



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 02:17 AM EDT

PDB ID : 1SMJ  
Title : Structure of the A264E mutant of cytochrome P450 BM3 complexed with palmitoleate  
Authors : Joyce, M.G.; Girvan, H.M.; Munro, A.W.; Leys, D.  
Deposited on : 2004-03-09  
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

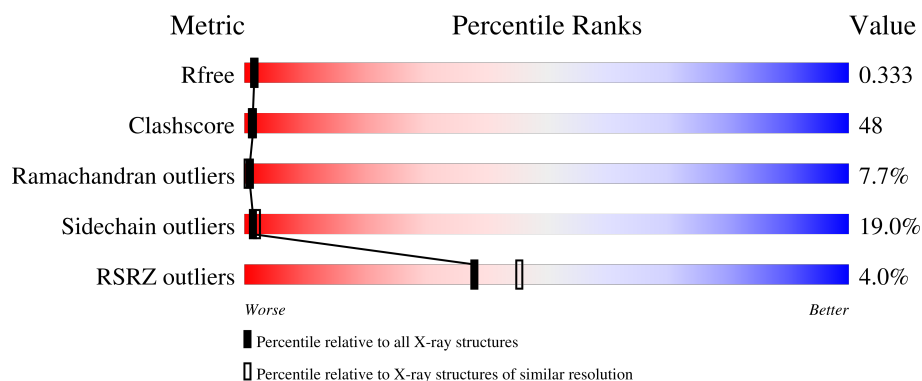
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	
1	C	471	
1	D	471	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14913 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 Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3662	2340	621	684	17			
1	B	455	Total	C	N	O	S	0	0	0
			3670	2344	622	687	17			
1	C	455	Total	C	N	O	S	0	0	0
			3670	2344	622	687	17			
1	D	454	Total	C	N	O	S	0	0	0
			3667	2343	622	685	17			

There are 4 discrepancies between the modelled and reference sequences:

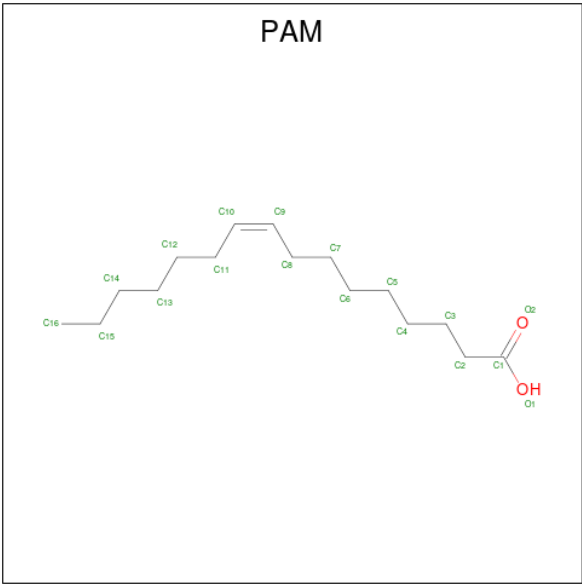
Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLU	ALA	engineered mutation	UNP P14779
B	264	GLU	ALA	engineered mutation	UNP P14779
C	264	GLU	ALA	engineered mutation	UNP P14779
D	264	GLU	ALA	engineered mutation	UNP P14779

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



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

- Molecule 3 is PALMITOLEIC ACID (three-letter code: PAM) (formula: C<sub>16</sub>H<sub>30</sub>O<sub>2</sub>).

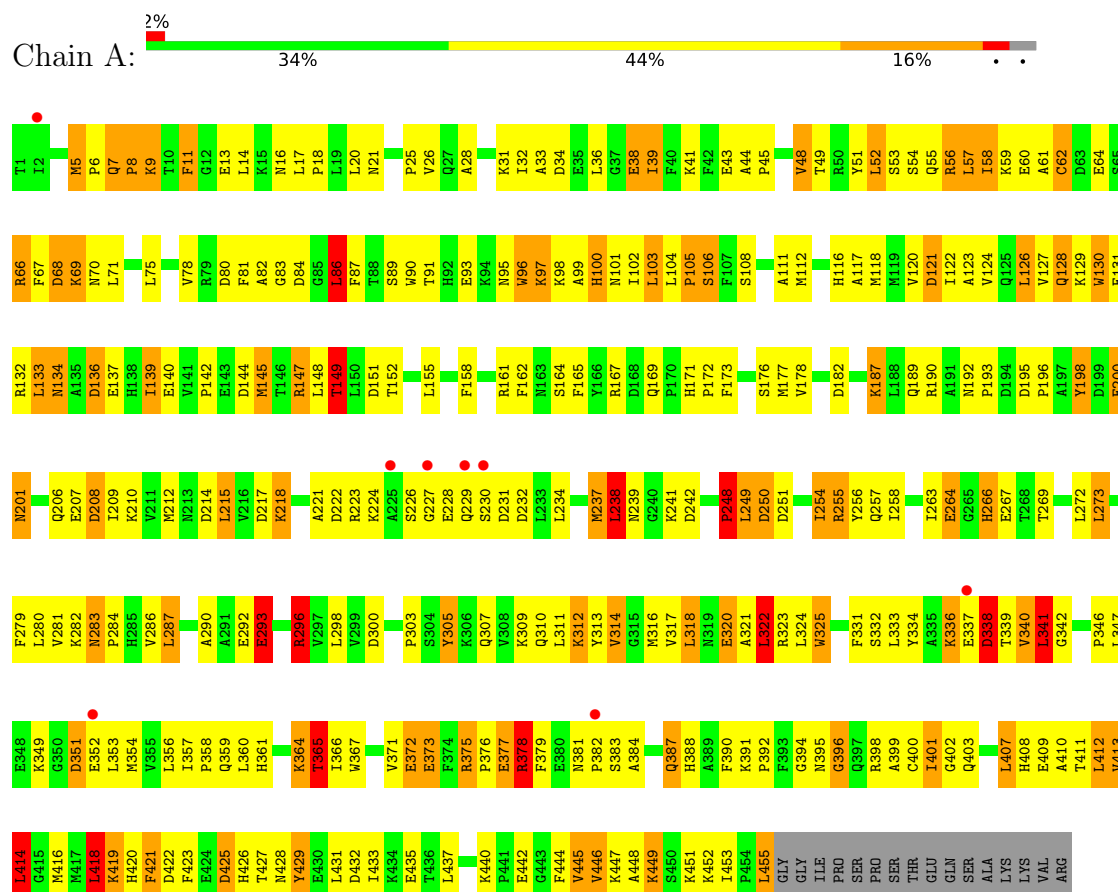


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 18	C 16	O 2	0	0
3	B	1	Total 18	C 16	O 2	0	0
3	C	1	Total 18	C 16	O 2	0	0
3	D	1	Total 18	C 16	O 2	0	0

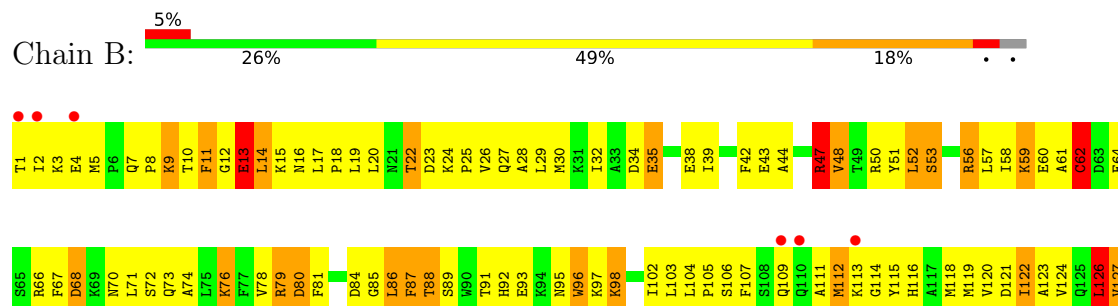
### 3 Residue-property plots

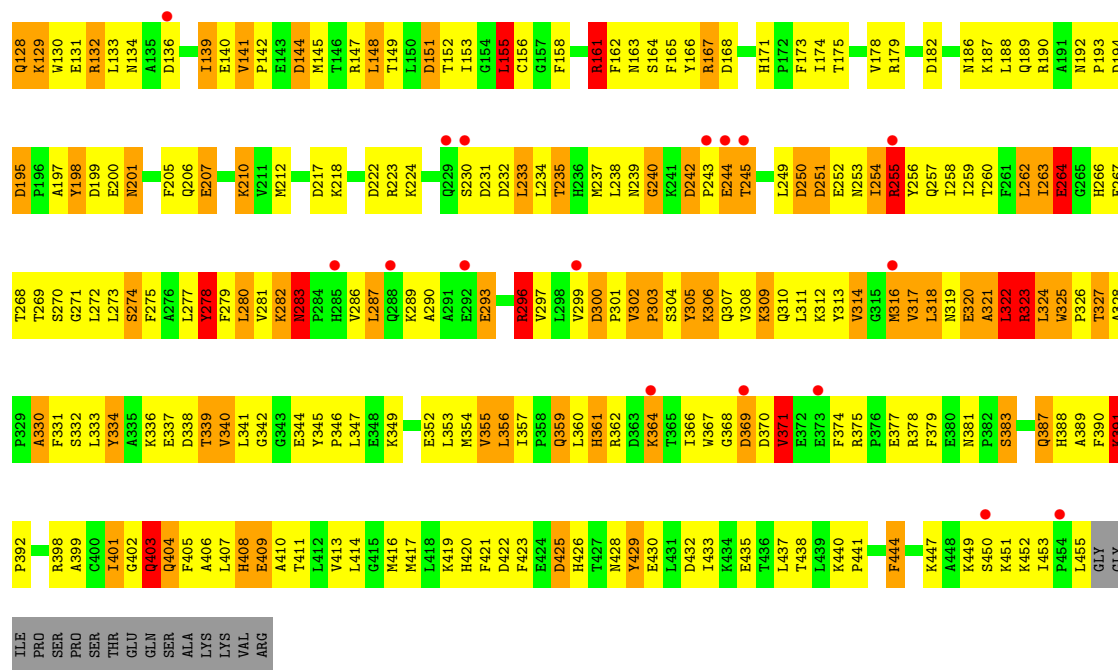
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional P-450:NADPH-P450 reductase

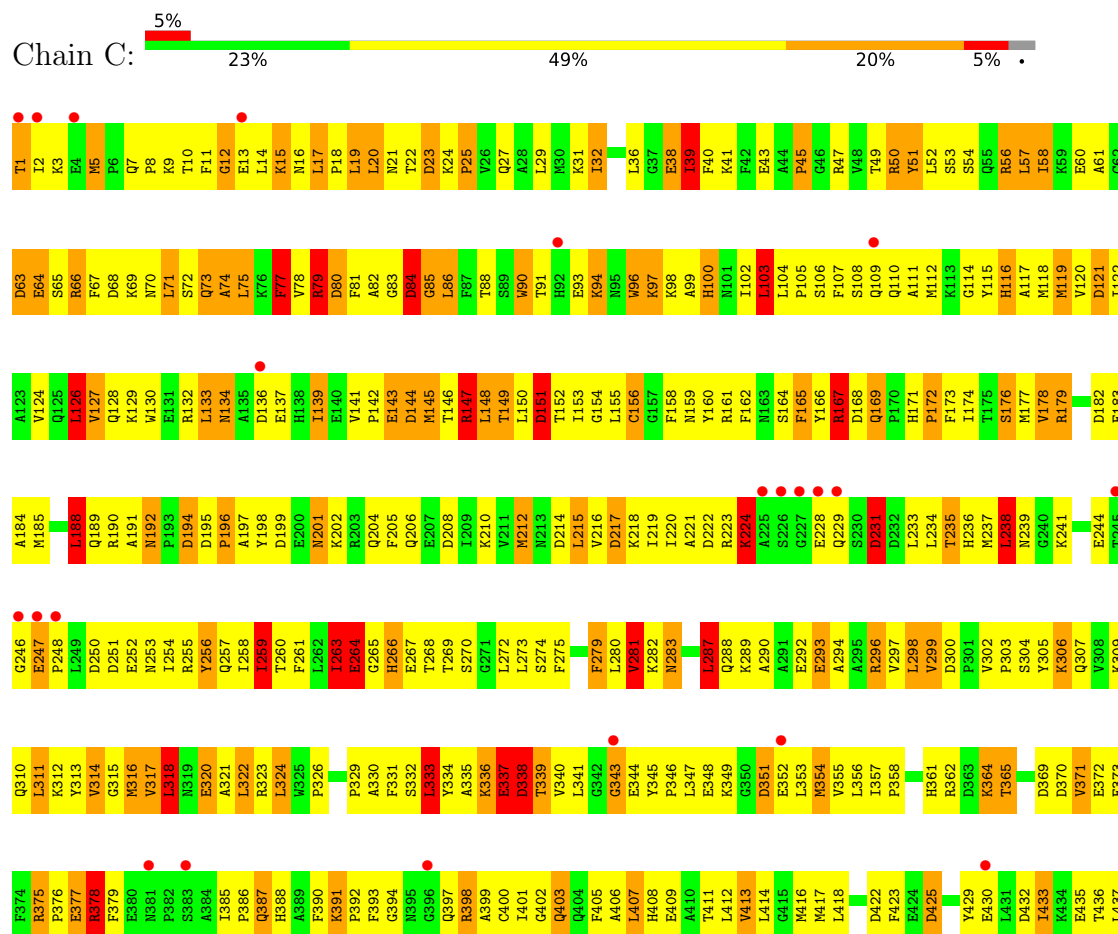


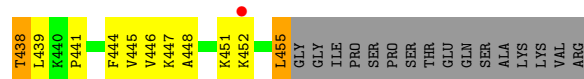
#### • Molecule 1: Bifunctional P-450:NADPH-P450 reductase



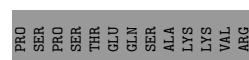
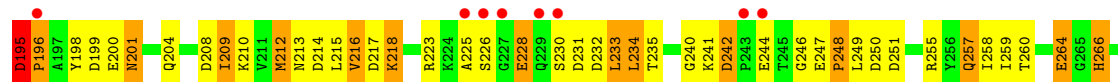
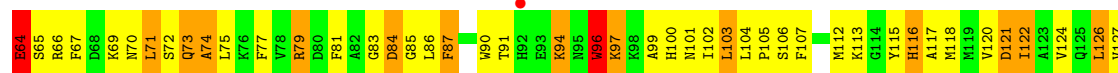


• Molecule 1: Bifunctional P-450:NADPH-P450 reductase





● Molecule 1: Bifunctional P-450:NADPH-P450 reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.31Å 166.89Å 224.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75 15.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.75) 99.1 (15.00-2.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.253 , 0.338 0.244 , 0.333	Depositor DCC
$R_{free}$ test set	2645 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.67	36/3747 (1.0%)	1.59	47/5068 (0.9%)
1	B	1.55	23/3755 (0.6%)	1.48	39/5078 (0.8%)
1	C	1.63	38/3755 (1.0%)	1.57	57/5078 (1.1%)
1	D	1.45	14/3752 (0.4%)	1.51	49/5072 (1.0%)
All	All	1.58	111/15009 (0.7%)	1.54	192/20296 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	1
All	All	0	8

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	GLU	CD-OE2	13.82	1.40	1.25
1	C	373	GLU	CD-OE2	13.80	1.40	1.25
1	C	373	GLU	CD-OE1	13.44	1.40	1.25
1	B	244	GLU	CD-OE1	12.02	1.38	1.25
1	C	247	GLU	CD-OE2	10.70	1.37	1.25
1	C	281	VAL	CB-CG1	-9.24	1.33	1.52
1	A	82	ALA	CA-CB	-8.32	1.34	1.52
1	B	255	ARG	CZ-NH1	8.28	1.43	1.33
1	C	247	GLU	CD-OE1	8.00	1.34	1.25
1	A	264	GLU	CD-OE2	7.93	1.34	1.25
1	A	264	GLU	CD-OE1	7.69	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	GLU	CD-OE1	7.63	1.34	1.25
1	C	77	PHE	CD2-CE2	7.45	1.54	1.39
1	C	23	ASP	CG-OD2	7.42	1.42	1.25
1	C	255	ARG	CZ-NH1	7.40	1.42	1.33
1	D	195	ASP	CG-OD2	7.39	1.42	1.25
1	B	242	ASP	CB-CG	7.38	1.67	1.51
1	C	74	ALA	CA-CB	-7.36	1.36	1.52
1	D	264	GLU	CD-OE2	7.14	1.33	1.25
1	A	421	PHE	CE2-CZ	7.11	1.50	1.37
1	C	255	ARG	CZ-NH2	7.10	1.42	1.33
1	A	256	TYR	CD1-CE1	-7.00	1.28	1.39
1	A	250	ASP	CB-CG	7.00	1.66	1.51
1	C	23	ASP	CA-C	6.99	1.71	1.52
1	A	384	ALA	CA-CB	6.93	1.67	1.52
1	B	207	GLU	CG-CD	6.92	1.62	1.51
1	A	48	VAL	CB-CG1	-6.91	1.38	1.52
1	A	26	VAL	CB-CG1	-6.87	1.38	1.52
1	B	13	GLU	CD-OE2	6.85	1.33	1.25
1	A	250	ASP	CG-OD2	6.77	1.41	1.25
1	C	255	ARG	NE-CZ	6.76	1.41	1.33
1	C	279	PHE	CD2-CE2	-6.73	1.25	1.39
1	D	264	GLU	CD-OE1	6.73	1.33	1.25
1	B	205	PHE	CE1-CZ	6.64	1.50	1.37
1	B	255	ARG	CZ-NH2	6.62	1.41	1.33
1	A	296	ARG	CZ-NH1	6.60	1.41	1.33
1	A	130	TRP	CE3-CZ3	6.55	1.49	1.38
1	B	250	ASP	CB-CG	6.42	1.65	1.51
1	C	166	TYR	CD1-CE1	6.41	1.49	1.39
1	A	178	VAL	CA-CB	6.40	1.68	1.54
1	D	199	ASP	CB-CG	6.34	1.65	1.51
1	C	166	TYR	CD2-CE2	6.28	1.48	1.39
1	D	430	GLU	CG-CD	6.20	1.61	1.51
1	C	445	VAL	CB-CG1	-6.15	1.40	1.52
1	C	85	GLY	C-O	6.11	1.33	1.23
1	B	255	ARG	NE-CZ	6.10	1.41	1.33
1	D	279	PHE	CD2-CE2	6.08	1.51	1.39
1	A	321	ALA	CA-CB	-6.04	1.39	1.52
1	C	228	GLU	CD-OE2	6.03	1.32	1.25
1	D	87	PHE	CE2-CZ	6.00	1.48	1.37
1	C	264	GLU	CD-OE2	5.99	1.32	1.25
1	A	241	LYS	CD-CE	5.98	1.66	1.51
1	A	178	VAL	CB-CG2	-5.98	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	ARG	CZ-NH1	5.95	1.40	1.33
1	A	352	GLU	CG-CD	5.94	1.60	1.51
1	A	31	LYS	CD-CE	5.90	1.66	1.51
1	D	430	GLU	CD-OE1	5.85	1.32	1.25
1	C	1	THR	CA-CB	5.85	1.68	1.53
1	C	264	GLU	CD-OE1	5.81	1.32	1.25
1	D	143	GLU	CD-OE2	5.76	1.31	1.25
1	C	50	ARG	C-O	5.74	1.34	1.23
1	C	279	PHE	CE2-CZ	5.74	1.48	1.37
1	C	25	PRO	C-O	5.74	1.34	1.23
1	B	131	GLU	CD-OE1	5.73	1.31	1.25
1	D	393	PHE	CB-CG	-5.72	1.41	1.51
1	A	325	TRP	CE3-CZ3	5.72	1.48	1.38
1	C	265	GLY	C-O	5.71	1.32	1.23
1	B	198	TYR	CD1-CE1	5.71	1.48	1.39
1	B	205	PHE	CB-CG	-5.70	1.41	1.51
1	A	273	LEU	N-CA	-5.64	1.35	1.46
1	B	264	GLU	CD-OE2	5.60	1.31	1.25
1	B	87	PHE	CE1-CZ	5.56	1.48	1.37
1	C	314	VAL	CB-CG2	-5.56	1.41	1.52
1	A	200	GLU	CD-OE2	5.51	1.31	1.25
1	C	281	VAL	CA-CB	-5.50	1.43	1.54
1	C	409	GLU	CD-OE1	5.48	1.31	1.25
1	B	334	TYR	CB-CG	-5.44	1.43	1.51
1	C	263	ILE	CA-CB	-5.43	1.42	1.54
1	A	352	GLU	CB-CG	5.42	1.62	1.52
1	D	297	VAL	CB-CG2	-5.41	1.41	1.52
1	B	264	GLU	CD-OE1	5.35	1.31	1.25
1	A	241	LYS	CE-NZ	5.33	1.62	1.49
1	D	182	ASP	CB-CG	5.32	1.62	1.51
1	A	314	VAL	CB-CG2	-5.29	1.41	1.52
1	C	337	GLU	CD-OE1	5.26	1.31	1.25
1	A	449	LYS	CB-CG	5.26	1.66	1.52
1	A	433	ILE	C-O	5.24	1.33	1.23
1	C	169	GLN	CG-CD	5.24	1.63	1.51
1	A	250	ASP	CA-CB	5.23	1.65	1.53
1	B	245	THR	CA-CB	5.23	1.67	1.53
1	A	429	TYR	CD2-CE2	-5.22	1.31	1.39
1	D	244	GLU	CD-OE1	5.21	1.31	1.25
1	A	373	GLU	CD-OE2	5.19	1.31	1.25
1	A	372	GLU	CD-OE1	5.17	1.31	1.25
1	A	200	GLU	CG-CD	5.17	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	GLU	CD-OE2	5.16	1.31	1.25
1	B	205	PHE	CA-CB	-5.15	1.42	1.53
1	A	413	VAL	CB-CG1	-5.13	1.42	1.52
1	C	84	ASP	CB-CG	5.13	1.62	1.51
1	C	179	ARG	C-O	5.12	1.33	1.23
1	B	278	TYR	CG-CD1	5.12	1.45	1.39
1	A	198	TYR	N-CA	-5.09	1.36	1.46
1	C	143	GLU	CG-CD	5.09	1.59	1.51
1	A	90	TRP	CB-CG	-5.08	1.41	1.50
1	C	51	TYR	CE1-CZ	5.08	1.45	1.38
1	D	87	PHE	CD1-CE1	5.08	1.49	1.39
1	A	26	VAL	CA-CB	-5.07	1.44	1.54
1	C	90	TRP	CE3-CZ3	5.06	1.47	1.38
1	A	339	THR	CA-CB	5.06	1.66	1.53
1	B	330	ALA	CA-CB	-5.03	1.41	1.52
1	B	4	GLU	CG-CD	5.03	1.59	1.51

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	ASP	CB-CG-OD2	16.00	132.70	118.30
1	A	250	ASP	CB-CG-OD2	14.22	131.10	118.30
1	C	23	ASP	CB-CG-OD1	-13.91	105.78	118.30
1	A	322	LEU	CB-CG-CD2	-12.58	89.62	111.00
1	C	351	ASP	CB-CG-OD2	12.05	129.15	118.30
1	C	231	ASP	CB-CG-OD2	11.61	128.75	118.30
1	D	250	ASP	CB-CG-OD2	11.03	128.22	118.30
1	B	144	ASP	CB-CG-OD2	10.92	128.12	118.30
1	D	168	ASP	CB-CG-OD1	10.90	128.11	118.30
1	C	250	ASP	CB-CG-OD2	10.83	128.05	118.30
1	C	144	ASP	CB-CG-OD2	10.78	128.00	118.30
1	B	34	ASP	CB-CG-OD2	10.32	127.59	118.30
1	A	455	LEU	CB-CG-CD1	-10.32	93.46	111.00
1	A	338	ASP	CB-CG-OD2	10.22	127.49	118.30
1	D	23	ASP	CB-CG-OD2	9.92	127.23	118.30
1	C	121	ASP	CB-CG-OD2	9.77	127.09	118.30
1	D	121	ASP	CB-CG-OD2	9.69	127.02	118.30
1	A	121	ASP	CB-CG-OD2	9.61	126.95	118.30
1	B	195	ASP	CB-CG-OD2	9.47	126.82	118.30
1	D	195	ASP	CB-CG-OD1	-9.47	109.78	118.30
1	A	151	ASP	CB-CG-OD2	9.40	126.76	118.30
1	C	84	ASP	CB-CG-OD2	9.24	126.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ASP	CB-CG-OD2	9.09	126.48	118.30
1	A	214	ASP	CB-CG-OD2	9.06	126.45	118.30
1	D	151	ASP	CB-CG-OD2	8.97	126.38	118.30
1	B	151	ASP	CB-CG-OD2	8.86	126.27	118.30
1	D	182	ASP	CB-CG-OD2	8.73	126.16	118.30
1	B	182	ASP	CB-CG-OD2	8.73	126.16	118.30
1	A	455	LEU	CA-CB-CG	8.72	135.37	115.30
1	B	300	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	296	ARG	NE-CZ-NH1	-8.63	115.99	120.30
1	C	17	LEU	CB-CG-CD2	-8.60	96.38	111.00
1	A	182	ASP	CB-CG-OD2	8.59	126.03	118.30
1	C	156	CYS	CA-CB-SG	-8.54	98.63	114.00
1	C	167	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	B	323	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	A	121	ASP	CB-CG-OD1	-8.35	110.79	118.30
1	B	338	ASP	CB-CG-OD2	8.33	125.79	118.30
1	C	333	LEU	CB-CG-CD1	8.28	125.07	111.00
1	C	20	LEU	CA-CB-CG	-8.23	96.37	115.30
1	A	414	LEU	CB-CG-CD1	8.17	124.89	111.00
1	D	79	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	D	407	LEU	CB-CG-CD2	7.92	124.46	111.00
1	D	425	ASP	CB-CG-OD2	7.91	125.42	118.30
1	C	168	ASP	CB-CG-OD1	7.91	125.42	118.30
1	D	369	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	238	LEU	CA-CB-CG	7.89	133.45	115.30
1	A	66	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	D	79	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	338	ASP	CB-CG-OD2	7.81	125.33	118.30
1	B	250	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	208	ASP	CB-CG-OD2	7.72	125.25	118.30
1	B	217	ASP	CB-CG-OD2	7.66	125.20	118.30
1	A	96	TRP	CA-CB-CG	-7.64	99.18	113.70
1	D	145	MET	CG-SD-CE	7.62	112.39	100.20
1	A	375	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	D	212	MET	CG-SD-CE	-7.59	88.06	100.20
1	D	362	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	231	ASP	CB-CG-OD2	7.42	124.98	118.30
1	A	250	ASP	CB-CA-C	7.37	125.14	110.40
1	C	182	ASP	CB-CG-OD2	7.32	124.89	118.30
1	C	351	ASP	CB-CG-OD1	-7.26	111.76	118.30
1	D	84	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	96	TRP	CA-CB-CG	-7.11	100.19	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	80	ASP	CB-CG-OD2	7.11	124.69	118.30
1	C	144	ASP	OD1-CG-OD2	-7.09	109.83	123.30
1	B	167	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	D	136	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	242	ASP	CB-CG-OD2	7.06	124.66	118.30
1	B	287	LEU	CA-CB-CG	7.05	131.52	115.30
1	A	217	ASP	CB-CG-OD2	7.04	124.64	118.30
1	D	84	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	351	ASP	CB-CG-OD2	6.98	124.58	118.30
1	C	212	MET	CG-SD-CE	-6.97	89.05	100.20
1	D	234	LEU	CB-CG-CD1	6.96	122.84	111.00
1	B	242	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	249	LEU	CA-CB-CG	6.83	131.02	115.30
1	D	179	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	250	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	C	238	LEU	CA-CB-CG	6.72	130.76	115.30
1	D	56	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	324	LEU	CA-CB-CG	6.68	130.66	115.30
1	C	147	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	354	MET	CG-SD-CE	-6.64	89.58	100.20
1	C	311	LEU	CA-CB-CG	-6.61	100.10	115.30
1	C	322	LEU	CB-CG-CD1	-6.59	99.79	111.00
1	D	362	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	231	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	375	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	45	PRO	N-CD-CG	-6.48	93.49	103.20
1	C	19	LEU	CB-CG-CD2	6.47	122.00	111.00
1	C	80	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	208	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	14	LEU	CA-CB-CG	6.45	130.13	115.30
1	B	122	ILE	CG1-CB-CG2	-6.45	97.22	111.40
1	B	167	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	68	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	251	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	56	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	D	300	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	199	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	251	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	132	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	75	LEU	CB-CG-CD2	6.16	121.47	111.00
1	D	231	ASP	CB-CG-OD2	6.15	123.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	249	LEU	CB-CG-CD2	6.13	121.43	111.00
1	C	57	LEU	CB-CG-CD2	6.11	121.39	111.00
1	B	250	ASP	OD1-CG-OD2	-6.07	111.77	123.30
1	D	96	TRP	CA-CB-CG	-6.05	102.20	113.70
1	D	168	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	369	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	251	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	103	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	433	ILE	CG1-CB-CG2	-5.87	98.48	111.40
1	D	144	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	277	LEU	CA-CB-CG	-5.81	101.94	115.30
1	A	144	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	161	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	178	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	D	63	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	238	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	B	47	ARG	CG-CD-NE	5.77	123.91	111.80
1	C	300	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	103	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	A	322	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	296	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	133	LEU	CB-CG-CD1	5.72	120.73	111.00
1	A	284	PRO	N-CD-CG	-5.72	94.63	103.20
1	B	68	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	187	LYS	CD-CE-NZ	-5.69	98.60	111.70
1	A	296	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	255	ARG	CB-CA-C	5.66	121.72	110.40
1	D	338	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	407	LEU	CB-CA-C	5.61	120.86	110.20
1	A	86	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	B	325	TRP	CA-CB-CG	-5.56	103.13	113.70
1	D	113	LYS	CD-CE-NZ	5.54	124.44	111.70
1	A	341	LEU	CB-CG-CD1	5.52	120.39	111.00
1	C	333	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	455	LEU	CB-CG-CD1	-5.51	101.62	111.00
1	D	257	GLN	CB-CA-C	5.51	121.42	110.40
1	C	318	LEU	CB-CG-CD2	5.50	120.35	111.00
1	A	149	THR	OG1-CB-CG2	-5.49	97.38	110.00
1	C	149	THR	OG1-CB-CG2	-5.47	97.42	110.00
1	A	167	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	244	GLU	OE1-CD-OE2	-5.45	116.76	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	LEU	CA-CB-CG	-5.45	102.77	115.30
1	D	322	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	C	378	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	430	GLU	CA-CB-CG	5.43	125.36	113.40
1	B	47	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	C	5	MET	CG-SD-CE	-5.42	91.53	100.20
1	C	314	VAL	CB-CA-C	-5.39	101.16	111.40
1	B	432	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	281	VAL	CA-CB-CG1	-5.36	102.85	110.90
1	C	75	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	B	98	LYS	CD-CE-NZ	-5.35	99.40	111.70
1	B	34	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	D	214	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	188	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	407	LEU	CB-CG-CD2	5.31	120.02	111.00
1	D	432	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	52	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	75	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	C	217	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	255	ARG	CB-CA-C	5.29	120.97	110.40
1	D	336	LYS	CA-CB-CG	5.26	124.98	113.40
1	D	351	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	262	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	D	250	ASP	OD1-CG-OD2	-5.25	113.32	123.30
1	A	161	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	167	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	66	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	214	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	B	222	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	31	LYS	CD-CE-NZ	5.15	123.54	111.70
1	C	151	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	422	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	63	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	120	VAL	CG1-CB-CG2	-5.13	102.70	110.90
1	A	446	VAL	CB-CA-C	-5.08	101.74	111.40
1	D	14	LEU	CA-CB-CG	5.07	126.97	115.30
1	D	302	VAL	CB-CA-C	-5.07	101.76	111.40
1	C	251	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	438	THR	OG1-CB-CG2	-5.05	98.39	110.00
1	D	47	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	199	ASP	OD1-CG-OD2	-5.04	113.72	123.30
1	C	39	ILE	CG1-CB-CG2	5.03	122.47	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	CG-CD-NE	5.02	122.34	111.80
1	A	418	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ASN	Peptide
1	A	292	GLU	Peptide
1	A	341	LEU	Peptide
1	B	283	ASN	Peptide
1	B	303	PRO	Peptide
1	B	316	MET	Peptide
1	B	320	GLU	Peptide
1	C	343	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3662	0	3625	312	2
1	B	3670	0	3635	359	1
1	C	3670	0	3636	393	1
1	D	3667	0	3636	337	0
2	A	43	0	30	14	0
2	B	43	0	30	15	0
2	C	43	0	30	4	0
2	D	43	0	30	13	0
3	A	18	0	29	3	0
3	B	18	0	29	0	0
3	C	18	0	29	6	0
3	D	18	0	29	2	0
All	All	14913	0	14768	1423	2

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 48.

All (1423) 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:C:107:PHE:CD2	1:C:401:ILE:HG22	1.45	1.49
1:C:85:GLY:HA2	1:C:257:GLN:NE2	1.50	1.24
1:C:100:HIS:CE1	1:C:104:LEU:HD22	1.72	1.22
1:B:313:TYR:HA	1:B:316:MET:CE	1.71	1.20
1:B:281:VAL:CG1	1:B:425:ASP:HB2	1.71	1.20
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.21	1.17
1:B:118:MET:HB3	1:B:155:LEU:HD23	1.19	1.15
1:C:107:PHE:CE2	1:C:401:ILE:HG22	1.80	1.15
1:B:224:LYS:HE2	1:B:224:LYS:HA	1.26	1.14
1:C:100:HIS:HE1	1:C:104:LEU:HD22	0.98	1.13
1:D:218:LYS:HE3	1:D:218:LYS:HA	1.23	1.13
1:B:242:ASP:HB3	1:B:245:THR:OG1	1.50	1.12
1:A:387:GLN:NE2	1:A:388:HIS:H	1.48	1.11
1:B:272:LEU:HD13	1:B:322:LEU:CD1	1.79	1.11
1:A:313:TYR:HA	1:A:316:MET:HE3	1.17	1.11
1:C:326:PRO:HG2	1:C:358:PRO:HD3	1.29	1.10
1:B:272:LEU:HD13	1:B:322:LEU:HD12	1.13	1.09
1:A:118:MET:HB3	1:A:155:LEU:HD23	1.34	1.09
1:A:272:LEU:HD13	1:A:322:LEU:HD12	1.34	1.09
1:C:149:THR:HG21	1:C:266:HIS:O	1.52	1.08
1:C:107:PHE:CD2	1:C:401:ILE:CG2	2.36	1.08
1:B:147:ARG:HG2	1:B:164:SER:HB3	1.36	1.07
1:A:313:TYR:HA	1:A:316:MET:CE	1.82	1.07
1:D:25:PRO:HD2	1:D:435:GLU:OE1	1.53	1.07
1:A:228:GLU:HG3	1:A:229:GLN:H	0.94	1.06
1:C:21:ASN:HA	1:C:189:GLN:OE1	1.55	1.06
1:D:141:VAL:HG12	1:D:142:PRO:HD3	1.34	1.06
1:C:107:PHE:HD2	1:C:401:ILE:CG2	1.71	1.04
1:A:364:LYS:H	1:A:364:LYS:HD2	1.22	1.03
1:C:272:LEU:HD13	1:C:322:LEU:HD13	1.37	1.03
1:B:147:ARG:CG	1:B:164:SER:HB3	1.88	1.02
1:B:57:LEU:HD12	1:B:341:LEU:HG	1.38	1.01
1:C:11:PHE:CD1	1:C:18:PRO:HG2	1.96	1.01
1:B:242:ASP:CB	1:B:245:THR:OG1	2.09	1.00
1:B:281:VAL:HG11	1:B:425:ASP:HB2	1.06	1.00
1:D:341:LEU:HB3	1:D:345:TYR:HB2	1.41	1.00
1:B:313:TYR:HA	1:B:316:MET:HE3	1.02	0.99
1:C:51:TYR:CE2	1:C:354:MET:HG2	1.97	0.99
1:C:272:LEU:HD13	1:C:322:LEU:CD1	1.92	0.99
1:A:147:ARG:HG3	1:A:164:SER:HB3	1.41	0.99
1:A:228:GLU:CG	1:A:229:GLN:H	1.72	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:HG3	1:A:229:GLN:N	1.77	0.98
1:C:64:GLU:OE2	1:C:397:GLN:HG2	1.62	0.98
1:D:147:ARG:HG3	1:D:164:SER:HB3	1.46	0.98
1:C:223:ARG:NH2	1:C:234:LEU:HD23	1.77	0.98
1:D:122:ILE:HG22	1:D:148:LEU:HD12	1.43	0.98
1:D:201:ASN:N	1:D:201:ASN:HD22	1.60	0.97
1:A:272:LEU:HD22	1:A:322:LEU:CD1	1.94	0.97
1:C:39:ILE:HG13	1:C:52:LEU:HD12	1.44	0.97
1:C:149:THR:HG22	1:C:266:HIS:HB2	1.45	0.97
1:C:74:ALA:O	1:C:78:VAL:HG23	1.66	0.96
1:B:201:ASN:N	1:B:201:ASN:HD22	1.58	0.96
1:D:141:VAL:HG11	1:D:444:PHE:CD2	2.00	0.96
1:A:33:ALA:HB3	1:A:359:GLN:NE2	1.82	0.95
1:D:326:PRO:HD2	1:D:358:PRO:HB3	1.49	0.95
1:A:33:ALA:CB	1:A:359:GLN:HE21	1.78	0.95
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.32	0.94
1:D:66:ARG:NH2	1:D:339:THR:OG1	1.99	0.94
1:B:201:ASN:HD22	1:B:201:ASN:H	1.02	0.94
1:D:201:ASN:HD22	1:D:201:ASN:H	1.09	0.94
1:C:63:ASP:OD2	1:C:66:ARG:HG3	1.66	0.94
1:C:85:GLY:HA2	1:C:257:GLN:HE22	1.07	0.94
1:C:100:HIS:HE1	1:C:104:LEU:CD2	1.81	0.94
1:A:33:ALA:HB3	1:A:359:GLN:HE21	1.32	0.93
1:B:451:LYS:O	1:B:453:ILE:HG13	1.68	0.93
1:D:39:ILE:HG13	1:D:52:LEU:HD12	1.47	0.93
1:A:68:ASP:HB3	1:A:334:TYR:CE1	2.04	0.93
1:A:377:GLU:O	1:A:379:PHE:N	2.02	0.93
1:B:362:ARG:O	1:B:371:VAL:HG11	1.70	0.92
2:B:472:HEM:HMC2	2:B:472:HEM:HBC2	1.49	0.92
1:C:223:ARG:CZ	1:C:234:LEU:HD23	2.00	0.92
1:C:223:ARG:NE	1:C:234:LEU:HD23	1.85	0.92
1:D:331:PHE:HE2	1:D:394:GLY:HA2	1.35	0.91
1:C:196:PRO:HB3	1:C:199:ASP:OD2	1.70	0.91
1:A:218:LYS:HE2	1:A:218:LYS:CA	1.98	0.91
1:D:86:LEU:HD11	1:D:99:ALA:HB1	1.50	0.91
1:D:331:PHE:CE2	1:D:394:GLY:HA2	2.05	0.90
1:A:139:ILE:HD11	1:A:446:VAL:HG22	1.53	0.90
1:B:78:VAL:HG13	1:B:81:PHE:CZ	2.07	0.90
1:C:279:PHE:O	1:C:283:ASN:ND2	2.05	0.89
1:D:122:ILE:HD13	1:D:122:ILE:N	1.87	0.89
1:C:82:ALA:O	1:C:256:TYR:CD1	2.26	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:PRO:O	1:D:195:ASP:N	2.05	0.89
1:D:398:ARG:NH2	2:D:472:HEM:O2D	2.06	0.89
1:C:436:THR:O	1:C:437:LEU:HB2	1.73	0.89
1:C:18:PRO:O	1:C:21:ASN:N	2.07	0.88
1:A:201:ASN:HD22	1:A:201:ASN:N	1.70	0.88
1:A:320:GLU:OE2	1:A:323:ARG:NE	2.07	0.88
2:B:472:HEM:CMB	2:B:472:HEM:HBB2	2.04	0.88
1:C:94:LYS:HE3	1:C:94:LYS:HA	1.56	0.88
1:C:219:ILE:O	1:C:222:ASP:HB3	1.74	0.88
1:A:313:TYR:O	1:A:316:MET:HB2	1.75	0.87
1:A:139:ILE:CD1	1:A:446:VAL:HG22	2.05	0.87
1:C:56:ARG:HG3	1:C:56:ARG:O	1.74	0.87
1:D:61:ALA:HA	1:D:67:PHE:CD2	2.09	0.87
1:A:134:ASN:H	1:A:134:ASN:ND2	1.69	0.87
1:A:139:ILE:CD1	1:A:446:VAL:CG2	2.53	0.87
1:B:58:ILE:HD12	1:B:355:VAL:HG22	1.55	0.87
1:C:223:ARG:HH21	1:C:234:LEU:HD23	1.38	0.86
1:C:201:ASN:H	1:C:201:ASN:HD22	1.23	0.86
1:A:224:LYS:HE2	1:A:224:LYS:HA	1.56	0.86
1:B:10:THR:C	1:B:11:PHE:HD1	1.77	0.86
1:A:139:ILE:HD11	1:A:446:VAL:CG2	2.06	0.86
1:B:282:LYS:HE2	1:B:425:ASP:OD2	1.75	0.86
1:A:310:GLN:O	1:A:312:LYS:HG3	1.76	0.85
1:A:290:ALA:HB2	1:A:313:TYR:CD2	2.12	0.85
1:B:44:ALA:HB3	1:B:47:ARG:HG3	1.57	0.85
1:D:296:ARG:O	1:D:299:VAL:HG13	1.76	0.85
1:A:52:LEU:HD23	1:A:58:ILE:HD13	1.58	0.85
1:C:107:PHE:CE2	1:C:401:ILE:CG2	2.57	0.85
1:C:116:HIS:HD2	1:C:408:HIS:NE2	1.74	0.85
1:C:176:SER:HB3	1:C:208:ASP:HB3	1.58	0.84
1:D:141:VAL:HG11	1:D:444:PHE:CE2	2.12	0.84
1:C:145:MET:HA	1:C:145:MET:CE	2.07	0.84
1:D:140:GLU:HB3	1:D:143:GLU:OE1	1.78	0.84
1:C:124:VAL:HG12	1:C:128:GLN:HG3	1.60	0.83
1:B:10:THR:C	1:B:11:PHE:CD1	2.50	0.83
1:B:282:LYS:C	1:B:283:ASN:HD22	1.81	0.83
1:B:281:VAL:HG11	1:B:425:ASP:CB	2.01	0.83
1:D:297:VAL:HG12	1:D:298:LEU:HD23	1.59	0.83
1:B:71:LEU:O	1:B:76:LYS:HE3	1.79	0.83
1:D:141:VAL:HG12	1:D:142:PRO:CD	2.08	0.83
2:D:472:HEM:HBC2	2:D:472:HEM:CMC	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:THR:HG22	1:C:266:HIS:CB	2.08	0.82
1:A:134:ASN:ND2	1:A:134:ASN:N	2.27	0.82
1:B:313:TYR:O	1:B:316:MET:HB2	1.78	0.82
1:C:10:THR:HA	1:C:15:LYS:O	1.80	0.82
1:B:313:TYR:CA	1:B:316:MET:HE3	1.99	0.82
1:D:51:TYR:CE2	1:D:354:MET:HG2	2.15	0.81
1:A:134:ASN:H	1:A:134:ASN:HD22	1.26	0.81
1:C:98:LYS:O	1:C:102:ILE:HD12	1.80	0.81
1:D:179:ARG:HE	1:D:204:GLN:NE2	1.78	0.81
1:B:57:LEU:HD12	1:B:341:LEU:CG	2.11	0.81
1:C:39:ILE:HG13	1:C:52:LEU:CD1	2.11	0.81
1:A:38:GLU:HB3	1:A:54:SER:HB3	1.61	0.81
1:C:82:ALA:O	1:C:256:TYR:HD1	1.60	0.81
1:D:25:PRO:CD	1:D:435:GLU:OE1	2.28	0.81
1:B:142:PRO:HB2	1:B:440:LYS:HE3	1.62	0.81
1:C:223:ARG:HE	1:C:234:LEU:HD23	1.44	0.81
2:B:472:HEM:HBB2	2:B:472:HEM:HMB2	1.61	0.81
1:C:129:LYS:NZ	1:C:144:ASP:OD1	2.14	0.81
1:B:264:GLU:OE1	1:B:264:GLU:HA	1.81	0.80
1:C:122:ILE:HG22	1:C:148:LEU:HD12	1.62	0.80
1:D:218:LYS:HA	1:D:218:LYS:CE	2.07	0.80
1:D:47:ARG:HD3	1:D:73:GLN:HG2	1.63	0.80
1:B:286:VAL:HG13	1:B:313:TYR:OH	1.81	0.80
1:A:140:GLU:HA	1:A:445:VAL:HG12	1.64	0.80
1:C:145:MET:HA	1:C:145:MET:HE2	1.61	0.80
1:A:118:MET:HB3	1:A:155:LEU:CD2	2.12	0.80
1:D:8:PRO:HD3	1:D:36:LEU:CD1	2.12	0.80
1:D:264:GLU:HB2	3:D:4465:PAM:H141	1.63	0.80
1:A:377:GLU:C	1:A:379:PHE:H	1.84	0.79
1:B:212:MET:HE2	1:B:263:ILE:HD11	1.65	0.79
1:C:149:THR:HG22	1:C:266:HIS:HA	1.65	0.79
1:A:38:GLU:CB	1:A:54:SER:HB3	2.12	0.79
1:C:339:THR:O	1:C:340:VAL:HG23	1.82	0.79
1:D:62:CYS:HB2	1:D:388:HIS:CE1	2.17	0.79
1:C:331:PHE:CE2	1:C:394:GLY:HA2	2.18	0.79
1:C:147:ARG:HG3	1:C:164:SER:HB3	1.64	0.79
1:A:177:MET:HA	1:A:212:MET:HE3	1.65	0.78
1:D:116:HIS:HD2	1:D:408:HIS:NE2	1.81	0.78
1:D:385:ILE:HG22	1:D:386:PRO:O	1.83	0.78
1:B:310:GLN:O	1:B:312:LYS:HG3	1.84	0.78
1:C:107:PHE:HD2	1:C:401:ILE:HG22	0.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ALA:O	1:B:323:ARG:N	2.17	0.78
1:D:421:PHE:HB2	1:D:423:PHE:CZ	2.18	0.78
1:B:147:ARG:HG2	1:B:164:SER:CB	2.13	0.78
1:D:192:ASN:O	1:D:195:ASP:HB2	1.83	0.78
1:B:61:ALA:HA	1:B:67:PHE:CE2	2.19	0.77
1:C:83:GLY:HA3	1:C:256:TYR:CE1	2.19	0.77
1:A:364:LYS:HD2	1:A:364:LYS:N	1.96	0.77
1:B:171:HIS:HD2	1:B:173:PHE:H	1.30	0.77
1:C:98:LYS:C	1:C:102:ILE:HD12	2.04	0.77
1:D:52:LEU:HB3	1:D:58:ILE:CD1	2.15	0.77
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.67	0.77
1:B:304:SER:OG	1:B:307:GLN:HB2	1.85	0.77
1:D:271:GLY:HA2	1:D:440:LYS:HG3	1.66	0.77
1:A:293:GLU:HA	1:A:296:ARG:NH1	2.00	0.77
1:A:145:MET:HE2	1:A:145:MET:HA	1.67	0.77
1:A:61:ALA:HA	1:A:67:PHE:CD2	2.19	0.76
1:C:244:GLU:O	1:C:244:GLU:CG	2.34	0.76
1:C:90:TRP:HD1	1:C:93:GLU:OE1	1.67	0.76
1:C:326:PRO:CG	1:C:358:PRO:HD3	2.14	0.76
1:C:331:PHE:CD2	1:C:394:GLY:HA2	2.20	0.76
1:A:272:LEU:CD2	1:A:322:LEU:HD13	2.14	0.76
1:D:75:LEU:HD11	1:D:87:PHE:HE1	1.50	0.76
1:A:381:ASN:ND2	1:A:383:SER:HB3	2.01	0.76
1:C:149:THR:HG22	1:C:266:HIS:CA	2.16	0.76
1:B:387:GLN:OE1	1:B:388:HIS:CD2	2.39	0.76
1:D:158:PHE:HE1	1:D:258:ILE:HG12	1.50	0.76
1:A:68:ASP:OD2	1:A:91:THR:HB	1.86	0.76
1:A:293:GLU:OE1	1:A:313:TYR:N	2.18	0.75
1:C:126:LEU:O	1:C:129:LYS:N	2.18	0.75
1:A:147:ARG:HG3	1:A:164:SER:CB	2.14	0.75
1:D:134:ASN:ND2	1:D:137:GLU:OE1	2.18	0.75
1:B:89:SER:HB2	1:B:93:GLU:OE1	1.86	0.75
1:B:201:ASN:N	1:B:201:ASN:ND2	2.34	0.75
1:A:238:LEU:O	1:A:239:ASN:ND2	2.20	0.75
1:B:16:ASN:HB3	1:B:19:LEU:HD12	1.66	0.75
1:A:98:LYS:HE2	1:A:248:PRO:O	1.85	0.75
2:B:472:HEM:HBC2	2:B:472:HEM:CMC	2.12	0.75
1:C:258:ILE:O	1:C:259:ILE:C	2.24	0.75
1:A:264:GLU:O	1:A:264:GLU:CD	2.25	0.75
1:A:272:LEU:HD13	1:A:322:LEU:CD1	2.16	0.75
1:A:296:ARG:HG2	1:A:296:ARG:NH1	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:TYR:CE2	1:D:431:LEU:HA	2.21	0.74
1:A:272:LEU:HD22	1:A:322:LEU:HD11	1.69	0.74
1:A:388:HIS:CD2	1:A:391:LYS:HE2	2.22	0.74
1:C:5:MET:HE1	1:C:50:ARG:HG2	1.69	0.74
1:C:364:LYS:H	1:C:364:LYS:HD2	1.53	0.74
2:D:472:HEM:HBC2	2:D:472:HEM:HMC1	1.67	0.74
1:D:62:CYS:CB	1:D:388:HIS:CE1	2.71	0.74
1:C:85:GLY:CA	1:C:257:GLN:HE22	1.95	0.74
1:B:283:ASN:HD22	1:B:283:ASN:N	1.85	0.74
1:C:214:ASP:O	1:C:218:LYS:HG2	1.88	0.74
1:B:304:SER:O	1:B:306:LYS:N	2.21	0.74
1:B:331:PHE:CZ	1:B:355:VAL:HG11	2.23	0.74
1:A:266:HIS:CD2	1:A:267:GLU:H	2.06	0.73
1:D:8:PRO:HD3	1:D:36:LEU:HD12	1.69	0.73
1:B:91:THR:OG1	1:B:398:ARG:HD3	1.89	0.73
1:D:162:PHE:HE1	1:D:215:LEU:HD21	1.53	0.73
1:A:298:LEU:CD2	1:A:303:PRO:HB3	2.18	0.73
1:D:370:ASP:OD2	1:D:375:ARG:NH2	2.22	0.73
1:D:26:VAL:O	1:D:29:LEU:N	2.18	0.73
1:D:273:LEU:HD21	1:D:413:VAL:HG12	1.70	0.73
1:B:147:ARG:HG3	1:B:164:SER:HB3	1.70	0.72
1:D:327:THR:O	1:D:329:PRO:HD3	1.89	0.72
1:B:253:ASN:O	1:B:257:GLN:HG2	1.87	0.72
1:D:85:GLY:HA2	1:D:257:GLN:NE2	2.04	0.72
1:C:314:VAL:HG23	1:C:315:GLY:N	2.05	0.72
1:B:53:SER:HB3	1:B:359:GLN:CB	2.20	0.72
1:C:238:LEU:C	1:C:239:ASN:HD22	1.93	0.72
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.53	0.72
1:A:282:LYS:HE2	1:A:425:ASP:OD2	1.90	0.72
1:A:272:LEU:CD2	1:A:322:LEU:CD1	2.65	0.71
1:B:201:ASN:H	1:B:201:ASN:ND2	1.84	0.71
1:B:416:MET:O	1:B:420:HIS:HD2	1.72	0.71
1:D:296:ARG:HG3	1:D:297:VAL:N	2.05	0.71
1:B:124:VAL:O	1:B:128:GLN:HG3	1.90	0.71
1:C:5:MET:CE	1:C:50:ARG:HG2	2.20	0.71
1:C:326:PRO:HG2	1:C:358:PRO:CD	2.15	0.71
1:D:311:LEU:HB3	1:D:314:VAL:HG22	1.73	0.71
1:B:356:LEU:O	1:B:357:ILE:C	2.29	0.71
1:B:59:LYS:HG3	1:B:60:GLU:N	2.05	0.71
1:D:149:THR:HG21	1:D:266:HIS:O	1.89	0.71
1:D:293:GLU:OE1	1:D:313:TYR:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TYR:CA	1:B:316:MET:CE	2.62	0.71
1:D:75:LEU:HD11	1:D:87:PHE:CE1	2.25	0.71
1:C:247:GLU:OE1	1:C:248:PRO:HD2	1.90	0.71
1:C:346:PRO:O	1:C:347:LEU:HD23	1.91	0.71
1:C:375:ARG:O	1:C:378:ARG:HG3	1.91	0.71
1:D:102:ILE:HD12	1:D:249:LEU:HG	1.72	0.71
1:D:62:CYS:HB3	1:D:388:HIS:NE2	2.06	0.70
1:D:59:LYS:HA	1:D:388:HIS:ND1	2.07	0.70
1:A:103:LEU:HD11	1:A:237:MET:CG	2.20	0.70
1:A:177:MET:HA	1:A:212:MET:CE	2.22	0.70
1:A:290:ALA:HB2	1:A:313:TYR:HD2	1.51	0.70
1:B:128:GLN:O	1:B:132:ARG:HG3	1.91	0.70
1:C:212:MET:CE	1:C:263:ILE:HD11	2.20	0.70
1:A:60:GLU:HG2	1:A:66:ARG:HH12	1.56	0.70
1:B:115:TYR:HA	1:B:118:MET:CE	2.21	0.70
1:D:122:ILE:HD13	1:D:122:ILE:H	1.55	0.70
1:A:139:ILE:HD13	1:A:446:VAL:CG2	2.20	0.70
1:A:201:ASN:HD22	1:A:201:ASN:H	1.37	0.70
1:D:335:ALA:O	1:D:349:LYS:HG3	1.92	0.70
1:A:218:LYS:HA	1:A:218:LYS:CE	2.13	0.70
1:B:212:MET:CE	1:B:263:ILE:HD11	2.20	0.70
1:C:281:VAL:HG12	1:C:281:VAL:O	1.89	0.70
1:B:61:ALA:HA	1:B:67:PHE:CD2	2.27	0.70
1:D:39:ILE:HG12	1:D:40:PHE:N	2.06	0.70
1:A:103:LEU:HD11	1:A:237:MET:HG3	1.73	0.70
1:C:201:ASN:H	1:C:201:ASN:ND2	1.90	0.70
1:A:298:LEU:HD22	1:A:303:PRO:HB3	1.73	0.69
1:D:218:LYS:HE3	1:D:218:LYS:CA	2.14	0.69
1:A:177:MET:CA	1:A:212:MET:HE3	2.21	0.69
1:A:381:ASN:HD21	1:A:383:SER:HB3	1.57	0.69
1:C:147:ARG:NH1	1:C:167:ARG:O	2.24	0.69
1:C:149:THR:CG2	1:C:266:HIS:HB2	2.22	0.69
1:A:17:LEU:HD13	1:A:44:ALA:HB1	1.74	0.69
1:D:326:PRO:CD	1:D:358:PRO:HB3	2.20	0.69
1:A:201:ASN:N	1:A:201:ASN:ND2	2.39	0.69
1:A:145:MET:HA	1:A:145:MET:CE	2.22	0.69
1:B:87:PHE:HE2	1:B:264:GLU:CD	1.96	0.69
1:D:86:LEU:HD11	1:D:99:ALA:CB	2.21	0.69
1:B:316:MET:HG2	1:B:379:PHE:HB2	1.74	0.69
1:C:298:LEU:HD21	1:C:311:LEU:HD11	1.74	0.69
1:D:17:LEU:HD22	1:D:45:PRO:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:THR:CG2	1:C:266:HIS:HA	2.22	0.68
1:C:323:ARG:HG2	1:C:361:HIS:HB3	1.73	0.68
1:B:78:VAL:CG1	1:B:81:PHE:CZ	2.76	0.68
1:D:149:THR:HG22	1:D:266:HIS:HA	1.75	0.68
1:A:423:PHE:CE1	1:A:448:ALA:HB2	2.28	0.68
1:C:112:MET:HB2	1:C:305:TYR:HE2	1.59	0.68
1:A:375:ARG:O	1:A:378:ARG:HG2	1.93	0.68
1:B:84:ASP:O	1:B:89:SER:HB3	1.94	0.68
1:D:56:ARG:O	1:D:59:LYS:HG2	1.93	0.68
1:D:201:ASN:N	1:D:201:ASN:ND2	2.34	0.68
1:A:97:LYS:HD2	1:A:101:ASN:HD21	1.58	0.68
1:B:272:LEU:CD1	1:B:322:LEU:CD1	2.65	0.68
1:A:356:LEU:C	1:A:358:PRO:HD2	2.14	0.68
1:B:130:TRP:CZ2	1:B:139:ILE:HD12	2.28	0.68
1:C:147:ARG:HD3	1:C:164:SER:O	1.94	0.68
1:C:387:GLN:O	1:C:388:HIS:HB2	1.93	0.68
1:C:78:VAL:HG13	1:C:81:PHE:CZ	2.28	0.67
1:A:387:GLN:NE2	1:A:388:HIS:N	2.33	0.67
1:B:296:ARG:HG3	1:B:297:VAL:N	2.09	0.67
1:B:325:TRP:HA	1:B:325:TRP:CE3	2.29	0.67
1:D:66:ARG:HH21	1:D:339:THR:HG1	1.42	0.67
1:B:62:CYS:SG	1:B:391:LYS:HD2	2.35	0.67
1:D:5:MET:HE3	1:D:39:ILE:HD11	1.76	0.67
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.30	0.67
1:C:5:MET:HG2	1:C:41:LYS:HB2	1.76	0.67
1:C:91:THR:HG23	1:C:96:TRP:CZ3	2.30	0.67
1:A:206:GLN:O	1:A:210:LYS:HG2	1.94	0.67
1:B:87:PHE:CE2	1:B:264:GLU:CD	2.68	0.67
1:A:391:LYS:HE3	1:A:395:ASN:OD1	1.95	0.67
1:C:338:ASP:O	1:C:339:THR:HB	1.94	0.67
1:D:91:THR:OG1	1:D:398:ARG:HD3	1.94	0.67
1:D:370:ASP:O	1:D:373:GLU:HB2	1.94	0.67
1:C:244:GLU:O	1:C:244:GLU:HG2	1.94	0.67
1:D:120:VAL:CG2	1:D:412:LEU:HD21	2.24	0.67
1:D:158:PHE:CE1	1:D:258:ILE:HG12	2.29	0.67
1:A:272:LEU:CD1	1:A:322:LEU:HD12	2.19	0.67
1:D:139:ILE:CD1	1:D:446:VAL:CG2	2.73	0.67
1:A:357:ILE:N	1:A:358:PRO:HD2	2.10	0.67
1:B:320:GLU:OE2	1:B:378:ARG:HD2	1.95	0.67
1:C:171:HIS:HD2	1:C:173:PHE:H	1.41	0.67
1:D:85:GLY:HA2	1:D:257:GLN:HE22	1.61	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HB2	1:B:345:TYR:CE1	2.30	0.66
1:B:7:GLN:HB2	1:B:8:PRO:HD2	1.76	0.66
1:D:103:LEU:O	1:D:106:SER:HB2	1.94	0.66
1:D:296:ARG:HG3	1:D:297:VAL:H	1.59	0.66
1:C:313:TYR:O	1:C:316:MET:N	2.27	0.66
1:A:376:PRO:O	1:A:377:GLU:C	2.33	0.66
1:C:128:GLN:O	1:C:132:ARG:HG3	1.95	0.66
1:A:310:GLN:O	1:A:312:LYS:N	2.23	0.66
1:A:310:GLN:C	1:A:312:LYS:H	1.99	0.66
1:B:264:GLU:HG3	2:B:472:HEM:C4C	2.30	0.66
1:B:390:PHE:O	1:B:392:PRO:HD2	1.95	0.66
1:C:111:ALA:O	1:C:114:GLY:N	2.28	0.66
1:D:69:LYS:HB2	1:D:398:ARG:HG3	1.78	0.66
1:B:59:LYS:HG3	1:B:60:GLU:H	1.59	0.66
1:C:38:GLU:HB3	1:C:54:SER:HB3	1.77	0.66
1:C:149:THR:CG2	1:C:266:HIS:CA	2.74	0.66
1:D:39:ILE:HG13	1:D:52:LEU:CD1	2.23	0.66
1:D:96:TRP:CZ2	1:D:100:HIS:HD2	2.13	0.66
2:B:472:HEM:HMB2	2:B:472:HEM:CBB	2.25	0.66
1:D:201:ASN:H	1:D:201:ASN:ND2	1.87	0.66
1:C:323:ARG:NH2	1:C:324:LEU:HD22	2.10	0.65
1:B:102:ILE:HD12	1:B:249:LEU:CD2	2.26	0.65
1:C:91:THR:CG2	1:C:96:TRP:CZ3	2.80	0.65
1:A:281:VAL:HG13	1:A:425:ASP:HB2	1.79	0.65
1:A:313:TYR:CA	1:A:316:MET:HE3	2.10	0.65
1:B:289:LYS:HG2	1:B:313:TYR:CE2	2.32	0.65
1:C:176:SER:HB3	1:C:208:ASP:CB	2.26	0.65
1:A:177:MET:O	1:A:177:MET:HG2	1.96	0.65
1:B:57:LEU:CD1	1:B:341:LEU:HG	2.22	0.65
1:B:72:SER:HB3	1:B:354:MET:HE1	1.79	0.65
1:B:332:SER:HB2	1:B:354:MET:HE2	1.79	0.65
1:C:17:LEU:HD22	1:C:45:PRO:HD3	1.79	0.65
1:C:334:TYR:HA	1:C:351:ASP:O	1.96	0.65
1:A:55:GLN:C	1:A:55:GLN:OE1	2.35	0.65
1:B:79:ARG:O	1:B:81:PHE:N	2.30	0.65
1:C:40:PHE:CE2	1:C:51:TYR:HB2	2.32	0.65
1:B:70:ASN:HB2	1:B:334:TYR:CD1	2.31	0.65
1:D:382:PRO:O	1:D:384:ALA:N	2.30	0.65
1:D:293:GLU:HG3	1:D:313:TYR:CB	2.27	0.64
1:A:139:ILE:HD13	1:A:446:VAL:HG23	1.77	0.64
1:A:357:ILE:N	1:A:358:PRO:CD	2.59	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:MET:HB3	1:B:305:TYR:HE2	1.61	0.64
1:C:38:GLU:CB	1:C:54:SER:HB3	2.27	0.64
1:C:149:THR:OG1	1:C:270:SER:HB3	1.98	0.64
1:A:33:ALA:O	1:A:36:LEU:N	2.29	0.64
1:D:242:ASP:O	1:D:246:GLY:N	2.25	0.64
1:B:210:LYS:N	1:B:210:LYS:HD2	2.12	0.64
1:C:32:ILE:HG22	1:C:36:LEU:HD12	1.78	0.64
1:D:139:ILE:HD13	1:D:446:VAL:HG23	1.78	0.64
1:D:271:GLY:O	1:D:275:PHE:HD2	1.80	0.64
1:B:61:ALA:O	1:B:67:PHE:HD2	1.79	0.64
1:C:237:MET:HE1	1:C:258:ILE:HG12	1.80	0.64
1:D:141:VAL:CG1	1:D:142:PRO:HD3	2.21	0.64
1:D:400:CYS:HB2	2:D:472:HEM:NA	2.12	0.64
1:D:139:ILE:HD11	1:D:446:VAL:CG2	2.27	0.64
1:A:418:LEU:N	1:A:418:LEU:HD23	2.09	0.64
1:C:63:ASP:O	1:C:66:ARG:N	2.30	0.64
1:C:100:HIS:ND1	1:C:100:HIS:C	2.51	0.64
1:C:341:LEU:HD22	1:C:353:LEU:HD21	1.79	0.64
1:D:179:ARG:NE	1:D:204:GLN:NE2	2.46	0.64
1:B:264:GLU:HG3	2:B:472:HEM:CHD	2.27	0.64
1:B:272:LEU:HD22	1:B:322:LEU:HD13	1.79	0.64
1:C:82:ALA:C	1:C:256:TYR:HD1	2.02	0.64
1:C:142:PRO:HG2	1:C:143:GLU:OE1	1.98	0.64
1:A:38:GLU:HB2	1:A:54:SER:CB	2.28	0.64
1:B:171:HIS:CD2	1:B:173:PHE:H	2.14	0.64
1:D:426:HIS:CD2	1:D:447:LYS:HG3	2.32	0.64
1:B:58:ILE:HG13	1:B:360:LEU:HD22	1.79	0.63
1:B:421:PHE:HB2	1:B:423:PHE:CZ	2.32	0.63
1:C:63:ASP:OD2	1:C:66:ARG:CG	2.44	0.63
2:C:472:HEM:HBC2	2:C:472:HEM:HMC1	1.80	0.63
1:D:336:LYS:O	1:D:349:LYS:HD2	1.97	0.63
1:B:71:LEU:HD21	1:B:88:THR:O	1.98	0.63
1:B:128:GLN:O	1:B:132:ARG:CG	2.47	0.63
1:B:305:TYR:CD1	1:B:305:TYR:O	2.50	0.63
1:C:167:ARG:HG3	1:C:169:GLN:O	1.97	0.63
1:D:223:ARG:HH21	1:D:234:LEU:HB3	1.64	0.63
1:A:99:ALA:O	1:A:103:LEU:HB2	1.99	0.63
1:A:62:CYS:HG	1:A:391:LYS:HE3	1.63	0.63
1:B:224:LYS:HE2	1:B:224:LYS:CA	2.14	0.63
1:C:202:LYS:O	1:C:206:GLN:HG2	1.98	0.63
1:A:33:ALA:CB	1:A:359:GLN:NE2	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:HE1	1:A:448:ALA:HB2	1.61	0.63
1:A:78:VAL:HG11	3:A:1465:PAM:H152	1.80	0.63
1:B:282:LYS:C	1:B:283:ASN:ND2	2.53	0.63
1:B:320:GLU:HB3	1:B:374:PHE:CE1	2.33	0.63
1:A:38:GLU:HB2	1:A:54:SER:OG	1.98	0.62
1:A:402:GLY:HA3	2:A:472:HEM:C3C	2.33	0.62
1:C:223:ARG:HH21	1:C:234:LEU:CD2	2.10	0.62
1:C:317:VAL:HG12	1:C:318:LEU:N	2.12	0.62
1:C:11:PHE:CE1	1:C:18:PRO:HB2	2.34	0.62
1:A:171:HIS:HD2	1:A:173:PHE:H	1.48	0.62
1:C:8:PRO:O	1:C:16:ASN:ND2	2.33	0.62
1:C:223:ARG:HE	1:C:234:LEU:CD2	2.11	0.62
1:D:293:GLU:HG3	1:D:313:TYR:HB3	1.80	0.62
1:C:183:GLU:OE1	1:C:190:ARG:NH2	2.32	0.62
1:D:107:PHE:CD2	1:D:401:ILE:HG22	2.34	0.62
1:B:239:ASN:O	1:B:240:GLY:O	2.18	0.62
1:B:102:ILE:HD12	1:B:249:LEU:HD21	1.81	0.62
1:B:224:LYS:HA	1:B:224:LYS:CE	2.16	0.62
1:A:272:LEU:O	1:A:273:LEU:C	2.35	0.62
1:B:313:TYR:O	1:B:316:MET:N	2.32	0.62
1:A:365:THR:O	1:A:365:THR:OG1	2.16	0.61
1:B:237:MET:HE1	1:B:258:ILE:HG12	1.82	0.61
1:C:212:MET:HE1	1:C:263:ILE:HD11	1.81	0.61
1:B:218:LYS:HE2	1:B:218:LYS:HA	1.80	0.61
1:C:72:SER:O	1:C:74:ALA:N	2.34	0.61
3:A:1465:PAM:H42	3:A:1465:PAM:O1	2.00	0.61
1:B:87:PHE:HD2	1:B:264:GLU:HG2	1.65	0.61
1:C:82:ALA:C	1:C:256:TYR:CD1	2.74	0.61
1:B:330:ALA:HA	1:B:357:ILE:HG13	1.81	0.61
2:A:472:HEM:HBC2	2:A:472:HEM:CMC	2.30	0.61
1:D:152:THR:HG21	1:D:409:GLU:OE2	2.01	0.61
1:D:298:LEU:HD21	1:D:311:LEU:HD11	1.83	0.61
1:C:7:GLN:HB3	1:C:41:LYS:HB3	1.82	0.61
1:C:323:ARG:O	1:C:361:HIS:ND1	2.33	0.61
1:D:337:GLU:O	1:D:338:ASP:O	2.19	0.61
1:B:281:VAL:CG1	1:B:425:ASP:CB	2.65	0.61
1:D:264:GLU:O	1:D:264:GLU:CG	2.49	0.61
1:B:87:PHE:HE2	1:B:264:GLU:OE2	1.84	0.60
1:C:96:TRP:CZ2	1:C:100:HIS:HD2	2.19	0.60
1:C:332:SER:O	1:C:333:LEU:HD13	2.01	0.60
1:B:381:ASN:C	1:B:383:SER:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LYS:HG2	1:B:420:HIS:CD2	2.36	0.60
1:D:87:PHE:O	1:D:87:PHE:CD1	2.54	0.60
1:D:128:GLN:O	1:D:129:LYS:C	2.38	0.60
1:D:426:HIS:CG	1:D:447:LYS:HG3	2.37	0.60
1:C:149:THR:HG21	1:C:266:HIS:C	2.20	0.60
1:A:176:SER:HB3	1:A:208:ASP:HB3	1.82	0.60
1:B:12:GLY:O	1:B:14:LEU:N	2.34	0.60
1:B:331:PHE:CE1	1:B:333:LEU:HD21	2.37	0.60
1:C:340:VAL:HG22	1:C:346:PRO:HA	1.82	0.60
1:B:74:ALA:O	1:B:78:VAL:HG23	2.01	0.60
1:C:273:LEU:HD11	1:C:413:VAL:HG11	1.84	0.60
1:D:377:GLU:O	1:D:380:GLU:HB2	2.01	0.60
1:B:97:LYS:O	1:B:98:LYS:C	2.38	0.60
1:C:27:GLN:OE1	1:C:433:ILE:HB	2.01	0.60
1:D:279:PHE:O	1:D:283:ASN:ND2	2.35	0.60
1:B:339:THR:OG1	1:B:340:VAL:N	2.34	0.60
1:C:69:LYS:HD3	1:C:398:ARG:NH1	2.16	0.60
1:C:223:ARG:HH21	1:C:234:LEU:HB3	1.67	0.60
1:A:293:GLU:HA	1:A:296:ARG:HH12	1.67	0.59
1:B:58:ILE:CD1	1:B:355:VAL:HG22	2.30	0.59
1:B:305:TYR:CE1	1:B:309:LYS:HE2	2.37	0.59
1:D:308:VAL:HG13	1:D:411:THR:HG22	1.84	0.59
1:A:286:VAL:O	1:A:287:LEU:C	2.41	0.59
1:C:77:PHE:CE2	1:C:188:LEU:HD23	2.38	0.59
1:D:56:ARG:O	1:D:59:LYS:CG	2.50	0.59
1:D:332:SER:O	1:D:333:LEU:HD13	2.01	0.59
1:A:17:LEU:N	1:A:18:PRO:CD	2.65	0.59
1:B:340:VAL:HG12	1:B:340:VAL:O	2.03	0.59
1:C:289:LYS:HG2	1:C:313:TYR:CE2	2.38	0.59
1:D:11:PHE:O	1:D:12:GLY:O	2.21	0.59
1:D:81:PHE:HB3	1:D:209:ILE:HD13	1.84	0.59
1:B:242:ASP:HB2	1:B:245:THR:OG1	2.00	0.59
1:D:421:PHE:HB2	1:D:423:PHE:CE2	2.36	0.59
1:A:337:GLU:HA	1:A:349:LYS:HB2	1.84	0.59
1:B:104:LEU:N	1:B:105:PRO:HD2	2.18	0.59
1:B:275:PHE:CE2	1:B:441:PRO:HD3	2.38	0.59
1:C:272:LEU:CD1	1:C:322:LEU:HD13	2.24	0.59
1:D:16:ASN:O	1:D:42:PHE:CZ	2.56	0.59
1:C:280:LEU:HB3	1:C:287:LEU:HG	1.84	0.59
1:A:69:LYS:HD3	1:A:398:ARG:NH1	2.18	0.59
1:B:331:PHE:HE1	1:B:333:LEU:HD21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ASN:O	1:B:323:ARG:HB2	2.02	0.59
1:B:22:THR:OG1	1:B:23:ASP:N	2.35	0.59
1:B:401:ILE:HG12	2:B:472:HEM:HBD2	1.83	0.59
1:D:39:ILE:HG23	1:D:39:ILE:O	2.03	0.59
1:D:425:ASP:OD2	1:D:428:ASN:HA	2.03	0.59
1:C:24:LYS:N	1:C:25:PRO:HD3	2.18	0.58
1:D:416:MET:O	1:D:420:HIS:HD2	1.86	0.58
1:A:25:PRO:HD2	1:A:435:GLU:OE1	2.03	0.58
1:A:149:THR:HG21	1:A:269:THR:HB	1.84	0.58
1:A:282:LYS:CE	1:A:425:ASP:OD2	2.51	0.58
1:B:314:VAL:O	1:B:317:VAL:HB	2.03	0.58
1:C:72:SER:O	1:C:73:GLN:C	2.41	0.58
1:C:263:ILE:HG22	1:C:264:GLU:N	2.17	0.58
1:C:390:PHE:O	1:C:392:PRO:HD2	2.03	0.58
1:A:59:LYS:HA	1:A:388:HIS:ND1	2.17	0.58
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.84	0.58
1:A:413:VAL:HG13	1:A:414:LEU:N	2.19	0.58
1:A:38:GLU:HB2	1:A:54:SER:HB3	1.86	0.58
1:A:177:MET:HB2	1:A:212:MET:HE3	1.85	0.58
1:B:271:GLY:HA3	1:B:327:THR:HG21	1.84	0.58
1:D:120:VAL:HG23	1:D:412:LEU:HD21	1.84	0.58
1:B:56:ARG:HH21	1:B:342:GLY:HA2	1.69	0.58
1:B:62:CYS:SG	1:B:391:LYS:CD	2.92	0.58
1:B:79:ARG:O	1:B:80:ASP:C	2.37	0.58
1:A:139:ILE:HG12	1:A:139:ILE:O	2.02	0.58
1:B:320:GLU:OE2	1:B:323:ARG:NE	2.36	0.58
1:C:11:PHE:CD1	1:C:18:PRO:CG	2.82	0.58
1:C:212:MET:HE2	1:C:263:ILE:HD11	1.85	0.58
1:D:30:MET:O	1:D:33:ALA:N	2.37	0.58
1:D:62:CYS:HB3	1:D:388:HIS:CE1	2.38	0.58
1:C:20:LEU:O	1:C:189:GLN:CD	2.42	0.58
1:D:62:CYS:CB	1:D:388:HIS:NE2	2.66	0.58
1:B:171:HIS:HD2	1:B:173:PHE:N	2.01	0.58
1:B:268:THR:HG21	1:B:328:ALA:HB2	1.84	0.58
1:D:63:ASP:OD2	1:D:66:ARG:HG3	2.04	0.58
1:D:149:THR:HG22	1:D:266:HIS:HB2	1.84	0.58
1:A:116:HIS:HD2	1:A:408:HIS:HE2	1.52	0.58
1:D:149:THR:HG22	1:D:266:HIS:CA	2.34	0.58
1:D:52:LEU:HB3	1:D:58:ILE:HD11	1.85	0.57
1:B:87:PHE:CD2	1:B:264:GLU:HG2	2.39	0.57
1:C:195:ASP:O	1:C:197:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ARG:NE	1:C:234:LEU:CD2	2.65	0.57
1:D:39:ILE:HG12	1:D:40:PHE:H	1.68	0.57
1:D:323:ARG:HA	1:D:361:HIS:HD1	1.69	0.57
1:A:17:LEU:HD13	1:A:44:ALA:CB	2.34	0.57
1:A:223:ARG:NH2	1:A:232:ASP:OD1	2.38	0.57
1:C:22:THR:N	1:C:189:GLN:OE1	2.34	0.57
1:A:266:HIS:CG	1:A:267:GLU:N	2.72	0.57
1:A:419:LYS:O	1:A:419:LYS:HG3	2.04	0.57
1:B:53:SER:HB3	1:B:359:GLN:HB3	1.86	0.57
1:C:264:GLU:HB2	3:C:3465:PAM:H141	1.86	0.57
1:C:70:ASN:ND2	1:C:352:GLU:HG2	2.18	0.57
1:C:134:ASN:ND2	1:C:134:ASN:H	2.03	0.57
1:D:150:LEU:HD22	1:D:174:ILE:HD11	1.85	0.57
1:A:305:TYR:O	1:A:309:LYS:HG2	2.05	0.57
1:B:332:SER:HB2	1:B:354:MET:CE	2.35	0.57
1:C:85:GLY:HA2	1:C:257:GLN:CD	2.23	0.57
1:C:212:MET:O	1:C:215:LEU:N	2.37	0.57
1:B:293:GLU:OE2	1:B:311:LEU:HD23	2.05	0.57
1:D:273:LEU:CD2	1:D:413:VAL:HG12	2.34	0.57
1:B:321:ALA:N	1:B:374:PHE:HE1	2.02	0.57
1:D:15:LYS:HG3	1:D:43:GLU:HG2	1.87	0.57
1:A:282:LYS:NZ	1:A:429:TYR:O	2.29	0.57
1:B:60:GLU:O	1:B:67:PHE:HE2	1.88	0.57
1:B:331:PHE:CE2	1:B:355:VAL:HG11	2.40	0.57
1:A:237:MET:HE1	1:A:258:ILE:HG13	1.87	0.57
1:A:399:ALA:O	1:A:401:ILE:N	2.38	0.57
1:B:194:ASP:O	1:B:195:ASP:C	2.41	0.57
1:B:301:PRO:HB2	1:B:455:LEU:HA	1.87	0.57
1:C:39:ILE:CG1	1:C:52:LEU:HD12	2.30	0.57
1:C:174:ILE:O	1:C:178:VAL:HG22	2.05	0.57
1:C:429:TYR:CZ	1:C:444:PHE:HB2	2.40	0.57
1:D:304:SER:OG	1:D:307:GLN:HG3	2.04	0.57
1:D:420:HIS:N	1:D:420:HIS:CD2	2.72	0.57
1:A:152:THR:CB	1:A:409:GLU:OE2	2.53	0.56
1:C:273:LEU:CD1	1:C:413:VAL:HG11	2.35	0.56
1:D:124:VAL:O	1:D:128:GLN:CG	2.53	0.56
1:D:366:ILE:HG23	1:D:386:PRO:HG2	1.87	0.56
1:A:177:MET:CB	1:A:212:MET:HE3	2.35	0.56
1:A:334:TYR:HA	1:A:351:ASP:O	2.05	0.56
1:A:400:CYS:HB2	2:A:472:HEM:NA	2.21	0.56
1:A:429:TYR:CE2	1:A:431:LEU:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:O	1:A:453:ILE:HG13	2.05	0.56
1:B:218:LYS:HE2	1:B:218:LYS:CA	2.35	0.56
1:B:279:PHE:HB3	1:B:374:PHE:CE2	2.41	0.56
1:C:179:ARG:NE	1:C:204:GLN:NE2	2.54	0.56
1:C:337:GLU:O	1:C:338:ASP:O	2.23	0.56
1:D:147:ARG:NH1	1:D:167:ARG:O	2.39	0.56
1:D:400:CYS:SG	1:D:403:GLN:N	2.78	0.56
1:A:266:HIS:CD2	1:A:267:GLU:N	2.73	0.56
1:B:155:LEU:HD11	1:B:161:ARG:CZ	2.35	0.56
1:C:179:ARG:HE	1:C:204:GLN:NE2	2.03	0.56
1:C:314:VAL:CG2	1:C:315:GLY:N	2.67	0.56
1:B:218:LYS:HA	1:B:218:LYS:CE	2.35	0.56
1:B:254:ILE:O	1:B:257:GLN:N	2.38	0.56
1:C:219:ILE:HG22	1:C:220:ILE:N	2.20	0.56
1:D:309:LYS:NZ	1:D:404:GLN:NE2	2.54	0.56
1:A:228:GLU:CG	1:A:229:GLN:N	2.43	0.56
1:C:84:ASP:OD1	1:C:253:ASN:ND2	2.37	0.56
1:C:293:GLU:O	1:C:293:GLU:OE2	2.23	0.56
1:D:215:LEU:O	1:D:216:VAL:C	2.44	0.56
1:A:8:PRO:HD2	1:A:16:ASN:ND2	2.19	0.56
1:A:131:GLU:HG2	1:A:421:PHE:HZ	1.71	0.56
1:A:387:GLN:OE1	1:A:388:HIS:CD2	2.58	0.56
1:B:30:MET:CE	1:B:325:TRP:CH2	2.88	0.56
1:B:52:LEU:HD13	1:B:353:LEU:HD23	1.87	0.56
1:B:321:ALA:C	1:B:323:ARG:H	2.09	0.56
1:B:336:LYS:O	1:B:349:LYS:HD2	2.06	0.56
1:C:400:CYS:SG	1:C:403:GLN:N	2.78	0.56
1:A:103:LEU:HD11	1:A:237:MET:HG2	1.88	0.56
1:A:281:VAL:CG1	1:A:425:ASP:HB2	2.35	0.56
1:B:148:LEU:HB2	1:B:165:PHE:HZ	1.71	0.56
1:C:269:THR:O	1:C:272:LEU:HB3	2.05	0.56
1:D:337:GLU:O	1:D:338:ASP:C	2.44	0.56
1:B:7:GLN:CB	1:B:8:PRO:HD2	2.35	0.56
1:C:160:TYR:HE2	1:C:215:LEU:HD11	1.69	0.56
1:B:264:GLU:OE1	1:B:264:GLU:CA	2.50	0.56
1:B:387:GLN:OE1	1:B:388:HIS:N	2.39	0.56
1:C:281:VAL:HG11	1:C:425:ASP:HB2	1.88	0.56
1:C:107:PHE:HE2	1:C:401:ILE:CG2	2.18	0.55
1:B:316:MET:HG2	1:B:379:PHE:CB	2.37	0.55
1:D:38:GLU:HA	1:D:53:SER:HB2	1.87	0.55
1:A:38:GLU:CB	1:A:54:SER:CB	2.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:C	1:A:121:ASP:OD1	2.44	0.55
1:A:312:LYS:O	1:A:316:MET:HG3	2.07	0.55
1:C:326:PRO:HG3	1:C:357:ILE:HG22	1.88	0.55
1:D:118:MET:HB3	1:D:155:LEU:HD23	1.89	0.55
1:A:68:ASP:HB3	1:A:334:TYR:CZ	2.42	0.55
1:B:68:ASP:OD2	1:B:91:THR:HB	2.05	0.55
1:C:108:SER:O	1:C:111:ALA:N	2.38	0.55
1:D:86:LEU:CD1	1:D:99:ALA:HB1	2.29	0.55
1:D:142:PRO:HG3	1:D:441:PRO:O	2.07	0.55
1:D:293:GLU:OE1	1:D:313:TYR:CB	2.55	0.55
1:B:29:LEU:HD13	1:B:51:TYR:CE2	2.42	0.55
1:B:268:THR:CG2	1:B:328:ALA:HB2	2.37	0.55
1:D:17:LEU:O	1:D:20:LEU:N	2.40	0.55
1:D:264:GLU:O	1:D:264:GLU:HG3	2.06	0.55
1:D:323:ARG:NH1	1:D:361:HIS:O	2.39	0.55
1:A:7:GLN:HB2	1:A:41:LYS:O	2.07	0.55
1:C:335:ALA:HB3	1:C:348:GLU:O	2.05	0.55
1:C:423:PHE:CE1	1:C:448:ALA:HB2	2.42	0.55
1:B:72:SER:CB	1:B:354:MET:HE1	2.36	0.55
1:A:131:GLU:HG2	1:A:421:PHE:CZ	2.42	0.55
1:A:427:THR:O	1:A:428:ASN:C	2.41	0.55
1:B:149:THR:HG22	1:B:266:HIS:HA	1.88	0.55
1:C:66:ARG:O	1:C:336:LYS:HB2	2.07	0.55
1:C:134:ASN:HD21	1:C:137:GLU:CD	2.10	0.55
1:C:323:ARG:HA	1:C:361:HIS:HD1	1.72	0.55
1:D:5:MET:HE3	1:D:50:ARG:HG2	1.88	0.55
1:D:38:GLU:O	1:D:53:SER:N	2.35	0.55
1:D:273:LEU:CD2	1:D:413:VAL:CG1	2.85	0.55
1:C:337:GLU:O	1:C:338:ASP:C	2.45	0.55
1:D:100:HIS:CE1	1:D:104:LEU:HD22	2.42	0.55
1:D:324:LEU:HD12	1:D:362:ARG:NH2	2.21	0.55
1:B:272:LEU:HD13	1:B:322:LEU:HD13	1.81	0.55
1:C:387:GLN:OE1	1:C:388:HIS:CD2	2.60	0.55
1:A:410:ALA:O	1:A:414:LEU:HB2	2.07	0.54
1:B:25:PRO:HD2	1:B:435:GLU:OE1	2.05	0.54
1:C:38:GLU:O	1:C:53:SER:HB2	2.07	0.54
1:D:280:LEU:C	1:D:287:LEU:HD12	2.28	0.54
1:A:402:GLY:HA3	2:A:472:HEM:C2C	2.42	0.54
1:B:234:LEU:O	1:B:235:THR:C	2.44	0.54
1:C:79:ARG:O	1:C:83:GLY:N	2.40	0.54
1:A:290:ALA:HB2	1:A:313:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HG3	1:B:57:LEU:HD22	1.90	0.54
1:C:116:HIS:CD2	1:C:408:HIS:NE2	2.65	0.54
1:C:164:SER:O	1:C:167:ARG:HG2	2.08	0.54
1:D:104:LEU:N	1:D:105:PRO:HD2	2.22	0.54
1:A:407:LEU:CD1	1:A:407:LEU:N	2.69	0.54
1:B:66:ARG:O	1:B:336:LYS:HB2	2.07	0.54
1:B:313:TYR:O	1:B:316:MET:CB	2.55	0.54
1:C:223:ARG:NH2	1:C:234:LEU:HB3	2.22	0.54
1:B:272:LEU:HD22	1:B:322:LEU:CD1	2.37	0.54
1:B:272:LEU:CD2	1:B:322:LEU:HD13	2.37	0.54
1:A:290:ALA:CB	1:A:313:TYR:HD2	2.20	0.54
1:A:376:PRO:O	1:A:378:ARG:N	2.41	0.54
1:A:377:GLU:C	1:A:379:PHE:N	2.55	0.54
1:A:422:ASP:N	1:A:449:LYS:O	2.19	0.54
1:B:98:LYS:O	1:B:102:ILE:HG13	2.08	0.54
1:B:300:ASP:OD2	1:B:307:GLN:NE2	2.41	0.54
1:C:185:MET:O	1:C:185:MET:HG2	2.06	0.54
1:D:185:MET:O	1:D:188:LEU:HB2	2.07	0.54
1:B:58:ILE:O	1:B:61:ALA:HB3	2.07	0.54
1:B:147:ARG:NH1	1:B:167:ARG:O	2.41	0.54
1:D:297:VAL:HG21	1:D:310:GLN:HB3	1.89	0.54
1:C:115:TYR:O	1:C:118:MET:N	2.40	0.54
1:C:126:LEU:O	1:C:127:VAL:C	2.47	0.54
1:C:306:LYS:O	1:C:309:LYS:N	2.41	0.54
1:D:281:VAL:HG13	1:D:425:ASP:HB2	1.90	0.54
1:A:407:LEU:HD13	1:A:407:LEU:H	1.73	0.54
1:C:93:GLU:O	1:C:94:LYS:C	2.46	0.54
1:C:400:CYS:SG	1:C:402:GLY:N	2.81	0.54
1:D:154:GLY:O	1:D:158:PHE:HB2	2.08	0.54
1:A:62:CYS:SG	1:A:391:LYS:HD2	2.48	0.53
1:A:190:ARG:HG2	1:A:198:TYR:CE2	2.44	0.53
1:A:272:LEU:CD1	1:A:322:LEU:CD1	2.83	0.53
1:A:303:PRO:HA	1:A:307:GLN:OE1	2.08	0.53
1:C:108:SER:O	1:C:110:GLN:N	2.41	0.53
1:A:124:VAL:O	1:A:128:GLN:HG2	2.07	0.53
1:D:322:LEU:HD12	1:D:326:PRO:HA	1.90	0.53
1:A:33:ALA:HB1	1:A:359:GLN:HE21	1.68	0.53
1:C:334:TYR:CA	1:C:351:ASP:O	2.57	0.53
1:D:12:GLY:O	1:D:14:LEU:N	2.42	0.53
1:D:120:VAL:HG22	1:D:412:LEU:HD21	1.89	0.53
1:A:61:ALA:HB2	1:A:353:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:CYS:HB3	1:A:388:HIS:CE1	2.43	0.53
1:C:3:LYS:HB2	1:C:345:TYR:CE1	2.44	0.53
1:D:116:HIS:CD2	1:D:408:HIS:NE2	2.70	0.53
1:A:57:LEU:HD12	1:A:341:LEU:HG	1.89	0.53
1:B:9:LYS:HB3	1:B:11:PHE:HE1	1.74	0.53
1:C:158:PHE:HE1	1:C:237:MET:HE1	1.73	0.53
1:D:87:PHE:O	1:D:87:PHE:HD1	1.92	0.53
1:D:323:ARG:HG2	1:D:361:HIS:HB3	1.89	0.53
1:A:423:PHE:CE1	1:A:448:ALA:CB	2.92	0.53
1:B:11:PHE:CD1	1:B:11:PHE:N	2.75	0.53
1:C:85:GLY:CA	1:C:257:GLN:NE2	2.45	0.53
1:C:194:ASP:HA	1:C:202:LYS:NZ	2.23	0.53
1:A:419:LYS:HG2	1:A:420:HIS:CD2	2.43	0.53
1:C:171:HIS:CD2	1:C:172:PRO:HD2	2.44	0.53
1:C:171:HIS:CD2	1:C:173:PHE:H	2.23	0.53
1:D:73:GLN:O	1:D:74:ALA:C	2.46	0.53
1:D:71:LEU:HD22	1:D:90:TRP:CE2	2.44	0.53
1:D:122:ILE:N	1:D:122:ILE:CD1	2.60	0.53
1:C:38:GLU:HA	1:C:53:SER:HB2	1.91	0.53
1:C:84:ASP:CG	1:C:253:ASN:HD22	2.12	0.53
1:D:8:PRO:HD3	1:D:36:LEU:HD11	1.90	0.53
1:A:97:LYS:HD2	1:A:101:ASN:ND2	2.24	0.52
1:B:26:VAL:H	1:B:435:GLU:CD	2.12	0.52
1:B:56:ARG:NH2	1:B:342:GLY:CA	2.72	0.52
1:B:334:TYR:CD1	1:B:334:TYR:N	2.74	0.52
1:C:235:THR:HA	1:C:238:LEU:HD12	1.89	0.52
1:C:402:GLY:HA3	2:C:472:HEM:C3C	2.44	0.52
1:D:55:GLN:C	1:D:55:GLN:OE1	2.48	0.52
1:D:124:VAL:O	1:D:128:GLN:HG2	2.09	0.52
1:D:129:LYS:HE2	1:D:144:ASP:OD1	2.09	0.52
1:A:310:GLN:O	1:A:312:LYS:CG	2.55	0.52
1:B:272:LEU:O	1:B:273:LEU:C	2.45	0.52
1:C:72:SER:C	1:C:74:ALA:N	2.61	0.52
1:C:139:ILE:HD11	1:C:446:VAL:CG2	2.40	0.52
1:D:318:LEU:CD1	1:D:414:LEU:HD12	2.39	0.52
1:D:402:GLY:HA3	2:D:472:HEM:C4C	2.45	0.52
1:A:371:VAL:HG23	1:A:372:GLU:N	2.23	0.52
1:B:237:MET:CE	1:B:258:ILE:HG12	2.40	0.52
1:B:305:TYR:CE1	1:B:309:LYS:CE	2.92	0.52
1:D:331:PHE:HE1	1:D:355:VAL:HG21	1.74	0.52
1:B:9:LYS:HB3	1:B:11:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:HB2	1:B:378:ARG:HE	1.73	0.52
1:D:240:GLY:O	1:D:248:PRO:HA	2.10	0.52
1:A:116:HIS:CD2	1:A:408:HIS:HE2	2.27	0.52
1:B:272:LEU:CD1	1:B:322:LEU:HD13	2.38	0.52
1:B:323:ARG:HG3	1:B:390:PHE:CE1	2.44	0.52
1:B:403:GLN:CG	1:B:404:GLN:N	2.70	0.52
1:D:141:VAL:CG1	1:D:444:PHE:CD2	2.85	0.52
1:A:145:MET:CE	1:A:145:MET:CA	2.87	0.52
1:B:30:MET:HE1	1:B:325:TRP:HH2	1.74	0.52
1:B:78:VAL:CG1	1:B:81:PHE:CE2	2.93	0.52
1:C:183:GLU:CD	1:C:190:ARG:HH22	2.11	0.52
1:D:158:PHE:HD1	1:D:234:LEU:HD22	1.75	0.52
1:B:92:HIS:HE1	1:B:336:LYS:HE2	1.74	0.52
1:B:190:ARG:HD3	1:B:198:TYR:CZ	2.45	0.52
1:B:368:GLY:O	1:B:370:ASP:N	2.38	0.52
1:D:209:ILE:HG22	1:D:213:ASN:ND2	2.25	0.52
1:D:306:LYS:HE2	1:D:306:LYS:H	1.74	0.52
2:D:472:HEM:HBB2	2:D:472:HEM:CMB	2.39	0.52
1:A:134:ASN:HD22	1:A:137:GLU:CD	2.13	0.52
1:B:270:SER:O	1:B:274:SER:HB2	2.10	0.52
1:C:60:GLU:OE1	1:C:341:LEU:HD12	2.09	0.52
1:D:311:LEU:HB3	1:D:314:VAL:CG2	2.39	0.52
1:A:340:VAL:HG23	1:A:346:PRO:HA	1.91	0.52
1:B:290:ALA:HB2	1:B:313:TYR:CE2	2.45	0.52
1:C:21:ASN:CA	1:C:189:GLN:OE1	2.44	0.52
1:C:104:LEU:N	1:C:105:PRO:HD2	2.25	0.52
1:D:183:GLU:O	1:D:186:ASN:HB2	2.10	0.52
1:D:190:ARG:HD3	1:D:198:TYR:CE2	2.45	0.52
1:A:340:VAL:CG2	1:A:346:PRO:HA	2.41	0.51
1:C:122:ILE:HG22	1:C:148:LEU:CD1	2.38	0.51
1:C:194:ASP:N	1:C:194:ASP:OD2	2.44	0.51
1:A:264:GLU:O	1:A:264:GLU:CG	2.56	0.51
1:B:3:LYS:HB2	1:B:345:TYR:HE1	1.74	0.51
1:C:83:GLY:HA3	1:C:256:TYR:CD1	2.46	0.51
1:C:341:LEU:C	1:C:343:GLY:N	2.63	0.51
1:D:7:GLN:NE2	1:D:41:LYS:O	2.43	0.51
1:D:44:ALA:HB3	1:D:47:ARG:CG	2.40	0.51
1:B:17:LEU:N	1:B:18:PRO:HD2	2.25	0.51
1:B:73:GLN:HA	1:B:76:LYS:HG3	1.92	0.51
1:D:100:HIS:HE1	1:D:104:LEU:HD22	1.75	0.51
1:D:141:VAL:CG1	1:D:142:PRO:CD	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:HG2	1:B:313:TYR:CZ	2.45	0.51
1:B:304:SER:O	1:B:305:TYR:C	2.47	0.51
1:B:451:LYS:O	1:B:452:LYS:C	2.48	0.51
1:C:145:MET:CE	1:C:145:MET:CA	2.86	0.51
1:D:17:LEU:HD22	1:D:45:PRO:CD	2.39	0.51
1:D:99:ALA:O	1:D:103:LEU:HD22	2.11	0.51
1:D:118:MET:HE3	1:D:156:CYS:HA	1.91	0.51
1:D:193:PRO:C	1:D:195:ASP:H	2.13	0.51
1:D:313:TYR:O	1:D:316:MET:HB2	2.11	0.51
1:A:28:ALA:O	1:A:32:ILE:HG13	2.10	0.51
2:A:472:HEM:HBC2	2:A:472:HEM:HMC1	1.93	0.51
1:B:11:PHE:HD1	1:B:11:PHE:N	2.08	0.51
1:C:160:TYR:CE2	1:C:215:LEU:HD11	2.46	0.51
1:A:280:LEU:HD21	1:A:317:VAL:HG11	1.93	0.51
1:B:78:VAL:HG12	1:B:81:PHE:CE2	2.46	0.51
1:B:118:MET:CB	1:B:155:LEU:HD23	2.13	0.51
1:C:69:LYS:CB	1:C:398:ARG:HG3	2.40	0.51
1:C:79:ARG:HA	1:C:83:GLY:H	1.75	0.51
1:B:410:ALA:O	1:B:413:VAL:HG12	2.10	0.51
2:C:472:HEM:HBC2	2:C:472:HEM:CMC	2.40	0.51
1:D:61:ALA:HB2	1:D:353:LEU:HD23	1.92	0.51
1:B:79:ARG:C	1:B:81:PHE:N	2.61	0.51
1:B:381:ASN:O	1:B:383:SER:N	2.44	0.51
1:B:72:SER:O	1:B:73:GLN:C	2.49	0.51
1:C:7:GLN:HB2	1:C:8:PRO:HD2	1.93	0.51
1:C:112:MET:CB	1:C:305:TYR:HE2	2.24	0.51
1:B:89:SER:CB	1:B:93:GLU:OE1	2.58	0.51
1:D:273:LEU:HD22	1:D:413:VAL:CG1	2.41	0.51
1:D:291:ALA:O	1:D:295:ALA:HB2	2.11	0.51
1:A:263:ILE:HG22	1:A:264:GLU:N	2.26	0.50
1:B:112:MET:HB3	1:B:305:TYR:CE2	2.45	0.50
1:C:341:LEU:C	1:C:343:GLY:H	2.13	0.50
1:D:85:GLY:O	1:D:86:LEU:C	2.50	0.50
1:C:52:LEU:N	1:C:354:MET:O	2.33	0.50
1:C:97:LYS:O	1:C:98:LYS:C	2.50	0.50
1:D:436:THR:O	1:D:438:THR:N	2.44	0.50
1:B:56:ARG:NH2	1:B:342:GLY:HA2	2.26	0.50
1:B:308:VAL:HG11	1:B:408:HIS:CE1	2.47	0.50
1:C:311:LEU:O	1:C:314:VAL:HG22	2.11	0.50
1:A:139:ILE:CD1	1:A:446:VAL:HG23	2.35	0.50
1:A:413:VAL:O	1:A:414:LEU:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ARG:HD3	1:C:164:SER:C	2.31	0.50
1:C:376:PRO:O	1:C:378:ARG:N	2.44	0.50
1:B:27:GLN:HG3	1:B:435:GLU:OE2	2.11	0.50
1:C:283:ASN:ND2	1:C:283:ASN:N	2.59	0.50
1:C:311:LEU:HB3	1:C:314:VAL:CG2	2.41	0.50
1:A:387:GLN:HE22	1:A:388:HIS:H	1.52	0.50
1:A:388:HIS:HD2	1:A:391:LYS:HE2	1.76	0.50
1:B:107:PHE:CZ	1:B:233:LEU:HD11	2.46	0.50
1:B:163:ASN:O	1:B:167:ARG:HD2	2.12	0.50
1:B:262:LEU:O	1:B:266:HIS:HD2	1.95	0.50
1:B:290:ALA:HB2	1:B:313:TYR:CD2	2.47	0.50
1:C:400:CYS:O	1:C:401:ILE:C	2.48	0.50
1:D:193:PRO:C	1:D:195:ASP:N	2.65	0.50
1:B:444:PHE:CD1	1:B:444:PHE:C	2.81	0.50
1:C:194:ASP:HA	1:C:202:LYS:HZ1	1.77	0.50
1:D:183:GLU:OE1	1:D:190:ARG:NH2	2.44	0.50
1:D:360:LEU:HD21	1:D:389:ALA:O	2.12	0.50
1:B:107:PHE:HZ	1:B:233:LEU:HD11	1.77	0.50
1:D:5:MET:SD	1:D:6:PRO:HD2	2.52	0.50
1:D:402:GLY:HA3	2:D:472:HEM:C3C	2.46	0.50
1:A:250:ASP:O	1:A:254:ILE:HG13	2.12	0.50
1:B:305:TYR:CZ	1:B:309:LYS:HE2	2.46	0.50
1:C:324:LEU:HD12	1:C:362:ARG:CZ	2.41	0.49
1:D:190:ARG:HD3	1:D:198:TYR:CD2	2.47	0.49
1:A:100:HIS:CE1	1:A:104:LEU:HD22	2.46	0.49
1:A:264:GLU:HG2	2:A:472:HEM:CHD	2.42	0.49
1:B:61:ALA:O	1:B:67:PHE:CD2	2.62	0.49
1:C:58:ILE:CD1	1:C:355:VAL:HG13	2.42	0.49
1:C:244:GLU:O	1:C:244:GLU:HG3	2.10	0.49
1:C:324:LEU:HD12	1:C:362:ARG:NH2	2.26	0.49
1:D:112:MET:HE1	1:D:405:PHE:HD2	1.77	0.49
1:D:319:ASN:O	1:D:323:ARG:N	2.45	0.49
1:A:100:HIS:HE1	1:A:104:LEU:HD22	1.77	0.49
1:B:24:LYS:HE2	1:B:433:ILE:O	2.13	0.49
1:B:124:VAL:O	1:B:128:GLN:CG	2.60	0.49
1:D:120:VAL:HG23	1:D:412:LEU:CD2	2.42	0.49
1:B:145:MET:O	1:B:149:THR:N	2.31	0.49
1:B:403:GLN:HG2	1:B:404:GLN:N	2.27	0.49
1:D:50:ARG:NH2	1:D:351:ASP:HB3	2.28	0.49
1:D:388:HIS:HD2	1:D:391:LYS:NZ	2.10	0.49
1:A:128:GLN:O	1:A:132:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD21	1:A:317:VAL:CG1	2.42	0.49
1:D:431:LEU:HD12	1:D:432:ASP:N	2.27	0.49
1:B:52:LEU:HD21	1:B:57:LEU:HB3	1.94	0.49
1:C:20:LEU:C	1:C:189:GLN:HG2	2.33	0.49
1:C:316:MET:HB3	1:C:379:PHE:HB2	1.94	0.49
1:C:339:THR:O	1:C:340:VAL:CG2	2.56	0.49
1:D:431:LEU:HD12	1:D:432:ASP:H	1.78	0.49
1:A:55:GLN:HE22	1:A:59:LYS:HD3	1.77	0.49
1:A:91:THR:OG1	1:A:398:ARG:HD3	2.12	0.49
1:A:377:GLU:O	1:A:378:ARG:C	2.48	0.49
1:A:432:ASP:O	1:A:442:GLU:N	2.42	0.49
1:C:306:LYS:O	1:C:307:GLN:C	2.51	0.49
1:D:124:VAL:O	1:D:128:GLN:HG3	2.13	0.49
1:A:218:LYS:CA	1:A:218:LYS:CE	2.80	0.49
1:A:272:LEU:HD21	1:A:322:LEU:HD13	1.95	0.49
1:B:86:LEU:HB3	2:B:472:HEM:HMD1	1.94	0.49
1:B:155:LEU:O	1:B:156:CYS:C	2.51	0.49
1:C:24:LYS:HA	1:C:435:GLU:HG3	1.94	0.49
1:C:115:TYR:O	1:C:116:HIS:C	2.50	0.49
1:C:139:ILE:CD1	1:C:446:VAL:HG23	2.43	0.49
1:D:337:GLU:C	1:D:338:ASP:O	2.50	0.49
1:A:257:GLN:O	1:A:258:ILE:C	2.48	0.49
1:B:297:VAL:HG13	1:B:310:GLN:NE2	2.27	0.49
1:B:403:GLN:HG2	1:B:404:GLN:H	1.78	0.49
1:C:403:GLN:O	1:C:406:ALA:HB3	2.13	0.49
1:A:62:CYS:SG	1:A:391:LYS:CE	3.01	0.49
1:B:264:GLU:HG2	2:B:472:HEM:C1D	2.47	0.49
2:B:472:HEM:HMC2	2:B:472:HEM:CBC	2.32	0.49
1:C:100:HIS:O	1:C:104:LEU:HB2	2.13	0.49
1:D:44:ALA:HB3	1:D:47:ARG:HG3	1.95	0.49
1:A:51:TYR:CE2	1:A:354:MET:HG2	2.48	0.48
1:B:30:MET:CE	1:B:325:TRP:HH2	2.23	0.48
1:B:86:LEU:HB3	2:B:472:HEM:CMD	2.42	0.48
1:C:86:LEU:CD1	1:C:99:ALA:HB3	2.43	0.48
1:C:86:LEU:O	1:C:398:ARG:NH2	2.45	0.48
1:C:201:ASN:O	1:C:205:PHE:HB2	2.13	0.48
1:D:360:LEU:CD2	1:D:389:ALA:O	2.61	0.48
1:D:361:HIS:CD2	1:D:361:HIS:N	2.80	0.48
1:A:60:GLU:HB3	1:A:341:LEU:HD12	1.94	0.48
1:B:321:ALA:C	1:B:323:ARG:N	2.66	0.48
1:B:323:ARG:O	1:B:361:HIS:ND1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:TRP:CZ2	1:D:100:HIS:CD2	2.98	0.48
1:A:61:ALA:HA	1:A:67:PHE:CE2	2.48	0.48
1:A:237:MET:CE	1:A:258:ILE:HG13	2.43	0.48
1:B:206:GLN:O	1:B:210:LYS:HG2	2.13	0.48
1:B:403:GLN:O	1:B:406:ALA:HB3	2.13	0.48
1:C:192:ASN:O	1:C:198:TYR:HE2	1.95	0.48
1:A:423:PHE:HE1	1:A:448:ALA:CB	2.25	0.48
1:C:12:GLY:O	1:C:15:LYS:N	2.45	0.48
1:C:96:TRP:CZ2	1:C:100:HIS:CD2	3.00	0.48
1:D:75:LEU:HD21	1:D:87:PHE:CE1	2.48	0.48
1:D:450:SER:OG	1:D:452:LYS:HG3	2.13	0.48
1:B:5:MET:HE3	1:B:39:ILE:HD11	1.95	0.48
1:B:35:GLU:O	1:B:35:GLU:CG	2.61	0.48
1:B:168:ASP:OD1	1:B:168:ASP:N	2.43	0.48
1:B:173:PHE:CE1	1:B:212:MET:HG2	2.49	0.48
1:B:387:GLN:CD	1:B:388:HIS:H	2.17	0.48
1:D:182:ASP:O	1:D:186:ASN:ND2	2.47	0.48
1:D:410:ALA:O	1:D:411:THR:C	2.50	0.48
1:A:296:ARG:NH1	1:A:296:ARG:CG	2.71	0.48
1:B:28:ALA:O	1:B:32:ILE:HG13	2.14	0.48
1:B:53:SER:CB	1:B:359:GLN:HB3	2.44	0.48
1:C:51:TYR:OH	3:C:3465:PAM:O1	2.27	0.48
1:C:91:THR:HG23	1:C:96:TRP:CE3	2.48	0.48
1:A:11:PHE:N	1:A:11:PHE:CD1	2.82	0.48
1:A:332:SER:C	1:A:333:LEU:HD22	2.34	0.48
1:C:15:LYS:HB2	1:C:43:GLU:O	2.13	0.48
1:C:22:THR:OG1	1:C:23:ASP:N	2.46	0.48
1:A:61:ALA:CB	1:A:353:LEU:HD23	2.44	0.48
3:A:1465:PAM:O1	3:A:1465:PAM:C4	2.61	0.48
1:B:297:VAL:HG13	1:B:310:GLN:HE21	1.78	0.48
1:B:323:ARG:HG3	1:B:390:PHE:CD1	2.49	0.48
1:C:77:PHE:HE2	1:C:188:LEU:HD23	1.78	0.48
1:C:174:ILE:O	1:C:178:VAL:HG13	2.14	0.48
1:D:7:GLN:NE2	1:D:41:LYS:HG2	2.27	0.48
1:D:26:VAL:O	1:D:29:LEU:HB2	2.14	0.48
1:A:264:GLU:CG	2:A:472:HEM:CHD	2.91	0.48
1:C:231:ASP:CG	1:C:236:HIS:HE1	2.17	0.48
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.48	0.48
1:D:341:LEU:N	1:D:345:TYR:O	2.21	0.48
1:A:171:HIS:CD2	1:A:173:PHE:H	2.31	0.48
1:B:17:LEU:HB3	1:B:18:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:O	1:B:124:VAL:HG23	2.14	0.48
1:C:311:LEU:HB3	1:C:314:VAL:HG22	1.95	0.48
1:D:7:GLN:HA	1:D:8:PRO:HD2	1.63	0.48
1:D:271:GLY:HA2	1:D:440:LYS:CG	2.42	0.48
1:A:8:PRO:HD2	1:A:16:ASN:HD21	1.78	0.47
1:A:147:ARG:HD3	1:A:164:SER:O	2.14	0.47
1:B:52:LEU:HD21	1:B:341:LEU:HD21	1.96	0.47
1:B:210:LYS:N	1:B:210:LYS:CD	2.74	0.47
1:B:273:LEU:CD1	1:B:413:VAL:HG11	2.44	0.47
1:D:79:ARG:NH2	1:D:84:ASP:HB3	2.29	0.47
1:A:134:ASN:ND2	1:A:137:GLU:CD	2.67	0.47
1:B:126:LEU:O	1:B:127:VAL:C	2.52	0.47
1:C:118:MET:O	1:C:120:VAL:N	2.47	0.47
1:C:126:LEU:HB3	1:C:127:VAL:H	1.38	0.47
1:C:223:ARG:NH2	1:C:234:LEU:CD2	2.63	0.47
1:C:253:ASN:O	1:C:254:ILE:C	2.53	0.47
1:A:264:GLU:HG2	2:A:472:HEM:C1D	2.50	0.47
1:B:356:LEU:HD13	1:B:359:GLN:HG2	1.96	0.47
1:C:210:LYS:N	1:C:210:LYS:HD2	2.29	0.47
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.73	0.47
1:B:52:LEU:CD2	1:B:57:LEU:HB3	2.43	0.47
1:B:95:ASN:O	1:B:96:TRP:O	2.32	0.47
1:B:149:THR:CG2	1:B:266:HIS:HA	2.45	0.47
1:B:282:LYS:HA	1:B:282:LYS:HD3	1.63	0.47
1:C:237:MET:SD	1:C:257:GLN:HB2	2.54	0.47
1:C:306:LYS:HE2	1:C:306:LYS:H	1.78	0.47
1:C:323:ARG:CA	1:C:361:HIS:HD1	2.28	0.47
1:A:147:ARG:HD2	1:A:165:PHE:CD1	2.50	0.47
1:B:58:ILE:HG21	1:B:360:LEU:HD22	1.95	0.47
1:B:129:LYS:HE3	1:B:144:ASP:OD2	2.15	0.47
1:B:296:ARG:HG3	1:B:297:VAL:H	1.80	0.47
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.80	0.47
1:C:397:GLN:HG3	1:C:398:ARG:N	2.30	0.47
1:C:411:THR:O	1:C:412:LEU:C	2.49	0.47
1:A:20:LEU:O	1:A:189:GLN:HG2	2.13	0.47
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.54	0.47
1:B:429:TYR:CD1	1:B:444:PHE:HA	2.50	0.47
1:B:451:LYS:O	1:B:453:ILE:CG1	2.52	0.47
1:C:370:ASP:O	1:C:371:VAL:C	2.53	0.47
1:D:112:MET:CE	1:D:405:PHE:HD2	2.28	0.47
1:D:126:LEU:O	1:D:127:VAL:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:VAL:O	1:D:414:LEU:C	2.52	0.47
1:C:297:VAL:HG21	1:C:310:GLN:O	2.15	0.47
1:D:29:LEU:O	1:D:30:MET:C	2.52	0.47
1:D:70:ASN:HB3	1:D:332:SER:HB3	1.97	0.47
1:A:320:GLU:O	1:A:323:ARG:N	2.45	0.47
1:B:263:ILE:HG22	1:B:264:GLU:N	2.30	0.47
1:B:273:LEU:HD11	1:B:413:VAL:HG11	1.97	0.47
1:C:27:GLN:HG3	1:C:435:GLU:OE2	2.15	0.47
1:C:290:ALA:HA	1:C:313:TYR:HD2	1.79	0.47
1:D:26:VAL:O	1:D:28:ALA:N	2.48	0.47
1:D:39:ILE:HA	1:D:51:TYR:O	2.15	0.47
1:A:124:VAL:O	1:A:128:GLN:CG	2.63	0.47
1:A:396:GLY:O	1:A:399:ALA:HB2	2.15	0.47
1:C:302:VAL:HG12	1:C:303:PRO:O	2.14	0.47
1:C:436:THR:O	1:C:437:LEU:CB	2.49	0.47
1:B:2:ILE:HG12	1:B:346:PRO:CG	2.45	0.46
1:B:39:ILE:HA	1:B:51:TYR:O	2.15	0.46
1:C:264:GLU:O	1:C:264:GLU:CG	2.62	0.46
1:C:274:SER:O	1:C:275:PHE:C	2.51	0.46
1:C:282:LYS:HE2	1:C:425:ASP:OD2	2.14	0.46
1:D:338:ASP:O	1:D:339:THR:HB	2.15	0.46
1:B:5:MET:HE3	1:B:50:ARG:HG2	1.97	0.46
1:B:8:PRO:HB2	1:B:19:LEU:HD13	1.96	0.46
1:B:30:MET:HE1	1:B:325:TRP:CH2	2.50	0.46
1:B:390:PHE:CE2	1:B:392:PRO:HG3	2.51	0.46
1:C:79:ARG:HG3	1:C:83:GLY:O	2.14	0.46
1:C:258:ILE:O	1:C:259:ILE:O	2.32	0.46
1:C:38:GLU:HB2	1:C:54:SER:HB3	1.97	0.46
1:A:59:LYS:HB3	1:A:388:HIS:HB2	1.98	0.46
1:B:339:THR:O	1:B:340:VAL:HG23	2.16	0.46
1:C:63:ASP:OD2	1:C:66:ARG:CD	2.63	0.46
1:D:204:GLN:O	1:D:204:GLN:HG3	2.15	0.46
1:D:215:LEU:O	1:D:217:ASP:N	2.48	0.46
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.65	0.46
1:D:364:LYS:HB3	1:D:364:LYS:HE3	1.72	0.46
1:C:318:LEU:HD12	1:C:318:LEU:HA	1.80	0.46
1:D:149:THR:HG22	1:D:266:HIS:CB	2.44	0.46
1:A:68:ASP:HB3	1:A:334:TYR:HE1	1.70	0.46
1:A:187:LYS:HG2	1:A:190:ARG:NH1	2.30	0.46
1:A:313:TYR:HA	1:A:316:MET:HE2	1.87	0.46
1:C:241:LYS:HD3	1:C:246:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ALA:HB3	3:C:3465:PAM:H42	1.97	0.46
1:C:393:PHE:O	1:C:399:ALA:HB1	2.16	0.46
1:C:403:GLN:HE21	1:C:403:GLN:HB2	1.53	0.46
1:D:17:LEU:N	1:D:18:PRO:CD	2.79	0.46
1:D:169:GLN:O	1:D:170:PRO:C	2.54	0.46
1:D:425:ASP:CG	1:D:425:ASP:O	2.53	0.46
2:D:472:HEM:CMC	2:D:472:HEM:CBC	2.85	0.46
1:A:210:LYS:HD2	1:A:210:LYS:HA	1.62	0.46
1:A:399:ALA:O	1:A:400:CYS:C	2.49	0.46
1:B:53:SER:HB3	1:B:359:GLN:HB2	1.94	0.46
1:C:38:GLU:C	1:C:53:SER:HB2	2.36	0.46
1:C:149:THR:CG2	1:C:266:HIS:CB	2.86	0.46
1:D:55:GLN:O	1:D:59:LYS:HG2	2.15	0.46
1:A:7:GLN:NE2	1:A:41:LYS:HG2	2.31	0.46
1:A:84:ASP:OD2	1:A:95:ASN:OD1	2.33	0.46
1:A:338:ASP:HA	1:A:347:LEU:O	2.16	0.46
1:A:360:LEU:O	1:A:360:LEU:HG	2.16	0.46
1:B:130:TRP:CZ3	1:B:417:MET:HG2	2.51	0.46
1:B:278:TYR:O	1:B:281:VAL:N	2.49	0.46
1:C:10:THR:CA	1:C:15:LYS:O	2.59	0.46
1:C:134:ASN:ND2	1:C:134:ASN:N	2.63	0.46
1:D:96:TRP:O	1:D:97:LYS:C	2.53	0.46
1:B:259:ILE:HG22	1:B:260:THR:N	2.30	0.46
1:B:305:TYR:CD1	1:B:305:TYR:C	2.88	0.46
1:B:344:GLU:O	1:B:346:PRO:HD2	2.15	0.46
1:C:334:TYR:CB	1:C:351:ASP:O	2.64	0.46
1:D:381:ASN:ND2	1:D:384:ALA:HB2	2.31	0.46
1:D:400:CYS:HB2	2:D:472:HEM:C1A	2.50	0.46
1:A:310:GLN:C	1:A:312:LYS:N	2.65	0.46
1:B:399:ALA:O	2:B:472:HEM:HBD1	2.15	0.46
1:C:237:MET:CE	1:C:258:ILE:HG12	2.44	0.46
1:A:17:LEU:HD22	1:A:45:PRO:CD	2.46	0.45
1:A:401:ILE:HG12	2:A:472:HEM:HBD1	1.98	0.45
1:B:262:LEU:N	1:B:262:LEU:HD23	2.21	0.45
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.62	0.45
1:B:381:ASN:C	1:B:383:SER:N	2.69	0.45
1:C:133:LEU:HD21	1:C:139:ILE:HG22	1.98	0.45
1:D:400:CYS:HA	2:D:472:HEM:CHA	2.46	0.45
1:A:177:MET:HB2	1:A:212:MET:CE	2.46	0.45
1:A:381:ASN:CG	1:A:383:SER:HB3	2.36	0.45
1:B:360:LEU:HD11	1:B:389:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PRO:O	1:C:20:LEU:N	2.50	0.45
1:C:112:MET:HB2	1:C:305:TYR:CE2	2.45	0.45
1:C:385:ILE:HG22	1:C:386:PRO:O	2.15	0.45
1:C:407:LEU:HD12	1:C:407:LEU:HA	1.52	0.45
1:D:387:GLN:HE22	1:D:391:LYS:HZ1	1.62	0.45
1:A:139:ILE:HD13	1:A:446:VAL:HG22	1.88	0.45
1:B:158:PHE:HE1	1:B:237:MET:HE1	1.82	0.45
1:D:38:GLU:HG3	1:D:39:ILE:HG22	1.99	0.45
1:A:142:PRO:HB2	1:A:440:LYS:HE3	1.98	0.45
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.56	0.45
1:C:5:MET:HE1	1:C:50:ARG:CG	2.42	0.45
1:C:5:MET:HB2	1:C:5:MET:HE2	1.71	0.45
1:C:218:LYS:O	1:C:222:ASP:HB2	2.16	0.45
1:C:304:SER:O	1:C:305:TYR:C	2.55	0.45
1:A:176:SER:HB3	1:A:208:ASP:CB	2.45	0.45
1:A:375:ARG:O	1:A:378:ARG:CG	2.61	0.45
1:B:11:PHE:O	1:B:14:LEU:HB2	2.16	0.45
1:B:186:ASN:O	1:B:188:LEU:N	2.49	0.45
1:B:192:ASN:O	1:B:198:TYR:HE2	1.99	0.45
3:C:3465:PAM:H111	3:C:3465:PAM:H81	1.60	0.45
1:D:3:LYS:HG2	1:D:344:GLU:HB3	1.98	0.45
1:D:277:LEU:HD12	1:D:277:LEU:HA	1.64	0.45
1:D:115:TYR:HA	1:D:118:MET:HE2	1.97	0.45
1:D:381:ASN:HA	1:D:382:PRO:HD3	1.76	0.45
1:A:108:SER:O	1:A:111:ALA:N	2.45	0.45
1:A:126:LEU:O	1:A:129:LYS:N	2.48	0.45
1:C:75:LEU:HA	1:C:75:LEU:HD23	1.67	0.45
1:C:91:THR:HG22	1:C:96:TRP:CZ3	2.51	0.45
1:C:220:ILE:O	1:C:221:ALA:C	2.52	0.45
1:C:260:THR:O	1:C:260:THR:CG2	2.64	0.45
1:C:320:GLU:HG3	1:C:376:PRO:HA	1.97	0.45
1:D:133:LEU:HD12	1:D:133:LEU:HA	1.39	0.45
1:A:272:LEU:HD22	1:A:322:LEU:HD13	1.72	0.45
1:B:152:THR:HB	1:B:409:GLU:OE2	2.17	0.45
1:B:323:ARG:HB2	1:B:390:PHE:HE1	1.82	0.45
1:C:72:SER:C	1:C:74:ALA:H	2.20	0.45
1:C:124:VAL:O	1:C:128:GLN:HB2	2.16	0.45
1:A:212:MET:HE2	1:A:263:ILE:HD11	1.98	0.45
1:B:130:TRP:HH2	1:B:417:MET:HE3	1.81	0.45
1:B:428:ASN:O	1:B:429:TYR:C	2.55	0.45
1:C:229:GLN:HA	1:C:229:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLU:O	1:C:321:ALA:C	2.56	0.45
1:C:341:LEU:O	1:C:343:GLY:N	2.50	0.45
1:D:97:LYS:HD2	1:D:97:LYS:HA	1.74	0.45
1:D:112:MET:HE1	1:D:115:TYR:HD2	1.82	0.45
1:D:139:ILE:CD1	1:D:446:VAL:HG23	2.37	0.45
1:D:304:SER:O	1:D:305:TYR:C	2.54	0.45
1:D:308:VAL:CG1	1:D:411:THR:HG22	2.47	0.45
1:D:397:GLN:H	1:D:397:GLN:HG3	1.53	0.45
2:D:472:HEM:HBD1	2:D:472:HEM:HHA	1.98	0.45
1:A:6:PRO:O	1:A:7:GLN:HB3	2.17	0.45
1:B:95:ASN:O	1:B:96:TRP:C	2.53	0.45
1:B:175:THR:O	1:B:178:VAL:HG22	2.17	0.45
1:C:153:ILE:HA	1:C:153:ILE:HD12	1.50	0.45
1:C:183:GLU:O	1:C:184:ALA:C	2.51	0.45
1:D:292:GLU:O	1:D:295:ALA:N	2.50	0.45
1:A:5:MET:SD	1:A:39:ILE:HG12	2.57	0.44
1:A:152:THR:HG21	1:A:409:GLU:OE2	2.17	0.44
1:C:118:MET:O	1:C:119:MET:C	2.54	0.44
1:C:338:ASP:O	1:C:339:THR:CB	2.64	0.44
1:C:357:ILE:HB	1:C:358:PRO:CD	2.46	0.44
1:D:314:VAL:CG2	1:D:411:THR:HG23	2.46	0.44
1:A:413:VAL:CG1	1:A:414:LEU:N	2.79	0.44
1:B:10:THR:O	1:B:11:PHE:CD1	2.69	0.44
1:B:164:SER:O	1:B:166:TYR:N	2.50	0.44
1:C:61:ALA:HA	1:C:67:PHE:CD2	2.52	0.44
1:D:96:TRP:CH2	1:D:100:HIS:HD2	2.34	0.44
1:D:341:LEU:HB3	1:D:345:TYR:CB	2.30	0.44
1:C:115:TYR:O	1:C:117:ALA:N	2.50	0.44
1:D:97:LYS:CE	1:D:101:ASN:HD21	2.30	0.44
1:D:283:ASN:HB3	1:D:286:VAL:HG23	2.00	0.44
1:A:323:ARG:HD3	1:A:367:TRP:CZ3	2.53	0.44
1:A:331:PHE:CE2	1:A:394:GLY:HA2	2.51	0.44
1:B:186:ASN:O	1:B:187:LYS:C	2.55	0.44
1:B:267:GLU:HG2	1:B:438:THR:HG21	2.00	0.44
1:C:141:VAL:HG11	1:C:444:PHE:CE2	2.51	0.44
1:C:281:VAL:CG1	1:C:425:ASP:HB2	2.48	0.44
1:C:432:ASP:O	1:C:441:PRO:HA	2.18	0.44
1:D:258:ILE:O	1:D:259:ILE:C	2.54	0.44
1:A:130:TRP:HA	1:A:133:LEU:HD22	2.00	0.44
1:C:20:LEU:HA	1:C:20:LEU:HD12	1.25	0.44
1:C:51:TYR:HE2	1:C:354:MET:HG2	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:O	1:C:106:SER:HB2	2.18	0.44
1:C:150:LEU:O	1:C:151:ASP:C	2.56	0.44
2:C:472:HEM:CMB	2:C:472:HEM:HBB2	2.47	0.44
1:D:215:LEU:C	1:D:217:ASP:N	2.69	0.44
1:D:270:SER:C	1:D:272:LEU:N	2.71	0.44
1:D:293:GLU:OE1	1:D:313:TYR:HB3	2.18	0.44
1:D:293:GLU:HG3	1:D:313:TYR:HB2	1.99	0.44
1:A:96:TRP:NE1	2:A:472:HEM:O1D	2.45	0.44
1:A:104:LEU:C	1:A:106:SER:H	2.21	0.44
1:B:277:LEU:HD22	1:B:417:MET:CE	2.48	0.44
1:C:71:LEU:HD12	1:C:71:LEU:HA	1.81	0.44
1:C:119:MET:HE2	1:C:405:PHE:CE2	2.52	0.44
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.82	0.44
1:C:259:ILE:HG22	1:C:260:THR:N	2.32	0.44
1:C:323:ARG:HA	1:C:361:HIS:ND1	2.31	0.44
1:A:96:TRP:CZ2	1:A:100:HIS:HD2	2.36	0.44
1:B:57:LEU:O	1:B:58:ILE:C	2.55	0.44
1:B:60:GLU:HG2	1:B:66:ARG:HH12	1.82	0.44
1:B:318:LEU:N	1:B:318:LEU:CD1	2.81	0.44
1:C:72:SER:O	1:C:75:LEU:N	2.51	0.44
1:C:126:LEU:HA	1:C:126:LEU:HD23	1.77	0.44
1:C:152:THR:O	1:C:153:ILE:C	2.56	0.44
1:C:194:ASP:O	1:C:195:ASP:C	2.56	0.44
1:A:118:MET:O	1:A:121:ASP:HB3	2.18	0.44
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.18	0.44
1:A:381:ASN:HA	1:A:382:PRO:HD2	1.93	0.44
1:B:57:LEU:HD12	1:B:341:LEU:CD2	2.48	0.44
1:B:264:GLU:CG	2:B:472:HEM:CHD	2.96	0.44
1:C:70:ASN:HD21	1:C:352:GLU:HG2	1.81	0.44
1:D:30:MET:HE3	1:D:30:MET:HB3	1.86	0.44
1:A:102:ILE:HD12	1:A:249:LEU:CD2	2.48	0.44
1:A:320:GLU:HG3	1:A:376:PRO:HA	1.99	0.44
1:A:373:GLU:O	1:A:378:ARG:NH2	2.51	0.44
1:C:130:TRP:HZ3	1:C:417:MET:HG2	1.82	0.44
1:D:324:LEU:O	1:D:362:ARG:NH1	2.48	0.44
1:A:17:LEU:HD22	1:A:45:PRO:HD2	1.99	0.43
1:A:313:TYR:HD1	1:A:316:MET:HE1	1.82	0.43
1:B:111:ALA:O	1:B:114:GLY:N	2.51	0.43
1:C:69:LYS:HB2	1:C:398:ARG:HG3	1.99	0.43
1:C:223:ARG:O	1:C:224:LYS:C	2.57	0.43
1:C:296:ARG:HG2	1:C:297:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:MET:CE	1:D:156:CYS:HA	2.47	0.43
1:D:283:ASN:HA	1:D:284:PRO:HD3	1.56	0.43
1:B:301:PRO:CB	1:B:455:LEU:HA	2.48	0.43
1:B:433:ILE:HG21	1:B:433:ILE:HD13	1.79	0.43
1:C:91:THR:CG2	1:C:96:TRP:CE3	3.02	0.43
1:C:323:ARG:C	1:C:361:HIS:HD1	2.20	0.43
1:D:17:LEU:N	1:D:18:PRO:HD2	2.32	0.43
1:B:17:LEU:HB3	1:B:18:PRO:CD	2.47	0.43
1:B:425:ASP:OD1	1:B:425:ASP:C	2.56	0.43
1:D:64:GLU:OE2	1:D:397:GLN:HG3	2.18	0.43
1:D:318:LEU:HD11	1:D:414:LEU:HD12	1.99	0.43
1:A:104:LEU:HB3	1:A:105:PRO:HD3	2.01	0.43
1:A:390:PHE:O	1:A:392:PRO:HD2	2.18	0.43
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.76	0.43
1:B:25:PRO:HD2	1:B:435:GLU:CD	2.39	0.43
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.38	0.43
1:C:281:VAL:O	1:C:281:VAL:CG1	2.58	0.43
1:C:293:GLU:HG3	1:C:313:TYR:HB2	2.00	0.43
1:C:336:LYS:HD2	1:C:336:LYS:HA	1.41	0.43
1:D:20:LEU:HD12	1:D:20:LEU:HA	1.90	0.43
1:D:388:HIS:HA	1:D:391:LYS:HD2	2.00	0.43
1:C:329:PRO:HG3	1:C:439:LEU:HG	2.00	0.43
1:D:69:LYS:CB	1:D:398:ARG:HG3	2.48	0.43
1:D:115:TYR:O	1:D:116:HIS:C	2.56	0.43
1:D:274:SER:HB3	1:D:441:PRO:HG2	2.00	0.43
1:A:102:ILE:HD12	1:A:249:LEU:HD23	2.01	0.43
1:A:102:ILE:O	1:A:105:PRO:HD2	2.18	0.43
1:A:221:ALA:O	1:A:224:LYS:HB2	2.18	0.43
1:C:118:MET:O	1:C:121:ASP:N	2.52	0.43
1:D:355:VAL:O	1:D:357:ILE:N	2.52	0.43
1:A:84:ASP:HB2	1:A:89:SER:HB3	2.00	0.43
1:A:158:PHE:N	1:A:158:PHE:CD2	2.87	0.43
1:A:264:GLU:CG	2:A:472:HEM:C4C	3.01	0.43
1:A:387:GLN:NE2	1:A:387:GLN:HA	2.33	0.43
1:A:407:LEU:N	1:A:407:LEU:HD13	2.33	0.43
1:B:278:TYR:O	1:B:279:PHE:C	2.57	0.43
1:B:304:SER:OG	1:B:304:SER:O	2.36	0.43
1:C:79:ARG:O	1:C:81:PHE:N	2.52	0.43
1:A:9:LYS:HD3	1:A:9:LYS:HA	1.67	0.43
1:A:325:TRP:CE3	1:A:325:TRP:HA	2.54	0.43
1:B:262:LEU:O	1:B:266:HIS:CD2	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:LYS:O	1:B:368:GLY:N	2.50	0.43
1:C:393:PHE:HB3	1:C:400:CYS:HB3	2.01	0.43
1:D:79:ARG:O	1:D:83:GLY:N	2.44	0.43
1:A:16:ASN:HB2	1:A:43:GLU:O	2.19	0.43
1:A:134:ASN:N	1:A:134:ASN:HD22	2.00	0.43
1:B:15:LYS:HB3	1:B:43:GLU:HB3	2.00	0.43
1:B:20:LEU:HD22	1:B:42:PHE:CZ	2.54	0.43
1:B:149:THR:HG21	1:B:269:THR:HB	2.00	0.43
1:B:302:VAL:HA	1:B:303:PRO:HD3	1.77	0.43
1:D:11:PHE:O	1:D:12:GLY:C	2.57	0.43
1:D:38:GLU:HB2	1:D:54:SER:OG	2.19	0.43
1:D:56:ARG:HG3	1:D:57:LEU:HD13	1.99	0.43
1:D:147:ARG:HD2	1:D:165:PHE:CD1	2.53	0.43
1:D:223:ARG:C	1:D:225:ALA:H	2.21	0.43
1:D:400:CYS:HA	2:D:472:HEM:C4D	2.54	0.43
3:D:4465:PAM:H152	3:D:4465:PAM:H122	1.88	0.43
1:C:147:ARG:HG3	1:C:164:SER:CB	2.41	0.43
1:C:196:PRO:CB	1:C:199:ASP:OD2	2.55	0.43
1:D:8:PRO:CD	1:D:36:LEU:CD1	2.93	0.43
1:D:232:ASP:O	1:D:233:LEU:C	2.54	0.43
1:A:371:VAL:CG2	1:A:372:GLU:N	2.82	0.42
1:B:5:MET:CE	1:B:39:ILE:HD11	2.48	0.42
1:B:27:GLN:HG3	1:B:27:GLN:H	1.36	0.42
1:B:280:LEU:HD21	1:B:317:VAL:HG13	2.01	0.42
1:B:323:ARG:CB	1:B:390:PHE:HE1	2.32	0.42
1:D:5:MET:HE3	1:D:39:ILE:CD1	2.47	0.42
1:A:118:MET:CB	1:A:155:LEU:HD23	2.25	0.42
1:A:158:PHE:CE1	1:A:258:ILE:HG12	2.54	0.42
1:A:300:ASP:CG	1:A:307:GLN:HE22	2.23	0.42
1:A:387:GLN:OE1	1:A:388:HIS:HD2	2.00	0.42
1:B:58:ILE:HG21	1:B:360:LEU:CD2	2.49	0.42
1:C:94:LYS:HE3	1:C:94:LYS:CA	2.37	0.42
1:C:323:ARG:O	1:C:361:HIS:CB	2.68	0.42
1:D:56:ARG:NH2	1:D:342:GLY:O	2.52	0.42
1:B:140:GLU:O	1:B:141:VAL:C	2.57	0.42
1:C:24:LYS:HA	1:C:435:GLU:CG	2.49	0.42
1:C:68:ASP:O	1:C:333:LEU:HA	2.19	0.42
1:C:238:LEU:C	1:C:239:ASN:ND2	2.66	0.42
1:D:241:LYS:HG2	1:D:246:GLY:O	2.19	0.42
1:D:264:GLU:O	1:D:264:GLU:CD	2.58	0.42
1:D:286:VAL:HG13	1:D:313:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:THR:O	1:A:412:LEU:C	2.58	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.46	0.42
1:B:328:ALA:O	1:B:357:ILE:HD12	2.19	0.42
1:C:158:PHE:C	1:C:160:TYR:N	2.71	0.42
1:C:234:LEU:O	1:C:237:MET:HB2	2.19	0.42
1:C:337:GLU:C	1:C:338:ASP:O	2.57	0.42
1:D:77:PHE:CE2	1:D:187:LYS:HB3	2.54	0.42
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.79	0.42
1:B:116:HIS:CD2	1:B:305:TYR:HA	2.55	0.42
1:C:17:LEU:N	1:C:18:PRO:CD	2.82	0.42
1:C:266:HIS:C	1:C:266:HIS:ND1	2.72	0.42
1:C:296:ARG:CG	1:C:297:VAL:N	2.82	0.42
1:D:13:GLU:HG3	1:D:14:LEU:HD22	2.01	0.42
1:C:24:LYS:N	1:C:25:PRO:CD	2.82	0.42
1:C:188:LEU:HD13	3:C:3465:PAM:O2	2.18	0.42
1:C:264:GLU:O	1:C:264:GLU:CD	2.58	0.42
1:C:289:LYS:HE3	1:C:313:TYR:CZ	2.54	0.42
1:D:323:ARG:O	1:D:361:HIS:ND1	2.52	0.42
1:A:147:ARG:HG2	1:A:165:PHE:CD1	2.54	0.42
1:A:192:ASN:HA	1:A:193:PRO:HD2	1.84	0.42
1:A:195:ASP:OD1	1:A:196:PRO:HD2	2.20	0.42
1:A:401:ILE:HG12	1:A:401:ILE:H	1.45	0.42
1:C:377:GLU:C	1:C:379:PHE:H	2.18	0.42
1:D:86:LEU:CD1	1:D:99:ALA:CB	2.94	0.42
1:D:115:TYR:O	1:D:117:ALA:N	2.53	0.42
1:D:141:VAL:CB	1:D:142:PRO:CD	2.97	0.42
1:D:174:ILE:O	1:D:177:MET:N	2.50	0.42
1:D:314:VAL:HG21	1:D:411:THR:HG23	2.00	0.42
2:D:472:HEM:HBC2	2:D:472:HEM:HMC3	1.97	0.42
1:B:2:ILE:HG12	1:B:346:PRO:HG3	2.00	0.42
1:B:3:LYS:HB3	1:B:3:LYS:HE3	1.59	0.42
1:B:153:ILE:HD12	1:B:153:ILE:HA	1.87	0.42
1:B:186:ASN:C	1:B:188:LEU:N	2.71	0.42
1:A:177:MET:CB	1:A:212:MET:CE	2.98	0.42
1:A:323:ARG:HG2	1:A:361:HIS:HB3	2.01	0.42
1:B:27:GLN:O	1:B:28:ALA:C	2.58	0.42
1:B:174:ILE:HD12	1:B:174:ILE:HG23	1.74	0.42
1:C:40:PHE:CZ	1:C:51:TYR:CB	3.03	0.42
1:C:129:LYS:O	1:C:132:ARG:N	2.46	0.42
1:C:188:LEU:CD1	3:C:3465:PAM:O2	2.68	0.42
1:D:94:LYS:O	1:D:94:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:PRO:HB3	1:D:455:LEU:HA	2.00	0.42
1:D:311:LEU:HD23	1:D:311:LEU:HA	1.72	0.42
1:D:316:MET:HB3	1:D:376:PRO:HB3	2.01	0.42
1:A:264:GLU:HG3	2:A:472:HEM:C4C	2.55	0.42
1:B:178:VAL:HG23	1:B:179:ARG:N	2.35	0.42
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.99	0.42
1:C:15:LYS:CB	1:C:43:GLU:O	2.68	0.42
1:C:115:TYR:HA	1:C:118:MET:HE3	2.02	0.42
1:C:322:LEU:HA	1:C:322:LEU:HD12	1.84	0.42
1:D:122:ILE:HG22	1:D:148:LEU:CD1	2.32	0.42
1:D:322:LEU:HD12	1:D:322:LEU:HA	1.74	0.42
1:A:55:GLN:O	1:A:59:LYS:HG2	2.20	0.41
1:A:428:ASN:O	1:A:429:TYR:C	2.58	0.41
1:B:7:GLN:HB2	1:B:8:PRO:CD	2.45	0.41
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.90	0.41
1:B:337:GLU:O	1:B:339:THR:HG22	2.19	0.41
1:C:233:LEU:HD11	1:C:261:PHE:CE2	2.56	0.41
1:D:73:GLN:HA	1:D:73:GLN:NE2	2.35	0.41
1:D:193:PRO:O	1:D:194:ASP:C	2.56	0.41
1:D:216:VAL:HG13	1:D:258:ILE:HD13	2.02	0.41
1:A:58:ILE:O	1:A:61:ALA:N	2.53	0.41
1:A:126:LEU:O	1:A:127:VAL:C	2.59	0.41
1:B:323:ARG:HA	1:B:361:HIS:HD1	1.85	0.41
1:C:1:THR:CG2	1:C:2:ILE:H	2.33	0.41
1:C:223:ARG:HH21	1:C:234:LEU:CB	2.32	0.41
1:C:294:ALA:O	1:C:298:LEU:HD12	2.20	0.41
1:C:299:VAL:H	1:C:299:VAL:HG22	1.39	0.41
1:C:397:GLN:HG3	1:C:398:ARG:H	1.83	0.41
1:D:215:LEU:HD12	1:D:215:LEU:HA	1.84	0.41
1:D:400:CYS:C	1:D:402:GLY:H	2.23	0.41
1:A:62:CYS:SG	1:A:391:LYS:CD	3.09	0.41
1:A:279:PHE:O	1:A:283:ASN:ND2	2.50	0.41
1:A:318:LEU:HD13	1:A:414:LEU:HD12	2.01	0.41
1:B:239:ASN:O	1:B:240:GLY:C	2.58	0.41
1:C:150:LEU:HD21	1:C:162:PHE:CD1	2.55	0.41
1:D:29:LEU:O	1:D:30:MET:O	2.38	0.41
1:D:33:ALA:HB2	1:D:40:PHE:HE1	1.86	0.41
1:D:270:SER:C	1:D:272:LEU:H	2.22	0.41
1:B:17:LEU:HD12	1:B:17:LEU:HA	1.90	0.41
1:C:147:ARG:HG2	1:C:165:PHE:CE1	2.55	0.41
1:C:377:GLU:C	1:C:379:PHE:N	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:VAL:HG12	1:D:27:GLN:N	2.35	0.41
1:D:33:ALA:HB3	1:D:359:GLN:HE21	1.85	0.41
1:D:345:TYR:HA	1:D:346:PRO:HD3	1.78	0.41
1:D:381:ASN:HD22	1:D:384:ALA:HB2	1.84	0.41
1:A:234:LEU:HA	1:A:237:MET:HE2	2.02	0.41
1:B:195:ASP:C	1:B:197:ALA:N	2.74	0.41
1:B:264:GLU:CG	2:B:472:HEM:C1D	3.04	0.41
1:B:319:ASN:O	1:B:379:PHE:CE1	2.74	0.41
1:B:401:ILE:HG12	1:B:401:ILE:H	1.79	0.41
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.95	0.41
1:C:58:ILE:HD13	1:C:355:VAL:HG13	2.02	0.41
1:C:124:VAL:HG12	1:C:128:GLN:CG	2.40	0.41
1:D:177:MET:HB2	1:D:212:MET:CE	2.50	0.41
1:B:47:ARG:HH11	1:B:47:ARG:HD2	1.65	0.41
1:B:151:ASP:OD1	1:B:162:PHE:HB2	2.21	0.41
1:B:318:LEU:O	1:B:322:LEU:HB2	2.19	0.41
1:C:17:LEU:HD22	1:C:45:PRO:CD	2.50	0.41
1:A:58:ILE:HD13	1:A:58:ILE:HA	1.82	0.41
1:A:401:ILE:CG1	2:A:472:HEM:HBD1	2.51	0.41
2:A:472:HEM:CMC	2:A:472:HEM:CBC	2.97	0.41
1:B:126:LEU:HD21	1:B:130:TRP:CE2	2.56	0.41
1:B:275:PHE:CZ	1:B:441:PRO:HD3	2.55	0.41
1:B:323:ARG:HD3	1:B:367:TRP:CZ3	2.56	0.41
1:C:418:LEU:HD23	1:C:418:LEU:HA	1.43	0.41
1:D:316:MET:HG2	1:D:379:PHE:O	2.21	0.41
1:D:422:ASP:OD1	1:D:451:LYS:HE2	2.20	0.41
1:B:128:GLN:O	1:B:132:ARG:HG2	2.20	0.41
1:B:272:LEU:N	1:B:327:THR:HG21	2.36	0.41
1:B:277:LEU:HD22	1:B:417:MET:HE1	2.03	0.41
1:C:17:LEU:N	1:C:18:PRO:HD2	2.35	0.41
1:C:216:VAL:O	1:C:218:LYS:N	2.54	0.41
1:D:17:LEU:O	1:D:18:PRO:C	2.59	0.41
1:D:388:HIS:HD2	1:D:391:LYS:HZ3	1.68	0.41
1:B:421:PHE:HA	1:B:449:LYS:O	2.21	0.41
1:C:134:ASN:HD22	1:C:134:ASN:C	2.25	0.41
1:D:101:ASN:O	1:D:102:ILE:C	2.54	0.41
1:A:64:GLU:OE2	1:A:396:GLY:HA3	2.21	0.40
1:A:66:ARG:O	1:A:336:LYS:HB2	2.21	0.40
1:B:255:ARG:HD2	1:B:256:TYR:N	2.36	0.40
1:B:314:VAL:CG2	1:B:411:THR:HG23	2.51	0.40
1:B:402:GLY:O	1:B:405:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ARG:NH1	1:C:49:THR:HG21	2.36	0.40
1:C:127:VAL:HG21	1:C:416:MET:HE2	2.03	0.40
1:D:177:MET:HB2	1:D:212:MET:HE3	2.02	0.40
1:D:289:LYS:HE3	1:D:313:TYR:OH	2.21	0.40
1:A:55:GLN:OE1	1:A:56:ARG:N	2.54	0.40
1:A:86:LEU:HD11	1:A:99:ALA:HB3	2.03	0.40
1:A:257:GLN:H	1:A:257:GLN:HG2	1.79	0.40
1:B:113:LYS:HA	1:B:305:TYR:CD2	2.57	0.40
1:C:147:ARG:CG	1:C:164:SER:HB3	2.42	0.40
1:D:281:VAL:CG1	1:D:425:ASP:HB2	2.51	0.40
1:A:218:LYS:HE2	1:A:218:LYS:N	2.35	0.40
1:B:321:ALA:O	1:B:322:LEU:C	2.60	0.40
1:C:1:THR:CG2	1:C:2:ILE:N	2.84	0.40
1:D:5:MET:CE	1:D:39:ILE:HD11	2.49	0.40
1:D:193:PRO:O	1:D:198:TYR:HD2	2.03	0.40
1:D:242:ASP:N	1:D:247:GLU:O	2.53	0.40
1:A:418:LEU:HD22	1:A:418:LEU:HA	1.61	0.40
1:B:122:ILE:C	1:B:124:VAL:N	2.75	0.40
1:B:223:ARG:HH22	1:B:232:ASP:CG	2.19	0.40
1:B:390:PHE:C	1:B:392:PRO:CD	2.90	0.40
1:A:116:HIS:O	1:A:117:ALA:C	2.59	0.40
1:B:126:LEU:O	1:B:128:GLN:N	2.55	0.40
1:C:158:PHE:O	1:C:160:TYR:N	2.53	0.40
1:C:340:VAL:HG12	1:C:343:GLY:HA2	2.03	0.40
1:C:393:PHE:CE1	1:C:403:GLN:HA	2.57	0.40
1:D:2:ILE:HA	1:D:344:GLU:O	2.22	0.40
1:D:13:GLU:HG3	1:D:14:LEU:N	2.36	0.40
1:D:51:TYR:CD2	1:D:354:MET:HB3	2.57	0.40
1:D:377:GLU:O	1:D:379:PHE:N	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD2	1:C:23:ASP:OD2[2_664]	1.70	0.50
1:A:207:GLU:OE2	1:B:207:GLU:OE2[6_664]	2.04	0.16

## 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	453/471 (96%)	358 (79%)	66 (15%)	29 (6%)	1	1
1	B	453/471 (96%)	326 (72%)	89 (20%)	38 (8%)	1	0
1	C	453/471 (96%)	307 (68%)	102 (22%)	44 (10%)	0	0
1	D	452/471 (96%)	351 (78%)	72 (16%)	29 (6%)	1	1
All	All	1811/1884 (96%)	1342 (74%)	329 (18%)	140 (8%)	1	0

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	GLY
1	A	365	THR
1	A	377	GLU
1	A	425	ASP
1	A	452	LYS
1	B	13	GLU
1	B	62	CYS
1	B	141	VAL
1	B	240	GLY
1	B	264	GLU
1	B	317	VAL
1	B	322	LEU
1	B	391	LYS
1	B	425	ASP
1	C	19	LEU
1	C	116	HIS
1	C	126	LEU
1	C	127	VAL
1	C	165	PHE
1	C	338	ASP
1	C	377	GLU
1	C	452	LYS

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Mol	Chain	Res	Type
1	D	12	GLY
1	D	13	GLU
1	D	27	GLN
1	D	38	GLU
1	D	116	HIS
1	D	193	PRO
1	D	194	ASP
1	D	338	ASP
1	D	378	ARG
1	D	383	SER
1	D	403	GLN
1	D	437	LEU
1	A	58	ILE
1	A	83	GLY
1	A	93	GLU
1	A	254	ILE
1	A	293	GLU
1	A	311	LEU
1	A	378	ARG
1	A	396	GLY
1	B	85	GLY
1	B	126	LEU
1	B	127	VAL
1	B	251	ASP
1	B	305	TYR
1	B	321	ALA
1	B	327	THR
1	B	340	VAL
1	B	361	HIS
1	B	369	ASP
1	B	371	VAL
1	B	377	GLU
1	B	426	HIS
1	B	429	TYR
1	C	9	LYS
1	C	15	LYS
1	C	73	GLN
1	C	79	ARG
1	C	119	MET
1	C	154	GLY
1	C	217	ASP
1	C	256	TYR

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Mol	Chain	Res	Type
1	C	263	ILE
1	C	264	GLU
1	D	8	PRO
1	D	26	VAL
1	D	64	GLU
1	D	74	ALA
1	A	34	ASP
1	A	100	HIS
1	A	366	ILE
1	A	403	GLN
1	B	47	ARG
1	B	155	LEU
1	B	193	PRO
1	B	263	ILE
1	C	80	ASP
1	C	109	GLN
1	C	155	LEU
1	C	159	ASN
1	C	287	LEU
1	C	372	GLU
1	C	451	LYS
1	D	158	PHE
1	D	356	LEU
1	D	382	PRO
1	A	227	GLY
1	A	237	MET
1	A	238	LEU
1	A	412	LEU
1	A	437	LEU
1	B	96	TRP
1	B	123	ALA
1	B	409	GLU
1	C	77	PHE
1	C	136	ASP
1	C	188	LEU
1	C	339	THR
1	C	369	ASP
1	D	96	TRP
1	D	410	ALA
1	D	438	THR
1	A	62	CYS
1	A	105	PRO

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Mol	Chain	Res	Type
1	A	123	ALA
1	B	403	GLN
1	B	408	HIS
1	B	437	LEU
1	C	146	THR
1	C	156	CYS
1	C	191	ALA
1	C	196	PRO
1	C	224	LYS
1	C	259	ILE
1	C	281	VAL
1	C	288	GLN
1	C	425	ASP
1	D	289	LYS
1	D	293	GLU
1	A	248	PRO
1	A	305	TYR
1	A	418	LEU
1	B	119	MET
1	B	252	GLU
1	C	151	ASP
1	C	365	THR
1	C	391	LYS
1	D	228	GLU
1	D	248	PRO
1	B	243	PRO
1	B	326	PRO
1	C	12	GLY
1	C	317	VAL
1	B	48	VAL
1	D	216	VAL
1	A	8	PRO
1	D	153	ILE
1	D	196	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	397/413 (96%)	327 (82%)	70 (18%)	2	3
1	B	399/413 (97%)	320 (80%)	79 (20%)	1	1
1	C	399/413 (97%)	327 (82%)	72 (18%)	1	2
1	D	399/413 (97%)	317 (79%)	82 (21%)	1	1
All	All	1594/1652 (96%)	1291 (81%)	303 (19%)	1	2

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	7	GLN
1	A	9	LYS
1	A	11	PHE
1	A	13	GLU
1	A	14	LEU
1	A	21	ASN
1	A	38	GLU
1	A	39	ILE
1	A	48	VAL
1	A	49	THR
1	A	53	SER
1	A	56	ARG
1	A	57	LEU
1	A	69	LYS
1	A	70	ASN
1	A	71	LEU
1	A	86	LEU
1	A	87	PHE
1	A	97	LYS
1	A	103	LEU
1	A	106	SER
1	A	112	MET
1	A	126	LEU
1	A	128	GLN
1	A	133	LEU
1	A	134	ASN
1	A	136	ASP
1	A	139	ILE
1	A	145	MET
1	A	147	ARG
1	A	149	THR
1	A	172	PRO

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Mol	Chain	Res	Type
1	A	200	GLU
1	A	201	ASN
1	A	215	LEU
1	A	218	LYS
1	A	222	ASP
1	A	226	SER
1	A	230	SER
1	A	248	PRO
1	A	255	ARG
1	A	266	HIS
1	A	287	LEU
1	A	293	GLU
1	A	296	ARG
1	A	312	LYS
1	A	314	VAL
1	A	318	LEU
1	A	320	GLU
1	A	322	LEU
1	A	324	LEU
1	A	336	LYS
1	A	338	ASP
1	A	340	VAL
1	A	364	LYS
1	A	365	THR
1	A	378	ARG
1	A	387	GLN
1	A	401	ILE
1	A	407	LEU
1	A	414	LEU
1	A	416	MET
1	A	418	LEU
1	A	419	LYS
1	A	426	HIS
1	A	444	PHE
1	A	445	VAL
1	A	447	LYS
1	A	455	LEU
1	B	1	THR
1	B	9	LYS
1	B	11	PHE
1	B	13	GLU
1	B	22	THR

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Mol	Chain	Res	Type
1	B	35	GLU
1	B	38	GLU
1	B	48	VAL
1	B	52	LEU
1	B	53	SER
1	B	56	ARG
1	B	59	LYS
1	B	62	CYS
1	B	64	GLU
1	B	76	LYS
1	B	79	ARG
1	B	86	LEU
1	B	88	THR
1	B	106	SER
1	B	109	GLN
1	B	112	MET
1	B	121	ASP
1	B	126	LEU
1	B	128	GLN
1	B	129	LYS
1	B	133	LEU
1	B	134	ASN
1	B	136	ASP
1	B	139	ILE
1	B	148	LEU
1	B	155	LEU
1	B	161	ARG
1	B	189	GLN
1	B	200	GLU
1	B	201	ASN
1	B	210	LYS
1	B	230	SER
1	B	233	LEU
1	B	235	THR
1	B	244	GLU
1	B	250	ASP
1	B	254	ILE
1	B	255	ARG
1	B	274	SER
1	B	278	TYR
1	B	280	LEU
1	B	282	LYS

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Mol	Chain	Res	Type
1	B	283	ASN
1	B	287	LEU
1	B	293	GLU
1	B	296	ARG
1	B	299	VAL
1	B	302	VAL
1	B	306	LYS
1	B	309	LYS
1	B	314	VAL
1	B	318	LEU
1	B	322	LEU
1	B	323	ARG
1	B	324	LEU
1	B	339	THR
1	B	352	GLU
1	B	355	VAL
1	B	356	LEU
1	B	359	GLN
1	B	364	LYS
1	B	366	ILE
1	B	371	VAL
1	B	383	SER
1	B	387	GLN
1	B	391	LYS
1	B	401	ILE
1	B	403	GLN
1	B	404	GLN
1	B	414	LEU
1	B	422	ASP
1	B	444	PHE
1	B	447	LYS
1	B	450	SER
1	C	13	GLU
1	C	14	LEU
1	C	32	ILE
1	C	38	GLU
1	C	39	ILE
1	C	56	ARG
1	C	57	LEU
1	C	58	ILE
1	C	64	GLU
1	C	65	SER

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Mol	Chain	Res	Type
1	C	71	LEU
1	C	79	ARG
1	C	84	ASP
1	C	86	LEU
1	C	88	THR
1	C	94	LYS
1	C	97	LYS
1	C	100	HIS
1	C	103	LEU
1	C	126	LEU
1	C	134	ASN
1	C	139	ILE
1	C	145	MET
1	C	147	ARG
1	C	148	LEU
1	C	167	ARG
1	C	172	PRO
1	C	176	SER
1	C	177	MET
1	C	192	ASN
1	C	194	ASP
1	C	201	ASN
1	C	224	LYS
1	C	231	ASP
1	C	235	THR
1	C	238	LEU
1	C	252	GLU
1	C	259	ILE
1	C	266	HIS
1	C	268	THR
1	C	283	ASN
1	C	287	LEU
1	C	293	GLU
1	C	296	ARG
1	C	298	LEU
1	C	299	VAL
1	C	306	LYS
1	C	312	LYS
1	C	316	MET
1	C	318	LEU
1	C	320	GLU
1	C	324	LEU

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Mol	Chain	Res	Type
1	C	333	LEU
1	C	336	LYS
1	C	337	GLU
1	C	344	GLU
1	C	349	LYS
1	C	364	LYS
1	C	365	THR
1	C	371	VAL
1	C	378	ARG
1	C	387	GLN
1	C	391	LYS
1	C	398	ARG
1	C	403	GLN
1	C	407	LEU
1	C	413	VAL
1	C	414	LEU
1	C	430	GLU
1	C	438	THR
1	C	447	LYS
1	C	455	LEU
1	D	7	GLN
1	D	17	LEU
1	D	31	LYS
1	D	39	ILE
1	D	48	VAL
1	D	55	GLN
1	D	56	ARG
1	D	57	LEU
1	D	59	LYS
1	D	64	GLU
1	D	65	SER
1	D	71	LEU
1	D	72	SER
1	D	73	GLN
1	D	94	LYS
1	D	97	LYS
1	D	103	LEU
1	D	121	ASP
1	D	122	ILE
1	D	126	LEU
1	D	128	GLN
1	D	133	LEU

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Mol	Chain	Res	Type
1	D	134	ASN
1	D	136	ASP
1	D	137	GLU
1	D	139	ILE
1	D	141	VAL
1	D	153	ILE
1	D	167	ARG
1	D	195	ASP
1	D	196	PRO
1	D	200	GLU
1	D	201	ASN
1	D	209	ILE
1	D	210	LYS
1	D	218	LYS
1	D	226	SER
1	D	228	GLU
1	D	230	SER
1	D	233	LEU
1	D	235	THR
1	D	242	ASP
1	D	255	ARG
1	D	260	THR
1	D	266	HIS
1	D	281	VAL
1	D	286	VAL
1	D	287	LEU
1	D	293	GLU
1	D	296	ARG
1	D	306	LYS
1	D	310	GLN
1	D	318	LEU
1	D	320	GLU
1	D	322	LEU
1	D	324	LEU
1	D	331	PHE
1	D	332	SER
1	D	336	LYS
1	D	338	ASP
1	D	344	GLU
1	D	352	GLU
1	D	362	ARG
1	D	364	LYS

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Mol	Chain	Res	Type
1	D	365	THR
1	D	370	ASP
1	D	371	VAL
1	D	383	SER
1	D	391	LYS
1	D	392	PRO
1	D	397	GLN
1	D	398	ARG
1	D	403	GLN
1	D	407	LEU
1	D	413	VAL
1	D	414	LEU
1	D	420	HIS
1	D	427	THR
1	D	430	GLU
1	D	438	THR
1	D	440	LYS
1	D	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	27	GLN
1	A	70	ASN
1	A	73	GLN
1	A	95	ASN
1	A	100	HIS
1	A	101	ASN
1	A	116	HIS
1	A	134	ASN
1	A	171	HIS
1	A	192	ASN
1	A	201	ASN
1	A	239	ASN
1	A	266	HIS
1	A	359	GLN
1	A	387	GLN
1	A	388	HIS
1	A	403	GLN
1	A	426	HIS
1	B	7	GLN

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Mol	Chain	Res	Type
1	B	92	HIS
1	B	116	HIS
1	B	171	HIS
1	B	192	ASN
1	B	201	ASN
1	B	239	ASN
1	B	266	HIS
1	B	283	ASN
1	B	310	GLN
1	B	388	HIS
1	B	403	GLN
1	B	420	HIS
1	C	7	GLN
1	C	100	HIS
1	C	116	HIS
1	C	134	ASN
1	C	171	HIS
1	C	201	ASN
1	C	204	GLN
1	C	236	HIS
1	C	239	ASN
1	C	319	ASN
1	C	388	HIS
1	C	403	GLN
1	D	73	GLN
1	D	100	HIS
1	D	101	ASN
1	D	110	GLN
1	D	116	HIS
1	D	171	HIS
1	D	201	ASN
1	D	204	GLN
1	D	239	ASN
1	D	388	HIS
1	D	403	GLN
1	D	404	GLN
1	D	420	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEM	C	472	1	27,50,50	2.07	10 (37%)	17,82,82	3.83	9 (52%)
2	HEM	B	472	1	27,50,50	2.78	10 (37%)	17,82,82	2.51	7 (41%)
2	HEM	D	472	1	27,50,50	2.12	6 (22%)	17,82,82	2.24	6 (35%)
3	PAM	B	2465	-	14,17,17	1.12	1 (7%)	13,17,17	1.08	0
3	PAM	D	4465	-	14,17,17	1.17	1 (7%)	13,17,17	1.12	0
3	PAM	C	3465	-	14,17,17	1.19	1 (7%)	13,17,17	1.26	2 (15%)
3	PAM	A	1465	-	14,17,17	1.08	1 (7%)	13,17,17	1.11	0
2	HEM	A	472	1	27,50,50	1.89	8 (29%)	17,82,82	3.27	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	472	1	-	2/6/54/54	-
2	HEM	B	472	1	-	0/6/54/54	-
2	HEM	D	472	1	-	2/6/54/54	-
3	PAM	B	2465	-	-	12/13/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PAM	D	4465	-	-	10/13/15/15	-
3	PAM	C	3465	-	-	7/13/15/15	-
3	PAM	A	1465	-	-	5/13/15/15	-
2	HEM	A	472	1	-	0/6/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	C3B-C2B	-8.24	1.28	1.40
2	B	472	HEM	C3C-C2C	-5.72	1.32	1.40
2	D	472	HEM	C3C-C2C	-5.48	1.32	1.40
2	D	472	HEM	CAA-C2A	5.45	1.60	1.52
2	B	472	HEM	C1A-CHA	-5.28	1.26	1.41
2	C	472	HEM	C3B-C2B	-4.42	1.34	1.40
2	A	472	HEM	C3B-C2B	-4.39	1.34	1.40
2	C	472	HEM	C3D-C2D	4.36	1.50	1.37
3	C	3465	PAM	C10-C9	4.11	1.55	1.31
3	D	4465	PAM	C10-C9	4.05	1.55	1.31
2	D	472	HEM	C3D-C2D	3.89	1.49	1.37
3	B	2465	PAM	C10-C9	3.87	1.54	1.31
3	A	1465	PAM	C10-C9	3.77	1.53	1.31
2	C	472	HEM	C3C-C2C	-3.71	1.35	1.40
2	A	472	HEM	C3C-C2C	-3.57	1.35	1.40
2	B	472	HEM	C4A-CHB	-3.34	1.31	1.41
2	B	472	HEM	CMA-C3A	3.34	1.58	1.51
2	C	472	HEM	C3C-CAC	3.32	1.54	1.47
2	C	472	HEM	C3B-CAB	3.23	1.54	1.47
2	C	472	HEM	CMB-C2B	3.22	1.59	1.51
2	A	472	HEM	C3D-C2D	3.08	1.46	1.37
2	A	472	HEM	C3B-CAB	3.05	1.54	1.47
2	B	472	HEM	C1B-C2B	2.98	1.49	1.42
2	B	472	HEM	C1C-C2C	2.98	1.49	1.42
2	B	472	HEM	C3C-CAC	2.87	1.53	1.47
2	B	472	HEM	C3D-C2D	2.80	1.46	1.37
2	D	472	HEM	CAD-C3D	2.74	1.57	1.52
2	D	472	HEM	CMB-C2B	2.66	1.57	1.51
2	A	472	HEM	C3C-CAC	2.46	1.52	1.47
2	C	472	HEM	C4A-CHB	-2.37	1.34	1.41
2	B	472	HEM	C1D-ND	2.23	1.40	1.36
2	A	472	HEM	C4A-NA	2.22	1.40	1.36
2	C	472	HEM	CMA-C3A	2.19	1.56	1.51
2	A	472	HEM	C1D-CHD	-2.14	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	472	HEM	C1A-NA	2.09	1.40	1.36
2	C	472	HEM	C1A-CHA	-2.08	1.35	1.41
2	D	472	HEM	CMA-C3A	2.05	1.55	1.51
2	A	472	HEM	CMA-C3A	2.00	1.55	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	472	HEM	CAD-CBD-CGD	-7.52	100.06	112.67
2	A	472	HEM	CAA-CBA-CGA	-6.93	101.05	112.67
2	C	472	HEM	CAA-CBA-CGA	-6.80	101.26	112.67
2	C	472	HEM	CBD-CAD-C3D	-6.70	100.13	112.48
2	A	472	HEM	CAD-CBD-CGD	-6.26	102.17	112.67
2	B	472	HEM	CBA-CAA-C2A	-5.80	101.79	112.49
2	A	472	HEM	CMB-C2B-C3B	5.35	134.68	124.68
2	C	472	HEM	CMA-C3A-C4A	-5.32	120.29	128.46
2	A	472	HEM	C1D-C2D-C3D	-5.02	103.50	107.00
2	D	472	HEM	CMA-C3A-C4A	-4.67	121.29	128.46
2	C	472	HEM	CMB-C2B-C3B	4.28	132.69	124.68
2	A	472	HEM	CMD-C2D-C1D	4.27	135.03	128.46
2	C	472	HEM	CBA-CAA-C2A	4.15	120.13	112.49
2	B	472	HEM	CBD-CAD-C3D	-4.01	105.09	112.48
2	D	472	HEM	CAD-CBD-CGD	-3.61	106.61	112.67
2	C	472	HEM	C4A-C3A-C2A	3.49	109.43	107.00
2	B	472	HEM	C4A-C3A-C2A	-3.49	104.57	107.00
2	D	472	HEM	CMB-C2B-C3B	3.38	131.01	124.68
2	D	472	HEM	CMA-C3A-C2A	3.29	131.15	124.94
2	B	472	HEM	CMA-C3A-C2A	3.26	131.09	124.94
2	C	472	HEM	C1D-C2D-C3D	-3.24	104.74	107.00
2	D	472	HEM	C3B-C4B-NB	-3.18	105.10	109.21
2	D	472	HEM	C4C-C3C-C2C	3.01	109.00	106.90
2	B	472	HEM	CMA-C3A-C4A	-2.71	124.30	128.46
2	C	472	HEM	CMA-C3A-C2A	2.69	130.01	124.94
2	B	472	HEM	CMB-C2B-C3B	2.60	129.54	124.68
2	A	472	HEM	C4A-C3A-C2A	-2.50	105.25	107.00
3	C	3465	PAM	C7-C6-C5	-2.43	102.11	114.42
3	C	3465	PAM	C11-C10-C9	-2.42	106.15	124.73
2	B	472	HEM	CMD-C2D-C1D	2.35	132.08	128.46
2	A	472	HEM	CMA-C3A-C2A	2.15	128.99	124.94

There are no chirality outliers.

All (38) torsion outliers are listed below:

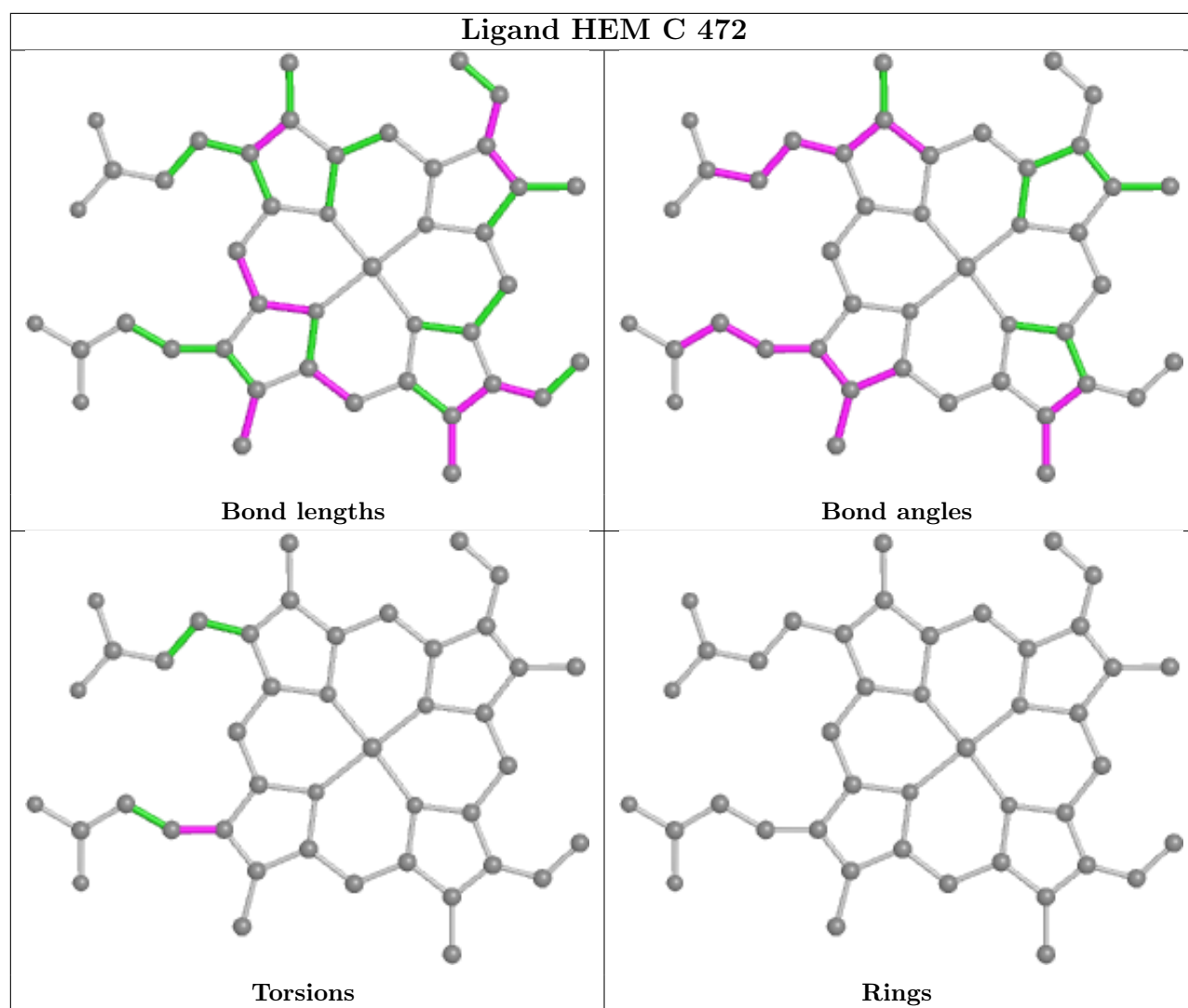
Mol	Chain	Res	Type	Atoms
2	D	472	HEM	C2D-C3D-CAD-CBD
2	D	472	HEM	C4D-C3D-CAD-CBD
3	A	1465	PAM	C1-C2-C3-C4
3	B	2465	PAM	C1-C2-C3-C4
3	D	4465	PAM	C1-C2-C3-C4
3	D	4465	PAM	C10-C11-C12-C13
3	D	4465	PAM	C12-C13-C14-C15
3	B	2465	PAM	C11-C10-C9-C8
3	B	2465	PAM	C2-C3-C4-C5
3	D	4465	PAM	C2-C3-C4-C5
3	D	4465	PAM	C4-C5-C6-C7
3	A	1465	PAM	C12-C13-C14-C15
3	B	2465	PAM	C3-C4-C5-C6
3	C	3465	PAM	C2-C3-C4-C5
3	D	4465	PAM	C6-C7-C8-C9
3	B	2465	PAM	C5-C6-C7-C8
3	B	2465	PAM	C11-C12-C13-C14
3	C	3465	PAM	C12-C13-C14-C15
3	B	2465	PAM	C10-C11-C12-C13
3	A	1465	PAM	C3-C4-C5-C6
3	C	3465	PAM	C10-C11-C12-C13
3	C	3465	PAM	C11-C12-C13-C14
3	D	4465	PAM	C11-C10-C9-C8
3	A	1465	PAM	C13-C14-C15-C16
3	C	3465	PAM	C4-C5-C6-C7
3	D	4465	PAM	C3-C4-C5-C6
3	B	2465	PAM	C12-C13-C14-C15
3	B	2465	PAM	C6-C7-C8-C9
3	B	2465	PAM	C4-C5-C6-C7
2	C	472	HEM	C1A-C2A-CAA-CBA
2	C	472	HEM	C3A-C2A-CAA-CBA
3	B	2465	PAM	C13-C14-C15-C16
3	C	3465	PAM	C9-C10-C11-C12
3	D	4465	PAM	C7-C8-C9-C10
3	D	4465	PAM	C9-C10-C11-C12
3	A	1465	PAM	C9-C10-C11-C12
3	C	3465	PAM	C1-C2-C3-C4
3	B	2465	PAM	C7-C8-C9-C10

There are no ring outliers.

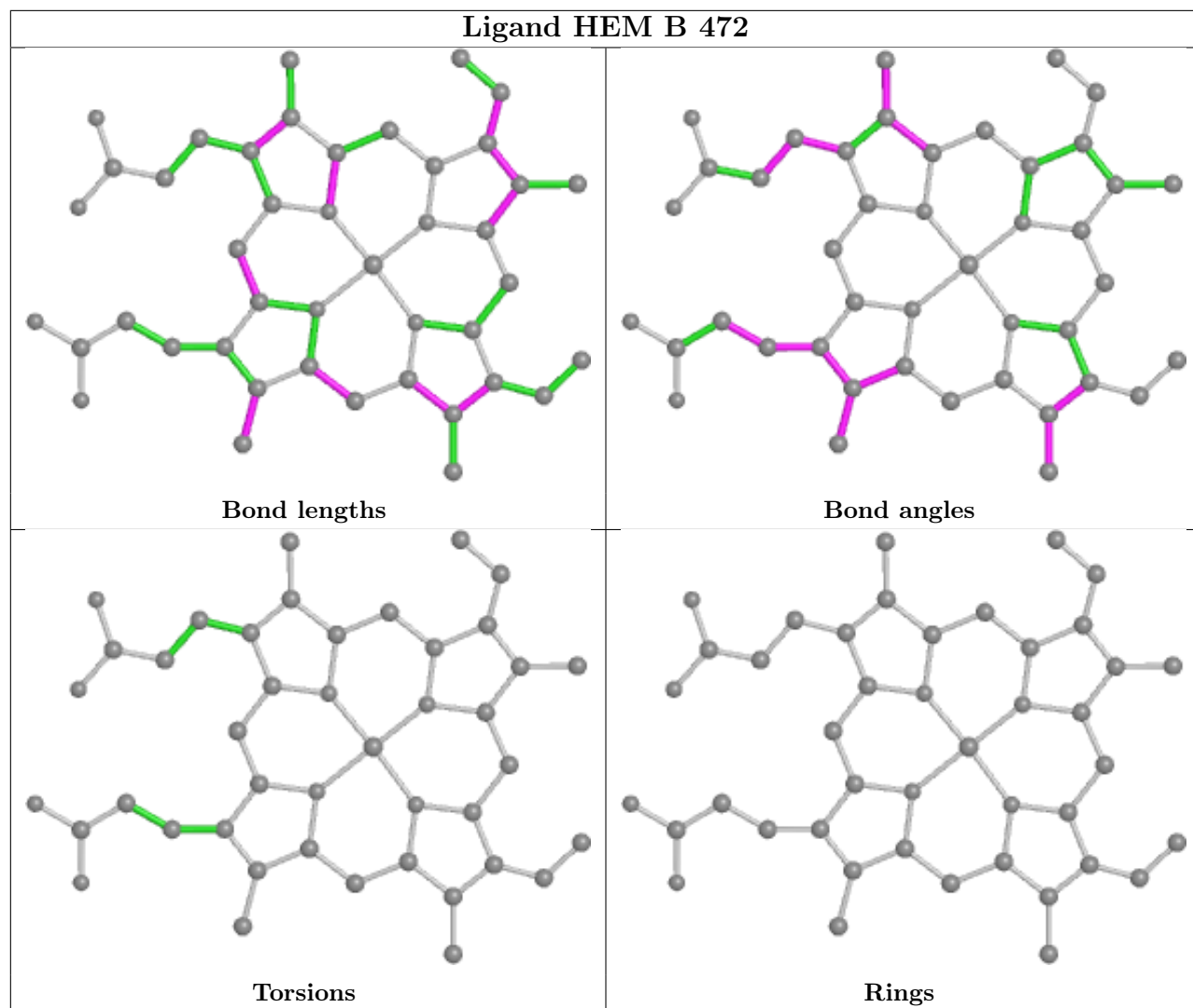
7 monomers are involved in 57 short contacts:

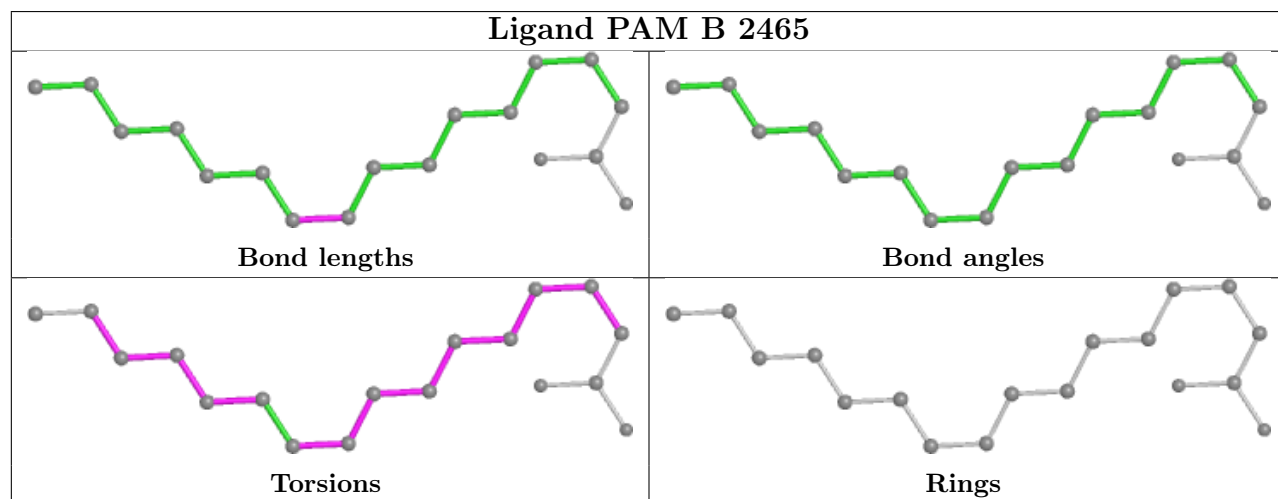
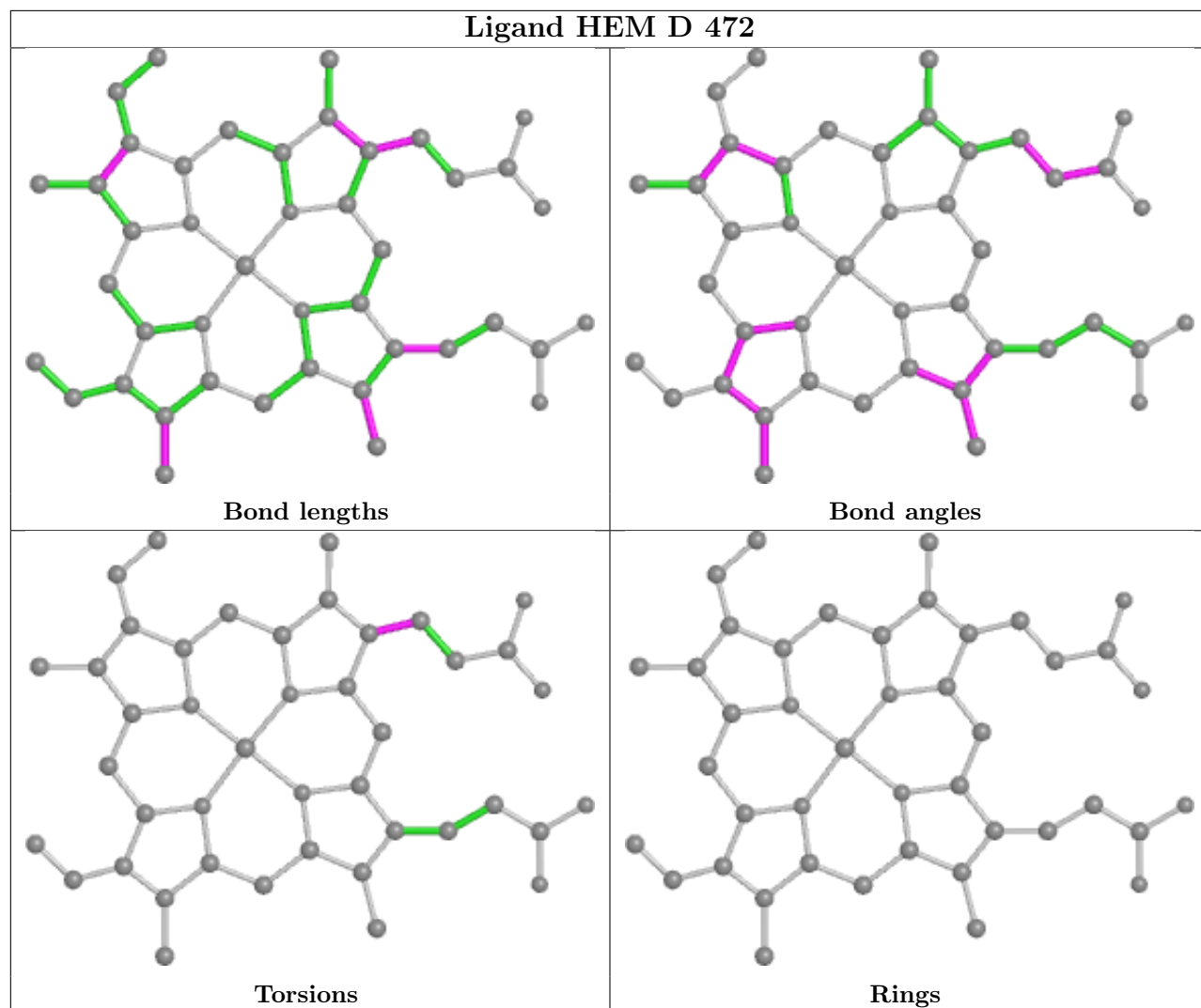
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	472	HEM	4	0
2	B	472	HEM	15	0
2	D	472	HEM	13	0
3	D	4465	PAM	2	0
3	C	3465	PAM	6	0
3	A	1465	PAM	3	0
2	A	472	HEM	14	0

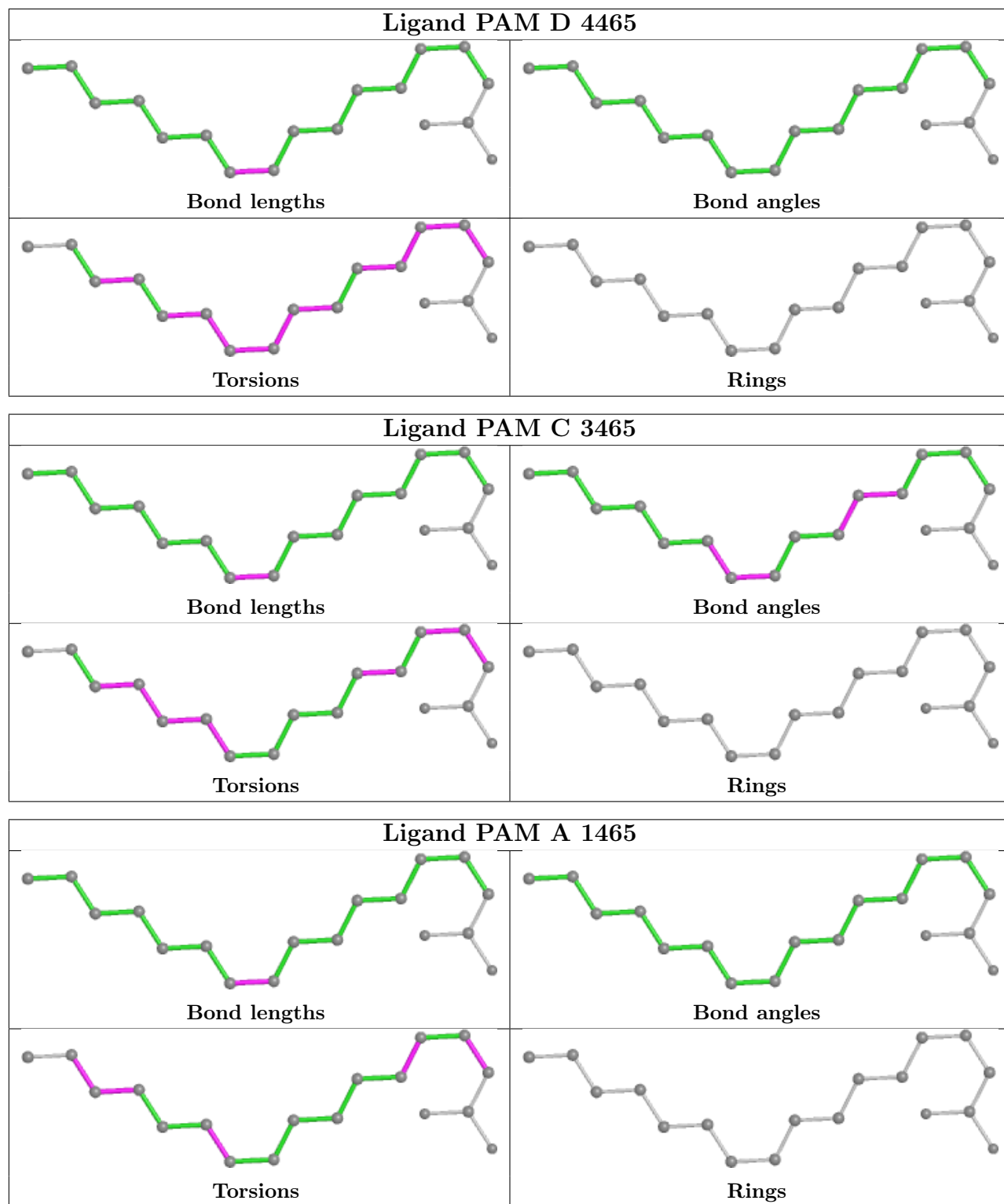
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

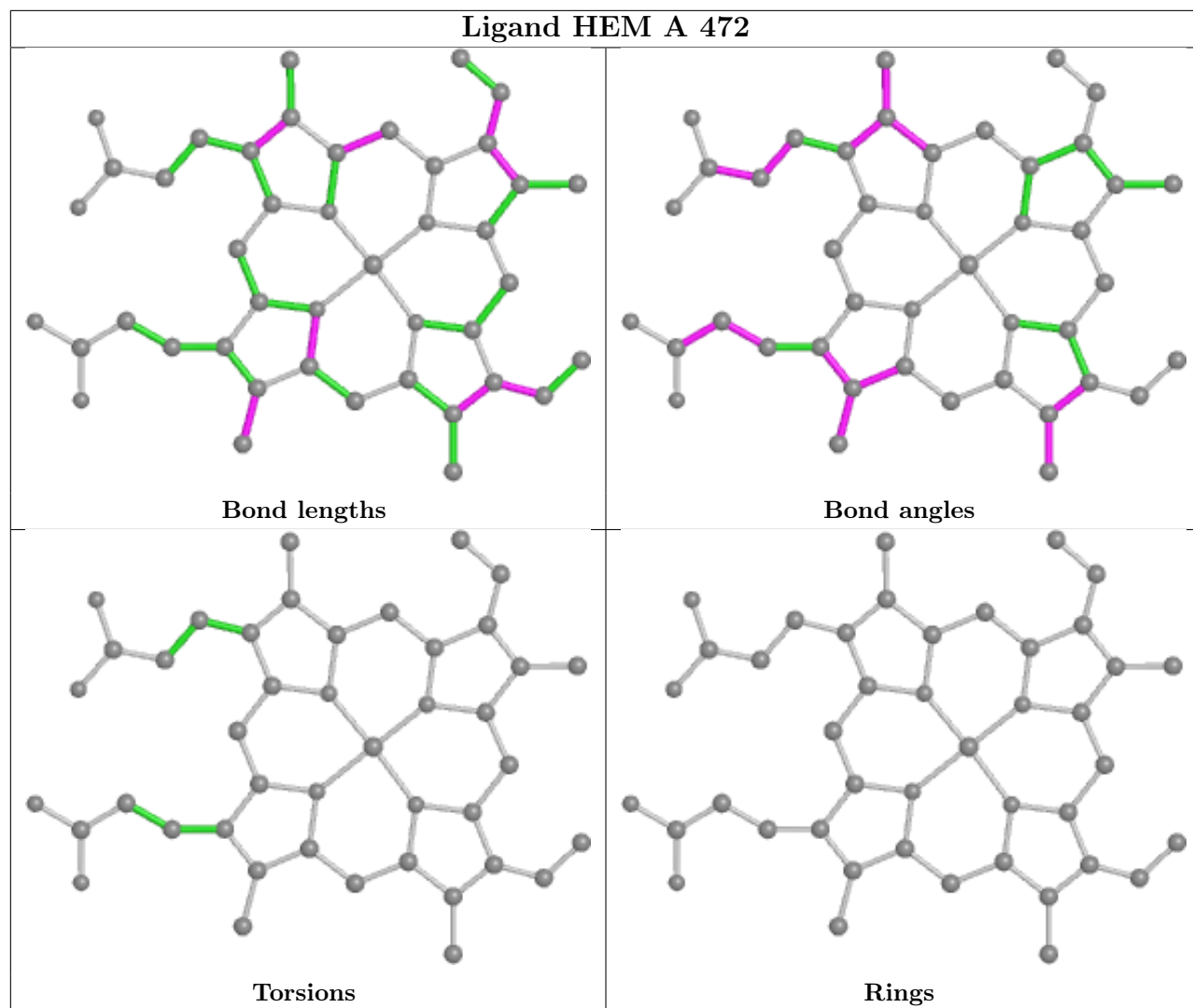












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	455/471 (96%)	-0.15	8 (1%) 68 76	24, 46, 66, 87	0
1	B	455/471 (96%)	0.17	23 (5%) 28 34	31, 58, 83, 96	0
1	C	455/471 (96%)	0.18	23 (5%) 28 34	32, 58, 80, 90	0
1	D	454/471 (96%)	0.21	19 (4%) 36 43	38, 62, 80, 92	0
All	All	1819/1884 (96%)	0.10	73 (4%) 38 45	24, 56, 80, 96	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	THR	7.1
1	C	1	THR	6.3
1	D	2	ILE	5.4
1	B	229	GLN	5.3
1	B	292	GLU	4.4
1	A	227	GLY	4.3
1	C	229	GLN	4.1
1	A	229	GLN	4.0
1	C	226	SER	3.5
1	C	247	GLU	3.5
1	B	113	LYS	3.5
1	D	225	ALA	3.5
1	D	243	PRO	3.4
1	C	2	ILE	3.4
1	B	243	PRO	3.3
1	C	92	HIS	3.3
1	B	110	GLN	3.3
1	D	229	GLN	3.3
1	D	92	HIS	3.3
1	C	352	GLU	3.2
1	C	136	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	244	GLU	3.2
1	D	227	GLY	3.2
1	B	288	GLN	3.2
1	C	245	THR	3.1
1	C	228	GLU	3.1
1	B	109	GLN	3.1
1	B	2	ILE	3.0
1	C	4	GLU	2.9
1	D	226	SER	2.9
1	B	285	HIS	2.8
1	B	299	VAL	2.8
1	D	4	GLU	2.8
1	D	285	HIS	2.8
1	B	450	SER	2.7
1	C	246	GLY	2.7
1	D	310	GLN	2.7
1	C	381	ASN	2.7
1	C	227	GLY	2.6
1	D	244	GLU	2.6
1	C	248	PRO	2.6
1	C	383	SER	2.6
1	B	255	ARG	2.6
1	D	360	LEU	2.6
1	D	361	HIS	2.5
1	C	225	ALA	2.5
1	D	196	PRO	2.5
1	D	3	LYS	2.5
1	B	373	GLU	2.4
1	B	136	ASP	2.4
1	B	230	SER	2.4
1	D	169	GLN	2.3
1	A	230	SER	2.3
1	A	2	ILE	2.3
1	C	452	LYS	2.3
1	A	352	GLU	2.2
1	B	4	GLU	2.2
1	C	13	GLU	2.2
1	C	396	GLY	2.2
1	B	316	MET	2.2
1	D	230	SER	2.2
1	D	452	LYS	2.1
1	B	245	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	382	PRO	2.1
1	B	364	LYS	2.1
1	C	430	GLU	2.1
1	B	454	PRO	2.1
1	D	336	LYS	2.0
1	A	225	ALA	2.0
1	C	343	GLY	2.0
1	A	337	GLU	2.0
1	B	369	ASP	2.0
1	C	109	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

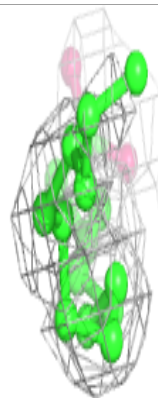
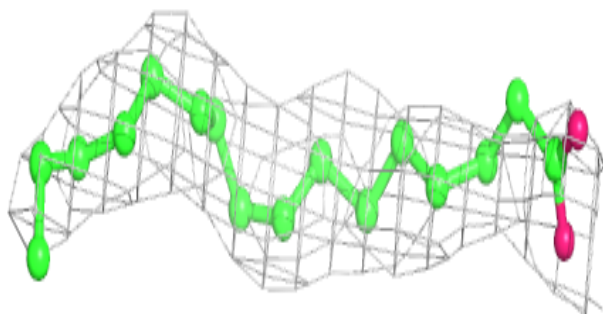
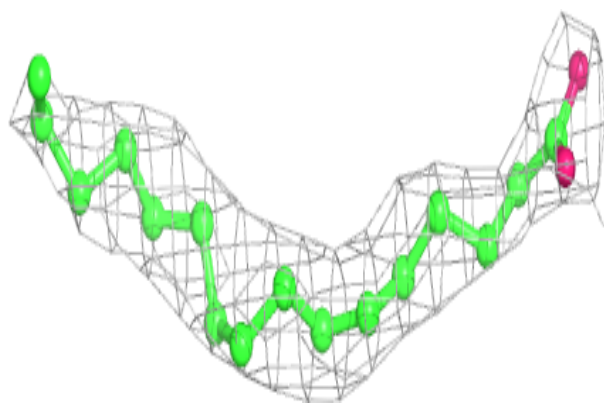
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PAM	B	2465	18/18	0.89	0.21	57,68,74,76	0
3	PAM	D	4465	18/18	0.91	0.22	45,59,78,79	0
3	PAM	C	3465	18/18	0.92	0.20	43,50,71,73	0
3	PAM	A	1465	18/18	0.92	0.15	30,45,62,64	0
2	HEM	C	472	43/43	0.97	0.14	23,30,48,54	0
2	HEM	D	472	43/43	0.97	0.14	29,40,55,60	0
2	HEM	B	472	43/43	0.97	0.14	27,35,59,68	0
2	HEM	A	472	43/43	0.98	0.13	18,27,38,43	0

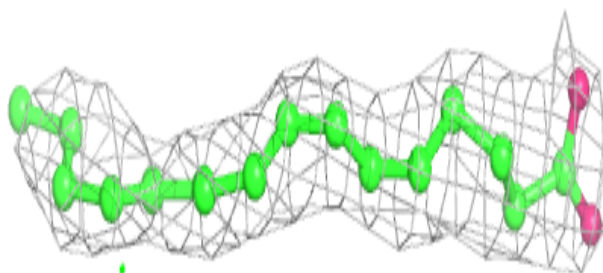
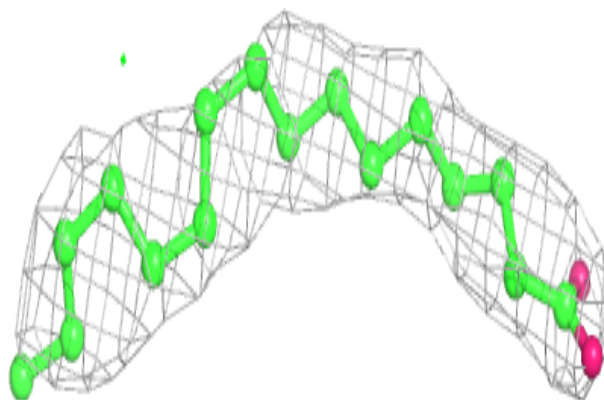
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PAM B 2465:**

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

**Electron density around PAM D 4465:**

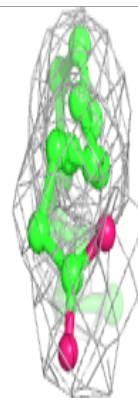
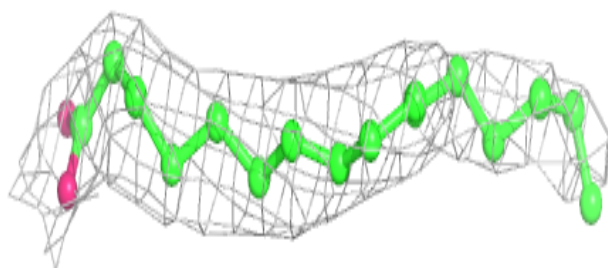
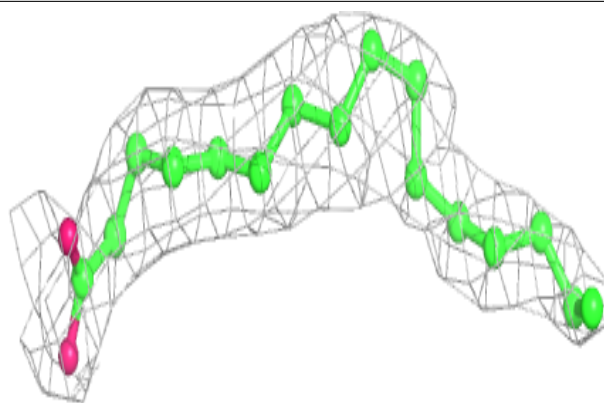
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



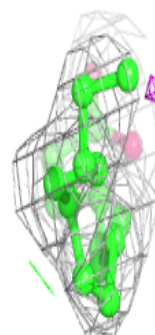
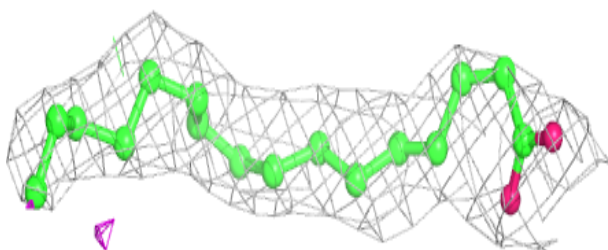
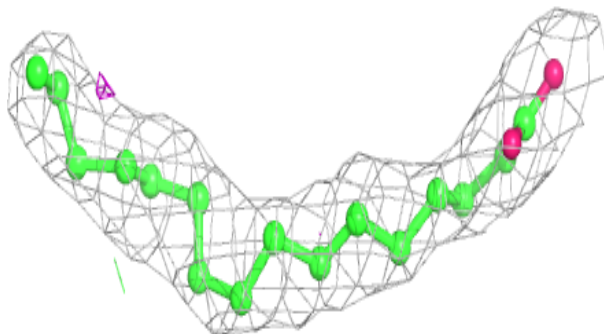


**Electron density around PAM C 3465:**

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

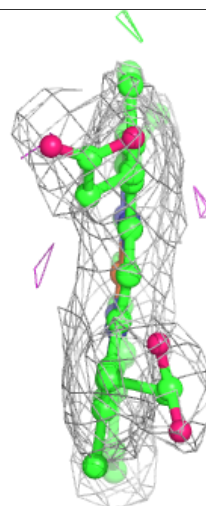
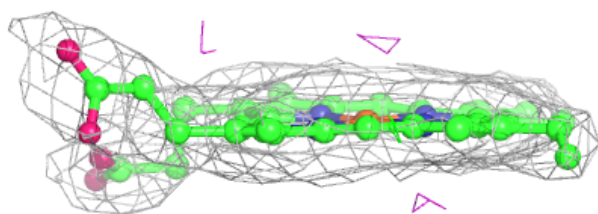
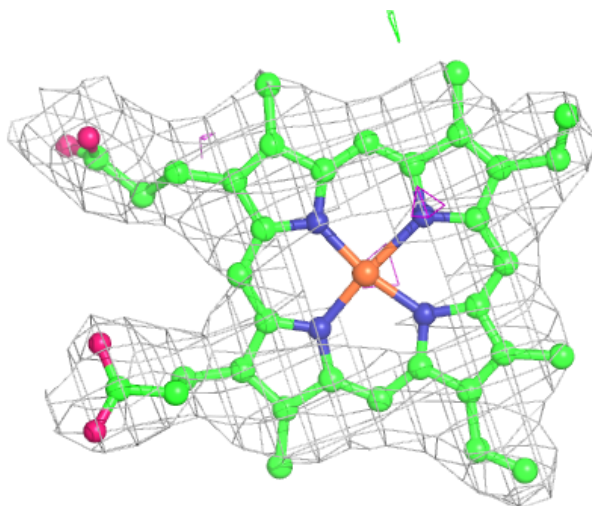
**Electron density around PAM A 1465:**

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



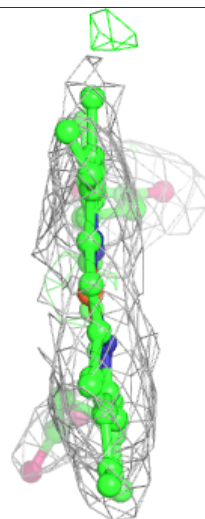
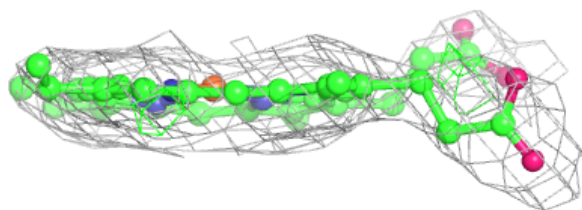
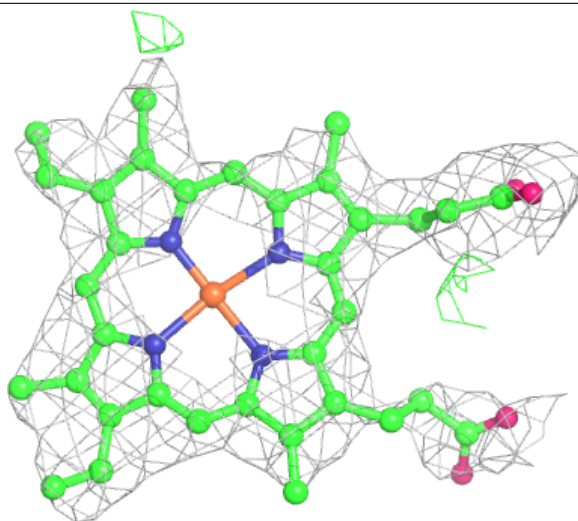
**Electron density around HEM C 472:**

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



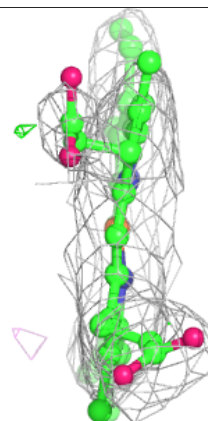
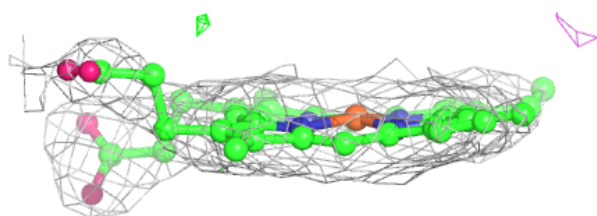
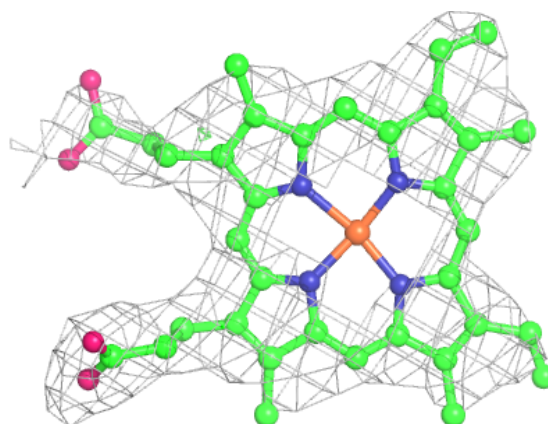
**Electron density around HEM D 472:**

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



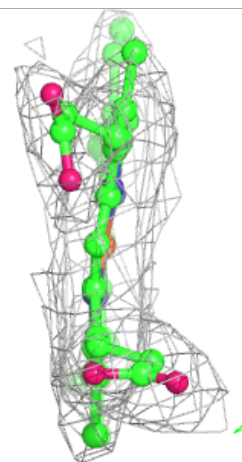
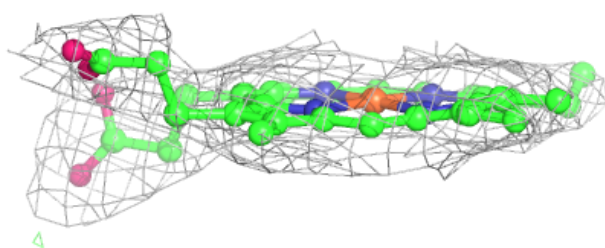
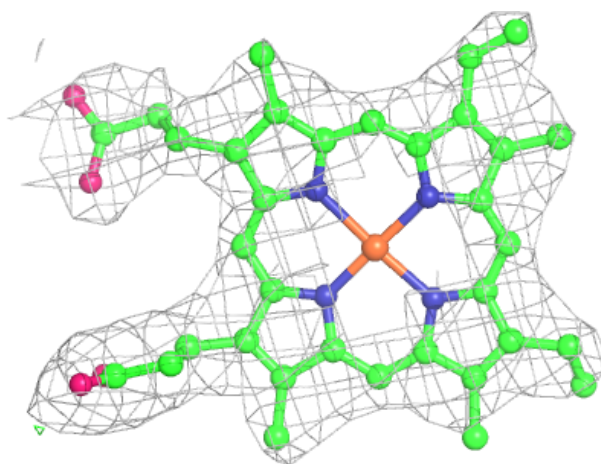
**Electron density around HEM B 472:**

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



**Electron density around HEM A 472:**

$2mF_o-DF_c$  (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.