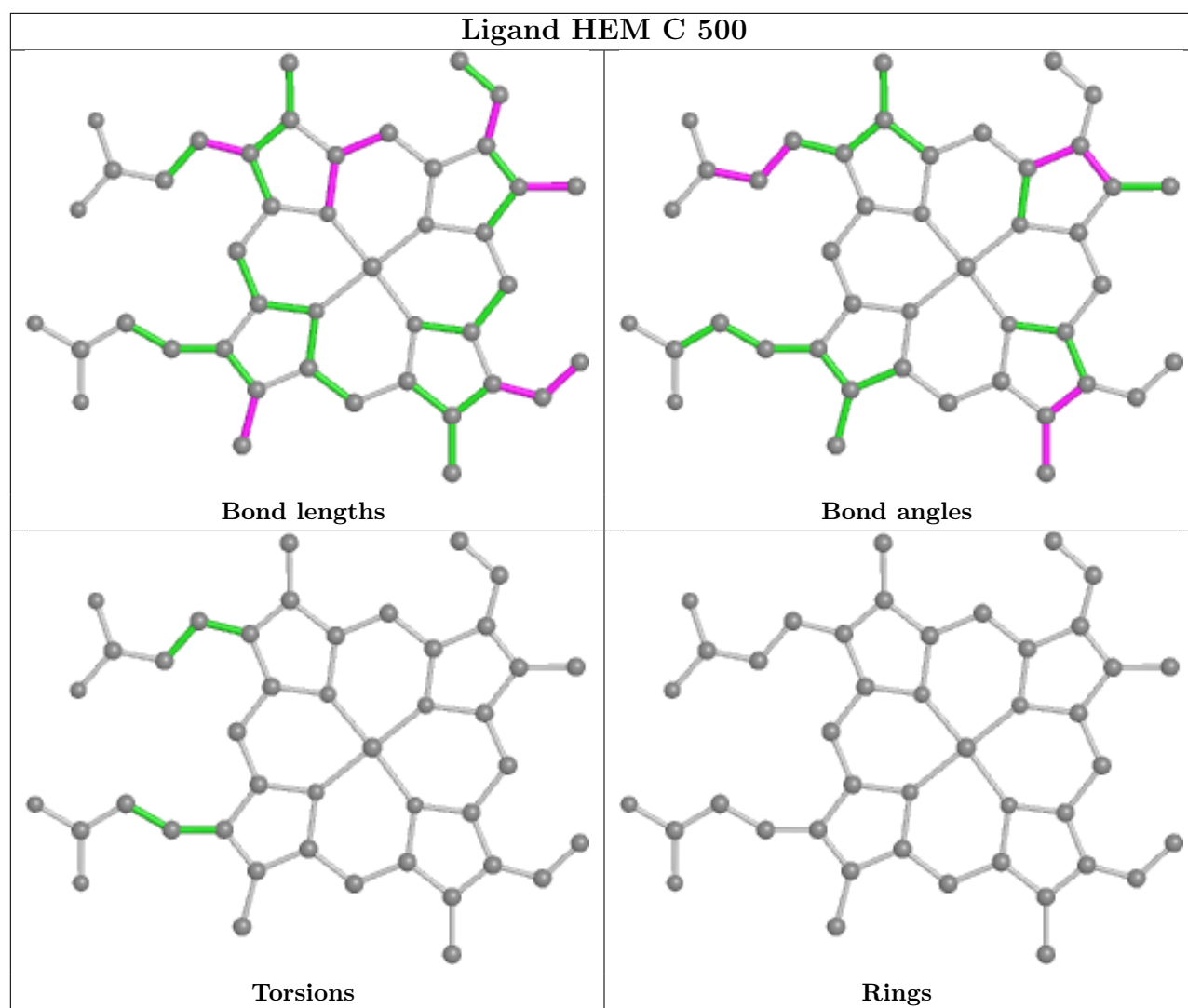
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	HEM	4	0
3	E	501	1CI	1	0
3	D	501	1CI	2	0
2	F	500	HEM	7	0
3	F	501	1CI	3	0
2	A	500	HEM	2	0
2	E	500	HEM	8	0
3	A	501	1CI	1	0

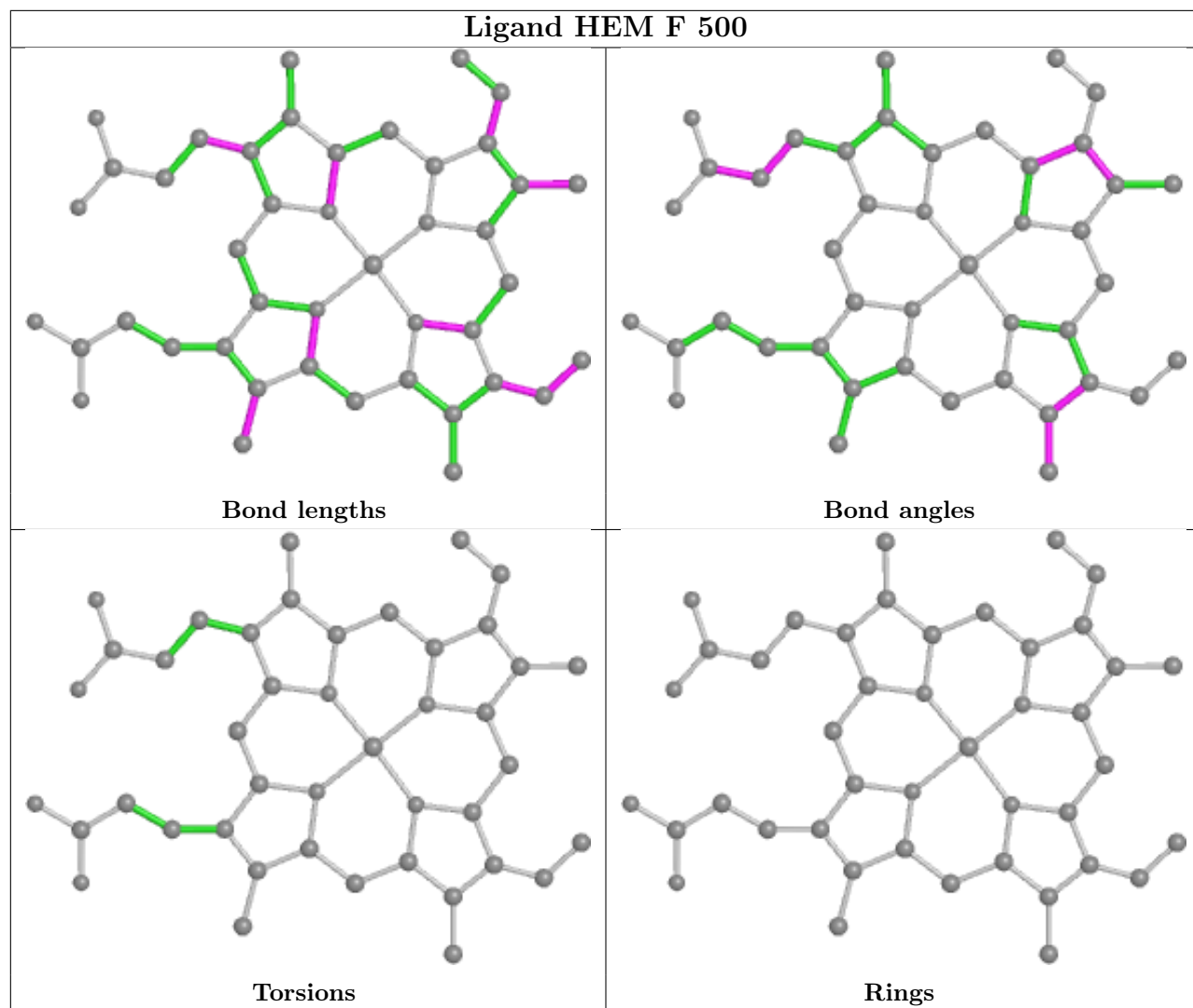
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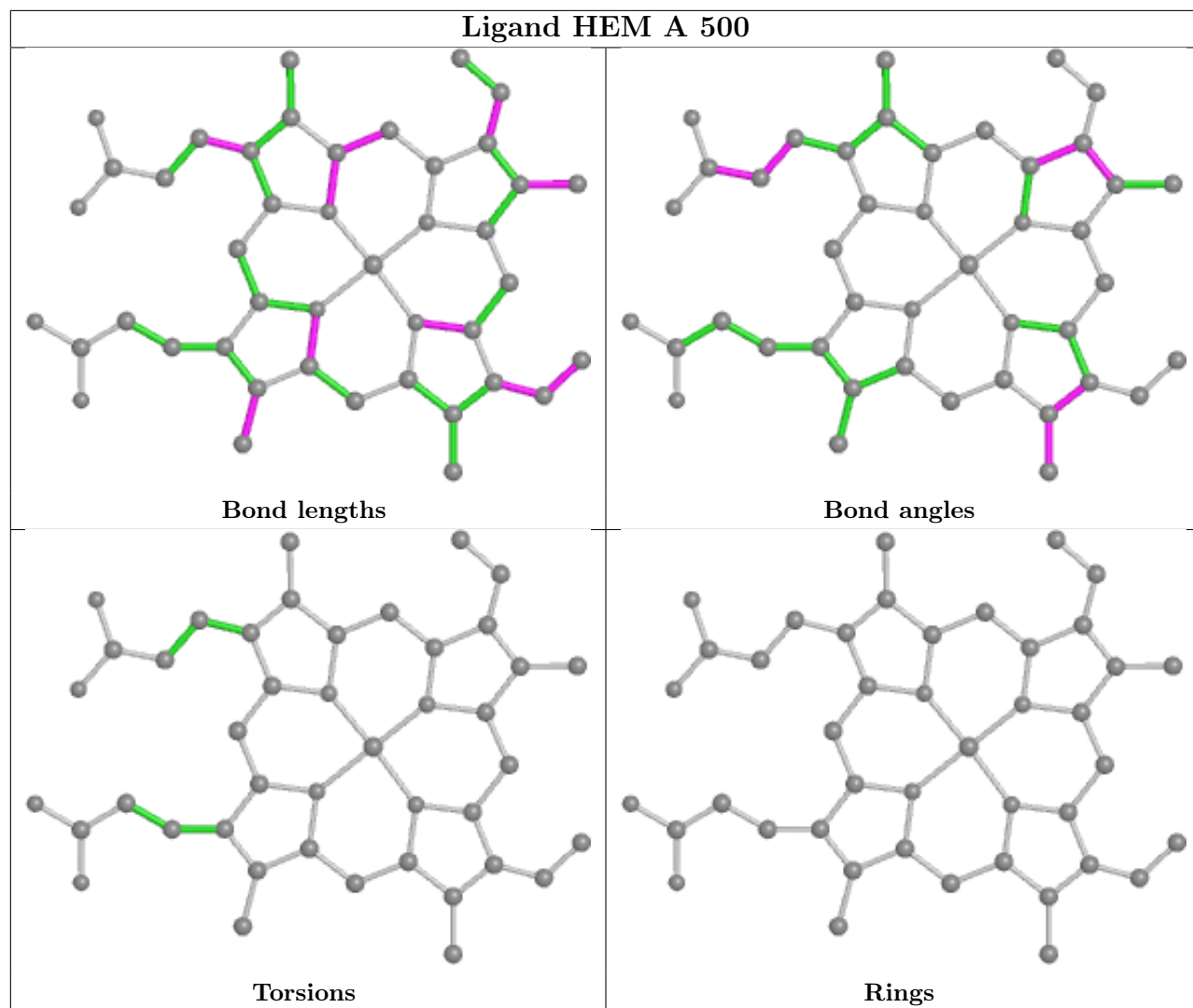
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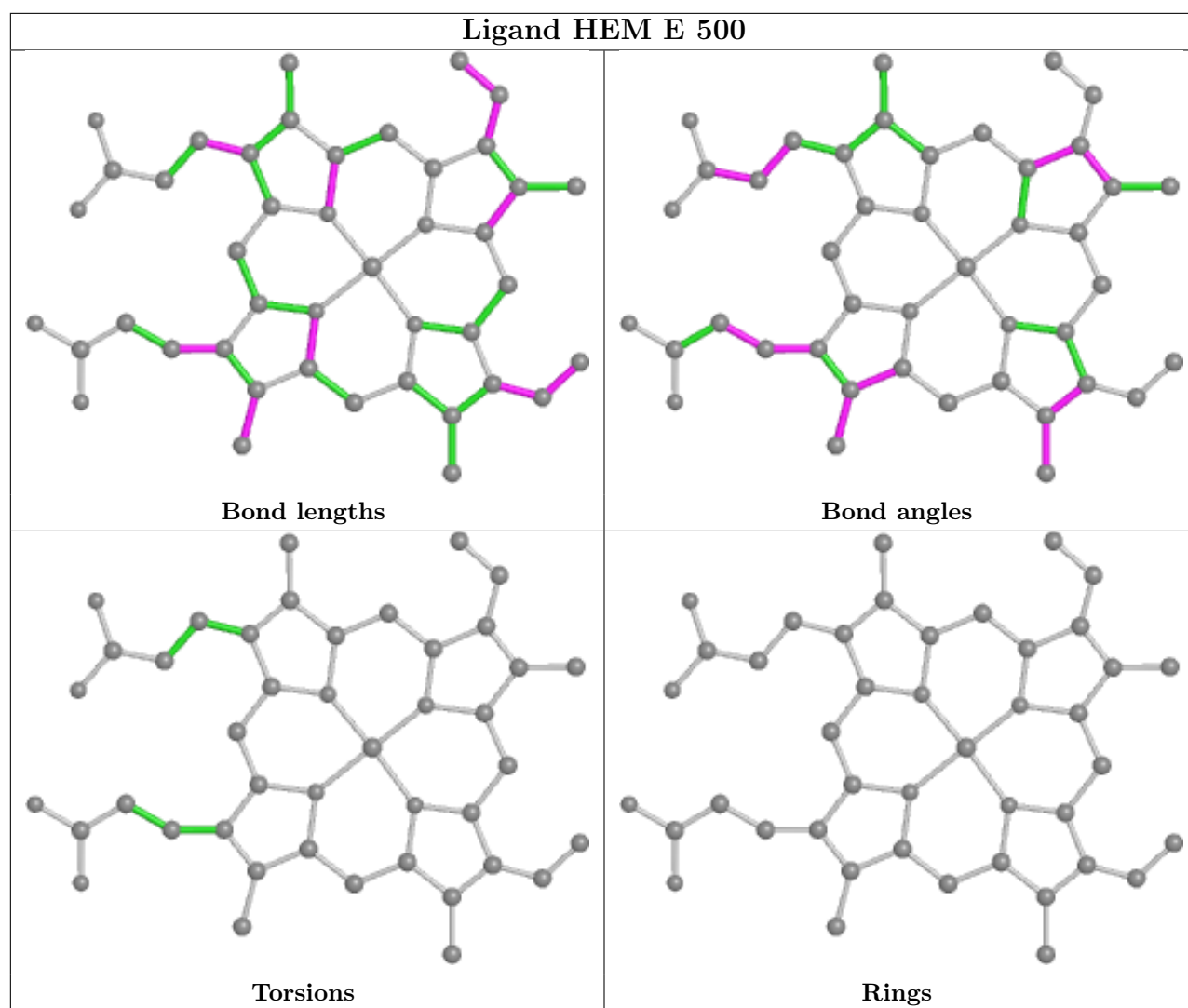
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	501	1CI	4	0
2	G	500	HEM	4	0
3	C	501	1CI	3	0
2	D	500	HEM	6	0
3	B	501	1CI	3	0
2	B	500	HEM	3	0

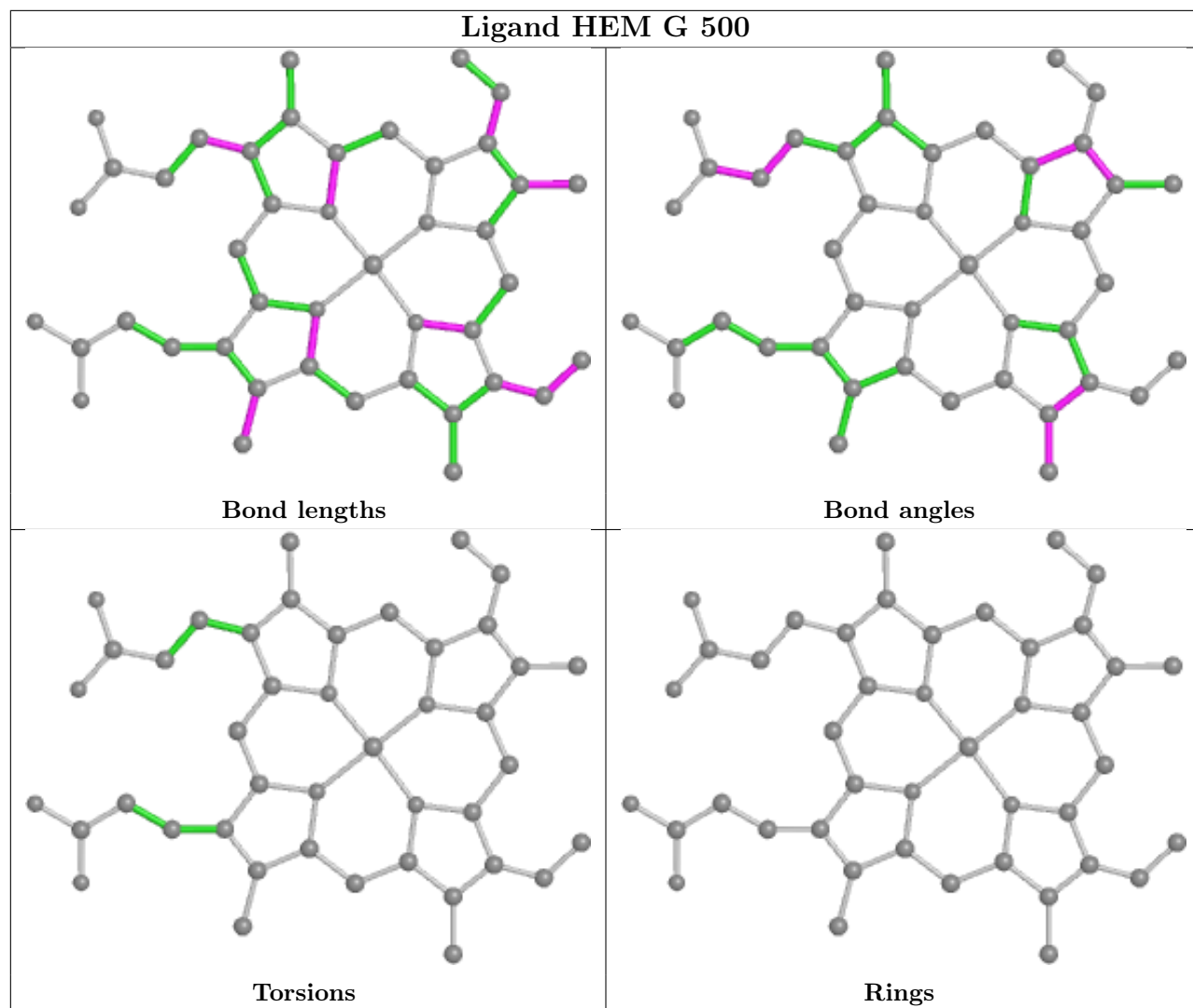
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

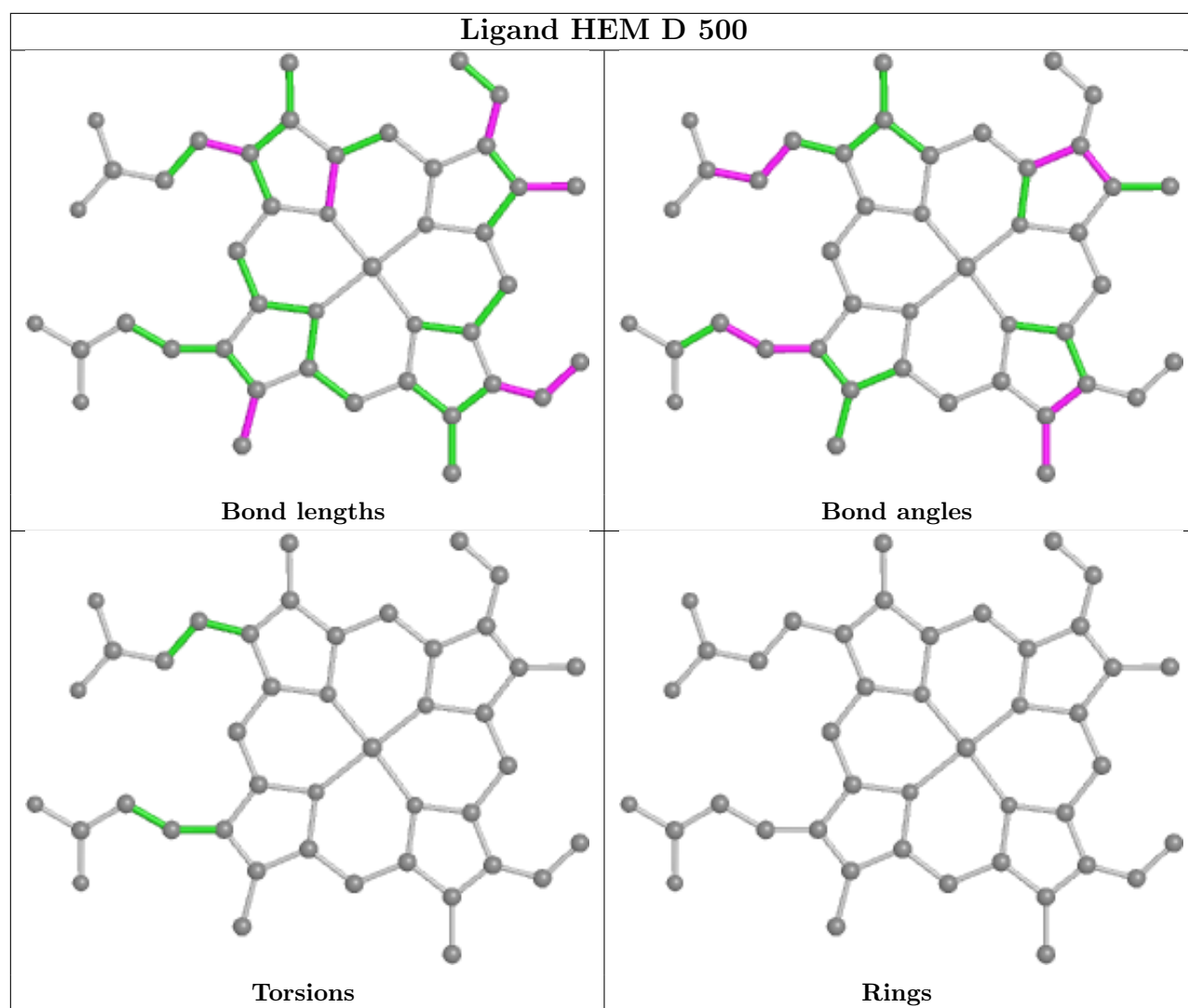


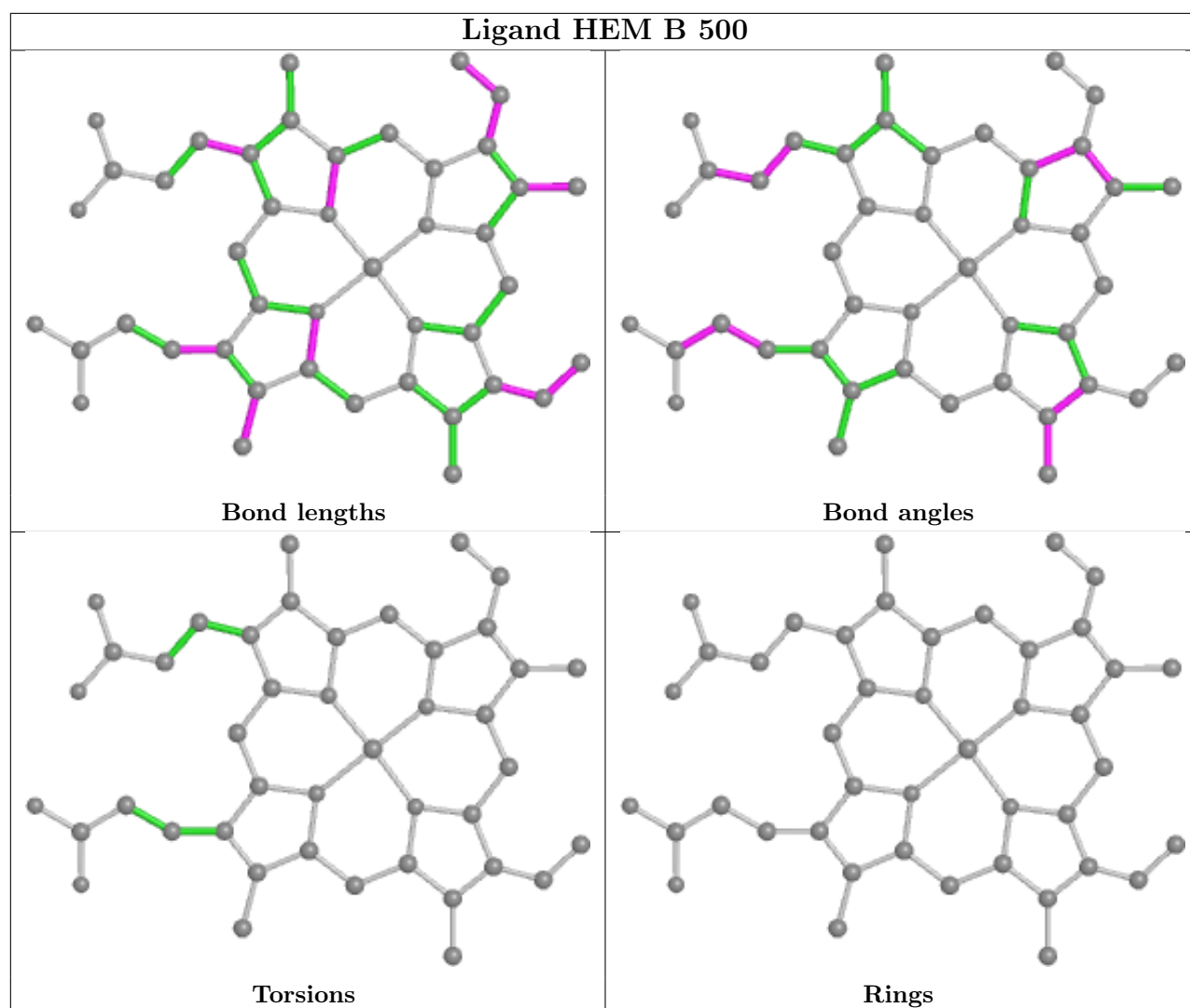












## 5.7 Other polymers [i](#)

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	465/478 (97%)	0.63	19 (4%) 37 24	48, 86, 120, 169	0
1	B	465/478 (97%)	0.78	46 (9%) 7 4	70, 103, 144, 202	0
1	C	465/478 (97%)	0.78	51 (10%) 5 3	64, 112, 156, 186	0
1	D	465/478 (97%)	0.69	32 (6%) 16 9	64, 100, 144, 202	0
1	E	465/478 (97%)	0.87	63 (13%) 3 2	62, 115, 158, 202	0
1	F	465/478 (97%)	1.03	81 (17%) 1 1	70, 119, 165, 197	0
1	G	465/478 (97%)	0.99	80 (17%) 1 1	63, 119, 173, 202	0
All	All	3255/3346 (97%)	0.82	372 (11%) 5 3	48, 108, 160, 202	0

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	138	GLY	9.1
1	F	84	ILE	7.3
1	G	137	MET	7.2
1	C	259	SER	7.2
1	G	136	GLY	7.0
1	F	377	PHE	7.0
1	E	130	ALA	6.9
1	G	375	THR	6.8
1	G	45	GLN	6.7
1	F	252	HIS	6.1
1	C	175	THR	6.1
1	F	369	HIS	6.0
1	F	423	ASN	5.9
1	F	138	GLY	5.9
1	C	258	PRO	5.9
1	E	286	GLN	5.8
1	G	86	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	88	LEU	5.7
1	F	63	GLY	5.6
1	E	284	HIS	5.3
1	F	139	LYS	5.3
1	F	131	THR	5.2
1	G	30	LEU	5.1
1	G	102	ALA	5.1
1	G	139	LYS	5.1
1	C	177	ASN	5.0
1	G	49	LYS	5.0
1	G	177	ASN	4.9
1	C	368	PRO	4.9
1	F	436	CYS	4.9
1	B	83	ALA	4.9
1	C	248	SER	4.9
1	F	42	ASN	4.8
1	D	77	VAL	4.8
1	G	67	THR	4.7
1	D	305	THR	4.7
1	G	397	HIS	4.7
1	G	178	ILE	4.6
1	F	119	GLU	4.6
1	F	59	ARG	4.6
1	E	431	LEU	4.5
1	G	354	HIS	4.4
1	F	121	TRP	4.4
1	G	435	ILE	4.3
1	G	32	PRO	4.3
1	B	301	GLU	4.3
1	E	278	ASP	4.3
1	G	382	ILE	4.3
1	E	272	MET	4.3
1	B	273	GLU	4.3
1	G	219	LEU	4.2
1	G	376	GLN	4.2
1	F	368	PRO	4.2
1	E	145	ARG	4.2
1	A	398	ASP	4.1
1	C	67	THR	4.1
1	B	418	GLY	4.1
1	G	77	VAL	4.1
1	G	54	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	137	MET	4.0
1	C	301	GLU	3.9
1	F	273	GLU	3.9
1	C	387	GLU	3.9
1	G	179	ILE	3.9
1	A	304	SER	3.9
1	D	136	GLY	3.8
1	G	84	ILE	3.8
1	G	364	PRO	3.8
1	C	270	LEU	3.8
1	E	436	CYS	3.7
1	E	71	GLY	3.7
1	F	72	SER	3.7
1	G	101	ILE	3.7
1	G	75	VAL	3.7
1	F	85	ARG	3.7
1	F	410	PRO	3.6
1	E	290	LEU	3.6
1	G	368	PRO	3.6
1	F	412	HIS	3.6
1	F	128	SER	3.6
1	D	306	THR	3.6
1	E	245	ILE	3.5
1	F	254	ALA	3.5
1	F	460	ALA	3.5
1	E	365	PHE	3.5
1	F	314	MET	3.5
1	F	206	PHE	3.5
1	A	144	GLU	3.4
1	G	210	SER	3.4
1	A	393	SER	3.4
1	F	96	SER	3.4
1	F	437	LEU	3.4
1	G	429	PHE	3.4
1	D	445	GLU	3.4
1	G	355	GLU	3.4
1	C	267	VAL	3.4
1	E	303	THR	3.4
1	B	181	SER	3.3
1	G	215	GLN	3.3
1	F	276	LYS	3.3
1	G	302	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	28	GLY	3.3
1	E	260	ASN	3.3
1	B	129	LEU	3.3
1	B	172	HIS	3.3
1	F	482	PRO	3.3
1	F	459	ILE	3.2
1	C	412	HIS	3.2
1	C	268	TYR	3.2
1	G	217	PHE	3.2
1	F	132	MET	3.2
1	B	177	ASN	3.2
1	E	265	ILE	3.2
1	E	70	LEU	3.2
1	E	152	CYS	3.2
1	G	70	LEU	3.2
1	E	34	PRO	3.2
1	F	137	MET	3.2
1	D	285	HIS	3.2
1	E	138	GLY	3.2
1	C	176	SER	3.2
1	E	139	LYS	3.1
1	E	158	ARG	3.1
1	G	388	VAL	3.1
1	E	462	PRO	3.1
1	C	272	MET	3.1
1	E	465	PRO	3.1
1	E	432	GLY	3.1
1	F	411	GLY	3.1
1	B	206	PHE	3.1
1	G	247	GLN	3.1
1	F	83	ALA	3.1
1	F	388	VAL	3.0
1	C	353	ILE	3.0
1	E	364	PRO	3.0
1	F	353	ILE	3.0
1	A	116	ALA	3.0
1	B	155	GLU	3.0
1	G	48	ARG	3.0
1	A	433	LYS	3.0
1	B	175	THR	3.0
1	G	104	VAL	3.0
1	F	329	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	353	ILE	2.9
1	E	456	ASN	2.9
1	G	74	PRO	2.9
1	B	264	PHE	2.9
1	F	426	PHE	2.9
1	B	373	LYS	2.9
1	G	377	PHE	2.9
1	E	450	PHE	2.9
1	C	302	THR	2.9
1	G	389	PHE	2.9
1	B	84	ILE	2.9
1	E	308	ARG	2.9
1	E	287	ASN	2.9
1	G	152	CYS	2.9
1	D	390	PRO	2.9
1	G	390	PRO	2.9
1	C	173	SER	2.8
1	C	179	ILE	2.8
1	E	243	THR	2.8
1	D	270	LEU	2.8
1	B	76	VAL	2.8
1	B	335	HIS	2.8
1	D	387	GLU	2.8
1	E	457	PHE	2.8
1	B	263	ASP	2.8
1	A	286	GLN	2.8
1	D	298	ALA	2.8
1	C	99	GLY	2.8
1	F	390	PRO	2.8
1	D	441	ILE	2.8
1	A	247	GLN	2.8
1	C	202	PHE	2.7
1	C	261	PRO	2.7
1	G	319	HIS	2.7
1	F	115	PHE	2.7
1	E	188	PHE	2.7
1	F	489	LEU	2.7
1	G	180	CYS	2.7
1	E	285	HIS	2.7
1	D	457	PHE	2.7
1	G	370	THR	2.7
1	G	29	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	437	LEU	2.7
1	C	94	ALA	2.7
1	D	175	THR	2.7
1	C	188	PHE	2.7
1	C	279	PRO	2.7
1	C	469	ASP	2.7
1	B	29	LYS	2.7
1	B	137	MET	2.7
1	D	292	VAL	2.7
1	F	414	LEU	2.7
1	G	176	SER	2.6
1	G	242	ASN	2.6
1	G	365	PHE	2.6
1	E	489	LEU	2.6
1	B	186	LYS	2.6
1	B	69	TYR	2.6
1	B	372	THR	2.6
1	G	100	LYS	2.6
1	C	415	ASP	2.6
1	G	315	LEU	2.6
1	F	140	ARG	2.6
1	B	361	ASP	2.6
1	E	33	GLY	2.6
1	F	294	SER	2.6
1	F	116	ALA	2.5
1	D	283	PHE	2.5
1	E	81	THR	2.5
1	A	269	LEU	2.5
1	A	361	ASP	2.5
1	F	202	PHE	2.5
1	F	104	VAL	2.5
1	E	430	SER	2.5
1	F	461	SER	2.5
1	E	94	ALA	2.5
1	G	206	PHE	2.5
1	F	112	GLY	2.5
1	A	141	SER	2.5
1	E	216	VAL	2.5
1	G	284	HIS	2.5
1	E	167	ASN	2.5
1	F	179	ILE	2.5
1	F	458	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.5
1	E	305	THR	2.5
1	G	287	ASN	2.5
1	B	381	VAL	2.5
1	B	362	LEU	2.4
1	F	113	VAL	2.4
1	C	354	HIS	2.4
1	C	125	ARG	2.4
1	G	395	ALA	2.4
1	F	310	GLY	2.4
1	C	181	SER	2.4
1	F	319	HIS	2.4
1	E	293	LEU	2.4
1	F	427	MET	2.4
1	F	80	GLY	2.4
1	F	272	MET	2.4
1	E	387	GLU	2.4
1	D	100	LYS	2.4
1	F	339	ALA	2.4
1	G	53	ARG	2.4
1	G	55	PHE	2.4
1	B	397	HIS	2.4
1	C	369	HIS	2.4
1	C	414	LEU	2.4
1	A	479	ASN	2.4
1	C	388	VAL	2.3
1	D	352	VAL	2.3
1	E	257	ASP	2.3
1	G	61	LYS	2.3
1	B	265	ILE	2.3
1	F	118	GLY	2.3
1	E	274	LYS	2.3
1	D	196	LEU	2.3
1	F	255	THR	2.3
1	A	278	ASP	2.3
1	C	207	SER	2.3
1	D	304	SER	2.3
1	E	356	ILE	2.3
1	G	114	ILE	2.3
1	G	185	GLY	2.3
1	B	319	HIS	2.3
1	D	492	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	180	CYS	2.3
1	B	78	LEU	2.3
1	G	381	VAL	2.3
1	E	425	GLY	2.3
1	D	375	THR	2.3
1	D	78	LEU	2.3
1	B	105	ASP	2.3
1	D	429	PHE	2.3
1	B	445	GLU	2.3
1	C	401	TYR	2.3
1	G	408	PHE	2.3
1	A	333	GLY	2.3
1	F	330	GLN	2.3
1	E	175	THR	2.3
1	G	135	PHE	2.3
1	G	243	THR	2.3
1	F	207	SER	2.3
1	F	392	LEU	2.3
1	G	88	LEU	2.3
1	E	224	LEU	2.3
1	C	283	PHE	2.3
1	E	449	PHE	2.3
1	B	405	PRO	2.2
1	E	261	PRO	2.2
1	G	227	PHE	2.2
1	C	485	GLN	2.2
1	G	87	ALA	2.2
1	F	66	PHE	2.2
1	G	202	PHE	2.2
1	F	86	GLU	2.2
1	F	387	GLU	2.2
1	B	393	SER	2.2
1	C	111	TYR	2.2
1	F	364	PRO	2.2
1	C	421	LYS	2.2
1	B	77	VAL	2.2
1	D	183	VAL	2.2
1	F	327	GLU	2.2
1	B	116	ALA	2.2
1	G	111	TYR	2.2
1	E	149	GLU	2.2
1	A	182	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	387	GLU	2.2
1	G	123	ALA	2.2
1	F	485	GLN	2.2
1	G	66	PHE	2.2
1	D	286	GLN	2.2
1	B	302	THR	2.2
1	F	321	THR	2.2
1	C	288	LEU	2.1
1	F	288	LEU	2.1
1	D	135	PHE	2.1
1	B	428	PRO	2.1
1	E	75	VAL	2.1
1	A	303	THR	2.1
1	G	392	LEU	2.1
1	E	426	PHE	2.1
1	E	331	VAL	2.1
1	E	414	LEU	2.1
1	C	323	ARG	2.1
1	C	476	GLY	2.1
1	F	454	LEU	2.1
1	C	84	ILE	2.1
1	E	259	SER	2.1
1	B	190	TYR	2.1
1	B	300	THR	2.1
1	B	355	GLU	2.1
1	E	178	ILE	2.1
1	B	364	PRO	2.1
1	D	235	TYR	2.1
1	B	183	VAL	2.1
1	D	338	PRO	2.1
1	B	254	ALA	2.1
1	C	419	ALA	2.1
1	F	200	ASP	2.1
1	G	64	ASP	2.1
1	C	118	GLY	2.1
1	F	302	THR	2.1
1	C	75	VAL	2.1
1	C	128	SER	2.1
1	E	332	ILE	2.1
1	F	50	GLY	2.1
1	D	428	PRO	2.1
1	A	364	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	ILE	2.1
1	C	284	HIS	2.1
1	F	281	SER	2.0
1	G	96	SER	2.0
1	F	68	VAL	2.0
1	G	69	TYR	2.0
1	B	133	ARG	2.0
1	D	200	ASP	2.0
1	E	398	ASP	2.0
1	F	146	ILE	2.0
1	D	177	ASN	2.0
1	E	410	PRO	2.0
1	B	268	TYR	2.0
1	F	76	VAL	2.0
1	D	410	PRO	2.0
1	C	422	ARG	2.0
1	E	173	SER	2.0
1	E	366	GLY	2.0
1	F	428	PRO	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1CI	E	501	12/12	0.73	0.81	107,107,107,107	0
3	1CI	G	501	12/12	0.79	0.51	107,107,107,107	0
3	1CI	A	501	12/12	0.80	0.54	107,107,107,107	0
3	1CI	C	501	12/12	0.81	0.56	107,107,107,107	0

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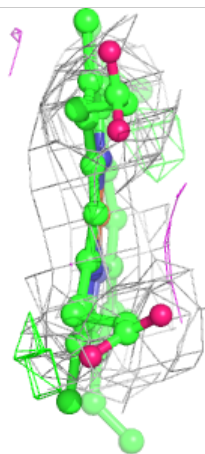
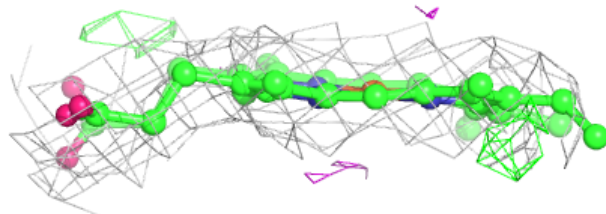
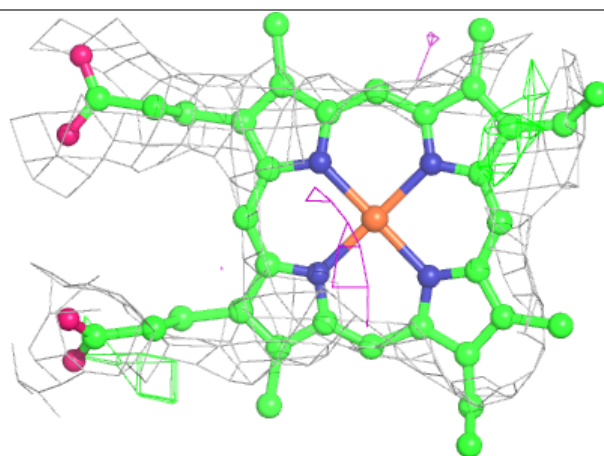
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1CI	B	501	12/12	0.82	0.41	107,107,107,107	0
3	1CI	F	501	12/12	0.88	0.39	107,107,107,107	0
3	1CI	D	501	12/12	0.88	0.36	107,107,107,107	0
2	HEM	F	500	43/43	0.93	0.38	111,111,111,111	0
2	HEM	B	500	43/43	0.93	0.39	78,78,78,78	0
2	HEM	G	500	43/43	0.94	0.39	109,109,109,109	0
2	HEM	D	500	43/43	0.94	0.35	102,102,102,102	0
2	HEM	C	500	43/43	0.95	0.32	93,93,93,93	0
2	HEM	A	500	43/43	0.95	0.39	78,78,78,78	0
2	HEM	E	500	43/43	0.95	0.34	69,69,69,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

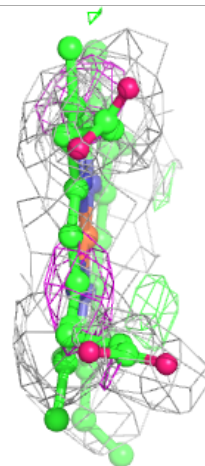
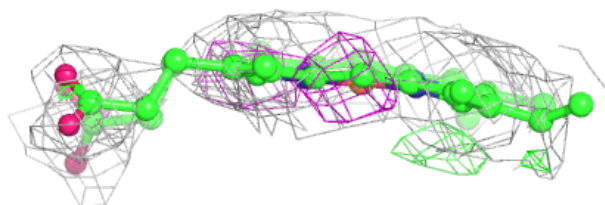
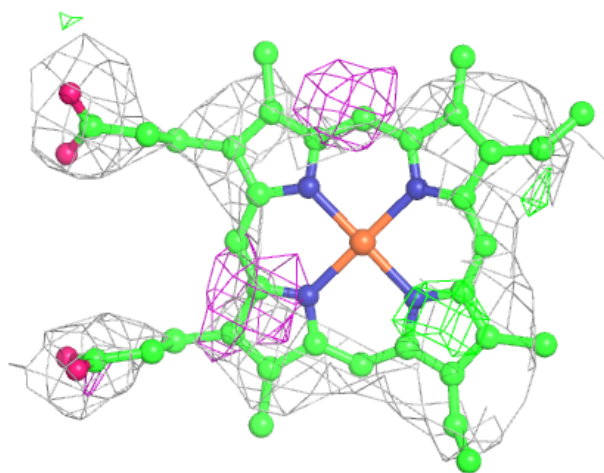
#### Electron density around HEM F 500:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



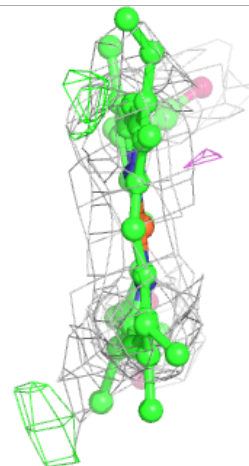
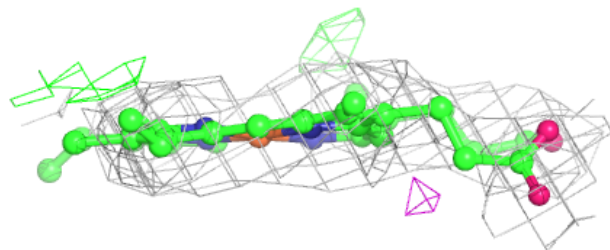
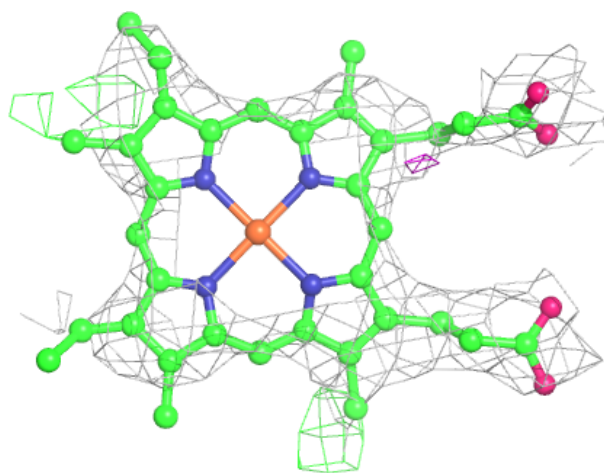
**Electron density around HEM B 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



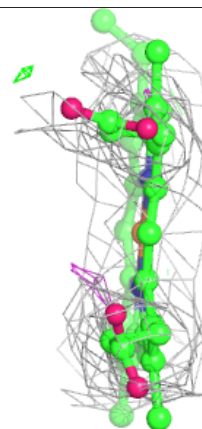
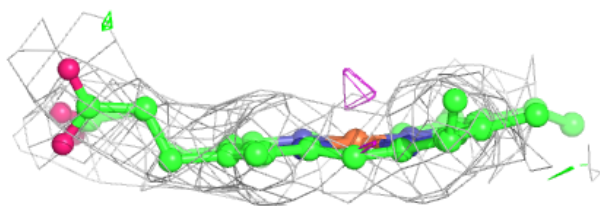
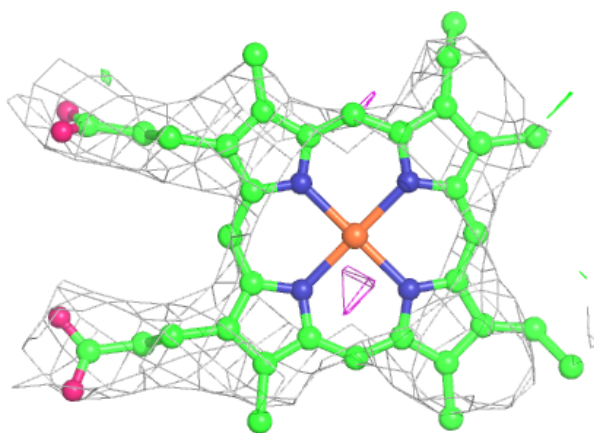
**Electron density around HEM G 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



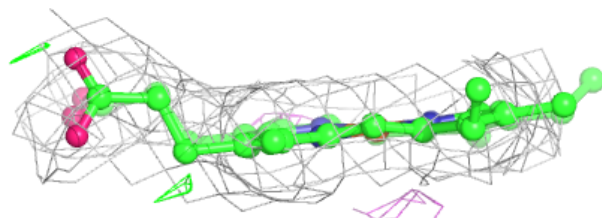
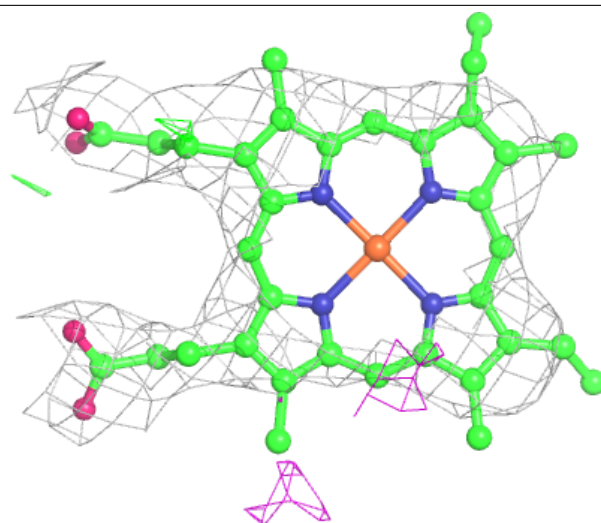
**Electron density around HEM D 500:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



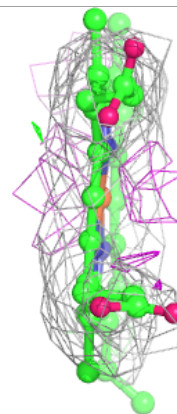
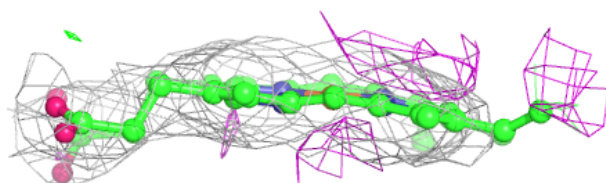
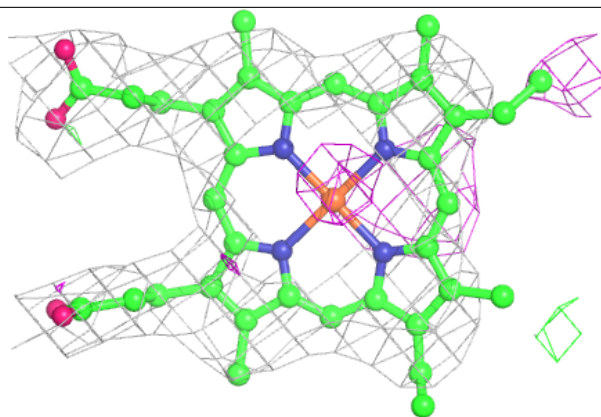
**Electron density around HEM C 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



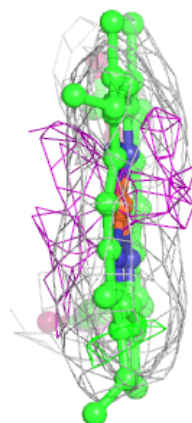
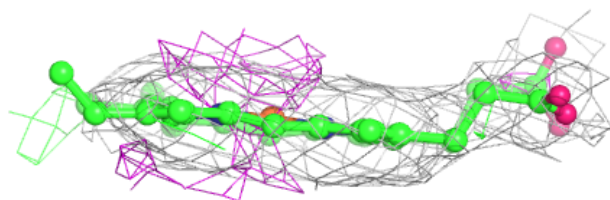
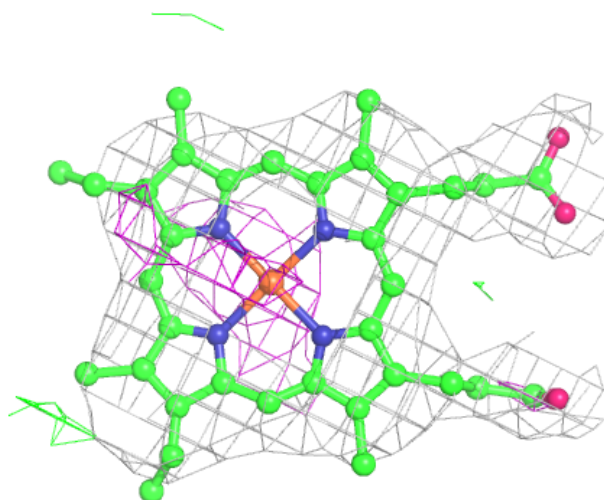
**Electron density around HEM A 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM E 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.