



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 02:56 AM EDT

PDB ID : 3H1J  
Title : Stigmatellin-bound cytochrome bc1 complex from chicken  
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.; Crofts, A.R.; Berry, E.A.; Kim, S.-H.  
Deposited on : unknown  
Resolution : 3.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

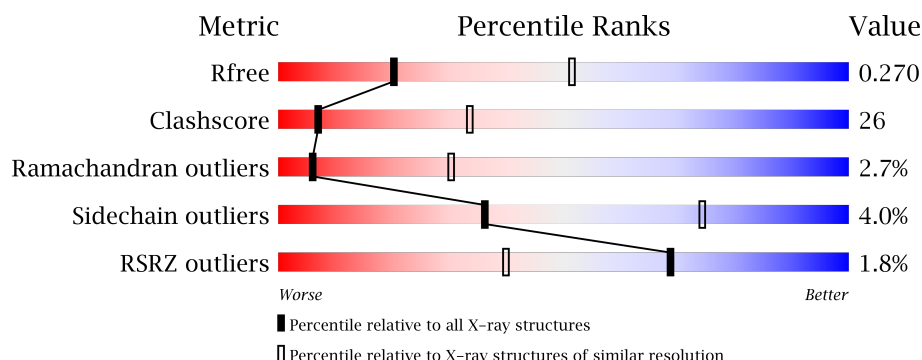
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.




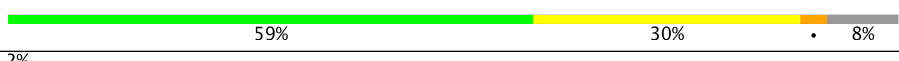
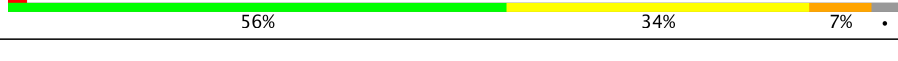
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	
1	N	446	
2	B	441	
2	O	441	
3	C	380	

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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	UNL	A	3016	-	-	-	X
11	UNL	C	2010	-	-	-	X
11	UNL	E	3103	-	-	-	X
11	UNL	R	2103	-	-	-	X
14	UQ	C	2002	-	-	-	X
14	UQ	P	3002	-	-	-	X
15	PEE	C	2007	-	-	-	X
15	PEE	C	2008	-	-	-	X
15	PEE	E	2005	-	-	-	X
15	PEE	N	3008	-	X	-	-
15	PEE	P	3007	-	-	-	X
15	PEE	R	3005	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	GOL	C	2011	-	-	-	X
16	GOL	P	3011	-	-	-	X
18	CDL	G	2004	-	-	-	X
18	CDL	S	3003	-	-	-	X
20	PLC	E	2009	-	-	-	X
20	PLC	R	3009	-	-	-	X

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32679 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	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	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
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	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- 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	70	Total	C	N	O	S	0	0	0
			574	350	105	114	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			

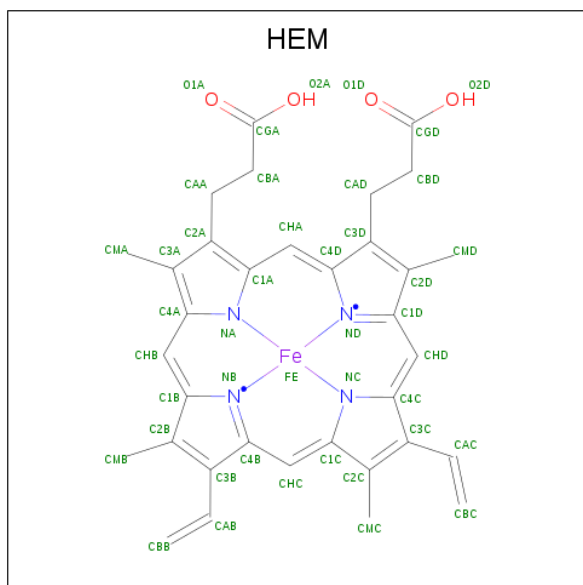
- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	3	Total	O	0	0
			3	3		
11	R	1	Total	O	0	0
			1	1		
11	A	1	Total	O	0	0
			1	1		
11	C	3	Total	O	0	0
			3	3		
11	E	2	Total	O	0	0
			2	2		

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



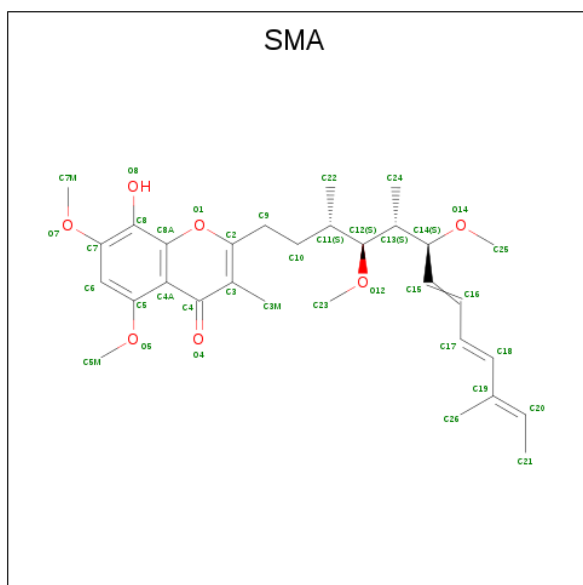
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

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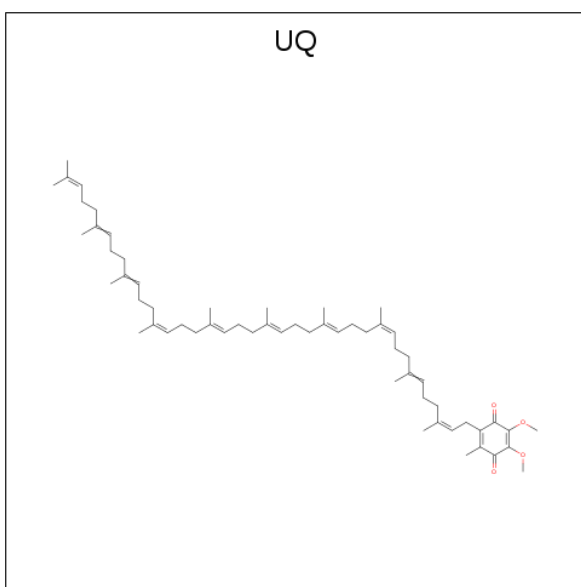
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).



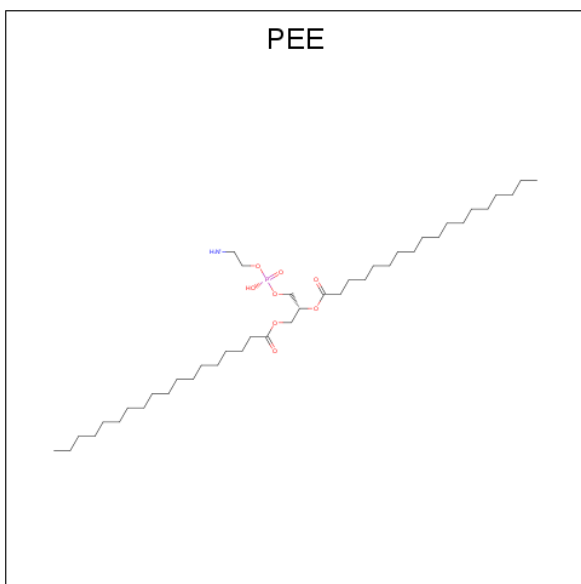
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			37	30	7		
13	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 14 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula:  $C_{59}H_{90}O_4$ ).



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

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



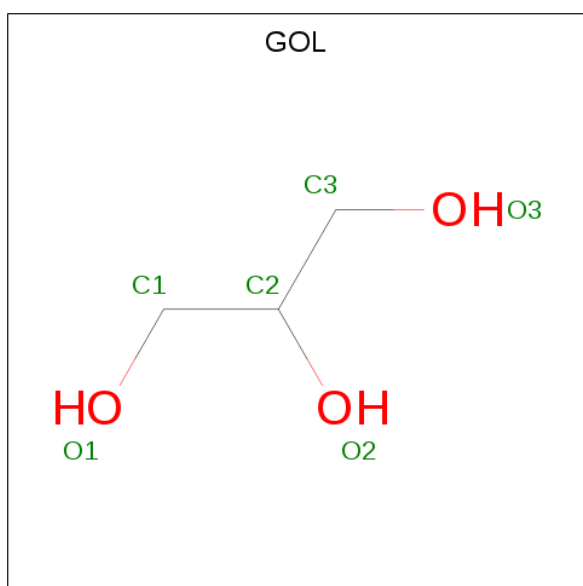
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

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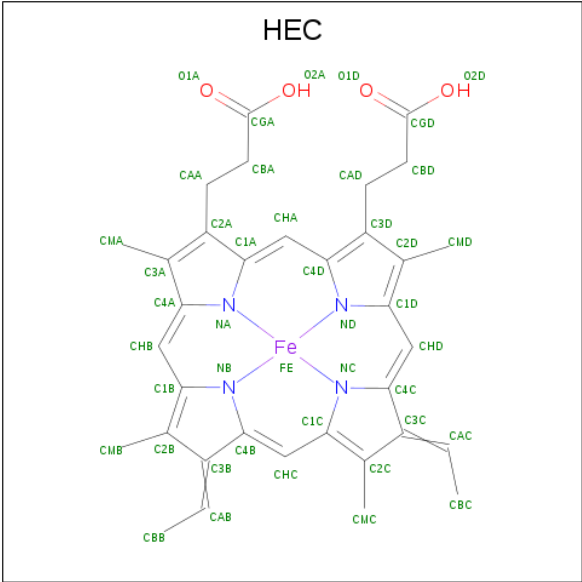
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	N	1	Total	O	P			0	0
			5	4	1				
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



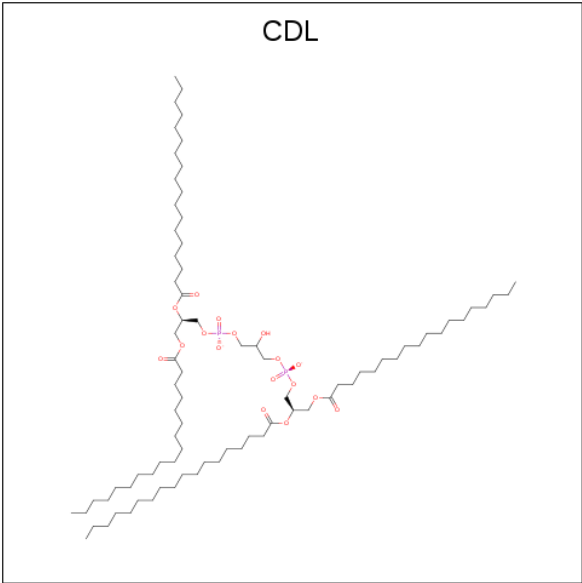
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).

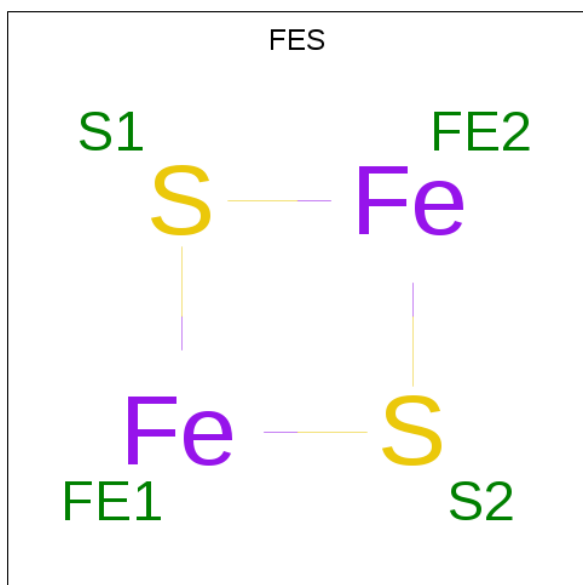


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			50	31	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		

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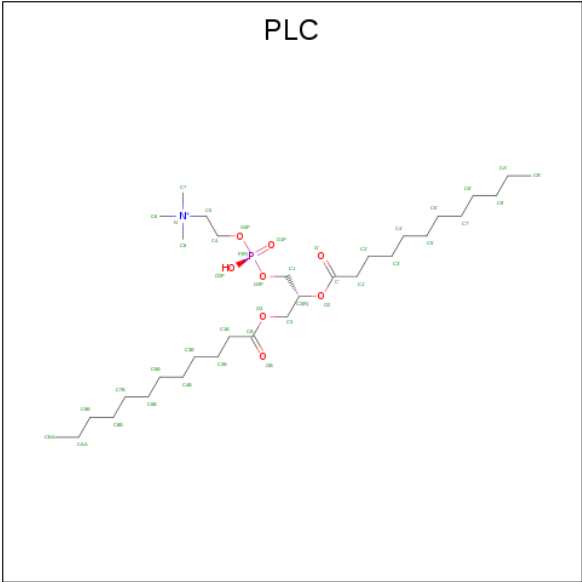
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			40	21	17	2		
18	S	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

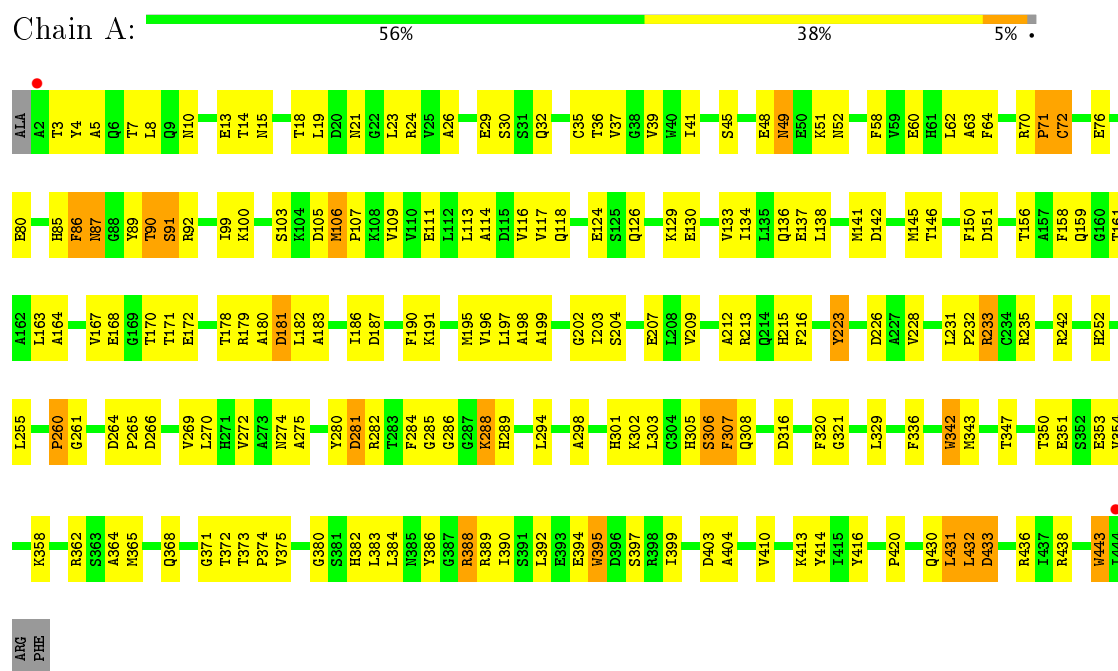
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	O	0	0
			1	1		
21	C	6	Total	O	0	0
			6	6		
21	P	6	Total	O	0	0
			6	6		
21	U	1	Total	O	0	0
			1	1		

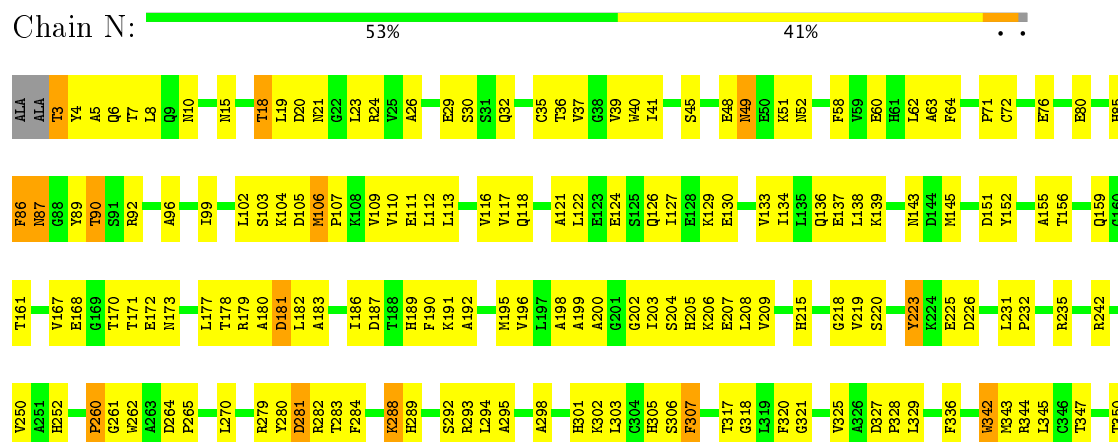
### 3 Residue-property plots

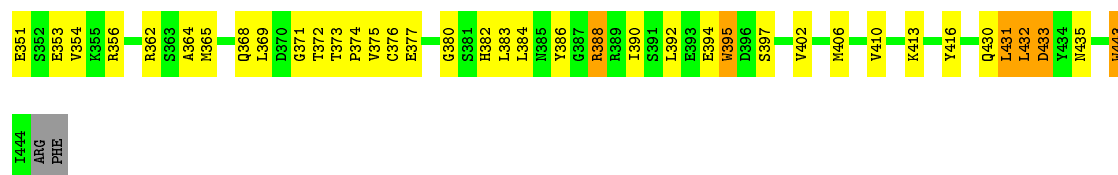
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I



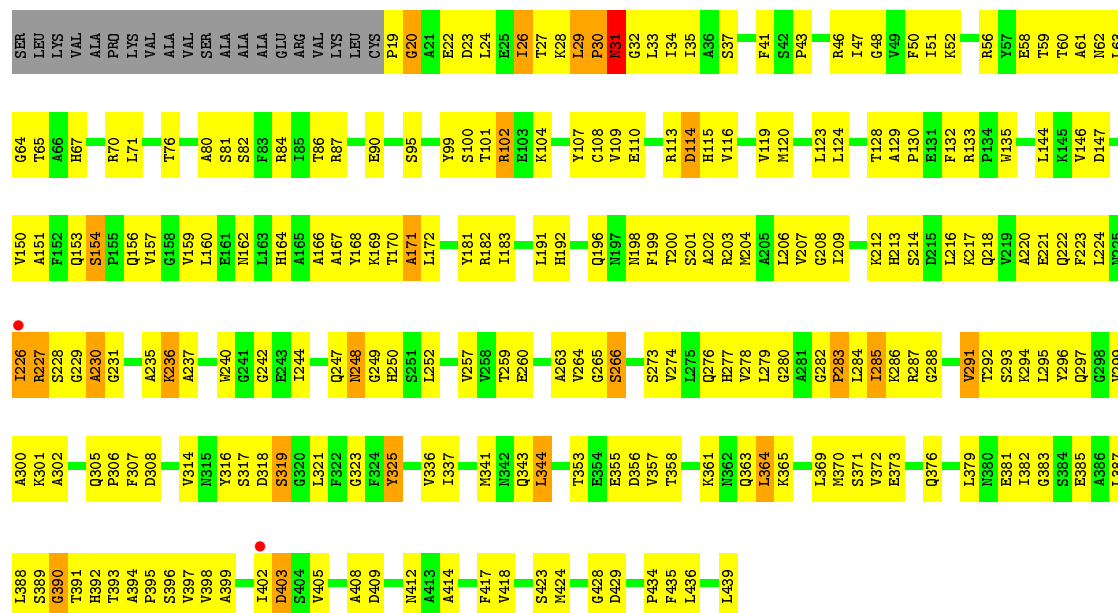
#### • Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I





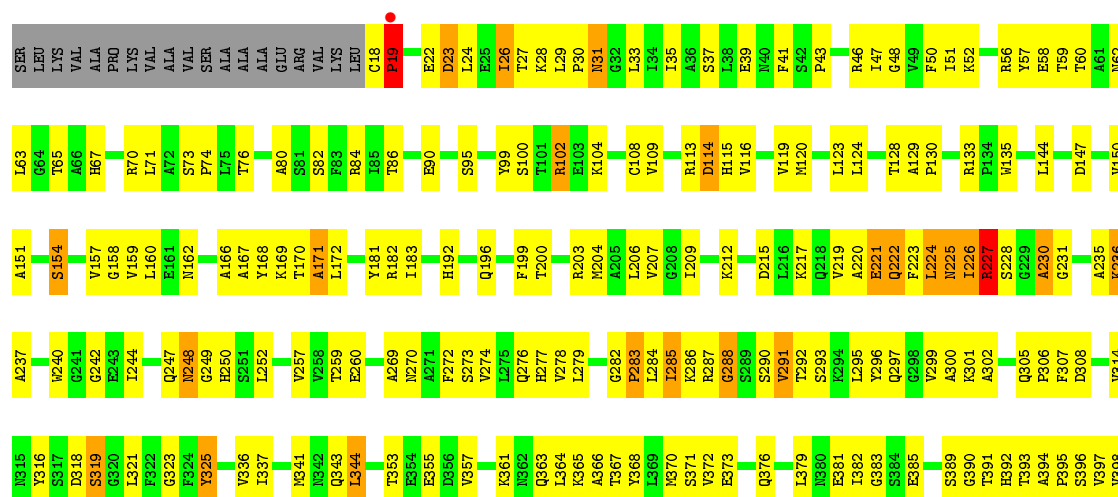
## • Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

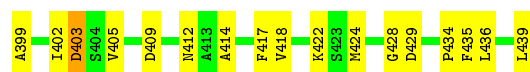
Chain B: 43% 47% 5% 5%



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

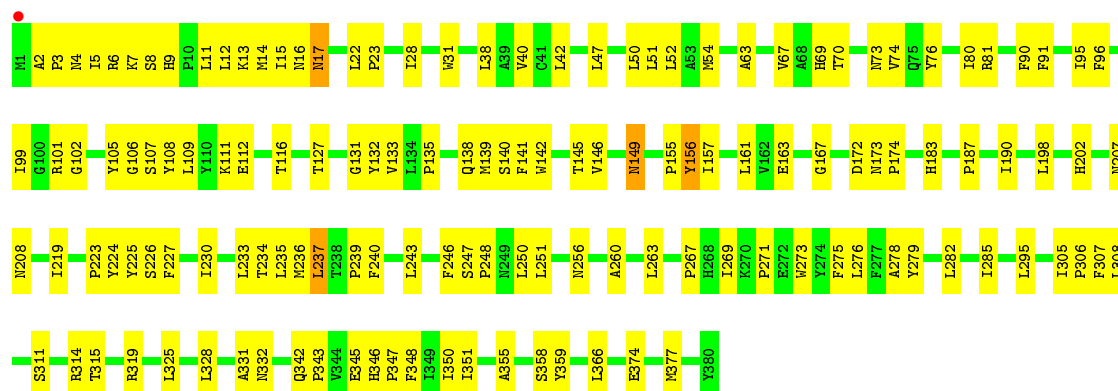
Chain O: 48% 42% 5% 5%





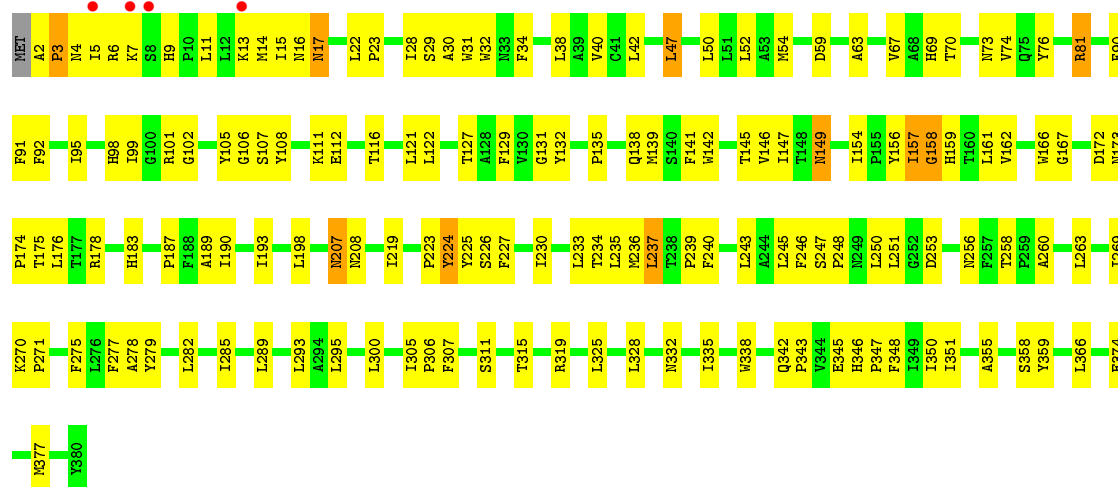
• Molecule 3: Cytochrome b

Chain C: 63% 36% .



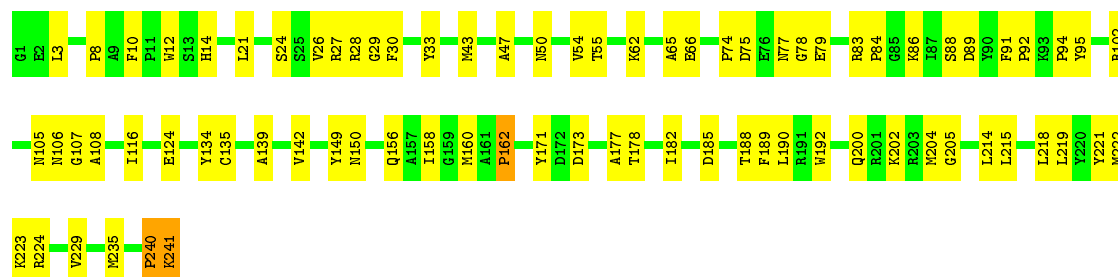
• Molecule 3: Cytochrome b

Chain P: 59% 38% .

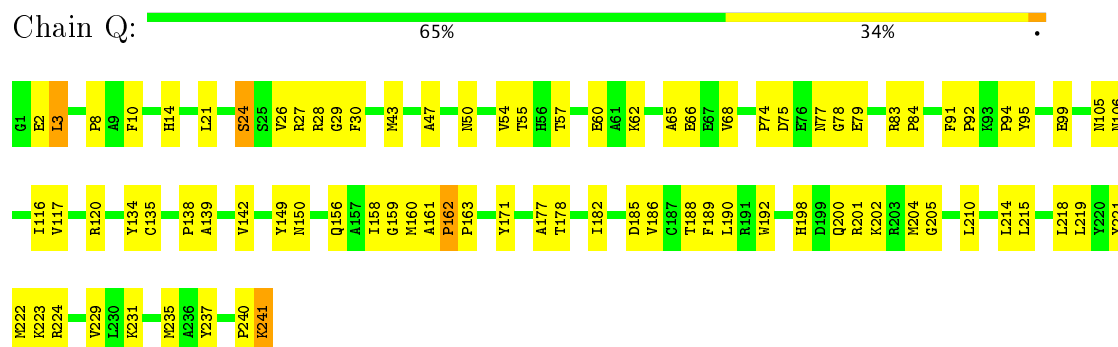


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

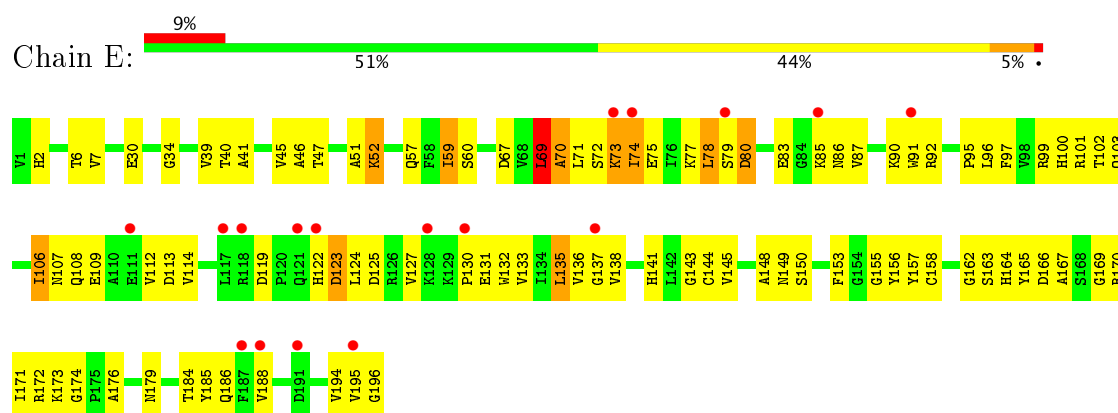
Chain D: 68% 31% .



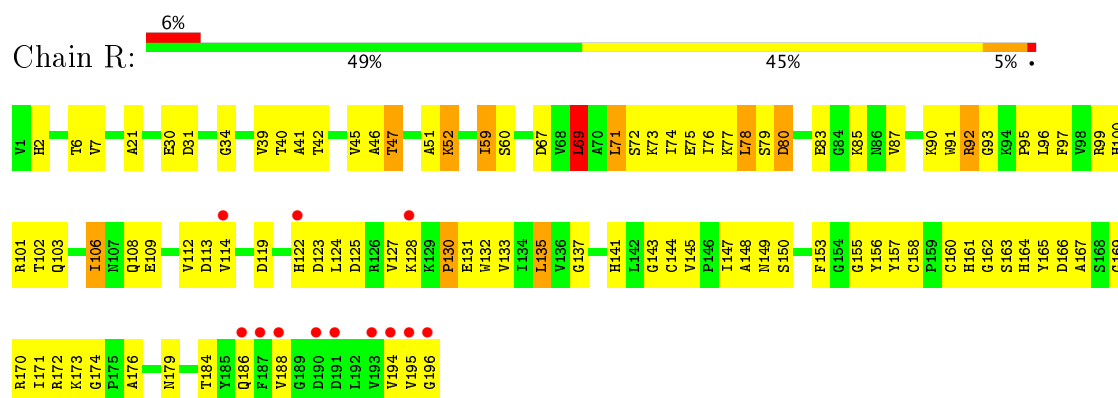
- Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



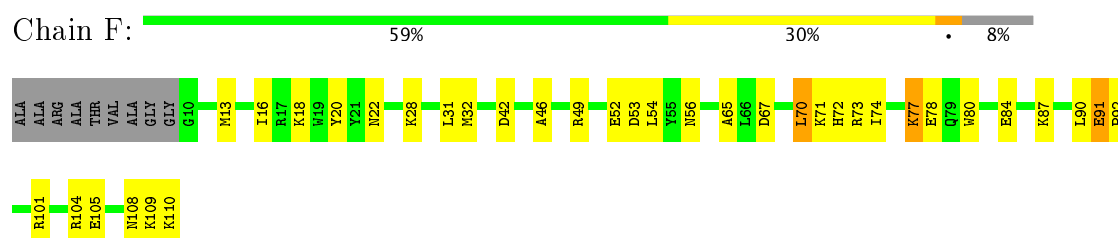
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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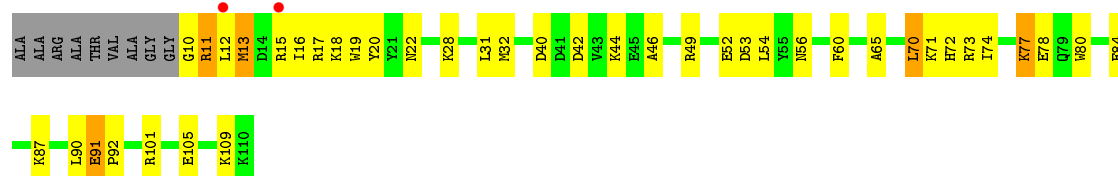


- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



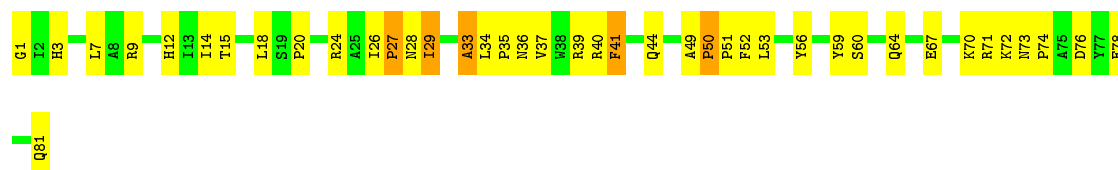
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S: 



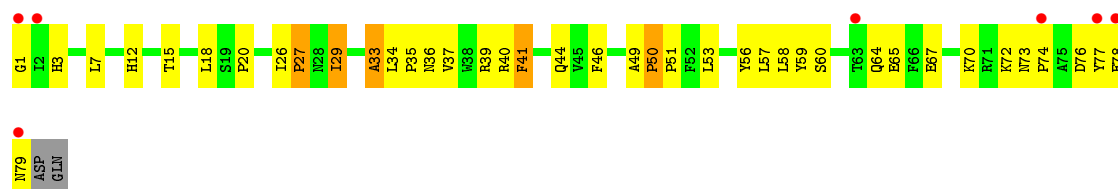
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



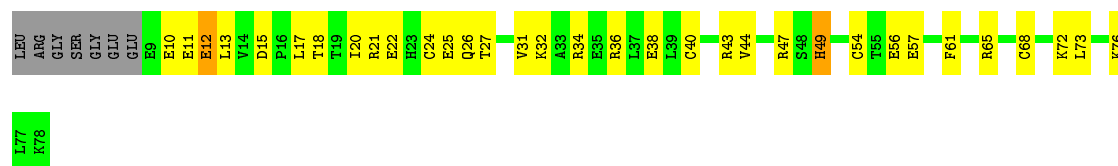
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T: 



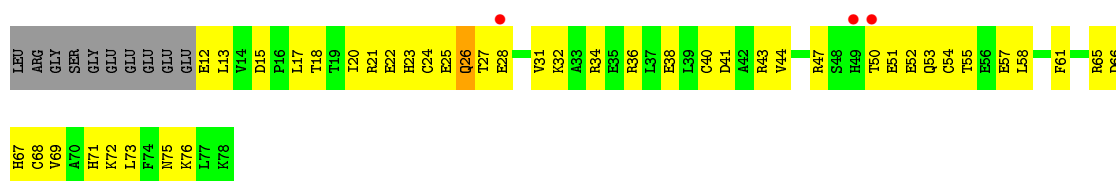
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H: 



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

Chain U: 



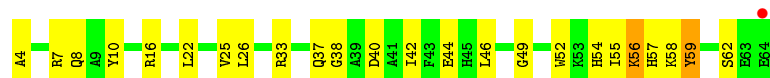
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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- 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, $\alpha$ , $\beta$ , $\gamma$	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.68-3.00) 92.5 (42.68-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.277 0.236 , 0.270	Depositor DCC
$R_{free}$ test set	2796 reflections (2.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, UNL, UQ, PLC, FES, HEC, HEM, PEE, SMA

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	0.43	0/3511	0.65	0/4757
1	N	0.43	0/3508	0.65	1/4753 (0.0%)
2	B	0.38	0/3196	0.63	0/4334
2	O	0.40	0/3202	0.63	0/4343
3	C	0.52	0/3122	0.67	0/4273
3	P	0.46	0/3114	0.65	0/4263
4	D	0.45	0/1956	0.64	0/2658
4	Q	0.40	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.64	1/2103 (0.0%)
5	R	0.39	0/1547	0.68	2/2103 (0.1%)
6	F	0.52	0/911	0.71	0/1219
6	S	0.43	0/911	0.63	0/1219
7	G	0.50	0/698	0.68	0/946
7	T	0.44	0/680	0.65	0/923
8	H	0.47	0/582	0.59	0/779
8	U	0.34	0/561	0.57	0/751
9	I	0.40	0/218	0.65	0/293
9	V	0.41	0/218	0.66	0/293
10	J	0.44	0/508	0.63	0/682
10	W	0.41	0/489	0.61	0/658
All	All	0.43	0/32435	0.65	4/44008 (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	P	0	1
4	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	E	143	GLY	N-CA-C	6.29	128.82	113.10
5	R	143	GLY	N-CA-C	6.28	128.80	113.10
1	N	218	GLY	N-CA-C	-5.19	100.11	113.10
5	R	71	LEU	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	33	TYR	Sidechain
3	P	224	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	169	0
1	N	3437	0	3349	192	0
2	B	3141	0	3142	255	0
2	O	3147	0	3146	228	0
3	C	3020	0	3070	136	0
3	P	3012	0	3058	152	0
4	D	1898	0	1846	63	0
4	Q	1898	0	1846	83	0
5	E	1513	0	1478	91	0
5	R	1513	0	1478	93	0
6	F	891	0	893	36	0
6	S	891	0	893	40	0
7	G	676	0	659	46	0
7	T	658	0	647	46	0
8	H	574	0	548	31	0
8	U	553	0	535	46	0
9	I	285	0	237	50	0
9	V	275	0	238	42	0
10	J	497	0	490	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	478	0	478	29	0
11	A	1	0	0	0	0
11	C	3	0	0	0	0
11	E	2	0	0	0	0
11	P	3	0	0	0	0
11	R	1	0	0	0	0
12	C	86	0	60	11	0
12	P	86	0	60	11	0
13	C	37	0	42	4	0
13	P	37	0	42	4	0
14	C	19	0	17	5	0
14	P	19	0	17	1	0
15	C	70	0	85	1	0
15	E	50	0	77	4	0
15	N	5	0	0	0	0
15	P	49	0	72	1	0
15	R	50	0	77	4	0
16	C	6	0	8	0	0
16	P	6	0	8	1	0
17	D	43	0	30	1	0
17	Q	43	0	30	1	0
18	D	50	0	44	1	0
18	G	40	0	24	1	0
18	P	40	0	24	3	0
18	S	50	0	44	2	0
19	E	4	0	0	0	0
19	R	4	0	0	1	0
20	E	32	0	38	3	0
20	R	32	0	38	2	0
21	B	1	0	0	0	0
21	C	6	0	0	0	0
21	P	6	0	0	1	0
21	U	1	0	0	1	0
All	All	32679	0	32221	1656	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 26.

All (1656) 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:353:THR:HG22	2:B:355:GLU:H	1.15	1.08
3:C:17:ASN:HD21	7:G:1:GLY:HA2	0.98	1.07
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.35	1.06
2:O:353:THR:HG22	2:O:355:GLU:H	1.19	1.06
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.37	1.06
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.37	1.06
2:O:76:THR:HG22	2:O:82:SER:H	1.17	1.05
2:O:22:GLU:HG3	2:O:39:GLU:HB3	1.37	1.05
2:B:76:THR:HG22	2:B:82:SER:H	1.22	1.01
3:P:90:PHE:HB3	3:P:236:MET:HE3	1.41	1.01
3:P:157:ILE:HG13	3:P:158:GLY:H	1.23	1.01
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.09	0.97
3:C:90:PHE:HB3	3:C:236:MET:HE3	1.45	0.96
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.45	0.96
7:T:29:ILE:HD12	7:T:29:ILE:H	1.28	0.96
9:V:28:UNK:CB	9:V:72:ALA:HB2	1.95	0.95
6:S:13:MET:HA	6:S:16:ILE:HB	1.46	0.95
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.29	0.94
3:C:17:ASN:ND2	7:G:1:GLY:HA2	1.82	0.94
1:A:178:THR:HB	1:A:181:ASP:OD1	1.68	0.93
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.34	0.92
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.50	0.92
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.52	0.91
6:S:32:MET:HE3	6:S:87:LYS:H	1.37	0.90
7:G:29:ILE:HD12	7:G:29:ILE:H	1.35	0.90
6:F:32:MET:CE	6:F:87:LYS:H	1.84	0.90
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.89
1:N:136:GLN:HE22	9:V:50:LEU:HD12	1.38	0.89
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.54	0.89
3:P:207:ASN:ND2	3:P:208:ASN:H	1.70	0.88
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.56	0.88
3:C:13:LYS:O	3:C:17:ASN:HB2	1.74	0.88
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.40	0.87
6:S:52:GLU:HG2	6:S:56:ASN:HD21	1.39	0.87
6:F:32:MET:CE	6:F:87:LYS:HG2	2.04	0.87
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.57	0.86
2:O:128:THR:HA	2:O:226:ILE:HD11	1.57	0.86
1:N:49:ASN:C	1:N:49:ASN:HD22	1.79	0.85
3:C:207:ASN:ND2	3:C:208:ASN:H	1.73	0.85
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.41	0.85
2:B:393:THR:HG23	2:B:397:VAL:HB	1.57	0.85
6:F:52:GLU:HG2	6:F:56:ASN:HD21	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:HD22	2:B:32:GLY:N	1.74	0.84
9:V:65:VAL:HB	9:V:77:ARG:HD3	1.58	0.84
2:O:393:THR:HG23	2:O:397:VAL:HB	1.58	0.84
3:P:101:ARG:C	3:P:101:ARG:HD2	1.97	0.84
5:R:73:LYS:HB3	5:R:195:VAL:O	1.77	0.83
6:F:32:MET:HE3	6:F:87:LYS:H	1.42	0.83
1:N:178:THR:HB	1:N:181:ASP:OD1	1.76	0.83
9:I:71:ASN:HD22	9:I:71:ASN:H	1.26	0.83
1:N:178:THR:HG22	1:N:180:ALA:H	1.41	0.83
6:S:52:GLU:HG2	6:S:56:ASN:ND2	1.94	0.83
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.42	0.83
3:P:13:LYS:O	3:P:17:ASN:HB2	1.77	0.83
1:A:178:THR:HG22	1:A:180:ALA:H	1.44	0.82
1:A:49:ASN:C	1:A:49:ASN:HD22	1.82	0.82
5:R:101:ARG:NH2	5:R:127:VAL:HG21	1.94	0.82
6:F:52:GLU:HG2	6:F:56:ASN:ND2	1.95	0.81
2:B:212:LYS:HD3	2:B:213:HIS:N	1.96	0.81
2:B:227:ARG:HD3	2:B:228:SER:H	1.45	0.80
1:A:187:ASP:O	1:A:191:LYS:HE3	1.82	0.80
3:C:101:ARG:C	3:C:101:ARG:HD2	2.02	0.80
2:O:62:ASN:O	2:O:65:THR:HG22	1.81	0.80
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.63	0.80
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.64	0.80
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.64	0.80
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.64	0.80
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.22	0.79
2:B:62:ASN:O	2:B:65:THR:HG22	1.82	0.79
6:S:32:MET:CE	6:S:87:LYS:H	1.96	0.79
5:E:101:ARG:NH2	5:E:127:VAL:HG21	1.97	0.79
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.63	0.79
2:B:47:ILE:HG12	2:B:120:MET:CE	2.13	0.79
2:O:76:THR:HG22	2:O:82:SER:N	1.95	0.79
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.78
1:N:187:ASP:O	1:N:191:LYS:HE3	1.84	0.78
1:N:99:ILE:HD12	1:N:109:VAL:HG13	1.65	0.78
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.18	0.78
2:B:76:THR:HG22	2:B:82:SER:N	1.97	0.78
1:A:99:ILE:HD12	1:A:109:VAL:HG13	1.67	0.77
2:B:227:ARG:HE	2:B:227:ARG:HA	1.48	0.76
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.67	0.76
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:CG2	2:B:82:SER:H	1.97	0.76
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.66	0.76
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.50	0.76
2:B:102:ARG:HH11	2:B:102:ARG:HG2	1.50	0.76
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.15	0.76
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.68	0.76
2:O:226:ILE:HG22	2:O:227:ARG:N	2.01	0.75
2:B:154:SER:O	2:B:157:VAL:HG12	1.86	0.75
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.26	0.75
6:F:32:MET:HE2	6:F:87:LYS:HG2	1.66	0.75
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.21	0.75
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.51	0.75
4:D:224:ARG:HE	7:G:26:ILE:HG12	1.52	0.75
9:I:32:UNK:N	9:I:73:PRO:HG2	2.01	0.75
2:O:47:ILE:HG12	2:O:120:MET:HE3	1.69	0.75
2:B:201:SER:OG	2:B:228:SER:HB3	1.87	0.74
1:A:136:GLN:NE2	9:I:50:LEU:HB2	2.02	0.74
2:B:47:ILE:HG12	2:B:120:MET:HE3	1.69	0.74
7:T:29:ILE:HD12	7:T:29:ILE:N	2.01	0.74
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.69	0.74
2:B:385:GLU:OE1	2:B:392:HIS:HA	1.87	0.74
1:N:373:THR:HB	1:N:374:PRO:HD3	1.68	0.74
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.70	0.74
3:P:157:ILE:HG13	3:P:158:GLY:N	2.01	0.74
2:O:219:VAL:O	2:O:223:PHE:HB2	1.88	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.70	0.73
2:O:47:ILE:HG12	2:O:120:MET:CE	2.18	0.73
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.70	0.73
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.69	0.73
2:B:248:ASN:HD22	2:B:248:ASN:C	1.90	0.73
7:G:29:ILE:CD1	7:G:29:ILE:H	1.93	0.73
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.70	0.73
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.23	0.73
2:O:154:SER:O	2:O:157:VAL:HG12	1.89	0.73
2:B:218:GLN:HG3	2:B:222:GLN:NE2	2.04	0.73
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.71	0.73
2:O:361:LYS:O	2:O:365:LYS:HG3	1.87	0.73
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.19	0.72
2:B:389:SER:O	2:B:391:THR:HG23	1.88	0.72
2:O:220:ALA:O	2:O:224:LEU:HB2	1.89	0.72
2:O:76:THR:CG2	2:O:82:SER:H	1.99	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:32:LYS:O	8:U:36:ARG:HG3	1.89	0.72
1:N:136:GLN:NE2	9:V:50:LEU:HB2	2.04	0.72
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.18	0.72
3:C:139:MET:HE1	3:C:269:ILE:HA	1.70	0.72
2:B:31:ASN:HB3	2:B:227:ARG:HH22	1.54	0.72
7:G:29:ILE:HD12	7:G:29:ILE:N	2.04	0.72
9:I:71:ASN:H	9:I:71:ASN:ND2	1.88	0.72
2:O:389:SER:O	2:O:391:THR:HG23	1.90	0.72
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.84	0.72
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.24	0.72
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.55	0.71
3:C:4:ASN:HD21	3:C:7:LYS:NZ	1.87	0.71
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.72	0.71
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.26	0.71
1:N:182:LEU:O	1:N:186:ILE:HG13	1.91	0.71
8:U:27:THR:O	8:U:31:VAL:HG23	1.89	0.71
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.30	0.71
2:O:22:GLU:HG3	2:O:39:GLU:CB	2.18	0.71
2:O:29:LEU:HD12	2:O:33:LEU:HD23	1.72	0.71
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.72	0.71
2:O:248:ASN:HD22	2:O:248:ASN:C	1.91	0.71
2:B:227:ARG:NE	2:B:227:ARG:HA	2.05	0.71
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.56	0.71
9:V:64:LEU:HD12	9:V:77:ARG:O	1.89	0.71
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.72	0.71
8:H:43:ARG:HD2	8:H:47:ARG:NH1	2.06	0.71
3:P:285:ILE:N	3:P:285:ILE:HD12	2.06	0.71
2:B:203:ARG:CD	2:B:230:ALA:HA	2.19	0.71
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.72	0.71
4:D:75:ASP:OD2	4:D:79:GLU:HB2	1.90	0.70
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.71	0.70
2:B:212:LYS:HD2	2:B:214:SER:OG	1.91	0.70
9:I:55:MET:O	9:I:58:ARG:HG2	1.92	0.70
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.27	0.70
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.06	0.70
7:T:29:ILE:CD1	7:T:29:ILE:H	1.90	0.70
1:N:90:THR:O	1:N:167:VAL:HG11	1.91	0.70
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.06	0.70
2:B:124:LEU:HD21	2:B:223:PHE:HB3	1.73	0.70
1:N:388:ARG:HG3	1:N:388:ARG:HH21	1.56	0.70
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.74	0.70
3:P:346:HIS:ND1	3:P:347:PRO:HA	2.06	0.70
2:B:353:THR:HG22	2:B:355:GLU:N	2.00	0.69
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.73	0.69
2:O:385:GLU:OE1	2:O:392:HIS:HA	1.92	0.69
3:P:187:PRO:HG2	12:P:501:HEM:HMC3	1.72	0.69
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.91	0.69
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.69
3:P:17:ASN:HD21	7:T:1:GLY:HA3	1.57	0.69
1:A:288:LYS:HE3	1:A:289:HIS:NE2	2.07	0.69
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.74	0.69
3:P:207:ASN:ND2	3:P:208:ASN:N	2.40	0.69
2:O:33:LEU:HD21	2:O:220:ALA:HB1	1.74	0.69
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.58	0.69
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.73	0.69
2:B:24:LEU:HD12	2:B:37:SER:O	1.92	0.69
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.73	0.69
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.75	0.68
1:A:10:ASN:HD21	2:B:19:PRO:HD3	1.56	0.68
2:B:31:ASN:HD22	2:B:32:GLY:H	1.39	0.68
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.08	0.68
1:A:281:ASP:HB3	1:A:284:PHE:CE1	2.29	0.68
1:A:45:SER:HA	1:A:48:GLU:HG3	1.74	0.68
9:I:31:UNK:C	9:I:73:PRO:HG2	2.23	0.68
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.28	0.68
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.75	0.68
5:R:91:TRP:CE3	5:R:96:LEU:HD22	2.28	0.68
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.75	0.68
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	1.94	0.68
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.20	0.68
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.23	0.68
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.29	0.68
1:A:373:THR:HB	1:A:374:PRO:HD3	1.75	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.58	0.68
1:A:350:THR:OG1	1:A:353:GLU:HG3	1.93	0.67
5:E:40:THR:HG21	15:E:2005:PEE:O2P	1.94	0.67
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.20	0.67
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.59	0.67
2:O:192:HIS:O	2:O:196:GLN:HG3	1.94	0.67
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.10	0.67
2:B:295:LEU:HA	2:B:343:GLN:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.60	0.67
3:P:226:SER:O	3:P:230:ILE:HG12	1.95	0.67
3:P:271:PRO:HA	13:P:3001:SMA:H10	1.75	0.67
3:P:247:SER:OG	3:P:250:LEU:HB2	1.95	0.67
2:O:217:LYS:O	2:O:221:GLU:HG2	1.95	0.67
6:F:70:LEU:HD12	6:F:70:LEU:C	2.15	0.67
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.67
3:P:4:ASN:HD21	3:P:7:LYS:NZ	1.92	0.67
2:O:227:ARG:HA	2:O:227:ARG:HH11	1.59	0.67
6:S:11:ARG:O	6:S:11:ARG:HG2	1.95	0.67
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.76	0.66
2:O:274:VAL:O	2:O:278:VAL:HG23	1.96	0.66
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.78	0.66
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.28	0.66
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.59	0.66
1:N:30:SER:O	1:N:202:GLY:HA2	1.95	0.66
3:C:187:PRO:HG2	12:C:501:HEM:HMC3	1.78	0.66
8:H:34:ARG:O	8:H:38:GLU:HG2	1.96	0.66
1:N:432:LEU:HD23	1:N:433:ASP:N	2.11	0.66
8:H:27:THR:O	8:H:31:VAL:HG23	1.95	0.66
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.76	0.66
2:B:199:PHE:O	2:B:226:ILE:HG12	1.95	0.66
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.60	0.66
3:P:345:GLU:O	3:P:348:PHE:HB2	1.95	0.66
6:S:70:LEU:HD12	6:S:70:LEU:C	2.16	0.66
9:V:64:LEU:HA	9:V:77:ARG:O	1.96	0.66
2:B:43:PRO:O	2:B:113:ARG:HG3	1.96	0.65
3:C:202:HIS:NE2	14:C:2002:UQ:O4	2.29	0.65
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.78	0.65
15:P:3007:PEE:H7	7:T:44:GLN:HE21	1.60	0.65
8:H:32:LYS:O	8:H:36:ARG:HG3	1.96	0.65
2:O:95:SER:HB3	9:V:28:UNK:H2	1.61	0.65
1:N:49:ASN:C	1:N:49:ASN:ND2	2.50	0.65
2:O:95:SER:HB3	9:V:28:UNK:N	2.11	0.65
1:N:136:GLN:NE2	9:V:50:LEU:HD12	2.10	0.65
2:B:229:GLY:O	2:B:231:GLY:N	2.28	0.65
3:C:207:ASN:ND2	3:C:208:ASN:N	2.45	0.65
2:O:124:LEU:HD13	2:O:224:LEU:HD23	1.79	0.65
1:A:156:THR:O	1:A:159:GLN:HG2	1.97	0.65
2:B:361:LYS:O	2:B:365:LYS:HG3	1.96	0.65
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:MET:HE1	6:F:87:LYS:H	1.62	0.65
2:O:250:HIS:HE1	2:O:252:LEU:HB2	1.61	0.65
3:P:347:PRO:O	3:P:351:ILE:HG13	1.97	0.65
3:C:285:ILE:N	3:C:285:ILE:HD12	2.10	0.64
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.79	0.64
4:D:200:GLN:HE21	20:E:2009:PLC:H51	1.62	0.64
2:O:357:VAL:O	2:O:361:LYS:HG3	1.97	0.64
5:E:83:GLU:HA	5:E:100:HIS:CG	2.32	0.64
2:B:307:PHE:H	9:I:52:ARG:HG2	1.61	0.64
4:Q:200:GLN:HE21	20:R:3009:PLC:H51	1.62	0.64
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.79	0.64
8:H:17:LEU:O	8:H:21:ARG:HG3	1.97	0.64
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.62	0.64
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.13	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.12	0.64
1:N:180:ALA:O	1:N:183:ALA:HB3	1.98	0.64
2:B:113:ARG:O	2:B:116:VAL:HG23	1.98	0.64
2:O:24:LEU:HD12	2:O:37:SER:O	1.97	0.64
1:N:288:LYS:HE3	1:N:289:HIS:NE2	2.13	0.64
1:N:351:GLU:O	1:N:354:VAL:HG22	1.98	0.64
1:N:45:SER:HA	1:N:48:GLU:HG3	1.79	0.64
2:B:409:ASP:HA	2:B:412:ASN:HD22	1.63	0.64
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.78	0.64
3:C:226:SER:O	3:C:230:ILE:HG12	1.98	0.64
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.98	0.64
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.79	0.64
2:B:357:VAL:O	2:B:361:LYS:HG3	1.98	0.64
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.33	0.64
2:O:409:ASP:HA	2:O:412:ASN:HD22	1.63	0.64
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.32	0.64
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.13	0.64
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.64	0.63
2:B:124:LEU:CD2	2:B:223:PHE:HB3	2.27	0.63
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.13	0.63
2:O:222:GLN:O	2:O:223:PHE:HD2	1.79	0.63
3:P:146:VAL:HG21	13:P:3001:SMA:H6	1.79	0.63
3:P:355:ALA:O	3:P:358:SER:HB3	1.98	0.63
2:B:370:MET:O	2:B:373:GLU:HG3	1.97	0.63
1:N:87:ASN:OD1	2:O:286:LYS:HD2	1.99	0.63
1:A:182:LEU:O	1:A:186:ILE:HG13	1.97	0.63
3:C:247:SER:OG	3:C:250:LEU:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:LEU:HD21	3:C:251:LEU:HD11	1.79	0.63
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.62	0.63
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.28	0.63
1:A:4:TYR:HA	2:B:113:ARG:HD3	1.81	0.63
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.33	0.63
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.13	0.63
20:R:3009:PLC:H1A1	20:R:3009:PLC:H1'1	1.79	0.63
5:R:83:GLU:HA	5:R:100:HIS:CG	2.33	0.63
2:O:325:TYR:HD1	9:V:60:ALA:HB2	1.64	0.63
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.79	0.63
3:C:346:HIS:ND1	3:C:347:PRO:HA	2.14	0.63
3:C:90:PHE:HB3	3:C:236:MET:CE	2.26	0.63
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.32	0.63
15:C:2007:PEE:H7	7:G:44:GLN:HE21	1.64	0.63
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.81	0.63
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.13	0.63
5:E:41:ALA:O	5:E:45:VAL:HG23	1.99	0.63
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.29	0.63
1:N:136:GLN:HG2	9:V:51:CYS:HB3	1.81	0.63
1:A:371:GLY:O	1:A:375:VAL:HG23	1.99	0.62
2:B:250:HIS:HE1	2:B:252:LEU:HB2	1.64	0.62
2:O:226:ILE:CG2	2:O:227:ARG:N	2.62	0.62
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.80	0.62
7:G:81:GLN:O	8:H:47:ARG:HA	2.00	0.62
1:N:126:GLN:NE2	1:N:129:LYS:HD3	2.15	0.62
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.63	0.62
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.35	0.62
1:N:103:SER:HB3	1:N:202:GLY:O	1.99	0.62
3:P:207:ASN:HD22	3:P:208:ASN:H	1.45	0.62
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.34	0.62
6:F:53:ASP:OD1	6:F:54:LEU:N	2.31	0.62
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.82	0.62
2:B:26:ILE:O	2:B:26:ILE:HG12	1.98	0.62
7:G:40:ARG:HD2	18:G:2004:CDL:OA4	1.99	0.62
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.83	0.62
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.81	0.62
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.29	0.62
1:A:30:SER:O	1:A:202:GLY:HA2	2.00	0.62
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.35	0.62
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.81	0.62
2:O:26:ILE:O	2:O:26:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG23	2:B:151:ALA:N	2.15	0.62
2:B:274:VAL:O	2:B:278:VAL:HG23	2.00	0.62
3:C:173:ASN:N	3:C:174:PRO:HD2	2.15	0.62
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.82	0.62
6:S:52:GLU:CG	6:S:56:ASN:HD21	2.11	0.62
7:T:29:ILE:O	7:T:34:LEU:HG	2.00	0.62
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.00	0.62
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.81	0.61
1:A:103:SER:HB3	1:A:202:GLY:O	2.00	0.61
1:A:49:ASN:ND2	1:A:49:ASN:C	2.53	0.61
6:F:18:LYS:O	6:F:22:ASN:ND2	2.32	0.61
8:U:52:GLU:HG2	8:U:53:GLN:N	2.14	0.61
2:B:86:THR:O	2:B:90:GLU:HG3	2.00	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.97	0.61
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.35	0.61
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.31	0.61
2:O:199:PHE:O	2:O:226:ILE:HG21	2.00	0.61
2:O:259:THR:HG22	2:O:260:GLU:N	2.16	0.61
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.82	0.61
4:D:47:ALA:H	4:D:50:ASN:ND2	1.91	0.61
7:G:74:PRO:O	7:G:78:GLU:HG3	2.01	0.61
2:O:221:GLU:O	2:O:223:PHE:N	2.33	0.61
2:B:306:PRO:HA	9:I:52:ARG:CG	2.31	0.61
8:U:17:LEU:O	8:U:21:ARG:HG3	2.01	0.61
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.82	0.61
2:B:28:LYS:O	2:B:29:LEU:O	2.19	0.61
1:N:279:ARG:NH2	9:V:31:UNK:O	2.33	0.61
2:O:227:ARG:NH1	2:O:228:SER:H	1.98	0.61
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.82	0.60
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.35	0.60
1:A:76:GLU:HG2	2:B:285:ILE:HD12	1.82	0.60
20:E:2009:PLC:H1'1	20:E:2009:PLC:H1A1	1.83	0.60
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.36	0.60
10:W:52:TRP:O	10:W:56:LYS:HB2	2.01	0.60
2:B:409:ASP:O	2:B:412:ASN:HB2	2.01	0.60
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.82	0.60
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.31	0.60
1:A:159:GLN:HE22	7:G:18:LEU:HD21	1.64	0.60
4:D:43:MET:HE3	4:D:189:PHE:CZ	2.35	0.60
1:N:76:GLU:HG2	2:O:285:ILE:HD12	1.81	0.60
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.32	0.60
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.16	0.60
2:O:27:THR:HG22	2:O:28:LYS:N	2.17	0.60
5:R:102:THR:O	5:R:106:ILE:HG13	2.02	0.60
2:B:259:THR:HG22	2:B:260:GLU:N	2.17	0.60
9:I:65:VAL:HB	9:I:77:ARG:HD2	1.83	0.60
5:R:40:THR:HG21	15:R:3005:PEE:O2P	2.01	0.60
8:U:13:LEU:HD23	8:U:13:LEU:H	1.66	0.60
1:A:90:THR:O	1:A:167:VAL:HG11	2.02	0.60
4:Q:224:ARG:HE	7:T:26:ILE:HG12	1.67	0.60
8:U:34:ARG:O	8:U:38:GLU:HG2	2.01	0.60
2:O:409:ASP:O	2:O:412:ASN:HB2	2.02	0.60
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.84	0.60
2:B:227:ARG:CD	2:B:228:SER:H	2.15	0.60
3:C:347:PRO:O	3:C:351:ILE:HG13	2.02	0.60
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.20	0.60
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.31	0.60
2:O:287:ARG:HD3	9:V:53:GLU:CG	2.32	0.59
2:B:56:ARG:HA	2:B:171:ALA:O	2.02	0.59
5:E:52:LYS:C	5:E:52:LYS:HD3	2.22	0.59
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.66	0.59
1:A:272:VAL:O	1:A:275:ALA:HB3	2.02	0.59
3:C:282:LEU:HD23	3:C:282:LEU:C	2.22	0.59
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.84	0.59
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.84	0.59
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.17	0.59
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.85	0.59
1:N:105:ASP:O	1:N:109:VAL:HG23	2.02	0.59
3:P:285:ILE:H	3:P:285:ILE:HD12	1.66	0.59
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.85	0.59
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.31	0.59
5:E:108:GLN:O	5:E:112:VAL:HG23	2.02	0.59
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.36	0.59
7:T:29:ILE:O	7:T:33:ALA:HB3	2.02	0.59
9:I:71:ASN:N	9:I:71:ASN:ND2	2.45	0.59
1:N:432:LEU:HD23	1:N:433:ASP:H	1.67	0.59
7:T:73:ASN:HB3	7:T:76:ASP:OD2	2.02	0.59
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.84	0.59
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.18	0.59
2:O:150:VAL:HG23	2:O:151:ALA:N	2.18	0.58
9:I:71:ASN:N	9:I:71:ASN:HD22	1.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.03	0.58
6:S:13:MET:CA	6:S:16:ILE:HB	2.28	0.58
2:B:292:THR:O	2:B:292:THR:HG22	2.03	0.58
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.85	0.58
2:B:47:ILE:HD12	2:B:47:ILE:N	2.17	0.58
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.39	0.58
2:O:113:ARG:O	2:O:116:VAL:HG23	2.02	0.58
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.02	0.58
1:N:371:GLY:O	1:N:375:VAL:HG23	2.02	0.58
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.03	0.58
6:S:32:MET:CE	6:S:87:LYS:HG2	2.33	0.58
1:A:380:GLY:O	1:A:384:LEU:HB2	2.04	0.58
5:E:90:LYS:HD3	3:P:263:LEU:HD11	1.84	0.58
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.86	0.58
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.39	0.58
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.58
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.83	0.58
2:B:279:LEU:HD13	2:B:344:LEU:HD11	1.86	0.58
3:C:146:VAL:HG21	13:C:2001:SMA:H6	1.85	0.58
5:E:102:THR:O	5:E:106:ILE:HG13	2.03	0.58
5:E:103:GLN:HA	5:E:106:ILE:HD12	1.86	0.58
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.04	0.58
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.22	0.58
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.17	0.58
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.38	0.58
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.38	0.58
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.04	0.58
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.33	0.58
4:Q:28:ARG:HD2	4:Q:185:ASP:OD2	2.04	0.58
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.34	0.58
2:B:31:ASN:ND2	2:B:33:LEU:H	2.00	0.58
8:H:18:THR:O	8:H:22:GLU:HG3	2.04	0.58
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.84	0.58
4:D:88:SER:HB2	5:E:69:LEU:HD22	1.85	0.57
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.39	0.57
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.85	0.57
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.84	0.57
2:B:229:GLY:C	2:B:231:GLY:H	2.07	0.57
3:C:269:ILE:HG23	3:C:269:ILE:O	2.04	0.57
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:370:MET:O	2:O:373:GLU:HG3	2.04	0.57
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.18	0.57
5:E:109:GLU:CG	5:E:167:ALA:HB3	2.34	0.57
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.39	0.57
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.69	0.57
5:R:51:ALA:HA	15:R:3005:PEE:H42	1.86	0.57
1:A:156:THR:HA	5:E:7:VAL:HG21	1.86	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.86	0.57
2:O:95:SER:CB	9:V:28:UNK:H2	2.17	0.57
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.52	0.57
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.03	0.57
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.05	0.57
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.19	0.57
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.86	0.57
2:O:250:HIS:CE1	2:O:252:LEU:HB2	2.39	0.57
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.35	0.57
2:B:144:LEU:HB3	2:B:183:ILE:HD12	1.86	0.57
2:B:402:ILE:O	2:B:405:VAL:HG23	2.05	0.57
10:J:52:TRP:O	10:J:56:LYS:HB2	2.05	0.57
1:N:35:CYS:HA	1:N:372:THR:HG21	1.87	0.57
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.05	0.57
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.39	0.57
1:A:388:ARG:NH2	1:A:388:ARG:HG3	2.20	0.57
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.17	0.57
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.40	0.57
2:B:144:LEU:HB2	2:B:183:ILE:HG23	1.87	0.57
1:N:156:THR:HA	5:R:7:VAL:HG21	1.86	0.57
3:P:243:LEU:HD21	3:P:251:LEU:HD11	1.86	0.57
1:A:106:MET:HE2	1:A:107:PRO:HA	1.87	0.56
6:S:46:ALA:HB1	6:S:90:LEU:HD11	1.86	0.56
2:O:86:THR:O	2:O:90:GLU:HG3	2.05	0.56
8:U:65:ARG:O	8:U:68:CYS:HB3	2.04	0.56
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.16	0.56
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.87	0.56
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.40	0.56
1:A:130:GLU:O	1:A:134:ILE:HG13	2.05	0.56
1:A:343:MET:O	1:A:347:THR:HG23	2.06	0.56
5:E:73:LYS:HB3	5:E:195:VAL:O	2.04	0.56
3:P:139:MET:HB2	3:P:256:ASN:OD1	2.05	0.56
2:B:264:VAL:HG11	2:B:388:LEU:CD1	2.36	0.56
8:H:11:GLU:O	8:H:12:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:CYS:O	8:H:44:VAL:HG23	2.05	0.56
1:N:219:VAL:HG12	1:N:220:SER:H	1.71	0.56
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.29	0.56
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.40	0.56
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.86	0.56
3:C:15:ILE:HD12	3:C:15:ILE:N	2.20	0.56
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.04	0.56
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.86	0.56
6:S:10:GLY:C	6:S:12:LEU:H	2.08	0.56
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.88	0.56
2:B:212:LYS:HD2	2:B:214:SER:H	1.69	0.56
6:F:77:LYS:CE	6:F:78:GLU:HG3	2.36	0.56
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.87	0.56
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.04	0.56
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.41	0.56
1:A:180:ALA:O	1:A:183:ALA:HB3	2.06	0.56
1:A:29:GLU:HG3	1:A:203:ILE:O	2.05	0.56
1:A:432:LEU:HD23	1:A:433:ASP:N	2.21	0.56
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.46	0.56
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.88	0.56
15:E:2005:PEE:H67	10:J:25:VAL:HG22	1.87	0.56
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.87	0.56
7:G:60:SER:HB3	7:G:64:GLN:NE2	2.21	0.56
3:C:101:ARG:NH2	12:C:502:HEM:HBD2	2.22	0.55
5:E:112:VAL:HG11	5:E:172:ARG:NH2	2.21	0.55
2:B:230:ALA:O	2:B:231:GLY:C	2.45	0.55
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.41	0.55
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.88	0.55
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.41	0.55
5:R:153:PHE:HD2	5:R:172:ARG:NH1	2.04	0.55
7:T:53:LEU:O	7:T:56:TYR:HB3	2.06	0.55
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.41	0.55
1:N:431:LEU:HG	1:N:432:LEU:N	2.22	0.55
1:A:233:ARG:NH1	1:A:233:ARG:HG3	2.20	0.55
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.21	0.55
7:G:24:ARG:NH2	7:G:28:ASN:H	2.05	0.55
10:J:33:ARG:O	10:J:37:GLN:HG3	2.06	0.55
5:R:112:VAL:HG11	5:R:172:ARG:NH2	2.21	0.55
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.42	0.55
9:V:28:UNK:CB	9:V:71:ASN:ND2	2.70	0.55
10:W:38:GLY:O	10:W:42:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:HG22	1:A:171:THR:N	2.22	0.55
1:A:351:GLU:O	1:A:354:VAL:HG22	2.07	0.55
4:Q:94:PRO:HG2	4:Q:95:TYR:CD1	2.42	0.55
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.88	0.55
7:G:53:LEU:O	7:G:56:TYR:HB3	2.07	0.55
1:A:305:HIS:O	1:A:306:SER:HB3	2.07	0.55
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.88	0.55
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.21	0.55
3:C:38:LEU:HB3	12:C:502:HEM:CMB	2.37	0.55
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.37	0.55
3:P:90:PHE:CZ	3:P:240:PHE:HA	2.42	0.55
5:R:108:GLN:O	5:R:112:VAL:HG23	2.06	0.55
5:R:78:LEU:HD22	5:R:132:TRP:CD2	2.42	0.55
7:T:41:PHE:CD2	7:T:41:PHE:C	2.80	0.55
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.22	0.55
3:C:5:ILE:O	3:C:5:ILE:HG22	2.07	0.55
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.42	0.55
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.06	0.55
5:R:52:LYS:HD3	5:R:52:LYS:C	2.26	0.55
2:B:252:LEU:CD1	9:I:49:LEU:HB2	2.36	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.42	0.55
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.07	0.55
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.72	0.54
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.72	0.54
5:E:195:VAL:HG12	5:E:196:GLY:N	2.22	0.54
2:O:47:ILE:HD12	2:O:47:ILE:N	2.22	0.54
2:O:70:ARG:HD3	2:O:100:SER:OG	2.06	0.54
3:P:5:ILE:O	3:P:5:ILE:HG22	2.06	0.54
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.42	0.54
3:C:111:LYS:HE2	3:C:307:PHE:CE1	2.42	0.54
1:N:130:GLU:O	1:N:134:ILE:HG13	2.08	0.54
5:R:47:THR:HG21	15:R:3005:PEE:H23	1.89	0.54
6:S:105:GLU:O	6:S:109:LYS:HG3	2.07	0.54
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.07	0.54
2:O:226:ILE:CG2	2:O:227:ARG:H	2.20	0.54
3:P:332:ASN:ND2	3:P:358:SER:OG	2.40	0.54
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.89	0.54
2:B:248:ASN:ND2	2:B:248:ASN:C	2.60	0.54
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.89	0.54
1:N:301:HIS:HB2	1:N:303:LEU:HG	1.90	0.54
3:C:207:ASN:HD22	3:C:208:ASN:H	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.88	0.54
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.43	0.54
1:N:223:TYR:HD2	1:N:223:TYR:H	1.56	0.54
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.38	0.54
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.89	0.54
7:T:67:GLU:O	7:T:70:LYS:HB2	2.08	0.54
9:V:32:UNK:C	9:V:73:PRO:HG2	2.38	0.54
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.43	0.54
3:P:17:ASN:HD21	7:T:1:GLY:CA	2.20	0.54
2:B:250:HIS:CE1	2:B:252:LEU:HB2	2.41	0.54
2:B:59:THR:HG22	2:B:60:THR:N	2.23	0.54
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.37	0.54
3:C:2:ALA:CB	3:C:8:SER:HB3	2.38	0.54
2:B:287:ARG:HB3	9:I:53:GLU:CG	2.38	0.54
2:O:47:ILE:O	2:O:108:CYS:HB2	2.07	0.54
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.41	0.54
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.23	0.54
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.38	0.54
2:B:58:GLU:OE1	2:B:64:GLY:N	2.37	0.54
3:C:271:PRO:HG2	3:C:279:TYR:CG	2.42	0.54
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.43	0.54
1:N:15:ASN:O	1:N:26:ALA:HA	2.07	0.54
2:O:162:ASN:O	2:O:244:ILE:HD12	2.08	0.54
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.41	0.54
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.37	0.54
4:D:94:PRO:HG2	4:D:95:TYR:CD1	2.43	0.53
1:N:10:ASN:HD21	2:O:18:CYS:HB3	1.73	0.53
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.89	0.53
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.77	0.53
5:R:69:LEU:HD12	5:R:71:LEU:HG	1.90	0.53
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.08	0.53
1:N:170:THR:HG22	1:N:171:THR:N	2.23	0.53
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.89	0.53
6:S:18:LYS:O	6:S:22:ASN:ND2	2.42	0.53
2:B:47:ILE:HG22	2:B:48:GLY:N	2.23	0.53
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.53
2:B:47:ILE:O	2:B:108:CYS:HB2	2.08	0.53
4:D:150:ASN:O	4:D:156:GLN:HA	2.08	0.53
6:F:46:ALA:CB	6:F:90:LEU:HD11	2.39	0.53
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.73	0.53
1:A:223:TYR:HD2	1:A:223:TYR:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:ILE:H	3:C:285:ILE:HD12	1.71	0.53
2:O:385:GLU:CD	2:O:392:HIS:HA	2.29	0.53
2:O:47:ILE:HG22	2:O:48:GLY:N	2.24	0.53
3:P:38:LEU:HB3	12:P:502:HEM:CMB	2.38	0.53
3:P:4:ASN:HD21	3:P:7:LYS:CE	2.21	0.53
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.90	0.53
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.91	0.53
4:D:86:LYS:NZ	5:E:71:LEU:HD13	2.24	0.53
1:N:260:PRO:HG2	1:N:261:GLY:H	1.73	0.53
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.91	0.53
1:A:364:ALA:O	1:A:368:GLN:HG2	2.09	0.53
2:B:102:ARG:NH1	2:B:164:HIS:CD2	2.76	0.53
2:B:280:GLY:HA3	2:B:293:SER:OG	2.08	0.53
2:B:167:ALA:HB1	2:B:321:LEU:HD21	1.91	0.53
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.44	0.53
5:E:100:HIS:HB2	5:E:132:TRP:CZ3	2.43	0.53
2:O:279:LEU:HD13	2:O:344:LEU:HD11	1.90	0.53
5:R:135:LEU:CD2	5:R:169:GLY:HA3	2.39	0.53
7:T:60:SER:HB3	7:T:64:GLN:NE2	2.24	0.53
3:C:90:PHE:CZ	3:C:240:PHE:HA	2.44	0.53
5:E:78:LEU:HD22	5:E:132:TRP:CD2	2.44	0.53
2:O:318:ASP:O	2:O:319:SER:HB2	2.08	0.53
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.90	0.53
3:C:345:GLU:O	3:C:348:PHE:HB2	2.09	0.53
1:N:219:VAL:HG12	1:N:220:SER:N	2.24	0.53
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.73	0.53
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.24	0.53
1:N:80:GLU:OE2	2:O:291:VAL:HG23	2.09	0.53
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.25	0.53
2:B:67:HIS:O	2:B:70:ARG:HB3	2.09	0.53
5:E:150:SER:OG	5:E:157:TYR:HB3	2.08	0.53
2:O:222:GLN:HG2	2:O:222:GLN:O	2.08	0.53
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.90	0.53
3:P:30:ALA:HB1	18:S:3003:CDL:H111	1.92	0.52
5:R:195:VAL:HG12	5:R:196:GLY:N	2.24	0.52
1:A:289:HIS:O	2:B:87:ARG:NE	2.35	0.52
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.08	0.52
3:C:263:LEU:HD11	5:R:90:LYS:HD3	1.91	0.52
3:C:4:ASN:HD21	3:C:7:LYS:CE	2.22	0.52
2:O:227:ARG:NH1	2:O:228:SER:N	2.57	0.52
3:P:271:PRO:HG2	3:P:279:TYR:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:47:ARG:HG2	8:U:47:ARG:HH11	1.74	0.52
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.40	0.52
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.39	0.52
3:P:31:TRP:O	3:P:101:ARG:HG3	2.09	0.52
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.43	0.52
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.40	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.75	0.52
1:A:431:LEU:HG	1:A:432:LEU:N	2.23	0.52
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.89	0.52
1:N:181:ASP:N	1:N:181:ASP:OD1	2.43	0.52
1:N:49:ASN:ND2	1:N:51:LYS:N	2.57	0.52
2:O:217:LYS:HE2	2:O:221:GLU:OE1	2.10	0.52
2:O:168:TYR:CD2	2:O:237:ALA:HB1	2.44	0.52
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.25	0.52
3:P:101:ARG:O	3:P:101:ARG:HD2	2.08	0.52
9:V:77:ARG:HD2	9:V:77:ARG:N	2.24	0.52
2:B:385:GLU:CD	2:B:392:HIS:HA	2.29	0.52
10:J:38:GLY:O	10:J:42:ILE:HG13	2.09	0.52
2:O:56:ARG:HA	2:O:171:ALA:O	2.10	0.52
3:P:9:HIS:CE1	3:P:11:LEU:HB2	2.43	0.52
18:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.09	0.52
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.91	0.52
2:O:29:LEU:CD1	2:O:33:LEU:HD23	2.39	0.52
5:R:100:HIS:HB2	5:R:132:TRP:CZ3	2.44	0.52
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.45	0.52
1:A:301:HIS:HB2	1:A:303:LEU:HG	1.91	0.52
1:A:49:ASN:ND2	1:A:52:ASN:OD1	2.42	0.52
3:P:15:ILE:N	3:P:15:ILE:HD12	2.25	0.52
3:P:42:LEU:HD22	3:P:190:ILE:HG22	1.91	0.52
7:T:41:PHE:HD2	7:T:41:PHE:C	2.13	0.52
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.21	0.52
2:B:389:SER:O	2:B:391:THR:N	2.43	0.52
7:G:67:GLU:O	7:G:70:LYS:HB2	2.10	0.52
1:N:161:THR:HG21	1:N:235:ARG:H	1.74	0.52
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.74	0.52
1:A:394:GLU:O	1:A:397:SER:HB3	2.10	0.52
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.91	0.52
1:N:106:MET:HE2	1:N:107:PRO:HA	1.92	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.52
10:W:33:ARG:O	10:W:37:GLN:HG3	2.08	0.52
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LYS:HE2	2:B:221:GLU:OE1	2.10	0.52
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.92	0.52
4:D:178:THR:HG23	8:H:13:LEU:HD11	1.92	0.52
1:N:380:GLY:O	1:N:384:LEU:HB2	2.09	0.52
3:P:187:PRO:HG2	12:P:501:HEM:CMC	2.39	0.52
5:R:114:VAL:HG12	5:R:114:VAL:O	2.10	0.52
6:S:53:ASP:OD1	6:S:54:LEU:N	2.39	0.52
2:B:162:ASN:O	2:B:244:ILE:HD12	2.10	0.51
2:B:318:ASP:O	2:B:319:SER:HB2	2.10	0.51
6:F:46:ALA:HB1	6:F:90:LEU:HD11	1.91	0.51
1:N:136:GLN:HE22	9:V:50:LEU:CD1	2.19	0.51
8:U:20:ILE:HD11	8:U:76:LYS:CD	2.38	0.51
2:B:26:ILE:HA	2:B:35:ILE:O	2.11	0.51
3:C:271:PRO:HA	13:C:2001:SMA:H10	1.93	0.51
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.92	0.51
4:D:158:ILE:HG12	4:D:160:MET:H	1.74	0.51
6:F:13:MET:HA	6:F:13:MET:CE	2.40	0.51
2:O:219:VAL:HG13	2:O:223:PHE:CD1	2.45	0.51
2:O:203:ARG:HD2	2:O:230:ALA:HA	1.92	0.51
2:O:248:ASN:C	2:O:248:ASN:ND2	2.62	0.51
5:R:45:VAL:HG13	10:W:28:ALA:N	2.24	0.51
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.92	0.51
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.46	0.51
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.92	0.51
1:N:305:HIS:O	1:N:306:SER:HB3	2.10	0.51
2:O:59:THR:HG22	2:O:60:THR:N	2.25	0.51
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.09	0.51
14:P:3002:UQ:C8	14:P:3002:UQ:HM51	2.40	0.51
2:O:306:PRO:HG2	9:V:51:CYS:HA	1.92	0.51
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.41	0.51
10:J:4:ALA:O	10:J:8:GLN:HG3	2.11	0.51
2:O:102:ARG:CG	2:O:102:ARG:HH11	2.15	0.51
2:O:297:GLN:O	2:O:301:LYS:HG3	2.09	0.51
2:O:226:ILE:HG22	2:O:227:ARG:H	1.74	0.51
3:P:131:GLY:HA3	3:P:183:HIS:CE1	2.45	0.51
3:P:154:ILE:HG21	3:P:157:ILE:HD11	1.93	0.51
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.11	0.51
2:O:306:PRO:HB3	9:V:52:ARG:N	2.25	0.51
10:W:42:ILE:O	10:W:46:LEU:HG	2.10	0.51
1:A:191:LYS:C	1:A:195:MET:HE2	2.31	0.51
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:262:TRP:O	1:N:386:TYR:HE1	1.93	0.51
3:P:285:ILE:N	3:P:285:ILE:CD1	2.74	0.51
1:A:181:ASP:N	1:A:181:ASP:OD1	2.44	0.51
1:A:260:PRO:HG2	1:A:261:GLY:H	1.75	0.51
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.40	0.51
8:H:65:ARG:O	8:H:68:CYS:HB3	2.11	0.51
7:T:56:TYR:O	7:T:59:TYR:HB3	2.10	0.51
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.40	0.51
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.92	0.51
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.46	0.51
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.11	0.51
4:D:43:MET:HE3	4:D:189:PHE:CE2	2.46	0.51
5:E:51:ALA:HA	15:E:2005:PEE:H42	1.93	0.51
3:P:173:ASN:N	3:P:174:PRO:HD2	2.25	0.51
7:T:74:PRO:O	7:T:78:GLU:HG3	2.11	0.51
1:A:10:ASN:ND2	2:B:19:PRO:HD3	2.23	0.51
1:A:178:THR:HG22	1:A:180:ALA:N	2.19	0.51
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.75	0.51
1:A:86:PHE:HD1	1:A:87:ASN:H	1.58	0.51
2:B:109:VAL:HG21	2:B:119:VAL:HG23	1.93	0.51
2:B:192:HIS:O	2:B:196:GLN:HG3	2.10	0.51
9:I:49:LEU:HB3	9:I:55:MET:HG2	1.93	0.51
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.92	0.51
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	1.91	0.51
7:G:41:PHE:CD2	7:G:41:PHE:C	2.83	0.51
1:N:159:GLN:HE22	7:T:18:LEU:HD21	1.76	0.51
3:P:223:PRO:O	3:P:227:PHE:HB2	2.10	0.51
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.93	0.51
1:A:410:VAL:O	1:A:413:LYS:HB3	2.11	0.50
2:B:308:ASP:OD1	9:I:56:SER:HA	2.11	0.50
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.93	0.50
2:B:306:PRO:HB3	9:I:52:ARG:N	2.26	0.50
5:R:103:GLN:HA	5:R:106:ILE:HB	1.92	0.50
5:R:41:ALA:O	5:R:45:VAL:HG23	2.10	0.50
1:A:432:LEU:HD23	1:A:433:ASP:H	1.76	0.50
1:N:63:ALA:HB1	1:N:116:VAL:CG1	2.41	0.50
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.46	0.50
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.90	0.50
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.94	0.50
5:R:90:LYS:O	5:R:91:TRP:HB2	2.11	0.50
1:A:8:LEU:HD22	1:A:392:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:CYS:O	8:H:27:THR:HB	2.11	0.50
2:B:325:TYR:HD1	9:I:60:ALA:CB	2.22	0.50
2:O:67:HIS:O	2:O:70:ARG:HB3	2.12	0.50
3:P:145:THR:O	3:P:149:ASN:HB2	2.12	0.50
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.11	0.50
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.40	0.50
1:N:179:ARG:HG2	1:N:179:ARG:HH11	1.75	0.50
1:A:386:TYR:CD2	1:A:390:ILE:HD12	2.46	0.50
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.47	0.50
1:A:45:SER:HA	1:A:48:GLU:CG	2.40	0.50
1:A:49:ASN:ND2	1:A:51:LYS:H	2.09	0.50
2:B:116:VAL:O	2:B:120:MET:HB2	2.11	0.50
2:B:414:ALA:O	2:B:418:VAL:HG23	2.11	0.50
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.46	0.50
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.93	0.50
2:O:26:ILE:HA	2:O:35:ILE:O	2.10	0.50
1:A:308:GLN:HG3	1:A:308:GLN:O	2.11	0.50
3:C:38:LEU:HB3	12:C:502:HEM:HMB1	1.94	0.50
6:F:71:LYS:O	6:F:72:HIS:HB2	2.10	0.50
9:I:38:UNK:C	9:I:40:UNK:N	2.72	0.50
1:N:388:ARG:NH2	1:N:388:ARG:HG3	2.26	0.50
2:B:212:LYS:CD	2:B:214:SER:H	2.24	0.50
4:D:224:ARG:HH21	7:G:26:ILE:HG23	1.77	0.50
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.12	0.50
3:P:285:ILE:H	3:P:285:ILE:CD1	2.25	0.50
6:S:71:LYS:O	6:S:72:HIS:HB2	2.12	0.50
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.92	0.50
5:E:103:GLN:HA	5:E:106:ILE:HB	1.94	0.50
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.45	0.50
7:G:73:ASN:HB3	7:G:76:ASP:OD2	2.11	0.50
1:N:156:THR:O	1:N:159:GLN:HG2	2.12	0.50
2:O:227:ARG:HG3	2:O:228:SER:H	1.76	0.50
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.93	0.50
3:P:135:PRO:HG3	12:P:501:HEM:O1D	2.12	0.50
6:S:46:ALA:CB	6:S:90:LEU:HD11	2.41	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.50
8:U:24:CYS:O	8:U:27:THR:HB	2.12	0.50
2:B:297:GLN:O	2:B:301:LYS:HG3	2.12	0.50
2:B:153:GLN:HE22	9:I:34:UNK:CB	2.24	0.50
2:O:402:ILE:O	2:O:405:VAL:HG23	2.10	0.50
3:P:101:ARG:NH2	12:P:502:HEM:HBD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:38:LEU:HB3	12:P:502:HEM:HMB1	1.94	0.50
8:U:12:GLU:N	21:U:1233:HOH:O	2.45	0.50
8:U:52:GLU:CG	8:U:53:GLN:N	2.75	0.50
2:B:257:VAL:O	2:B:323:GLY:HA3	2.12	0.49
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.11	0.49
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.20	0.49
10:J:42:ILE:O	10:J:46:LEU:HG	2.12	0.49
2:O:144:LEU:HB3	2:O:183:ILE:HD12	1.93	0.49
3:P:70:THR:HA	3:P:74:VAL:HG23	1.93	0.49
10:W:40:ASP:O	10:W:44:GLU:HG3	2.12	0.49
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.47	0.49
3:C:42:LEU:HD22	3:C:190:ILE:HG22	1.93	0.49
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.47	0.49
5:E:171:ILE:HG23	5:E:171:ILE:O	2.13	0.49
1:N:112:LEU:O	1:N:116:VAL:HG23	2.12	0.49
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.39	0.49
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.94	0.49
9:I:55:MET:O	9:I:56:SER:C	2.50	0.49
1:N:152:TYR:HA	1:N:155:ALA:HB3	1.94	0.49
2:O:227:ARG:HG3	2:O:228:SER:N	2.27	0.49
2:O:341:MET:HG3	2:O:439:LEU:HB3	1.94	0.49
2:O:381:GLU:OE1	2:O:381:GLU:HA	2.11	0.49
3:P:158:GLY:O	3:P:161:LEU:N	2.41	0.49
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.26	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.52	0.49
2:B:300:ALA:C	2:B:302:ALA:H	2.14	0.49
3:C:9:HIS:CE1	3:C:11:LEU:HB2	2.47	0.49
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.47	0.49
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.94	0.49
1:A:233:ARG:NH1	1:A:233:ARG:CG	2.74	0.49
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.93	0.49
1:N:178:THR:HG22	1:N:180:ALA:N	2.19	0.49
1:N:329:LEU:HA	1:N:430:GLN:NE2	2.27	0.49
2:O:159:VAL:HG23	2:O:160:LEU:N	2.27	0.49
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.77	0.49
6:S:12:LEU:O	6:S:15:ARG:HG2	2.13	0.49
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.42	0.49
2:B:95:SER:HA	9:I:71:ASN:OD1	2.11	0.49
2:O:124:LEU:HD22	2:O:223:PHE:HB3	1.95	0.49
2:O:283:PRO:CG	9:V:56:SER:HB2	2.43	0.49
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:ASN:HD21	3:C:359:TYR:N	2.10	0.49
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.43	0.49
5:E:155:GLY:HA3	5:E:166:ASP:C	2.33	0.49
7:G:56:TYR:O	7:G:59:TYR:HB3	2.13	0.49
1:N:49:ASN:ND2	1:N:52:ASN:OD1	2.46	0.49
10:W:49:GLY:N	10:W:54:HIS:ND1	2.60	0.49
2:B:212:LYS:HD3	2:B:213:HIS:H	1.77	0.49
3:C:243:LEU:HD21	3:C:251:LEU:CD1	2.42	0.49
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.47	0.49
8:U:40:CYS:O	8:U:44:VAL:HG23	2.12	0.49
8:U:25:GLU:HG2	8:U:61:PHE:HZ	1.78	0.49
4:D:14:HIS:O	4:D:202:LYS:NZ	2.46	0.49
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.48	0.49
7:T:77:TYR:C	7:T:79:ASN:H	2.16	0.49
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.94	0.48
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.27	0.48
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.48
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.94	0.48
2:O:389:SER:O	2:O:391:THR:N	2.46	0.48
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.48	0.48
4:Q:43:MET:HE3	4:Q:189:PHE:CZ	2.48	0.48
5:R:77:LYS:HB3	5:R:80:ASP:OD2	2.13	0.48
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.27	0.48
2:B:168:TYR:CD2	2:B:237:ALA:HB1	2.48	0.48
2:B:248:ASN:HD22	2:B:249:GLY:N	2.11	0.48
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.12	0.48
1:N:394:GLU:O	1:N:397:SER:HB3	2.13	0.48
1:N:86:PHE:HD1	1:N:87:ASN:H	1.62	0.48
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.94	0.48
13:C:2001:SMA:H4	5:R:160:CYS:HB3	1.94	0.48
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.26	0.48
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.95	0.48
8:H:43:ARG:HD2	8:H:47:ARG:HH12	1.78	0.48
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.95	0.48
1:N:5:ALA:O	1:N:8:LEU:HB2	2.13	0.48
2:O:170:THR:O	2:O:172:LEU:N	2.46	0.48
3:P:81:ARG:HH22	16:P:3011:GOL:H2	1.76	0.48
2:B:167:ALA:HA	2:B:423:SER:OG	2.13	0.48
2:B:285:ILE:O	2:B:288:GLY:N	2.46	0.48
2:B:70:ARG:HD3	2:B:100:SER:OG	2.14	0.48
2:B:76:THR:HG22	2:B:81:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:LYS:C	1:N:195:MET:HE2	2.33	0.48
2:O:50:PHE:CE1	2:O:207:VAL:HB	2.48	0.48
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.48	0.48
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.13	0.48
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.48	0.48
4:D:28:ARG:HG2	4:D:171:TYR:CD2	2.48	0.48
7:G:41:PHE:HD2	7:G:41:PHE:C	2.16	0.48
1:A:305:HIS:HB3	9:I:35:UNK:CB	2.42	0.48
1:N:19:LEU:HD12	1:N:23:LEU:HD23	1.94	0.48
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.78	0.48
2:O:353:THR:HG22	2:O:355:GLU:N	2.04	0.48
3:P:111:LYS:HE2	3:P:307:PHE:CE1	2.49	0.48
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.96	0.48
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.48	0.48
1:A:133:VAL:O	1:A:137:GLU:HG3	2.14	0.48
2:B:170:THR:O	2:B:172:LEU:N	2.47	0.48
1:A:80:GLU:OE2	2:B:291:VAL:HG23	2.14	0.48
2:B:47:ILE:CG2	2:B:48:GLY:N	2.77	0.48
1:N:191:LYS:CA	1:N:195:MET:HE2	2.44	0.48
1:N:206:LYS:O	1:N:209:VAL:HG12	2.13	0.48
2:O:370:MET:O	2:O:372:VAL:N	2.47	0.48
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.48	0.48
3:P:95:ILE:O	3:P:99:ILE:HG13	2.13	0.48
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.14	0.48
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.48
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.14	0.48
2:B:156:GLN:NE2	9:I:77:ARG:C	2.67	0.48
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.49	0.48
5:R:122:HIS:CE1	5:R:124:LEU:HG	2.48	0.48
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.96	0.48
1:A:233:ARG:NH2	1:A:316:ASP:O	2.43	0.48
5:E:127:VAL:HG11	5:E:133:VAL:HA	1.94	0.48
1:N:19:LEU:O	1:N:21:ASN:N	2.47	0.48
1:N:205:HIS:O	1:N:208:LEU:HB3	2.14	0.48
2:O:212:LYS:HB2	2:O:215:ASP:OD2	2.14	0.48
3:P:132:TYR:HA	12:P:501:HEM:HAA2	1.96	0.48
3:P:141:PHE:HB2	3:P:260:ALA:CB	2.43	0.48
3:P:282:LEU:HD23	3:P:282:LEU:C	2.33	0.48
3:C:236:MET:HA	18:D:2003:CDL:H162	1.94	0.48
4:D:235:MET:HB3	7:G:15:THR:HG22	1.96	0.48
5:E:114:VAL:O	5:E:114:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.49	0.48
2:O:113:ARG:O	2:O:115:HIS:N	2.47	0.48
8:U:47:ARG:NH1	8:U:47:ARG:HG2	2.28	0.48
1:A:35:CYS:HA	1:A:372:THR:HG21	1.95	0.48
2:B:220:ALA:O	2:B:224:LEU:HB2	2.14	0.48
2:B:59:THR:HG22	2:B:60:THR:H	1.78	0.48
3:C:135:PRO:HG3	12:C:501:HEM:O1D	2.14	0.48
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.95	0.48
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.49	0.48
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.29	0.48
3:P:142:TRP:O	3:P:146:VAL:HG23	2.13	0.48
2:B:28:LYS:HG2	2:B:28:LYS:O	2.14	0.47
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.28	0.47
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.70	0.47
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.96	0.47
1:A:15:ASN:O	1:A:26:ALA:HA	2.13	0.47
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.49	0.47
2:B:398:VAL:O	2:B:402:ILE:HG13	2.14	0.47
3:C:285:ILE:H	3:C:285:ILE:CD1	2.27	0.47
3:P:245:LEU:O	4:Q:201:ARG:HG2	2.14	0.47
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.47
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.95	0.47
1:N:280:TYR:CG	1:N:281:ASP:N	2.82	0.47
1:N:35:CYS:HB2	1:N:200:ALA:O	2.14	0.47
3:P:112:GLU:O	3:P:116:THR:HG23	2.14	0.47
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.49	0.47
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.49	0.47
2:B:35:ILE:O	2:B:213:HIS:HE1	1.98	0.47
3:C:63:ALA:O	3:C:67:VAL:HG23	2.15	0.47
6:F:77:LYS:HE3	6:F:78:GLU:HG3	1.95	0.47
1:N:223:TYR:CD2	1:N:223:TYR:N	2.82	0.47
3:P:189:ALA:O	3:P:193:ILE:HG13	2.15	0.47
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.96	0.47
2:B:147:ASP:O	2:B:150:VAL:HG22	2.15	0.47
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.28	0.47
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.49	0.47
5:E:90:LYS:O	5:E:91:TRP:HB2	2.15	0.47
1:N:179:ARG:HG2	1:N:179:ARG:NH1	2.29	0.47
1:N:26:ALA:O	1:N:198:ALA:HA	2.14	0.47
3:P:271:PRO:HA	13:P:3001:SMA:C7M	2.41	0.47
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:GLU:HG2	8:H:61:PHE:HZ	1.78	0.47
2:O:29:LEU:HB2	2:O:31:ASN:HD21	1.80	0.47
2:O:300:ALA:C	2:O:302:ALA:H	2.18	0.47
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.44	0.47
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.14	0.47
1:A:329:LEU:HA	1:A:430:GLN:NE2	2.29	0.47
3:C:347:PRO:O	3:C:350:ILE:HG22	2.15	0.47
4:D:135:CYS:O	4:D:149:TYR:HB3	2.15	0.47
10:J:57:HIS:O	10:J:62:SER:HB2	2.14	0.47
1:N:410:VAL:O	1:N:413:LYS:HB3	2.14	0.47
2:O:27:THR:CG2	2:O:28:LYS:N	2.77	0.47
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.76	0.47
3:P:158:GLY:O	3:P:161:LEU:HB2	2.14	0.47
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.97	0.47
4:D:171:TYR:OH	4:D:182:ILE:HA	2.14	0.47
5:E:57:GLN:OE1	20:E:2009:PLC:H12	2.14	0.47
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.96	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.95	0.47
5:R:171:ILE:HG23	5:R:171:ILE:O	2.15	0.47
6:S:73:ARG:HA	6:S:73:ARG:HD3	1.74	0.47
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.15	0.47
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.15	0.47
3:C:101:ARG:HD2	3:C:102:GLY:N	2.30	0.47
3:C:157:ILE:O	3:C:161:LEU:HD12	2.14	0.47
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.96	0.47
5:R:164:HIS:HB2	5:R:173:LYS:HB3	1.96	0.47
15:R:3005:PEE:H54	10:W:21:ALA:HA	1.97	0.47
2:B:150:VAL:CG2	2:B:151:ALA:N	2.77	0.47
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.45	0.47
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.50	0.47
2:B:50:PHE:CE1	2:B:207:VAL:HB	2.50	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.49	0.47
5:E:69:LEU:HB2	5:E:70:ALA:H	1.34	0.47
8:H:43:ARG:HD2	8:H:47:ARG:CZ	2.44	0.47
1:N:382:HIS:O	1:N:386:TYR:N	2.48	0.47
2:O:306:PRO:CG	9:V:51:CYS:HA	2.45	0.47
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.62	0.47
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.44	0.47
2:B:341:MET:HG3	2:B:439:LEU:HB3	1.96	0.46
4:D:214:LEU:HD11	4:D:218:LEU:HD11	1.97	0.46
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:101:ARG:N	5:R:131:GLU:O	2.45	0.46
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.97	0.46
1:A:18:THR:HG23	1:A:24:ARG:HG2	1.97	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.15	0.46
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.15	0.46
2:O:47:ILE:CG2	2:O:48:GLY:N	2.78	0.46
3:P:332:ASN:HD21	3:P:359:TYR:N	2.13	0.46
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.97	0.46
8:U:50:THR:OG1	8:U:51:GLU:N	2.48	0.46
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.31	0.46
1:A:191:LYS:CA	1:A:195:MET:HE2	2.45	0.46
2:B:209:ILE:HD12	2:B:379:LEU:HB2	1.97	0.46
3:C:243:LEU:CD2	3:C:251:LEU:HD11	2.45	0.46
4:D:21:LEU:HD13	4:D:192:TRP:HB2	1.97	0.46
10:J:40:ASP:O	10:J:44:GLU:HG3	2.15	0.46
4:Q:62:LYS:O	4:Q:65:ALA:HB3	2.15	0.46
1:A:285:GLY:O	1:A:286:GLY:C	2.54	0.46
2:B:113:ARG:O	2:B:115:HIS:N	2.47	0.46
5:E:148:ALA:HA	5:E:156:TYR:CD2	2.50	0.46
2:B:86:THR:OG1	9:I:70:LEU:HD11	2.16	0.46
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.50	0.46
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.96	0.46
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.50	0.46
1:A:416:TYR:HE1	1:A:443:TRP:H	1.64	0.46
3:C:285:ILE:N	3:C:285:ILE:CD1	2.77	0.46
5:E:101:ARG:N	5:E:131:GLU:O	2.45	0.46
7:G:29:ILE:O	7:G:33:ALA:HB3	2.15	0.46
1:N:364:ALA:O	1:N:368:GLN:HG2	2.16	0.46
1:N:365:MET:HG2	1:N:392:LEU:HD22	1.98	0.46
5:R:155:GLY:HA3	5:R:166:ASP:C	2.36	0.46
8:U:18:THR:O	8:U:22:GLU:HG3	2.16	0.46
1:A:63:ALA:HB1	1:A:116:VAL:CG1	2.45	0.46
1:A:124:GLU:O	1:A:124:GLU:HG2	2.16	0.46
2:B:102:ARG:CG	2:B:102:ARG:NH1	2.78	0.46
3:C:325:LEU:HD11	3:C:366:LEU:HD12	1.98	0.46
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.51	0.46
3:P:101:ARG:CD	3:P:101:ARG:C	2.74	0.46
2:B:109:VAL:CG1	2:B:123:LEU:HB2	2.46	0.46
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.96	0.46
2:B:394:ALA:O	2:B:396:SER:N	2.48	0.46
2:B:99:TYR:HA	9:I:67:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:355:ALA:O	3:C:358:SER:HB3	2.16	0.46
3:C:374:GLU:HG2	6:F:20:TYR:CZ	2.51	0.46
4:D:27:ARG:NH1	4:D:55:THR:O	2.48	0.46
2:O:167:ALA:HB1	2:O:321:LEU:HD21	1.98	0.46
3:P:70:THR:HA	3:P:74:VAL:CG2	2.46	0.46
5:R:150:SER:OG	5:R:157:TYR:HB3	2.15	0.46
2:B:159:VAL:HG23	2:B:160:LEU:N	2.30	0.46
3:C:133:VAL:O	3:C:133:VAL:HG12	2.15	0.46
3:C:141:PHE:HB2	3:C:260:ALA:CB	2.46	0.46
1:A:223:TYR:CD2	1:A:223:TYR:N	2.84	0.46
1:A:389:ARG:HD2	1:A:390:ILE:H	1.81	0.46
1:A:5:ALA:O	1:A:8:LEU:HB2	2.16	0.46
3:C:246:PHE:C	3:C:248:PRO:HD3	2.36	0.46
3:C:350:ILE:HG23	3:C:351:ILE:N	2.31	0.46
2:O:102:ARG:CG	2:O:102:ARG:NH1	2.75	0.46
2:O:235:ALA:O	2:O:236:LYS:O	2.34	0.46
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.97	0.46
3:P:346:HIS:CG	3:P:347:PRO:HA	2.50	0.46
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.15	0.46
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.51	0.46
2:B:203:ARG:HD2	2:B:230:ALA:CA	2.26	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.51	0.46
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.81	0.46
2:O:116:VAL:O	2:O:120:MET:HB2	2.16	0.46
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.50	0.46
5:R:67:ASP:O	5:R:69:LEU:HD23	2.15	0.46
6:S:77:LYS:CE	6:S:78:GLU:HG3	2.46	0.46
7:T:34:LEU:HA	7:T:37:VAL:HG23	1.97	0.46
1:A:255:LEU:HD11	1:A:420:PRO:HB2	1.97	0.45
1:A:7:THR:HB	2:B:41:PHE:O	2.16	0.45
3:C:31:TRP:O	3:C:101:ARG:HG3	2.15	0.45
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.47	0.45
1:N:373:THR:HB	1:N:374:PRO:CD	2.43	0.45
2:O:394:ALA:O	2:O:396:SER:N	2.49	0.45
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.16	0.45
3:C:142:TRP:CH2	5:R:145:VAL:HG23	2.51	0.45
5:R:148:ALA:O	5:R:149:ASN:HB2	2.16	0.45
2:B:394:ALA:C	2:B:396:SER:H	2.20	0.45
3:C:223:PRO:O	3:C:227:PHE:HB2	2.16	0.45
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.46	0.45
9:I:38:UNK:O	9:I:39:UNK:C	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:LEU:HB3	9:I:55:MET:CG	2.46	0.45
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.31	0.45
2:O:73:SER:OG	2:O:74:PRO:HD3	2.16	0.45
4:Q:2:GLU:HG2	4:Q:2:GLU:O	2.16	0.45
5:E:136:VAL:HG12	5:E:138:VAL:HG23	1.98	0.45
1:N:145:MET:CB	1:N:252:HIS:CD2	2.99	0.45
2:O:109:VAL:CG1	2:O:123:LEU:HB2	2.45	0.45
2:O:209:ILE:HD12	2:O:379:LEU:HB2	1.97	0.45
5:R:91:TRP:O	5:R:93:GLY:N	2.50	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.15	0.45
2:B:101:THR:HG22	9:I:65:VAL:HG22	1.99	0.45
2:B:102:ARG:HH11	2:B:102:ARG:CG	2.21	0.45
2:B:60:THR:CG2	2:B:61:ALA:N	2.80	0.45
3:C:237:LEU:HD12	3:C:237:LEU:HA	1.68	0.45
5:E:122:HIS:CE1	5:E:124:LEU:HG	2.51	0.45
6:F:28:LYS:HB3	6:F:74:ILE:HD12	1.97	0.45
7:G:29:ILE:O	7:G:34:LEU:HG	2.17	0.45
1:N:121:ALA:O	1:N:122:LEU:HB2	2.15	0.45
1:N:126:GLN:HE22	1:N:129:LYS:HD3	1.79	0.45
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.45	0.45
2:O:150:VAL:CG2	2:O:151:ALA:N	2.80	0.45
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.68	0.45
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.99	0.45
3:C:70:THR:HA	3:C:74:VAL:HG23	1.99	0.45
4:D:102:ARG:NH1	4:D:107:GLY:O	2.47	0.45
5:E:59:ILE:HG22	5:E:60:SER:N	2.31	0.45
1:N:416:TYR:HE1	1:N:443:TRP:H	1.64	0.45
3:P:157:ILE:CG1	3:P:158:GLY:H	2.07	0.45
3:P:269:ILE:HG23	3:P:269:ILE:O	2.16	0.45
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	1.99	0.45
8:U:52:GLU:CG	8:U:53:GLN:H	2.30	0.45
1:A:212:ALA:O	1:A:216:PHE:HB2	2.16	0.45
2:B:198:ASN:HB3	2:B:203:ARG:HH21	1.81	0.45
3:C:132:TYR:HA	12:C:501:HEM:HAA2	1.98	0.45
5:E:145:VAL:HG23	3:P:142:TRP:CH2	2.52	0.45
7:G:9:ARG:HH11	7:G:9:ARG:HG3	1.82	0.45
1:N:145:MET:CB	1:N:252:HIS:NE2	2.80	0.45
1:N:36:THR:HG21	1:N:373:THR:HA	1.99	0.45
2:O:269:ALA:O	2:O:272:PHE:N	2.49	0.45
3:P:342:GLN:HE21	3:P:342:GLN:CA	2.25	0.45
6:S:13:MET:HA	6:S:16:ILE:CB	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.99	0.45
2:B:212:LYS:C	2:B:212:LYS:HD3	2.37	0.45
2:B:27:THR:H	2:B:213:HIS:CE1	2.34	0.45
2:B:279:LEU:HA	2:B:294:LYS:HB2	1.99	0.45
3:C:23:PRO:HG2	7:G:3:HIS:CB	2.47	0.45
5:E:148:ALA:O	5:E:149:ASN:HB2	2.17	0.45
8:H:32:LYS:HD3	8:H:32:LYS:HA	1.82	0.45
10:W:59:TYR:CD1	10:W:59:TYR:N	2.84	0.45
1:A:161:THR:HG21	1:A:235:ARG:H	1.82	0.45
3:C:155:PRO:O	3:C:156:TYR:HB2	2.17	0.45
5:E:85:LYS:HG2	5:E:86:ASN:N	2.31	0.45
2:B:308:ASP:CG	9:I:56:SER:HA	2.37	0.45
9:I:69:SER:CB	9:I:72:ALA:HB3	2.46	0.45
1:N:364:ALA:HB2	9:V:29:UNK:CB	2.47	0.45
1:N:80:GLU:OE1	2:O:290:SER:HA	2.16	0.45
2:O:31:ASN:N	2:O:31:ASN:HD22	2.14	0.45
2:O:367:THR:HG22	2:O:368:TYR:N	2.30	0.45
2:O:414:ALA:O	2:O:418:VAL:HG23	2.16	0.45
3:P:325:LEU:HD11	3:P:366:LEU:HD12	1.99	0.45
3:P:76:TYR:HE2	4:Q:204:MET:CE	2.30	0.45
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.99	0.45
8:U:52:GLU:HG2	8:U:53:GLN:H	1.80	0.45
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.32	0.45
2:B:107:TYR:O	2:B:108:CYS:HB3	2.17	0.45
7:G:71:ARG:NH2	8:H:56:GLU:OE1	2.50	0.45
10:J:49:GLY:N	10:J:54:HIS:ND1	2.65	0.45
1:N:29:GLU:HG3	1:N:203:ILE:O	2.17	0.45
1:N:294:LEU:HD23	1:N:307:PHE:CE1	2.52	0.45
1:N:386:TYR:CD2	1:N:390:ILE:HD12	2.52	0.45
2:O:398:VAL:O	2:O:402:ILE:HG13	2.17	0.45
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.98	0.45
5:R:153:PHE:CE2	5:R:172:ARG:HB3	2.52	0.45
2:B:394:ALA:C	2:B:396:SER:N	2.70	0.45
3:C:12:LEU:C	3:C:14:MET:N	2.70	0.45
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.99	0.45
1:N:106:MET:HB3	1:N:107:PRO:CD	2.47	0.45
2:O:221:GLU:C	2:O:223:PHE:H	2.20	0.45
2:O:259:THR:CG2	2:O:260:GLU:N	2.80	0.45
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.52	0.45
5:R:122:HIS:ND1	5:R:124:LEU:HG	2.32	0.45
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:VAL:HG13	2:B:399:ALA:N	2.33	0.44
5:E:69:LEU:HD13	5:E:71:LEU:HD21	1.99	0.44
6:F:31:LEU:HD21	6:F:65:ALA:HB2	1.99	0.44
6:F:52:GLU:CG	6:F:56:ASN:HD21	2.21	0.44
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.00	0.44
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.52	0.44
4:Q:120:ARG:HH11	4:Q:120:ARG:HG2	1.81	0.44
5:R:135:LEU:HD22	5:R:169:GLY:HA3	1.99	0.44
1:A:228:VAL:O	1:A:228:VAL:HG13	2.18	0.44
2:B:51:ILE:HG22	2:B:52:LYS:N	2.33	0.44
9:I:32:UNK:N	9:I:73:PRO:CG	2.75	0.44
2:O:144:LEU:HB2	2:O:183:ILE:HG23	1.97	0.44
3:P:107:SER:HB3	12:P:502:HEM:HAD1	1.99	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
6:F:105:GLU:O	6:F:109:LYS:HG3	2.17	0.44
7:G:71:ARG:CZ	8:H:56:GLU:OE1	2.65	0.44
8:H:20:ILE:HD12	8:H:73:LEU:HA	1.99	0.44
2:O:230:ALA:O	2:O:231:GLY:C	2.55	0.44
2:O:344:LEU:HD23	2:O:417:PHE:CD2	2.53	0.44
3:P:47:LEU:O	3:P:47:LEU:HD12	2.17	0.44
2:B:202:ALA:HB3	2:B:229:GLY:H	1.83	0.44
2:B:47:ILE:CD1	2:B:47:ILE:N	2.80	0.44
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.51	0.44
5:E:185:TYR:HB3	5:E:195:VAL:HG13	2.00	0.44
1:N:189:HIS:O	1:N:191:LYS:N	2.49	0.44
1:N:342:TRP:O	1:N:345:LEU:HB2	2.18	0.44
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.98	0.44
4:Q:214:LEU:HD11	4:Q:218:LEU:HD11	1.98	0.44
5:R:128:LYS:O	5:R:130:PRO:HD3	2.17	0.44
2:B:129:ALA:N	2:B:130:PRO:CD	2.81	0.44
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.98	0.44
1:N:343:MET:O	1:N:347:THR:HG23	2.17	0.44
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.73	0.44
2:O:287:ARG:HD3	9:V:53:GLU:HG2	1.98	0.44
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.16	0.44
5:R:77:LYS:C	5:R:79:SER:H	2.21	0.44
1:A:86:PHE:HD1	1:A:87:ASN:N	2.15	0.44
1:A:91:SER:OG	1:A:92:ARG:N	2.49	0.44
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.52	0.44
3:C:51:LEU:HD23	3:C:51:LEU:HA	1.88	0.44
1:N:242:ARG:NH1	1:N:432:LEU:HA	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:166:ALA:HB1	2:O:242:GLY:C	2.38	0.44
3:P:141:PHE:HB2	3:P:260:ALA:HB1	1.98	0.44
6:S:77:LYS:HE3	6:S:78:GLU:HG3	2.00	0.44
8:U:72:LYS:HA	8:U:75:ASN:HD22	1.83	0.44
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.47	0.44
2:B:209:ILE:HG13	2:B:379:LEU:HD13	1.98	0.44
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.18	0.44
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.53	0.44
3:P:289:LEU:HG	3:P:293:LEU:HD11	2.00	0.44
3:P:198:LEU:HD21	12:P:502:HEM:CMA	2.47	0.44
4:Q:178:THR:HG21	8:U:15:ASP:HA	1.99	0.44
4:Q:55:THR:O	10:W:52:TRP:CZ3	2.71	0.44
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.99	0.44
2:B:291:VAL:C	2:B:293:SER:H	2.21	0.44
5:E:165:TYR:HA	5:E:170:ARG:O	2.16	0.44
2:O:291:VAL:C	2:O:293:SER:H	2.21	0.44
2:O:394:ALA:C	2:O:396:SER:N	2.72	0.44
3:P:166:TRP:HA	3:P:175:THR:HG23	1.99	0.44
3:P:235:LEU:O	3:P:239:PRO:HD2	2.18	0.44
3:P:300:LEU:HA	3:P:300:LEU:HD23	1.84	0.44
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.47	0.44
5:R:171:ILE:N	5:R:179:ASN:OD1	2.49	0.44
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.82	0.44
1:A:87:ASN:OD1	2:B:286:LYS:HD2	2.17	0.44
3:C:132:TYR:O	3:C:135:PRO:HD2	2.18	0.44
3:C:187:PRO:HG2	12:C:501:HEM:CMC	2.46	0.44
4:D:27:ARG:O	4:D:30:PHE:HB3	2.17	0.44
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.33	0.44
1:N:18:THR:HG23	1:N:24:ARG:CG	2.40	0.44
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.99	0.44
1:N:382:HIS:HB3	1:N:388:ARG:O	2.18	0.44
1:N:45:SER:HA	1:N:48:GLU:CG	2.46	0.44
2:O:248:ASN:HD22	2:O:249:GLY:N	2.15	0.44
3:P:132:TYR:O	3:P:135:PRO:HD2	2.18	0.44
4:Q:241:LYS:CA	4:Q:241:LYS:HE3	2.43	0.44
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	2.00	0.44
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.74	0.43
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.32	0.43
1:N:170:THR:HG22	1:N:172:GLU:H	1.82	0.43
3:P:138:GLN:N	3:P:258:THR:O	2.48	0.43
6:S:40:ASP:O	6:S:44:LYS:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:O	1:A:109:VAL:HG23	2.18	0.43
3:C:198:LEU:HD13	14:C:2002:UQ:HM53	2.00	0.43
4:D:3:LEU:HA	4:D:3:LEU:HD23	1.83	0.43
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.53	0.43
1:N:220:SER:HA	1:N:225:GLU:OE1	2.18	0.43
2:O:129:ALA:N	2:O:130:PRO:CD	2.82	0.43
3:P:30:ALA:C	3:P:32:TRP:H	2.21	0.43
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.39	0.43
5:R:99:ARG:HB3	5:R:133:VAL:HG12	1.99	0.43
8:U:73:LEU:HD12	8:U:73:LEU:O	2.18	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.39	0.43
2:O:235:ALA:O	2:O:236:LYS:C	2.55	0.43
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.48	0.43
3:P:159:HIS:O	3:P:162:VAL:N	2.52	0.43
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.43
7:T:56:TYR:HD2	7:T:57:LEU:HD23	1.82	0.43
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.48	0.43
2:B:229:GLY:C	2:B:231:GLY:N	2.71	0.43
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.52	0.43
2:B:393:THR:CG2	2:B:397:VAL:HB	2.39	0.43
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.86	0.43
5:R:148:ALA:HA	5:R:156:TYR:CD2	2.53	0.43
6:S:28:LYS:HB3	6:S:74:ILE:HD12	2.01	0.43
8:U:23:HIS:O	8:U:26:GLN:HB2	2.19	0.43
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.81	0.43
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.53	0.43
1:A:362:ARG:O	1:A:365:MET:HB3	2.18	0.43
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.48	0.43
2:B:344:LEU:HD23	2:B:417:PHE:CD2	2.53	0.43
3:C:52:LEU:HD21	3:C:80:ILE:HG22	2.01	0.43
5:E:109:GLU:O	5:E:123:ASP:HB2	2.18	0.43
1:N:133:VAL:O	1:N:137:GLU:HG3	2.18	0.43
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.53	0.43
1:N:62:LEU:C	1:N:64:PHE:H	2.22	0.43
2:O:22:GLU:HB3	2:O:23:ASP:H	1.61	0.43
3:P:105:TYR:O	3:P:315:THR:HG22	2.18	0.43
1:A:358:LYS:HE3	1:A:399:ILE:O	2.19	0.43
3:C:101:ARG:CZ	12:C:502:HEM:HBD2	2.48	0.43
3:C:282:LEU:HD23	3:C:282:LEU:O	2.18	0.43
5:E:163:SER:HA	5:E:174:GLY:HA3	2.00	0.43
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:TYR:HA	2:O:113:ARG:HD3	2.01	0.43
2:O:257:VAL:O	2:O:323:GLY:HA3	2.18	0.43
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.18	0.43
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.40	0.43
5:R:109:GLU:O	5:R:123:ASP:HB2	2.19	0.43
7:T:46:PHE:O	7:T:50:PRO:HG2	2.18	0.43
2:B:166:ALA:HB1	2:B:242:GLY:C	2.39	0.43
2:B:31:ASN:CB	2:B:227:ARG:HH22	2.29	0.43
3:C:112:GLU:O	3:C:116:THR:HG23	2.19	0.43
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.82	0.43
4:D:83:ARG:HB2	4:D:84:PRO:HD2	1.99	0.43
5:E:59:ILE:CG2	5:E:60:SER:N	2.81	0.43
5:E:69:LEU:O	5:E:70:ALA:HB2	2.19	0.43
2:O:147:ASP:O	2:O:150:VAL:HG22	2.18	0.43
3:P:243:LEU:HD21	3:P:251:LEU:CD1	2.49	0.43
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.18	0.43
8:U:25:GLU:HG2	8:U:61:PHE:CZ	2.54	0.43
2:B:385:GLU:O	2:B:387:LEU:N	2.52	0.43
3:C:52:LEU:CD2	3:C:80:ILE:HG22	2.48	0.43
5:E:135:LEU:HD22	5:E:169:GLY:HA3	2.00	0.43
5:E:85:LYS:HE2	5:E:87:VAL:CG2	2.45	0.43
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.00	0.43
3:P:246:PHE:C	3:P:248:PRO:HD3	2.39	0.43
3:P:34:PHE:HB2	21:P:381:HOH:O	2.19	0.43
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.83	0.43
4:Q:60:GLU:OE1	10:W:59:TYR:HB3	2.18	0.43
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.54	0.43
3:C:131:GLY:HA3	3:C:183:HIS:CE1	2.54	0.43
4:D:142:VAL:O	4:D:142:VAL:HG23	2.18	0.43
6:F:13:MET:CE	6:F:16:ILE:HD12	2.49	0.43
1:N:293:ARG:HH21	1:N:344:ARG:NE	2.17	0.43
1:N:433:ASP:OD2	1:N:435:ASN:N	2.52	0.43
5:R:165:TYR:HA	5:R:170:ARG:O	2.19	0.43
7:T:77:TYR:CD2	8:U:52:GLU:HB2	2.54	0.43
1:A:26:ALA:O	1:A:198:ALA:HA	2.19	0.43
1:A:7:THR:HG21	2:B:113:ARG:CD	2.49	0.43
2:B:235:ALA:O	2:B:236:LYS:C	2.57	0.43
3:C:107:SER:HB3	12:C:502:HEM:HAD1	2.01	0.43
4:D:62:LYS:HE2	4:D:66:GLU:OE2	2.19	0.43
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.84	0.43
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:THR:HG21	1:N:235:ARG:N	2.34	0.43
3:P:139:MET:HE3	3:P:270:LYS:H	1.84	0.43
3:P:275:PHE:CD2	13:P:3001:SMA:H11	2.54	0.43
3:P:2:ALA:HA	3:P:3:PRO:O	2.19	0.43
5:R:186:GLN:NE2	5:R:188:VAL:HG12	2.34	0.43
2:B:353:THR:HB	2:B:356:ASP:CG	2.39	0.42
5:E:72:SER:HB2	5:E:73:LYS:H	1.62	0.42
1:N:220:SER:HB2	1:N:226:ASP:OD1	2.19	0.42
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.78	0.42
1:N:86:PHE:HD1	1:N:87:ASN:N	2.17	0.42
1:A:159:GLN:HE22	7:G:18:LEU:CD2	2.30	0.42
2:B:146:VAL:HG12	2:B:147:ASP:N	2.34	0.42
3:C:101:ARG:O	3:C:101:ARG:HD2	2.18	0.42
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.18	0.42
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.54	0.42
3:P:101:ARG:HD2	3:P:102:GLY:N	2.31	0.42
3:P:139:MET:HE2	3:P:253:ASP:OD2	2.18	0.42
4:Q:14:HIS:O	4:Q:202:LYS:NZ	2.52	0.42
2:O:147:ASP:OD1	9:V:68:ILE:HD11	2.19	0.42
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.83	0.42
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.83	0.42
5:E:47:THR:HG21	15:E:2005:PEE:H23	2.01	0.42
1:N:86:PHE:O	2:O:285:ILE:HA	2.19	0.42
3:P:2:ALA:HA	3:P:3:PRO:C	2.37	0.42
6:S:16:ILE:O	6:S:19:TRP:HB3	2.19	0.42
2:B:385:GLU:C	2:B:387:LEU:N	2.73	0.42
3:C:95:ILE:CG2	3:C:96:PHE:N	2.82	0.42
5:E:122:HIS:ND1	5:E:124:LEU:HG	2.35	0.42
7:G:34:LEU:HA	7:G:37:VAL:HG23	2.01	0.42
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.87	0.42
7:T:73:ASN:HA	7:T:74:PRO:HD2	1.90	0.42
3:C:235:LEU:O	3:C:239:PRO:HD2	2.19	0.42
3:C:95:ILE:O	3:C:99:ILE:HG13	2.20	0.42
4:Q:210:LEU:HD23	4:Q:210:LEU:HA	1.82	0.42
4:Q:62:LYS:HE2	4:Q:66:GLU:OE2	2.19	0.42
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.99	0.42
9:V:64:LEU:HD12	9:V:77:ARG:C	2.39	0.42
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.55	0.42
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.88	0.42
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.55	0.42
3:C:101:ARG:CD	3:C:101:ARG:C	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.84	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.64	0.42
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.52	0.42
5:E:69:LEU:HD12	5:E:71:LEU:HG	2.01	0.42
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.59	0.42
8:H:73:LEU:O	8:H:73:LEU:HD12	2.20	0.42
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.54	0.42
1:N:433:ASP:C	1:N:433:ASP:OD2	2.58	0.42
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.02	0.42
3:P:158:GLY:O	3:P:159:HIS:C	2.58	0.42
1:A:76:GLU:O	1:A:80:GLU:HG3	2.19	0.42
2:B:116:VAL:HG12	2:B:120:MET:HE2	2.02	0.42
3:C:133:VAL:HA	3:C:140:SER:HB3	2.01	0.42
4:D:105:ASN:O	4:D:106:ASN:HB2	2.20	0.42
3:C:246:PHE:CZ	4:D:205:GLY:HA3	2.55	0.42
8:H:15:ASP:O	8:H:17:LEU:N	2.52	0.42
8:H:57:GLU:CD	8:H:57:GLU:H	2.23	0.42
9:I:52:ARG:O	9:I:56:SER:HB3	2.19	0.42
2:O:157:VAL:HG13	2:O:158:GLY:N	2.34	0.42
2:O:225:ASN:O	2:O:226:ILE:O	2.36	0.42
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.32	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.65	0.42
1:A:365:MET:HG2	1:A:392:LEU:HD22	2.02	0.42
3:C:141:PHE:HB2	3:C:260:ALA:HB1	2.02	0.42
3:C:50:LEU:O	3:C:54:MET:HG3	2.20	0.42
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.55	0.42
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.50	0.42
1:N:39:VAL:HG11	1:N:117:VAL:CG1	2.49	0.42
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.20	0.42
2:O:59:THR:HG22	2:O:60:THR:H	1.85	0.42
3:P:335:ILE:HD13	7:T:58:LEU:HD23	2.01	0.42
1:A:26:ALA:CB	1:A:383:LEU:HD11	2.49	0.42
1:A:388:ARG:NH2	1:A:388:ARG:CG	2.83	0.42
1:A:403:ASP:O	1:A:404:ALA:C	2.58	0.42
2:B:305:GLN:HB3	2:B:306:PRO:HD2	2.01	0.42
4:D:222:MET:HE1	5:E:40:THR:HG23	2.00	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.19	0.42
7:G:81:GLN:OXT	8:H:49:HIS:N	2.53	0.42
1:N:178:THR:CG2	1:N:179:ARG:N	2.82	0.42
2:O:394:ALA:C	2:O:396:SER:H	2.22	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:59:ILE:HG22	5:R:60:SER:N	2.35	0.42
3:C:105:TYR:O	3:C:315:THR:HG22	2.20	0.42
6:F:84:GLU:CD	6:F:84:GLU:H	2.24	0.42
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.83	0.42
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.32	0.42
3:P:187:PRO:O	3:P:190:ILE:HB	2.20	0.42
3:P:270:LYS:HA	3:P:271:PRO:HD3	1.84	0.42
4:Q:74:PRO:HA	4:Q:79:GLU:O	2.20	0.42
5:R:109:GLU:CD	5:R:167:ALA:HB3	2.41	0.42
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.49	0.42
7:T:41:PHE:HD2	7:T:41:PHE:O	2.02	0.42
1:A:13:GLU:HG2	1:A:14:THR:N	2.35	0.41
2:B:100:SER:HA	2:B:104:LYS:O	2.20	0.41
2:B:109:VAL:HG21	2:B:119:VAL:CG2	2.50	0.41
2:B:265:GLY:O	2:B:266:SER:C	2.58	0.41
3:C:76:TYR:HE2	4:D:204:MET:CE	2.33	0.41
4:D:28:ARG:NH1	4:D:173:ASP:OD2	2.53	0.41
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.50	0.41
1:N:37:VAL:HG12	1:N:199:ALA:HB2	2.00	0.41
1:N:63:ALA:O	1:N:116:VAL:HG13	2.20	0.41
3:P:237:LEU:HD12	3:P:237:LEU:HA	1.70	0.41
6:S:13:MET:O	6:S:17:ARG:HG3	2.21	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.54	0.41
9:V:55:MET:HA	9:V:58:ARG:HG3	2.01	0.41
1:A:158:PHE:O	1:A:164:ALA:HB2	2.19	0.41
4:D:62:LYS:O	4:D:65:ALA:HB3	2.20	0.41
6:F:91:GLU:N	6:F:92:PRO:HD2	2.35	0.41
7:G:9:ARG:NH1	7:G:9:ARG:HG3	2.35	0.41
4:Q:28:ARG:HG3	4:Q:28:ARG:HH11	1.85	0.41
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.50	0.41
5:R:31:ASP:OD1	10:W:7:ARG:HG3	2.20	0.41
1:A:126:GLN:NE2	1:A:129:LYS:HD3	2.35	0.41
2:B:128:THR:HG21	2:B:224:LEU:CD2	2.50	0.41
3:C:275:PHE:CD2	13:C:2001:SMA:H11	2.55	0.41
9:I:49:LEU:O	9:I:50:LEU:HD23	2.19	0.41
1:N:136:GLN:O	1:N:139:LYS:N	2.54	0.41
2:O:43:PRO:C	2:O:113:ARG:HG3	2.38	0.41
3:P:31:TRP:HE1	18:P:3004:CDL:H1	1.85	0.41
7:T:34:LEU:HA	7:T:37:VAL:CG2	2.50	0.41
8:U:57:GLU:CD	8:U:57:GLU:H	2.24	0.41
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PRO:HD3	1:A:414:TYR:CE2	2.55	0.41
1:A:242:ARG:NH1	1:A:432:LEU:HA	2.20	0.41
2:B:24:LEU:HD23	2:B:392:HIS:CE1	2.55	0.41
3:C:15:ILE:CD1	3:C:15:ILE:N	2.82	0.41
3:C:273:TRP:HA	3:C:276:LEU:HG	2.02	0.41
5:E:103:GLN:O	5:E:107:ASN:ND2	2.53	0.41
5:E:67:ASP:O	5:E:69:LEU:HD23	2.19	0.41
1:N:402:VAL:HA	1:N:406:MET:SD	2.61	0.41
1:N:99:ILE:HD12	1:N:109:VAL:CG1	2.43	0.41
2:O:47:ILE:CD1	2:O:47:ILE:N	2.84	0.41
3:P:59:ASP:HA	3:P:173:ASN:OD1	2.20	0.41
5:R:69:LEU:H	5:R:69:LEU:HD23	1.84	0.41
8:U:67:HIS:ND1	8:U:67:HIS:C	2.73	0.41
5:E:77:LYS:C	5:E:79:SER:H	2.23	0.41
9:I:64:LEU:HD12	9:I:77:ARG:O	2.20	0.41
1:N:21:ASN:O	1:N:192:ALA:HB3	2.20	0.41
1:N:252:HIS:CE1	1:N:325:VAL:HG22	2.55	0.41
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.20	0.41
2:O:50:PHE:HE1	2:O:207:VAL:HB	1.85	0.41
1:N:356:ARG:HG3	2:O:90:GLU:O	2.21	0.41
3:P:172:ASP:HB3	3:P:174:PRO:HD2	2.02	0.41
8:U:13:LEU:CD2	8:U:13:LEU:H	2.30	0.41
8:U:51:GLU:HA	8:U:51:GLU:OE1	2.20	0.41
8:U:58:LEU:HD12	8:U:58:LEU:O	2.21	0.41
10:W:14:PHE:HA	10:W:20:PHE:HD2	1.85	0.41
1:A:30:SER:OG	1:A:32:GLN:HB2	2.20	0.41
2:B:207:VAL:HG12	2:B:208:GLY:N	2.34	0.41
4:D:10:PHE:N	4:D:10:PHE:CD1	2.87	0.41
10:J:59:TYR:CD1	10:J:59:TYR:N	2.88	0.41
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.02	0.41
2:O:100:SER:HA	2:O:104:LYS:O	2.21	0.41
2:O:398:VAL:HG13	2:O:399:ALA:N	2.35	0.41
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.20	0.41
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.51	0.41
9:V:77:ARG:N	9:V:77:ARG:CD	2.83	0.41
1:A:99:ILE:HG22	1:A:100:LYS:N	2.35	0.41
1:A:204:SER:HB3	1:A:207:GLU:HB2	2.02	0.41
1:A:49:ASN:ND2	1:A:51:LYS:N	2.68	0.41
3:C:40:VAL:HG11	3:C:233:LEU:HD11	2.03	0.41
6:F:109:LYS:O	6:F:110:LYS:C	2.59	0.41
9:I:49:LEU:HD22	9:I:55:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:ARG:HB3	10:J:7:ARG:CZ	2.50	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
1:N:329:LEU:C	1:N:430:GLN:HE22	2.23	0.41
2:O:269:ALA:O	2:O:270:ASN:C	2.59	0.41
3:P:122:LEU:HD23	3:P:122:LEU:HA	1.86	0.41
4:Q:158:ILE:HG12	4:Q:159:GLY:N	2.35	0.41
5:R:75:GLU:C	5:R:76:ILE:HG13	2.41	0.41
1:A:136:GLN:HE22	9:I:50:LEU:CD1	2.34	0.41
1:A:280:TYR:CD2	1:A:281:ASP:N	2.89	0.41
1:A:233:ARG:NH2	1:A:316:ASP:HB2	2.36	0.41
2:B:259:THR:HG22	2:B:260:GLU:H	1.84	0.41
3:C:308:LEU:HD23	3:C:308:LEU:HA	1.85	0.41
5:E:195:VAL:HG12	5:E:196:GLY:H	1.83	0.41
4:Q:27:ARG:NH2	10:W:59:TYR:CD2	2.88	0.41
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.88	0.41
9:V:49:LEU:HD22	9:V:55:MET:HG2	2.03	0.41
4:Q:57:THR:HG23	10:W:59:TYR:HB2	2.03	0.41
1:A:209:VAL:O	1:A:213:ARG:HG3	2.21	0.41
1:A:242:ARG:O	7:G:14:ILE:HA	2.20	0.41
2:B:263:ALA:HB1	2:B:317:SER:O	2.21	0.41
2:B:33:LEU:HD21	2:B:220:ALA:HB1	2.02	0.41
2:B:369:LEU:O	2:B:372:VAL:HG22	2.21	0.41
2:B:26:ILE:HD11	2:B:390:GLY:O	2.21	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.55	0.41
5:E:133:VAL:HG13	5:E:133:VAL:O	2.21	0.41
6:F:32:MET:HE3	6:F:87:LYS:N	2.22	0.41
1:N:368:GLN:O	1:N:369:LEU:HD23	2.20	0.41
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.85	0.41
2:O:29:LEU:HB2	2:O:31:ASN:ND2	2.36	0.41
2:B:429:ASP:OD1	2:O:60:THR:HG21	2.20	0.41
3:P:40:VAL:HG11	3:P:233:LEU:HD11	2.02	0.41
3:P:50:LEU:O	3:P:54:MET:HG3	2.21	0.41
5:R:166:ASP:HB3	5:R:172:ARG:HH11	1.85	0.41
1:A:23:LEU:HD22	1:A:216:PHE:HB3	2.02	0.41
1:A:266:ASP:O	1:A:269:VAL:N	2.54	0.41
2:B:43:PRO:C	2:B:113:ARG:HG3	2.40	0.41
6:F:104:ARG:O	6:F:108:ASN:ND2	2.53	0.41
3:C:331:ALA:HB2	7:G:52:PHE:CD2	2.56	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.50	0.41
1:N:106:MET:HE2	1:N:106:MET:O	2.21	0.41
1:N:317:THR:OG1	1:N:318:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:203:ARG:CD	2:O:230:ALA:HA	2.51	0.41
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.33	0.41
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.55	0.41
6:S:10:GLY:C	6:S:12:LEU:N	2.74	0.41
2:O:307:PHE:H	9:V:52:ARG:HG2	1.86	0.41
1:A:146:THR:O	1:A:150:PHE:HD1	2.03	0.41
1:A:10:ASN:ND2	2:B:19:PRO:CD	2.84	0.41
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.50	0.41
3:C:145:THR:O	3:C:149:ASN:HB2	2.21	0.41
1:N:102:LEU:C	1:N:104:LYS:N	2.74	0.41
1:N:45:SER:OG	1:N:92:ARG:HA	2.20	0.41
2:O:124:LEU:CD2	2:O:223:PHE:HB3	2.51	0.41
2:O:56:ARG:HG3	2:O:57:TYR:CD1	2.56	0.41
3:P:167:GLY:HA3	3:P:178:ARG:NH2	2.36	0.41
3:P:42:LEU:CD2	3:P:190:ILE:HG22	2.51	0.41
3:P:207:ASN:HD22	3:P:208:ASN:N	2.10	0.41
3:P:243:LEU:CD2	3:P:251:LEU:HD11	2.50	0.41
3:P:347:PRO:O	3:P:350:ILE:HG22	2.21	0.41
1:A:39:VAL:O	1:A:39:VAL:HG13	2.21	0.40
3:C:163:GLU:O	3:C:167:GLY:N	2.52	0.40
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.85	0.40
6:F:67:ASP:O	6:F:70:LEU:HG	2.21	0.40
1:N:292:SER:O	1:N:295:ALA:HB3	2.22	0.40
1:N:30:SER:OG	1:N:32:GLN:HB2	2.22	0.40
1:N:362:ARG:O	1:N:365:MET:HB3	2.21	0.40
2:O:209:ILE:HG13	2:O:379:LEU:HD13	2.01	0.40
3:P:236:MET:HA	18:S:3003:CDL:H162	2.02	0.40
3:P:29:SER:HB2	18:P:3004:CDL:HB21	2.03	0.40
3:P:63:ALA:O	3:P:67:VAL:HG23	2.21	0.40
5:R:69:LEU:CD1	5:R:71:LEU:HD11	2.51	0.40
6:S:77:LYS:HE2	6:S:78:GLU:OE2	2.21	0.40
6:S:91:GLU:N	6:S:92:PRO:HD2	2.36	0.40
4:Q:235:MET:CB	7:T:15:THR:HG22	2.51	0.40
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.04	0.40
4:Q:138:PRO:HD3	8:U:58:LEU:HD23	2.02	0.40
1:A:62:LEU:C	1:A:64:PHE:H	2.25	0.40
2:B:19:PRO:O	2:B:20:GLY:O	2.39	0.40
2:B:259:THR:CG2	2:B:260:GLU:N	2.83	0.40
2:B:300:ALA:C	2:B:302:ALA:N	2.74	0.40
2:B:408:ALA:O	2:B:409:ASP:C	2.60	0.40
3:C:11:LEU:O	3:C:14:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:267:PRO:HA	5:R:147:ILE:HD11	2.03	0.40
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.03	0.40
1:N:223:TYR:HD2	1:N:223:TYR:N	2.17	0.40
2:O:307:PHE:CD1	2:O:308:ASP:N	2.89	0.40
2:O:366:ALA:O	2:O:367:THR:C	2.59	0.40
2:O:51:ILE:HG22	2:O:52:LYS:N	2.36	0.40
3:P:11:LEU:O	3:P:14:MET:HB2	2.21	0.40
4:Q:161:ALA:O	4:Q:163:PRO:HD3	2.22	0.40
6:S:84:GLU:H	6:S:84:GLU:CD	2.25	0.40
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.86	0.40
3:C:109:LEU:HB2	3:C:314:ARG:HH21	1.86	0.40
3:C:70:THR:HA	3:C:74:VAL:CG2	2.51	0.40
5:E:103:GLN:CA	5:E:106:ILE:HD12	2.50	0.40
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.04	0.40
1:N:37:VAL:HG23	1:N:113:LEU:HD11	2.03	0.40
1:N:173:ASN:O	1:N:177:LEU:HG	2.21	0.40
1:N:281:ASP:O	1:N:283:THR:N	2.54	0.40
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.55	0.40
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	3.04	0.40
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.50	0.40
5:R:127:VAL:HG11	5:R:133:VAL:HG23	2.03	0.40
4:Q:139:ALA:HB2	8:U:41:ASP:HA	2.02	0.40
2:B:128:THR:C	2:B:130:PRO:HD2	2.42	0.40
2:B:56:ARG:HB2	2:B:171:ALA:HB1	2.02	0.40
4:D:105:ASN:O	4:D:108:ALA:HB3	2.21	0.40
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.57	0.40
5:E:103:GLN:HA	5:E:106:ILE:CG1	2.52	0.40
2:O:19:PRO:HB3	2:O:41:PHE:CG	2.57	0.40
3:P:338:TRP:CZ2	3:P:348:PHE:HE2	2.38	0.40
3:P:76:TYR:HE2	4:Q:204:MET:HE3	1.86	0.40
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.37	0.40
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.56	0.40
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.40
5:R:91:TRP:C	5:R:93:GLY:N	2.75	0.40
7:T:65:GLU:OE1	7:T:65:GLU:HA	2.22	0.40
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.62	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.84	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.76	0.40
1:A:36:THR:HG21	1:A:373:THR:HA	2.04	0.40
1:A:4:TYR:O	1:A:5:ALA:C	2.59	0.40
2:B:34:ILE:HD13	2:B:390:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ARG:HD3	3:C:16:ASN:OD1	2.22	0.40
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.51	0.40
4:D:139:ALA:HB3	8:H:54:CYS:SG	2.62	0.40
4:D:47:ALA:HB1	4:D:89:ASP:O	2.21	0.40
5:E:52:LYS:O	5:E:52:LYS:HD3	2.21	0.40
8:H:20:ILE:HD11	8:H:76:LYS:CD	2.44	0.40
1:N:15:ASN:HB3	1:N:205:HIS:CD2	2.57	0.40
2:O:109:VAL:HG21	2:O:119:VAL:HG23	2.02	0.40
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.04	0.40
2:O:422:LYS:O	2:O:436:LEU:HD21	2.21	0.40
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.51	0.40
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	2.04	0.40
5:R:103:GLN:HA	5:R:106:ILE:CG1	2.51	0.40
5:R:34:GLY:HA2	10:W:10:TYR:HB2	2.04	0.40
10:W:7:ARG:HB3	10:W:7:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	393 (89%)	40 (9%)	8 (2%)	10	43
1	N	440/446 (99%)	397 (90%)	36 (8%)	7 (2%)	11	46
2	B	419/441 (95%)	339 (81%)	63 (15%)	17 (4%)	3	19
2	O	420/441 (95%)	336 (80%)	66 (16%)	18 (4%)	3	18
3	C	378/380 (100%)	358 (95%)	18 (5%)	2 (0%)	32	74
3	P	377/380 (99%)	349 (93%)	24 (6%)	4 (1%)	17	56
4	D	239/241 (99%)	217 (91%)	20 (8%)	2 (1%)	22	64
4	Q	239/241 (99%)	214 (90%)	22 (9%)	3 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	194/196 (99%)	157 (81%)	24 (12%)	13 (7%)	1	7
5	R	194/196 (99%)	161 (83%)	21 (11%)	12 (6%)	2	10
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	18	59
7	G	79/81 (98%)	66 (84%)	9 (11%)	4 (5%)	2	14
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	2	14
8	H	68/77 (88%)	57 (84%)	8 (12%)	3 (4%)	3	17
8	U	65/77 (84%)	48 (74%)	16 (25%)	1 (2%)	12	48
9	I	29/47 (62%)	19 (66%)	7 (24%)	3 (10%)	0	3
9	V	29/47 (62%)	20 (69%)	7 (24%)	2 (7%)	1	7
10	J	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	11	44
10	W	57/61 (93%)	45 (79%)	8 (14%)	4 (7%)	1	7
All	All	4002/4160 (96%)	3475 (87%)	418 (10%)	109 (3%)	6	30

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	114	ASP
2	B	171	ALA
2	B	230	ALA
2	B	236	LYS
5	E	69	LEU
5	E	70	ALA
5	E	95	PRO
7	G	7	LEU
8	H	12	GLU
10	J	56	LYS
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	114	ASP
2	O	171	ALA
2	O	222	GLN
2	O	225	ASN
2	O	226	ILE

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Mol	Chain	Res	Type
2	O	236	LYS
3	P	157	ILE
5	R	69	LEU
5	R	72	SER
5	R	95	PRO
7	T	7	LEU
10	W	56	LYS
1	A	71	PRO
1	A	72	CYS
1	A	282	ARG
1	A	433	ASP
2	B	31	ASN
2	B	226	ILE
2	B	283	PRO
2	B	371	SER
2	B	390	GLY
5	E	74	ILE
5	E	113	ASP
5	E	137	GLY
7	G	33	ALA
8	H	49	HIS
9	I	56	SER
1	N	20	ASP
1	N	72	CYS
1	N	282	ARG
2	O	221	GLU
2	O	230	ALA
2	O	283	PRO
2	O	371	SER
2	O	390	GLY
3	P	158	GLY
4	Q	177	ALA
5	R	113	ASP
7	T	33	ALA
2	B	30	PRO
3	C	3	PRO
5	E	73	LYS
5	E	78	LEU
5	E	141	HIS
8	H	72	LYS
9	I	55	MET
1	N	71	PRO

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Mol	Chain	Res	Type
1	N	288	LYS
2	O	224	LEU
3	P	3	PRO
3	P	156	TYR
5	R	92	ARG
6	S	11	ARG
10	W	60	GLU
1	A	3	THR
1	A	306	SER
3	C	156	TYR
5	E	92	ARG
5	E	130	PRO
9	I	63	ASP
2	O	227	ARG
4	Q	198	HIS
5	R	78	LEU
5	R	141	HIS
10	W	57	HIS
10	W	61	ALA
1	A	288	LYS
2	B	22	GLU
2	B	266	SER
2	B	382	ILE
4	D	177	ALA
5	E	123	ASP
4	Q	162	PRO
5	R	21	ALA
5	R	74	ILE
5	R	130	PRO
5	R	137	GLY
9	V	63	ASP
2	B	319	SER
1	N	260	PRO
2	O	319	SER
5	R	106	ILE
7	T	27	PRO
8	U	28	GLU
1	A	260	PRO
5	E	106	ILE
7	G	27	PRO
2	O	382	ILE
7	G	50	PRO

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Mol	Chain	Res	Type
7	T	50	PRO
9	V	76	VAL
2	O	288	GLY
4	D	162	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	344 (94%)	21 (6%)	23	61
1	N	365/368 (99%)	344 (94%)	21 (6%)	23	61
2	B	332/347 (96%)	318 (96%)	14 (4%)	34	73
2	O	333/347 (96%)	319 (96%)	14 (4%)	34	73
3	C	329/329 (100%)	323 (98%)	6 (2%)	64	89
3	P	328/329 (100%)	321 (98%)	7 (2%)	59	87
4	D	200/200 (100%)	196 (98%)	4 (2%)	60	87
4	Q	200/200 (100%)	196 (98%)	4 (2%)	60	87
5	E	166/166 (100%)	157 (95%)	9 (5%)	26	64
5	R	166/166 (100%)	157 (95%)	9 (5%)	26	64
6	F	93/96 (97%)	90 (97%)	3 (3%)	44	79
6	S	93/96 (97%)	89 (96%)	4 (4%)	33	72
7	G	71/71 (100%)	68 (96%)	3 (4%)	34	73
7	T	69/71 (97%)	66 (96%)	3 (4%)	33	72
8	H	65/71 (92%)	63 (97%)	2 (3%)	45	80
8	U	63/71 (89%)	61 (97%)	2 (3%)	44	79
9	I	23/26 (88%)	22 (96%)	1 (4%)	33	72
9	V	23/26 (88%)	22 (96%)	1 (4%)	33	72
10	J	49/49 (100%)	45 (92%)	4 (8%)	13	44
10	W	47/49 (96%)	44 (94%)	3 (6%)	20	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3380/3446 (98%)	3245 (96%)	135 (4%)	36 74

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	72	CYS
1	A	86	PHE
1	A	87	ASN
1	A	90	THR
1	A	91	SER
1	A	106	MET
1	A	181	ASP
1	A	223	TYR
1	A	226	ASP
1	A	233	ARG
1	A	281	ASP
1	A	302	LYS
1	A	307	PHE
1	A	342	TRP
1	A	388	ARG
1	A	395	TRP
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	102	ARG
2	B	154	SER
2	B	227	ARG
2	B	248	ASN
2	B	285	ILE
2	B	291	VAL
2	B	296	TYR
2	B	325	TYR
2	B	344	LEU
2	B	358	THR
2	B	364	LEU
2	B	403	ASP
3	C	17	ASN
3	C	47	LEU

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Mol	Chain	Res	Type
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	237	LEU
4	D	24	SER
4	D	77	ASN
4	D	240	PRO
4	D	241	LYS
5	E	6	THR
5	E	52	LYS
5	E	59	ILE
5	E	69	LEU
5	E	74	ILE
5	E	80	ASP
5	E	125	ASP
5	E	135	LEU
5	E	184	THR
6	F	70	LEU
6	F	77	LYS
6	F	91	GLU
7	G	27	PRO
7	G	29	ILE
7	G	41	PHE
8	H	10	GLU
8	H	26	GLN
9	I	71	ASN
10	J	16	ARG
10	J	22	LEU
10	J	26	LEU
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	87	ASN
1	N	90	THR
1	N	106	MET
1	N	124	GLU
1	N	181	ASP
1	N	223	TYR
1	N	281	ASP

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Mol	Chain	Res	Type
1	N	302	LYS
1	N	307	PHE
1	N	342	TRP
1	N	376	CYS
1	N	388	ARG
1	N	395	TRP
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	23	ASP
2	O	31	ASN
2	O	99	TYR
2	O	102	ARG
2	O	154	SER
2	O	227	ARG
2	O	248	ASN
2	O	285	ILE
2	O	291	VAL
2	O	296	TYR
2	O	325	TYR
2	O	344	LEU
2	O	403	ASP
3	P	17	ASN
3	P	47	LEU
3	P	81	ARG
3	P	91	PHE
3	P	149	ASN
3	P	207	ASN
3	P	237	LEU
4	Q	3	LEU
4	Q	24	SER
4	Q	77	ASN
4	Q	241	LYS
5	R	6	THR
5	R	47	THR
5	R	52	LYS
5	R	59	ILE
5	R	69	LEU
5	R	80	ASP
5	R	125	ASP
5	R	135	LEU

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Mol	Chain	Res	Type
5	R	184	THR
6	S	13	MET
6	S	70	LEU
6	S	77	LYS
6	S	91	GLU
7	T	27	PRO
7	T	29	ILE
7	T	41	PHE
8	U	26	GLN
8	U	71	HIS
9	V	70	LEU
10	W	22	LEU
10	W	26	LEU
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	126	GLN
1	A	136	GLN
1	A	147	ASN
1	A	159	GLN
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
1	A	360	HIS
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	222	GLN
2	B	248	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	362	ASN
2	B	363	GLN
2	B	400	GLN
2	B	412	ASN

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Mol	Chain	Res	Type
3	C	4	ASN
3	C	17	ASN
3	C	69	HIS
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	200	GLN
5	E	86	ASN
5	E	107	ASN
5	E	164	HIS
5	E	186	GLN
6	F	56	ASN
6	F	72	HIS
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	64	GLN
7	G	79	ASN
7	G	81	GLN
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	126	GLN
1	N	136	GLN
1	N	143	ASN
1	N	147	ASN
1	N	159	GLN
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
1	N	360	HIS
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN

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Mol	Chain	Res	Type
2	O	192	HIS
2	O	222	GLN
2	O	225	ASN
2	O	248	ASN
2	O	270	ASN
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	329	GLN
2	O	362	ASN
2	O	363	GLN
2	O	400	GLN
2	O	412	ASN
3	P	4	ASN
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	200	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
6	S	56	ASN
6	S	72	HIS
6	S	79	GLN
7	T	23	GLN
7	T	44	GLN
7	T	64	GLN
8	U	71	HIS
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, 10 are unknown - leaving 26 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
13	SMA	C	2001	-	36,38,38	1.87	8 (22%)	44,52,52	1.84	6 (13%)
14	UQ	C	2002	-	19,19,63	2.54	9 (47%)	23,26,79	1.02	2 (8%)
15	PEE	C	2007	-	48,48,50	1.33	7 (14%)	50,53,55	0.99	5 (10%)
15	PEE	C	2008	-	20,20,50	1.72	6 (30%)	22,25,55	0.65	0
16	GOL	C	2011	-	5,5,5	1.27	0	5,5,5	0.57	0
12	HEM	C	501	3	28,50,50	2.10	10 (35%)	17,82,82	1.76	4 (23%)
12	HEM	C	502	3	28,50,50	1.82	7 (25%)	17,82,82	1.91	7 (41%)
18	CDL	D	2003	-	49,49,99	1.13	1 (2%)	51,61,111	1.05	3 (5%)
17	HEC	D	501	4	28,50,50	2.00	7 (25%)	16,82,82	1.96	3 (18%)
15	PEE	E	2005	-	49,49,50	1.40	10 (20%)	51,54,55	0.96	5 (9%)
20	PLC	E	2009	-	31,31,41	1.66	6 (19%)	36,39,49	0.68	1 (2%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
18	CDL	G	2004	-	39,39,99	1.33	5 (12%)	41,51,111	1.20	4 (9%)
15	PEE	N	3008	-	4,4,50	3.47	4 (100%)	6,6,55	0.55	0
13	SMA	P	3001	-	36,38,38	1.95	9 (25%)	44,52,52	1.79	6 (13%)
14	UQ	P	3002	-	19,19,63	2.50	9 (47%)	23,26,79	1.04	2 (8%)
18	CDL	P	3004	-	39,39,99	1.24	4 (10%)	41,51,111	1.21	4 (9%)
15	PEE	P	3007	-	48,48,50	1.30	7 (14%)	50,53,55	0.93	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	GOL	P	3011	-	5,5,5	1.46	1 (20%)	5,5,5	0.68	0
12	HEM	P	501	3	28,50,50	1.91	7 (25%)	17,82,82	1.48	4 (23%)
12	HEM	P	502	3	28,50,50	1.80	7 (25%)	17,82,82	1.71	6 (35%)
17	HEC	Q	501	4	28,50,50	2.11	4 (14%)	16,82,82	1.74	3 (18%)
15	PEE	R	3005	-	49,49,50	1.42	9 (18%)	51,54,55	0.95	5 (9%)
20	PLC	R	3009	-	31,31,41	1.59	7 (22%)	36,39,49	0.65	1 (2%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
18	CDL	S	3003	-	49,49,99	1.12	2 (4%)	51,61,111	1.05	3 (5%)

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
13	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
14	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
15	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
15	PEE	C	2008	-	-	0/24/24/54	0/0/0/0
16	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
12	HEM	C	501	3	-	0/6/54/54	0/0/8/8
12	HEM	C	502	3	-	0/6/54/54	0/0/8/8
18	CDL	D	2003	-	-	0/59/59/110	0/0/0/0
17	HEC	D	501	4	-	0/6/54/54	0/0/8/8
15	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
20	PLC	E	2009	-	-	0/35/35/45	0/0/0/0
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
18	CDL	G	2004	-	-	0/49/49/110	0/0/0/0
15	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
13	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
14	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
18	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
15	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
16	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
12	HEM	P	501	3	-	0/6/54/54	0/0/8/8
12	HEM	P	502	3	-	0/6/54/54	0/0/8/8
17	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
15	PEE	R	3005	-	-	0/53/53/54	0/0/0/0
20	PLC	R	3009	-	-	0/35/35/45	0/0/0/0
19	FES	R	501	5	-	0/0/4/4	0/1/1/1
18	CDL	S	3003	-	-	0/59/59/110	0/0/0/0

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3B-C2B	-7.54	1.32	1.40
17	D	501	HEC	C3B-C2B	-6.27	1.34	1.40
17	D	501	HEC	C3C-C2C	-5.06	1.35	1.40
12	C	501	HEM	C3B-CAB	-4.84	1.38	1.47
12	P	501	HEM	C3B-CAB	-4.59	1.38	1.47
12	P	501	HEM	C3C-CAC	-4.39	1.39	1.47
17	Q	501	HEC	C3C-C2C	-3.93	1.36	1.40
12	P	502	HEM	C3B-CAB	-3.73	1.40	1.47
12	P	502	HEM	C3C-CAC	-3.64	1.40	1.47
12	C	502	HEM	C3C-CAC	-3.60	1.40	1.47
12	C	501	HEM	C3C-CAC	-3.50	1.40	1.47
12	C	502	HEM	C3B-CAB	-3.49	1.40	1.47
12	P	501	HEM	C3B-C2B	-3.35	1.35	1.40
12	P	502	HEM	C3C-C2C	-2.93	1.36	1.40
15	E	2005	PEE	C19-C18	-2.93	1.34	1.51
15	R	3005	PEE	C19-C18	-2.92	1.35	1.51
15	R	3005	PEE	C22-C21	-2.77	1.35	1.51
15	E	2005	PEE	C22-C21	-2.76	1.35	1.51
12	C	502	HEM	C3C-C2C	-2.71	1.36	1.40
12	C	501	HEM	C1D-CHD	-2.67	1.33	1.40
15	P	3007	PEE	C22-C21	-2.66	1.36	1.51
15	P	3007	PEE	C19-C18	-2.63	1.36	1.51
15	C	2007	PEE	C22-C21	-2.59	1.36	1.51
15	C	2007	PEE	C19-C18	-2.49	1.37	1.51
12	C	501	HEM	C1A-CHA	-2.47	1.33	1.40
12	C	501	HEM	C3C-C2C	-2.46	1.37	1.40
12	C	501	HEM	C3B-C2B	-2.38	1.37	1.40
18	G	2004	CDL	OA8-CA6	-2.06	1.40	1.45
18	P	3004	CDL	OA8-CA6	-2.06	1.40	1.45
15	E	2005	PEE	P-O4P	2.01	1.67	1.59
17	D	501	HEC	C1C-NC	2.01	1.40	1.36
15	E	2005	PEE	C11-C10	2.03	1.56	1.50
18	S	3003	CDL	OA6-CA5	2.04	1.40	1.34
13	C	2001	SMA	C6-C7	2.11	1.42	1.38
18	P	3004	CDL	CB3-CB4	2.11	1.56	1.50
20	R	3009	PLC	C1B-CB	2.12	1.56	1.50
13	C	2001	SMA	O1-C8A	2.12	1.40	1.36
15	C	2007	PEE	C11-C10	2.13	1.56	1.50
15	C	2008	PEE	C11-C10	2.14	1.56	1.50
13	P	3001	SMA	C6-C5	2.14	1.44	1.37
18	P	3004	CDL	CA3-CA4	2.15	1.56	1.50
15	P	3007	PEE	C11-C10	2.16	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	3008	PEE	P-O2P	2.16	1.62	1.54
15	C	2008	PEE	C3-C2	2.18	1.56	1.50
16	P	3011	GOL	O2-C2	2.19	1.49	1.43
12	P	501	HEM	C4C-NC	2.23	1.39	1.36
13	C	2001	SMA	C11-C12	2.24	1.57	1.53
15	R	3005	PEE	C11-C10	2.26	1.57	1.50
12	C	502	HEM	C1C-NC	2.28	1.39	1.36
18	G	2004	CDL	CB3-CB4	2.29	1.57	1.50
15	P	3007	PEE	C3-C2	2.29	1.57	1.50
17	D	501	HEC	C1A-NA	2.32	1.39	1.36
13	P	3001	SMA	C6-C7	2.34	1.43	1.38
17	D	501	HEC	C3C-C4C	2.35	1.47	1.43
15	R	3005	PEE	C3-C2	2.36	1.57	1.50
14	P	3002	UQ	C5-C4	2.38	1.56	1.47
20	R	3009	PLC	O2-C2	2.38	1.52	1.46
13	P	3001	SMA	O5-C5	2.39	1.41	1.36
15	E	2005	PEE	C3-C2	2.41	1.57	1.50
20	R	3009	PLC	C3-C2	2.42	1.57	1.50
18	P	3004	CDL	O1-C1	2.42	1.50	1.43
15	C	2008	PEE	C1-C2	2.42	1.57	1.50
12	P	502	HEM	C4D-ND	2.42	1.39	1.36
15	R	3005	PEE	C1-C2	2.43	1.57	1.50
13	P	3001	SMA	O1-C8A	2.45	1.40	1.36
13	C	2001	SMA	O7-C7	2.46	1.41	1.37
20	E	2009	PLC	C3-C2	2.46	1.57	1.50
15	C	2007	PEE	C3-C2	2.49	1.57	1.50
14	C	2002	UQ	C5-C4	2.49	1.56	1.47
18	G	2004	CDL	O1-C1	2.50	1.50	1.43
15	R	3005	PEE	C31-C30	2.51	1.58	1.50
17	D	501	HEC	C4B-NB	2.52	1.39	1.36
18	S	3003	CDL	O1-C1	2.52	1.50	1.43
15	E	2005	PEE	C31-C30	2.54	1.58	1.50
15	C	2007	PEE	P-O1P	2.55	1.60	1.50
13	P	3001	SMA	O7-C7	2.55	1.41	1.37
18	G	2004	CDL	OA6-CA5	2.58	1.41	1.34
20	R	3009	PLC	C1-C2	2.58	1.58	1.50
18	D	2003	CDL	O1-C1	2.59	1.51	1.43
15	E	2005	PEE	O2-C10	2.63	1.41	1.34
14	C	2002	UQ	C3-C4	2.66	1.56	1.48
14	C	2002	UQ	CM5-C5	2.66	1.56	1.50
15	E	2005	PEE	C1-C2	2.67	1.58	1.50
17	D	501	HEC	C4A-NA	2.67	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	501	HEM	C1C-NC	2.68	1.39	1.36
18	G	2004	CDL	CA3-CA4	2.68	1.58	1.50
14	P	3002	UQ	CM5-C5	2.69	1.56	1.50
14	P	3002	UQ	C3-C4	2.70	1.56	1.48
15	P	3007	PEE	P-O1P	2.75	1.61	1.50
12	C	501	HEM	CBB-CAB	2.76	1.48	1.28
15	C	2008	PEE	O3-C30	2.77	1.41	1.33
15	P	3007	PEE	O3-C30	2.81	1.41	1.33
14	P	3002	UQ	O2-C2	2.81	1.43	1.36
20	E	2009	PLC	O2-C2	2.81	1.53	1.46
14	P	3002	UQ	C2-C1	2.82	1.57	1.48
15	C	2007	PEE	O3-C30	2.83	1.41	1.33
15	N	3008	PEE	P-O3P	2.91	1.64	1.54
15	N	3008	PEE	P-O4P	2.91	1.64	1.54
20	E	2009	PLC	O3-CB	2.91	1.41	1.33
20	E	2009	PLC	C1-C2	2.92	1.59	1.50
14	C	2002	UQ	C2-C1	2.92	1.57	1.48
15	C	2007	PEE	O2-C10	2.93	1.42	1.34
12	C	502	HEM	CBC-CAC	2.94	1.49	1.28
12	P	501	HEM	CBB-CAB	2.97	1.49	1.28
20	R	3009	PLC	O3-CB	2.98	1.42	1.33
15	C	2008	PEE	P-O1P	2.98	1.62	1.50
15	C	2008	PEE	O2-C10	3.03	1.43	1.34
15	P	3007	PEE	O2-C10	3.07	1.43	1.34
12	C	501	HEM	C4D-ND	3.15	1.40	1.36
14	P	3002	UQ	O3-C3	3.16	1.44	1.36
15	R	3005	PEE	O2-C10	3.16	1.43	1.34
15	E	2005	PEE	P-O1P	3.18	1.62	1.50
14	C	2002	UQ	O2-C2	3.20	1.44	1.36
15	R	3005	PEE	P-O1P	3.20	1.62	1.50
12	P	502	HEM	CBB-CAB	3.21	1.51	1.28
20	R	3009	PLC	P-O1P	3.23	1.63	1.50
20	E	2009	PLC	P-O1P	3.24	1.63	1.50
17	Q	501	HEC	C4A-NA	3.32	1.40	1.36
12	P	501	HEM	CBC-CAC	3.35	1.52	1.28
12	C	501	HEM	CBC-CAC	3.40	1.52	1.28
15	R	3005	PEE	O3-C30	3.40	1.43	1.33
15	E	2005	PEE	O3-C30	3.41	1.43	1.33
12	C	502	HEM	CBB-CAB	3.43	1.53	1.28
13	P	3001	SMA	C4-C3	3.44	1.51	1.41
12	P	502	HEM	C1B-NB	3.44	1.40	1.36
12	P	502	HEM	CBC-CAC	3.46	1.53	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C4D-ND	3.49	1.40	1.36
13	C	2001	SMA	C4-C3	3.57	1.51	1.41
20	R	3009	PLC	O2-C'	3.65	1.44	1.34
14	C	2002	UQ	O3-C3	3.77	1.46	1.36
14	P	3002	UQ	C6-C1	3.78	1.57	1.46
14	C	2002	UQ	C6-C1	3.95	1.57	1.46
14	C	2002	UQ	C6-C5	4.01	1.44	1.35
20	E	2009	PLC	O2-C'	4.02	1.46	1.34
17	Q	501	HEC	C1A-NA	4.11	1.41	1.36
14	P	3002	UQ	C6-C5	4.26	1.44	1.35
13	P	3001	SMA	C7-C8	4.29	1.46	1.40
13	C	2001	SMA	O1-C2	4.44	1.41	1.35
12	C	501	HEM	C1B-NB	4.71	1.42	1.36
14	C	2002	UQ	C7-C6	4.83	1.59	1.51
13	C	2001	SMA	C7-C8	5.15	1.47	1.40
15	N	3008	PEE	P-O1P	5.17	1.61	1.50
14	P	3002	UQ	C7-C6	5.20	1.60	1.51
13	P	3001	SMA	O1-C2	5.20	1.42	1.35
13	C	2001	SMA	C4-C4A	5.47	1.49	1.41
13	P	3001	SMA	C4-C4A	6.11	1.50	1.41

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	HEM	CBA-CAA-C2A	-4.50	103.89	112.48
13	C	2001	SMA	C3-C4-C4A	-4.42	115.38	121.25
13	P	3001	SMA	C9-C10-C11	-4.23	109.03	114.72
13	P	3001	SMA	C3-C4-C4A	-4.06	115.86	121.25
13	C	2001	SMA	C9-C10-C11	-4.05	109.26	114.72
18	P	3004	CDL	CB4-OB6-CB5	-3.64	109.27	117.88
18	G	2004	CDL	CB4-OB6-CB5	-3.55	109.48	117.88
17	D	501	HEC	CAA-C2A-C3A	-3.40	119.29	129.00
12	P	501	HEM	CBA-CAA-C2A	-3.31	106.16	112.48
12	P	502	HEM	C4C-C3C-C2C	-3.23	104.64	106.90
17	Q	501	HEC	CAA-C2A-C3A	-3.22	119.80	129.00
13	P	3001	SMA	O1-C2-C9	-3.20	108.00	111.94
13	C	2001	SMA	O1-C2-C9	-3.16	108.05	111.94
18	D	2003	CDL	CA6-CA4-CA3	-2.90	105.33	111.86
12	C	502	HEM	C4C-C3C-C2C	-2.81	104.94	106.90
18	S	3003	CDL	CA6-CA4-CA3	-2.77	105.61	111.86
18	D	2003	CDL	CB4-OB6-CB5	-2.63	111.66	117.88
12	C	502	HEM	C4A-C3A-C2A	-2.60	105.19	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	502	HEM	CMD-C2D-C1D	-2.53	124.57	128.46
14	P	3002	UQ	C7-C6-C1	-2.49	115.28	118.47
18	G	2004	CDL	CB6-CB4-CB3	-2.47	106.29	111.86
18	P	3004	CDL	CB6-CB4-CB3	-2.42	106.39	111.86
18	S	3003	CDL	CB4-OB6-CB5	-2.37	112.27	117.88
18	P	3004	CDL	CA6-CA4-CA3	-2.37	106.51	111.86
14	C	2002	UQ	C7-C6-C1	-2.33	115.49	118.47
13	C	2001	SMA	C7-C8-C8A	-2.31	118.15	120.18
18	G	2004	CDL	CA6-CA4-CA3	-2.24	106.81	111.86
12	C	502	HEM	CMD-C2D-C1D	-2.08	125.26	128.46
18	S	3003	CDL	CB6-CB4-CB3	-2.08	107.17	111.86
18	D	2003	CDL	CB6-CB4-CB3	-2.06	107.22	111.86
17	Q	501	HEC	CBD-CAD-C3D	2.01	116.33	112.48
13	P	3001	SMA	C7M-O7-C7	2.02	120.44	117.54
12	P	502	HEM	C3B-C4B-NB	2.04	111.85	109.21
15	P	3007	PEE	O3-C3-C2	2.07	113.86	108.66
12	P	501	HEM	C3B-C4B-NB	2.09	111.92	109.21
12	C	502	HEM	CMA-C3A-C2A	2.13	128.96	124.94
12	C	501	HEM	CMC-C2C-C3C	2.17	128.91	124.89
20	E	2009	PLC	O3-C3-C2	2.19	114.15	108.66
20	R	3009	PLC	O3-C3-C2	2.21	114.20	108.66
12	C	502	HEM	CMB-C2B-C3B	2.25	129.06	124.89
12	C	501	HEM	C3B-C4B-NB	2.30	112.18	109.21
17	D	501	HEC	CBD-CAD-C3D	2.33	116.94	112.48
18	P	3004	CDL	OB6-CB4-CB3	2.33	116.92	108.44
12	P	501	HEM	CMC-C2C-C3C	2.37	129.29	124.89
18	G	2004	CDL	OB6-CB4-CB3	2.38	117.10	108.44
15	E	2005	PEE	C19-C18-C17	2.43	126.98	114.45
12	P	501	HEM	CBD-CAD-C3D	2.44	117.12	112.47
12	P	502	HEM	CBA-CAA-C2A	2.46	117.18	112.48
15	P	3007	PEE	C22-C21-C20	2.47	127.19	114.45
15	R	3005	PEE	C22-C21-C20	2.47	127.20	114.45
15	E	2005	PEE	C23-C22-C21	2.49	127.29	114.45
15	R	3005	PEE	O3-C3-C2	2.50	114.95	108.66
15	C	2007	PEE	C22-C21-C20	2.51	127.40	114.45
15	R	3005	PEE	C23-C22-C21	2.52	127.42	114.45
15	R	3005	PEE	C19-C18-C17	2.52	127.44	114.45
15	P	3007	PEE	C23-C22-C21	2.53	127.48	114.45
15	E	2005	PEE	C22-C21-C20	2.55	127.58	114.45
15	C	2007	PEE	O3-C3-C2	2.55	115.07	108.66
15	E	2005	PEE	O3-C3-C2	2.57	115.10	108.66
15	C	2007	PEE	C23-C22-C21	2.57	127.71	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	502	HEM	C1D-C2D-C3D	2.64	108.83	107.00
12	P	502	HEM	CMB-C2B-C3B	2.67	129.85	124.89
13	P	3001	SMA	O7-C7-C8	2.69	117.15	114.49
12	C	502	HEM	CBA-CAA-C2A	2.73	117.71	112.48
15	P	3007	PEE	C20-C19-C18	2.75	128.62	114.45
15	C	2007	PEE	C19-C18-C17	2.80	128.87	114.45
15	R	3005	PEE	C20-C19-C18	2.81	128.92	114.45
15	P	3007	PEE	C19-C18-C17	2.82	128.97	114.45
15	E	2005	PEE	C20-C19-C18	2.84	129.12	114.45
15	C	2007	PEE	C20-C19-C18	2.88	129.31	114.45
12	C	501	HEM	CBD-CAD-C3D	2.89	117.99	112.47
14	C	2002	UQ	C8-C7-C6	2.96	120.15	111.85
14	P	3002	UQ	C8-C7-C6	2.96	120.18	111.85
13	C	2001	SMA	O7-C7-C8	3.80	118.25	114.49
12	C	502	HEM	C1D-C2D-C3D	3.88	109.69	107.00
17	Q	501	HEC	CBA-CAA-C2A	5.10	122.19	112.47
17	D	501	HEC	CBA-CAA-C2A	5.70	123.33	112.47
13	C	2001	SMA	C9-C2-C3	7.79	129.68	120.35
13	P	3001	SMA	C9-C2-C3	7.83	129.72	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	2001	SMA	4	0
14	C	2002	UQ	5	0
15	C	2007	PEE	1	0
12	C	501	HEM	5	0
12	C	502	HEM	6	0
18	D	2003	CDL	1	0
17	D	501	HEC	1	0
15	E	2005	PEE	4	0
20	E	2009	PLC	3	0
18	G	2004	CDL	1	0
13	P	3001	SMA	4	0
14	P	3002	UQ	1	0
18	P	3004	CDL	3	0
15	P	3007	PEE	1	0
16	P	3011	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	501	HEM	5	0
12	P	502	HEM	6	0
17	Q	501	HEC	1	0
15	R	3005	PEE	4	0
20	R	3009	PLC	2	0
19	R	501	FES	1	0
18	S	3003	CDL	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/446 (99%)	-0.34	2 (0%) 90 74	44, 77, 105, 114	0
1	N	442/446 (99%)	-0.31	0 100 100	54, 80, 102, 110	0
2	B	421/441 (95%)	-0.26	2 (0%) 90 74	66, 93, 122, 140	0
2	O	422/441 (95%)	-0.29	1 (0%) 94 85	52, 85, 111, 124	0
3	C	380/380 (100%)	-0.49	1 (0%) 93 82	33, 49, 84, 140	0
3	P	379/380 (99%)	-0.31	4 (1%) 80 55	44, 75, 99, 119	0
4	D	241/241 (100%)	-0.51	0 100 100	42, 55, 86, 114	0
4	Q	241/241 (100%)	-0.25	0 100 100	59, 86, 112, 127	0
5	E	196/196 (100%)	0.28	17 (8%) 11 4	48, 114, 165, 172	0
5	R	196/196 (100%)	0.04	12 (6%) 22 8	54, 85, 134, 151	0
6	F	101/110 (91%)	-0.64	0 100 100	37, 53, 67, 99	0
6	S	101/110 (91%)	-0.24	2 (1%) 65 36	64, 84, 112, 141	0
7	G	81/81 (100%)	-0.27	0 100 100	48, 62, 94, 113	0
7	T	79/81 (97%)	0.18	7 (8%) 10 4	69, 95, 147, 164	0
8	H	70/77 (90%)	-0.44	0 100 100	48, 73, 90, 133	0
8	U	67/77 (87%)	0.18	3 (4%) 34 13	102, 125, 148, 154	0
9	I	31/47 (65%)	1.31	9 (29%) 1 0	94, 127, 172, 178	0
9	V	31/47 (65%)	1.58	11 (35%) 0 0	93, 125, 184, 184	0
10	J	61/61 (100%)	-0.43	1 (1%) 72 44	57, 71, 109, 151	0
10	W	59/61 (96%)	-0.01	1 (1%) 70 42	69, 85, 101, 117	0
All	All	4042/4160 (97%)	-0.25	73 (1%) 69 40	33, 79, 125, 184	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	GLY	5.7
8	U	50	THR	5.3
9	V	51	CYS	5.2
7	T	78	GLU	4.7
7	T	2	ILE	4.1
5	E	187	PHE	4.1
5	R	187	PHE	3.9
3	P	8	SER	3.8
3	C	1	MET	3.7
10	W	62	SER	3.7
9	I	48	PRO	3.6
5	R	114	VAL	3.4
5	E	191	ASP	3.3
9	V	56	SER	3.3
1	A	2	ALA	3.3
7	T	79	ASN	3.2
9	V	53	GLU	3.2
9	V	57	GLY	3.1
5	R	194	VAL	3.1
5	R	190	ASP	3.0
5	R	191	ASP	3.0
9	V	59	SER	3.0
9	V	62	ARG	2.9
9	V	50	LEU	2.9
9	I	53	GLU	2.9
6	S	12	LEU	2.9
5	R	195	VAL	2.8
9	V	61	ARG	2.8
7	T	74	PRO	2.8
2	O	19	PRO	2.8
3	P	7	LYS	2.8
5	R	196	GLY	2.7
9	I	58	ARG	2.7
9	I	63	ASP	2.7
5	E	195	VAL	2.6
5	R	186	GLN	2.6
9	I	62	ARG	2.6
9	I	77	ARG	2.6
5	E	121	GLN	2.6
5	R	122	HIS	2.6
5	E	130	PRO	2.6
5	R	193	VAL	2.6
9	I	57	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	444	ILE	2.6
5	E	85	LYS	2.5
5	E	122	HIS	2.4
9	V	49	LEU	2.3
5	E	128	LYS	2.3
8	U	49	HIS	2.3
2	B	402	ILE	2.3
5	E	188	VAL	2.3
5	E	73	LYS	2.2
8	U	28	GLU	2.2
5	E	79	SER	2.2
5	R	128	LYS	2.2
5	E	74	ILE	2.2
10	J	64	GLU	2.2
7	T	77	TYR	2.2
9	V	77	ARG	2.2
3	P	5	ILE	2.1
9	V	63	ASP	2.1
9	I	51	CYS	2.1
5	R	188	VAL	2.1
9	I	47	ARG	2.1
5	E	137	GLY	2.1
3	P	13	LYS	2.1
5	E	111	GLU	2.1
5	E	118	ARG	2.1
6	S	15	ARG	2.1
5	E	117	LEU	2.1
7	T	63	THR	2.0
5	E	91	TRP	2.0
2	B	226	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	UNL	C	2010	1/-	0.59	1.52	52.71	53,53,53,53	0
11	UNL	R	2103	1/-	0.79	0.62	23.86	45,45,45,45	0
16	GOL	C	2011	6/6	0.84	0.35	7.54	79,81,82,83	0
15	PEE	R	3005	50/51	0.78	0.38	4.79	95,108,116,119	0
15	PEE	E	2005	50/51	0.78	0.34	4.32	76,90,95,95	0
18	CDL	S	3003	50/100	0.75	0.39	4.16	126,140,153,153	0
15	PEE	C	2007	49/51	0.92	0.28	3.92	52,68,87,89	0
20	PLC	E	2009	32/42	0.82	0.32	3.52	67,83,97,98	0
11	UNL	E	3103	1/-	0.65	0.43	3.43	45,45,45,45	0
11	UNL	A	3016	1/-	0.74	0.40	3.29	55,55,55,55	0
15	PEE	P	3007	49/51	0.87	0.34	3.29	73,98,107,108	0
15	PEE	C	2008	21/51	0.76	0.33	3.05	139,142,144,144	0
14	UQ	C	2002	19/63	0.84	0.28	3.00	85,88,90,91	0
16	GOL	P	3011	6/6	0.91	0.27	2.80	69,71,72,72	0
20	PLC	R	3009	32/42	0.82	0.35	2.55	91,99,116,116	0
14	UQ	P	3002	19/63	0.85	0.30	2.26	116,121,122,122	0
18	CDL	G	2004	40/100	0.90	0.26	2.11	81,90,97,98	0
18	CDL	D	2003	50/100	0.85	0.27	1.59	79,112,130,131	0
13	SMA	P	3001	37/37	0.94	0.23	0.92	67,73,75,78	0
12	HEM	P	501	43/43	0.98	0.21	0.91	56,61,69,75	0
18	CDL	P	3004	40/100	0.85	0.27	0.88	106,114,120,121	0
13	SMA	C	2001	37/37	0.97	0.20	0.79	41,44,46,52	0
12	HEM	C	501	43/43	0.98	0.20	0.71	44,48,50,53	0
12	HEM	P	502	43/43	0.99	0.20	0.16	59,63,71,77	0
12	HEM	C	502	43/43	0.99	0.19	0.02	34,40,50,54	0
19	FES	R	501	4/4	1.00	0.16	0.00	52,54,56,57	0
17	HEC	D	501	43/43	0.98	0.17	-0.29	44,46,50,53	0
17	HEC	Q	501	43/43	0.96	0.19	-0.46	67,71,76,78	0
19	FES	E	501	4/4	0.98	0.15	-1.26	92,93,95,95	0
11	UNL	P	3010	1/-	0.65	0.88	-	67,67,67,67	0
11	UNL	C	2104	1/-	0.67	0.63	-	71,71,71,71	0
15	PEE	N	3008	5/51	0.82	0.34	-	135,135,136,136	0
11	UNL	E	2105	1/-	0.51	0.39	-	62,62,62,62	0
11	UNL	C	3015	1/-	0.72	0.48	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
11	UNL	P	2015	1/-	0.72	0.39	-	33,33,33,33	0
11	UNL	P	3104	1/-	0.76	0.55	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.