



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:54 pm BST

PDB ID : 1OCZ  
Title : BOVINE HEART CYTOCHROME C OXIDASE IN AZIDE-BOUND STATE  
Authors : Tsukihara, T.; Yao, M.  
Deposited on : 1998-07-13  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

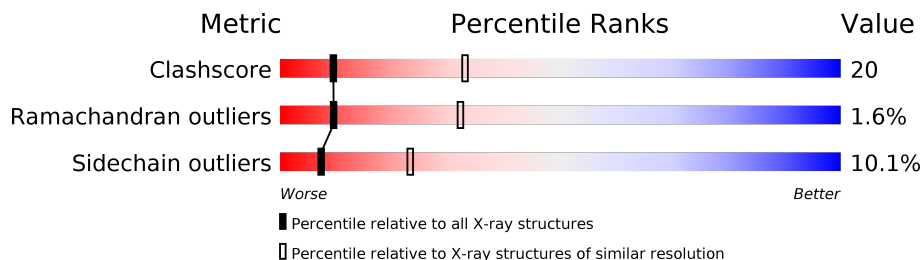
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	63% 34% .
1	N	514	63% 35% .
2	B	227	51% 42% 6%
2	O	227	51% 43% 6%
3	C	261	68% 25% 6% .
3	P	261	65% 29% 5% .
4	D	147	58% 35% 5% .
4	Q	147	56% 37% 5% .

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Mol	Chain	Length	Quality of chain
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
17	AZI	N	521	-	-	X	-
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 28818 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	0	0
			4025	2690	623	677	35			
1	N	514	Total	C	N	O	S	0	0	0
			4025	2690	623	677	35			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	5	0
			1863	1207	288	350	18			
2	O	227	Total	C	N	O	S	0	5	0
			1863	1207	288	350	18			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	261	Total	C	N	O	S	0	0	0
			2124	1420	338	353	13			
3	P	261	Total	C	N	O	S	0	0	0
			2124	1420	338	353	13			

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	109	Total 878	C 558	N 150	O 168	S 2	0	0	0
5	R	109	Total 878	C 558	N 150	O 168	S 2	0	0	0

- Molecule 6 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	98	Total 748	C 464	N 134	O 145	S 5	0	0	0
6	S	98	Total 748	C 464	N 134	O 145	S 5	0	0	0

- Molecule 7 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	84	Total 672	C 431	N 129	O 111	S 1	0	0	0
7	T	84	Total 672	C 431	N 129	O 111	S 1	0	0	0

- Molecule 8 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	75	Total 628	C 395	N 114	O 114	S 5	0	0	0
8	U	75	Total 628	C 395	N 114	O 114	S 5	0	0	0

- Molecule 9 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	73	Total 598	C 388	N 107	O 99	S 4	0	0	0
9	V	73	Total 598	C 388	N 107	O 99	S 4	0	0	0

- Molecule 10 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	56	Total 441	C 285	N 73	O 80	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

- Molecule 11 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			386	257	65	62	2			
12	Y	47	Total	C	N	O	S	0	0	0
			386	257	65	62	2			

- Molecule 13 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	O	2	Total	Cu	0	0
			2	2		
14	B	2	Total	Cu	0	0
			2	2		
14	A	1	Total	Cu	0	0
			1	1		
14	N	1	Total	Cu	0	0
			1	1		

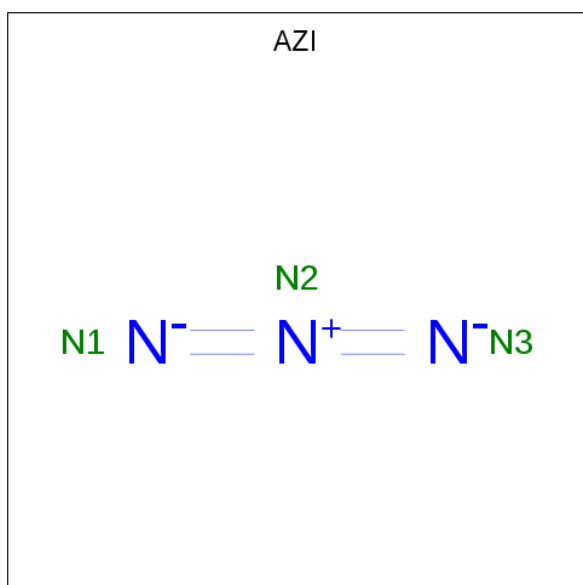
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

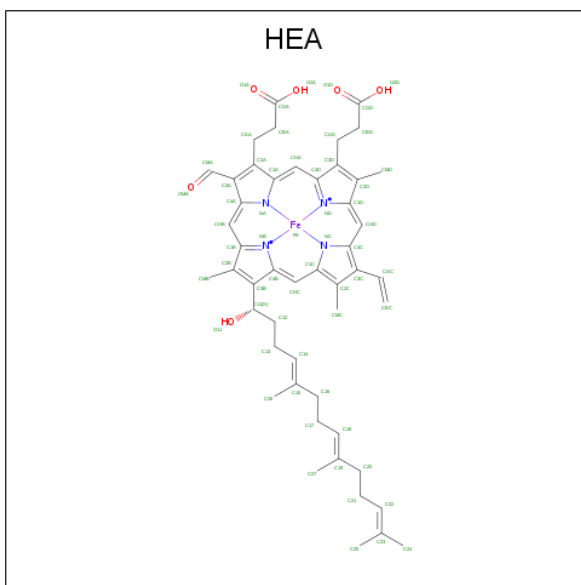
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total N 3 3	0	0
17	A	1	Total N 3 3	0	0
17	N	1	Total N 3 3	0	0
17	N	1	Total N 3 3	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
18	A	1	60	49	1	4	6	0	0
18	A	1	60	49	1	4	6	0	0
18	N	1	60	49	1	4	6	0	0
18	N	1	60	49	1	4	6	0	0

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	S	1	Total	Zn	0	0
			1	1		
19	F	1	Total	Zn	0	0
			1	1		

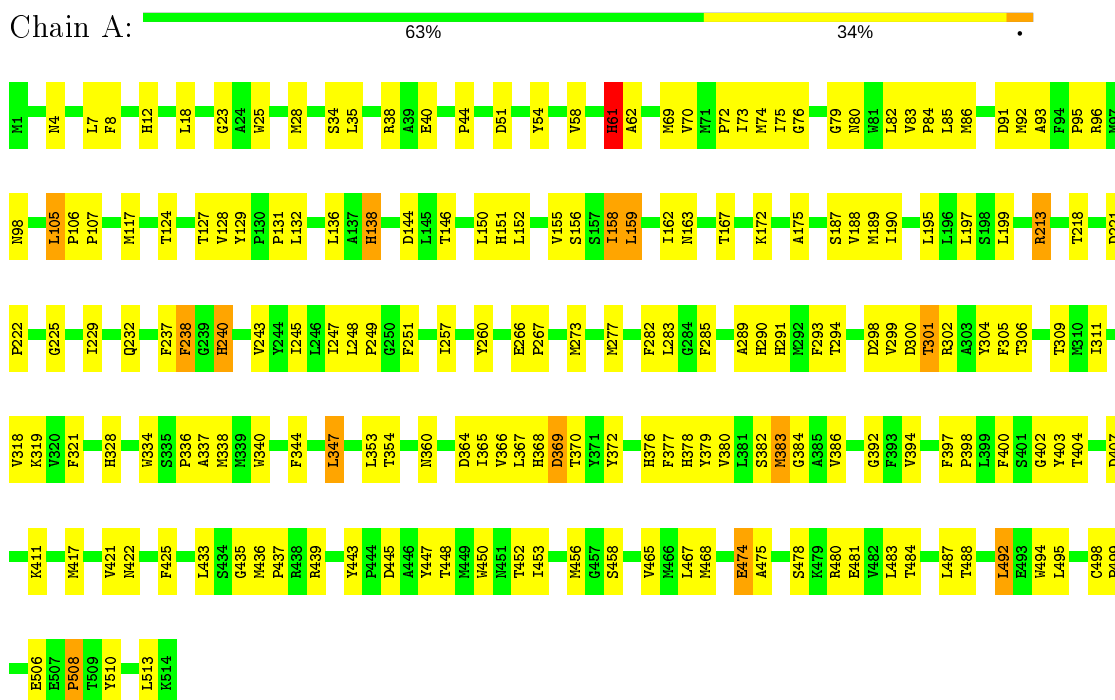


### 3 Residue-property plots

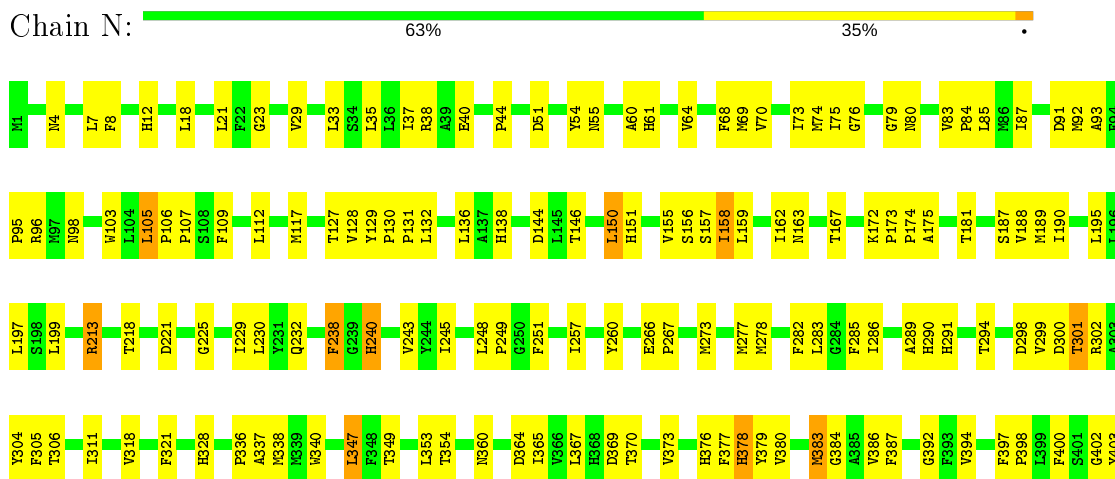
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

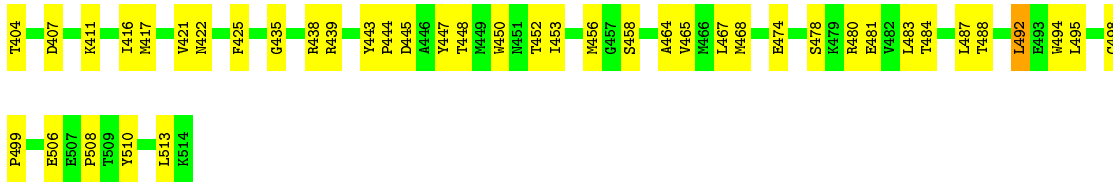
Note EDS was not executed.

- Molecule 1: CYTOCHROME C OXIDASE



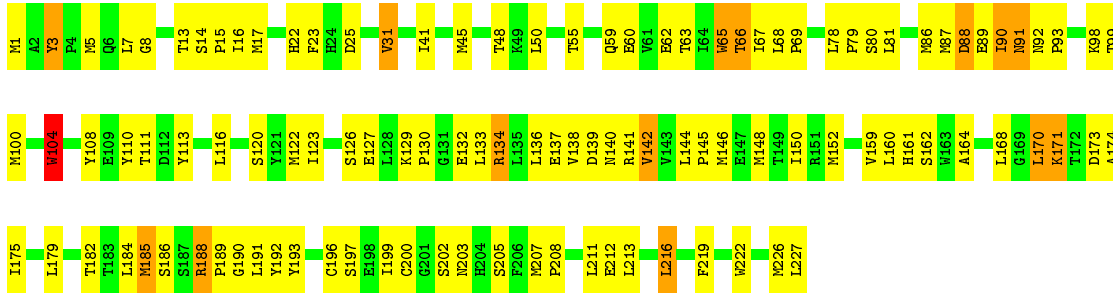
- Molecule 1: CYTOCHROME C OXIDASE





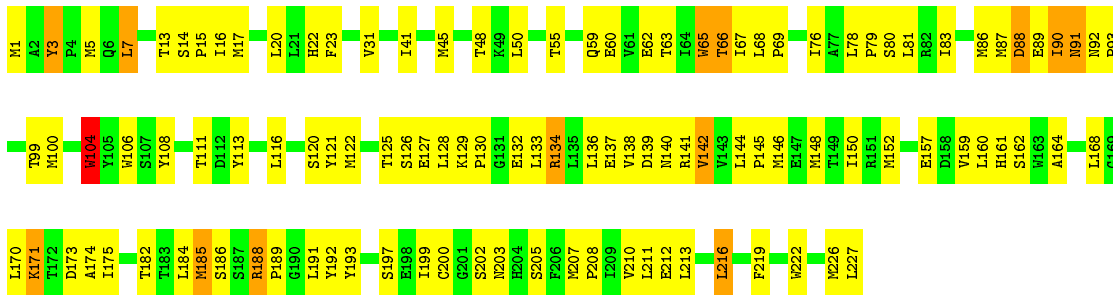
- Molecule 2: CYTOCHROME C OXIDASE

Chain B: 51% 42% 6%



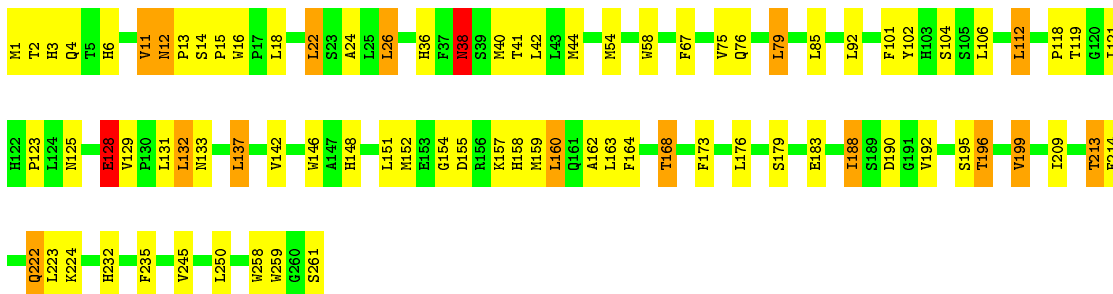
- Molecule 2: CYTOCHROME C OXIDASE

Chain O: 51% 43% 6%



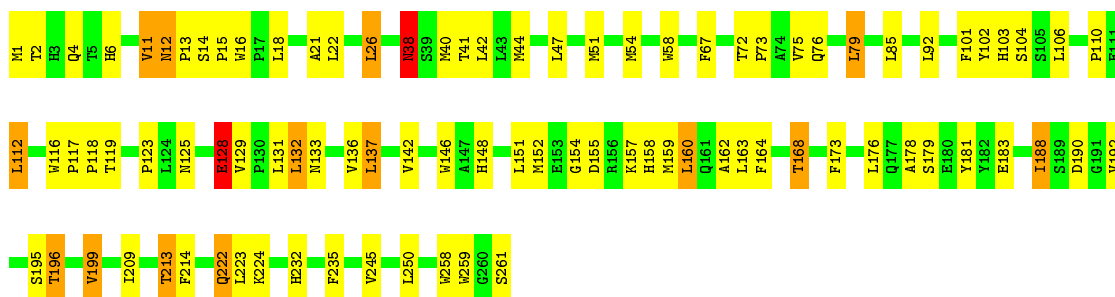
- Molecule 3: CYTOCHROME C OXIDASE

Chain C: 68% 25% 6%

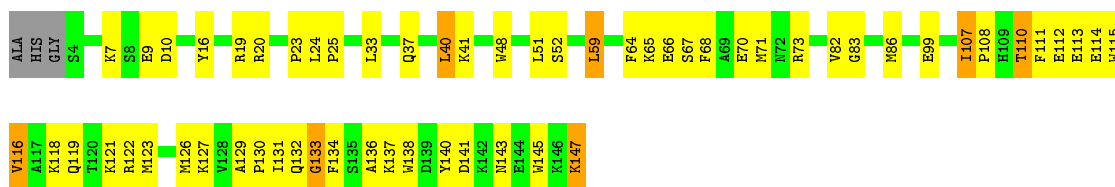


- Molecule 3: CYTOCHROME C OXIDASE

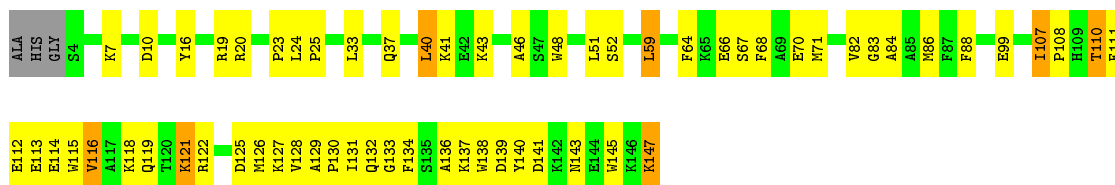
Chain P: 65% 29% 5%



- Molecule 4: CYTOCHROME C OXIDASE



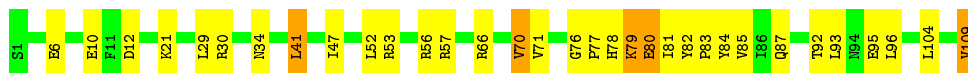
- Molecule 4: CYTOCHROME C OXIDASE



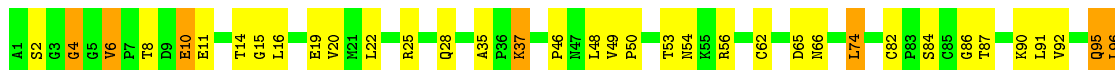
- Molecule 5: CYTOCHROME C OXIDASE



- Molecule 5: CYTOCHROME C OXIDASE



- Molecule 6: CYTOCHROME C OXIDASE



A97  
H98

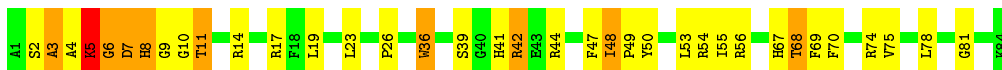
- Molecule 6: CYTOCHROME C OXIDASE

Chain S: 57% 34% 9%

A97  
H98

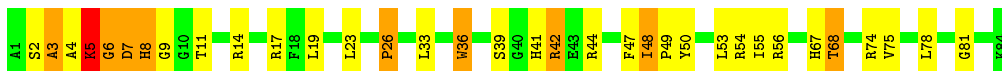
- Molecule 7: CYTOCHROME C OXIDASE

Chain G: 57% 31% 11%



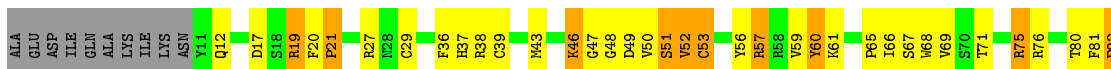
- Molecule 7: CYTOCHROME C OXIDASE

Chain T: 60% 29% 11%



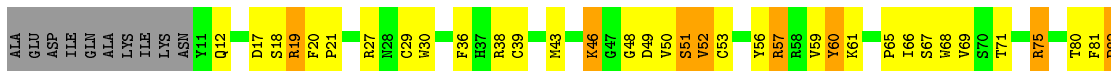
- Molecule 8: CYTOCHROME C OXIDASE

Chain H: 44% 33% 12% 12%

G83  
R84  
I85

- Molecule 8: CYTOCHROME C OXIDASE

Chain U: 45% 34% 9% 12%

G83  
R84  
I85

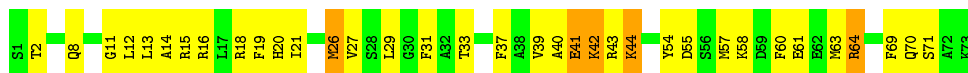
- Molecule 9: CYTOCHROME C OXIDASE

Chain I: 51% 44% 5%



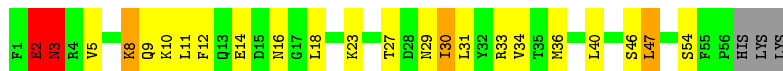
- Molecule 9: CYTOCHROME C OXIDASE

Chain V:  52% 41% 7%



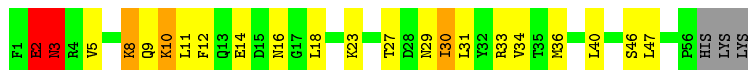
- Molecule 10: CYTOCHROME C OXIDASE

Chain J:  56% 31% 5% 5%



- Molecule 10: CYTOCHROME C OXIDASE

Chain W:  58% 29% 5% 5%



- Molecule 11: CYTOCHROME C OXIDASE

Chain K:  59% 25% 13%



- Molecule 11: CYTOCHROME C OXIDASE

Chain X:  57% 25% 5% 13%



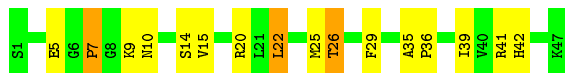
- Molecule 12: CYTOCHROME C OXIDASE

Chain L:  68% 28% 4%



- Molecule 12: CYTOCHROME C OXIDASE

Chain Y:  66% 28% 6%



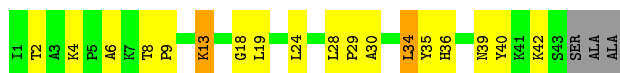
- Molecule 13: CYTOCHROME C OXIDASE

Chain M:  57% 35% 7%



● Molecule 13: CYTOCHROME C OXIDASE

Chain Z:  54% 35% 7%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.20Å 210.60Å 178.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90	Depositor
% Data completeness (in resolution range)	80.2 (7.00-2.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, $R_{free}$	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, MG, NA, ZN, HEA, CU

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	0.70	1/4164 (0.0%)	0.84	2/5688 (0.0%)
1	N	0.64	1/4164 (0.0%)	0.82	1/5688 (0.0%)
2	B	0.66	0/1909	0.89	2/2601 (0.1%)
2	O	0.62	0/1909	0.85	1/2601 (0.0%)
3	C	0.65	0/2211	0.77	1/3023 (0.0%)
3	P	0.61	0/2211	0.75	1/3023 (0.0%)
4	D	0.63	0/1229	0.71	1/1658 (0.1%)
4	Q	0.59	0/1229	0.69	1/1658 (0.1%)
5	E	0.60	0/898	0.72	0/1218
5	R	0.55	0/898	0.71	0/1218
6	F	0.63	0/765	0.86	0/1038
6	S	0.58	0/765	0.85	0/1038
7	G	0.59	0/699	0.81	1/950 (0.1%)
7	T	0.61	0/699	0.83	1/950 (0.1%)
8	H	0.62	0/648	0.73	0/877
8	U	0.62	0/648	0.73	0/877
9	I	0.65	0/611	0.70	0/810
9	V	0.64	0/611	0.70	0/810
10	J	0.64	0/451	0.73	0/610
10	W	0.62	0/451	0.70	0/610
11	K	0.68	0/398	0.70	0/546
11	X	0.54	0/398	0.69	0/546
12	L	0.65	0/399	0.68	0/534
12	Y	0.61	0/399	0.67	0/534
13	M	0.61	0/345	0.76	0/470
13	Z	0.57	0/345	0.73	0/470
All	All	0.64	2/29454 (0.0%)	0.79	12/40046 (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
1	A	0	4
1	N	0	3
2	B	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	378	HIS	CG-CD2	6.05	1.46	1.35
1	A	334	TRP	CB-CG	-5.31	1.40	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	LEU	CA-CB-CG	-7.17	98.81	115.30
3	P	92	LEU	CA-CB-CG	-6.78	99.71	115.30
4	D	133	GLY	N-CA-C	5.96	127.99	113.10
7	G	7	ASP	N-CA-C	5.90	126.93	111.00
1	N	435	GLY	N-CA-C	5.77	127.52	113.10
1	A	435	GLY	N-CA-C	5.61	127.12	113.10
7	T	7	ASP	N-CA-C	5.54	125.94	111.00
4	Q	133	GLY	N-CA-C	5.49	126.83	113.10
1	A	61	HIS	CG-CD2-NE2	-5.16	99.40	109.20
2	B	170	LEU	CA-CB-CG	5.08	126.98	115.30
2	O	134	ARG	N-CA-C	5.06	124.66	111.00
2	B	134	ARG	N-CA-C	5.04	124.60	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	A	372	TYR	Sidechain
1	A	61	HIS	Sidechain
2	B	110	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
1	N	61	HIS	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	4025	0	4002	164	0
1	N	4025	0	4002	167	0
2	B	1863	0	1867	100	0
2	O	1863	0	1867	104	0
3	C	2124	0	2044	75	0
3	P	2124	0	2044	82	0
4	D	1195	0	1183	57	0
4	Q	1195	0	1183	60	0
5	E	878	0	868	31	0
5	R	878	0	868	30	0
6	F	748	0	728	32	0
6	S	748	0	728	38	0
7	G	672	0	645	53	0
7	T	672	0	645	50	0
8	H	628	0	582	49	0
8	U	628	0	582	51	0
9	I	598	0	612	37	0
9	V	598	0	612	36	0
10	J	441	0	439	20	0
10	W	441	0	439	22	0
11	K	384	0	366	12	0
11	X	384	0	366	15	0
12	L	386	0	388	13	0
12	Y	386	0	388	15	0
13	M	335	0	352	13	0
13	Z	335	0	352	14	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
14	N	1	0	0	0	0
14	O	2	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	6	0	0	1	0
17	N	6	0	0	3	0
18	A	120	0	108	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	120	0	108	15	0
19	F	1	0	0	0	0
19	S	1	0	0	0	0
All	All	28818	0	28368	1117	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 20.

All (1117) 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:O:86:MET:O	2:O:89[B]:GLU:HG2	1.20	1.32
2:B:86:MET:O	2:B:89[B]:GLU:HG2	1.32	1.27
2:B:59:GLN:HA	2:B:62:GLU:HB2	1.30	1.07
2:O:59:GLN:HA	2:O:62:GLU:HB2	1.32	1.06
3:P:12:ASN:HD22	3:P:12:ASN:H	1.02	0.99
2:O:86:MET:O	2:O:89[B]:GLU:CG	2.11	0.98
3:C:12:ASN:H	3:C:12:ASN:HD22	0.99	0.98
1:A:506:GLU:HB2	3:C:1:MET:SD	2.11	0.91
3:P:12:ASN:ND2	3:P:12:ASN:H	1.68	0.91
8:H:39:CYS:HG	8:H:53:CYS:HG	0.93	0.91
1:N:492:LEU:HD23	1:N:495:LEU:HD12	1.53	0.91
3:C:12:ASN:ND2	3:C:12:ASN:H	1.69	0.90
2:B:86:MET:O	2:B:89[B]:GLU:CG	2.19	0.89
1:N:506:GLU:HB2	3:P:1:MET:SD	2.15	0.85
3:P:183:GLU:HB3	7:T:42:ARG:HH22	1.41	0.85
4:D:147:LYS:HE3	4:D:147:LYS:HA	1.59	0.84
3:C:183:GLU:HB3	7:G:42:ARG:HH22	1.41	0.84
1:A:492:LEU:HD23	1:A:495:LEU:HD12	1.61	0.82
18:A:515:HEA:HBC1	18:A:515:HEA:HMC1	1.62	0.82
1:N:92:MET:HE2	1:N:167:THR:HG21	1.60	0.81
1:N:347:LEU:HD11	17:N:521:AZI:N1	1.96	0.81
4:Q:147:LYS:HA	4:Q:147:LYS:HE3	1.61	0.80
8:H:39:CYS:HG	8:H:53:CYS:CB	1.94	0.80
1:A:218:THR:HG21	7:G:55:ILE:HD12	1.63	0.80
8:U:71:THR:O	8:U:75:ARG:HD3	1.82	0.80
4:Q:40:LEU:HD13	4:Q:59:LEU:HD13	1.63	0.80
4:D:40:LEU:HD13	4:D:59:LEU:HD13	1.64	0.80
3:P:155:ASP:HA	6:S:4:GLY:HA3	1.63	0.79
1:A:282:PHE:HB2	7:T:5:LYS:HB3	1.64	0.79
1:A:380:VAL:HG23	18:A:516:HEA:HBC1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:HB3	1:N:282:PHE:HB2	1.65	0.79
6:F:95:GLN:HE21	6:F:96:LEU:HD13	1.48	0.79
8:U:57:ARG:HB3	8:U:57:ARG:HH11	1.48	0.78
2:O:13:THR:HB	2:O:168:LEU:HD23	1.65	0.78
1:N:218:THR:HG21	7:T:55:ILE:HD12	1.66	0.78
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.66	0.78
3:C:12:ASN:HD22	3:C:12:ASN:N	1.81	0.77
1:N:127:THR:HB	1:N:129:TYR:CE1	2.19	0.77
6:S:95:GLN:HE21	6:S:96:LEU:HD13	1.48	0.77
1:N:92:MET:CE	1:N:167:THR:HG21	2.13	0.77
2:B:59:GLN:H	2:B:62:GLU:HG3	1.50	0.76
9:V:15:ARG:HD2	9:V:18:ARG:HH22	1.50	0.76
8:U:39:CYS:HG	8:U:53:CYS:HG	0.86	0.76
8:H:71:THR:O	8:H:75:ARG:HD3	1.84	0.76
3:P:209:ILE:O	3:P:213:THR:HG22	1.86	0.76
3:C:155:ASP:HA	6:F:4:GLY:HA3	1.66	0.76
8:H:57:ARG:HH11	8:H:57:ARG:HB3	1.49	0.76
2:B:152:MET:HB2	2:B:182:THR:HG23	1.68	0.75
9:I:15:ARG:HD2	9:I:18:ARG:HH22	1.51	0.75
2:O:59:GLN:H	2:O:62:GLU:HG3	1.51	0.75
2:O:152:MET:HB2	2:O:182:THR:HG23	1.68	0.75
1:N:380:VAL:HG23	18:N:516:HEA:HBC1	1.69	0.75
2:B:78:LEU:HB2	2:B:79:PRO:HD3	1.70	0.74
9:V:64:ARG:HH11	9:V:64:ARG:HB3	1.51	0.74
1:N:195:LEU:HD23	1:N:245:ILE:HD13	1.70	0.74
1:A:92:MET:CE	1:A:167:THR:HG21	2.18	0.73
1:A:92:MET:HE2	1:A:167:THR:HG21	1.69	0.73
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.70	0.73
5:E:79:LYS:H	5:E:79:LYS:HD3	1.53	0.73
1:N:172:LYS:HB2	1:N:172:LYS:NZ	2.02	0.73
4:Q:130:PRO:O	4:Q:136:ALA:HB2	1.88	0.73
3:C:209:ILE:O	3:C:213:THR:HG22	1.89	0.73
1:N:298:ASP:HB2	1:N:301:THR:HG23	1.70	0.73
7:T:42:ARG:HD2	7:T:74:ARG:NH2	2.04	0.73
8:H:39:CYS:SG	8:H:53:CYS:CB	2.77	0.72
6:F:53:THR:HG22	6:F:54:ASN:OD1	1.90	0.71
3:P:154:GLY:HA2	6:S:6:VAL:HG22	1.70	0.71
7:G:42:ARG:HD2	7:G:74:ARG:NH2	2.05	0.71
6:S:48:LEU:O	6:S:50:PRO:HD3	1.90	0.71
3:P:112:LEU:HG	3:P:118:PRO:HB3	1.73	0.71
4:Q:16:TYR:CE1	4:Q:25:PRO:HG3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:53:THR:HG22	6:S:54:ASN:OD1	1.90	0.70
8:U:39:CYS:SG	8:U:53:CYS:CB	2.79	0.70
2:B:22:HIS:CE1	9:I:44:LYS:HD3	2.26	0.70
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.71	0.70
6:F:48:LEU:O	6:F:50:PRO:HD3	1.90	0.70
7:G:9:GLY:HA2	7:G:19:LEU:HD11	1.73	0.70
5:R:79:LYS:HD3	5:R:79:LYS:H	1.55	0.70
7:T:42:ARG:HD2	7:T:74:ARG:HH22	1.57	0.70
1:N:132:LEU:HD22	2:O:200:CYS:HA	1.73	0.70
2:B:59:GLN:HA	2:B:62:GLU:CB	2.18	0.70
6:F:16:LEU:O	6:F:20:VAL:HG13	1.93	0.69
3:P:164:PHE:O	3:P:168:THR:HG23	1.92	0.69
1:A:298:ASP:HB2	1:A:301:THR:HG23	1.73	0.69
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.73	0.69
2:O:78:LEU:HB2	2:O:79:PRO:HD3	1.74	0.69
1:A:127:THR:HB	1:A:129:TYR:CE1	2.28	0.69
4:D:16:TYR:CE1	4:D:25:PRO:HG3	2.28	0.68
3:P:157:LYS:HE3	3:P:158:HIS:CD2	2.27	0.68
3:C:112:LEU:HG	3:C:118:PRO:HB3	1.74	0.68
6:S:53:THR:HG22	6:S:54:ASN:H	1.59	0.68
10:W:29:ASN:O	10:W:33:ARG:HG3	1.94	0.68
2:B:13:THR:HB	2:B:168:LEU:HD23	1.76	0.68
4:D:130:PRO:O	4:D:136:ALA:HB2	1.94	0.68
7:G:48:ILE:CD1	8:H:80:THR:HG22	2.24	0.68
3:P:183:GLU:HB3	7:T:42:ARG:NH2	2.09	0.68
9:I:64:ARG:HH11	9:I:64:ARG:HB3	1.59	0.67
2:B:129:LYS:O	2:B:132:GLU:HG3	1.94	0.67
1:A:172:LYS:NZ	1:A:172:LYS:HB2	2.09	0.67
2:B:188:ARG:HG3	9:I:54:TYR:OH	1.95	0.67
12:L:25:MET:HE3	12:L:29:PHE:HE2	1.60	0.67
8:U:39:CYS:HG	8:U:53:CYS:CB	2.06	0.67
7:G:42:ARG:HD2	7:G:74:ARG:HH22	1.58	0.67
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.09	0.67
7:T:48:ILE:CD1	8:U:80:THR:HG22	2.24	0.67
6:S:28:GLN:OE1	6:S:96:LEU:HD21	1.95	0.66
9:I:55:ASP:HB3	9:I:58:LYS:HB3	1.77	0.66
3:C:183:GLU:HB3	7:G:42:ARG:NH2	2.09	0.66
2:B:1:MET:SD	2:B:133:LEU:HD11	2.34	0.66
10:J:36:MET:O	10:J:40:LEU:HG	1.95	0.66
2:B:132:GLU:HA	4:D:122:ARG:NH1	2.11	0.66
6:F:53:THR:HG22	6:F:54:ASN:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:24:PHE:O	11:X:28:VAL:HG23	1.96	0.66
7:T:67:HIS:CD2	7:T:78:LEU:HD11	2.31	0.65
1:A:197:LEU:HD12	7:T:4:ALA:HB2	1.76	0.65
10:W:30:ILE:HG13	10:W:31:LEU:N	2.12	0.65
10:W:30:ILE:O	10:W:34:VAL:HG23	1.97	0.65
1:N:452:THR:O	1:N:456:MET:HG3	1.95	0.65
1:A:294:THR:HG21	2:B:171:LYS:HG2	1.77	0.65
6:F:53:THR:HG22	6:F:54:ASN:N	2.12	0.65
10:W:36:MET:O	10:W:40:LEU:HG	1.96	0.65
6:S:16:LEU:O	6:S:20:VAL:HG13	1.96	0.65
9:V:55:ASP:HB3	9:V:58:LYS:HB3	1.77	0.65
1:N:422:ASN:OD1	17:N:521:AZI:N3	2.29	0.65
1:N:484:THR:HB	13:Z:2:THR:CG2	2.26	0.64
3:C:157:LYS:HE3	3:C:158:HIS:CD2	2.32	0.64
8:H:39:CYS:SG	8:H:53:CYS:HB3	2.37	0.64
10:J:3:ASN:ND2	10:J:5:VAL:HG12	2.12	0.64
9:V:15:ARG:HD2	9:V:18:ARG:NH2	2.13	0.64
12:Y:25:MET:HE3	12:Y:29:PHE:HE2	1.62	0.64
3:C:154:GLY:HA2	6:F:6:VAL:HG22	1.80	0.64
4:Q:82:VAL:O	4:Q:86:MET:HG3	1.97	0.64
3:C:164:PHE:O	3:C:168:THR:HG23	1.98	0.64
11:K:24:PHE:O	11:K:28:VAL:HG23	1.97	0.64
2:O:1:MET:SD	2:O:133:LEU:HD11	2.37	0.64
10:W:3:ASN:ND2	10:W:5:VAL:HG12	2.12	0.64
1:A:98:ASN:HB2	1:A:163:ASN:ND2	2.12	0.64
4:D:130:PRO:HG2	4:D:131:ILE:HG13	1.79	0.64
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.80	0.64
1:A:132:LEU:HD22	2:B:200:CYS:HA	1.78	0.64
3:C:160:LEU:HD13	3:C:222:GLN:HG2	1.79	0.64
2:O:188:ARG:HG3	9:V:54:TYR:OH	1.98	0.64
1:A:243:VAL:HB	18:A:516:HEA:HAC	1.79	0.64
2:O:1:MET:SD	2:O:133:LEU:CD1	2.86	0.64
2:O:188:ARG:HH11	2:O:188:ARG:HG2	1.63	0.64
7:T:36:TRP:HA	7:T:39:SER:HB3	1.80	0.64
1:A:92:MET:HA	1:A:92:MET:HE3	1.79	0.63
10:J:30:ILE:O	10:J:34:VAL:HG23	1.98	0.63
1:A:484:THR:HB	13:M:2:THR:CG2	2.28	0.63
7:G:4:ALA:HB2	1:N:197:LEU:HD12	1.80	0.63
1:N:243:VAL:HB	18:N:516:HEA:HAC	1.81	0.63
4:Q:67:SER:OG	4:Q:70:GLU:HG3	1.98	0.63
4:Q:130:PRO:HG2	4:Q:131:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:HZ3	1:A:172:LYS:HB2	1.63	0.63
1:A:506:GLU:CB	3:C:1:MET:SD	2.84	0.63
2:O:22:HIS:CE1	9:V:44:LYS:HD3	2.32	0.63
8:H:53:CYS:HA	8:U:46:LYS:HZ1	1.64	0.63
2:O:90[A]:ILE:H	2:O:90[A]:ILE:HD12	1.64	0.63
3:P:12:ASN:HD22	3:P:12:ASN:N	1.83	0.63
8:U:39:CYS:SG	8:U:53:CYS:HB3	2.39	0.63
1:N:225:GLY:HA3	3:P:112:LEU:CD1	2.29	0.62
2:B:164:ALA:HB2	2:B:171:LYS:HD3	1.80	0.62
9:I:15:ARG:HD2	9:I:18:ARG:NH2	2.14	0.62
9:I:40:ALA:O	9:I:44:LYS:HE2	1.99	0.62
4:Q:64:PHE:CE1	5:R:66:ARG:HD2	2.35	0.62
6:S:37:LYS:H	6:S:37:LYS:CD	2.11	0.62
1:N:92:MET:HE2	1:N:167:THR:CG2	2.30	0.62
3:P:104:SER:HB3	3:P:192:VAL:HG11	1.81	0.62
2:B:226:MET:O	2:B:227:LEU:HB2	1.98	0.62
1:A:398:PRO:O	1:A:498:CYS:HB3	1.99	0.62
4:D:23:PRO:O	5:E:66:ARG:HD3	1.98	0.62
1:N:294:THR:HG21	2:O:171:LYS:HG2	1.82	0.62
3:P:154:GLY:C	6:S:6:VAL:HG13	2.20	0.62
2:B:13:THR:HG21	2:B:192:TYR:CE2	2.35	0.62
1:A:488:THR:HG22	1:A:494:TRP:HB2	1.82	0.62
1:A:76:GLY:O	1:A:80:ASN:HB2	2.00	0.62
2:B:50:LEU:HD21	5:E:77:PRO:HD2	1.81	0.62
3:C:104:SER:HB3	3:C:192:VAL:HG11	1.82	0.61
3:P:160:LEU:HD13	3:P:222:GLN:HG2	1.80	0.61
10:J:30:ILE:HG13	10:J:31:LEU:N	2.14	0.61
7:G:6:GLY:HA3	1:N:190:ILE:HG12	1.81	0.61
8:H:75:ARG:HH11	8:H:75:ARG:HG2	1.63	0.61
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.82	0.61
6:S:10:GLU:HG2	6:S:25:ARG:HH22	1.64	0.61
6:S:53:THR:HG22	6:S:54:ASN:N	2.15	0.61
13:M:13:LYS:HD3	13:M:13:LYS:H	1.66	0.61
1:A:225:GLY:HA3	3:C:112:LEU:CD1	2.31	0.61
3:C:148:HIS:O	3:C:152:MET:HG2	2.01	0.61
4:Q:132:GLN:NE2	9:V:42:LYS:HE3	2.15	0.61
7:T:47:PHE:CE2	7:T:81:GLY:HA2	2.36	0.61
9:V:11:GLY:O	9:V:15:ARG:HD3	2.01	0.61
1:A:291:HIS:CE1	17:A:520:AZI:N3	2.68	0.61
2:O:164:ALA:HB2	2:O:171:LYS:HD3	1.83	0.61
2:O:59:GLN:HA	2:O:62:GLU:CB	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:PRO:HG3	1:N:92:MET:HE3	1.83	0.61
6:F:48:LEU:HB3	6:F:92:VAL:HG21	1.82	0.60
7:G:42:ARG:HD3	7:G:75:VAL:HG11	1.82	0.60
2:O:189:PRO:HG2	9:V:63:MET:HE3	1.83	0.60
2:B:1:MET:SD	2:B:133:LEU:CD1	2.90	0.60
7:G:67:HIS:CD2	7:G:78:LEU:HD11	2.36	0.60
8:H:53:CYS:HA	8:U:46:LYS:NZ	2.15	0.60
1:N:240:HIS:O	1:N:243:VAL:HG22	2.01	0.60
1:N:84:PRO:HG3	1:N:92:MET:CE	2.31	0.60
2:O:226:MET:O	2:O:227:LEU:HB2	2.01	0.60
1:A:452:THR:O	1:A:456:MET:HG3	2.01	0.60
3:P:119:THR:HG21	8:U:82:PRO:O	2.02	0.60
2:B:90[A]:ILE:HD12	2:B:90[A]:ILE:H	1.65	0.60
8:H:51:SER:HB3	8:U:48:GLY:O	2.00	0.60
4:Q:37:GLN:O	4:Q:41:LYS:HG2	2.02	0.60
2:B:87:MET:O	2:B:89[B]:GLU:N	2.32	0.60
2:B:189:PRO:HG2	9:I:63:MET:HE3	1.84	0.60
4:D:82:VAL:O	4:D:86:MET:HG3	2.01	0.60
6:F:28:GLN:OE1	6:F:96:LEU:HD21	2.01	0.60
7:G:36:TRP:HA	7:G:39:SER:HB3	1.82	0.60
1:N:398:PRO:O	1:N:498:CYS:HB3	2.02	0.60
4:Q:130:PRO:HG2	4:Q:131:ILE:H	1.67	0.60
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.84	0.60
13:Z:6:ALA:O	13:Z:9:PRO:HD3	2.02	0.60
7:G:47:PHE:CE2	7:G:81:GLY:HA2	2.37	0.60
1:N:76:GLY:O	1:N:80:ASN:HB2	2.01	0.60
4:Q:66:GLU:O	5:R:66:ARG:NH2	2.35	0.60
1:N:172:LYS:HB2	1:N:172:LYS:HZ3	1.65	0.60
2:B:90[B]:ILE:HD11	2:B:93:PRO:HD3	1.84	0.59
1:N:195:LEU:CD2	1:N:245:ILE:HD13	2.31	0.59
3:P:4:GLN:NE2	3:P:6:HIS:O	2.35	0.59
1:A:240:HIS:O	1:A:243:VAL:HG22	2.03	0.59
4:D:130:PRO:HG2	4:D:131:ILE:H	1.67	0.59
9:I:41:GLU:OE1	9:I:41:GLU:HA	2.02	0.59
2:O:216:LEU:O	2:O:219:PHE:HB3	2.01	0.59
1:A:380:VAL:CG2	18:A:516:HEA:HBC1	2.31	0.59
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.37	0.59
1:N:488:THR:HG22	1:N:494:TRP:HB2	1.83	0.59
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.32	0.59
4:D:132:GLN:NE2	9:I:42:LYS:HE3	2.16	0.59
11:X:26:VAL:O	11:X:30:VAL:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:41:GLU:OE1	9:V:41:GLU:HA	2.02	0.59
3:C:12:ASN:ND2	3:C:12:ASN:N	2.47	0.59
1:A:117:MET:HE3	12:L:39:ILE:HG23	1.84	0.59
2:B:216:LEU:O	2:B:219:PHE:HB3	2.01	0.59
7:T:9:GLY:HA2	7:T:19:LEU:HD11	1.85	0.59
2:B:68:LEU:HB3	2:B:69:PRO:HD3	1.83	0.59
6:F:10:GLU:HG2	6:F:25:ARG:HH22	1.66	0.59
1:N:422:ASN:OD1	17:N:521:AZI:N1	2.36	0.59
7:T:42:ARG:HD3	7:T:75:VAL:HG11	1.84	0.59
1:A:117:MET:CE	12:L:39:ILE:HG23	2.33	0.59
6:S:22:LEU:O	6:S:25:ARG:HG2	2.03	0.59
8:H:19:ARG:HG3	8:H:20:PHE:CE2	2.38	0.59
1:A:190:ILE:HG12	7:T:6:GLY:HA3	1.85	0.59
8:U:81:PHE:CE2	8:U:85:ILE:HD11	2.37	0.59
6:F:37:LYS:CD	6:F:37:LYS:H	2.14	0.58
7:G:7:ASP:O	7:G:8:HIS:HB2	2.03	0.58
5:R:95:GLU:HG2	5:R:96:LEU:HD23	1.85	0.58
8:U:39:CYS:O	8:U:43:MET:HG2	2.03	0.58
9:V:42:LYS:HE2	9:V:43:ARG:N	2.18	0.58
10:J:29:ASN:O	10:J:33:ARG:HG3	2.02	0.58
2:O:111:THR:HG21	8:U:66:ILE:HD11	1.83	0.58
3:P:54:MET:HB3	3:P:58:TRP:CZ3	2.38	0.58
1:A:187:SER:HB2	1:A:277:MET:HE1	1.86	0.58
6:F:62:CYS:SG	6:F:84:SER:OG	2.59	0.58
7:G:4:ALA:O	7:G:6:GLY:N	2.36	0.58
6:S:62:CYS:SG	6:S:84:SER:OG	2.62	0.58
7:T:4:ALA:O	7:T:6:GLY:N	2.37	0.58
3:P:76:GLN:HA	3:P:79:LEU:HD12	1.85	0.58
8:U:75:ARG:HH11	8:U:75:ARG:HG2	1.68	0.58
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.58
2:B:120:SER:OG	2:B:138:VAL:HG21	2.03	0.58
3:C:67:PHE:HA	10:J:9:GLN:HG2	1.85	0.58
2:O:116:LEU:HD11	2:O:226:MET:HG3	1.84	0.58
3:C:54:MET:HB3	3:C:58:TRP:CZ3	2.38	0.58
4:D:37:GLN:O	4:D:41:LYS:HG2	2.04	0.58
5:R:41:LEU:O	5:R:41:LEU:HD12	2.03	0.58
7:T:42:ARG:NH1	7:T:74:ARG:HH21	2.00	0.58
8:H:46:LYS:NZ	8:U:53:CYS:HA	2.19	0.58
2:O:191:LEU:HB2	4:Q:126:MET:HE3	1.86	0.58
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.86	0.58
1:N:144:ASP:OD1	1:N:213:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:42:ARG:NH1	7:G:74:ARG:HH21	2.02	0.57
9:I:11:GLY:O	9:I:15:ARG:HD3	2.03	0.57
1:N:92:MET:HA	1:N:92:MET:HE3	1.86	0.57
2:B:141:ARG:HD2	2:B:212:GLU:OE1	2.04	0.57
1:A:484:THR:HB	13:M:2:THR:HG23	1.86	0.57
3:P:154:GLY:HA2	6:S:6:VAL:CG2	2.34	0.57
8:U:57:ARG:HB3	8:U:57:ARG:NH1	2.18	0.57
1:N:450:TRP:HE3	1:N:453:ILE:HD12	1.69	0.57
1:A:84:PRO:HG3	1:A:92:MET:CE	2.35	0.57
3:C:101:PHE:CE2	3:C:259:TRP:HZ3	2.23	0.57
8:U:38:ARG:HG2	8:U:85:ILE:HA	1.87	0.57
2:O:120:SER:OG	2:O:138:VAL:HG21	2.04	0.57
8:U:19:ARG:HG3	8:U:20:PHE:CE2	2.40	0.57
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.87	0.57
4:D:33:LEU:HD22	4:D:37:GLN:HB3	1.86	0.57
13:Z:13:LYS:H	13:Z:13:LYS:HD3	1.70	0.57
2:B:188:ARG:HH11	2:B:188:ARG:HG2	1.69	0.57
9:I:27:VAL:HG12	9:I:31:PHE:HE2	1.70	0.57
1:N:484:THR:HB	13:Z:2:THR:HG23	1.86	0.57
2:O:141:ARG:HD2	2:O:212:GLU:OE1	2.05	0.57
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.87	0.57
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.40	0.57
8:U:36:PHE:HB2	8:U:56:TYR:CB	2.35	0.57
1:A:62:ALA:HB2	18:A:515:HEA:HBD1	1.86	0.56
3:C:76:GLN:HA	3:C:79:LEU:HD12	1.86	0.56
4:D:24:LEU:HB3	5:E:30:ARG:HG2	1.86	0.56
6:S:37:LYS:H	6:S:37:LYS:HD3	1.70	0.56
7:G:44:ARG:HD2	7:G:74:ARG:O	2.04	0.56
7:T:7:ASP:O	7:T:8:HIS:HB2	2.05	0.56
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.39	0.56
4:D:66:GLU:O	5:E:66:ARG:NH2	2.37	0.56
9:I:42:LYS:HE2	9:I:43:ARG:N	2.21	0.56
4:D:67:SER:OG	4:D:70:GLU:HG3	2.05	0.56
5:E:53:ARG:HG2	5:E:96:LEU:HD11	1.88	0.56
10:J:2:GLU:CG	10:J:3:ASN:H	2.17	0.56
2:O:13:THR:HG21	2:O:192:TYR:CE2	2.41	0.56
3:C:154:GLY:C	6:F:6:VAL:HG13	2.25	0.56
8:H:17:ASP:OD1	8:H:19:ARG:HG2	2.05	0.56
3:P:195:SER:O	3:P:199:VAL:HG13	2.04	0.56
5:R:53:ARG:NH1	5:R:92:THR:HG23	2.21	0.56
9:V:27:VAL:HG12	9:V:31:PHE:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:LEU:HD22	3:C:173:PHE:CE2	2.41	0.56
8:H:36:PHE:HB2	8:H:56:TYR:CB	2.35	0.56
3:P:148:HIS:HB2	3:P:235:PHE:HE2	1.70	0.56
3:P:101:PHE:CE2	3:P:259:TRP:HZ3	2.23	0.56
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.88	0.56
3:P:148:HIS:O	3:P:152:MET:HG2	2.05	0.56
3:C:148:HIS:HB2	3:C:235:PHE:HE2	1.69	0.56
2:O:129:LYS:O	2:O:132:GLU:HG3	2.06	0.56
6:S:48:LEU:HB3	6:S:92:VAL:HG21	1.86	0.56
7:T:56:ARG:HG2	7:T:56:ARG:HH11	1.71	0.56
7:G:23:LEU:O	7:G:26:PRO:HD2	2.05	0.56
8:H:57:ARG:NH1	8:H:57:ARG:HB3	2.18	0.56
2:O:90[B]:ILE:HD11	2:O:93:PRO:HD3	1.87	0.56
8:H:46:LYS:HZ2	8:U:53:CYS:HA	1.71	0.56
1:A:12:HIS:HD2	1:A:80:ASN:O	1.88	0.56
8:H:48:GLY:O	8:U:51:SER:HB3	2.05	0.56
3:C:190:ASP:HB3	7:G:53:LEU:HD22	1.87	0.55
8:U:18:SER:O	8:U:21:PRO:HD3	2.06	0.55
10:W:2:GLU:CG	10:W:3:ASN:H	2.19	0.55
6:F:22:LEU:O	6:F:25:ARG:HG2	2.06	0.55
1:N:127:THR:HB	1:N:129:TYR:CD1	2.40	0.55
1:A:450:TRP:HE3	1:A:453:ILE:HD12	1.71	0.55
1:N:380:VAL:CG2	18:N:516:HEA:HBC1	2.35	0.55
1:A:92:MET:HE2	1:A:167:THR:CG2	2.36	0.55
3:P:137:LEU:HD22	3:P:173:PHE:CE2	2.42	0.55
4:Q:137:LYS:O	4:Q:145:TRP:HE3	1.89	0.55
9:V:40:ALA:O	9:V:44:LYS:HE2	2.07	0.55
1:N:513:LEU:HD22	6:S:35:ALA:HB3	1.87	0.55
1:A:513:LEU:HD22	6:F:35:ALA:HB3	1.88	0.55
3:C:4:GLN:NE2	3:C:6:HIS:O	2.40	0.55
8:H:65:PRO:HG2	8:H:68:TRP:CD1	2.42	0.55
2:O:87:MET:O	2:O:89[B]:GLU:N	2.38	0.55
6:S:95:GLN:HB2	6:S:96:LEU:HD12	1.89	0.55
1:A:197:LEU:HD12	7:T:4:ALA:CB	2.36	0.55
2:B:189:PRO:O	9:I:63:MET:HE1	2.07	0.55
3:C:222:GLN:HE21	3:C:222:GLN:HA	1.72	0.55
4:D:40:LEU:CD1	4:D:59:LEU:HD13	2.35	0.55
1:A:257:ILE:HD11	1:A:392:GLY:HA2	1.88	0.55
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.89	0.55
2:O:184:LEU:HD11	2:O:211:LEU:HD21	1.88	0.55
7:G:48:ILE:HD11	8:H:80:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:98:ASN:HB2	1:N:163:ASN:ND2	2.22	0.54
2:O:106:TRP:NE1	2:O:207:MET:HE3	2.22	0.54
5:E:78:HIS:CE1	9:I:12:LEU:HD22	2.42	0.54
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.88	0.54
1:A:189:MET:SD	7:T:7:ASP:HB2	2.46	0.54
1:A:74:MET:HE3	1:A:249:PRO:HB2	1.89	0.54
2:O:76:ILE:O	2:O:79:PRO:HD2	2.07	0.54
2:O:161:HIS:HB2	2:O:174:ALA:HB3	1.89	0.54
2:O:3:TYR:N	2:O:3:TYR:CD1	2.76	0.54
5:E:95:GLU:HG2	5:E:96:LEU:HD23	1.88	0.54
2:B:111:THR:HG21	8:H:66:ILE:HD11	1.88	0.54
11:K:26:VAL:O	11:K:30:VAL:HB	2.07	0.54
1:N:257:ILE:HD11	1:N:392:GLY:HA2	1.89	0.54
1:A:225:GLY:HA3	3:C:112:LEU:HD11	1.90	0.54
2:O:136:LEU:HB3	2:O:193:TYR:CD2	2.42	0.54
4:Q:23:PRO:O	5:R:66:ARG:HD3	2.08	0.54
4:D:64:PHE:CE1	5:E:66:ARG:HD2	2.42	0.54
1:N:506:GLU:CB	3:P:1:MET:SD	2.91	0.54
3:C:224:LYS:HB3	3:C:224:LYS:NZ	2.23	0.54
1:N:299:VAL:HA	1:N:302:ARG:NH1	2.23	0.54
1:N:367:LEU:O	1:N:370:THR:HG23	2.08	0.54
1:A:299:VAL:HA	1:A:302:ARG:NH1	2.23	0.53
2:B:191:LEU:HB2	4:D:126:MET:HE3	1.90	0.53
1:N:151:HIS:O	1:N:155:VAL:HG23	2.08	0.53
4:D:48:TRP:HA	4:D:51:LEU:HD12	1.91	0.53
1:A:367:LEU:O	1:A:370:THR:HG23	2.08	0.53
2:B:3:TYR:CD1	2:B:3:TYR:N	2.77	0.53
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	1.89	0.53
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.38	0.53
6:F:95:GLN:HB2	6:F:96:LEU:HD12	1.91	0.53
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.91	0.53
5:R:80:GLU:CD	5:R:80:GLU:H	2.11	0.53
1:A:510:TYR:HB2	6:F:56:ARG:NH1	2.24	0.53
2:O:41:ILE:O	2:O:45:MET:HG2	2.08	0.53
3:P:224:LYS:HB3	3:P:224:LYS:NZ	2.24	0.53
7:T:44:ARG:HD2	7:T:74:ARG:O	2.08	0.53
11:X:53:TRP:O	11:X:54:ARG:HB3	2.08	0.53
5:R:53:ARG:HG2	5:R:96:LEU:HD11	1.90	0.53
1:N:478:SER:HA	13:Z:8:THR:O	2.08	0.53
2:B:145:PRO:HG3	2:B:148:MET:HE1	1.91	0.53
7:G:7:ASP:HB2	1:N:189:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:22:LEU:O	12:L:26:THR:HB	2.09	0.53
6:F:48:LEU:HD23	6:F:90:LYS:HB3	1.90	0.53
1:N:128:VAL:O	1:N:128:VAL:HG22	2.09	0.53
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.09	0.53
1:N:75:ILE:O	1:N:79:GLY:HA3	2.09	0.53
1:N:117:MET:HA	1:N:117:MET:HE2	1.91	0.52
1:A:92:MET:CE	1:A:92:MET:HA	2.39	0.52
1:N:225:GLY:HA3	3:P:112:LEU:HD11	1.91	0.52
8:U:65:PRO:HG2	8:U:68:TRP:CD1	2.44	0.52
8:U:65:PRO:HG2	8:U:68:TRP:CG	2.44	0.52
4:D:83:GLY:HA3	11:K:18:LEU:HA	1.92	0.52
5:E:41:LEU:O	5:E:41:LEU:HD12	2.08	0.52
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.45	0.52
1:N:225:GLY:HA3	3:P:112:LEU:HD13	1.91	0.52
6:S:82:CYS:N	6:S:86:GLY:O	2.42	0.52
4:Q:107:ILE:HB	4:Q:108:PRO:HD2	1.91	0.52
4:Q:24:LEU:HB3	5:R:30:ARG:HG2	1.92	0.52
4:D:129:ALA:HB3	4:D:134:PHE:H	1.73	0.52
1:A:407:ASP:O	1:A:411:LYS:HG3	2.09	0.52
1:A:450:TRP:CE3	1:A:453:ILE:HD12	2.44	0.52
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.91	0.52
9:V:29:LEU:O	9:V:33:THR:HG23	2.10	0.52
1:A:84:PRO:HG3	1:A:92:MET:HE3	1.92	0.52
3:C:119:THR:HG21	8:H:82:PRO:O	2.10	0.52
6:F:82:CYS:N	6:F:86:GLY:O	2.43	0.52
8:H:38:ARG:HG2	8:H:85:ILE:HA	1.90	0.52
9:I:39:VAL:O	9:I:42:LYS:HE2	2.09	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.10	0.52
4:Q:138:TRP:CD1	4:Q:140:TYR:CD1	2.98	0.52
1:A:386:VAL:HG11	18:A:515:HEA:H261	1.92	0.52
4:D:137:LYS:O	4:D:145:TRP:HE3	1.91	0.52
4:D:68:PHE:HA	4:D:71:MET:HG2	1.92	0.52
5:E:53:ARG:NH1	5:E:92:THR:HG23	2.24	0.52
8:U:36:PHE:HB2	8:U:56:TYR:HB2	1.91	0.52
1:A:82:LEU:O	1:A:86:MET:HG3	2.10	0.52
1:N:266:GLU:HB2	1:N:267:PRO:HD2	1.92	0.52
2:B:152:MET:HB2	2:B:182:THR:CG2	2.39	0.51
2:B:16:ILE:HD12	2:B:17:MET:N	2.25	0.51
1:N:450:TRP:CE3	1:N:453:ILE:HD12	2.44	0.51
1:A:483:LEU:HB2	13:M:2:THR:OG1	2.10	0.51
1:N:416:ILE:HG22	1:N:464:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:136:LEU:HB3	2:O:193:TYR:HD2	1.75	0.51
4:Q:129:ALA:HB3	4:Q:134:PHE:H	1.74	0.51
1:N:187:SER:HB2	1:N:277:MET:HE1	1.93	0.51
6:S:48:LEU:HD23	6:S:90:LYS:HB3	1.92	0.51
1:A:51:ASP:HB2	2:B:202:SER:O	2.10	0.51
1:A:513:LEU:HD22	6:F:35:ALA:CB	2.40	0.51
7:G:48:ILE:HG13	7:G:50:TYR:CD2	2.45	0.51
10:J:3:ASN:C	10:J:3:ASN:HD22	2.13	0.51
4:D:107:ILE:HB	4:D:108:PRO:HD2	1.91	0.51
8:H:57:ARG:O	8:H:61:LYS:HB2	2.11	0.51
11:X:31:TYR:CD2	11:X:35:GLN:HB2	2.46	0.51
2:B:184:LEU:HD11	2:B:211:LEU:HD21	1.92	0.51
2:B:116:LEU:HD11	2:B:226:MET:HG3	1.92	0.51
1:N:403:TYR:CE1	12:Y:7:PRO:HB3	2.46	0.51
1:N:380:VAL:HG21	18:N:516:HEA:C2C	2.41	0.51
1:N:92:MET:CE	1:N:92:MET:HA	2.40	0.51
4:Q:110:THR:HG22	4:Q:115:TRP:CE2	2.46	0.51
10:W:30:ILE:HG13	10:W:31:LEU:H	1.75	0.51
12:Y:22:LEU:O	12:Y:26:THR:HB	2.10	0.51
2:O:144:LEU:HD22	2:O:150:ILE:HD13	1.93	0.51
3:P:12:ASN:N	3:P:12:ASN:ND2	2.45	0.51
4:Q:118:LYS:HA	11:X:51:LYS:O	2.11	0.51
7:T:48:ILE:HD12	7:T:49:PRO:N	2.25	0.51
8:U:38:ARG:HG2	8:U:85:ILE:HG23	1.92	0.51
9:V:39:VAL:O	9:V:42:LYS:HE2	2.11	0.51
2:B:146:MET:SD	2:B:189:PRO:HB3	2.51	0.51
13:M:6:ALA:O	13:M:9:PRO:HD3	2.11	0.51
3:P:222:GLN:HA	3:P:222:GLN:HE21	1.76	0.51
7:T:23:LEU:O	7:T:26:PRO:HD2	2.10	0.51
2:B:189:PRO:HG2	9:I:63:MET:CE	2.41	0.51
4:Q:128:VAL:O	4:Q:134:PHE:HB3	2.10	0.51
10:W:14:GLU:O	10:W:23:LYS:HE3	2.11	0.51
12:Y:5:GLU:O	12:Y:9:LYS:HD2	2.11	0.51
4:D:127:LYS:O	4:D:130:PRO:HD3	2.11	0.51
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.93	0.50
8:H:65:PRO:HG2	8:H:68:TRP:CG	2.46	0.50
2:O:104:TRP:N	2:O:104:TRP:CD1	2.79	0.50
5:R:6:GLU:HB2	5:R:10:GLU:HB2	1.93	0.50
4:D:40:LEU:HD22	4:D:59:LEU:HD13	1.93	0.50
7:G:4:ALA:CB	1:N:197:LEU:HD12	2.41	0.50
13:Z:30:ALA:O	13:Z:34:LEU:HD12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
3:C:133:ASN:HD21	3:C:176:LEU:HB3	1.76	0.50
3:P:154:GLY:HA2	6:S:6:VAL:HG13	1.94	0.50
8:U:57:ARG:O	8:U:61:LYS:HB2	2.12	0.50
5:E:6:GLU:HB2	5:E:10:GLU:HB2	1.93	0.50
1:N:51:ASP:HB2	2:O:202:SER:O	2.10	0.50
3:P:133:ASN:HD21	3:P:176:LEU:HB3	1.77	0.50
12:L:22:LEU:HD11	13:M:18:GLY:HA2	1.92	0.50
12:Y:41:ARG:HG3	13:Z:40:TYR:CE2	2.45	0.50
11:K:53:TRP:O	11:K:54:ARG:HB3	2.12	0.50
2:O:160:LEU:HD21	2:O:175:ILE:HG23	1.94	0.50
2:O:48:THR:HB	9:V:16:ARG:CZ	2.42	0.50
1:A:8:PHE:CE2	3:C:15:PRO:HB3	2.46	0.50
1:N:377:PHE:CD2	18:N:516:HEA:HAD1	2.47	0.50
1:N:302:ARG:O	1:N:306:THR:HG23	2.10	0.50
1:A:95:PRO:HB2	3:C:11:VAL:HG13	1.93	0.50
1:N:7:LEU:C	1:N:8:PHE:HD1	2.15	0.50
1:N:510:TYR:HB2	6:S:56:ARG:NH1	2.27	0.50
1:N:456:MET:SD	11:X:40:TRP:HH2	2.35	0.50
5:E:80:GLU:H	5:E:80:GLU:CD	2.15	0.49
1:A:456:MET:SD	11:K:40:TRP:HH2	2.35	0.49
1:N:23:GLY:HA3	1:N:73:ILE:HG13	1.94	0.49
2:O:13:THR:HG22	2:O:13:THR:O	2.12	0.49
2:O:5:MET:HE2	11:X:42:PRO:HA	1.94	0.49
1:A:378:HIS:CD2	1:A:425:PHE:CZ	3.00	0.49
1:A:69:MET:CE	1:A:70:VAL:HG23	2.42	0.49
3:C:151:LEU:HD21	3:C:232:HIS:CG	2.47	0.49
2:O:189:PRO:HG2	9:V:63:MET:CE	2.42	0.49
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.49
2:B:13:THR:O	2:B:13:THR:HG22	2.13	0.49
1:N:12:HIS:HD2	1:N:80:ASN:O	1.94	0.49
1:N:340:TRP:HH2	1:N:417:MET:HG2	1.77	0.49
2:O:145:PRO:HG3	2:O:148:MET:HE1	1.94	0.49
3:P:67:PHE:O	6:S:14:THR:HG21	2.12	0.49
13:Z:35:TYR:HD2	13:Z:36:HIS:CE1	2.30	0.49
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.93	0.49
1:A:481:GLU:HB2	13:M:4:LYS:HD2	1.95	0.49
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.48	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.12	0.49
5:E:53:ARG:O	5:E:56:ARG:HB3	2.13	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:51:SER:O	8:U:52:VAL:HG13	2.12	0.49
2:B:63:THR:O	2:B:66:THR:HG22	2.12	0.49
2:B:90[B]:ILE:HD11	2:B:93:PRO:CD	2.43	0.49
4:D:16:TYR:HE1	4:D:25:PRO:HG3	1.75	0.49
1:N:60:ALA:O	1:N:64:VAL:HG23	2.13	0.49
5:R:78:HIS:CE1	9:V:12:LEU:HD22	2.48	0.49
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.48	0.49
8:H:36:PHE:HB2	8:H:56:TYR:HB2	1.94	0.49
2:O:90[B]:ILE:HG23	2:O:91[B]:ASN:H	1.78	0.49
7:T:48:ILE:HG13	7:T:50:TYR:CD2	2.48	0.49
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.95	0.49
18:A:515:HEA:HMC1	18:A:515:HEA:CBC	2.38	0.49
1:A:7:LEU:C	1:A:8:PHE:HD1	2.15	0.49
2:O:134:ARG:HD2	4:Q:110:THR:OG1	2.12	0.49
4:D:66:GLU:HA	4:D:70:GLU:OE1	2.12	0.49
9:I:60:PHE:CE1	9:I:69:PHE:CE2	3.01	0.49
1:A:302:ARG:O	1:A:306:THR:HG23	2.13	0.49
2:B:89[B]:GLU:HB2	2:B:91[B]:ASN:ND2	2.28	0.49
2:B:87:MET:C	2:B:89[B]:GLU:H	2.12	0.49
10:J:16:ASN:OD1	10:J:18:LEU:HB2	2.13	0.49
1:N:402:GLY:HA3	1:N:499:PRO:HD3	1.95	0.48
4:Q:114:GLU:O	4:Q:118:LYS:HG2	2.13	0.48
8:H:39:CYS:O	8:H:43:MET:HG2	2.12	0.48
2:O:87:MET:C	2:O:89[B]:GLU:H	2.15	0.48
4:Q:83:GLY:HA3	11:X:18:LEU:HA	1.95	0.48
7:T:48:ILE:HD11	8:U:80:THR:HA	1.94	0.48
2:O:152:MET:HB2	2:O:182:THR:CG2	2.40	0.48
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.95	0.48
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.13	0.48
7:T:42:ARG:HH11	7:T:74:ARG:NH2	2.12	0.48
1:A:127:THR:HB	1:A:129:TYR:CD1	2.49	0.48
1:A:175:ALA:HB1	1:A:513:LEU:HD13	1.95	0.48
1:A:266:GLU:HB2	1:A:267:PRO:HD2	1.95	0.48
18:A:516:HEA:HMD1	18:A:516:HEA:HBD2	1.94	0.48
4:D:40:LEU:HD13	4:D:59:LEU:CD1	2.40	0.48
6:F:49:VAL:HG21	6:F:74:LEU:HD12	1.96	0.48
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.48
3:P:102:TYR:O	3:P:106:LEU:HB2	2.13	0.48
3:P:157:LYS:HE3	3:P:158:HIS:NE2	2.28	0.48
1:A:225:GLY:HA3	3:C:112:LEU:HD13	1.94	0.48
3:C:128:GLU:HB3	3:C:129:VAL:H	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ARG:HD2	4:D:110:THR:OG1	2.14	0.48
12:L:41:ARG:HG3	13:M:40:TYR:CE2	2.49	0.48
1:N:230:LEU:HB2	3:P:103:HIS:CD2	2.48	0.48
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.95	0.48
1:A:34:SER:HB3	1:A:61:HIS:CD2	2.48	0.48
1:N:172:LYS:HB2	1:N:172:LYS:HZ2	1.79	0.48
1:N:443:TYR:CD2	1:N:447:TYR:HB2	2.48	0.48
2:O:50:LEU:HB2	9:V:13:LEU:HD13	1.95	0.48
4:Q:113:GLU:O	4:Q:116:VAL:HG22	2.14	0.48
7:T:56:ARG:HG2	7:T:56:ARG:NH1	2.29	0.48
11:X:22:ALA:O	11:X:26:VAL:HG12	2.14	0.48
1:A:144:ASP:OD1	1:A:213:ARG:HD3	2.14	0.48
1:A:12:HIS:CD2	1:A:80:ASN:O	2.66	0.48
3:C:101:PHE:CE2	3:C:259:TRP:CZ3	3.01	0.48
10:J:30:ILE:HG13	10:J:31:LEU:H	1.77	0.48
18:N:515:HEA:HMC1	18:N:515:HEA:CBC	2.43	0.48
1:N:230:LEU:HD13	3:P:103:HIS:CG	2.49	0.48
4:Q:40:LEU:CD1	4:Q:59:LEU:HD13	2.38	0.48
7:T:48:ILE:HD12	7:T:48:ILE:C	2.34	0.48
6:F:37:LYS:HD3	6:F:37:LYS:H	1.77	0.48
9:I:61:GLU:OE1	9:I:64:ARG:NH1	2.47	0.48
10:W:8:LYS:HZ1	10:W:12:PHE:HE2	1.61	0.48
1:A:40:GLU:HG2	1:A:54:TYR:CD1	2.49	0.48
8:H:75:ARG:NH1	8:H:75:ARG:HG2	2.27	0.48
2:B:212:GLU:OE1	9:I:70:GLN:HG2	2.13	0.48
1:N:513:LEU:HD22	6:S:35:ALA:CB	2.44	0.48
8:H:49:ASP:HB2	8:U:49:ASP:HB2	1.96	0.48
1:A:44:PRO:HG3	4:D:111:PHE:CE2	2.49	0.48
2:B:14:SER:HB2	2:B:15:PRO:HD2	1.95	0.48
2:B:185:MET:SD	2:B:185:MET:C	2.92	0.48
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.48	0.48
1:N:117:MET:HE3	12:Y:39:ILE:HG23	1.96	0.48
2:O:89[B]:GLU:HB2	2:O:91[B]:ASN:ND2	2.28	0.48
5:R:81:ILE:O	5:R:85:VAL:HG23	2.14	0.48
7:T:42:ARG:HH11	7:T:75:VAL:HG11	1.79	0.48
3:C:22:LEU:HD12	3:C:22:LEU:HA	1.73	0.47
8:H:53:CYS:CA	8:U:46:LYS:NZ	2.76	0.47
9:I:29:LEU:O	9:I:33:THR:HG23	2.14	0.47
3:P:16:TRP:HE3	3:P:16:TRP:HA	1.79	0.47
1:N:403:TYR:CZ	12:Y:7:PRO:HB3	2.49	0.47
1:A:403:TYR:CE1	12:L:7:PRO:HB3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:404:THR:O	1:N:480:ARG:NH1	2.47	0.47
2:O:63:THR:O	2:O:66:THR:HG22	2.14	0.47
10:W:3:ASN:HD22	10:W:3:ASN:C	2.16	0.47
7:G:47:PHE:CZ	7:G:81:GLY:HA2	2.49	0.47
9:I:21:ILE:HD12	9:I:21:ILE:HA	1.77	0.47
1:N:175:ALA:HB1	1:N:513:LEU:HD13	1.97	0.47
1:N:380:VAL:HG21	18:N:516:HEA:C3C	2.44	0.47
1:N:38:ARG:HG3	1:N:458:SER:HB3	1.97	0.47
6:S:8:THR:OG1	6:S:11:GLU:HG2	2.14	0.47
1:A:443:TYR:CD2	1:A:447:TYR:HB2	2.50	0.47
2:B:5:MET:HE2	11:K:42:PRO:HA	1.96	0.47
1:N:248:LEU:O	1:N:251:PHE:HB2	2.13	0.47
1:N:481:GLU:HB2	13:Z:4:LYS:HD2	1.96	0.47
1:N:83:VAL:HG21	1:N:188:VAL:HG11	1.95	0.47
8:U:17:ASP:OD1	8:U:19:ARG:HG2	2.14	0.47
1:A:197:LEU:CD1	7:T:4:ALA:HB2	2.43	0.47
5:E:78:HIS:ND1	9:I:12:LEU:HD22	2.29	0.47
3:P:123:PRO:HB2	3:P:261:SER:HB3	1.96	0.47
4:Q:16:TYR:HE1	4:Q:25:PRO:HG3	1.75	0.47
10:W:11:LEU:HD23	10:W:11:LEU:C	2.35	0.47
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.49	0.47
7:G:56:ARG:HG2	7:G:56:ARG:HH11	1.79	0.47
1:N:40:GLU:HG2	1:N:54:TYR:CD1	2.50	0.47
3:P:101:PHE:CE2	3:P:259:TRP:CZ3	3.02	0.47
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.50	0.47
4:Q:112:GLU:O	4:Q:116:VAL:HG13	2.14	0.47
7:T:42:ARG:NH1	7:T:75:VAL:HG11	2.29	0.47
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.49	0.47
1:A:299:VAL:HG13	1:A:300:ASP:N	2.29	0.47
7:G:48:ILE:HD12	7:G:49:PRO:N	2.30	0.47
7:G:5:LYS:HE3	7:G:23:LEU:HD13	1.97	0.47
1:N:69:MET:CE	1:N:70:VAL:HG23	2.45	0.47
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.50	0.47
2:B:89[A]:GLU:HG2	2:B:90[A]:ILE:N	2.30	0.47
8:H:19:ARG:HG3	8:H:20:PHE:CD2	2.50	0.47
8:H:36:PHE:HB2	8:H:56:TYR:HB3	1.97	0.47
1:N:283:LEU:HD13	1:N:311:ILE:HG13	1.96	0.47
2:O:146:MET:SD	2:O:189:PRO:HB3	2.55	0.47
2:O:212:GLU:OE1	9:V:70:GLN:HG2	2.14	0.47
2:O:89[A]:GLU:HG2	2:O:90[A]:ILE:N	2.30	0.47
3:P:75:VAL:O	3:P:79:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:104:LEU:HA	5:R:104:LEU:HD23	1.77	0.47
7:T:42:ARG:HD3	7:T:75:VAL:CG1	2.45	0.47
7:G:36:TRP:C	7:G:36:TRP:CD1	2.87	0.47
1:N:439:ARG:HD3	2:O:199:ILE:HB	1.95	0.47
9:V:21:ILE:HA	9:V:21:ILE:HD12	1.82	0.47
1:A:248:LEU:O	1:A:251:PHE:HB2	2.15	0.46
2:B:104:TRP:CD1	2:B:104:TRP:N	2.81	0.46
4:D:70:GLU:HA	5:E:109:VAL:CG1	2.45	0.46
7:G:42:ARG:HH11	7:G:74:ARG:NH2	2.13	0.46
1:A:400:PHE:O	12:L:10:ASN:ND2	2.47	0.46
13:M:35:TYR:HD2	13:M:36:HIS:CE1	2.34	0.46
6:F:8:THR:OG1	6:F:11:GLU:HG2	2.15	0.46
7:G:42:ARG:HD3	7:G:75:VAL:CG1	2.45	0.46
1:N:438:ARG:NH2	18:N:515:HEA:O2D	2.48	0.46
3:P:125:ASN:HB3	3:P:128:GLU:OE1	2.15	0.46
8:U:75:ARG:NH1	8:U:75:ARG:HG2	2.31	0.46
4:D:108:PRO:HG2	4:D:111:PHE:CE2	2.50	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
1:A:283:LEU:HD13	1:A:311:ILE:HG13	1.97	0.46
3:C:154:GLY:HA2	6:F:6:VAL:CG2	2.45	0.46
3:P:132:LEU:HD13	3:P:176:LEU:HD11	1.96	0.46
1:A:243:VAL:HB	18:A:516:HEA:CAC	2.45	0.46
8:H:51:SER:O	8:H:52:VAL:HG13	2.16	0.46
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.50	0.46
2:O:14:SER:HB2	2:O:15:PRO:HD2	1.97	0.46
4:Q:132:GLN:HE22	9:V:43:ARG:HB2	1.81	0.46
9:V:61:GLU:OE1	9:V:64:ARG:NH1	2.49	0.46
1:A:309:THR:CG2	18:A:516:HEA:HMB2	2.45	0.46
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.46
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.97	0.46
8:U:19:ARG:HG3	8:U:20:PHE:CD2	2.50	0.46
1:A:151:HIS:O	1:A:155:VAL:HG23	2.16	0.46
3:C:123:PRO:HB2	3:C:261:SER:HB3	1.97	0.46
3:P:129:VAL:HG13	3:P:176:LEU:HD22	1.98	0.46
1:N:8:PHE:CE2	3:P:15:PRO:HB3	2.51	0.46
2:B:90[B]:ILE:HG23	2:B:91[B]:ASN:H	1.81	0.46
3:C:154:GLY:HA2	6:F:6:VAL:HG13	1.97	0.46
3:C:137:LEU:HD22	3:C:173:PHE:CD2	2.51	0.46
4:D:138:TRP:CD1	4:D:140:TYR:CD1	3.04	0.46
5:E:21:LYS:O	5:E:57:ARG:NH1	2.49	0.46
7:G:48:ILE:HD12	8:H:80:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:TYR:CD2	11:K:35:GLN:HB2	2.50	0.46
1:N:68:PHE:HE2	1:N:112:LEU:HD22	1.81	0.46
1:N:29:VAL:HG13	12:Y:36:PRO:HG3	1.97	0.46
12:Y:39:ILE:O	12:Y:42:HIS:HB3	2.16	0.46
1:A:439:ARG:HD3	2:B:199:ILE:HB	1.98	0.46
1:N:260:TYR:CD1	1:N:487:LEU:HD12	2.51	0.46
3:P:40:MET:O	3:P:44:MET:HG2	2.15	0.46
5:R:53:ARG:O	5:R:56:ARG:HB3	2.16	0.46
7:T:5:LYS:HE3	7:T:23:LEU:HD13	1.98	0.46
3:C:125:ASN:HB3	3:C:128:GLU:OE1	2.15	0.45
2:O:90[B]:ILE:HD11	2:O:93:PRO:CD	2.45	0.45
6:S:86:GLY:O	6:S:87:THR:O	2.34	0.45
7:T:36:TRP:CD1	7:T:36:TRP:C	2.89	0.45
1:A:285:PHE:CE2	7:T:4:ALA:HB3	2.52	0.45
1:A:189:MET:SD	7:T:7:ASP:CB	3.04	0.45
12:Y:14:SER:HB3	12:Y:20:ARG:HH12	1.81	0.45
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.52	0.45
1:A:421:VAL:HG23	1:A:422:ASN:N	2.30	0.45
1:A:98:ASN:HB2	1:A:163:ASN:HD21	1.80	0.45
2:B:162:SER:HB3	2:B:197:SER:O	2.16	0.45
3:C:250:LEU:HD23	3:C:250:LEU:HA	1.71	0.45
7:G:48:ILE:HD11	8:H:80:THR:HG22	1.96	0.45
10:J:47:LEU:HD12	10:J:47:LEU:HA	1.66	0.45
1:N:378:HIS:CD2	1:N:425:PHE:CZ	3.04	0.45
2:O:139:ASP:OD1	2:O:140:ASN:N	2.49	0.45
1:N:117:MET:CE	12:Y:39:ILE:HG23	2.47	0.45
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.03	0.45
1:A:69:MET:HE2	1:A:70:VAL:HG23	1.98	0.45
2:B:98:LYS:HB2	2:B:98:LYS:HE3	1.78	0.45
3:C:137:LEU:HA	3:C:137:LEU:HD12	1.77	0.45
3:C:160:LEU:HD21	3:C:223:LEU:HD23	1.98	0.45
1:N:129:TYR:CE2	1:N:232:GLN:HG2	2.51	0.45
1:N:44:PRO:HG3	4:Q:111:PHE:CE2	2.50	0.45
2:O:186:SER:HB3	2:O:213:LEU:HD22	1.99	0.45
4:Q:43:LYS:O	4:Q:46:ALA:HB3	2.16	0.45
10:W:11:LEU:O	10:W:11:LEU:HD23	2.17	0.45
1:A:222:PRO:O	1:A:225:GLY:N	2.48	0.45
7:G:2:SER:H	1:N:286:ILE:HG22	1.80	0.45
4:Q:108:PRO:HG2	4:Q:111:PHE:CE2	2.52	0.45
4:Q:114:GLU:HG3	11:X:51:LYS:CE	2.46	0.45
2:B:99:THR:C	2:B:100:MET:HG2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:386:VAL:HG11	18:N:515:HEA:H261	1.98	0.45
2:O:184:LEU:HD11	2:O:211:LEU:CD2	2.46	0.45
2:O:5:MET:CE	11:X:43:SER:H	2.30	0.45
6:S:18:ARG:HG3	6:S:21:MET:HE1	1.98	0.45
9:V:60:PHE:CE1	9:V:69:PHE:CE2	3.04	0.45
10:W:8:LYS:NZ	10:W:12:PHE:HE2	2.15	0.45
1:A:187:SER:HB2	1:A:277:MET:CE	2.46	0.45
3:C:195:SER:O	3:C:199:VAL:HG13	2.17	0.45
4:D:114:GLU:O	4:D:118:LYS:HG2	2.16	0.45
8:H:59:VAL:HG12	8:H:60:TYR:N	2.31	0.45
2:B:50:LEU:HB2	9:I:13:LEU:HD13	1.99	0.45
1:N:243:VAL:HB	18:N:516:HEA:CAC	2.46	0.45
7:T:42:ARG:NH1	7:T:74:ARG:NH2	2.64	0.45
1:A:4:ASN:HA	1:A:8:PHE:HB2	1.99	0.45
1:A:69:MET:O	1:A:72:PRO:HD2	2.17	0.45
1:A:92:MET:HE2	1:A:167:THR:CB	2.46	0.45
2:B:136:LEU:HB3	2:B:193:TYR:HD2	1.80	0.45
2:B:48:THR:HB	9:I:16:ARG:CZ	2.47	0.45
4:D:114:GLU:HG3	11:K:51:LYS:CE	2.47	0.45
4:Q:84:ALA:O	4:Q:88:PHE:HD2	1.99	0.45
1:A:260:TYR:CD1	1:A:487:LEU:HD12	2.52	0.45
1:A:474:GLU:HG3	1:A:475:ALA:N	2.32	0.45
2:B:186:SER:HB3	2:B:213:LEU:HD22	1.99	0.45
3:C:38:ASN:HD22	3:C:38:ASN:C	2.20	0.45
6:F:49:VAL:O	6:F:91:LEU:HD12	2.17	0.45
12:L:41:ARG:HD2	13:M:40:TYR:CZ	2.52	0.45
2:O:16:ILE:HD12	2:O:17:MET:N	2.32	0.45
6:S:85:CYS:SG	6:S:87:THR:OG1	2.71	0.45
2:B:66:THR:CG2	2:B:67:ILE:N	2.80	0.45
5:E:52:LEU:HA	5:E:52:LEU:HD23	1.67	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.45
2:B:222:TRP:HB2	9:I:71:SER:HB2	1.98	0.45
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.52	0.45
1:N:95:PRO:HB2	3:P:11:VAL:HG13	1.98	0.45
5:R:70:VAL:HG12	5:R:71:VAL:N	2.31	0.45
3:C:16:TRP:HA	3:C:16:TRP:HE3	1.81	0.45
1:N:445:ASP:OD1	2:O:134:ARG:NH1	2.49	0.45
3:P:42:LEU:HD21	10:W:46:SER:HB3	1.99	0.45
3:P:72:THR:HB	3:P:73:PRO:HD2	1.98	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CD2	2.52	0.45
6:F:16:LEU:O	6:F:20:VAL:CG1	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:MET:HE2	1:A:117:MET:HA	1.98	0.44
1:A:124:THR:HG22	1:A:138:HIS:CE1	2.52	0.44
2:B:162:SER:HA	2:B:173:ASP:HA	1.99	0.44
5:E:81:ILE:O	5:E:85:VAL:HG23	2.18	0.44
1:N:495:LEU:HD23	1:N:495:LEU:HA	1.78	0.44
2:O:108:TYR:N	2:O:108:TYR:CD1	2.85	0.44
3:P:160:LEU:HD21	3:P:223:LEU:HD23	1.99	0.44
4:Q:126:MET:O	4:Q:127:LYS:HB2	2.16	0.44
4:Q:66:GLU:HA	4:Q:70:GLU:OE1	2.17	0.44
3:C:157:LYS:HE3	3:C:158:HIS:NE2	2.32	0.44
1:N:131:PRO:HB2	2:O:159:VAL:HA	1.99	0.44
4:Q:70:GLU:HA	5:R:109:VAL:CG1	2.47	0.44
2:B:193:TYR:HE1	4:D:126:MET:HE3	1.83	0.44
1:N:299:VAL:HG13	1:N:300:ASP:N	2.31	0.44
2:O:100:MET:CE	2:O:157:GLU:HG3	2.47	0.44
3:P:192:VAL:O	3:P:196:THR:HB	2.18	0.44
4:Q:115:TRP:O	4:Q:119:GLN:HB2	2.17	0.44
5:R:52:LEU:HD23	5:R:52:LEU:HA	1.60	0.44
7:T:48:ILE:HD12	8:U:80:THR:HG22	1.99	0.44
9:V:57:MET:O	9:V:60:PHE:HB3	2.18	0.44
1:A:293:PHE:CZ	1:A:306:THR:HG22	2.52	0.44
1:A:289:ALA:HB3	1:A:305:PHE:CD1	2.53	0.44
3:C:102:TYR:O	3:C:106:LEU:HB2	2.18	0.44
7:G:4:ALA:HB2	1:N:197:LEU:CD1	2.47	0.44
12:L:14:SER:HB3	12:L:20:ARG:HH12	1.82	0.44
1:N:8:PHE:CZ	3:P:15:PRO:HB3	2.52	0.44
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.17	0.44
1:A:282:PHE:HE1	7:T:3:ALA:CB	2.31	0.44
4:Q:121:LYS:HD2	11:X:50:PRO:HB2	2.00	0.44
1:A:404:THR:O	1:A:480:ARG:NH1	2.48	0.44
3:C:36:HIS:C	3:C:38:ASN:H	2.21	0.44
7:G:48:ILE:C	7:G:48:ILE:HD12	2.38	0.44
2:O:62:GLU:O	2:O:66:THR:HB	2.18	0.44
3:C:192:VAL:O	3:C:196:THR:HB	2.18	0.44
7:G:48:ILE:HD12	7:G:49:PRO:CD	2.48	0.44
1:A:117:MET:HB3	10:J:54:SER:OG	2.17	0.44
10:J:8:LYS:HZ1	10:J:12:PHE:HE2	1.64	0.44
3:P:188:ILE:HG13	3:P:188:ILE:H	1.61	0.44
7:T:2:SER:O	7:T:3:ALA:HB2	2.17	0.44
7:T:47:PHE:CZ	7:T:81:GLY:HA2	2.53	0.44
2:B:139:ASP:OD1	2:B:140:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASP:OD1	9:I:43:ARG:NH1	2.51	0.44
2:O:1:MET:SD	2:O:133:LEU:HD13	2.56	0.44
3:P:250:LEU:HA	3:P:250:LEU:HD23	1.75	0.44
9:V:37:PHE:HA	9:V:41:GLU:HB2	2.00	0.44
10:W:18:LEU:HD23	10:W:18:LEU:HA	1.80	0.44
1:N:21:LEU:HA	1:N:21:LEU:HD23	1.76	0.44
2:O:62:GLU:HA	2:O:65:TRP:CD1	2.53	0.44
5:R:84:TYR:O	5:R:87:GLN:HB3	2.18	0.44
6:S:35:ALA:HA	6:S:36:PRO:HD3	1.87	0.44
8:U:59:VAL:HG12	8:U:60:TYR:N	2.33	0.44
1:A:285:PHE:CD2	7:T:4:ALA:HB3	2.53	0.43
1:A:433:LEU:HD13	2:B:8:GLY:HA2	1.99	0.43
8:H:57:ARG:HA	8:H:60:TYR:CD2	2.53	0.43
4:Q:132:GLN:HE21	9:V:42:LYS:HE3	1.82	0.43
12:Y:22:LEU:HD11	13:Z:18:GLY:HA2	2.00	0.43
1:A:347:LEU:HG	1:A:383:MET:CE	2.48	0.43
2:B:190:GLY:O	2:B:191:LEU:HD23	2.18	0.43
1:A:353:LEU:HG	2:B:31:VAL:HB	2.00	0.43
2:B:62:GLU:O	2:B:66:THR:HB	2.17	0.43
8:H:84:LYS:HA	8:H:84:LYS:HD2	1.67	0.43
1:N:417:MET:HE2	1:N:421:VAL:HG13	2.01	0.43
1:N:4:ASN:HA	1:N:8:PHE:HB2	1.99	0.43
1:N:513:LEU:HA	1:N:513:LEU:HD12	1.57	0.43
2:O:59:GLN:O	2:O:63:THR:HG23	2.18	0.43
4:Q:122:ARG:O	4:Q:125:ASP:HB2	2.18	0.43
8:U:84:LYS:HA	8:U:84:LYS:HD2	1.63	0.43
9:V:19:PHE:HD2	9:V:20:HIS:ND1	2.15	0.43
10:W:16:ASN:OD1	10:W:18:LEU:HB2	2.18	0.43
1:A:8:PHE:CZ	3:C:15:PRO:HB3	2.53	0.43
4:D:113:GLU:O	4:D:116:VAL:HG22	2.19	0.43
8:H:38:ARG:NH1	8:H:84:LYS:O	2.51	0.43
1:N:298:ASP:HB2	1:N:301:THR:CG2	2.43	0.43
2:O:189:PRO:O	9:V:63:MET:HE1	2.17	0.43
4:Q:145:TRP:CZ2	11:X:45:VAL:HA	2.53	0.43
4:Q:147:LYS:CA	4:Q:147:LYS:HE3	2.42	0.43
9:V:14:ALA:CB	9:V:18:ARG:HH21	2.31	0.43
1:A:129:TYR:CE2	1:A:232:GLN:HG2	2.54	0.43
1:A:319:LYS:HE3	1:A:319:LYS:HB3	1.79	0.43
1:A:38:ARG:HG3	1:A:458:SER:HB3	1.99	0.43
3:C:42:LEU:HD21	10:J:46:SER:HB3	1.99	0.43
5:E:90:ARG:HD3	5:E:90:ARG:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:LEU:HD12	1:N:105:LEU:HA	1.73	0.43
2:O:162:SER:HA	2:O:173:ASP:HA	2.00	0.43
3:P:110:PRO:HB2	8:U:30:TRP:CE3	2.52	0.43
3:P:154:GLY:CA	6:S:6:VAL:HG13	2.48	0.43
3:P:178:ALA:O	3:P:181:TYR:HB2	2.19	0.43
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.18	0.43
5:R:21:LYS:O	5:R:57:ARG:NH1	2.52	0.43
1:A:347:LEU:HD12	1:A:347:LEU:HA	1.81	0.43
1:A:360:ASN:O	1:A:364:ASP:N	2.50	0.43
4:D:7:LYS:O	4:D:10:ASP:HB2	2.18	0.43
7:G:42:ARG:HH11	7:G:75:VAL:HG11	1.82	0.43
8:H:37:HIS:CD2	8:H:76:ARG:NH1	2.86	0.43
1:N:157:SER:HB2	1:N:199:LEU:CD2	2.49	0.43
2:O:5:MET:HE3	11:X:43:SER:H	1.83	0.43
1:N:103:TRP:O	3:P:21:ALA:HB1	2.19	0.43
4:Q:48:TRP:NE1	5:R:56:ARG:NH2	2.66	0.43
18:A:515:HEA:H11	18:A:515:HEA:HMB1	1.84	0.43
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.53	0.43
3:C:121:ILE:HD13	3:C:121:ILE:HA	1.73	0.43
2:O:125:THR:HA	2:O:128:LEU:CD1	2.49	0.43
1:A:237:PHE:HZ	7:T:2:SER:HB2	1.83	0.43
1:A:397:PHE:HB3	1:A:398:PRO:HD3	2.01	0.43
2:B:184:LEU:HD11	2:B:211:LEU:CD2	2.48	0.43
8:H:43:MET:O	8:H:47:GLY:N	2.52	0.43
1:A:403:TYR:CZ	12:L:7:PRO:HB3	2.54	0.43
7:G:3:ALA:CB	1:N:282:PHE:HE1	2.30	0.43
10:J:8:LYS:NZ	10:J:12:PHE:HE2	2.15	0.43
1:N:172:LYS:HD3	1:N:181:THR:HG21	2.01	0.43
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.49	0.43
2:O:50:LEU:HD21	5:R:77:PRO:HD2	1.99	0.43
9:V:19:PHE:HD2	9:V:20:HIS:CE1	2.37	0.43
10:W:31:LEU:HD23	10:W:31:LEU:HA	1.77	0.43
1:A:158:ILE:O	1:A:162:ILE:HG13	2.19	0.43
2:B:62:GLU:HA	2:B:65:TRP:CD1	2.54	0.43
3:C:188:ILE:HD11	7:G:68:THR:HG22	2.01	0.43
7:G:42:ARG:O	7:G:42:ARG:HD2	2.19	0.43
4:D:132:GLN:HE22	9:I:43:ARG:HB2	1.83	0.43
1:N:83:VAL:CG2	1:N:188:VAL:HG11	2.49	0.43
1:N:129:TYR:CZ	1:N:232:GLN:HG2	2.54	0.43
7:T:42:ARG:O	7:T:42:ARG:HD2	2.19	0.43
1:A:152:LEU:CD2	3:C:24:ALA:HB1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:HIS:O	1:A:382:SER:HB2	2.19	0.43
5:E:12:ASP:HA	5:E:47:ILE:HD11	2.01	0.43
10:J:11:LEU:HD23	10:J:11:LEU:C	2.38	0.43
1:N:92:MET:HE2	1:N:167:THR:CB	2.48	0.43
3:P:42:LEU:HA	3:P:42:LEU:HD12	1.93	0.43
8:U:39:CYS:CB	8:U:53:CYS:SG	3.07	0.43
10:W:29:ASN:ND2	10:W:33:ARG:HD2	2.34	0.43
3:C:16:TRP:HA	3:C:16:TRP:CE3	2.52	0.42
3:C:26:LEU:HA	3:C:26:LEU:HD12	1.85	0.42
4:D:73:ARG:CZ	4:D:73:ARG:HB3	2.49	0.42
5:E:70:VAL:HG12	5:E:71:VAL:N	2.32	0.42
3:C:67:PHE:O	6:F:14:THR:HG21	2.18	0.42
8:H:19:ARG:C	8:H:21:PRO:HD3	2.40	0.42
3:P:151:LEU:HD21	3:P:232:HIS:CG	2.53	0.42
7:T:48:ILE:HD12	7:T:49:PRO:CD	2.49	0.42
1:A:506:GLU:HB3	3:C:1:MET:CG	2.49	0.42
2:B:160:LEU:HD21	2:B:175:ILE:HG23	2.01	0.42
2:B:5:MET:CE	11:K:43:SER:H	2.32	0.42
4:D:112:GLU:O	4:D:116:VAL:HG13	2.19	0.42
7:G:42:ARG:NH1	7:G:74:ARG:NH2	2.65	0.42
11:K:53:TRP:CD1	11:K:53:TRP:N	2.86	0.42
5:R:12:ASP:HA	5:R:47:ILE:HD11	2.01	0.42
5:R:78:HIS:ND1	9:V:12:LEU:HD22	2.34	0.42
6:S:16:LEU:O	6:S:20:VAL:CG1	2.65	0.42
11:X:53:TRP:N	11:X:53:TRP:CD1	2.86	0.42
2:B:196:CYS:HB2	2:B:207:MET:HE2	2.01	0.42
3:C:129:VAL:HG13	3:C:176:LEU:HD22	2.01	0.42
1:A:506:GLU:HB3	3:C:1:MET:HB3	2.01	0.42
4:D:129:ALA:HB1	4:D:133:GLY:HA3	2.01	0.42
5:E:104:LEU:HA	5:E:104:LEU:HD23	1.75	0.42
9:I:14:ALA:CB	9:I:18:ARG:HH21	2.33	0.42
1:N:379:TYR:CD2	1:N:383:MET:HE2	2.54	0.42
1:N:51:ASP:O	1:N:55:ASN:HB2	2.20	0.42
2:O:186:SER:CB	2:O:213:LEU:HD22	2.48	0.42
3:P:137:LEU:HD22	3:P:173:PHE:CD2	2.53	0.42
3:P:190:ASP:HB3	7:T:53:LEU:HD22	1.99	0.42
3:P:38:ASN:HD22	3:P:38:ASN:C	2.21	0.42
5:E:81:ILE:HA	9:I:7:PRO:HG3	2.01	0.42
1:N:87:ILE:O	1:N:173:PRO:HD3	2.19	0.42
18:N:515:HEA:HMB1	18:N:515:HEA:H11	1.85	0.42
4:Q:139:ASP:O	4:Q:143:ASN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:48:ILE:HD11	8:U:80:THR:HG22	2.00	0.42
1:A:402:GLY:HA3	1:A:499:PRO:HD3	2.00	0.42
1:A:92:MET:HE2	1:A:167:THR:OG1	2.18	0.42
2:B:113:TYR:OH	8:H:12:GLN:HA	2.20	0.42
3:C:132:LEU:HD13	3:C:176:LEU:HD11	2.00	0.42
7:G:48:ILE:HG13	7:G:50:TYR:CE2	2.55	0.42
8:H:46:LYS:NZ	8:U:53:CYS:CA	2.82	0.42
2:O:184:LEU:HD23	2:O:185:MET:N	2.34	0.42
5:R:79:LYS:HE2	5:R:79:LYS:HB2	1.76	0.42
5:R:93:LEU:HD23	5:R:93:LEU:HA	1.75	0.42
6:S:14:THR:OG1	6:S:15:GLY:N	2.53	0.42
8:U:57:ARG:HG3	8:U:60:TYR:CE2	2.54	0.42
1:A:83:VAL:HG21	1:A:188:VAL:HG11	2.01	0.42
1:A:58:VAL:HG13	18:A:515:HEA:HBD2	2.02	0.42
4:D:108:PRO:HG2	4:D:111:PHE:CD2	2.54	0.42
9:I:19:PHE:HD2	9:I:20:HIS:ND1	2.18	0.42
10:J:31:LEU:HD23	10:J:31:LEU:HA	1.72	0.42
1:N:218:THR:HB	1:N:221:ASP:HB3	2.01	0.42
1:N:443:TYR:HB2	1:N:447:TYR:HD2	1.85	0.42
1:N:468:MET:SD	18:N:515:HEA:H243	2.59	0.42
2:O:116:LEU:HD11	2:O:226:MET:CG	2.47	0.42
1:A:199:LEU:HD12	1:A:238:PHE:CE1	2.55	0.42
1:A:379:TYR:CD2	1:A:383:MET:HE2	2.54	0.42
3:C:104:SER:CB	3:C:192:VAL:HG11	2.49	0.42
6:F:53:THR:CG2	6:F:54:ASN:N	2.82	0.42
1:N:12:HIS:CD2	1:N:80:ASN:O	2.72	0.42
7:G:4:ALA:HB3	1:N:285:PHE:CD2	2.54	0.42
2:O:160:LEU:HD22	2:O:175:ILE:HG12	2.02	0.42
2:O:185:MET:SD	2:O:185:MET:C	2.98	0.42
8:U:36:PHE:HB2	8:U:56:TYR:HB3	2.01	0.42
1:A:247:ILE:HA	1:A:247:ILE:HD12	1.86	0.42
3:C:188:ILE:H	3:C:188:ILE:HG13	1.58	0.42
9:I:29:LEU:HA	9:I:29:LEU:HD23	1.75	0.42
1:A:478:SER:HA	13:M:8:THR:O	2.20	0.42
6:S:49:VAL:HG21	6:S:74:LEU:HD12	2.00	0.42
9:V:14:ALA:HB3	9:V:18:ARG:HH21	1.85	0.42
1:A:377:PHE:HB3	18:A:516:HEA:C1D	2.49	0.42
1:A:468:MET:SD	18:A:515:HEA:H243	2.59	0.42
1:A:75:ILE:O	1:A:79:GLY:HA3	2.20	0.42
7:G:49:PRO:HG2	8:H:80:THR:CG2	2.50	0.42
1:N:199:LEU:HD12	1:N:238:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:347:LEU:HG	1:N:383:MET:CE	2.50	0.42
1:N:383:MET:HA	1:N:387:PHE:CD1	2.55	0.42
2:O:66:THR:CG2	2:O:67:ILE:N	2.83	0.42
3:P:26:LEU:HA	3:P:26:LEU:HD12	1.79	0.42
8:U:39:CYS:CB	8:U:53:CYS:HG	2.32	0.42
1:A:445:ASP:OD1	2:B:134:ARG:NH1	2.49	0.42
2:B:87:MET:C	2:B:89[B]:GLU:N	2.73	0.42
7:G:42:ARG:NH1	7:G:75:VAL:HG11	2.34	0.42
1:N:443:TYR:HE2	1:N:448:THR:HA	1.85	0.42
1:N:92:MET:HE2	1:N:167:THR:OG1	2.20	0.42
5:R:76:GLY:HA3	5:R:77:PRO:HD2	1.87	0.42
6:S:95:GLN:NE2	6:S:96:LEU:HD13	2.27	0.42
7:T:78:LEU:HD12	7:T:78:LEU:HA	1.85	0.42
9:V:26:MET:HA	9:V:26:MET:CE	2.50	0.42
10:W:3:ASN:HD22	10:W:5:VAL:HG12	1.84	0.42
1:N:158:ILE:O	1:N:162:ILE:HG13	2.21	0.41
2:O:133:LEU:HA	2:O:133:LEU:HD23	1.82	0.41
3:P:188:ILE:HD11	7:T:68:THR:HG22	2.02	0.41
8:U:17:ASP:OD2	8:U:19:ARG:NH1	2.52	0.41
1:A:508:PRO:HB2	6:F:56:ARG:HH21	1.85	0.41
18:A:515:HEA:H272	18:A:515:HEA:H172	1.78	0.41
2:B:123:ILE:HD12	2:B:137:GLU:HB3	2.01	0.41
3:C:173:PHE:C	3:C:173:PHE:CD1	2.93	0.41
4:D:147:LYS:HE3	4:D:147:LYS:CA	2.39	0.41
3:P:137:LEU:HD12	3:P:137:LEU:HA	1.82	0.41
4:Q:40:LEU:HD22	4:Q:59:LEU:HD13	2.02	0.41
1:A:309:THR:HG22	18:A:516:HEA:HMB2	2.02	0.41
7:G:10:GLY:O	7:G:11:THR:O	2.37	0.41
12:L:4:GLU:HB3	12:L:9:LYS:HD3	2.02	0.41
1:N:400:PHE:O	12:Y:10:ASN:ND2	2.50	0.41
2:O:142:VAL:HG13	2:O:210:VAL:O	2.20	0.41
3:P:47:LEU:O	3:P:51:MET:HG2	2.20	0.41
1:A:131:PRO:HB2	2:B:159:VAL:HA	2.02	0.41
1:A:380:VAL:HG21	18:A:516:HEA:C3C	2.49	0.41
2:B:186:SER:CB	2:B:213:LEU:HD22	2.51	0.41
4:D:16:TYR:CE2	4:D:65:LYS:HB2	2.55	0.41
8:H:38:ARG:HG2	8:H:85:ILE:HG23	2.01	0.41
10:W:10:LYS:HE3	10:W:10:LYS:O	2.21	0.41
1:A:376:HIS:CD2	18:A:516:HEA:ND	2.88	0.41
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.62	0.41
1:A:93:ALA:O	1:A:95:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD22	3:C:24:ALA:HB1	2.01	0.41
9:I:14:ALA:HB3	9:I:18:ARG:HH21	1.84	0.41
6:S:74:LEU:HD11	6:S:89:TYR:HB3	2.03	0.41
7:T:48:ILE:HG13	7:T:50:TYR:CE2	2.56	0.41
1:A:218:THR:HB	1:A:221:ASP:HB3	2.01	0.41
1:A:25:TRP:O	1:A:28:MET:HB2	2.21	0.41
1:A:85:LEU:O	1:A:492:LEU:HD13	2.20	0.41
3:C:3:HIS:CD2	6:F:97:ALA:HB1	2.56	0.41
1:N:150:LEU:HA	1:N:150:LEU:HD12	1.83	0.41
1:N:421:VAL:HG23	1:N:422:ASN:N	2.35	0.41
1:N:93:ALA:O	1:N:95:PRO:HD3	2.20	0.41
2:O:122:MET:HA	2:O:137:GLU:O	2.21	0.41
3:P:154:GLY:HA2	6:S:6:VAL:CG1	2.50	0.41
1:A:105:LEU:HA	1:A:105:LEU:HD12	1.76	0.41
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.78	0.41
1:A:417:MET:HE2	1:A:421:VAL:HG13	2.02	0.41
2:B:108:TYR:CD1	2:B:108:TYR:N	2.89	0.41
2:B:188:ARG:HD3	9:I:51:TYR:HE1	1.85	0.41
3:C:224:LYS:HB3	3:C:224:LYS:HZ3	1.84	0.41
3:C:40:MET:O	3:C:44:MET:HG2	2.20	0.41
5:E:44:GLU:OE1	5:E:45:PRO:HD2	2.20	0.41
4:D:48:TRP:NE1	5:E:56:ARG:NH2	2.69	0.41
9:I:60:PHE:HE1	9:I:69:PHE:CE2	2.38	0.41
10:J:3:ASN:O	10:J:3:ASN:ND2	2.53	0.41
7:G:4:ALA:HB3	1:N:285:PHE:CE2	2.56	0.41
1:N:321:PHE:HB3	2:O:65:TRP:CE3	2.55	0.41
2:O:113:TYR:OH	8:U:12:GLN:HA	2.21	0.41
8:U:19:ARG:C	8:U:21:PRO:HD3	2.41	0.41
7:G:7:ASP:CB	1:N:189:MET:SD	3.09	0.41
3:P:116:TRP:HA	3:P:117:PRO:C	2.41	0.41
3:P:132:LEU:HD13	3:P:176:LEU:CD1	2.51	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.94	0.41
1:A:8:PHE:CD1	1:A:8:PHE:N	2.89	0.41
2:B:108:TYR:CE2	2:B:142:VAL:HG11	2.56	0.41
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.95	0.41
2:B:184:LEU:HD23	2:B:185:MET:N	2.35	0.41
5:E:79:LYS:HE2	5:E:79:LYS:HB2	1.76	0.41
7:G:2:SER:O	7:G:3:ALA:HB2	2.20	0.41
7:G:69:PHE:HD2	7:G:70:PHE:CE1	2.38	0.41
8:H:81:PHE:CE2	8:H:85:ILE:HD11	2.56	0.41
10:J:14:GLU:O	10:J:23:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.56	0.41
1:N:506:GLU:OE1	3:P:1:MET:HB3	2.20	0.41
2:O:193:TYR:HE1	4:Q:126:MET:HE3	1.86	0.41
10:W:29:ASN:HD21	10:W:33:ARG:HD2	1.86	0.41
4:D:9:GLU:H	4:D:9:GLU:CD	2.24	0.41
5:E:93:LEU:HD23	5:E:93:LEU:HA	1.77	0.41
2:O:99:THR:C	2:O:100:MET:HG2	2.41	0.41
3:P:173:PHE:C	3:P:173:PHE:CD1	2.94	0.41
1:A:128:VAL:O	1:A:128:VAL:HG22	2.21	0.41
1:A:443:TYR:HE2	1:A:448:THR:HA	1.85	0.41
4:D:141:ASP:C	4:D:143:ASN:H	2.25	0.41
13:M:19:LEU:C	13:M:19:LEU:HD23	2.42	0.41
1:N:260:TYR:CE1	1:N:487:LEU:HD12	2.56	0.41
1:N:349:THR:O	1:N:353:LEU:HB2	2.21	0.41
1:N:506:GLU:HB3	3:P:1:MET:CG	2.51	0.41
1:N:69:MET:HE1	1:N:70:VAL:HG23	2.02	0.41
2:O:162:SER:HB3	2:O:197:SER:O	2.20	0.41
5:E:52:LEU:O	5:E:55:CYS:HB2	2.21	0.40
8:H:17:ASP:OD2	8:H:19:ARG:NH1	2.53	0.40
9:I:37:PHE:HA	9:I:41:GLU:HB2	2.03	0.40
11:K:22:ALA:O	11:K:26:VAL:HG12	2.21	0.40
1:N:187:SER:HB2	1:N:277:MET:CE	2.50	0.40
1:N:85:LEU:O	1:N:492:LEU:HD13	2.21	0.40
9:V:60:PHE:HE1	9:V:69:PHE:CE2	2.39	0.40
4:D:118:LYS:HA	11:K:51:LYS:O	2.22	0.40
4:D:132:GLN:HE21	9:I:42:LYS:HE3	1.85	0.40
1:N:74:MET:CE	1:N:249:PRO:HB2	2.52	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.22	0.40
2:O:20:LEU:CD2	2:O:83:ILE:HG21	2.52	0.40
3:P:132:LEU:O	3:P:136:VAL:HG23	2.21	0.40
4:Q:138:TRP:HD1	4:Q:140:TYR:CD1	2.38	0.40
8:U:38:ARG:NH1	8:U:84:LYS:O	2.51	0.40
13:Z:19:LEU:C	13:Z:19:LEU:HD23	2.42	0.40
1:A:302:ARG:HD3	1:A:302:ARG:HH11	1.73	0.40
1:A:436:MET:HA	1:A:437:PRO:HD3	1.88	0.40
7:G:36:TRP:O	7:G:36:TRP:HD1	2.04	0.40
10:J:2:GLU:HG3	10:J:3:ASN:H	1.85	0.40
1:N:98:ASN:HB2	1:N:163:ASN:HD21	1.85	0.40
1:N:376:HIS:CD2	18:N:516:HEA:ND	2.89	0.40
1:N:443:TYR:CD1	1:N:443:TYR:N	2.87	0.40
1:N:377:PHE:HB3	18:N:516:HEA:C1D	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:HD12	2:O:68:LEU:HA	1.94	0.40
4:Q:139:ASP:O	4:Q:143:ASN:N	2.54	0.40
4:Q:59:LEU:HA	4:Q:59:LEU:HD12	1.95	0.40
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.71	0.40
4:D:119:GLN:O	4:D:123:MET:HG3	2.21	0.40
4:D:130:PRO:HG2	4:D:131:ILE:N	2.34	0.40
4:D:131:ILE:H	4:D:131:ILE:HG13	1.68	0.40
1:N:33:LEU:O	1:N:37:ILE:HG13	2.21	0.40
1:N:360:ASN:O	1:N:364:ASP:N	2.51	0.40
1:N:400:PHE:O	1:N:499:PRO:HB3	2.20	0.40
1:N:8:PHE:CD1	1:N:8:PHE:N	2.89	0.40
2:O:7:LEU:HA	2:O:7:LEU:HD12	1.79	0.40
4:Q:141:ASP:C	4:Q:143:ASN:H	2.25	0.40
6:S:49:VAL:O	6:S:91:LEU:HD12	2.21	0.40
1:A:340:TRP:HH2	1:A:417:MET:HG2	1.86	0.40
2:B:144:LEU:HD22	2:B:150:ILE:HD13	2.04	0.40
3:C:75:VAL:O	3:C:79:LEU:HD12	2.22	0.40
2:B:1:MET:SD	4:D:123:MET:HE3	2.62	0.40
7:G:56:ARG:HG2	7:G:56:ARG:NH1	2.36	0.40
3:P:106:LEU:HD23	3:P:106:LEU:HA	1.92	0.40
3:P:104:SER:CB	3:P:192:VAL:HG11	2.50	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	512/514 (100%)	469 (92%)	39 (8%)	4 (1%)	19	51
1	N	512/514 (100%)	470 (92%)	38 (7%)	4 (1%)	19	51
2	B	230/227 (101%)	197 (86%)	27 (12%)	6 (3%)	5	20
2	O	230/227 (101%)	197 (86%)	27 (12%)	6 (3%)	5	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	259/261 (99%)	249 (96%)	7 (3%)	3 (1%)	13	40
3	P	259/261 (99%)	248 (96%)	8 (3%)	3 (1%)	13	40
4	D	142/147 (97%)	131 (92%)	10 (7%)	1 (1%)	22	54
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	22	54
5	E	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
5	R	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	82 (85%)	7 (7%)	7 (7%)	1	3
6	S	96/98 (98%)	79 (82%)	10 (10%)	7 (7%)	1	3
7	G	82/84 (98%)	64 (78%)	13 (16%)	5 (6%)	1	4
7	T	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	1	4
8	H	73/85 (86%)	61 (84%)	10 (14%)	2 (3%)	5	19
8	U	73/85 (86%)	61 (84%)	10 (14%)	2 (3%)	5	19
9	I	71/73 (97%)	67 (94%)	3 (4%)	1 (1%)	11	36
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	54/59 (92%)	47 (87%)	5 (9%)	2 (4%)	3	13
10	W	54/59 (92%)	47 (87%)	5 (9%)	2 (4%)	3	13
11	K	47/56 (84%)	35 (74%)	12 (26%)	0	100	100
11	X	47/56 (84%)	36 (77%)	11 (23%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3518/3612 (97%)	3169 (90%)	288 (8%)	61 (2%)	9	31

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	HIS
2	B	88[A]	ASP
2	B	88[B]	ASP
2	B	91[A]	ASN
2	B	91[B]	ASN
3	C	38	ASN
6	F	2	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	87	THR
6	F	97	ALA
7	G	5	LYS
7	G	11	THR
10	J	2	GLU
1	N	328	HIS
2	O	88[A]	ASP
2	O	88[B]	ASP
2	O	91[A]	ASN
2	O	91[B]	ASN
3	P	38	ASN
6	S	2	SER
6	S	87	THR
6	S	97	ALA
7	T	5	LYS
7	T	11	THR
10	W	2	GLU
2	B	104	TRP
6	F	66	ASN
6	F	96	LEU
8	H	46	LYS
2	O	104	TRP
2	O	127	GLU
6	S	66	ASN
6	S	96	LEU
8	U	46	LYS
2	B	127	GLU
3	C	2	THR
4	D	20	ARG
6	F	15	GLY
7	G	6	GLY
7	G	8	HIS
10	J	3	ASN
3	P	2	THR
4	Q	20	ARG
6	S	15	GLY
7	T	8	HIS
10	W	3	ASN
1	A	508	PRO
3	C	128	GLU
7	G	3	ALA
7	T	3	ALA

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Mol	Chain	Res	Type
7	T	6	GLY
1	A	91	ASP
1	N	91	ASP
3	P	128	GLU
1	A	384	GLY
9	I	36	LYS
8	H	50	VAL
8	U	50	VAL
6	F	4	GLY
1	N	384	GLY
1	N	508	PRO
6	S	4	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/427 (100%)	399 (93%)	28 (7%)	16	44
1	N	427/427 (100%)	394 (92%)	33 (8%)	13	35
2	B	216/211 (102%)	192 (89%)	24 (11%)	6	19
2	O	216/211 (102%)	192 (89%)	24 (11%)	6	19
3	C	226/226 (100%)	196 (87%)	30 (13%)	4	11
3	P	226/226 (100%)	196 (87%)	30 (13%)	4	11
4	D	128/129 (99%)	118 (92%)	10 (8%)	12	34
4	Q	128/129 (99%)	118 (92%)	10 (8%)	12	34
5	E	95/95 (100%)	89 (94%)	6 (6%)	18	46
5	R	95/95 (100%)	89 (94%)	6 (6%)	18	46
6	F	81/81 (100%)	72 (89%)	9 (11%)	6	19
6	S	81/81 (100%)	73 (90%)	8 (10%)	8	24
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	12
7	T	68/68 (100%)	57 (84%)	11 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	67/75 (89%)	54 (81%)	13 (19%)	1	4
8	U	67/75 (89%)	56 (84%)	11 (16%)	2	7
9	I	58/58 (100%)	52 (90%)	6 (10%)	7	22
9	V	58/58 (100%)	51 (88%)	7 (12%)	5	15
10	J	47/50 (94%)	40 (85%)	7 (15%)	3	9
10	W	47/50 (94%)	40 (85%)	7 (15%)	3	9
11	K	39/46 (85%)	35 (90%)	4 (10%)	7	22
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	22
12	L	40/40 (100%)	37 (92%)	3 (8%)	13	37
12	Y	40/40 (100%)	36 (90%)	4 (10%)	7	23
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	11
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	11
All	All	3058/3088 (99%)	2744 (90%)	314 (10%)	7	22

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	35	LEU
1	A	96	ARG
1	A	105	LEU
1	A	136	LEU
1	A	138	HIS
1	A	146	THR
1	A	150	LEU
1	A	156	SER
1	A	158	ILE
1	A	159	LEU
1	A	213	ARG
1	A	238	PHE
1	A	273	MET
1	A	301	THR
1	A	318	VAL
1	A	336	PRO
1	A	338	MET
1	A	347	LEU
1	A	354	THR
1	A	365	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	366	VAL
1	A	369	ASP
1	A	383	MET
1	A	465	VAL
1	A	467	LEU
1	A	474	GLU
1	A	492	LEU
2	B	3	TYR
2	B	7	LEU
2	B	31	VAL
2	B	55	THR
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	81	LEU
2	B	88[A]	ASP
2	B	88[B]	ASP
2	B	90[A]	ILE
2	B	90[B]	ILE
2	B	92[A]	ASN
2	B	92[B]	ASN
2	B	104	TRP
2	B	126	SER
2	B	130	PRO
2	B	142	VAL
2	B	170	LEU
2	B	171	LYS
2	B	185	MET
2	B	188	ARG
2	B	205	SER
2	B	216	LEU
3	C	11	VAL
3	C	12	ASN
3	C	13	PRO
3	C	14	SER
3	C	18	LEU
3	C	22	LEU
3	C	26	LEU
3	C	38	ASN
3	C	41	THR
3	C	79	LEU
3	C	85	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	112	LEU
3	C	128	GLU
3	C	131	LEU
3	C	132	LEU
3	C	137	LEU
3	C	142	VAL
3	C	159	MET
3	C	160	LEU
3	C	163	LEU
3	C	168	THR
3	C	179	SER
3	C	188	ILE
3	C	196	THR
3	C	199	VAL
3	C	213	THR
3	C	214	PHE
3	C	222	GLN
3	C	245	VAL
3	C	258	TRP
4	D	19	ARG
4	D	40	LEU
4	D	52	SER
4	D	59	LEU
4	D	99	GLU
4	D	107	ILE
4	D	110	THR
4	D	116	VAL
4	D	121	LYS
4	D	147	LYS
5	E	29	LEU
5	E	41	LEU
5	E	70	VAL
5	E	79	LYS
5	E	80	GLU
5	E	109	VAL
6	F	6	VAL
6	F	10	GLU
6	F	19	GLU
6	F	37	LYS
6	F	46	PRO
6	F	65	ASP
6	F	74	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	95	GLN
6	F	98	HIS
7	G	5	LYS
7	G	14	ARG
7	G	17	ARG
7	G	36	TRP
7	G	41	HIS
7	G	42	ARG
7	G	48	ILE
7	G	54	ARG
7	G	68	THR
8	H	19	ARG
8	H	21	PRO
8	H	27	ARG
8	H	29	CYS
8	H	51	SER
8	H	52	VAL
8	H	53	CYS
8	H	57	ARG
8	H	60	TYR
8	H	67	SER
8	H	69	VAL
8	H	75	ARG
8	H	82	PRO
9	I	8	GLN
9	I	26	MET
9	I	41	GLU
9	I	42	LYS
9	I	44	LYS
9	I	64	ARG
10	J	2	GLU
10	J	3	ASN
10	J	8	LYS
10	J	10	LYS
10	J	27	THR
10	J	30	ILE
10	J	47	LEU
11	K	7	PRO
11	K	26	VAL
11	K	45	VAL
11	K	54	ARG
12	L	15	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	L	22	LEU
12	L	26	THR
13	M	13	LYS
13	M	24	LEU
13	M	34	LEU
13	M	39	ASN
13	M	42	LYS
1	N	18	LEU
1	N	35	LEU
1	N	96	ARG
1	N	105	LEU
1	N	109	PHE
1	N	130	PRO
1	N	136	LEU
1	N	138	HIS
1	N	146	THR
1	N	150	LEU
1	N	156	SER
1	N	158	ILE
1	N	159	LEU
1	N	174	PRO
1	N	213	ARG
1	N	238	PHE
1	N	273	MET
1	N	278	MET
1	N	301	THR
1	N	318	VAL
1	N	336	PRO
1	N	338	MET
1	N	347	LEU
1	N	354	THR
1	N	365	ILE
1	N	369	ASP
1	N	373	VAL
1	N	383	MET
1	N	444	PRO
1	N	465	VAL
1	N	467	LEU
1	N	474	GLU
1	N	492	LEU
2	O	3	TYR
2	O	7	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	O	31	VAL
2	O	55	THR
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	81	LEU
2	O	88[A]	ASP
2	O	88[B]	ASP
2	O	90[A]	ILE
2	O	90[B]	ILE
2	O	92[A]	ASN
2	O	92[B]	ASN
2	O	104	TRP
2	O	126	SER
2	O	130	PRO
2	O	142	VAL
2	O	170	LEU
2	O	171	LYS
2	O	185	MET
2	O	188	ARG
2	O	205	SER
2	O	216	LEU
3	P	11	VAL
3	P	12	ASN
3	P	13	PRO
3	P	14	SER
3	P	18	LEU
3	P	22	LEU
3	P	26	LEU
3	P	38	ASN
3	P	41	THR
3	P	79	LEU
3	P	85	LEU
3	P	112	LEU
3	P	128	GLU
3	P	131	LEU
3	P	132	LEU
3	P	137	LEU
3	P	142	VAL
3	P	159	MET
3	P	160	LEU
3	P	163	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	P	168	THR
3	P	179	SER
3	P	188	ILE
3	P	196	THR
3	P	199	VAL
3	P	213	THR
3	P	214	PHE
3	P	222	GLN
3	P	245	VAL
3	P	258	TRP
4	Q	19	ARG
4	Q	40	LEU
4	Q	52	SER
4	Q	59	LEU
4	Q	99	GLU
4	Q	107	ILE
4	Q	110	THR
4	Q	116	VAL
4	Q	121	LYS
4	Q	147	LYS
5	R	29	LEU
5	R	41	LEU
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	109	VAL
6	S	6	VAL
6	S	10	GLU
6	S	19	GLU
6	S	37	LYS
6	S	65	ASP
6	S	74	LEU
6	S	95	GLN
6	S	98	HIS
7	T	5	LYS
7	T	14	ARG
7	T	17	ARG
7	T	26	PRO
7	T	33	LEU
7	T	36	TRP
7	T	41	HIS
7	T	42	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	T	48	ILE
7	T	54	ARG
7	T	68	THR
8	U	19	ARG
8	U	27	ARG
8	U	29	CYS
8	U	51	SER
8	U	52	VAL
8	U	57	ARG
8	U	60	TYR
8	U	67	SER
8	U	69	VAL
8	U	75	ARG
8	U	82	PRO
9	V	2	THR
9	V	8	GLN
9	V	26	MET
9	V	41	GLU
9	V	42	LYS
9	V	44	LYS
9	V	64	ARG
10	W	2	GLU
10	W	3	ASN
10	W	8	LYS
10	W	10	LYS
10	W	27	THR
10	W	30	ILE
10	W	47	LEU
11	X	7	PRO
11	X	26	VAL
11	X	45	VAL
11	X	54	ARG
12	Y	7	PRO
12	Y	15	VAL
12	Y	22	LEU
12	Y	26	THR
13	Z	13	LYS
13	Z	24	LEU
13	Z	34	LEU
13	Z	39	ASN
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	61	HIS
1	A	368	HIS
1	A	512	ASN
3	C	3	HIS
3	C	4	GLN
3	C	12	ASN
3	C	38	ASN
3	C	50	ASN
3	C	133	ASN
3	C	222	GLN
4	D	132	GLN
6	F	95	GLN
9	I	53	ASN
10	J	3	ASN
12	L	42	HIS
1	N	12	HIS
1	N	61	HIS
1	N	368	HIS
1	N	512	ASN
3	P	3	HIS
3	P	4	GLN
3	P	12	ASN
3	P	38	ASN
3	P	50	ASN
3	P	133	ASN
3	P	222	GLN
4	Q	132	GLN
4	Q	143	ASN
6	S	95	GLN
9	V	53	ASN
10	W	3	ASN
12	Y	42	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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
18	HEA	N	515	1	44,67,67	1.79	7 (15%)	37,103,103	1.97	12 (32%)
17	AZI	N	521	1	0,2,2	0.00	-	0,1,1	0.00	-
18	HEA	A	516	1,17	44,67,67	1.91	8 (18%)	37,103,103	1.75	9 (24%)
18	HEA	N	516	1,17	44,67,67	1.74	8 (18%)	37,103,103	1.79	8 (21%)
18	HEA	A	515	1	44,67,67	1.59	7 (15%)	37,103,103	2.49	14 (37%)
17	AZI	N	520	18,14	0,2,2	0.00	-	0,1,1	0.00	-
17	AZI	A	520	18,14	0,2,2	0.00	-	0,1,1	0.00	-
17	AZI	A	521	-	0,2,2	0.00	-	0,1,1	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HEA	N	516	1,17	1/1/7/16	4/24/76/76	-
18	HEA	N	515	1	3/3/7/16	4/24/76/76	-
18	HEA	A	515	1	3/3/7/16	4/24/76/76	-
18	HEA	A	516	1,17	1/1/7/16	5/24/76/76	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	515	HEA	C3B-C11	-7.93	1.46	1.52
18	A	515	HEA	C3B-C11	-6.73	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	516	HEA	C3B-C11	-5.88	1.48	1.52
18	A	516	HEA	C3C-C2C	-5.74	1.32	1.40
18	N	516	HEA	C3C-C2C	-5.17	1.33	1.40
18	A	516	HEA	CAA-C2A	5.10	1.61	1.52
18	A	516	HEA	C3A-C2A	-4.55	1.34	1.40
18	A	516	HEA	C3B-C11	-4.53	1.49	1.52
18	N	515	HEA	CAD-C3D	3.91	1.57	1.52
18	A	516	HEA	C3A-CMA	-3.25	1.38	1.46
18	A	515	HEA	C3A-CMA	-3.19	1.39	1.46
18	N	515	HEA	C3A-C2A	-3.05	1.36	1.40
18	N	516	HEA	C3B-C2B	-2.96	1.31	1.41
18	N	516	HEA	CAA-C2A	2.82	1.57	1.52
18	N	516	HEA	C3A-CMA	-2.74	1.40	1.46
18	N	515	HEA	C3C-CAC	2.68	1.53	1.47
18	A	516	HEA	C1D-C2D	2.64	1.48	1.42
18	N	515	HEA	C1B-CHB	-2.58	1.33	1.41
18	N	515	HEA	C3A-CMA	-2.54	1.40	1.46
18	A	515	HEA	C4B-C3B	2.54	1.48	1.42
18	N	516	HEA	C1A-C2A	2.53	1.48	1.42
18	A	515	HEA	C1B-CHB	-2.46	1.34	1.41
18	A	516	HEA	C17-C18	2.38	1.58	1.50
18	N	516	HEA	C3A-C2A	-2.22	1.37	1.40
18	N	515	HEA	C4B-C3B	2.21	1.47	1.42
18	N	516	HEA	C4B-C3B	2.20	1.47	1.42
18	A	515	HEA	C3A-C2A	-2.19	1.37	1.40
18	A	515	HEA	CAD-C3D	2.16	1.55	1.52
18	A	516	HEA	C1A-C2A	2.07	1.47	1.42
18	A	515	HEA	C1C-NC	2.02	1.40	1.36

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C4B-C3B-C2B	-7.64	101.53	106.87
18	N	516	HEA	C4B-C3B-C2B	-5.78	102.83	106.87
18	A	515	HEA	C1B-C2B-C3B	5.63	110.91	107.00
18	A	516	HEA	CBD-CAD-C3D	5.09	121.87	112.49
18	A	516	HEA	C4B-C3B-C2B	-4.75	103.55	106.87
18	N	515	HEA	C13-C14-C15	-4.51	116.81	127.66
18	A	515	HEA	C13-C14-C15	-4.32	117.25	127.66
18	N	515	HEA	C17-C18-C19	-4.20	117.55	127.66
18	N	515	HEA	C1B-C2B-C3B	4.00	109.78	107.00
18	N	515	HEA	C4B-C3B-C2B	-3.90	104.14	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C17-C18-C19	-3.73	118.68	127.66
18	A	515	HEA	C27-C19-C20	3.60	121.32	115.27
18	A	515	HEA	C27-C19-C18	-3.44	114.85	123.68
18	N	516	HEA	CBA-CAA-C2A	3.41	118.77	112.48
18	A	516	HEA	C1B-C2B-C3B	3.40	109.36	107.00
18	A	515	HEA	CMB-C2B-C1B	-3.33	123.34	128.46
18	A	515	HEA	C3C-C4C-NC	3.28	113.46	109.21
18	N	516	HEA	C1B-C2B-C3B	3.26	109.26	107.00
18	A	515	HEA	CBA-CAA-C2A	3.20	118.38	112.48
18	A	515	HEA	C17-C16-C15	-3.18	102.50	112.98
18	N	515	HEA	C17-C16-C15	-3.13	102.68	112.98
18	N	516	HEA	CMD-C2D-C3D	3.11	130.80	124.94
18	N	515	HEA	C27-C19-C18	-2.97	116.05	123.68
18	N	516	HEA	CBD-CAD-C3D	2.97	117.96	112.49
18	N	515	HEA	C27-C19-C20	2.96	120.25	115.27
18	A	515	HEA	C16-C17-C18	-2.94	102.23	111.88
18	N	516	HEA	C25-C23-C24	2.89	120.99	114.60
18	N	515	HEA	CMB-C2B-C1B	-2.84	124.09	128.46
18	N	516	HEA	C17-C18-C19	-2.83	120.86	127.66
18	A	516	HEA	C25-C23-C24	2.73	120.62	114.60
18	N	515	HEA	C3C-C4C-NC	2.65	112.64	109.21
18	A	516	HEA	CBA-CAA-C2A	2.47	117.03	112.48
18	N	515	HEA	C12-C13-C14	-2.44	105.80	112.23
18	A	516	HEA	C17-C18-C19	-2.44	121.80	127.66
18	N	515	HEA	C16-C17-C18	-2.35	104.15	111.88
18	A	515	HEA	C26-C15-C16	2.18	118.94	115.27
18	N	515	HEA	C20-C21-C22	-2.17	104.76	111.88
18	A	516	HEA	O11-C11-C12	-2.11	101.40	109.55
18	A	515	HEA	C12-C13-C14	-2.09	106.71	112.23
18	N	516	HEA	O11-C11-C12	-2.05	101.62	109.55
18	A	516	HEA	C17-C16-C15	2.05	119.73	112.98
18	A	516	HEA	C26-C15-C14	-2.04	118.45	123.68
18	A	515	HEA	CBD-CAD-C3D	2.02	116.20	112.49

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	516	HEA	NB
18	A	516	HEA	NB
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB

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Mol	Chain	Res	Type	Atom
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	N	516	HEA	C2D-C3D-CAD-CBD
18	N	516	HEA	C4D-C3D-CAD-CBD
18	N	516	HEA	C21-C22-C23-C25
18	A	516	HEA	C2D-C3D-CAD-CBD
18	A	516	HEA	C4D-C3D-CAD-CBD
18	A	516	HEA	C21-C22-C23-C25
18	N	515	HEA	C21-C22-C23-C25
18	N	516	HEA	C21-C22-C23-C24
18	A	516	HEA	C21-C22-C23-C24
18	A	515	HEA	C21-C22-C23-C25
18	N	515	HEA	C21-C22-C23-C24
18	N	515	HEA	C15-C16-C17-C18
18	A	515	HEA	C15-C16-C17-C18
18	A	515	HEA	C21-C22-C23-C24
18	N	515	HEA	C13-C14-C15-C26
18	A	515	HEA	C13-C14-C15-C26
18	A	516	HEA	C26-C15-C16-C17

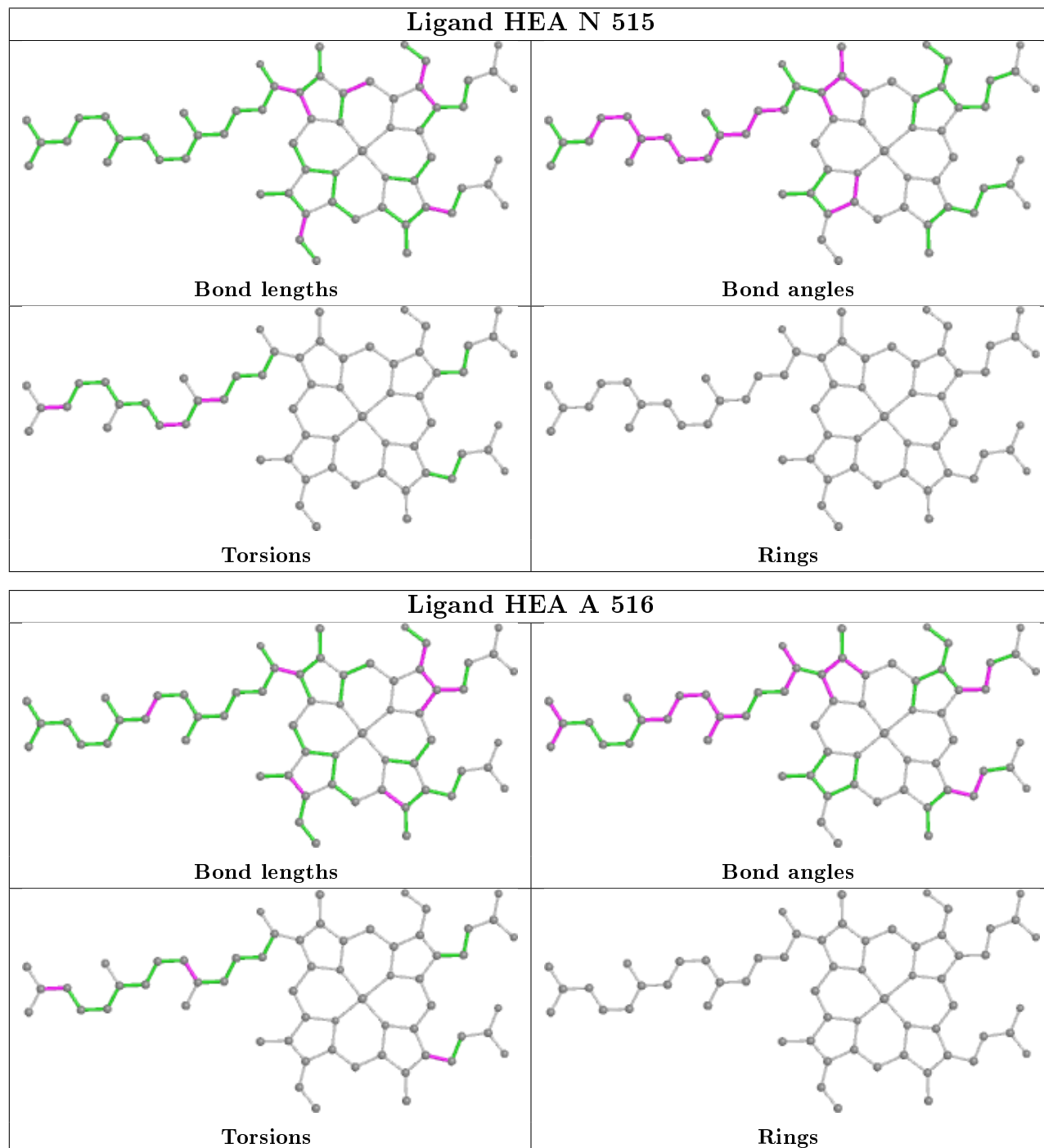
There are no ring outliers.

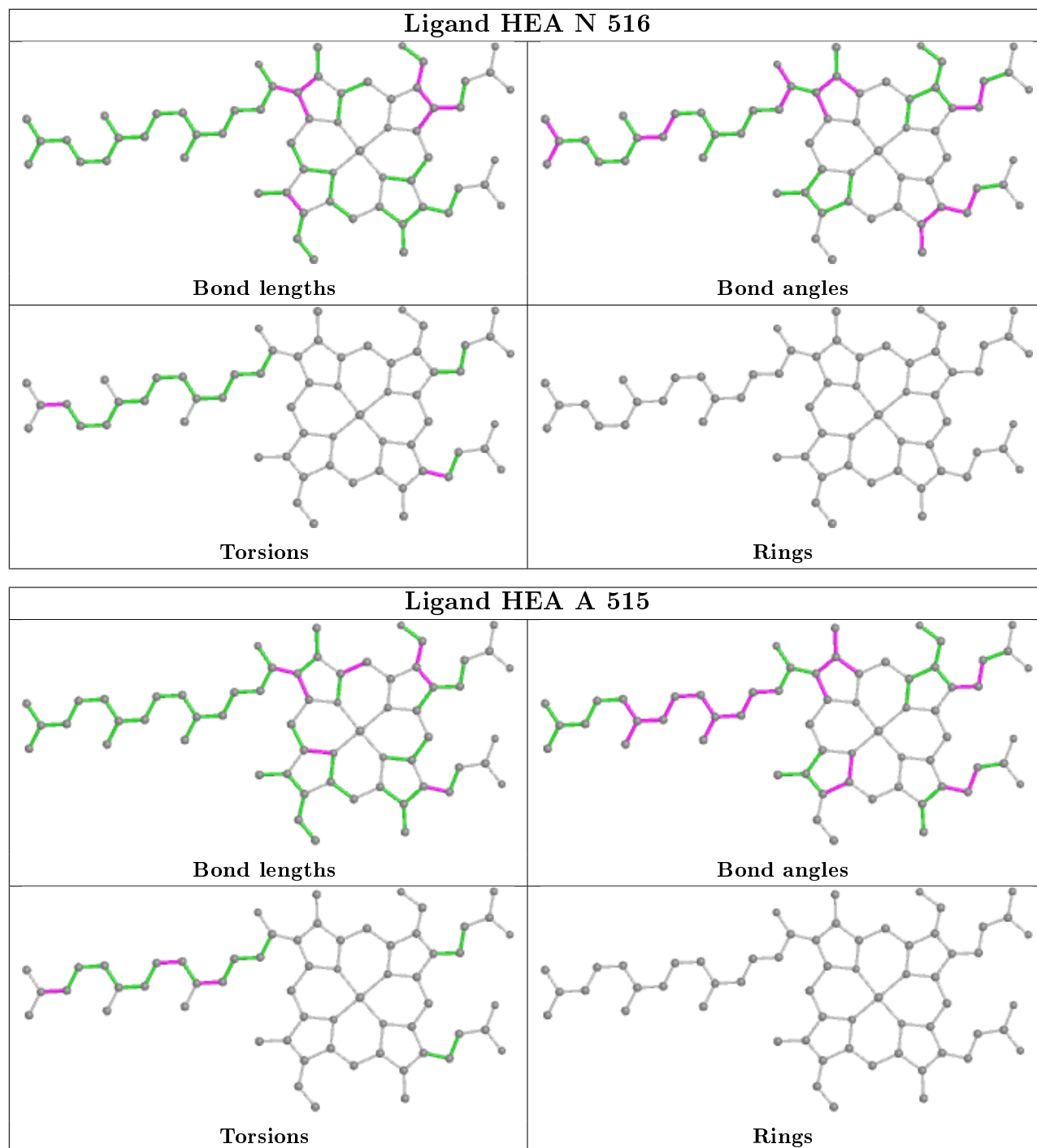
6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	515	HEA	6	0
17	N	521	AZI	3	0
18	A	516	HEA	10	0
18	N	516	HEA	9	0
18	A	515	HEA	8	0
17	A	520	AZI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.