



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:15 PM EDT

PDB ID : 2Q6N / pdb_00002q6n
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

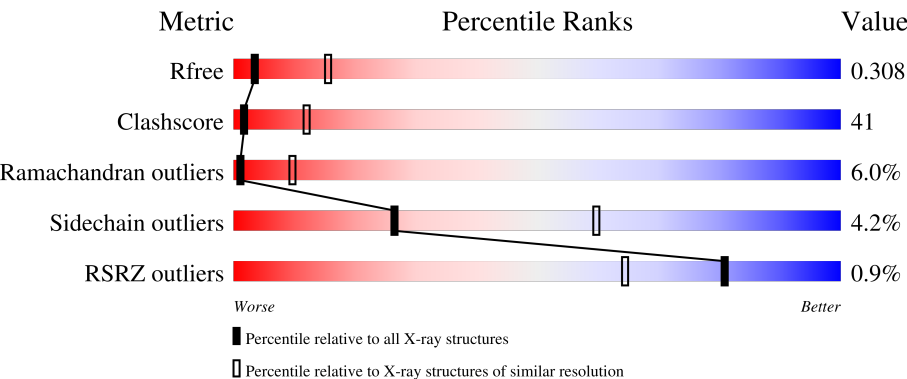
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 ≥ 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	42%48%7% . .
1	B	478	% 40%50%7% .
1	C	478	% 31%57%9% .
1	D	478	% 36%53%9% .
1	E	478	% 33%56%8% . .

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Mol	Chain	Length	Quality of chain
1	F	478	% 32% 54% 11%
1	G	478	2% 31% 57% 8%

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	G	501	-	-	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
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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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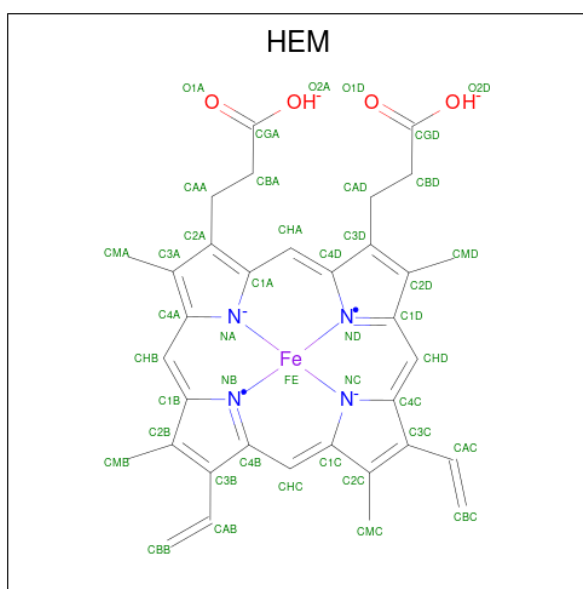
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP P00178
F	?	-	PHE	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	ALA	deletion	UNP P00178
F	?	-	GLY	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



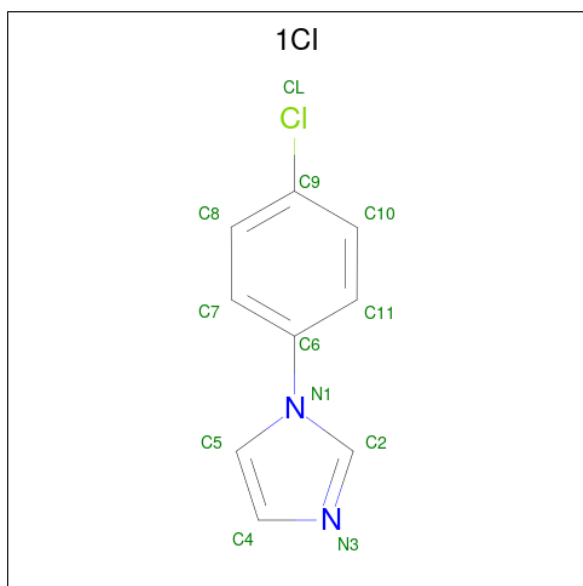
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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

- Molecule 3 is 1-(4-CHLOROPHENYL)-1H-IMIDAZOLE (CCD ID: 1CI) (formula: C₉H₇ClN₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	E	1	Total	C	Cl	N	0	0
			12	9	1	2		

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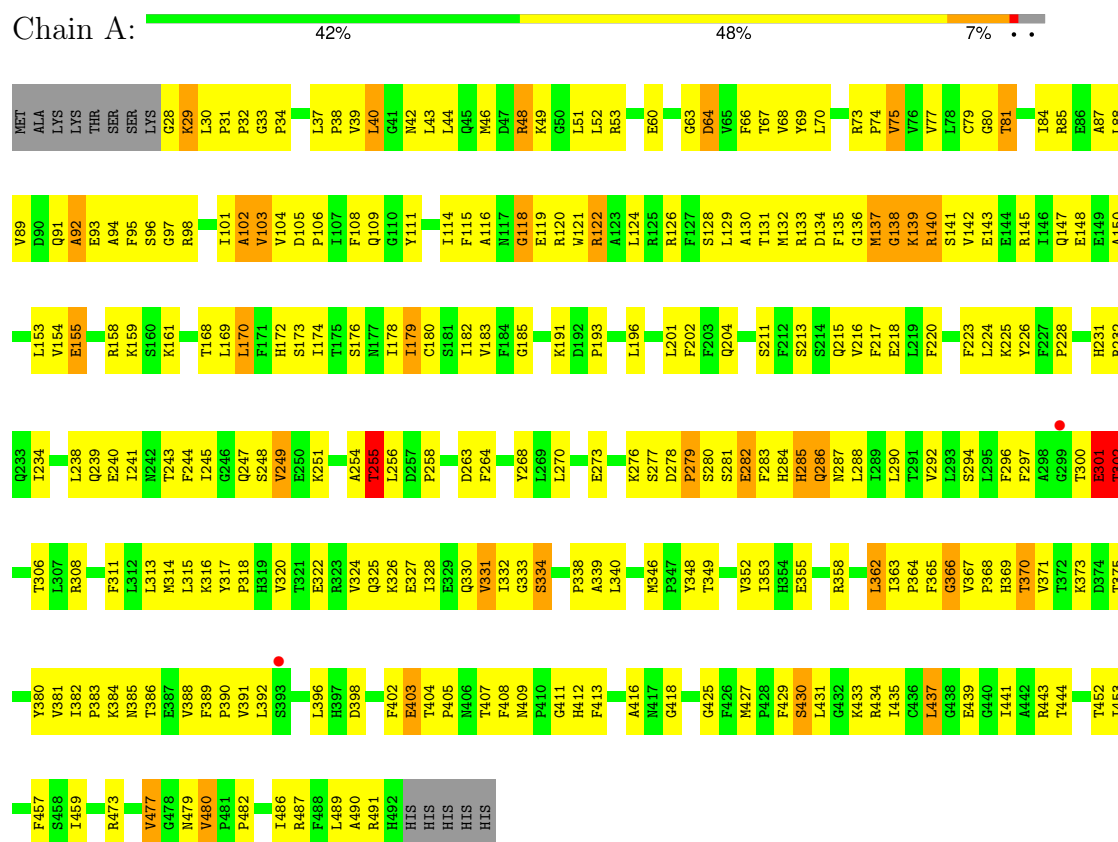
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	G	1	Total	C	Cl	N	0	0
			12	9	1	2		

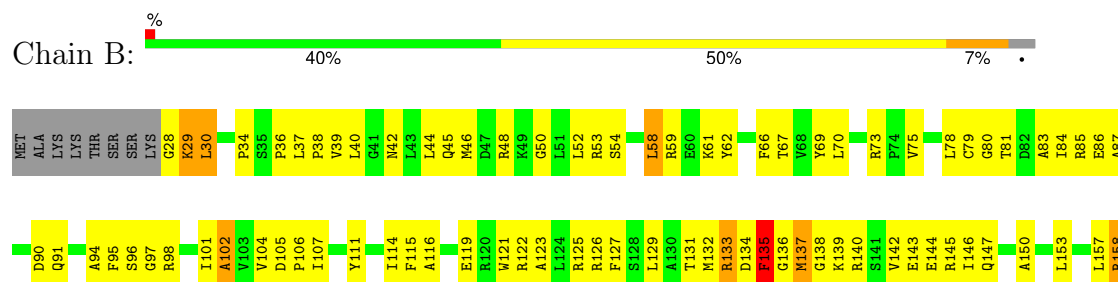
3 Residue-property plots

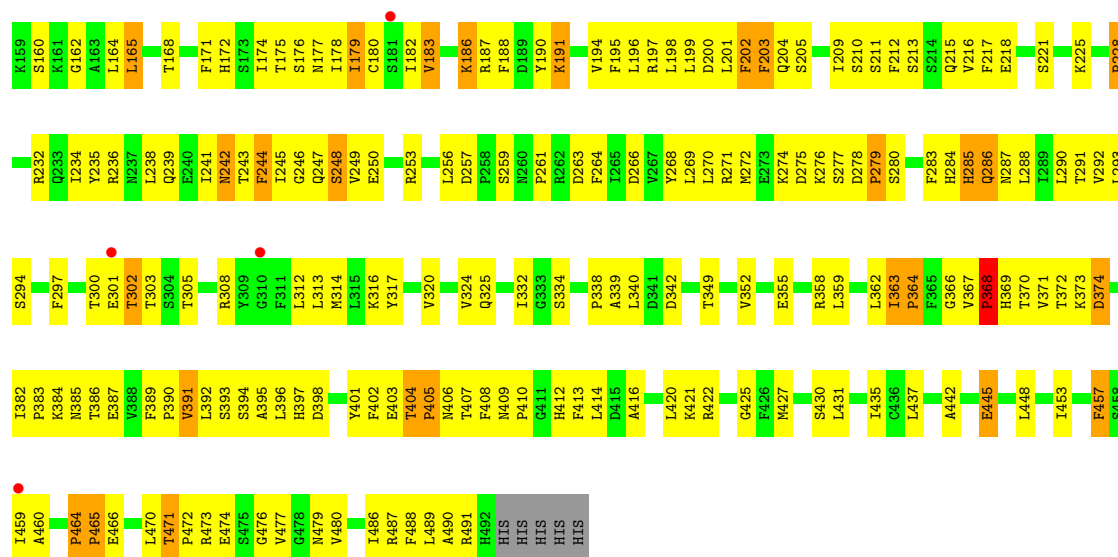
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

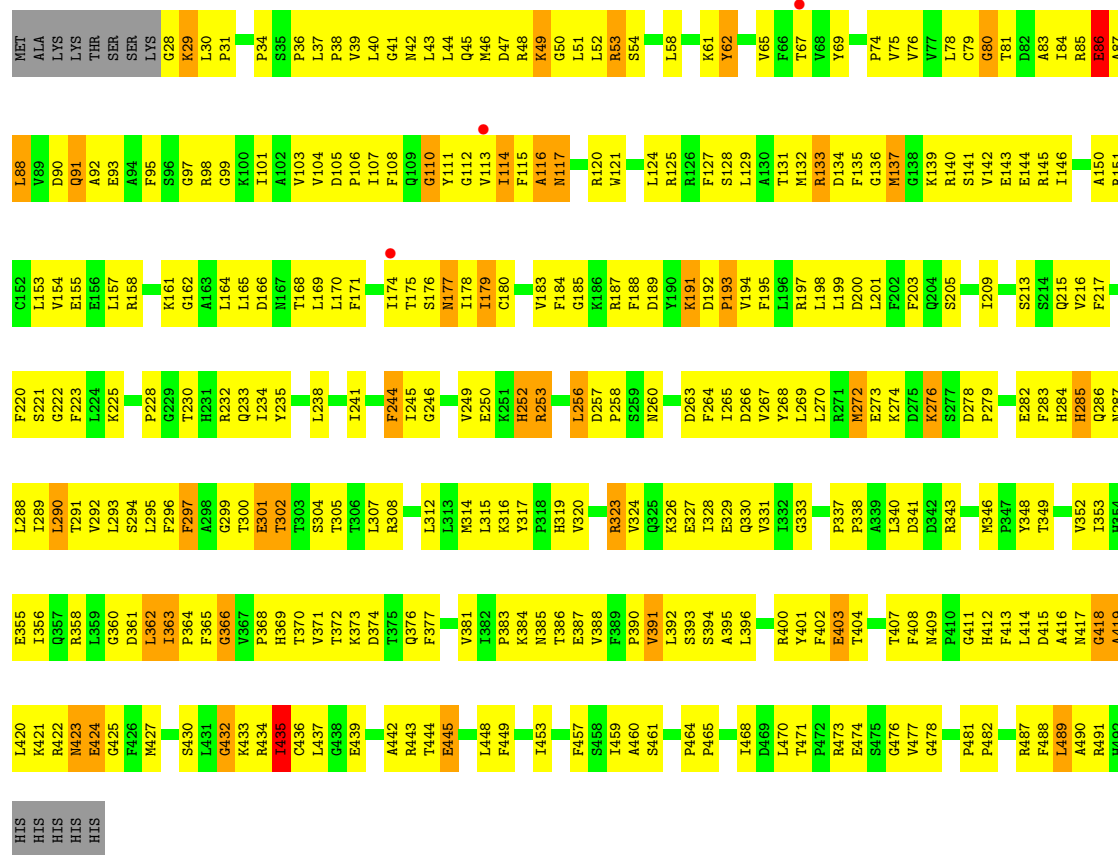


• Molecule 1: Cytochrome P450 2B4



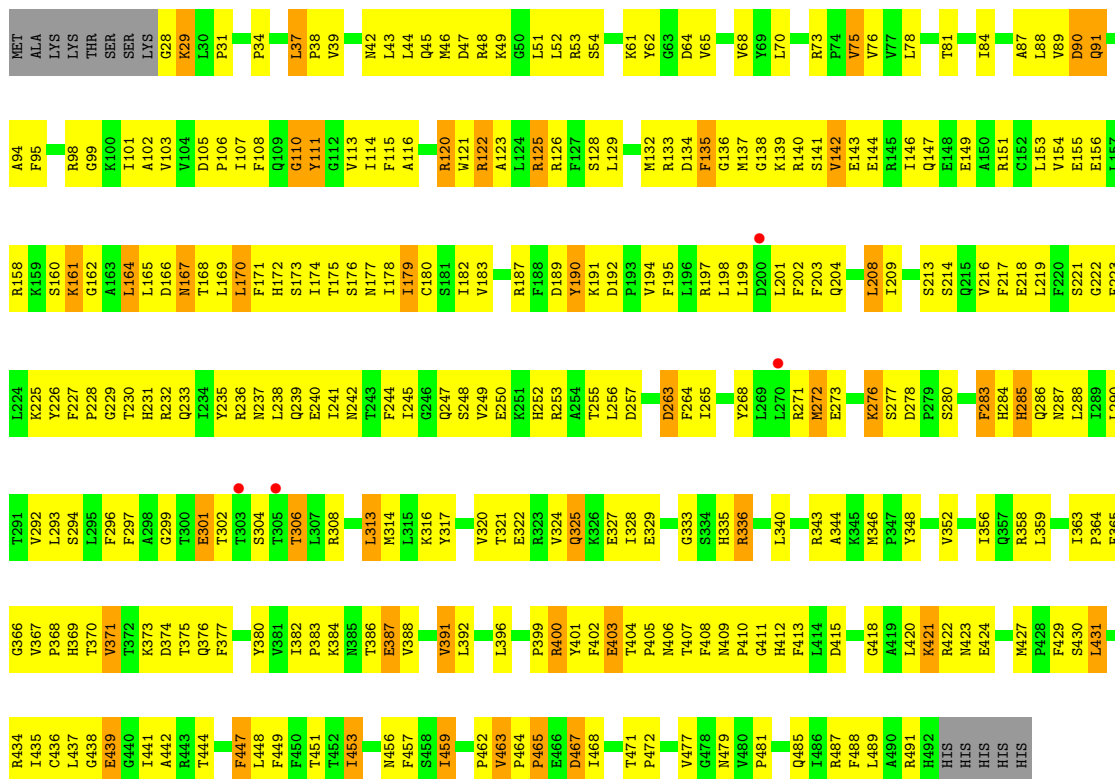


• Molecule 1: Cytochrome P450 2B4

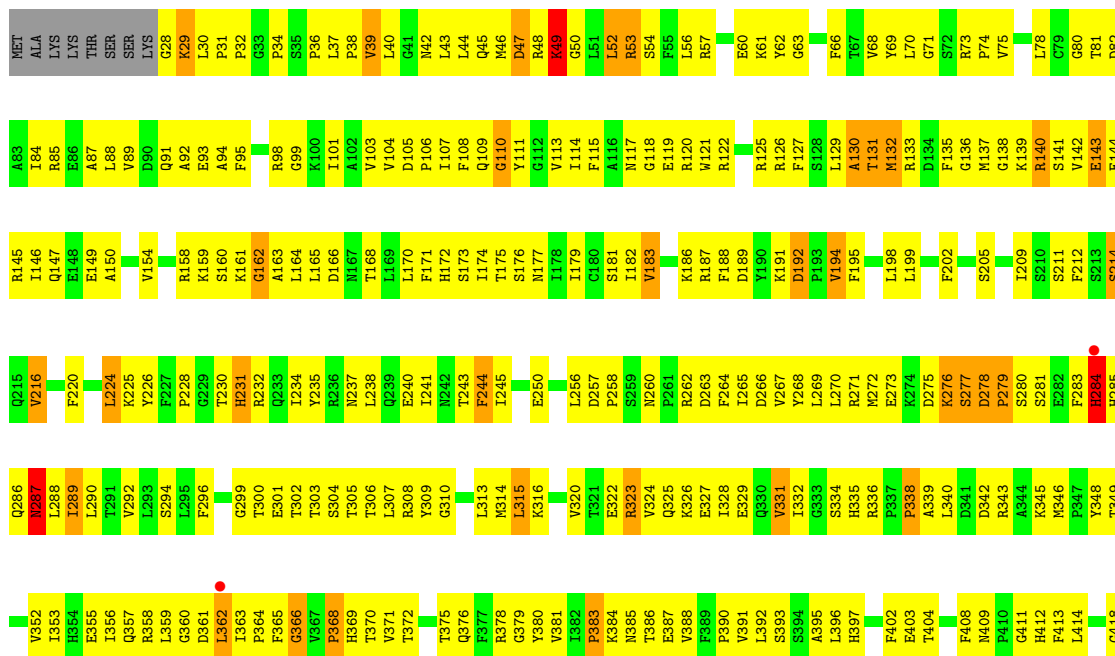


• Molecule 1: Cytochrome P450 2B4

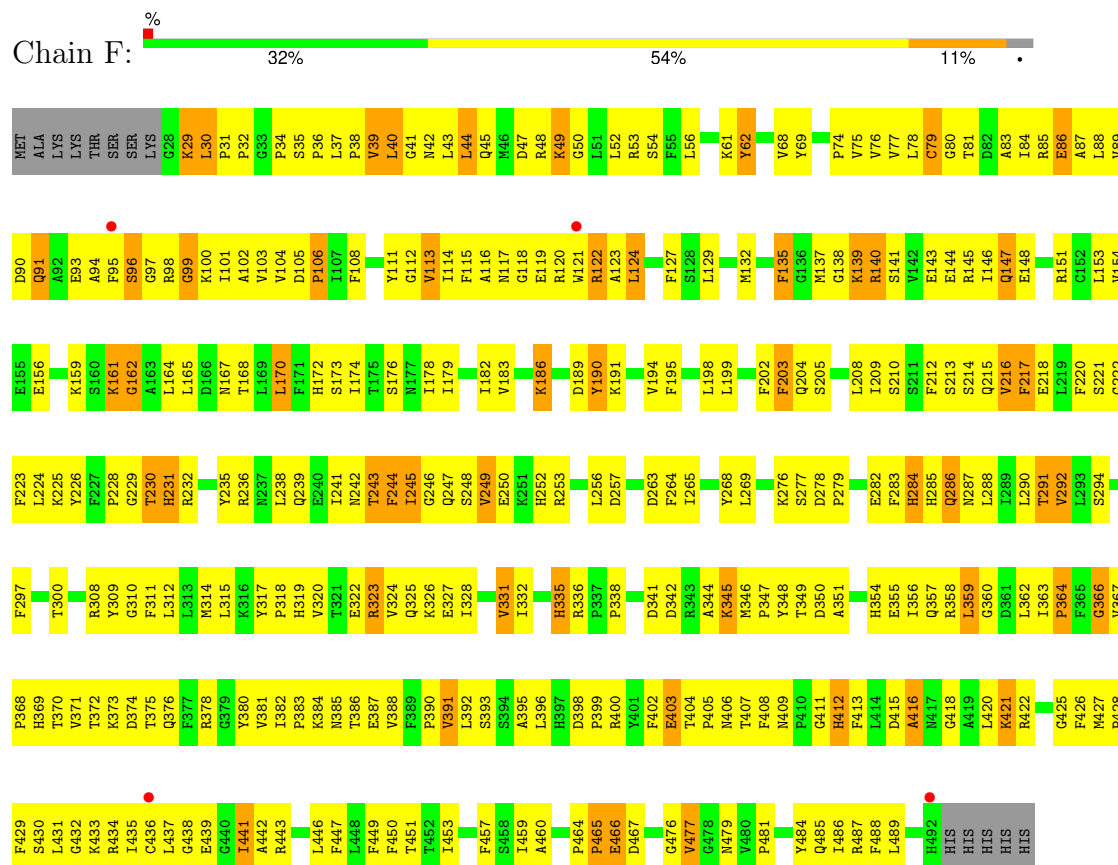




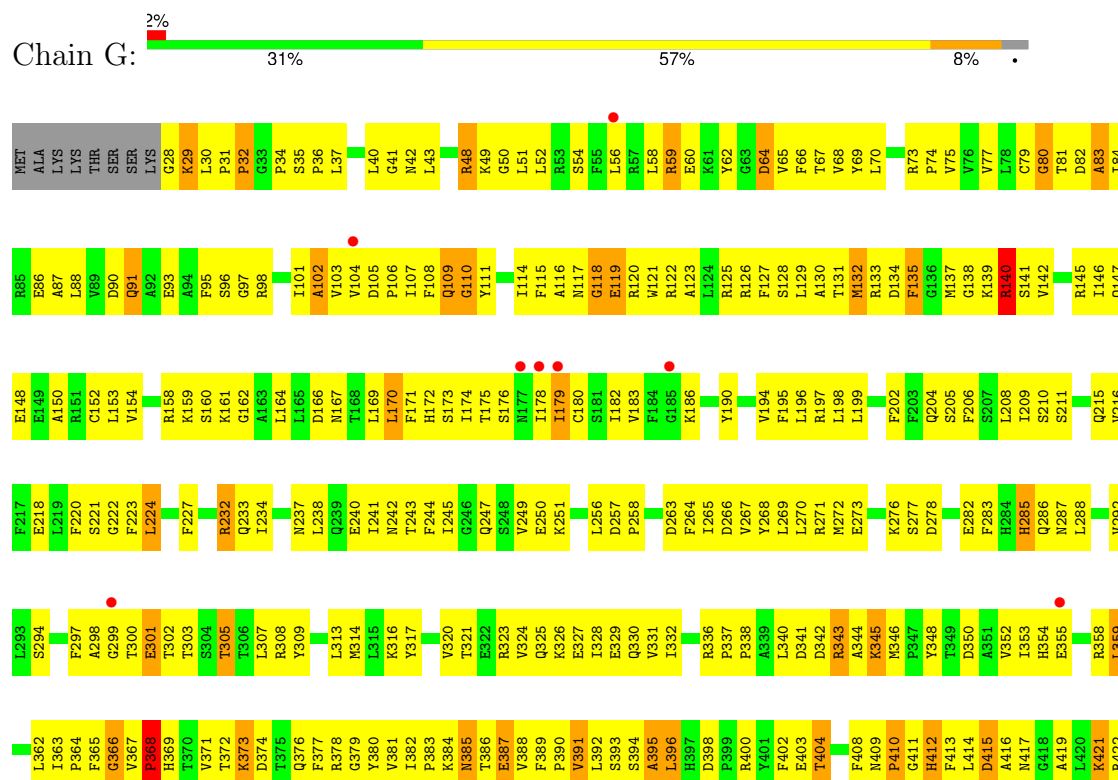
- Molecule 1: Cytochrome P450 2B4



● Molecule 1: Cytochrome P450 2B4



● Molecule 1: Cytochrome P450 2B4



M423	E424	G425	L431	G432	K433	R434	I435	C436	L437	G438	E439	G440	I441	T444	E445	I446	F447	L448	F449	F450	T451	T452	I453	L454	Q455	I459	A460	S461	P462	I468	R473	E474	V477	G478	N479	V480	P481	I486	R487	R491	R492	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.00Å 147.31Å 238.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-3.20) 99.0 (30.00-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.311 0.233 , 0.308	Depositor DCC
R_{free} test set	4077 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26523	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.41	0/3828	0.97	16/5181 (0.3%)
1	B	0.37	0/3828	0.93	18/5181 (0.3%)
1	C	0.35	0/3828	0.90	19/5181 (0.4%)
1	D	0.37	0/3828	0.96	21/5181 (0.4%)
1	E	0.35	0/3828	0.94	12/5181 (0.2%)
1	F	0.35	0/3828	0.91	13/5181 (0.3%)
1	G	0.35	0/3828	0.94	15/5181 (0.3%)
All	All	0.37	0/26796	0.94	114/36267 (0.3%)

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	PHE	N-CA-C	-9.69	98.17	110.19
1	G	51	LEU	N-CA-C	-8.81	102.66	113.41
1	F	96	SER	N-CA-C	-8.03	103.98	113.21
1	A	302	THR	N-CA-C	8.02	119.71	110.97
1	E	183	VAL	N-CA-C	7.94	118.83	111.45
1	D	313	LEU	N-CA-C	-7.92	103.22	113.12
1	B	302	THR	N-CA-C	7.89	120.58	111.11
1	G	59	ARG	N-CA-C	-7.88	103.81	113.50
1	G	272	MET	N-CA-C	-7.85	104.19	114.31
1	A	224	LEU	N-CA-C	7.84	119.91	111.36
1	A	403	GLU	N-CA-C	-7.70	99.64	110.50
1	C	331	VAL	N-CA-C	7.51	117.59	110.53
1	F	249	VAL	N-CA-C	-7.42	102.47	113.39
1	A	398	ASP	CA-C-N	7.24	126.94	119.56
1	A	398	ASP	C-N-CA	7.24	126.94	119.56
1	F	243	THR	N-CA-C	-7.19	104.94	113.21
1	F	291	THR	N-CA-C	-7.16	104.70	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	LEU	N-CA-C	-7.14	105.09	113.88
1	D	217	PHE	N-CA-C	-7.13	104.21	113.12
1	G	396	LEU	N-CA-C	-6.95	105.34	114.31
1	F	44	LEU	N-CA-C	6.89	119.63	111.71
1	D	301	GLU	N-CA-C	6.82	119.34	111.02
1	C	144	GLU	N-CA-C	-6.79	103.95	111.36
1	D	403	GLU	N-CA-C	-6.76	99.56	110.32
1	G	273	GLU	N-CA-C	-6.64	105.18	113.28
1	D	272	MET	N-CA-C	-6.62	104.84	113.12
1	B	248	SER	N-CA-C	-6.58	104.17	112.93
1	D	302	THR	N-CA-C	6.58	118.14	110.97
1	B	457	PHE	N-CA-C	6.55	117.77	108.74
1	C	403	GLU	N-CA-C	-6.31	99.35	109.96
1	G	133	ARG	N-CA-C	-6.30	104.51	111.82
1	G	404	THR	CA-C-N	6.28	127.69	119.84
1	G	404	THR	C-N-CA	6.28	127.69	119.84
1	E	225	LYS	N-CA-C	-6.27	105.57	113.72
1	F	403	GLU	N-CA-C	-6.20	102.35	110.53
1	B	183	VAL	N-CA-C	6.19	116.88	111.56
1	B	471	THR	CA-C-N	6.10	126.12	119.89
1	B	471	THR	C-N-CA	6.10	126.12	119.89
1	F	245	ILE	N-CA-C	-6.09	105.37	112.98
1	B	473	ARG	N-CA-C	-6.04	105.95	113.38
1	E	306	THR	N-CA-C	-6.01	105.44	112.89
1	C	252	HIS	N-CA-C	-5.99	106.52	113.88
1	A	103	VAL	N-CA-C	5.98	120.50	111.89
1	B	135	PHE	N-CA-C	-5.96	103.92	113.28
1	B	363	ILE	CA-C-N	5.95	127.28	119.84
1	B	363	ILE	C-N-CA	5.95	127.28	119.84
1	C	317	TYR	CA-C-N	5.95	125.33	118.85
1	C	317	TYR	C-N-CA	5.95	125.33	118.85
1	D	142	VAL	N-CA-C	-5.93	105.28	113.00
1	D	263	ASP	N-CA-C	5.93	116.11	108.34
1	C	312	LEU	N-CA-C	-5.88	104.88	111.28
1	A	346	MET	CA-C-N	5.86	125.53	119.56
1	A	346	MET	C-N-CA	5.86	125.53	119.56
1	F	217	PHE	N-CA-C	-5.83	105.01	111.71
1	G	166	ASP	N-CA-C	-5.82	100.51	109.76
1	D	363	ILE	CA-C-N	5.78	127.07	119.84
1	D	363	ILE	C-N-CA	5.78	127.07	119.84
1	E	433	LYS	N-CA-C	-5.78	106.19	113.18
1	C	363	ILE	CA-C-N	5.76	127.05	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	ILE	C-N-CA	5.76	127.05	119.84
1	C	445	GLU	N-CA-C	-5.75	105.01	111.28
1	A	480	VAL	N-CA-C	5.72	113.53	107.76
1	C	272	MET	N-CA-C	-5.71	106.45	113.41
1	E	473	ARG	N-CA-C	-5.70	106.18	113.01
1	A	40	LEU	N-CA-C	5.67	118.40	111.82
1	D	367	VAL	CA-C-N	5.67	126.92	119.84
1	D	367	VAL	C-N-CA	5.67	126.92	119.84
1	B	445	GLU	N-CA-C	-5.64	105.21	111.36
1	E	276	LYS	N-CA-C	-5.62	105.53	112.38
1	E	459	ILE	N-CA-C	5.58	117.93	109.12
1	A	477	VAL	N-CA-C	-5.53	105.81	113.00
1	G	147	GLN	N-CA-C	-5.51	104.66	111.33
1	C	274	LYS	N-CA-C	-5.50	104.69	111.40
1	G	395	ALA	N-CA-C	-5.47	106.45	114.39
1	C	62	TYR	N-CA-C	5.45	119.23	112.59
1	D	120	ARG	N-CA-C	-5.44	105.04	110.97
1	D	459	ILE	N-CA-C	5.43	117.47	108.99
1	D	421	LYS	N-CA-C	5.42	113.23	108.78
1	C	302	THR	N-CA-C	5.41	119.38	112.34
1	C	88	LEU	N-CA-C	5.33	119.85	113.23
1	B	464	PRO	CA-C-N	5.28	126.44	119.84
1	B	464	PRO	C-N-CA	5.28	126.44	119.84
1	C	253	ARG	N-CA-C	-5.27	106.82	113.20
1	E	315	LEU	N-CA-C	-5.27	106.98	113.41
1	B	158	ARG	N-CA-C	-5.26	105.54	111.28
1	E	192	ASP	CA-C-N	5.26	124.71	119.24
1	E	192	ASP	C-N-CA	5.26	124.71	119.24
1	F	231	HIS	N-CA-C	-5.26	107.52	114.31
1	D	64	ASP	N-CA-C	-5.23	106.74	113.02
1	C	290	LEU	N-CA-C	5.22	116.66	111.07
1	F	244	PHE	N-CA-C	-5.22	106.24	113.18
1	A	396	LEU	N-CA-C	-5.22	106.76	113.23
1	G	342	ASP	N-CA-C	-5.21	106.98	113.19
1	B	242	ASN	N-CA-C	-5.21	106.92	113.28
1	D	306	THR	N-CA-C	-5.18	105.25	112.45
1	A	249	VAL	N-CA-C	-5.18	105.36	111.00
1	E	287	ASN	N-CA-C	-5.16	107.12	113.41
1	C	114	ILE	CB-CA-C	-5.16	107.33	111.71
1	F	292	VAL	N-CA-C	-5.14	105.40	111.00
1	E	244	PHE	N-CA-C	-5.13	105.58	111.07
1	D	374	ASP	N-CA-C	-5.11	100.75	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	216	VAL	N-CA-C	-5.11	105.41	110.62
1	D	37	LEU	N-CA-C	-5.10	103.04	110.08
1	A	301	GLU	N-CA-C	5.09	121.65	110.80
1	A	158	ARG	N-CA-C	-5.08	105.83	111.36
1	D	182	ILE	N-CA-C	-5.08	106.98	113.22
1	F	174	ILE	N-CA-C	5.08	115.29	110.42
1	G	251	LYS	N-CA-C	-5.07	105.83	111.36
1	D	421	LYS	CA-C-O	5.07	120.88	117.94
1	A	315	LEU	N-CA-C	-5.06	107.24	113.41
1	G	473	ARG	N-CA-C	-5.05	106.54	113.30
1	B	244	PHE	N-CA-C	-5.04	104.78	112.04
1	F	147	GLN	N-CA-C	-5.01	105.29	111.40
1	C	58	LEU	N-CA-C	-5.01	106.34	112.90

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	259	0
1	B	3734	0	3744	278	0
1	C	3734	0	3744	334	0
1	D	3734	0	3744	293	0
1	E	3734	0	3745	347	0
1	F	3734	0	3744	345	0
1	G	3734	0	3744	325	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2149	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 41.

All (2149) 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:C:132:MET:HG3	1:C:137:MET:HE2	1.50	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:C:253:ARG:HH22	1:C:272:MET:HE1	1.34	0.90
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
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:B:253:ARG:HH22	1:B:272:MET:HE1	1.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:395:ALA:HB1	1:C:427:MET:HE3	1.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:328:ILE:HG12	1:E:346:MET:HE1	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:ILE:HB	1:F:104:VAL:HG22	1.68	0.74
1:F:132:MET:HE1	1:F:441:ILE:HD11	1.69	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:415:ASP:CG	1:G:416:ALA:H	1.96	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:G:139:LYS:C	1:G:140:ARG:HG3	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:LYS:HD2	1:F:276:LYS:C	2.15	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: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:E:272:MET:HE1	1:E:283:PHE:HD2	1.56	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:A:137:MET:O	1:A:138:GLY:C	2.33	0.71
1:F:143:GLU:O	1:F:147:GLN:HG3	1.91	0.71
1:A:132:MET:HE2	1:A:137:MET:HE3	1.72	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:D:132:MET:C	1:D:134:ASP:H	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:HB3	1:A:223:PHE:HB3	1.74	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:F:95:PHE:C	1:F:97:GLY:H	1.99	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:C:253:ARG:HH22	1:C:272:MET:CE	2.03	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: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:A:126:ARG:HE	1:A:130:ALA:HB2	1.58	0.68
1:B:284:HIS:O	1:B:285:HIS:C	2.37	0.67
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:C:395:ALA:CB	1:C:427:MET:HE3	2.25	0.67
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:F:186:LYS:HD2	1:F:186:LYS:H	1.60	0.66
1:A:129:LEU:C	1:A:129:LEU:HD23	2.21	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:E:114:ILE:HD11	2:E:500:HEM:HMD3	1.77	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:E:314:MET:HE3	1:E:356:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:73:ARG:HH21	1:D:387:GLU:CD	2.05	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:G:344:ALA:C	1:G:346:MET:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:PHE:C	1:G:97:GLY:H	2.06	0.64
1:G:137:MET:HG3	1:G:138:GLY:H	1.63	0.64
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:E:29:LYS:C	1:E:30:LEU:HD12	2.22	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	1.64	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: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: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:E:272:MET:HE1	1:E:283:PHE:CD2	2.34	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:G:299:GLY:HA2	2:G:500:HEM:HMC3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:179:ILE:HD13	1:D:179:ILE:C	2.24	0.62
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: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:G:82:ASP:C	1:G:84:ILE:H	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:ILE:HG12	1:G:346:MET:HE1	1.82	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
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:F:242:ASN:C	1:F:244:PHE:H	2.09	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:F:250:GLU:C	1:F:252:HIS:H	2.08	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:G:423:ASN:C	1:G:425:GLY:H	2.10	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:C:244:PHE:CD1	1:C:244:PHE:C	2.80	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:B:285:HIS:O	1:B:286:GLN:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:56:LEU:C	1:G:58:LEU:H	2.10	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:D:427:MET:HE2	1:D:431:LEU:HD21	1.83	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: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:34:PRO:HG2	1:E:42:ASN:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:398:ASP:OD2	1:F:400:ARG:HB2	2.04	0.58
1:G:376:GLN:CD	1:G:376:GLN:H	2.11	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:D:314:MET:HE2	1:D:314:MET:HA	1.85	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:225:LYS:C	1:D:227:PHE:H	2.10	0.58
1:D:236:ARG:O	1:D:239:GLN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:138:GLY:C	1:A:139:LYS:HD2	2.28	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
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:B:248:SER:C	1:B:250:GLU:H	2.12	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:F:229:GLY:C	1:F:231:HIS:H	2.12	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:B:253:ARG:NH2	1:B:272:MET:HE1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:161:LYS:O	1:E:162:GLY:C	2.49	0.56
1:E:171:PHE:CD2	1:E:307:LEU:HB3	2.40	0.56
1:E:271:ARG:C	1:E:272:MET:HE2	2.31	0.56
1:E:358:ARG:HD2	1:E:396:LEU:O	2.06	0.56
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:41:GLY:C	1:G:43:LEU:H	2.13	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:G:341:ASP:C	1:G:343:ARG:H	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:421:LYS:CG	1:C:422:ARG:H	2.17	0.56
1:C:437:LEU:C	1:C:437:LEU:HD23	2.31	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: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
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:F:415:ASP:CG	1:F:416:ALA:N	2.64	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: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:F:246:GLY:C	1:F:248:SER:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:ASP:C	1:B:136:GLY:H	2.14	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: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
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: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:A:60:GLU:OE2	1:A:60:GLU:HA	2.06	0.54
1:A:362:LEU:C	1:A:363:ILE:HD12	2.32	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:132:MET:C	1:D:134:ASP:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLY:HA2	1:C:225:LYS:HE3	1.89	0.54
1:C:223:PHE:C	1:C:223:PHE:CD2	2.85	0.54
1:F:29:LYS:C	1:F:30:LEU:HD23	2.32	0.54
1:G:400:ARG:HG2	1:G:400:ARG:HH11	1.71	0.54
1:B:142:VAL:C	1:B:144:GLU:N	2.64	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:F:403:GLU:O	1:F:404:THR:C	2.51	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:HD23	1:C:437:LEU:O	2.07	0.54
1:A:429:PHE:O	1:A:430:SER:HB3	2.08	0.54
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:34:PRO:HG2	1:E:42:ASN:CG	2.33	0.54
1:E:129:LEU:HG	1:E:437:LEU:HD11	1.89	0.54
1:A:136:GLY:C	1:A:142:VAL:HG23	2.33	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:F:223:PHE:C	1:F:223:PHE:CD2	2.85	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:D:438:GLY:O	1:D:439:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:403:GLU:O	1:G:404:THR:C	2.51	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:170:LEU:HD23	1:C:170:LEU:C	2.33	0.53
1:C:442:ALA:HB1	2:C:500:HEM:CBB	2.39	0.53
1:D:108:PHE:C	1:D:110:GLY:H	2.14	0.53
1:D:409:ASN:C	1:D:411:GLY:H	2.16	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:A:278:ASP:C	1:A:280:SER:H	2.16	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
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:A:213:SER:C	1:A:215:GLN:H	2.16	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:F:415:ASP:CG	1:F:416:ALA:H	2.16	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:C:187:ARG:O	1:C:187:ARG:HG3	2.07	0.53
1:F:409:ASN:HB3	1:F:412:HIS:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:HIS:ND1	1:G:300:THR:HG22	2.23	0.53
1:G:415:ASP:CG	1:G:416:ALA:N	2.66	0.53
1:A:487:ARG:CD	1:A:489:LEU:HD11	2.39	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: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:D:129:LEU:C	1:D:129:LEU:HD23	2.33	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:244:PHE:CD1	1:G:244:PHE:C	2.86	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
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:A:223:PHE:C	1:A:223:PHE:CD2	2.88	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:F:250:GLU:C	1:F:252:HIS:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:373:LYS:O	1:C:374:ASP:C	2.52	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:137:MET:HE2	1:A:441:ILE:CD1	2.39	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:132:MET:O	1:B:133:ARG:C	2.53	0.52
1:B:212:PHE:CD1	1:B:212:PHE:C	2.87	0.52
1:B:257:ASP:C	1:B:259:SER:H	2.18	0.52
1:B:373:LYS:O	1:B:374:ASP:C	2.52	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:180:CYS:C	1:G:182:ILE:H	2.17	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
1:D:285:HIS:O	1:D:286:GLN:C	2.52	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:VAL:C	1:D:91:GLN:H	2.18	0.52
1:E:78:LEU:O	1:E:84:ILE:HD11	2.09	0.52
1:E:324:VAL:O	1:E:328:ILE:HG13	2.10	0.52
1:A:34:PRO:HG2	1:A:42:ASN:CG	2.35	0.52
1:B:457:PHE:CD1	1:B:490:ALA:HA	2.45	0.52
1:D:189:ASP:C	1:D:191:LYS:H	2.17	0.52
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.45	0.52
1:E:375:THR:HG22	1:E:376:GLN:N	2.25	0.52
1:F:165:LEU:C	1:F:165:LEU:HD12	2.35	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:F:285:HIS:O	1:F:286:GLN:C	2.53	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:F:223:PHE:C	1:F:223:PHE:HD2	2.18	0.51
1:G:80:GLY:O	1:G:84:ILE:HG12	2.10	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
1:D:111:TYR:HB2	1:D:290:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:127:PHE:C	1:B:127:PHE:CD1	2.89	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:E:138:GLY:C	1:E:139:LYS:HD3	2.35	0.51
1:E:435:ILE:O	1:E:436:CYS:C	2.53	0.51
1:F:52:LEU:C	1:F:54:SER:H	2.17	0.51
1:G:341:ASP:C	1:G:343:ARG:N	2.69	0.51
1:A:49:LYS:CE	1:A:53:ARG:HE	2.24	0.51
1:B:248:SER:C	1:B:250:GLU:N	2.65	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:D:149:GLU:CD	1:D:187:ARG:HH21	2.19	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: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:B:73:ARG:NH2	1:B:387:GLU:CD	2.69	0.51
1:D:316:LYS:O	1:D:465:PRO:HB3	2.10	0.51
1:D:409:ASN:C	1:D:411:GLY:N	2.69	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:285:HIS:O	1:A:286:GLN:C	2.52	0.51
1:A:487:ARG:HD2	1:A:489:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLY:C	1:C:142:VAL:HB	2.36	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:235:TYR:O	1:F:236:ARG:C	2.54	0.51
1:F:246:GLY:O	1:F:249:VAL:HG12	2.11	0.51
1:G:459:ILE:O	1:G:460:ALA:HB2	2.10	0.51
1:A:213:SER:C	1:A:215:GLN:N	2.68	0.50
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:E:129:LEU:O	1:E:130:ALA:C	2.55	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:127:PHE:C	1:E:127:PHE:CD1	2.89	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: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:D:160:SER:O	1:D:161:LYS:C	2.54	0.50
1:F:47:ASP:HB3	1:F:54:SER:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:ARG:HA	1:F:282:GLU:HG3	1.93	0.50
1:F:328:ILE:HG12	1:F:346:MET:HE1	1.94	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:D:201:LEU:HD11	1:D:240:GLU:CD	2.37	0.50
1:E:195:PHE:CZ	1:E:199:LEU:HD11	2.47	0.50
1:E:395:ALA:HB1	1:E:427:MET:HE3	1.94	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: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:B:395:ALA:HB1	1:B:427:MET:HE3	1.94	0.50
1:C:28:GLY:O	1:C:29:LYS:HG2	2.11	0.50
1:C:38:PRO:C	1:C:40:LEU:H	2.18	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:E:476:GLY:C	1:E:478:GLY:H	2.20	0.50
1:F:39:VAL:O	1:F:41:GLY:N	2.44	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:328:ILE:HG12	1:C:346:MET:HE1	1.92	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: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:B:165:LEU:HD12	1:B:486:ILE:O	2.11	0.49

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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	0.49
1:C:30:LEU:HD21	1:C:383:PRO:HD2	1.94	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: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: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
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:390:PRO:O	1:F:391:VAL:C	2.55	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: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:F:405:PRO:C	1:F:407:THR:H	2.20	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:328:ILE:HA	1:C:346:MET:HE3	1.95	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:263:ASP:OD1	1:E:265:ILE:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:LEU:HD21	1:F:369:HIS:NE2	2.27	0.49
1:F:189:ASP:C	1:F:191:LYS:H	2.21	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:427:MET:HE2	1:A:431:LEU:HD11	1.95	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
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:C:434:ARG:O	1:C:435:ILE:C	2.55	0.49
1:D:229:GLY:C	1:D:231:HIS:H	2.20	0.49
1:D:413:PHE:O	1:D:420:LEU:HD12	2.13	0.49
1:E:42:ASN:ND2	1:E:69:TYR:HB2	2.28	0.49
1:E:277:SER:O	1:E:278:ASP:C	2.56	0.49
1:F:99:GLY:H	1:F:368:PRO:C	2.20	0.49
1:G:65:VAL:HG21	1:G:377:PHE:CE2	2.47	0.49
1:G:355:GLU:CD	1:G:358:ARG:HH21	2.21	0.49
1:A:284:HIS:O	1:A:285:HIS:C	2.55	0.49
1:B:316:LYS:HD3	1:B:317:TYR:HE1	1.76	0.49
1:B:340:LEU:C	1:B:342:ASP:H	2.20	0.49
1:C:49:LYS:HE3	1:C:53:ARG:HH12	1.74	0.49
1:D:137:MET:HE3	1:D:138:GLY:N	2.27	0.49
1:D:139:LYS:HG3	1:D:139:LYS:O	2.12	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:E:121:TRP:CZ2	1:E:434:ARG:HD3	2.47	0.49
1:E:131:THR:OG1	1:E:135:PHE:HD1	1.95	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: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:D:411:GLY:C	1:D:413:PHE:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ALA:C	1:D:346:MET:H	2.20	0.48
1:D:449:PHE:O	1:D:453:ILE:HG13	2.14	0.48
1:E:137:MET:HA	1:E:137:MET:HE3	1.95	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:314:MET:HE2	1:A:314:MET:HA	1.95	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:F:268:TYR:CE1	1:F:288:LEU:HB2	2.48	0.48
1:F:373:LYS:C	1:F:375:THR:H	2.21	0.48
1:G:325:GLN:NE2	1:G:491:ARG:HH11	2.09	0.48
1:A:28:GLY:C	1:A:29:LYS:HG2	2.38	0.48
1:C:360:GLY:O	1:C:361:ASP:C	2.56	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:327:GLU:CD	1:F:346:MET:HA	2.39	0.48
1:G:364:PRO:HG3	1:G:479:ASN:HD22	1.77	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:A:409:ASN:C	1:A:411:GLY:H	2.21	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:C:476:GLY:C	1:C:478:GLY:H	2.21	0.48
1:D:37:LEU:HD13	1:D:44:LEU:HD13	1.95	0.48
1:E:108:PHE:C	1:E:110:GLY:H	2.21	0.48
1:F:61:LYS:HD3	1:F:62:TYR:CE2	2.48	0.48
1:G:197:ARG:HH21	1:G:240:GLU:CD	2.20	0.48
1:A:136:GLY:HA3	1:A:145:ARG:HH12	1.79	0.48
1:B:211:SER:HA	1:B:474:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:327:GLU:O	1:E:346:MET:HE3	2.13	0.48
1:F:39:VAL:C	1:F:41:GLY:H	2.22	0.48
1:F:411:GLY:C	1:F:413:PHE:N	2.72	0.48
1:F:465:PRO:C	1:F:467:ASP:H	2.20	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
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:E:139:LYS:O	1:E:140:ARG:C	2.57	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: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:225:LYS:C	1:D:227:PHE:N	2.71	0.48
1:D:247:GLN:O	1:D:250:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:407:THR:O	1:A:408:PHE:C	2.55	0.48
1:B:142:VAL:C	1:B:144:GLU:H	2.20	0.48
1:C:52:LEU:C	1:C:54:SER:H	2.21	0.48
1:C:188:PHE:HB2	1:C:195:PHE:CG	2.48	0.48
1:D:358:ARG:HG3	1:D:396:LEU:HB3	1.94	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:B:480:VAL:O	1:B:480:VAL:HG13	2.13	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:E:52:LEU:HD23	1:E:53:ARG:HH12	1.78	0.47
1:E:244:PHE:CD1	1:E:244:PHE:C	2.91	0.47
1:F:162:GLY:HA2	1:F:488:PHE:O	2.14	0.47
1:G:477:VAL:HG13	1:G:478:GLY:N	2.29	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:122:ARG:C	1:E:126:ARG:HD3	2.39	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:90:ASP:O	1:F:91:GLN:CB	2.61	0.47
1:F:312:LEU:HD13	1:F:484:TYR:CD2	2.48	0.47
1:A:140:ARG:O	1:A:141:SER:C	2.57	0.47
1:A:153:LEU:HB2	1:A:174:ILE:HG21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:376:GLN:CD	1:E:376:GLN:C	2.82	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:277:SER:O	1:G:278:ASP:C	2.57	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:203:PHE:C	1:F:205:SER:H	2.23	0.47
1:F:384:LYS:O	1:F:385:ASN:HB2	2.13	0.47
1:G:82:ASP:C	1:G:84:ILE:N	2.72	0.47
1:B:54:SER:O	1:B:58:LEU:HG	2.15	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:B:275:ASP:O	1:B:276:LYS:C	2.57	0.47
1:B:407:THR:O	1:B:408:PHE:C	2.58	0.47
1:C:270:LEU:C	1:C:272:MET:H	2.23	0.47
1:D:141:SER:C	1:D:143:GLU:N	2.70	0.47
1:D:288:LEU:O	1:D:292:VAL:HG23	2.15	0.47
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:223:PHE:C	1:A:223:PHE:HD2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:PHE:C	1:D:244:PHE:CD1	2.93	0.47
1:D:371:VAL:C	1:D:373:LYS:H	2.22	0.47
1:E:129:LEU:HG	1:E:437:LEU:CD1	2.45	0.47
1:E:275:ASP:C	1:E:277:SER:N	2.71	0.47
1:E:310:GLY:O	1:E:314:MET:HG2	2.15	0.47
1:F:85:ARG:O	1:F:86:GLU:C	2.57	0.47
1:G:118:GLY:O	1:G:119:GLU:C	2.58	0.47
1:G:146:ILE:HG12	1:G:178:ILE:HD12	1.97	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:108:PHE:C	1:D:110:GLY:N	2.71	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: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
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:D:287:ASN:O	1:D:288:LEU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:95:PHE:C	1:G:97:GLY:N	2.72	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:E:104:VAL:O	1:E:105:ASP:C	2.58	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:F:286:GLN:O	1:F:287:ASN:C	2.58	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: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:158:ARG:C	1:E:160:SER:H	2.23	0.46
1:E:250:GLU:OE2	1:E:250:GLU:HA	2.15	0.46
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:B:287:ASN:O	1:B:291:THR:HB	2.15	0.46
1:B:362:LEU:C	1:B:363:ILE:HG13	2.40	0.46
1:D:141:SER:C	1:D:143:GLU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASN:C	1:A:411:GLY:N	2.73	0.46
1:B:466:GLU:OE1	1:B:466:GLU:N	2.37	0.46
1:C:46:MET:HE3	1:C:54:SER:OG	2.15	0.46
1:C:253:ARG:NH2	1:C:272:MET:HE1	2.15	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:F:364:PRO:HD2	1:F:477:VAL:C	2.41	0.46
1:G:116:ALA:HB1	1:G:120:ARG:HD2	1.97	0.46
1:G:134:ASP:O	1:G:135:PHE:C	2.58	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:215:GLN:C	1:A:217:PHE:N	2.72	0.46
1:A:281:SER:C	1:A:283:PHE:H	2.23	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:399:PRO:C	1:D:401:TYR:N	2.74	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:F:119:GLU:C	1:F:121:TRP:N	2.73	0.46
1:G:298:ALA:C	1:G:300:THR:N	2.72	0.46
1:G:422:ARG:CG	1:G:423:ASN:N	2.79	0.46
1:C:43:LEU:HD22	1:C:220:PHE:CZ	2.50	0.46
1:C:139:LYS:HZ2	1:C:140:ARG:HD3	1.81	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:212:PHE:CD1	1:E:212:PHE:C	2.93	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:355:GLU:CD	1:E:358:ARG:HH21	2.23	0.46
1:F:52:LEU:C	1:F:54:SER:N	2.72	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:A:244:PHE:C	1:A:244:PHE:CD1	2.93	0.46
1:B:101:ILE:O	1:B:102:ALA:C	2.58	0.46
1:B:121:TRP:C	1:B:123:ALA:N	2.73	0.46
1:D:189:ASP:C	1:D:191:LYS:N	2.74	0.46
1:E:93:GLU:O	1:E:94:ALA:C	2.58	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:F:432:GLY:C	1:F:434:ARG:H	2.24	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:166:ASP:OD1	1:E:168:THR:HB	2.15	0.46
1:E:231:HIS:ND1	1:E:231:HIS:C	2.73	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: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:B:38:PRO:C	1:B:40:LEU:H	2.24	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:324:VAL:C	1:E:326:LYS:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:447:PHE:O	1:D:448:LEU:C	2.59	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:E:241:ILE:C	1:E:243:THR:N	2.73	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: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:F:284:HIS:O	1:F:285:HIS:C	2.60	0.45
1:F:404:THR:HG1	1:F:407:THR:HB	1.80	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:B:157:LEU:O	1:B:160:SER:OG	2.29	0.45
1:C:164:LEU:HD23	1:C:487:ARG:HB3	1.98	0.45
1:D:43:LEU:C	1:D:45:GLN:H	2.25	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:262:ARG:HH21	1:E:266:ASP:CG	2.24	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:C:52:LEU:C	1:C:54:SER:N	2.72	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:134:ASP:C	1:B:136:GLY:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:176:SER:O	1:C:180:CYS:CB	2.65	0.45
1:C:285:HIS:O	1:C:286:GLN:C	2.60	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:B:135:PHE:C	1:B:135:PHE:CD1	2.94	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:D:329:GLU:CD	1:D:333:GLY:HA2	2.42	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: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:244:PHE:C	1:B:246:GLY:H	2.24	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:D:411:GLY:C	1:D:413:PHE:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:O	1:D:173:SER:HB2	2.17	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
1:G:129:LEU:C	1:G:131:THR:N	2.74	0.44
1:A:327:GLU:CD	1:A:348:TYR:HB3	2.42	0.44
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:D:435:ILE:O	1:D:436:CYS:C	2.59	0.44
1:F:276:LYS:NZ	1:F:277:SER:HB2	2.33	0.44
1:G:325:GLN:HE21	1:G:491:ARG:NH1	2.13	0.44
1:A:137:MET:HE2	1:A:441:ILE:HD11	2.00	0.44
1:C:223:PHE:C	1:C:223:PHE:HD2	2.25	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:F:256:LEU:HG	1:F:257:ASP:N	2.32	0.44
1:G:41:GLY:C	1:G:43:LEU:N	2.76	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:D:53:ARG:HA	1:D:53:ARG:NH1	2.21	0.44
1:D:221:SER:C	1:D:223:PHE:N	2.75	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: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:116:ALA:C	1:F:121:TRP:HB2	2.43	0.44
1:A:281:SER:C	1:A:283:PHE:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:ASN:C	1:F:244:PHE:N	2.75	0.44
1:F:411:GLY:C	1:F:413:PHE:H	2.25	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: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:B:410:PRO:C	1:B:414:LEU:HD12	2.42	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
1:F:121:TRP:O	1:F:123:ALA:N	2.51	0.44
1:F:244:PHE:CD1	1:F:244:PHE:C	2.94	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:417:ASN:C	1:G:419:ALA:H	2.26	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:C:418:GLY:O	1:C:419:ALA:C	2.60	0.44
1:D:111:TYR:N	1:D:111:TYR:CD1	2.86	0.44
1:D:223:PHE:C	1:D:223:PHE:CD2	2.95	0.44
1:D:239:GLN:OE1	1:D:239:GLN:HA	2.18	0.44
1:E:324:VAL:C	1:E:326:LYS:N	2.76	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:158:ARG:C	1:G:160:SER:H	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:ARG:HG3	1:E:272:MET:HE2	2.00	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: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: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:B:30:LEU:HD22	1:B:383:PRO:HD3	2.00	0.43
1:B:201:LEU:C	1:B:202:PHE:O	2.58	0.43
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: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:98:ARG:H	1:F:117:ASN:CG	2.26	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:213:SER:HA	1:C:228:PRO:HB3	2.00	0.43
1:B:244:PHE:C	1:B:244:PHE:CD1	2.96	0.43
1:B:367:VAL:O	1:B:368:PRO:C	2.60	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:G:364:PRO:CG	1:G:479:ASN:ND2	2.80	0.43
1:B:137:MET:C	1:B:139:LYS:H	2.27	0.43
1:B:249:VAL:HG11	1:B:288:LEU:CD2	2.48	0.43
1:B:257:ASP:C	1:B:259:SER:N	2.76	0.43
1:B:373:LYS:HD2	1:B:373:LYS:C	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:MET:HE2	1:C:51:LEU:HD23	2.00	0.43
1:C:90:ASP:O	1:C:91:GLN:CG	2.61	0.43
1:C:139:LYS:HZ3	1:C:143:GLU:CD	2.26	0.43
1:C:166:ASP:C	1:C:168:THR:H	2.26	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:E:409:ASN:C	1:E:411:GLY:H	2.25	0.43
1:E:409:ASN:C	1:E:411:GLY:N	2.75	0.43
1:B:50:GLY:O	1:B:54:SER:HB2	2.19	0.43
1:B:153:LEU:CD2	1:B:174:ILE:HD13	2.45	0.43
1:C:188:PHE:HB3	1:C:195:PHE:HB2	2.00	0.43
1:C:270:LEU:C	1:C:272:MET:N	2.75	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:99:GLY:HA3	1:E:368:PRO:C	2.44	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:203:PHE:C	1:F:205:SER:N	2.74	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:438:GLY:O	1:G:439:GLU:C	2.61	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:371:VAL:C	1:D:373:LYS:N	2.76	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:344:ALA:C	1:G:346:MET:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:226:TYR:O	1:E:216:VAL:HG21	2.18	0.43
1:E:135:PHE:C	1:E:135:PHE:CD2	2.94	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:F:344:ALA:C	1:F:346:MET:H	2.26	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:253:ARG:HH22	1:B:272:MET:CE	2.21	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
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: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:135:PHE:HZ	1:B:263:ASP:C	2.27	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: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: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:101:ILE:O	1:A:102:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:ILE:O	1:A:182:ILE:HD13	2.19	0.43
1:B:85:ARG:O	1:B:86:GLU:C	2.61	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:39:VAL:C	1:F:41:GLY:N	2.76	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
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:166:ASP:C	1:C:168:THR:N	2.75	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:C:489:LEU:O	1:C:490:ALA:C	2.62	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:91:GLN:O	1:E:93:GLU:N	2.52	0.42
1:E:241:ILE:C	1:E:243:THR:H	2.26	0.42
1:E:309:TYR:HE2	1:E:313:LEU:HD12	1.84	0.42
1:F:369:HIS:HE1	2:F:500:HEM:O2A	2.02	0.42
1:A:287:ASN:O	1:A:288:LEU:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:ARG:HG3	1:E:272:MET:CE	2.49	0.42
1:F:119:GLU:C	1:F:121:TRP:H	2.27	0.42
1:F:121:TRP:O	1:F:122:ARG:C	2.62	0.42
1:F:127:PHE:C	1:F:129:LEU:H	2.26	0.42
1:F:139:LYS:O	1:F:140:ARG:C	2.61	0.42
1:F:399:PRO:HA	1:F:402:PHE:O	2.20	0.42
1:G:137:MET:CG	1:G:138:GLY:H	2.25	0.42
1:G:409:ASN:C	1:G:411:GLY:H	2.27	0.42
1:A:95:PHE:C	1:A:97:GLY:H	2.27	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: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
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:B:96:SER:HB3	1:B:372:THR:CG2	2.49	0.42
1:C:176:SER:C	1:C:178:ILE:H	2.27	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: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:G:127:PHE:O	1:G:128:SER:C	2.62	0.42
1:G:423:ASN:C	1:G:425:GLY:N	2.74	0.42
1:A:103:VAL:HG23	1:A:104:VAL:HG13	2.00	0.42
1:B:266:ASP:O	1:B:270:LEU:HG	2.19	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:179:ILE:HD13	1:D:179:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLN:NE2	1:D:237:ASN:OD1	2.52	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:264:PHE:CD1	1:G:264:PHE:C	2.97	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
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:A:215:GLN:C	1:A:217:PHE:H	2.25	0.42
1:B:268:TYR:CG	1:B:288:LEU:HD13	2.55	0.42
1:C:36:PRO:C	1:C:37:LEU:HD12	2.45	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:C:470:LEU:O	1:C:471:THR:C	2.63	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:F:159:LYS:C	1:F:161:LYS:H	2.28	0.42
1:F:189:ASP:C	1:F:191:LYS:N	2.76	0.42
1:G:153:LEU:HD13	1:G:170:LEU:HD22	2.02	0.42
1:G:256:LEU:HD12	1:G:256:LEU:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:407:THR:HG22	1:C:408:PHE:N	2.35	0.42
1:C:416:ALA:HB3	1:G:267:VAL:HG11	2.01	0.42
1:D:403:GLU:O	1:D:404:THR:C	2.61	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: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:199:LEU:O	1:C:200:ASP:C	2.63	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
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:D:139:LYS:C	1:D:144:GLU:HG3	2.45	0.42
1:E:29:LYS:O	1:E:30:LEU:HD12	2.19	0.42
1:E:82:ASP:O	1:E:85:ARG:HB2	2.20	0.42
1:F:36:PRO:O	1:F:37:LEU:C	2.62	0.42
1:F:98:ARG:HD3	1:F:368:PRO:O	2.20	0.42
1:F:322:GLU:O	1:F:326:LYS:HB2	2.20	0.42
1:F:441:ILE:O	1:F:442:ALA:C	2.63	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:221:SER:C	1:G:223:PHE:N	2.78	0.42
1:G:353:ILE:CD1	1:G:447:PHE:HA	2.50	0.42
1:A:63:GLY:O	1:A:64:ASP:C	2.63	0.42
1:A:143:GLU:O	1:A:147:GLN:HG3	2.19	0.42
1:A:277:SER:C	1:A:279:PRO:HD3	2.45	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:E:270:LEU:C	1:E:272:MET:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:ARG:O	1:E:435:ILE:C	2.63	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:91:GLN:C	1:A:93:GLU:H	2.27	0.41
1:A:487:ARG:HG3	1:A:489:LEU:CD1	2.49	0.41
1:C:265:ILE:O	1:C:266:ASP:C	2.62	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: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:211:SER:HA	1:G:474:GLU:CD	2.45	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:390:PRO:O	1:G:391:VAL:C	2.61	0.41
1:A:434:ARG:O	1:A:435:ILE:C	2.64	0.41
1:B:61:LYS:C	1:B:62:TYR:CD2	2.99	0.41
1:C:176:SER:C	1:C:178:ILE:N	2.78	0.41
1:C:403:GLU:O	1:C:403:GLU:HG3	2.20	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:G:42:ASN:HD22	1:G:42:ASN:N	2.18	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:136:GLY:O	1:A:137:MET:C	2.62	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: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:43:LEU:C	1:E:45:GLN:H	2.27	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:113:VAL:C	1:E:114:ILE:HD12	2.45	0.41
1:E:273:GLU:C	1:E:275:ASP:H	2.28	0.41
1:E:464:PRO:HA	1:E:465:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:367:VAL:O	1:G:368:PRO:C	2.64	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:E:85:ARG:C	1:E:87:ALA:N	2.77	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: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: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
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:C:403:GLU:C	1:C:404:THR:HG22	2.45	0.41
1:F:42:ASN:O	1:F:43:LEU:C	2.63	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: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:278:ASP:C	1:D:280:SER:H	2.28	0.41
1:E:40:LEU:C	1:E:71:GLY:HA2	2.46	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:460:ALA:O	1:F:487:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:PHE:O	1:A:218:GLU:C	2.64	0.41
1:A:439:GLU:O	1:A:443:ARG:HG3	2.21	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:253:ARG:C	1:D:255:THR:H	2.29	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
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:51:LEU:O	1:A:52:LEU:C	2.62	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:A:411:GLY:C	1:A:413:PHE:N	2.78	0.41
1:A:416:ALA:C	1:A:418:GLY:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:ASP:OD1	1:E:364:PRO:HA	2.21	0.41
1:F:95:PHE:C	1:F:97:GLY:N	2.66	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:314:MET:HE2	1:G:314:MET:N	2.36	0.41
1:G:350:ASP:O	1:G:354:HIS:ND1	2.53	0.41
1:G:393:SER:C	1:G:395:ALA:H	2.28	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:B:404:THR:C	1:B:406:ASN:H	2.29	0.41
1:C:197:ARG:O	1:C:198:LEU:C	2.64	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
1:G:451:THR:O	1:G:452:THR:C	2.64	0.41
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.21	0.40
1:A:403:GLU:O	1:A:404:THR:C	2.65	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:100:LYS:HE2	1:F:105:ASP:CG	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:C	1:A:87:ALA:N	2.79	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: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:276:LYS:C	1:D:278:ASP:H	2.30	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:209:ILE:O	1:F:209:ILE:HG22	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:G:411:GLY:C	1:G:413:PHE:N	2.78	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:81:THR:HG23	1:B:427:MET:HE3	2.03	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:250:GLU:C	1:C:252:HIS:H	2.30	0.40
1:C:370:THR:HG23	1:C:386:THR:H	1.87	0.40
1:C:393:SER:C	1:C:395:ALA:N	2.78	0.40
1:F:441:ILE:H	1:F:441:ILE:HG13	1.69	0.40
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: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:B:277:SER:O	1:B:278:ASP:C	2.64	0.40
1:C:47:ASP:O	1:C:48:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:304:SER:C	1:D:306:THR:H	2.30	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:E:322:GLU:O	1:E:323:ARG:C	2.64	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:203:PHE:O	1:B:204:GLN:C	2.65	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: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:E:359:LEU:O	1:E:360:GLY:C	2.65	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:F:318:PRO:O	1:F:319:HIS:C	2.64	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
1:G:139:LYS:C	1:G:141:SER:H	2.30	0.40
1:G:221:SER:C	1:G:223:PHE:H	2.30	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%)	1	13
1	B	463/478 (97%)	365 (79%)	76 (16%)	22 (5%)	2	14
1	C	463/478 (97%)	356 (77%)	80 (17%)	27 (6%)	1	10
1	D	463/478 (97%)	360 (78%)	82 (18%)	21 (4%)	2	15
1	E	463/478 (97%)	366 (79%)	69 (15%)	28 (6%)	1	10
1	F	463/478 (97%)	327 (71%)	97 (21%)	39 (8%)	0	4
1	G	463/478 (97%)	339 (73%)	88 (19%)	36 (8%)	1	5
All	All	3241/3346 (97%)	2493 (77%)	552 (17%)	196 (6%)	1	10

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
1	D	336	ARG
1	E	301	GLU

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Mol	Chain	Res	Type
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
1	F	122	ARG
1	F	230	THR

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Mol	Chain	Res	Type
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
1	G	32	PRO
1	G	83	ALA

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Mol	Chain	Res	Type
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
1	E	368	PRO
1	E	385	ASN

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Mol	Chain	Res	Type
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
1	F	162	GLY
1	F	364	PRO

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Mol	Chain	Res	Type
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%)	24	58
1	B	411/423 (97%)	402 (98%)	9 (2%)	45	71
1	C	411/423 (97%)	394 (96%)	17 (4%)	27	60
1	D	411/423 (97%)	390 (95%)	21 (5%)	21	54
1	E	411/423 (97%)	388 (94%)	23 (6%)	19	52
1	F	411/423 (97%)	392 (95%)	19 (5%)	24	58
1	G	411/423 (97%)	399 (97%)	12 (3%)	37	67
All	All	2877/2961 (97%)	2757 (96%)	120 (4%)	26	60

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	73	ARG
1	A	75	VAL
1	A	81	THR
1	A	122	ARG
1	A	139	LYS
1	A	155	GLU
1	A	169	LEU
1	A	170	LEU
1	A	179	ILE
1	A	201	LEU
1	A	204	GLN
1	A	255	THR
1	A	302	THR
1	A	306	THR

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Mol	Chain	Res	Type
1	A	362	LEU
1	A	370	THR
1	A	437	LEU
1	A	477	VAL
1	B	30	LEU
1	B	135	PHE
1	B	165	LEU
1	B	179	ILE
1	B	186	LYS
1	B	191	LYS
1	B	359	LEU
1	B	368	PRO
1	B	465	PRO
1	C	53	ARG
1	C	86	GLU
1	C	165	LEU
1	C	169	LEU
1	C	179	ILE
1	C	191	LYS
1	C	244	PHE
1	C	276	LYS
1	C	323	ARG
1	C	341	ASP
1	C	362	LEU
1	C	423	ASN
1	C	424	GLU
1	C	435	ILE
1	C	439	GLU
1	C	474	GLU
1	C	489	LEU
1	D	75	VAL
1	D	111	TYR
1	D	122	ARG
1	D	125	ARG
1	D	135	PHE
1	D	164	LEU
1	D	165	LEU
1	D	170	LEU
1	D	179	ILE
1	D	208	LEU
1	D	230	THR
1	D	276	LYS

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Mol	Chain	Res	Type
1	D	325	GLN
1	D	359	LEU
1	D	371	VAL
1	D	387	GLU
1	D	431	LEU
1	D	451	THR
1	D	463	VAL
1	D	465	PRO
1	D	467	ASP
1	E	47	ASP
1	E	49	LYS
1	E	52	LEU
1	E	53	ARG
1	E	131	THR
1	E	132	MET
1	E	143	GLU
1	E	165	LEU
1	E	179	ILE
1	E	186	LYS
1	E	191	LYS
1	E	194	VAL
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
1	E	335	HIS
1	E	362	LEU
1	E	441	ILE
1	E	467	ASP
1	F	30	LEU
1	F	62	TYR
1	F	76	VAL
1	F	113	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

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Mol	Chain	Res	Type
1	F	204	GLN
1	F	216	VAL
1	F	284	HIS
1	F	323	ARG
1	F	335	HIS
1	F	341	ASP
1	F	359	LEU
1	F	466	GLU
1	F	477	VAL
1	G	132	MET
1	G	140	ARG
1	G	170	LEU
1	G	179	ILE
1	G	186	LYS
1	G	224	LEU
1	G	232	ARG
1	G	302	THR
1	G	305	THR
1	G	359	LEU
1	G	368	PRO
1	G	479	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	147	GLN
1	A	204	GLN
1	A	233	GLN
1	A	287	ASN
1	A	325	GLN
1	A	369	HIS
1	A	385	ASN
1	A	479	ASN
1	B	172	HIS
1	B	242	ASN
1	B	286	GLN
1	B	287	ASN
1	B	325	GLN
1	B	369	HIS
1	B	385	ASN
1	B	397	HIS

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Mol	Chain	Res	Type
1	B	479	ASN
1	B	492	HIS
1	C	117	ASN
1	C	215	GLN
1	C	247	GLN
1	C	260	ASN
1	C	285	HIS
1	C	330	GLN
1	C	335	HIS
1	C	369	HIS
1	C	385	ASN
1	C	412	HIS
1	C	492	HIS
1	D	45	GLN
1	D	204	GLN
1	D	233	GLN
1	D	237	ASN
1	D	284	HIS
1	D	325	GLN
1	D	354	HIS
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
1	E	325	GLN
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	167	ASN
1	F	204	GLN
1	F	233	GLN
1	F	237	ASN
1	F	319	HIS
1	F	325	GLN
1	F	330	GLN
1	F	357	GLN

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Mol	Chain	Res	Type
1	F	376	GLN
1	F	485	GLN
1	G	42	ASN
1	G	45	GLN
1	G	204	GLN
1	G	233	GLN
1	G	285	HIS
1	G	325	GLN
1	G	369	HIS
1	G	479	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	500	1,3	50,50,50	2.38	24 (48%)	67,82,82	1.38	11 (16%)
3	1CI	A	501	2	13,13,13	1.90	2 (15%)	17,17,17	0.73	0
3	1CI	C	501	2	13,13,13	1.89	2 (15%)	17,17,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	500	1,3	50,50,50	2.41	23 (46%)	67,82,82	1.42	14 (20%)
2	HEM	G	500	1,3	50,50,50	2.41	23 (46%)	67,82,82	1.48	14 (20%)
2	HEM	C	500	1,3	50,50,50	2.36	25 (50%)	67,82,82	1.40	11 (16%)
3	1CI	F	501	2	13,13,13	1.91	2 (15%)	17,17,17	0.74	0
3	1CI	G	501	2	13,13,13	1.88	2 (15%)	17,17,17	0.73	0
3	1CI	B	501	2	13,13,13	1.90	2 (15%)	17,17,17	0.78	0
2	HEM	D	500	1,3	50,50,50	2.39	21 (42%)	67,82,82	1.39	11 (16%)
2	HEM	E	500	-	50,50,50	2.47	23 (46%)	67,82,82	1.40	13 (19%)
3	1CI	D	501	2	13,13,13	1.90	2 (15%)	17,17,17	0.75	0
2	HEM	F	500	1,3	50,50,50	2.39	22 (44%)	67,82,82	1.40	13 (19%)
3	1CI	E	501	-	13,13,13	1.89	2 (15%)	17,17,17	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1,3	-	5/14/54/54	-
3	1CI	A	501	2	-	0/4/4/4	0/2/2/2
3	1CI	C	501	2	-	0/4/4/4	0/2/2/2
2	HEM	B	500	1,3	-	6/14/54/54	-
2	HEM	G	500	1,3	-	8/14/54/54	-
2	HEM	C	500	1,3	-	6/14/54/54	-
3	1CI	F	501	2	-	0/4/4/4	0/2/2/2
3	1CI	G	501	2	-	0/4/4/4	0/2/2/2
3	1CI	B	501	2	-	0/4/4/4	0/2/2/2
2	HEM	D	500	1,3	-	4/14/54/54	-
2	HEM	E	500	-	-	8/14/54/54	-
3	1CI	D	501	2	-	0/4/4/4	0/2/2/2
2	HEM	F	500	1,3	-	8/14/54/54	-
3	1CI	E	501	-	-	0/4/4/4	0/2/2/2

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	1CI	C6-N1	-5.96	1.33	1.43
3	D	501	1CI	C6-N1	-5.94	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	1CI	C6-N1	-5.91	1.33	1.43
3	E	501	1CI	C6-N1	-5.91	1.33	1.43
3	A	501	1CI	C6-N1	-5.90	1.33	1.43
3	C	501	1CI	C6-N1	-5.86	1.33	1.43
3	G	501	1CI	C6-N1	-5.83	1.33	1.43
2	E	500	HEM	C4A-NA	-4.73	1.30	1.39
2	E	500	HEM	C1D-ND	-4.67	1.29	1.38
2	A	500	HEM	C1B-NB	-4.57	1.32	1.40
2	B	500	HEM	C4A-NA	-4.45	1.31	1.39
2	F	500	HEM	C1D-ND	-4.45	1.30	1.38
2	D	500	HEM	C1D-ND	-4.41	1.30	1.38
2	G	500	HEM	C1D-ND	-4.41	1.30	1.38
2	C	500	HEM	C1D-ND	-4.38	1.30	1.38
2	A	500	HEM	C1D-ND	-4.35	1.30	1.38
2	D	500	HEM	C1B-NB	-4.33	1.32	1.40
2	E	500	HEM	C1B-NB	-4.26	1.32	1.40
2	F	500	HEM	C1B-NB	-4.25	1.32	1.40
2	G	500	HEM	C4D-ND	-4.21	1.33	1.40
2	B	500	HEM	C1C-NC	-4.21	1.31	1.39
2	B	500	HEM	C1D-ND	-4.17	1.30	1.38
2	B	500	HEM	C1B-NB	-4.15	1.33	1.40
2	A	500	HEM	C4A-NA	-4.13	1.31	1.39
2	G	500	HEM	C4A-NA	-4.08	1.31	1.39
2	F	500	HEM	C4A-NA	-4.07	1.32	1.39
2	D	500	HEM	CAC-C3C	-4.06	1.36	1.47
2	G	500	HEM	C1B-NB	-4.01	1.33	1.40
2	D	500	HEM	C4A-NA	-4.00	1.32	1.39
2	G	500	HEM	C1C-NC	-3.98	1.32	1.39
2	G	500	HEM	FE-NB	3.93	2.07	1.94
2	E	500	HEM	C1C-NC	-3.92	1.32	1.39
2	B	500	HEM	FE-ND	3.91	2.06	1.94
2	A	500	HEM	C1C-NC	-3.91	1.32	1.39
2	D	500	HEM	FE-NB	3.91	2.06	1.94
2	C	500	HEM	FE-NB	3.90	2.06	1.94
2	C	500	HEM	C1C-NC	-3.89	1.32	1.39
2	D	500	HEM	CBB-CAB	3.85	1.48	1.30
2	F	500	HEM	C1C-NC	-3.85	1.32	1.39
2	E	500	HEM	C4D-ND	-3.84	1.33	1.40
2	F	500	HEM	CAC-C3C	-3.83	1.37	1.47
2	G	500	HEM	CBB-CAB	3.80	1.48	1.30
2	C	500	HEM	CBB-CAB	3.79	1.48	1.30
2	E	500	HEM	CAC-C3C	-3.79	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	HEM	CAC-C3C	-3.78	1.37	1.47
2	F	500	HEM	CBB-CAB	3.77	1.48	1.30
2	F	500	HEM	C4D-ND	-3.76	1.33	1.40
2	C	500	HEM	C1B-NB	-3.75	1.33	1.40
2	B	500	HEM	CBB-CAB	3.75	1.48	1.30
2	E	500	HEM	CMA-C3A	3.75	1.58	1.50
2	E	500	HEM	C1C-C2C	-3.75	1.37	1.45
2	A	500	HEM	CMA-C3A	3.75	1.58	1.50
2	C	500	HEM	C4A-NA	-3.74	1.32	1.39
2	A	500	HEM	FE-NB	3.74	2.06	1.94
2	A	500	HEM	CAC-C3C	-3.73	1.37	1.47
2	E	500	HEM	FE-NB	3.72	2.06	1.94
2	F	500	HEM	FE-ND	3.69	2.06	1.94
2	A	500	HEM	CBB-CAB	3.69	1.48	1.30
2	C	500	HEM	C4D-ND	-3.68	1.33	1.40
2	E	500	HEM	CBB-CAB	3.68	1.48	1.30
2	B	500	HEM	CAC-C3C	-3.68	1.37	1.47
2	B	500	HEM	CMA-C3A	3.66	1.58	1.50
2	D	500	HEM	CMA-C3A	3.65	1.58	1.50
2	G	500	HEM	CMA-C3A	3.64	1.58	1.50
2	G	500	HEM	FE-ND	3.62	2.06	1.94
2	C	500	HEM	CAC-C3C	-3.62	1.37	1.47
2	D	500	HEM	C1C-C2C	-3.62	1.38	1.45
2	G	500	HEM	FE-NC	3.62	2.07	1.95
2	C	500	HEM	CMA-C3A	3.60	1.58	1.50
2	D	500	HEM	FE-NC	3.59	2.07	1.95
2	A	500	HEM	C4B-NB	-3.59	1.31	1.38
2	D	500	HEM	FE-ND	3.58	2.05	1.94
2	F	500	HEM	CMA-C3A	3.58	1.58	1.50
2	A	500	HEM	FE-ND	3.58	2.05	1.94
2	A	500	HEM	C1C-C2C	-3.56	1.38	1.45
2	E	500	HEM	FE-NC	3.55	2.06	1.95
2	F	500	HEM	FE-NB	3.54	2.05	1.94
2	D	500	HEM	C1C-NC	-3.53	1.33	1.39
2	D	500	HEM	C4D-ND	-3.53	1.34	1.40
2	C	500	HEM	FE-NA	3.50	2.06	1.95
2	C	500	HEM	FE-ND	3.50	2.05	1.94
2	F	500	HEM	C4B-NB	-3.50	1.32	1.38
2	B	500	HEM	FE-NA	3.50	2.06	1.95
2	B	500	HEM	C1C-C2C	-3.49	1.38	1.45
2	G	500	HEM	C4B-NB	-3.47	1.32	1.38
2	F	500	HEM	FE-NC	3.47	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	HEM	C1C-C2C	-3.45	1.38	1.45
2	G	500	HEM	FE-NA	3.45	2.06	1.95
2	E	500	HEM	FE-ND	3.44	2.05	1.94
2	B	500	HEM	FE-NB	3.42	2.05	1.94
2	D	500	HEM	FE-NA	3.40	2.06	1.95
2	F	500	HEM	FE-NA	3.40	2.06	1.95
2	E	500	HEM	C4B-NB	-3.35	1.32	1.38
2	B	500	HEM	C4B-NB	-3.35	1.32	1.38
2	C	500	HEM	C1C-C2C	-3.34	1.38	1.45
2	C	500	HEM	C4B-NB	-3.33	1.32	1.38
2	A	500	HEM	C4D-ND	-3.33	1.34	1.40
2	F	500	HEM	C1C-C2C	-3.32	1.38	1.45
2	B	500	HEM	FE-NC	3.31	2.06	1.95
2	B	500	HEM	C4D-ND	-3.29	1.34	1.40
2	A	500	HEM	FE-NC	3.28	2.06	1.95
2	C	500	HEM	FE-NC	3.26	2.05	1.95
2	D	500	HEM	C4B-NB	-3.24	1.32	1.38
2	E	500	HEM	FE-NA	3.11	2.05	1.95
2	A	500	HEM	FE-NA	3.09	2.05	1.95
2	E	500	HEM	C4C-NC	-3.02	1.33	1.39
2	F	500	HEM	CMC-C2C	3.01	1.56	1.50
2	B	500	HEM	CMC-C2C	2.94	1.56	1.50
2	A	500	HEM	CMC-C2C	2.91	1.56	1.50
2	G	500	HEM	CMC-C2C	2.90	1.56	1.50
2	B	500	HEM	C3B-C2B	2.89	1.43	1.37
2	D	500	HEM	CMC-C2C	2.84	1.56	1.50
2	C	500	HEM	CMC-C2C	2.84	1.56	1.50
2	E	500	HEM	CMC-C2C	2.71	1.56	1.50
2	F	500	HEM	O2A-CGA	-2.70	1.21	1.30
2	B	500	HEM	C4C-NC	-2.69	1.34	1.39
2	A	500	HEM	C4C-NC	-2.69	1.34	1.39
2	C	500	HEM	O2A-CGA	-2.69	1.21	1.30
2	C	500	HEM	C4C-NC	-2.65	1.34	1.39
2	E	500	HEM	CBD-CGD	2.64	1.56	1.50
2	D	500	HEM	O2A-CGA	-2.62	1.22	1.30
2	B	500	HEM	O2A-CGA	-2.62	1.22	1.30
2	C	500	HEM	C3B-C2B	2.61	1.42	1.37
2	B	500	HEM	CBC-CAC	2.61	1.42	1.30
2	A	500	HEM	O2A-CGA	-2.60	1.22	1.30
2	D	500	HEM	C4C-NC	-2.59	1.34	1.39
2	D	500	HEM	C3B-C2B	2.59	1.42	1.37
2	F	500	HEM	CAD-C3D	2.58	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CAD-C3D	2.57	1.58	1.51
2	E	500	HEM	CAD-C3D	2.57	1.57	1.51
2	G	500	HEM	C4C-NC	-2.54	1.34	1.39
2	E	500	HEM	CBC-CAC	2.53	1.42	1.30
3	B	501	1CI	C5-N1	-2.51	1.33	1.38
3	G	501	1CI	C5-N1	-2.51	1.33	1.38
2	G	500	HEM	C3B-C2B	2.51	1.42	1.37
3	A	501	1CI	C5-N1	-2.49	1.33	1.38
2	C	500	HEM	CBC-CAC	2.48	1.42	1.30
2	F	500	HEM	C4C-NC	-2.46	1.35	1.39
2	E	500	HEM	C3B-C2B	2.46	1.42	1.37
3	D	501	1CI	C5-N1	-2.46	1.33	1.38
3	C	501	1CI	C5-N1	-2.46	1.33	1.38
2	A	500	HEM	CBC-CAC	2.45	1.42	1.30
3	F	501	1CI	C5-N1	-2.44	1.33	1.38
2	G	500	HEM	CBC-CAC	2.44	1.42	1.30
2	E	500	HEM	C3C-C4C	-2.43	1.41	1.46
3	E	501	1CI	C5-N1	-2.43	1.33	1.38
2	F	500	HEM	CBC-CAC	2.41	1.42	1.30
2	G	500	HEM	CAD-C3D	2.40	1.57	1.51
2	G	500	HEM	C4D-C3D	-2.38	1.41	1.45
2	F	500	HEM	C3B-C2B	2.36	1.42	1.37
2	D	500	HEM	CBC-CAC	2.35	1.41	1.30
2	B	500	HEM	C3C-C4C	-2.33	1.42	1.46
2	G	500	HEM	O2A-CGA	-2.30	1.23	1.30
2	A	500	HEM	C3B-C2B	2.29	1.41	1.37
2	C	500	HEM	C3C-C4C	-2.29	1.42	1.46
2	D	500	HEM	C4D-C3D	-2.28	1.41	1.45
2	C	500	HEM	CBD-CGD	2.25	1.55	1.50
2	D	500	HEM	CAD-C3D	2.24	1.57	1.51
2	C	500	HEM	CAD-C3D	2.23	1.57	1.51
2	E	500	HEM	C4D-C3D	-2.23	1.41	1.45
2	F	500	HEM	CBD-CGD	2.20	1.55	1.50
2	A	500	HEM	C3C-C4C	-2.18	1.42	1.46
2	B	500	HEM	CBD-CGD	2.18	1.55	1.50
2	B	500	HEM	C4D-C3D	-2.16	1.41	1.45
2	A	500	HEM	C4D-C3D	-2.15	1.41	1.45
2	C	500	HEM	CMD-C2D	2.10	1.55	1.50
2	G	500	HEM	CBD-CGD	2.10	1.55	1.50
2	G	500	HEM	O2D-CGD	-2.09	1.23	1.30
2	E	500	HEM	C1D-C2D	-2.06	1.40	1.44
2	C	500	HEM	C3C-C2C	2.06	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	CAB-C3B	-2.06	1.41	1.47
2	A	500	HEM	C1D-C2D	-2.04	1.40	1.44
2	A	500	HEM	CAB-C3B	-2.04	1.41	1.47
2	F	500	HEM	C3C-C4C	-2.04	1.42	1.46
2	A	500	HEM	C3C-C2C	2.03	1.41	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CHD-C4C-NC	-4.58	119.47	124.45
2	F	500	HEM	CHD-C4C-NC	-3.95	120.15	124.45
2	G	500	HEM	CHD-C4C-NC	-3.82	120.29	124.45
2	G	500	HEM	CHB-C1B-NB	-3.78	119.69	124.37
2	B	500	HEM	CHD-C4C-NC	-3.56	120.57	124.45
2	D	500	HEM	CHD-C4C-NC	-3.53	120.61	124.45
2	E	500	HEM	CHD-C4C-NC	-3.43	120.72	124.45
2	A	500	HEM	CHD-C4C-NC	-3.35	120.81	124.45
2	E	500	HEM	CHB-C1B-NB	-3.07	120.57	124.37
2	B	500	HEM	C1B-NB-C4B	3.03	108.79	105.21
2	F	500	HEM	CHB-C1B-NB	-2.98	120.68	124.37
2	C	500	HEM	C1C-CHC-C4B	2.93	132.24	126.02
2	G	500	HEM	C1B-NB-C4B	2.85	108.58	105.21
2	E	500	HEM	C1B-NB-C4B	2.82	108.54	105.21
2	A	500	HEM	CHB-C1B-NB	-2.79	120.92	124.37
2	D	500	HEM	C4B-C3B-C2B	-2.73	104.77	107.28
2	G	500	HEM	C4C-C3C-C2C	-2.71	104.47	106.81
2	F	500	HEM	C1B-NB-C4B	2.71	108.41	105.21
2	D	500	HEM	CHB-C1B-NB	-2.71	121.02	124.37
2	B	500	HEM	C4B-C3B-C2B	-2.70	104.80	107.28
2	A	500	HEM	C3B-C2B-C1B	-2.70	104.39	106.41
2	B	500	HEM	C4C-C3C-C2C	-2.69	104.48	106.81
2	A	500	HEM	C3B-C4B-NB	2.67	111.39	109.47
2	E	500	HEM	C4D-ND-C1D	2.67	108.36	105.21
2	B	500	HEM	CHC-C4B-NB	-2.63	121.59	124.42
2	G	500	HEM	CAD-CBD-CGD	2.62	120.60	113.67
2	E	500	HEM	C1C-CHC-C4B	2.61	131.57	126.02
2	A	500	HEM	C4C-C3C-C2C	-2.61	104.56	106.81
2	E	500	HEM	C4B-C3B-C2B	-2.60	104.89	107.28
2	D	500	HEM	C4D-ND-C1D	2.60	108.28	105.21
2	G	500	HEM	C4B-C3B-C2B	-2.59	104.90	107.28
2	F	500	HEM	C1C-CHC-C4B	2.57	131.48	126.02
2	A	500	HEM	C4B-C3B-C2B	-2.56	104.92	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	HEM	C4B-C3B-C2B	-2.56	104.92	107.28
2	D	500	HEM	C1C-CHC-C4B	2.56	131.46	126.02
2	B	500	HEM	C1C-CHC-C4B	2.52	131.38	126.02
2	B	500	HEM	C4D-ND-C1D	2.52	108.19	105.21
2	C	500	HEM	C1B-NB-C4B	2.51	108.18	105.21
2	E	500	HEM	C4C-C3C-C2C	-2.49	104.66	106.81
2	D	500	HEM	C3B-C4B-NB	2.48	111.25	109.47
2	D	500	HEM	C3B-C2B-C1B	-2.48	104.55	106.41
2	A	500	HEM	C1C-CHC-C4B	2.46	131.26	126.02
2	C	500	HEM	C3B-C2B-C1B	-2.45	104.57	106.41
2	B	500	HEM	C4A-CHB-C1B	2.45	132.01	126.25
2	A	500	HEM	C4D-ND-C1D	2.42	108.07	105.21
2	G	500	HEM	C4D-ND-C1D	2.42	108.07	105.21
2	C	500	HEM	C4C-C3C-C2C	-2.42	104.72	106.81
2	G	500	HEM	CHD-C4C-C3C	2.41	129.26	125.21
2	F	500	HEM	C3B-C4B-NB	2.40	111.19	109.47
2	A	500	HEM	C1B-NB-C4B	2.40	108.05	105.21
2	C	500	HEM	CHB-C1B-NB	-2.40	121.40	124.37
2	C	500	HEM	C4D-ND-C1D	2.39	108.04	105.21
2	B	500	HEM	CHB-C1B-NB	-2.37	121.44	124.37
2	D	500	HEM	C4C-C3C-C2C	-2.37	104.76	106.81
2	F	500	HEM	C3B-C2B-C1B	-2.36	104.64	106.41
2	B	500	HEM	C3B-C2B-C1B	-2.36	104.64	106.41
2	E	500	HEM	CAD-CBD-CGD	2.35	119.91	113.67
2	C	500	HEM	C4B-C3B-C2B	-2.34	105.13	107.28
2	B	500	HEM	CHD-C4C-C3C	2.34	129.16	125.21
2	F	500	HEM	C4C-CHD-C1D	2.34	130.99	126.02
2	D	500	HEM	C1B-NB-C4B	2.30	107.93	105.21
2	F	500	HEM	CHC-C1C-NC	-2.30	121.95	124.45
2	G	500	HEM	C3B-C4B-NB	2.28	111.10	109.47
2	G	500	HEM	C1C-CHC-C4B	2.27	130.83	126.02
2	F	500	HEM	C4A-CHB-C1B	2.26	131.57	126.25
2	G	500	HEM	O2A-CGA-CBA	2.26	121.14	114.00
2	G	500	HEM	CHC-C4B-NB	-2.23	122.02	124.42
2	A	500	HEM	CAD-C3D-C4D	2.23	128.58	124.70
2	E	500	HEM	CHD-C4C-C3C	2.22	128.96	125.21
2	B	500	HEM	CAD-CBD-CGD	2.22	119.55	113.67
2	E	500	HEM	O2A-CGA-CBA	2.21	120.99	114.00
2	A	500	HEM	CHC-C1C-NC	-2.21	122.05	124.45
2	G	500	HEM	CHC-C1C-NC	-2.20	122.06	124.45
2	F	500	HEM	O2A-CGA-CBA	2.18	120.89	114.00
2	D	500	HEM	CHD-C4C-C3C	2.17	128.86	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	HEM	C4A-CHB-C1B	2.17	131.34	126.25
2	G	500	HEM	C3B-C2B-C1B	-2.15	104.79	106.41
2	F	500	HEM	C4D-ND-C1D	2.14	107.75	105.21
2	C	500	HEM	C4A-CHB-C1B	2.14	131.28	126.25
2	D	500	HEM	O2A-CGA-CBA	2.13	120.74	114.00
2	F	500	HEM	C4C-C3C-C2C	-2.13	104.97	106.81
2	C	500	HEM	O2A-CGA-CBA	2.12	120.69	114.00
2	E	500	HEM	C3B-C2B-C1B	-2.11	104.83	106.41
2	B	500	HEM	O2A-CGA-CBA	2.08	120.57	114.00
2	E	500	HEM	C4D-C3D-C2D	-2.07	103.89	106.89
2	C	500	HEM	C3B-C4B-NB	2.06	110.94	109.47
2	B	500	HEM	C3B-C4B-NB	2.04	110.93	109.47

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	C2C-C3C-CAC-CBC
2	E	500	HEM	C2B-C3B-CAB-CBB
2	E	500	HEM	C4B-C3B-CAB-CBB
2	F	500	HEM	C2C-C3C-CAC-CBC
2	F	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	E	500	HEM	C2C-C3C-CAC-CBC
2	F	500	HEM	C2B-C3B-CAB-CBB
2	G	500	HEM	C2C-C3C-CAC-CBC
2	E	500	HEM	C4C-C3C-CAC-CBC
2	G	500	HEM	C4C-C3C-CAC-CBC
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A
2	G	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	E	500	HEM	CAA-CBA-CGA-O1A
2	E	500	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	A	500	HEM	CAA-CBA-CGA-O1A
2	G	500	HEM	CAA-CBA-CGA-O2A
2	E	500	HEM	CAD-CBD-CGD-O2D
2	F	500	HEM	CAA-CBA-CGA-O1A
2	F	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAD-CBD-CGD-O2D
2	E	500	HEM	CAD-CBD-CGD-O1D
2	C	500	HEM	C4B-C3B-CAB-CBB
2	F	500	HEM	C4B-C3B-CAB-CBB
2	G	500	HEM	C4B-C3B-CAB-CBB
2	B	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	F	500	HEM	CAD-CBD-CGD-O1D
2	F	500	HEM	CAD-CBD-CGD-O2D
2	G	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAD-CBD-CGD-O2D
2	C	500	HEM	C2B-C3B-CAB-CBB
2	G	500	HEM	C2B-C3B-CAB-CBB
2	G	500	HEM	CAD-CBD-CGD-O1D

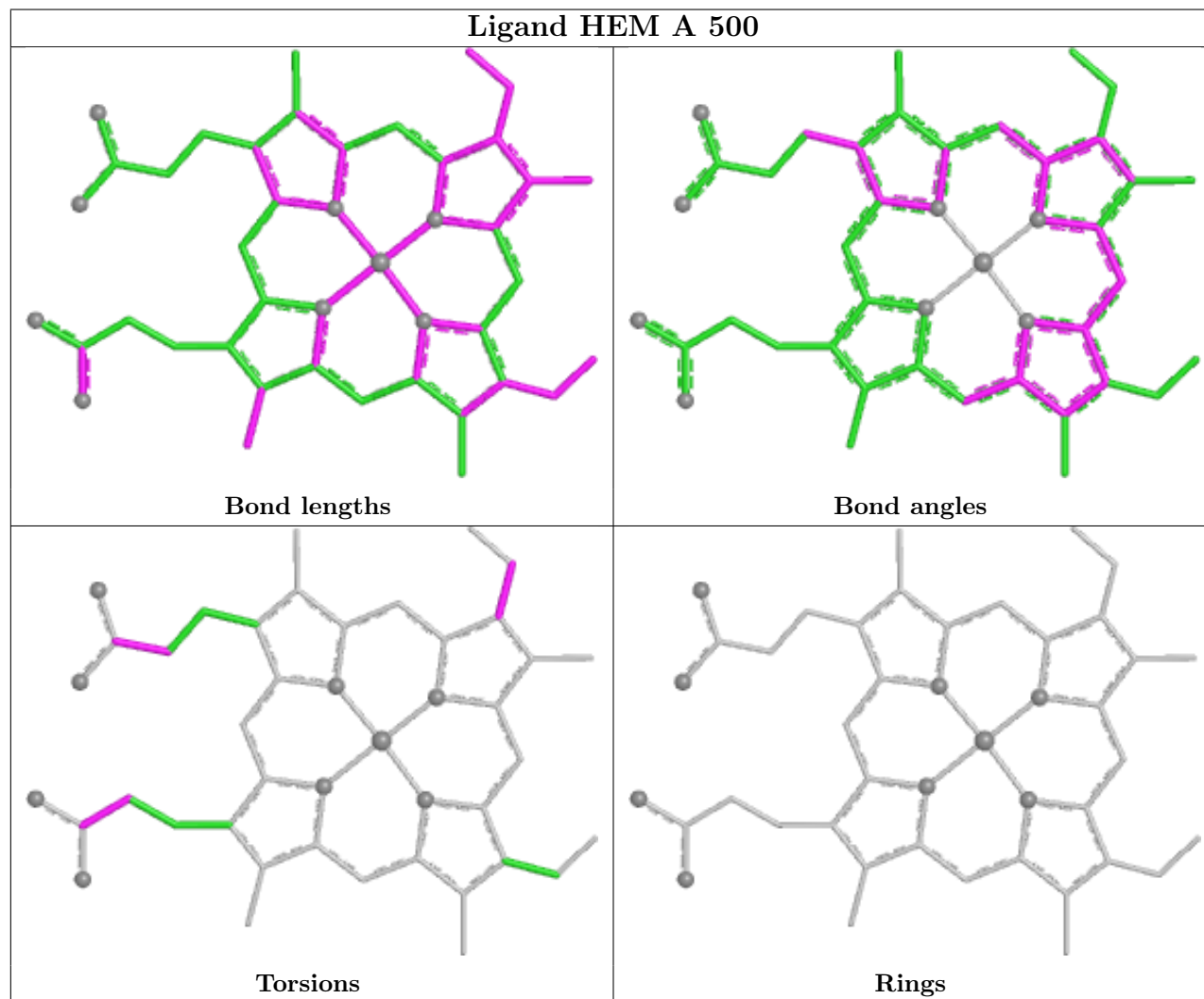
There are no ring outliers.

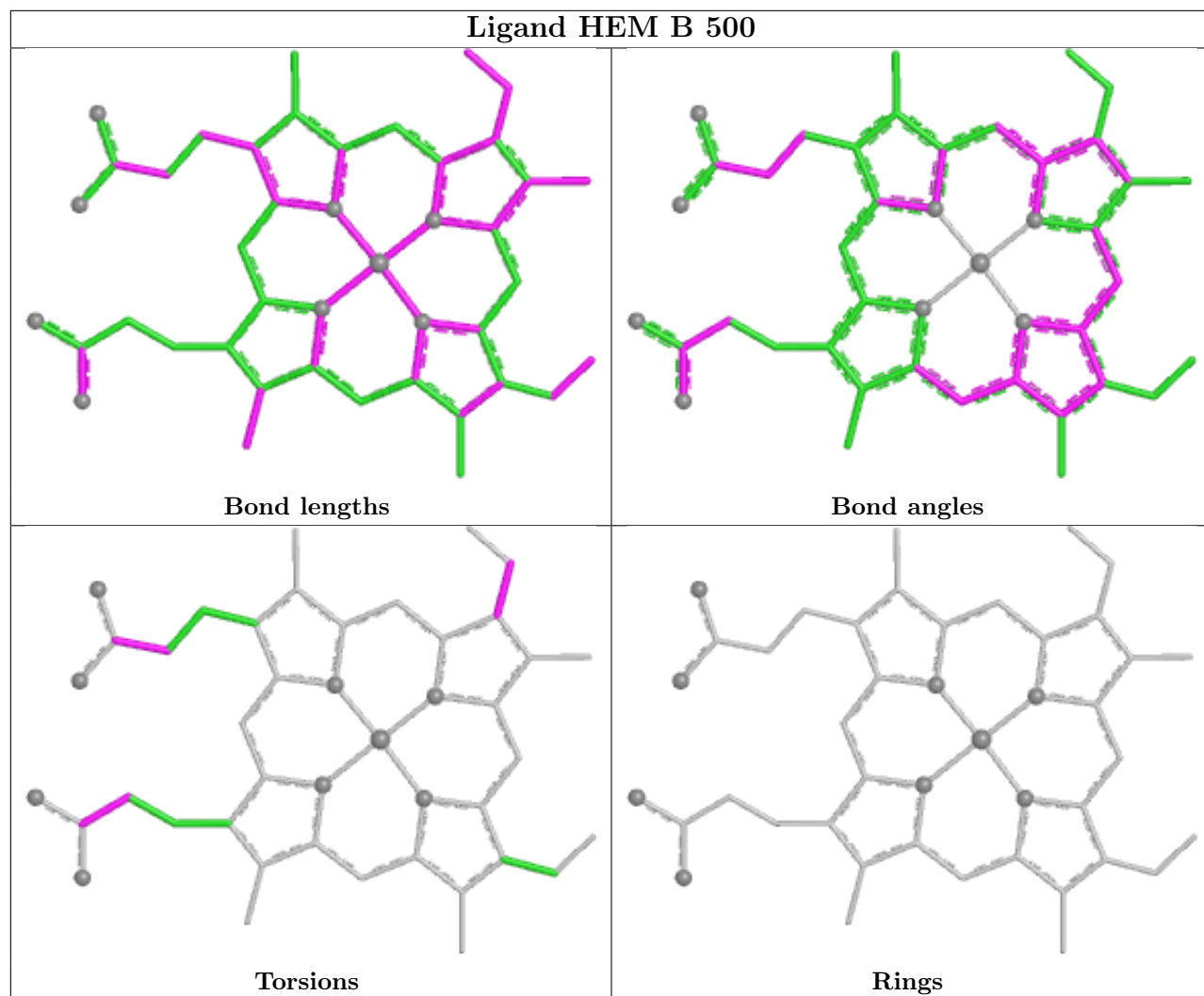
14 monomers are involved in 48 short contacts:

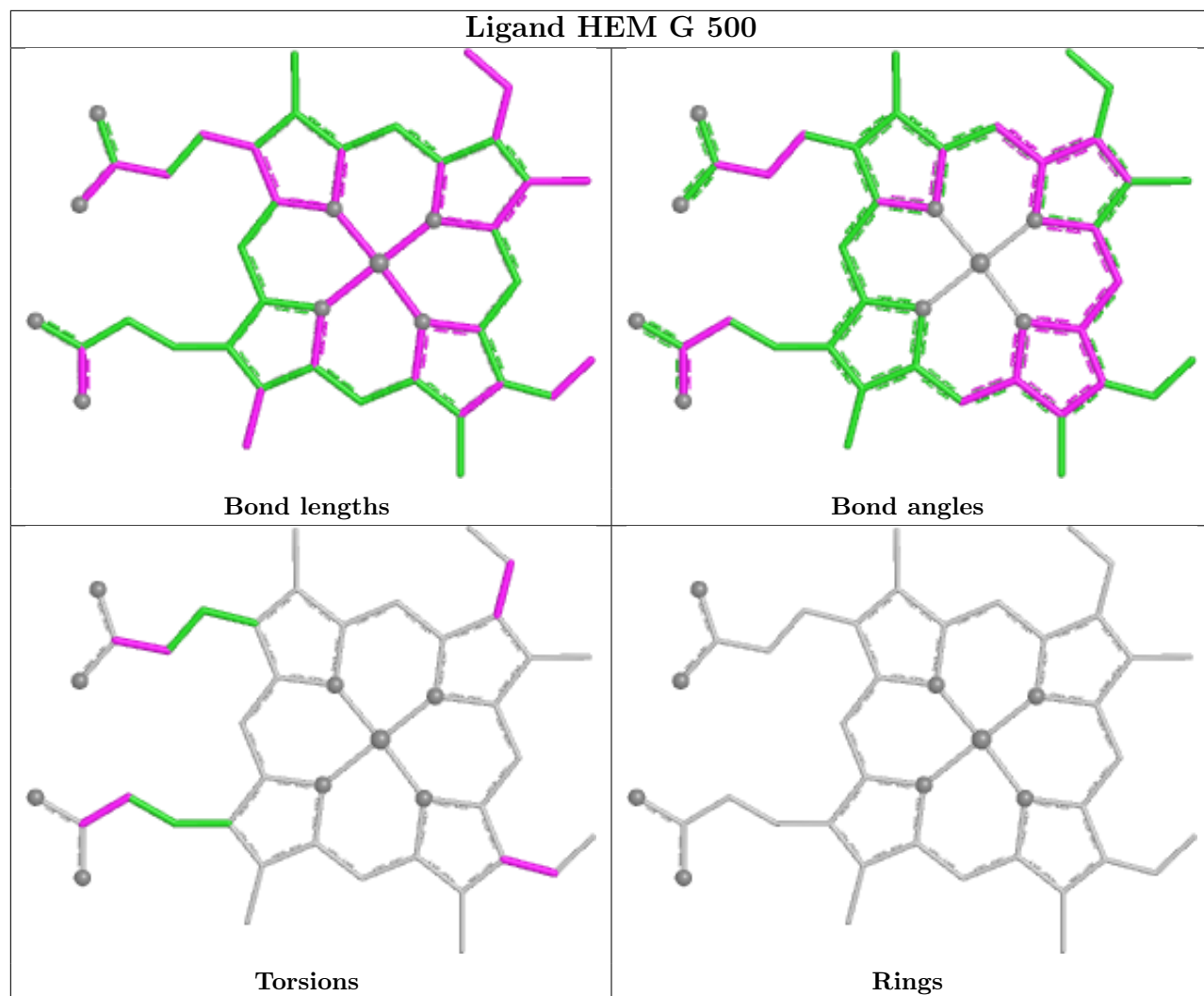
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	2	0
3	A	501	1CI	1	0
3	C	501	1CI	3	0
2	B	500	HEM	3	0
2	G	500	HEM	4	0
2	C	500	HEM	4	0
3	F	501	1CI	3	0
3	G	501	1CI	4	0
3	B	501	1CI	3	0
2	D	500	HEM	6	0
2	E	500	HEM	8	0
3	D	501	1CI	2	0
2	F	500	HEM	7	0
3	E	501	1CI	1	0

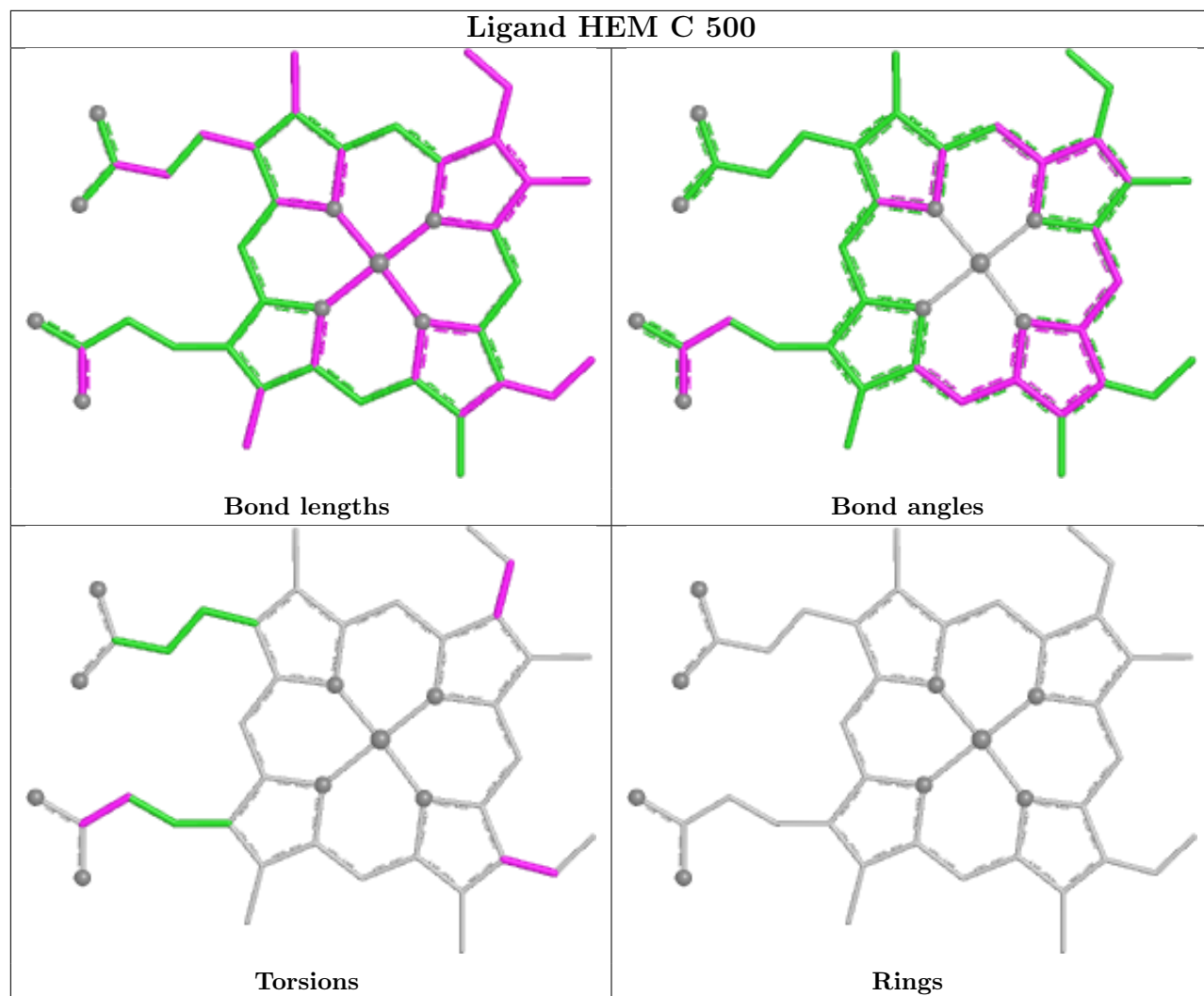
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

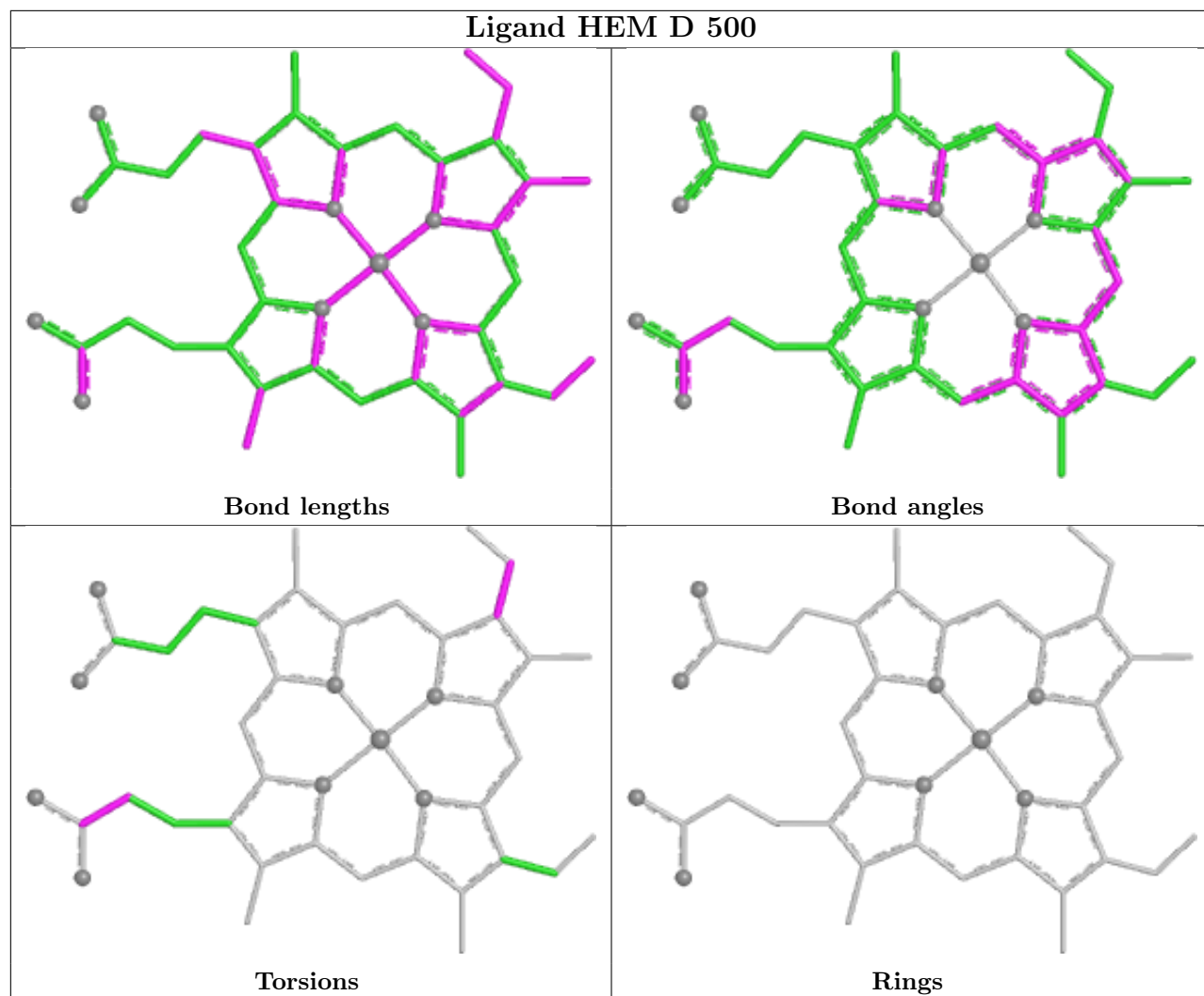
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

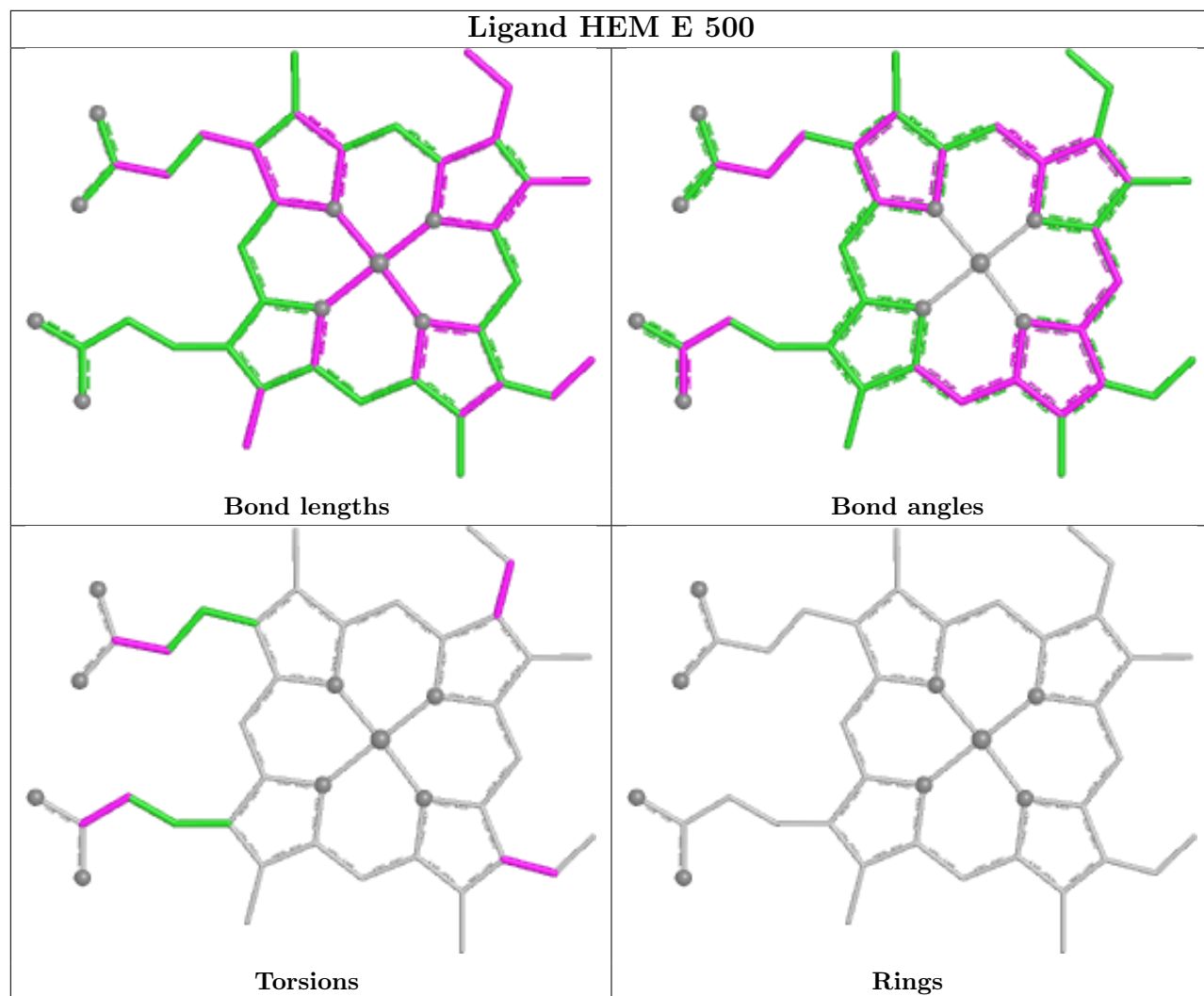


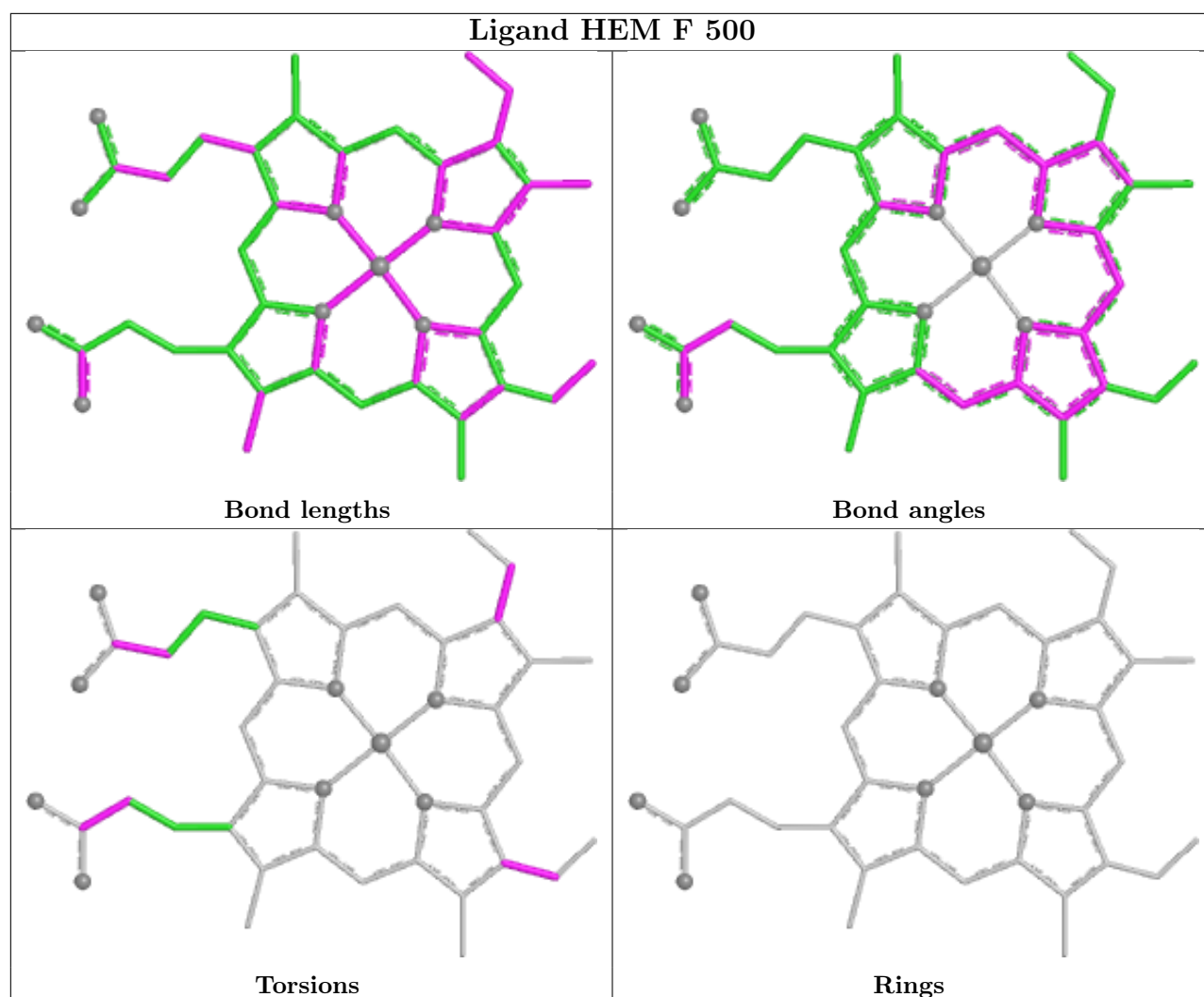












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/478 (97%)	-0.10	2 (0%) 88 79	48, 86, 120, 169	0
1	B	465/478 (97%)	-0.02	4 (0%) 81 64	70, 103, 144, 202	0
1	C	465/478 (97%)	-0.06	3 (0%) 85 73	64, 112, 156, 186	0
1	D	465/478 (97%)	-0.06	4 (0%) 81 64	64, 100, 144, 202	0
1	E	465/478 (97%)	0.06	3 (0%) 85 73	62, 115, 158, 202	0
1	F	465/478 (97%)	0.05	4 (0%) 81 64	70, 119, 165, 197	0
1	G	465/478 (97%)	0.05	8 (1%) 69 49	63, 119, 173, 202	0
All	All	3255/3346 (97%)	-0.01	28 (0%) 81 64	48, 108, 160, 202	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	SER	3.4
1	C	67	THR	3.3
1	G	299	GLY	3.1
1	B	301	GLU	3.1
1	E	362	LEU	3.0
1	F	95	PHE	2.9
1	G	178	ILE	2.8
1	D	305	THR	2.7
1	E	462	PRO	2.7
1	G	104	VAL	2.6
1	E	284	HIS	2.5
1	G	56	LEU	2.5
1	F	492	HIS	2.5
1	D	270	LEU	2.4
1	B	181	SER	2.4
1	G	355	GLU	2.4
1	C	113	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	299	GLY	2.3
1	D	303	THR	2.3
1	D	200	ASP	2.2
1	F	436	CYS	2.2
1	B	459	ILE	2.2
1	B	310	GLY	2.2
1	G	185	GLY	2.1
1	G	177	ASN	2.1
1	F	121	TRP	2.1
1	C	174	ILE	2.0
1	G	179	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

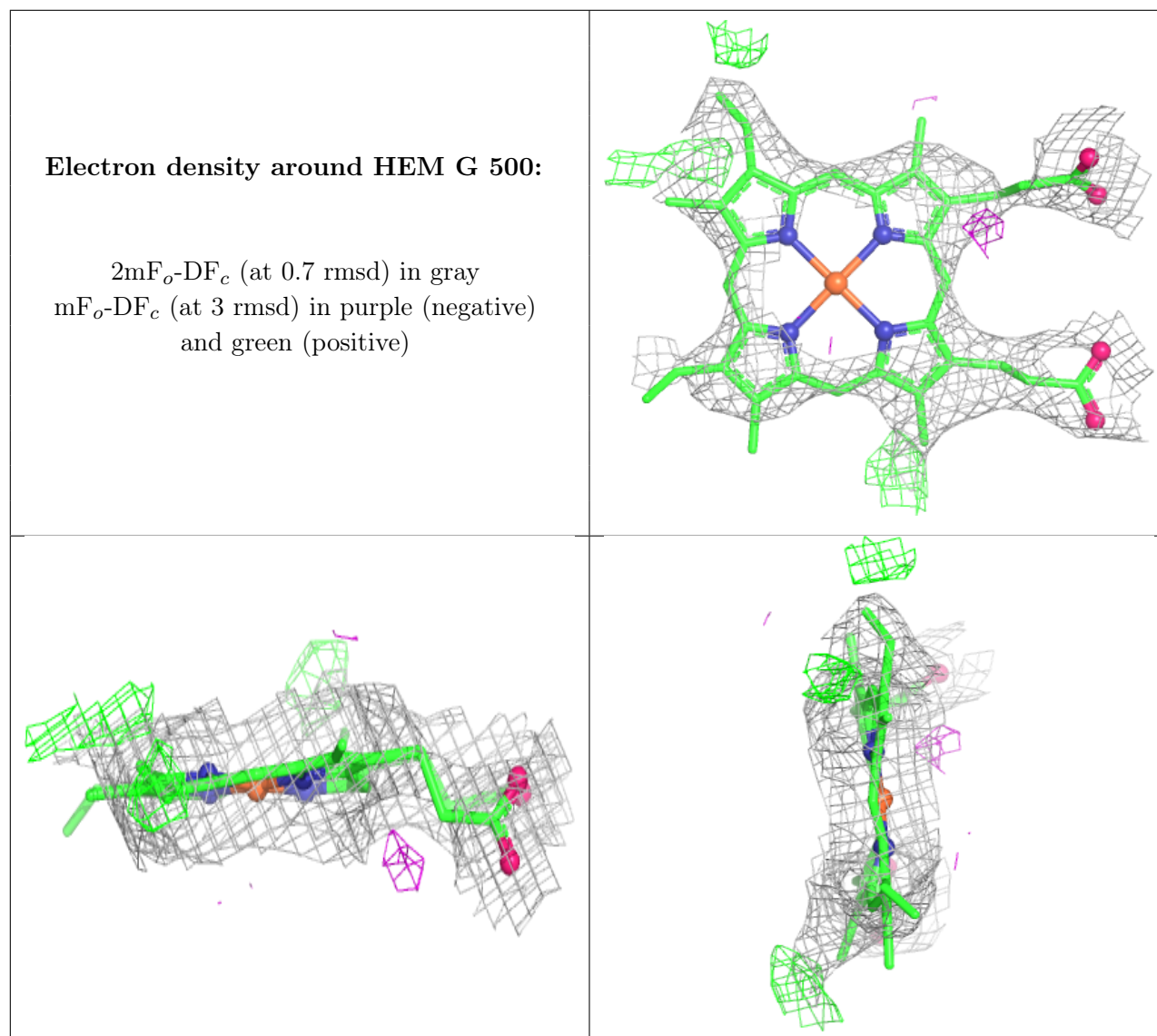
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	1CI	E	501	12/12	0.62	0.20	107,107,107,107	0
3	1CI	G	501	12/12	0.66	0.17	107,107,107,107	0
3	1CI	A	501	12/12	0.75	0.17	107,107,107,107	0
3	1CI	B	501	12/12	0.75	0.19	107,107,107,107	0
3	1CI	F	501	12/12	0.77	0.16	107,107,107,107	0
3	1CI	D	501	12/12	0.81	0.15	107,107,107,107	0
3	1CI	C	501	12/12	0.82	0.14	107,107,107,107	0
2	HEM	G	500	43/43	0.91	0.12	109,109,109,109	0
2	HEM	F	500	43/43	0.92	0.14	111,111,111,111	0
2	HEM	E	500	43/43	0.93	0.11	69,69,69,69	0
2	HEM	B	500	43/43	0.93	0.12	78,78,78,78	0
2	HEM	C	500	43/43	0.94	0.10	93,93,93,93	0

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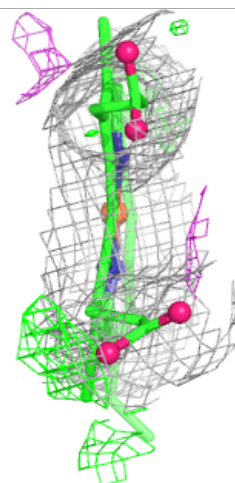
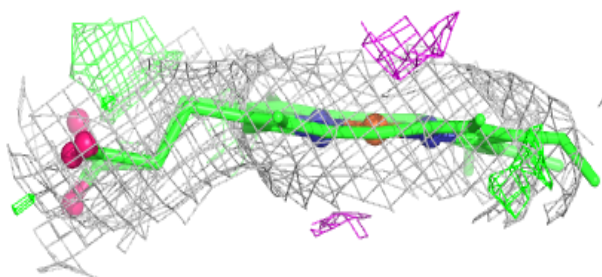
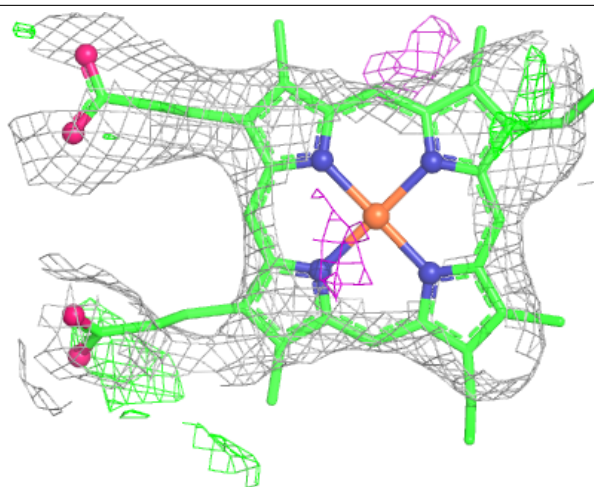
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	500	43/43	0.94	0.12	102,102,102,102	0
2	HEM	A	500	43/43	0.95	0.10	78,78,78,78	0

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.



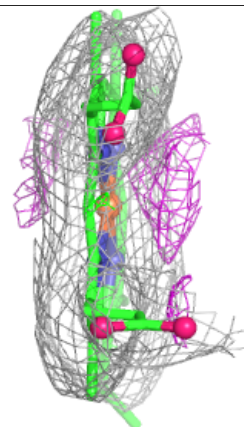
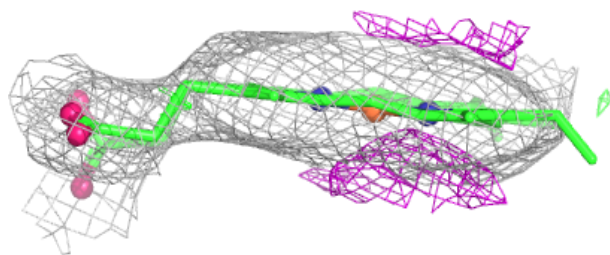
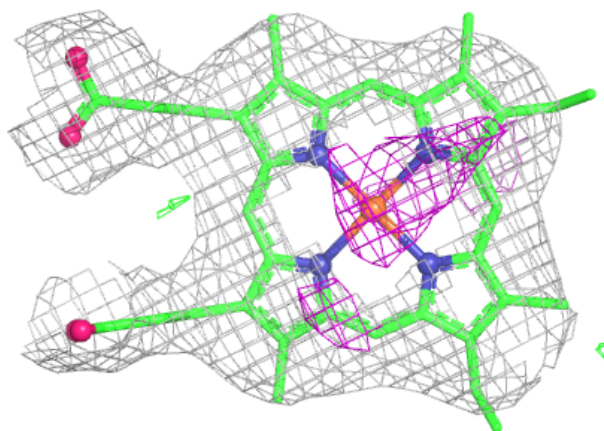
Electron density around HEM F 500:

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



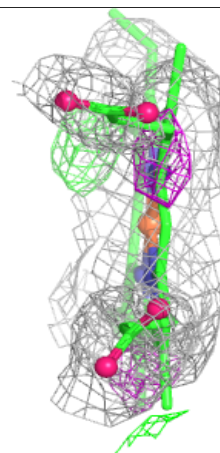
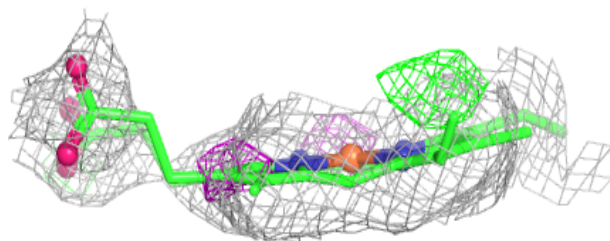
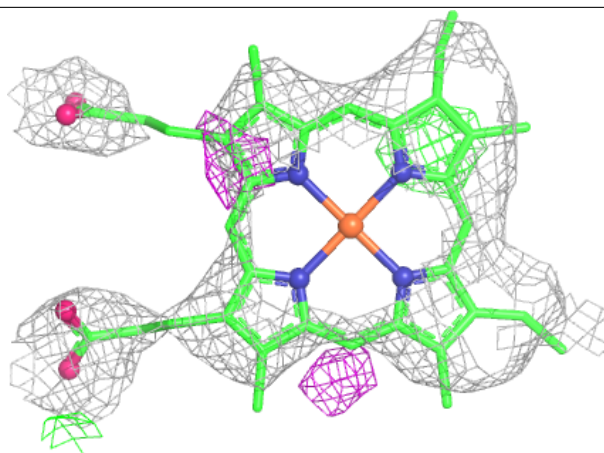
Electron density around HEM E 500:

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



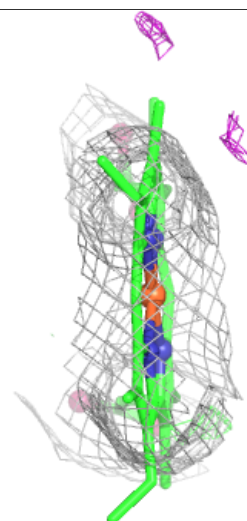
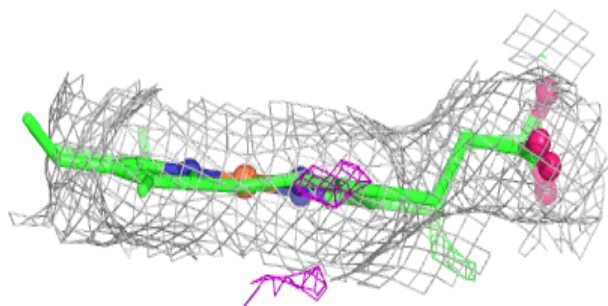
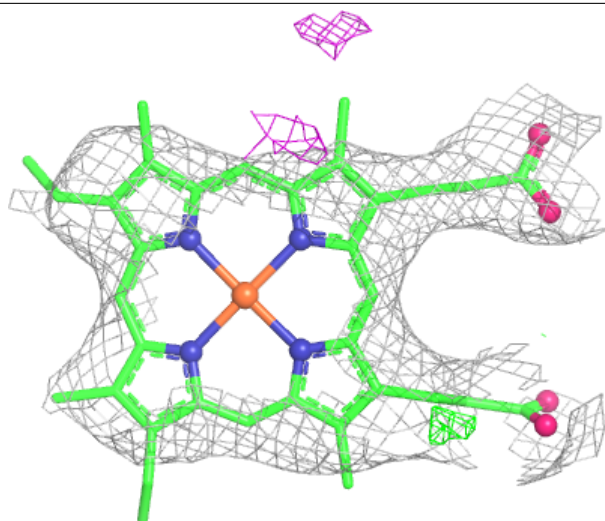
Electron density around HEM B 500:

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



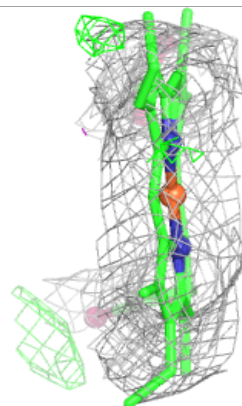
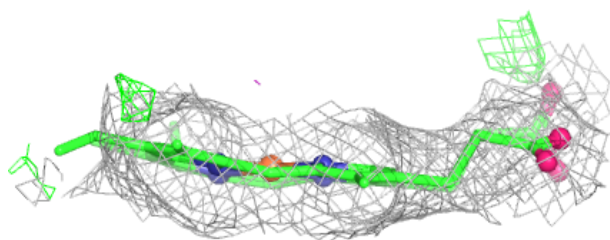
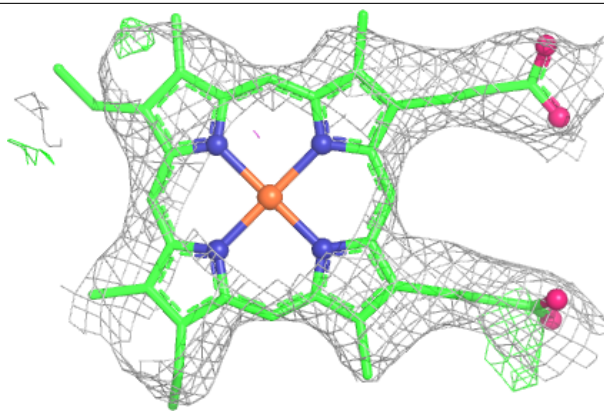
Electron density around HEM C 500:

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

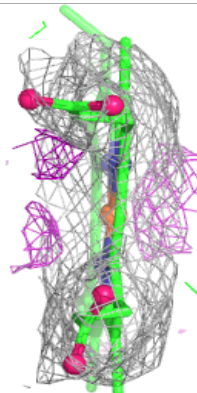
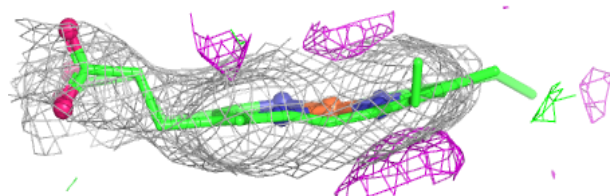
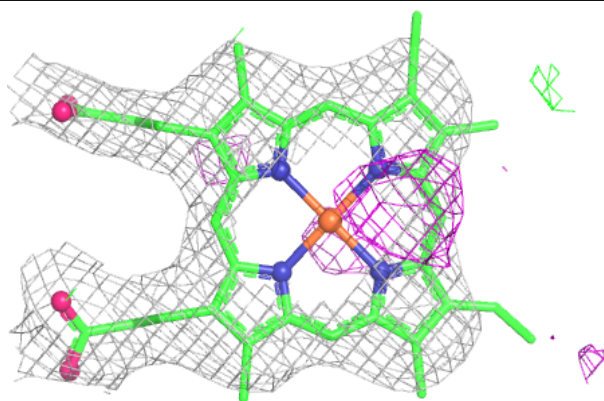


Electron density around HEM D 500:

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

**Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.