



# Full wwPDB X-ray Structure Validation Report

Oct 21, 2014 – 08:42 PM EDT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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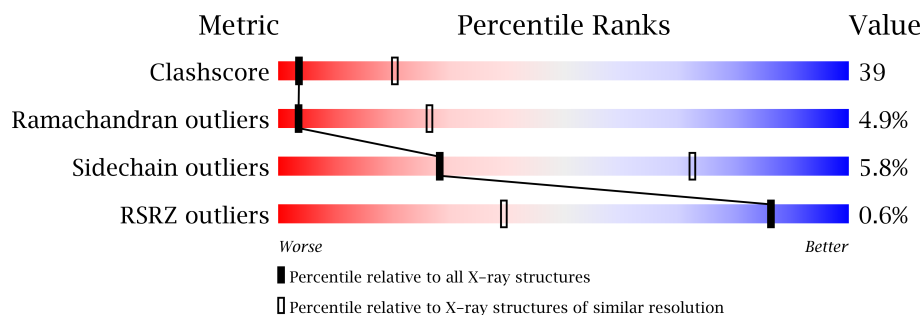
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

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	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	422	
3	C	380	
4	D	241	
5	E	196	
6	F	109	
7	G	81	
8	H	78	
9	I	33	
10	J	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
14	U10	C	383	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
15	PEE	C	384	-	X
15	PEE	E	198	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15719 atoms, of which 0 are hydrogen and 0 are deuterium.

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
2	B	406	Total	C	N	O	S	0	0	0
			2994	1878	518	591	7			

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
3	C	379	Total	C	N	O	S	0	0	0
			3002	2013	473	504	12			

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

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

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
5	E	196	Total	C	N	O	S	0	0	0
			1512	953	266	285	8			

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
6	F	100	Total	C	N	O	S	0	0	0
			875	557	153	162	3			

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
7	G	78	Total	C	N	O	S	0	0	0
			626	411	114	100	1			

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
8	H	66	Total	C	N	O	S	0	0	0
			490	301	88	96	5			

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
9	I	33	Total	C	N	O	0	0	0
			159	92	33	34			

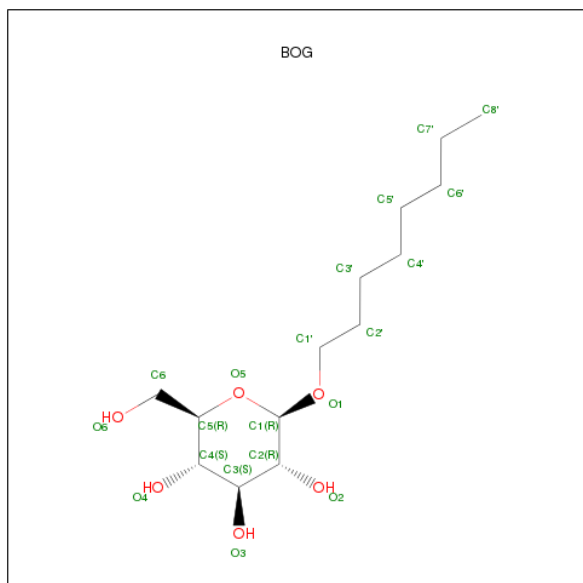
- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

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

There is a discrepancy between the modelled and reference sequences:

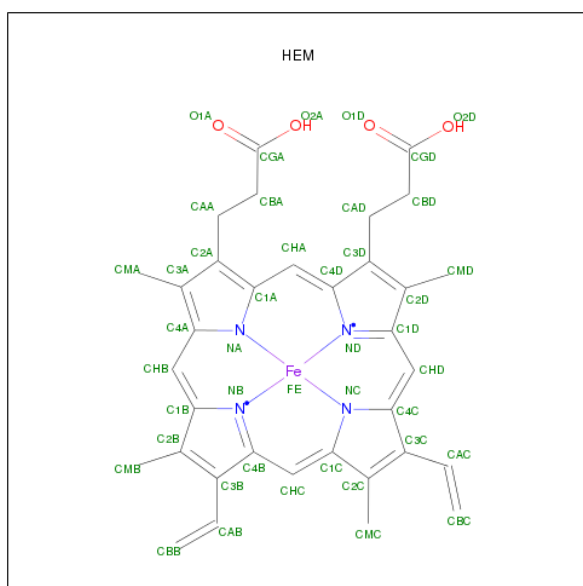
Chain	Residue	Modelled	Actual	Comment	Reference
J	30	LEU	PHE	CONFLICT	UNP P00130

- Molecule 11 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



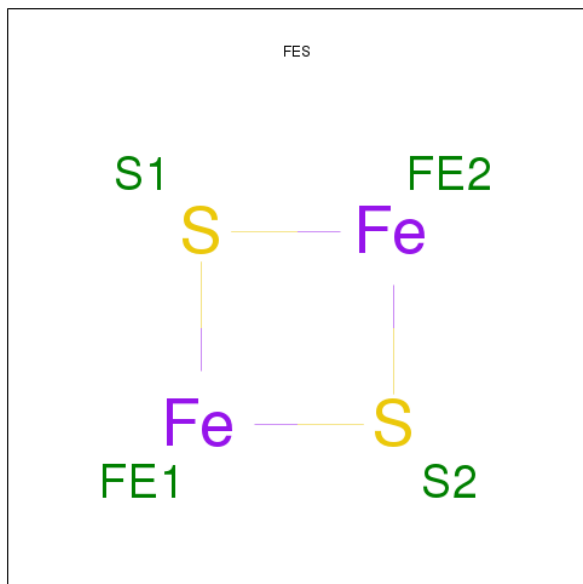
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



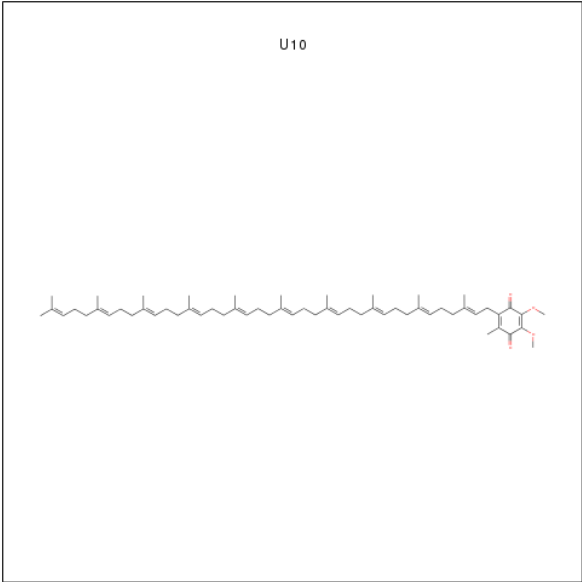
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



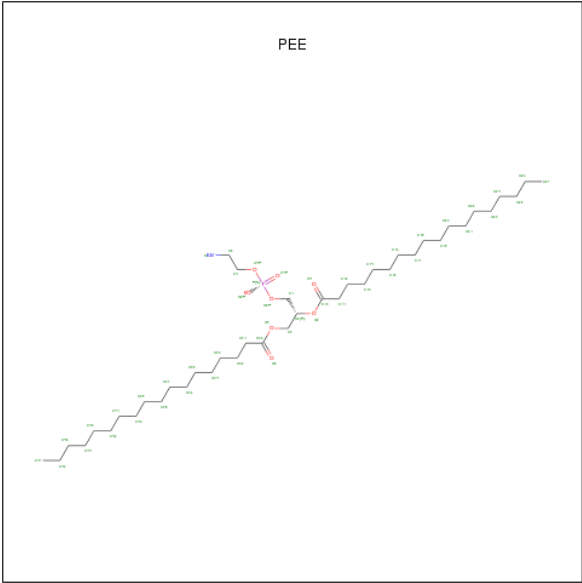
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula:  $\text{C}_{59}\text{H}_{90}\text{O}_4$ ).



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

- Molecule 15 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



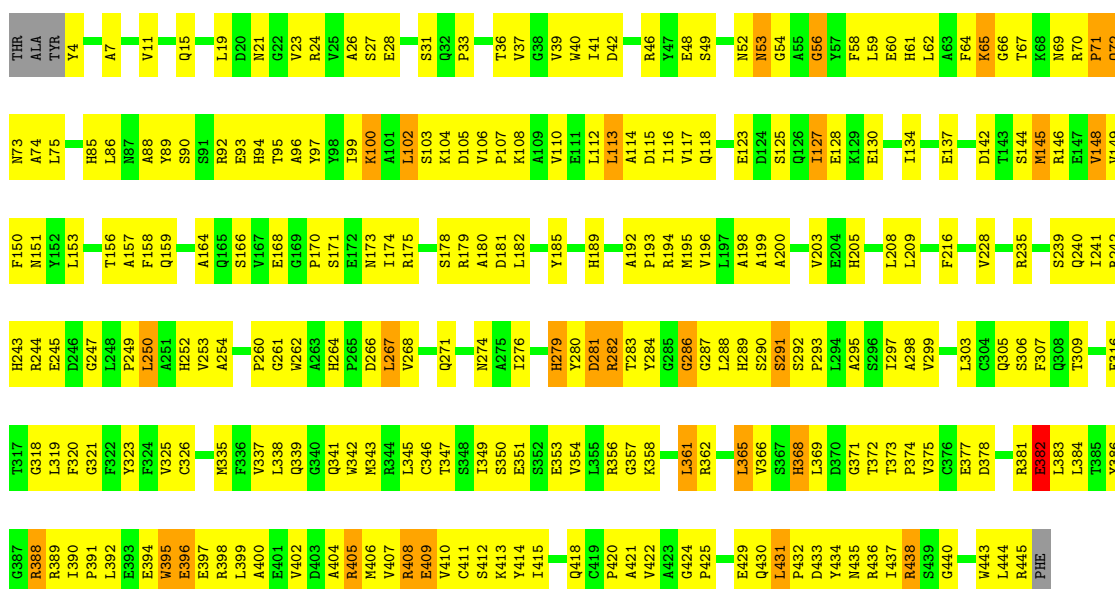
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

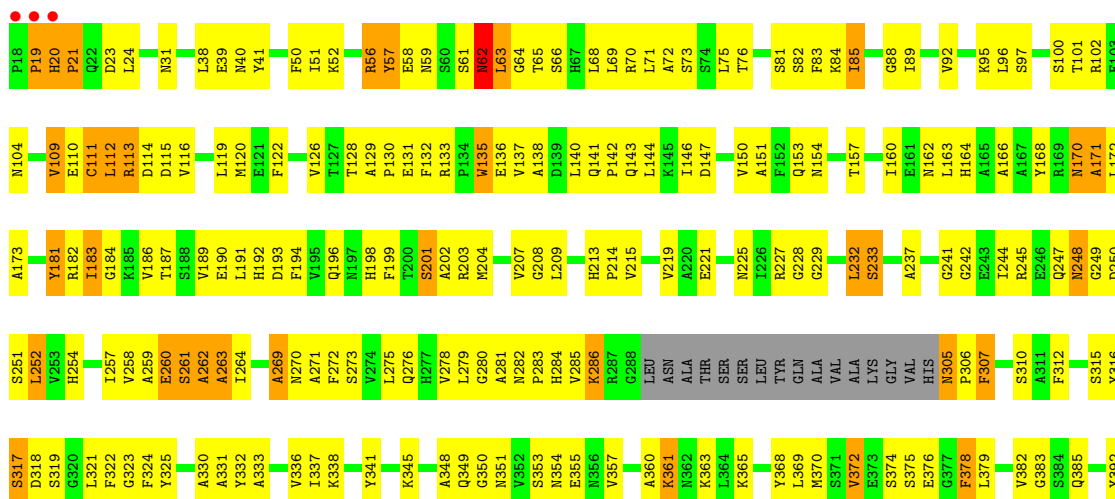
#### • Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain A:



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

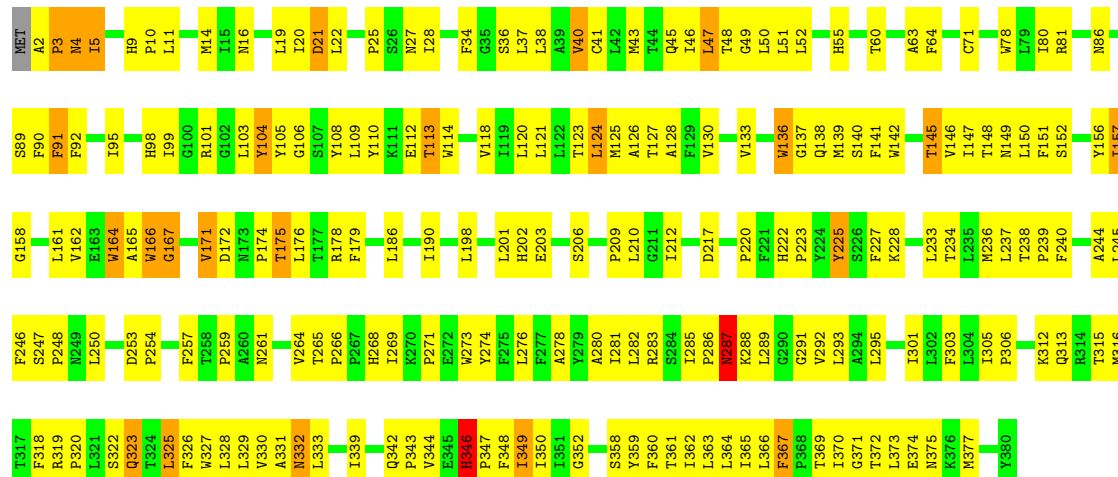
Chain B:





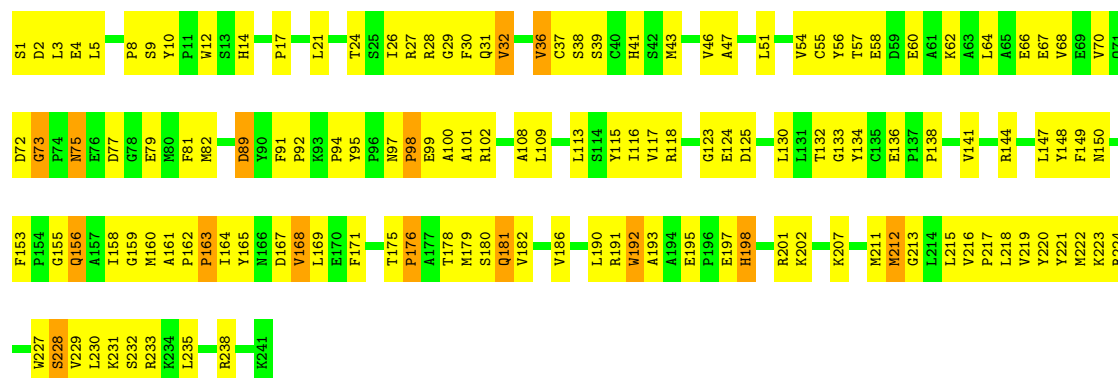
• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain C:



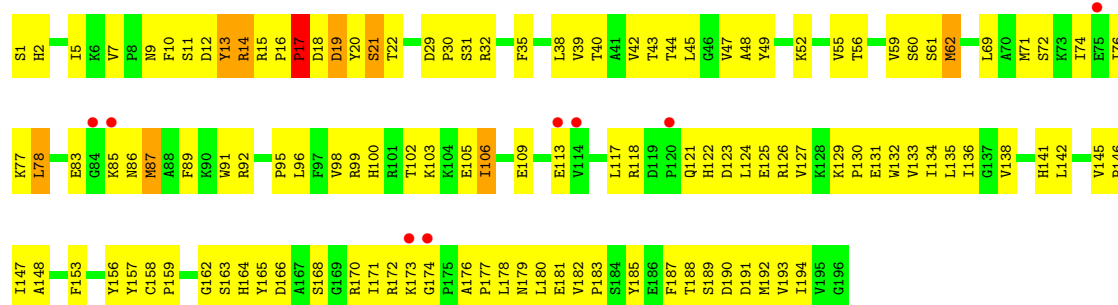
• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain D:



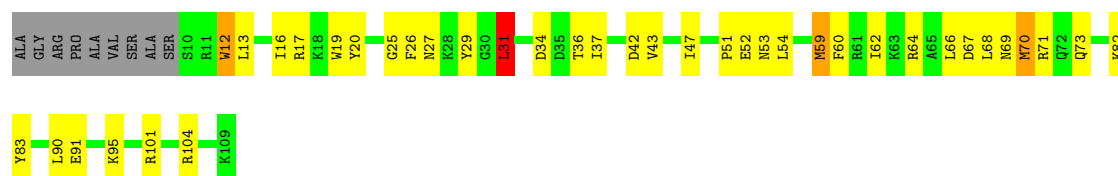
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain E:



• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain F: 



• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain G: 



• Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain H: 



• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I: 



• Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain J: 



## 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)	Xtriage
Refinement program	CNS 0.1	Depositor
R, $R_{free}$	0.270 , 0.310 0.285 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	90.1	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 123774 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	15719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage'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.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	D	20	0	28	2	0
12	C	86	0	60	12	0
12	D	43	0	30	0	0
13	E	4	0	0	1	0
14	C	29	0	33	4	0
15	C	49	0	70	2	0
15	E	49	0	70	1	0
All	All	15719	0	15167	1200	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (1200) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:B:76:THR:HG22	2:B:82:SER:H	1.23	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	12: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	12: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:83:GLU:HA	5:E:100:HIS:HB3	1.68	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
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	11: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	15:E:198:PEE:H162	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
4:D:224:ARG:HH21	7:G:26:PHE:HA	1.56	0.69
5:E:62:MET:CE	5:E:62:MET:HA	2.22	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	12: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:288:LEU:HD22	2:B:83:PHE:HD1	1.61	0.65
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.77	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	12: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	12:C:382:HEM:CMA	2.27	0.64
4:D:51:LEU:O	4:D:54:VAL:HG12	1.98	0.64
15:C:384:PEE:O5	7:G:48:VAL:HG21	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	13: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
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
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.34	0.63
2:B:70:ARG:HD3	2:B:100:SER:HB3	1.78	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:34:PHE:HD1	3:C:37:LEU:HD12	1.63	0.63
1:A:429:GLU:OE2	7:G:7:LEU:HB2	1.99	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
5:E:16:PRO:HD3	7:G:23:GLN:HA	1.81	0.62
4:D:218:LEU:HD11	5:E:42:VAL:HG12	1.82	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
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:170:ASN:HD21	2:B:237:ALA:HA	1.66	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:166:ALA:HB1	2:B:242:GLY:HA3	1.82	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
14:C:383:U10:H8	14: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
14:C:383:U10:C8	14: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
3:C:301:ILE:HD11	3:C:364:LEU:HD11	1.85	0.59
3:C:45:GLN:CB	12: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	12:C:382:HEM:HAB	2.33	0.59
4:D:227:TRP:O	4:D:229:VAL:N	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:361:LYS:HA	2:B:402:ILE:HD11	1.85	0.58
2:B:341:TYR:OH	2:B:422:LYS:HE3	2.02	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	12: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:45:LEU:HD13	5:E:45:LEU:C	2.24	0.58
5:E:78:LEU:HG	5:E:191:ASP:C	2.23	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:78:LEU:HB3	5:E:132:TRP:CZ2	2.40	0.56
5:E:17:PRO:HD3	7:G:24:ARG:NE	2.20	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:N	1:A:250:LEU:HD13	2.20	0.56
1:A:250:LEU:HD22	1:A:250:LEU:C	2.25	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	12: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:61:HIS:HD2	1:A:134:ILE:HG12	1.69	0.56
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.87	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
1:A:33:PRO:HG3	2:B:369:LEU:HD22	1.87	0.56
2:B:109:VAL:CG2	2:B:119:LEU:HD11	2.35	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:319:ARG:HH12	3:C:371:GLY:HA2	1.72	0.55
3:C:209:PRO:HG2	6:F:69:ASN:HD21	1.71	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	12: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
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
4:D:181:GLN:CB	8:H:77:LEU:HD22	2.37	0.54
5:E:103:LYS:HA	5:E:106:ILE:HD12	1.89	0.54
1:A:284:TYR:HE1	9:I:112:UNK:O	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:374:PRO:O	1:A:377:GLU:HB3	2.07	0.54
1:A:58:PHE:CE1	1:A:127:ILE:HG23	2.42	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
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:105:TYR:CE1	3:C:209:PRO:HA	2.43	0.54
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.89	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.91	0.53
4:D:75:ASN:H	4:D:79:GLU:H	1.57	0.53
4:D:75:ASN:ND2	4:D:79:GLU:O	2.42	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
1:A:242:ARG:O	7:G:14:ILE:HA	2.09	0.52
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: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
3:C:206:SER:HB2	14: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:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.52
2:B:307:PHE:C	2:B:307:PHE:CD1	2.83	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.93	0.50
5:E:117:LEU:HD12	5:E:121:GLN:H	1.74	0.50
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.93	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
1:A:106:VAL:CG2	1:A:203:VAL:HG22	2.41	0.50
1:A:106:VAL:HG21	1:A:203:VAL:CG1	2.40	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:349:ILE:HG22	1:A:408:ARG:HG3	1.93	0.49
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.75	0.49
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.94	0.49
4:D:27:ARG:CZ	10:J:59:TYR:CE2	2.95	0.49
5:E:147:ILE:HD11	5:E:159:PRO:HG3	1.94	0.49
5:E:135:LEU:HD13	5:E:180:LEU:HD12	1.95	0.49
5:E:52:LYS:C	5:E:52:LYS:HD3	2.33	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
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
3:C:318:PHE:CG	6:F:26:PHE:HB3	2.48	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
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
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.95	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:227:PHE:HE1	4:D:222:MET:HE2	1.78	0.48
3:C:312:LYS:HG2	3:C:375:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:153:PHE:CG	4:D:158:ILE:HG12	2.49	0.48
4:D:211:MET:CG	11: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
1:A:65:LYS:HZ3	9:I:311:UNK:HA	1.78	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: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
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: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
4:D:141:VAL:HG21	8:H:55:THR:HG23	1.95	0.47
1:A:373:THR:N	1:A:374:PRO:HD2	2.29	0.47
1:A:254:ALA:O	1:A:422:VAL:HA	2.14	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:65:LYS:NZ	9:I:311:UNK:N	2.63	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: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
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.50	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.51	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
1:A:382:GLU:HA	1:A:386:TYR:HD2	1.79	0.46
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.96	0.46
2:B:259:ALA:O	2:B:260:GLU:C	2.53	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
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
4:D:221:TYR:CE1	7:G:25:PRO:HG2	2.51	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.51	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
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:132:THR:HA	4:D:179:MET:CE	2.46	0.45
4:D:98:PRO:O	4:D:101:ALA:N	2.48	0.45
5:E:17:PRO:HG3	7:G:24:ARG:HH21	1.81	0.45
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	15:C:384:PEE:H31	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:306:SER:HB2	9:I:206:UNK:CB	2.47	0.45
1:A:366:VAL:C	1:A:368:HIS:N	2.71	0.45
4:D:118:ARG:HD3	4:D:191:ARG:HH12	1.82	0.45
4:D:181:GLN:CG	8:H:77:LEU:HD22	2.47	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:92:ARG:HH12	1:A:166:SER:HA	1.81	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
10:J:33:ARG:O	10:J:37:GLN:HG3	2.17	0.45
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.45	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
1:A:239:SER:O	1:A:421:ALA:HA	2.16	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:182:VAL:HA	5:E:183:PRO:HD2	1.83	0.45
5:E:9:ASN:OD1	5:E:11:SER:HB2	2.17	0.45
6:F:34:ASP:OD2	6:F:90:LEU:HB3	2.17	0.45
4:D:231:LYS:HD3	6:F:70:MET:CE	2.47	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:143:GLN:O	2:B:146:ILE:HG12	2.18	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
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.99	0.44
1:A:266:ASP:O	1:A:268:VAL:N	2.50	0.44
1:A:100:LYS:HG3	2:B:370:MET:HE1	1.99	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:67:THR:HG21	1:A:115:ASP:OD2	2.18	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.47	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
3:C:327:TRP:NE1	7:G:48:VAL:HG22	2.33	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
5:E:136:ILE:HG12	5:E:181:GLU:O	2.17	0.43
5:E:134:ILE:HD12	5:E:185:TYR:CE2	2.53	0.43
5:E:16:PRO:HG3	5:E:32:ARG:HH11	1.82	0.43
4:D:231:LYS:HD3	6:F:70:MET:HE1	2.00	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:230:LEU:HB3	6:F:70:MET:SD	2.58	0.43
4:D:21:LEU:HB3	4:D:26:ILE:HD11	1.99	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
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:51:LEU:HD11	5:E:61:SER:OG	2.19	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:55:HIS:HE1	5:E:61:SER:O	2.01	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:65:LYS:HZ3	9:I:311:UNK:CA	2.32	0.42
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.19	0.42
1:A:159:GLN:NE2	5:E:7:VAL:HG11	2.33	0.42
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.97	0.42
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.54	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
5:E:17:PRO:CD	7:G:24:ARG:HH21	2.32	0.42
1:A:15:GLN:O	1:A:26:ALA:HA	2.19	0.42
1:A:178:SER:C	1:A:180:ALA:N	2.68	0.42
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.01	0.42
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	12: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
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:218:LEU:HD22	5:E:39:VAL:HG13	2.02	0.42
4:D:28:ARG:O	4:D:29:GLY:C	2.58	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
14:C:383:U10:H8	14: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
4:D:41:HIS:HB3	4:D:113:LEU:HD13	2.02	0.41
4:D:144:ARG:HG3	4:D:147:LEU:HD23	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: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
5:E:17:PRO:HD3	7:G:24:ARG:NH2	2.35	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
12:C:381:HEM:O2D	12: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:235:ARG:NH1	5:E:15:ARG:CZ	2.84	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
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
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

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/446 (99%)	348 (79%)	73 (17%)	19 (4%)	4	30
2	B	404/422 (96%)	291 (72%)	74 (18%)	39 (10%)	1	7
3	C	377/380 (99%)	299 (79%)	64 (17%)	14 (4%)	5	34
4	D	239/241 (99%)	195 (82%)	31 (13%)	13 (5%)	3	23
5	E	194/196 (99%)	167 (86%)	23 (12%)	4 (2%)	11	53
6	F	98/109 (90%)	83 (85%)	15 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	76/81 (94%)	61 (80%)	10 (13%)	5 (7%)	2	16
8	H	64/78 (82%)	50 (78%)	14 (22%)	0	100	100
10	J	57/62 (92%)	43 (75%)	12 (21%)	2 (4%)	6	37
All	All	1949/2015 (97%)	1537 (79%)	316 (16%)	96 (5%)	3	26

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	30	74
2	B	307/336 (91%)	286 (93%)	21 (7%)	22	65
3	C	326/329 (99%)	308 (94%)	18 (6%)	30	74
4	D	201/207 (97%)	190 (94%)	11 (6%)	30	74
5	E	165/169 (98%)	156 (94%)	9 (6%)	30	74
6	F	90/98 (92%)	85 (94%)	5 (6%)	30	74
7	G	60/72 (83%)	54 (90%)	6 (10%)	11	41
8	H	51/74 (69%)	49 (96%)	2 (4%)	43	84
10	J	41/52 (79%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1600/1713 (93%)	1508 (94%)	92 (6%)	28	72

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	HEM	C	381	3	42,50,50	2.74	13 (30%)	27,82,82	2.42	7 (25%)
12	HEM	C	382	3	42,50,50	3.10	10 (23%)	27,82,82	3.02	7 (25%)
14	U10	C	383	-	29,29,63	2.48	9 (31%)	37,38,79	1.87	12 (32%)
15	PEE	C	384	-	48,48,50	2.42	12 (25%)	53,53,55	4.23	25 (47%)
11	BOG	D	242	-	20,20,20	0.73	0	25,25,25	0.92	1 (4%)
12	HEM	D	243	4	42,50,50	3.82	14 (33%)	27,82,82	2.49	9 (33%)
13	FES	E	197	5	0,4,4	0.00	-	0,4,4	0.00	-
15	PEE	E	198	-	48,48,50	2.31	10 (20%)	53,53,55	4.24	22 (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	HEM	C	381	3	-	0/14/114/114	0/0/8/8
12	HEM	C	382	3	-	0/14/114/114	0/0/8/8
14	U10	C	383	-	-	0/23/47/87	0/1/1/1
15	PEE	C	384	-	1/1/4/4	0/52/52/54	0/0/0/0
11	BOG	D	242	-	-	0/11/31/31	0/1/1/1
12	HEM	D	243	4	-	0/14/114/114	0/0/8/8
13	FES	E	197	5	-	0/0/4/4	0/1/1/1
15	PEE	E	198	-	1/1/4/4	0/52/52/54	0/0/0/0

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	243	HEM	C3C-C2C	-16.34	1.32	1.45
12	C	382	HEM	C3C-C2C	-14.60	1.34	1.45
12	D	243	HEM	C3B-C2B	-12.66	1.33	1.45
15	E	198	PEE	O5-C30	11.40	1.56	1.22
15	C	384	PEE	O5-C30	11.12	1.55	1.22
12	C	381	HEM	C3C-C2C	-10.66	1.37	1.45
12	C	382	HEM	C3B-C2B	-7.26	1.38	1.45
12	C	381	HEM	C3B-C2B	-6.71	1.39	1.45
14	C	383	U10	C22-C21	-6.56	1.52	1.55
14	C	383	U10	C6-C1	5.78	1.48	1.35
12	C	381	HEM	CMB-C2B	4.89	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	383	U10	C7-C6	4.81	1.60	1.51
12	C	382	HEM	CMB-C2B	4.76	1.53	1.45
15	E	198	PEE	O2-C10	4.69	1.48	1.34
12	C	382	HEM	FE-ND	-4.63	1.77	1.95
12	C	381	HEM	CMC-C2C	4.60	1.53	1.45
12	C	381	HEM	CHC-C4B	-4.44	1.34	1.39
12	C	382	HEM	C3D-C2D	-4.33	1.32	1.43
12	D	243	HEM	FE-ND	-4.26	1.79	1.95
14	C	383	U10	C18-C19	4.25	1.41	1.32
15	C	384	PEE	C26-C25	4.19	1.56	1.55
12	C	382	HEM	CMC-C2C	4.16	1.52	1.45
15	C	384	PEE	O2-C10	4.14	1.46	1.34
12	C	381	HEM	CMD-C2D	4.04	1.52	1.45
12	D	243	HEM	CHC-C4B	-4.04	1.35	1.39
12	D	243	HEM	CBB-CAB	3.96	1.51	1.29
15	E	198	PEE	C26-C25	3.87	1.56	1.55
15	C	384	PEE	C11-C10	3.84	1.62	1.50
15	C	384	PEE	C1-C2	3.83	1.61	1.50
12	D	243	HEM	CBC-CAC	3.78	1.50	1.29
12	D	243	HEM	C3D-C2D	-3.77	1.33	1.43
14	C	383	U10	C13-C14	3.71	1.40	1.32
15	C	384	PEE	C46-C45	3.65	1.56	1.55
12	D	243	HEM	C3B-CAB	3.65	1.52	1.40
12	C	381	HEM	FE-NB	-3.53	1.82	1.95
12	D	243	HEM	CMD-C2D	3.45	1.51	1.45
12	D	243	HEM	C3C-CAC	3.39	1.51	1.40
15	E	198	PEE	C11-C10	3.38	1.60	1.50
12	D	243	HEM	C1B-C2B	-3.20	1.42	1.45
12	D	243	HEM	CMC-C2C	3.20	1.50	1.45
12	C	381	HEM	C3D-C2D	-3.19	1.35	1.43
12	D	243	HEM	CMB-C2B	3.18	1.50	1.45
15	E	198	PEE	C22-C21	-2.99	1.33	1.51
14	C	383	U10	C8-C9	2.97	1.38	1.32
15	E	198	PEE	C31-C30	-2.92	1.41	1.50
15	E	198	PEE	C42-C41	-2.90	1.34	1.51
12	C	381	HEM	C1D-ND	2.85	1.40	1.33
15	C	384	PEE	C22-C21	-2.82	1.34	1.51
15	C	384	PEE	C42-C41	-2.76	1.34	1.51
12	C	382	HEM	FE-NC	-2.74	1.85	1.95
15	C	384	PEE	C31-C30	-2.69	1.42	1.50
14	C	383	U10	C3-C2	-2.59	1.41	1.48
12	C	381	HEM	C1B-C2B	2.57	1.47	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	198	PEE	C5-C4	2.50	1.58	1.50
15	C	384	PEE	P-O3P	2.48	1.70	1.59
12	C	382	HEM	C1C-NC	2.42	1.39	1.33
15	E	198	PEE	C1-C2	2.40	1.57	1.50
12	C	381	HEM	FE-NC	-2.39	1.86	1.95
15	C	384	PEE	C5-C4	2.39	1.57	1.50
12	D	243	HEM	C1C-NC	2.30	1.39	1.33
12	C	382	HEM	CMD-C2D	2.30	1.49	1.45
12	C	382	HEM	C1B-C2B	-2.28	1.43	1.45
15	C	384	PEE	O2-C2	-2.21	1.41	1.46
14	C	383	U10	O4-C4M	-2.11	1.40	1.45
12	C	381	HEM	C4C-NC	2.10	1.39	1.33
14	C	383	U10	C7-C8	-2.08	1.47	1.50
15	E	198	PEE	C3-C2	2.05	1.56	1.50
12	C	381	HEM	C4D-ND	2.02	1.38	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	198	PEE	O4-C10-C11	-17.94	51.02	123.78
15	C	384	PEE	O4-C10-C11	-17.92	51.11	123.78
15	E	198	PEE	O3-C30-C31	13.09	151.98	111.90
15	C	384	PEE	O3-C30-C31	12.82	151.15	111.90
15	C	384	PEE	O3-C30-O5	-10.94	94.89	123.48
15	E	198	PEE	O3-C30-O5	-10.80	95.27	123.48
15	E	198	PEE	O2-C2-C3	7.66	136.86	108.50
12	C	382	HEM	C4A-NA-C1A	-7.65	98.40	107.93
15	C	384	PEE	O2-C2-C3	7.56	136.47	108.50
15	E	198	PEE	O2-C10-C11	7.24	126.96	111.54
12	C	382	HEM	CBA-CAA-C2A	6.89	124.09	112.63
12	D	243	HEM	C3A-C4A-NA	6.64	113.93	109.50
15	C	384	PEE	O2-C10-C11	6.50	125.40	111.54
12	C	382	HEM	C3A-C4A-NA	6.44	113.80	109.50
12	C	381	HEM	CAD-C3D-C4D	6.06	134.14	125.60
15	E	198	PEE	C12-C11-C10	-6.03	90.09	113.51
15	C	384	PEE	O2-C10-O4	-5.82	108.13	123.66
12	C	381	HEM	C4A-NA-C1A	-5.66	100.88	107.93
15	E	198	PEE	O2-C10-O4	-5.61	108.69	123.66
15	C	384	PEE	C12-C11-C10	-5.57	91.91	113.51
12	D	243	HEM	C4A-NA-C1A	-5.46	101.13	107.93
12	C	382	HEM	C2A-C1A-NA	5.46	117.31	109.73
15	C	384	PEE	O3-C3-C2	5.43	123.07	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEM	CBA-CAA-C2A	5.09	121.10	112.63
12	D	243	HEM	CAD-C3D-C4D	5.02	132.68	125.60
15	E	198	PEE	O3-C3-C2	5.00	121.94	108.80
14	C	383	U10	C10-C9-C8	-4.89	113.79	123.52
12	C	382	HEM	CBD-CAD-C3D	4.85	125.04	114.51
12	C	382	HEM	C1A-C2A-C3A	-4.57	102.19	106.92
12	D	243	HEM	C4A-C3A-C2A	-3.87	104.30	107.00
12	C	381	HEM	C3A-C4A-NA	3.83	112.05	109.50
14	C	383	U10	C1-C6-C5	-3.80	115.49	120.26
15	C	384	PEE	C4-C5-N	3.75	117.88	110.92
15	E	198	PEE	C4-C5-N	3.72	117.83	110.92
14	C	383	U10	C15-C14-C13	-3.65	116.26	123.52
15	C	384	PEE	O3P-C1-C2	3.63	120.26	108.54
12	C	381	HEM	CAD-C3D-C2D	-3.46	118.36	127.19
12	C	381	HEM	C2A-C1A-NA	3.39	114.44	109.73
11	D	242	BOG	C1'-O1-C1	3.33	119.79	113.91
15	E	198	PEE	O3P-C1-C2	3.31	119.22	108.54
12	D	243	HEM	CMA-C3A-C4A	3.06	133.16	128.46
15	E	198	PEE	C33-C32-C31	3.05	124.56	113.28
12	C	381	HEM	C1A-C2A-C3A	-2.98	103.83	106.92
15	C	384	PEE	C42-C41-C40	2.98	130.40	114.56
14	C	383	U10	C15-C14-C16	2.96	119.89	115.39
15	E	198	PEE	C22-C21-C20	2.96	130.27	114.56
15	E	198	PEE	C34-C33-C32	-2.93	99.00	114.56
15	C	384	PEE	C14-C13-C12	-2.92	99.07	114.56
15	E	198	PEE	C42-C41-C40	2.91	130.01	114.56
14	C	383	U10	C11-C9-C8	2.89	126.61	121.06
14	C	383	U10	C20-C19-C18	-2.84	117.86	123.52
15	C	384	PEE	C33-C32-C31	2.84	123.81	113.28
15	C	384	PEE	C22-C21-C20	2.80	129.43	114.56
14	C	383	U10	C10-C9-C11	2.77	119.60	115.39
15	C	384	PEE	C3-O3-C30	-2.77	109.09	116.99
15	C	384	PEE	C34-C33-C32	-2.74	99.99	114.56
15	E	198	PEE	O5-C30-C31	-2.72	112.74	123.78
15	C	384	PEE	O4P-P-O3P	2.71	112.42	104.68
15	C	384	PEE	O4P-C4-C5	-2.67	105.06	109.37
12	D	243	HEM	CBA-CAA-C2A	2.62	116.99	112.63
15	E	198	PEE	C46-C45-C44	-2.60	105.50	112.94
15	E	198	PEE	C14-C13-C12	-2.58	100.87	114.56
15	E	198	PEE	C26-C25-C24	-2.47	105.87	112.94
12	D	243	HEM	C2A-C1A-NA	2.45	113.14	109.73
15	C	384	PEE	O5-C30-C31	-2.44	113.88	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	198	PEE	C3-C2-C1	-2.38	106.40	111.86
15	C	384	PEE	C46-C45-C44	-2.34	106.24	112.94
15	C	384	PEE	C23-C24-C25	2.34	123.16	113.73
15	E	198	PEE	C3-O3-C30	-2.33	110.34	116.99
15	C	384	PEE	C3-C2-C1	-2.30	106.57	111.86
12	C	382	HEM	C4A-C3A-C2A	-2.30	105.39	107.00
15	C	384	PEE	O2-C2-C1	2.27	116.92	108.50
14	C	383	U10	O2-C2-C3	-2.25	116.00	121.05
12	D	243	HEM	CAD-C3D-C2D	-2.23	121.48	127.19
15	E	198	PEE	O2-C2-C1	2.22	116.73	108.50
14	C	383	U10	C4-C5-C6	2.21	122.16	117.87
12	D	243	HEM	CBD-CAD-C3D	2.17	119.21	114.51
15	C	384	PEE	C26-C25-C24	-2.15	106.79	112.94
14	C	383	U10	C7-C8-C9	2.14	130.37	126.76
14	C	383	U10	O5-C5-C4	-2.12	116.30	121.05
14	C	383	U10	C3-C2-C1	2.07	121.90	117.87
15	C	384	PEE	C16-C15-C14	-2.04	103.71	114.56
15	E	198	PEE	C36-C35-C34	-2.02	103.81	114.56

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	442/446 (99%)	-0.15	0 100 100	47, 84, 100, 100	0
2	B	406/422 (96%)	-0.03	3 (0%) 84 35	60, 93, 100, 100	0
3	C	379/380 (99%)	-0.24	0 100 100	33, 64, 96, 100	0
4	D	241/241 (100%)	-0.14	0 100 100	50, 76, 99, 100	0
5	E	196/196 (100%)	0.39	8 (4%) 35 6	54, 100, 100, 100	0
6	F	100/109 (91%)	-0.17	0 100 100	50, 73, 98, 100	0
7	G	78/81 (96%)	-0.06	0 100 100	51, 85, 100, 100	0
8	H	66/78 (84%)	-0.24	0 100 100	76, 95, 99, 100	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	-0.14	1 (1%) 67 17	66, 80, 99, 100	0
All	All	1967/2048 (96%)	-0.09	12 (0%) 86 39	33, 83, 100, 100	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	PRO	4.8
5	E	114	VAL	3.5
5	E	85	LYS	2.9
2	B	19	PRO	2.7
5	E	174	GLY	2.4
5	E	84	GLY	2.3
10	J	62	LYS	2.3
5	E	173	LYS	2.1
5	E	75	GLU	2.1
2	B	20	HIS	2.1
5	E	120	PRO	2.1
5	E	113	GLU	2.1

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	PEE	E	198	49/51	0.49	5.59	24,45,64,65	49
15	PEE	C	384	49/51	0.36	4.47	20,39,54,55	49
14	U10	C	383	29/63	0.38	4.34	77,83,100,100	29
11	BOG	D	242	20/20	0.25	1.23	37,59,70,72	20
12	HEM	C	381	43/43	0.23	0.88	43,51,59,62	0
12	HEM	C	382	43/43	0.21	0.81	43,46,59,62	0
12	HEM	D	243	43/43	0.18	-0.63	46,58,69,74	0
13	FES	E	197	4/4	0.21	-0.90	100,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.