



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:47 PM BST

PDB ID : 1BCC  
Title : CYTOCHROME BC1 COMPLEX FROM CHICKEN  
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.; Crofts, A.R.; Berry, E.A.; Kim, S.-H.  
Deposited on : 1998-03-23  
Resolution : 3.16 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 : 2.13.1  
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) : 2.13.1

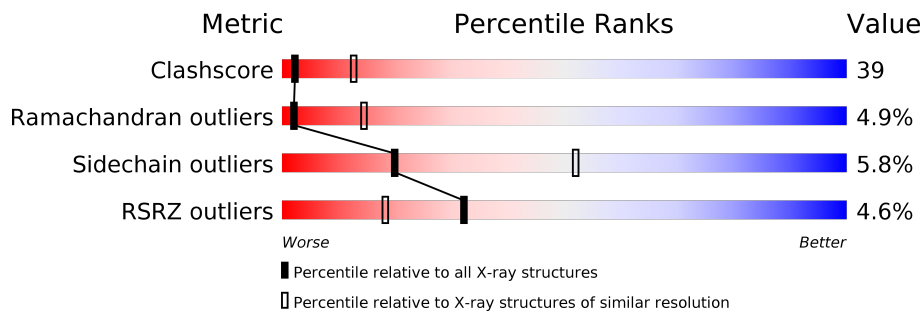
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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))
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	446	 2% 42% 50% 7%
2	B	422	 4% 40% 47% 9%
3	C	380	 2% 45% 48% 6%
4	D	241	 3% 44% 50% 6%
5	E	196	 23% 38% 58%
6	F	109	 2% 56% 32% 8%
7	G	81	 2% 47% 40% 10%

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Mol	Chain	Length	Quality of chain
8	H	78	<p>%</p> <p>51% 32% 15%</p>
9	I	33	<p>64% 36%</p>
10	J	62	<p>3%</p> <p>56% 37% 5%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	PEE	C	384	X	-	-	-
13	PEE	E	198	X	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15719 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3423	2147	601	657	18	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	THR	conflict	UNP P13272
A	23	VAL	LEU	conflict	UNP P13272
A	59	LEU	VAL	conflict	UNP P13272
A	72	GLN	GLY	conflict	UNP P13272
A	91	SER	THR	conflict	UNP P13272
A	106	VAL	LEU	conflict	UNP P13272
A	135	VAL	LEU	conflict	UNP P13272
A	136	ARG	GLN	conflict	UNP P13272
A	147	GLU	ASP	conflict	UNP P13272
A	162	GLY	PRO	conflict	UNP P13272
A	174	ILE	VAL	conflict	UNP P13272
A	188	THR	ARG	conflict	UNP P13272
A	191	THR	LYS	conflict	UNP P13272
A	203	VAL	LEU	conflict	UNP P13272
A	206	GLN	ARG	conflict	UNP P13272
A	210	GLU	ASP	conflict	UNP P13272
A	217	GLY	SER	conflict	UNP P13272
A	219	VAL	LEU	conflict	UNP P13272
A	220	PRO	SER	conflict	UNP P13272
A	221	PHE	GLY	conflict	UNP P13272
A	225	ASP	GLU	conflict	UNP P13272
A	233	LYS	PRO	conflict	UNP P13272
A	242	ARG	CYS	conflict	UNP P13272
A	267	LEU	ASN	conflict	UNP P13272
A	282	ARG	CYS	conflict	UNP P13272
A	288	LEU	ALA	conflict	UNP P13272
A	290	SER	LEU	conflict	UNP P13272

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	VAL	ALA	conflict	UNP P13272
A	311	SER	ASN	conflict	UNP P13272
A	315	SER	ALA	conflict	UNP P13272
A	316	GLU	ASP	conflict	UNP P13272
A	320	PHE	LEU	conflict	UNP P13272
A	322	PHE	ALA	conflict	UNP P13272
A	323	TYR	HIS	conflict	UNP P13272
A	328	ARG	HIS	conflict	UNP P13272
A	349	ILE	ALA	conflict	UNP P13272
A	350	SER	THR	conflict	UNP P13272
A	360	PHE	LEU	conflict	UNP P13272
A	382	GLU	SER	conflict	UNP P13272
A	393	GLU	ALA	conflict	UNP P13272
A	397	GLU	SER	conflict	UNP P13272
A	399	LEU	ILE	conflict	UNP P13272
A	406	MET	VAL	conflict	UNP P13272
A	415	ILE	PHE	conflict	UNP P13272
A	425	PRO	PHE	conflict	UNP P13272

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	406	2994	1878	518	591	7	0	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ILE	PHE	conflict	UNP P23004
B	28	LYS	ARG	conflict	UNP P23004
B	42	SER	ALA	conflict	UNP P23004
B	44	GLY	ALA	conflict	UNP P23004
B	46	THR	ARG	conflict	UNP P23004
B	49	VAL	LEU	conflict	UNP P23004
B	61	SER	ASN	conflict	UNP P23004
B	99	GLU	THR	conflict	UNP P23004
B	117	GLU	ASP	conflict	UNP P23004
B	134	PRO	ARG	conflict	UNP P23004
B	139	ASP	ALA	conflict	UNP P23004
B	145	LYS	ARG	conflict	UNP P23004
B	152	PHE	LEU	conflict	UNP P23004
B	157	THR	ALA	conflict	UNP P23004

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Chain	Residue	Modelled	Actual	Comment	Reference
B	174	ASP	ASN	conflict	UNP P23004
B	188	SER	PRO	conflict	UNP P23004
B	194	PHE	TYR	conflict	UNP P23004
B	207	VAL	ILE	conflict	UNP P23004
B	218	ASN	GLN	conflict	UNP P23004
B	223	LEU	PHE	conflict	UNP P23004
B	240	ARG	HIS	conflict	UNP P23004
B	257	ILE	LEU	conflict	UNP P23004
B	266	GLY	SER	conflict	UNP P23004
B	282	ASN	GLY	conflict	UNP P23004
B	321	LEU	SER	conflict	UNP P23004
B	332	TYR	SER	conflict	UNP P23004
B	335	GLN	ASP	conflict	UNP P23004
B	352	VAL	LEU	conflict	UNP P23004
B	355	GLU	PRO	conflict	UNP P23004
B	356	ASN	ASP	conflict	UNP P23004
B	367	LYS	GLY	conflict	UNP P23004
B	380	GLU	ASP	conflict	UNP P23004
B	393	ASN	THR	conflict	UNP P23004
B	412	LYS	ASN	conflict	UNP P23004
B	420	ARG	GLY	conflict	UNP P23004
B	421	GLN	ARG	conflict	UNP P23004
B	436	VAL	ILE	conflict	UNP P23004

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3002	2013	473	504	12	0	0	0

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1899	1214	326	345	14	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PRO	LEU	conflict	UNP P00125
D	143	VAL	LEU	conflict	UNP P00125
D	167	ASP	GLU	conflict	UNP P00125

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	VAL	LEU	conflict	UNP P00125
D	221	TYR	ALA	conflict	UNP P00125

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1512	953	266	285	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ASN	ASP	conflict	UNP P13272
E	17	PRO	GLU	conflict	UNP P13272
E	18	ASP	VAL	conflict	UNP P13272
E	19	ASP	LEU	conflict	UNP P13272
E	20	TYR	ASP	conflict	UNP P13272
E	26	ARG	LYS	conflict	UNP P13272
E	29	ASP	SER	conflict	UNP P13272
E	30	PRO	GLU	conflict	UNP P13272
E	31	SER	ALA	conflict	UNP P13272
E	42	VAL	THR	conflict	UNP P13272
E	45	LEU	VAL	conflict	UNP P13272
E	56	THR	SER	conflict	UNP P13272

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	100	875	557	153	162	3	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	TYR	LEU	conflict	UNP P00129
F	38	TYR	HIS	conflict	UNP P00129
F	59	MET	VAL	conflict	UNP P00129
F	69	ASN	SER	conflict	UNP P00129
F	87	VAL	LYS	conflict	UNP P00129
F	88	PRO	SER	conflict	UNP P00129
F	108	ASP	ALA	conflict	UNP P00129

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	78	626	411	114	100	1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	LEU	VAL	conflict	UNP P13271
G	25	PRO	ALA	conflict	UNP P13271
G	34	VAL	ILE	conflict	UNP P13271
G	38	TRP	LEU	conflict	UNP P13271
G	41	LEU	THR	conflict	UNP P13271
G	53	LEU	VAL	conflict	UNP P13271
G	58	LEU	VAL	conflict	UNP P13271
G	78	VAL	GLU	conflict	UNP P13271

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	66	490	301	88	96	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	59	PHE	LEU	conflict	UNP P00126

- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	33	159	92	33	34	0	0	0

- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

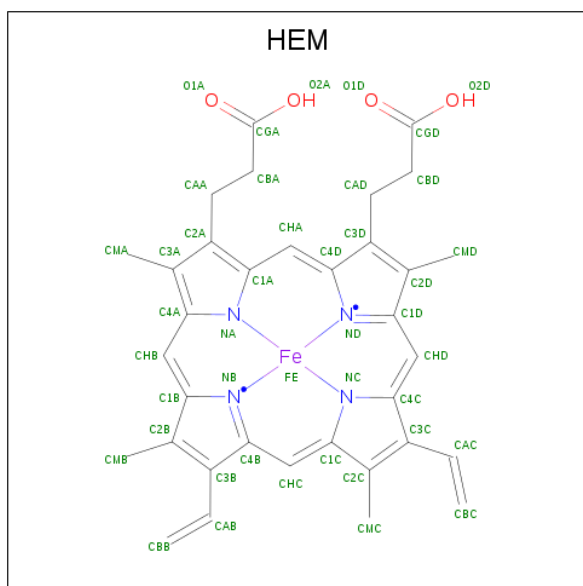
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	59	459	299	78	82	0	0	0

There is a discrepancy between the modelled and reference sequences:



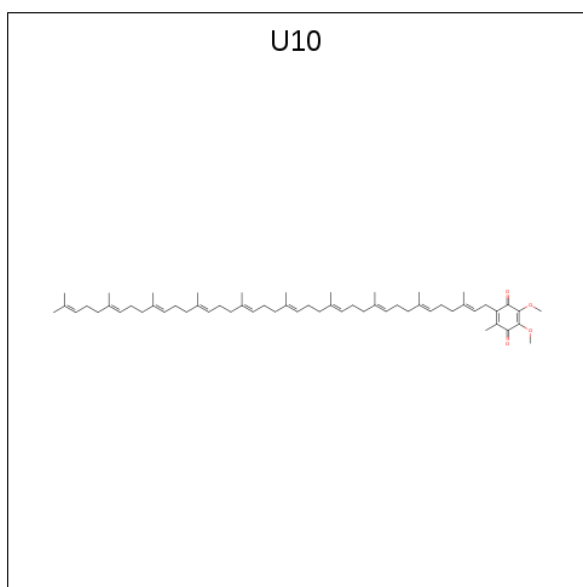
Chain	Residue	Modelled	Actual	Comment	Reference
J	30	LEU	PHE	conflict	UNP P00130

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



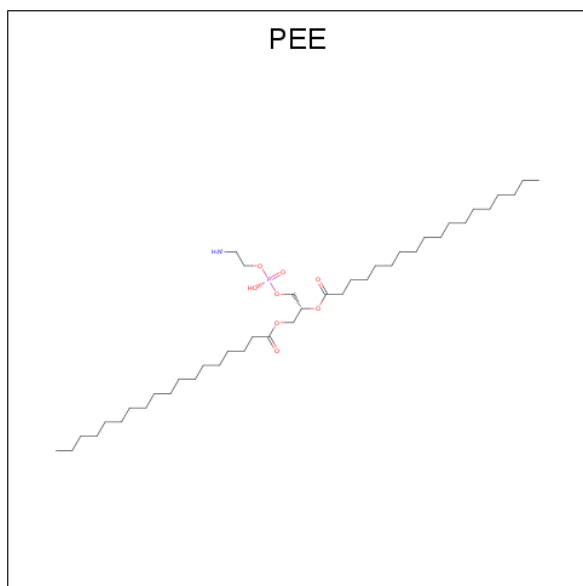
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
11	C	1	43	34	1	4	4	0	0
11	C	1	43	34	1	4	4	0	0
11	D	1	43	34	1	4	4	0	0

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



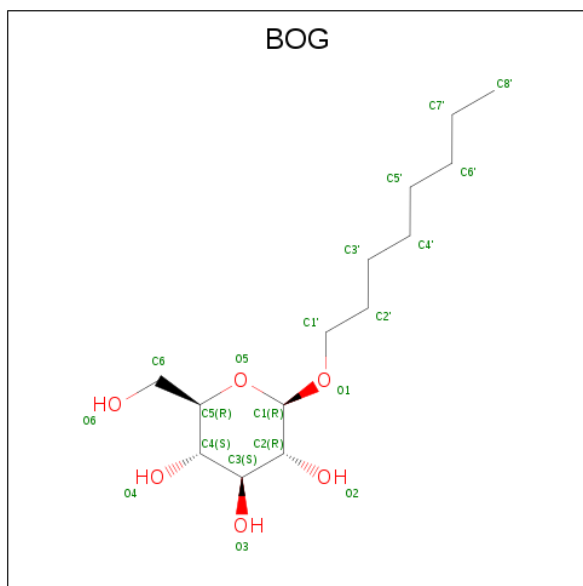
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	C	1	29	25	4	0	0

- Molecule 13 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



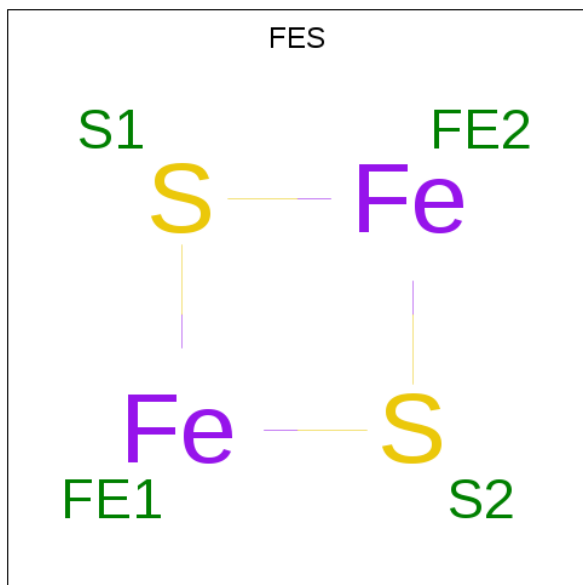
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	C	1	49	39	1	8	1	0	0
13	E	1	49	39	1	8	1	0	0

- Molecule 14 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
14	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).

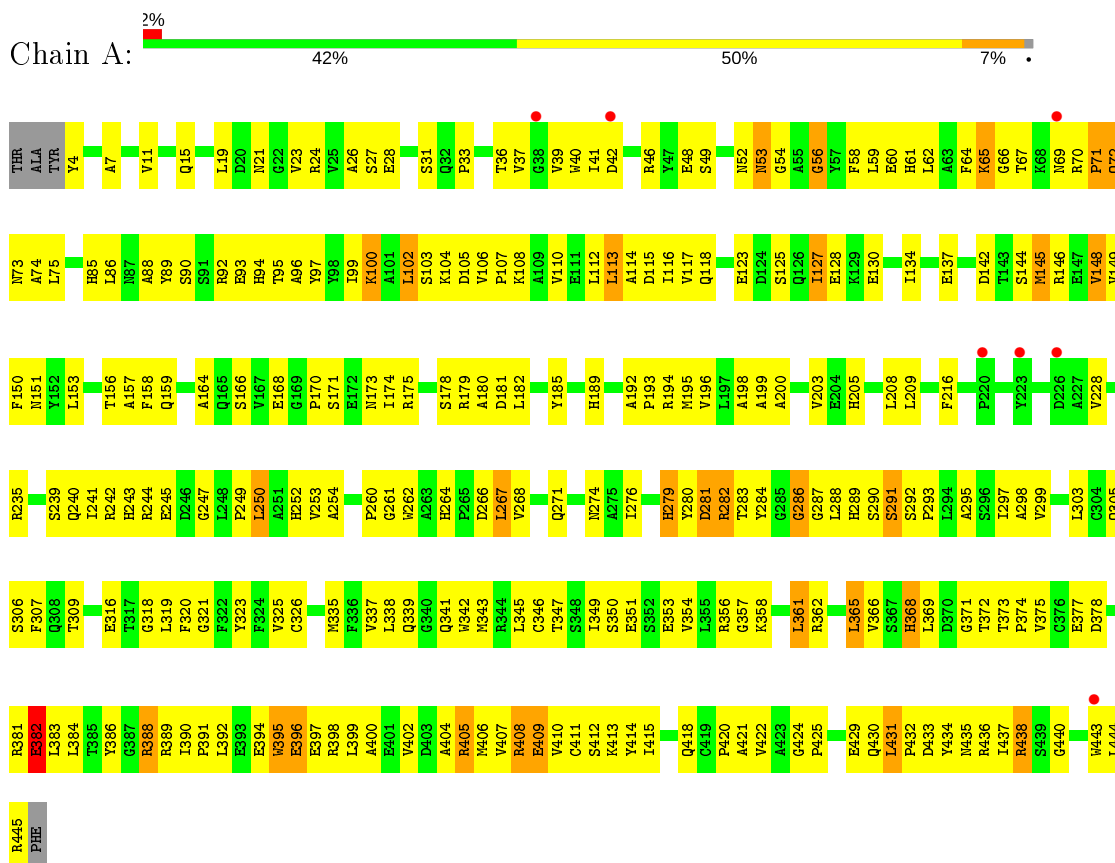


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
15	E	1	Total	Fe	S	0	0
			4	2	2		

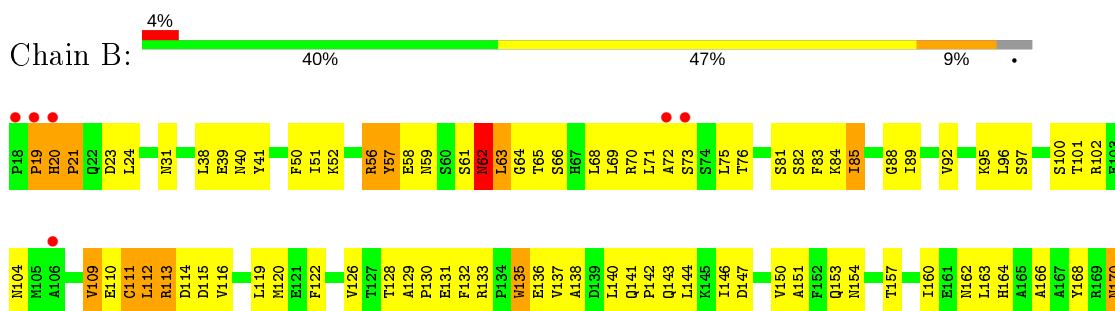
### 3 Residue-property plots i

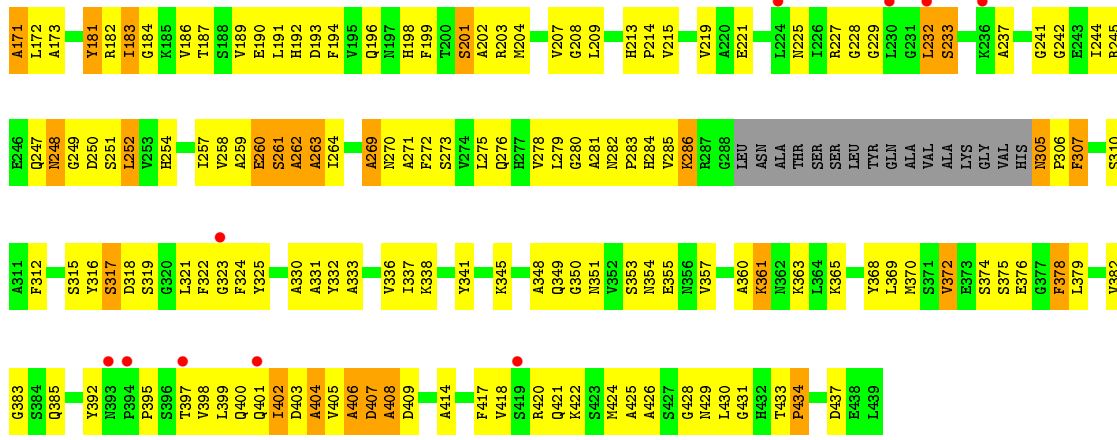
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

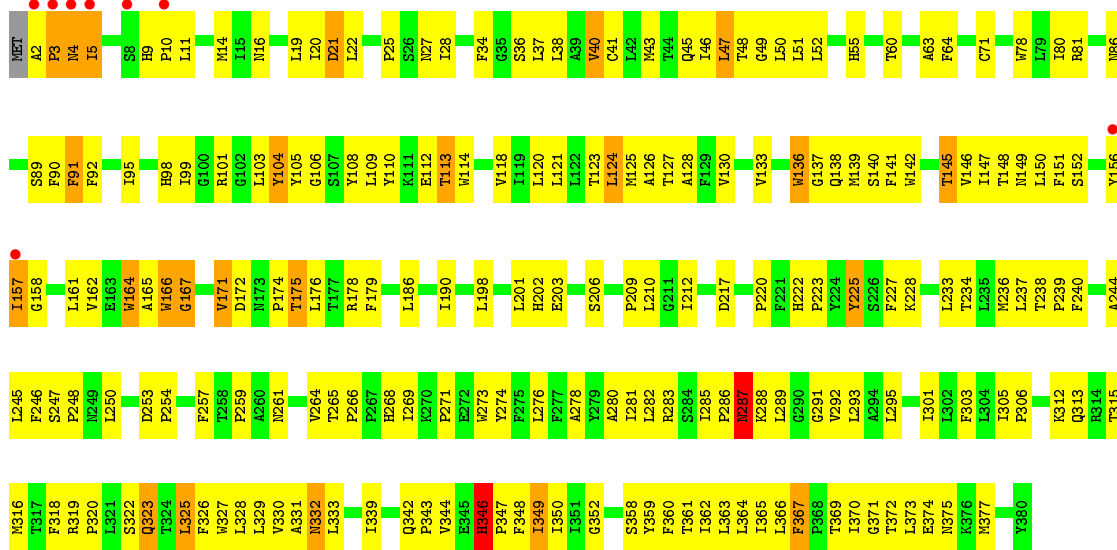


#### • Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

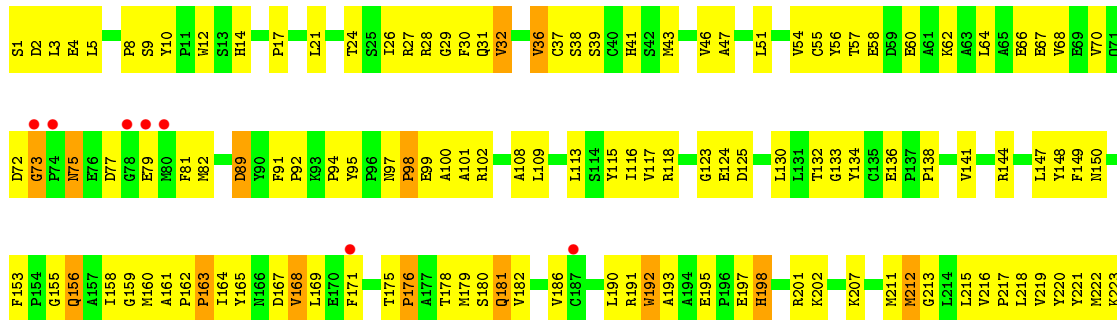




• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

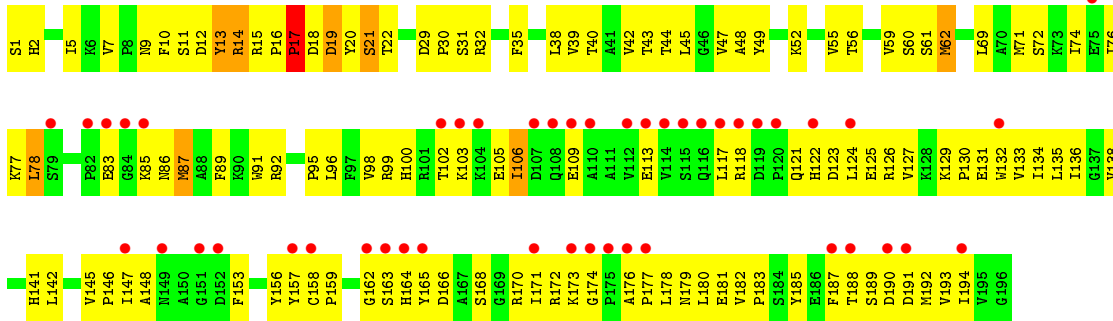


• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

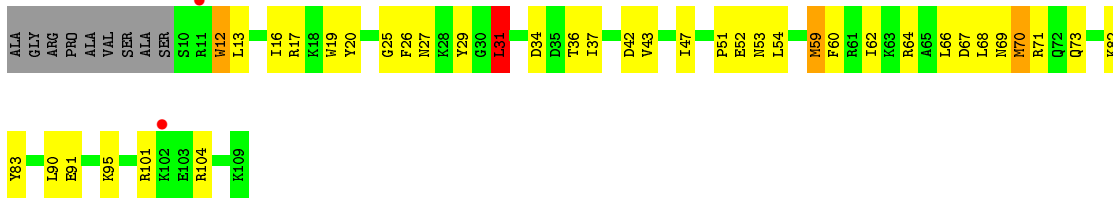




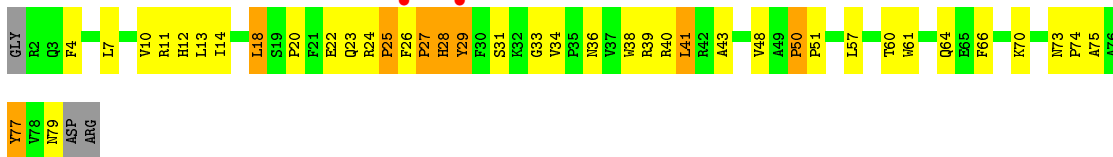
- Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



- Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



- Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

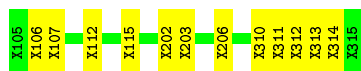


- Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



- Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE





- Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.59Å 182.52Å 240.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.16 27.93 – 3.16	Depositor EDS
% Data completeness (in resolution range)	85.5 (12.00-3.16) 90.8 (27.93-3.16)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 3.17Å)	Xtrriage
Refinement program	CNS 0.1	Depositor
R, $R_{free}$	0.270 , 0.310 0.288 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.1	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	15719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: U10, PEE, FES, HEM, BOG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/3495	0.73	1/4742 (0.0%)
2	B	0.45	0/3046	0.70	0/4132
3	C	0.51	0/3104	0.77	1/4252 (0.0%)
4	D	0.49	0/1960	0.75	1/2665 (0.0%)
5	E	0.58	0/1548	0.77	0/2095
6	F	0.50	0/896	0.74	1/1206 (0.1%)
7	G	0.54	0/648	0.75	1/882 (0.1%)
8	H	0.42	0/495	0.64	0/669
10	J	0.46	0/470	0.69	0/635
All	All	0.50	0/15662	0.74	5/21278 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLY	N-CA-C	-5.71	98.83	113.10
4	D	235	LEU	CA-CB-CG	5.50	127.96	115.30
6	F	31	LEU	CA-CB-CG	5.49	127.92	115.30
7	G	18	LEU	CA-CB-CG	5.43	127.78	115.30
3	C	346	HIS	N-CA-C	5.24	125.15	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	225	TYR	Sidechain

## 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	3423	0	3286	291	0
2	B	2994	0	2906	278	0
3	C	3002	0	3036	251	0
4	D	1899	0	1822	158	0
5	E	1512	0	1485	159	0
6	F	875	0	839	49	0
7	G	626	0	591	51	0
8	H	490	0	445	35	0
9	I	159	0	42	19	0
10	J	459	0	424	21	0
11	C	86	0	60	12	0
11	D	43	0	30	0	0
12	C	29	0	33	4	0
13	C	49	0	70	2	0
13	E	49	0	70	1	0
14	D	20	0	28	2	0
15	E	4	0	0	1	0
All	All	15719	0	15167	1200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:ILE:HG22	4:D:160:MET:H	1.07	1.15
1:A:282:ARG:NH1	9:I:202:UNK:H	1.47	1.11
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.33	1.10
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.56	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG22	2:B:82:SER:H	1.23	1.01
1:A:88:ALA:HB1	1:A:96:ALA:O	1.62	1.00
2:B:241:GLY:HA3	2:B:421:GLN:HE21	1.26	0.99
2:B:280:GLY:H	2:B:283:PRO:HD2	1.30	0.96
3:C:99:ILE:HD13	11:C:382:HEM:HBC2	1.49	0.95
1:A:42:ASP:HB3	1:A:194:ARG:HB3	1.48	0.93
3:C:167:GLY:H	3:C:175:THR:HG22	1.34	0.93
1:A:49:SER:H	1:A:52:ASN:HB3	1.35	0.91
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.53	0.89
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.54	0.89
2:B:20:HIS:N	2:B:21:PRO:HD3	1.85	0.89
2:B:162:ASN:HB3	2:B:244:ILE:HD11	1.54	0.88
8:H:47:ARG:HD3	8:H:48:SER:H	1.38	0.88
4:D:32:VAL:O	4:D:36:VAL:HG13	1.73	0.87
4:D:130:LEU:HD11	4:D:158:ILE:HD11	1.57	0.87
3:C:238:THR:HG23	3:C:239:PRO:HD3	1.57	0.86
4:D:164:ILE:HD11	4:D:182:VAL:HG13	1.57	0.85
3:C:104:TYR:CE2	3:C:316:MET:HB2	2.11	0.85
4:D:158:ILE:HG22	4:D:160:MET:N	1.92	0.85
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.40	0.85
1:A:88:ALA:HB2	1:A:97:TYR:HA	1.59	0.83
1:A:282:ARG:NH1	9:I:202:UNK:N	2.26	0.83
1:A:286:GLY:HA3	1:A:289:HIS:CD2	2.13	0.83
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.58	0.83
5:E:14:ARG:HG2	5:E:14:ARG:HH11	1.42	0.83
1:A:291:SER:HB2	1:A:356:ARG:NH2	1.94	0.83
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.59	0.82
5:E:121:GLN:HB3	5:E:126:ARG:HD2	1.59	0.82
6:F:43:VAL:O	6:F:47:ILE:HG13	1.80	0.81
1:A:361:LEU:HD13	1:A:399:LEU:HD22	1.61	0.81
2:B:129:ALA:N	2:B:130:PRO:HD3	1.93	0.81
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.80	0.80
3:C:99:ILE:CD1	11:C:382:HEM:HBC2	2.10	0.80
5:E:11:SER:HA	5:E:15:ARG:HD2	1.62	0.80
3:C:27:ASN:HB2	6:F:69:ASN:ND2	1.97	0.80
1:A:94:HIS:NE2	1:A:381:ARG:HG2	1.97	0.80
4:D:98:PRO:HG2	4:D:99:GLU:OE2	1.81	0.80
1:A:433:ASP:OD2	1:A:435:ASN:HB2	1.82	0.80
4:D:54:VAL:HG21	4:D:192:TRP:CZ3	2.18	0.79
2:B:232:LEU:HG	2:B:233:SER:H	1.49	0.78
2:B:128:THR:C	2:B:130:PRO:HD3	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:LEU:HD11	3:C:366:LEU:HB3	1.66	0.78
1:A:281:ASP:O	1:A:283:THR:N	2.17	0.78
3:C:27:ASN:HD22	6:F:69:ASN:HD22	1.32	0.78
3:C:123:THR:O	3:C:127:THR:HG23	1.84	0.77
5:E:157:TYR:HE1	5:E:162:GLY:HA2	1.48	0.77
3:C:238:THR:OG1	4:D:212:MET:HG3	1.84	0.77
8:H:50:THR:HG22	8:H:52:GLU:H	1.50	0.77
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.65	0.76
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.16	0.76
1:A:145:MET:HA	1:A:148:VAL:CG1	2.16	0.76
2:B:227:ARG:O	2:B:229:GLY:N	2.18	0.76
5:E:136:ILE:HG13	5:E:181:GLU:HG2	1.67	0.76
1:A:282:ARG:HH12	9:I:202:UNK:H	1.32	0.76
5:E:45:LEU:HD21	10:J:28:ALA:N	2.00	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.67	0.75
3:C:325:LEU:HD22	3:C:362:ILE:HG23	1.66	0.75
1:A:362:ARG:HG3	1:A:399:LEU:HD11	1.68	0.75
3:C:172:ASP:O	3:C:175:THR:HG23	1.85	0.75
1:A:85:HIS:HB2	1:A:100:LYS:CG	2.17	0.75
10:J:42:ILE:O	10:J:46:ILE:HG13	1.87	0.75
5:E:122:HIS:O	5:E:125:GLU:HG2	1.87	0.75
5:E:11:SER:O	5:E:13:TYR:N	2.19	0.75
5:E:83:GLU:HA	5:E:100:HIS:HB3	1.68	0.75
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.20	0.75
5:E:123:ASP:HB2	5:E:170:ARG:NH2	2.02	0.75
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.68	0.74
4:D:211:MET:HG3	14:D:242:BOG:H5'1	1.69	0.74
5:E:45:LEU:HD21	10:J:27:GLY:C	2.07	0.74
2:B:399:LEU:HA	2:B:402:ILE:HG22	1.69	0.74
3:C:127:THR:HG22	3:C:186:LEU:HB3	1.69	0.74
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.67	0.74
7:G:36:ASN:O	7:G:40:ARG:HG3	1.87	0.74
1:A:85:HIS:HB2	1:A:100:LYS:HG3	1.69	0.74
1:A:23:VAL:HG23	1:A:192:ALA:HB1	1.70	0.73
1:A:178:SER:HB2	1:A:181:ASP:OD1	1.87	0.73
1:A:291:SER:HB2	1:A:356:ARG:HH22	1.52	0.73
4:D:167:ASP:O	4:D:169:LEU:N	2.21	0.73
3:C:360:PHE:O	3:C:364:LEU:HB2	1.89	0.73
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.24	0.72
2:B:241:GLY:HA3	2:B:421:GLN:NE2	2.04	0.72
4:D:167:ASP:C	4:D:169:LEU:H	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG21	1:A:203:VAL:HG13	1.70	0.72
2:B:405:VAL:HG12	2:B:406:ALA:H	1.54	0.72
3:C:167:GLY:H	3:C:175:THR:CG2	2.00	0.72
3:C:52:LEU:HD13	3:C:80:ILE:HG22	1.70	0.72
10:J:12:LEU:O	10:J:19:THR:HG21	1.89	0.72
1:A:102:LEU:N	1:A:102:LEU:HD12	2.05	0.72
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.71	0.72
2:B:111:CYS:SG	2:B:119:LEU:HD22	2.30	0.72
2:B:280:GLY:N	2:B:283:PRO:HD2	2.03	0.71
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.70	0.71
3:C:148:THR:HG22	3:C:162:VAL:HG13	1.72	0.71
1:A:295:ALA:O	1:A:299:VAL:HG23	1.90	0.71
1:A:354:VAL:O	1:A:358:LYS:HG3	1.90	0.71
3:C:238:THR:CG2	3:C:239:PRO:HD3	2.20	0.71
2:B:280:GLY:H	2:B:283:PRO:CD	2.02	0.71
4:D:21:LEU:HD13	4:D:26:ILE:HD11	1.73	0.71
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.55	0.71
5:E:47:VAL:HG21	13:E:198:PEE:H24	1.73	0.71
1:A:243:HIS:O	1:A:425:PRO:HA	1.91	0.71
4:D:212:MET:O	4:D:216:VAL:HG22	1.90	0.71
1:A:282:ARG:HH11	9:I:202:UNK:H	1.39	0.71
5:E:60:SER:C	5:E:62:MET:H	1.93	0.71
1:A:267:LEU:O	1:A:271:GLN:HB2	1.91	0.71
1:A:382:GLU:HG2	1:A:389:ARG:HA	1.73	0.71
2:B:81:SER:O	2:B:85:ILE:HG22	1.90	0.71
2:B:264:ILE:HG12	2:B:316:TYR:O	1.91	0.70
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.73	0.70
4:D:116:ILE:HG23	4:D:117:VAL:N	2.07	0.70
7:G:50:PRO:HG2	7:G:51:PRO:HD2	1.73	0.70
1:A:4:TYR:HB2	2:B:113:ARG:HB3	1.73	0.70
2:B:92:VAL:CG1	2:B:115:ASP:HB3	2.20	0.70
3:C:320:PRO:HA	3:C:323:GLN:HE21	1.55	0.70
1:A:106:VAL:O	1:A:110:VAL:HG23	1.90	0.70
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.57	0.70
3:C:370:ILE:O	3:C:374:GLU:HB2	1.91	0.70
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.27	0.70
2:B:95:LYS:O	2:B:109:VAL:HA	1.92	0.69
5:E:62:MET:CE	5:E:62:MET:HA	2.22	0.69
4:D:224:ARG:HH21	7:G:26:PHE:HA	1.56	0.69
1:A:399:LEU:O	1:A:399:LEU:HD12	1.93	0.69
1:A:282:ARG:HB2	9:I:203:UNK:CB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:PHE:CE2	2:B:191:LEU:HB3	2.28	0.69
3:C:142:TRP:CH2	3:C:265:THR:HG22	2.27	0.69
4:D:30:PHE:CE2	4:D:64:LEU:HD21	2.28	0.69
2:B:109:VAL:HG22	2:B:119:LEU:HD21	1.73	0.69
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.75	0.68
5:E:17:PRO:HD3	7:G:24:ARG:HE	1.59	0.68
3:C:27:ASN:ND2	6:F:69:ASN:ND2	2.36	0.68
1:A:64:PHE:O	1:A:75:LEU:HD23	1.93	0.68
2:B:132:PHE:CD2	2:B:191:LEU:HB3	2.28	0.68
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.76	0.68
2:B:76:THR:CG2	2:B:82:SER:H	2.04	0.68
5:E:13:TYR:O	5:E:14:ARG:HD3	1.93	0.68
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.24	0.68
2:B:424:MET:HG2	2:B:425:ALA:N	2.08	0.68
1:A:40:TRP:CH2	1:A:377:GLU:HA	2.28	0.67
4:D:165:TYR:CE2	4:D:168:VAL:HG22	2.30	0.67
1:A:292:SER:N	1:A:293:PRO:HD3	2.07	0.67
3:C:316:MET:SD	3:C:319:ARG:NE	2.67	0.67
6:F:70:MET:HE2	6:F:71:ARG:HG2	1.75	0.67
2:B:395:PRO:O	2:B:398:VAL:HG12	1.94	0.67
3:C:198:LEU:HD21	11:C:382:HEM:HMA1	1.75	0.67
1:A:58:PHE:HB3	1:A:182:LEU:HD11	1.77	0.67
2:B:258:VAL:HG12	2:B:259:ALA:N	2.09	0.67
3:C:110:TYR:HB3	3:C:113:THR:CG2	2.24	0.67
3:C:238:THR:CB	4:D:212:MET:HG3	2.25	0.67
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.29	0.67
1:A:23:VAL:HG23	1:A:192:ALA:CB	2.25	0.67
1:A:371:GLY:O	1:A:375:VAL:HG23	1.95	0.67
2:B:38:LEU:HD23	2:B:378:PHE:HZ	1.60	0.67
1:A:205:HIS:NE2	1:A:209:LEU:HD21	2.09	0.67
3:C:127:THR:HG22	3:C:186:LEU:CB	2.25	0.67
5:E:15:ARG:HH11	5:E:19:ASP:HB3	1.58	0.67
5:E:43:THR:O	5:E:47:VAL:HG23	1.95	0.67
1:A:36:THR:HG22	1:A:100:LYS:CB	2.26	0.66
2:B:407:ASP:C	2:B:409:ASP:H	1.98	0.66
1:A:110:VAL:HA	1:A:113:LEU:HD12	1.77	0.66
2:B:162:ASN:HB3	2:B:244:ILE:CD1	2.23	0.66
2:B:333:ALA:O	2:B:337:ILE:HG13	1.95	0.66
5:E:86:ASN:HB3	5:E:148:ALA:HB1	1.77	0.66
6:F:13:LEU:O	6:F:17:ARG:HG3	1.95	0.66
3:C:27:ASN:ND2	6:F:69:ASN:HD22	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ASN:O	2:B:157:THR:HG22	1.96	0.66
2:B:405:VAL:HG12	2:B:406:ALA:N	2.11	0.66
3:C:28:ILE:HD12	3:C:225:TYR:CZ	2.30	0.66
3:C:167:GLY:HA3	3:C:174:PRO:HG2	1.77	0.66
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.61	0.66
7:G:79:ASN:O	8:H:47:ARG:NH1	2.29	0.65
2:B:111:CYS:SG	2:B:116:VAL:HA	2.37	0.65
5:E:136:ILE:HG12	5:E:183:PRO:HD3	1.78	0.65
2:B:353:SER:C	2:B:355:GLU:H	1.99	0.65
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.76	0.65
3:C:146:VAL:O	3:C:150:LEU:HD13	1.96	0.65
3:C:5:ILE:O	3:C:5:ILE:HG22	1.97	0.65
1:A:102:LEU:H	1:A:102:LEU:HD12	1.62	0.65
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.77	0.65
1:A:288:LEU:HD22	2:B:83:PHE:HD1	1.61	0.65
2:B:248:ASN:HD22	2:B:248:ASN:C	1.99	0.65
4:D:164:ILE:HD11	4:D:182:VAL:CG1	2.27	0.65
3:C:104:TYR:CE2	3:C:316:MET:CB	2.80	0.64
5:E:16:PRO:HD2	7:G:22:GLU:O	1.96	0.64
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.77	0.64
3:C:120:LEU:HG	11:C:382:HEM:HAB	1.79	0.64
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.96	0.64
2:B:100:SER:O	9:I:106:UNK:HA	1.97	0.64
4:D:192:TRP:CD1	4:D:193:ALA:N	2.65	0.64
1:A:362:ARG:HH22	2:B:113:ARG:NH1	1.95	0.64
3:C:198:LEU:HD21	11:C:382:HEM:CMA	2.27	0.64
13:C:384:PEE:O5	7:G:48:VAL:HG21	1.98	0.64
4:D:51:LEU:O	4:D:54:VAL:HG12	1.98	0.64
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.12	0.64
2:B:357:VAL:HG11	2:B:406:ALA:HB1	1.80	0.64
3:C:104:TYR:CZ	3:C:316:MET:HG3	2.33	0.64
4:D:195:GLU:O	4:D:195:GLU:HG3	1.97	0.64
5:E:162:GLY:O	5:E:164:HIS:HD2	1.81	0.64
5:E:142:LEU:HB2	15:E:197:FES:S2	2.37	0.64
4:D:238:ARG:HD2	5:E:5:ILE:HD11	1.79	0.64
2:B:310:SER:O	2:B:324:PHE:HB2	1.99	0.63
2:B:272:PHE:O	2:B:276:GLN:N	2.26	0.63
2:B:96:LEU:HD23	2:B:97:SER:N	2.12	0.63
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.63
5:E:109:GLU:OE1	5:E:166:ASP:HB2	1.98	0.63
2:B:39:GLU:HG3	2:B:41:TYR:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:LEU:O	3:C:103:LEU:HD13	1.99	0.63
4:D:216:VAL:HG23	4:D:217:PRO:HD3	1.81	0.63
1:A:378:ASP:O	1:A:382:GLU:HB2	1.98	0.63
1:A:53:ASN:HD22	1:A:54:GLY:N	1.97	0.63
1:A:429:GLU:OE2	7:G:7:LEU:HB2	1.99	0.63
2:B:70:ARG:HD3	2:B:100:SER:HB3	1.78	0.63
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.34	0.63
3:C:34:PHE:HD1	3:C:37:LEU:HD12	1.63	0.63
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.62
5:E:122:HIS:CE1	5:E:124:LEU:HB2	2.34	0.62
1:A:245:GLU:HG3	7:G:11:ARG:HG2	1.80	0.62
1:A:108:LYS:HE3	1:A:108:LYS:HA	1.80	0.62
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.34	0.62
3:C:332:ASN:HD22	3:C:332:ASN:C	2.03	0.62
2:B:31:ASN:HB3	2:B:201:SER:HB2	1.81	0.62
2:B:202:ALA:HB3	2:B:229:GLY:O	2.00	0.62
5:E:44:THR:HB	10:J:24:ILE:HD12	1.80	0.62
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.80	0.62
4:D:149:PHE:HA	4:D:156:GLN:O	2.00	0.62
5:E:147:ILE:O	5:E:156:TYR:HA	2.00	0.62
1:A:245:GLU:HG2	1:A:247:GLY:H	1.64	0.62
4:D:218:LEU:HD11	5:E:42:VAL:HG12	1.82	0.62
5:E:16:PRO:HD3	7:G:23:GLN:HA	1.81	0.62
3:C:167:GLY:N	3:C:175:THR:HG22	2.12	0.62
1:A:284:TYR:CE1	9:I:112:UNK:O	2.53	0.62
2:B:163:LEU:HD21	2:B:258:VAL:HG21	1.80	0.61
3:C:247:SER:HB3	3:C:250:LEU:HB2	1.82	0.61
8:H:50:THR:HG22	8:H:52:GLU:N	2.15	0.61
3:C:25:PRO:HD2	3:C:28:ILE:HD11	1.82	0.61
5:E:123:ASP:HB2	5:E:170:ARG:CZ	2.30	0.61
1:A:342:TRP:O	1:A:345:LEU:HB3	1.99	0.61
2:B:92:VAL:HG11	2:B:115:ASP:HB3	1.81	0.61
3:C:124:LEU:HD22	3:C:124:LEU:O	2.00	0.61
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.82	0.61
2:B:207:VAL:HG12	2:B:208:GLY:N	2.15	0.61
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.30	0.61
5:E:183:PRO:O	5:E:185:TYR:HD1	1.84	0.61
1:A:56:GLY:HA2	1:A:185:TYR:CE2	2.35	0.61
2:B:360:ALA:O	2:B:363:LYS:N	2.31	0.61
3:C:104:TYR:OH	3:C:322:SER:HB2	1.99	0.61
5:E:14:ARG:O	7:G:24:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:TRP:HB2	3:C:175:THR:HG21	1.81	0.61
3:C:125:MET:O	3:C:128:ALA:N	2.33	0.61
3:C:222:HIS:O	3:C:223:PRO:C	2.38	0.61
3:C:238:THR:HG23	3:C:239:PRO:CD	2.31	0.61
5:E:102:THR:O	5:E:106:ILE:HG13	2.01	0.61
2:B:122:PHE:O	2:B:126:VAL:HG23	2.01	0.60
2:B:166:ALA:HB1	2:B:242:GLY:HA3	1.82	0.60
2:B:170:ASN:HD21	2:B:237:ALA:HA	1.66	0.60
3:C:142:TRP:O	3:C:146:VAL:HG22	2.01	0.60
3:C:209:PRO:O	3:C:315:THR:HG21	2.01	0.60
12:C:383:U10:H8	12:C:383:U10:H1M1	1.82	0.60
2:B:260:GLU:O	2:B:261:SER:HB3	2.01	0.60
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.83	0.60
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.82	0.60
5:E:59:VAL:O	5:E:59:VAL:HG12	2.01	0.60
3:C:112:GLU:N	3:C:112:GLU:OE1	2.34	0.60
12:C:383:U10:C8	12:C:383:U10:H1M1	2.31	0.60
5:E:99:ARG:H	5:E:133:VAL:HG12	1.65	0.60
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.31	0.60
4:D:55:CYS:HG	4:D:56:TYR:HD2	1.50	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.02	0.60
1:A:252:HIS:CE1	1:A:325:VAL:HG22	2.37	0.59
2:B:101:THR:HG22	2:B:102:ARG:N	2.17	0.59
2:B:405:VAL:O	2:B:406:ALA:HB2	2.02	0.59
2:B:52:LYS:O	2:B:203:ARG:NH2	2.27	0.59
4:D:167:ASP:O	4:D:169:LEU:HD23	2.02	0.59
4:D:32:VAL:CG1	4:D:186:VAL:HG22	2.31	0.59
1:A:279:HIS:HA	1:A:307:PHE:CE1	2.36	0.59
2:B:24:LEU:H	2:B:24:LEU:HD23	1.67	0.59
2:B:258:VAL:CG1	2:B:321:LEU:HB3	2.29	0.59
3:C:110:TYR:HB3	3:C:113:THR:HG23	1.83	0.59
4:D:116:ILE:CG2	4:D:117:VAL:N	2.65	0.59
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.31	0.59
2:B:95:LYS:HB2	2:B:110:GLU:CG	2.32	0.59
3:C:136:TRP:CD1	3:C:176:LEU:HD13	2.37	0.59
3:C:27:ASN:HD22	6:F:69:ASN:HD21	1.43	0.59
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.37	0.59
1:A:102:LEU:O	1:A:104:LYS:N	2.35	0.59
1:A:61:HIS:CD2	1:A:134:ILE:HG12	2.37	0.59
2:B:101:THR:HB	2:B:104:ASN:OD1	2.02	0.59
2:B:207:VAL:HG11	2:B:382:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:ILE:HD11	3:C:364:LEU:HD11	1.85	0.59
3:C:45:GLN:CB	11:C:381:HEM:HAB	2.32	0.59
5:E:16:PRO:HD3	7:G:23:GLN:CA	2.33	0.59
2:B:406:ALA:O	2:B:408:ALA:N	2.35	0.59
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.38	0.59
1:A:252:HIS:ND1	1:A:325:VAL:HG22	2.18	0.59
3:C:120:LEU:CG	11:C:382:HEM:HAB	2.33	0.59
4:D:227:TRP:O	4:D:229:VAL:N	2.36	0.59
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.84	0.59
10:J:13:LEU:HA	10:J:19:THR:HG21	1.85	0.58
2:B:341:TYR:OH	2:B:422:LYS:HE3	2.02	0.58
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.85	0.58
4:D:182:VAL:O	4:D:186:VAL:HG23	2.03	0.58
3:C:175:THR:HA	3:C:178:ARG:HG2	1.86	0.58
3:C:225:TYR:HA	3:C:228:LYS:HB3	1.86	0.58
3:C:346:HIS:O	3:C:350:ILE:HG12	2.02	0.58
5:E:96:LEU:HD12	5:E:135:LEU:O	2.04	0.58
3:C:45:GLN:HB3	11:C:381:HEM:HAB	1.86	0.58
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.51	0.58
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.85	0.58
3:C:347:PRO:HG3	7:G:66:PHE:HB2	1.86	0.58
5:E:78:LEU:HG	5:E:191:ASP:C	2.23	0.58
5:E:45:LEU:HD13	5:E:45:LEU:C	2.24	0.58
2:B:357:VAL:HG12	2:B:361:LYS:CD	2.34	0.58
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.33	0.57
3:C:64:PHE:CD2	3:C:259:PRO:HG3	2.39	0.57
4:D:171:PHE:HE2	4:D:181:GLN:HE22	1.50	0.57
5:E:76:ILE:O	5:E:193:VAL:HG12	2.04	0.57
2:B:146:ILE:HG13	2:B:147:ASP:N	2.19	0.57
5:E:85:LYS:HD2	5:E:87:MET:SD	2.44	0.57
1:A:7:ALA:O	1:A:11:VAL:HG23	2.04	0.57
3:C:220:PRO:HG2	3:C:223:PRO:HG2	1.86	0.57
2:B:112:LEU:N	2:B:112:LEU:HD23	2.19	0.57
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.36	0.57
6:F:59:MET:HA	6:F:59:MET:CE	2.34	0.57
4:D:2:ASP:OD2	7:G:70:LYS:HE2	2.04	0.57
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.57
1:A:88:ALA:CB	1:A:97:TYR:HA	2.32	0.57
2:B:258:VAL:HG13	2:B:322:PHE:H	1.68	0.57
4:D:155:GLY:C	4:D:156:GLN:NE2	2.58	0.57
1:A:130:GLU:O	1:A:134:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:CB	2:B:113:ARG:HB3	2.35	0.57
2:B:250:ASP:O	2:B:251:SER:HB3	2.05	0.57
4:D:165:TYR:O	4:D:168:VAL:HG23	2.05	0.57
4:D:3:LEU:HD23	4:D:4:GLU:N	2.20	0.57
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.87	0.57
3:C:245:LEU:O	4:D:201:ARG:HD3	2.04	0.57
3:C:330:VAL:CG2	3:C:331:ALA:N	2.68	0.57
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.87	0.57
4:D:232:SER:CB	7:G:23:GLN:HE22	2.17	0.57
7:G:77:TYR:CE1	8:H:52:GLU:HB2	2.39	0.57
1:A:297:ILE:HG21	1:A:337:VAL:HG11	1.85	0.56
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.68	0.56
5:E:17:PRO:HD3	7:G:24:ARG:NE	2.20	0.56
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.40	0.56
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.86	0.56
3:C:95:ILE:O	3:C:99:ILE:HG12	2.05	0.56
1:A:250:LEU:HD22	1:A:250:LEU:C	2.25	0.56
1:A:250:LEU:N	1:A:250:LEU:HD13	2.20	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.05	0.56
3:C:64:PHE:CE2	3:C:259:PRO:HG3	2.40	0.56
4:D:32:VAL:HG21	4:D:186:VAL:CG2	2.35	0.56
8:H:35:GLU:O	8:H:39:LEU:HD13	2.05	0.56
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.56
3:C:81:ARG:NH1	11:C:381:HEM:O1D	2.38	0.56
1:A:205:HIS:O	1:A:208:LEU:HB3	2.06	0.56
2:B:257:ILE:O	2:B:323:GLY:HA3	2.05	0.56
3:C:146:VAL:HG23	3:C:147:ILE:N	2.21	0.56
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.70	0.56
6:F:67:ASP:O	6:F:71:ARG:HG3	2.06	0.56
2:B:56:ARG:HB2	2:B:102:ARG:O	2.06	0.56
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.87	0.56
1:A:61:HIS:HD2	1:A:134:ILE:HG12	1.69	0.56
2:B:101:THR:HG22	2:B:102:ARG:H	1.70	0.56
2:B:20:HIS:N	2:B:21:PRO:CD	2.64	0.56
2:B:258:VAL:HA	2:B:322:PHE:O	2.06	0.56
1:A:252:HIS:CE1	1:A:323:TYR:HH	2.24	0.56
3:C:293:LEU:N	3:C:293:LEU:HD22	2.21	0.56
3:C:373:LEU:HD23	3:C:373:LEU:O	2.05	0.56
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.41	0.56
1:A:102:LEU:C	1:A:104:LYS:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:CG2	2:B:119:LEU:HD11	2.35	0.56
1:A:33:PRO:HG3	2:B:369:LEU:HD22	1.87	0.56
2:B:372:VAL:O	2:B:372:VAL:HG12	2.06	0.56
2:B:397:THR:O	2:B:401:GLN:HG2	2.05	0.56
3:C:157:ILE:O	3:C:157:ILE:HG12	2.06	0.55
3:C:209:PRO:HG2	6:F:69:ASN:HD21	1.71	0.55
3:C:319:ARG:HH12	3:C:371:GLY:HA2	1.72	0.55
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.87	0.55
2:B:353:SER:C	2:B:355:GLU:N	2.59	0.55
3:C:167:GLY:HA3	3:C:174:PRO:CG	2.36	0.55
4:D:207:LYS:O	4:D:211:MET:HG2	2.06	0.55
5:E:100:HIS:CD2	5:E:131:GLU:HB2	2.42	0.55
9:I:310:UNK:O	9:I:311:UNK:C	2.54	0.55
3:C:261:ASN:HD21	3:C:264:VAL:HG23	1.71	0.55
3:C:49:GLY:C	11:C:381:HEM:HAC	2.27	0.55
4:D:68:VAL:HG11	4:D:92:PRO:HG2	1.89	0.55
1:A:108:LYS:O	1:A:112:LEU:HG	2.06	0.55
1:A:39:VAL:HA	1:A:196:VAL:O	2.06	0.55
2:B:126:VAL:O	2:B:130:PRO:HG3	2.06	0.55
3:C:105:TYR:CD1	3:C:209:PRO:HA	2.41	0.55
4:D:167:ASP:C	4:D:169:LEU:N	2.59	0.55
5:E:98:VAL:HA	5:E:133:VAL:O	2.05	0.55
2:B:76:THR:HG22	2:B:82:SER:N	2.07	0.55
3:C:273:TRP:HA	3:C:276:LEU:HG	1.88	0.55
3:C:293:LEU:H	3:C:293:LEU:HD22	1.72	0.55
4:D:215:LEU:O	4:D:219:VAL:HG22	2.06	0.55
4:D:213:GLY:O	4:D:217:PRO:CD	2.54	0.55
4:D:75:ASN:HB2	4:D:77:ASP:H	1.70	0.55
7:G:11:ARG:O	7:G:12:HIS:HB2	2.07	0.55
1:A:291:SER:CB	1:A:356:ARG:HH22	2.17	0.55
2:B:248:ASN:HD22	2:B:249:GLY:N	2.05	0.55
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.07	0.55
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.16	0.55
4:D:130:LEU:HD11	4:D:158:ILE:CD1	2.35	0.55
6:F:12:TRP:HA	6:F:12:TRP:HE3	1.72	0.55
6:F:91:GLU:O	6:F:95:LYS:HG3	2.07	0.55
3:C:27:ASN:HB2	6:F:69:ASN:HD22	1.71	0.55
1:A:280:TYR:CG	1:A:281:ASP:N	2.75	0.55
3:C:3:PRO:HG2	3:C:4:ASN:H	1.71	0.55
5:E:77:LYS:HA	5:E:191:ASP:O	2.07	0.55
1:A:26:ALA:O	1:A:198:ALA:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:CYS:HB3	1:A:411:CYS:CB	2.36	0.54
3:C:293:LEU:H	3:C:293:LEU:CD2	2.21	0.54
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.42	0.54
10:J:13:LEU:HA	10:J:19:THR:CG2	2.37	0.54
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.73	0.54
1:A:349:ILE:HD12	1:A:407:VAL:HG11	1.89	0.54
1:A:381:ARG:O	1:A:382:GLU:C	2.46	0.54
3:C:358:SER:O	3:C:362:ILE:HG13	2.06	0.54
5:E:103:LYS:HA	5:E:106:ILE:HD12	1.89	0.54
4:D:181:GLN:CB	8:H:77:LEU:HD22	2.37	0.54
1:A:58:PHE:CE1	1:A:127:ILE:HG23	2.42	0.54
1:A:374:PRO:O	1:A:377:GLU:HB3	2.07	0.54
1:A:85:HIS:O	1:A:99:ILE:HA	2.07	0.54
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.70	0.54
5:E:189:SER:OG	5:E:192:MET:HB2	2.08	0.54
1:A:284:TYR:HE1	9:I:112:UNK:O	1.90	0.54
3:C:166:TRP:HB2	3:C:175:THR:CG2	2.38	0.54
3:C:289:LEU:O	3:C:293:LEU:HD23	2.07	0.54
4:D:216:VAL:HG23	4:D:217:PRO:CD	2.37	0.54
2:B:414:ALA:O	2:B:417:PHE:HB3	2.08	0.54
2:B:109:VAL:HG22	2:B:119:LEU:HD11	1.88	0.54
4:D:62:LYS:O	4:D:66:GLU:HG2	2.07	0.54
3:C:133:VAL:HA	3:C:140:SER:HB3	1.90	0.54
2:B:400:GLN:O	2:B:404:ALA:HB2	2.06	0.54
4:D:165:TYR:CD2	4:D:168:VAL:HG22	2.43	0.54
1:A:15:GLN:HB3	1:A:205:HIS:ND1	2.22	0.54
2:B:143:GLN:OE1	2:B:146:ILE:HD11	2.07	0.54
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.89	0.54
3:C:105:TYR:CE1	3:C:209:PRO:HA	2.43	0.54
5:E:164:HIS:CB	5:E:173:LYS:HB3	2.34	0.54
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.38	0.54
6:F:59:MET:HE3	6:F:59:MET:HA	1.88	0.54
8:H:47:ARG:CD	8:H:48:SER:H	2.14	0.54
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.23	0.54
4:D:148:TYR:CD1	4:D:148:TYR:N	2.76	0.54
5:E:147:ILE:HD12	5:E:159:PRO:HD3	1.90	0.54
1:A:318:GLY:O	1:A:319:LEU:HD23	2.08	0.53
2:B:129:ALA:N	2:B:130:PRO:CD	2.69	0.53
3:C:34:PHE:CD1	3:C:37:LEU:HD12	2.42	0.53
4:D:117:VAL:O	4:D:123:GLY:HA2	2.08	0.53
1:A:40:TRP:CD1	1:A:40:TRP:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ALA:C	2:B:173:ALA:H	2.10	0.53
5:E:12:ASP:O	5:E:13:TYR:C	2.46	0.53
10:J:13:LEU:HG	10:J:23:THR:HG21	1.90	0.53
1:A:362:ARG:HH22	2:B:113:ARG:HH12	1.56	0.53
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.41	0.53
5:E:62:MET:HA	5:E:62:MET:HE2	1.90	0.53
3:C:127:THR:CG2	3:C:186:LEU:HB3	2.37	0.53
2:B:213:HIS:N	2:B:214:PRO:HD2	2.24	0.53
2:B:305:ASN:CB	2:B:306:PRO:HD2	2.38	0.53
3:C:20:ILE:O	3:C:22:LEU:N	2.42	0.53
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.44	0.53
6:F:71:ARG:O	6:F:73:GLN:HG2	2.09	0.53
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.91	0.53
4:D:75:ASN:ND2	4:D:79:GLU:O	2.42	0.53
4:D:75:ASN:H	4:D:79:GLU:H	1.57	0.53
1:A:189:HIS:CD2	1:A:194:ARG:HH12	2.26	0.53
5:E:177:PRO:O	5:E:178:LEU:HD23	2.09	0.53
2:B:109:VAL:HG13	2:B:119:LEU:HD21	1.91	0.52
2:B:353:SER:O	2:B:355:GLU:N	2.42	0.52
4:D:32:VAL:HG21	4:D:186:VAL:HG22	1.91	0.52
6:F:16:ILE:O	6:F:19:TRP:HB3	2.09	0.52
6:F:91:GLU:HG2	6:F:95:LYS:HE3	1.89	0.52
1:A:242:ARG:O	7:G:14:ILE:HA	2.09	0.52
1:A:253:VAL:O	1:A:323:TYR:HD1	1.92	0.52
2:B:150:VAL:HG23	2:B:151:ALA:N	2.24	0.52
2:B:361:LYS:NZ	2:B:403:ASP:HA	2.25	0.52
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.73	0.52
1:A:356:ARG:O	1:A:357:GLY:C	2.47	0.52
1:A:88:ALA:CB	1:A:96:ALA:O	2.48	0.52
2:B:140:LEU:C	2:B:142:PRO:HD2	2.30	0.52
3:C:89:SER:O	3:C:90:PHE:C	2.47	0.52
5:E:78:LEU:CD1	5:E:187:PHE:HE1	2.21	0.52
8:H:47:ARG:HD3	8:H:48:SER:N	2.17	0.52
1:A:114:ALA:HB2	1:A:216:PHE:CE1	2.45	0.52
1:A:293:PRO:O	1:A:297:ILE:N	2.37	0.52
2:B:19:PRO:C	2:B:21:PRO:HD3	2.29	0.52
2:B:40:ASN:O	2:B:41:TYR:HB2	2.09	0.52
1:A:274:ASN:O	1:A:309:THR:HG21	2.09	0.52
2:B:280:GLY:O	2:B:283:PRO:HG2	2.08	0.52
2:B:66:SER:O	2:B:69:LEU:HB3	2.09	0.52
3:C:157:ILE:O	3:C:161:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:SER:HB2	12:C:383:U10:H3M1	1.92	0.52
1:A:286:GLY:HA3	1:A:289:HIS:NE2	2.24	0.52
1:A:297:ILE:HG22	1:A:303:LEU:HD11	1.92	0.52
2:B:202:ALA:HB2	2:B:229:GLY:HA2	1.92	0.52
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.92	0.52
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.44	0.52
1:A:250:LEU:HB2	1:A:326:CYS:O	2.10	0.52
2:B:258:VAL:CG1	2:B:259:ALA:N	2.71	0.52
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.25	0.52
3:C:281:ILE:HG22	3:C:281:ILE:O	2.10	0.52
5:E:118:ARG:HH11	5:E:118:ARG:HB3	1.75	0.52
2:B:307:PHE:C	2:B:307:PHE:CD1	2.83	0.52
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.52
1:A:171:SER:O	1:A:175:ARG:HG3	2.10	0.52
1:A:431:LEU:HD23	1:A:432:PRO:HD2	1.91	0.52
1:A:350:SER:OG	1:A:353:GLU:HG3	2.09	0.51
3:C:164:TRP:CD1	3:C:165:ALA:N	2.78	0.51
4:D:12:TRP:HB3	4:D:14:HIS:CE1	2.46	0.51
7:G:77:TYR:CZ	8:H:52:GLU:HB2	2.45	0.51
2:B:113:ARG:HG3	2:B:114:ASP:H	1.75	0.51
2:B:399:LEU:CA	2:B:402:ILE:HG22	2.40	0.51
3:C:3:PRO:O	3:C:5:ILE:HG13	2.10	0.51
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.46	0.51
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.46	0.51
4:D:117:VAL:HG23	4:D:190:LEU:HB3	1.92	0.51
6:F:16:ILE:O	6:F:19:TRP:N	2.43	0.51
1:A:178:SER:O	1:A:182:LEU:HD23	2.11	0.51
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.11	0.51
2:B:262:ALA:O	2:B:263:ALA:HB2	2.10	0.51
3:C:156:TYR:C	3:C:158:GLY:H	2.13	0.51
3:C:233:LEU:O	3:C:237:LEU:HB2	2.10	0.51
4:D:29:GLY:O	4:D:32:VAL:HG13	2.11	0.51
5:E:86:ASN:ND2	5:E:156:TYR:HE2	2.09	0.51
1:A:250:LEU:CD2	1:A:325:VAL:HG13	2.40	0.51
2:B:132:PHE:CD2	2:B:191:LEU:CB	2.94	0.51
3:C:20:ILE:C	3:C:22:LEU:H	2.14	0.51
3:C:48:THR:O	3:C:52:LEU:HB2	2.11	0.51
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.46	0.51
4:D:3:LEU:HD22	8:H:59:PHE:HE2	1.75	0.51
1:A:388:ARG:HG2	1:A:389:ARG:N	2.26	0.51
1:A:382:GLU:HG2	1:A:389:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:CYS:O	4:D:39:SER:N	2.43	0.51
4:D:57:THR:HB	4:D:60:GLU:HB2	1.93	0.51
1:A:86:LEU:O	9:I:312:UNK:O	2.28	0.51
1:A:343:MET:O	1:A:347:THR:HG22	2.11	0.51
1:A:444:LEU:O	1:A:445:ARG:O	2.28	0.51
2:B:162:ASN:CB	2:B:244:ILE:HD11	2.34	0.51
2:B:395:PRO:C	2:B:398:VAL:HG12	2.31	0.51
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.41	0.51
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.26	0.51
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.76	0.51
1:A:48:GLU:CD	1:A:53:ASN:HA	2.31	0.51
2:B:278:VAL:O	2:B:282:ASN:ND2	2.44	0.51
3:C:372:THR:O	3:C:375:ASN:N	2.43	0.51
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.46	0.51
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.11	0.51
5:E:78:LEU:HD21	5:E:193:VAL:HB	1.93	0.51
1:A:100:LYS:HE3	2:B:370:MET:CE	2.41	0.50
2:B:245:ARG:HB3	2:B:430:LEU:HD13	1.93	0.50
3:C:142:TRP:HA	3:C:145:THR:OG1	2.11	0.50
3:C:146:VAL:HG23	3:C:147:ILE:H	1.76	0.50
4:D:72:ASP:O	4:D:73:GLY:O	2.29	0.50
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.41	0.50
1:A:42:ASP:CB	1:A:194:ARG:HB3	2.30	0.50
1:A:252:HIS:HB2	1:A:425:PRO:HD2	1.93	0.50
2:B:164:HIS:H	2:B:164:HIS:HD1	1.60	0.50
2:B:207:VAL:HG12	2:B:208:GLY:H	1.76	0.50
10:J:59:TYR:CD1	10:J:59:TYR:N	2.78	0.50
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.94	0.50
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.93	0.50
3:C:246:PHE:C	3:C:248:PRO:HD3	2.32	0.50
3:C:377:MET:HE2	6:F:20:TYR:CG	2.46	0.50
5:E:117:LEU:HD12	5:E:121:GLN:H	1.74	0.50
4:D:28:ARG:HD2	4:D:171:PHE:CE2	2.46	0.50
5:E:38:LEU:O	5:E:42:VAL:HG23	2.12	0.50
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.93	0.50
1:A:106:VAL:HG21	1:A:203:VAL:CG1	2.40	0.50
1:A:106:VAL:CG2	1:A:203:VAL:HG22	2.41	0.50
1:A:266:ASP:C	1:A:268:VAL:H	2.15	0.50
1:A:307:PHE:C	1:A:307:PHE:CD1	2.84	0.50
1:A:4:TYR:HB2	2:B:113:ARG:CB	2.40	0.50
2:B:109:VAL:HG13	2:B:109:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:TYR:O	2:B:372:VAL:HG23	2.12	0.50
2:B:407:ASP:C	2:B:409:ASP:N	2.64	0.50
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.93	0.50
1:A:15:GLN:HB3	1:A:205:HIS:CE1	2.47	0.50
1:A:253:VAL:HG11	1:A:335:MET:CE	2.41	0.50
1:A:49:SER:N	1:A:52:ASN:HB3	2.16	0.50
5:E:12:ASP:N	5:E:20:TYR:HE2	2.10	0.50
1:A:291:SER:O	1:A:292:SER:C	2.48	0.50
2:B:232:LEU:HG	2:B:233:SER:N	2.23	0.50
3:C:86:ASN:OD1	3:C:244:ALA:HA	2.12	0.50
10:J:36:ASP:O	10:J:37:GLN:C	2.50	0.50
1:A:444:LEU:HD12	1:A:444:LEU:H	1.76	0.50
1:A:95:THR:HG22	1:A:96:ALA:N	2.27	0.50
2:B:62:ASN:O	2:B:65:THR:CG2	2.59	0.50
5:E:9:ASN:HD21	5:E:11:SER:HB3	1.76	0.50
1:A:290:SER:O	1:A:291:SER:C	2.49	0.50
2:B:143:GLN:O	2:B:144:LEU:C	2.49	0.50
5:E:14:ARG:HG2	5:E:14:ARG:NH1	2.17	0.50
9:I:313:UNK:CB	9:I:314:UNK:CD	2.90	0.50
2:B:131:GLU:O	2:B:131:GLU:HG3	2.11	0.49
1:A:100:LYS:HB2	1:A:100:LYS:HZ2	1.77	0.49
1:A:292:SER:N	1:A:293:PRO:CD	2.71	0.49
5:E:136:ILE:HG22	5:E:138:VAL:HG23	1.92	0.49
5:E:48:ALA:O	5:E:49:TYR:C	2.51	0.49
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.94	0.49
10:J:57:HIS:HB2	10:J:62:LYS:CB	2.42	0.49
1:A:106:VAL:HB	1:A:107:PRO:CD	2.42	0.49
1:A:339:GLN:OE1	1:A:437:ILE:O	2.30	0.49
3:C:9:HIS:HD2	3:C:10:PRO:CD	2.23	0.49
4:D:150:ASN:O	4:D:156:GLN:HA	2.13	0.49
4:D:43:MET:CE	4:D:46:VAL:HG21	2.37	0.49
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.18	0.49
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.75	0.49
1:A:349:ILE:HG22	1:A:408:ARG:HG3	1.93	0.49
4:D:27:ARG:CZ	10:J:59:TYR:CE2	2.95	0.49
5:E:135:LEU:HD13	5:E:180:LEU:HD12	1.95	0.49
5:E:147:ILE:HD11	5:E:159:PRO:HG3	1.94	0.49
5:E:52:LYS:C	5:E:52:LYS:HD3	2.33	0.49
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.94	0.49
2:B:120:MET:HE2	2:B:219:VAL:HG11	1.94	0.49
5:E:29:ASP:OD1	5:E:32:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:70:MET:HE2	6:F:71:ARG:CG	2.42	0.49
7:G:60:THR:O	7:G:61:TRP:C	2.50	0.49
1:A:106:VAL:N	1:A:107:PRO:HD2	2.27	0.49
1:A:338:LEU:O	1:A:341:GLN:N	2.45	0.49
1:A:394:GLU:O	1:A:395:TRP:C	2.51	0.49
2:B:170:ASN:H	2:B:170:ASN:HD22	1.60	0.49
5:E:60:SER:C	5:E:62:MET:N	2.61	0.49
3:C:377:MET:CE	6:F:20:TYR:HB2	2.43	0.49
3:C:318:PHE:CG	6:F:26:PHE:HB3	2.48	0.49
2:B:372:VAL:O	2:B:378:PHE:HB2	2.13	0.49
2:B:56:ARG:O	2:B:56:ARG:HD3	2.13	0.49
3:C:141:PHE:HE1	3:C:171:VAL:O	1.96	0.49
3:C:147:ILE:HD11	3:C:271:PRO:HB3	1.94	0.49
3:C:344:VAL:O	3:C:344:VAL:HG23	2.12	0.49
8:H:49:GLN:HG2	8:H:49:GLN:O	2.11	0.49
2:B:24:LEU:N	2:B:24:LEU:HD23	2.27	0.49
2:B:59:ASN:C	2:B:61:SER:N	2.65	0.49
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.95	0.49
3:C:120:LEU:CD1	3:C:190:ILE:HG23	2.43	0.49
5:E:136:ILE:HG13	5:E:181:GLU:CG	2.41	0.49
5:E:42:VAL:O	5:E:45:LEU:HB3	2.13	0.49
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.46	0.49
1:A:320:PHE:CE2	1:A:415:ILE:HD11	2.48	0.48
1:A:240:GLN:OE1	1:A:434:TYR:HB2	2.13	0.48
2:B:58:GLU:OE2	2:B:65:THR:HG22	2.13	0.48
3:C:130:VAL:HG13	3:C:179:PHE:CG	2.48	0.48
4:D:97:ASN:O	4:D:100:ALA:HB3	2.12	0.48
5:E:15:ARG:NH1	5:E:19:ASP:HB3	2.28	0.48
7:G:73:ASN:O	7:G:75:ALA:N	2.46	0.48
2:B:61:SER:O	2:B:62:ASN:OD1	2.31	0.48
3:C:130:VAL:HG13	3:C:179:PHE:CB	2.42	0.48
3:C:283:ARG:NH2	3:C:339:ILE:O	2.46	0.48
1:A:102:LEU:C	1:A:104:LYS:N	2.67	0.48
1:A:266:ASP:C	1:A:268:VAL:N	2.66	0.48
1:A:288:LEU:HD22	2:B:83:PHE:CD1	2.45	0.48
1:A:305:GLN:O	1:A:306:SER:HB3	2.13	0.48
1:A:366:VAL:C	1:A:368:HIS:H	2.17	0.48
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.13	0.48
2:B:429:ASN:O	2:B:430:LEU:HB2	2.13	0.48
4:D:21:LEU:CD1	4:D:26:ILE:HD11	2.42	0.48
6:F:70:MET:O	6:F:70:MET:HE3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:CZ3	1:A:377:GLU:CD	2.87	0.48
2:B:89:ILE:CD1	2:B:96:LEU:HB2	2.44	0.48
3:C:220:PRO:HG2	3:C:223:PRO:CG	2.43	0.48
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.48	0.48
3:C:333:LEU:HD11	3:C:359:TYR:CE1	2.48	0.48
7:G:29:TYR:CD1	7:G:29:TYR:N	2.80	0.48
1:A:431:LEU:HD23	1:A:432:PRO:CD	2.43	0.48
2:B:399:LEU:O	2:B:402:ILE:HG22	2.13	0.48
3:C:110:TYR:CB	3:C:113:THR:HG23	2.44	0.48
3:C:19:LEU:C	3:C:20:ILE:HG13	2.33	0.48
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.95	0.48
5:E:35:PHE:O	5:E:38:LEU:HB3	2.13	0.48
6:F:13:LEU:HD12	6:F:13:LEU:N	2.28	0.48
8:H:62:LEU:O	8:H:66:ASP:OD1	2.32	0.48
1:A:391:PRO:O	1:A:394:GLU:N	2.40	0.48
3:C:312:LYS:HG2	3:C:375:ASN:OD1	2.13	0.48
4:D:153:PHE:CG	4:D:158:ILE:HG12	2.49	0.48
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.78	0.48
4:D:211:MET:CG	14:D:242:BOG:H5'1	2.42	0.48
5:E:11:SER:CA	5:E:15:ARG:HD2	2.40	0.48
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.96	0.48
2:B:348:ALA:C	2:B:350:GLY:H	2.17	0.48
2:B:402:ILE:HD13	2:B:402:ILE:C	2.33	0.48
1:A:288:LEU:HD13	2:B:83:PHE:HA	1.96	0.48
2:B:232:LEU:CG	2:B:233:SER:H	2.20	0.48
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.29	0.48
4:D:220:TYR:O	4:D:224:ARG:HG2	2.13	0.48
4:D:68:VAL:HG11	4:D:92:PRO:CG	2.44	0.48
5:E:21:SER:O	5:E:22:THR:OG1	2.23	0.48
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.24	0.48
2:B:141:GLN:N	2:B:142:PRO:HD2	2.29	0.48
2:B:39:GLU:HG3	2:B:41:TYR:CD1	2.48	0.48
3:C:369:THR:C	3:C:371:GLY:N	2.67	0.48
8:H:50:THR:CG2	8:H:52:GLU:H	2.23	0.48
1:A:65:LYS:HZ3	9:I:311:UNK:HA	1.78	0.48
1:A:444:LEU:N	1:A:444:LEU:HD12	2.29	0.47
1:A:59:LEU:O	1:A:59:LEU:HD12	2.14	0.47
2:B:430:LEU:O	2:B:433:THR:N	2.36	0.47
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.49	0.47
5:E:29:ASP:N	5:E:30:PRO:HD2	2.28	0.47
1:A:281:ASP:C	1:A:283:THR:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HG3	1:A:323:TYR:OH	2.15	0.47
2:B:166:ALA:HB1	2:B:242:GLY:CA	2.44	0.47
2:B:214:PRO:HG2	2:B:215:VAL:H	1.79	0.47
2:B:248:ASN:ND2	2:B:248:ASN:C	2.67	0.47
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.94	0.47
3:C:285:ILE:HG23	3:C:291:GLY:HA2	1.97	0.47
4:D:141:VAL:HG21	8:H:55:THR:HG23	1.95	0.47
4:D:222:MET:CE	5:E:40:THR:HG23	2.45	0.47
8:H:20:VAL:O	8:H:20:VAL:HG12	2.13	0.47
1:A:373:THR:N	1:A:374:PRO:HD2	2.29	0.47
1:A:292:SER:O	1:A:295:ALA:N	2.44	0.47
1:A:349:ILE:CD1	1:A:407:VAL:HG11	2.44	0.47
1:A:254:ALA:O	1:A:422:VAL:HA	2.14	0.47
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.49	0.47
2:B:395:PRO:CA	2:B:398:VAL:HG12	2.44	0.47
3:C:103:LEU:C	3:C:103:LEU:HD13	2.34	0.47
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.48	0.47
3:C:118:VAL:HB	3:C:303:PHE:CE1	2.49	0.47
1:A:65:LYS:NZ	9:I:311:UNK:N	2.63	0.47
2:B:31:ASN:HB3	2:B:201:SER:CB	2.43	0.47
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.15	0.47
3:C:148:THR:HG21	3:C:166:TRP:CE3	2.50	0.47
3:C:326:PHE:O	3:C:329:LEU:HB3	2.15	0.47
7:G:57:LEU:H	7:G:57:LEU:HD22	1.79	0.47
1:A:418:GLN:O	1:A:420:PRO:HD3	2.14	0.47
2:B:75:LEU:HD11	2:B:140:LEU:HD22	1.96	0.47
2:B:258:VAL:HG11	2:B:321:LEU:CB	2.37	0.47
3:C:342:GLN:CA	3:C:342:GLN:HE21	2.27	0.47
3:C:325:LEU:CD2	3:C:362:ILE:HG23	2.42	0.47
4:D:43:MET:HE3	4:D:46:VAL:CG2	2.38	0.47
5:E:123:ASP:HA	5:E:126:ARG:HD3	1.97	0.47
2:B:170:ASN:H	2:B:170:ASN:ND2	2.13	0.47
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.50	0.47
2:B:264:ILE:HG12	2:B:316:TYR:C	2.35	0.47
2:B:361:LYS:O	2:B:365:LYS:HG3	2.14	0.47
3:C:292:VAL:O	3:C:295:LEU:HB3	2.15	0.47
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.97	0.47
5:E:124:LEU:HA	5:E:127:VAL:HG22	1.96	0.47
3:C:78:TRP:CG	4:D:197:GLU:HG2	2.50	0.47
5:E:14:ARG:CG	5:E:14:ARG:NH1	2.74	0.47
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:LEU:O	7:G:41:LEU:HD13	2.15	0.47
1:A:149:VAL:HG13	1:A:150:PHE:N	2.30	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.15	0.47
3:C:139:MET:CE	3:C:269:ILE:HA	2.44	0.47
4:D:102:ARG:HG2	4:D:109:LEU:HB2	1.96	0.47
4:D:165:TYR:O	4:D:168:VAL:CG2	2.63	0.47
2:B:252:LEU:N	2:B:252:LEU:HD23	2.29	0.47
2:B:317:SER:OG	2:B:318:ASP:N	2.47	0.47
3:C:278:ALA:HB1	3:C:295:LEU:HD12	1.96	0.47
3:C:51:LEU:HG	3:C:80:ILE:HD13	1.97	0.47
4:D:227:TRP:O	4:D:228:SER:C	2.52	0.47
4:D:3:LEU:HD22	8:H:59:PHE:CE2	2.49	0.47
1:A:240:GLN:NE2	1:A:242:ARG:HE	2.13	0.47
2:B:281:ALA:O	2:B:285:VAL:HB	2.15	0.47
3:C:103:LEU:HD12	3:C:326:PHE:CE1	2.50	0.47
4:D:75:ASN:CB	4:D:77:ASP:H	2.27	0.47
1:A:40:TRP:HZ3	1:A:377:GLU:OE2	1.97	0.46
2:B:323:GLY:O	2:B:324:PHE:HB3	2.15	0.46
2:B:338:LYS:O	2:B:341:TYR:HB3	2.16	0.46
5:E:16:PRO:O	5:E:18:ASP:N	2.47	0.46
6:F:60:PHE:CD1	7:G:13:LEU:HD22	2.49	0.46
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.51	0.46
1:A:382:GLU:HA	1:A:386:TYR:HD2	1.79	0.46
2:B:259:ALA:O	2:B:260:GLU:C	2.53	0.46
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.96	0.46
5:E:17:PRO:HD3	7:G:24:ARG:HH21	1.80	0.46
1:A:144:SER:O	1:A:146:ARG:N	2.48	0.46
2:B:70:ARG:HD3	2:B:100:SER:CB	2.45	0.46
3:C:330:VAL:HG23	3:C:331:ALA:N	2.30	0.46
3:C:38:LEU:HD11	3:C:95:ILE:HA	1.97	0.46
4:D:54:VAL:HG11	4:D:192:TRP:CH2	2.50	0.46
1:A:27:SER:HA	1:A:199:ALA:O	2.15	0.46
1:A:438:ARG:C	1:A:440:GLY:H	2.19	0.46
2:B:361:LYS:HZ2	2:B:403:ASP:HA	1.79	0.46
2:B:84:LYS:O	2:B:88:GLY:N	2.48	0.46
4:D:221:TYR:CE1	7:G:25:PRO:HG2	2.51	0.46
5:E:129:LYS:HA	5:E:130:PRO:HD3	1.73	0.46
5:E:99:ARG:HB3	5:E:133:VAL:HG11	1.96	0.46
5:E:163:SER:OG	5:E:176:ALA:HB2	2.16	0.46
1:A:48:GLU:OE1	1:A:53:ASN:ND2	2.49	0.46
2:B:379:LEU:O	2:B:382:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:CD1	2:B:57:TYR:N	2.84	0.46
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.80	0.46
1:A:19:LEU:C	1:A:21:ASN:H	2.18	0.46
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.84	0.46
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.45	0.46
2:B:433:THR:HG23	2:B:434:PRO:HD2	1.98	0.46
1:A:268:VAL:CG1	1:A:399:LEU:HB3	2.45	0.46
1:A:362:ARG:NH2	2:B:113:ARG:NH1	2.63	0.46
2:B:258:VAL:HG12	2:B:259:ALA:H	1.80	0.46
2:B:258:VAL:HG13	2:B:322:PHE:N	2.30	0.46
2:B:405:VAL:CG1	2:B:406:ALA:H	2.26	0.46
3:C:373:LEU:HD23	3:C:373:LEU:C	2.36	0.46
5:E:163:SER:HA	5:E:174:GLY:HA3	1.97	0.46
6:F:62:ILE:O	6:F:66:LEU:HG	2.15	0.46
7:G:38:TRP:C	7:G:40:ARG:N	2.69	0.46
8:H:73:LEU:O	8:H:73:LEU:HD23	2.16	0.46
1:A:153:LEU:C	1:A:153:LEU:HD23	2.36	0.46
1:A:444:LEU:C	1:A:445:ARG:O	2.54	0.46
3:C:350:ILE:HD13	3:C:350:ILE:N	2.31	0.46
1:A:156:THR:HG23	1:A:157:ALA:N	2.30	0.46
1:A:24:ARG:HH11	1:A:24:ARG:HG3	1.81	0.46
1:A:253:VAL:HG11	1:A:335:MET:HE2	1.98	0.46
2:B:282:ASN:HB2	2:B:283:PRO:CD	2.46	0.46
5:E:141:HIS:HA	5:E:177:PRO:HD2	1.97	0.46
10:J:4:THR:O	10:J:5:LEU:C	2.53	0.46
1:A:48:GLU:OE2	1:A:54:GLY:N	2.44	0.46
2:B:199:PHE:CA	2:B:204:MET:HE2	2.46	0.46
3:C:301:ILE:HD11	3:C:364:LEU:CD1	2.45	0.46
4:D:132:THR:HG21	4:D:180:SER:HA	1.97	0.46
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.84	0.46
5:E:123:ASP:H	5:E:170:ARG:NH1	2.14	0.46
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.51	0.46
8:H:59:PHE:O	8:H:62:LEU:N	2.49	0.46
8:H:73:LEU:C	8:H:73:LEU:CD2	2.84	0.46
1:A:245:GLU:C	1:A:247:GLY:H	2.18	0.45
2:B:168:TYR:CE2	2:B:172:LEU:HD23	2.50	0.45
2:B:258:VAL:HG11	2:B:321:LEU:HD22	1.98	0.45
2:B:397:THR:HA	2:B:400:GLN:CB	2.46	0.45
4:D:98:PRO:O	4:D:101:ALA:N	2.48	0.45
4:D:132:THR:HA	4:D:179:MET:CE	2.46	0.45
5:E:17:PRO:HG3	7:G:24:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:CG2	1:A:100:LYS:HB3	2.38	0.45
1:A:65:LYS:HD2	1:A:65:LYS:N	2.30	0.45
2:B:137:VAL:CG2	2:B:138:ALA:N	2.78	0.45
2:B:166:ALA:HB1	2:B:242:GLY:C	2.36	0.45
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.35	0.45
4:D:75:ASN:OD1	4:D:79:GLU:HB2	2.16	0.45
5:E:52:LYS:O	5:E:56:THR:HG23	2.17	0.45
1:A:430:GLN:O	1:A:430:GLN:HG2	2.15	0.45
2:B:258:VAL:CG1	2:B:259:ALA:H	2.30	0.45
1:A:192:ALA:N	1:A:193:PRO:HD2	2.31	0.45
1:A:249:PRO:HG2	1:A:250:LEU:HD13	1.98	0.45
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.98	0.45
2:B:130:PRO:HB3	2:B:132:PHE:CE1	2.51	0.45
3:C:137:GLY:H	3:C:140:SER:HB2	1.81	0.45
3:C:327:TRP:HZ2	13:C:384:PEE:H7	1.81	0.45
5:E:12:ASP:N	5:E:20:TYR:CE2	2.84	0.45
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.80	0.45
1:A:405:ARG:CA	1:A:408:ARG:HH21	2.30	0.45
3:C:210:LEU:O	3:C:212:ILE:HG23	2.16	0.45
4:D:164:ILE:O	4:D:179:MET:HG3	2.17	0.45
3:C:40:VAL:HG21	3:C:233:LEU:HD21	1.98	0.45
4:D:28:ARG:O	4:D:31:GLN:HB2	2.17	0.45
7:G:36:ASN:HA	7:G:39:ARG:HB2	1.99	0.45
1:A:306:SER:HB2	9:I:206:UNK:CB	2.47	0.45
1:A:365:LEU:O	1:A:365:LEU:HD22	2.17	0.45
3:C:27:ASN:CB	6:F:69:ASN:HD22	2.29	0.45
1:A:366:VAL:C	1:A:368:HIS:N	2.71	0.45
4:D:181:GLN:CG	8:H:77:LEU:HD22	2.47	0.45
4:D:118:ARG:HD3	4:D:191:ARG:HH12	1.82	0.45
4:D:37:CYS:C	4:D:39:SER:H	2.20	0.45
5:E:121:GLN:OE1	5:E:126:ARG:NH1	2.44	0.45
5:E:78:LEU:HD11	5:E:187:PHE:CE1	2.52	0.45
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.51	0.45
6:F:25:GLY:C	6:F:27:ASN:H	2.21	0.45
1:A:170:PRO:HG2	1:A:173:ASN:HB2	1.97	0.45
1:A:36:THR:HG23	1:A:372:THR:OG1	2.17	0.45
1:A:92:ARG:HH12	1:A:166:SER:HA	1.81	0.45
10:J:33:ARG:O	10:J:37:GLN:HG3	2.17	0.45
1:A:239:SER:O	1:A:421:ALA:HA	2.16	0.45
1:A:391:PRO:O	1:A:392:LEU:C	2.53	0.45
1:A:396:GLU:O	1:A:400:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.45	0.45
2:B:137:VAL:HG23	2:B:138:ALA:N	2.30	0.45
3:C:261:ASN:ND2	3:C:264:VAL:CG2	2.80	0.45
5:E:9:ASN:OD1	5:E:11:SER:HB2	2.17	0.45
5:E:182:VAL:HA	5:E:183:PRO:HD2	1.83	0.45
4:D:231:LYS:HD3	6:F:70:MET:CE	2.47	0.45
6:F:34:ASP:OD2	6:F:90:LEU:HB3	2.17	0.45
2:B:232:LEU:O	2:B:233:SER:HB3	2.16	0.44
3:C:319:ARG:NH1	3:C:374:GLU:HB3	2.32	0.44
4:D:116:ILE:CG2	4:D:190:LEU:HD13	2.47	0.44
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.52	0.44
5:E:69:LEU:O	5:E:72:SER:HB3	2.17	0.44
3:C:27:ASN:CB	6:F:69:ASN:ND2	2.77	0.44
8:H:73:LEU:C	8:H:73:LEU:HD23	2.38	0.44
1:A:410:VAL:O	1:A:413:LYS:N	2.49	0.44
2:B:399:LEU:HA	2:B:402:ILE:CG2	2.43	0.44
2:B:65:THR:O	2:B:69:LEU:HB2	2.17	0.44
3:C:145:THR:O	3:C:149:ASN:HB2	2.18	0.44
3:C:361:THR:HA	3:C:365:ILE:HG22	2.00	0.44
4:D:138:PRO:HB3	8:H:58:LEU:HD22	1.99	0.44
4:D:32:VAL:CG2	4:D:186:VAL:HG22	2.47	0.44
5:E:109:GLU:CD	5:E:166:ASP:HB2	2.38	0.44
5:E:59:VAL:O	5:E:59:VAL:CG1	2.66	0.44
2:B:70:ARG:NE	9:I:107:UNK:CB	2.80	0.44
1:A:365:LEU:CD1	1:A:392:LEU:HD22	2.47	0.44
2:B:24:LEU:HD11	2:B:392:TYR:CD1	2.52	0.44
2:B:59:ASN:O	2:B:61:SER:O	2.35	0.44
2:B:89:ILE:HD11	2:B:96:LEU:HD12	1.99	0.44
3:C:104:TYR:CD2	3:C:316:MET:HB2	2.52	0.44
5:E:121:GLN:NE2	5:E:126:ARG:HG3	2.32	0.44
5:E:55:VAL:O	5:E:59:VAL:HG23	2.17	0.44
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.45	0.44
1:A:114:ALA:CB	1:A:216:PHE:CE1	3.01	0.44
1:A:369:LEU:HD21	1:A:378:ASP:OD2	2.18	0.44
1:A:65:LYS:NZ	9:I:311:UNK:HA	2.32	0.44
2:B:402:ILE:O	2:B:402:ILE:HD13	2.17	0.44
8:H:37:LEU:C	8:H:37:LEU:HD13	2.37	0.44
1:A:105:ASP:O	1:A:106:VAL:C	2.55	0.44
1:A:123:GLU:HG3	1:A:125:SER:OG	2.18	0.44
1:A:349:ILE:HG22	1:A:408:ARG:CD	2.47	0.44
1:A:48:GLU:CD	1:A:54:GLY:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLN:O	2:B:146:ILE:HG12	2.18	0.44
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.99	0.44
3:C:41:CYS:SG	3:C:91:PHE:HA	2.57	0.44
4:D:178:THR:O	4:D:182:VAL:HG12	2.17	0.44
1:A:100:LYS:HG3	2:B:370:MET:HE1	1.99	0.44
1:A:266:ASP:O	1:A:268:VAL:N	2.50	0.44
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.98	0.44
4:D:175:THR:HA	4:D:176:PRO:HD3	1.73	0.44
4:D:57:THR:HG22	4:D:58:GLU:N	2.32	0.44
5:E:171:ILE:HG12	5:E:176:ALA:O	2.18	0.44
6:F:29:TYR:HB2	6:F:31:LEU:CD2	2.48	0.44
7:G:24:ARG:HA	7:G:25:PRO:HD3	1.68	0.44
1:A:114:ALA:HA	1:A:216:PHE:HE1	1.82	0.44
2:B:170:ASN:N	2:B:170:ASN:HD22	2.15	0.44
3:C:161:LEU:O	3:C:164:TRP:HD1	2.00	0.44
4:D:116:ILE:CG2	4:D:117:VAL:H	2.30	0.44
4:D:55:CYS:SG	4:D:56:TYR:HD2	2.40	0.44
8:H:63:HIS:ND1	8:H:63:HIS:O	2.51	0.44
1:A:276:ILE:CD1	1:A:349:ILE:HD11	2.48	0.44
1:A:346:CYS:HB2	1:A:412:SER:N	2.33	0.44
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.18	0.44
1:A:74:ALA:O	1:A:75:LEU:C	2.55	0.44
3:C:125:MET:O	3:C:126:ALA:C	2.57	0.44
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.47	0.44
3:C:327:TRP:NE1	7:G:48:VAL:HG22	2.33	0.44
3:C:359:TYR:HD2	3:C:360:PHE:CE1	2.36	0.44
3:C:92:PHE:O	3:C:95:ILE:HG22	2.18	0.44
4:D:147:LEU:N	4:D:147:LEU:HD22	2.32	0.44
4:D:181:GLN:NE2	4:D:181:GLN:C	2.71	0.44
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.83	0.44
1:A:228:VAL:HG13	1:A:228:VAL:O	2.17	0.44
1:A:281:ASP:O	1:A:284:TYR:CD1	2.71	0.44
1:A:373:THR:HB	1:A:374:PRO:CD	2.47	0.44
1:A:64:PHE:O	1:A:66:GLY:N	2.51	0.44
2:B:332:TYR:O	2:B:336:VAL:HG23	2.18	0.44
5:E:19:ASP:C	5:E:20:TYR:CD1	2.91	0.44
2:B:250:ASP:O	2:B:251:SER:CB	2.66	0.43
2:B:241:GLY:CA	2:B:421:GLN:HE21	2.12	0.43
2:B:424:MET:HG2	2:B:425:ALA:H	1.78	0.43
3:C:329:LEU:O	3:C:332:ASN:HB3	2.18	0.43
3:C:346:HIS:ND1	3:C:347:PRO:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:231:LYS:HD3	6:F:70:MET:HE1	2.00	0.43
5:E:134:ILE:HD12	5:E:185:TYR:CE2	2.53	0.43
5:E:136:ILE:HG12	5:E:181:GLU:O	2.17	0.43
5:E:16:PRO:HG3	5:E:32:ARG:HH11	1.82	0.43
7:G:36:ASN:HA	7:G:39:ARG:CB	2.48	0.43
1:A:284:TYR:HD2	1:A:289:HIS:CE1	2.37	0.43
1:A:349:ILE:CG2	1:A:408:ARG:HG3	2.48	0.43
1:A:40:TRP:HZ3	1:A:377:GLU:CD	2.21	0.43
2:B:150:VAL:CG2	2:B:151:ALA:N	2.81	0.43
2:B:194:PHE:O	2:B:198:HIS:ND1	2.40	0.43
3:C:344:VAL:O	3:C:349:ILE:HD11	2.18	0.43
4:D:28:ARG:O	4:D:31:GLN:N	2.51	0.43
1:A:41:ILE:HD12	1:A:195:MET:SD	2.59	0.43
2:B:150:VAL:HA	2:B:153:GLN:HE21	1.84	0.43
2:B:72:ALA:O	2:B:73:SER:C	2.56	0.43
3:C:139:MET:HE1	3:C:269:ILE:HA	1.99	0.43
6:F:101:ARG:HG3	6:F:104:ARG:HH21	1.82	0.43
1:A:408:ARG:O	1:A:409:GLU:C	2.56	0.43
1:A:410:VAL:O	1:A:413:LYS:HB3	2.18	0.43
2:B:112:LEU:O	2:B:113:ARG:C	2.57	0.43
2:B:24:LEU:CD2	2:B:24:LEU:H	2.29	0.43
3:C:280:ALA:C	3:C:282:LEU:N	2.71	0.43
3:C:329:LEU:O	3:C:330:VAL:C	2.57	0.43
3:C:227:PHE:CE1	4:D:222:MET:HE2	2.54	0.43
2:B:260:GLU:O	2:B:261:SER:CB	2.66	0.43
2:B:405:VAL:CG1	2:B:406:ALA:N	2.81	0.43
4:D:21:LEU:HB3	4:D:26:ILE:HD11	1.99	0.43
4:D:230:LEU:HB3	6:F:70:MET:SD	2.58	0.43
5:E:118:ARG:HH11	5:E:118:ARG:CB	2.31	0.43
1:A:24:ARG:NH1	1:A:24:ARG:HG3	2.33	0.43
2:B:109:VAL:HG13	2:B:119:LEU:CD2	2.49	0.43
2:B:63:LEU:C	2:B:65:THR:H	2.22	0.43
3:C:285:ILE:CG2	3:C:291:GLY:HA2	2.48	0.43
3:C:319:ARG:CZ	3:C:374:GLU:OE1	2.66	0.43
1:A:19:LEU:C	1:A:21:ASN:N	2.69	0.43
2:B:192:HIS:O	2:B:196:GLN:HG3	2.19	0.43
2:B:89:ILE:CD1	2:B:96:LEU:HD12	2.49	0.43
3:C:9:HIS:HA	3:C:10:PRO:HD2	1.90	0.43
4:D:102:ARG:HA	4:D:108:ALA:O	2.18	0.43
4:D:29:GLY:O	4:D:30:PHE:C	2.57	0.43
5:E:29:ASP:C	5:E:31:SER:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:PHE:HA	2:B:204:MET:HE2	2.01	0.43
2:B:360:ALA:O	2:B:361:LYS:C	2.57	0.43
1:A:149:VAL:HG13	1:A:150:PHE:H	1.84	0.43
1:A:153:LEU:HD23	1:A:157:ALA:HB2	2.01	0.43
3:C:103:LEU:HD13	3:C:104:TYR:HD1	1.84	0.43
3:C:55:HIS:HE1	5:E:61:SER:O	2.01	0.43
4:D:10:TYR:CD1	4:D:10:TYR:N	2.87	0.43
3:C:234:THR:OG1	4:D:216:VAL:HG12	2.18	0.43
5:E:118:ARG:NH1	5:E:118:ARG:CB	2.82	0.43
5:E:166:ASP:OD1	5:E:168:SER:N	2.50	0.43
5:E:45:LEU:HD21	10:J:28:ALA:CA	2.49	0.43
3:C:51:LEU:HD11	5:E:61:SER:OG	2.19	0.43
1:A:241:ILE:HG23	1:A:241:ILE:O	2.19	0.43
1:A:245:GLU:C	1:A:247:GLY:N	2.73	0.43
2:B:114:ASP:C	2:B:116:VAL:H	2.22	0.43
2:B:135:TRP:CD1	2:B:135:TRP:N	2.87	0.43
2:B:170:ASN:O	2:B:171:ALA:O	2.36	0.43
2:B:50:PHE:HZ	2:B:379:LEU:HD13	1.84	0.43
3:C:201:LEU:O	3:C:203:GLU:N	2.52	0.43
8:H:72:LYS:O	8:H:73:LEU:C	2.56	0.43
1:A:397:GLU:O	1:A:398:ARG:C	2.57	0.42
1:A:320:PHE:HE2	1:A:415:ILE:HD11	1.83	0.42
1:A:65:LYS:HZ3	9:I:311:UNK:CA	2.32	0.42
1:A:93:GLU:O	1:A:94:HIS:HB2	2.19	0.42
2:B:113:ARG:HG3	2:B:114:ASP:N	2.34	0.42
2:B:353:SER:OG	2:B:355:GLU:HB3	2.19	0.42
4:D:32:VAL:HG21	4:D:186:VAL:HG21	2.01	0.42
5:E:45:LEU:HD22	5:E:45:LEU:HA	1.83	0.42
7:G:26:PHE:HE1	7:G:29:TYR:HB3	1.84	0.42
8:H:59:PHE:O	8:H:60:ASP:C	2.57	0.42
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.19	0.42
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.54	0.42
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.97	0.42
1:A:85:HIS:HB2	1:A:100:LYS:HG2	1.97	0.42
4:D:102:ARG:HH11	4:D:109:LEU:HB2	1.84	0.42
5:E:105:GLU:O	5:E:109:GLU:HG2	2.19	0.42
1:A:159:GLN:NE2	5:E:7:VAL:HG11	2.33	0.42
5:E:17:PRO:CD	7:G:24:ARG:HH21	2.32	0.42
1:A:178:SER:C	1:A:180:ALA:N	2.68	0.42
1:A:15:GLN:O	1:A:26:ALA:HA	2.19	0.42
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:HIS:NE2	2:B:232:LEU:CD2	2.83	0.42
3:C:101:ARG:O	3:C:105:TYR:HD2	2.02	0.42
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.82	0.42
3:C:237:LEU:HD12	3:C:240:PHE:HD2	1.83	0.42
3:C:293:LEU:N	3:C:293:LEU:CD2	2.81	0.42
3:C:104:TYR:OH	3:C:316:MET:HG3	2.19	0.42
3:C:362:ILE:HA	3:C:366:LEU:HB2	2.01	0.42
3:C:92:PHE:HA	3:C:95:ILE:CG2	2.43	0.42
5:E:17:PRO:HA	5:E:20:TYR:HE1	1.83	0.42
2:B:312:PHE:H	2:B:324:PHE:HA	1.84	0.42
2:B:385:GLN:NE2	2:B:392:TYR:HA	2.35	0.42
2:B:405:VAL:O	2:B:406:ALA:CB	2.67	0.42
3:C:145:THR:HG23	3:C:171:VAL:HB	2.00	0.42
4:D:46:VAL:HG12	4:D:47:ALA:N	2.34	0.42
5:E:153:PHE:CE2	5:E:172:ARG:NH1	2.87	0.42
5:E:12:ASP:CA	5:E:20:TYR:OH	2.67	0.42
1:A:339:GLN:HG2	1:A:440:GLY:O	2.20	0.42
1:A:65:LYS:CD	1:A:65:LYS:N	2.83	0.42
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.50	0.42
4:D:55:CYS:O	4:D:56:TYR:CD2	2.72	0.42
2:B:56:ARG:O	2:B:171:ALA:HB1	2.19	0.42
3:C:130:VAL:HG13	3:C:179:PHE:HB3	2.01	0.42
4:D:54:VAL:HG13	4:D:55:CYS:N	2.34	0.42
5:E:86:ASN:HB2	5:E:99:ARG:NE	2.35	0.42
6:F:31:LEU:H	6:F:31:LEU:HD23	1.84	0.42
1:A:274:ASN:ND2	1:A:320:PHE:CZ	2.88	0.42
3:C:268:HIS:CD2	3:C:268:HIS:N	2.87	0.42
6:F:82:LYS:O	6:F:83:TYR:C	2.57	0.42
10:J:20:PHE:CE1	10:J:24:ILE:HD11	2.55	0.42
10:J:5:LEU:O	10:J:6:THR:C	2.57	0.42
2:B:284:HIS:O	2:B:286:LYS:N	2.48	0.42
3:C:2:ALA:HB1	3:C:3:PRO:HD2	2.01	0.42
3:C:43:MET:CE	3:C:43:MET:HA	2.50	0.42
7:G:25:PRO:C	7:G:27:PRO:HD3	2.40	0.42
8:H:72:LYS:HA	8:H:75:ASN:HD21	1.85	0.42
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.40	0.42
1:A:365:LEU:HD13	1:A:392:LEU:HD22	2.02	0.42
1:A:48:GLU:HB3	1:A:53:ASN:HA	2.02	0.42
3:C:98:HIS:HD2	11:C:382:HEM:C1C	2.38	0.42
9:I:107:UNK:HA	9:I:115:UNK:O	2.19	0.42
1:A:282:ARG:HD3	9:I:203:UNK:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD21	1:A:325:VAL:CG1	2.49	0.42
3:C:46:ILE:O	3:C:50:LEU:HB2	2.19	0.42
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.42
4:D:28:ARG:O	4:D:29:GLY:C	2.58	0.42
4:D:218:LEU:HD22	5:E:39:VAL:HG13	2.02	0.42
1:A:244:ARG:NE	7:G:10:VAL:HB	2.35	0.42
1:A:424:GLY:HA2	1:A:425:PRO:HD3	1.73	0.41
2:B:146:ILE:O	2:B:147:ASP:C	2.57	0.41
2:B:275:LEU:O	2:B:279:LEU:HB2	2.19	0.41
4:D:178:THR:O	4:D:179:MET:C	2.57	0.41
3:C:238:THR:HB	4:D:212:MET:HG3	2.01	0.41
1:A:102:LEU:H	1:A:102:LEU:CD1	2.31	0.41
2:B:59:ASN:C	2:B:61:SER:H	2.22	0.41
3:C:9:HIS:HD2	3:C:10:PRO:HG2	1.86	0.41
3:C:112:GLU:CD	3:C:112:GLU:H	2.13	0.41
3:C:250:LEU:O	3:C:250:LEU:HD13	2.20	0.41
4:D:75:ASN:ND2	4:D:81:PHE:HD2	2.19	0.41
5:E:176:ALA:HA	5:E:177:PRO:HD2	1.85	0.41
6:F:52:GLU:O	6:F:53:ASN:C	2.58	0.41
1:A:391:PRO:HG2	1:A:394:GLU:HB2	2.02	0.41
2:B:189:VAL:O	2:B:192:HIS:N	2.53	0.41
2:B:258:VAL:HG13	2:B:322:PHE:O	2.21	0.41
12:C:383:U10:H8	12:C:383:U10:C1M	2.50	0.41
3:C:92:PHE:CA	3:C:95:ILE:HG22	2.43	0.41
4:D:70:VAL:HG21	4:D:89:ASP:OD2	2.20	0.41
5:E:32:ARG:HA	5:E:32:ARG:HD2	1.76	0.41
1:A:145:MET:HA	1:A:148:VAL:HG13	2.00	0.41
2:B:170:ASN:C	2:B:170:ASN:HD22	2.24	0.41
3:C:150:LEU:O	3:C:151:PHE:C	2.59	0.41
3:C:346:HIS:C	3:C:346:HIS:ND1	2.72	0.41
1:A:142:ASP:OD2	5:E:1:SER:HA	2.20	0.41
1:A:189:HIS:HD2	1:A:194:ARG:HH12	1.69	0.41
1:A:28:GLU:O	1:A:200:ALA:HA	2.21	0.41
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.20	0.41
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.73	0.41
1:A:72:GLN:O	1:A:73:ASN:C	2.59	0.41
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.50	0.41
2:B:264:ILE:HG23	2:B:315:SER:O	2.20	0.41
3:C:16:ASN:OD1	3:C:16:ASN:O	2.39	0.41
3:C:285:ILE:HA	3:C:286:PRO:HD3	1.83	0.41
3:C:5:ILE:CG2	3:C:5:ILE:O	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:144:ARG:HG3	4:D:147:LEU:HD23	2.02	0.41
4:D:41:HIS:HB3	4:D:113:LEU:HD13	2.02	0.41
4:D:232:SER:OG	5:E:14:ARG:HG3	2.20	0.41
10:J:25:VAL:O	10:J:28:ALA:N	2.52	0.41
10:J:54:HIS:N	10:J:54:HIS:CD2	2.88	0.41
1:A:250:LEU:N	1:A:250:LEU:CD1	2.83	0.41
2:B:407:ASP:OD1	2:B:408:ALA:N	2.52	0.41
4:D:161:ALA:O	4:D:163:PRO:HD3	2.21	0.41
1:A:410:VAL:O	1:A:411:CYS:C	2.59	0.41
3:C:280:ALA:C	3:C:282:LEU:H	2.24	0.41
1:A:402:VAL:HA	1:A:406:MET:SD	2.61	0.41
1:A:260:PRO:HD3	1:A:414:TYR:CE2	2.55	0.41
2:B:318:ASP:O	2:B:319:SER:HB2	2.20	0.41
2:B:50:PHE:CD1	2:B:50:PHE:N	2.89	0.41
3:C:166:TRP:O	3:C:167:GLY:O	2.39	0.41
3:C:348:PHE:O	3:C:349:ILE:C	2.59	0.41
3:C:348:PHE:O	3:C:350:ILE:N	2.54	0.41
4:D:124:GLU:O	4:D:125:ASP:C	2.59	0.41
2:B:269:ALA:O	2:B:271:ALA:N	2.54	0.41
2:B:374:SER:O	2:B:376:GLU:N	2.54	0.41
4:D:17:PRO:O	4:D:202:LYS:HD3	2.21	0.41
5:E:17:PRO:HD3	7:G:24:ARG:NH2	2.35	0.41
5:E:74:ILE:O	5:E:194:ILE:HA	2.21	0.41
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.21	0.41
1:A:108:LYS:CE	1:A:108:LYS:HA	2.50	0.41
1:A:90:SER:HB3	1:A:95:THR:HG23	2.03	0.41
3:C:151:PHE:HB2	3:C:162:VAL:CG2	2.51	0.41
3:C:156:TYR:O	3:C:158:GLY:N	2.51	0.41
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.86	0.41
3:C:273:TRP:CD2	3:C:274:TYR:N	2.89	0.41
3:C:305:ILE:HB	3:C:306:PRO:HD3	2.02	0.41
5:E:158:CYS:HA	5:E:159:PRO:HD2	1.76	0.41
1:A:264:HIS:HD2	1:A:266:ASP:HB2	1.86	0.41
2:B:254:HIS:O	2:B:426:ALA:HA	2.20	0.41
2:B:414:ALA:O	2:B:418:VAL:HG23	2.20	0.41
3:C:120:LEU:HD13	3:C:120:LEU:HA	1.87	0.41
3:C:164:TRP:O	3:C:165:ALA:C	2.60	0.41
3:C:253:ASP:HA	3:C:254:PRO:HD2	1.90	0.41
3:C:287:ASN:O	3:C:288:LYS:C	2.58	0.41
3:C:325:LEU:HD22	3:C:362:ILE:CG2	2.44	0.41
3:C:366:LEU:O	3:C:367:PHE:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:VAL:O	8:H:73:LEU:HB2	2.21	0.41
1:A:116:ILE:C	1:A:118:GLN:H	2.25	0.40
1:A:261:GLY:O	1:A:262:TRP:C	2.60	0.40
1:A:389:ARG:HD2	1:A:390:ILE:H	1.86	0.40
2:B:160:ILE:HG23	2:B:164:HIS:CE1	2.57	0.40
2:B:24:LEU:O	2:B:24:LEU:HG	2.21	0.40
3:C:305:ILE:HD11	3:C:363:LEU:HD22	2.03	0.40
11:C:381:HEM:O2D	11:C:381:HEM:HHA	2.20	0.40
1:A:53:ASN:ND2	1:A:54:GLY:N	2.67	0.40
2:B:183:ILE:HG22	2:B:184:GLY:N	2.36	0.40
3:C:105:TYR:HA	3:C:315:THR:HG22	2.03	0.40
3:C:37:LEU:O	3:C:41:CYS:HB2	2.21	0.40
5:E:165:TYR:HE2	5:E:179:ASN:HA	1.86	0.40
5:E:89:PHE:O	5:E:95:PRO:HA	2.20	0.40
6:F:64:ARG:O	6:F:68:LEU:HD13	2.21	0.40
1:A:245:GLU:HA	7:G:11:ARG:HA	2.04	0.40
1:A:349:ILE:HG12	1:A:350:SER:N	2.36	0.40
2:B:109:VAL:O	2:B:109:VAL:CG1	2.69	0.40
2:B:199:PHE:O	2:B:204:MET:HE3	2.22	0.40
2:B:273:SER:O	2:B:276:GLN:HB3	2.21	0.40
2:B:382:VAL:HG23	2:B:383:GLY:N	2.36	0.40
2:B:407:ASP:O	2:B:409:ASP:N	2.54	0.40
2:B:92:VAL:HG12	2:B:92:VAL:O	2.21	0.40
2:B:95:LYS:HB2	2:B:110:GLU:HG3	2.01	0.40
3:C:150:LEU:O	3:C:152:SER:N	2.55	0.40
3:C:71:CYS:SG	3:C:81:ARG:HD3	2.62	0.40
4:D:158:ILE:HG22	4:D:159:GLY:N	2.35	0.40
4:D:118:ARG:NH1	4:D:195:GLU:OE1	2.54	0.40
5:E:11:SER:C	5:E:13:TYR:N	2.75	0.40
7:G:38:TRP:C	7:G:40:ARG:H	2.23	0.40
8:H:40:CYS:O	8:H:44:VAL:HG23	2.22	0.40
1:A:178:SER:O	1:A:179:ARG:C	2.58	0.40
1:A:250:LEU:C	1:A:250:LEU:CD2	2.90	0.40
2:B:51:ILE:HG22	2:B:52:LYS:N	2.35	0.40
3:C:101:ARG:O	3:C:101:ARG:HD2	2.21	0.40
4:D:218:LEU:O	4:D:222:MET:HG3	2.21	0.40
4:D:1:SER:C	4:D:3:LEU:H	2.24	0.40
5:E:100:HIS:HD2	5:E:131:GLU:O	2.04	0.40
1:A:235:ARG:NH1	5:E:15:ARG:CZ	2.84	0.40
4:D:141:VAL:HG23	8:H:53:ASP:HB3	2.03	0.40
1:A:182:LEU:N	1:A:182:LEU:HD22	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:LEU:O	3:C:14:MET:HB2	2.22	0.40
3:C:350:ILE:C	3:C:352:GLY:N	2.75	0.40
4:D:164:ILE:HG23	4:D:164:ILE:O	2.22	0.40
4:D:222:MET:HE2	4:D:222:MET:HB3	1.96	0.40
5:E:19:ASP:O	5:E:20:TYR:CG	2.74	0.40
5:E:83:GLU:HA	5:E:100:HIS:CB	2.46	0.40
7:G:29:TYR:O	7:G:34:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/446 (99%)	348 (79%)	73 (17%)	19 (4%)	2	17
2	B	404/422 (96%)	291 (72%)	74 (18%)	39 (10%)	0	3
3	C	377/380 (99%)	299 (79%)	64 (17%)	14 (4%)	3	19
4	D	239/241 (99%)	195 (82%)	31 (13%)	13 (5%)	2	12
5	E	194/196 (99%)	167 (86%)	23 (12%)	4 (2%)	7	33
6	F	98/109 (90%)	83 (85%)	15 (15%)	0	100	100
7	G	76/81 (94%)	61 (80%)	10 (13%)	5 (7%)	1	8
8	H	64/78 (82%)	50 (78%)	14 (22%)	0	100	100
10	J	57/62 (92%)	43 (75%)	12 (21%)	2 (4%)	3	21
All	All	1949/2015 (97%)	1537 (79%)	316 (16%)	96 (5%)	2	14

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	65	LYS
1	A	103	SER
1	A	282	ARG
1	A	291	SER
2	B	113	ARG
2	B	171	ALA
2	B	183	ILE
2	B	228	GLY
2	B	263	ALA
2	B	286	LYS
2	B	330	ALA
2	B	375	SER
2	B	407	ASP
4	D	73	GLY
4	D	198	HIS
4	D	228	SER
4	D	233	ARG
5	E	21	SER
1	A	145	MET
2	B	23	ASP
2	B	109	VAL
2	B	111	CYS
2	B	233	SER
2	B	404	ALA
2	B	431	GLY
3	C	21	ASP
3	C	157	ILE
3	C	167	GLY
3	C	171	VAL
3	C	202	HIS
4	D	8	PRO
4	D	38	SER
4	D	75	ASN
5	E	17	PRO
5	E	106	ILE
7	G	43	ALA
10	J	5	LEU
1	A	71	PRO
1	A	128	GLU
2	B	21	PRO
2	B	63	LEU
2	B	261	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	270	ASN
2	B	317	SER
2	B	345	LYS
2	B	349	GLN
2	B	354	ASN
2	B	406	ALA
2	B	408	ALA
2	B	420	ARG
3	C	63	ALA
3	C	346	HIS
3	C	349	ILE
4	D	168	VAL
10	J	61	ASN
1	A	72	GLN
1	A	281	ASP
1	A	382	GLU
1	A	396	GLU
1	A	408	ARG
2	B	201	SER
2	B	269	ALA
2	B	361	LYS
2	B	372	VAL
3	C	60	THR
3	C	287	ASN
4	D	9	SER
4	D	67	GLU
4	D	176	PRO
5	E	13	TYR
1	A	405	ARG
2	B	19	PRO
2	B	20	HIS
2	B	260	GLU
2	B	262	ALA
2	B	331	ALA
3	C	47	LEU
7	G	25	PRO
7	G	50	PRO
1	A	56	GLY
1	A	113	LEU
1	A	267	LEU
2	B	62	ASN
2	B	232	LEU

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Mol	Chain	Res	Type
3	C	3	PRO
3	C	36	SER
7	G	74	PRO
1	A	127	ILE
1	A	286	GLY
2	B	64	GLY
3	C	5	ILE
4	D	133	GLY
7	G	33	GLY
4	D	98	PRO
2	B	305	ASN

### 5.3.2 Protein sidechains [i](#)

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	359/376 (96%)	339 (94%)	20 (6%)	21	53
2	B	307/336 (91%)	286 (93%)	21 (7%)	16	46
3	C	326/329 (99%)	308 (94%)	18 (6%)	21	54
4	D	201/207 (97%)	190 (94%)	11 (6%)	21	54
5	E	165/169 (98%)	156 (94%)	9 (6%)	21	54
6	F	90/98 (92%)	85 (94%)	5 (6%)	21	53
7	G	60/72 (83%)	54 (90%)	6 (10%)	7	28
8	H	51/74 (69%)	49 (96%)	2 (4%)	32	64
10	J	41/52 (79%)	41 (100%)	0	100	100
All	All	1600/1713 (93%)	1508 (94%)	92 (6%)	20	52

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	69	ASN
1	A	100	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	102	LEU
1	A	148	VAL
1	A	168	GLU
1	A	250	LEU
1	A	279	HIS
1	A	316	GLU
1	A	361	LEU
1	A	365	LEU
1	A	368	HIS
1	A	382	GLU
1	A	384	LEU
1	A	388	ARG
1	A	395	TRP
1	A	409	GLU
1	A	431	LEU
1	A	438	ARG
1	A	443	TRP
2	B	56	ARG
2	B	57	TYR
2	B	62	ASN
2	B	85	ILE
2	B	112	LEU
2	B	135	TRP
2	B	170	ASN
2	B	181	TYR
2	B	193	ASP
2	B	221	GLU
2	B	225	ASN
2	B	247	GLN
2	B	248	ASN
2	B	252	LEU
2	B	307	PHE
2	B	325	TYR
2	B	351	ASN
2	B	378	PHE
2	B	402	ILE
2	B	434	PRO
2	B	437	ASP
3	C	4	ASN
3	C	40	VAL
3	C	47	LEU
3	C	91	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	104	TYR
3	C	113	THR
3	C	124	LEU
3	C	136	TRP
3	C	145	THR
3	C	164	TRP
3	C	166	TRP
3	C	175	THR
3	C	217	ASP
3	C	287	ASN
3	C	323	GLN
3	C	325	LEU
3	C	332	ASN
3	C	367	PHE
4	D	24	THR
4	D	32	VAL
4	D	36	VAL
4	D	82	MET
4	D	89	ASP
4	D	136	GLU
4	D	156	GLN
4	D	163	PRO
4	D	181	GLN
4	D	192	TRP
4	D	212	MET
5	E	14	ARG
5	E	17	PRO
5	E	19	ASP
5	E	62	MET
5	E	71	MET
5	E	78	LEU
5	E	87	MET
5	E	113	GLU
5	E	188	THR
6	F	12	TRP
6	F	31	LEU
6	F	37	ILE
6	F	59	MET
6	F	70	MET
7	G	4	PHE
7	G	27	PRO
7	G	28	HIS

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Mol	Chain	Res	Type
7	G	29	TYR
7	G	41	LEU
7	G	77	TYR
8	H	41	ASP
8	H	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	118	GLN
1	A	141	ASN
1	A	151	ASN
1	A	165	GLN
1	A	274	ASN
1	A	289	HIS
1	A	339	GLN
1	A	341	GLN
2	B	22	GLN
2	B	153	GLN
2	B	170	ASN
2	B	225	ASN
2	B	248	ASN
2	B	282	ASN
2	B	343	GLN
2	B	351	ASN
2	B	356	ASN
2	B	421	GLN
2	B	429	ASN
3	C	4	ASN
3	C	9	HIS
3	C	55	HIS
3	C	73	ASN
3	C	82	ASN
3	C	261	ASN
3	C	268	HIS
3	C	287	ASN
3	C	313	GLN
3	C	323	GLN
3	C	342	GLN

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Mol	Chain	Res	Type
4	D	35	GLN
4	D	75	ASN
4	D	156	GLN
4	D	181	GLN
5	E	86	ASN
5	E	122	HIS
5	E	164	HIS
6	F	69	ASN
7	G	23	GLN
7	G	64	GLN
8	H	75	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
12	U10	C	383	-	29,29,63	2.31	9 (31%)	35,38,79	1.77	10 (28%)
15	FES	E	197	5	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	HEM	D	243	4	27,50,50	2.18	10 (37%)	17,82,82	2.11	6 (35%)
13	PEE	C	384	-	48,48,50	2.31	9 (18%)	51,53,55	4.28	18 (35%)
11	HEM	C	381	3	27,50,50	1.77	8 (29%)	17,82,82	2.43	6 (35%)
13	PEE	E	198	-	48,48,50	2.27	9 (18%)	51,53,55	4.31	17 (33%)
14	BOG	D	242	-	20,20,20	0.75	0	25,25,25	0.93	1 (4%)
11	HEM	C	382	3	27,50,50	1.88	4 (14%)	17,82,82	2.69	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
12	U10	C	383	-	-	8/23/47/87	0/1/1/1
15	FES	E	197	5	-	-	0/1/1/1
11	HEM	D	243	4	-	1/6/54/54	-
13	PEE	C	384	-	1/1/4/4	23/52/52/54	-
11	HEM	C	381	3	-	0/6/54/54	-
13	PEE	E	198	-	1/1/4/4	28/52/52/54	-
14	BOG	D	242	-	-	5/11/31/31	0/1/1/1
11	HEM	C	382	3	-	1/6/54/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	198	PEE	O5-C30	11.49	1.56	1.22
13	C	384	PEE	O5-C30	11.21	1.55	1.22
12	C	383	U10	C6-C1	7.48	1.48	1.35
11	D	243	HEM	C3C-C2C	-5.57	1.32	1.40
12	C	383	U10	C7-C6	5.54	1.60	1.51
11	D	243	HEM	C3B-C2B	-5.08	1.33	1.40
13	E	198	PEE	O2-C10	5.02	1.48	1.34
11	C	381	HEM	C3B-CAB	-4.94	1.37	1.47
11	C	382	HEM	C3C-C2C	-4.60	1.34	1.40
13	C	384	PEE	O2-C10	4.43	1.46	1.34
11	C	382	HEM	C1A-CHA	-4.11	1.29	1.41
13	C	384	PEE	C11-C10	3.93	1.62	1.50
11	C	382	HEM	C3C-CAC	-3.90	1.39	1.47
11	C	382	HEM	C3B-CAB	-3.58	1.40	1.47
12	C	383	U10	C18-C19	3.51	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	PEE	C1-C2	3.49	1.61	1.50
13	E	198	PEE	C11-C10	3.45	1.60	1.50
11	D	243	HEM	CBB-CAB	3.36	1.51	1.29
13	E	198	PEE	C22-C21	-3.21	1.33	1.51
11	D	243	HEM	CBC-CAC	3.20	1.50	1.29
11	C	381	HEM	C3C-CAC	-3.17	1.41	1.47
13	E	198	PEE	C42-C41	-3.12	1.34	1.51
12	C	383	U10	C13-C14	3.06	1.40	1.33
13	E	198	PEE	C31-C30	-3.05	1.41	1.50
13	C	384	PEE	C22-C21	-3.03	1.34	1.51
13	C	384	PEE	C42-C41	-2.97	1.34	1.51
13	C	384	PEE	C31-C30	-2.82	1.42	1.50
13	C	384	PEE	P-O3P	2.74	1.70	1.59
11	D	243	HEM	C4A-CHB	-2.72	1.33	1.41
12	C	383	U10	C3-C2	-2.63	1.41	1.48
11	D	243	HEM	C1D-CHD	-2.58	1.33	1.41
12	C	383	U10	C8-C9	2.44	1.38	1.33
11	C	381	HEM	C3C-C2C	-2.40	1.37	1.40
11	C	381	HEM	C1D-CHD	-2.37	1.34	1.41
11	C	381	HEM	C1A-CHA	-2.33	1.34	1.41
11	C	381	HEM	C4B-CHC	-2.32	1.34	1.41
11	D	243	HEM	C1A-CHA	-2.29	1.34	1.41
11	C	381	HEM	C1D-ND	2.28	1.40	1.36
11	D	243	HEM	CAA-C2A	-2.25	1.48	1.52
13	C	384	PEE	O2-C2	-2.22	1.41	1.46
13	E	198	PEE	C1-C2	2.20	1.57	1.50
12	C	383	U10	O4-C4M	-2.18	1.40	1.45
12	C	383	U10	C7-C8	-2.18	1.47	1.50
11	D	243	HEM	C4B-CHC	-2.14	1.35	1.41
11	D	243	HEM	C3B-CAB	2.14	1.52	1.47
12	C	383	U10	C16-C14	2.09	1.55	1.51
11	C	381	HEM	C1B-C2B	2.09	1.47	1.42
13	E	198	PEE	C5-C4	2.04	1.58	1.50
13	E	198	PEE	O2-C2	-2.00	1.41	1.46

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	198	PEE	O4-C10-C11	-18.64	51.02	123.73
13	C	384	PEE	O4-C10-C11	-18.62	51.11	123.73
13	E	198	PEE	O3-C30-C31	12.77	151.98	111.91
13	C	384	PEE	O3-C30-C31	12.50	151.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	384	PEE	O3-C30-O5	-11.37	94.89	123.59
13	E	198	PEE	O3-C30-O5	-11.22	95.27	123.59
13	E	198	PEE	O2-C2-C3	7.86	136.86	108.40
13	C	384	PEE	O2-C2-C3	7.75	136.47	108.40
13	E	198	PEE	O2-C10-C11	7.17	126.96	111.50
11	C	382	HEM	CBD-CAD-C3D	6.82	125.04	112.48
13	E	198	PEE	C12-C11-C10	-6.47	90.09	113.62
13	C	384	PEE	O2-C10-C11	6.45	125.40	111.50
13	C	384	PEE	O2-C10-O4	-6.45	108.13	123.70
11	C	382	HEM	CBA-CAA-C2A	6.29	124.09	112.49
13	E	198	PEE	O2-C10-O4	-6.21	108.69	123.70
13	C	384	PEE	C12-C11-C10	-5.97	91.91	113.62
11	C	381	HEM	C4C-C3C-C2C	-5.54	103.03	106.90
13	C	384	PEE	O3-C3-C2	5.03	123.07	108.43
11	C	381	HEM	CBA-CAA-C2A	4.67	121.10	112.49
13	E	198	PEE	O3-C3-C2	4.64	121.94	108.43
12	C	383	U10	C1-C6-C5	-4.35	115.49	119.58
11	D	243	HEM	C4A-C3A-C2A	-3.87	104.30	107.00
12	C	383	U10	C10-C9-C8	-3.86	113.79	123.68
11	C	381	HEM	C1D-C2D-C3D	-3.84	104.33	107.00
11	D	243	HEM	CBD-CAD-C3D	3.66	119.21	112.48
11	D	243	HEM	C3B-C4B-NB	3.61	113.88	109.21
14	D	242	BOG	C1'-O1-C1	3.59	119.79	113.84
11	C	381	HEM	C3B-C4B-NB	3.56	113.81	109.21
13	E	198	PEE	C33-C32-C31	3.16	124.56	113.19
13	C	384	PEE	C42-C41-C40	3.15	130.40	114.42
13	E	198	PEE	C22-C21-C20	3.12	130.27	114.42
11	C	381	HEM	CAD-C3D-C2D	-3.09	118.36	127.25
13	E	198	PEE	C42-C41-C40	3.07	130.01	114.42
11	D	243	HEM	CMA-C3A-C4A	3.06	133.16	128.46
13	E	198	PEE	C34-C33-C32	-3.04	99.00	114.42
13	C	384	PEE	C14-C13-C12	-3.03	99.07	114.42
13	C	384	PEE	C22-C21-C20	2.95	129.43	114.42
13	C	384	PEE	C33-C32-C31	2.95	123.81	113.19
12	C	383	U10	C15-C14-C13	-2.89	116.26	123.68
13	C	384	PEE	C34-C33-C32	-2.84	99.99	114.42
13	E	198	PEE	O5-C30-C31	-2.82	112.74	123.73
12	C	383	U10	C15-C14-C16	2.74	119.89	115.27
12	C	383	U10	C11-C9-C8	2.71	126.61	121.12
11	C	382	HEM	C1D-C2D-C3D	-2.68	105.13	107.00
13	E	198	PEE	C14-C13-C12	-2.67	100.87	114.42
12	C	383	U10	C10-C9-C11	2.57	119.60	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	384	PEE	O5-C30-C31	-2.52	113.88	123.73
11	C	382	HEM	CMB-C2B-C3B	2.46	129.29	124.68
11	D	243	HEM	CBA-CAA-C2A	2.44	116.99	112.49
11	C	382	HEM	C4C-C3C-C2C	-2.42	105.21	106.90
13	C	384	PEE	O2-C2-C1	2.35	116.92	108.40
11	C	381	HEM	C3C-C4C-NC	2.35	115.38	110.94
12	C	383	U10	O2-C2-C3	-2.32	116.00	120.93
11	C	382	HEM	C4A-C3A-C2A	-2.30	105.39	107.00
13	E	198	PEE	O2-C2-C1	2.30	116.73	108.40
11	C	382	HEM	C3B-C4B-NB	2.28	112.16	109.21
13	E	198	PEE	C3-C2-C1	-2.28	106.40	111.79
12	C	383	U10	C20-C19-C18	-2.27	117.86	123.68
13	C	384	PEE	C3-C2-C1	-2.21	106.57	111.79
12	C	383	U10	O5-C5-C4	-2.18	116.30	120.93
13	C	384	PEE	C3-O3-C30	-2.17	109.09	117.12
12	C	383	U10	C7-C8-C9	2.15	130.37	126.79
13	C	384	PEE	C16-C15-C14	-2.11	103.71	114.42
13	E	198	PEE	C36-C35-C34	-2.09	103.81	114.42
11	D	243	HEM	CAD-C3D-C2D	-2.01	121.48	127.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	384	PEE	C2
13	E	198	PEE	C2

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	383	U10	C1-C6-C7-C8
12	C	383	U10	C5-C6-C7-C8
12	C	383	U10	C14-C16-C17-C18
11	D	243	HEM	C2D-C3D-CAD-CBD
13	C	384	PEE	O4-C10-O2-C2
13	E	198	PEE	O4-C10-O2-C2
13	E	198	PEE	C31-C30-O3-C3
13	E	198	PEE	O5-C30-O3-C3
11	C	382	HEM	C4D-C3D-CAD-CBD
13	C	384	PEE	O5-C30-O3-C3
12	C	383	U10	C12-C11-C9-C10
13	C	384	PEE	C22-C23-C24-C25
13	E	198	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
13	C	384	PEE	C31-C30-O3-C3
13	E	198	PEE	C30-C31-C32-C33
14	D	242	BOG	C2-C1-O1-C1'
12	C	383	U10	C12-C11-C9-C8
14	D	242	BOG	O5-C1-O1-C1'
13	E	198	PEE	C35-C36-C37-C38
13	E	198	PEE	C39-C40-C41-C42
13	E	198	PEE	C16-C17-C18-C19
13	C	384	PEE	C3-C2-O2-C10
13	E	198	PEE	C12-C13-C14-C15
13	C	384	PEE	C37-C38-C39-C40
13	C	384	PEE	C20-C21-C22-C23
13	E	198	PEE	C14-C15-C16-C17
13	E	198	PEE	C19-C20-C21-C22
13	E	198	PEE	C33-C34-C35-C36
13	C	384	PEE	C13-C14-C15-C16
14	D	242	BOG	C2'-C3'-C4'-C5'
13	E	198	PEE	C31-C32-C33-C34
13	E	198	PEE	C21-C22-C23-C24
13	C	384	PEE	C17-C18-C19-C20
13	C	384	PEE	C38-C39-C40-C41
13	E	198	PEE	C11-C12-C13-C14
14	D	242	BOG	C3'-C4'-C5'-C6'
13	C	384	PEE	C12-C13-C14-C15
13	E	198	PEE	C17-C18-C19-C20
13	E	198	PEE	C18-C19-C20-C21
13	C	384	PEE	C40-C41-C42-C43
13	E	198	PEE	C1-C2-C3-O3
13	E	198	PEE	C37-C38-C39-C40
13	C	384	PEE	C14-C15-C16-C17
13	E	198	PEE	C41-C42-C43-C44
13	C	384	PEE	C39-C40-C41-C42
13	E	198	PEE	O3P-C1-C2-O2
13	C	384	PEE	C23-C24-C25-C26
12	C	383	U10	C9-C11-C12-C13
13	C	384	PEE	C41-C42-C43-C44
13	C	384	PEE	O3P-C1-C2-O2
13	C	384	PEE	O2-C2-C3-O3
13	C	384	PEE	C4-O4P-P-O3P
13	E	198	PEE	C4-O4P-P-O3P
13	E	198	PEE	C40-C41-C42-C43
13	E	198	PEE	O4P-C4-C5-N

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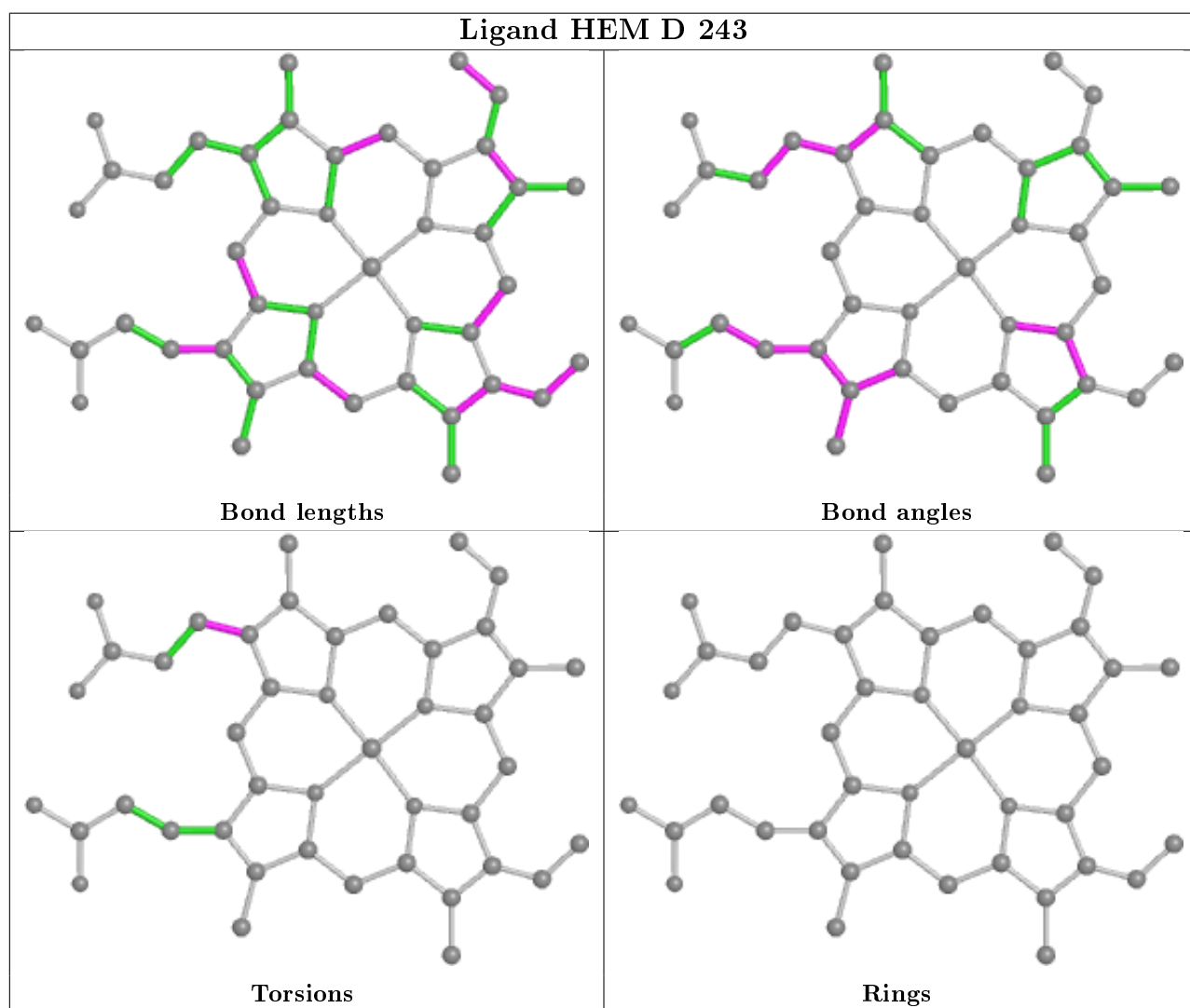
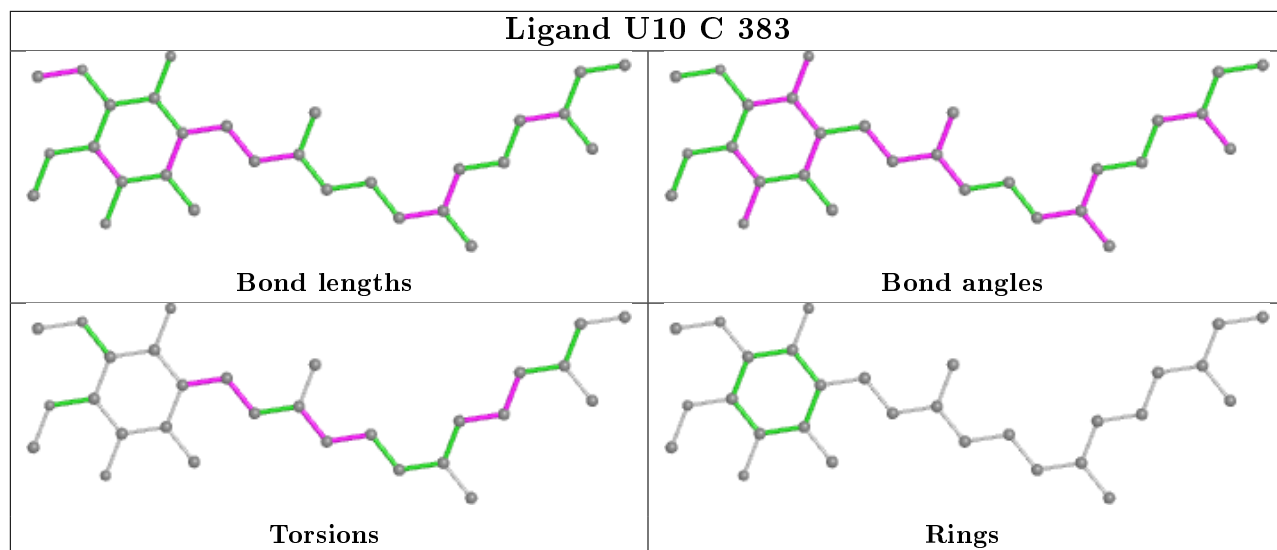
Mol	Chain	Res	Type	Atoms
13	E	198	PEE	C20-C21-C22-C23
13	E	198	PEE	C42-C43-C44-C45
14	D	242	BOG	C4'-C5'-C6'-C7'
13	C	384	PEE	C18-C19-C20-C21
13	C	384	PEE	O3P-C1-C2-C3
12	C	383	U10	C16-C17-C18-C19
12	C	383	U10	C6-C7-C8-C9
13	C	384	PEE	C4-O4P-P-O1P
13	C	384	PEE	C5-C4-O4P-P
13	E	198	PEE	C3-C2-O2-C10
13	E	198	PEE	O3-C30-C31-C32

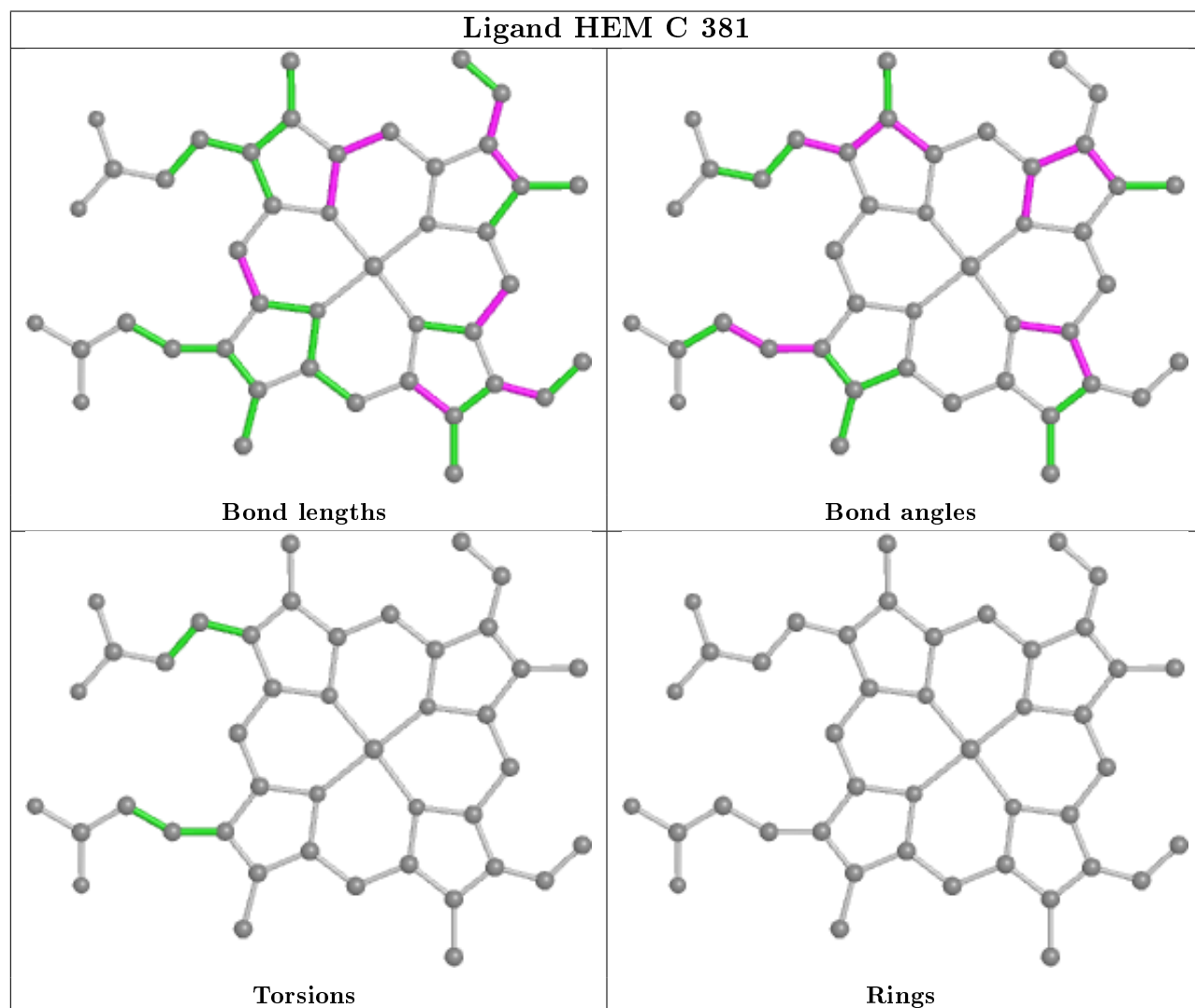
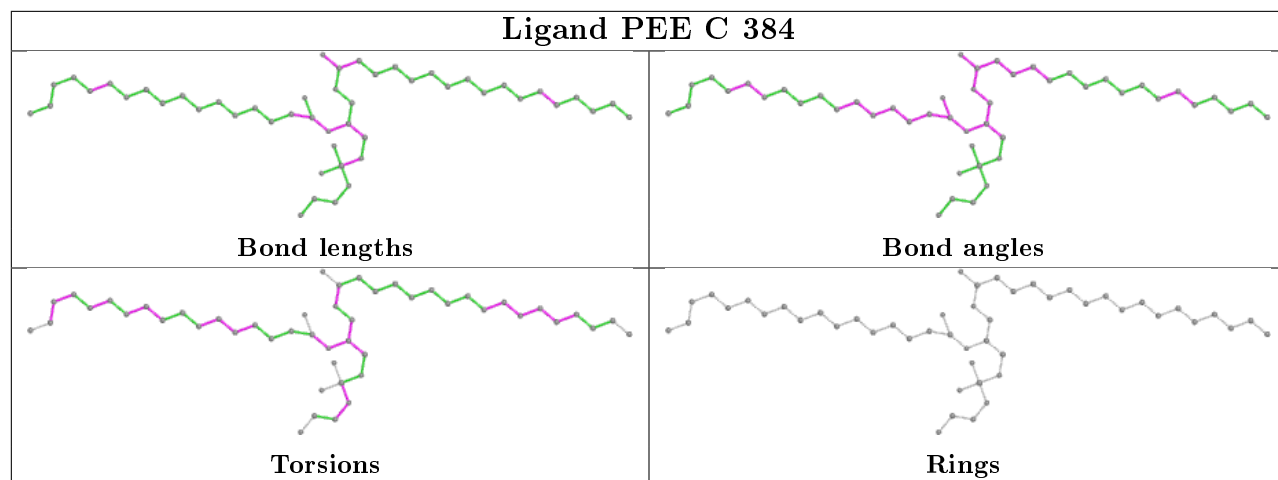
There are no ring outliers.

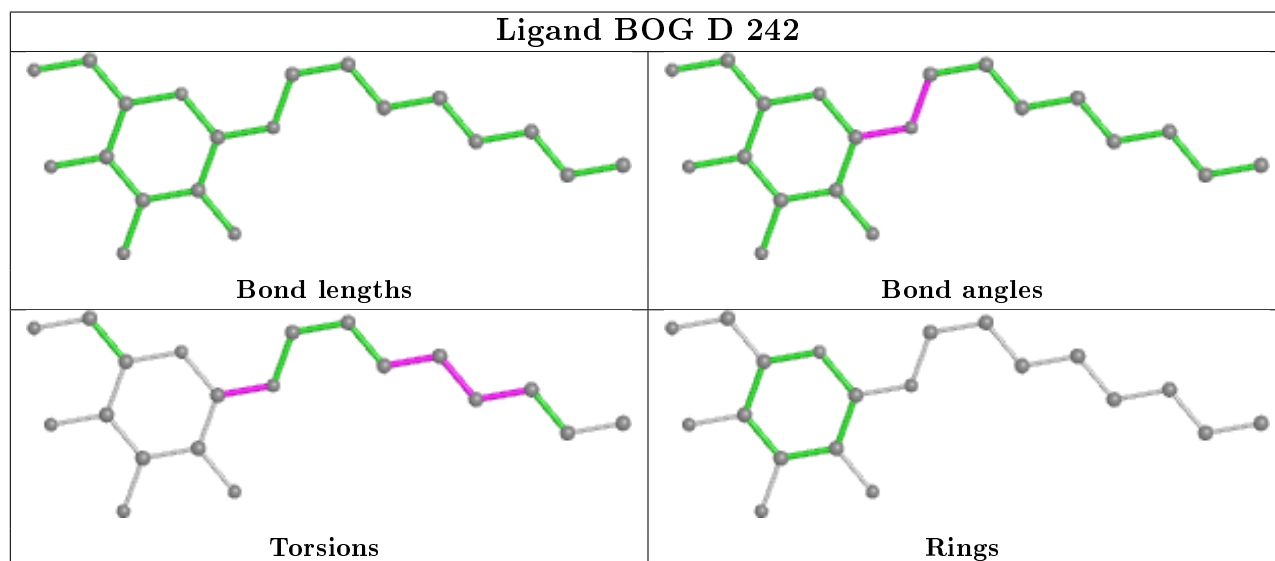
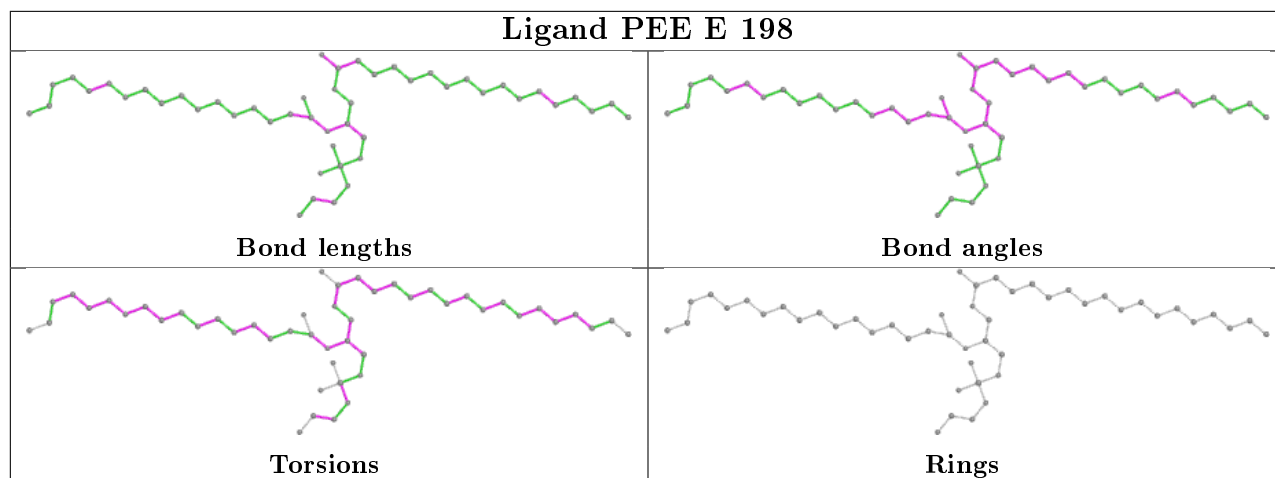
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	383	U10	4	0
15	E	197	FES	1	0
13	C	384	PEE	2	0
11	C	381	HEM	5	0
13	E	198	PEE	1	0
14	D	242	BOG	2	0
11	C	382	HEM	7	0

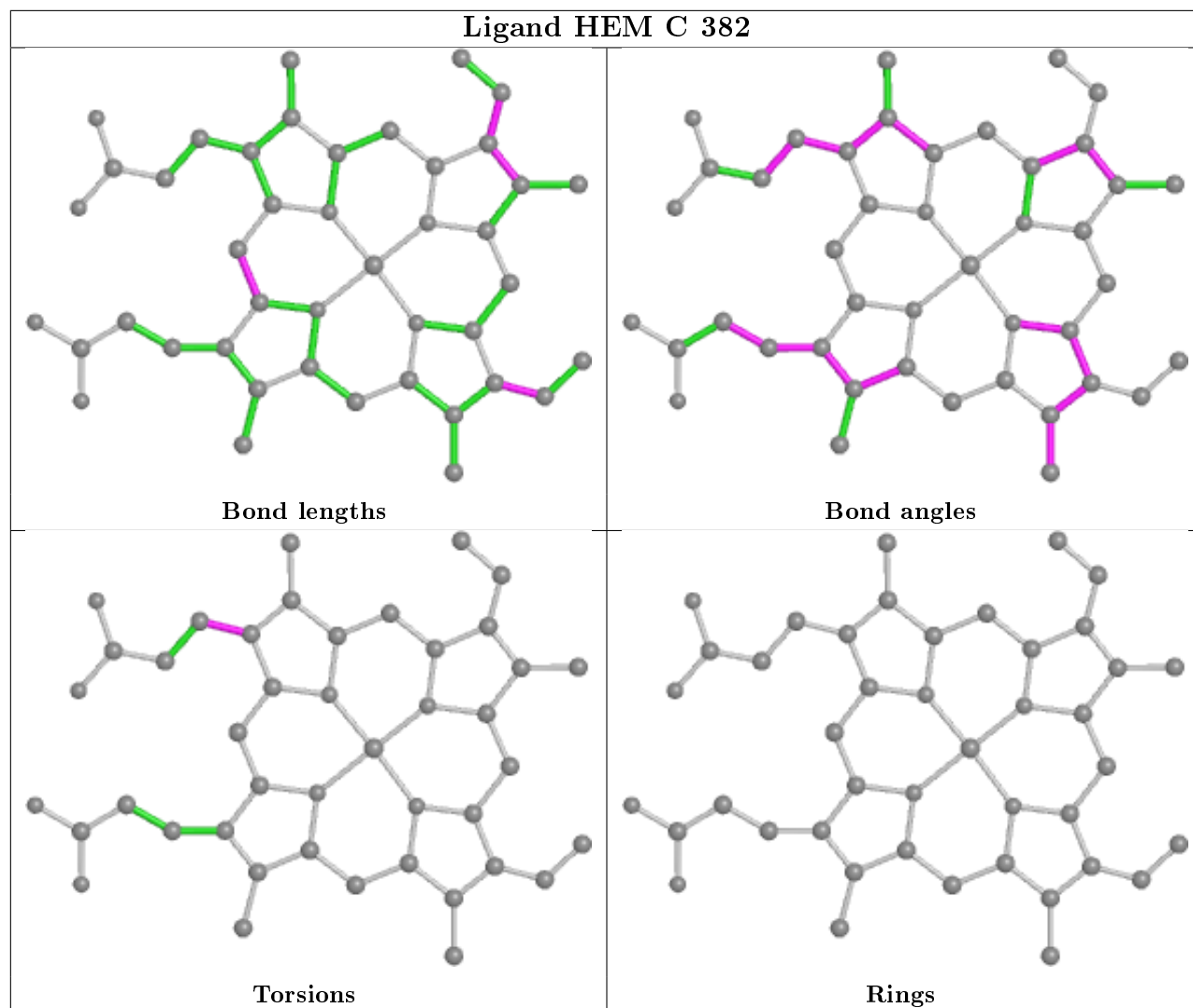
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	121:UNK	C	202:UNK	N	29.43

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	442/446 (99%)	-0.10	7 (1%) 72 59	47, 84, 100, 100	0
2	B	406/422 (96%)	0.09	16 (3%) 39 24	60, 93, 100, 100	0
3	C	379/380 (99%)	-0.24	8 (2%) 63 49	33, 64, 96, 100	0
4	D	241/241 (100%)	-0.03	7 (2%) 51 35	50, 76, 99, 100	0
5	E	196/196 (100%)	0.90	46 (23%) 0 0	54, 100, 100, 100	0
6	F	100/109 (91%)	-0.10	2 (2%) 65 50	50, 73, 98, 100	0
7	G	78/81 (96%)	0.09	2 (2%) 56 40	51, 85, 100, 100	0
8	H	66/78 (84%)	-0.19	1 (1%) 73 61	76, 95, 99, 100	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	-0.05	2 (3%) 45 28	66, 80, 99, 100	0
All	All	1967/2048 (96%)	0.03	91 (4%) 32 18	33, 83, 100, 100	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	114	VAL	6.6
5	E	163	SER	6.3
2	B	18	PRO	5.8
5	E	174	GLY	5.2
10	J	62	LYS	4.6
10	J	61	ASN	4.5
5	E	115	SER	4.4
5	E	84	GLY	4.4
2	B	19	PRO	4.3
5	E	176	ALA	4.1
5	E	120	PRO	4.0
3	C	8	SER	3.9
5	E	173	LYS	3.9
5	E	82	PRO	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	E	85	LYS	3.8
5	E	117	LEU	3.8
5	E	165	TYR	3.7
5	E	104	LYS	3.7
5	E	162	GLY	3.6
5	E	175	PRO	3.6
1	A	223	TYR	3.6
5	E	124	LEU	3.4
5	E	157	TYR	3.3
5	E	113	GLU	3.3
5	E	164	HIS	3.3
5	E	190	ASP	3.2
1	A	38	GLY	3.2
5	E	158	CYS	3.2
2	B	419	SER	3.1
1	A	220	PRO	3.1
5	E	83	GLU	3.1
3	C	10	PRO	3.1
2	B	397	THR	3.1
2	B	20	HIS	3.1
3	C	4	ASN	3.1
2	B	393	ASN	3.0
3	C	156	TYR	3.0
5	E	119	ASP	3.0
5	E	171	ILE	2.9
4	D	78	GLY	2.9
5	E	102	THR	2.9
5	E	194	ILE	2.8
5	E	188	THR	2.8
2	B	73	SER	2.8
5	E	152	ASP	2.8
5	E	177	PRO	2.8
5	E	108	GLN	2.7
5	E	122	HIS	2.7
5	E	187	PHE	2.7
4	D	73	GLY	2.7
4	D	187	CYS	2.6
2	B	230	LEU	2.6
2	B	232	LEU	2.6
2	B	236	LYS	2.5
5	E	118	ARG	2.5
1	A	226	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	2	ALA	2.5
6	F	11	ARG	2.4
1	A	69	ASN	2.4
5	E	103	LYS	2.4
5	E	116	GLN	2.4
1	A	443	TRP	2.4
5	E	149	ASN	2.4
4	D	74	PRO	2.3
4	D	80	MET	2.3
5	E	107	ASP	2.3
3	C	157	ILE	2.3
3	C	3	PRO	2.3
2	B	106	ALA	2.3
5	E	191	ASP	2.3
2	B	323	GLY	2.2
2	B	72	ALA	2.2
5	E	79	SER	2.2
5	E	132	TRP	2.2
4	D	79	GLU	2.2
8	H	40	CYS	2.2
3	C	5	ILE	2.2
5	E	147	ILE	2.2
2	B	394	PRO	2.2
7	G	26	PHE	2.2
7	G	29	TYR	2.2
2	B	401	GLN	2.2
1	A	42	ASP	2.2
5	E	112	VAL	2.1
4	D	171	PHE	2.1
5	E	75	GLU	2.1
2	B	224	LEU	2.1
5	E	110	ALA	2.1
5	E	109	GLU	2.0
5	E	151	GLY	2.0
6	F	102	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no monosaccharides in this entry.

### 6.4 Ligands

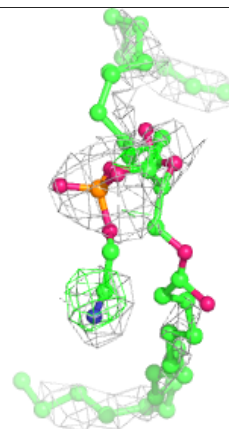
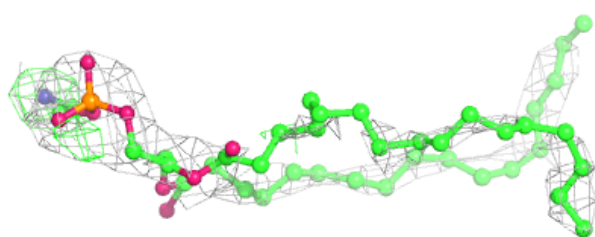
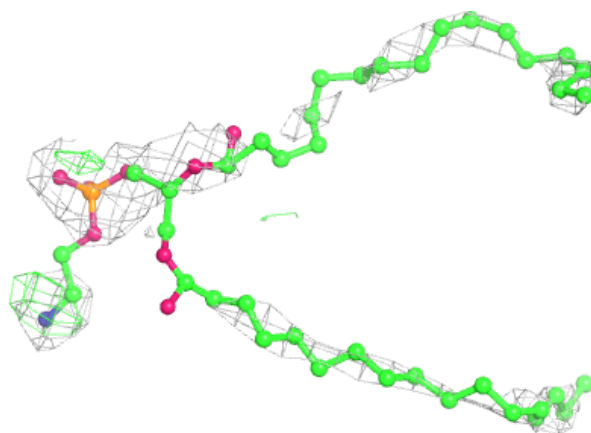
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	PEE	E	198	49/51	0.65	0.49	24,45,64,65	49
12	U10	C	383	29/63	0.77	0.39	77,83,100,100	29
13	PEE	C	384	49/51	0.82	0.40	20,39,54,55	49
14	BOG	D	242	20/20	0.90	0.25	37,59,70,72	20
15	FES	E	197	4/4	0.97	0.28	100,100,100,100	0
11	HEM	D	243	43/43	0.98	0.18	46,58,69,74	0
11	HEM	C	381	43/43	0.98	0.23	43,51,59,62	0
11	HEM	C	382	43/43	0.98	0.21	43,46,59,62	0

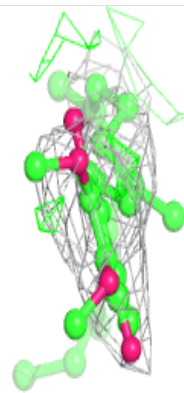
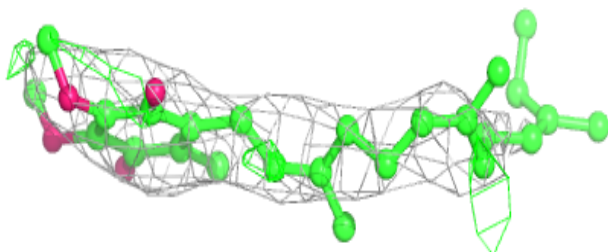
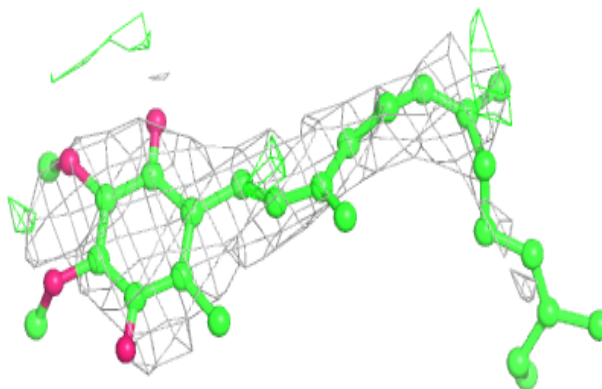
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PEE E 198:**

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

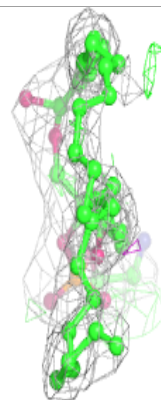
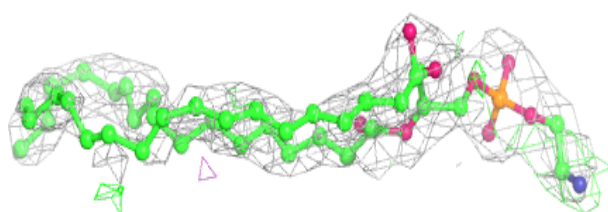
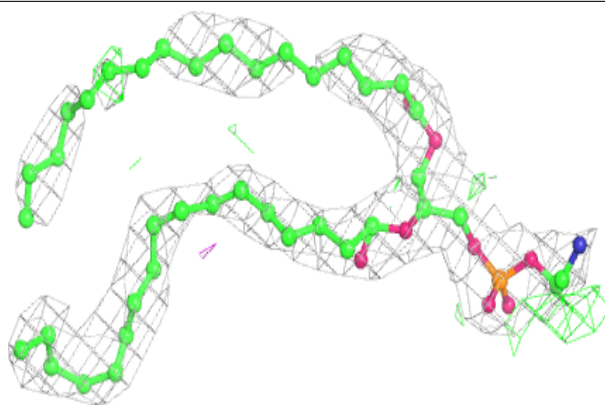
**Electron density around U10 C 383:**

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

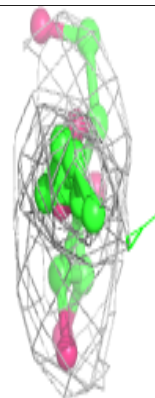
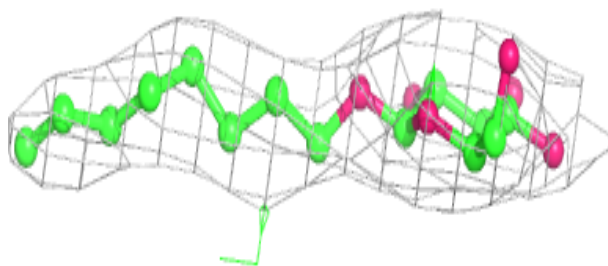
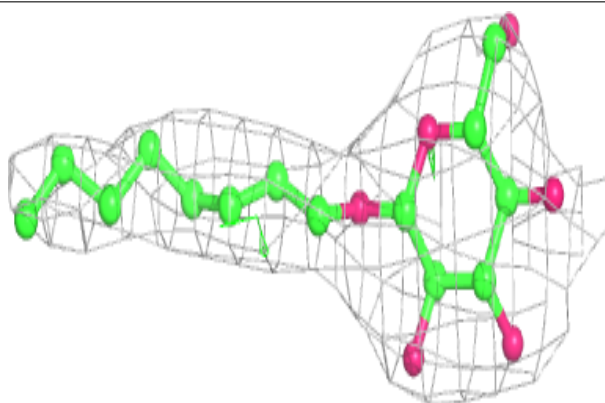


**Electron density around PEE C 384:**

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

**Electron density around BOG D 242:**

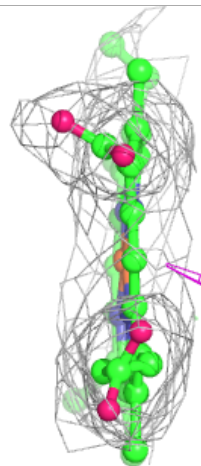
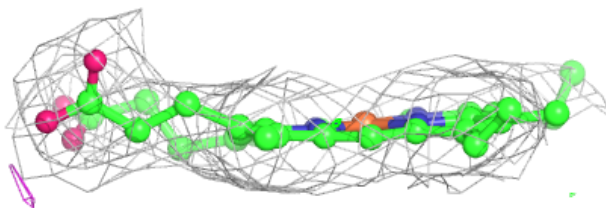
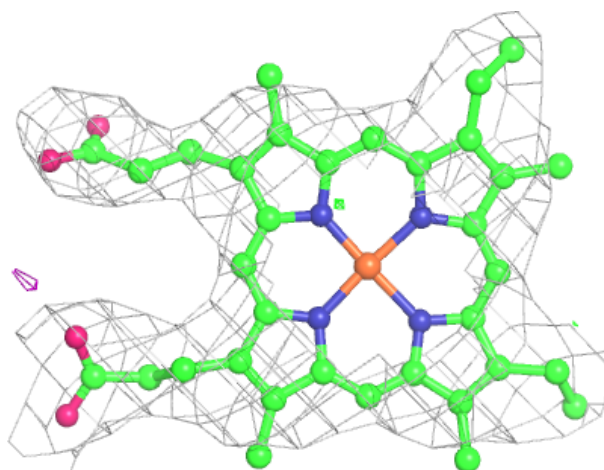
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





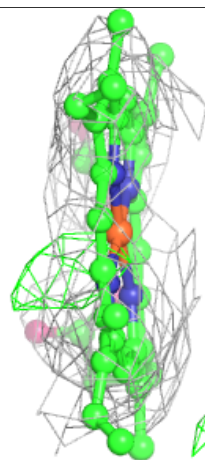
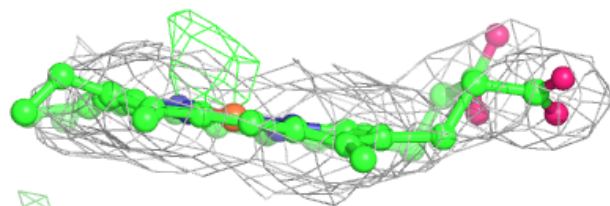
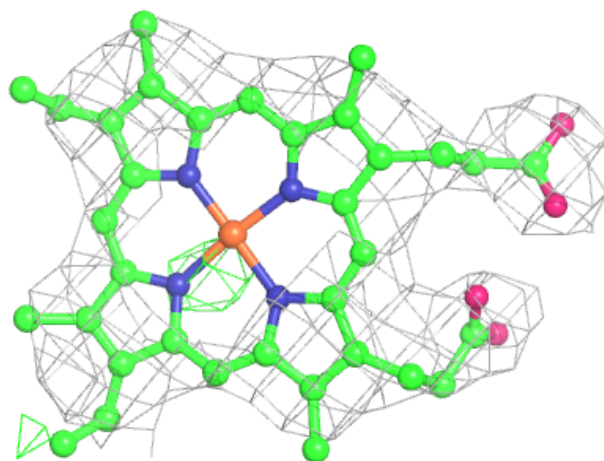
**Electron density around HEM D 243:**

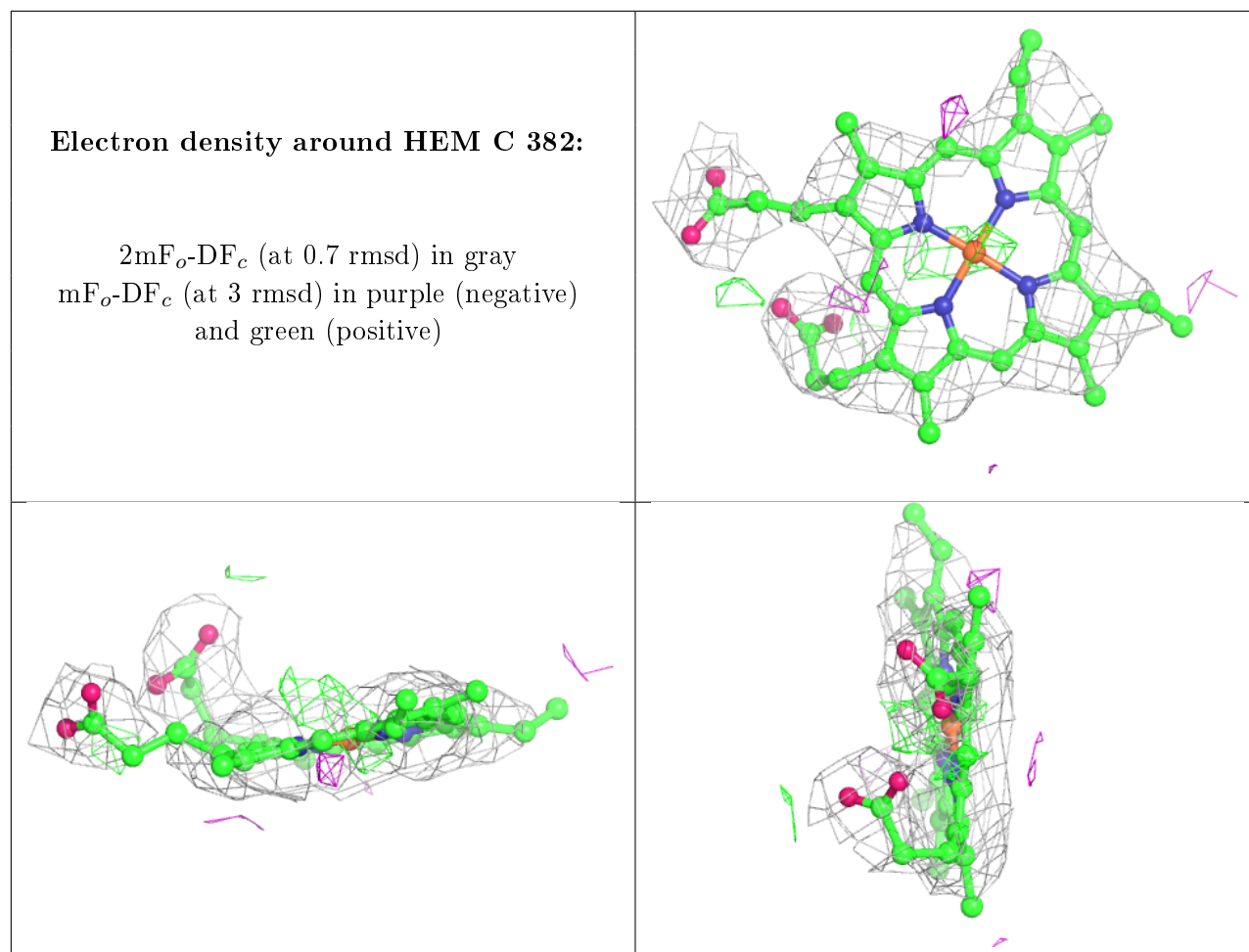
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 381:**

$2mF_o-DF_c$  (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.