



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:14 AM UTC

PDB ID : 1OCO / pdb\_00001oco  
Title : BOVINE HEART CYTOCHROME C OXIDASE IN CARBON MONOXIDE-  
BOUND STATE  
Authors : Tsukihara, T.; Yao, M.  
Deposited on : 1998-07-09  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

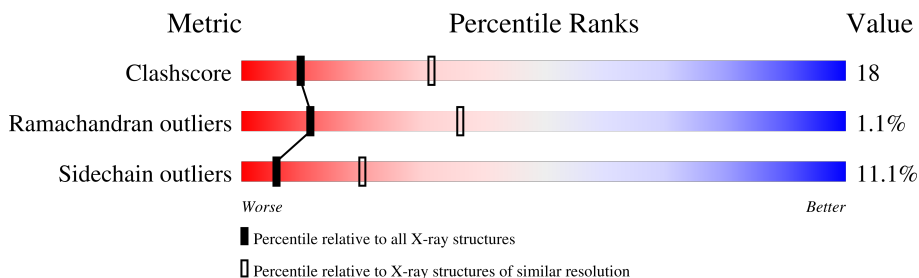
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 of 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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	

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Mol	Chain	Length	Quality of chain
5	E	109	60% 30% 10%
5	R	109	59% 35% 6%
6	F	98	54% 36% 8% .
6	S	98	49% 40% 9% .
7	G	84	58% 29% 13%
7	T	84	58% 31% 11%
8	H	85	46% 31% 12% 12%
8	U	85	48% 29% 11% 12%
9	I	73	58% 37% 5%
9	V	73	51% 42% 7%
10	J	59	58% 27% 10% 5%
10	W	59	63% 22% 7% . 5%
11	K	56	61% 23% . 12%
11	X	56	55% 27% 5% 12%
12	L	47	60% 34% 6%
12	Y	47	62% 34% .
13	M	46	61% 30% . 7%
13	Z	46	63% 28% . 7%

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 28810 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	4025	2690	623	677	35	0	0	0
1	N	514	4025	2690	623	677	35	0	0	0

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 5 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 6 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 7 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 8 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 9 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 10 is a protein called CYTOCHROME C OXIDASE.

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

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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 (CCD ID: CU) (formula: Cu).

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

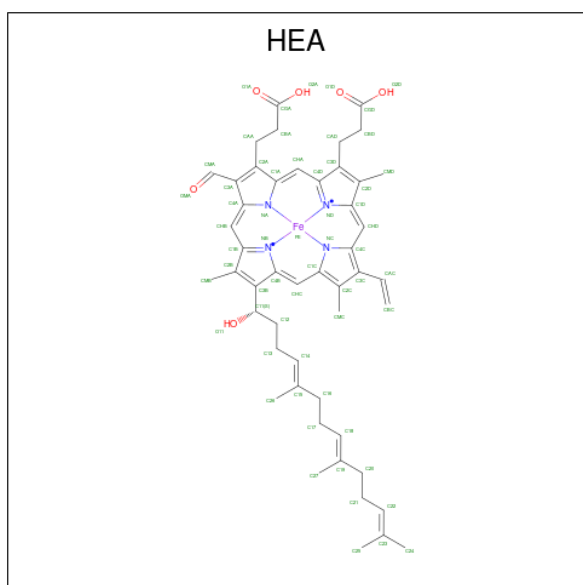
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: NA) (formula: Na).

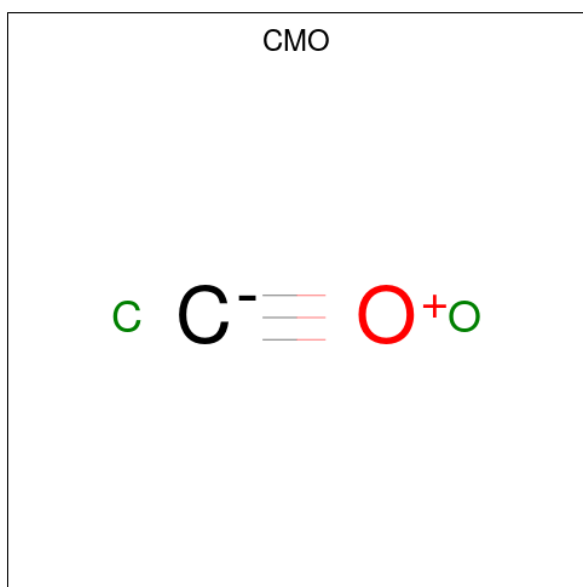
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

- Molecule 18 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

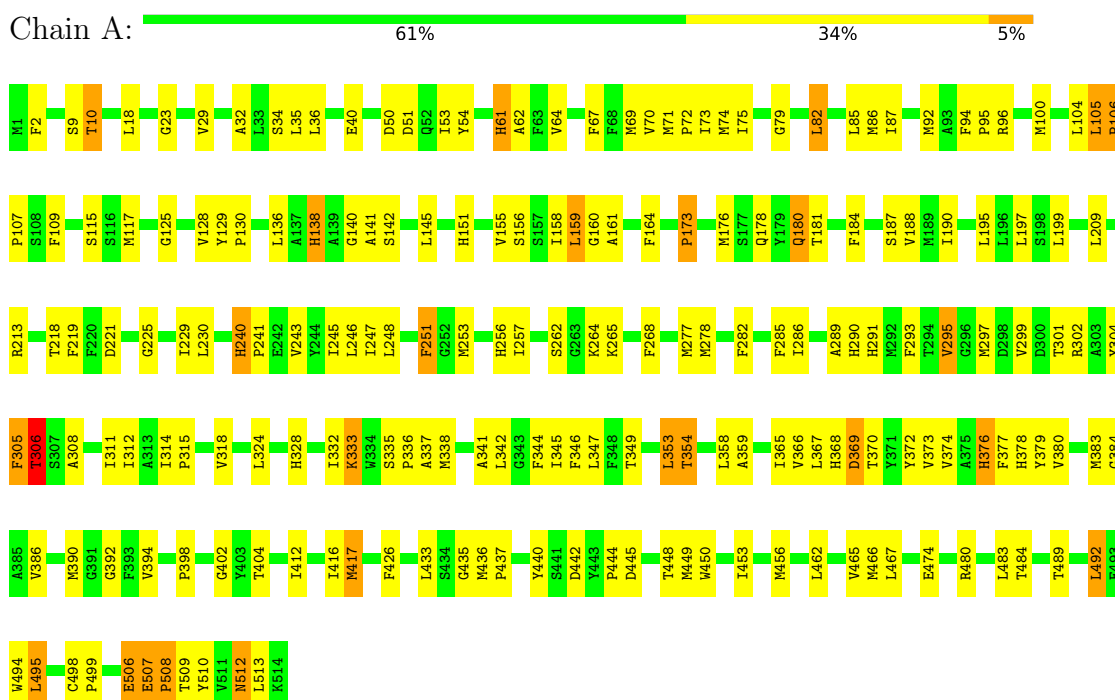
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	1	Total Zn 1 1	0	0
19	S	1	Total Zn 1 1	0	0

### 3 Residue-property plots [i](#)

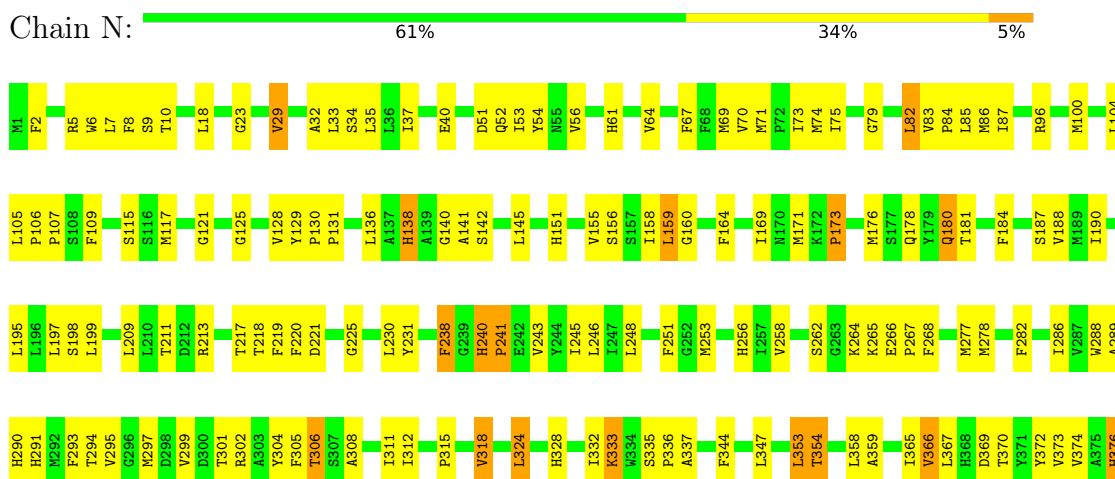
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

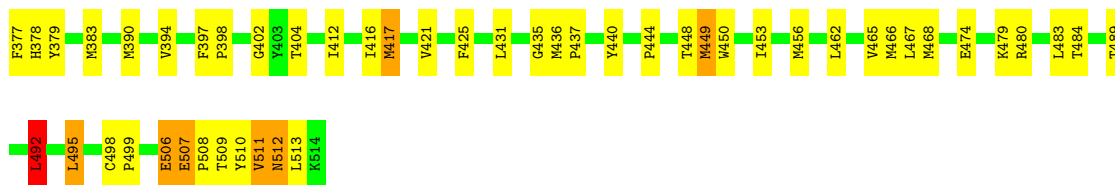
Note EDS was not executed.

- Molecule 1: CYTOCHROME C OXIDASE



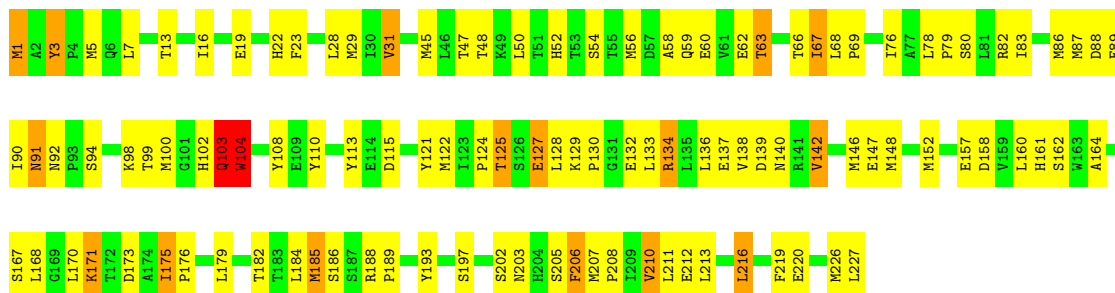
- Molecule 1: CYTOCHROME C OXIDASE





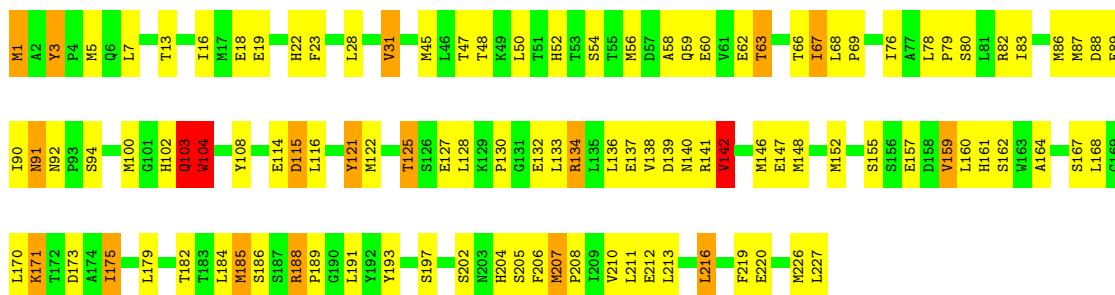
• Molecule 2: CYTOCHROME C OXIDASE

Chain B: 52% 41% 7%



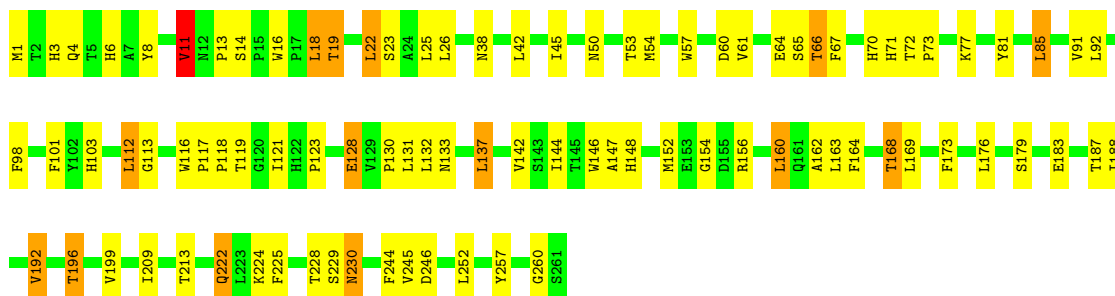
• Molecule 2: CYTOCHROME C OXIDASE

Chain O: 52% 39% 7%



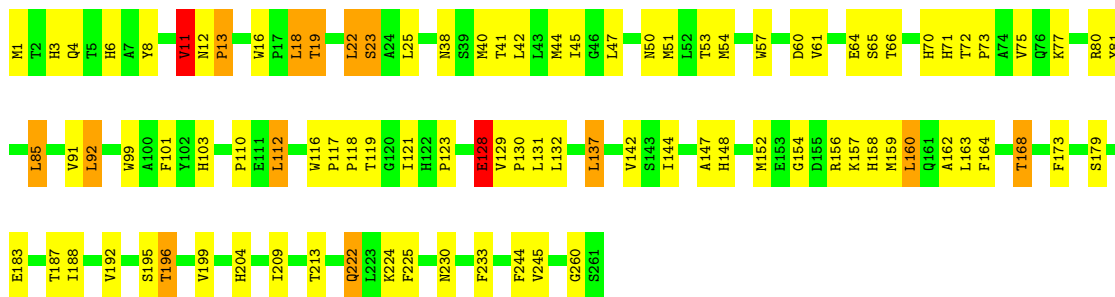
• Molecule 3: CYTOCHROME C OXIDASE

Chain C: 65% 29% 5%



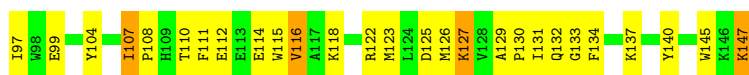
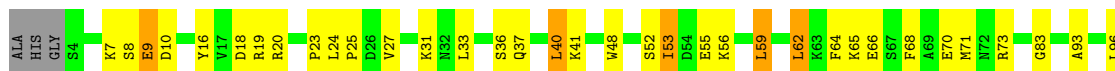
• Molecule 3: CYTOCHROME C OXIDASE

Chain P: 64% 30% 5%



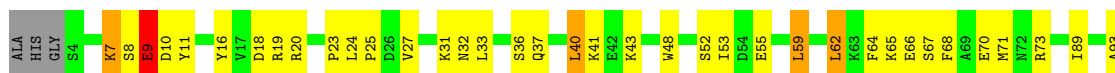
- Molecule 4: CYTOCHROME C OXIDASE

Chain D: 56% 36% 6%



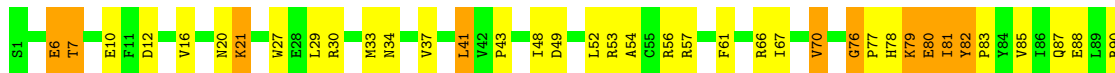
- Molecule 4: CYTOCHROME C OXIDASE

Chain Q: 56% 36% 5%



- Molecule 5: CYTOCHROME C OXIDASE

Chain E: 60% 30% 10%



- Molecule 5: CYTOCHROME C OXIDASE

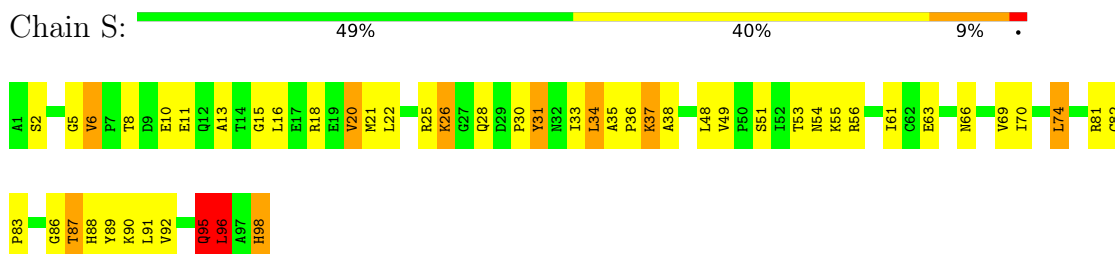
Chain R: 59% 35% 6%



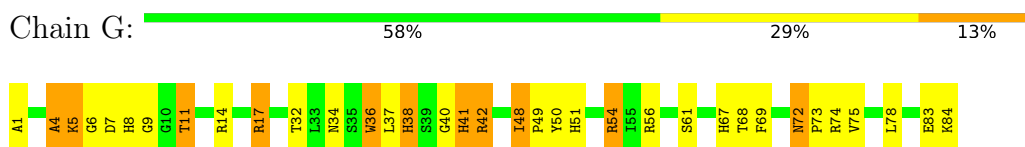
- Molecule 6: CYTOCHROME C OXIDASE



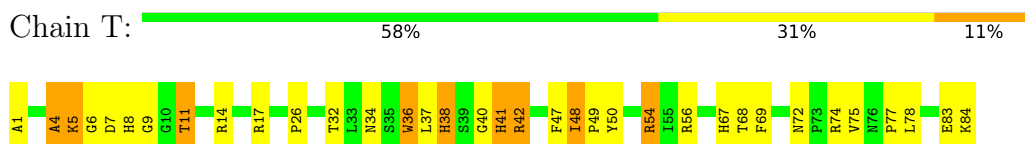
- Molecule 6: CYTOCHROME C OXIDASE



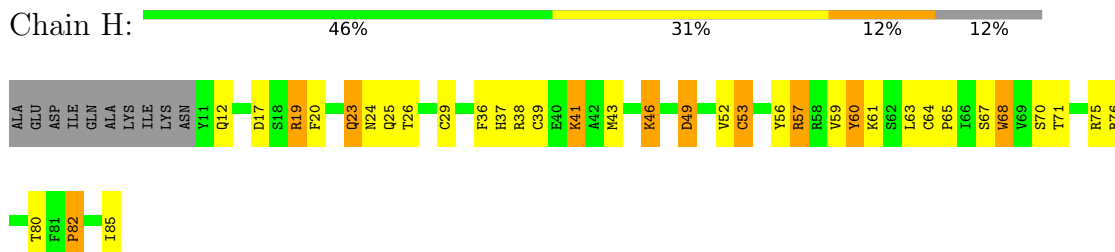
- Molecule 7: CYTOCHROME C OXIDASE



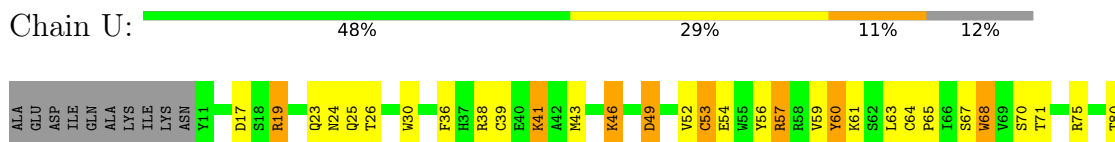
- Molecule 7: CYTOCHROME C OXIDASE



- Molecule 8: CYTOCHROME C OXIDASE



- Molecule 8: CYTOCHROME C OXIDASE





- Molecule 9: CYTOCHROME C OXIDASE

Chain I: 58% 37% 5%



- Molecule 9: CYTOCHROME C OXIDASE

Chain V: 51% 42% 7%



- Molecule 10: CYTOCHROME C OXIDASE

Chain J: 58% 27% 10% 5%



- Molecule 10: CYTOCHROME C OXIDASE

Chain W: 63% 22% 7% 8%



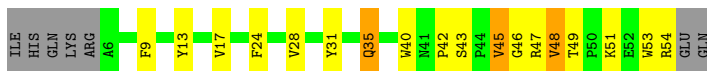
- Molecule 11: CYTOCHROME C OXIDASE

Chain K: 61% 23% 12%



- Molecule 11: CYTOCHROME C OXIDASE

Chain X: 55% 27% 5% 12%



- Molecule 12: CYTOCHROME C OXIDASE

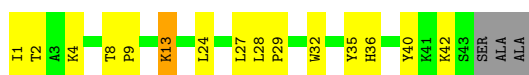
Chain L: 60% 34% 6%



- Molecule 12: CYTOCHROME C OXIDASE



- Molecule 13: CYTOCHROME C OXIDASE



- Molecule 13: CYTOCHROME C OXIDASE



## 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, $\alpha$ , $\beta$ , $\gamma$	189.10Å 210.50Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.3 (7.00-2.80)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, $R_{free}$	0.213 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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: HEA, ZN, NA, CMO, CU, MG

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	1.02	5/4164 (0.1%)	1.28	44/5688 (0.8%)
1	N	0.90	5/4164 (0.1%)	1.25	41/5688 (0.7%)
2	B	0.92	2/1909 (0.1%)	1.21	8/2601 (0.3%)
2	O	0.82	2/1909 (0.1%)	1.19	11/2601 (0.4%)
3	C	0.85	0/2211	1.12	11/3023 (0.4%)
3	P	0.80	0/2211	1.10	8/3023 (0.3%)
4	D	0.79	0/1229	1.07	5/1658 (0.3%)
4	Q	0.66	0/1229	1.06	9/1658 (0.5%)
5	E	0.75	0/898	1.09	9/1218 (0.7%)
5	R	0.68	0/898	1.07	6/1218 (0.5%)
6	F	0.91	0/765	1.16	4/1038 (0.4%)
6	S	0.84	0/765	1.20	4/1038 (0.4%)
7	G	0.82	0/699	1.22	6/950 (0.6%)
7	T	0.76	0/699	1.23	5/950 (0.5%)
8	H	0.80	0/648	1.20	9/877 (1.0%)
8	U	0.71	0/648	1.20	10/877 (1.1%)
9	I	0.80	0/611	1.07	4/810 (0.5%)
9	V	0.76	0/611	1.04	4/810 (0.5%)
10	J	0.80	0/451	1.06	2/610 (0.3%)
10	W	0.72	1/451 (0.2%)	1.04	1/610 (0.2%)
11	K	0.83	0/398	1.02	2/546 (0.4%)
11	X	0.71	0/398	1.04	2/546 (0.4%)
12	L	0.89	0/399	1.01	3/534 (0.6%)
12	Y	0.73	0/399	1.00	2/534 (0.4%)
13	M	0.89	0/345	1.15	1/470 (0.2%)
13	Z	0.69	0/345	1.06	1/470 (0.2%)
All	All	0.85	15/29454 (0.1%)	1.17	212/40046 (0.5%)

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	2
1	N	0	2
2	B	0	2
2	O	0	1
3	C	0	1
3	P	0	1
5	E	0	1
5	R	0	1
All	All	0	11

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	378	HIS	ND1-CE1	8.78	1.41	1.32
1	N	61	HIS	CG-CD2	8.62	1.45	1.35
1	N	378	HIS	CG-CD2	8.30	1.45	1.35
1	A	61	HIS	CG-CD2	7.92	1.44	1.35
1	A	378	HIS	ND1-CE1	6.72	1.39	1.32
1	N	511	VAL	CA-CB	6.01	1.62	1.54
1	A	494	TRP	CA-C	5.94	1.60	1.52
2	B	175	ILE	CA-CB	5.91	1.59	1.54
1	N	61	HIS	ND1-CE1	5.66	1.38	1.32
2	B	210	VAL	CA-CB	-5.66	1.47	1.54
10	W	5	VAL	CA-CB	5.53	1.62	1.54
1	A	376	HIS	ND1-CE1	5.50	1.38	1.32
1	A	295	VAL	CA-CB	5.25	1.60	1.54
2	O	142	VAL	CA-CB	5.15	1.59	1.53
2	O	175	ILE	CA-CB	5.04	1.58	1.54

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	61	HIS	ND1-CE1-NE2	10.92	119.32	108.40
1	A	378	HIS	ND1-CE1-NE2	10.08	118.48	108.40
1	A	61	HIS	ND1-CE1-NE2	9.81	118.21	108.40
1	N	332	ILE	N-CA-C	9.46	121.70	108.93
13	Z	27	LEU	N-CA-C	9.41	121.62	111.36
1	A	378	HIS	CE1-NE2-CD2	-9.09	99.91	109.00
1	A	332	ILE	N-CA-C	8.91	120.61	108.84
7	T	72	ASN	CA-C-N	8.76	129.63	119.47
7	T	72	ASN	C-N-CA	8.76	129.63	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	GLY	N-CA-C	8.74	126.28	114.92
13	M	27	LEU	N-CA-C	8.52	120.64	111.36
8	U	52	VAL	N-CA-C	8.51	121.14	108.46
8	H	52	VAL	N-CA-C	8.42	121.01	108.46
1	N	130	PRO	N-CA-C	-8.42	100.43	110.70
7	G	72	ASN	CA-C-N	8.10	128.86	119.47
7	G	72	ASN	C-N-CA	8.10	128.86	119.47
1	N	435	GLY	N-CA-C	8.00	125.31	114.92
1	A	130	PRO	N-CA-C	-7.92	101.04	110.70
6	S	5	GLY	N-CA-C	7.90	123.88	114.48
2	B	134	ARG	N-CA-C	7.74	124.14	111.37
1	N	61	HIS	CB-CG-CD2	-7.74	121.14	131.20
9	V	20	HIS	N-CA-C	7.74	120.80	111.82
1	N	378	HIS	ND1-CE1-NE2	7.54	115.94	108.40
1	N	495	LEU	N-CA-C	7.52	121.72	112.54
5	R	76	GLY	CA-C-N	7.46	127.63	119.87
5	R	76	GLY	C-N-CA	7.46	127.63	119.87
5	E	76	GLY	CA-C-N	7.38	127.54	119.87
5	E	76	GLY	C-N-CA	7.38	127.54	119.87
1	A	507	GLU	CA-C-N	7.37	129.05	119.84
1	A	507	GLU	C-N-CA	7.37	129.05	119.84
1	A	9	SER	N-CA-C	7.34	120.05	110.43
1	A	125	GLY	N-CA-C	-7.24	103.56	112.68
2	O	206	PHE	N-CA-C	7.16	119.35	109.54
3	C	113	GLY	N-CA-C	-7.11	105.04	115.63
2	B	206	PHE	N-CA-C	7.07	119.23	109.54
4	D	129	ALA	CA-C-N	7.05	126.68	119.56
4	D	129	ALA	C-N-CA	7.05	126.68	119.56
9	I	20	HIS	N-CA-C	7.04	119.98	111.82
9	I	68	ILE	N-CA-C	6.99	117.78	110.72
1	N	507	GLU	CA-C-N	6.95	128.53	119.84
1	N	507	GLU	C-N-CA	6.95	128.53	119.84
9	I	24	ALA	N-CA-C	-6.86	103.73	111.14
9	V	24	ALA	N-CA-C	-6.85	103.89	111.36
1	N	125	GLY	N-CA-C	-6.82	104.09	112.68
5	R	81	ILE	N-CA-C	6.81	116.96	110.42
2	B	161	HIS	N-CA-C	-6.75	99.35	108.86
4	Q	129	ALA	CA-C-N	6.74	126.37	119.56
4	Q	129	ALA	C-N-CA	6.74	126.37	119.56
7	T	69	PHE	N-CA-C	6.73	119.19	111.11
1	A	495	LEU	N-CA-C	6.69	120.55	112.38
1	N	61	HIS	CG-ND1-CE1	-6.66	97.98	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	134	ARG	N-CA-C	6.66	124.98	110.80
1	A	448	THR	N-CA-C	6.61	118.48	111.28
1	N	9	SER	N-CA-C	6.60	119.33	110.35
3	C	66	THR	N-CA-C	6.58	118.53	111.36
1	N	262	SER	N-CA-C	-6.54	104.54	113.30
4	D	133	GLY	N-CA-C	6.51	128.60	113.18
2	O	127	GLU	N-CA-C	6.49	119.85	112.97
5	E	81	ILE	N-CA-C	6.48	116.64	110.42
8	U	63	LEU	N-CA-C	6.47	119.64	111.69
2	B	127	GLU	N-CA-C	6.45	119.81	112.97
1	A	376	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	N	376	HIS	CB-CG-CD2	-6.45	122.82	131.20
7	G	69	PHE	N-CA-C	6.42	118.85	111.02
2	O	161	HIS	N-CA-C	-6.41	99.82	108.86
1	N	492	LEU	N-CA-C	6.37	120.62	112.34
3	P	70	HIS	N-CA-C	6.36	120.30	112.54
8	U	81	PHE	CA-C-N	6.36	126.49	119.87
8	U	81	PHE	C-N-CA	6.36	126.49	119.87
3	C	244	PHE	N-CA-C	-6.33	104.30	111.07
1	N	448	THR	N-CA-C	6.29	118.22	111.36
1	A	10	THR	N-CA-C	-6.29	103.79	112.03
1	A	262	SER	N-CA-C	-6.27	104.89	113.30
8	H	20	PHE	N-CA-C	-6.19	99.84	108.76
10	J	24	GLY	N-CA-C	6.18	122.33	114.66
1	N	2	PHE	N-CA-C	-6.18	104.08	111.69
11	X	48	VAL	N-CA-C	6.05	116.64	108.17
8	H	63	LEU	N-CA-C	6.02	119.10	111.69
4	Q	133	GLY	N-CA-C	6.00	127.41	113.18
2	B	104	TRP	N-CA-C	6.00	123.57	110.80
1	A	142	SER	N-CA-C	5.97	117.48	110.97
11	X	35	GLN	N-CA-C	5.95	120.15	113.01
9	V	68	ILE	N-CA-C	5.93	116.71	110.72
3	P	66	THR	N-CA-C	5.91	117.81	111.36
5	R	21	LYS	CA-C-N	5.91	125.61	119.05
5	R	21	LYS	C-N-CA	5.91	125.61	119.05
1	N	140	GLY	N-CA-C	5.89	117.55	111.95
2	O	47	THR	N-CA-C	5.89	120.04	112.26
1	A	2	PHE	N-CA-C	-5.86	104.48	111.69
7	G	9	GLY	N-CA-C	-5.86	99.28	113.18
2	B	47	THR	N-CA-C	5.86	119.99	112.26
3	C	70	HIS	N-CA-C	5.85	119.68	112.54
11	K	35	GLN	N-CA-C	5.85	120.15	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	89	ILE	N-CA-C	-5.82	104.84	110.72
1	N	412	ILE	N-CA-C	-5.81	105.07	110.53
7	T	9	GLY	N-CA-C	-5.79	99.46	113.18
1	N	67	PHE	N-CA-C	5.78	119.51	112.23
12	Y	6	GLY	CA-C-N	5.76	127.04	119.84
12	Y	6	GLY	C-N-CA	5.76	127.04	119.84
2	O	104	TRP	N-CA-C	5.76	123.06	110.80
1	A	412	ILE	N-CA-C	-5.75	105.12	110.53
5	E	21	LYS	CA-C-N	5.72	125.40	119.05
5	E	21	LYS	C-N-CA	5.72	125.40	119.05
1	N	142	SER	N-CA-C	5.71	117.19	110.97
3	P	244	PHE	N-CA-C	-5.70	105.07	111.28
1	N	479	LYS	N-CA-C	5.69	118.96	111.28
3	P	225	PHE	N-CA-C	5.68	119.79	112.86
1	A	67	PHE	N-CA-C	5.64	119.88	112.89
1	A	466	MET	N-CA-C	-5.60	104.56	111.40
8	H	59	VAL	N-CA-C	5.59	115.72	110.30
1	A	105	LEU	CA-C-N	-5.59	114.63	120.38
1	A	105	LEU	C-N-CA	-5.59	114.63	120.38
1	N	509	THR	N-CA-C	-5.58	102.66	110.35
1	A	509	THR	N-CA-C	-5.54	102.71	110.35
8	U	64	CYS	CA-C-N	-5.53	114.27	119.85
8	U	64	CYS	C-N-CA	-5.53	114.27	119.85
3	C	11	VAL	N-CA-C	5.52	116.70	109.58
1	A	251	PHE	N-CA-C	-5.52	105.17	111.07
8	H	52	VAL	CA-C-N	5.51	130.72	122.23
8	H	52	VAL	C-N-CA	5.51	130.72	122.23
3	C	225	PHE	N-CA-C	5.51	119.58	112.86
1	A	129	TYR	CB-CA-C	-5.51	100.78	109.42
4	Q	32	ASN	N-CA-C	5.50	117.27	108.41
1	A	94	PHE	CA-C-N	5.49	124.95	119.24
1	A	94	PHE	C-N-CA	5.49	124.95	119.24
4	D	104	TYR	N-CA-C	5.49	117.66	109.25
1	N	158	ILE	N-CA-C	-5.49	105.02	110.62
1	N	169	ILE	N-CA-C	5.49	116.53	111.81
10	W	24	GLY	N-CA-C	5.48	121.45	114.66
2	O	204	HIS	N-CA-C	-5.48	105.41	111.71
3	C	257	TYR	N-CA-C	5.47	117.33	111.36
3	C	246	ASP	CB-CA-C	-5.46	102.27	110.90
6	S	31	TYR	N-CA-C	5.45	118.94	112.72
1	A	305	PHE	N-CA-C	5.45	119.03	112.38
2	O	207	MET	CA-C-N	5.45	126.65	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	207	MET	C-N-CA	5.45	126.65	119.84
7	T	11	THR	N-CA-C	5.45	122.40	110.80
1	A	173	PRO	N-CA-C	-5.44	104.06	110.70
3	P	75	VAL	N-CA-C	5.42	116.20	110.72
3	C	245	VAL	N-CA-C	5.41	116.14	110.62
3	P	159	MET	N-CA-C	-5.41	105.38	111.28
10	J	20	VAL	N-CA-C	5.41	118.64	111.17
1	A	158	ILE	N-CA-C	-5.40	105.11	110.62
11	K	48	VAL	N-CA-C	5.40	115.73	108.17
12	L	6	GLY	CA-C-N	5.40	126.59	119.84
12	L	6	GLY	C-N-CA	5.40	126.59	119.84
1	A	50	ASP	N-CA-C	5.39	118.26	109.59
1	A	140	GLY	N-CA-C	5.37	117.52	112.04
1	N	288	TRP	N-CA-C	5.35	122.20	110.80
8	U	52	VAL	CA-C-N	5.35	130.47	122.23
8	U	52	VAL	C-N-CA	5.35	130.47	122.23
4	Q	103	VAL	N-CA-C	5.35	116.41	111.81
1	N	82	LEU	N-CA-C	5.33	119.88	112.90
1	N	425	PHE	N-CA-C	5.32	119.83	113.23
8	U	59	VAL	N-CA-C	5.32	115.46	110.30
3	P	11	VAL	N-CA-C	5.32	116.44	109.58
8	U	68	TRP	N-CA-C	-5.32	105.13	111.03
1	N	305	PHE	N-CA-C	5.30	118.85	112.38
4	D	118	LYS	N-CA-C	-5.29	105.59	111.36
6	F	38	ALA	N-CA-C	5.29	117.51	110.53
1	N	449	MET	N-CA-C	5.29	116.73	110.97
6	F	35	ALA	CA-C-N	5.26	125.20	119.78
6	F	35	ALA	C-N-CA	5.26	125.20	119.78
1	N	171	MET	N-CA-C	5.26	118.83	111.30
2	O	18	GLU	N-CA-C	-5.26	105.46	111.14
5	E	79	LYS	N-CA-C	5.25	119.18	112.87
1	A	82	LEU	N-CA-C	5.25	119.77	112.90
1	A	338	MET	N-CA-C	-5.24	105.74	111.82
7	G	11	THR	N-CA-C	5.24	121.96	110.80
1	A	433	LEU	N-CA-C	-5.24	105.57	111.28
1	N	466	MET	N-CA-C	-5.22	105.50	111.14
9	I	2	THR	N-CA-C	5.22	117.92	108.69
3	C	98	PHE	N-CA-C	-5.21	105.66	112.23
1	A	506	GLU	N-CA-C	-5.21	105.72	111.71
1	N	129	TYR	CB-CA-C	-5.21	101.25	109.42
6	S	38	ALA	N-CA-C	5.20	117.39	110.53
5	E	21	LYS	N-CA-C	-5.20	102.33	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	211	THR	N-CA-C	-5.19	105.69	112.23
5	E	7	THR	N-CA-C	-5.18	103.84	110.53
3	P	99	TRP	N-CA-C	-5.18	105.55	111.14
8	H	64	CYS	CA-C-N	-5.14	114.62	119.76
8	H	64	CYS	C-N-CA	-5.14	114.62	119.76
1	A	161	ALA	N-CA-C	-5.14	105.76	111.36
3	C	246	ASP	N-CA-CB	5.12	117.50	110.07
1	N	173	PRO	N-CA-C	-5.11	104.47	110.70
1	A	141	ALA	N-CA-C	5.10	119.13	113.01
12	L	21	LEU	N-CA-C	-5.10	105.63	111.14
8	H	68	TRP	N-CA-C	-5.09	105.38	111.03
1	N	506	GLU	N-CA-C	-5.09	105.86	111.71
1	A	36	LEU	N-CA-C	-5.07	105.83	111.36
5	E	6	GLU	N-CA-C	5.07	118.03	110.52
1	N	421	VAL	N-CA-C	5.06	115.78	110.62
2	O	202	SER	N-CA-C	5.05	119.71	111.37
5	R	6	GLU	N-CA-C	5.05	117.92	110.59
7	G	51	HIS	N-CA-C	5.05	119.16	112.89
1	N	217	THR	N-CA-C	-5.05	103.27	110.59
1	A	306	THR	N-CA-C	-5.05	106.29	112.90
1	N	29	VAL	CB-CA-C	-5.05	105.51	111.97
2	B	76	ILE	N-CA-C	-5.04	106.88	111.67
6	F	26	LYS	N-CA-C	-5.04	107.10	113.20
4	Q	104	TYR	N-CA-C	5.04	116.95	109.25
2	B	202	SER	N-CA-C	5.03	119.67	111.37
1	A	436	MET	CA-C-N	5.03	125.01	120.03
1	A	436	MET	C-N-CA	5.03	125.01	120.03
6	S	26	LYS	N-CA-C	-5.03	107.12	113.20
1	N	436	MET	CA-C-N	5.02	125.00	120.03
1	N	436	MET	C-N-CA	5.02	125.00	120.03
4	Q	9	GLU	N-CA-C	-5.02	107.11	113.18
9	V	2	THR	N-CA-C	5.02	117.24	108.76
1	A	426	PHE	CA-C-N	5.02	125.04	119.32
1	A	426	PHE	C-N-CA	5.02	125.04	119.32
4	Q	7	LYS	N-CA-C	5.01	117.08	108.90

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	110	TYR	Sidechain
2	B	121	TYR	Sidechain
3	C	8	TYR	Sidechain
5	E	82	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
2	O	121	TYR	Sidechain
3	P	8	TYR	Sidechain
5	R	82	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	4025	0	4002	142	0
1	N	4025	0	4002	145	0
2	B	1863	0	1867	92	0
2	O	1863	0	1867	91	0
3	C	2124	0	2044	69	0
3	P	2124	0	2044	75	0
4	D	1195	0	1183	48	0
4	Q	1195	0	1183	49	0
5	E	878	0	868	36	0
5	R	878	0	868	33	0
6	F	748	0	728	40	0
6	S	748	0	728	47	0
7	G	672	0	645	37	0
7	T	672	0	645	35	0
8	H	628	0	582	53	0
8	U	628	0	582	52	0
9	I	598	0	612	28	0
9	V	598	0	612	30	0
10	J	441	0	439	13	0
10	W	441	0	439	11	0
11	K	384	0	366	11	0
11	X	384	0	366	15	0
12	L	386	0	388	15	0
12	Y	386	0	388	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	335	0	352	16	0
13	Z	335	0	352	15	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	120	0	107	13	0
17	N	120	0	107	10	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	F	1	0	0	0	0
19	S	1	0	0	0	0
All	All	28810	0	28366	1002	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 18.

All (1002) 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)
8:H:57:ARG:HH11	8:H:57:ARG:HB3	1.23	1.03
8:U:57:ARG:HH11	8:U:57:ARG:HB3	1.20	1.01
1:N:187:SER:HB2	1:N:277:MET:HE1	1.45	0.97
2:B:86:MET:O	2:B:89[B]:GLU:HG2	1.65	0.96
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.53	0.90
1:A:187:SER:HB2	1:A:277:MET:HE1	1.53	0.90
2:O:86:MET:O	2:O:89[B]:GLU:HG2	1.71	0.89
2:O:78:LEU:HB2	2:O:79:PRO:HD3	1.55	0.88
2:B:78:LEU:HB2	2:B:79:PRO:HD3	1.55	0.87
8:H:39:CYS:SG	8:H:53:CYS:CB	2.64	0.86
8:U:39:CYS:SG	8:U:53:CYS:CB	2.65	0.84
8:H:39:CYS:SG	8:H:53:CYS:HB3	2.17	0.84
1:A:282:PHE:HB2	7:T:5:LYS:HB3	1.59	0.83
1:N:365:ILE:HG13	2:O:87:MET:HE1	1.60	0.83
7:G:5:LYS:HB3	1:N:282:PHE:HB2	1.60	0.82
3:P:209:ILE:O	3:P:213:THR:HG23	1.80	0.82
8:U:39:CYS:SG	8:U:53:CYS:HB3	2.20	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:184:PHE:H	1:N:256:HIS:HE1	1.27	0.81
2:O:103:GLN:HG2	2:O:104:TRP:CE2	2.15	0.81
1:A:365:ILE:HG13	2:B:87:MET:HE1	1.61	0.80
2:B:103:GLN:HG2	2:B:104:TRP:CE2	2.16	0.80
7:G:1:ALA:HB1	1:N:286:ILE:HG22	1.63	0.80
1:A:286:ILE:HG22	7:T:1:ALA:HB1	1.64	0.79
7:G:6:GLY:HA3	1:N:190:ILE:HG12	1.63	0.78
1:N:506:GLU:HG3	3:P:1:MET:SD	2.24	0.78
1:N:35:LEU:HD11	1:N:462:LEU:HD13	1.65	0.77
3:C:209:ILE:O	3:C:213:THR:HG23	1.84	0.77
3:P:18:LEU:HD22	3:P:22:LEU:HD22	1.67	0.77
2:O:13:THR:HB	2:O:168:LEU:HD23	1.67	0.77
1:A:190:ILE:HG12	7:T:6:GLY:HA3	1.66	0.76
6:F:33:ILE:HG22	6:F:34:LEU:HD12	1.67	0.76
1:A:506:GLU:HG3	3:C:1:MET:SD	2.24	0.76
4:Q:147:LYS:HE3	4:Q:147:LYS:HA	1.68	0.75
2:B:13:THR:HB	2:B:168:LEU:HD23	1.68	0.75
1:A:187:SER:CB	1:A:277:MET:HE1	2.17	0.74
2:B:59:GLN:H	2:B:62:GLU:HG3	1.52	0.74
4:D:147:LYS:HE3	4:D:147:LYS:HA	1.68	0.74
2:B:1:MET:SD	2:B:133:LEU:CD1	2.76	0.74
2:O:152:MET:HB2	2:O:182:THR:HG23	1.70	0.73
1:A:176:MET:HE3	1:A:181:THR:HG22	1.70	0.73
6:F:30:PRO:HB3	6:F:96:LEU:HB3	1.70	0.73
2:B:188:ARG:HG3	9:I:54:TYR:OH	1.89	0.73
8:H:39:CYS:HG	8:H:53:CYS:HG	0.78	0.73
1:N:187:SER:CB	1:N:277:MET:HE1	2.18	0.72
10:W:29:ASN:O	10:W:33:ARG:HG3	1.89	0.72
13:M:13:LYS:H	13:M:13:LYS:HD3	1.54	0.72
8:H:43:MET:HE1	8:U:43:MET:HE1	1.72	0.72
1:A:184:PHE:H	1:A:256:HIS:HE1	1.38	0.71
1:A:306:THR:HB	1:A:359:ALA:O	1.90	0.71
8:H:53:CYS:HA	8:U:46:LYS:NZ	2.06	0.71
1:N:306:THR:HB	1:N:359:ALA:O	1.90	0.71
3:P:60:ASP:O	3:P:64:GLU:HG3	1.91	0.71
1:N:176:MET:HE3	1:N:181:THR:HG22	1.72	0.71
6:S:30:PRO:HB3	6:S:96:LEU:HB3	1.71	0.71
2:B:59:GLN:HA	2:B:62:GLU:HB2	1.72	0.70
2:B:152:MET:HB2	2:B:182:THR:HG23	1.73	0.70
1:A:506:GLU:HB2	3:C:1:MET:SD	2.32	0.70
8:H:46:LYS:NZ	8:U:53:CYS:HA	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:506:GLU:HB2	3:P:1:MET:HA	1.74	0.70
9:I:27:VAL:HG13	9:I:31:PHE:HE2	1.57	0.69
3:C:60:ASP:O	3:C:64:GLU:HG3	1.91	0.69
2:O:188:ARG:HG3	9:V:54:TYR:OH	1.92	0.69
2:O:59:GLN:HA	2:O:62:GLU:HB2	1.74	0.69
4:D:23:PRO:O	5:E:66:ARG:HD3	1.93	0.69
8:U:71:THR:O	8:U:75:ARG:HD3	1.92	0.69
1:A:506:GLU:HB2	3:C:1:MET:HA	1.74	0.69
2:O:186:SER:HB3	2:O:213:LEU:HD22	1.75	0.69
10:J:29:ASN:O	10:J:33:ARG:HG3	1.93	0.68
8:U:39:CYS:HG	8:U:53:CYS:HG	0.69	0.68
8:H:71:THR:O	8:H:75:ARG:HD3	1.92	0.68
7:G:4:ALA:HB2	1:N:197:LEU:HD12	1.76	0.68
2:O:1:MET:SD	2:O:133:LEU:CD1	2.82	0.68
2:O:59:GLN:H	2:O:62:GLU:HG3	1.58	0.67
8:H:41:LYS:NZ	8:H:41:LYS:HB3	2.09	0.67
1:A:197:LEU:HD12	7:T:4:ALA:HB2	1.77	0.66
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.76	0.66
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.78	0.66
9:V:27:VAL:HG13	9:V:31:PHE:HE2	1.60	0.66
2:B:193:TYR:CE1	4:D:126:MET:HE1	2.31	0.66
1:N:184:PHE:H	1:N:256:HIS:CE1	2.11	0.66
6:S:33:ILE:HG22	6:S:34:LEU:HD12	1.76	0.66
2:B:103:GLN:HG2	2:B:104:TRP:CZ2	2.30	0.66
8:H:39:CYS:HG	8:H:53:CYS:CB	2.08	0.66
3:C:19:THR:HG23	3:C:53:THR:OG1	1.96	0.66
7:G:54:ARG:HD3	7:G:54:ARG:N	2.10	0.66
2:O:1:MET:SD	2:O:133:LEU:HD13	2.36	0.65
8:U:41:LYS:NZ	8:U:41:LYS:HB3	2.12	0.65
3:C:164:PHE:O	3:C:168:THR:HG23	1.97	0.65
7:G:4:ALA:CB	1:N:197:LEU:HD12	2.26	0.65
4:D:24:LEU:HB3	5:E:30:ARG:HG2	1.78	0.65
4:D:40:LEU:HD22	4:D:59:LEU:HD13	1.77	0.65
4:Q:24:LEU:HB3	5:R:30:ARG:HG2	1.79	0.65
13:Z:13:LYS:H	13:Z:13:LYS:HD3	1.61	0.64
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.78	0.64
8:H:17:ASP:OD1	8:H:19:ARG:HG2	1.98	0.64
3:P:164:PHE:O	3:P:168:THR:HG23	1.97	0.64
1:A:184:PHE:H	1:A:256:HIS:CE1	2.15	0.64
8:U:65:PRO:HG2	8:U:68:TRP:CG	2.33	0.64
7:G:4:ALA:HB2	1:N:197:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:32:TRP:O	13:M:36:HIS:HD2	1.80	0.64
2:O:103:GLN:HG2	2:O:104:TRP:CZ2	2.33	0.64
13:Z:32:TRP:O	13:Z:36:HIS:HD2	1.79	0.64
3:C:18:LEU:HD22	3:C:22:LEU:HD22	1.79	0.64
1:A:510:TYR:HB2	6:F:56:ARG:NH1	2.12	0.64
2:B:1:MET:SD	2:B:133:LEU:HD11	2.38	0.64
2:O:90[A]:ILE:HD12	2:O:90[A]:ILE:H	1.63	0.64
1:N:390:MET:CE	17:N:515:HEA:H242	2.27	0.64
1:A:197:LEU:HD12	7:T:4:ALA:CB	2.28	0.63
1:A:248:LEU:HD22	1:A:277:MET:HE2	1.80	0.63
6:S:8:THR:OG1	6:S:11:GLU:HG2	1.98	0.63
2:B:90[A]:ILE:H	2:B:90[A]:ILE:HD12	1.63	0.63
1:A:197:LEU:CD1	7:T:4:ALA:HB2	2.29	0.63
7:T:67:HIS:CD2	7:T:78:LEU:HD11	2.34	0.63
2:B:22:HIS:CE1	9:I:44:LYS:HD3	2.34	0.62
2:B:193:TYR:HE1	4:D:126:MET:HE1	1.64	0.62
2:O:193:TYR:CE1	4:Q:126:MET:HE1	2.34	0.62
4:Q:40:LEU:HD22	4:Q:59:LEU:HD13	1.80	0.62
2:B:186:SER:HB3	2:B:213:LEU:HD22	1.81	0.62
7:G:67:HIS:CD2	7:G:78:LEU:HD11	2.34	0.62
2:B:50:LEU:HD21	5:E:77:PRO:HD2	1.82	0.62
10:J:50:LEU:HD22	10:J:50:LEU:O	1.99	0.62
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.00	0.62
6:S:10:GLU:HG2	6:S:25:ARG:HH22	1.63	0.62
6:F:13:ALA:O	6:F:18:ARG:HD2	1.99	0.62
6:F:10:GLU:HG2	6:F:25:ARG:HH22	1.64	0.62
2:O:136:LEU:HB3	2:O:193:TYR:CD2	2.35	0.62
6:S:53:THR:HG22	6:S:54:ASN:H	1.64	0.62
8:U:57:ARG:HH11	8:U:57:ARG:CB	2.05	0.62
3:C:154:GLY:HA2	6:F:6:VAL:HG22	1.82	0.62
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.82	0.61
6:F:8:THR:OG1	6:F:11:GLU:HG2	2.00	0.61
10:J:12:PHE:O	10:J:23:LYS:HE2	2.01	0.61
7:T:54:ARG:HD3	7:T:54:ARG:N	2.15	0.61
3:P:19:THR:HG23	3:P:53:THR:OG1	2.00	0.61
6:F:53:THR:HG22	6:F:54:ASN:H	1.64	0.61
1:N:219:PHE:HZ	3:P:199:VAL:HG21	1.63	0.61
4:Q:23:PRO:O	5:R:66:ARG:HD3	2.00	0.61
9:I:39:VAL:O	9:I:42:LYS:HE2	2.00	0.61
1:A:333:LYS:HE2	1:A:335:SER:HB3	1.81	0.61
7:G:42:ARG:CZ	7:G:74:ARG:HH21	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:510:TYR:HB2	6:S:56:ARG:NH1	2.16	0.61
10:W:12:PHE:O	10:W:23:LYS:HE2	2.01	0.61
1:N:71:MET:HE3	1:N:245:ILE:HG21	1.83	0.61
1:N:128:VAL:HG22	1:N:128:VAL:O	2.00	0.60
3:C:222:GLN:HE21	3:C:222:GLN:HA	1.65	0.60
1:N:333:LYS:HE2	1:N:335:SER:HB3	1.84	0.60
2:O:90[B]:ILE:HG23	2:O:91[B]:ASN:H	1.65	0.60
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.82	0.60
7:T:42:ARG:CZ	7:T:74:ARG:HH21	2.15	0.60
10:W:27:THR:O	10:W:30:ILE:HG12	2.01	0.60
8:U:38:ARG:HG2	8:U:85:ILE:HG23	1.83	0.60
6:S:13:ALA:O	6:S:18:ARG:HD2	2.02	0.60
1:N:219:PHE:CZ	3:P:199:VAL:HG21	2.37	0.59
2:O:179:LEU:HD21	8:U:65:PRO:HD3	1.83	0.59
3:P:154:GLY:C	6:S:6:VAL:HG13	2.27	0.59
3:P:222:GLN:HE21	3:P:222:GLN:HA	1.66	0.59
8:U:17:ASP:OD1	8:U:19:ARG:HG2	2.02	0.59
2:B:90[B]:ILE:HG23	2:B:91[B]:ASN:H	1.68	0.59
4:D:68:PHE:HA	4:D:71:MET:HG2	1.84	0.59
1:N:225:GLY:HA3	3:P:112:LEU:CD1	2.33	0.59
2:O:226:MET:O	2:O:227:LEU:HB2	2.02	0.59
8:H:65:PRO:HG2	8:H:68:TRP:CG	2.38	0.59
1:N:506:GLU:HB2	3:P:1:MET:SD	2.42	0.59
9:V:26:MET:HE3	9:V:26:MET:HA	1.84	0.59
1:A:225:GLY:HA3	3:C:112:LEU:CD1	2.33	0.58
8:H:57:ARG:HB3	8:H:57:ARG:NH1	2.08	0.58
3:C:148:HIS:O	3:C:152:MET:HG3	2.02	0.58
4:Q:130:PRO:HG2	4:Q:131:ILE:HG13	1.85	0.58
1:A:128:VAL:HG22	1:A:128:VAL:O	2.03	0.58
2:B:48:THR:HB	9:I:16:ARG:CZ	2.33	0.58
2:B:179:LEU:HD21	8:H:65:PRO:HD3	1.84	0.58
10:W:50:LEU:O	10:W:50:LEU:HD22	2.02	0.58
2:B:226:MET:O	2:B:227:LEU:HB2	2.03	0.58
2:O:76:ILE:O	2:O:79:PRO:HD2	2.04	0.58
1:A:82:LEU:O	1:A:86:MET:HG3	2.03	0.58
2:B:83:ILE:O	2:B:87:MET:HG3	2.02	0.58
4:D:64:PHE:CE1	5:E:66:ARG:HD2	2.39	0.58
4:D:130:PRO:HG2	4:D:131:ILE:HG13	1.85	0.58
2:O:22:HIS:CE1	9:V:44:LYS:HD3	2.38	0.58
2:B:152:MET:HB2	2:B:182:THR:CG2	2.33	0.58
4:D:70:GLU:HA	5:E:109:VAL:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:MET:HE2	5:E:67:ILE:HG23	1.86	0.58
1:N:87:ILE:O	1:N:173:PRO:HD3	2.04	0.58
9:V:29:LEU:O	9:V:33:THR:HG23	2.03	0.58
9:V:39:VAL:O	9:V:42:LYS:HE2	2.03	0.58
1:A:87:ILE:O	1:A:173:PRO:HD3	2.03	0.58
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.39	0.58
9:I:15:ARG:HD2	9:I:18:ARG:NH2	2.19	0.58
1:N:219:PHE:HZ	3:P:199:VAL:CG2	2.17	0.58
1:N:390:MET:HE1	17:N:515:HEA:H242	1.86	0.58
2:O:146:MET:SD	2:O:189:PRO:HB3	2.43	0.58
1:N:248:LEU:HD22	1:N:277:MET:HE2	1.86	0.57
3:P:154:GLY:HA2	6:S:6:VAL:HG22	1.86	0.57
5:R:6:GLU:HB2	5:R:10:GLU:HB2	1.86	0.57
5:R:7:THR:OG1	5:R:10:GLU:HG3	2.04	0.57
8:U:57:ARG:O	8:U:61:LYS:HB2	2.04	0.57
2:B:1:MET:SD	2:B:133:LEU:HD13	2.44	0.57
2:B:63:THR:O	2:B:66:THR:HG22	2.04	0.57
6:F:53:THR:HG22	6:F:54:ASN:OD1	2.05	0.57
2:O:125:THR:HA	2:O:128:LEU:HG	1.86	0.57
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.04	0.57
1:A:75:ILE:O	1:A:79:GLY:HA3	2.05	0.57
8:H:57:ARG:HA	8:H:60:TYR:CD2	2.39	0.57
1:N:29:VAL:HG13	12:Y:36:PRO:HG3	1.87	0.57
1:A:398:PRO:O	1:A:498:CYS:HB3	2.05	0.57
9:I:15:ARG:HD2	9:I:18:ARG:HH22	1.69	0.57
1:N:492:LEU:HD23	1:N:495:LEU:HD12	1.86	0.57
4:Q:70:GLU:HA	5:R:109:VAL:HG12	1.85	0.57
8:U:39:CYS:CB	8:U:53:CYS:SG	2.93	0.57
1:A:506:GLU:CG	3:C:1:MET:SD	2.93	0.57
10:W:29:ASN:ND2	10:W:33:ARG:HD2	2.19	0.57
9:I:29:LEU:O	9:I:33:THR:HG23	2.04	0.57
2:O:48:THR:HB	9:V:16:ARG:CZ	2.35	0.57
2:O:83:ILE:O	2:O:87:MET:HG3	2.04	0.57
10:W:36:MET:O	10:W:40:LEU:HG	2.05	0.57
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.86	0.57
1:N:456:MET:HE1	11:X:40:TRP:CH2	2.40	0.57
4:Q:67:SER:HG	4:Q:70:GLU:HG3	1.70	0.57
2:B:102:HIS:O	2:B:104:TRP:N	2.38	0.56
4:Q:137:LYS:O	4:Q:145:TRP:HE3	1.88	0.56
1:A:240:HIS:O	1:A:243:VAL:HG22	2.05	0.56
12:L:41:ARG:HD2	13:M:40:TYR:CZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.40	0.56
2:B:125:THR:HA	2:B:128:LEU:HG	1.87	0.56
2:O:3:TYR:CD1	2:O:3:TYR:N	2.73	0.56
1:A:53:ILE:HD11	12:L:43:GLN:HB3	1.86	0.56
1:A:506:GLU:CB	3:C:1:MET:SD	2.93	0.56
1:N:53:ILE:HD11	12:Y:43:GLN:HB3	1.88	0.56
2:B:86:MET:O	2:B:89[B]:GLU:CG	2.49	0.56
9:I:26:MET:HE3	9:I:26:MET:HA	1.87	0.56
12:L:41:ARG:HG3	13:M:40:TYR:CE2	2.41	0.56
1:N:398:PRO:O	1:N:498:CYS:HB3	2.04	0.56
5:R:33:MET:HE2	5:R:67:ILE:HG23	1.87	0.56
4:D:137:LYS:O	4:D:145:TRP:HE3	1.89	0.56
3:P:154:GLY:HA2	6:S:6:VAL:CG2	2.36	0.56
8:H:39:CYS:CB	8:H:53:CYS:SG	2.93	0.56
9:V:15:ARG:HD2	9:V:18:ARG:HH22	1.71	0.56
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.41	0.56
4:Q:8:SER:OG	13:Z:4:LYS:HE3	2.06	0.56
2:O:193:TYR:HE1	4:Q:126:MET:HE1	1.70	0.55
1:A:35:LEU:CD1	1:A:462:LEU:HD13	2.33	0.55
4:D:7:LYS:O	4:D:10:ASP:HB2	2.07	0.55
1:N:35:LEU:CD1	1:N:462:LEU:HD13	2.35	0.55
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.94	0.55
1:N:506:GLU:CG	3:P:1:MET:SD	2.93	0.55
3:P:148:HIS:O	3:P:152:MET:HG3	2.05	0.55
4:Q:64:PHE:CE1	5:R:66:ARG:HD2	2.40	0.55
5:R:80:GLU:H	5:R:80:GLU:CD	2.13	0.55
8:H:49:ASP:HB2	8:U:49:ASP:HB2	1.88	0.55
1:N:115:SER:HA	1:N:145:LEU:HD12	1.89	0.55
2:O:63:THR:O	2:O:66:THR:HG22	2.07	0.55
6:F:16:LEU:O	6:F:20:VAL:HG13	2.06	0.55
7:T:42:ARG:HG3	7:T:42:ARG:HH11	1.72	0.55
3:C:121:ILE:HG22	3:C:123:PRO:HD3	1.89	0.55
2:O:152:MET:HB2	2:O:182:THR:CG2	2.37	0.55
8:U:57:ARG:HB3	8:U:57:ARG:NH1	2.05	0.55
2:O:94:SER:OG	2:O:148:MET:HE3	2.07	0.55
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.89	0.55
2:B:78:LEU:HB2	2:B:79:PRO:CD	2.34	0.55
2:O:142:VAL:HG13	2:O:210:VAL:O	2.06	0.55
12:Y:41:ARG:HG3	13:Z:40:TYR:CE2	2.42	0.55
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.42	0.55
1:N:230:LEU:HB2	3:P:103:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:HE1	11:K:40:TRP:CH2	2.42	0.55
3:C:156:ARG:HG3	3:C:156:ARG:HH11	1.72	0.55
1:N:328:HIS:HB2	2:O:45:MET:HE3	1.88	0.54
9:V:15:ARG:HD2	9:V:18:ARG:NH2	2.21	0.54
11:X:24:PHE:O	11:X:28:VAL:HG23	2.07	0.54
7:G:42:ARG:NH1	7:G:74:ARG:HH21	2.04	0.54
3:P:137:LEU:HD13	3:P:173:PHE:CD2	2.43	0.54
1:A:390:MET:CE	17:A:515:HEA:H242	2.38	0.54
3:C:154:GLY:C	6:F:6:VAL:HG13	2.33	0.54
8:H:43:MET:HE1	8:U:43:MET:SD	2.47	0.54
1:N:33:LEU:O	1:N:37:ILE:HG13	2.07	0.54
1:N:449:MET:SD	2:O:5:MET:HE2	2.46	0.54
2:B:28:LEU:HD23	9:I:35:TYR:CZ	2.43	0.54
4:D:52:SER:OG	4:D:55:GLU:HG3	2.06	0.54
7:G:41:HIS:CD2	7:G:42:ARG:HH12	2.26	0.54
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.22	0.54
3:P:154:GLY:HA2	6:S:6:VAL:HG13	1.89	0.54
6:F:62:CYS:SG	6:F:84:SER:OG	2.65	0.54
8:H:43:MET:CE	8:U:43:MET:HE1	2.38	0.54
2:O:164:ALA:HB2	2:O:171:LYS:HD3	1.89	0.54
2:O:184:LEU:HD11	2:O:211:LEU:HD21	1.89	0.54
1:A:115:SER:HA	1:A:145:LEU:HD12	1.89	0.54
1:A:219:PHE:HZ	3:C:199:VAL:HG21	1.73	0.54
2:B:3:TYR:N	2:B:3:TYR:CD1	2.75	0.54
5:E:6:GLU:HB2	5:E:10:GLU:HB2	1.88	0.54
8:H:57:ARG:HH11	8:H:57:ARG:CB	2.08	0.54
2:O:66:THR:HG23	2:O:67:ILE:HD13	1.90	0.54
2:O:139:ASP:OD1	2:O:140:ASN:N	2.40	0.54
1:A:225:GLY:HA3	3:C:112:LEU:HD11	1.90	0.54
3:P:81:TYR:O	3:P:85:LEU:HD22	2.08	0.54
4:Q:127:LYS:HD3	9:V:63:MET:HE2	1.90	0.54
7:T:49:PRO:HG2	8:U:80:THR:HG21	1.90	0.54
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.89	0.54
1:A:71:MET:HE3	1:A:245:ILE:HG21	1.90	0.54
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.43	0.54
10:J:36:MET:O	10:J:40:LEU:HG	2.07	0.54
3:P:154:GLY:HA2	6:S:6:VAL:CG1	2.37	0.54
8:U:41:LYS:HB3	8:U:41:LYS:HZ2	1.72	0.54
2:B:94:SER:OG	2:B:148:MET:HE3	2.08	0.54
1:N:225:GLY:HA3	3:P:112:LEU:HD11	1.89	0.54
5:E:80:GLU:CD	5:E:80:GLU:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:75:ILE:O	1:N:79:GLY:HA3	2.08	0.53
6:S:87:THR:HG22	6:S:89:TYR:CE2	2.43	0.53
8:U:65:PRO:HG2	8:U:68:TRP:CD1	2.43	0.53
3:P:16:TRP:CE3	3:P:19:THR:HG21	2.43	0.53
13:Z:1:ILE:HG23	13:Z:1:ILE:O	2.08	0.53
3:P:4:GLN:NE2	3:P:6:HIS:O	2.41	0.53
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.91	0.53
1:A:219:PHE:HZ	3:C:199:VAL:CG2	2.22	0.53
1:N:264:LYS:NZ	2:O:56:MET:HE2	2.24	0.53
7:T:42:ARG:NH1	7:T:74:ARG:HH21	2.06	0.53
5:E:12:ASP:O	5:E:16:VAL:HG23	2.08	0.53
10:J:27:THR:O	10:J:30:ILE:HG12	2.09	0.53
4:Q:33:LEU:HD13	4:Q:41:LYS:HG3	1.90	0.53
8:H:38:ARG:HG2	8:H:85:ILE:HG23	1.90	0.53
8:H:43:MET:SD	8:U:43:MET:HE1	2.49	0.53
9:I:27:VAL:HG13	9:I:31:PHE:CE2	2.41	0.53
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.08	0.53
2:B:146:MET:SD	2:B:189:PRO:HB3	2.49	0.53
6:S:49:VAL:O	6:S:91:LEU:HD12	2.09	0.53
6:S:53:THR:HG22	6:S:54:ASN:OD1	2.08	0.53
4:D:40:LEU:CD2	4:D:59:LEU:HD13	2.39	0.53
5:E:7:THR:OG1	5:E:10:GLU:HG3	2.08	0.53
7:T:36:TRP:O	7:T:36:TRP:HD1	1.92	0.53
2:B:164:ALA:HB2	2:B:171:LYS:HD3	1.91	0.53
1:N:289:ALA:HB1	1:N:297:MET:HE1	1.90	0.53
1:N:484:THR:HB	13:Z:2:THR:CG2	2.39	0.53
10:J:29:ASN:ND2	10:J:33:ARG:HD2	2.24	0.52
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.91	0.52
8:U:24:ASN:ND2	8:U:26:THR:H	2.07	0.52
1:N:367:LEU:O	1:N:370:THR:HG23	2.09	0.52
5:R:95:GLU:HG2	5:R:96:LEU:HD23	1.92	0.52
11:X:47:ARG:HG3	11:X:48:VAL:HG23	1.92	0.52
1:A:264:LYS:NZ	2:B:56:MET:HE2	2.25	0.52
1:A:513:LEU:HD22	6:F:35:ALA:HB3	1.91	0.52
3:C:154:GLY:HA2	6:F:6:VAL:CG2	2.39	0.52
6:F:49:VAL:O	6:F:91:LEU:HD12	2.09	0.52
1:N:240:HIS:O	1:N:243:VAL:HG22	2.09	0.52
1:N:402:GLY:HA3	1:N:499:PRO:HD3	1.91	0.52
1:A:367:LEU:O	1:A:370:THR:HG23	2.10	0.52
2:B:108:TYR:N	2:B:108:TYR:CD1	2.77	0.52
1:N:437:PRO:HG2	1:N:440:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:LEU:HD11	2:B:211:LEU:HD21	1.92	0.52
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.90	0.52
11:K:13:TYR:O	11:K:17:VAL:HG23	2.09	0.52
1:A:176:MET:CE	1:A:181:THR:HG22	2.39	0.52
7:G:36:TRP:HD1	7:G:36:TRP:O	1.93	0.52
2:O:102:HIS:O	2:O:104:TRP:N	2.43	0.52
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.45	0.52
10:W:30:ILE:O	10:W:34:VAL:HG23	2.10	0.52
1:A:219:PHE:CZ	3:C:199:VAL:HG21	2.44	0.52
8:H:41:LYS:HB3	8:H:41:LYS:HZ2	1.72	0.52
13:M:1:ILE:HG23	13:M:1:ILE:O	2.09	0.52
7:G:49:PRO:HG2	8:H:80:THR:HG21	1.91	0.52
2:B:216:LEU:O	2:B:219:PHE:HB3	2.10	0.52
8:H:65:PRO:HG2	8:H:68:TRP:CD1	2.45	0.52
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.92	0.52
6:F:33:ILE:HG22	6:F:34:LEU:CD1	2.37	0.51
8:H:43:MET:HE1	8:U:43:MET:CE	2.37	0.51
10:W:27:THR:HG22	10:W:30:ILE:HD11	1.91	0.51
2:B:68:LEU:HB3	2:B:69:PRO:HD3	1.91	0.51
4:D:73:ARG:CZ	4:D:73:ARG:HB3	2.40	0.51
8:H:57:ARG:O	8:H:61:LYS:HB2	2.09	0.51
2:O:13:THR:HG22	2:O:13:THR:O	2.10	0.51
3:P:16:TRP:HE3	3:P:19:THR:HG21	1.73	0.51
7:T:41:HIS:CD2	7:T:42:ARG:HH12	2.28	0.51
7:T:42:ARG:HG3	7:T:42:ARG:NH1	2.25	0.51
1:A:333:LYS:CE	1:A:335:SER:HB3	2.40	0.51
8:H:46:LYS:HZ3	8:U:53:CYS:HA	1.73	0.51
7:G:48:ILE:HD13	7:G:50:TYR:CZ	2.46	0.51
13:M:35:TYR:HD2	13:M:36:HIS:CD2	2.28	0.51
2:O:50:LEU:HD21	5:R:77:PRO:HD2	1.93	0.51
2:B:185:MET:SD	2:B:185:MET:C	2.93	0.51
3:C:173:PHE:CD1	3:C:173:PHE:C	2.89	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.91	0.51
2:O:28:LEU:HD23	9:V:35:TYR:CZ	2.46	0.51
4:Q:41:LYS:HD3	4:Q:62:LEU:HD23	1.93	0.51
5:R:12:ASP:O	5:R:16:VAL:HG23	2.11	0.51
2:B:5:MET:CE	11:K:42:PRO:HA	2.40	0.51
2:B:139:ASP:OD1	2:B:140:ASN:N	2.43	0.51
7:G:5:LYS:O	7:G:6:GLY:C	2.51	0.51
4:Q:114:GLU:HG3	11:X:51:LYS:HE2	1.93	0.51
1:A:483:LEU:HB2	13:M:2:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HG2	1:A:54:TYR:CD1	2.46	0.51
1:A:328:HIS:HB2	2:B:45:MET:HE3	1.93	0.50
17:A:515:HEA:HBC1	17:A:515:HEA:HMC1	1.92	0.50
2:B:132:GLU:HA	4:D:122:ARG:NH1	2.24	0.50
2:O:108:TYR:CD1	2:O:108:TYR:N	2.79	0.50
6:F:87:THR:HG22	6:F:89:TYR:CE2	2.45	0.50
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.75	0.50
9:I:40:ALA:O	9:I:44:LYS:HE2	2.11	0.50
1:N:74:MET:HE1	1:N:246:LEU:O	2.10	0.50
1:N:506:GLU:OE2	3:P:1:MET:HG3	2.11	0.50
4:Q:16:TYR:CE1	4:Q:25:PRO:HG3	2.46	0.50
5:R:20:ASN:HA	5:R:57:ARG:HH22	1.76	0.50
1:A:117:MET:HE3	12:L:39:ILE:HG23	1.93	0.50
10:J:30:ILE:O	10:J:34:VAL:HG23	2.11	0.50
1:N:290:HIS:HA	1:N:293:PHE:CZ	2.46	0.50
6:S:16:LEU:O	6:S:20:VAL:HG13	2.12	0.50
1:A:230:LEU:HB2	3:C:103:HIS:CD2	2.46	0.50
4:D:40:LEU:HD22	4:D:59:LEU:CD1	2.41	0.50
5:E:20:ASN:HA	5:E:57:ARG:HH22	1.76	0.50
5:E:21:LYS:O	5:E:57:ARG:NH1	2.45	0.50
1:N:468:MET:HE1	17:N:515:HEA:C21	2.41	0.50
2:O:78:LEU:HB2	2:O:79:PRO:CD	2.35	0.50
4:Q:128:VAL:O	4:Q:134:PHE:HB3	2.11	0.50
4:Q:37:GLN:O	4:Q:41:LYS:HG2	2.12	0.50
3:P:156:ARG:HG3	3:P:156:ARG:HH11	1.77	0.50
8:U:17:ASP:OD2	8:U:19:ARG:NH1	2.44	0.50
1:A:248:LEU:O	1:A:251:PHE:HB2	2.12	0.50
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.93	0.50
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.93	0.50
2:O:162:SER:HA	2:O:173:ASP:HA	1.93	0.50
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.94	0.50
2:B:66:THR:HG23	2:B:67:ILE:HD13	1.93	0.49
1:A:268:PHE:CZ	2:B:58:ALA:HA	2.47	0.49
1:N:268:PHE:CZ	2:O:58:ALA:HA	2.47	0.49
3:C:160:LEU:HD13	3:C:222:GLN:HG2	1.94	0.49
6:F:95:GLN:NE2	6:F:96:LEU:H	2.09	0.49
8:H:53:CYS:HA	8:U:46:LYS:HZ3	1.75	0.49
1:N:85:LEU:O	1:N:492:LEU:HD13	2.12	0.49
1:N:176:MET:CE	1:N:181:THR:HG22	2.40	0.49
8:U:24:ASN:HD22	8:U:25:GLN:N	2.10	0.49
10:W:11:LEU:C	10:W:11:LEU:HD23	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:GLU:HG2	1:N:54:TYR:CD1	2.47	0.49
2:O:188:ARG:HH11	2:O:188:ARG:HG2	1.77	0.49
6:S:37:LYS:HD3	6:S:37:LYS:N	2.28	0.49
1:A:10:THR:HG21	3:C:11:VAL:HG22	1.95	0.49
1:A:484:THR:HB	13:M:2:THR:CG2	2.41	0.49
7:G:7:ASP:CG	7:G:8:HIS:H	2.21	0.49
8:H:37:HIS:CD2	8:H:76:ARG:NH1	2.80	0.49
2:O:216:LEU:O	2:O:219:PHE:HB3	2.12	0.49
2:B:125:THR:HB	2:B:134:ARG:HG3	1.95	0.49
4:D:107:ILE:HB	4:D:108:PRO:HD2	1.95	0.49
5:E:78:HIS:CE1	9:I:12:LEU:HD22	2.48	0.49
7:G:42:ARG:NH1	7:G:42:ARG:HG3	2.28	0.49
1:N:358:LEU:HD21	1:N:372:TYR:HD2	1.77	0.49
2:O:5:MET:CE	11:X:42:PRO:HA	2.42	0.49
2:O:125:THR:HB	2:O:134:ARG:HG3	1.95	0.49
3:P:173:PHE:CD1	3:P:173:PHE:C	2.90	0.49
8:H:17:ASP:OD2	8:H:19:ARG:NH1	2.45	0.49
1:N:513:LEU:HD22	6:S:35:ALA:HB3	1.95	0.49
2:B:189:PRO:O	9:I:63:MET:HE1	2.13	0.49
4:D:37:GLN:O	4:D:41:LYS:HG2	2.12	0.49
10:J:27:THR:HG22	10:J:30:ILE:HD11	1.94	0.49
1:N:71:MET:CE	1:N:195:LEU:HD21	2.43	0.49
1:N:506:GLU:CB	3:P:1:MET:SD	3.00	0.49
6:S:18:ARG:NH1	6:S:21:MET:HE1	2.28	0.49
11:X:13:TYR:O	11:X:17:VAL:HG23	2.13	0.49
4:D:33:LEU:HD13	4:D:41:LYS:HG3	1.94	0.48
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.48
6:S:48:LEU:HB3	6:S:92:VAL:HG21	1.94	0.48
7:T:5:LYS:O	7:T:6:GLY:C	2.51	0.48
3:C:228:THR:O	3:C:230:ASN:N	2.46	0.48
9:I:36:LYS:O	9:I:40:ALA:HB3	2.12	0.48
2:O:116:LEU:HD11	2:O:226:MET:HG3	1.94	0.48
7:T:42:ARG:NH2	7:T:75:VAL:HG11	2.28	0.48
1:A:358:LEU:HD21	1:A:372:TYR:HD2	1.77	0.48
4:Q:9:GLU:CD	4:Q:9:GLU:H	2.22	0.48
6:S:81:ARG:HG2	6:S:88:HIS:CD2	2.48	0.48
1:A:379:TYR:O	1:A:383:MET:HB2	2.13	0.48
3:C:66:THR:HG22	3:C:67:PHE:CD1	2.49	0.48
3:P:160:LEU:HD13	3:P:222:GLN:HG2	1.94	0.48
4:D:114:GLU:HG3	11:K:51:LYS:HE2	1.96	0.48
6:F:30:PRO:CB	6:F:96:LEU:HB3	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:42:ARG:NH2	7:G:75:VAL:HG11	2.29	0.48
5:R:87:GLN:OE1	9:V:4:LEU:HD23	2.13	0.48
9:V:27:VAL:HG13	9:V:31:PHE:CE2	2.44	0.48
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.48	0.48
6:F:55:LYS:HA	6:F:74:LEU:O	2.13	0.48
1:N:333:LYS:CE	1:N:335:SER:HB3	2.43	0.48
3:P:128:GLU:HB3	3:P:129:VAL:H	1.56	0.48
4:Q:67:SER:OG	4:Q:70:GLU:HG3	2.13	0.48
2:B:124:PRO:HB2	2:B:127:GLU:HG2	1.96	0.48
2:B:142:VAL:HG13	2:B:210:VAL:O	2.13	0.48
3:C:147:ALA:HB2	3:C:162:ALA:HB3	1.95	0.48
11:K:47:ARG:HG3	11:K:48:VAL:HG23	1.95	0.48
4:Q:11:TYR:CD1	4:Q:11:TYR:C	2.91	0.48
8:U:38:ARG:HG2	8:U:85:ILE:HA	1.95	0.48
1:A:69:MET:O	1:A:72:PRO:HD2	2.13	0.48
3:P:16:TRP:HA	3:P:19:THR:HG22	1.96	0.48
4:Q:132:GLN:HE22	9:V:43:ARG:HB2	1.78	0.48
6:S:33:ILE:HG22	6:S:34:LEU:CD1	2.43	0.48
3:C:57:TRP:O	3:C:61:VAL:HG23	2.14	0.48
3:C:77:LYS:HE2	3:C:81:TYR:OH	2.14	0.48
6:F:61:ILE:HG12	6:F:69:VAL:HG22	1.95	0.48
5:R:81:ILE:O	5:R:85:VAL:HG23	2.14	0.48
6:S:61:ILE:HG12	6:S:69:VAL:HG22	1.94	0.48
7:T:47:PHE:CD2	7:T:77:PRO:HB2	2.49	0.48
13:Z:35:TYR:HD2	13:Z:36:HIS:CD2	2.31	0.48
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.61	0.48
7:G:5:LYS:O	1:N:278:MET:HG2	2.13	0.48
2:O:1:MET:HE2	4:Q:123:MET:HE3	1.96	0.48
5:R:80:GLU:O	5:R:83:PRO:HD2	2.14	0.48
9:V:26:MET:HA	9:V:26:MET:CE	2.43	0.48
8:H:38:ARG:HG2	8:H:85:ILE:HA	1.96	0.47
11:K:9:PHE:CD1	11:K:9:PHE:C	2.92	0.47
1:N:328:HIS:HB2	2:O:45:MET:CE	2.44	0.47
2:O:100:MET:HE3	2:O:100:MET:HB3	1.73	0.47
6:S:31:TYR:HE2	6:S:98:HIS:CE1	2.32	0.47
2:B:59:GLN:N	2:B:62:GLU:HG3	2.26	0.47
2:B:188:ARG:HG2	2:B:188:ARG:HH11	1.79	0.47
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.96	0.47
3:P:77:LYS:HE2	3:P:81:TYR:OH	2.14	0.47
3:P:195:SER:O	3:P:199:VAL:HG22	2.14	0.47
7:T:38:HIS:C	7:T:40:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:O	1:A:164:PHE:HD2	1.97	0.47
1:A:290:HIS:HA	1:A:293:PHE:CZ	2.50	0.47
5:E:87:GLN:OE1	9:I:4:LEU:HD23	2.14	0.47
1:N:248:LEU:O	1:N:251:PHE:HB2	2.14	0.47
1:N:365:ILE:HD13	1:N:365:ILE:HA	1.66	0.47
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.47
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.47
1:A:365:ILE:HD13	1:A:365:ILE:HA	1.71	0.47
1:A:449:MET:SD	2:B:5:MET:HE2	2.55	0.47
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.97	0.47
2:O:86:MET:O	2:O:89[B]:GLU:CG	2.55	0.47
3:P:119:THR:HG21	8:U:82:PRO:O	2.15	0.47
6:S:82:CYS:N	6:S:86:GLY:O	2.48	0.47
1:A:218:THR:HB	1:A:221:ASP:HB3	1.95	0.47
2:B:162:SER:HA	2:B:173:ASP:HA	1.97	0.47
3:C:4:GLN:NE2	3:C:6:HIS:O	2.48	0.47
3:C:137:LEU:HD13	3:C:173:PHE:CD2	2.50	0.47
5:E:95:GLU:HG2	5:E:96:LEU:HD23	1.95	0.47
3:P:147:ALA:HB2	3:P:162:ALA:HB3	1.96	0.47
3:P:183:GLU:O	7:T:42:ARG:NH2	2.47	0.47
4:Q:18:ASP:OD2	4:Q:66:GLU:HG2	2.13	0.47
4:Q:73:ARG:CZ	4:Q:73:ARG:HB3	2.43	0.47
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.95	0.47
10:W:29:ASN:HD21	10:W:33:ARG:HD2	1.79	0.47
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	1.96	0.47
1:A:209:LEU:O	1:A:213:ARG:HG3	2.15	0.47
4:D:24:LEU:CB	5:E:30:ARG:HG2	2.45	0.47
4:D:93:ALA:O	4:D:97:ILE:HG13	2.15	0.47
1:N:100:MET:HE2	1:N:159:LEU:HD21	1.97	0.47
2:O:89[B]:GLU:HB2	2:O:91[B]:ASN:ND2	2.30	0.47
3:P:154:GLY:CA	6:S:6:VAL:HG13	2.45	0.47
3:P:192:VAL:O	3:P:196:THR:HB	2.14	0.47
4:Q:145:TRP:CE2	11:X:45:VAL:HA	2.49	0.47
6:S:95:GLN:NE2	6:S:96:LEU:H	2.12	0.47
8:U:24:ASN:HD22	8:U:24:ASN:C	2.22	0.47
1:A:492:LEU:O	1:A:492:LEU:HD22	2.14	0.47
2:B:19:GLU:CD	2:B:82:ARG:HH22	2.23	0.47
8:H:36:PHE:HB2	8:H:56:TYR:CB	2.45	0.47
1:N:100:MET:HE2	1:N:159:LEU:CD2	2.45	0.47
1:N:117:MET:HA	1:N:117:MET:HE2	1.96	0.47
3:P:187:THR:HG21	7:T:68:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:24:LEU:CB	5:R:30:ARG:HG2	2.43	0.47
1:A:69:MET:HE2	1:A:70:VAL:N	2.30	0.47
2:B:129:LYS:O	2:B:132:GLU:HG3	2.15	0.47
8:H:49:ASP:CB	8:U:49:ASP:HB2	2.45	0.47
9:I:26:MET:HA	9:I:26:MET:CE	2.45	0.47
11:X:9:PHE:CD1	11:X:9:PHE:C	2.92	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.03	0.47
3:C:187:THR:HG21	7:G:68:THR:HG21	1.97	0.47
5:E:78:HIS:ND1	9:I:12:LEU:HD22	2.30	0.47
3:P:112:LEU:HG	3:P:118:PRO:HB3	1.95	0.47
1:A:506:GLU:OE2	3:C:1:MET:HG3	2.15	0.46
12:L:41:ARG:HD2	13:M:40:TYR:OH	2.15	0.46
1:N:160:GLY:O	1:N:164:PHE:HD2	1.99	0.46
7:T:54:ARG:HH11	7:T:54:ARG:HB2	1.80	0.46
4:D:16:TYR:CE1	4:D:25:PRO:HG3	2.49	0.46
1:N:117:MET:HE3	12:Y:39:ILE:HG23	1.97	0.46
1:N:138:HIS:O	1:N:213:ARG:NH2	2.48	0.46
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.16	0.46
12:Y:4:GLU:HB3	12:Y:9:LYS:HD3	1.97	0.46
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.50	0.46
12:L:4:GLU:HB3	12:L:9:LYS:HD3	1.97	0.46
7:T:83:GLU:O	7:T:84:LYS:HB2	2.15	0.46
3:C:183:GLU:O	7:G:42:ARG:NH2	2.48	0.46
4:D:68:PHE:CZ	5:E:70:VAL:HG23	2.50	0.46
6:F:82:CYS:N	6:F:86:GLY:O	2.49	0.46
10:J:11:LEU:HD23	10:J:11:LEU:C	2.40	0.46
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.50	0.46
2:O:63:THR:HA	2:O:66:THR:HG22	1.98	0.46
1:A:344:PHE:CD1	1:A:344:PHE:C	2.94	0.46
1:A:390:MET:HE1	17:A:515:HEA:H242	1.98	0.46
4:D:9:GLU:CD	4:D:9:GLU:H	2.23	0.46
13:M:13:LYS:HD3	13:M:13:LYS:N	2.25	0.46
3:C:16:TRP:CE3	3:C:19:THR:HG21	2.51	0.46
3:C:146:TRP:CE2	7:G:17:ARG:HB2	2.51	0.46
5:E:49:ASP:O	5:E:53:ARG:HG3	2.16	0.46
8:H:39:CYS:HB3	8:H:53:CYS:SG	2.56	0.46
8:H:46:LYS:HZ3	8:U:53:CYS:CA	2.28	0.46
9:I:61:GLU:OE1	9:I:64:ARG:NH1	2.48	0.46
1:N:468:MET:SD	17:N:515:HEA:H243	2.55	0.46
4:Q:40:LEU:CD2	4:Q:59:LEU:HD13	2.45	0.46
1:A:29:VAL:HG13	12:L:36:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:TRP:HE3	3:C:19:THR:HG21	1.81	0.46
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.97	0.46
2:O:160:LEU:HD21	2:O:175:ILE:HG23	1.98	0.46
3:P:72:THR:HB	3:P:73:PRO:CD	2.46	0.46
1:A:71:MET:HE3	1:A:245:ILE:CG2	2.45	0.46
2:B:50:LEU:CD2	5:E:77:PRO:HD2	2.45	0.46
7:G:38:HIS:C	7:G:40:GLY:H	2.23	0.46
5:R:49:ASP:O	5:R:53:ARG:HG3	2.15	0.46
8:U:36:PHE:HB2	8:U:56:TYR:CB	2.44	0.46
12:Y:41:ARG:HD2	13:Z:40:TYR:OH	2.16	0.46
1:A:404:THR:O	1:A:480:ARG:NH1	2.49	0.46
2:B:160:LEU:HD23	2:B:175:ILE:HA	1.97	0.46
2:B:160:LEU:CD2	2:B:175:ILE:HG12	2.46	0.46
6:F:31:TYR:HE2	6:F:98:HIS:CE1	2.34	0.46
1:N:377:PHE:CD2	17:N:516:HEA:HAD1	2.51	0.46
1:A:484:THR:HB	13:M:2:THR:HG23	1.98	0.46
2:B:100:MET:HE3	2:B:100:MET:HB3	1.72	0.46
5:E:90:ARG:HA	5:E:90:ARG:HD3	1.62	0.46
6:F:37:LYS:HD3	6:F:37:LYS:N	2.31	0.46
7:G:83:GLU:O	7:G:84:LYS:HB2	2.15	0.46
1:N:417:MET:HB2	1:N:417:MET:HE2	1.84	0.46
6:S:31:TYR:HE2	6:S:98:HIS:HE1	1.64	0.46
9:V:61:GLU:OE1	9:V:64:ARG:NH1	2.49	0.46
1:A:117:MET:HE3	12:L:39:ILE:HG12	1.98	0.45
2:B:89[B]:GLU:HB2	2:B:91[B]:ASN:ND2	2.31	0.45
1:N:71:MET:HE3	1:N:245:ILE:CG2	2.45	0.45
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.98	0.45
3:P:40:MET:O	3:P:44:MET:HG2	2.16	0.45
3:P:204:HIS:HE1	3:P:245:VAL:O	1.99	0.45
13:Z:13:LYS:H	13:Z:13:LYS:CD	2.28	0.45
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.98	0.45
1:A:402:GLY:HA3	1:A:499:PRO:HD3	1.97	0.45
2:B:98:LYS:HE3	2:B:98:LYS:HB2	1.70	0.45
4:D:145:TRP:CE2	11:K:45:VAL:HA	2.52	0.45
7:G:42:ARG:CZ	7:G:74:ARG:NH2	2.80	0.45
13:M:13:LYS:H	13:M:13:LYS:CD	2.23	0.45
1:N:353:LEU:HG	2:O:31:VAL:HB	1.98	0.45
7:T:7:ASP:CG	7:T:8:HIS:H	2.23	0.45
8:U:54:GLU:CD	8:U:57:ARG:NH1	2.75	0.45
12:Y:15:VAL:HG23	12:Y:21:LEU:HD22	1.98	0.45
1:A:71:MET:CE	1:A:195:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:HG2	4:D:96:LEU:HD13	1.97	0.45
3:C:22:LEU:HD12	3:C:22:LEU:HA	1.74	0.45
4:D:41:LYS:HD3	4:D:62:LEU:HD23	1.97	0.45
2:O:116:LEU:HD11	2:O:226:MET:CG	2.46	0.45
1:N:5:ARG:HG2	1:N:6:TRP:NE1	2.32	0.45
2:O:19:GLU:CD	2:O:82:ARG:HH22	2.25	0.45
3:C:112:LEU:HG	3:C:118:PRO:HB3	1.98	0.45
1:N:115:SER:O	1:N:121:GLY:HA2	2.16	0.45
3:P:101:PHE:HZ	3:P:260:GLY:HA3	1.81	0.45
3:P:118:PRO:HG2	3:P:121:ILE:HG13	1.99	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.15	0.45
13:Z:13:LYS:HD3	13:Z:13:LYS:N	2.29	0.45
4:D:108:PRO:HG2	4:D:111:PHE:CE2	2.52	0.45
3:P:12:ASN:O	3:P:13:PRO:C	2.60	0.45
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.99	0.45
1:A:64:VAL:HG22	1:A:109:PHE:HE1	1.82	0.45
2:B:13:THR:O	2:B:13:THR:HG22	2.15	0.45
1:A:353:LEU:HG	2:B:31:VAL:HB	1.98	0.45
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.98	0.45
10:J:3:ASN:OD1	10:J:5:VAL:HG12	2.16	0.45
1:N:10:THR:HG21	3:P:11:VAL:HG22	1.98	0.45
3:P:1:MET:O	3:P:3:HIS:N	2.49	0.45
7:T:48:ILE:HG13	8:U:80:THR:HG22	1.99	0.45
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.98	0.45
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.99	0.45
3:C:72:THR:HB	3:C:73:PRO:CD	2.47	0.45
8:H:24:ASN:ND2	8:H:26:THR:H	2.14	0.45
1:N:52:GLN:O	1:N:56:VAL:HG23	2.17	0.45
1:N:218:THR:HB	1:N:221:ASP:HB3	1.98	0.45
3:P:16:TRP:CE3	3:P:16:TRP:HA	2.52	0.45
3:P:50:ASN:OD1	3:P:54:MET:HE2	2.17	0.45
1:A:354:THR:HG21	1:A:376:HIS:HA	1.99	0.44
4:D:83:GLY:HA3	11:K:18:LEU:HA	1.99	0.44
4:D:112:GLU:O	4:D:116:VAL:HG13	2.17	0.44
1:N:404:THR:O	1:N:480:ARG:NH1	2.51	0.44
2:O:100:MET:HE3	2:O:157:GLU:HG3	1.99	0.44
3:P:57:TRP:O	3:P:61:VAL:HG23	2.17	0.44
4:Q:108:PRO:HG2	4:Q:111:PHE:CE2	2.52	0.44
8:U:39:CYS:HB3	8:U:53:CYS:SG	2.57	0.44
8:U:60:TYR:CD1	8:U:60:TYR:C	2.96	0.44
5:E:52:LEU:HD23	5:E:52:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:21:LEU:O	12:L:22:LEU:C	2.61	0.44
1:N:513:LEU:HD12	1:N:513:LEU:HA	1.56	0.44
4:Q:68:PHE:CZ	5:R:70:VAL:HG23	2.52	0.44
6:S:30:PRO:CB	6:S:96:LEU:HB3	2.42	0.44
7:T:36:TRP:CD1	7:T:36:TRP:C	2.94	0.44
10:W:3:ASN:OD1	10:W:5:VAL:HG12	2.16	0.44
1:A:100:MET:HE2	1:A:159:LEU:CD2	2.47	0.44
2:O:1:MET:SD	2:O:133:LEU:HD11	2.55	0.44
4:Q:107:ILE:HB	4:Q:108:PRO:HD2	2.00	0.44
6:S:31:TYR:CE2	6:S:98:HIS:HE1	2.35	0.44
1:A:34:SER:HB2	17:A:515:HEA:C2B	2.47	0.44
1:A:92:MET:HE1	1:A:164:PHE:CD1	2.52	0.44
1:A:417:MET:O	1:A:417:MET:HG3	2.18	0.44
1:A:437:PRO:HG2	1:A:440:TYR:CE2	2.52	0.44
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.71	0.44
4:D:18:ASP:OD2	4:D:66:GLU:HG2	2.17	0.44
1:N:315:PRO:O	1:N:318:VAL:HG22	2.18	0.44
2:O:160:LEU:CD2	2:O:175:ILE:HG12	2.47	0.44
5:R:21:LYS:O	5:R:57:ARG:NH1	2.50	0.44
1:A:74:MET:HE1	1:A:246:LEU:O	2.17	0.44
1:A:315:PRO:O	1:A:318:VAL:HG22	2.18	0.44
1:A:374:VAL:HA	1:A:377:PHE:CE2	2.53	0.44
3:C:116:TRP:HA	3:C:117:PRO:C	2.42	0.44
3:C:224:LYS:NZ	3:C:224:LYS:HB3	2.32	0.44
6:F:31:TYR:HE2	6:F:98:HIS:HE1	1.65	0.44
8:H:49:ASP:HB2	8:U:49:ASP:CB	2.46	0.44
4:Q:145:TRP:CZ2	11:X:45:VAL:HA	2.52	0.44
1:A:225:GLY:HA3	3:C:112:LEU:HD13	1.99	0.44
8:H:60:TYR:CD1	8:H:60:TYR:C	2.95	0.44
1:N:5:ARG:HG2	1:N:6:TRP:CE2	2.52	0.44
1:N:104:LEU:C	1:N:107:PRO:HD2	2.42	0.44
6:S:98:HIS:ND1	6:S:98:HIS:N	2.66	0.44
7:T:48:ILE:HD13	7:T:50:TYR:CZ	2.52	0.44
13:Z:32:TRP:O	13:Z:36:HIS:CD2	2.65	0.44
1:A:314:ILE:HB	1:A:315:PRO:CD	2.48	0.44
17:A:515:HEA:HBC1	17:A:515:HEA:CMC	2.48	0.44
5:E:20:ASN:O	5:E:21:LYS:C	2.60	0.44
9:I:27:VAL:CG1	9:I:31:PHE:HE2	2.26	0.44
1:N:344:PHE:CD1	1:N:344:PHE:C	2.95	0.44
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.44
12:L:46:LYS:O	12:L:47:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MET:HE1	1:A:195:LEU:HD21	2.00	0.44
1:A:456:MET:CE	11:K:40:TRP:CH2	3.01	0.44
2:B:5:MET:HE3	2:B:5:MET:HB2	1.73	0.44
3:C:154:GLY:HA2	6:F:6:VAL:HG13	1.99	0.44
7:G:6:GLY:CA	1:N:190:ILE:HG12	2.43	0.44
7:G:48:ILE:HG13	8:H:80:THR:HG22	1.99	0.44
8:H:24:ASN:HD22	8:H:25:GLN:N	2.15	0.44
1:N:324:LEU:O	2:O:45:MET:HE3	2.17	0.44
1:A:386:VAL:HG11	17:A:515:HEA:H261	1.99	0.43
3:C:192:VAL:O	3:C:196:THR:HB	2.18	0.43
7:G:36:TRP:CD1	7:G:36:TRP:C	2.96	0.43
11:K:24:PHE:O	11:K:28:VAL:HG23	2.17	0.43
3:P:224:LYS:NZ	3:P:224:LYS:HB3	2.33	0.43
6:S:48:LEU:HD23	6:S:90:LYS:HB3	2.00	0.43
4:D:56:LYS:HB3	5:E:61:PHE:CE2	2.53	0.43
6:F:18:ARG:NH1	6:F:21:MET:HE1	2.33	0.43
1:N:484:THR:HB	13:Z:2:THR:HG23	2.00	0.43
1:N:492:LEU:HD22	1:N:492:LEU:O	2.17	0.43
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.52	0.43
3:P:110:PRO:HB3	8:U:30:TRP:CD2	2.53	0.43
4:Q:40:LEU:HD22	4:Q:59:LEU:CD1	2.47	0.43
5:R:87:GLN:HG2	5:R:88:GLU:OE2	2.18	0.43
6:S:8:THR:H	6:S:11:GLU:HG2	1.82	0.43
8:U:39:CYS:HG	8:U:53:CYS:CB	2.12	0.43
4:D:123:MET:HE2	4:D:134:PHE:CE2	2.53	0.43
7:G:42:ARG:C	7:G:42:ARG:HD2	2.43	0.43
1:N:159:LEU:HD12	1:N:159:LEU:HA	1.85	0.43
11:X:43:SER:OG	11:X:45:VAL:HG12	2.18	0.43
1:A:308:ALA:O	1:A:311:ILE:HG12	2.18	0.43
3:C:42:LEU:HD21	10:J:46:SER:HB3	2.01	0.43
5:E:76:GLY:HA3	5:E:77:PRO:HD2	1.86	0.43
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.99	0.43
1:N:69:MET:HE2	1:N:70:VAL:N	2.34	0.43
2:O:114:GLU:HG3	2:O:115:ASP:H	1.84	0.43
2:O:212:GLU:OE1	9:V:70:GLN:HG2	2.18	0.43
3:P:16:TRP:HE3	3:P:16:TRP:HA	1.82	0.43
12:Y:15:VAL:O	12:Y:15:VAL:HG13	2.18	0.43
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.00	0.43
1:A:299:VAL:HA	1:A:302:ARG:NH1	2.33	0.43
1:A:492:LEU:HD23	1:A:495:LEU:HD12	2.01	0.43
3:C:1:MET:O	3:C:3:HIS:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:PRO:HA	6:F:92:VAL:O	2.18	0.43
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.01	0.43
6:F:8:THR:H	6:F:11:GLU:HG2	1.83	0.43
1:N:225:GLY:HA3	3:P:112:LEU:HD13	2.00	0.43
6:S:51:SER:HB2	6:S:91:LEU:HD11	1.99	0.43
1:A:138:HIS:O	1:A:213:ARG:NH2	2.51	0.43
2:B:63:THR:HA	2:B:66:THR:HG22	2.00	0.43
3:C:224:LYS:HB3	3:C:224:LYS:HZ3	1.84	0.43
3:C:228:THR:C	3:C:230:ASN:H	2.27	0.43
4:D:132:GLN:HE22	9:I:43:ARG:HB2	1.84	0.43
5:E:41:LEU:O	5:E:41:LEU:HD12	2.18	0.43
1:N:390:MET:HE1	17:N:515:HEA:H211	2.00	0.43
2:O:100:MET:SD	2:O:155:SER:HB3	2.58	0.43
2:O:136:LEU:HD22	2:O:193:TYR:HB3	2.01	0.43
5:R:53:ARG:O	5:R:54:ALA:C	2.61	0.43
8:U:36:PHE:HB2	8:U:56:TYR:HB3	2.00	0.43
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.53	0.43
2:B:212:GLU:OE1	9:I:70:GLN:HG2	2.19	0.43
1:N:197:LEU:O	3:P:92:LEU:HD22	2.18	0.43
2:O:5:MET:HB2	2:O:5:MET:HE3	1.76	0.43
5:R:53:ARG:O	5:R:56:ARG:HB3	2.19	0.43
1:A:278:MET:HG2	7:T:5:LYS:O	2.19	0.43
6:F:53:THR:HG22	6:F:54:ASN:N	2.32	0.43
7:G:84:LYS:HB3	7:G:84:LYS:HE3	1.86	0.43
1:N:456:MET:CE	11:X:40:TRP:CH2	3.02	0.43
1:N:508:PRO:HG3	3:P:6:HIS:HB3	2.00	0.43
2:O:216:LEU:O	2:O:219:PHE:N	2.52	0.43
4:Q:145:TRP:CD1	11:X:46:GLY:H	2.37	0.43
5:R:90:ARG:HA	5:R:90:ARG:HD3	1.63	0.43
8:U:65:PRO:HG2	8:U:68:TRP:CD2	2.54	0.43
9:V:27:VAL:CG1	9:V:31:PHE:HE2	2.28	0.43
1:A:95:PRO:HB2	3:C:11:VAL:HG13	2.00	0.43
1:A:450:TRP:CE3	1:A:453:ILE:HD12	2.54	0.43
1:N:82:LEU:O	1:N:86:MET:HG3	2.19	0.43
1:N:353:LEU:HD12	1:N:353:LEU:HA	1.92	0.43
7:T:42:ARG:CZ	7:T:74:ARG:NH2	2.82	0.43
1:A:159:LEU:HA	1:A:159:LEU:HD12	1.72	0.42
4:D:108:PRO:HG2	4:D:111:PHE:CD2	2.54	0.42
8:H:53:CYS:CA	8:U:46:LYS:NZ	2.79	0.42
1:N:311:ILE:HG21	1:N:311:ILE:HD13	1.65	0.42
1:N:390:MET:HE2	17:N:515:HEA:H242	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.00	0.42
5:R:20:ASN:O	5:R:21:LYS:C	2.62	0.42
8:U:57:ARG:HA	8:U:60:TYR:CE2	2.54	0.42
17:A:516:HEA:HHC	17:A:516:HEA:O11	2.19	0.42
3:C:26:LEU:HD23	3:C:45:ILE:HG22	2.01	0.42
4:D:145:TRP:CD1	11:K:46:GLY:H	2.37	0.42
5:E:27:TRP:CH2	6:F:86:GLY:HA2	2.54	0.42
5:E:87:GLN:HG2	5:E:88:GLU:OE2	2.20	0.42
6:F:31:TYR:CE2	6:F:98:HIS:HE1	2.36	0.42
1:N:176:MET:HG3	1:N:180:GLN:HB3	2.01	0.42
1:N:198:SER:HB2	1:N:238:PHE:HA	2.01	0.42
2:O:193:TYR:CD1	2:O:193:TYR:N	2.87	0.42
5:R:42:VAL:HG13	5:R:71:VAL:HG13	1.99	0.42
7:T:47:PHE:CD2	7:T:77:PRO:CB	3.02	0.42
1:A:85:LEU:O	1:A:492:LEU:HD13	2.19	0.42
1:A:285:PHE:CE2	7:T:4:ALA:HB3	2.54	0.42
2:B:100:MET:HE3	2:B:157:GLU:HG3	2.02	0.42
3:C:101:PHE:HZ	3:C:260:GLY:HA3	1.84	0.42
3:C:133:ASN:ND2	3:C:176:LEU:HD13	2.34	0.42
9:I:21:ILE:HD12	9:I:21:ILE:HA	1.74	0.42
1:N:308:ALA:O	1:N:311:ILE:HG12	2.19	0.42
2:O:185:MET:SD	2:O:185:MET:C	3.03	0.42
7:T:42:ARG:HD2	7:T:42:ARG:C	2.44	0.42
11:X:31:TYR:CD2	11:X:35:GLN:HB2	2.53	0.42
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.54	0.42
1:A:104:LEU:C	1:A:107:PRO:HD2	2.44	0.42
1:A:498:CYS:HA	1:A:499:PRO:HA	1.90	0.42
7:G:1:ALA:HB1	1:N:286:ILE:CG2	2.42	0.42
6:S:35:ALA:HA	6:S:36:PRO:HD3	1.89	0.42
8:U:54:GLU:CD	8:U:57:ARG:HH12	2.28	0.42
2:B:158:ASP:O	2:B:176:PRO:HG3	2.19	0.42
7:G:42:ARG:NH1	7:G:74:ARG:NH2	2.66	0.42
9:I:15:ARG:NH1	9:I:18:ARG:HH22	2.18	0.42
9:V:15:ARG:NH1	9:V:18:ARG:HH22	2.18	0.42
3:C:118:PRO:HG2	3:C:121:ILE:HG13	2.01	0.42
4:D:18:ASP:OD2	4:D:65:LYS:HB3	2.20	0.42
5:E:53:ARG:O	5:E:56:ARG:HB3	2.20	0.42
5:E:81:ILE:O	5:E:85:VAL:HG23	2.20	0.42
2:O:162:SER:HB3	2:O:197:SER:C	2.45	0.42
1:A:61:HIS:HE1	17:A:515:HEA:C4B	2.33	0.42
2:B:104:TRP:HA	2:B:207:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:SER:HB3	2:B:197:SER:C	2.43	0.42
3:C:16:TRP:CE3	3:C:16:TRP:HA	2.55	0.42
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.01	0.42
2:O:141:ARG:HD2	2:O:212:GLU:OE1	2.20	0.42
3:P:42:LEU:HD12	3:P:42:LEU:HA	1.86	0.42
5:R:53:ARG:O	5:R:56:ARG:N	2.52	0.42
12:Y:21:LEU:O	12:Y:22:LEU:C	2.62	0.42
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.89	0.42
1:A:377:PHE:CD2	17:A:516:HEA:HAD1	2.55	0.42
6:F:48:LEU:HD23	6:F:90:LYS:HB3	2.01	0.42
9:I:36:LYS:HD2	9:I:37:PHE:CE2	2.54	0.42
1:N:489:THR:HB	6:S:70:ILE:HG23	2.01	0.42
1:N:512:ASN:HD22	1:N:512:ASN:HA	1.69	0.42
9:V:11:GLY:O	9:V:15:ARG:HD3	2.19	0.42
9:V:21:ILE:HD12	9:V:21:ILE:HA	1.86	0.42
7:G:54:ARG:HD3	7:G:54:ARG:H	1.82	0.42
8:H:24:ASN:HD22	8:H:24:ASN:C	2.28	0.42
8:H:46:LYS:NZ	8:U:53:CYS:CA	2.80	0.42
1:N:390:MET:HE1	17:N:515:HEA:C24	2.49	0.42
5:R:52:LEU:HD11	5:R:68:LEU:HD21	2.01	0.42
1:A:510:TYR:HB2	6:F:56:ARG:HH11	1.83	0.42
2:B:193:TYR:CD1	2:B:193:TYR:N	2.87	0.42
5:E:81:ILE:HA	9:I:7:PRO:HG3	2.01	0.42
8:H:53:CYS:CA	8:U:46:LYS:HZ3	2.33	0.42
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.02	0.42
9:V:36:LYS:O	9:V:40:ALA:HB3	2.19	0.42
1:A:241:PRO:O	1:A:245:ILE:HG13	2.20	0.41
4:D:23:PRO:HD2	5:E:34:ASN:OD1	2.20	0.41
7:G:72:ASN:HA	7:G:73:PRO:HD3	1.84	0.41
13:M:32:TRP:O	13:M:36:HIS:CD2	2.65	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.01	0.41
2:O:136:LEU:HB3	2:O:193:TYR:HD2	1.79	0.41
2:O:191:LEU:CD2	2:O:212:GLU:HG3	2.49	0.41
1:A:100:MET:HE2	1:A:159:LEU:HD21	2.02	0.41
17:A:515:HEA:H272	17:A:515:HEA:H172	1.87	0.41
2:B:179:LEU:HD21	8:H:65:PRO:CD	2.50	0.41
3:C:16:TRP:HE3	3:C:16:TRP:HA	1.86	0.41
3:C:169:LEU:HD23	3:C:169:LEU:HA	1.93	0.41
8:H:36:PHE:HB2	8:H:56:TYR:HB3	2.01	0.41
12:L:15:VAL:HG23	12:L:21:LEU:HD22	2.02	0.41
1:N:7:LEU:C	1:N:8:PHE:HD1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:GLN:C	1:N:180:GLN:H	2.28	0.41
1:N:354:THR:HG21	1:N:376:HIS:HA	2.01	0.41
3:P:72:THR:HB	3:P:73:PRO:HD2	2.02	0.41
3:P:192:VAL:HA	3:P:195:SER:HB2	2.02	0.41
2:B:189:PRO:HG2	9:I:63:MET:CE	2.50	0.41
3:C:154:GLY:HA2	6:F:6:VAL:CG1	2.51	0.41
4:D:96:LEU:HD23	4:D:96:LEU:HA	1.92	0.41
6:F:61:ILE:O	6:F:62:CYS:C	2.63	0.41
13:M:8:THR:O	13:M:9:PRO:C	2.63	0.41
1:N:195:LEU:CD2	1:N:245:ILE:HD13	2.50	0.41
1:N:416:ILE:HD12	1:N:467:LEU:HD12	2.02	0.41
4:Q:43:LYS:HE2	4:Q:43:LYS:HB3	1.80	0.41
7:T:54:ARG:HH11	7:T:54:ARG:CG	2.34	0.41
11:X:53:TRP:O	11:X:54:ARG:CB	2.68	0.41
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.20	0.41
1:A:314:ILE:HB	1:A:315:PRO:HD2	2.02	0.41
1:A:442:ASP:OD2	2:B:134:ARG:NH2	2.53	0.41
2:B:1:MET:HE2	4:D:123:MET:HE3	2.01	0.41
2:B:203:ASN:HD22	2:B:206:PHE:HD2	1.68	0.41
3:C:50:ASN:OD1	3:C:54:MET:HE2	2.19	0.41
3:C:119:THR:HG21	8:H:82:PRO:O	2.21	0.41
7:G:54:ARG:HH11	7:G:54:ARG:CG	2.33	0.41
2:O:104:TRP:HA	2:O:207:MET:SD	2.61	0.41
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.20	0.41
7:T:54:ARG:HD3	7:T:54:ARG:H	1.83	0.41
8:U:39:CYS:O	8:U:43:MET:HG2	2.21	0.41
1:A:346:PHE:O	1:A:349:THR:HB	2.20	0.41
7:G:54:ARG:HH11	7:G:54:ARG:HB2	1.85	0.41
8:H:57:ARG:HA	8:H:60:TYR:CE2	2.56	0.41
1:N:266:GLU:HB2	1:N:267:PRO:HD2	2.02	0.41
6:S:37:LYS:N	6:S:37:LYS:CD	2.84	0.41
1:A:512:ASN:HD22	1:A:512:ASN:HA	1.69	0.41
2:B:99:THR:C	2:B:100:MET:HG2	2.46	0.41
4:D:8:SER:OG	13:M:4:LYS:HE3	2.20	0.41
9:I:15:ARG:HH11	9:I:18:ARG:HH22	1.68	0.41
1:N:131:PRO:HB2	2:O:159:VAL:HA	2.02	0.41
2:O:59:GLN:N	2:O:62:GLU:HG3	2.32	0.41
3:P:22:LEU:HD12	3:P:22:LEU:HA	1.85	0.41
6:S:26:LYS:HB3	6:S:28:GLN:NE2	2.35	0.41
1:A:257:ILE:HD11	1:A:392:GLY:HA2	2.03	0.41
1:A:341:ALA:O	1:A:345:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ILE:HD12	1:A:467:LEU:HD12	2.02	0.41
1:N:64:VAL:HG22	1:N:109:PHE:HE1	1.85	0.41
1:N:151:HIS:O	1:N:155:VAL:HG23	2.21	0.41
1:N:209:LEU:O	1:N:213:ARG:HG3	2.21	0.41
1:N:241:PRO:O	1:N:245:ILE:HG13	2.21	0.41
1:A:380:VAL:HG21	17:A:516:HEA:C3C	2.51	0.41
1:A:489:THR:HB	6:F:70:ILE:HG23	2.01	0.41
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.56	0.41
1:N:366:VAL:O	1:N:366:VAL:HG23	2.20	0.41
1:N:450:TRP:CE3	1:N:453:ILE:HD12	2.55	0.41
3:P:47:LEU:O	3:P:51:MET:HG2	2.21	0.41
4:Q:108:PRO:HG2	4:Q:111:PHE:CD2	2.56	0.41
6:S:22:LEU:HA	6:S:25:ARG:HG2	2.02	0.41
6:S:81:ARG:HB3	6:S:86:GLY:O	2.21	0.41
12:Y:22:LEU:HA	12:Y:22:LEU:HD23	1.71	0.41
1:A:508:PRO:HG3	3:C:6:HIS:HB3	2.02	0.41
2:B:52:HIS:C	2:B:52:HIS:CD2	2.98	0.41
4:D:52:SER:O	4:D:53:ILE:C	2.62	0.41
4:D:127:LYS:HG3	4:D:140:TYR:OH	2.21	0.41
5:E:53:ARG:O	5:E:54:ALA:C	2.64	0.41
6:F:49:VAL:HG21	6:F:74:LEU:HD12	2.03	0.41
10:J:29:ASN:HD21	10:J:33:ARG:HD2	1.85	0.41
1:N:294:THR:HG22	1:N:365:ILE:HD13	2.03	0.41
1:N:299:VAL:HA	1:N:302:ARG:NH1	2.36	0.41
2:O:146:MET:HE1	9:V:56:SER:HB2	2.02	0.41
3:P:19:THR:O	3:P:23:SER:HB2	2.21	0.41
6:S:31:TYR:CE2	6:S:98:HIS:CE1	3.08	0.41
6:S:63:GLU:HB2	6:S:66:ASN:ND2	2.36	0.41
9:V:60:PHE:CE1	9:V:69:PHE:CE2	3.09	0.41
1:A:178:GLN:C	1:A:180:GLN:H	2.28	0.41
1:A:289:ALA:HB3	1:A:305:PHE:CD2	2.56	0.41
2:B:103:GLN:HE21	2:B:104:TRP:HZ2	1.69	0.41
8:H:23:GLN:HE21	8:H:23:GLN:HB2	1.70	0.41
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.03	0.41
4:Q:18:ASP:OD2	4:Q:65:LYS:HB3	2.21	0.41
4:Q:132:GLN:NE2	9:V:42:LYS:HE3	2.36	0.41
9:V:36:LYS:HD2	9:V:37:PHE:CE2	2.56	0.41
1:A:328:HIS:HB2	2:B:45:MET:CE	2.51	0.40
1:A:390:MET:HE2	17:A:515:HEA:H242	2.04	0.40
3:C:14:SER:HG	3:C:16:TRP:CD1	2.38	0.40
3:C:22:LEU:O	3:C:26:LEU:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:ARG:O	4:D:125:ASP:HB2	2.20	0.40
1:N:34:SER:HB2	17:N:515:HEA:C2B	2.51	0.40
1:N:128:VAL:O	1:N:128:VAL:CG2	2.67	0.40
1:N:511:VAL:O	6:S:36:PRO:HD2	2.22	0.40
3:P:137:LEU:HD22	3:P:173:PHE:CE2	2.56	0.40
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.03	0.40
2:B:59:GLN:CA	2:B:62:GLU:HB2	2.47	0.40
2:B:113:TYR:OH	8:H:12:GLN:HA	2.20	0.40
8:H:76:ARG:HH11	8:H:76:ARG:HD2	1.75	0.40
2:O:50:LEU:HB2	9:V:13:LEU:HD13	2.03	0.40
3:P:157:LYS:HE3	3:P:158:HIS:CD2	2.56	0.40
4:Q:112:GLU:O	4:Q:116:VAL:HG13	2.21	0.40
5:R:78:HIS:CE1	9:V:12:LEU:HD22	2.56	0.40
1:A:69:MET:HE2	1:A:70:VAL:HA	2.04	0.40
1:A:151:HIS:O	1:A:155:VAL:HG23	2.21	0.40
1:A:176:MET:HG3	1:A:180:GLN:HB3	2.03	0.40
2:B:29:MET:HE2	2:B:29:MET:HB3	1.96	0.40
3:C:81:TYR:O	3:C:85:LEU:HD22	2.22	0.40
3:C:252:LEU:HA	3:C:252:LEU:HD23	1.86	0.40
12:L:22:LEU:HA	12:L:22:LEU:HD23	1.74	0.40
6:S:82:CYS:HA	6:S:83:PRO:HD3	1.95	0.40
7:T:42:ARG:NH1	7:T:74:ARG:NH2	2.69	0.40
1:A:195:LEU:HG	1:A:245:ILE:HD13	2.03	0.40
1:A:247:ILE:HD12	1:A:247:ILE:HA	1.94	0.40
6:F:98:HIS:ND1	6:F:98:HIS:N	2.68	0.40
10:J:30:ILE:HG13	10:J:31:LEU:N	2.36	0.40
1:N:141:ALA:O	1:N:145:LEU:HG	2.21	0.40
2:O:52:HIS:CD2	2:O:52:HIS:C	2.98	0.40
3:P:41:THR:O	3:P:45:ILE:HG13	2.21	0.40
3:P:80:ARG:HG2	3:P:233:PHE:CE1	2.56	0.40
3:P:137:LEU:HD12	3:P:137:LEU:HA	1.91	0.40
9:V:30:GLY:O	9:V:31:PHE:C	2.64	0.40
1:A:445:ASP:OD1	2:B:134:ARG:NH1	2.54	0.40
12:L:25:MET:O	12:L:29:PHE:HD1	2.04	0.40
1:N:220:PHE:CD1	1:N:231:TYR:HB2	2.57	0.40
1:N:379:TYR:HA	1:N:383:MET:HE3	2.04	0.40
2:O:1:MET:HE1	4:Q:123:MET:SD	2.62	0.40
2:O:160:LEU:HD23	2:O:175:ILE:HA	2.04	0.40
3:P:121:ILE:HG22	3:P:123:PRO:HD3	2.04	0.40
6:S:8:THR:H	6:S:11:GLU:CG	2.35	0.40
6:S:53:THR:HG22	6:S:54:ASN:N	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:31:TYR:CE2	11:X:35:GLN:CB	3.04	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%)	477 (93%)	33 (6%)	2 (0%)	30	60
1	N	512/514 (100%)	476 (93%)	36 (7%)	0	100	100
2	B	230/227 (101%)	202 (88%)	24 (10%)	4 (2%)	7	25
2	O	230/227 (101%)	202 (88%)	23 (10%)	5 (2%)	5	19
3	C	259/261 (99%)	249 (96%)	8 (3%)	2 (1%)	16	44
3	P	259/261 (99%)	250 (96%)	8 (3%)	1 (0%)	30	60
4	D	142/147 (97%)	134 (94%)	7 (5%)	1 (1%)	18	47
4	Q	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	18	47
5	E	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
5	R	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	85 (88%)	6 (6%)	5 (5%)	1	5
6	S	96/98 (98%)	86 (90%)	5 (5%)	5 (5%)	1	5
7	G	82/84 (98%)	65 (79%)	14 (17%)	3 (4%)	2	9
7	T	82/84 (98%)	64 (78%)	16 (20%)	2 (2%)	4	17
8	H	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	30
8	U	73/85 (86%)	62 (85%)	10 (14%)	1 (1%)	9	30
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	54/59 (92%)	49 (91%)	2 (4%)	3 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	W	54/59 (92%)	50 (93%)	1 (2%)	3 (6%)	1	4
11	K	47/56 (84%)	40 (85%)	7 (15%)	0	100	100
11	X	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
12	L	45/47 (96%)	41 (91%)	4 (9%)	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%)	0	1 (2%)	4	17
All	All	3518/3612 (97%)	3230 (92%)	248 (7%)	40 (1%)	11	36

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	91[A]	ASN
2	B	91[B]	ASN
4	D	20	ARG
6	F	87	THR
6	F	96	LEU
7	G	11	THR
10	J	2	GLU
10	J	3	ASN
2	O	91[A]	ASN
2	O	91[B]	ASN
4	Q	20	ARG
6	S	87	THR
6	S	96	LEU
7	T	11	THR
10	W	2	GLU
10	W	3	ASN
2	B	104	TRP
6	F	2	SER
6	F	15	GLY
6	F	95	GLN
7	G	4	ALA
8	H	46	LYS
2	O	104	TRP
6	S	2	SER
6	S	15	GLY
6	S	95	GLN
7	T	4	ALA
8	U	46	LYS

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Mol	Chain	Res	Type
1	A	508	PRO
3	C	128	GLU
3	P	128	GLU
10	W	23	LYS
2	B	103	GLN
2	O	103	GLN
3	C	229	SER
10	J	23	LYS
7	G	61	SER
1	A	384	GLY
2	O	159	VAL
13	Z	9	PRO

### 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%)	393 (92%)	34 (8%)	11 34
1	N	427/427 (100%)	390 (91%)	37 (9%)	9 30
2	B	216/211 (102%)	189 (88%)	27 (12%)	4 15
2	O	216/211 (102%)	189 (88%)	27 (12%)	4 15
3	C	226/226 (100%)	199 (88%)	27 (12%)	5 17
3	P	226/226 (100%)	200 (88%)	26 (12%)	5 18
4	D	128/129 (99%)	114 (89%)	14 (11%)	6 21
4	Q	128/129 (99%)	114 (89%)	14 (11%)	6 21
5	E	95/95 (100%)	85 (90%)	10 (10%)	6 22
5	R	95/95 (100%)	86 (90%)	9 (10%)	8 26
6	F	81/81 (100%)	72 (89%)	9 (11%)	6 20
6	S	81/81 (100%)	73 (90%)	8 (10%)	7 24
7	G	68/68 (100%)	55 (81%)	13 (19%)	1 5
7	T	68/68 (100%)	54 (79%)	14 (21%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	67/75 (89%)	56 (84%)	11 (16%)	2	8
8	U	67/75 (89%)	57 (85%)	10 (15%)	3	10
9	I	58/58 (100%)	52 (90%)	6 (10%)	7	23
9	V	58/58 (100%)	52 (90%)	6 (10%)	7	23
10	J	47/50 (94%)	39 (83%)	8 (17%)	2	7
10	W	47/50 (94%)	38 (81%)	9 (19%)	1	5
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	54
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	54
12	L	40/40 (100%)	34 (85%)	6 (15%)	3	10
12	Y	40/40 (100%)	33 (82%)	7 (18%)	2	7
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	33
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	33
All	All	3058/3088 (99%)	2716 (89%)	342 (11%)	6	19

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	51	ASP
1	A	96	ARG
1	A	105	LEU
1	A	106	PRO
1	A	136	LEU
1	A	138	HIS
1	A	156	SER
1	A	159	LEU
1	A	180	GLN
1	A	188	VAL
1	A	199	LEU
1	A	253	MET
1	A	265	LYS
1	A	295	VAL
1	A	301	THR
1	A	306	THR
1	A	312	ILE
1	A	324	LEU
1	A	333	LYS
1	A	336	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	347	LEU
1	A	353	LEU
1	A	354	THR
1	A	366	VAL
1	A	369	ASP
1	A	373	VAL
1	A	417	MET
1	A	444	PRO
1	A	465	VAL
1	A	474	GLU
1	A	492	LEU
1	A	507	GLU
1	A	512	ASN
2	B	1	MET
2	B	3	TYR
2	B	7	LEU
2	B	16	ILE
2	B	31	VAL
2	B	54	SER
2	B	60	GLU
2	B	63	THR
2	B	67	ILE
2	B	88[A]	ASP
2	B	88[B]	ASP
2	B	92[A]	ASN
2	B	92[B]	ASN
2	B	103	GLN
2	B	115	ASP
2	B	125	THR
2	B	130	PRO
2	B	138	VAL
2	B	142	VAL
2	B	147	GLU
2	B	167	SER
2	B	170	LEU
2	B	171	LYS
2	B	185	MET
2	B	205	SER
2	B	216	LEU
2	B	220	GLU
3	C	11	VAL
3	C	13	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	18	LEU
3	C	19	THR
3	C	22	LEU
3	C	23	SER
3	C	38	ASN
3	C	85	LEU
3	C	91	VAL
3	C	92	LEU
3	C	112	LEU
3	C	128	GLU
3	C	130	PRO
3	C	131	LEU
3	C	132	LEU
3	C	137	LEU
3	C	142	VAL
3	C	144	ILE
3	C	160	LEU
3	C	163	LEU
3	C	168	THR
3	C	179	SER
3	C	188	ILE
3	C	192	VAL
3	C	196	THR
3	C	222	GLN
3	C	230	ASN
4	D	9	GLU
4	D	19	ARG
4	D	27	VAL
4	D	31	LYS
4	D	36	SER
4	D	40	LEU
4	D	53	ILE
4	D	59	LEU
4	D	62	LEU
4	D	99	GLU
4	D	107	ILE
4	D	116	VAL
4	D	127	LYS
4	D	147	LYS
5	E	29	LEU
5	E	37	VAL
5	E	41	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	70	VAL
5	E	79	LYS
5	E	80	GLU
5	E	99	SER
5	E	101	PRO
5	E	103	GLU
5	E	109	VAL
6	F	6	VAL
6	F	20	VAL
6	F	34	LEU
6	F	37	LYS
6	F	52	ILE
6	F	74	LEU
6	F	95	GLN
6	F	96	LEU
6	F	98	HIS
7	G	5	LYS
7	G	14	ARG
7	G	17	ARG
7	G	32	THR
7	G	34	ASN
7	G	36	TRP
7	G	37	LEU
7	G	38	HIS
7	G	41	HIS
7	G	42	ARG
7	G	48	ILE
7	G	54	ARG
7	G	56	ARG
8	H	19	ARG
8	H	23	GLN
8	H	29	CYS
8	H	41	LYS
8	H	49	ASP
8	H	53	CYS
8	H	57	ARG
8	H	60	TYR
8	H	67	SER
8	H	70	SER
8	H	82	PRO
9	I	2	THR
9	I	8	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	21	ILE
9	I	26	MET
9	I	41	GLU
9	I	64	ARG
10	J	1	PHE
10	J	2	GLU
10	J	5	VAL
10	J	8	LYS
10	J	10	LYS
10	J	27	THR
10	J	47	LEU
10	J	50	LEU
11	K	45	VAL
11	K	49	THR
12	L	11	ILE
12	L	15	VAL
12	L	20	ARG
12	L	22	LEU
12	L	26	THR
12	L	27	LEU
13	M	13	LYS
13	M	24	LEU
13	M	42	LYS
1	N	18	LEU
1	N	51	ASP
1	N	96	ARG
1	N	105	LEU
1	N	136	LEU
1	N	138	HIS
1	N	156	SER
1	N	159	LEU
1	N	180	GLN
1	N	188	VAL
1	N	199	LEU
1	N	238	PHE
1	N	241	PRO
1	N	253	MET
1	N	258	VAL
1	N	265	LYS
1	N	295	VAL
1	N	301	THR
1	N	306	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	N	312	ILE
1	N	318	VAL
1	N	324	LEU
1	N	333	LYS
1	N	336	PRO
1	N	347	LEU
1	N	353	LEU
1	N	354	THR
1	N	366	VAL
1	N	369	ASP
1	N	373	VAL
1	N	417	MET
1	N	444	PRO
1	N	465	VAL
1	N	474	GLU
1	N	492	LEU
1	N	507	GLU
1	N	512	ASN
2	O	1	MET
2	O	3	TYR
2	O	7	LEU
2	O	16	ILE
2	O	31	VAL
2	O	54	SER
2	O	60	GLU
2	O	63	THR
2	O	67	ILE
2	O	88[A]	ASP
2	O	88[B]	ASP
2	O	92[A]	ASN
2	O	92[B]	ASN
2	O	103	GLN
2	O	115	ASP
2	O	125	THR
2	O	130	PRO
2	O	142	VAL
2	O	147	GLU
2	O	167	SER
2	O	170	LEU
2	O	171	LYS
2	O	185	MET
2	O	188	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	O	205	SER
2	O	216	LEU
2	O	220	GLU
3	P	11	VAL
3	P	13	PRO
3	P	18	LEU
3	P	19	THR
3	P	22	LEU
3	P	23	SER
3	P	38	ASN
3	P	85	LEU
3	P	91	VAL
3	P	92	LEU
3	P	112	LEU
3	P	128	GLU
3	P	130	PRO
3	P	131	LEU
3	P	132	LEU
3	P	137	LEU
3	P	142	VAL
3	P	144	ILE
3	P	160	LEU
3	P	163	LEU
3	P	168	THR
3	P	179	SER
3	P	188	ILE
3	P	196	THR
3	P	222	GLN
3	P	230	ASN
4	Q	9	GLU
4	Q	19	ARG
4	Q	27	VAL
4	Q	31	LYS
4	Q	36	SER
4	Q	40	LEU
4	Q	53	ILE
4	Q	59	LEU
4	Q	62	LEU
4	Q	99	GLU
4	Q	107	ILE
4	Q	116	VAL
4	Q	127	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	Q	147	LYS
5	R	29	LEU
5	R	37	VAL
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	99	SER
5	R	101	PRO
5	R	103	GLU
5	R	109	VAL
6	S	6	VAL
6	S	20	VAL
6	S	34	LEU
6	S	37	LYS
6	S	74	LEU
6	S	95	GLN
6	S	96	LEU
6	S	98	HIS
7	T	5	LYS
7	T	14	ARG
7	T	17	ARG
7	T	26	PRO
7	T	32	THR
7	T	34	ASN
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	41	HIS
7	T	42	ARG
7	T	48	ILE
7	T	54	ARG
7	T	56	ARG
8	U	19	ARG
8	U	23	GLN
8	U	41	LYS
8	U	49	ASP
8	U	53	CYS
8	U	57	ARG
8	U	60	TYR
8	U	67	SER
8	U	70	SER
8	U	82	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	V	2	THR
9	V	8	GLN
9	V	21	ILE
9	V	26	MET
9	V	41	GLU
9	V	64	ARG
10	W	1	PHE
10	W	2	GLU
10	W	5	VAL
10	W	8	LYS
10	W	10	LYS
10	W	23	LYS
10	W	27	THR
10	W	47	LEU
10	W	50	LEU
11	X	45	VAL
11	X	49	THR
12	Y	11	ILE
12	Y	15	VAL
12	Y	20	ARG
12	Y	22	LEU
12	Y	26	THR
12	Y	27	LEU
12	Y	44	LEU
13	Z	13	LYS
13	Z	24	LEU
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	4	ASN
1	A	256	HIS
1	A	413	HIS
1	A	512	ASN
2	B	181	GLN
2	B	203	ASN
3	C	71	HIS
3	C	133	ASN
3	C	204	HIS
3	C	222	GLN
4	D	132	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	2	HIS
6	F	66	ASN
7	G	41	HIS
8	H	23	GLN
8	H	24	ASN
8	H	28	ASN
8	H	31	GLN
8	H	32	ASN
9	I	20	HIS
9	I	53	ASN
9	I	70	GLN
10	J	21	HIS
10	J	29	ASN
11	K	10	HIS
13	M	36	HIS
13	M	39	ASN
1	N	4	ASN
1	N	43	GLN
1	N	256	HIS
1	N	512	ASN
2	O	181	GLN
2	O	203	ASN
3	P	71	HIS
3	P	133	ASN
3	P	204	HIS
3	P	222	GLN
4	Q	132	GLN
5	R	2	HIS
6	S	66	ASN
6	S	94	HIS
7	T	41	HIS
8	U	23	GLN
8	U	24	ASN
8	U	28	ASN
8	U	32	ASN
9	V	53	ASN
9	V	70	GLN
10	W	21	HIS
11	X	10	HIS
13	Z	36	HIS
13	Z	39	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
17	HEA	N	515	1	67,67,67	1.19	7 (10%)	81,103,103	1.96	20 (24%)
17	HEA	N	516	18,1	67,67,67	1.47	13 (19%)	81,103,103	1.88	27 (33%)
18	CMO	N	520	17,14	0,1,1	-	-	-	-	-
18	CMO	A	520	17,14	0,1,1	-	-	-	-	-
17	HEA	A	515	1	67,67,67	1.28	7 (10%)	81,103,103	1.99	18 (22%)
17	HEA	A	516	18,1	67,67,67	1.54	12 (17%)	81,103,103	2.00	32 (39%)

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
17	HEA	N	515	1	-	11/36/76/76	-
17	HEA	N	516	18,1	-	10/36/76/76	-
17	HEA	A	515	1	-	12/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEA	A	516	18,1	-	9/36/76/76	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	516	HEA	FE-ND	-3.77	1.83	1.94
17	N	516	HEA	C3C-C2C	-3.49	1.29	1.41
17	A	515	HEA	CMA-C3A	-3.39	1.37	1.45
17	N	516	HEA	FE-NB	-3.29	1.84	1.94
17	A	516	HEA	CMA-C3A	-3.26	1.38	1.45
17	A	516	HEA	C1D-ND	-3.22	1.34	1.40
17	A	515	HEA	C4B-NB	3.21	1.45	1.40
17	N	515	HEA	C11-C3B	-3.16	1.47	1.51
17	A	516	HEA	C3B-C2B	-3.11	1.27	1.34
17	A	516	HEA	FE-NA	2.98	2.05	1.95
17	N	515	HEA	CMA-C3A	-2.91	1.38	1.45
17	A	516	HEA	CHD-C4C	-2.86	1.33	1.39
17	N	516	HEA	CAA-C2A	2.80	1.58	1.51
17	N	516	HEA	CMD-C2D	2.77	1.56	1.50
17	A	516	HEA	CAA-C2A	2.75	1.58	1.51
17	N	516	HEA	CMA-C3A	-2.75	1.39	1.45
17	A	516	HEA	C3C-C2C	-2.71	1.32	1.41
17	A	515	HEA	C1A-NA	2.70	1.44	1.39
17	N	516	HEA	CHC-C4B	-2.65	1.33	1.38
17	A	515	HEA	CHB-C1B	-2.64	1.33	1.39
17	N	516	HEA	CHA-C1A	-2.56	1.33	1.38
17	N	515	HEA	C4A-NA	-2.54	1.34	1.39
17	A	515	HEA	C11-C3B	-2.50	1.48	1.51
17	A	516	HEA	C1B-C2B	2.38	1.49	1.44
17	N	516	HEA	C26-C15	-2.33	1.45	1.50
17	N	515	HEA	C4B-C3B	2.30	1.48	1.44
17	A	516	HEA	C3D-C2D	-2.29	1.31	1.36
17	N	515	HEA	CHA-C1A	2.19	1.42	1.38
17	N	516	HEA	FE-ND	-2.16	1.88	1.94
17	A	516	HEA	C1B-NB	-2.14	1.34	1.38
17	A	515	HEA	C27-C19	-2.13	1.45	1.50
17	A	515	HEA	FE-ND	-2.13	1.88	1.94
17	N	516	HEA	C1D-C2D	2.13	1.48	1.44
17	A	516	HEA	C20-C19	-2.12	1.46	1.51
17	N	516	HEA	C20-C19	-2.12	1.46	1.51
17	N	516	HEA	C16-C15	-2.07	1.47	1.51
17	N	515	HEA	C3B-C2B	2.06	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	CHB-C4A	-2.06	1.34	1.38
17	N	516	HEA	C4B-C3B	2.01	1.48	1.44

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	515	HEA	C12-C11-C3B	7.35	123.61	112.12
17	A	515	HEA	C12-C11-C3B	6.49	122.26	112.12
17	A	516	HEA	CMB-C2B-C3B	-5.68	119.30	130.28
17	N	515	HEA	C13-C14-C15	-5.38	115.31	127.62
17	A	515	HEA	C13-C14-C15	-5.16	115.81	127.62
17	N	516	HEA	CMB-C2B-C3B	-5.07	120.48	130.28
17	A	515	HEA	C3B-C4B-NB	4.59	115.12	109.84
17	A	515	HEA	C4B-C3B-C2B	-4.58	99.73	107.44
17	A	515	HEA	O11-C11-C12	-4.46	97.32	109.14
17	A	515	HEA	C1B-C2B-C3B	4.38	111.87	106.80
17	A	515	HEA	C17-C18-C19	-4.37	117.63	127.62
17	A	516	HEA	CHA-C1A-NA	-4.25	119.83	124.45
17	N	515	HEA	C3A-C2A-C1A	-4.10	103.17	107.05
17	N	516	HEA	C25-C23-C24	3.88	123.53	114.59
17	N	516	HEA	CMB-C2B-C1B	3.86	131.07	125.03
17	A	515	HEA	C4B-NB-C1B	-3.82	100.69	105.21
17	N	515	HEA	C3B-C4B-NB	3.80	114.21	109.84
17	A	516	HEA	CMB-C2B-C1B	3.79	130.95	125.03
17	N	515	HEA	C4B-C3B-C2B	-3.76	101.11	107.44
17	A	516	HEA	CHB-C4A-NA	-3.74	120.38	124.45
17	A	516	HEA	C4B-NB-C1B	-3.71	100.82	105.21
17	A	516	HEA	CMD-C2D-C1D	3.69	130.79	125.03
17	N	516	HEA	C3C-C4C-NC	3.61	112.84	109.80
17	N	516	HEA	C1D-C2D-C3D	-3.51	103.29	106.98
17	A	516	HEA	CHA-C4D-ND	3.37	128.05	124.42
17	A	516	HEA	O11-C11-C3B	-3.24	105.32	111.26
17	N	515	HEA	O11-C11-C12	-3.22	100.61	109.14
17	A	516	HEA	C3B-C4B-NB	3.19	113.51	109.84
17	N	516	HEA	CHA-C1A-NA	-3.18	121.00	124.45
17	N	516	HEA	C20-C19-C18	-3.09	114.23	121.17
17	N	515	HEA	C3C-C4C-NC	3.07	112.38	109.80
17	A	516	HEA	C25-C23-C24	3.03	121.55	114.59
17	N	516	HEA	CAD-C3D-C2D	-3.02	122.20	127.87
17	N	515	HEA	C12-C13-C14	-3.00	104.29	112.16
17	N	516	HEA	C4C-NC-C1C	-2.99	100.95	105.82
17	N	515	HEA	C1B-C2B-C3B	2.95	110.21	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	515	HEA	C4A-C3A-C2A	2.93	109.35	106.81
17	A	516	HEA	CAD-C3D-C2D	-2.92	122.40	127.87
17	A	515	HEA	C26-C15-C14	-2.87	116.26	123.63
17	A	516	HEA	CBA-CAA-C2A	2.87	120.46	112.53
17	A	515	HEA	C12-C13-C14	-2.87	104.63	112.16
17	A	515	HEA	C26-C15-C16	2.84	120.16	115.23
17	N	516	HEA	CHD-C1D-ND	2.79	127.82	124.37
17	N	516	HEA	CBA-CAA-C2A	2.72	120.05	112.53
17	A	516	HEA	C20-C19-C18	-2.67	115.18	121.17
17	N	515	HEA	CHC-C1C-C2C	-2.66	119.70	127.43
17	A	516	HEA	C3A-C2A-C1A	-2.66	104.53	107.05
17	A	516	HEA	C4C-NC-C1C	-2.66	101.49	105.82
17	N	516	HEA	CHD-C1D-C2D	-2.64	119.43	126.95
17	A	516	HEA	C17-C16-C15	2.64	121.93	113.19
17	N	516	HEA	CHB-C4A-NA	-2.57	121.65	124.45
17	N	516	HEA	C3B-C4B-NB	2.56	112.78	109.84
17	A	516	HEA	C3C-C4C-NC	2.55	111.95	109.80
17	N	516	HEA	O11-C11-C3B	-2.55	106.59	111.26
17	N	515	HEA	C17-C18-C19	-2.50	121.89	127.62
17	A	516	HEA	C2D-C1D-ND	2.50	112.72	109.84
17	A	515	HEA	C4C-NC-C1C	-2.48	101.78	105.82
17	A	516	HEA	C2B-C1B-NB	2.46	112.74	109.90
17	N	516	HEA	C17-C16-C15	2.45	121.31	113.19
17	N	515	HEA	C26-C15-C14	-2.43	117.38	123.63
17	A	516	HEA	C1D-C2D-C3D	-2.43	104.43	106.98
17	N	516	HEA	C2A-C1A-NA	2.43	112.67	110.32
17	A	516	HEA	CHD-C1D-C2D	-2.39	120.17	126.95
17	A	516	HEA	CHA-C4D-C3D	-2.35	121.34	124.77
17	A	515	HEA	C1D-ND-C4D	-2.34	102.44	105.21
17	A	516	HEA	C4A-NA-C1A	-2.33	102.02	105.82
17	A	515	HEA	CMB-C2B-C1B	-2.33	121.40	125.03
17	N	515	HEA	C4B-NB-C1B	-2.32	102.46	105.21
17	N	516	HEA	CHA-C4D-ND	2.32	126.92	124.42
17	A	515	HEA	C3C-C4C-NC	2.29	111.73	109.80
17	N	515	HEA	C2C-C1C-NC	2.29	113.81	110.14
17	N	516	HEA	CMC-C2C-C1C	2.28	128.89	125.42
17	N	516	HEA	CAA-C2A-C1A	2.26	129.44	124.85
17	N	515	HEA	C27-C19-C18	-2.26	117.83	123.63
17	A	515	HEA	C20-C19-C18	2.25	126.22	121.17
17	N	516	HEA	CHC-C4B-C3B	-2.24	120.15	125.80
17	N	516	HEA	C2D-C1D-ND	2.24	112.41	109.84
17	A	516	HEA	CHD-C4C-NC	-2.22	119.83	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	516	HEA	CHC-C4B-C3B	-2.22	120.20	125.80
17	N	516	HEA	C3A-C2A-C1A	-2.22	104.95	107.05
17	N	515	HEA	C20-C19-C18	2.17	126.05	121.17
17	N	515	HEA	C25-C23-C24	2.16	119.57	114.59
17	A	515	HEA	C2D-C1D-ND	2.16	112.32	109.84
17	N	516	HEA	CMD-C2D-C1D	2.12	128.35	125.03
17	A	516	HEA	CAD-C3D-C4D	2.12	128.39	124.70
17	N	515	HEA	CHC-C4B-NB	-2.11	121.75	124.37
17	A	515	HEA	C2B-C1B-NB	2.10	112.33	109.90
17	A	516	HEA	C27-C19-C20	2.10	118.87	115.23
17	N	516	HEA	C4D-C3D-C2D	2.09	109.93	106.89
17	A	516	HEA	O2A-CGA-CBA	2.07	120.54	114.00
17	A	516	HEA	C2A-C1A-NA	2.06	112.31	110.32
17	A	516	HEA	CMC-C2C-C1C	2.06	128.55	125.42
17	N	516	HEA	C4B-NB-C1B	-2.06	102.77	105.21
17	N	515	HEA	O2D-CGD-CBD	2.04	120.43	114.00
17	N	516	HEA	O1D-CGD-CBD	-2.01	116.72	123.09
17	A	516	HEA	O1A-CGA-CBA	-2.01	116.72	123.09
17	A	516	HEA	C4A-C3A-C2A	2.00	108.55	106.81

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	515	HEA	C2A-C3A-CMA-OMA
17	A	515	HEA	C4A-C3A-CMA-OMA
17	A	515	HEA	C12-C11-C3B-C2B
17	N	515	HEA	C2A-C3A-CMA-OMA
17	N	515	HEA	C4A-C3A-CMA-OMA
17	N	515	HEA	C12-C11-C3B-C2B
17	N	515	HEA	C15-C16-C17-C18
17	A	515	HEA	C15-C16-C17-C18
17	N	515	HEA	C13-C14-C15-C26
17	A	516	HEA	C2C-C3C-CAC-CBC
17	N	516	HEA	C2C-C3C-CAC-CBC
17	A	515	HEA	C13-C14-C15-C26
17	A	516	HEA	C4C-C3C-CAC-CBC
17	N	516	HEA	C4C-C3C-CAC-CBC
17	A	515	HEA	O11-C11-C12-C13
17	A	516	HEA	C13-C14-C15-C26
17	A	516	HEA	C4A-C3A-CMA-OMA
17	N	516	HEA	C4A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
17	N	516	HEA	C13-C14-C15-C26
17	N	515	HEA	O11-C11-C12-C13
17	N	516	HEA	CAA-CBA-CGA-O2A
17	A	516	HEA	CAA-CBA-CGA-O2A
17	A	515	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAA-CBA-CGA-O1A
17	A	516	HEA	CAA-CBA-CGA-O1A
17	A	515	HEA	C26-C15-C16-C17
17	A	515	HEA	CAD-CBD-CGD-O2D
17	N	516	HEA	CAD-CBD-CGD-O2D
17	N	516	HEA	CAD-CBD-CGD-O1D
17	A	516	HEA	CAD-CBD-CGD-O1D
17	A	516	HEA	CAD-CBD-CGD-O2D
17	N	516	HEA	C2A-C3A-CMA-OMA
17	A	516	HEA	C26-C15-C16-C17
17	N	515	HEA	C26-C15-C16-C17
17	A	515	HEA	C2C-C3C-CAC-CBC
17	N	515	HEA	CAD-CBD-CGD-O1D
17	A	515	HEA	CAA-CBA-CGA-O1A
17	N	515	HEA	CAA-CBA-CGA-O1A
17	A	515	HEA	CAA-CBA-CGA-O2A
17	N	515	HEA	CAA-CBA-CGA-O2A
17	N	516	HEA	C26-C15-C16-C17
17	N	515	HEA	CAD-CBD-CGD-O2D

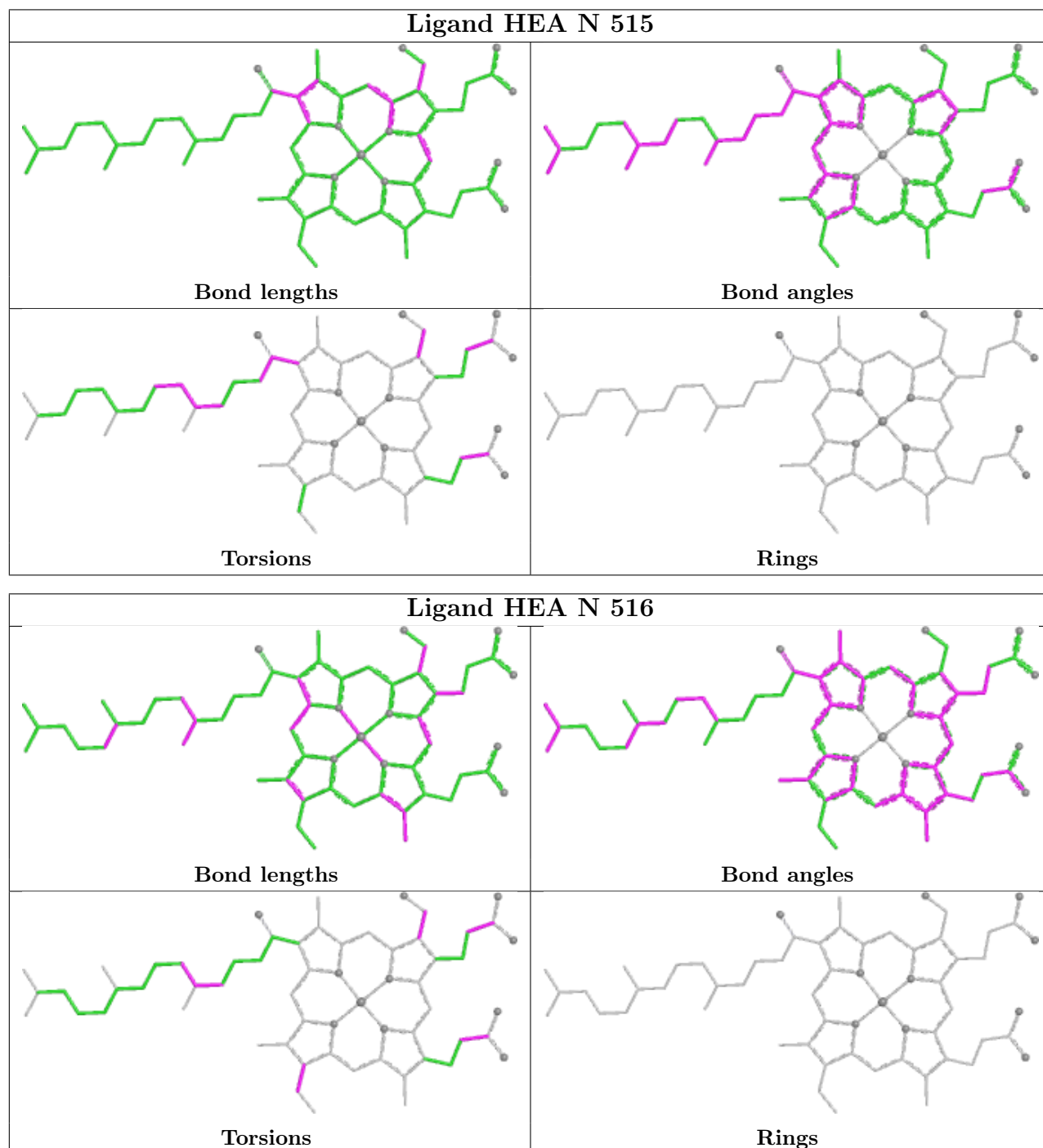
There are no ring outliers.

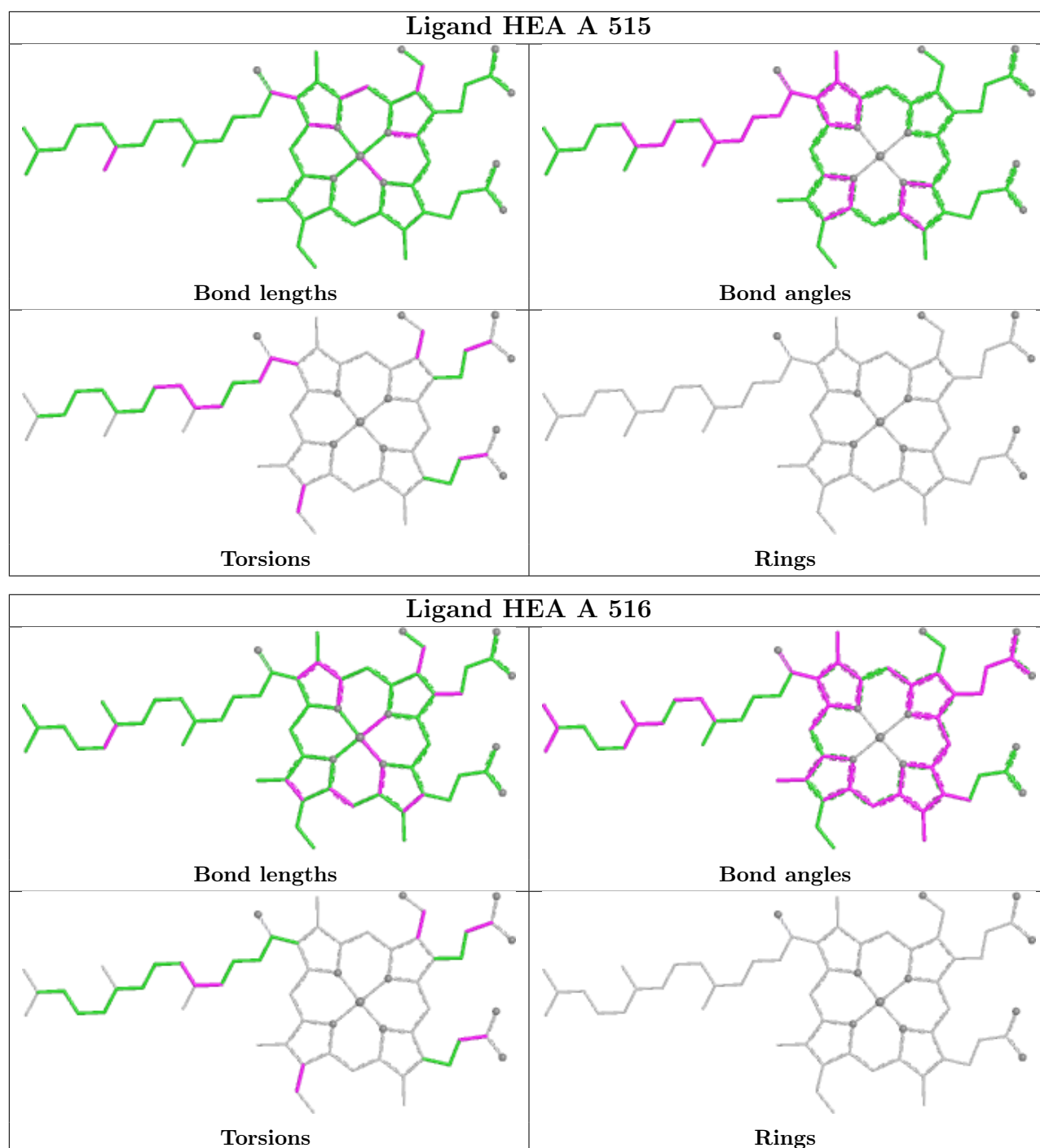
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	515	HEA	9	0
17	N	516	HEA	1	0
17	A	515	HEA	10	0
17	A	516	HEA	3	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.