



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

PDB ID : 3H1K  
Title : Chicken cytochrome BC1 complex with ZN++ and an iodinated derivative of kresoxim-methyl bound  
Authors : Berry, E.A.; Zhang, Z.; Bellamy, H.D.; Huang, L.S.  
Deposited on : 2009-04-12  
Resolution : 3.48 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

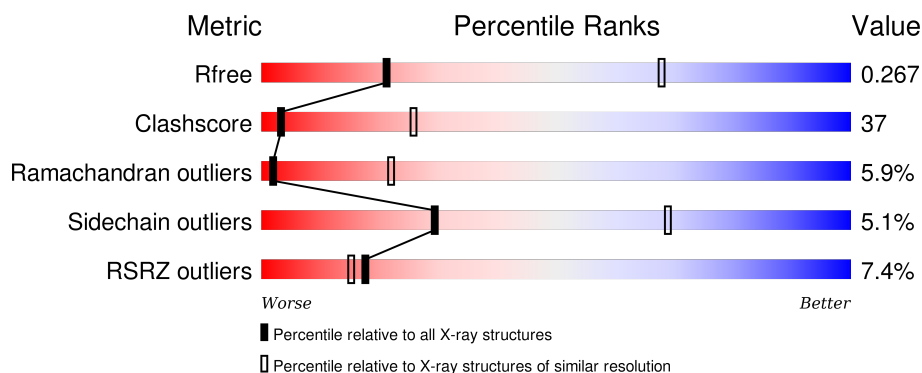
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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. 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	<div> <div>2%</div> <div>44%</div> <div>50%</div> <div>5%</div> <div>..</div> </div>
1	N	446	<div> <div>4%</div> <div>40%</div> <div>54%</div> <div>5%</div> <div>..</div> </div>
2	B	441	<div> <div>5%</div> <div>36%</div> <div>51%</div> <div>10%</div> <div>.</div> </div>
2	O	441	<div> <div>2%</div> <div>34%</div> <div>52%</div> <div>9%</div> <div>.</div> </div>
3	C	380	<div> <div>2%</div> <div>44%</div> <div>50%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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
11	PEE	A	2008	-	-	-	X
11	PEE	E	2005	-	-	-	X
11	PEE	P	3008	-	X	-	-
11	PEE	R	3005	-	-	-	X
12	UNL	A	3284	-	-	-	X
16	CDL	D	2003	-	-	-	X
16	CDL	Q	3003	-	-	-	X
18	GOL	C	2011	-	-	-	X
20	BOG	D	2009	-	-	-	X
20	BOG	D	2091	-	-	-	X
20	BOG	P	2010	-	-	-	X
20	BOG	Q	3009	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	FES	E	501	-	-	X	-
21	FES	R	501	-	-	X	-

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 32673 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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3164	1987	551	616	10			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	S	0	0	0
			571	348	105	113	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

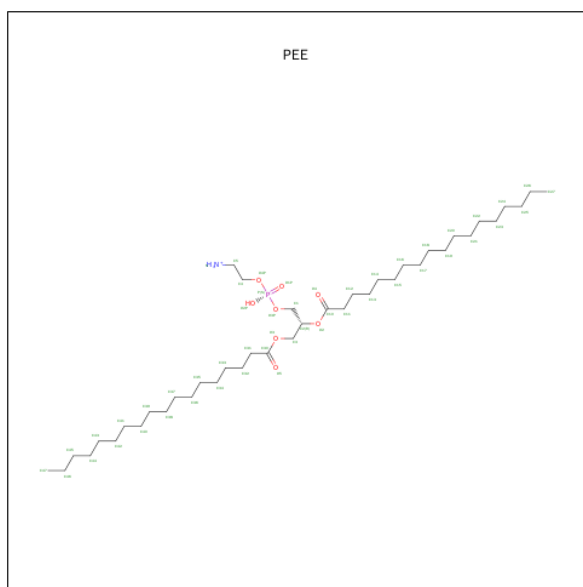
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	2			

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	P	0	0
			18	9	8	1		
11	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	E	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	P	1	Total	O	P		0	0
			5	4	1			
11	R	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

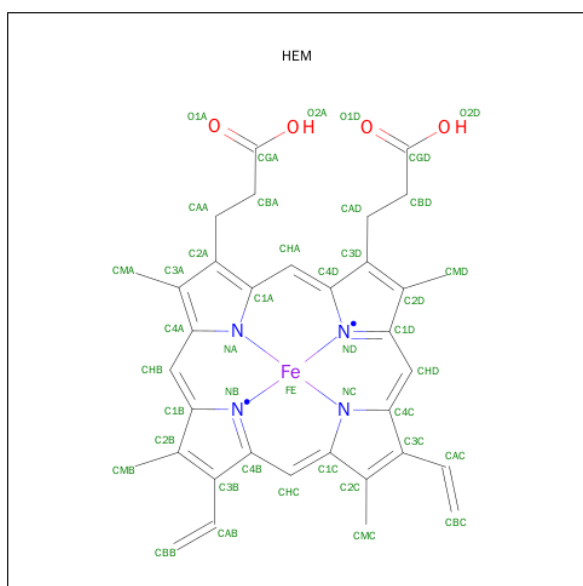
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	P	1	Total 1 O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	O	0	0
			2	2		
12	C	1	Total	O	0	0
			1	1		
12	N	1	Total	O	0	0
			1	1		

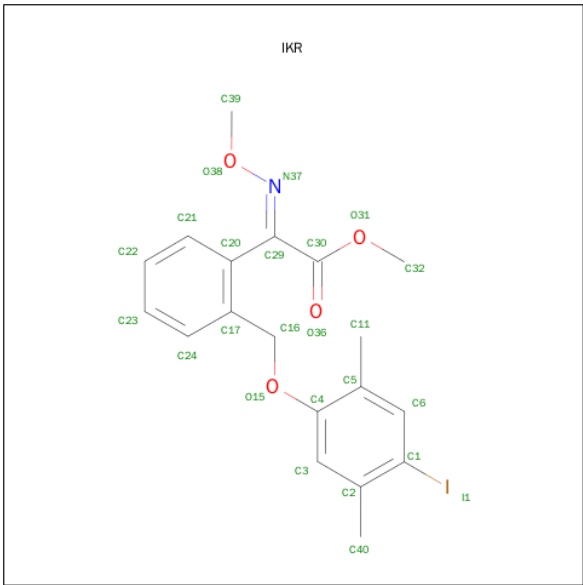
- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

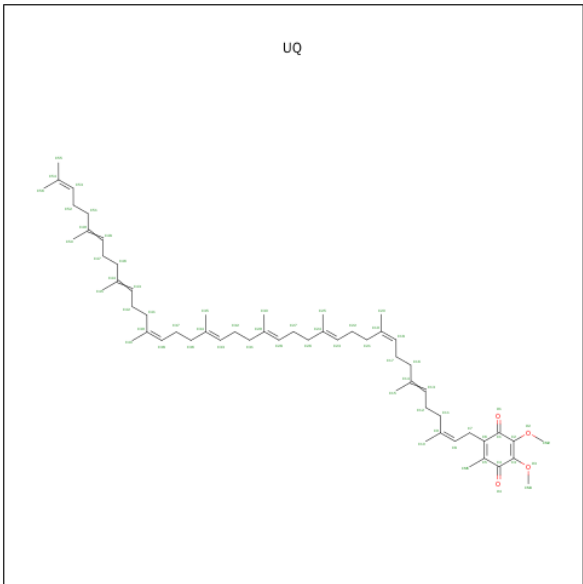
- Molecule 14 is METHYL (2E)-{2-[(4-iodo-2,5-dimethylphenoxy)methyl]phenyl}(methoxyimino)ethanoate (three-letter code: IKR) (formula:  $C_{19}H_{20}INO_4$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
14	P	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

- Molecule 15 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



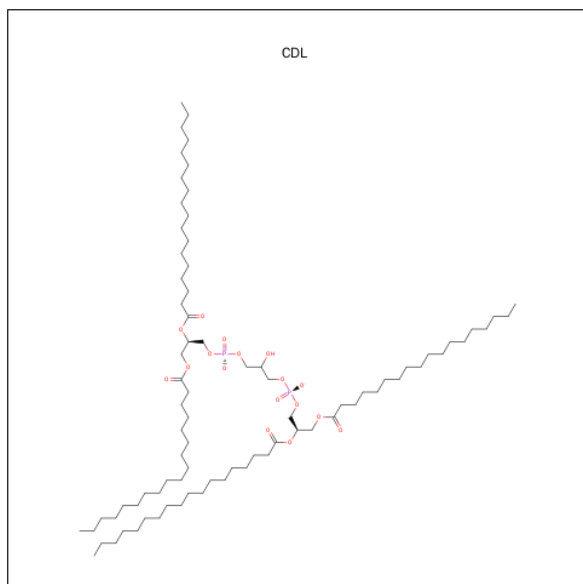
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			19	15	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).

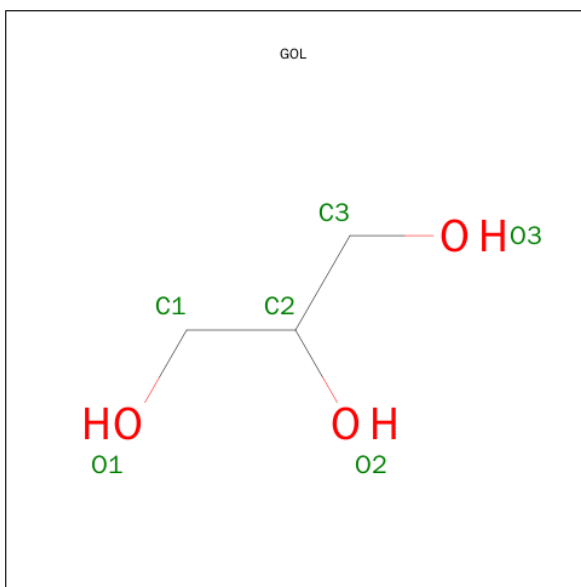


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	O	P	0	0
			40	21	17	2		
16	D	1	Total	C	O	P	0	0
			42	23	17	2		
16	P	1	Total	C	O	P	0	0
			40	21	17	2		
16	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

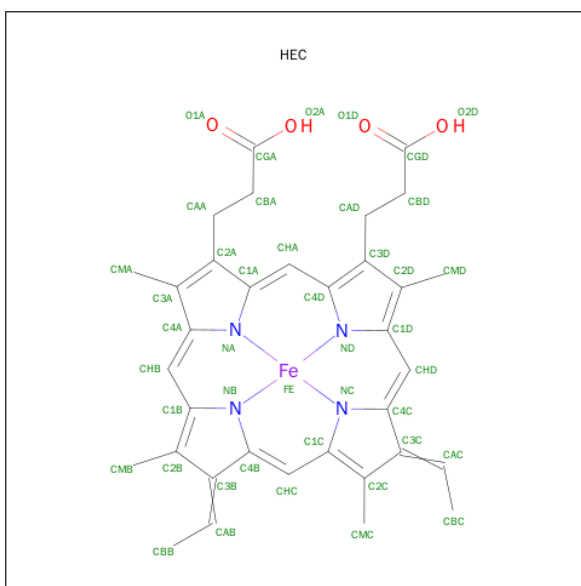
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	P	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		

- Molecule 18 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



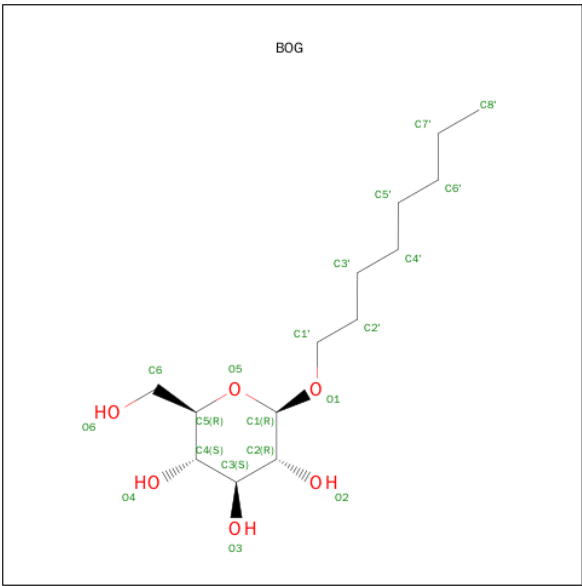
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total 6	C 3	O 3	0	0
18	P	1	Total 6	C 3	O 3	0	0

- Molecule 19 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



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

- Molecule 20 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total	C	O	0	0
			20	14	6		
20	D	1	Total	C	O	0	0
			13	7	6		
20	P	1	Total	C	O	0	0
			12	6	6		
20	P	1	Total	C	O	0	0
			13	7	6		
20	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

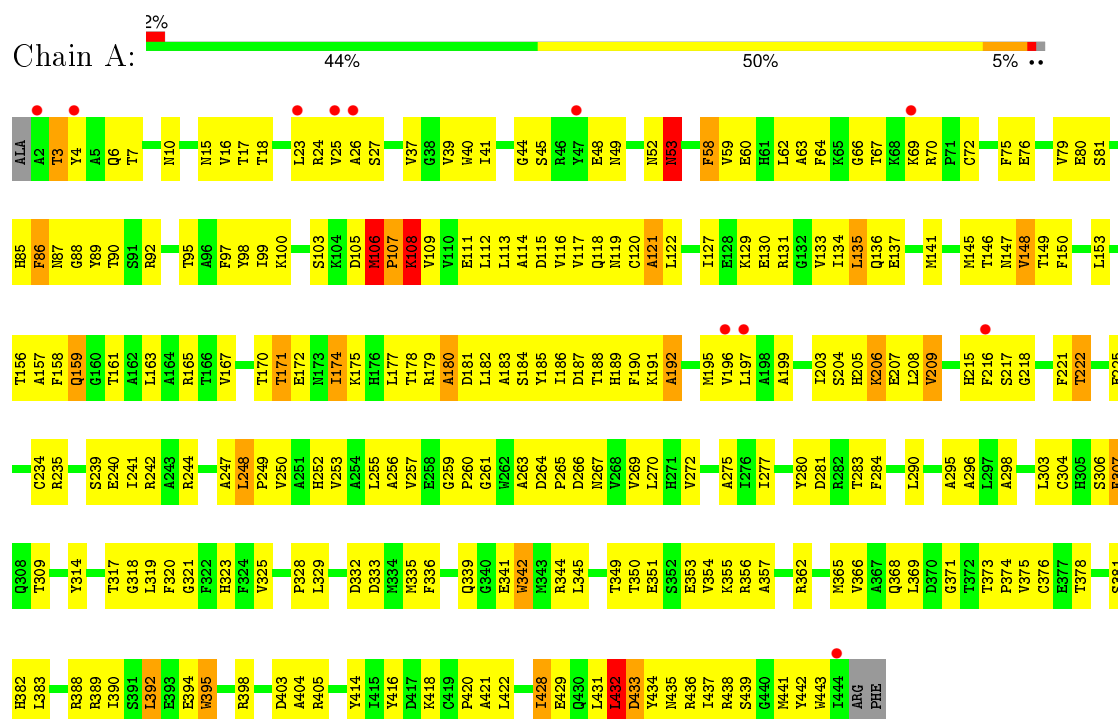
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	O	0	0
			1	1		
22	C	7	Total	O	0	0
			7	7		
22	E	1	Total	O	0	0
			1	1		
22	P	7	Total	O	0	0
			7	7		
22	R	1	Total	O	0	0
			1	1		

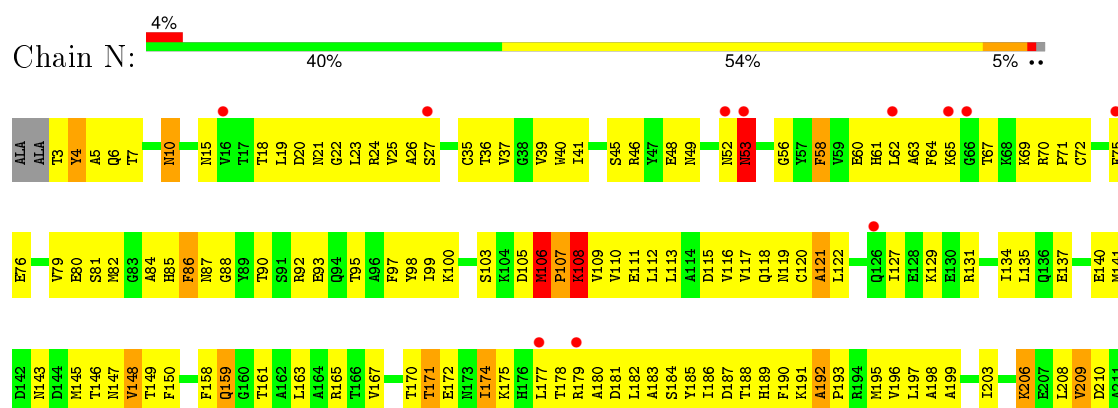
### 3 Residue-property plots

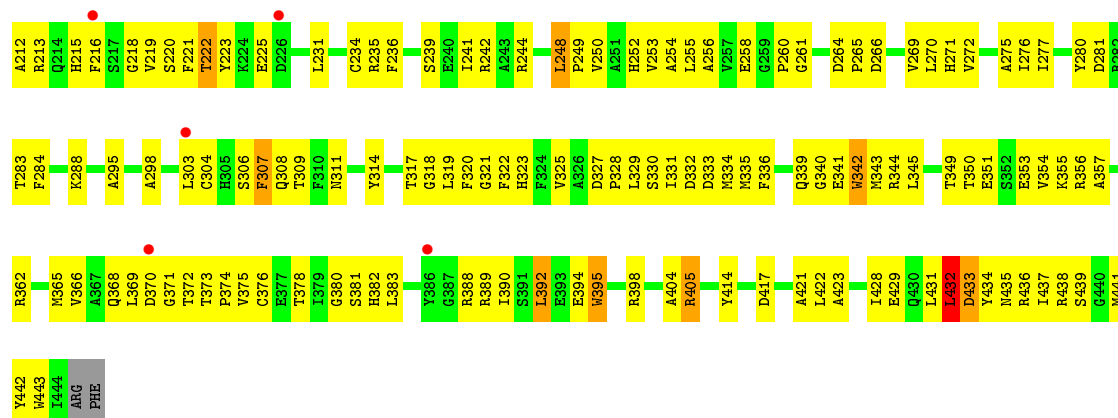
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

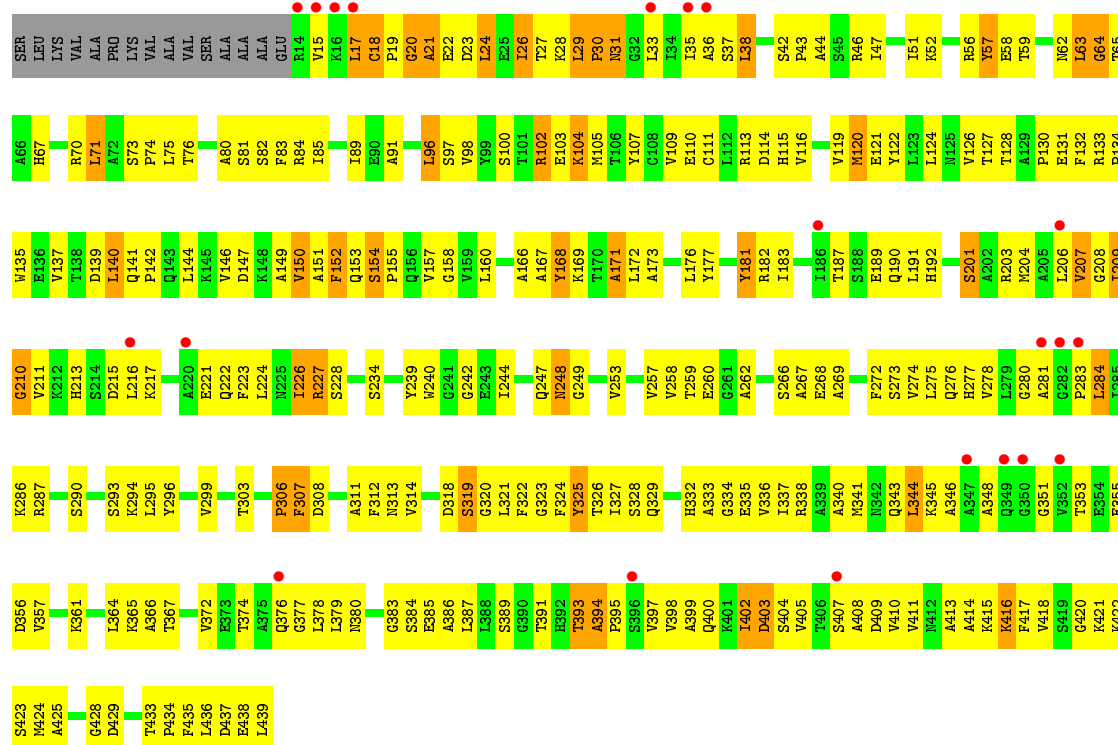


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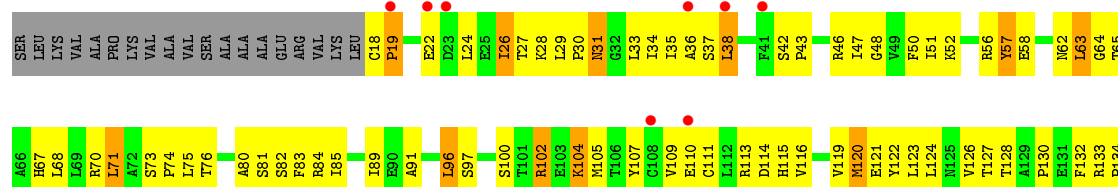


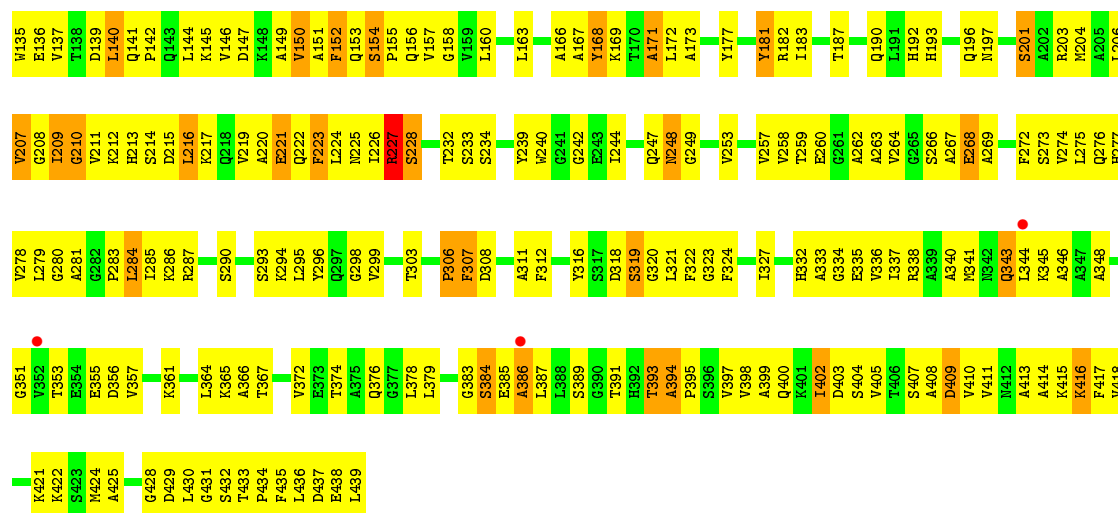


### • Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

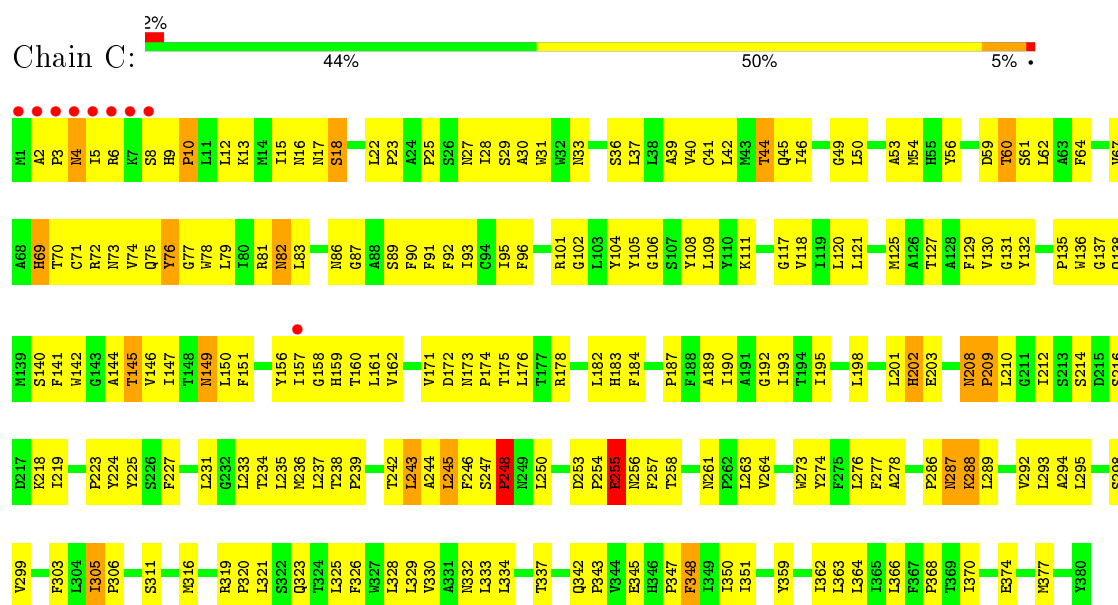


### • Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

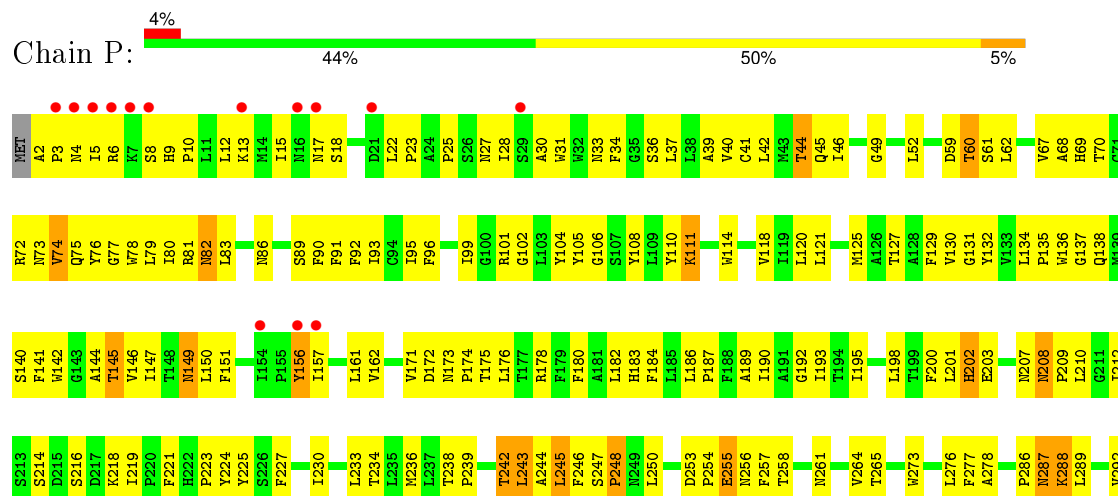




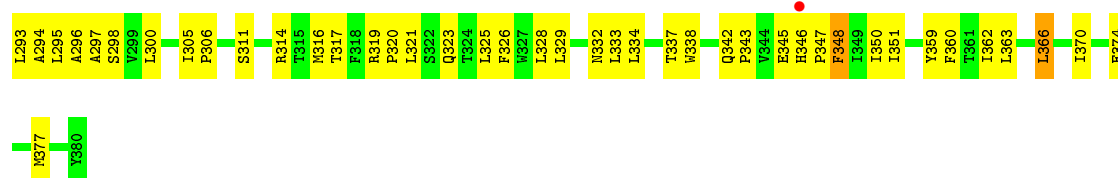
• Molecule 3: Cytochrome b



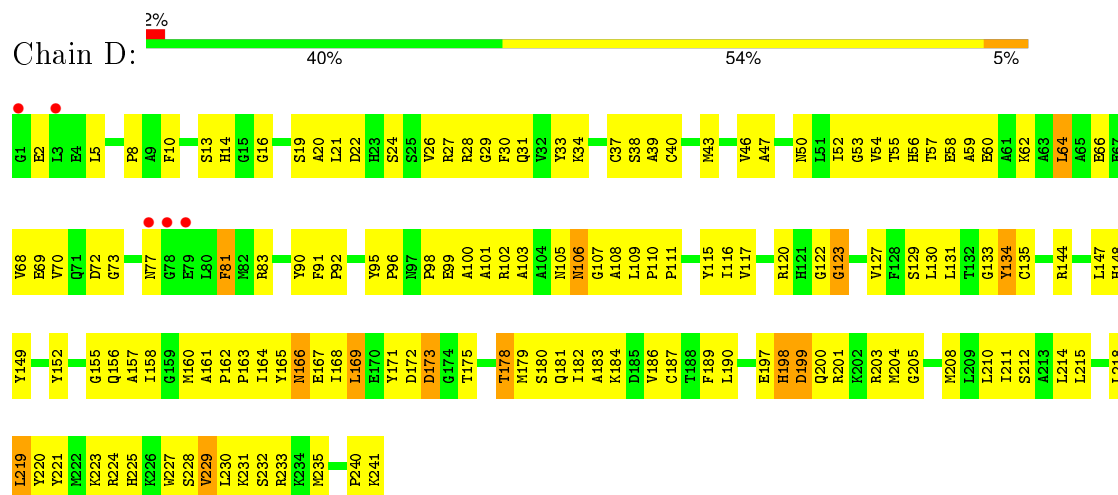
• Molecule 3: Cytochrome b



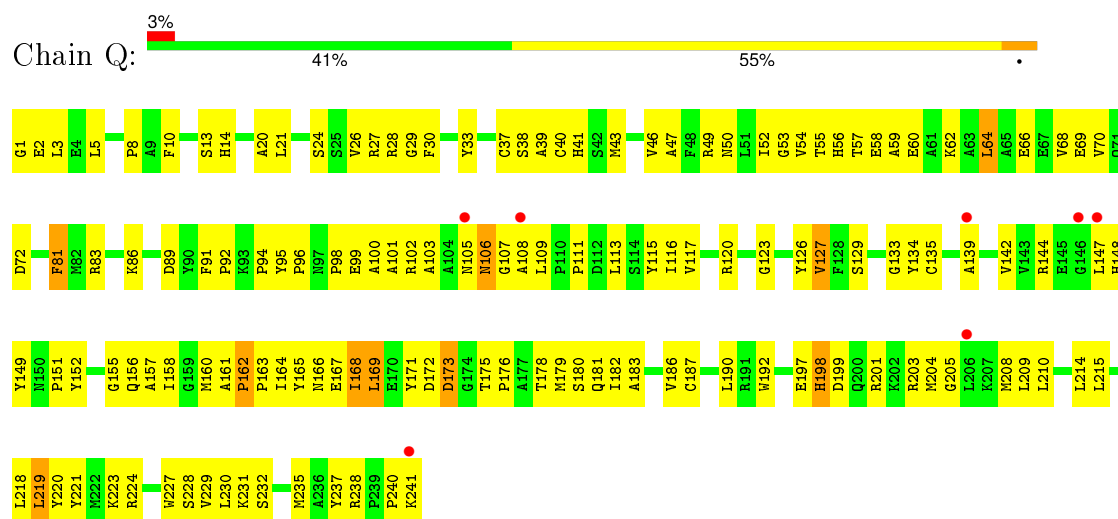




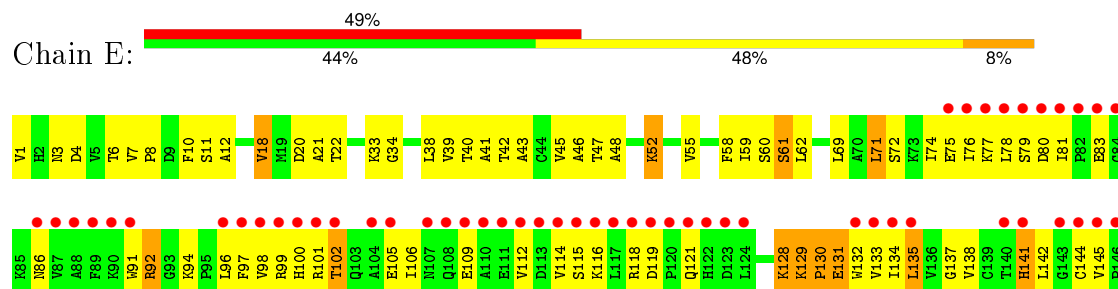
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

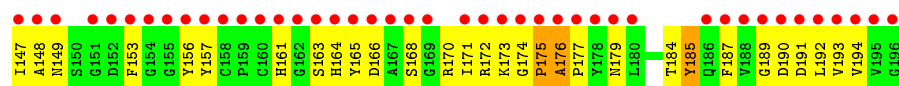


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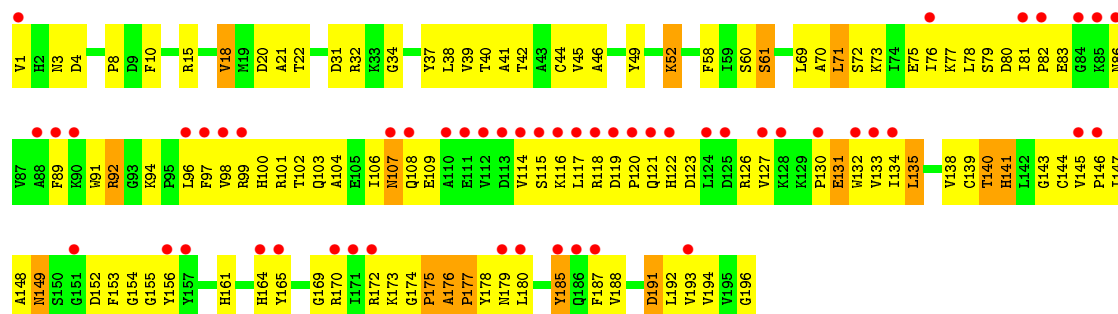
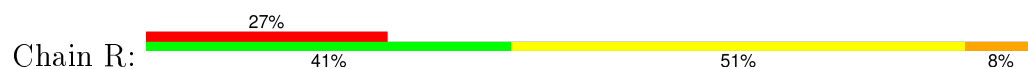


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

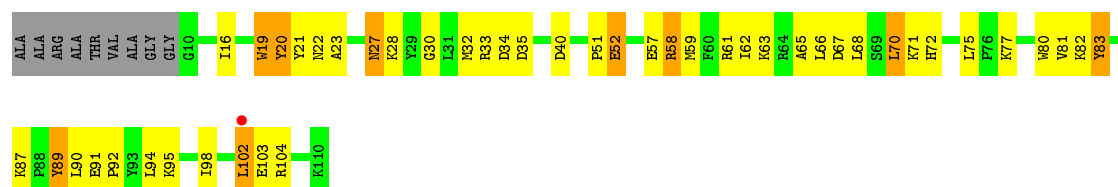




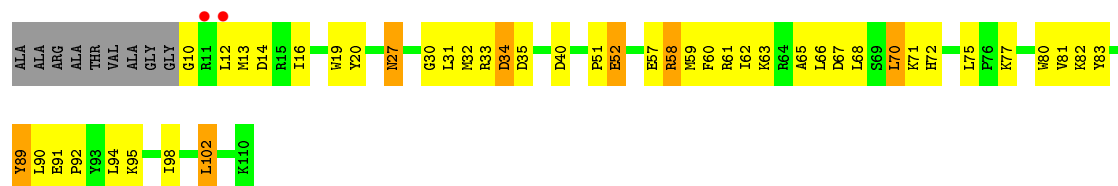
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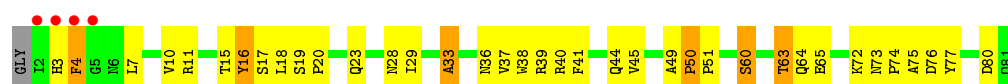
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



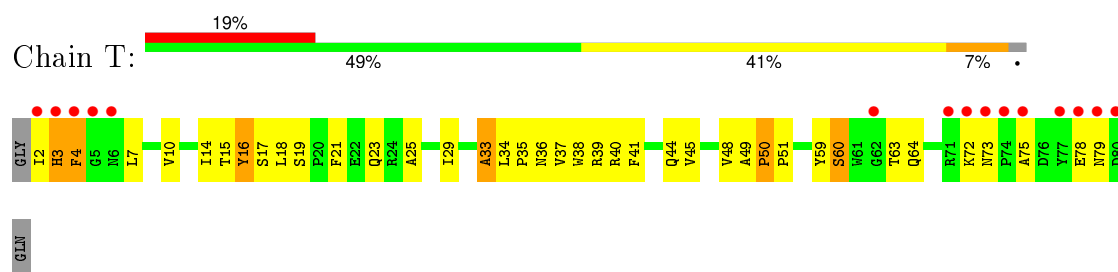
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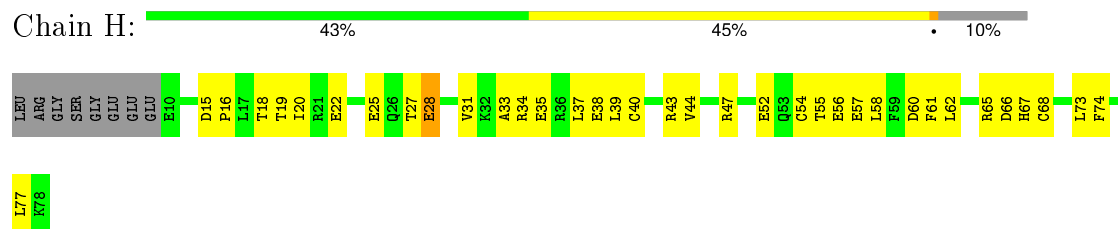
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



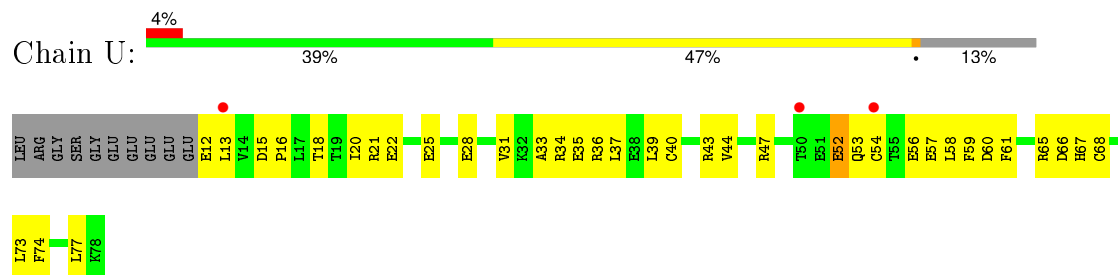
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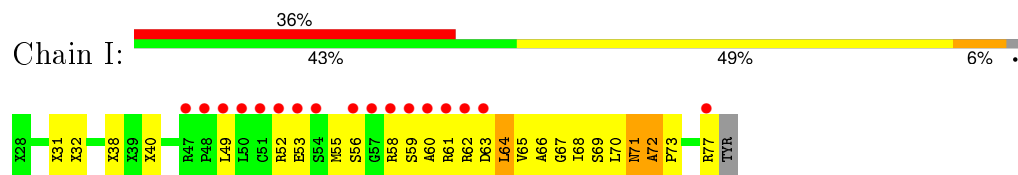
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



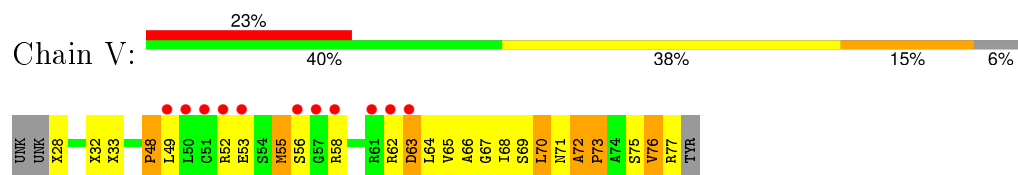
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

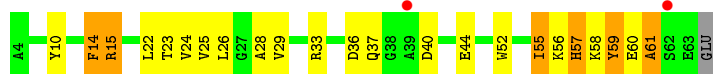


- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN





- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.72Å 181.30Å 241.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.48 42.60 – 3.48	Depositor EDS
% Data completeness (in resolution range)	89.7 (18.00-3.48) 89.7 (42.60-3.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.284 0.226 , 0.267	Depositor DCC
$R_{free}$ test set	2558 reflections (3.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 83.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 86926 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	32673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, IKR, CDL, UQ, FES, HEC, PEE, UNL, 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	0.48	0/3513	0.70	1/4760 (0.0%)
1	N	0.50	0/3508	0.70	1/4753 (0.0%)
2	B	0.41	0/3219	0.64	0/4364
2	O	0.46	0/3202	0.67	0/4343
3	C	0.54	0/3122	0.70	0/4273
3	P	0.48	0/3114	0.67	0/4263
4	D	0.52	0/1956	0.68	0/2658
4	Q	0.44	0/1956	0.65	0/2658
5	E	0.37	0/1547	0.56	0/2103
5	R	0.39	0/1547	0.59	0/2103
6	F	0.52	0/911	0.67	0/1219
6	S	0.45	0/911	0.61	0/1219
7	G	0.54	0/694	0.72	0/941
7	T	0.49	0/684	0.71	0/929
8	H	0.50	0/579	0.68	0/775
8	U	0.40	0/561	0.60	0/751
9	I	0.37	0/218	0.64	0/293
9	V	0.40	0/218	0.66	0/293
10	J	0.50	0/508	0.60	0/682
10	W	0.43	0/490	0.61	0/660
All	All	0.47	0/32458	0.66	2/44040 (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	2
4	D	0	1
6	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	432	LEU	N-CA-C	5.68	126.33	111.00
1	N	432	LEU	N-CA-C	5.29	125.30	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	56	TYR	Sidechain
3	C	76	TYR	Sidechain
4	D	134	TYR	Sidechain
6	F	20	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	3442	0	3354	261	0
1	N	3437	0	3349	280	0
2	B	3164	0	3158	303	0
2	O	3147	0	3146	336	0
3	C	3020	0	3070	240	0
3	P	3012	0	3058	231	0
4	D	1898	0	1846	167	0
4	Q	1898	0	1846	169	0
5	E	1513	0	1478	111	0
5	R	1513	0	1478	118	0
6	F	891	0	893	50	0
6	S	891	0	893	50	0
7	G	672	0	653	38	0
7	T	662	0	645	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	571	0	547	33	0
8	U	553	0	535	41	0
9	I	285	0	238	37	0
9	V	275	0	238	39	0
10	J	497	0	490	28	0
10	W	479	0	478	32	0
11	A	18	0	11	0	0
11	C	49	0	72	3	0
11	E	50	0	77	0	0
11	P	54	0	72	4	0
11	R	50	0	77	0	0
12	A	2	0	0	0	0
12	C	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
13	C	86	0	60	19	0
13	P	86	0	60	20	0
14	C	25	0	20	5	0
14	P	25	0	20	4	0
15	C	19	0	17	6	0
15	P	19	0	17	6	0
16	C	40	0	24	2	0
16	D	42	0	28	1	0
16	P	40	0	24	2	0
16	Q	42	0	28	3	0
17	C	1	0	0	0	0
17	P	1	0	0	0	0
18	C	6	0	8	1	0
18	P	6	0	8	1	0
19	D	43	0	30	2	0
19	Q	43	0	30	2	0
20	D	33	0	39	1	0
20	P	25	0	22	0	0
20	Q	20	0	28	0	0
21	E	4	0	0	3	0
21	R	4	0	0	2	0
22	A	1	0	0	0	0
22	C	7	0	0	1	0
22	E	1	0	0	0	0
22	P	7	0	0	3	0
22	R	1	0	0	1	0
All	All	32673	0	32165	2414	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 37.

All (2414) 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)
2:B:209:ILE:HG22	2:B:210:GLY:H	1.08	1.09
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.28	1.07
2:O:209:ILE:HG22	2:O:210:GLY:H	1.09	1.07
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.38	1.06
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.26	0.99
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.45	0.98
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.43	0.98
3:C:120:LEU:HD13	13:C:502:HEM:HBB2	1.44	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	0.97
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.47	0.97
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.45	0.96
4:D:158:ILE:HG12	4:D:160:MET:H	1.31	0.94
5:R:148:ALA:HA	5:R:156:TYR:HA	1.49	0.94
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.48	0.94
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.48	0.94
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.50	0.93
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.51	0.93
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.50	0.91
2:B:207:VAL:HG12	2:B:208:GLY:H	1.35	0.91
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.50	0.91
2:O:71:LEU:O	2:O:74:PRO:HD2	1.71	0.91
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.51	0.91
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.49	0.91
2:O:76:THR:HG22	2:O:82:SER:H	1.35	0.91
5:E:147:ILE:HG22	5:E:148:ALA:H	1.33	0.90
4:Q:43:MET:HE2	4:Q:46:VAL:HG21	1.52	0.90
1:A:206:LYS:O	1:A:209:VAL:HG12	1.71	0.90
2:B:327:ILE:HD11	9:I:58:ARG:O	1.71	0.90
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.52	0.90
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.52	0.89
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.37	0.89
4:D:57:THR:HG22	4:D:59:ALA:H	1.36	0.89
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.35	0.89
2:O:96:LEU:HB2	2:O:109:VAL:HG12	1.55	0.88
2:B:209:ILE:HG22	2:B:210:GLY:N	1.87	0.88
1:A:248:LEU:HD13	1:A:249:PRO:HD2	1.54	0.88
9:V:49:LEU:HB3	9:V:55:MET:HG2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.88
2:O:209:ILE:HG22	2:O:210:GLY:N	1.87	0.88
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.56	0.88
1:N:328:PRO:HG2	1:N:329:LEU:HD12	1.55	0.88
4:D:47:ALA:H	4:D:50:ASN:HD22	1.19	0.87
7:T:29:ILE:O	7:T:33:ALA:HB3	1.73	0.87
2:O:207:VAL:HG12	2:O:208:GLY:H	1.37	0.87
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.37	0.87
9:I:32:UNK:N	9:I:73:PRO:HG2	1.89	0.87
5:R:58:PHE:O	5:R:61:SER:HB3	1.75	0.86
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.38	0.86
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.40	0.86
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.55	0.86
2:B:102:ARG:HH11	2:B:102:ARG:HG2	1.38	0.86
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.38	0.86
1:N:248:LEU:HD13	1:N:249:PRO:HD2	1.56	0.85
2:B:71:LEU:O	2:B:74:PRO:HD2	1.75	0.85
2:O:201:SER:HB3	2:O:227:ARG:HB2	1.56	0.85
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.40	0.85
2:B:96:LEU:HB2	2:B:109:VAL:HG12	1.57	0.85
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.59	0.84
3:C:125:MET:HE2	14:C:2001:IKR:I1	2.48	0.84
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.60	0.83
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.13	0.83
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.60	0.83
1:N:206:LYS:O	1:N:209:VAL:HG12	1.77	0.83
3:C:125:MET:CE	14:C:2001:IKR:I1	2.96	0.82
3:C:253:ASP:OD1	3:C:255:GLU:HG2	1.79	0.82
2:O:201:SER:H	2:O:227:ARG:HB3	1.41	0.82
2:O:353:THR:HG22	2:O:355:GLU:H	1.43	0.82
2:O:209:ILE:CG2	2:O:210:GLY:H	1.91	0.81
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.63	0.81
2:O:353:THR:HB	2:O:356:ASP:OD1	1.81	0.81
2:B:209:ILE:CG2	2:B:210:GLY:H	1.91	0.81
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.77	0.81
2:O:100:SER:HB3	2:O:105:MET:HG2	1.61	0.81
6:S:89:TYR:HD1	6:S:90:LEU:N	1.79	0.81
3:C:118:VAL:N	13:C:502:HEM:HBC2	1.96	0.81
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.46	0.81
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.62	0.81
2:B:353:THR:HG22	2:B:355:GLU:H	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.22	0.80
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.46	0.80
2:B:71:LEU:HD11	2:B:144:LEU:HD23	1.62	0.80
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.63	0.80
9:V:49:LEU:HD22	9:V:55:MET:HB3	1.62	0.80
1:N:105:ASP:O	1:N:109:VAL:HG23	1.82	0.80
1:A:161:THR:HB	1:A:234:CYS:SG	2.22	0.80
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.62	0.80
1:N:161:THR:HB	1:N:234:CYS:SG	2.21	0.80
5:E:116:LYS:HD2	5:E:116:LYS:H	1.46	0.80
1:N:382:HIS:ND1	1:N:389:ARG:HD2	1.98	0.79
3:P:120:LEU:HD13	13:P:502:HEM:HBB2	1.65	0.79
2:B:100:SER:HB3	2:B:105:MET:HG2	1.63	0.79
7:G:29:ILE:O	7:G:33:ALA:HB3	1.81	0.79
3:P:138:GLN:HB2	3:P:255:GLU:O	1.83	0.79
1:N:134:ILE:HG21	1:N:174:ILE:HG12	1.65	0.78
3:P:253:ASP:OD1	3:P:255:GLU:HG2	1.83	0.78
2:B:122:TYR:O	2:B:126:VAL:HG23	1.83	0.78
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.23	0.78
1:A:328:PRO:HG2	1:A:329:LEU:HD12	1.64	0.78
2:O:221:GLU:HG3	2:O:222:GLN:H	1.48	0.78
4:Q:127:VAL:HG12	4:Q:187:CYS:SG	2.23	0.78
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.13	0.78
5:E:114:VAL:HG21	5:E:172:ARG:NH1	1.97	0.78
6:F:89:TYR:HD1	6:F:90:LEU:N	1.81	0.78
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.66	0.78
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.49	0.78
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.66	0.78
5:R:188:VAL:O	5:R:192:LEU:HB2	1.83	0.78
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.66	0.78
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.67	0.77
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.67	0.77
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.66	0.77
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.66	0.77
2:O:102:ARG:HG2	2:O:102:ARG:NH1	1.98	0.77
3:C:61:SER:O	3:C:62:LEU:HG	1.84	0.77
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.67	0.77
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.48	0.77
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.19	0.77
2:O:160:LEU:HB3	9:V:64:LEU:HD22	1.68	0.77
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:277:ILE:HD11	1:N:345:LEU:HD11	1.66	0.76
3:P:12:LEU:HD23	3:P:15:ILE:HD12	1.67	0.76
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.67	0.76
3:C:120:LEU:CD1	13:C:502:HEM:HBB2	2.15	0.76
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.47	0.76
3:P:145:THR:O	3:P:149:ASN:HB2	1.85	0.76
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.50	0.76
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.50	0.76
2:O:37:SER:HB2	2:O:213:HIS:ND1	2.01	0.76
2:O:156:GLN:HE22	9:V:77:ARG:C	1.88	0.76
2:O:341:MET:HE2	2:O:341:MET:HA	1.66	0.75
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.01	0.75
3:C:120:LEU:HB3	13:C:502:HEM:CBB	2.16	0.75
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.01	0.75
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.51	0.75
4:D:43:MET:CE	4:D:46:VAL:HG21	2.16	0.75
3:P:118:VAL:N	13:P:502:HEM:HBC2	2.02	0.75
1:N:170:THR:HG22	1:N:171:THR:H	1.51	0.75
2:B:353:THR:HB	2:B:356:ASP:OD1	1.87	0.74
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.52	0.74
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.04	0.74
1:A:362:ARG:O	1:A:365:MET:HG2	1.87	0.74
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.03	0.74
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.69	0.74
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.52	0.74
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.17	0.74
3:C:59:ASP:O	3:C:61:SER:N	2.20	0.74
1:N:80:GLU:HA	2:O:284:LEU:HD12	1.68	0.74
2:B:89:ILE:CD1	2:B:96:LEU:HD23	2.17	0.74
4:D:116:ILE:HG23	4:D:117:VAL:N	2.02	0.74
5:E:58:PHE:O	5:E:61:SER:HB3	1.88	0.74
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.70	0.74
3:P:173:ASN:N	3:P:174:PRO:HD2	2.03	0.74
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.21	0.74
1:N:106:MET:HG2	1:N:203:ILE:HD13	1.70	0.74
6:S:91:GLU:HB3	6:S:92:PRO:HD3	1.70	0.74
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.70	0.74
5:R:1:VAL:HG23	5:R:3:ASN:H	1.50	0.74
9:I:49:LEU:HD11	9:I:58:ARG:NH1	2.03	0.73
2:O:225:ASN:O	2:O:227:ARG:HG3	1.87	0.73
9:V:49:LEU:HB3	9:V:55:MET:CG	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD21	1:A:431:LEU:HD21	1.69	0.73
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.68	0.73
2:O:113:ARG:O	2:O:116:VAL:HG23	1.88	0.73
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.53	0.73
2:O:374:THR:HG22	2:O:376:GLN:H	1.53	0.73
1:A:106:MET:HG2	1:A:203:ILE:HD13	1.69	0.73
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.52	0.73
4:Q:43:MET:CE	4:Q:46:VAL:HG21	2.19	0.73
10:W:56:LYS:HG2	10:W:60:GLU:OE1	1.89	0.73
2:B:100:SER:CB	2:B:105:MET:HG2	2.19	0.73
19:Q:501:HEC:HMB1	19:Q:501:HEC:HBB3	1.71	0.73
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.71	0.72
2:O:295:LEU:O	2:O:299:VAL:HG23	1.89	0.72
3:P:214:SER:HB2	3:P:218:LYS:NZ	2.03	0.72
2:O:150:VAL:O	2:O:153:GLN:HB2	1.88	0.72
2:O:71:LEU:N	2:O:71:LEU:HD23	2.04	0.72
1:A:134:ILE:HG21	1:A:174:ILE:HG12	1.71	0.72
1:N:58:PHE:HB3	1:N:182:LEU:HD21	1.69	0.72
3:C:245:LEU:O	4:D:201:ARG:HD3	1.88	0.72
3:P:127:THR:O	3:P:130:VAL:HG22	1.90	0.72
2:O:100:SER:CB	2:O:105:MET:HG2	2.20	0.72
2:B:96:LEU:HG	9:I:70:LEU:HD13	1.71	0.72
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.23	0.72
2:O:122:TYR:O	2:O:126:VAL:HG23	1.90	0.72
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.53	0.72
9:I:49:LEU:HD22	9:I:55:MET:HG2	1.72	0.72
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.24	0.72
3:P:120:LEU:HB3	13:P:502:HEM:CBB	2.20	0.72
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.25	0.72
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.25	0.72
2:B:113:ARG:O	2:B:116:VAL:HG23	1.88	0.72
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.71	0.72
5:E:147:ILE:HG22	5:E:148:ALA:N	2.05	0.72
2:B:209:ILE:O	2:B:211:VAL:HG22	1.90	0.71
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.53	0.71
2:B:402:ILE:HG23	2:B:403:ASP:H	1.55	0.71
3:C:214:SER:HB2	3:C:218:LYS:NZ	2.05	0.71
2:O:274:VAL:O	2:O:278:VAL:HG23	1.90	0.71
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.24	0.71
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.25	0.71
5:E:1:VAL:HG23	5:E:3:ASN:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.30	0.71
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.26	0.71
3:C:92:PHE:O	3:C:95:ILE:HG22	1.90	0.71
3:C:236:MET:O	3:C:239:PRO:HD2	1.90	0.71
2:B:226:ILE:HG23	2:B:227:ARG:HD3	1.71	0.71
2:B:374:THR:HG22	2:B:376:GLN:H	1.56	0.71
1:N:37:VAL:HG12	1:N:199:ALA:HB2	1.73	0.71
2:B:18:CYS:HB3	2:B:19:PRO:HD3	1.70	0.71
3:C:173:ASN:N	3:C:174:PRO:HD2	2.05	0.71
2:B:295:LEU:O	2:B:299:VAL:HG23	1.91	0.71
2:B:280:GLY:HA3	2:B:293:SER:OG	1.91	0.70
2:O:361:LYS:O	2:O:365:LYS:HG3	1.90	0.70
2:O:154:SER:O	2:O:157:VAL:HG12	1.90	0.70
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.26	0.70
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.27	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.70
1:N:422:LEU:HD21	1:N:431:LEU:HD21	1.73	0.70
1:N:365:MET:HG3	1:N:366:VAL:N	2.07	0.70
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.71	0.70
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.91	0.70
5:R:148:ALA:HB2	5:R:156:TYR:CD2	2.27	0.70
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.73	0.70
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.06	0.70
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.74	0.70
4:D:57:THR:HB	4:D:60:GLU:HG3	1.74	0.70
3:C:138:GLN:HB2	3:C:255:GLU:O	1.92	0.70
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.73	0.70
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.73	0.70
1:A:342:TRP:O	1:A:345:LEU:HB2	1.92	0.69
2:B:76:THR:CG2	2:B:82:SER:H	2.04	0.69
2:B:341:MET:HE2	2:B:341:MET:HA	1.72	0.69
3:P:125:MET:HE2	14:P:3001:IKR:I1	2.61	0.69
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.07	0.69
3:P:247:SER:OG	3:P:250:LEU:HB2	1.92	0.69
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.07	0.69
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.07	0.69
3:C:238:THR:HB	3:C:239:PRO:HD3	1.74	0.69
2:O:287:ARG:HA	9:V:53:GLU:HG3	1.72	0.69
5:R:71:LEU:HD23	5:R:71:LEU:N	2.08	0.69
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.74	0.69
3:P:101:ARG:C	3:P:101:ARG:HD2	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.74	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.73	0.69
3:P:92:PHE:O	3:P:95:ILE:HG22	1.92	0.69
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.23	0.69
2:O:89:ILE:CD1	2:O:96:LEU:HD23	2.22	0.69
3:C:70:THR:HA	3:C:74:VAL:HG23	1.75	0.69
2:O:76:THR:CG2	2:O:82:SER:H	2.04	0.69
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.26	0.69
3:P:61:SER:O	3:P:62:LEU:HG	1.92	0.69
1:N:239:SER:HB2	7:T:17:SER:O	1.93	0.69
2:O:402:ILE:HG23	2:O:403:ASP:H	1.58	0.68
1:N:170:THR:HG22	1:N:171:THR:N	2.07	0.68
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.74	0.68
5:E:98:VAL:HG22	5:E:134:ILE:HG12	1.75	0.68
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.07	0.68
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.75	0.68
3:C:145:THR:O	3:C:149:ASN:HB2	1.94	0.68
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.75	0.68
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.27	0.68
10:W:40:ASP:O	10:W:44:GLU:HG3	1.94	0.68
1:A:106:MET:O	1:A:106:MET:HE2	1.94	0.68
1:N:369:LEU:HD12	1:N:392:LEU:HD21	1.74	0.68
2:O:201:SER:HB3	2:O:227:ARG:CB	2.24	0.68
1:A:433:ASP:OD2	1:A:435:ASN:HB2	1.94	0.68
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.75	0.68
3:C:12:LEU:HD23	3:C:15:ILE:HD12	1.76	0.68
5:R:98:VAL:HG22	5:R:134:ILE:HG12	1.73	0.68
1:A:170:THR:HG22	1:A:171:THR:H	1.59	0.68
1:A:45:SER:OG	1:A:92:ARG:HA	1.94	0.68
2:O:27:THR:HG22	2:O:28:LYS:N	2.08	0.68
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.59	0.68
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.76	0.68
1:N:106:MET:HE2	1:N:106:MET:O	1.94	0.67
4:D:20:ALA:HB1	4:D:199:ASP:OD2	1.94	0.67
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.76	0.67
1:A:117:VAL:HG23	1:A:118:GLN:N	2.09	0.67
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.24	0.67
1:N:439:SER:HA	1:N:442:TYR:CE2	2.28	0.67
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.88	0.67
2:O:35:ILE:O	2:O:213:HIS:HE1	1.77	0.67
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.28	0.67
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.75	0.67
1:N:161:THR:HG21	1:N:235:ARG:H	1.58	0.67
9:I:38:UNK:C	9:I:40:UNK:H	2.06	0.67
3:P:31:TRP:O	3:P:101:ARG:HG3	1.94	0.67
4:Q:52:ILE:O	4:Q:54:VAL:HG23	1.94	0.67
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.25	0.67
2:O:62:ASN:O	2:O:65:THR:HG22	1.94	0.67
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.77	0.67
2:B:274:VAL:O	2:B:278:VAL:HG23	1.95	0.67
2:B:97:SER:HB3	9:I:69:SER:HA	1.76	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.10	0.67
1:N:342:TRP:O	1:N:345:LEU:HB2	1.94	0.66
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.31	0.66
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.13	0.66
2:B:154:SER:O	2:B:157:VAL:HG12	1.95	0.66
1:A:80:GLU:HA	2:B:284:LEU:HD12	1.76	0.66
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.25	0.66
1:N:253:VAL:HG11	1:N:335:MET:HE1	1.77	0.66
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.24	0.66
2:B:306:PRO:HB3	9:I:52:ARG:HG3	1.77	0.66
3:C:125:MET:HE1	14:C:2001:IKR:I1	2.66	0.66
1:A:249:PRO:HG2	1:A:250:VAL:H	1.60	0.66
3:P:82:ASN:HD22	3:P:82:ASN:N	1.93	0.66
3:P:70:THR:HA	3:P:74:VAL:HG23	1.76	0.66
2:B:102:ARG:NH1	2:B:102:ARG:HG2	2.09	0.66
19:D:501:HEC:HBB3	19:D:501:HEC:HMB1	1.78	0.66
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.78	0.66
4:D:52:ILE:O	4:D:54:VAL:HG23	1.96	0.66
3:C:137:GLY:H	3:C:140:SER:HB2	1.61	0.66
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.26	0.66
3:C:36:SER:O	3:C:40:VAL:HG23	1.96	0.66
3:P:236:MET:O	3:P:239:PRO:HD2	1.95	0.66
5:R:69:LEU:O	5:R:72:SER:HB3	1.95	0.66
1:A:187:ASP:O	1:A:191:LYS:HE3	1.96	0.66
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	1.78	0.65
1:N:317:THR:HG23	1:N:318:GLY:N	2.10	0.65
1:N:10:ASN:OD1	2:O:19:PRO:HD2	1.96	0.65
2:O:262:ALA:O	2:O:320:GLY:HA3	1.96	0.65
1:A:365:MET:HG3	1:A:366:VAL:N	2.10	0.65
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.77	0.65
2:O:152:PHE:HE1	2:O:177:TYR:HD1	1.44	0.65
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.11	0.65
1:N:23:LEU:HD23	1:N:24:ARG:N	2.11	0.65
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.25	0.65
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.62	0.65
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.77	0.65
1:A:23:LEU:HD23	1:A:24:ARG:N	2.10	0.65
6:S:13:MET:HA	6:S:16:ILE:HD12	1.76	0.65
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.11	0.65
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.32	0.65
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.60	0.65
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.32	0.65
3:C:247:SER:OG	3:C:250:LEU:HB2	1.97	0.65
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.79	0.65
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.77	0.65
2:B:19:PRO:O	2:B:22:GLU:N	2.28	0.65
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.27	0.65
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.32	0.65
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.79	0.65
2:O:141:GLN:N	2:O:142:PRO:HD2	2.12	0.65
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.31	0.65
5:E:161:HIS:HB2	21:E:501:FES:S1	2.37	0.65
6:F:89:TYR:CD1	6:F:90:LEU:N	2.65	0.65
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.32	0.65
2:O:96:LEU:HG	9:V:70:LEU:HD13	1.78	0.64
1:A:27:SER:HA	1:A:199:ALA:O	1.97	0.64
6:F:89:TYR:HD1	6:F:90:LEU:H	1.45	0.64
2:O:209:ILE:O	2:O:211:VAL:HG22	1.97	0.64
4:D:47:ALA:H	4:D:50:ASN:ND2	1.91	0.64
2:B:150:VAL:O	2:B:153:GLN:HB2	1.96	0.64
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.79	0.64
10:J:14:PHE:CD2	10:J:14:PHE:N	2.64	0.64
3:C:198:LEU:HD13	15:C:2002:UQ:HM53	1.79	0.64
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.32	0.64
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.97	0.64
5:E:18:VAL:O	5:E:18:VAL:HG23	1.95	0.64
10:W:26:LEU:O	10:W:29:VAL:HB	1.97	0.64
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.27	0.64
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.79	0.64
5:R:161:HIS:HB2	21:R:501:FES:S1	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.78	0.64
5:R:78:LEU:HB2	5:R:191:ASP:HA	1.78	0.64
3:C:239:PRO:HA	3:C:242:THR:HB	1.79	0.64
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.26	0.64
2:O:438:GLU:O	2:O:439:LEU:HD23	1.97	0.64
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.27	0.64
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	1.79	0.64
3:P:238:THR:HB	3:P:239:PRO:HD3	1.77	0.64
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.80	0.64
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.80	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.31	0.64
7:T:41:PHE:O	7:T:45:VAL:HG23	1.96	0.64
5:E:71:LEU:HD23	5:E:71:LEU:N	2.13	0.64
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.80	0.64
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.80	0.64
4:D:186:VAL:O	4:D:190:LEU:HG	1.97	0.64
2:O:219:VAL:O	2:O:223:PHE:HB2	1.98	0.64
7:G:77:TYR:HA	7:G:80:ASP:OD2	1.98	0.64
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.24	0.63
5:E:78:LEU:HD12	5:E:190:ASP:O	1.97	0.63
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.99	0.63
1:N:362:ARG:O	1:N:365:MET:HG2	1.97	0.63
5:E:77:LYS:HE2	5:E:79:SER:OG	1.98	0.63
1:N:199:ALA:HA	1:N:376:CYS:SG	2.38	0.63
2:B:160:LEU:HB3	9:I:64:LEU:HD22	1.80	0.63
3:C:101:ARG:C	3:C:101:ARG:HD2	2.17	0.63
3:C:120:LEU:HD22	13:C:502:HEM:HBB2	1.79	0.63
2:B:144:LEU:HB2	2:B:183:ILE:CD1	2.28	0.63
1:N:342:TRP:HA	1:N:345:LEU:HD12	1.79	0.63
10:W:14:PHE:CD2	10:W:14:PHE:N	2.63	0.63
3:P:70:THR:HA	3:P:74:VAL:CG2	2.27	0.63
3:P:239:PRO:HA	3:P:242:THR:HB	1.78	0.63
3:C:323:GLN:O	3:C:326:PHE:HB3	1.98	0.63
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.29	0.63
5:R:148:ALA:O	5:R:149:ASN:HB2	1.96	0.63
1:N:103:SER:O	1:N:106:MET:HB2	1.99	0.63
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.33	0.63
4:D:102:ARG:NH1	4:D:107:GLY:O	2.32	0.63
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.78	0.63
4:D:33:TYR:HD1	4:D:37:CYS:HB2	1.63	0.63
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.97	0.63
3:C:127:THR:O	3:C:130:VAL:HG22	1.99	0.63
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.80	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.32	0.63
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.81	0.63
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.63
1:N:433:ASP:OD2	1:N:435:ASN:HB2	1.97	0.63
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.28	0.63
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.78	0.63
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.80	0.63
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.34	0.63
9:V:49:LEU:HD22	9:V:55:MET:CB	2.27	0.63
1:N:45:SER:OG	1:N:92:ARG:HA	1.98	0.63
6:S:89:TYR:CD1	6:S:90:LEU:N	2.65	0.62
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.81	0.62
5:E:69:LEU:O	5:E:72:SER:HB3	1.99	0.62
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.82	0.62
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.81	0.62
1:N:368:GLN:O	1:N:374:PRO:HB2	1.99	0.62
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.34	0.62
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.98	0.62
7:G:36:ASN:O	7:G:40:ARG:HG3	2.00	0.62
3:P:323:GLN:O	3:P:326:PHE:HB3	1.99	0.62
2:O:168:TYR:HB2	2:O:173:ALA:CB	2.27	0.62
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.26	0.62
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.82	0.62
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.15	0.62
5:R:126:ARG:HH21	5:R:170:ARG:HG2	1.65	0.62
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.34	0.62
2:O:31:ASN:N	2:O:31:ASN:HD22	1.98	0.62
3:C:82:ASN:HD22	3:C:82:ASN:N	1.97	0.62
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.82	0.62
1:N:112:LEU:O	1:N:116:VAL:HG23	2.00	0.62
2:B:402:ILE:HG23	2:B:403:ASP:N	2.14	0.62
4:Q:147:LEU:HD13	4:Q:157:ALA:HB1	1.81	0.62
1:A:163:LEU:HD22	1:A:314:TYR:CE1	2.35	0.62
4:D:232:SER:HB3	7:G:23:GLN:NE2	2.13	0.62
3:P:125:MET:CE	14:P:3001:IKR:I1	3.17	0.62
1:N:178:THR:HG22	1:N:179:ARG:N	2.15	0.62
3:C:59:ASP:C	3:C:61:SER:H	2.03	0.61
1:A:383:LEU:HD23	1:A:388:ARG:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:30:PHE:HE2	4:Q:64:LEU:HD11	1.65	0.61
3:C:254:PRO:O	3:C:256:ASN:N	2.32	0.61
9:V:65:VAL:HG12	9:V:66:ALA:N	2.15	0.61
3:P:234:THR:HG21	4:Q:219:LEU:HD13	1.82	0.61
1:N:270:LEU:HB3	1:N:320:PHE:HE1	1.64	0.61
3:P:242:THR:N	4:Q:208:MET:HE1	2.14	0.61
9:I:65:VAL:HG12	9:I:66:ALA:N	2.15	0.61
3:C:286:PRO:O	3:C:287:ASN:HB2	2.00	0.61
4:D:62:LYS:O	4:D:66:GLU:HG3	1.99	0.61
2:B:385:GLU:C	2:B:387:LEU:H	2.03	0.61
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.82	0.61
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.61
6:S:89:TYR:HD1	6:S:90:LEU:H	1.46	0.61
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.33	0.61
2:O:402:ILE:HG23	2:O:403:ASP:N	2.16	0.61
5:E:141:HIS:HB3	21:E:501:FES:S2	2.40	0.61
5:E:78:LEU:HD13	5:E:129:LYS:HE3	1.82	0.61
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.36	0.61
1:N:106:MET:HB3	1:N:107:PRO:CD	2.30	0.61
1:N:27:SER:HA	1:N:199:ALA:O	2.00	0.61
4:D:197:GLU:O	4:D:198:HIS:C	2.39	0.61
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.16	0.61
5:R:18:VAL:HG23	5:R:18:VAL:O	1.99	0.61
1:A:103:SER:O	1:A:106:MET:HB2	2.01	0.61
4:D:60:GLU:O	4:D:64:LEU:HB2	2.01	0.61
2:B:226:ILE:HD13	2:B:227:ARG:NH1	2.16	0.61
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.65	0.61
2:B:361:LYS:O	2:B:365:LYS:HG3	2.01	0.61
3:P:370:ILE:O	3:P:374:GLU:HB2	2.01	0.61
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.47	0.61
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.35	0.61
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.36	0.61
2:O:156:GLN:NE2	9:V:77:ARG:C	2.53	0.61
3:C:70:THR:HA	3:C:74:VAL:CG2	2.31	0.61
1:A:106:MET:HB3	1:A:107:PRO:CD	2.31	0.61
4:D:37:CYS:C	4:D:39:ALA:H	2.04	0.61
4:D:221:TYR:CD2	5:E:39:VAL:HG21	2.36	0.61
5:E:129:LYS:HE2	5:E:187:PHE:HE2	1.65	0.60
1:A:112:LEU:O	1:A:116:VAL:HG23	2.01	0.60
8:H:40:CYS:O	8:H:44:VAL:HG23	2.00	0.60
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:40:CYS:O	8:U:44:VAL:HG23	2.00	0.60
3:P:82:ASN:H	3:P:82:ASN:HD22	1.47	0.60
1:N:45:SER:HA	1:N:48:GLU:HG3	1.82	0.60
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.83	0.60
2:B:24:LEU:O	2:B:24:LEU:HD23	2.01	0.60
2:B:385:GLU:O	2:B:387:LEU:N	2.34	0.60
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.01	0.60
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.24	0.60
2:O:385:GLU:C	2:O:387:LEU:H	2.03	0.60
2:O:402:ILE:HD13	2:O:402:ILE:C	2.21	0.60
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.82	0.60
1:N:63:ALA:O	1:N:116:VAL:HG13	2.00	0.60
1:A:161:THR:HG21	1:A:235:ARG:H	1.66	0.60
2:B:141:GLN:N	2:B:142:PRO:HD2	2.16	0.60
2:B:187:THR:OG1	2:B:190:GLN:HG3	2.02	0.60
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.37	0.60
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.37	0.60
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.36	0.60
1:A:67:THR:HA	1:A:121:ALA:H	1.66	0.60
13:P:502:HEM:HBD1	22:P:384:HOH:O	2.02	0.60
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.01	0.60
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.16	0.60
4:D:197:GLU:HG2	4:D:198:HIS:N	2.15	0.60
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.34	0.60
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.84	0.60
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.01	0.60
2:O:402:ILE:O	2:O:405:VAL:HG23	2.00	0.60
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.84	0.60
7:G:41:PHE:O	7:G:45:VAL:HG23	2.01	0.60
2:O:76:THR:HG22	2:O:82:SER:N	2.13	0.60
2:B:76:THR:HG22	2:B:82:SER:N	2.14	0.60
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.84	0.60
4:Q:95:TYR:CE2	4:Q:101:ALA:HA	2.36	0.60
2:O:67:HIS:O	2:O:70:ARG:HB3	2.00	0.60
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.67	0.60
9:V:52:ARG:O	9:V:56:SER:HB3	2.02	0.60
2:B:67:HIS:O	2:B:70:ARG:HB3	2.02	0.60
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.22	0.60
4:D:158:ILE:CD1	4:D:160:MET:HB3	2.32	0.60
10:W:56:LYS:HE3	10:W:60:GLU:OE1	2.02	0.60
4:Q:37:CYS:C	4:Q:39:ALA:H	2.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:LEU:CG	13:C:502:HEM:HBB2	2.31	0.60
2:O:385:GLU:O	2:O:387:LEU:N	2.35	0.60
2:O:96:LEU:O	9:V:70:LEU:HD22	2.01	0.60
2:O:144:LEU:HB2	2:O:183:ILE:CD1	2.32	0.60
5:E:114:VAL:CG2	5:E:172:ARG:HH12	2.13	0.60
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.66	0.60
1:A:178:THR:HG22	1:A:179:ARG:N	2.17	0.60
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.66	0.59
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.66	0.59
5:E:94:LYS:HD3	5:E:138:VAL:HG21	1.82	0.59
4:Q:197:GLU:O	4:Q:198:HIS:C	2.40	0.59
8:U:35:GLU:O	8:U:39:LEU:HG	2.02	0.59
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.32	0.59
2:O:187:THR:OG1	2:O:190:GLN:HG3	2.01	0.59
15:C:2002:UQ:HM51	15:C:2002:UQ:C8	2.31	0.59
1:A:7:THR:HG21	2:B:113:ARG:NE	2.17	0.59
2:B:17:LEU:O	2:B:18:CYS:HB3	2.01	0.59
15:P:3002:UQ:HM51	15:P:3002:UQ:C8	2.32	0.59
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.34	0.59
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.84	0.59
3:P:129:PHE:HB2	14:P:3001:IKR:H40	1.83	0.59
6:F:71:LYS:O	6:F:72:HIS:HB2	2.01	0.59
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.83	0.59
6:F:27:ASN:O	6:F:30:GLY:N	2.30	0.59
1:A:317:THR:HG23	1:A:318:GLY:N	2.18	0.59
2:B:71:LEU:N	2:B:71:LEU:HD23	2.16	0.59
3:P:101:ARG:NH2	13:P:502:HEM:HBD2	2.18	0.59
1:N:187:ASP:O	1:N:191:LYS:HE3	2.03	0.59
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.33	0.59
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.37	0.59
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.32	0.59
2:B:152:PHE:HE1	2:B:177:TYR:HD1	1.50	0.59
9:I:31:UNK:C	9:I:73:PRO:HG2	2.32	0.59
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.16	0.59
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.37	0.59
1:A:48:GLU:HB3	1:A:52:ASN:OD1	2.03	0.59
1:N:90:THR:O	1:N:90:THR:HG23	2.02	0.59
5:R:169:GLY:O	5:R:179:ASN:HB3	2.02	0.59
4:D:220:TYR:OH	4:D:224:ARG:HD3	2.02	0.59
3:C:347:PRO:O	3:C:350:ILE:HG22	2.02	0.59
2:O:132:PHE:HB2	2:O:192:HIS:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:PHE:CD2	3:P:184:PHE:CD2	2.91	0.59
1:A:105:ASP:O	1:A:109:VAL:HG23	2.02	0.59
1:N:261:GLY:HA2	1:N:317:THR:O	2.03	0.59
1:A:18:THR:HG23	1:A:24:ARG:HG2	1.85	0.59
3:P:294:ALA:O	3:P:298:SER:HB3	2.03	0.59
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.68	0.58
2:B:402:ILE:HD13	2:B:402:ILE:C	2.23	0.58
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.03	0.58
5:E:144:CYS:HB2	21:E:501:FES:S2	2.43	0.58
1:N:163:LEU:HD22	1:N:314:TYR:CE1	2.38	0.58
2:B:438:GLU:O	2:B:439:LEU:HD23	2.03	0.58
5:E:52:LYS:C	5:E:52:LYS:HD3	2.23	0.58
2:B:57:TYR:CD1	2:B:57:TYR:N	2.70	0.58
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.18	0.58
2:B:306:PRO:CB	9:I:52:ARG:HG3	2.33	0.58
2:O:75:LEU:HD11	2:O:140:LEU:CD2	2.32	0.58
3:P:316:MET:HG2	3:P:319:ARG:HH21	1.68	0.58
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.19	0.58
4:D:223:LYS:HD3	4:D:223:LYS:C	2.24	0.58
3:C:294:ALA:O	3:C:298:SER:HB3	2.03	0.58
2:O:156:GLN:NE2	9:V:77:ARG:O	2.36	0.58
9:I:63:ASP:CG	9:I:64:LEU:H	2.05	0.58
1:N:249:PRO:HG2	1:N:250:VAL:H	1.67	0.58
2:B:20:GLY:O	2:B:21:ALA:HB3	2.03	0.58
1:N:307:PHE:CD1	1:N:307:PHE:C	2.77	0.58
3:P:347:PRO:O	3:P:350:ILE:HG22	2.04	0.58
3:P:286:PRO:O	3:P:287:ASN:HB2	2.03	0.58
4:D:231:LYS:O	6:F:71:LYS:HE3	2.03	0.58
2:B:96:LEU:O	9:I:70:LEU:HD22	2.03	0.58
1:N:86:PHE:CD2	1:N:99:ILE:HD11	2.37	0.58
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.86	0.58
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.21	0.58
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.69	0.58
3:P:137:GLY:H	3:P:140:SER:HB2	1.68	0.58
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.33	0.58
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.38	0.58
4:Q:43:MET:HE2	4:Q:46:VAL:CG2	2.28	0.58
2:B:281:ALA:HB2	2:B:311:ALA:HB3	1.86	0.58
1:A:239:SER:HB2	7:G:17:SER:O	2.04	0.58
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.34	0.58
2:B:402:ILE:O	2:B:405:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:PHE:CD1	2:B:308:ASP:N	2.72	0.58
1:A:90:THR:O	1:A:90:THR:HG23	2.04	0.58
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.18	0.58
5:R:52:LYS:HD3	5:R:52:LYS:C	2.23	0.58
4:Q:180:SER:OG	8:U:77:LEU:HD21	2.03	0.58
2:B:394:ALA:HB1	2:B:395:PRO:HD2	1.85	0.58
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.38	0.58
3:C:320:PRO:HG2	3:C:321:LEU:H	1.67	0.58
1:A:368:GLN:O	1:A:374:PRO:HB2	2.02	0.58
2:O:318:ASP:O	2:O:319:SER:HB2	2.04	0.58
6:S:65:ALA:O	6:S:68:LEU:HB2	2.04	0.58
3:P:214:SER:HB2	3:P:218:LYS:HZ1	1.69	0.58
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.18	0.58
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.39	0.58
3:C:82:ASN:H	3:C:82:ASN:HD22	1.52	0.58
2:O:247:GLN:HE21	2:O:249:GLY:H	1.50	0.58
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.19	0.58
1:A:261:GLY:HA2	1:A:317:THR:O	2.04	0.58
1:N:354:VAL:HG23	1:N:355:LYS:N	2.19	0.58
9:V:49:LEU:HD13	9:V:55:MET:HB3	1.85	0.57
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.03	0.57
3:P:2:ALA:CB	3:P:8:SER:HB3	2.33	0.57
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.85	0.57
2:B:37:SER:HB2	2:B:213:HIS:ND1	2.19	0.57
3:C:362:ILE:HG22	3:C:363:LEU:N	2.19	0.57
1:A:137:GLU:O	1:A:141:MET:HG3	2.04	0.57
6:S:71:LYS:O	6:S:72:HIS:HB2	2.04	0.57
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.39	0.57
3:P:101:ARG:HD2	3:P:102:GLY:N	2.18	0.57
1:N:439:SER:C	1:N:441:MET:H	2.06	0.57
3:C:370:ILE:O	3:C:374:GLU:HB2	2.03	0.57
4:D:235:MET:HB3	7:G:15:THR:HG22	1.85	0.57
3:C:187:PRO:HG2	13:C:501:HEM:HMC3	1.85	0.57
4:D:57:THR:CB	4:D:60:GLU:HG3	2.35	0.57
2:O:57:TYR:CE2	2:O:234:SER:HB2	2.38	0.57
2:O:96:LEU:C	2:O:96:LEU:HD12	2.25	0.57
2:O:294:LYS:HE3	2:O:356:ASP:OD2	2.05	0.57
8:U:73:LEU:O	8:U:73:LEU:HD12	2.03	0.57
4:Q:181:GLN:CA	8:U:77:LEU:HD22	2.34	0.57
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.84	0.57
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.40	0.57
2:O:399:ALA:O	2:O:402:ILE:HG22	2.05	0.57
9:V:72:ALA:HB1	9:V:73:PRO:HD3	1.87	0.57
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.33	0.57
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.34	0.57
6:S:75:LEU:O	6:S:80:TRP:NE1	2.31	0.57
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.87	0.57
4:Q:5:LEU:HG	4:Q:152:TYR:HE1	1.69	0.57
1:N:307:PHE:HA	1:N:323:HIS:O	2.04	0.57
2:O:407:SER:O	2:O:411:VAL:HG23	2.04	0.57
1:A:439:SER:HA	1:A:442:TYR:CE2	2.39	0.57
2:B:262:ALA:O	2:B:320:GLY:HA3	2.05	0.57
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.86	0.57
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.04	0.57
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.86	0.57
1:N:117:VAL:HG23	1:N:118:GLN:N	2.19	0.57
2:B:207:VAL:HG12	2:B:208:GLY:N	2.12	0.57
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.87	0.57
3:C:147:ILE:HG13	14:C:2001:IKR:H16A	1.87	0.57
3:P:59:ASP:C	3:P:61:SER:H	2.08	0.57
1:A:90:THR:O	1:A:167:VAL:HG11	2.04	0.57
5:R:116:LYS:O	5:R:117:LEU:HG	2.05	0.57
3:C:64:PHE:CE1	18:C:2011:GOL:H2	2.39	0.57
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.39	0.57
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.86	0.57
5:E:12:ALA:HB1	7:G:28:ASN:HD21	1.70	0.57
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.87	0.57
2:O:96:LEU:CB	2:O:109:VAL:HG12	2.32	0.57
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.85	0.57
2:B:150:VAL:CG2	2:B:151:ALA:N	2.68	0.57
2:O:57:TYR:N	2:O:57:TYR:CD1	2.73	0.56
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	2.88	0.56
3:P:59:ASP:O	3:P:61:SER:N	2.38	0.56
3:P:198:LEU:HD13	15:P:3002:UQ:HM53	1.87	0.56
2:O:394:ALA:HB1	2:O:395:PRO:HD2	1.87	0.56
1:N:280:TYR:O	1:N:306:SER:HA	2.04	0.56
3:C:261:ASN:ND2	3:C:264:VAL:H	2.03	0.56
4:Q:221:TYR:HE1	7:T:25:ALA:CB	2.18	0.56
2:B:393:THR:HG22	2:B:397:VAL:HB	1.86	0.56
5:E:94:LYS:HB3	5:E:138:VAL:CG2	2.36	0.56
5:R:94:LYS:HD3	5:R:138:VAL:HG21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:O	1:A:79:VAL:HG23	2.05	0.56
4:Q:43:MET:HG2	4:Q:46:VAL:HG23	1.87	0.56
1:A:63:ALA:O	1:A:116:VAL:HG13	2.06	0.56
3:P:120:LEU:HD22	13:P:502:HEM:HBB2	1.87	0.56
2:O:268:GLU:O	2:O:268:GLU:HG2	2.05	0.56
1:A:365:MET:CG	1:A:366:VAL:N	2.68	0.56
1:A:7:THR:HG21	2:B:113:ARG:CD	2.35	0.56
2:B:306:PRO:HA	9:I:52:ARG:HE	1.71	0.56
1:A:307:PHE:CD1	1:A:307:PHE:C	2.78	0.56
4:Q:33:TYR:HD1	4:Q:37:CYS:HB2	1.70	0.56
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.39	0.56
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.41	0.56
1:A:280:TYR:O	1:A:306:SER:HA	2.04	0.56
2:O:281:ALA:HB2	2:O:311:ALA:HB3	1.87	0.56
4:Q:60:GLU:O	4:Q:64:LEU:HB2	2.05	0.56
2:O:424:MET:HG2	2:O:425:ALA:N	2.20	0.56
2:B:168:TYR:N	2:B:168:TYR:CD1	2.72	0.56
3:C:129:PHE:HB2	14:C:2001:IKR:H40	1.87	0.56
2:O:403:ASP:C	2:O:405:VAL:H	2.08	0.56
2:O:437:ASP:OD1	2:O:438:GLU:HG3	2.06	0.56
1:A:344:ARG:NH2	1:A:353:GLU:OE2	2.38	0.56
1:A:266:ASP:HA	1:A:269:VAL:HG23	1.87	0.56
3:C:33:ASN:HB3	22:C:1008:HOH:O	2.05	0.56
2:B:168:TYR:N	2:B:168:TYR:HD1	2.04	0.56
5:R:99:ARG:NH2	5:R:149:ASN:HD22	2.04	0.56
3:P:95:ILE:CD1	3:P:121:LEU:HD13	2.30	0.56
4:Q:30:PHE:CE2	4:Q:64:LEU:HD11	2.40	0.56
2:B:294:LYS:HE3	2:B:356:ASP:OD2	2.05	0.56
8:U:44:VAL:HG22	8:U:52:GLU:OE1	2.06	0.56
1:A:270:LEU:HD13	1:A:320:PHE:CD1	2.41	0.56
2:O:146:VAL:O	2:O:149:ALA:N	2.33	0.56
10:J:26:LEU:O	10:J:29:VAL:HB	2.06	0.56
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.72	0.56
2:O:207:VAL:HG12	2:O:208:GLY:N	2.15	0.56
2:B:247:GLN:HE21	2:B:249:GLY:H	1.53	0.56
1:N:365:MET:CG	1:N:366:VAL:N	2.67	0.56
2:O:75:LEU:HD11	2:O:140:LEU:HD23	1.88	0.56
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.88	0.56
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.87	0.56
9:I:49:LEU:HD13	9:I:55:MET:CE	2.35	0.56
10:W:57:HIS:HA	10:W:60:GLU:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.36	0.56
1:A:350:THR:OG1	1:A:353:GLU:HG3	2.05	0.56
1:A:242:ARG:NH2	1:A:432:LEU:HA	2.21	0.56
1:N:277:ILE:HB	1:N:309:THR:HG21	1.88	0.56
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.88	0.56
1:A:277:ILE:HB	1:A:309:THR:HG21	1.88	0.56
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.06	0.56
2:O:37:SER:CB	2:O:213:HIS:ND1	2.69	0.56
9:V:65:VAL:CG1	9:V:66:ALA:N	2.69	0.56
5:R:76:ILE:HG23	5:R:89:PHE:CZ	2.41	0.56
1:A:16:VAL:O	1:A:17:THR:HG23	2.06	0.56
2:B:345:LYS:O	2:B:348:ALA:N	2.39	0.56
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.88	0.56
10:J:59:TYR:CD1	10:J:59:TYR:N	2.73	0.55
4:Q:40:CYS:HA	4:Q:95:TYR:HE1	1.70	0.55
5:E:101:ARG:HB3	5:E:105:GLU:OE1	2.07	0.55
5:R:100:HIS:CD2	5:R:131:GLU:HB2	2.41	0.55
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.21	0.55
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.42	0.55
1:A:180:ALA:O	1:A:183:ALA:HB3	2.06	0.55
4:D:100:ALA:O	4:D:103:ALA:HB3	2.06	0.55
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.41	0.55
2:O:280:GLY:HA3	2:O:293:SER:OG	2.06	0.55
6:F:75:LEU:O	6:F:80:TRP:NE1	2.32	0.55
1:A:199:ALA:HA	1:A:376:CYS:SG	2.46	0.55
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.88	0.55
6:F:61:ARG:HG3	6:F:61:ARG:HH11	1.72	0.55
2:O:259:THR:HG22	2:O:260:GLU:N	2.22	0.55
1:A:270:LEU:HB3	1:A:320:PHE:HE1	1.71	0.55
5:R:82:PRO:O	5:R:100:HIS:HB3	2.05	0.55
1:A:354:VAL:HG23	1:A:355:LYS:N	2.22	0.55
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.89	0.55
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.87	0.55
4:Q:231:LYS:HA	6:S:71:LYS:HG2	1.88	0.55
1:N:143:ASN:HA	1:N:145:MET:HE1	1.88	0.55
9:I:65:VAL:CG1	9:I:66:ALA:N	2.69	0.55
4:Q:167:GLU:C	4:Q:169:LEU:H	2.10	0.55
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.06	0.55
3:P:36:SER:O	3:P:40:VAL:HG23	2.06	0.55
4:Q:20:ALA:HB1	4:Q:199:ASP:OD2	2.05	0.55
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:70:LEU:HD23	9:V:71:ASN:N	2.21	0.55
3:P:172:ASP:C	3:P:174:PRO:HD2	2.26	0.55
1:A:433:ASP:O	1:A:437:ILE:HG13	2.06	0.55
2:O:307:PHE:H	9:V:52:ARG:HG2	1.72	0.55
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.86	0.55
4:D:24:SER:OG	10:J:55:ILE:HG21	2.07	0.55
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.89	0.55
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.42	0.55
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.89	0.55
2:O:27:THR:HG22	2:O:28:LYS:H	1.72	0.55
1:N:253:VAL:HG11	1:N:335:MET:CE	2.35	0.55
5:E:55:VAL:O	5:E:59:ILE:HG12	2.06	0.55
8:H:43:ARG:HD2	8:H:47:ARG:CZ	2.37	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.42	0.55
8:H:65:ARG:O	8:H:68:CYS:HB3	2.07	0.55
3:C:120:LEU:HB3	13:C:502:HEM:HBB2	1.87	0.55
1:N:134:ILE:HG21	1:N:174:ILE:CG1	2.35	0.55
1:N:67:THR:HA	1:N:121:ALA:H	1.70	0.55
2:O:166:ALA:HA	2:O:240:TRP:CZ3	2.42	0.55
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.35	0.55
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.42	0.55
3:C:377:MET:CE	6:F:20:TYR:HB2	2.37	0.55
1:A:87:ASN:HB3	1:A:98:TYR:CZ	2.42	0.55
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.42	0.55
9:V:65:VAL:H	9:V:77:ARG:HB2	1.72	0.55
2:B:424:MET:HG2	2:B:425:ALA:N	2.21	0.55
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.42	0.55
3:C:350:ILE:HG23	3:C:351:ILE:N	2.22	0.55
4:D:171:TYR:HD1	4:D:175:THR:HB	1.72	0.55
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.71	0.55
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.55
3:P:95:ILE:O	3:P:99:ILE:HG13	2.07	0.55
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.71	0.55
9:V:32:UNK:O	9:V:33:UNK:C	2.54	0.55
4:Q:100:ALA:O	4:Q:103:ALA:HB3	2.06	0.55
2:B:58:GLU:OE1	2:B:64:GLY:N	2.39	0.55
3:C:31:TRP:O	3:C:101:ARG:HG3	2.07	0.54
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.36	0.54
10:W:59:TYR:N	10:W:59:TYR:CD1	2.74	0.54
1:N:107:PRO:O	1:N:109:VAL:N	2.40	0.54
3:C:214:SER:HB2	3:C:218:LYS:HZ1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:GLY:N	3:C:140:SER:HB2	2.22	0.54
4:Q:148:HIS:CD2	4:Q:148:HIS:N	2.75	0.54
4:D:116:ILE:CG2	4:D:117:VAL:N	2.70	0.54
3:P:244:ALA:O	3:P:245:LEU:HD23	2.08	0.54
1:A:45:SER:HA	1:A:48:GLU:HG3	1.87	0.54
1:N:333:ASP:O	1:N:336:PHE:HB3	2.07	0.54
1:N:212:ALA:O	1:N:216:PHE:HB2	2.07	0.54
2:O:97:SER:HB3	9:V:69:SER:HA	1.88	0.54
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.72	0.54
1:N:266:ASP:HA	1:N:269:VAL:HG23	1.89	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.89	0.54
1:N:90:THR:O	1:N:167:VAL:HG11	2.07	0.54
5:R:118:ARG:NH2	5:R:174:GLY:O	2.41	0.54
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.42	0.54
1:N:19:LEU:O	1:N:21:ASN:N	2.40	0.54
1:N:22:GLY:O	1:N:193:PRO:HA	2.08	0.54
6:F:32:MET:CE	6:F:87:LYS:HG2	2.37	0.54
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.07	0.54
2:B:115:HIS:O	2:B:119:VAL:HG23	2.07	0.54
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.07	0.54
4:Q:10:PHE:HD2	8:U:74:PHE:CE2	2.26	0.54
1:N:90:THR:HA	1:N:95:THR:HA	1.88	0.54
2:B:146:VAL:O	2:B:149:ALA:N	2.35	0.54
3:C:141:PHE:O	3:C:144:ALA:HB3	2.07	0.54
1:N:107:PRO:HG2	1:N:108:LYS:H	1.73	0.54
1:N:62:LEU:CD1	1:N:127:ILE:HG12	2.37	0.54
2:O:374:THR:HG22	2:O:376:GLN:N	2.22	0.54
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.28	0.54
2:O:107:TYR:CG	2:O:127:THR:HG22	2.43	0.54
5:R:99:ARG:NH2	5:R:149:ASN:ND2	2.55	0.54
2:B:399:ALA:O	2:B:402:ILE:HG22	2.07	0.54
2:B:403:ASP:C	2:B:405:VAL:H	2.10	0.54
5:E:142:LEU:O	3:P:265:THR:N	2.39	0.54
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.89	0.54
2:B:318:ASP:O	2:B:319:SER:HB2	2.08	0.54
1:A:304:CYS:HB2	1:A:325:VAL:O	2.08	0.54
1:N:75:PHE:O	1:N:79:VAL:HG23	2.08	0.54
8:H:20:ILE:HD12	8:H:73:LEU:HA	1.88	0.54
2:B:333:ALA:O	2:B:337:ILE:HG13	2.08	0.54
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.37	0.54
5:E:76:ILE:O	5:E:193:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:LEU:HD13	4:D:157:ALA:HB1	1.89	0.54
8:U:25:GLU:HG2	8:U:61:PHE:HZ	1.71	0.54
5:E:116:LYS:HD2	5:E:116:LYS:N	2.19	0.54
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.43	0.54
6:S:13:MET:HA	6:S:16:ILE:CD1	2.37	0.54
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.42	0.54
6:F:51:PRO:O	6:F:52:GLU:C	2.45	0.54
4:D:56:HIS:HB3	4:D:60:GLU:HB2	1.90	0.54
3:P:189:ALA:O	3:P:193:ILE:HG13	2.08	0.54
8:H:35:GLU:O	8:H:39:LEU:HG	2.08	0.54
9:I:49:LEU:HB3	9:I:55:MET:SD	2.48	0.54
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.38	0.54
2:B:259:THR:HG22	2:B:260:GLU:N	2.22	0.54
1:N:25:VAL:HG22	1:N:197:LEU:HB3	1.90	0.54
2:O:115:HIS:O	2:O:119:VAL:HG23	2.08	0.53
3:C:244:ALA:O	3:C:245:LEU:HD23	2.09	0.53
4:Q:5:LEU:HG	4:Q:152:TYR:CE1	2.43	0.53
3:P:147:ILE:HG13	14:P:3001:IKR:H16A	1.89	0.53
3:C:9:HIS:HD2	3:C:12:LEU:H	1.56	0.53
1:N:48:GLU:HB3	1:N:52:ASN:OD1	2.08	0.53
1:A:307:PHE:HA	1:A:323:HIS:O	2.09	0.53
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.89	0.53
2:O:393:THR:HG22	2:O:397:VAL:HB	1.89	0.53
2:B:201:SER:OG	2:B:228:SER:HA	2.08	0.53
1:A:3:THR:HG23	1:A:6:GLN:OE1	2.08	0.53
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.43	0.53
4:D:27:ARG:O	4:D:30:PHE:HB3	2.08	0.53
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.35	0.53
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.89	0.53
5:R:109:GLU:OE1	5:R:123:ASP:HB2	2.08	0.53
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.90	0.53
2:O:306:PRO:HB3	9:V:52:ARG:N	2.23	0.53
3:C:254:PRO:C	3:C:256:ASN:N	2.61	0.53
1:N:383:LEU:HD23	1:N:388:ARG:O	2.09	0.53
2:B:227:ARG:N	2:B:227:ARG:HD3	2.23	0.53
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.53
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.39	0.53
2:B:31:ASN:HD22	2:B:31:ASN:N	2.05	0.53
1:N:147:ASN:O	1:N:148:VAL:C	2.47	0.53
3:C:254:PRO:C	3:C:256:ASN:H	2.12	0.53
3:P:78:TRP:CD2	3:P:79:LEU:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:170:ARG:HG2	5:R:179:ASN:ND2	2.24	0.53
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.90	0.53
2:O:201:SER:CB	2:O:227:ARG:HB2	2.32	0.53
1:N:158:PHE:O	1:N:159:GLN:O	2.27	0.53
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.44	0.53
2:O:26:ILE:HG23	2:O:26:ILE:O	2.08	0.53
2:O:287:ARG:CA	9:V:53:GLU:HG3	2.39	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.44	0.53
1:N:318:GLY:O	1:N:319:LEU:HD23	2.08	0.53
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.39	0.53
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.44	0.53
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.90	0.53
3:C:130:VAL:HG23	3:C:131:GLY:N	2.23	0.53
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.53
3:P:142:TRP:HA	3:P:145:THR:OG1	2.08	0.53
2:B:19:PRO:O	2:B:20:GLY:C	2.45	0.53
4:Q:52:ILE:O	4:Q:54:VAL:N	2.41	0.53
4:D:28:ARG:O	4:D:31:GLN:N	2.42	0.53
1:A:145:MET:HB2	1:A:252:HIS:NE2	2.24	0.53
8:H:73:LEU:HD12	8:H:73:LEU:O	2.09	0.53
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.43	0.53
3:P:273:TRP:HA	3:P:276:LEU:HG	1.91	0.53
4:D:148:HIS:CE1	4:D:161:ALA:HA	2.42	0.53
3:P:243:LEU:HD12	3:P:243:LEU:C	2.27	0.53
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.90	0.53
6:S:70:LEU:HG	6:S:71:LYS:N	2.23	0.53
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.09	0.53
1:N:433:ASP:O	1:N:437:ILE:HG13	2.07	0.53
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.44	0.53
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.91	0.53
16:P:3004:CDL:HA31	7:T:40:ARG:HB3	1.90	0.53
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.44	0.53
8:U:20:ILE:HD12	8:U:73:LEU:HA	1.91	0.53
1:N:277:ILE:CD1	1:N:345:LEU:HD11	2.39	0.53
3:C:4:ASN:O	3:C:5:ILE:HD13	2.09	0.53
4:Q:27:ARG:CZ	10:W:59:TYR:HE2	2.21	0.53
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.91	0.53
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.44	0.53
1:N:134:ILE:CG2	1:N:174:ILE:HG12	2.36	0.53
3:P:9:HIS:HD2	3:P:12:LEU:H	1.57	0.53
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:52:ASN:O	1:N:53:ASN:C	2.46	0.53
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.90	0.53
5:R:15:ARG:HD2	7:T:21:PHE:O	2.09	0.53
7:G:63:THR:HG22	7:G:64:GLN:N	2.23	0.53
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.44	0.53
3:C:101:ARG:HD2	3:C:102:GLY:N	2.23	0.53
4:D:180:SER:OG	8:H:77:LEU:HD21	2.08	0.53
3:P:120:LEU:CD1	13:P:502:HEM:HBB2	2.38	0.53
6:S:16:ILE:O	6:S:19:TRP:HB3	2.09	0.53
3:C:350:ILE:CG2	3:C:351:ILE:N	2.72	0.53
3:P:261:ASN:HD22	3:P:264:VAL:HB	1.74	0.53
4:Q:24:SER:OG	10:W:55:ILE:HG21	2.09	0.53
4:D:27:ARG:CZ	10:J:59:TYR:CE2	2.91	0.52
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.74	0.52
2:B:226:ILE:HD13	2:B:227:ARG:HH12	1.73	0.52
1:A:117:VAL:CG2	1:A:118:GLN:N	2.72	0.52
5:R:107:ASN:O	5:R:109:GLU:N	2.39	0.52
2:B:107:TYR:CG	2:B:127:THR:HG22	2.44	0.52
3:C:13:LYS:HG2	3:C:13:LYS:O	2.09	0.52
1:A:277:ILE:HD11	1:A:345:LEU:HD11	1.90	0.52
4:D:43:MET:HG2	4:D:46:VAL:CG2	2.39	0.52
2:O:258:VAL:HG11	2:O:312:PHE:CD2	2.41	0.52
1:A:253:VAL:HG11	1:A:335:MET:CE	2.39	0.52
2:B:437:ASP:OD1	2:B:438:GLU:HG3	2.08	0.52
1:N:19:LEU:C	1:N:21:ASN:H	2.12	0.52
1:A:255:LEU:HD13	1:A:422:LEU:CD1	2.39	0.52
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.08	0.52
2:B:20:GLY:O	2:B:21:ALA:CB	2.57	0.52
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.40	0.52
2:O:152:PHE:CE1	2:O:177:TYR:HD1	2.26	0.52
5:R:141:HIS:HB3	21:R:501:FES:S2	2.49	0.52
4:Q:215:LEU:HD13	5:R:46:ALA:CB	2.40	0.52
4:Q:165:TYR:O	4:Q:168:ILE:HB	2.09	0.52
2:B:26:ILE:O	2:B:26:ILE:HG23	2.09	0.52
6:S:61:ARG:HG3	6:S:61:ARG:HH11	1.74	0.52
4:Q:186:VAL:CG1	4:Q:187:CYS:N	2.72	0.52
1:A:373:THR:N	1:A:374:PRO:HD2	2.25	0.52
10:J:40:ASP:O	10:J:44:GLU:HG3	2.08	0.52
2:O:124:LEU:C	2:O:124:LEU:HD23	2.29	0.52
1:N:15:ASN:O	1:N:26:ALA:HA	2.09	0.52
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:165:TYR:O	4:D:168:ILE:HB	2.08	0.52
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.74	0.52
3:C:120:LEU:CD2	13:C:502:HEM:HBB2	2.39	0.52
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.90	0.52
2:O:168:TYR:N	2:O:168:TYR:CD1	2.75	0.52
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.25	0.52
3:P:326:PHE:O	3:P:329:LEU:HB3	2.09	0.52
1:N:147:ASN:O	1:N:149:THR:N	2.43	0.52
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.45	0.52
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.45	0.52
5:R:107:ASN:C	5:R:109:GLU:H	2.13	0.52
5:R:140:THR:O	5:R:141:HIS:C	2.48	0.52
1:A:332:ASP:O	1:A:333:ASP:C	2.48	0.52
2:O:73:SER:N	2:O:74:PRO:HD2	2.25	0.52
4:D:57:THR:HG22	4:D:58:GLU:N	2.23	0.52
7:T:36:ASN:O	7:T:40:ARG:HG3	2.10	0.52
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.45	0.52
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.52
1:N:255:LEU:HD13	1:N:422:LEU:CD1	2.39	0.52
2:B:43:PRO:O	2:B:113:ARG:HG3	2.09	0.52
2:B:166:ALA:HA	2:B:240:TRP:CE3	2.45	0.52
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.45	0.52
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.45	0.52
1:A:284:PHE:CD2	9:I:71:ASN:HA	2.45	0.52
3:P:120:LEU:HB3	13:P:502:HEM:HBB2	1.90	0.52
4:D:43:MET:HE2	4:D:46:VAL:CG2	2.38	0.52
3:P:329:LEU:O	3:P:332:ASN:HB3	2.09	0.52
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.25	0.52
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.44	0.52
4:D:81:PHE:HD2	4:D:81:PHE:H	1.57	0.52
3:P:13:LYS:HG2	3:P:13:LYS:O	2.09	0.52
6:F:70:LEU:HG	6:F:71:LYS:N	2.25	0.52
2:O:119:VAL:HG12	2:O:119:VAL:O	2.10	0.52
2:B:110:GLU:O	2:B:111:CYS:HB3	2.09	0.52
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.92	0.52
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.52
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.10	0.52
2:B:155:PRO:O	2:B:158:GLY:N	2.40	0.52
4:Q:235:MET:HE1	6:S:63:LYS:HG2	1.91	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.52
2:O:264:VAL:HG23	2:O:316:TYR:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:267:ALA:C	2:O:269:ALA:H	2.13	0.52
4:D:167:GLU:C	4:D:169:LEU:H	2.13	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HB2	2.46	0.51
2:B:96:LEU:C	2:B:96:LEU:HD12	2.30	0.51
4:D:40:CYS:HA	4:D:95:TYR:HE1	1.75	0.51
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.45	0.51
2:O:290:SER:CB	2:O:293:SER:HB3	2.40	0.51
2:O:168:TYR:N	2:O:168:TYR:HD1	2.08	0.51
2:O:73:SER:OG	2:O:74:PRO:HD3	2.09	0.51
2:O:333:ALA:O	2:O:337:ILE:HG13	2.10	0.51
1:N:171:THR:HB	5:R:4:ASP:OD2	2.11	0.51
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.46	0.51
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.75	0.51
5:E:142:LEU:HD12	5:E:161:HIS:HE1	1.74	0.51
3:P:137:GLY:N	3:P:140:SER:HB2	2.25	0.51
1:A:242:ARG:HH22	1:A:432:LEU:HA	1.76	0.51
9:I:59:SER:O	9:I:60:ALA:HB3	2.11	0.51
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.91	0.51
3:C:86:ASN:ND2	3:C:243:LEU:HD11	2.26	0.51
7:T:78:GLU:C	7:T:79:ASN:HD22	2.13	0.51
2:O:341:MET:HE3	2:O:417:PHE:CZ	2.46	0.51
3:P:142:TRP:O	3:P:146:VAL:HG23	2.09	0.51
2:B:374:THR:HG22	2:B:376:GLN:N	2.25	0.51
4:D:148:HIS:ND1	4:D:161:ALA:HA	2.25	0.51
8:H:57:GLU:O	8:H:60:ASP:HB2	2.10	0.51
3:P:130:VAL:HG23	3:P:131:GLY:N	2.26	0.51
1:A:255:LEU:HD12	1:A:421:ALA:O	2.10	0.51
2:O:201:SER:H	2:O:227:ARG:CB	2.17	0.51
2:B:341:MET:O	2:B:344:LEU:HB2	2.11	0.51
1:A:158:PHE:O	1:A:159:GLN:O	2.28	0.51
5:R:76:ILE:O	5:R:193:VAL:HG12	2.10	0.51
9:V:28:UNK:HA	9:V:72:ALA:HB2	1.93	0.51
4:D:171:TYR:OH	4:D:182:ILE:HA	2.11	0.51
2:B:259:THR:HG23	2:B:421:LYS:O	2.11	0.51
1:A:333:ASP:O	1:A:336:PHE:HB3	2.10	0.51
3:P:132:TYR:O	3:P:135:PRO:HD2	2.11	0.51
3:P:187:PRO:HG2	13:P:501:HEM:HMC3	1.93	0.51
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.40	0.51
2:O:341:MET:CE	2:O:417:PHE:CE2	2.93	0.51
1:A:163:LEU:HD22	1:A:314:TYR:HE1	1.74	0.51
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.45	0.51
6:F:81:VAL:HG12	6:F:82:LYS:N	2.26	0.51
1:A:106:MET:HB3	1:A:107:PRO:HD3	1.93	0.51
2:O:415:LYS:O	2:O:417:PHE:N	2.44	0.51
1:A:381:SER:O	1:A:382:HIS:C	2.49	0.51
4:D:52:ILE:C	4:D:54:VAL:H	2.13	0.51
4:D:134:TYR:CD2	4:D:162:PRO:HG3	2.45	0.51
1:N:221:PHE:O	1:N:222:THR:O	2.28	0.51
3:C:78:TRP:CD2	3:C:79:LEU:N	2.79	0.51
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.91	0.51
1:N:106:MET:HB3	1:N:107:PRO:HD3	1.93	0.51
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.25	0.51
6:F:61:ARG:NH1	6:F:61:ARG:HG3	2.26	0.51
5:R:101:ARG:NH2	5:R:127:VAL:HG11	2.26	0.51
5:R:101:ARG:HH21	5:R:127:VAL:HG21	1.74	0.51
2:O:42:SER:O	2:O:113:ARG:HD2	2.10	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
1:N:373:THR:N	1:N:374:PRO:HD2	2.24	0.51
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.31	0.51
5:R:133:VAL:HG13	5:R:133:VAL:O	2.11	0.51
1:A:206:LYS:O	1:A:207:GLU:C	2.49	0.51
6:S:58:ARG:HG3	6:S:89:TYR:OH	2.11	0.51
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.26	0.51
1:N:255:LEU:O	1:N:321:GLY:HA3	2.11	0.51
8:U:52:GLU:HG2	8:U:53:GLN:N	2.26	0.51
3:C:216:SER:HB3	6:F:59:MET:CE	2.41	0.51
3:C:243:LEU:HD12	3:C:243:LEU:C	2.31	0.51
1:A:221:PHE:O	1:A:222:THR:O	2.29	0.51
2:O:102:ARG:CG	2:O:102:ARG:NH1	2.66	0.51
2:O:203:ARG:O	2:O:387:LEU:HD11	2.11	0.51
2:B:424:MET:HG2	2:B:425:ALA:H	1.75	0.51
3:C:198:LEU:HD21	13:C:502:HEM:CMA	2.41	0.50
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.92	0.50
2:O:168:TYR:CE2	2:O:172:LEU:HB2	2.45	0.50
5:E:129:LYS:HD2	5:E:132:TRP:CD1	2.46	0.50
3:C:89:SER:O	3:C:90:PHE:C	2.49	0.50
3:C:95:ILE:CG2	3:C:96:PHE:N	2.74	0.50
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.94	0.50
2:O:58:GLU:OE1	2:O:64:GLY:N	2.43	0.50
4:Q:52:ILE:C	4:Q:54:VAL:H	2.15	0.50
1:N:180:ALA:O	1:N:183:ALA:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:65:ARG:O	8:U:68:CYS:HB3	2.10	0.50
3:P:75:GLN:O	3:P:77:GLY:N	2.44	0.50
5:E:81:ILE:HD12	5:E:132:TRP:CZ3	2.46	0.50
4:D:57:THR:H	4:D:60:GLU:HG3	1.75	0.50
2:O:221:GLU:HG3	2:O:222:GLN:N	2.23	0.50
2:O:341:MET:O	2:O:344:LEU:HB2	2.11	0.50
4:Q:10:PHE:HD2	8:U:74:PHE:HE2	1.59	0.50
3:P:320:PRO:HG2	3:P:321:LEU:H	1.76	0.50
1:A:64:PHE:HA	1:A:75:PHE:HE2	1.76	0.50
10:J:60:GLU:O	10:J:61:ALA:HB3	2.11	0.50
3:C:175:THR:O	3:C:178:ARG:HG2	2.11	0.50
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.75	0.50
2:O:109:VAL:HG23	2:O:109:VAL:O	2.11	0.50
1:A:105:ASP:O	1:A:106:MET:C	2.49	0.50
2:B:81:SER:C	2:B:83:PHE:N	2.64	0.50
2:O:225:ASN:C	2:O:227:ARG:H	2.14	0.50
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.73	0.50
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.92	0.50
4:D:37:CYS:O	4:D:39:ALA:N	2.45	0.50
1:A:261:GLY:O	1:A:267:ASN:ND2	2.45	0.50
2:O:395:PRO:O	2:O:398:VAL:HG12	2.11	0.50
2:B:378:LEU:O	2:B:378:LEU:HD12	2.11	0.50
3:P:4:ASN:O	3:P:5:ILE:HD13	2.11	0.50
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.40	0.50
4:Q:186:VAL:HG13	4:Q:187:CYS:N	2.25	0.50
4:D:208:MET:O	4:D:212:SER:HB2	2.12	0.50
1:A:90:THR:HA	1:A:95:THR:HA	1.93	0.50
6:S:10:GLY:O	6:S:14:ASP:HB2	2.10	0.50
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.92	0.50
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.42	0.50
2:O:378:LEU:HD12	2:O:378:LEU:O	2.12	0.50
2:O:341:MET:CE	2:O:417:PHE:HE2	2.23	0.50
4:Q:221:TYR:HE1	7:T:25:ALA:HB2	1.75	0.50
1:N:253:VAL:CG1	1:N:335:MET:HE1	2.41	0.50
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.46	0.50
2:O:152:PHE:HE1	2:O:177:TYR:CD1	2.28	0.50
2:B:150:VAL:HG22	2:B:151:ALA:N	2.26	0.50
3:C:29:SER:HB2	16:C:2004:CDL:OB4	2.12	0.50
5:R:126:ARG:HH21	5:R:179:ASN:ND2	2.10	0.50
2:O:209:ILE:HD11	2:O:378:LEU:HG	1.93	0.50
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:CB	2:B:109:VAL:HG12	2.37	0.50
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.41	0.50
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.11	0.50
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.94	0.50
1:A:418:LYS:O	1:A:420:PRO:HD3	2.12	0.50
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.94	0.50
8:U:18:THR:O	8:U:22:GLU:HG3	2.12	0.50
16:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.11	0.50
1:N:107:PRO:O	1:N:108:LYS:C	2.49	0.50
6:S:57:GLU:HB3	6:S:61:ARG:HH12	1.76	0.50
3:C:345:GLU:O	3:C:348:PHE:HB2	2.10	0.50
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.47	0.50
8:U:57:GLU:O	8:U:60:ASP:HB2	2.12	0.50
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.94	0.50
1:N:87:ASN:OD1	1:N:88:GLY:N	2.37	0.50
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.92	0.50
3:C:247:SER:N	3:C:248:PRO:HD3	2.27	0.50
3:C:316:MET:HG2	3:C:319:ARG:NH2	2.26	0.50
1:A:344:ARG:HB3	1:A:344:ARG:CZ	2.42	0.50
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.94	0.50
2:O:259:THR:HG23	2:O:421:LYS:O	2.11	0.50
4:D:52:ILE:O	4:D:54:VAL:N	2.45	0.50
4:Q:148:HIS:CE1	4:Q:161:ALA:HA	2.46	0.50
2:O:345:LYS:O	2:O:348:ALA:N	2.45	0.50
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.12	0.50
3:C:329:LEU:O	3:C:332:ASN:HB3	2.11	0.50
3:C:158:GLY:C	3:C:160:THR:N	2.65	0.50
1:N:105:ASP:O	1:N:106:MET:C	2.50	0.50
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.93	0.50
2:O:85:ILE:HA	2:O:122:TYR:CD2	2.47	0.50
9:I:63:ASP:O	9:I:64:LEU:HB2	2.12	0.50
3:C:287:ASN:O	3:C:288:LYS:C	2.50	0.50
4:Q:235:MET:HE1	6:S:63:LYS:C	2.31	0.50
3:C:210:LEU:HD12	6:F:66:LEU:HD23	1.92	0.50
5:E:130:PRO:HG2	5:E:131:GLU:H	1.77	0.50
1:A:429:GLU:HG2	1:A:429:GLU:O	2.11	0.50
9:V:49:LEU:CD2	9:V:55:MET:HB3	2.39	0.49
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.42	0.49
1:A:365:MET:CG	1:A:366:VAL:H	2.25	0.49
8:U:37:LEU:O	8:U:40:CYS:N	2.44	0.49
7:T:79:ASN:N	7:T:79:ASN:HD22	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LEU:C	2:B:124:LEU:HD23	2.31	0.49
4:Q:81:PHE:HD2	4:Q:81:PHE:H	1.60	0.49
2:O:263:ALA:O	2:O:266:SER:HB3	2.12	0.49
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.43	0.49
2:O:268:GLU:HG2	2:O:272:PHE:HE1	1.77	0.49
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.11	0.49
4:D:109:LEU:O	4:D:111:PRO:HD3	2.12	0.49
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.77	0.49
2:O:100:SER:HA	2:O:104:LYS:O	2.12	0.49
4:Q:57:THR:H	4:Q:60:GLU:HG3	1.76	0.49
1:A:67:THR:HA	1:A:121:ALA:N	2.27	0.49
8:H:43:ARG:HD2	8:H:47:ARG:NH2	2.26	0.49
1:N:365:MET:CG	1:N:366:VAL:H	2.23	0.49
3:P:70:THR:O	3:P:74:VAL:HG23	2.12	0.49
2:O:290:SER:HB3	2:O:293:SER:HB3	1.94	0.49
1:N:147:ASN:C	1:N:149:THR:N	2.66	0.49
2:O:124:LEU:O	2:O:128:THR:HG23	2.12	0.49
5:E:20:ASP:C	5:E:22:THR:H	2.16	0.49
6:S:61:ARG:HG3	6:S:61:ARG:NH1	2.28	0.49
2:O:283:PRO:C	2:O:284:LEU:HD23	2.32	0.49
1:N:253:VAL:O	1:N:323:HIS:HA	2.11	0.49
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.48	0.49
8:H:18:THR:O	8:H:22:GLU:HG3	2.12	0.49
9:I:32:UNK:N	9:I:73:PRO:CG	2.70	0.49
3:C:245:LEU:O	4:D:201:ARG:CD	2.60	0.49
1:A:171:THR:HB	5:E:4:ASP:OD2	2.12	0.49
3:P:86:ASN:ND2	3:P:243:LEU:HD11	2.27	0.49
2:B:313:ASN:O	9:I:62:ARG:O	2.31	0.49
6:S:68:LEU:O	6:S:71:LYS:N	2.46	0.49
2:O:27:THR:CG2	2:O:28:LYS:N	2.74	0.49
3:C:277:PHE:CG	3:C:278:ALA:N	2.80	0.49
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.77	0.49
1:N:4:TYR:O	1:N:6:GLN:N	2.46	0.49
2:B:385:GLU:C	2:B:387:LEU:N	2.66	0.49
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.48	0.49
4:Q:158:ILE:CD1	4:Q:160:MET:HB3	2.42	0.49
5:R:81:ILE:HB	5:R:132:TRP:HH2	1.77	0.49
2:B:283:PRO:C	2:B:284:LEU:HD23	2.33	0.49
3:C:137:GLY:H	3:C:140:SER:CB	2.26	0.49
4:D:10:PHE:N	4:D:10:PHE:CD1	2.81	0.49
2:O:120:MET:O	2:O:121:GLU:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.49
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.94	0.49
1:A:107:PRO:O	1:A:108:LYS:C	2.50	0.49
1:A:40:TRP:CH2	1:A:376:CYS:HB3	2.48	0.49
4:D:27:ARG:CZ	10:J:59:TYR:HE2	2.25	0.49
1:A:122:LEU:HD11	1:A:186:ILE:CD1	2.43	0.49
5:R:1:VAL:HG23	5:R:3:ASN:N	2.24	0.49
2:B:306:PRO:HB3	9:I:52:ARG:N	2.28	0.49
2:B:395:PRO:O	2:B:398:VAL:HG12	2.12	0.49
1:N:343:MET:O	1:N:344:ARG:C	2.50	0.49
5:R:15:ARG:HH11	5:R:32:ARG:HB3	1.76	0.49
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.95	0.49
8:H:25:GLU:HG2	8:H:61:PHE:HZ	1.78	0.49
6:F:68:LEU:O	6:F:71:LYS:N	2.46	0.49
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.78	0.49
1:N:170:THR:HG22	1:N:172:GLU:H	1.78	0.49
2:O:150:VAL:CG2	2:O:151:ALA:N	2.75	0.49
7:G:77:TYR:CD1	8:H:52:GLU:HB2	2.48	0.49
1:N:178:THR:CG2	1:N:179:ARG:N	2.76	0.49
3:P:287:ASN:O	3:P:288:LYS:C	2.52	0.49
7:G:60:SER:O	7:G:64:GLN:HB2	2.13	0.49
1:A:147:ASN:O	1:A:148:VAL:C	2.51	0.49
1:A:244:ARG:NE	7:G:10:VAL:HB	2.27	0.49
1:N:281:ASP:OD1	1:N:281:ASP:O	2.31	0.49
3:C:189:ALA:O	3:C:193:ILE:HG13	2.12	0.49
4:D:116:ILE:HG23	4:D:117:VAL:H	1.75	0.49
4:D:117:VAL:HG13	4:D:190:LEU:HB3	1.95	0.49
1:A:134:ILE:CG2	1:A:174:ILE:HG12	2.42	0.49
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.80	0.49
2:O:424:MET:HG2	2:O:425:ALA:H	1.77	0.49
3:P:82:ASN:H	3:P:82:ASN:ND2	2.11	0.49
5:R:141:HIS:HB2	5:R:176:ALA:CB	2.43	0.49
4:D:235:MET:HE1	6:F:63:LYS:HG2	1.94	0.49
2:B:372:VAL:O	2:B:372:VAL:HG12	2.12	0.49
1:A:434:TYR:CE2	7:G:19:SER:HB2	2.48	0.49
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.94	0.49
1:N:371:GLY:O	1:N:375:VAL:HG23	2.13	0.49
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.13	0.48
3:P:104:TYR:HD2	3:P:105:TYR:CE1	2.30	0.48
4:Q:117:VAL:HG13	4:Q:190:LEU:HB3	1.95	0.48
3:C:172:ASP:C	3:C:174:PRO:HD2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:O	1:A:53:ASN:C	2.51	0.48
6:S:51:PRO:O	6:S:52:GLU:C	2.51	0.48
5:E:129:LYS:HG2	5:E:187:PHE:CZ	2.48	0.48
2:B:415:LYS:O	2:B:417:PHE:N	2.45	0.48
2:O:415:LYS:C	2:O:417:PHE:N	2.66	0.48
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.48
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.49	0.48
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	3.01	0.48
3:C:273:TRP:HA	3:C:276:LEU:HG	1.94	0.48
4:D:240:PRO:O	4:D:241:LYS:C	2.51	0.48
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.95	0.48
4:D:47:ALA:N	4:D:50:ASN:HD22	2.00	0.48
1:A:342:TRP:HA	1:A:345:LEU:HD12	1.94	0.48
3:P:253:ASP:OD1	3:P:254:PRO:N	2.46	0.48
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.91	0.48
3:P:150:LEU:HB3	3:P:292:VAL:CG2	2.43	0.48
1:A:433:ASP:OD2	1:A:435:ASN:N	2.47	0.48
1:A:53:ASN:OD1	1:A:165:ARG:HD3	2.14	0.48
2:B:157:VAL:O	2:B:157:VAL:HG22	2.14	0.48
1:N:271:HIS:NE2	1:N:311:ASN:HB3	2.28	0.48
4:Q:98:PRO:HG2	4:Q:99:GLU:OE1	2.13	0.48
3:P:175:THR:O	3:P:178:ARG:HG2	2.12	0.48
2:O:385:GLU:C	2:O:387:LEU:N	2.66	0.48
2:B:203:ARG:O	2:B:387:LEU:HD11	2.14	0.48
1:A:87:ASN:HB3	1:A:98:TYR:CE1	2.48	0.48
4:D:187:CYS:O	4:D:190:LEU:HB2	2.14	0.48
3:C:41:CYS:SG	3:C:91:PHE:HA	2.54	0.48
3:C:242:THR:N	4:D:208:MET:HE1	2.27	0.48
4:D:218:LEU:HD13	5:E:43:ALA:HA	1.94	0.48
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.47	0.48
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.93	0.48
5:R:83:GLU:HA	5:R:100:HIS:O	2.14	0.48
1:N:349:THR:HA	1:N:353:GLU:OE1	2.13	0.48
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.12	0.48
3:P:175:THR:O	3:P:176:LEU:C	2.51	0.48
3:P:297:ALA:HA	3:P:300:LEU:HB2	1.96	0.48
5:E:163:SER:HA	5:E:174:GLY:HA3	1.96	0.48
5:E:129:LYS:HG2	5:E:187:PHE:CE2	2.48	0.48
2:B:415:LYS:C	2:B:417:PHE:N	2.66	0.48
2:O:166:ALA:O	2:O:242:GLY:N	2.46	0.48
1:A:53:ASN:CG	1:A:165:ARG:HD3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:C	1:A:195:MET:HE2	2.33	0.48
1:N:178:THR:C	1:N:180:ALA:N	2.64	0.48
4:D:164:ILE:HG21	4:D:182:ILE:HG21	1.94	0.48
2:O:220:ALA:O	2:O:224:LEU:HB2	2.14	0.48
5:R:118:ARG:O	5:R:120:PRO:HD3	2.13	0.48
1:N:281:ASP:OD1	1:N:281:ASP:C	2.52	0.48
4:Q:43:MET:HG2	4:Q:46:VAL:CG2	2.44	0.48
1:N:106:MET:HE1	1:N:208:LEU:HD13	1.96	0.48
1:N:158:PHE:HB3	1:N:161:THR:OG1	2.13	0.48
1:A:4:TYR:OH	1:A:362:ARG:HD3	2.12	0.48
3:P:78:TRP:CG	3:P:79:LEU:N	2.82	0.48
3:C:132:TYR:O	3:C:135:PRO:HD2	2.13	0.48
4:D:135:CYS:O	4:D:149:TYR:HB3	2.14	0.48
1:N:64:PHE:HA	1:N:75:PHE:HE2	1.79	0.48
1:A:356:ARG:HG3	2:B:91:ALA:HA	1.95	0.48
1:N:242:ARG:NH2	1:N:432:LEU:HA	2.28	0.48
2:B:57:TYR:CE2	2:B:234:SER:HB2	2.49	0.48
2:O:81:SER:C	2:O:83:PHE:N	2.65	0.48
2:B:76:THR:HG22	2:B:81:SER:HA	1.95	0.48
3:C:72:ARG:HG2	3:C:72:ARG:NH1	2.29	0.48
3:C:61:SER:C	3:C:62:LEU:HG	2.34	0.48
2:O:258:VAL:HG21	2:O:321:LEU:HD22	1.95	0.48
3:P:60:THR:HG23	3:P:173:ASN:HA	1.95	0.48
2:O:43:PRO:O	2:O:113:ARG:HG3	2.13	0.48
3:C:60:THR:HG23	3:C:173:ASN:HA	1.96	0.48
1:N:317:THR:HG23	1:N:318:GLY:H	1.78	0.48
5:R:175:PRO:HG2	5:R:176:ALA:H	1.79	0.48
1:N:270:LEU:HD13	1:N:320:PHE:HD1	1.79	0.48
4:D:171:TYR:C	4:D:173:ASP:H	2.17	0.48
3:P:277:PHE:CG	3:P:278:ALA:N	2.82	0.48
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.96	0.48
10:W:10:TYR:CD2	10:W:10:TYR:O	2.67	0.48
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.35	0.48
1:N:122:LEU:HD11	1:N:186:ILE:CD1	2.44	0.48
1:N:184:SER:O	1:N:187:ASP:HB2	2.14	0.48
2:O:312:PHE:O	2:O:322:PHE:HA	2.14	0.48
1:N:40:TRP:CH2	1:N:376:CYS:HB3	2.49	0.48
8:U:43:ARG:O	8:U:47:ARG:HG3	2.14	0.48
1:N:87:ASN:HB3	1:N:98:TYR:CZ	2.48	0.48
4:D:218:LEU:CD1	5:E:43:ALA:HA	2.44	0.48
5:R:20:ASP:C	5:R:22:THR:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:201:LEU:C	3:P:203:GLU:H	2.17	0.48
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.71	0.48
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
10:J:15:ARG:HH11	10:J:15:ARG:HG2	1.77	0.48
6:F:67:ASP:HA	6:F:70:LEU:CD2	2.32	0.48
2:B:56:ARG:HG2	2:B:234:SER:OG	2.13	0.48
3:C:147:ILE:HA	3:C:150:LEU:HD12	1.96	0.48
1:A:134:ILE:HG21	1:A:174:ILE:CG1	2.43	0.48
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.18	0.48
2:B:248:ASN:HD22	2:B:248:ASN:C	2.16	0.48
2:O:137:VAL:O	2:O:140:LEU:HB3	2.14	0.48
1:A:178:THR:HG22	1:A:180:ALA:H	1.79	0.48
5:R:15:ARG:NH1	5:R:32:ARG:HB3	2.29	0.48
2:B:47:ILE:HD13	2:B:120:MET:CE	2.43	0.48
10:W:23:THR:O	10:W:24:VAL:C	2.53	0.48
5:E:133:VAL:HG13	5:E:133:VAL:O	2.13	0.48
3:P:184:PHE:CE2	13:P:501:HEM:HBC1	2.49	0.48
5:E:147:ILE:CG2	5:E:148:ALA:H	2.15	0.48
10:W:52:TRP:O	10:W:56:LYS:HB2	2.13	0.48
5:E:116:LYS:CD	5:E:116:LYS:H	2.20	0.48
8:H:37:LEU:O	8:H:40:CYS:N	2.47	0.48
1:N:277:ILE:HG22	1:N:277:ILE:O	2.12	0.48
5:E:40:THR:O	5:E:41:ALA:C	2.53	0.48
3:P:141:PHE:O	3:P:144:ALA:HB3	2.13	0.48
2:O:422:LYS:O	2:O:436:LEU:HD21	2.14	0.48
4:Q:220:TYR:OH	4:Q:224:ARG:HD3	2.14	0.48
2:O:24:LEU:HD23	2:O:24:LEU:O	2.14	0.48
3:C:67:VAL:CG2	13:C:501:HEM:HBD2	2.44	0.47
5:R:99:ARG:NH2	5:R:148:ALA:HB1	2.28	0.47
2:O:383:GLY:O	2:O:384:SER:C	2.52	0.47
4:Q:56:HIS:HB3	4:Q:60:GLU:HB2	1.96	0.47
2:B:109:VAL:O	2:B:109:VAL:HG23	2.14	0.47
3:C:95:ILE:HG23	3:C:96:PHE:N	2.29	0.47
5:R:76:ILE:HD13	5:R:89:PHE:CE1	2.49	0.47
5:R:139:CYS:O	5:R:141:HIS:N	2.47	0.47
5:R:73:LYS:HB3	5:R:196:GLY:HA3	1.95	0.47
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.49	0.47
2:O:247:GLN:NE2	2:O:249:GLY:H	2.12	0.47
4:D:186:VAL:HG13	4:D:187:CYS:N	2.27	0.47
1:A:182:LEU:O	1:A:186:ILE:HG13	2.14	0.47
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:222:GLN:O	2:O:223:PHE:CG	2.67	0.47
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.79	0.47
1:A:378:THR:O	1:A:382:HIS:N	2.43	0.47
3:C:142:TRP:O	3:C:146:VAL:HG23	2.14	0.47
3:C:316:MET:HG2	3:C:319:ARG:HH21	1.78	0.47
2:B:132:PHE:HB2	2:B:192:HIS:CE1	2.49	0.47
4:D:72:ASP:HB3	4:D:81:PHE:CE2	2.50	0.47
3:P:75:GLN:C	3:P:77:GLY:H	2.18	0.47
3:C:175:THR:O	3:C:176:LEU:C	2.50	0.47
7:T:63:THR:HG22	7:T:64:GLN:N	2.28	0.47
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.14	0.47
2:O:209:ILE:CG2	2:O:210:GLY:N	2.60	0.47
4:Q:106:ASN:C	4:Q:108:ALA:H	2.18	0.47
8:U:52:GLU:CG	8:U:53:GLN:N	2.77	0.47
1:N:439:SER:C	1:N:441:MET:N	2.68	0.47
1:A:270:LEU:HD13	1:A:320:PHE:HD1	1.77	0.47
3:C:45:GLN:O	3:C:49:GLY:N	2.38	0.47
2:O:248:ASN:HD22	2:O:248:ASN:C	2.17	0.47
5:E:96:LEU:HD12	5:E:135:LEU:O	2.14	0.47
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.27	0.47
2:B:407:SER:O	2:B:411:VAL:HG23	2.14	0.47
4:D:122:GLY:O	4:D:123:GLY:C	2.52	0.47
2:B:253:VAL:HG11	2:B:433:THR:OG1	2.13	0.47
3:C:120:LEU:CB	13:C:502:HEM:HBB2	2.43	0.47
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.49	0.47
2:O:385:GLU:HB3	2:O:391:THR:O	2.15	0.47
10:W:60:GLU:O	10:W:61:ALA:HB2	2.15	0.47
2:O:215:ASP:C	2:O:217:LYS:N	2.67	0.47
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.96	0.47
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.47
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.78	0.47
2:O:306:PRO:HB3	9:V:52:ARG:H	1.80	0.47
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.79	0.47
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.97	0.47
3:C:208:ASN:OD1	3:C:208:ASN:C	2.53	0.47
5:E:81:ILE:HD12	5:E:132:TRP:CH2	2.50	0.47
2:O:71:LEU:O	2:O:74:PRO:CD	2.55	0.47
4:D:186:VAL:CG1	4:D:187:CYS:N	2.77	0.47
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.96	0.47
4:Q:221:TYR:CD2	5:R:39:VAL:HG21	2.50	0.47
4:Q:108:ALA:HB1	19:Q:501:HEC:HMD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:HIS:O	2:B:336:VAL:HG23	2.14	0.47
2:O:257:VAL:CG2	2:O:424:MET:HG3	2.42	0.47
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.54	0.47
1:A:15:ASN:HB2	1:A:205:HIS:ND1	2.30	0.47
2:B:266:SER:OG	2:B:267:ALA:N	2.47	0.47
2:B:209:ILE:O	2:B:211:VAL:N	2.48	0.47
2:B:383:GLY:O	2:B:384:SER:C	2.52	0.47
3:P:30:ALA:HB1	16:Q:3003:CDL:H111	1.96	0.47
1:N:106:MET:C	1:N:106:MET:HE2	2.35	0.47
1:N:378:THR:O	1:N:382:HIS:N	2.42	0.47
1:N:121:ALA:O	1:N:122:LEU:HB2	2.13	0.47
5:R:79:SER:C	5:R:81:ILE:H	2.18	0.47
2:O:272:PHE:O	2:O:276:GLN:N	2.39	0.47
2:O:215:ASP:O	2:O:217:LYS:N	2.47	0.47
2:O:151:ALA:C	2:O:153:GLN:H	2.18	0.47
1:N:365:MET:HG3	1:N:366:VAL:H	1.80	0.47
1:A:23:LEU:HA	1:A:192:ALA:O	2.15	0.47
5:R:170:ARG:HA	5:R:179:ASN:CG	2.35	0.47
2:B:152:PHE:CE1	2:B:177:TYR:HD1	2.31	0.47
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.96	0.47
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.15	0.47
4:D:106:ASN:C	4:D:108:ALA:H	2.17	0.47
5:E:175:PRO:O	5:E:176:ALA:C	2.53	0.47
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.50	0.47
3:C:30:ALA:HB1	16:D:2003:CDL:H111	1.95	0.47
1:N:254:ALA:HB3	1:N:423:ALA:HB3	1.96	0.47
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.50	0.47
3:C:254:PRO:O	3:C:257:PHE:N	2.47	0.47
1:N:58:PHE:HA	1:N:134:ILE:HD11	1.96	0.47
1:A:44:GLY:HA3	1:A:92:ARG:O	2.15	0.47
1:N:256:ALA:HA	1:N:320:PHE:O	2.15	0.47
5:E:101:ARG:HD2	5:E:105:GLU:HB3	1.96	0.47
1:N:344:ARG:HG3	1:N:344:ARG:NH1	2.30	0.47
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.50	0.47
3:C:187:PRO:O	3:C:190:ILE:HB	2.14	0.47
2:O:109:VAL:CG2	2:O:119:VAL:HG12	2.45	0.47
2:B:73:SER:N	2:B:74:PRO:HD2	2.29	0.47
2:B:73:SER:OG	2:B:74:PRO:HD3	2.15	0.47
2:B:119:VAL:O	2:B:119:VAL:HG12	2.15	0.47
3:P:254:PRO:O	3:P:256:ASN:N	2.48	0.47
5:R:185:TYR:CD2	5:R:185:TYR:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:332:ASP:O	1:N:333:ASP:C	2.51	0.47
4:D:73:GLY:N	4:D:81:PHE:HE2	2.13	0.47
1:A:15:ASN:O	1:A:26:ALA:HA	2.15	0.47
6:F:16:ILE:O	6:F:19:TRP:HB3	2.15	0.47
4:D:98:PRO:HG2	4:D:99:GLU:OE1	2.15	0.47
3:P:184:PHE:HA	13:P:501:HEM:HBC2	1.97	0.47
3:C:72:ARG:HG2	3:C:72:ARG:HH11	1.78	0.47
1:N:191:LYS:N	1:N:195:MET:HE2	2.30	0.47
6:F:90:LEU:O	6:F:91:GLU:C	2.51	0.47
1:A:52:ASN:C	1:A:52:ASN:OD1	2.52	0.47
4:D:28:ARG:O	4:D:29:GLY:C	2.53	0.47
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.79	0.47
6:F:32:MET:O	6:F:33:ARG:C	2.52	0.47
1:N:394:GLU:O	1:N:395:TRP:C	2.53	0.47
4:D:70:VAL:HG23	4:D:83:ARG:HG2	1.97	0.47
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.46
1:N:67:THR:HA	1:N:121:ALA:N	2.30	0.46
2:B:85:ILE:HA	2:B:122:TYR:CD2	2.51	0.46
2:O:272:PHE:HA	2:O:275:LEU:HB3	1.96	0.46
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.80	0.46
1:N:65:LYS:NZ	2:O:287:ARG:O	2.41	0.46
1:N:295:ALA:O	1:N:298:ALA:HB3	2.15	0.46
9:V:32:UNK:N	9:V:73:PRO:HG2	2.31	0.46
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.45	0.46
2:O:140:LEU:C	2:O:142:PRO:HD2	2.36	0.46
4:Q:148:HIS:ND1	4:Q:162:PRO:HD3	2.30	0.46
1:N:178:THR:HG22	1:N:180:ALA:H	1.80	0.46
2:O:34:ILE:HG21	2:O:386:ALA:O	2.15	0.46
3:C:120:LEU:HD21	3:C:193:ILE:HB	1.96	0.46
1:A:107:PRO:O	1:A:109:VAL:N	2.48	0.46
16:Q:3003:CDL:HA21	6:S:72:HIS:CD2	2.50	0.46
2:O:258:VAL:HG12	2:O:323:GLY:HA3	1.98	0.46
1:N:341:GLU:O	1:N:342:TRP:C	2.53	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.15	0.46
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.45	0.46
5:E:79:SER:OG	5:E:191:ASP:HB2	2.14	0.46
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.15	0.46
1:A:260:PRO:HB3	1:A:414:TYR:CE2	2.51	0.46
8:H:31:VAL:C	8:H:33:ALA:H	2.17	0.46
6:S:67:ASP:O	6:S:71:LYS:HG3	2.15	0.46
1:N:170:THR:CG2	1:N:171:THR:H	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.45	0.46
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.80	0.46
1:N:219:VAL:HG12	1:N:220:SER:N	2.30	0.46
5:R:44:CYS:HB3	10:W:24:VAL:HG11	1.97	0.46
2:B:341:MET:HE3	2:B:417:PHE:CZ	2.51	0.46
2:O:337:ILE:O	2:O:340:ALA:HB3	2.16	0.46
4:D:127:VAL:O	4:D:131:LEU:HG	2.14	0.46
3:P:253:ASP:OD1	3:P:254:PRO:CD	2.63	0.46
3:P:82:ASN:ND2	3:P:82:ASN:N	2.63	0.46
2:B:215:ASP:C	2:B:217:LYS:N	2.69	0.46
1:N:163:LEU:HD22	1:N:314:TYR:HE1	1.81	0.46
4:D:200:GLN:NE2	20:D:2091:BOG:H3	2.30	0.46
1:N:76:GLU:HA	2:O:285:ILE:HD11	1.96	0.46
9:I:77:ARG:HB2	9:I:77:ARG:HE	1.56	0.46
2:O:81:SER:O	2:O:83:PHE:N	2.48	0.46
3:C:72:ARG:NE	4:D:115:TYR:OH	2.48	0.46
1:A:58:PHE:HA	1:A:134:ILE:HD11	1.97	0.46
1:N:161:THR:HG21	1:N:234:CYS:HA	1.97	0.46
1:N:161:THR:HG21	1:N:235:ARG:N	2.29	0.46
1:N:382:HIS:HB3	1:N:389:ARG:HA	1.97	0.46
2:O:160:LEU:CB	9:V:64:LEU:HD22	2.42	0.46
3:C:92:PHE:O	3:C:93:ILE:C	2.51	0.46
2:B:18:CYS:CB	2:B:19:PRO:HD3	2.42	0.46
7:G:72:LYS:NZ	8:H:52:GLU:HG3	2.30	0.46
4:D:218:LEU:HD13	5:E:43:ALA:N	2.31	0.46
4:D:218:LEU:HB3	5:E:43:ALA:HB2	1.96	0.46
1:N:270:LEU:HB3	1:N:320:PHE:CE1	2.48	0.46
4:D:155:GLY:C	4:D:157:ALA:H	2.19	0.46
3:P:40:VAL:O	3:P:44:THR:OG1	2.32	0.46
3:P:261:ASN:ND2	3:P:264:VAL:H	2.14	0.46
3:C:158:GLY:C	3:C:160:THR:H	2.18	0.46
2:O:430:LEU:O	2:O:432:SER:N	2.49	0.46
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.31	0.46
4:Q:120:ARG:HH11	4:Q:120:ARG:HG2	1.80	0.46
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.50	0.46
4:D:158:ILE:HD11	4:D:160:MET:HB3	1.96	0.46
2:B:81:SER:O	2:B:83:PHE:N	2.48	0.46
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.45	0.46
3:P:147:ILE:HA	3:P:150:LEU:HD12	1.98	0.46
4:D:218:LEU:HD13	5:E:42:THR:HG22	1.96	0.46
4:D:184:LYS:HG2	8:H:74:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:272:VAL:O	1:N:275:ALA:HB3	2.16	0.46
10:W:55:ILE:HG13	10:W:55:ILE:O	2.15	0.46
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.98	0.46
5:R:20:ASP:O	5:R:22:THR:N	2.40	0.46
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.98	0.46
2:B:400:GLN:O	2:B:404:SER:HB3	2.16	0.46
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.79	0.46
2:O:102:ARG:H	2:O:102:ARG:HD2	1.80	0.46
2:O:168:TYR:HE2	2:O:172:LEU:HD12	1.80	0.46
1:A:249:PRO:HG2	1:A:250:VAL:N	2.28	0.46
2:B:341:MET:CE	2:B:417:PHE:HE2	2.28	0.46
4:Q:10:PHE:HD1	4:Q:10:PHE:H	1.64	0.46
3:P:89:SER:O	3:P:90:PHE:C	2.52	0.46
3:C:234:THR:HG21	4:D:219:LEU:HD13	1.98	0.46
5:E:38:LEU:HB2	10:J:14:PHE:HE1	1.81	0.46
3:C:319:ARG:HB3	3:C:374:GLU:OE1	2.16	0.46
1:A:178:THR:CG2	1:A:179:ARG:N	2.79	0.46
3:C:5:ILE:O	3:C:5:ILE:HG22	2.16	0.46
2:B:410:VAL:O	2:B:413:ALA:N	2.48	0.46
1:N:304:CYS:HB2	1:N:325:VAL:O	2.16	0.46
2:B:422:LYS:O	2:B:436:LEU:HD21	2.16	0.46
2:O:155:PRO:O	2:O:158:GLY:N	2.46	0.46
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.27	0.46
2:O:338:ARG:O	2:O:341:MET:N	2.48	0.46
2:O:415:LYS:O	2:O:418:VAL:N	2.49	0.46
5:R:139:CYS:O	5:R:140:THR:C	2.55	0.46
1:A:392:LEU:N	1:A:392:LEU:CD2	2.79	0.46
4:D:184:LYS:CG	8:H:74:PHE:CE1	2.99	0.46
2:B:24:LEU:C	2:B:24:LEU:HD23	2.36	0.46
2:B:152:PHE:HE1	2:B:177:TYR:CD1	2.33	0.46
8:H:58:LEU:HD11	8:H:62:LEU:CD1	2.46	0.46
1:A:272:VAL:O	1:A:275:ALA:HB3	2.16	0.46
2:B:124:LEU:O	2:B:128:THR:HG23	2.16	0.46
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.46	0.46
3:C:289:LEU:O	3:C:293:LEU:HG	2.16	0.46
3:C:253:ASP:OD1	3:C:254:PRO:N	2.49	0.46
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.16	0.46
3:C:238:THR:CB	3:C:239:PRO:HD3	2.44	0.46
3:C:142:TRP:HA	3:C:145:THR:OG1	2.15	0.46
3:C:247:SER:HG	3:C:250:LEU:HB2	1.81	0.46
4:Q:155:GLY:C	4:Q:157:ALA:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HH12	1:A:432:LEU:N	2.13	0.46
2:B:31:ASN:N	2:B:31:ASN:ND2	2.64	0.46
2:B:287:ARG:C	9:I:53:GLU:HG3	2.35	0.46
4:D:227:TRP:O	4:D:228:SER:C	2.54	0.46
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.73	0.46
8:U:21:ARG:HH11	8:U:21:ARG:HG3	1.81	0.46
2:B:341:MET:CE	2:B:417:PHE:CE2	2.98	0.46
3:P:79:LEU:O	3:P:79:LEU:HD12	2.15	0.46
5:R:139:CYS:HB3	5:R:143:GLY:O	2.16	0.46
1:A:344:ARG:NH1	1:A:344:ARG:CB	2.79	0.46
4:D:148:HIS:CD2	4:D:148:HIS:N	2.82	0.46
6:S:81:VAL:HG12	6:S:82:LYS:N	2.31	0.46
3:P:216:SER:HB3	6:S:59:MET:CE	2.46	0.46
8:U:12:GLU:HG2	8:U:13:LEU:N	2.31	0.46
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.50	0.45
5:E:128:LYS:HG3	5:E:129:LYS:N	2.32	0.45
3:P:366:LEU:HD22	3:P:366:LEU:N	2.31	0.45
4:Q:171:TYR:HD1	4:Q:175:THR:HB	1.81	0.45
2:B:290:SER:CB	2:B:293:SER:HB3	2.46	0.45
2:B:62:ASN:HD22	2:B:65:THR:HG21	1.81	0.45
4:Q:147:LEU:C	4:Q:148:HIS:HD2	2.19	0.45
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.45	0.45
1:A:178:THR:C	1:A:180:ALA:N	2.67	0.45
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.51	0.45
5:E:189:GLY:O	5:E:192:LEU:O	2.35	0.45
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.50	0.45
5:R:114:VAL:HG12	5:R:114:VAL:O	2.17	0.45
1:A:107:PRO:HG2	1:A:108:LYS:H	1.82	0.45
2:B:111:CYS:HB3	2:B:119:VAL:HG21	1.97	0.45
3:C:89:SER:O	3:C:92:PHE:N	2.48	0.45
2:B:42:SER:O	2:B:113:ARG:HD2	2.17	0.45
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.51	0.45
1:A:191:LYS:N	1:A:195:MET:HE2	2.32	0.45
2:B:107:TYR:CD2	2:B:127:THR:HG22	2.51	0.45
4:D:165:TYR:O	4:D:166:ASN:C	2.55	0.45
7:T:79:ASN:N	7:T:79:ASN:ND2	2.64	0.45
10:J:36:ASP:O	10:J:37:GLN:C	2.54	0.45
1:A:116:VAL:O	1:A:120:CYS:HB2	2.17	0.45
8:H:43:ARG:HG3	8:H:44:VAL:N	2.30	0.45
2:B:258:VAL:HG11	2:B:312:PHE:CD2	2.41	0.45
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.52	0.45
1:A:439:SER:C	1:A:441:MET:H	2.20	0.45
3:P:75:GLN:C	3:P:77:GLY:N	2.69	0.45
3:P:5:ILE:O	3:P:5:ILE:HG22	2.16	0.45
4:Q:72:ASP:HB3	4:Q:81:PHE:CE2	2.52	0.45
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.50	0.45
3:P:334:LEU:O	3:P:337:THR:HB	2.17	0.45
1:A:39:VAL:O	1:A:39:VAL:HG13	2.16	0.45
6:S:40:ASP:OD1	6:S:40:ASP:C	2.54	0.45
2:B:102:ARG:H	2:B:102:ARG:HD2	1.81	0.45
2:B:338:ARG:O	2:B:341:MET:N	2.49	0.45
6:S:90:LEU:O	6:S:91:GLU:C	2.55	0.45
2:B:272:PHE:O	2:B:276:GLN:N	2.39	0.45
2:O:332:HIS:O	2:O:336:VAL:HG23	2.17	0.45
2:B:70:ARG:NH2	2:B:177:TYR:CE2	2.85	0.45
1:A:259:GLY:N	1:A:318:GLY:O	2.47	0.45
2:B:146:VAL:HG12	2:B:147:ASP:N	2.31	0.45
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.15	0.45
4:D:210:LEU:O	4:D:211:ILE:C	2.54	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
1:N:429:GLU:O	1:N:429:GLU:HG2	2.16	0.45
3:C:101:ARG:NH2	13:C:502:HEM:HBD2	2.31	0.45
2:B:111:CYS:CB	2:B:119:VAL:HG21	2.46	0.45
6:S:58:ARG:HH11	6:S:58:ARG:HG3	1.82	0.45
8:H:37:LEU:O	8:H:38:GLU:C	2.55	0.45
5:R:187:PHE:O	5:R:188:VAL:HG13	2.16	0.45
2:O:215:ASP:C	2:O:217:LYS:H	2.20	0.45
2:O:27:THR:CG2	2:O:28:LYS:H	2.29	0.45
1:A:117:VAL:HG23	1:A:118:GLN:H	1.81	0.45
3:P:238:THR:CB	3:P:239:PRO:HD3	2.44	0.45
4:D:215:LEU:O	4:D:219:LEU:HD12	2.16	0.45
1:N:53:ASN:CG	1:N:165:ARG:HD3	2.36	0.45
8:H:58:LEU:O	8:H:58:LEU:HD12	2.16	0.45
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.98	0.45
6:S:12:LEU:C	6:S:14:ASP:H	2.19	0.45
8:U:66:ASP:O	8:U:67:HIS:C	2.53	0.45
3:C:75:GLN:C	3:C:77:GLY:H	2.20	0.45
3:C:75:GLN:C	3:C:77:GLY:N	2.70	0.45
2:O:400:GLN:O	2:O:404:SER:HB3	2.16	0.45
2:B:51:ILE:HG22	2:B:52:LYS:N	2.30	0.45
10:W:57:HIS:HA	10:W:60:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:120:LEU:HD21	3:P:193:ILE:HB	1.98	0.45
4:Q:171:TYR:C	4:Q:173:ASP:H	2.20	0.45
1:N:88:GLY:O	2:O:286:LYS:NZ	2.42	0.45
3:C:104:TYR:CD2	3:C:104:TYR:O	2.69	0.45
3:P:208:ASN:OD1	3:P:210:LEU:N	2.42	0.45
5:R:73:LYS:HG3	22:R:1240:HOH:O	2.17	0.45
1:N:76:GLU:HA	2:O:285:ILE:CD1	2.46	0.45
1:A:156:THR:HA	5:E:7:VAL:HG21	1.97	0.45
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.46	0.45
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.81	0.45
3:P:127:THR:O	3:P:130:VAL:CG2	2.64	0.45
1:A:106:MET:C	1:A:106:MET:HE2	2.37	0.45
3:P:92:PHE:O	3:P:93:ILE:C	2.53	0.45
1:A:67:THR:HB	1:A:119:ASN:O	2.16	0.45
3:P:253:ASP:OD1	3:P:254:PRO:HD2	2.17	0.45
3:P:254:PRO:C	3:P:256:ASN:N	2.70	0.45
2:B:303:THR:HB	2:B:336:VAL:HG22	1.97	0.45
3:P:247:SER:HG	3:P:250:LEU:HB2	1.82	0.45
3:P:223:PRO:O	3:P:227:PHE:HB2	2.17	0.45
4:Q:37:CYS:O	4:Q:39:ALA:N	2.48	0.45
3:P:86:ASN:HD21	3:P:243:LEU:HD11	1.82	0.45
2:O:253:VAL:HG11	2:O:433:THR:OG1	2.17	0.45
10:W:15:ARG:HH11	10:W:15:ARG:HG2	1.82	0.45
1:N:177:LEU:HD23	1:N:177:LEU:HA	1.80	0.45
7:G:4:PHE:HD2	7:G:4:PHE:HA	1.69	0.45
6:F:94:LEU:HG	6:F:98:ILE:HD11	1.98	0.45
4:Q:57:THR:CB	4:Q:60:GLU:HG3	2.47	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.31	0.45
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.64	0.45
2:O:181:TYR:CE1	2:O:182:ARG:CG	2.99	0.45
2:B:242:GLY:O	2:B:423:SER:HB2	2.17	0.45
3:C:247:SER:N	3:C:248:PRO:CD	2.79	0.45
3:C:158:GLY:O	3:C:160:THR:N	2.50	0.45
3:P:28:ILE:CG1	3:P:225:TYR:CE2	3.00	0.45
10:J:52:TRP:O	10:J:56:LYS:HB2	2.16	0.45
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.83	0.45
1:A:208:LEU:O	1:A:209:VAL:C	2.55	0.45
2:O:227:ARG:HB2	2:O:228:SER:H	1.48	0.45
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.25	0.45
2:O:272:PHE:O	2:O:273:SER:C	2.54	0.45
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:CG2	1:A:171:THR:N	2.80	0.45
3:C:39:ALA:O	3:C:42:LEU:N	2.50	0.45
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.52	0.45
1:A:257:VAL:HG23	1:A:320:PHE:HB3	1.99	0.45
4:Q:1:GLY:C	4:Q:3:LEU:H	2.20	0.45
8:U:31:VAL:C	8:U:33:ALA:H	2.20	0.45
7:G:16:TYR:CD1	7:G:16:TYR:N	2.84	0.45
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.99	0.45
3:C:117:GLY:O	3:C:120:LEU:HB2	2.17	0.45
1:A:86:PHE:HE2	1:A:116:VAL:HG21	1.82	0.45
1:A:284:PHE:HD2	9:I:71:ASN:HA	1.80	0.45
2:O:35:ILE:O	2:O:213:HIS:CE1	2.66	0.45
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.98	0.45
8:U:43:ARG:HG3	8:U:44:VAL:N	2.31	0.45
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.37	0.45
3:P:221:PHE:HE1	15:P:3002:UQ:O1	2.00	0.45
6:F:27:ASN:O	6:F:28:LYS:C	2.54	0.45
2:B:286:LYS:HE2	2:B:287:ARG:NH2	2.32	0.45
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.47	0.45
6:S:32:MET:O	6:S:33:ARG:C	2.55	0.45
4:Q:83:ARG:HH12	4:Q:86:LYS:HG2	1.82	0.45
6:S:98:ILE:O	6:S:102:LEU:HB2	2.17	0.45
3:P:67:VAL:CG2	13:P:501:HEM:HBD2	2.47	0.44
2:B:326:THR:C	2:B:327:ILE:HG13	2.38	0.44
2:B:415:LYS:O	2:B:418:VAL:N	2.50	0.44
1:N:109:VAL:O	1:N:112:LEU:N	2.50	0.44
1:N:382:HIS:CG	1:N:389:ARG:HD2	2.51	0.44
5:R:70:ALA:C	5:R:72:SER:H	2.20	0.44
3:P:137:GLY:H	3:P:140:SER:CB	2.29	0.44
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.35	0.44
1:N:137:GLU:O	1:N:141:MET:HG3	2.17	0.44
1:N:356:ARG:HG3	2:O:91:ALA:HA	1.99	0.44
6:S:94:LEU:O	6:S:95:LYS:C	2.55	0.44
2:B:385:GLU:HB3	2:B:391:THR:O	2.17	0.44
1:N:206:LYS:H	1:N:206:LYS:HD2	1.82	0.44
9:V:28:UNK:HA	9:V:72:ALA:CB	2.47	0.44
5:R:175:PRO:O	5:R:176:ALA:C	2.56	0.44
2:B:37:SER:O	2:B:38:LEU:CB	2.65	0.44
1:A:147:ASN:C	1:A:149:THR:N	2.70	0.44
2:O:408:ALA:O	2:O:410:VAL:N	2.50	0.44
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:LEU:O	3:C:87:GLY:N	2.46	0.44
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.46	0.44
10:J:58:LYS:C	10:J:59:TYR:CD1	2.91	0.44
4:D:47:ALA:N	4:D:50:ASN:ND2	2.62	0.44
3:C:150:LEU:HB3	3:C:292:VAL:HG22	2.00	0.44
3:P:114:TRP:HE3	13:P:502:HEM:HMD1	1.83	0.44
7:G:72:LYS:HZ3	8:H:52:GLU:HG3	1.83	0.44
3:C:104:TYR:HA	3:C:316:MET:SD	2.57	0.44
2:O:97:SER:HB3	9:V:69:SER:CB	2.47	0.44
2:O:135:TRP:O	2:O:136:GLU:C	2.55	0.44
2:B:98:VAL:O	9:I:67:GLY:HA2	2.18	0.44
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.48	0.44
3:C:82:ASN:O	3:C:83:LEU:C	2.54	0.44
3:C:202:HIS:NE2	15:C:2002:UQ:O4	2.49	0.44
1:A:255:LEU:O	1:A:321:GLY:HA3	2.18	0.44
1:N:7:THR:HG21	2:O:113:ARG:CD	2.47	0.44
1:N:438:ARG:O	1:N:441:MET:HG2	2.17	0.44
4:D:37:CYS:C	4:D:39:ALA:N	2.70	0.44
4:D:8:PRO:HG2	4:D:10:PHE:HE1	1.81	0.44
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.46	0.44
2:B:23:ASP:O	2:B:24:LEU:HB3	2.16	0.44
8:H:34:ARG:HB2	8:H:61:PHE:CE1	2.52	0.44
3:C:201:LEU:C	3:C:203:GLU:H	2.21	0.44
3:P:157:ILE:O	3:P:161:LEU:HB3	2.17	0.44
4:Q:126:TYR:CD2	4:Q:126:TYR:C	2.91	0.44
7:T:33:ALA:O	7:T:37:VAL:HG23	2.18	0.44
1:N:249:PRO:HG2	1:N:250:VAL:N	2.32	0.44
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.33	0.44
2:O:374:THR:HG22	2:O:376:GLN:HB3	1.99	0.44
2:O:303:THR:HB	2:O:336:VAL:HG22	1.98	0.44
3:P:70:THR:CA	3:P:74:VAL:HG23	2.45	0.44
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.53	0.44
5:R:126:ARG:HH22	5:R:179:ASN:HB2	1.82	0.44
4:D:68:VAL:HG12	4:D:69:GLU:N	2.32	0.44
2:B:259:THR:HG22	2:B:260:GLU:H	1.82	0.44
1:A:242:ARG:CZ	1:A:432:LEU:HA	2.48	0.44
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.86	0.44
9:I:67:GLY:O	9:I:68:ILE:HD13	2.18	0.44
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.82	0.44
5:E:109:GLU:HA	5:E:112:VAL:HG13	1.98	0.44
1:N:35:CYS:HA	1:N:372:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:GLU:OE1	4:D:2:GLU:HA	2.17	0.44
10:W:57:HIS:HA	10:W:60:GLU:CD	2.38	0.44
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.65	0.44
1:A:127:ILE:C	1:A:129:LYS:N	2.70	0.44
2:O:415:LYS:O	2:O:416:LYS:C	2.55	0.44
5:R:127:VAL:O	5:R:127:VAL:HG23	2.18	0.44
2:O:43:PRO:HA	2:O:113:ARG:HD2	2.00	0.44
1:A:295:ALA:O	1:A:298:ALA:N	2.51	0.44
1:N:52:ASN:OD1	1:N:52:ASN:C	2.56	0.44
1:N:39:VAL:O	1:N:39:VAL:HG13	2.16	0.44
2:O:393:THR:O	2:O:394:ALA:O	2.35	0.44
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.99	0.44
3:P:41:CYS:SG	3:P:91:PHE:HA	2.57	0.44
1:N:56:GLY:HA2	1:N:185:TYR:CE2	2.52	0.44
4:Q:151:PRO:HB2	8:U:59:PHE:HE1	1.83	0.44
3:P:156:TYR:CD2	3:P:156:TYR:N	2.85	0.44
2:O:81:SER:O	2:O:82:SER:C	2.56	0.44
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.81	0.44
1:A:121:ALA:O	1:A:122:LEU:HB2	2.18	0.44
2:B:290:SER:HB3	2:B:293:SER:HB3	1.99	0.44
3:C:135:PRO:HG2	3:C:140:SER:OG	2.18	0.44
1:N:36:THR:HG21	1:N:373:THR:HA	2.00	0.44
3:C:261:ASN:ND2	3:C:264:VAL:N	2.65	0.44
1:A:349:THR:HA	1:A:353:GLU:OE1	2.17	0.44
2:B:137:VAL:O	2:B:140:LEU:HB3	2.17	0.44
5:E:118:ARG:O	5:E:119:ASP:HB2	2.18	0.44
5:E:184:THR:HG22	5:E:185:TYR:N	2.33	0.44
3:C:334:LEU:O	3:C:337:THR:HB	2.18	0.44
2:O:193:HIS:O	2:O:197:ASN:ND2	2.51	0.44
4:D:34:LYS:HG2	4:D:34:LYS:O	2.18	0.44
3:C:81:ARG:O	3:C:82:ASN:C	2.56	0.44
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.00	0.44
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.53	0.44
1:N:182:LEU:O	1:N:186:ILE:HG13	2.16	0.44
2:B:29:LEU:CB	2:B:30:PRO:CD	2.96	0.44
1:N:370:ASP:OD2	2:O:374:THR:HG23	2.18	0.44
1:A:25:VAL:HG22	1:A:197:LEU:HB3	2.00	0.44
2:O:287:ARG:HB3	9:V:53:GLU:HG2	2.00	0.44
5:E:10:PHE:O	5:E:11:SER:C	2.56	0.44
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.44
7:T:2:ILE:O	7:T:3:HIS:CG	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:79:VAL:O	1:N:82:MET:HG2	2.18	0.44
6:F:94:LEU:O	6:F:95:LYS:C	2.56	0.44
3:P:192:GLY:O	3:P:195:ILE:HB	2.18	0.44
7:T:38:TRP:O	7:T:39:ARG:C	2.56	0.44
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.51	0.44
3:P:254:PRO:C	3:P:256:ASN:H	2.21	0.44
2:O:37:SER:OG	2:O:38:LEU:N	2.49	0.44
3:P:345:GLU:O	3:P:348:PHE:HB2	2.18	0.44
1:N:434:TYR:O	1:N:435:ASN:C	2.56	0.44
3:P:319:ARG:HA	3:P:320:PRO:HD2	1.84	0.44
5:E:52:LYS:C	5:E:52:LYS:CD	2.86	0.44
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.99	0.44
2:B:31:ASN:HB2	2:B:228:SER:HB3	2.00	0.44
5:E:33:LYS:HE3	10:J:10:TYR:OH	2.17	0.44
8:H:27:THR:O	8:H:28:GLU:C	2.56	0.44
5:E:106:ILE:O	5:E:106:ILE:HG22	2.17	0.44
2:B:415:LYS:O	2:B:416:LYS:C	2.55	0.43
1:N:208:LEU:O	1:N:209:VAL:C	2.56	0.43
1:A:133:VAL:O	1:A:134:ILE:C	2.54	0.43
8:U:73:LEU:HD11	8:U:77:LEU:HD11	2.00	0.43
3:C:59:ASP:C	3:C:61:SER:N	2.68	0.43
1:N:199:ALA:CA	1:N:376:CYS:SG	3.05	0.43
2:B:312:PHE:N	2:B:323:GLY:O	2.42	0.43
3:P:214:SER:HB2	3:P:218:LYS:HZ3	1.79	0.43
2:O:286:LYS:HZ3	2:O:287:ARG:HH22	1.66	0.43
2:B:169:LYS:HG3	2:B:240:TRP:HB2	2.00	0.43
5:R:141:HIS:HA	5:R:177:PRO:HD2	1.99	0.43
6:F:20:TYR:O	6:F:23:ALA:HB3	2.18	0.43
1:A:253:VAL:O	1:A:323:HIS:HA	2.17	0.43
4:Q:204:MET:O	4:Q:205:GLY:C	2.54	0.43
4:Q:70:VAL:HG23	4:Q:83:ARG:HG2	1.98	0.43
1:N:140:GLU:HG2	9:V:48:PRO:HB2	1.99	0.43
4:D:120:ARG:HH11	4:D:120:ARG:HG2	1.83	0.43
2:O:337:ILE:HD12	2:O:434:PRO:CD	2.41	0.43
1:N:40:TRP:CG	1:N:380:GLY:HA3	2.53	0.43
2:B:299:VAL:O	2:B:303:THR:HG22	2.18	0.43
3:C:40:VAL:O	3:C:44:THR:OG1	2.35	0.43
2:B:151:ALA:C	2:B:153:GLN:H	2.21	0.43
1:N:117:VAL:CG2	1:N:118:GLN:N	2.81	0.43
4:D:165:TYR:O	4:D:166:ASN:O	2.36	0.43
1:N:241:ILE:O	1:N:241:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:16:TYR:N	7:T:16:TYR:CD1	2.86	0.43
2:B:100:SER:HA	2:B:104:LYS:O	2.17	0.43
4:Q:28:ARG:O	4:Q:29:GLY:C	2.56	0.43
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.83	0.43
2:O:157:VAL:HG22	2:O:157:VAL:O	2.17	0.43
2:O:62:ASN:O	2:O:65:THR:CG2	2.64	0.43
1:A:90:THR:CB	1:A:95:THR:HG23	2.49	0.43
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.90	0.43
6:F:32:MET:HE1	6:F:87:LYS:HG2	2.00	0.43
2:B:120:MET:O	2:B:121:GLU:C	2.56	0.43
8:U:58:LEU:HD12	8:U:58:LEU:O	2.17	0.43
3:P:184:PHE:CD2	13:P:501:HEM:HBC1	2.53	0.43
1:A:106:MET:HE1	1:A:208:LEU:HD13	2.00	0.43
1:A:106:MET:CG	1:A:203:ILE:HD13	2.46	0.43
1:A:87:ASN:OD1	1:A:88:GLY:N	2.44	0.43
1:A:239:SER:O	1:A:421:ALA:HA	2.17	0.43
1:A:117:VAL:CG2	1:A:118:GLN:H	2.32	0.43
1:A:184:SER:HA	1:A:187:ASP:HB2	2.00	0.43
5:R:141:HIS:HB2	5:R:176:ALA:HB2	2.00	0.43
2:B:206:LEU:O	2:B:206:LEU:HG	2.18	0.43
3:P:137:GLY:O	3:P:140:SER:HB2	2.18	0.43
2:O:47:ILE:HD13	2:O:120:MET:CE	2.48	0.43
1:A:395:TRP:O	1:A:398:ARG:HB2	2.19	0.43
2:B:408:ALA:O	2:B:409:ASP:C	2.57	0.43
4:D:98:PRO:O	4:D:99:GLU:C	2.56	0.43
7:T:4:PHE:HA	7:T:4:PHE:HD2	1.71	0.43
2:O:167:ALA:HB3	2:O:168:TYR:HD1	1.83	0.43
2:B:56:ARG:HD3	2:B:103:GLU:HB3	2.01	0.43
2:B:341:MET:HA	2:B:341:MET:CE	2.46	0.43
3:C:316:MET:HA	3:C:319:ARG:HE	1.84	0.43
4:Q:167:GLU:C	4:Q:169:LEU:N	2.72	0.43
2:O:34:ILE:HD13	2:O:386:ALA:O	2.19	0.43
2:B:346:ALA:O	2:B:351:GLY:HA3	2.18	0.43
3:P:34:PHE:HB2	22:P:381:HOH:O	2.18	0.43
1:N:381:SER:O	1:N:382:HIS:C	2.57	0.43
3:P:101:ARG:CZ	13:P:502:HEM:HBD2	2.49	0.43
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.38	0.43
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.53	0.43
1:A:256:ALA:HA	1:A:320:PHE:O	2.18	0.43
3:C:78:TRP:CG	3:C:79:LEU:N	2.86	0.43
2:O:430:LEU:H	2:O:430:LEU:HG	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.54	0.43
6:F:98:ILE:O	6:F:102:LEU:HB2	2.17	0.43
9:V:67:GLY:O	9:V:68:ILE:HD13	2.18	0.43
8:H:55:THR:O	8:H:56:GLU:C	2.57	0.43
2:O:372:VAL:O	2:O:372:VAL:HG12	2.19	0.43
4:Q:47:ALA:HB1	4:Q:89:ASP:O	2.18	0.43
5:E:147:ILE:HG13	5:E:157:TYR:O	2.18	0.43
1:N:206:LYS:N	1:N:206:LYS:HD2	2.32	0.43
1:N:159:GLN:O	1:N:159:GLN:HG3	2.18	0.43
4:Q:175:THR:HA	4:Q:176:PRO:HD3	1.84	0.43
4:Q:26:VAL:CG1	4:Q:55:THR:HG21	2.45	0.43
2:B:244:ILE:O	2:B:425:ALA:HA	2.19	0.43
2:O:142:PRO:O	2:O:145:LYS:HB2	2.18	0.43
3:P:319:ARG:HB3	3:P:374:GLU:CD	2.39	0.43
3:C:263:LEU:O	5:R:143:GLY:HA3	2.19	0.43
1:A:318:GLY:O	1:A:319:LEU:HD23	2.19	0.43
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.52	0.43
1:A:247:ALA:HB2	7:G:11:ARG:HD2	2.00	0.43
3:C:86:ASN:HD21	3:C:243:LEU:HD11	1.83	0.43
1:N:185:TYR:HA	1:N:189:HIS:HD2	1.83	0.43
3:C:192:GLY:O	3:C:195:ILE:HB	2.19	0.43
6:S:27:ASN:O	6:S:30:GLY:N	2.41	0.43
6:F:21:TYR:C	6:F:21:TYR:CD2	2.92	0.43
1:A:438:ARG:HG3	1:A:438:ARG:HH11	1.81	0.43
1:N:23:LEU:HA	1:N:192:ALA:O	2.18	0.43
1:N:112:LEU:HG	1:N:112:LEU:H	1.53	0.43
2:O:258:VAL:HG12	2:O:323:GLY:CA	2.49	0.43
2:O:37:SER:O	2:O:38:LEU:CB	2.67	0.43
2:O:374:THR:CG2	2:O:376:GLN:HB3	2.48	0.43
1:A:76:GLU:O	1:A:80:GLU:HG3	2.19	0.43
1:A:242:ARG:NH1	1:A:432:LEU:HA	2.33	0.43
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.82	0.43
1:A:147:ASN:O	1:A:149:THR:N	2.51	0.43
1:N:76:GLU:HG2	2:O:285:ILE:HD13	2.00	0.43
3:C:75:GLN:O	3:C:77:GLY:N	2.52	0.43
10:J:63:GLU:O	10:J:64:GLU:HB3	2.19	0.43
4:Q:41:HIS:HB3	4:Q:113:LEU:HD12	2.00	0.43
3:P:33:ASN:HB3	22:P:385:HOH:O	2.18	0.43
1:A:241:ILE:O	1:A:241:ILE:HG23	2.18	0.43
2:O:275:LEU:O	2:O:279:LEU:HD12	2.19	0.43
1:A:114:ALA:O	1:A:117:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:163:LEU:HA	1:N:163:LEU:HD23	1.86	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.77	0.43
6:S:34:ASP:OD1	6:S:34:ASP:N	2.51	0.43
3:P:289:LEU:O	3:P:293:LEU:HG	2.17	0.43
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.99	0.43
1:N:116:VAL:O	1:N:120:CYS:HB2	2.19	0.43
2:O:268:GLU:OE1	2:O:416:LYS:NZ	2.48	0.43
5:E:98:VAL:HG22	5:E:134:ILE:HG23	2.01	0.43
2:B:166:ALA:O	2:B:242:GLY:N	2.51	0.43
3:P:79:LEU:HD11	3:P:83:LEU:HD11	2.01	0.43
2:O:70:ARG:NH2	2:O:177:TYR:CE2	2.87	0.43
4:Q:37:CYS:C	4:Q:39:ALA:N	2.72	0.43
5:R:138:VAL:O	5:R:180:LEU:HD22	2.19	0.43
1:A:242:ARG:HH12	1:A:432:LEU:H	1.65	0.43
4:D:167:GLU:C	4:D:169:LEU:N	2.73	0.43
3:C:305:ILE:HA	3:C:305:ILE:HD13	1.83	0.43
5:E:20:ASP:O	5:E:22:THR:N	2.45	0.43
6:F:103:GLU:O	6:F:104:ARG:C	2.57	0.43
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.37	0.43
2:B:167:ALA:HB3	2:B:168:TYR:HD1	1.84	0.42
2:O:51:ILE:N	2:O:105:MET:O	2.51	0.42
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.81	0.42
1:A:240:GLU:HB3	1:A:422:LEU:HB3	2.01	0.42
3:P:255:GLU:H	3:P:255:GLU:HG2	1.60	0.42
1:N:67:THR:HB	1:N:119:ASN:O	2.19	0.42
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.48	0.42
2:O:150:VAL:HG22	2:O:151:ALA:N	2.34	0.42
6:S:13:MET:HB2	6:S:16:ILE:HD12	2.01	0.42
2:B:215:ASP:C	2:B:217:LYS:H	2.23	0.42
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.18	0.42
1:A:253:VAL:CG1	1:A:335:MET:HE1	2.47	0.42
5:E:91:TRP:O	5:E:92:ARG:C	2.57	0.42
3:C:216:SER:HB3	6:F:59:MET:HE2	2.00	0.42
2:O:146:VAL:HG12	2:O:147:ASP:N	2.33	0.42
6:F:82:LYS:O	6:F:83:TYR:C	2.55	0.42
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.34	0.42
7:T:60:SER:O	7:T:64:GLN:HB2	2.19	0.42
1:N:404:ALA:O	1:N:405:ARG:C	2.57	0.42
2:O:298:GLY:HA3	2:O:343:GLN:HG3	2.00	0.42
2:O:346:ALA:O	2:O:351:GLY:HA3	2.18	0.42
2:O:56:ARG:HG2	2:O:234:SER:OG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:111:CYS:HB3	2:O:119:VAL:HG21	2.01	0.42
2:B:324:PHE:HE2	2:B:341:MET:HE2	1.84	0.42
4:Q:221:TYR:CE2	5:R:39:VAL:HG21	2.54	0.42
3:P:82:ASN:O	3:P:83:LEU:C	2.58	0.42
4:D:52:ILE:C	4:D:54:VAL:N	2.72	0.42
4:D:197:GLU:HG2	4:D:198:HIS:H	1.84	0.42
3:P:22:LEU:HA	3:P:23:PRO:HD3	1.88	0.42
3:P:346:HIS:CG	3:P:347:PRO:HA	2.54	0.42
6:S:12:LEU:C	6:S:14:ASP:N	2.73	0.42
5:R:145:VAL:HA	5:R:146:PRO:HD3	1.85	0.42
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.76	0.42
3:C:82:ASN:H	3:C:82:ASN:ND2	2.14	0.42
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.54	0.42
1:N:127:ILE:C	1:N:129:LYS:N	2.73	0.42
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.54	0.42
1:N:219:VAL:CG1	1:N:220:SER:N	2.82	0.42
3:P:4:ASN:HD22	3:P:6:ARG:H	1.68	0.42
2:O:24:LEU:HD23	2:O:24:LEU:C	2.40	0.42
3:P:68:ALA:HA	18:P:3011:GOL:O3	2.20	0.42
2:B:176:LEU:O	2:B:176:LEU:HD12	2.19	0.42
1:N:308:GLN:O	1:N:322:PHE:HA	2.19	0.42
9:I:49:LEU:HD13	9:I:55:MET:HE2	2.01	0.42
16:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.34	0.42
1:N:109:VAL:HA	1:N:112:LEU:CD1	2.47	0.42
6:F:58:ARG:HG3	6:F:89:TYR:OH	2.20	0.42
2:B:181:TYR:CE1	2:B:182:ARG:CG	3.00	0.42
3:P:230:ILE:O	3:P:233:LEU:HB3	2.19	0.42
5:E:1:VAL:HG23	5:E:3:ASN:N	2.27	0.42
2:B:248:ASN:ND2	2:B:248:ASN:C	2.73	0.42
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.50	0.42
2:B:215:ASP:O	2:B:217:LYS:N	2.52	0.42
4:Q:148:HIS:ND1	4:Q:161:ALA:HA	2.35	0.42
1:N:242:ARG:O	7:T:14:ILE:HA	2.19	0.42
1:A:156:THR:CG2	1:A:157:ALA:N	2.83	0.42
3:P:207:ASN:ND2	3:P:314:ARG:NH1	2.67	0.42
3:C:81:ARG:NH2	13:C:501:HEM:O1A	2.53	0.42
2:O:209:ILE:O	2:O:211:VAL:N	2.53	0.42
2:O:68:LEU:HA	2:O:144:LEU:HD21	2.00	0.42
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.48	0.42
2:B:337:ILE:O	2:B:340:ALA:HB3	2.20	0.42
2:O:272:PHE:HB3	2:O:322:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:SER:HB2	3:C:218:LYS:HZ3	1.81	0.42
1:N:340:GLY:O	1:N:343:MET:HB2	2.19	0.42
3:P:175:THR:HA	3:P:178:ARG:HG2	2.01	0.42
5:R:146:PRO:C	5:R:147:ILE:HG13	2.38	0.42
1:N:260:PRO:HB3	1:N:414:TYR:CE2	2.54	0.42
3:P:183:HIS:CE1	13:P:501:HEM:NB	2.87	0.42
5:R:156:TYR:HB2	5:R:165:TYR:HB2	2.00	0.42
6:F:89:TYR:C	6:F:89:TYR:CD1	2.93	0.42
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.55	0.42
3:P:173:ASN:N	3:P:174:PRO:CD	2.80	0.42
2:B:42:SER:C	2:B:44:ALA:H	2.23	0.42
1:A:170:THR:HG22	1:A:172:GLU:H	1.85	0.42
1:A:295:ALA:O	1:A:298:ALA:HB3	2.20	0.42
5:R:69:LEU:HD23	5:R:69:LEU:HA	1.92	0.42
16:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.20	0.42
5:E:71:LEU:CD2	5:E:71:LEU:N	2.83	0.42
8:U:34:ARG:HB2	8:U:61:PHE:CE1	2.54	0.42
1:A:204:SER:O	1:A:205:HIS:C	2.58	0.42
2:O:327:ILE:HD11	9:V:58:ARG:O	2.19	0.42
3:C:231:LEU:O	3:C:235:LEU:HG	2.19	0.42
2:B:268:GLU:O	2:B:269:ALA:C	2.58	0.42
1:A:109:VAL:O	1:A:112:LEU:N	2.52	0.42
2:O:201:SER:N	2:O:227:ARG:HB3	2.22	0.42
1:N:41:ILE:HG12	1:N:195:MET:HG2	2.01	0.42
3:C:59:ASP:O	3:C:62:LEU:N	2.47	0.42
3:C:273:TRP:CD2	3:C:274:TYR:N	2.88	0.42
3:P:350:ILE:HG23	3:P:351:ILE:N	2.34	0.42
7:G:73:ASN:HB3	7:G:76:ASP:OD2	2.20	0.42
2:O:267:ALA:O	2:O:269:ALA:N	2.52	0.42
1:N:242:ARG:HH12	1:N:432:LEU:N	2.18	0.42
5:E:175:PRO:HG2	5:E:176:ALA:H	1.84	0.42
2:O:80:ALA:HA	2:O:84:ARG:NH2	2.35	0.42
10:W:22:LEU:HD23	10:W:22:LEU:C	2.40	0.42
3:P:52:LEU:HD21	3:P:80:ILE:HG22	2.01	0.42
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.54	0.42
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.50	0.42
1:A:59:VAL:HG23	1:A:182:LEU:HD23	2.02	0.42
2:O:272:PHE:HB3	2:O:322:PHE:CD1	2.55	0.42
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.44	0.42
1:N:7:THR:HG21	2:O:113:ARG:NE	2.35	0.42
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PRO:HA	9:I:52:ARG:CG	2.50	0.42
4:D:102:ARG:HG2	4:D:107:GLY:O	2.18	0.42
1:A:60:GLU:OE2	1:A:89:TYR:C	2.58	0.42
3:C:160:THR:O	3:C:161:LEU:C	2.58	0.42
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.19	0.42
2:O:212:LYS:HG2	2:O:214:SER:OG	2.20	0.42
9:V:75:SER:O	9:V:76:VAL:HB	2.20	0.42
1:N:244:ARG:NE	7:T:10:VAL:HB	2.34	0.42
5:E:137:GLY:O	5:E:145:VAL:HG13	2.20	0.42
3:C:28:ILE:CG1	3:C:225:TYR:CE2	3.03	0.42
2:O:71:LEU:N	2:O:71:LEU:CD2	2.75	0.42
3:P:362:ILE:HG22	3:P:363:LEU:N	2.35	0.42
1:N:86:PHE:HE2	1:N:116:VAL:HG21	1.85	0.42
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.42
3:C:236:MET:O	3:C:238:THR:N	2.53	0.42
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.31	0.42
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.19	0.42
1:N:433:ASP:OD2	1:N:435:ASN:N	2.53	0.42
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.55	0.42
5:E:119:ASP:CG	5:E:179:ASN:ND2	2.74	0.42
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	2.01	0.42
5:E:33:LYS:HE3	10:J:10:TYR:CZ	2.55	0.42
10:W:36:ASP:O	10:W:37:GLN:C	2.57	0.42
2:O:232:THR:HG22	2:O:233:SER:N	2.35	0.42
5:E:156:TYR:HB2	5:E:165:TYR:HB2	2.01	0.42
4:Q:2:GLU:CD	4:Q:2:GLU:H	2.23	0.42
2:O:56:ARG:HH22	2:O:318:ASP:CG	2.24	0.42
2:B:100:SER:HB2	2:B:105:MET:HG2	1.99	0.42
5:R:77:LYS:HE3	5:R:191:ASP:OD2	2.20	0.42
2:B:43:PRO:HA	2:B:113:ARG:HD2	2.02	0.42
2:B:402:ILE:CG2	2:B:403:ASP:H	2.29	0.42
1:N:354:VAL:O	1:N:355:LYS:C	2.58	0.42
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.68	0.42
1:N:280:TYR:HA	1:N:284:PHE:CE1	2.55	0.42
4:D:204:MET:O	4:D:205:GLY:C	2.56	0.42
3:P:134:LEU:HD21	3:P:180:PHE:HA	2.01	0.42
2:O:366:ALA:O	2:O:367:THR:C	2.58	0.42
4:D:16:GLY:N	4:D:19:SER:OG	2.52	0.42
1:N:23:LEU:HD23	1:N:23:LEU:C	2.41	0.41
2:O:51:ILE:HG22	2:O:52:LYS:N	2.35	0.41
1:A:134:ILE:O	1:A:136:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:HD2	3:P:12:LEU:HG	1.80	0.41
2:B:19:PRO:O	2:B:22:GLU:CB	2.68	0.41
2:O:287:ARG:HA	9:V:53:GLU:CG	2.46	0.41
2:B:306:PRO:O	2:B:307:PHE:HB3	2.20	0.41
2:O:18:CYS:HA	2:O:19:PRO:HD3	1.84	0.41
3:C:326:PHE:O	3:C:330:VAL:HG23	2.20	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
4:D:81:PHE:CD2	4:D:81:PHE:N	2.87	0.41
1:N:220:SER:HA	1:N:225:GLU:OE1	2.19	0.41
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.49	0.41
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.20	0.41
3:C:130:VAL:HG23	3:C:183:HIS:HD1	1.85	0.41
2:B:402:ILE:CG2	2:B:403:ASP:N	2.83	0.41
4:Q:198:HIS:O	4:Q:201:ARG:HB3	2.20	0.41
1:A:172:GLU:O	1:A:175:LYS:HB2	2.20	0.41
3:P:81:ARG:O	3:P:82:ASN:C	2.57	0.41
3:C:39:ALA:O	3:C:40:VAL:C	2.57	0.41
6:F:20:TYR:HA	6:F:23:ALA:HB3	2.02	0.41
3:P:202:HIS:NE2	15:P:3002:UQ:O4	2.52	0.41
3:C:216:SER:O	6:F:63:LYS:HD2	2.19	0.41
4:D:161:ALA:O	4:D:163:PRO:HD3	2.19	0.41
5:E:100:HIS:NE2	5:E:131:GLU:HG3	2.35	0.41
4:Q:81:PHE:N	4:Q:81:PHE:CD2	2.88	0.41
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.20	0.41
3:C:333:LEU:HB3	11:C:2007:PEE:H75	2.02	0.41
1:A:86:PHE:CD2	1:A:99:ILE:HD11	2.55	0.41
1:A:341:GLU:O	1:A:342:TRP:C	2.59	0.41
4:D:178:THR:O	4:D:181:GLN:HB3	2.20	0.41
1:N:106:MET:HE1	1:N:208:LEU:CD1	2.50	0.41
1:A:127:ILE:C	1:A:129:LYS:H	2.22	0.41
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.02	0.41
2:O:163:LEU:HD12	2:O:425:ALA:CB	2.50	0.41
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.35	0.41
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.89	0.41
3:P:316:MET:HA	3:P:319:ARG:HE	1.85	0.41
4:Q:161:ALA:O	4:Q:163:PRO:N	2.54	0.41
2:B:393:THR:O	2:B:394:ALA:O	2.37	0.41
2:O:290:SER:HB2	2:O:293:SER:HB3	2.02	0.41
2:B:372:VAL:CG1	2:B:378:LEU:HD13	2.50	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.73	0.41
2:O:408:ALA:O	2:O:409:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:103:GLN:HA	5:R:106:ILE:HD12	2.01	0.41
3:C:127:THR:O	3:C:130:VAL:CG2	2.68	0.41
4:D:160:MET:HB2	19:D:501:HEC:C4D	2.50	0.41
2:B:51:ILE:CG2	2:B:52:LYS:N	2.83	0.41
1:A:99:ILE:HG13	1:A:113:LEU:HD21	2.02	0.41
3:P:95:ILE:CG2	3:P:96:PHE:N	2.82	0.41
1:A:240:GLU:CB	1:A:422:LEU:HB3	2.50	0.41
4:Q:232:SER:CB	7:T:23:GLN:HE22	2.20	0.41
2:B:247:GLN:NE2	2:B:249:GLY:H	2.19	0.41
4:D:183:ALA:O	4:D:186:VAL:HG12	2.20	0.41
3:P:104:TYR:CD2	11:P:3007:PEE:H14	2.55	0.41
5:R:37:TYR:HB3	10:W:14:PHE:HB3	2.02	0.41
2:O:299:VAL:O	2:O:303:THR:HG22	2.19	0.41
1:N:239:SER:O	1:N:421:ALA:HA	2.21	0.41
1:N:417:ASP:OD2	1:N:438:ARG:NH2	2.46	0.41
3:C:276:LEU:O	3:C:277:PHE:C	2.56	0.41
1:A:23:LEU:HD23	1:A:23:LEU:C	2.41	0.41
5:R:102:THR:C	5:R:104:ALA:N	2.73	0.41
4:D:230:LEU:HD23	4:D:230:LEU:HA	1.87	0.41
3:P:311:SER:CB	3:P:319:ARG:NH1	2.84	0.41
4:D:10:PHE:CD2	8:H:74:PHE:HE2	2.38	0.41
2:B:35:ILE:HG23	2:B:216:LEU:HG	2.02	0.41
3:C:311:SER:CB	3:C:319:ARG:NH1	2.82	0.41
1:N:39:VAL:HG11	1:N:117:VAL:HG11	2.03	0.41
4:Q:228:SER:OG	4:Q:229:VAL:N	2.54	0.41
1:N:210:ASP:O	1:N:213:ARG:N	2.54	0.41
1:A:86:PHE:HD1	1:A:87:ASN:N	2.19	0.41
6:S:58:ARG:HA	6:S:61:ARG:NH2	2.35	0.41
2:O:157:VAL:HG23	9:V:64:LEU:HD21	2.03	0.41
2:B:312:PHE:O	2:B:322:PHE:HA	2.21	0.41
8:U:36:ARG:CB	8:U:36:ARG:HH11	2.34	0.41
4:Q:94:PRO:HB2	4:Q:95:TYR:CD1	2.54	0.41
1:N:335:MET:O	1:N:336:PHE:C	2.59	0.41
1:A:23:LEU:HB2	1:A:192:ALA:HB1	2.02	0.41
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.55	0.41
4:D:33:TYR:HA	4:D:37:CYS:SG	2.60	0.41
4:Q:161:ALA:O	4:Q:163:PRO:HD3	2.20	0.41
3:C:246:PHE:CZ	4:D:205:GLY:HA3	2.55	0.41
3:P:366:LEU:CD2	3:P:366:LEU:N	2.83	0.41
10:J:57:HIS:ND1	10:J:58:LYS:HG3	2.36	0.41
1:N:86:PHE:CE2	1:N:116:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:239:TYR:CD2	2:O:240:TRP:N	2.89	0.41
2:O:324:PHE:HD2	2:O:344:LEU:HD12	1.85	0.41
2:B:272:PHE:HB3	2:B:322:PHE:CD1	2.55	0.41
4:D:26:VAL:CG1	4:D:55:THR:HG21	2.47	0.41
1:A:295:ALA:O	1:A:296:ALA:C	2.59	0.41
1:N:339:GLN:HE22	1:N:437:ILE:HG23	1.86	0.41
3:P:79:LEU:HD12	3:P:79:LEU:C	2.41	0.41
3:C:247:SER:O	3:C:248:PRO:C	2.59	0.41
3:P:36:SER:O	3:P:39:ALA:HB3	2.21	0.41
4:Q:120:ARG:NH1	4:Q:120:ARG:HG2	2.35	0.41
5:R:40:THR:O	5:R:41:ALA:C	2.56	0.41
8:H:66:ASP:O	8:H:67:HIS:C	2.56	0.41
8:U:15:ASP:HA	8:U:16:PRO:HD2	1.87	0.41
2:B:377:GLY:O	2:B:380:ASN:HB3	2.21	0.41
1:A:428:ILE:HG12	1:A:428:ILE:H	1.57	0.41
4:Q:210:LEU:HA	4:Q:210:LEU:HD23	1.88	0.41
3:C:50:LEU:O	3:C:53:ALA:N	2.54	0.41
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.84	0.41
2:B:81:SER:O	2:B:82:SER:C	2.58	0.41
1:N:184:SER:HA	1:N:187:ASP:HB2	2.02	0.41
2:O:222:GLN:O	2:O:223:PHE:CB	2.69	0.41
1:N:85:HIS:CD2	2:O:284:LEU:HB3	2.55	0.41
1:N:365:MET:SD	1:N:392:LEU:HD13	2.60	0.41
3:C:137:GLY:O	3:C:140:SER:HB2	2.21	0.41
3:C:320:PRO:HG2	3:C:321:LEU:N	2.33	0.41
1:N:354:VAL:CG2	1:N:355:LYS:N	2.82	0.41
2:B:131:GLU:O	2:B:132:PHE:C	2.59	0.41
1:N:242:ARG:CZ	1:N:432:LEU:HA	2.51	0.41
4:D:22:ASP:HA	10:J:50:LYS:HB3	2.02	0.41
2:B:366:ALA:O	2:B:367:THR:C	2.58	0.41
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.55	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.41	0.41
2:O:111:CYS:CB	2:O:119:VAL:HG21	2.50	0.41
1:N:86:PHE:CE1	1:N:97:PHE:HB3	2.55	0.41
3:P:317:THR:HG23	11:P:3007:PEE:H9	2.03	0.41
4:Q:164:ILE:HG21	4:Q:182:ILE:CG2	2.48	0.41
1:A:127:ILE:O	1:A:130:GLU:N	2.54	0.41
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.56	0.41
1:A:90:THR:HB	1:A:95:THR:HG23	2.03	0.41
7:G:44:GLN:O	7:G:45:VAL:C	2.59	0.41
2:B:70:ARG:NH2	2:B:177:TYR:HE2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:O	1:A:179:ARG:C	2.59	0.41
1:N:269:VAL:O	1:N:272:VAL:N	2.54	0.41
1:N:19:LEU:C	1:N:21:ASN:N	2.74	0.41
5:E:112:VAL:HG23	5:E:112:VAL:O	2.20	0.41
3:C:54:MET:SD	5:E:62:LEU:HD21	2.61	0.41
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.35	0.41
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.41
3:P:52:LEU:HD13	13:P:501:HEM:O2D	2.20	0.41
3:C:184:PHE:CZ	3:P:184:PHE:HB3	2.56	0.41
13:C:502:HEM:HHA	13:C:502:HEM:HBD1	2.02	0.41
1:A:86:PHE:CE1	1:A:97:PHE:HB3	2.56	0.41
3:C:253:ASP:OD1	3:C:254:PRO:CD	2.68	0.41
2:O:26:ILE:HA	2:O:35:ILE:O	2.21	0.41
1:N:171:THR:O	1:N:175:LYS:HG3	2.20	0.41
1:N:84:ALA:HA	1:N:100:LYS:O	2.21	0.41
3:P:59:ASP:C	3:P:61:SER:N	2.74	0.41
1:A:339:GLN:NE2	1:A:437:ILE:HG23	2.36	0.41
1:N:435:ASN:O	1:N:438:ARG:HB3	2.20	0.41
4:Q:52:ILE:C	4:Q:54:VAL:N	2.74	0.41
1:N:145:MET:O	1:N:146:THR:C	2.60	0.41
2:O:70:ARG:NH2	2:O:177:TYR:HE2	2.19	0.41
6:S:13:MET:CA	6:S:16:ILE:HD12	2.47	0.41
6:S:13:MET:CB	6:S:16:ILE:HD12	2.51	0.41
7:G:38:TRP:O	7:G:39:ARG:C	2.57	0.41
3:C:326:PHE:C	3:C:326:PHE:CD2	2.94	0.41
1:A:90:THR:CG2	1:A:90:THR:O	2.69	0.41
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.41
4:D:66:GLU:C	4:D:68:VAL:H	2.23	0.41
1:A:416:TYR:CE1	1:A:442:TYR:HA	2.56	0.41
2:O:206:LEU:HG	2:O:216:LEU:HD11	2.03	0.41
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.02	0.41
2:O:47:ILE:HG22	2:O:48:GLY:N	2.35	0.41
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.54	0.41
3:P:208:ASN:C	3:P:208:ASN:OD1	2.58	0.41
4:D:72:ASP:HB2	4:D:83:ARG:HE	1.84	0.41
4:Q:98:PRO:O	4:Q:99:GLU:C	2.59	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.90	0.41
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.34	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.76	0.41
3:P:45:GLN:O	3:P:49:GLY:N	2.44	0.41
2:B:33:LEU:HD21	2:B:224:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:330:SER:O	1:N:331:ILE:C	2.60	0.41
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.81	0.41
2:B:80:ALA:HA	2:B:84:ARG:NH2	2.36	0.41
1:A:150:PHE:O	1:A:153:LEU:HB3	2.21	0.41
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.41
2:B:102:ARG:NH1	2:B:172:LEU:O	2.54	0.41
1:A:277:ILE:CD1	1:A:345:LEU:HD11	2.51	0.41
2:O:225:ASN:C	2:O:227:ARG:HG3	2.40	0.41
4:Q:179:MET:O	4:Q:182:ILE:HB	2.21	0.41
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.21	0.41
3:C:70:THR:CA	3:C:74:VAL:HG23	2.49	0.41
1:N:434:TYR:CE2	7:T:19:SER:HB2	2.56	0.41
2:B:307:PHE:C	2:B:307:PHE:CD1	2.91	0.41
7:T:44:GLN:O	7:T:45:VAL:C	2.60	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.75	0.41
5:R:96:LEU:HD12	5:R:135:LEU:O	2.20	0.41
2:O:206:LEU:O	2:O:206:LEU:HG	2.20	0.41
1:A:64:PHE:C	1:A:66:GLY:H	2.25	0.41
1:N:149:THR:HG22	1:N:150:PHE:N	2.35	0.41
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.83	0.41
2:B:408:ALA:O	2:B:410:VAL:N	2.54	0.41
1:N:46:ARG:HD3	1:N:231:LEU:HD13	2.02	0.41
4:Q:209:LEU:HD23	4:Q:209:LEU:HA	1.77	0.41
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.21	0.41
1:A:403:ASP:O	1:A:404:ALA:C	2.59	0.41
3:P:254:PRO:O	3:P:257:PHE:N	2.52	0.40
6:F:57:GLU:HB3	6:F:61:ARG:HH12	1.85	0.40
2:B:272:PHE:O	2:B:273:SER:C	2.59	0.40
2:O:402:ILE:CG2	2:O:403:ASP:H	2.30	0.40
2:O:192:HIS:O	2:O:196:GLN:HG3	2.21	0.40
3:P:350:ILE:CG2	3:P:351:ILE:N	2.84	0.40
4:D:203:ARG:HD3	10:J:40:ASP:OD1	2.21	0.40
2:O:410:VAL:O	2:O:413:ALA:N	2.54	0.40
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.93	0.40
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.49	0.40
3:P:110:TYR:O	3:P:111:LYS:C	2.60	0.40
4:D:130:LEU:HD12	4:D:130:LEU:HA	1.92	0.40
3:C:67:VAL:HG22	13:C:501:HEM:HBD2	2.02	0.40
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	2.03	0.40
4:D:30:PHE:HE2	4:D:64:LEU:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HG	1:A:174:ILE:HG21	2.01	0.40
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.56	0.40
5:R:38:LEU:O	5:R:39:VAL:C	2.59	0.40
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.53	0.40
2:O:163:LEU:CD1	2:O:425:ALA:HB3	2.51	0.40
2:O:403:ASP:C	2:O:405:VAL:N	2.74	0.40
10:J:14:PHE:HD2	10:J:14:PHE:N	2.17	0.40
4:D:10:PHE:HD1	4:D:10:PHE:H	1.67	0.40
5:R:52:LYS:C	5:R:52:LYS:CD	2.88	0.40
4:D:164:ILE:O	4:D:179:MET:CE	2.69	0.40
2:O:107:TYR:CD2	2:O:127:THR:HG22	2.56	0.40
3:C:4:ASN:C	3:C:5:ILE:HD13	2.41	0.40
4:D:81:PHE:N	4:D:81:PHE:HD2	2.19	0.40
3:P:201:LEU:O	3:P:203:GLU:N	2.54	0.40
3:P:377:MET:HE2	6:S:20:TYR:HB2	2.04	0.40
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.77	0.40
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.39	0.40
3:C:364:LEU:O	3:C:368:PRO:HG3	2.21	0.40
5:R:80:ASP:O	5:R:80:ASP:OD1	2.38	0.40
3:C:28:ILE:HG12	3:C:225:TYR:CZ	2.56	0.40
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.52	0.40
6:F:65:ALA:O	6:F:68:LEU:HB2	2.21	0.40
4:D:233:ARG:HG3	7:G:17:SER:OG	2.21	0.40
7:G:33:ALA:O	7:G:37:VAL:HG23	2.21	0.40
2:O:166:ALA:HB1	2:O:242:GLY:C	2.42	0.40
2:O:169:LYS:HE3	2:O:240:TRP:HA	2.02	0.40
1:N:37:VAL:HA	1:N:198:ALA:O	2.22	0.40
5:R:38:LEU:CA	10:W:14:PHE:CE1	3.04	0.40
2:B:280:GLY:HA3	2:B:293:SER:CB	2.52	0.40
5:R:153:PHE:C	5:R:155:GLY:H	2.24	0.40
1:N:276:ILE:HG13	1:N:357:ALA:HB2	2.02	0.40
8:U:25:GLU:HG2	8:U:61:PHE:CZ	2.55	0.40
3:C:303:PHE:O	3:C:306:PRO:HD2	2.21	0.40
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.36	0.40
4:D:90:TYR:O	4:D:91:PHE:C	2.60	0.40
2:B:410:VAL:O	2:B:411:VAL:C	2.59	0.40
4:Q:227:TRP:O	4:Q:228:SER:C	2.60	0.40
3:C:10:PRO:HG2	3:P:200:PHE:CE1	2.56	0.40
3:C:16:ASN:O	3:C:18:SER:N	2.47	0.40
4:Q:238:ARG:HB3	4:Q:238:ARG:NH1	2.37	0.40
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PHE:CE2	1:A:116:VAL:HG21	2.57	0.40
1:A:106:MET:CE	1:A:208:LEU:HD13	2.52	0.40
1:A:127:ILE:O	1:A:129:LYS:N	2.54	0.40
2:O:341:MET:HE3	2:O:417:PHE:CE2	2.57	0.40
2:O:122:TYR:O	2:O:123:LEU:C	2.58	0.40
4:Q:49:ARG:O	4:Q:52:ILE:HG13	2.22	0.40
5:R:126:ARG:HH22	5:R:179:ASN:CB	2.35	0.40
15:P:3002:UQ:HM51	15:P:3002:UQ:H8	2.02	0.40
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.56	0.40
3:C:4:ASN:HD22	3:C:6:ARG:H	1.69	0.40
2:B:325:TYR:CD2	2:B:325:TYR:C	2.94	0.40
6:F:19:TRP:O	6:F:22:ASN:N	2.52	0.40
1:N:331:ILE:O	1:N:334:MET:HB3	2.21	0.40
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.86	0.40
7:T:34:LEU:HB2	7:T:35:PRO:HD3	2.03	0.40
1:N:223:TYR:CD1	1:N:223:TYR:C	2.94	0.40
6:F:40:ASP:OD1	6:F:40:ASP:C	2.58	0.40
3:P:42:LEU:CD2	3:P:190:ILE:HG22	2.52	0.40
2:O:110:GLU:O	2:O:111:CYS:HB3	2.21	0.40
3:P:362:ILE:HA	3:P:366:LEU:HB2	2.04	0.40
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.68	0.40
1:A:248:LEU:HA	1:A:248:LEU:HD22	1.89	0.40
2:B:324:PHE:HD2	2:B:344:LEU:HD12	1.84	0.40
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.50	0.40
4:Q:28:ARG:HH21	4:Q:181:GLN:NE2	2.19	0.40
4:Q:221:TYR:CE1	7:T:25:ALA:CB	3.02	0.40
3:C:236:MET:O	3:C:237:LEU:C	2.60	0.40
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.45	0.40
2:B:280:GLY:HA3	2:B:293:SER:HG	1.85	0.40
2:O:286:LYS:NZ	2:O:287:ARG:HH22	2.19	0.40
3:C:70:THR:O	3:C:74:VAL:HG23	2.22	0.40
1:N:295:ALA:O	1:N:298:ALA:N	2.54	0.40
4:Q:162:PRO:HA	4:Q:163:PRO:HD2	1.91	0.40
4:Q:168:ILE:HG23	4:Q:169:LEU:HD22	2.04	0.40
3:P:39:ALA:O	3:P:40:VAL:C	2.59	0.40
5:E:47:THR:O	5:E:48:ALA:C	2.59	0.40
2:B:328:SER:O	2:B:329:GLN:C	2.59	0.40
1:A:185:TYR:HA	1:A:189:HIS:HD2	1.86	0.40
10:J:16:ARG:C	10:J:18:SER:H	2.25	0.40
10:J:16:ARG:C	10:J:18:SER:N	2.75	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	441/446 (99%)	335 (76%)	84 (19%)	22 (5%)	3	26
1	N	440/446 (99%)	330 (75%)	87 (20%)	23 (5%)	2	25
2	B	424/441 (96%)	315 (74%)	78 (18%)	31 (7%)	1	16
2	O	420/441 (95%)	313 (74%)	78 (19%)	29 (7%)	1	18
3	C	378/380 (100%)	298 (79%)	61 (16%)	19 (5%)	3	26
3	P	377/380 (99%)	294 (78%)	67 (18%)	16 (4%)	3	31
4	D	239/241 (99%)	177 (74%)	51 (21%)	11 (5%)	3	29
4	Q	239/241 (99%)	181 (76%)	47 (20%)	11 (5%)	3	29
5	E	194/196 (99%)	119 (61%)	60 (31%)	15 (8%)	1	14
5	R	194/196 (99%)	122 (63%)	50 (26%)	22 (11%)	0	7
6	F	99/110 (90%)	74 (75%)	21 (21%)	4 (4%)	4	33
6	S	99/110 (90%)	77 (78%)	19 (19%)	3 (3%)	5	41
7	G	78/81 (96%)	59 (76%)	16 (20%)	3 (4%)	4	35
7	T	77/81 (95%)	57 (74%)	15 (20%)	5 (6%)	1	19
8	H	67/77 (87%)	44 (66%)	22 (33%)	1 (2%)	13	56
8	U	65/77 (84%)	43 (66%)	20 (31%)	2 (3%)	5	41
9	I	29/47 (62%)	15 (52%)	10 (34%)	4 (14%)	0	4
9	V	29/47 (62%)	15 (52%)	9 (31%)	5 (17%)	0	2
10	J	59/61 (97%)	38 (64%)	16 (27%)	5 (8%)	1	12
10	W	58/61 (95%)	39 (67%)	14 (24%)	5 (9%)	1	12
All	All	4006/4160 (96%)	2945 (74%)	825 (21%)	236 (6%)	2	22

All (236) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	222	THR
1	A	432	LEU
2	B	15	VAL
2	B	17	LEU
2	B	18	CYS
2	B	29	LEU
2	B	38	LEU
2	B	201	SER
2	B	210	GLY
2	B	221	GLU
2	B	386	ALA
3	C	18	SER
3	C	60	THR
3	C	111	LYS
3	C	248	PRO
3	C	287	ASN
4	D	166	ASN
4	D	198	HIS
5	E	102	THR
5	E	115	SER
5	E	130	PRO
5	E	177	PRO
7	G	7	LEU
7	G	33	ALA
9	I	56	SER
9	I	61	ARG
1	N	20	ASP
1	N	159	GLN
1	N	222	THR
1	N	432	LEU
2	O	19	PRO
2	O	38	LEU
2	O	201	SER
2	O	223	PHE
2	O	226	ILE
2	O	227	ARG
3	P	18	SER
3	P	60	THR
3	P	111	LYS
3	P	287	ASN
4	Q	166	ASN
4	Q	198	HIS

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Mol	Chain	Res	Type
5	R	8	PRO
5	R	107	ASN
5	R	130	PRO
5	R	140	THR
5	R	141	HIS
5	R	178	TYR
5	R	191	ASP
7	T	3	HIS
7	T	7	LEU
7	T	33	ALA
10	W	61	ALA
1	A	206	LYS
2	B	171	ALA
2	B	226	ILE
3	C	157	ILE
4	D	53	GLY
4	D	77	ASN
5	E	8	PRO
5	E	21	ALA
8	H	28	GLU
1	N	4	TYR
1	N	5	ALA
1	N	81	SER
1	N	108	LYS
1	N	433	ASP
2	O	171	ALA
2	O	210	GLY
2	O	268	GLU
2	O	386	ALA
3	P	76	TYR
3	P	202	HIS
4	Q	53	GLY
4	Q	172	ASP
5	R	21	ALA
5	R	108	GLN
5	R	115	SER
5	R	122	HIS
5	R	131	GLU
5	R	144	CYS
5	R	177	PRO
8	U	52	GLU
9	V	63	ASP

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Mol	Chain	Res	Type
9	V	72	ALA
9	V	76	VAL
10	W	25	VAL
1	A	72	CYS
1	A	81	SER
1	A	107	PRO
1	A	108	LYS
1	A	135	LEU
1	A	290	LEU
2	B	20	GLY
2	B	26	ILE
2	B	63	LEU
2	B	152	PHE
2	B	207	VAL
2	B	389	SER
3	C	3	PRO
3	C	156	TYR
3	C	202	HIS
3	C	255	GLU
4	D	38	SER
4	D	133	GLY
6	F	52	GLU
6	F	77	LYS
6	F	83	TYR
9	I	64	LEU
10	J	25	VAL
10	J	33	ARG
10	J	55	ILE
1	N	72	CYS
1	N	107	PRO
1	N	121	ALA
1	N	135	LEU
1	N	206	LYS
1	N	218	GLY
1	N	288	LYS
2	O	140	LEU
2	O	389	SER
2	O	431	GLY
3	P	248	PRO
4	Q	38	SER
4	Q	133	GLY
8	U	28	GLU

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Mol	Chain	Res	Type
10	W	15	ARG
10	W	33	ARG
10	W	55	ILE
1	A	121	ALA
1	A	180	ALA
1	A	217	SER
1	A	218	GLY
1	A	433	ASP
2	B	24	LEU
2	B	140	LEU
2	B	222	GLN
2	B	306	PRO
2	B	393	THR
3	C	288	LYS
3	C	348	PHE
4	D	172	ASP
5	E	92	ARG
5	E	128	LYS
5	E	176	ALA
10	J	15	ARG
2	O	63	LEU
2	O	152	PHE
2	O	221	GLU
2	O	393	THR
2	O	409	ASP
2	O	416	LYS
3	P	3	PRO
3	P	156	TYR
3	P	255	GLU
3	P	288	LYS
3	P	348	PHE
5	R	49	TYR
5	R	149	ASN
5	R	175	PRO
6	S	52	GLU
7	T	50	PRO
9	V	73	PRO
1	A	53	ASN
1	A	106	MET
1	A	192	ALA
2	B	21	ALA
2	B	30	PRO

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Mol	Chain	Res	Type
2	B	307	PHE
2	B	319	SER
2	B	394	ALA
2	B	416	LYS
3	C	4	ASN
3	C	17	ASN
3	C	76	TYR
3	C	159	HIS
4	D	96	PRO
4	D	123	GLY
5	E	80	ASP
5	E	141	HIS
5	E	149	ASN
6	F	19	TRP
7	G	50	PRO
10	J	32	GLU
1	N	192	ALA
2	O	26	ILE
2	O	207	VAL
2	O	216	LEU
2	O	228	SER
2	O	306	PRO
2	O	307	PHE
2	O	319	SER
2	O	394	ALA
3	P	17	ASN
3	P	296	ALA
3	P	366	LEU
4	Q	106	ASN
5	R	92	ARG
5	R	121	GLN
6	S	77	LYS
6	S	83	TYR
9	V	48	PRO
1	A	263	ALA
4	D	106	ASN
5	E	129	LYS
1	N	53	ASN
1	N	106	MET
1	N	148	VAL
2	O	384	SER
3	P	10	PRO

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Mol	Chain	Res	Type
3	C	10	PRO
5	E	175	PRO
1	N	209	VAL
4	Q	96	PRO
4	Q	162	PRO
5	R	176	ALA
1	A	209	VAL
2	B	209	ILE
2	B	420	GLY
9	I	72	ALA
2	O	209	ILE
5	R	18	VAL
7	T	48	VAL
1	A	148	VAL
2	B	64	GLY
3	C	209	PRO
4	D	229	VAL
1	N	428	ILE
5	E	18	VAL
4	Q	123	GLY
4	Q	168	ILE
5	R	154	GLY
1	A	428	ILE
3	C	305	ILE
1	N	110	VAL

### 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	365/368 (99%)	346 (95%)	19 (5%)	29	68
1	N	365/368 (99%)	346 (95%)	19 (5%)	29	68
2	B	333/347 (96%)	308 (92%)	25 (8%)	17	55
2	O	333/347 (96%)	312 (94%)	21 (6%)	22	63
3	C	329/329 (100%)	317 (96%)	12 (4%)	42	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	328/329 (100%)	318 (97%)	10 (3%)	48	81
4	D	200/200 (100%)	191 (96%)	9 (4%)	34	73
4	Q	200/200 (100%)	191 (96%)	9 (4%)	34	73
5	E	166/166 (100%)	158 (95%)	8 (5%)	31	71
5	R	166/166 (100%)	158 (95%)	8 (5%)	31	71
6	F	93/96 (97%)	87 (94%)	6 (6%)	21	62
6	S	93/96 (97%)	87 (94%)	6 (6%)	21	62
7	G	71/71 (100%)	66 (93%)	5 (7%)	19	59
7	T	70/71 (99%)	67 (96%)	3 (4%)	35	74
8	H	65/71 (92%)	64 (98%)	1 (2%)	72	90
8	U	63/71 (89%)	63 (100%)	0	100	100
9	I	23/26 (88%)	22 (96%)	1 (4%)	35	74
9	V	23/26 (88%)	19 (83%)	4 (17%)	2	14
10	J	49/49 (100%)	46 (94%)	3 (6%)	23	63
10	W	47/49 (96%)	44 (94%)	3 (6%)	22	62
All	All	3382/3446 (98%)	3210 (95%)	172 (5%)	29	69

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	10	ASN
1	A	49	ASN
1	A	53	ASN
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	108	LYS
1	A	171	THR
1	A	174	ILE
1	A	181	ASP
1	A	188	THR
1	A	248	LEU
1	A	283	THR
1	A	307	PHE
1	A	342	TRP
1	A	392	LEU

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Mol	Chain	Res	Type
1	A	395	TRP
1	A	405	ARG
2	B	31	ASN
2	B	57	TYR
2	B	59	THR
2	B	71	LEU
2	B	96	LEU
2	B	102	ARG
2	B	104	LYS
2	B	114	ASP
2	B	120	MET
2	B	139	ASP
2	B	150	VAL
2	B	154	SER
2	B	168	TYR
2	B	181	TYR
2	B	189	GLU
2	B	227	ARG
2	B	248	ASN
2	B	284	LEU
2	B	296	TYR
2	B	325	TYR
2	B	335	GLU
2	B	343	GLN
2	B	344	LEU
2	B	402	ILE
2	B	403	ASP
3	C	44	THR
3	C	69	HIS
3	C	82	ASN
3	C	145	THR
3	C	149	ASN
3	C	182	LEU
3	C	208	ASN
3	C	243	LEU
3	C	245	LEU
3	C	248	PRO
3	C	255	GLU
3	C	299	VAL
4	D	13	SER
4	D	64	LEU
4	D	81	PHE

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Mol	Chain	Res	Type
4	D	169	LEU
4	D	173	ASP
4	D	178	THR
4	D	199	ASP
4	D	214	LEU
4	D	219	LEU
5	E	6	THR
5	E	52	LYS
5	E	60	SER
5	E	61	SER
5	E	71	LEU
5	E	131	GLU
5	E	135	LEU
5	E	185	TYR
6	F	27	ASN
6	F	34	ASP
6	F	58	ARG
6	F	70	LEU
6	F	89	TYR
6	F	102	LEU
7	G	4	PHE
7	G	16	TYR
7	G	60	SER
7	G	63	THR
7	G	65	GLU
8	H	19	THR
9	I	71	ASN
10	J	14	PHE
10	J	57	HIS
10	J	59	TYR
1	N	3	THR
1	N	10	ASN
1	N	49	ASN
1	N	53	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	108	LYS
1	N	171	THR
1	N	174	ILE
1	N	181	ASP
1	N	188	THR

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Mol	Chain	Res	Type
1	N	248	LEU
1	N	283	THR
1	N	307	PHE
1	N	342	TRP
1	N	392	LEU
1	N	395	TRP
1	N	405	ARG
2	O	22	GLU
2	O	31	ASN
2	O	57	TYR
2	O	71	LEU
2	O	96	LEU
2	O	102	ARG
2	O	104	LYS
2	O	114	ASP
2	O	120	MET
2	O	139	ASP
2	O	150	VAL
2	O	154	SER
2	O	168	TYR
2	O	181	TYR
2	O	227	ARG
2	O	248	ASN
2	O	284	LEU
2	O	296	TYR
2	O	335	GLU
2	O	343	GLN
2	O	402	ILE
3	P	44	THR
3	P	74	VAL
3	P	82	ASN
3	P	145	THR
3	P	149	ASN
3	P	182	LEU
3	P	208	ASN
3	P	242	THR
3	P	243	LEU
3	P	245	LEU
4	Q	13	SER
4	Q	64	LEU
4	Q	81	PHE
4	Q	127	VAL

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Mol	Chain	Res	Type
4	Q	169	LEU
4	Q	173	ASP
4	Q	178	THR
4	Q	214	LEU
4	Q	219	LEU
5	R	31	ASP
5	R	52	LYS
5	R	60	SER
5	R	61	SER
5	R	71	LEU
5	R	135	LEU
5	R	152	ASP
5	R	185	TYR
6	S	27	ASN
6	S	34	ASP
6	S	58	ARG
6	S	70	LEU
6	S	89	TYR
6	S	102	LEU
7	T	4	PHE
7	T	16	TYR
7	T	60	SER
9	V	55	MET
9	V	62	ARG
9	V	63	ASP
9	V	70	LEU
10	W	14	PHE
10	W	57	HIS
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	173	ASN
1	A	271	HIS
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
1	A	435	ASN
2	B	31	ASN
2	B	156	GLN

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Mol	Chain	Res	Type
2	B	192	HIS
2	B	197	ASN
2	B	247	GLN
2	B	248	ASN
2	B	250	HIS
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	376	GLN
3	C	9	HIS
3	C	16	ASN
3	C	69	HIS
3	C	82	ASN
3	C	86	ASN
3	C	207	ASN
3	C	261	ASN
3	C	309	HIS
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	97	ASN
4	D	105	ASN
4	D	200	GLN
5	E	57	GLN
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	28	ASN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	21	ASN
1	N	32	GLN
1	N	118	GLN
1	N	126	GLN
1	N	173	ASN
1	N	274	ASN
1	N	305	HIS
1	N	308	GLN
1	N	339	GLN
1	N	435	ASN

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Mol	Chain	Res	Type
2	O	31	ASN
2	O	156	GLN
2	O	192	HIS
2	O	197	ASN
2	O	247	GLN
2	O	248	ASN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	376	GLN
3	P	9	HIS
3	P	16	ASN
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	261	ASN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	97	ASN
4	Q	105	ASN
5	R	57	GLN
5	R	107	ASN
5	R	149	ASN
5	R	164	HIS
5	R	186	GLN
7	T	23	GLN
7	T	28	ASN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	75	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 5 are unknown and 2 are monoatomic - leaving 29 for Mogul analysis.

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
11	PEE	A	2008	-	16,16,50	1.71	5 (31%)	16,20,55	0.50	0
14	IKR	C	2001	-	25,26,26	1.35	4 (16%)	31,35,35	1.29	4 (12%)
15	UQ	C	2002	-	19,19,63	2.35	10 (52%)	23,26,79	1.38	4 (17%)
16	CDL	C	2004	-	39,39,99	1.28	4 (10%)	41,51,111	1.18	5 (12%)
11	PEE	C	2007	-	48,48,50	1.25	6 (12%)	49,53,55	0.88	4 (8%)
18	GOL	C	2011	-	5,5,5	1.27	0	5,5,5	0.56	0
13	HEM	C	501	3	30,50,50	3.17	9 (30%)	24,82,82	3.13	13 (54%)
13	HEM	C	502	3	30,50,50	2.69	10 (33%)	24,82,82	2.01	8 (33%)
16	CDL	D	2003	-	41,41,99	1.14	1 (2%)	43,53,111	1.09	3 (6%)
20	BOG	D	2009	-	20,20,20	1.07	2 (10%)	25,25,25	0.93	2 (8%)
20	BOG	D	2091	-	13,13,20	1.44	3 (23%)	18,18,25	1.12	2 (11%)
19	HEC	D	501	4	24,50,50	2.33	4 (16%)	19,82,82	4.21	9 (47%)
11	PEE	E	2005	-	49,49,50	1.45	10 (20%)	50,54,55	0.96	5 (10%)
21	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
20	BOG	P	2010	-	12,12,20	1.53	3 (25%)	17,17,25	0.65	0
14	IKR	P	3001	-	25,26,26	1.34	4 (16%)	31,35,35	1.28	4 (12%)
15	UQ	P	3002	-	19,19,63	2.49	11 (57%)	23,26,79	1.38	4 (17%)
16	CDL	P	3004	-	39,39,99	1.24	4 (10%)	41,51,111	1.17	5 (12%)
11	PEE	P	3007	-	48,48,50	1.22	6 (12%)	49,53,55	0.86	4 (8%)
11	PEE	P	3008	-	4,4,50	3.62	4 (100%)	6,6,55	0.56	0
18	GOL	P	3011	-	5,5,5	1.28	0	5,5,5	0.63	0
20	BOG	P	3091	-	13,13,20	1.31	2 (15%)	18,18,25	1.06	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	HEM	P	501	3	30,50,50	3.12	8 (26%)	24,82,82	2.69	11 (45%)
13	HEM	P	502	3	30,50,50	3.07	11 (36%)	24,82,82	2.21	8 (33%)
16	CDL	Q	3003	-	41,41,99	1.14	0	43,53,111	1.10	5 (11%)
20	BOG	Q	3009	-	20,20,20	1.02	2 (10%)	25,25,25	1.01	2 (8%)
19	HEC	Q	501	4	24,50,50	2.50	4 (16%)	19,82,82	3.80	8 (42%)
11	PEE	R	3005	-	49,49,50	1.48	10 (20%)	50,54,55	0.95	5 (10%)
21	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-

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
11	PEE	A	2008	-	-	0/19/19/54	0/0/0/0
14	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
15	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
16	CDL	C	2004	-	-	0/49/49/110	0/0/0/0
11	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
18	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
13	HEM	C	501	3	-	0/10/54/54	0/0/8/8
13	HEM	C	502	3	-	0/10/54/54	0/0/8/8
16	CDL	D	2003	-	-	0/51/51/110	0/0/0/0
20	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
20	BOG	D	2091	-	-	0/4/24/31	0/1/1/1
19	HEC	D	501	4	-	0/6/54/54	0/0/8/8
11	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
21	FES	E	501	5	-	0/0/4/4	0/1/1/1
20	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
14	IKR	P	3001	-	-	0/18/18/18	0/2/2/2
15	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
16	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
11	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
11	PEE	P	3008	-	-	0/0/0/54	0/0/0/0
18	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
20	BOG	P	3091	-	-	0/4/24/31	0/1/1/1
13	HEM	P	501	3	-	0/10/54/54	0/0/8/8
13	HEM	P	502	3	-	0/10/54/54	0/0/8/8
16	CDL	Q	3003	-	-	0/51/51/110	0/0/0/0
20	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
19	HEC	Q	501	4	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEE	R	3005	-	-	0/53/53/54	0/0/0/0
21	FES	R	501	5	-	0/0/4/4	0/1/1/1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	501	HEC	C3B-C2B	-9.34	1.31	1.40
13	P	502	HEM	C3B-CAB	-7.57	1.37	1.51
13	C	501	HEM	C2D-C3D	-7.35	1.32	1.54
13	P	501	HEM	C2D-C3D	-7.13	1.33	1.54
13	P	501	HEM	C3B-CAB	-7.09	1.38	1.51
13	C	501	HEM	C3B-CAB	-7.05	1.38	1.51
19	D	501	HEC	C3C-C2C	-6.87	1.33	1.40
13	P	501	HEM	C3C-CAC	-6.87	1.38	1.51
19	D	501	HEC	C3B-C2B	-6.77	1.33	1.40
13	C	501	HEM	C3B-C4B	-6.76	1.45	1.51
13	P	502	HEM	C3C-CAC	-6.76	1.38	1.51
13	P	502	HEM	C3B-C4B	-6.61	1.46	1.51
13	C	502	HEM	C3B-CAB	-6.45	1.39	1.51
13	C	502	HEM	C2D-C3D	-6.19	1.36	1.54
13	P	501	HEM	C3B-C4B	-5.90	1.46	1.51
13	P	502	HEM	C2D-C3D	-5.81	1.37	1.54
13	C	502	HEM	C3C-CAC	-5.78	1.40	1.51
13	C	501	HEM	C2C-C1C	-5.64	1.41	1.52
19	Q	501	HEC	C3C-C2C	-5.62	1.34	1.40
13	P	501	HEM	C3D-C4D	-5.41	1.44	1.51
13	C	501	HEM	C3C-CAC	-5.39	1.41	1.51
13	P	502	HEM	C3D-C4D	-5.21	1.44	1.51
13	C	501	HEM	C3D-C4D	-4.73	1.45	1.51
13	P	501	HEM	C2C-C1C	-4.18	1.44	1.52
13	C	502	HEM	C3B-C4B	-4.17	1.48	1.51
13	P	502	HEM	C2C-C1C	-3.48	1.46	1.52
13	C	502	HEM	C2C-C1C	-3.23	1.46	1.52
13	C	502	HEM	C3D-C4D	-2.98	1.47	1.51
11	P	3007	PEE	C22-C21	-2.94	1.34	1.51
11	E	2005	PEE	C19-C18	-2.91	1.34	1.51
11	C	2007	PEE	C19-C18	-2.88	1.34	1.51
13	C	502	HEM	C4A-CHB	-2.87	1.31	1.39
11	E	2005	PEE	C22-C21	-2.80	1.35	1.51
11	P	3007	PEE	C19-C18	-2.80	1.35	1.51
11	C	2007	PEE	C22-C21	-2.79	1.35	1.51
11	R	3005	PEE	C19-C18	-2.78	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	3005	PEE	C22-C21	-2.77	1.35	1.51
19	Q	501	HEC	C4D-CHA	-2.47	1.33	1.39
13	C	501	HEM	FE-NC	-2.45	1.86	1.95
13	P	502	HEM	C4A-CHB	-2.37	1.33	1.39
16	P	3004	CDL	OA8-CA6	-2.36	1.39	1.45
13	P	502	HEM	C2D-C1D	-2.23	1.44	1.51
16	C	2004	CDL	OA8-CA6	-2.22	1.40	1.45
19	D	501	HEC	C4D-CHA	-2.14	1.34	1.39
13	C	502	HEM	FE-ND	-2.08	1.86	1.97
16	C	2004	CDL	OA5-CA3	-2.04	1.36	1.44
13	P	502	HEM	CAD-C3D	-2.03	1.50	1.54
11	C	2007	PEE	C3-C2	2.01	1.56	1.50
15	C	2002	UQ	O2-C2	2.01	1.42	1.37
20	D	2091	BOG	C1-C2	2.02	1.58	1.52
20	Q	3009	BOG	C4-C5	2.03	1.57	1.53
11	P	3007	PEE	C3-C2	2.04	1.56	1.50
20	D	2009	BOG	C1-C2	2.05	1.58	1.52
11	A	2008	PEE	C11-C10	2.05	1.56	1.50
15	P	3002	UQ	O2-C2	2.06	1.42	1.37
11	P	3008	PEE	P-O2P	2.06	1.62	1.54
16	D	2003	CDL	O1-C1	2.07	1.49	1.43
16	P	3004	CDL	OB8-CB7	2.10	1.39	1.33
19	Q	501	HEC	C1A-NA	2.12	1.39	1.36
15	C	2002	UQ	C7-C8	2.21	1.54	1.50
15	P	3002	UQ	C8-C9	2.22	1.37	1.33
11	E	2005	PEE	C31-C30	2.24	1.57	1.50
20	P	2010	BOG	O5-C1	2.26	1.47	1.43
20	P	3091	BOG	C4-C5	2.28	1.57	1.53
20	Q	3009	BOG	O5-C1	2.28	1.47	1.41
14	P	3001	IKR	C24-C17	2.30	1.43	1.39
16	P	3004	CDL	CB3-CB4	2.32	1.57	1.50
14	P	3001	IKR	C20-C17	2.32	1.43	1.40
16	P	3004	CDL	O1-C1	2.33	1.50	1.43
11	R	3005	PEE	O2-C2	2.34	1.52	1.46
11	E	2005	PEE	O2-C2	2.34	1.52	1.46
11	R	3005	PEE	C31-C30	2.34	1.57	1.50
11	A	2008	PEE	C3-C2	2.35	1.57	1.50
14	C	2001	IKR	C24-C17	2.35	1.43	1.39
15	P	3002	UQ	C3-C4	2.36	1.55	1.48
20	D	2091	BOG	O5-C1	2.36	1.47	1.41
19	D	501	HEC	C3C-C4C	2.40	1.48	1.42
11	R	3005	PEE	C11-C10	2.41	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	3091	BOG	O5-C1	2.44	1.48	1.41
11	E	2005	PEE	C1-C2	2.45	1.57	1.50
14	C	2001	IKR	C3-C4	2.45	1.43	1.38
20	D	2009	BOG	O5-C1	2.46	1.48	1.41
15	C	2002	UQ	C5-C4	2.47	1.56	1.47
15	C	2002	UQ	C2-C1	2.48	1.56	1.48
11	R	3005	PEE	C3-C2	2.49	1.57	1.50
14	C	2001	IKR	C20-C17	2.51	1.44	1.40
15	P	3002	UQ	C5-C4	2.52	1.56	1.47
14	P	3001	IKR	C3-C4	2.52	1.43	1.38
11	A	2008	PEE	C1-C2	2.53	1.57	1.50
15	C	2002	UQ	CM5-C5	2.56	1.56	1.50
11	R	3005	PEE	C1-C2	2.58	1.58	1.50
11	E	2005	PEE	C11-C10	2.58	1.58	1.50
11	P	3007	PEE	P-O1P	2.60	1.60	1.51
16	C	2004	CDL	CB3-CB4	2.61	1.58	1.50
15	P	3002	UQ	CM5-C5	2.62	1.56	1.50
11	P	3007	PEE	O2-C10	2.65	1.42	1.34
11	P	3008	PEE	P-O3P	2.65	1.64	1.54
15	C	2002	UQ	C3-C4	2.65	1.56	1.48
11	E	2005	PEE	C3-C2	2.67	1.58	1.50
15	P	3002	UQ	C2-C1	2.69	1.56	1.48
20	P	2010	BOG	C4-C5	2.71	1.58	1.53
15	P	3002	UQ	O3-C3	2.76	1.44	1.37
11	C	2007	PEE	O2-C10	2.77	1.42	1.34
11	C	2007	PEE	O3-C30	2.77	1.41	1.33
11	A	2008	PEE	O2-C10	2.80	1.42	1.34
11	P	3008	PEE	P-O4P	2.80	1.64	1.54
16	C	2004	CDL	O1-C1	2.82	1.52	1.43
11	C	2007	PEE	P-O1P	2.84	1.61	1.51
20	D	2091	BOG	C4-C5	2.90	1.59	1.53
11	P	3007	PEE	O3-C30	2.90	1.42	1.33
11	E	2005	PEE	P-O1P	2.90	1.61	1.51
15	P	3002	UQ	C7-C8	2.92	1.55	1.50
14	P	3001	IKR	C40-C2	2.96	1.57	1.51
11	A	2008	PEE	P-O1P	2.97	1.62	1.51
20	P	2010	BOG	C1-C2	2.97	1.58	1.52
11	E	2005	PEE	O3-C30	3.16	1.42	1.33
15	C	2002	UQ	O3-C3	3.20	1.45	1.37
14	C	2001	IKR	C40-C2	3.21	1.57	1.51
11	R	3005	PEE	P-O1P	3.21	1.62	1.51
11	E	2005	PEE	O2-C10	3.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	3005	PEE	O3-C30	3.43	1.43	1.33
11	R	3005	PEE	O2-C10	3.56	1.45	1.34
13	P	502	HEM	CBB-CAB	3.58	1.49	1.29
15	C	2002	UQ	C6-C5	3.60	1.43	1.35
15	P	3002	UQ	C6-C1	3.75	1.57	1.46
13	C	502	HEM	CBB-CAB	3.83	1.51	1.29
15	P	3002	UQ	C6-C5	3.89	1.44	1.35
15	C	2002	UQ	C6-C1	3.92	1.57	1.46
13	C	501	HEM	CBB-CAB	4.16	1.53	1.29
13	P	501	HEM	CBB-CAB	4.17	1.53	1.29
13	C	502	HEM	CBC-CAC	4.37	1.54	1.29
13	P	502	HEM	CBC-CAC	4.40	1.54	1.29
15	C	2002	UQ	C7-C6	4.48	1.59	1.51
13	P	501	HEM	CBC-CAC	4.52	1.55	1.29
15	P	3002	UQ	C7-C6	5.40	1.61	1.51
13	C	501	HEM	CBC-CAC	5.48	1.60	1.29
11	P	3008	PEE	P-O1P	5.77	1.61	1.50

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	501	HEC	CBC-CAC-C3C	-12.84	98.81	127.35
19	Q	501	HEC	CBC-CAC-C3C	-11.29	102.26	127.35
13	C	501	HEM	CBA-CAA-C2A	-7.16	99.70	112.53
19	D	501	HEC	CBB-CAB-C3B	-6.24	113.48	127.35
19	Q	501	HEC	CBB-CAB-C3B	-5.85	114.36	127.35
13	C	501	HEM	CMA-C3A-C4A	-5.30	119.59	128.36
13	P	501	HEM	CBA-CAA-C2A	-5.23	103.16	112.53
13	C	501	HEM	C3B-CAB-CBB	-4.69	117.26	124.46
13	P	501	HEM	C3C-CAC-CBC	-4.46	117.62	124.46
13	P	501	HEM	C3B-CAB-CBB	-3.71	118.76	124.46
13	C	501	HEM	C3C-CAC-CBC	-3.56	118.99	124.46
15	C	2002	UQ	C7-C6-C1	-3.34	114.63	118.56
15	P	3002	UQ	C7-C6-C1	-3.34	114.63	118.56
14	P	3001	IKR	C40-C2-C3	-3.32	113.31	119.49
13	P	501	HEM	CMA-C3A-C4A	-3.27	122.96	128.36
19	D	501	HEC	CAA-C2A-C3A	-3.21	119.83	129.00
14	C	2001	IKR	C40-C2-C3	-3.15	113.64	119.49
14	C	2001	IKR	O31-C30-C29	-3.04	108.66	111.73
16	P	3004	CDL	CB4-OB6-CB5	-2.97	110.77	117.89
15	C	2002	UQ	C10-C9-C8	-2.89	117.83	123.50
14	P	3001	IKR	O31-C30-C29	-2.82	108.87	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	HEM	C2C-C1C-CHC	-2.81	119.41	123.68
15	P	3002	UQ	C10-C9-C8	-2.81	117.99	123.50
16	P	3004	CDL	CA6-CA4-CA3	-2.79	105.55	112.07
16	C	2004	CDL	CB4-OB6-CB5	-2.79	111.20	117.89
16	C	2004	CDL	CA6-CA4-CA3	-2.70	105.76	112.07
16	D	2003	CDL	CB4-OB6-CB5	-2.67	111.49	117.89
19	Q	501	HEC	CAA-C2A-C3A	-2.67	121.38	129.00
16	Q	3003	CDL	CB4-OB6-CB5	-2.43	112.07	117.89
16	D	2003	CDL	CA6-CA4-CA3	-2.37	106.54	112.07
16	Q	3003	CDL	CA6-CA4-CA3	-2.26	106.79	112.07
16	Q	3003	CDL	CA4-OA6-CA5	-2.21	112.58	117.89
16	C	2004	CDL	CA4-OA6-CA5	-2.20	112.60	117.89
13	P	502	HEM	C3B-CAB-CBB	-2.14	121.18	124.46
16	P	3004	CDL	CA4-OA6-CA5	-2.12	112.81	117.89
16	Q	3003	CDL	CB6-CB4-CB3	-2.10	107.15	112.07
14	C	2001	IKR	C21-C20-C29	-2.10	115.95	119.62
13	C	502	HEM	CBD-CAD-C3D	-2.08	107.50	113.55
16	P	3004	CDL	CA6-OA8-CA7	-2.07	111.91	117.14
16	Q	3003	CDL	CA6-OA8-CA7	-2.07	111.91	117.14
19	D	501	HEC	C4B-C3B-C2B	-2.05	104.14	106.35
16	D	2003	CDL	CA4-OA6-CA5	-2.03	113.01	117.89
14	P	3001	IKR	C21-C20-C29	-2.02	116.08	119.62
16	C	2004	CDL	CA6-OA8-CA7	-2.00	112.07	117.14
15	P	3002	UQ	C11-C9-C8	2.11	125.45	120.74
15	C	2002	UQ	C11-C9-C8	2.15	125.55	120.74
11	R	3005	PEE	O3-C3-C2	2.16	114.50	108.69
19	Q	501	HEC	CMC-C2C-C1C	2.17	131.95	128.36
20	Q	3009	BOG	O1-C1-C2	2.21	110.83	108.04
11	E	2005	PEE	O3-C3-C2	2.27	114.80	108.69
11	C	2007	PEE	C22-C21-C20	2.28	126.28	114.53
11	P	3007	PEE	C22-C21-C20	2.28	126.31	114.53
13	C	501	HEM	CMA-C3A-C2A	2.28	130.01	125.24
13	P	501	HEM	CMA-C3A-C2A	2.29	130.02	125.24
13	P	501	HEM	CMD-C2D-C3D	2.32	124.59	114.35
11	R	3005	PEE	C23-C22-C21	2.32	126.51	114.53
16	C	2004	CDL	OB6-CB4-CB3	2.33	116.56	108.36
11	E	2005	PEE	C23-C22-C21	2.36	126.71	114.53
19	Q	501	HEC	CAD-C3D-C4D	2.36	129.57	127.01
11	P	3007	PEE	C23-C22-C21	2.37	126.78	114.53
20	P	3091	BOG	O1-C1-C2	2.37	111.01	108.21
16	P	3004	CDL	OB6-CB4-CB3	2.39	116.77	108.36
11	C	2007	PEE	C23-C22-C21	2.40	126.94	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	2007	PEE	C19-C18-C17	2.42	127.02	114.53
13	C	502	HEM	C2D-C3D-C4D	2.43	105.61	101.50
11	E	2005	PEE	C22-C21-C20	2.44	127.12	114.53
11	E	2005	PEE	C19-C18-C17	2.45	127.19	114.53
11	R	3005	PEE	C22-C21-C20	2.48	127.34	114.53
13	C	501	HEM	CMD-C2D-C3D	2.52	125.48	114.35
11	P	3007	PEE	C19-C18-C17	2.52	127.54	114.53
13	C	502	HEM	C2C-C1C-NC	2.53	114.47	110.21
11	R	3005	PEE	C19-C18-C17	2.53	127.59	114.53
11	E	2005	PEE	C20-C19-C18	2.64	128.14	114.53
20	D	2091	BOG	O1-C1-C2	2.64	111.33	108.21
20	D	2009	BOG	O1-C1-C2	2.69	111.43	108.04
11	P	3007	PEE	C20-C19-C18	2.70	128.48	114.53
11	C	2007	PEE	C20-C19-C18	2.71	128.54	114.53
11	R	3005	PEE	C20-C19-C18	2.71	128.55	114.53
19	D	501	HEC	CAD-C3D-C4D	2.79	130.03	127.01
14	C	2001	IKR	O31-C30-O36	2.85	129.23	123.56
13	P	501	HEM	CMB-C2B-C3B	2.85	123.66	116.53
14	P	3001	IKR	O31-C30-O36	2.88	129.30	123.56
13	C	502	HEM	CMB-C2B-C3B	2.93	123.85	116.53
19	D	501	HEC	CMC-C2C-C1C	2.94	133.23	128.36
13	C	502	HEM	CMD-C2D-C3D	2.96	127.42	114.35
13	C	501	HEM	CAA-C2A-C1A	3.06	130.33	127.01
20	D	2009	BOG	C1'-O1-C1	3.07	119.30	113.94
13	P	501	HEM	C2D-C3D-C4D	3.15	106.83	101.50
13	P	502	HEM	CBA-CAA-C2A	3.17	118.22	112.53
13	C	502	HEM	CAD-C3D-C2D	3.26	122.59	113.22
13	P	502	HEM	CMB-C2B-C3B	3.28	124.72	116.53
20	D	2091	BOG	C1'-O1-C1	3.29	118.67	113.29
13	P	502	HEM	CMD-C2D-C3D	3.30	128.93	114.35
20	P	3091	BOG	C1'-O1-C1	3.31	118.70	113.29
13	C	501	HEM	CMB-C2B-C3B	3.40	125.02	116.53
13	C	501	HEM	C2D-C3D-C4D	3.42	107.30	101.50
13	P	502	HEM	CAD-C3D-C2D	3.49	123.24	113.22
19	Q	501	HEC	CBD-CAD-C3D	3.56	118.91	112.53
13	C	501	HEM	CAD-C3D-C2D	3.69	123.84	113.22
15	C	2002	UQ	C8-C7-C6	3.77	122.96	111.64
15	P	3002	UQ	C8-C7-C6	3.79	123.02	111.64
13	C	502	HEM	CMC-C2C-C3C	3.84	126.11	116.53
20	Q	3009	BOG	C1'-O1-C1	3.87	120.70	113.94
13	P	502	HEM	C2D-C3D-C4D	3.88	108.08	101.50
19	D	501	HEC	CBD-CAD-C3D	4.00	119.69	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	501	HEM	CAD-C3D-C2D	4.08	124.93	113.22
13	P	501	HEM	CAD-C3D-C4D	4.40	128.00	112.47
13	P	502	HEM	CMC-C2C-C3C	4.47	127.68	116.53
13	C	501	HEM	CAD-C3D-C4D	4.48	128.28	112.47
13	P	502	HEM	CAD-C3D-C4D	4.59	128.66	112.47
19	Q	501	HEC	CAA-C2A-C1A	4.84	132.26	127.01
13	C	501	HEM	CMC-C2C-C3C	4.97	128.94	116.53
13	P	501	HEM	CMC-C2C-C3C	5.11	129.30	116.53
19	D	501	HEC	CAA-C2A-C1A	5.39	132.86	127.01
13	C	502	HEM	CAD-C3D-C4D	5.48	131.78	112.47
19	D	501	HEC	CBA-CAA-C2A	7.06	125.19	112.53
19	Q	501	HEC	CBA-CAA-C2A	7.19	125.41	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2001	IKR	5	0
15	C	2002	UQ	6	0
16	C	2004	CDL	2	0
11	C	2007	PEE	3	0
18	C	2011	GOL	1	0
13	C	501	HEM	6	0
13	C	502	HEM	13	0
16	D	2003	CDL	1	0
20	D	2091	BOG	1	0
19	D	501	HEC	2	0
21	E	501	FES	3	0
14	P	3001	IKR	4	0
15	P	3002	UQ	6	0
16	P	3004	CDL	2	0
11	P	3007	PEE	4	0
18	P	3011	GOL	1	0
13	P	501	HEM	9	0
13	P	502	HEM	11	0
16	Q	3003	CDL	3	0
19	Q	501	HEC	2	0
21	R	501	FES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/446 (99%)	-0.07	11 (2%) 61 51	56, 103, 147, 160	0
1	N	442/446 (99%)	-0.03	16 (3%) 46 38	65, 100, 132, 147	0
2	B	426/441 (96%)	0.23	21 (4%) 33 27	85, 126, 182, 218	0
2	O	422/441 (95%)	-0.02	11 (2%) 59 50	70, 108, 147, 161	0
3	C	380/380 (100%)	-0.28	9 (2%) 62 53	40, 64, 131, 204	0
3	P	379/380 (99%)	-0.08	15 (3%) 42 34	52, 97, 148, 187	0
4	D	241/241 (100%)	-0.20	5 (2%) 67 59	48, 72, 121, 138	0
4	Q	241/241 (100%)	0.03	7 (2%) 55 46	74, 108, 149, 167	0
5	E	196/196 (100%)	2.82	96 (48%) 0 0	57, 214, 260, 262	125 (63%)
5	R	196/196 (100%)	1.28	53 (27%) 1 1	64, 183, 229, 234	1 (0%)
6	F	101/110 (91%)	-0.33	1 (0%) 84 77	56, 75, 97, 117	0
6	S	101/110 (91%)	0.06	2 (1%) 68 60	87, 124, 174, 190	0
7	G	80/81 (98%)	0.10	4 (5%) 32 26	58, 86, 158, 166	0
7	T	79/81 (97%)	0.65	15 (18%) 2 2	81, 126, 222, 227	0
8	H	69/77 (89%)	-0.22	0 100 100	70, 98, 119, 154	0
8	U	67/77 (87%)	0.23	3 (4%) 37 30	133, 165, 209, 211	0
9	I	31/47 (65%)	3.52	17 (54%) 0 0	147, 185, 257, 259	0
9	V	31/47 (65%)	1.90	11 (35%) 0 0	121, 163, 242, 244	0
10	J	61/61 (100%)	0.11	2 (3%) 50 42	75, 93, 139, 177	0
10	W	60/61 (98%)	0.43	2 (3%) 50 42	84, 108, 157, 165	0
All	All	4046/4160 (97%)	0.22	301 (7%) 17 15	40, 104, 204, 262	126 (3%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	51	CYS	26.2
5	E	162	GLY	15.5
5	E	172	ARG	13.3
5	E	117	LEU	13.0
2	B	14	ARG	12.9
5	E	173	LYS	12.8
5	E	171	ILE	12.8
5	E	174	GLY	12.4
5	E	114	VAL	12.3
5	E	98	VAL	12.3
5	E	163	SER	12.2
2	B	15	VAL	11.9
5	E	120	PRO	11.8
5	E	115	SER	11.4
5	E	113	ASP	10.6
5	E	119	ASP	10.6
5	E	159	PRO	10.2
5	E	152	ASP	10.2
5	E	116	LYS	9.8
5	E	133	VAL	9.3
9	I	50	LEU	9.1
5	E	157	TYR	8.8
2	B	16	LYS	8.8
5	E	145	VAL	8.7
5	R	117	LEU	8.6
3	C	4	ASN	8.6
5	R	113	ASP	8.5
5	E	144	CYS	8.4
5	E	118	ARG	8.3
5	R	120	PRO	8.2
9	I	62	ARG	8.1
5	E	188	VAL	8.1
5	R	98	VAL	7.8
5	E	76	ILE	7.8
5	E	89	PHE	7.8
5	R	121	GLN	7.7
5	E	107	ASN	7.5
5	E	78	LEU	7.4
9	I	61	ARG	7.3
3	C	7	LYS	7.3
5	E	134	ILE	7.3
5	E	146	PRO	7.1
5	E	154	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
5	E	175	PRO	6.7
3	C	5	ILE	6.6
5	E	87	VAL	6.5
9	I	52	ARG	6.5
9	V	51	CYS	6.4
3	P	8	SER	6.4
3	C	8	SER	6.4
5	R	172	ARG	6.3
5	R	111	GLU	6.2
5	E	168	SER	6.2
5	R	116	LYS	6.1
5	E	193	VAL	6.1
5	R	186	GLN	6.1
5	R	112	VAL	5.9
5	E	105	GLU	5.9
3	C	6	ARG	5.8
5	E	121	GLN	5.8
5	E	164	HIS	5.8
5	R	119	ASP	5.8
5	R	171	ILE	5.8
5	E	75	GLU	5.7
8	U	50	THR	5.7
5	E	88	ALA	5.7
5	E	195	VAL	5.7
5	R	133	VAL	5.6
5	E	96	LEU	5.5
5	E	109	GLU	5.4
5	E	108	GLN	5.4
5	R	81	ILE	5.4
9	I	53	GLU	5.4
3	P	7	LYS	5.3
5	E	190	ASP	5.3
5	R	114	VAL	5.3
5	E	112	VAL	5.2
5	R	115	SER	5.2
5	R	157	TYR	5.1
7	T	74	PRO	5.1
5	E	81	ILE	5.1
5	E	180	LEU	5.1
5	E	158	CYS	5.0
3	P	6	ARG	5.0
5	E	178	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
5	R	122	HIS	5.0
5	E	160	CYS	5.0
5	E	165	TYR	4.9
5	E	151	GLY	4.9
9	I	58	ARG	4.9
5	R	193	VAL	4.9
5	E	147	ILE	4.8
5	E	132	TRP	4.8
4	D	1	GLY	4.7
5	E	140	THR	4.7
5	R	118	ARG	4.6
9	I	54	SER	4.6
5	R	97	PHE	4.6
2	B	216	LEU	4.6
5	R	146	PRO	4.5
5	E	156	TYR	4.5
5	E	100	HIS	4.4
3	C	2	ALA	4.4
9	V	50	LEU	4.4
7	T	3	HIS	4.4
3	P	4	ASN	4.3
5	E	99	ARG	4.3
5	E	176	ALA	4.2
5	E	77	LYS	4.2
5	E	79	SER	4.2
5	R	76	ILE	4.2
7	T	75	ALA	4.1
5	R	132	TRP	4.1
9	V	53	GLU	4.1
5	E	153	PHE	4.1
5	E	97	PHE	4.0
6	S	11	ARG	4.0
7	T	2	ILE	4.0
5	E	169	GLY	4.0
3	C	3	PRO	4.0
7	T	73	ASN	4.0
5	E	123	ASP	3.9
5	E	187	PHE	3.9
5	R	164	HIS	3.9
9	V	49	LEU	3.8
1	N	66	GLY	3.8
5	E	167	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
5	R	110	ALA	3.8
2	B	350	GLY	3.8
7	T	4	PHE	3.8
7	T	78	GLU	3.8
7	T	77	TYR	3.7
5	E	192	LEU	3.7
5	E	135	LEU	3.7
1	A	69	LYS	3.7
10	J	64	GLU	3.7
5	E	179	ASN	3.7
9	V	56	SER	3.7
5	R	82	PRO	3.7
5	E	196	GLY	3.6
7	T	6	ASN	3.6
7	T	5	GLY	3.6
5	R	156	TYR	3.6
5	R	85	LYS	3.6
5	E	122	HIS	3.6
9	I	77	ARG	3.5
5	R	127	VAL	3.5
5	R	134	ILE	3.5
5	R	96	LEU	3.5
5	R	165	TYR	3.5
5	R	88	ALA	3.5
5	E	82	PRO	3.4
1	A	444	ILE	3.4
3	P	156	TYR	3.4
3	P	29	SER	3.4
1	A	197	LEU	3.4
2	O	19	PRO	3.4
3	P	5	ILE	3.4
9	V	58	ARG	3.3
5	R	180	LEU	3.2
3	P	157	ILE	3.2
2	O	38	LEU	3.2
2	B	36	ALA	3.2
7	T	72	LYS	3.2
5	R	128	LYS	3.2
2	B	352	VAL	3.2
5	E	194	VAL	3.2
2	B	347	ALA	3.2
5	R	108	GLN	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	I	47	ARG	3.1
1	A	4	TYR	3.1
1	N	75	PHE	3.1
9	V	63	ASP	3.1
9	I	49	LEU	3.1
9	V	52	ARG	3.1
2	B	396	SER	3.0
5	E	148	ALA	3.0
5	R	151	GLY	3.0
9	V	61	ARG	3.0
2	B	17	LEU	3.0
9	I	56	SER	3.0
2	O	23	ASP	3.0
5	E	189	GLY	3.0
10	J	63	GLU	3.0
5	E	161	HIS	3.0
2	B	220	ALA	3.0
5	R	124	LEU	2.9
5	E	101	ARG	2.9
4	D	78	GLY	2.9
7	T	71	ARG	2.9
10	W	39	ALA	2.9
1	N	65	LYS	2.9
9	I	57	GLY	2.9
3	P	21	ASP	2.9
5	R	90	LYS	2.8
3	P	17	ASN	2.8
3	P	3	PRO	2.8
5	R	130	PRO	2.8
9	I	60	ALA	2.8
5	R	84	GLY	2.8
5	R	125	ASP	2.8
2	O	344	LEU	2.8
4	Q	105	ASN	2.8
1	A	2	ALA	2.8
2	B	282	GLY	2.8
5	E	102	THR	2.8
5	E	143	GLY	2.7
5	E	90	LYS	2.7
5	E	104	ALA	2.7
5	R	99	ARG	2.7
2	B	206	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	25	VAL	2.7
5	R	170	ARG	2.7
9	V	62	ARG	2.7
9	I	48	PRO	2.7
1	N	126	GLN	2.6
5	E	86	ASN	2.6
4	D	3	LEU	2.6
4	D	77	ASN	2.6
2	B	35	ILE	2.6
10	W	62	SER	2.6
1	N	62	LEU	2.5
5	E	91	TRP	2.5
5	E	110	ALA	2.5
7	G	3	HIS	2.5
5	E	111	GLU	2.5
4	Q	206	LEU	2.5
5	E	186	GLN	2.5
6	S	12	LEU	2.5
1	N	53	ASN	2.5
2	O	108	CYS	2.5
5	E	141	HIS	2.5
5	E	166	ASP	2.5
7	T	62	GLY	2.5
2	B	186	ILE	2.5
7	T	80	ASP	2.4
1	A	196	VAL	2.4
4	Q	108	ALA	2.4
3	C	1	MET	2.4
5	R	179	ASN	2.4
3	P	13	LYS	2.4
7	G	4	PHE	2.4
5	E	80	ASP	2.4
5	E	177	PRO	2.4
4	Q	241	LYS	2.4
2	B	349	GLN	2.4
1	N	386	TYR	2.4
5	E	191	ASP	2.3
4	D	79	GLU	2.3
5	R	1	VAL	2.3
3	P	346	HIS	2.3
7	T	79	ASN	2.3
2	O	352	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	Q	139	ALA	2.3
2	O	110	GLU	2.3
1	N	179	ARG	2.3
5	E	124	LEU	2.3
1	N	52	ASN	2.3
1	N	177	LEU	2.3
2	O	36	ALA	2.2
5	R	86	ASN	2.2
9	I	63	ASP	2.2
4	Q	146	GLY	2.2
3	P	16	ASN	2.2
2	B	376	GLN	2.2
3	C	157	ILE	2.2
5	E	83	GLU	2.2
4	Q	147	LEU	2.2
8	U	13	LEU	2.2
6	F	102	LEU	2.2
2	O	22	GLU	2.2
5	R	107	ASN	2.2
5	R	145	VAL	2.2
1	N	370	ASP	2.2
1	A	216	PHE	2.1
1	N	16	VAL	2.1
2	B	281	ALA	2.1
5	R	89	PHE	2.1
2	B	283	PRO	2.1
1	N	226	ASP	2.1
5	R	185	TYR	2.1
1	N	303	LEU	2.1
7	G	5	GLY	2.1
2	B	33	LEU	2.1
5	E	149	ASN	2.1
5	R	187	PHE	2.1
1	A	26	ALA	2.1
1	N	216	PHE	2.1
2	B	407	SER	2.1
9	I	59	SER	2.1
5	E	155	GLY	2.1
2	O	41	PHE	2.1
8	U	54	CYS	2.1
1	N	27	SER	2.1
1	A	23	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	2	ILE	2.0
9	V	57	GLY	2.0
3	P	154	ILE	2.0
5	E	84	GLY	2.0
1	A	47	TYR	2.0
2	O	386	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	PEE	A	2008	18/51	0.66	0.58	7.25	89,197,198,199	0
11	PEE	E	2005	50/51	0.78	0.52	4.59	113,127,137,139	0
18	GOL	C	2011	6/6	0.94	0.34	4.39	69,72,75,78	0
11	PEE	R	3005	50/51	0.68	0.48	4.24	114,131,139,141	0
20	BOG	D	2091	13/20	0.63	0.48	3.79	191,192,193,193	0
16	CDL	Q	3003	42/100	0.71	0.44	3.64	183,193,208,208	0
20	BOG	Q	3009	20/20	0.82	0.52	3.08	103,118,120,121	0
20	BOG	P	2010	12/20	0.41	0.56	2.95	248,249,250,250	0
20	BOG	D	2009	20/20	0.90	0.40	2.64	93,104,108,108	0
16	CDL	D	2003	42/100	0.87	0.33	2.61	134,141,153,153	0
11	PEE	P	3007	49/51	0.89	0.32	1.97	102,116,140,141	0
12	UNL	A	3284	1/-	0.83	0.49	1.88	31,31,31,31	0
15	UQ	C	2002	19/63	0.91	0.27	1.81	107,111,115,115	0
18	GOL	P	3011	6/6	0.87	0.29	1.66	103,108,109,110	0
15	UQ	P	3002	19/63	0.87	0.36	1.61	134,146,148,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	CDL	P	3004	40/100	0.76	0.38	1.55	147,157,162,162	0
16	CDL	C	2004	40/100	0.89	0.29	1.47	103,110,126,128	0
11	PEE	C	2007	49/51	0.93	0.24	1.11	68,80,102,104	0
13	HEM	P	501	43/43	0.98	0.25	0.94	65,72,79,81	0
14	IKR	P	3001	25/25	0.97	0.23	0.81	86,89,108,116	0
13	HEM	C	501	43/43	0.98	0.23	0.77	48,52,62,66	0
13	HEM	C	502	43/43	0.99	0.21	0.25	41,46,56,61	0
19	HEC	D	501	43/43	0.98	0.20	0.20	57,60,68,70	0
13	HEM	P	502	43/43	0.98	0.20	-0.12	68,73,82,82	0
14	IKR	C	2001	25/25	0.99	0.17	-0.24	65,67,75,79	0
19	HEC	Q	501	43/43	0.96	0.21	-0.57	87,91,97,99	0
21	FES	E	501	4/4	0.92	0.36	-0.89	257,257,257,257	4
21	FES	R	501	4/4	0.90	0.06	-1.37	201,201,201,202	0
12	UNL	C	4234	1/-	0.53	0.99	-	58,58,58,58	0
12	UNL	P	4236	1/-	0.69	0.76	-	94,94,94,94	0
17	ZN	C	2012	1/1	0.94	0.04	-	104,104,104,104	0
17	ZN	P	3012	1/1	0.98	0.04	-	121,121,121,121	0
11	PEE	P	3008	5/51	0.83	0.38	-	184,184,184,185	0
12	UNL	N	4231	1/-	0.37	0.59	-	90,90,90,90	0
20	BOG	P	3091	13/20	0.28	0.83	-	298,299,299,300	0
12	UNL	A	3231	1/-	0.75	0.82	-	45,45,45,45	0

## 6.5 Other polymers

There are no such residues in this entry.