



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:09 AM EDT

PDB ID : 1OCZ / pdb_00001ocz
Title : BOVINE HEART CYTOCHROME C OXIDASE IN AZIDE-BOUND STATE
Authors : Tsukihara, T.; Yao, M.
Deposited on : 1998-07-13
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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>.

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)
Xtriage (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)	:	2.50

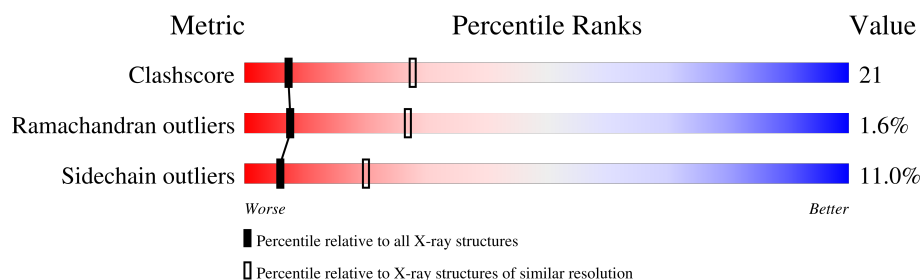
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

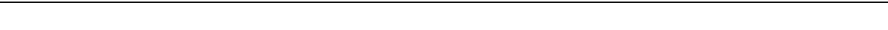
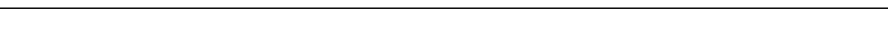
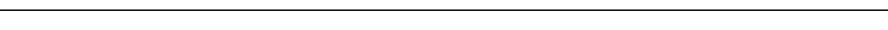
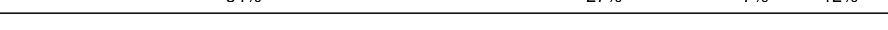
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
5	R	109	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	AZI	A	520	-	X	-	-
17	AZI	A	521	-	X	-	-
17	AZI	N	521	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 28818 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 5 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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		

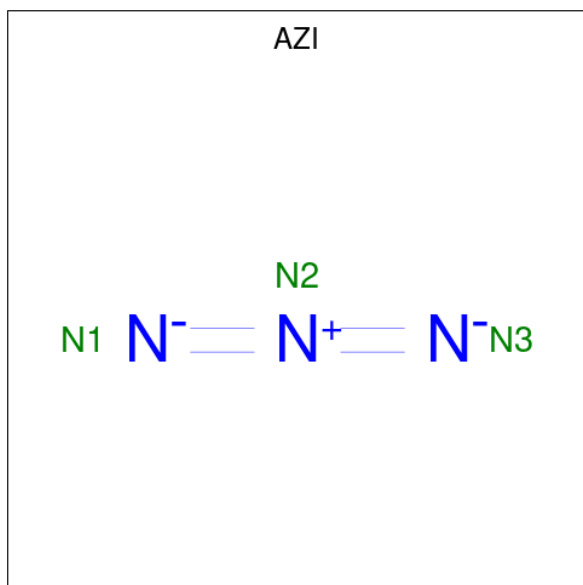
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

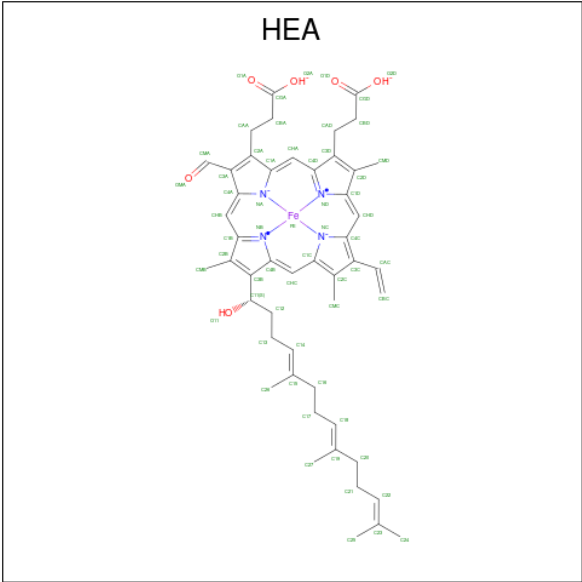
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is AZIDE ION (CCD ID: AZI) (formula: N₃).



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

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

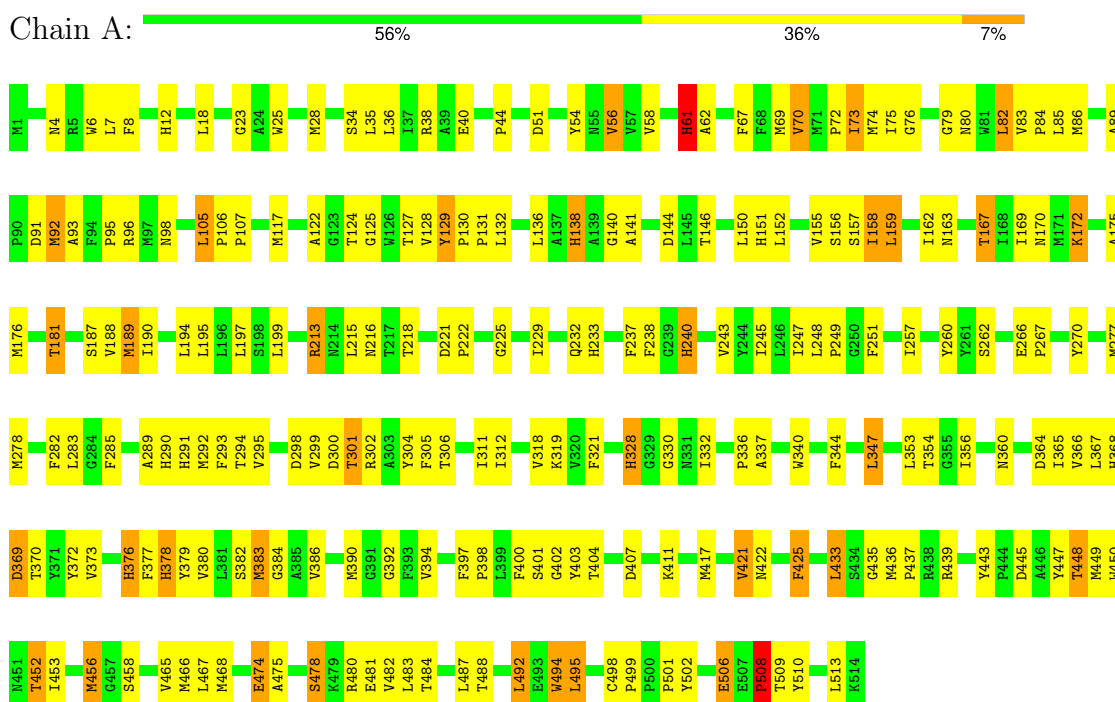
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	F	1	Total	Zn	0	0
			1	1		
19	S	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

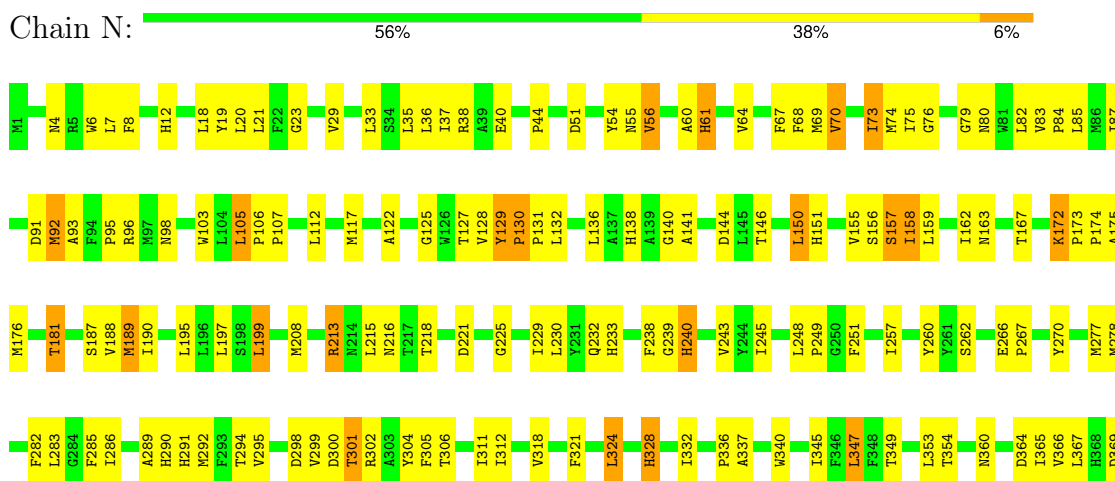
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

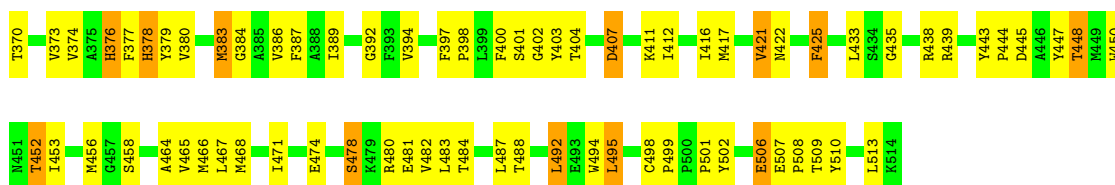
Note EDS was not executed.

• Molecule 1: CYTOCHROME C OXIDASE

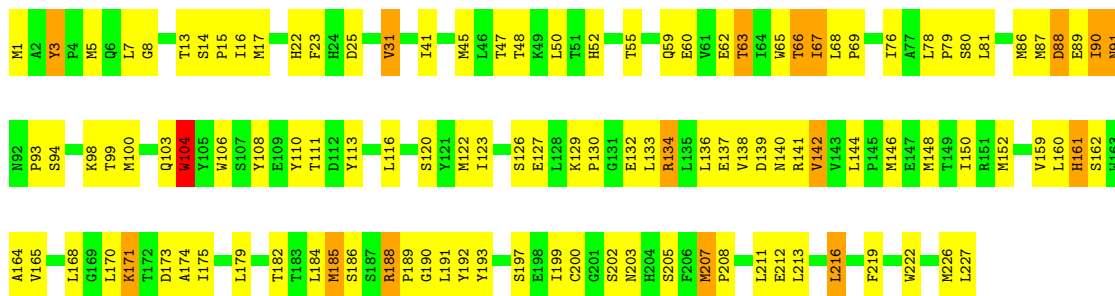


• Molecule 1: CYTOCHROME C OXIDASE

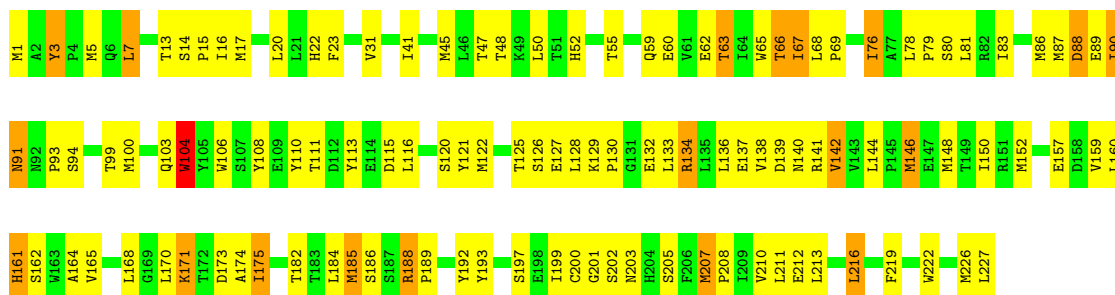




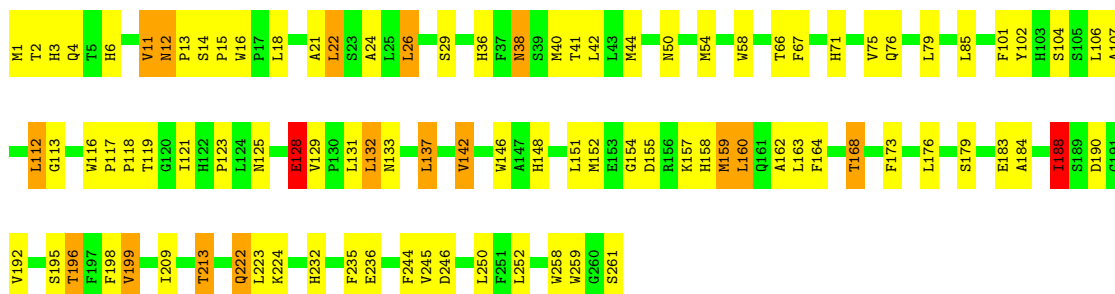
• Molecule 2: CYTOCHROME C OXIDASE



• Molecule 2: CYTOCHROME C OXIDASE

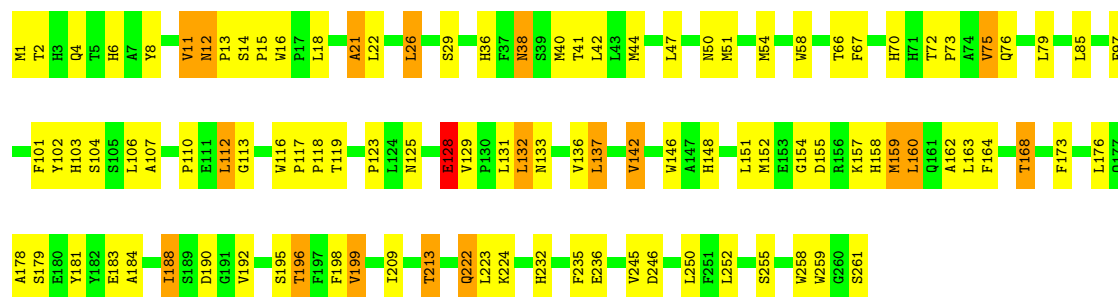


• Molecule 3: CYTOCHROME C OXIDASE

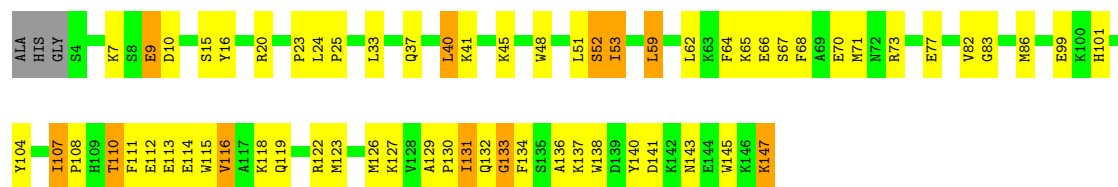


• Molecule 3: CYTOCHROME C OXIDASE

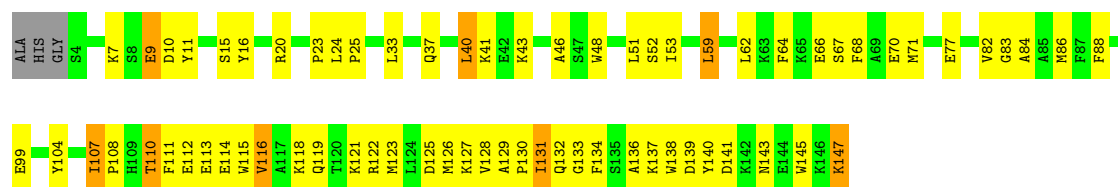




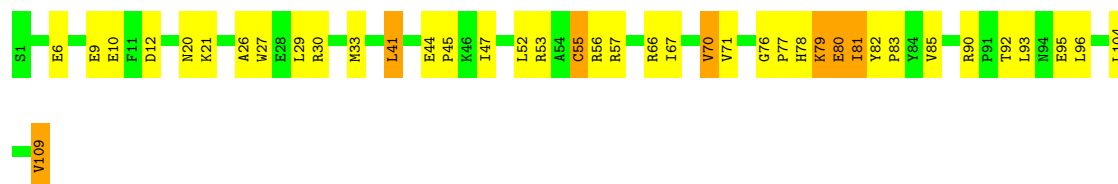
• Molecule 4: CYTOCHROME C OXIDASE



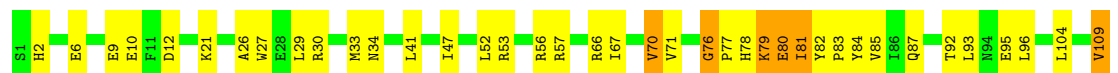
• Molecule 4: CYTOCHROME C OXIDASE



• Molecule 5: CYTOCHROME C OXIDASE

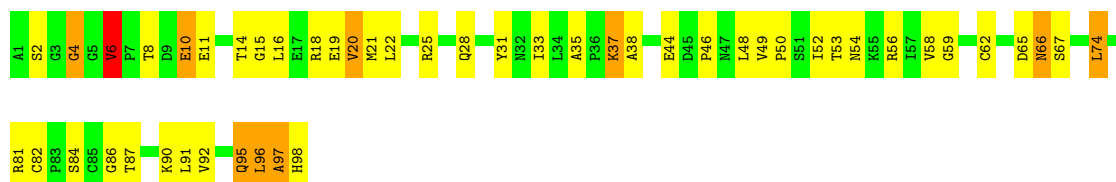


• Molecule 5: CYTOCHROME C OXIDASE



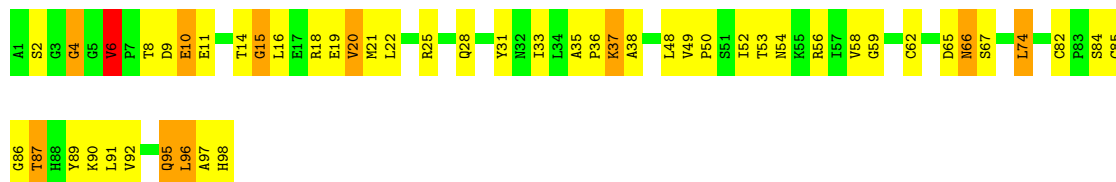
• Molecule 6: CYTOCHROME C OXIDASE





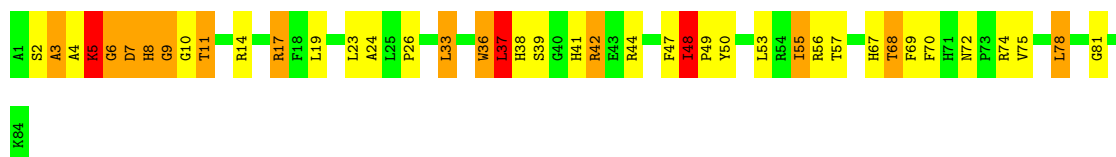
• Molecule 6: CYTOCHROME C OXIDASE

Chain S: 49% 40% 10% .



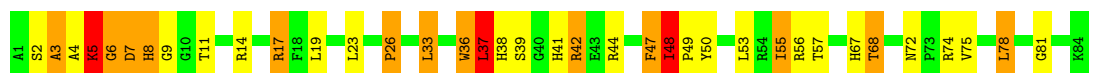
• Molecule 7: CYTOCHROME C OXIDASE

Chain G: 51% 30% 15% .



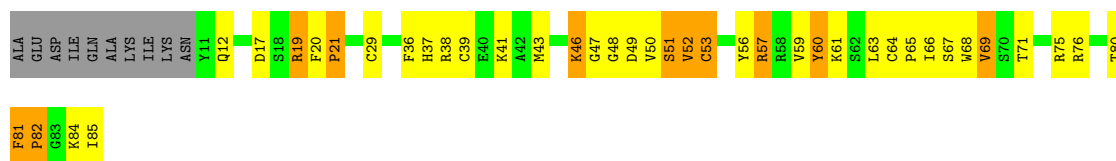
• Molecule 8: CYTOCHROME C OXIDASE

Chain T: 56% 25% 15% .



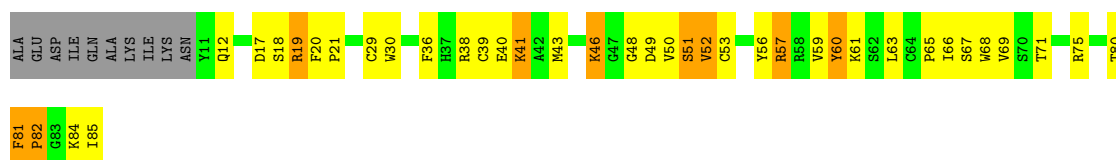
• Molecule 8: CYTOCHROME C OXIDASE

Chain H: 41% 34% 13% 12%

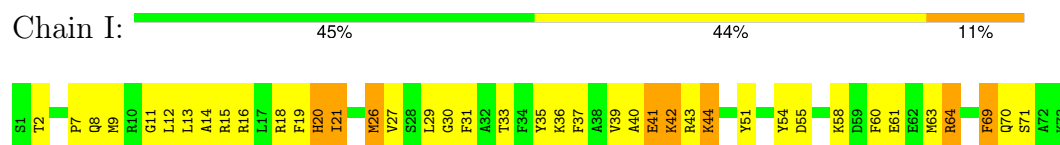


• Molecule 8: CYTOCHROME C OXIDASE

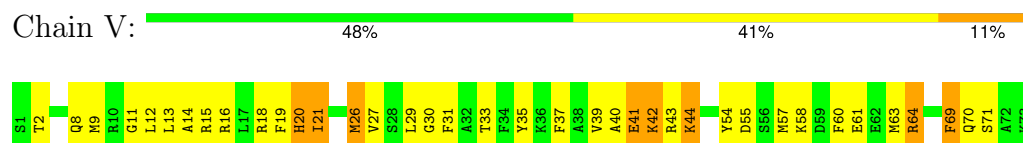
Chain U: 42% 35% 11% 12%



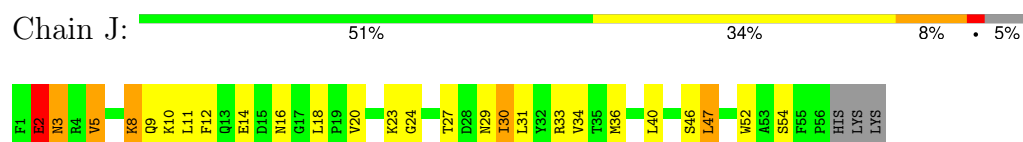
- Molecule 9: CYTOCHROME C OXIDASE



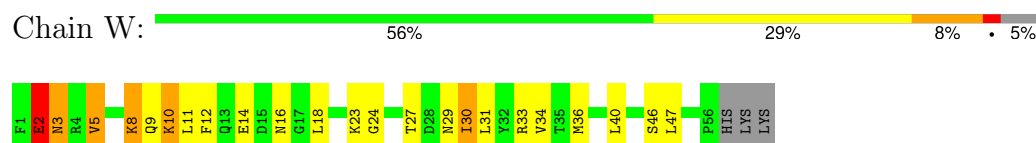
- Molecule 9: CYTOCHROME C OXIDASE



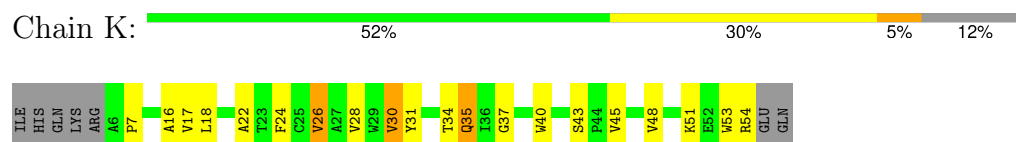
- Molecule 10: CYTOCHROME C OXIDASE



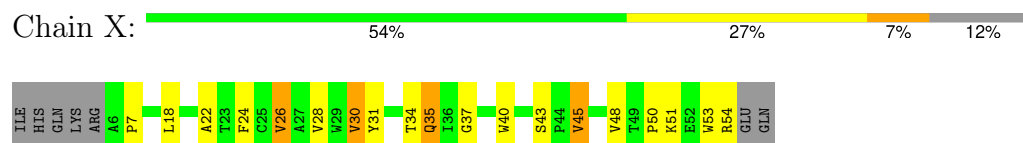
- Molecule 10: CYTOCHROME C OXIDASE



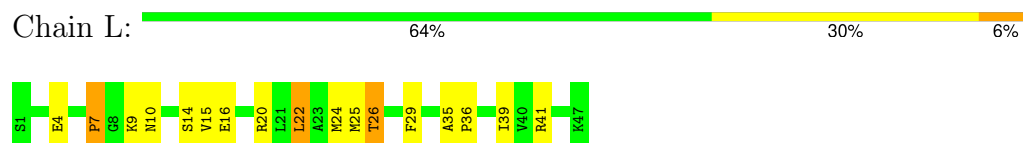
- Molecule 11: CYTOCHROME C OXIDASE



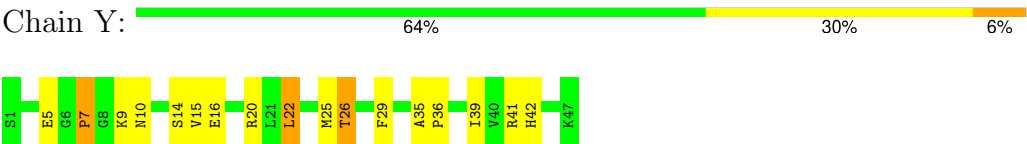
- Molecule 11: CYTOCHROME C OXIDASE



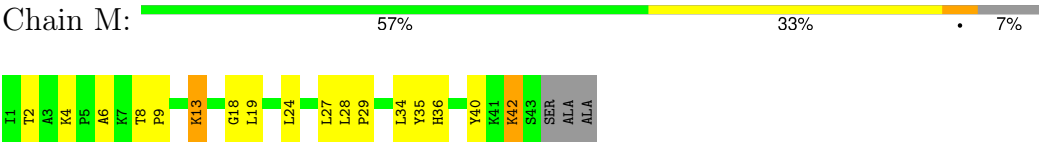
- Molecule 12: CYTOCHROME C OXIDASE



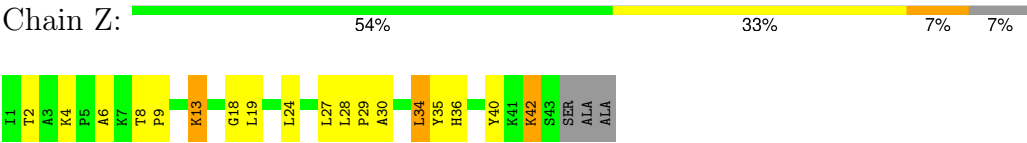
- Molecule 12: CYTOCHROME C OXIDASE



• Molecule 13: CYTOCHROME C OXIDASE



• Molecule 13: CYTOCHROME C OXIDASE



4 Data and refinement statistics

Xtriage (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, α , β , γ	189.20Å 210.60Å 178.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90	Depositor
% Data completeness (in resolution range)	80.2 (7.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28818	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, CU, ZN, HEA, NA, 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	0.97	9/4164 (0.2%)	1.27	43/5688 (0.8%)
1	N	0.85	7/4164 (0.2%)	1.23	44/5688 (0.8%)
2	B	0.88	0/1909	1.22	13/2601 (0.5%)
2	O	0.80	1/1909 (0.1%)	1.18	16/2601 (0.6%)
3	C	0.84	1/2211 (0.0%)	1.18	16/3023 (0.5%)
3	P	0.76	1/2211 (0.0%)	1.15	17/3023 (0.6%)
4	D	0.76	0/1229	1.08	7/1658 (0.4%)
4	Q	0.63	0/1229	1.04	5/1658 (0.3%)
5	E	0.78	0/898	1.08	4/1218 (0.3%)
5	R	0.69	0/898	1.06	3/1218 (0.2%)
6	F	0.80	0/765	1.21	8/1038 (0.8%)
6	S	0.75	0/765	1.21	7/1038 (0.7%)
7	G	0.75	0/699	1.26	10/950 (1.1%)
7	T	0.74	0/699	1.28	10/950 (1.1%)
8	H	0.76	1/648 (0.2%)	1.17	5/877 (0.6%)
8	U	0.69	0/648	1.14	3/877 (0.3%)
9	I	0.82	0/611	1.03	3/810 (0.4%)
9	V	0.71	0/611	1.02	3/810 (0.4%)
10	J	0.82	0/451	1.04	4/610 (0.7%)
10	W	0.70	0/451	1.01	2/610 (0.3%)
11	K	0.90	0/398	1.14	4/546 (0.7%)
11	X	0.67	0/398	1.12	4/546 (0.7%)
12	L	0.83	0/399	1.08	1/534 (0.2%)
12	Y	0.69	0/399	1.06	1/534 (0.2%)
13	M	0.88	0/345	1.16	2/470 (0.4%)
13	Z	0.66	0/345	1.14	2/470 (0.4%)
All	All	0.82	20/29454 (0.1%)	1.18	237/40046 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	3
2	B	0	1
All	All	0	8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	378	HIS	CG-CD2	9.26	1.46	1.35
1	A	61	HIS	CD2-NE2	9.00	1.47	1.37
1	N	378	HIS	ND1-CE1	8.53	1.41	1.32
1	N	61	HIS	CD2-NE2	7.87	1.46	1.37
1	A	378	HIS	ND1-CE1	6.76	1.39	1.32
1	A	61	HIS	CG-CD2	6.63	1.43	1.35
3	P	142	VAL	CA-CB	6.50	1.63	1.54
8	H	69	VAL	CA-CB	-6.39	1.47	1.54
1	A	378	HIS	CG-CD2	6.38	1.42	1.35
1	A	376	HIS	ND1-CE1	6.32	1.38	1.32
1	N	376	HIS	ND1-CE1	6.31	1.38	1.32
1	A	61	HIS	CG-ND1	6.22	1.45	1.38
1	N	378	HIS	CD2-NE2	6.06	1.44	1.37
2	O	175	ILE	CA-CB	5.75	1.58	1.54
1	N	376	HIS	CG-CD2	5.46	1.41	1.35
1	N	130	PRO	CA-C	5.28	1.57	1.52
3	C	142	VAL	CA-CB	5.21	1.61	1.54
1	A	376	HIS	CG-CD2	5.17	1.41	1.35
1	A	494	TRP	CA-C	5.11	1.59	1.52
1	A	130	PRO	CA-C	5.10	1.56	1.52

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	7	ASP	N-CA-C	10.59	126.93	109.24
7	T	7	ASP	N-CA-C	10.00	125.94	109.24
1	A	330	GLY	N-CA-C	9.22	122.53	111.93
1	N	435	GLY	N-CA-C	9.18	127.52	115.40
1	A	378	HIS	ND1-CE1-NE2	9.17	117.57	108.40
1	N	378	HIS	ND1-CE1-NE2	8.93	117.33	108.40
1	A	435	GLY	N-CA-C	8.88	127.12	115.40
1	N	332	ILE	N-CA-C	8.49	120.83	109.37
1	N	401	SER	N-CA-C	8.44	122.07	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	PRO	N-CA-C	-8.32	100.55	110.70
3	P	107	ALA	CA-C-N	8.32	128.63	119.90
3	P	107	ALA	C-N-CA	8.32	128.63	119.90
1	N	56	VAL	N-CA-C	-8.20	102.44	110.72
1	N	130	PRO	N-CA-C	-8.11	100.80	110.70
2	B	165	VAL	CA-C-N	8.08	129.94	119.84
2	B	165	VAL	C-N-CA	8.08	129.94	119.84
3	C	107	ALA	CA-C-N	8.08	128.38	119.90
3	C	107	ALA	C-N-CA	8.08	128.38	119.90
2	O	165	VAL	CA-C-N	8.06	129.91	119.84
2	O	165	VAL	C-N-CA	8.06	129.91	119.84
9	V	20	HIS	N-CA-C	7.96	120.87	111.71
1	N	378	HIS	CA-CB-CG	-7.94	105.86	113.80
1	A	332	ILE	N-CA-C	7.84	119.96	109.37
1	A	61	HIS	CG-CD2-NE2	-7.80	99.40	107.20
1	A	401	SER	N-CA-C	7.77	123.25	112.45
11	X	48	VAL	N-CA-C	7.75	119.73	108.58
5	R	76	GLY	CA-C-N	7.71	128.69	120.83
5	R	76	GLY	C-N-CA	7.71	128.69	120.83
5	R	81	ILE	N-CA-C	7.66	117.73	110.30
3	P	159	MET	N-CA-C	-7.61	102.67	110.97
5	E	76	GLY	CA-C-N	7.58	129.79	121.00
5	E	76	GLY	C-N-CA	7.58	129.79	121.00
4	Q	131	ILE	N-CA-C	7.57	120.51	111.05
1	N	448	THR	N-CA-C	7.55	119.15	111.07
9	I	20	HIS	N-CA-C	7.54	120.38	111.71
1	A	140	GLY	N-CA-C	7.46	119.62	112.08
4	D	131	ILE	N-CA-C	7.42	120.33	111.05
1	A	56	VAL	N-CA-C	-7.31	103.66	110.53
1	N	61	HIS	CG-CD2-NE2	-7.30	99.90	107.20
1	N	495	LEU	N-CA-C	7.30	122.02	113.18
1	A	448	THR	N-CA-C	7.30	118.88	111.07
5	E	81	ILE	N-CA-C	7.21	117.30	110.30
1	A	425	PHE	N-CA-C	7.18	122.34	113.50
1	N	67	PHE	N-CA-C	7.14	120.10	111.82
1	N	262	SER	N-CA-C	-7.14	104.60	113.38
1	A	67	PHE	N-CA-C	7.13	120.09	111.82
1	N	425	PHE	N-CA-C	7.08	122.21	113.50
11	K	48	VAL	N-CA-C	7.07	118.76	108.58
8	U	63	LEU	N-CA-C	7.06	120.38	111.69
7	T	72	ASN	CA-C-N	7.05	128.66	119.84
7	T	72	ASN	C-N-CA	7.05	128.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	37	GLY	N-CA-C	7.02	122.20	114.40
8	U	81	PHE	CA-C-N	7.01	127.91	120.12
8	U	81	PHE	C-N-CA	7.01	127.91	120.12
3	C	113	GLY	N-CA-C	-7.00	105.20	115.63
3	P	113	GLY	N-CA-C	-7.00	105.20	115.63
3	P	236	GLU	N-CA-C	-6.99	103.59	111.07
3	C	159	MET	N-CA-C	-6.97	103.37	110.97
1	A	262	SER	N-CA-C	-6.96	104.82	113.38
1	N	125	GLY	N-CA-C	-6.95	104.07	112.48
1	A	125	GLY	N-CA-C	-6.93	104.10	112.48
11	K	37	GLY	N-CA-C	6.89	122.05	114.40
1	A	70	VAL	N-CA-C	6.88	117.38	110.23
12	Y	16	GLU	N-CA-C	6.85	118.82	111.36
1	A	506	GLU	N-CA-C	-6.84	103.84	111.71
1	N	140	GLY	N-CA-C	6.83	118.98	112.08
6	S	31	TYR	N-CA-C	6.80	120.88	112.59
1	N	376	HIS	CB-CG-CD2	-6.78	122.38	131.20
3	P	246	ASP	CB-CA-C	-6.76	100.47	110.95
1	N	6	TRP	N-CA-C	6.75	121.52	113.28
1	A	433	LEU	N-CA-C	-6.73	104.02	111.36
8	H	81	PHE	CA-C-N	6.66	127.52	120.12
8	H	81	PHE	C-N-CA	6.66	127.52	120.12
1	A	6	TRP	N-CA-C	6.60	121.34	113.28
13	Z	27	LEU	N-CA-C	6.59	120.53	112.23
1	N	216	ASN	N-CA-C	6.57	120.48	111.54
3	C	246	ASP	CB-CA-C	-6.57	100.77	110.95
3	C	236	GLU	N-CA-C	-6.56	104.05	111.07
1	N	181	THR	CA-C-N	6.53	126.49	119.76
1	N	181	THR	C-N-CA	6.53	126.49	119.76
8	H	63	LEU	N-CA-C	6.52	119.71	111.69
2	O	134	ARG	N-CA-C	6.51	124.66	110.80
2	B	134	ARG	N-CA-C	6.48	124.60	110.80
9	I	35	TYR	N-CA-C	-6.39	104.31	111.28
7	G	72	ASN	CA-C-N	6.34	127.76	119.84
7	G	72	ASN	C-N-CA	6.34	127.76	119.84
1	A	82	LEU	N-CA-C	6.33	120.21	112.23
6	F	31	TYR	N-CA-C	6.33	120.31	112.59
1	A	378	HIS	CA-CB-CG	-6.31	107.49	113.80
1	A	181	THR	CA-C-N	6.30	126.25	119.76
1	A	181	THR	C-N-CA	6.30	126.25	119.76
1	A	376	HIS	CB-CG-CD2	-6.29	123.03	131.20
4	D	133	GLY	N-CA-C	6.25	127.99	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	61	HIS	CB-CG-ND1	-6.24	113.35	122.70
1	N	506	GLU	N-CA-C	-6.23	104.55	111.71
1	A	495	LEU	N-CA-C	6.21	120.70	113.18
8	H	64	CYS	CA-C-N	-6.21	113.58	119.85
8	H	64	CYS	C-N-CA	-6.21	113.58	119.85
7	T	17	ARG	N-CA-C	-6.19	104.62	111.36
2	B	103	GLN	CA-C-N	6.18	133.35	121.54
2	B	103	GLN	C-N-CA	6.18	133.35	121.54
1	N	478	SER	N-CA-C	6.17	118.08	111.36
6	F	67	SER	N-CA-C	-6.14	105.27	112.89
6	F	38	ALA	N-CA-C	6.14	118.44	110.53
2	B	104	TRP	N-CA-C	6.13	123.86	110.80
6	S	38	ALA	N-CA-C	6.13	118.44	110.53
1	A	36	LEU	N-CA-C	-6.13	104.52	111.14
6	S	67	SER	N-CA-C	-6.09	105.34	112.89
12	L	16	GLU	N-CA-C	6.08	117.99	111.36
1	N	82	LEU	N-CA-C	6.08	119.17	111.69
11	K	35	GLN	N-CA-C	6.00	121.65	113.37
1	N	509	THR	N-CA-C	-6.00	102.79	110.53
2	O	104	TRP	N-CA-C	5.99	123.56	110.80
1	N	466	MET	N-CA-C	-5.97	104.86	111.36
3	P	198	PHE	N-CA-C	5.94	118.71	111.82
3	C	244	PHE	N-CA-C	-5.88	104.78	111.07
7	T	33	LEU	N-CA-C	-5.87	104.78	111.07
1	A	378	HIS	CE1-NE2-CD2	-5.87	103.13	109.00
1	A	456	MET	N-CA-C	-5.86	104.89	111.28
1	A	509	THR	N-CA-C	-5.86	102.97	110.53
13	M	42	LYS	N-CA-C	-5.86	106.13	113.28
3	C	66	THR	N-CA-C	5.84	117.65	111.28
2	O	76	ILE	N-CA-C	-5.84	106.12	111.67
4	Q	104	TYR	N-CA-C	5.84	119.04	109.76
9	I	69	PHE	N-CA-C	5.81	118.03	110.53
9	V	35	TYR	N-CA-C	-5.81	104.95	111.28
9	V	69	PHE	N-CA-C	5.80	118.01	110.53
3	C	198	PHE	N-CA-C	5.79	118.54	111.82
1	A	216	ASN	N-CA-C	5.79	119.41	111.54
7	G	33	LEU	N-CA-C	-5.77	104.90	111.07
1	A	73	ILE	N-CA-C	5.76	115.95	110.42
4	Q	133	GLY	N-CA-C	5.76	126.83	113.18
2	O	110	TYR	N-CA-C	-5.75	99.16	108.52
6	F	81	ARG	N-CA-C	5.72	118.44	108.76
2	O	207	MET	CA-C-N	5.70	126.50	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	207	MET	C-N-CA	5.70	126.50	120.11
3	P	66	THR	N-CA-C	5.70	117.57	111.36
5	E	55	CYS	N-CA-C	-5.69	104.98	111.07
1	A	421	VAL	N-CA-C	5.69	115.88	110.42
1	N	36	LEU	N-CA-C	-5.69	105.00	111.14
2	O	47	THR	N-CA-C	5.69	120.57	111.81
4	Q	15	SER	N-CA-C	5.66	117.22	109.18
3	P	70	HIS	N-CA-C	5.66	120.03	113.18
2	O	201	GLY	N-CA-C	5.66	118.13	111.63
1	A	376	HIS	ND1-CE1-NE2	5.65	114.05	108.40
6	S	6	VAL	CA-C-N	5.65	125.60	119.78
6	S	6	VAL	C-N-CA	5.65	125.60	119.78
11	X	35	GLN	N-CA-C	5.65	121.17	113.37
1	N	328	HIS	N-CA-C	5.63	122.80	110.80
1	N	407	ASP	N-CA-C	5.63	118.14	111.33
1	A	328	HIS	N-CA-C	5.62	122.76	110.80
2	B	76	ILE	CB-CA-C	-5.60	106.12	111.44
6	F	6	VAL	CA-C-N	5.60	125.55	119.78
6	F	6	VAL	C-N-CA	5.60	125.55	119.78
3	C	21	ALA	N-CA-C	-5.59	105.10	111.14
7	G	37	LEU	N-CA-C	-5.59	106.50	113.15
7	G	57	THR	N-CA-C	-5.59	106.51	113.38
1	A	466	MET	N-CA-C	-5.57	105.28	111.36
1	N	70	VAL	N-CA-C	5.57	116.02	110.23
13	Z	42	LYS	N-CA-C	-5.56	106.49	113.28
6	F	66	ASN	N-CA-C	5.53	122.57	110.80
2	O	175	ILE	N-CA-C	5.52	114.18	107.61
3	C	184	ALA	CA-C-N	5.51	126.57	120.45
3	C	184	ALA	C-N-CA	5.51	126.57	120.45
4	D	15	SER	N-CA-C	5.51	117.00	109.18
3	C	29	SER	N-CA-C	-5.49	105.85	112.54
11	K	34	THR	N-CA-C	5.49	119.74	112.72
7	T	37	LEU	N-CA-C	-5.49	106.62	113.15
4	D	77	GLU	N-CA-C	5.48	116.93	111.07
4	D	101	HIS	N-CA-C	5.47	117.32	111.36
1	N	507	GLU	CA-C-N	5.46	126.66	119.84
1	N	507	GLU	C-N-CA	5.46	126.66	119.84
1	N	376	HIS	ND1-CE1-NE2	5.44	113.84	108.40
6	F	59	GLY	N-CA-C	-5.43	102.39	110.71
1	A	141	ALA	N-CA-C	5.41	119.37	112.87
2	B	76	ILE	N-CA-C	-5.41	106.91	111.56
3	P	21	ALA	N-CA-C	-5.38	105.33	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	161	HIS	N-CA-C	-5.37	101.33	108.74
3	P	29	SER	N-CA-C	-5.37	105.99	112.54
7	T	57	THR	N-CA-C	-5.33	106.83	113.38
2	B	207	MET	CA-C-N	5.30	126.05	120.11
2	B	207	MET	C-N-CA	5.30	126.05	120.11
1	N	345	ILE	N-CA-C	5.30	115.93	110.36
10	J	24	GLY	N-CA-C	5.30	122.26	115.32
10	J	2	GLU	N-CA-C	5.30	122.08	110.80
2	B	47	THR	N-CA-C	5.29	119.96	111.81
2	O	115	ASP	N-CA-C	5.29	117.17	109.71
6	S	59	GLY	N-CA-C	-5.27	102.64	110.71
6	S	66	ASN	N-CA-C	5.24	121.97	110.80
7	G	17	ARG	N-CA-C	-5.24	105.65	111.36
1	N	433	LEU	N-CA-C	-5.23	105.66	111.36
7	T	47	PHE	N-CA-C	5.23	117.25	109.25
1	N	239	GLY	N-CA-C	5.22	119.20	112.83
7	G	9	GLY	N-CA-C	-5.21	100.83	113.18
1	A	157	SER	N-CA-C	5.21	117.86	111.82
1	A	167	THR	CB-CA-C	-5.20	102.95	110.96
3	C	71	HIS	N-CA-C	5.17	117.38	109.62
4	D	45	LYS	N-CA-C	-5.17	106.48	112.89
1	A	478	SER	N-CA-C	5.17	116.99	111.36
10	W	2	GLU	N-CA-C	5.15	121.76	110.80
1	N	374	VAL	N-CA-C	-5.14	105.52	110.72
3	P	8	TYR	N-CA-C	5.14	117.49	110.55
1	A	122	ALA	N-CA-C	5.14	117.54	108.24
1	N	73	ILE	N-CA-C	5.14	115.28	110.30
4	D	104	TYR	N-CA-C	5.13	117.92	109.76
3	P	252	LEU	N-CA-C	-5.13	105.60	111.14
10	W	24	GLY	N-CA-C	5.12	121.01	114.66
3	C	252	LEU	N-CA-C	-5.11	105.62	111.14
7	T	48	ILE	CA-C-N	5.11	126.23	119.84
7	T	48	ILE	C-N-CA	5.11	126.23	119.84
1	A	89	ALA	CA-C-N	5.11	124.61	119.19
1	A	89	ALA	C-N-CA	5.11	124.61	119.19
1	N	157	SER	N-CA-C	5.10	117.58	111.71
1	A	356	ILE	N-CA-C	-5.10	105.16	112.35
4	Q	77	GLU	N-CA-C	5.10	116.53	111.07
3	C	188	ILE	CB-CA-C	-5.10	104.26	112.16
1	N	129	TYR	CB-CA-C	-5.09	101.08	109.27
11	X	34	THR	N-CA-C	5.08	119.23	112.72
1	A	129	TYR	CB-CA-C	-5.08	101.09	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	412	ILE	N-CA-C	-5.07	105.55	110.42
1	N	421	VAL	N-CA-C	5.07	115.28	110.42
3	P	255	SER	N-CA-C	5.06	117.76	111.24
2	O	63	THR	N-CA-C	-5.05	105.47	111.69
1	N	141	ALA	N-CA-C	5.05	118.93	112.87
2	B	63	THR	N-CA-C	-5.05	105.48	111.69
10	J	20	VAL	N-CA-C	5.04	119.83	109.34
7	G	48	ILE	CA-C-N	5.04	126.14	119.84
7	G	48	ILE	C-N-CA	5.04	126.14	119.84
1	N	122	ALA	N-CA-C	5.02	117.33	108.24
2	B	161	HIS	N-CA-C	-5.02	101.48	108.96
10	J	52	TRP	N-CA-C	-5.02	105.94	111.71
3	P	75	VAL	N-CA-C	5.02	115.79	110.72
3	P	184	ALA	CA-C-N	5.02	126.02	120.45
3	P	184	ALA	C-N-CA	5.02	126.02	120.45
2	O	103	GLN	CA-C-N	5.01	131.11	121.54
2	O	103	GLN	C-N-CA	5.01	131.11	121.54
13	M	27	LEU	N-CA-C	5.00	119.45	112.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	A	372	TYR	Sidechain
1	A	61	HIS	Sidechain
2	B	110	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
1	N	61	HIS	Sidechain

5.2 Too-close contacts ⓘ

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	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4025	0	4002	178	0
2	B	1863	0	1867	101	0
2	O	1863	0	1867	109	0
3	C	2124	0	2044	78	0
3	P	2124	0	2044	87	0
4	D	1195	0	1183	58	0
4	Q	1195	0	1183	63	0
5	E	878	0	868	37	0
5	R	878	0	868	34	0
6	F	748	0	728	34	0
6	S	748	0	728	41	0
7	G	672	0	645	55	0
7	T	672	0	645	51	0
8	H	628	0	582	53	0
8	U	628	0	582	57	0
9	I	598	0	612	41	0
9	V	598	0	612	39	0
10	J	441	0	439	20	0
10	W	441	0	439	22	0
11	K	384	0	366	13	0
11	X	384	0	366	15	0
12	L	386	0	388	16	0
12	Y	386	0	388	16	0
13	M	335	0	352	13	0
13	Z	335	0	352	14	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
14	N	1	0	0	0	0
14	O	2	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	6	0	0	1	0
17	N	6	0	0	4	0
18	A	120	0	108	14	0
18	N	120	0	108	13	0
19	F	1	0	0	0	0
19	S	1	0	0	0	0
All	All	28818	0	28368	1178	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 21.

All (1178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:86:MET:O	2:O:89[B]:GLU:HG2	1.20	1.32
2:B:86:MET:O	2:B:89[B]:GLU:HG2	1.32	1.27
2:B:59:GLN:HA	2:B:62:GLU:HB2	1.30	1.07
2:O:59:GLN:HA	2:O:62:GLU:HB2	1.32	1.06
1:A:84:PRO:HG3	1:A:92:MET:HE3	1.40	1.03
1:N:84:PRO:HG3	1:N:92:MET:HE3	1.36	1.03
3:P:12:ASN:H	3:P:12:ASN:HD22	1.02	0.99
2:O:86:MET:O	2:O:89[B]:GLU:CG	2.11	0.98
3:C:12:ASN:HD22	3:C:12:ASN:H	0.99	0.98
1:N:422:ASN:OD1	17:N:521:AZI:N2	1.99	0.95
1:A:506:GLU:HB2	3:C:1:MET:SD	2.11	0.91
1:N:492:LEU:HD23	1:N:495:LEU:HD12	1.53	0.91
3:C:12:ASN:H	3:C:12:ASN:ND2	1.69	0.90
1:A:187:SER:HB2	1:A:277:MET:HE1	1.51	0.90
2:B:86:MET:O	2:B:89[B]:GLU:CG	2.19	0.89
1:N:187:SER:HB2	1:N:277:MET:HE1	1.55	0.89
1:A:347:LEU:HG	1:A:383:MET:HE3	1.56	0.88
3:P:12:ASN:H	3:P:12:ASN:ND2	1.68	0.87
1:N:506:GLU:HB2	3:P:1:MET:SD	2.15	0.85
1:A:69:MET:HE2	1:A:70:VAL:HG23	1.57	0.85
1:N:69:MET:HE2	1:N:70:VAL:HG23	1.59	0.85
3:P:183:GLU:HB3	7:T:42:ARG:HH22	1.41	0.85
1:N:347:LEU:HG	1:N:383:MET:HE3	1.57	0.84
4:D:147:LYS:HE3	4:D:147:LYS:HA	1.59	0.84
3:C:183:GLU:HB3	7:G:42:ARG:HH22	1.41	0.84
8:H:43:MET:HE1	8:U:43:MET:HE1	1.60	0.83
8:H:39:CYS:HG	8:H:53:CYS:HG	0.86	0.82
1:A:492:LEU:HD23	1:A:495:LEU:HD12	1.61	0.82
1:N:347:LEU:HD11	17:N:521:AZI:N1	1.96	0.81
4:Q:147:LYS:HE3	4:Q:147:LYS:HA	1.61	0.80
1:A:218:THR:HG21	7:G:55:ILE:HD12	1.63	0.80
8:U:71:THR:O	8:U:75:ARG:HD3	1.82	0.80
4:Q:40:LEU:HD13	4:Q:59:LEU:HD13	1.63	0.80
4:D:40:LEU:HD13	4:D:59:LEU:HD13	1.64	0.80
3:P:155:ASP:HA	6:S:4:GLY:HA3	1.63	0.79
1:A:282:PHE:HB2	7:T:5:LYS:HB3	1.64	0.79
1:N:92:MET:HE2	1:N:92:MET:HA	1.65	0.79
1:A:380:VAL:HG23	18:A:516:HEA:HBC1	1.65	0.79
7:G:5:LYS:HB3	1:N:282:PHE:HB2	1.65	0.79
6:F:95:GLN:HE21	6:F:96:LEU:HD13	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:57:ARG:HH11	8:U:57:ARG:HB3	1.48	0.78
1:N:218:THR:HG21	7:T:55:ILE:HD12	1.66	0.78
2:O:13:THR:HB	2:O:168:LEU:HD23	1.65	0.78
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.66	0.78
3:C:12:ASN:HD22	3:C:12:ASN:N	1.81	0.77
1:N:127:THR:HB	1:N:129:TYR:CE1	2.19	0.77
6:S:95:GLN:HE21	6:S:96:LEU:HD13	1.48	0.77
1:N:417:MET:HE2	1:N:421:VAL:HG13	1.67	0.77
1:N:92:MET:CE	1:N:167:THR:HG21	2.13	0.77
1:A:92:MET:HA	1:A:92:MET:HE2	1.66	0.76
2:B:59:GLN:H	2:B:62:GLU:HG3	1.50	0.76
9:V:15:ARG:HD2	9:V:18:ARG:HH22	1.50	0.76
8:H:71:THR:O	8:H:75:ARG:HD3	1.84	0.76
1:A:187:SER:CB	1:A:277:MET:HE1	2.15	0.76
3:P:209:ILE:O	3:P:213:THR:HG22	1.86	0.76
3:C:155:ASP:HA	6:F:4:GLY:HA3	1.66	0.76
8:H:57:ARG:HH11	8:H:57:ARG:HB3	1.49	0.76
2:B:152:MET:HB2	2:B:182:THR:HG23	1.68	0.75
9:I:15:ARG:HD2	9:I:18:ARG:HH22	1.51	0.75
8:U:39:CYS:HG	8:U:53:CYS:HG	0.87	0.75
2:O:59:GLN:H	2:O:62:GLU:HG3	1.51	0.75
2:O:152:MET:HB2	2:O:182:THR:HG23	1.68	0.75
1:N:380:VAL:HG23	18:N:516:HEA:HBC1	1.69	0.75
2:B:78:LEU:HB2	2:B:79:PRO:HD3	1.70	0.74
9:V:64:ARG:HH11	9:V:64:ARG:HB3	1.51	0.74
1:N:117:MET:HA	1:N:117:MET:HE2	1.70	0.74
1:N:195:LEU:HD23	1:N:245:ILE:HD13	1.70	0.74
1:A:92:MET:CE	1:A:167:THR:HG21	2.18	0.73
1:N:187:SER:CB	1:N:277:MET:HE1	2.18	0.73
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.70	0.73
5:E:79:LYS:H	5:E:79:LYS:HD3	1.53	0.73
1:N:176:MET:HE3	1:N:181:THR:HG22	1.70	0.73
1:N:172:LYS:NZ	1:N:172:LYS:HB2	2.02	0.73
4:Q:130:PRO:O	4:Q:136:ALA:HB2	1.88	0.73
3:C:209:ILE:O	3:C:213:THR:HG22	1.89	0.73
2:B:193:TYR:HE1	4:D:126:MET:HE1	1.53	0.73
1:N:298:ASP:HB2	1:N:301:THR:HG23	1.70	0.73
7:T:42:ARG:HD2	7:T:74:ARG:NH2	2.04	0.73
8:H:39:CYS:SG	8:H:53:CYS:CB	2.77	0.72
5:E:81:ILE:HG23	9:I:9:MET:HE3	1.69	0.72
6:F:53:THR:HG22	6:F:54:ASN:OD1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:154:GLY:HA2	6:S:6:VAL:HG22	1.70	0.71
7:G:42:ARG:HD2	7:G:74:ARG:NH2	2.05	0.71
6:S:48:LEU:O	6:S:50:PRO:HD3	1.90	0.71
2:O:193:TYR:HE1	4:Q:126:MET:HE1	1.55	0.71
18:A:515:HEA:HBC1	18:A:515:HEA:HMC1	1.72	0.71
3:P:112:LEU:HG	3:P:118:PRO:HB3	1.73	0.71
4:Q:16:TYR:CE1	4:Q:25:PRO:HG3	2.26	0.71
6:S:53:THR:HG22	6:S:54:ASN:OD1	1.90	0.70
8:U:39:CYS:SG	8:U:53:CYS:CB	2.79	0.70
2:B:22:HIS:CE1	9:I:44:LYS:HD3	2.26	0.70
6:F:48:LEU:O	6:F:50:PRO:HD3	1.90	0.70
7:G:9:GLY:HA2	7:G:19:LEU:HD11	1.73	0.70
5:R:79:LYS:HD3	5:R:79:LYS:H	1.55	0.70
7:T:42:ARG:HD2	7:T:74:ARG:HH22	1.57	0.70
1:A:417:MET:HE2	1:A:421:VAL:HG13	1.71	0.70
1:N:132:LEU:HD22	2:O:200:CYS:HA	1.73	0.70
2:B:59:GLN:HA	2:B:62:GLU:CB	2.18	0.70
6:F:16:LEU:O	6:F:20:VAL:HG13	1.93	0.69
3:P:164:PHE:O	3:P:168:THR:HG23	1.92	0.69
1:A:298:ASP:HB2	1:A:301:THR:HG23	1.73	0.69
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.73	0.69
2:B:5:MET:HE3	11:K:43:SER:H	1.58	0.69
2:O:78:LEU:HB2	2:O:79:PRO:HD3	1.74	0.69
1:A:127:THR:HB	1:A:129:TYR:CE1	2.28	0.69
4:D:16:TYR:CE1	4:D:25:PRO:HG3	2.28	0.68
3:P:157:LYS:HE3	3:P:158:HIS:CD2	2.27	0.68
3:C:112:LEU:HG	3:C:118:PRO:HB3	1.74	0.68
6:S:53:THR:HG22	6:S:54:ASN:H	1.59	0.68
10:W:29:ASN:O	10:W:33:ARG:HG3	1.94	0.68
2:B:13:THR:HB	2:B:168:LEU:HD23	1.76	0.68
4:D:130:PRO:O	4:D:136:ALA:HB2	1.94	0.68
7:G:48:ILE:CD1	8:H:80:THR:HG22	2.24	0.68
3:P:183:GLU:HB3	7:T:42:ARG:NH2	2.09	0.68
9:I:64:ARG:HB3	9:I:64:ARG:HH11	1.59	0.67
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.74	0.67
2:B:129:LYS:O	2:B:132:GLU:HG3	1.94	0.67
1:A:172:LYS:HB2	1:A:172:LYS:NZ	2.09	0.67
2:B:188:ARG:HG3	9:I:54:TYR:OH	1.95	0.67
8:U:39:CYS:HG	8:U:53:CYS:CB	2.06	0.67
7:G:42:ARG:HD2	7:G:74:ARG:HH22	1.58	0.67
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:48:ILE:CD1	8:U:80:THR:HG22	2.24	0.67
2:B:189:PRO:O	9:I:63:MET:HE1	1.95	0.66
3:P:154:GLY:C	6:S:6:VAL:HG13	2.20	0.66
6:S:28:GLN:OE1	6:S:96:LEU:HD21	1.95	0.66
9:I:55:ASP:HB3	9:I:58:LYS:HB3	1.77	0.66
3:C:183:GLU:HB3	7:G:42:ARG:NH2	2.09	0.66
2:B:1:MET:SD	2:B:133:LEU:HD11	2.34	0.66
10:J:36:MET:O	10:J:40:LEU:HG	1.95	0.66
2:B:132:GLU:HA	4:D:122:ARG:NH1	2.11	0.66
6:F:53:THR:HG22	6:F:54:ASN:H	1.60	0.66
11:X:24:PHE:O	11:X:28:VAL:HG23	1.96	0.66
7:T:67:HIS:CD2	7:T:78:LEU:HD11	2.31	0.65
1:A:197:LEU:HD12	7:T:4:ALA:HB2	1.76	0.65
10:W:30:ILE:HG13	10:W:31:LEU:N	2.12	0.65
10:W:30:ILE:O	10:W:34:VAL:HG23	1.97	0.65
1:N:452:THR:O	1:N:456:MET:HG3	1.95	0.65
1:A:294:THR:HG21	2:B:171:LYS:HG2	1.77	0.65
6:F:53:THR:HG22	6:F:54:ASN:N	2.12	0.65
10:W:36:MET:O	10:W:40:LEU:HG	1.96	0.65
6:S:16:LEU:O	6:S:20:VAL:HG13	1.96	0.65
11:K:53:TRP:H	11:K:53:TRP:CD1	2.15	0.65
9:V:55:ASP:HB3	9:V:58:LYS:HB3	1.77	0.65
1:N:422:ASN:OD1	17:N:521:AZI:N3	2.29	0.65
1:N:484:THR:HB	13:Z:2:THR:CG2	2.26	0.64
3:C:157:LYS:HE3	3:C:158:HIS:CD2	2.32	0.64
8:H:39:CYS:SG	8:H:53:CYS:HB3	2.37	0.64
10:J:3:ASN:ND2	10:J:5:VAL:HG12	2.12	0.64
9:V:15:ARG:HD2	9:V:18:ARG:NH2	2.13	0.64
3:C:154:GLY:HA2	6:F:6:VAL:HG22	1.80	0.64
4:Q:82:VAL:O	4:Q:86:MET:HG3	1.97	0.64
3:C:164:PHE:O	3:C:168:THR:HG23	1.98	0.64
8:H:39:CYS:HG	8:H:53:CYS:CB	2.10	0.64
11:K:24:PHE:O	11:K:28:VAL:HG23	1.97	0.64
2:O:1:MET:SD	2:O:133:LEU:HD11	2.37	0.64
10:W:3:ASN:ND2	10:W:5:VAL:HG12	2.12	0.64
1:A:98:ASN:HB2	1:A:163:ASN:ND2	2.12	0.64
1:A:176:MET:HE3	1:A:181:THR:HG22	1.80	0.64
4:D:130:PRO:HG2	4:D:131:ILE:HG13	1.79	0.64
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.80	0.64
1:A:132:LEU:HD22	2:B:200:CYS:HA	1.78	0.64
3:C:160:LEU:HD13	3:C:222:GLN:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:188:ARG:HG3	9:V:54:TYR:OH	1.98	0.64
1:A:243:VAL:HB	18:A:516:HEA:HAC	1.79	0.64
2:O:1:MET:SD	2:O:133:LEU:CD1	2.86	0.64
11:X:53:TRP:CD1	11:X:53:TRP:H	2.14	0.64
1:A:379:TYR:CE2	1:A:383:MET:HE2	2.33	0.64
2:O:188:ARG:HH11	2:O:188:ARG:HG2	1.63	0.64
7:T:36:TRP:HA	7:T:39:SER:HB3	1.80	0.64
1:A:484:THR:HB	13:M:2:THR:CG2	2.28	0.63
10:J:30:ILE:O	10:J:34:VAL:HG23	1.98	0.63
7:G:4:ALA:HB2	1:N:197:LEU:HD12	1.80	0.63
1:N:243:VAL:HB	18:N:516:HEA:HAC	1.81	0.63
4:Q:67:SER:OG	4:Q:70:GLU:HG3	1.98	0.63
4:Q:130:PRO:HG2	4:Q:131:ILE:HG13	1.80	0.63
1:A:117:MET:HE2	1:A:117:MET:HA	1.81	0.63
1:A:172:LYS:HB2	1:A:172:LYS:HZ3	1.63	0.63
1:A:506:GLU:CB	3:C:1:MET:SD	2.84	0.63
5:R:81:ILE:HG23	9:V:9:MET:HE3	1.80	0.63
2:O:22:HIS:CE1	9:V:44:LYS:HD3	2.32	0.63
2:O:5:MET:HE3	11:X:43:SER:H	1.64	0.63
2:O:90[A]:ILE:HD12	2:O:90[A]:ILE:H	1.64	0.63
1:N:379:TYR:CE2	1:N:383:MET:HE2	2.34	0.63
3:P:12:ASN:HD22	3:P:12:ASN:N	1.83	0.63
8:U:39:CYS:SG	8:U:53:CYS:HB3	2.39	0.63
1:N:225:GLY:HA3	3:P:112:LEU:CD1	2.29	0.62
2:B:164:ALA:HB2	2:B:171:LYS:HD3	1.80	0.62
9:I:15:ARG:HD2	9:I:18:ARG:NH2	2.14	0.62
8:H:53:CYS:HA	8:U:46:LYS:HZ1	1.65	0.62
9:I:40:ALA:O	9:I:44:LYS:HE2	1.99	0.62
1:N:248:LEU:HD22	1:N:277:MET:HE2	1.81	0.62
4:Q:64:PHE:CE1	5:R:66:ARG:HD2	2.35	0.62
6:S:37:LYS:CD	6:S:37:LYS:H	2.11	0.62
1:N:92:MET:HE2	1:N:167:THR:HG21	1.81	0.62
3:P:104:SER:HB3	3:P:192:VAL:HG11	1.81	0.62
1:A:398:PRO:O	1:A:498:CYS:HB3	1.99	0.62
4:D:23:PRO:O	5:E:66:ARG:HD3	1.98	0.62
1:N:294:THR:HG21	2:O:171:LYS:HG2	1.82	0.62
2:B:13:THR:HG21	2:B:192:TYR:CE2	2.35	0.62
1:A:76:GLY:O	1:A:80:ASN:HB2	2.00	0.62
1:A:488:THR:HG22	1:A:494:TRP:HB2	1.82	0.62
2:B:50:LEU:HD21	5:E:77:PRO:HD2	1.81	0.62
2:B:226:MET:O	2:B:227:LEU:HB2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:SER:HB3	3:C:192:VAL:HG11	1.82	0.61
1:N:74:MET:HE3	1:N:249:PRO:HB2	1.81	0.61
3:P:160:LEU:HD13	3:P:222:GLN:HG2	1.80	0.61
10:J:30:ILE:HG13	10:J:31:LEU:N	2.14	0.61
7:G:6:GLY:HA3	1:N:190:ILE:HG12	1.81	0.61
8:H:75:ARG:HG2	8:H:75:ARG:HH11	1.63	0.61
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.82	0.61
6:S:10:GLU:HG2	6:S:25:ARG:HH22	1.64	0.61
6:S:53:THR:HG22	6:S:54:ASN:N	2.15	0.61
13:M:13:LYS:H	13:M:13:LYS:HD3	1.66	0.61
1:A:225:GLY:HA3	3:C:112:LEU:CD1	2.31	0.61
3:C:148:HIS:O	3:C:152:MET:HG2	2.01	0.61
4:Q:132:GLN:NE2	9:V:42:LYS:HE3	2.15	0.61
7:T:47:PHE:CE2	7:T:81:GLY:HA2	2.36	0.61
9:V:11:GLY:O	9:V:15:ARG:HD3	2.01	0.61
1:A:291:HIS:CE1	17:A:520:AZI:N3	2.68	0.61
1:A:379:TYR:CD2	1:A:383:MET:HE2	2.36	0.61
3:C:154:GLY:C	6:F:6:VAL:HG13	2.25	0.61
2:O:59:GLN:HA	2:O:62:GLU:CB	2.19	0.61
2:O:164:ALA:HB2	2:O:171:LYS:HD3	1.83	0.61
6:F:48:LEU:HB3	6:F:92:VAL:HG21	1.82	0.60
7:G:42:ARG:HD3	7:G:75:VAL:HG11	1.82	0.60
2:B:1:MET:SD	2:B:133:LEU:CD1	2.90	0.60
7:G:67:HIS:CD2	7:G:78:LEU:HD11	2.36	0.60
8:H:53:CYS:HA	8:U:46:LYS:NZ	2.15	0.60
1:N:240:HIS:O	1:N:243:VAL:HG22	2.01	0.60
2:O:226:MET:O	2:O:227:LEU:HB2	2.01	0.60
1:A:452:THR:O	1:A:456:MET:HG3	2.01	0.60
3:P:119:THR:HG21	8:U:82:PRO:O	2.02	0.60
2:B:90[A]:ILE:H	2:B:90[A]:ILE:HD12	1.65	0.60
8:H:51:SER:HB3	8:U:48:GLY:O	2.00	0.60
4:Q:37:GLN:O	4:Q:41:LYS:HG2	2.02	0.60
2:B:87:MET:O	2:B:89[B]:GLU:N	2.32	0.60
4:D:82:VAL:O	4:D:86:MET:HG3	2.01	0.60
6:F:28:GLN:OE1	6:F:96:LEU:HD21	2.01	0.60
7:G:36:TRP:HA	7:G:39:SER:HB3	1.82	0.60
1:N:398:PRO:O	1:N:498:CYS:HB3	2.02	0.60
4:Q:130:PRO:HG2	4:Q:131:ILE:H	1.67	0.60
13:Z:6:ALA:O	13:Z:9:PRO:HD3	2.02	0.60
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.84	0.60
7:G:47:PHE:CE2	7:G:81:GLY:HA2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:GLY:O	1:N:80:ASN:HB2	2.01	0.60
4:Q:66:GLU:O	5:R:66:ARG:NH2	2.35	0.60
1:N:172:LYS:HB2	1:N:172:LYS:HZ3	1.65	0.60
2:B:90[B]:ILE:HD11	2:B:93:PRO:HD3	1.84	0.59
1:N:195:LEU:CD2	1:N:245:ILE:HD13	2.31	0.59
3:P:4:GLN:NE2	3:P:6:HIS:O	2.35	0.59
1:A:240:HIS:O	1:A:243:VAL:HG22	2.03	0.59
4:D:130:PRO:HG2	4:D:131:ILE:H	1.67	0.59
9:I:41:GLU:HA	9:I:41:GLU:OE1	2.02	0.59
2:O:216:LEU:O	2:O:219:PHE:HB3	2.01	0.59
1:A:380:VAL:CG2	18:A:516:HEA:HBC1	2.31	0.59
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.37	0.59
1:N:488:THR:HG22	1:N:494:TRP:HB2	1.83	0.59
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.32	0.59
2:B:1:MET:SD	4:D:123:MET:HE3	2.42	0.59
4:D:132:GLN:NE2	9:I:42:LYS:HE3	2.16	0.59
11:X:26:VAL:O	11:X:30:VAL:HB	2.02	0.59
9:V:41:GLU:HA	9:V:41:GLU:OE1	2.02	0.59
3:C:12:ASN:ND2	3:C:12:ASN:N	2.47	0.59
2:B:216:LEU:O	2:B:219:PHE:HB3	2.01	0.59
1:N:233:HIS:CE1	1:N:292:MET:HE1	2.37	0.59
7:T:9:GLY:HA2	7:T:19:LEU:HD11	1.85	0.59
2:B:68:LEU:HB3	2:B:69:PRO:HD3	1.83	0.59
2:B:193:TYR:CE1	4:D:126:MET:HE1	2.36	0.59
6:F:10:GLU:HG2	6:F:25:ARG:HH22	1.66	0.59
1:N:422:ASN:OD1	17:N:521:AZI:N1	2.36	0.59
7:T:42:ARG:HD3	7:T:75:VAL:HG11	1.84	0.59
1:A:117:MET:CE	12:L:39:ILE:HG23	2.33	0.59
5:R:33:MET:HE2	5:R:67:ILE:HG23	1.83	0.59
6:S:22:LEU:O	6:S:25:ARG:HG2	2.03	0.59
1:A:190:ILE:HG12	7:T:6:GLY:HA3	1.85	0.59
8:H:19:ARG:HG3	8:H:20:PHE:CE2	2.38	0.59
8:U:81:PHE:CE2	8:U:85:ILE:HD11	2.37	0.59
6:F:37:LYS:H	6:F:37:LYS:CD	2.14	0.58
7:G:7:ASP:O	7:G:8:HIS:HB2	2.03	0.58
5:R:95:GLU:HG2	5:R:96:LEU:HD23	1.85	0.58
8:U:39:CYS:O	8:U:43:MET:HG2	2.03	0.58
9:V:42:LYS:HE2	9:V:43:ARG:N	2.18	0.58
10:J:29:ASN:O	10:J:33:ARG:HG3	2.02	0.58
2:O:111:THR:HG21	8:U:66:ILE:HD11	1.83	0.58
3:P:54:MET:HB3	3:P:58:TRP:CZ3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD22	1:A:277:MET:HE2	1.84	0.58
6:F:62:CYS:SG	6:F:84:SER:OG	2.59	0.58
7:G:4:ALA:O	7:G:6:GLY:N	2.36	0.58
6:S:62:CYS:SG	6:S:84:SER:OG	2.62	0.58
7:T:4:ALA:O	7:T:6:GLY:N	2.37	0.58
1:A:117:MET:HE3	12:L:39:ILE:HG23	1.85	0.58
3:P:76:GLN:HA	3:P:79:LEU:HD12	1.85	0.58
8:U:75:ARG:HG2	8:U:75:ARG:HH11	1.68	0.58
2:B:120:SER:OG	2:B:138:VAL:HG21	2.03	0.58
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.58
3:C:67:PHE:HA	10:J:9:GLN:HG2	1.85	0.58
2:O:116:LEU:HD11	2:O:226:MET:HG3	1.84	0.58
5:R:80:GLU:H	5:R:80:GLU:CD	2.11	0.58
3:C:54:MET:HB3	3:C:58:TRP:CZ3	2.38	0.58
4:D:37:GLN:O	4:D:41:LYS:HG2	2.04	0.58
5:R:41:LEU:HD12	5:R:41:LEU:O	2.03	0.58
7:T:42:ARG:NH1	7:T:74:ARG:HH21	2.00	0.58
8:H:46:LYS:NZ	8:U:53:CYS:HA	2.19	0.58
12:L:25:MET:HE3	12:L:29:PHE:HE2	1.67	0.58
1:N:417:MET:HE2	1:N:421:VAL:CG1	2.33	0.58
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.86	0.58
1:N:144:ASP:OD1	1:N:213:ARG:HD3	2.03	0.58
2:B:87:MET:C	2:B:89[B]:GLU:H	2.12	0.57
7:G:42:ARG:NH1	7:G:74:ARG:HH21	2.02	0.57
9:I:11:GLY:O	9:I:15:ARG:HD3	2.03	0.57
1:A:484:THR:HB	13:M:2:THR:HG23	1.86	0.57
2:B:141:ARG:HD2	2:B:212:GLU:OE1	2.04	0.57
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.20	0.57
3:P:154:GLY:HA2	6:S:6:VAL:CG2	2.34	0.57
8:U:57:ARG:HB3	8:U:57:ARG:NH1	2.18	0.57
1:N:450:TRP:HE3	1:N:453:ILE:HD12	1.69	0.57
3:C:101:PHE:CE2	3:C:259:TRP:HZ3	2.23	0.57
8:H:43:MET:HE1	8:U:43:MET:CE	2.34	0.57
8:U:38:ARG:HG2	8:U:85:ILE:HA	1.87	0.57
2:O:120:SER:OG	2:O:138:VAL:HG21	2.04	0.57
8:U:19:ARG:HG3	8:U:20:PHE:CE2	2.40	0.57
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.87	0.57
4:D:33:LEU:HD22	4:D:37:GLN:HB3	1.86	0.57
13:Z:13:LYS:H	13:Z:13:LYS:HD3	1.70	0.57
2:B:188:ARG:HG2	2:B:188:ARG:HH11	1.69	0.57
9:I:27:VAL:HG12	9:I:31:PHE:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:THR:HB	13:Z:2:THR:HG23	1.86	0.57
2:O:141:ARG:HD2	2:O:212:GLU:OE1	2.05	0.57
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.87	0.57
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.40	0.57
8:U:36:PHE:HB2	8:U:56:TYR:CB	2.35	0.57
1:A:62:ALA:HB2	18:A:515:HEA:HBD1	1.86	0.56
3:C:76:GLN:HA	3:C:79:LEU:HD12	1.86	0.56
9:V:26:MET:HE3	9:V:26:MET:HA	1.87	0.56
4:D:24:LEU:HB3	5:E:30:ARG:HG2	1.86	0.56
2:O:189:PRO:O	9:V:63:MET:HE1	2.04	0.56
6:S:37:LYS:H	6:S:37:LYS:HD3	1.70	0.56
4:D:66:GLU:O	5:E:66:ARG:NH2	2.37	0.56
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.39	0.56
5:E:33:MET:HE2	5:E:67:ILE:HG23	1.86	0.56
7:G:44:ARG:HD2	7:G:74:ARG:O	2.04	0.56
9:I:42:LYS:HE2	9:I:43:ARG:N	2.21	0.56
1:N:379:TYR:CD2	1:N:383:MET:HE2	2.40	0.56
4:D:67:SER:OG	4:D:70:GLU:HG3	2.05	0.56
5:E:53:ARG:HG2	5:E:96:LEU:HD11	1.88	0.56
10:J:2:GLU:CG	10:J:3:ASN:H	2.17	0.56
2:O:13:THR:HG21	2:O:192:TYR:CE2	2.41	0.56
8:H:17:ASP:OD1	8:H:19:ARG:HG2	2.05	0.56
3:P:195:SER:O	3:P:199:VAL:HG13	2.04	0.56
5:R:53:ARG:NH1	5:R:92:THR:HG23	2.21	0.56
9:V:27:VAL:HG12	9:V:31:PHE:HE2	1.70	0.56
3:C:137:LEU:HD22	3:C:173:PHE:CE2	2.41	0.56
8:H:36:PHE:HB2	8:H:56:TYR:CB	2.35	0.56
3:P:101:PHE:CE2	3:P:259:TRP:HZ3	2.23	0.56
3:P:148:HIS:HB2	3:P:235:PHE:HE2	1.70	0.56
10:J:3:ASN:C	10:J:3:ASN:HD22	2.13	0.56
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.88	0.56
3:P:148:HIS:O	3:P:152:MET:HG2	2.05	0.56
1:A:233:HIS:CE1	1:A:292:MET:HE1	2.41	0.56
3:C:148:HIS:HB2	3:C:235:PHE:HE2	1.69	0.56
2:O:129:LYS:O	2:O:132:GLU:HG3	2.06	0.56
6:S:48:LEU:HB3	6:S:92:VAL:HG21	1.86	0.56
7:T:56:ARG:HH11	7:T:56:ARG:HG2	1.71	0.56
7:G:23:LEU:O	7:G:26:PRO:HD2	2.05	0.56
8:H:46:LYS:HZ2	8:U:53:CYS:HA	1.71	0.56
8:H:57:ARG:HB3	8:H:57:ARG:NH1	2.18	0.56
2:O:90[B]:ILE:HD11	2:O:93:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:7:ASP:O	7:T:8:HIS:HB2	2.05	0.56
1:A:12:HIS:HD2	1:A:80:ASN:O	1.88	0.56
8:H:48:GLY:O	8:U:51:SER:HB3	2.05	0.56
3:C:190:ASP:HB3	7:G:53:LEU:HD22	1.87	0.55
8:U:18:SER:O	8:U:21:PRO:HD3	2.06	0.55
10:W:2:GLU:CG	10:W:3:ASN:H	2.19	0.55
6:F:22:LEU:O	6:F:25:ARG:HG2	2.06	0.55
1:N:127:THR:HB	1:N:129:TYR:CD1	2.40	0.55
1:A:450:TRP:HE3	1:A:453:ILE:HD12	1.71	0.55
1:N:380:VAL:CG2	18:N:516:HEA:HBC1	2.35	0.55
12:Y:25:MET:HE3	12:Y:29:PHE:HE2	1.70	0.55
1:A:92:MET:HE2	1:A:167:THR:HG21	1.89	0.55
3:P:137:LEU:HD22	3:P:173:PHE:CE2	2.42	0.55
4:Q:137:LYS:O	4:Q:145:TRP:HE3	1.89	0.55
9:V:40:ALA:O	9:V:44:LYS:HE2	2.07	0.55
1:N:513:LEU:HD22	6:S:35:ALA:HB3	1.87	0.55
1:A:513:LEU:HD22	6:F:35:ALA:HB3	1.88	0.55
3:C:4:GLN:NE2	3:C:6:HIS:O	2.40	0.55
8:H:65:PRO:HG2	8:H:68:TRP:CD1	2.42	0.55
2:O:87:MET:O	2:O:89[B]:GLU:N	2.38	0.55
6:S:95:GLN:HB2	6:S:96:LEU:HD12	1.89	0.55
1:A:197:LEU:HD12	7:T:4:ALA:CB	2.36	0.55
3:C:222:GLN:HE21	3:C:222:GLN:HA	1.72	0.55
4:D:40:LEU:CD1	4:D:59:LEU:HD13	2.35	0.55
1:A:257:ILE:HD11	1:A:392:GLY:HA2	1.88	0.55
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.89	0.55
2:O:184:LEU:HD11	2:O:211:LEU:HD21	1.88	0.55
1:A:417:MET:HE2	1:A:421:VAL:CG1	2.38	0.54
7:G:48:ILE:HD11	8:H:80:THR:HA	1.89	0.54
1:N:7:LEU:C	1:N:8:PHE:HD1	2.15	0.54
1:N:98:ASN:HB2	1:N:163:ASN:ND2	2.22	0.54
5:E:78:HIS:CE1	9:I:12:LEU:HD22	2.42	0.54
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.88	0.54
1:A:74:MET:HE3	1:A:249:PRO:HB2	1.89	0.54
1:A:189:MET:SD	7:T:7:ASP:HB2	2.46	0.54
2:O:76:ILE:O	2:O:79:PRO:HD2	2.07	0.54
2:O:3:TYR:CD1	2:O:3:TYR:N	2.76	0.54
2:O:161:HIS:HB2	2:O:174:ALA:HB3	1.89	0.54
2:B:111:THR:HG21	8:H:66:ILE:HD11	1.88	0.54
5:E:95:GLU:HG2	5:E:96:LEU:HD23	1.88	0.54
11:K:26:VAL:O	11:K:30:VAL:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:257:ILE:HD11	1:N:392:GLY:HA2	1.89	0.54
1:A:225:GLY:HA3	3:C:112:LEU:HD11	1.90	0.54
2:O:136:LEU:HB3	2:O:193:TYR:CD2	2.42	0.54
2:O:193:TYR:CE1	4:Q:126:MET:HE1	2.40	0.54
4:Q:23:PRO:O	5:R:66:ARG:HD3	2.08	0.54
4:D:64:PHE:CE1	5:E:66:ARG:HD2	2.42	0.54
1:N:506:GLU:CB	3:P:1:MET:SD	2.91	0.54
1:A:7:LEU:C	1:A:8:PHE:HD1	2.15	0.54
3:C:224:LYS:NZ	3:C:224:LYS:HB3	2.23	0.54
1:N:299:VAL:HA	1:N:302:ARG:NH1	2.23	0.54
1:N:367:LEU:O	1:N:370:THR:HG23	2.08	0.54
1:A:299:VAL:HA	1:A:302:ARG:NH1	2.23	0.53
2:O:189:PRO:HG2	9:V:63:MET:HE1	1.90	0.53
1:N:151:HIS:O	1:N:155:VAL:HG23	2.08	0.53
4:D:48:TRP:HA	4:D:51:LEU:HD12	1.91	0.53
2:O:87:MET:C	2:O:89[B]:GLU:H	2.15	0.53
10:W:3:ASN:C	10:W:3:ASN:HD22	2.16	0.53
1:A:367:LEU:O	1:A:370:THR:HG23	2.08	0.53
2:B:3:TYR:N	2:B:3:TYR:CD1	2.77	0.53
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	1.89	0.53
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.38	0.53
6:F:95:GLN:HB2	6:F:96:LEU:HD12	1.91	0.53
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.91	0.53
1:A:510:TYR:HB2	6:F:56:ARG:NH1	2.24	0.53
2:O:41:ILE:O	2:O:45:MET:HG2	2.08	0.53
3:P:224:LYS:NZ	3:P:224:LYS:HB3	2.24	0.53
7:T:44:ARG:HD2	7:T:74:ARG:O	2.08	0.53
11:X:53:TRP:O	11:X:54:ARG:HB3	2.08	0.53
1:N:92:MET:HE1	1:N:167:THR:HG21	1.87	0.53
1:N:478:SER:HA	13:Z:8:THR:O	2.08	0.53
5:R:53:ARG:HG2	5:R:96:LEU:HD11	1.90	0.53
5:E:80:GLU:CD	5:E:80:GLU:H	2.15	0.53
7:G:7:ASP:HB2	1:N:189:MET:SD	2.49	0.53
12:L:22:LEU:O	12:L:26:THR:HB	2.09	0.53
7:T:48:ILE:HD12	7:T:48:ILE:C	2.34	0.53
6:F:48:LEU:HD23	6:F:90:LYS:HB3	1.90	0.53
1:N:75:ILE:O	1:N:79:GLY:HA3	2.09	0.53
1:N:128:VAL:HG22	1:N:128:VAL:O	2.09	0.53
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.09	0.53
2:B:185:MET:SD	2:B:185:MET:C	2.92	0.52
1:N:225:GLY:HA3	3:P:112:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:65:PRO:HG2	8:U:68:TRP:CD1	2.44	0.52
8:U:65:PRO:HG2	8:U:68:TRP:CG	2.44	0.52
4:D:83:GLY:HA3	11:K:18:LEU:HA	1.92	0.52
5:E:41:LEU:O	5:E:41:LEU:HD12	2.08	0.52
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.45	0.52
1:N:225:GLY:HA3	3:P:112:LEU:HD13	1.91	0.52
6:S:82:CYS:N	6:S:86:GLY:O	2.42	0.52
2:B:189:PRO:HG2	9:I:63:MET:HE1	1.91	0.52
4:Q:24:LEU:HB3	5:R:30:ARG:HG2	1.92	0.52
4:Q:107:ILE:HB	4:Q:108:PRO:HD2	1.91	0.52
4:D:129:ALA:HB3	4:D:134:PHE:H	1.73	0.52
8:H:43:MET:CE	8:U:43:MET:HE1	2.34	0.52
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.44	0.52
1:A:407:ASP:O	1:A:411:LYS:HG3	2.09	0.52
1:A:450:TRP:CE3	1:A:453:ILE:HD12	2.44	0.52
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.91	0.52
9:V:29:LEU:O	9:V:33:THR:HG23	2.10	0.52
3:C:119:THR:HG21	8:H:82:PRO:O	2.10	0.52
6:F:82:CYS:N	6:F:86:GLY:O	2.43	0.52
8:H:38:ARG:HG2	8:H:85:ILE:HA	1.90	0.52
9:I:39:VAL:O	9:I:42:LYS:HE2	2.09	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.10	0.52
4:Q:138:TRP:CD1	4:Q:140:TYR:CD1	2.98	0.52
1:A:386:VAL:HG11	18:A:515:HEA:H261	1.92	0.52
4:D:68:PHE:HA	4:D:71:MET:HG2	1.92	0.52
4:D:137:LYS:O	4:D:145:TRP:HE3	1.91	0.52
5:E:53:ARG:NH1	5:E:92:THR:HG23	2.24	0.52
8:U:36:PHE:HB2	8:U:56:TYR:HB2	1.91	0.52
10:W:11:LEU:C	10:W:11:LEU:HD23	2.35	0.52
1:A:82:LEU:O	1:A:86:MET:HG3	2.10	0.52
1:N:266:GLU:HB2	1:N:267:PRO:HD2	1.92	0.52
2:B:16:ILE:HD12	2:B:17:MET:N	2.25	0.51
2:B:152:MET:HB2	2:B:182:THR:CG2	2.39	0.51
1:N:450:TRP:CE3	1:N:453:ILE:HD12	2.44	0.51
1:A:483:LEU:HB2	13:M:2:THR:OG1	2.10	0.51
1:N:416:ILE:HG22	1:N:464:ALA:HB2	1.92	0.51
2:O:136:LEU:HB3	2:O:193:TYR:HD2	1.75	0.51
4:Q:129:ALA:HB3	4:Q:134:PHE:H	1.74	0.51
7:G:36:TRP:CD1	7:G:36:TRP:C	2.87	0.51
6:S:48:LEU:HD23	6:S:90:LYS:HB3	1.92	0.51
1:A:51:ASP:HB2	2:B:202:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LEU:HD22	6:F:35:ALA:CB	2.40	0.51
7:G:48:ILE:HG13	7:G:50:TYR:CD2	2.45	0.51
4:D:107:ILE:HB	4:D:108:PRO:HD2	1.91	0.51
8:H:57:ARG:O	8:H:61:LYS:HB2	2.11	0.51
11:X:31:TYR:CD2	11:X:35:GLN:HB2	2.46	0.51
2:B:116:LEU:HD11	2:B:226:MET:HG3	1.92	0.51
2:B:184:LEU:HD11	2:B:211:LEU:HD21	1.92	0.51
1:N:380:VAL:HG21	18:N:516:HEA:C2C	2.41	0.51
1:N:403:TYR:CE1	12:Y:7:PRO:HB3	2.46	0.51
4:Q:110:THR:HG22	4:Q:115:TRP:CE2	2.46	0.51
10:W:30:ILE:HG13	10:W:31:LEU:H	1.75	0.51
12:Y:22:LEU:O	12:Y:26:THR:HB	2.10	0.51
2:O:144:LEU:HD22	2:O:150:ILE:HD13	1.93	0.51
3:P:12:ASN:ND2	3:P:12:ASN:N	2.45	0.51
4:Q:118:LYS:HA	11:X:51:LYS:O	2.11	0.51
7:T:48:ILE:HD12	7:T:49:PRO:N	2.25	0.51
8:U:38:ARG:HG2	8:U:85:ILE:HG23	1.92	0.51
9:V:39:VAL:O	9:V:42:LYS:HE2	2.11	0.51
2:B:146:MET:SD	2:B:189:PRO:HB3	2.51	0.51
13:M:6:ALA:O	13:M:9:PRO:HD3	2.11	0.51
3:P:222:GLN:HE21	3:P:222:GLN:HA	1.76	0.51
7:T:23:LEU:O	7:T:26:PRO:HD2	2.10	0.51
2:B:94:SER:OG	2:B:148:MET:HE3	2.10	0.51
2:B:189:PRO:HG2	9:I:63:MET:CE	2.41	0.51
4:Q:128:VAL:O	4:Q:134:PHE:HB3	2.10	0.51
10:W:14:GLU:O	10:W:23:LYS:HE3	2.11	0.51
12:Y:5:GLU:O	12:Y:9:LYS:HD2	2.11	0.51
4:D:127:LYS:O	4:D:130:PRO:HD3	2.11	0.51
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.93	0.50
8:H:65:PRO:HG2	8:H:68:TRP:CG	2.46	0.50
2:O:104:TRP:CD1	2:O:104:TRP:N	2.79	0.50
5:R:6:GLU:HB2	5:R:10:GLU:HB2	1.93	0.50
2:B:99:THR:C	2:B:100:MET:HG2	2.36	0.50
4:D:40:LEU:HD22	4:D:59:LEU:HD13	1.93	0.50
7:G:4:ALA:CB	1:N:197:LEU:HD12	2.41	0.50
13:Z:30:ALA:O	13:Z:34:LEU:HD12	2.10	0.50
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
3:C:133:ASN:HD21	3:C:176:LEU:HB3	1.76	0.50
2:O:189:PRO:HG2	9:V:63:MET:CE	2.42	0.50
3:P:154:GLY:HA2	6:S:6:VAL:HG13	1.94	0.50
8:U:57:ARG:O	8:U:61:LYS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:GLU:HB2	5:E:10:GLU:HB2	1.93	0.50
1:N:51:ASP:HB2	2:O:202:SER:O	2.10	0.50
3:P:133:ASN:HD21	3:P:176:LEU:HB3	1.77	0.50
7:T:36:TRP:CD1	7:T:36:TRP:C	2.89	0.50
1:A:92:MET:HA	1:A:92:MET:CE	2.39	0.50
12:L:22:LEU:HD11	13:M:18:GLY:HA2	1.92	0.50
12:Y:41:ARG:HG3	13:Z:40:TYR:CE2	2.45	0.50
2:O:48:THR:HB	9:V:16:ARG:CZ	2.42	0.50
2:O:160:LEU:HD21	2:O:175:ILE:HG23	1.94	0.50
1:A:8:PHE:CE2	3:C:15:PRO:HB3	2.46	0.50
1:A:92:MET:HE1	1:A:167:THR:HG21	1.91	0.50
1:N:377:PHE:CD2	18:N:516:HEA:HAD1	2.47	0.50
1:N:302:ARG:O	1:N:306:THR:HG23	2.10	0.50
1:A:95:PRO:HB2	3:C:11:VAL:HG13	1.93	0.50
1:N:456:MET:SD	11:X:40:TRP:HH2	2.35	0.50
1:N:510:TYR:HB2	6:S:56:ARG:NH1	2.27	0.50
2:O:1:MET:SD	4:Q:123:MET:HE3	2.52	0.50
1:A:456:MET:SD	11:K:40:TRP:HH2	2.35	0.49
5:E:81:ILE:CG2	9:I:9:MET:HE3	2.41	0.49
9:I:26:MET:HE3	9:I:26:MET:HA	1.94	0.49
1:N:23:GLY:HA3	1:N:73:ILE:HG13	1.94	0.49
2:O:13:THR:HG22	2:O:13:THR:O	2.12	0.49
1:A:378:HIS:CD2	1:A:425:PHE:CZ	3.00	0.49
3:C:38:ASN:C	3:C:38:ASN:HD22	2.20	0.49
3:C:151:LEU:HD21	3:C:232:HIS:CG	2.47	0.49
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.49
8:H:60:TYR:CD1	8:H:60:TYR:C	2.89	0.49
1:N:12:HIS:HD2	1:N:80:ASN:O	1.94	0.49
1:N:340:TRP:HH2	1:N:417:MET:HG2	1.77	0.49
3:P:67:PHE:O	6:S:14:THR:HG21	2.12	0.49
6:S:18:ARG:HG3	6:S:21:MET:HE2	1.94	0.49
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.27	0.49
13:Z:35:TYR:HD2	13:Z:36:HIS:CE1	2.30	0.49
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.93	0.49
1:A:481:GLU:HB2	13:M:4:LYS:HD2	1.95	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.12	0.49
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.48	0.49
5:E:53:ARG:O	5:E:56:ARG:HB3	2.13	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD12	1.94	0.49
8:U:51:SER:O	8:U:52:VAL:HG13	2.12	0.49
2:B:63:THR:O	2:B:66:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90[B]:ILE:HD11	2:B:93:PRO:CD	2.43	0.49
4:D:16:TYR:HE1	4:D:25:PRO:HG3	1.75	0.49
1:N:60:ALA:O	1:N:64:VAL:HG23	2.13	0.49
5:R:78:HIS:CE1	9:V:12:LEU:HD22	2.48	0.49
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.48	0.49
8:H:36:PHE:HB2	8:H:56:TYR:HB2	1.94	0.49
2:O:90[B]:ILE:HG23	2:O:91[B]:ASN:H	1.78	0.49
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.95	0.49
7:T:48:ILE:HG13	7:T:50:TYR:CD2	2.48	0.49
11:K:53:TRP:O	11:K:54:ARG:HB3	2.12	0.49
2:O:134:ARG:HD2	4:Q:110:THR:OG1	2.12	0.49
4:D:66:GLU:HA	4:D:70:GLU:OE1	2.12	0.49
9:I:60:PHE:CE1	9:I:69:PHE:CE2	3.01	0.49
3:P:38:ASN:C	3:P:38:ASN:HD22	2.21	0.49
1:A:302:ARG:O	1:A:306:THR:HG23	2.13	0.49
2:B:89[B]:GLU:HB2	2:B:91[B]:ASN:ND2	2.28	0.49
3:C:36:HIS:C	3:C:38:ASN:H	2.21	0.49
3:C:50:ASN:HD22	3:C:54:MET:HE2	1.78	0.49
7:G:48:ILE:C	7:G:48:ILE:HD12	2.38	0.49
10:J:16:ASN:OD1	10:J:18:LEU:HB2	2.13	0.49
10:J:11:LEU:HD23	10:J:11:LEU:C	2.38	0.48
1:N:402:GLY:HA3	1:N:499:PRO:HD3	1.95	0.48
4:Q:114:GLU:O	4:Q:118:LYS:HG2	2.13	0.48
2:B:13:THR:O	2:B:13:THR:HG22	2.13	0.48
8:H:39:CYS:O	8:H:43:MET:HG2	2.12	0.48
4:Q:83:GLY:HA3	11:X:18:LEU:HA	1.95	0.48
7:T:48:ILE:HD11	8:U:80:THR:HA	1.94	0.48
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.95	0.48
2:O:152:MET:HB2	2:O:182:THR:CG2	2.40	0.48
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.13	0.48
7:T:42:ARG:HH11	7:T:74:ARG:NH2	2.12	0.48
1:A:127:THR:HB	1:A:129:TYR:CD1	2.49	0.48
1:A:175:ALA:HB1	1:A:513:LEU:HD13	1.95	0.48
1:A:266:GLU:HB2	1:A:267:PRO:HD2	1.95	0.48
4:D:40:LEU:HD13	4:D:59:LEU:CD1	2.40	0.48
6:F:49:VAL:HG21	6:F:74:LEU:HD12	1.96	0.48
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.48
3:P:102:TYR:O	3:P:106:LEU:HB2	2.13	0.48
3:P:157:LYS:HE3	3:P:158:HIS:NE2	2.28	0.48
1:A:225:GLY:HA3	3:C:112:LEU:HD13	1.94	0.48
2:B:134:ARG:HD2	4:D:110:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:GLU:HB3	3:C:129:VAL:H	1.50	0.48
12:L:41:ARG:HG3	13:M:40:TYR:CE2	2.49	0.48
1:N:230:LEU:HB2	3:P:103:HIS:CD2	2.48	0.48
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.95	0.48
1:A:34:SER:HB3	1:A:61:HIS:CD2	2.48	0.48
1:N:172:LYS:HB2	1:N:172:LYS:HZ2	1.79	0.48
1:N:443:TYR:CD2	1:N:447:TYR:HB2	2.48	0.48
2:O:50:LEU:HB2	9:V:13:LEU:HD13	1.95	0.48
4:Q:113:GLU:O	4:Q:116:VAL:HG22	2.14	0.48
7:T:56:ARG:HG2	7:T:56:ARG:NH1	2.29	0.48
11:X:22:ALA:O	11:X:26:VAL:HG12	2.14	0.48
1:A:12:HIS:CD2	1:A:80:ASN:O	2.66	0.48
1:A:144:ASP:OD1	1:A:213:ARG:HD3	2.14	0.48
3:C:101:PHE:CE2	3:C:259:TRP:CZ3	3.01	0.48
10:J:30:ILE:HG13	10:J:31:LEU:H	1.77	0.48
1:N:117:MET:HE3	12:Y:39:ILE:HG23	1.95	0.48
1:N:230:LEU:HD13	3:P:103:HIS:CG	2.49	0.48
2:O:94:SER:OG	2:O:148:MET:HE3	2.14	0.48
4:Q:40:LEU:CD1	4:Q:59:LEU:HD13	2.38	0.48
6:F:37:LYS:H	6:F:37:LYS:HD3	1.77	0.48
9:I:61:GLU:OE1	9:I:64:ARG:NH1	2.47	0.48
10:W:8:LYS:HZ1	10:W:12:PHE:HE2	1.62	0.48
1:A:40:GLU:HG2	1:A:54:TYR:CD1	2.49	0.48
2:B:212:GLU:OE1	9:I:70:GLN:HG2	2.13	0.48
8:H:49:ASP:HB2	8:U:49:ASP:HB2	1.96	0.48
8:H:75:ARG:HG2	8:H:75:ARG:NH1	2.27	0.48
1:N:92:MET:HA	1:N:92:MET:CE	2.40	0.48
1:N:513:LEU:HD22	6:S:35:ALA:CB	2.44	0.48
1:A:44:PRO:HG3	4:D:111:PHE:CE2	2.49	0.48
2:B:14:SER:HB2	2:B:15:PRO:HD2	1.95	0.48
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.48	0.48
2:O:89[B]:GLU:HB2	2:O:91[B]:ASN:ND2	2.28	0.48
5:R:81:ILE:O	5:R:85:VAL:HG23	2.14	0.48
7:T:42:ARG:HH11	7:T:75:VAL:HG11	1.79	0.48
3:C:22:LEU:HD12	3:C:22:LEU:HA	1.73	0.47
8:H:53:CYS:CA	8:U:46:LYS:NZ	2.76	0.47
9:I:29:LEU:O	9:I:33:THR:HG23	2.14	0.47
1:N:403:TYR:CZ	12:Y:7:PRO:HB3	2.49	0.47
3:P:16:TRP:HE3	3:P:16:TRP:HA	1.79	0.47
1:A:403:TYR:CE1	12:L:7:PRO:HB3	2.48	0.47
1:N:404:THR:O	1:N:480:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:THR:O	2:O:66:THR:HG22	2.14	0.47
7:G:47:PHE:CZ	7:G:81:GLY:HA2	2.49	0.47
8:H:19:ARG:C	8:H:21:PRO:HD3	2.40	0.47
9:I:21:ILE:HD12	9:I:21:ILE:HA	1.77	0.47
1:N:38:ARG:HG3	1:N:458:SER:HB3	1.97	0.47
1:N:175:ALA:HB1	1:N:513:LEU:HD13	1.97	0.47
1:N:380:VAL:HG21	18:N:516:HEA:C3C	2.44	0.47
6:S:8:THR:OG1	6:S:11:GLU:HG2	2.14	0.47
1:A:443:TYR:CD2	1:A:447:TYR:HB2	2.50	0.47
1:N:83:VAL:HG21	1:N:188:VAL:HG11	1.95	0.47
1:N:248:LEU:O	1:N:251:PHE:HB2	2.13	0.47
1:N:481:GLU:HB2	13:Z:4:LYS:HD2	1.96	0.47
8:U:17:ASP:OD1	8:U:19:ARG:HG2	2.14	0.47
1:A:197:LEU:CD1	7:T:4:ALA:HB2	2.43	0.47
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.49	0.47
5:E:78:HIS:ND1	9:I:12:LEU:HD22	2.29	0.47
7:G:56:ARG:HG2	7:G:56:ARG:HH11	1.79	0.47
1:N:40:GLU:HG2	1:N:54:TYR:CD1	2.50	0.47
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.50	0.47
3:P:101:PHE:CE2	3:P:259:TRP:CZ3	3.02	0.47
3:P:123:PRO:HB2	3:P:261:SER:HB3	1.96	0.47
4:Q:16:TYR:HE1	4:Q:25:PRO:HG3	1.75	0.47
4:Q:112:GLU:O	4:Q:116:VAL:HG13	2.14	0.47
7:T:42:ARG:NH1	7:T:75:VAL:HG11	2.29	0.47
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.49	0.47
12:Y:25:MET:HE2	12:Y:25:MET:HB3	1.77	0.47
1:A:299:VAL:HG13	1:A:300:ASP:N	2.29	0.47
7:G:5:LYS:HE3	7:G:23:LEU:HD13	1.97	0.47
7:G:48:ILE:HD12	7:G:49:PRO:N	2.30	0.47
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.50	0.47
2:B:89[A]:GLU:HG2	2:B:90[A]:ILE:N	2.30	0.47
8:H:19:ARG:HG3	8:H:20:PHE:CD2	2.50	0.47
8:H:36:PHE:HB2	8:H:56:TYR:HB3	1.97	0.47
1:N:283:LEU:HD13	1:N:311:ILE:HG13	1.96	0.47
2:O:89[A]:GLU:HG2	2:O:90[A]:ILE:N	2.30	0.47
2:O:146:MET:SD	2:O:189:PRO:HB3	2.55	0.47
2:O:185:MET:SD	2:O:185:MET:C	2.98	0.47
2:O:212:GLU:OE1	9:V:70:GLN:HG2	2.14	0.47
3:P:75:VAL:O	3:P:79:LEU:HD12	2.14	0.47
5:R:104:LEU:HD23	5:R:104:LEU:HA	1.77	0.47
7:T:42:ARG:HD3	7:T:75:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:439:ARG:HD3	2:O:199:ILE:HB	1.95	0.47
9:V:21:ILE:HD12	9:V:21:ILE:HA	1.82	0.47
1:A:248:LEU:O	1:A:251:PHE:HB2	2.15	0.46
1:A:400:PHE:O	12:L:10:ASN:ND2	2.47	0.46
2:B:104:TRP:CD1	2:B:104:TRP:N	2.81	0.46
4:D:70:GLU:HA	5:E:109:VAL:CG1	2.45	0.46
7:G:42:ARG:HH11	7:G:74:ARG:NH2	2.13	0.46
13:M:35:TYR:HD2	13:M:36:HIS:CE1	2.34	0.46
6:F:8:THR:OG1	6:F:11:GLU:HG2	2.15	0.46
7:G:42:ARG:HD3	7:G:75:VAL:CG1	2.45	0.46
1:N:438:ARG:NH2	18:N:515:HEA:O2D	2.48	0.46
3:P:125:ASN:HB3	3:P:128:GLU:OE1	2.15	0.46
8:U:75:ARG:HG2	8:U:75:ARG:NH1	2.31	0.46
4:D:108:PRO:HG2	4:D:111:PHE:CE2	2.50	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
1:A:283:LEU:HD13	1:A:311:ILE:HG13	1.97	0.46
3:C:154:GLY:HA2	6:F:6:VAL:CG2	2.45	0.46
3:C:173:PHE:CD1	3:C:173:PHE:C	2.93	0.46
3:P:132:LEU:HD13	3:P:176:LEU:HD11	1.96	0.46
1:A:243:VAL:HB	18:A:516:HEA:CAC	2.45	0.46
8:H:51:SER:O	8:H:52:VAL:HG13	2.16	0.46
2:O:14:SER:HB2	2:O:15:PRO:HD2	1.97	0.46
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.50	0.46
4:Q:132:GLN:HE22	9:V:43:ARG:HB2	1.81	0.46
9:V:61:GLU:OE1	9:V:64:ARG:NH1	2.49	0.46
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.46
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.97	0.46
1:N:84:PRO:CG	1:N:92:MET:HE3	2.27	0.46
8:U:19:ARG:HG3	8:U:20:PHE:CD2	2.50	0.46
1:A:151:HIS:O	1:A:155:VAL:HG23	2.16	0.46
3:C:123:PRO:HB2	3:C:261:SER:HB3	1.97	0.46
1:N:8:PHE:CE2	3:P:15:PRO:HB3	2.51	0.46
3:P:129:VAL:HG13	3:P:176:LEU:HD22	1.98	0.46
8:U:19:ARG:C	8:U:21:PRO:HD3	2.41	0.46
2:B:90[B]:ILE:HG23	2:B:91[B]:ASN:H	1.81	0.46
3:C:154:GLY:HA2	6:F:6:VAL:HG13	1.97	0.46
3:P:50:ASN:HD22	3:P:54:MET:HE2	1.80	0.46
3:P:116:TRP:HA	3:P:117:PRO:C	2.41	0.46
3:C:137:LEU:HD22	3:C:173:PHE:CD2	2.51	0.46
4:D:138:TRP:CD1	4:D:140:TYR:CD1	3.04	0.46
5:E:21:LYS:O	5:E:57:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:48:ILE:HD12	8:H:80:THR:HG22	1.96	0.46
11:K:31:TYR:CD2	11:K:35:GLN:HB2	2.50	0.46
1:N:29:VAL:HG13	12:Y:36:PRO:HG3	1.97	0.46
1:N:68:PHE:HE2	1:N:112:LEU:HD22	1.81	0.46
12:Y:39:ILE:O	12:Y:42:HIS:HB3	2.16	0.46
1:A:439:ARG:HD3	2:B:199:ILE:HB	1.98	0.46
1:N:260:TYR:CD1	1:N:487:LEU:HD12	2.51	0.46
3:P:40:MET:O	3:P:44:MET:HG2	2.15	0.46
5:R:53:ARG:O	5:R:56:ARG:HB3	2.16	0.46
7:T:5:LYS:HE3	7:T:23:LEU:HD13	1.98	0.46
1:A:189:MET:SD	7:T:7:ASP:CB	3.04	0.45
1:A:285:PHE:CE2	7:T:4:ALA:HB3	2.52	0.45
1:A:344:PHE:CD1	1:A:344:PHE:C	2.94	0.45
3:C:125:ASN:HB3	3:C:128:GLU:OE1	2.15	0.45
2:O:90[B]:ILE:HD11	2:O:93:PRO:CD	2.45	0.45
6:S:86:GLY:O	6:S:87:THR:O	2.34	0.45
12:Y:14:SER:HB3	12:Y:20:ARG:HH12	1.81	0.45
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.52	0.45
1:A:98:ASN:HB2	1:A:163:ASN:HD21	1.80	0.45
1:A:421:VAL:HG23	1:A:422:ASN:N	2.30	0.45
2:B:162:SER:HB3	2:B:197:SER:O	2.16	0.45
3:C:250:LEU:HA	3:C:250:LEU:HD23	1.71	0.45
4:D:9:GLU:CD	4:D:9:GLU:H	2.24	0.45
7:G:48:ILE:HD11	8:H:80:THR:HG22	1.96	0.45
10:J:47:LEU:HD12	10:J:47:LEU:HA	1.66	0.45
1:N:117:MET:CE	12:Y:39:ILE:HG23	2.47	0.45
1:N:324:LEU:O	2:O:45:MET:HE3	2.16	0.45
1:N:378:HIS:CD2	1:N:425:PHE:CZ	3.04	0.45
2:O:99:THR:C	2:O:100:MET:HG2	2.41	0.45
2:O:139:ASP:OD1	2:O:140:ASN:N	2.49	0.45
3:P:173:PHE:CD1	3:P:173:PHE:C	2.94	0.45
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.03	0.45
2:B:98:LYS:HE3	2:B:98:LYS:HB2	1.78	0.45
3:C:137:LEU:HA	3:C:137:LEU:HD12	1.77	0.45
3:C:160:LEU:HD21	3:C:223:LEU:HD23	1.98	0.45
4:D:141:ASP:C	4:D:143:ASN:H	2.25	0.45
13:M:19:LEU:C	13:M:19:LEU:HD23	2.42	0.45
1:N:44:PRO:HG3	4:Q:111:PHE:CE2	2.50	0.45
1:N:129:TYR:CE2	1:N:232:GLN:HG2	2.51	0.45
2:O:186:SER:HB3	2:O:213:LEU:HD22	1.99	0.45
4:Q:43:LYS:O	4:Q:46:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:11:LEU:HD23	10:W:11:LEU:O	2.17	0.45
1:A:222:PRO:O	1:A:225:GLY:N	2.48	0.45
7:G:2:SER:H	1:N:286:ILE:HG22	1.80	0.45
3:P:36:HIS:C	3:P:38:ASN:H	2.24	0.45
4:Q:108:PRO:HG2	4:Q:111:PHE:CE2	2.52	0.45
4:Q:114:GLU:HG3	11:X:51:LYS:CE	2.46	0.45
1:N:386:VAL:HG11	18:N:515:HEA:H261	1.98	0.45
2:O:5:MET:CE	11:X:43:SER:H	2.30	0.45
2:O:184:LEU:HD11	2:O:211:LEU:CD2	2.46	0.45
9:V:60:PHE:CE1	9:V:69:PHE:CE2	3.04	0.45
10:W:8:LYS:NZ	10:W:12:PHE:HE2	2.15	0.45
2:B:50:LEU:HB2	9:I:13:LEU:HD13	1.99	0.45
3:C:195:SER:O	3:C:199:VAL:HG13	2.17	0.45
4:D:114:GLU:O	4:D:118:LYS:HG2	2.16	0.45
8:H:59:VAL:HG12	8:H:60:TYR:N	2.31	0.45
1:N:243:VAL:HB	18:N:516:HEA:CAC	2.46	0.45
7:T:42:ARG:NH1	7:T:74:ARG:NH2	2.64	0.45
1:A:4:ASN:HA	1:A:8:PHE:HB2	1.99	0.45
1:A:69:MET:O	1:A:72:PRO:HD2	2.17	0.45
2:B:48:THR:HB	9:I:16:ARG:CZ	2.47	0.45
2:B:136:LEU:HB3	2:B:193:TYR:HD2	1.80	0.45
4:D:114:GLU:HG3	11:K:51:LYS:CE	2.47	0.45
12:L:20:ARG:HG2	12:L:24:MET:HE2	1.99	0.45
4:Q:84:ALA:O	4:Q:88:PHE:HD2	1.99	0.45
4:Q:141:ASP:C	4:Q:143:ASN:H	2.25	0.45
1:A:117:MET:HE3	12:L:39:ILE:HG12	1.99	0.45
1:A:260:TYR:CD1	1:A:487:LEU:HD12	2.52	0.45
1:A:474:GLU:HG3	1:A:475:ALA:N	2.32	0.45
2:B:87:MET:C	2:B:89[B]:GLU:N	2.73	0.45
2:B:186:SER:HB3	2:B:213:LEU:HD22	1.99	0.45
6:F:49:VAL:O	6:F:91:LEU:HD12	2.17	0.45
12:L:41:ARG:HD2	13:M:40:TYR:CZ	2.52	0.45
2:O:16:ILE:HD12	2:O:17:MET:N	2.32	0.45
6:S:85:CYS:SG	6:S:87:THR:OG1	2.71	0.45
2:B:66:THR:CG2	2:B:67:ILE:N	2.80	0.45
2:B:222:TRP:HB2	9:I:71:SER:HB2	1.98	0.45
5:E:52:LEU:HA	5:E:52:LEU:HD23	1.67	0.45
1:N:95:PRO:HB2	3:P:11:VAL:HG13	1.98	0.45
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.52	0.45
5:R:70:VAL:HG12	5:R:71:VAL:N	2.31	0.45
3:C:16:TRP:HE3	3:C:16:TRP:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:445:ASP:OD1	2:O:134:ARG:NH1	2.49	0.45
3:P:42:LEU:HD21	10:W:46:SER:HB3	1.99	0.45
3:P:72:THR:HB	3:P:73:PRO:HD2	1.98	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CD2	2.52	0.45
6:F:16:LEU:O	6:F:20:VAL:CG1	2.64	0.44
1:A:124:THR:HG22	1:A:138:HIS:CE1	2.52	0.44
2:B:162:SER:HA	2:B:173:ASP:HA	1.99	0.44
5:E:81:ILE:O	5:E:85:VAL:HG23	2.18	0.44
1:N:495:LEU:HD23	1:N:495:LEU:HA	1.78	0.44
2:O:108:TYR:CD1	2:O:108:TYR:N	2.85	0.44
3:P:160:LEU:HD21	3:P:223:LEU:HD23	1.99	0.44
4:Q:66:GLU:HA	4:Q:70:GLU:OE1	2.17	0.44
4:Q:126:MET:O	4:Q:127:LYS:HB2	2.16	0.44
3:C:157:LYS:HE3	3:C:158:HIS:NE2	2.32	0.44
1:N:131:PRO:HB2	2:O:159:VAL:HA	1.99	0.44
4:Q:70:GLU:HA	5:R:109:VAL:CG1	2.47	0.44
1:N:299:VAL:HG13	1:N:300:ASP:N	2.31	0.44
2:O:100:MET:CE	2:O:157:GLU:HG3	2.47	0.44
3:P:192:VAL:O	3:P:196:THR:HB	2.18	0.44
4:Q:115:TRP:O	4:Q:119:GLN:HB2	2.17	0.44
5:R:52:LEU:HD23	5:R:52:LEU:HA	1.60	0.44
7:T:48:ILE:HD12	8:U:80:THR:HG22	1.99	0.44
9:V:57:MET:O	9:V:60:PHE:HB3	2.18	0.44
1:A:282:PHE:HE1	7:T:3:ALA:CB	2.31	0.44
1:A:289:ALA:HB3	1:A:305:PHE:CD1	2.53	0.44
1:A:293:PHE:CZ	1:A:306:THR:HG22	2.52	0.44
3:C:102:TYR:O	3:C:106:LEU:HB2	2.18	0.44
7:G:4:ALA:HB2	1:N:197:LEU:CD1	2.47	0.44
12:L:14:SER:HB3	12:L:20:ARG:HH12	1.82	0.44
1:N:8:PHE:CZ	3:P:15:PRO:HB3	2.52	0.44
4:Q:121:LYS:HD2	11:X:50:PRO:HB2	2.00	0.44
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.17	0.44
13:Z:19:LEU:HD23	13:Z:19:LEU:C	2.42	0.44
1:A:404:THR:O	1:A:480:ARG:NH1	2.48	0.44
2:O:62:GLU:O	2:O:66:THR:HB	2.18	0.44
8:U:60:TYR:CD1	8:U:60:TYR:C	2.96	0.44
1:A:117:MET:HB3	10:J:54:SER:OG	2.17	0.44
2:B:106:TRP:NE1	2:B:207:MET:HE3	2.33	0.44
3:C:192:VAL:O	3:C:196:THR:HB	2.18	0.44
7:G:48:ILE:HD12	7:G:49:PRO:CD	2.48	0.44
10:J:8:LYS:HZ1	10:J:12:PHE:HE2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:188:ILE:H	3:P:188:ILE:HG13	1.61	0.44
7:T:2:SER:O	7:T:3:ALA:HB2	2.17	0.44
7:T:47:PHE:CZ	7:T:81:GLY:HA2	2.53	0.44
2:B:25:ASP:OD1	9:I:43:ARG:NH1	2.51	0.44
2:B:139:ASP:OD1	2:B:140:ASN:N	2.50	0.44
11:K:16:ALA:O	11:K:17:VAL:C	2.60	0.44
2:O:1:MET:SD	2:O:133:LEU:HD13	2.56	0.44
3:P:250:LEU:HA	3:P:250:LEU:HD23	1.75	0.44
9:V:37:PHE:HA	9:V:41:GLU:HB2	2.00	0.44
10:W:18:LEU:HD23	10:W:18:LEU:HA	1.80	0.44
1:N:21:LEU:HA	1:N:21:LEU:HD23	1.76	0.44
2:O:62:GLU:HA	2:O:65:TRP:CD1	2.53	0.44
5:R:84:TYR:O	5:R:87:GLN:HB3	2.18	0.44
6:S:35:ALA:HA	6:S:36:PRO:HD3	1.87	0.44
8:U:59:VAL:HG12	8:U:60:TYR:N	2.33	0.44
1:A:285:PHE:CD2	7:T:4:ALA:HB3	2.53	0.43
1:A:433:LEU:HD13	2:B:8:GLY:HA2	1.99	0.43
8:H:57:ARG:HA	8:H:60:TYR:CD2	2.53	0.43
4:Q:132:GLN:HE21	9:V:42:LYS:HE3	1.82	0.43
12:Y:22:LEU:HD11	13:Z:18:GLY:HA2	2.00	0.43
1:A:353:LEU:HG	2:B:31:VAL:HB	2.00	0.43
2:B:62:GLU:O	2:B:66:THR:HB	2.17	0.43
2:B:190:GLY:O	2:B:191:LEU:HD23	2.18	0.43
3:C:152:MET:HE2	3:C:152:MET:HB3	1.83	0.43
8:H:84:LYS:HD2	8:H:84:LYS:HA	1.67	0.43
1:N:4:ASN:HA	1:N:8:PHE:HB2	1.99	0.43
1:N:513:LEU:HA	1:N:513:LEU:HD12	1.57	0.43
2:O:59:GLN:O	2:O:63:THR:HG23	2.18	0.43
4:Q:9:GLU:CD	4:Q:9:GLU:H	2.26	0.43
4:Q:122:ARG:O	4:Q:125:ASP:HB2	2.18	0.43
8:U:84:LYS:HA	8:U:84:LYS:HD2	1.63	0.43
9:V:19:PHE:HD2	9:V:20:HIS:ND1	2.15	0.43
10:W:16:ASN:OD1	10:W:18:LEU:HB2	2.18	0.43
1:A:8:PHE:CZ	3:C:15:PRO:HB3	2.53	0.43
4:D:113:GLU:O	4:D:116:VAL:HG22	2.19	0.43
8:H:38:ARG:NH1	8:H:84:LYS:O	2.51	0.43
1:N:298:ASP:HB2	1:N:301:THR:CG2	2.43	0.43
4:Q:145:TRP:CZ2	11:X:45:VAL:HA	2.53	0.43
4:Q:147:LYS:HE3	4:Q:147:LYS:CA	2.42	0.43
8:U:39:CYS:CB	8:U:53:CYS:HG	2.30	0.43
9:V:14:ALA:CB	9:V:18:ARG:HH21	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG3	1:A:458:SER:HB3	1.99	0.43
1:A:129:TYR:CE2	1:A:232:GLN:HG2	2.54	0.43
1:A:319:LYS:HE3	1:A:319:LYS:HB3	1.79	0.43
2:B:52:HIS:C	2:B:52:HIS:CD2	2.96	0.43
3:C:42:LEU:HD21	10:J:46:SER:HB3	1.99	0.43
5:E:90:ARG:HA	5:E:90:ARG:HD3	1.70	0.43
1:N:105:LEU:HD12	1:N:105:LEU:HA	1.73	0.43
2:O:52:HIS:CD2	2:O:52:HIS:C	2.96	0.43
2:O:162:SER:HA	2:O:173:ASP:HA	2.00	0.43
3:P:110:PRO:HB2	8:U:30:TRP:CE3	2.52	0.43
3:P:154:GLY:CA	6:S:6:VAL:HG13	2.48	0.43
3:P:178:ALA:O	3:P:181:TYR:HB2	2.19	0.43
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.18	0.43
5:R:21:LYS:O	5:R:57:ARG:NH1	2.52	0.43
1:A:347:LEU:HD12	1:A:347:LEU:HA	1.81	0.43
1:A:360:ASN:O	1:A:364:ASP:N	2.50	0.43
4:D:7:LYS:O	4:D:10:ASP:HB2	2.18	0.43
7:G:42:ARG:HH11	7:G:75:VAL:HG11	1.82	0.43
8:H:37:HIS:CD2	8:H:76:ARG:NH1	2.86	0.43
1:N:103:TRP:O	3:P:21:ALA:HB1	2.19	0.43
1:N:157:SER:HB2	1:N:199:LEU:CD2	2.49	0.43
4:Q:48:TRP:NE1	5:R:56:ARG:NH2	2.66	0.43
1:A:237:PHE:HZ	7:T:2:SER:HB2	1.83	0.43
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.53	0.43
3:C:121:ILE:HD13	3:C:121:ILE:HA	1.73	0.43
2:O:125:THR:HA	2:O:128:LEU:CD1	2.49	0.43
1:A:397:PHE:HB3	1:A:398:PRO:HD3	2.01	0.43
1:A:403:TYR:CZ	12:L:7:PRO:HB3	2.54	0.43
2:B:184:LEU:HD11	2:B:211:LEU:CD2	2.48	0.43
7:G:3:ALA:CB	1:N:282:PHE:HE1	2.30	0.43
8:H:43:MET:O	8:H:47:GLY:N	2.52	0.43
9:I:30:GLY:O	9:I:31:PHE:C	2.62	0.43
4:Q:11:TYR:CD1	4:Q:11:TYR:C	2.97	0.43
10:J:8:LYS:NZ	10:J:12:PHE:HE2	2.15	0.43
12:L:25:MET:HE2	12:L:25:MET:HB3	1.71	0.43
1:N:172:LYS:HD3	1:N:181:THR:HG21	2.01	0.43
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.49	0.43
2:O:50:LEU:HD21	5:R:77:PRO:HD2	1.99	0.43
9:V:19:PHE:HD2	9:V:20:HIS:CE1	2.37	0.43
10:W:31:LEU:HD23	10:W:31:LEU:HA	1.77	0.43
1:A:158:ILE:O	1:A:162:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:GLU:HA	2:B:65:TRP:CD1	2.54	0.43
3:C:188:ILE:HD11	7:G:68:THR:HG22	2.01	0.43
4:D:132:GLN:HE22	9:I:43:ARG:HB2	1.83	0.43
7:G:42:ARG:HD2	7:G:42:ARG:O	2.19	0.43
1:N:83:VAL:CG2	1:N:188:VAL:HG11	2.49	0.43
1:N:129:TYR:CZ	1:N:232:GLN:HG2	2.54	0.43
7:T:42:ARG:HD2	7:T:42:ARG:O	2.19	0.43
1:A:152:LEU:CD2	3:C:24:ALA:HB1	2.49	0.43
1:A:378:HIS:O	1:A:382:SER:HB2	2.19	0.43
5:E:12:ASP:HA	5:E:47:ILE:HD11	2.01	0.43
3:P:42:LEU:HD12	3:P:42:LEU:HA	1.93	0.43
8:U:39:CYS:CB	8:U:53:CYS:SG	3.07	0.43
10:W:29:ASN:ND2	10:W:33:ARG:HD2	2.34	0.43
3:C:16:TRP:HA	3:C:16:TRP:CE3	2.52	0.42
3:C:26:LEU:HD12	3:C:26:LEU:HA	1.85	0.42
3:C:67:PHE:O	6:F:14:THR:HG21	2.18	0.42
4:D:73:ARG:CZ	4:D:73:ARG:HB3	2.49	0.42
5:E:70:VAL:HG12	5:E:71:VAL:N	2.32	0.42
1:N:270:TYR:CD1	1:N:270:TYR:C	2.97	0.42
3:P:151:LEU:HD21	3:P:232:HIS:CG	2.53	0.42
7:T:48:ILE:HD12	7:T:49:PRO:CD	2.49	0.42
9:V:30:GLY:O	9:V:31:PHE:C	2.62	0.42
1:A:176:MET:HE3	1:A:181:THR:CG2	2.49	0.42
1:A:506:GLU:HB3	3:C:1:MET:CG	2.49	0.42
2:B:160:LEU:HD21	2:B:175:ILE:HG23	2.01	0.42
4:D:112:GLU:O	4:D:116:VAL:HG13	2.19	0.42
7:G:42:ARG:NH1	7:G:74:ARG:NH2	2.65	0.42
11:K:53:TRP:CD1	11:K:53:TRP:N	2.86	0.42
2:O:106:TRP:NE1	2:O:207:MET:HE3	2.34	0.42
2:O:152:MET:HE3	2:O:152:MET:HB3	1.91	0.42
5:R:12:ASP:HA	5:R:47:ILE:HD11	2.01	0.42
5:R:78:HIS:ND1	9:V:12:LEU:HD22	2.34	0.42
6:S:16:LEU:O	6:S:20:VAL:CG1	2.65	0.42
11:X:53:TRP:CD1	11:X:53:TRP:N	2.86	0.42
1:A:506:GLU:HB3	3:C:1:MET:HB3	2.01	0.42
3:C:116:TRP:HA	3:C:117:PRO:C	2.44	0.42
3:C:129:VAL:HG13	3:C:176:LEU:HD22	2.01	0.42
4:D:129:ALA:HB1	4:D:133:GLY:HA3	2.01	0.42
5:E:104:LEU:HA	5:E:104:LEU:HD23	1.75	0.42
9:I:14:ALA:CB	9:I:18:ARG:HH21	2.33	0.42
1:N:51:ASP:O	1:N:55:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:186:SER:CB	2:O:213:LEU:HD22	2.48	0.42
3:P:137:LEU:HD22	3:P:173:PHE:CD2	2.53	0.42
3:P:190:ASP:HB3	7:T:53:LEU:HD22	1.99	0.42
5:E:81:ILE:HA	9:I:7:PRO:HG3	2.01	0.42
1:N:87:ILE:O	1:N:173:PRO:HD3	2.19	0.42
4:Q:139:ASP:O	4:Q:143:ASN:HA	2.19	0.42
7:T:48:ILE:HD11	8:U:80:THR:HG22	2.00	0.42
1:A:402:GLY:HA3	1:A:499:PRO:HD3	2.00	0.42
2:B:113:TYR:OH	8:H:12:GLN:HA	2.20	0.42
3:C:132:LEU:HD13	3:C:176:LEU:HD11	2.00	0.42
7:G:48:ILE:HG13	7:G:50:TYR:CE2	2.55	0.42
8:H:46:LYS:NZ	8:U:53:CYS:CA	2.82	0.42
2:O:184:LEU:HD23	2:O:185:MET:N	2.34	0.42
5:R:79:LYS:HE2	5:R:79:LYS:HB2	1.76	0.42
5:R:93:LEU:HD23	5:R:93:LEU:HA	1.75	0.42
6:S:14:THR:OG1	6:S:15:GLY:N	2.53	0.42
6:S:18:ARG:NH1	6:S:21:MET:HE1	2.34	0.42
8:U:57:ARG:HG3	8:U:60:TYR:CE2	2.54	0.42
1:A:58:VAL:HG13	18:A:515:HEA:HBD2	2.02	0.42
1:A:83:VAL:HG21	1:A:188:VAL:HG11	2.01	0.42
4:D:108:PRO:HG2	4:D:111:PHE:CD2	2.54	0.42
9:I:19:PHE:HD2	9:I:20:HIS:ND1	2.18	0.42
10:J:31:LEU:HD23	10:J:31:LEU:HA	1.72	0.42
1:N:218:THR:HB	1:N:221:ASP:HB3	2.01	0.42
1:N:443:TYR:HB2	1:N:447:TYR:HD2	1.85	0.42
1:N:468:MET:SD	18:N:515:HEA:H243	2.59	0.42
1:N:501:PRO:O	1:N:502:TYR:C	2.62	0.42
2:O:116:LEU:HD11	2:O:226:MET:CG	2.47	0.42
1:A:84:PRO:CG	1:A:92:MET:HE3	2.30	0.42
1:A:199:LEU:HD12	1:A:238:PHE:CE1	2.55	0.42
3:C:104:SER:CB	3:C:192:VAL:HG11	2.49	0.42
6:F:18:ARG:HG3	6:F:21:MET:HE2	2.01	0.42
6:F:53:THR:CG2	6:F:54:ASN:N	2.82	0.42
7:G:4:ALA:HB3	1:N:285:PHE:CD2	2.54	0.42
1:N:12:HIS:CD2	1:N:80:ASN:O	2.72	0.42
2:O:160:LEU:HD22	2:O:175:ILE:HG12	2.02	0.42
8:U:36:PHE:HB2	8:U:56:TYR:HB3	2.01	0.42
1:A:247:ILE:HD12	1:A:247:ILE:HA	1.86	0.42
1:A:478:SER:HA	13:M:8:THR:O	2.20	0.42
3:C:188:ILE:H	3:C:188:ILE:HG13	1.58	0.42
9:I:29:LEU:HD23	9:I:29:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:49:VAL:HG21	6:S:74:LEU:HD12	2.00	0.42
9:V:14:ALA:HB3	9:V:18:ARG:HH21	1.85	0.42
1:A:75:ILE:O	1:A:79:GLY:HA3	2.20	0.42
1:A:377:PHE:HB3	18:A:516:HEA:C1D	2.49	0.42
1:A:449:MET:HE1	2:B:5:MET:HE2	2.01	0.42
1:A:468:MET:SD	18:A:515:HEA:H243	2.59	0.42
1:A:501:PRO:O	1:A:502:TYR:C	2.62	0.42
5:E:9:GLU:H	5:E:9:GLU:CD	2.28	0.42
7:G:49:PRO:HG2	8:H:80:THR:CG2	2.50	0.42
1:N:199:LEU:HD12	1:N:238:PHE:CE1	2.55	0.42
1:N:383:MET:HA	1:N:387:PHE:CD1	2.55	0.42
2:O:66:THR:CG2	2:O:67:ILE:N	2.83	0.42
3:P:26:LEU:HD12	3:P:26:LEU:HA	1.79	0.42
8:U:40:GLU:O	8:U:41:LYS:C	2.63	0.42
1:A:445:ASP:OD1	2:B:134:ARG:NH1	2.49	0.42
7:G:42:ARG:NH1	7:G:75:VAL:HG11	2.34	0.42
1:N:176:MET:HE3	1:N:181:THR:CG2	2.42	0.42
1:N:443:TYR:HE2	1:N:448:THR:HA	1.85	0.42
5:R:76:GLY:HA3	5:R:77:PRO:HD2	1.87	0.42
6:S:95:GLN:NE2	6:S:96:LEU:HD13	2.27	0.42
7:T:78:LEU:HA	7:T:78:LEU:HD12	1.85	0.42
9:V:26:MET:HA	9:V:26:MET:CE	2.50	0.42
10:W:3:ASN:HD22	10:W:5:VAL:HG12	1.84	0.42
1:A:468:MET:HE1	18:A:515:HEA:H211	2.02	0.41
1:N:158:ILE:O	1:N:162:ILE:HG13	2.21	0.41
2:O:133:LEU:HA	2:O:133:LEU:HD23	1.82	0.41
3:P:188:ILE:HD11	7:T:68:THR:HG22	2.02	0.41
7:T:37:LEU:C	7:T:38:HIS:HD1	2.28	0.41
8:U:17:ASP:OD2	8:U:19:ARG:NH1	2.52	0.41
1:A:508:PRO:HB2	6:F:56:ARG:HH21	1.85	0.41
18:A:515:HEA:H272	18:A:515:HEA:H172	1.78	0.41
2:B:123:ILE:HD12	2:B:137:GLU:HB3	2.01	0.41
4:D:52:SER:O	4:D:53:ILE:C	2.62	0.41
4:D:147:LYS:HE3	4:D:147:LYS:CA	2.39	0.41
3:P:137:LEU:HD12	3:P:137:LEU:HA	1.82	0.41
4:Q:40:LEU:HD22	4:Q:59:LEU:HD13	2.02	0.41
7:G:10:GLY:O	7:G:11:THR:O	2.37	0.41
12:L:4:GLU:HB3	12:L:9:LYS:HD3	2.02	0.41
1:N:400:PHE:O	12:Y:10:ASN:ND2	2.50	0.41
2:O:142:VAL:HG13	2:O:210:VAL:O	2.20	0.41
3:P:47:LEU:O	3:P:51:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:HB2	2:B:159:VAL:HA	2.02	0.41
1:A:170:ASN:CG	1:A:170:ASN:O	2.63	0.41
1:A:380:VAL:HG21	18:A:516:HEA:C3C	2.49	0.41
2:B:186:SER:CB	2:B:213:LEU:HD22	2.51	0.41
4:D:16:TYR:CE2	4:D:65:LYS:HB2	2.55	0.41
8:H:38:ARG:HG2	8:H:85:ILE:HG23	2.01	0.41
5:R:9:GLU:H	5:R:9:GLU:CD	2.28	0.41
10:W:10:LYS:HE3	10:W:10:LYS:O	2.21	0.41
1:A:93:ALA:O	1:A:95:PRO:HD3	2.20	0.41
1:A:152:LEU:HD22	3:C:24:ALA:HB1	2.01	0.41
1:A:376:HIS:CD2	18:A:516:HEA:ND	2.88	0.41
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.62	0.41
6:F:18:ARG:NH1	6:F:21:MET:HE1	2.36	0.41
9:I:14:ALA:HB3	9:I:18:ARG:HH21	1.84	0.41
1:N:208:MET:HE2	3:P:97:PHE:HD1	1.85	0.41
6:S:74:LEU:HD11	6:S:89:TYR:HB3	2.03	0.41
7:T:48:ILE:HG13	7:T:50:TYR:CE2	2.56	0.41
1:A:25:TRP:O	1:A:28:MET:HB2	2.21	0.41
1:A:85:LEU:O	1:A:492:LEU:HD13	2.20	0.41
1:A:218:THR:HB	1:A:221:ASP:HB3	2.01	0.41
1:A:390:MET:HE1	1:A:468:MET:SD	2.60	0.41
3:C:3:HIS:CD2	6:F:97:ALA:HB1	2.56	0.41
1:N:93:ALA:O	1:N:95:PRO:HD3	2.20	0.41
1:N:150:LEU:HA	1:N:150:LEU:HD12	1.83	0.41
1:N:421:VAL:HG23	1:N:422:ASN:N	2.35	0.41
2:O:122:MET:HA	2:O:137:GLU:O	2.21	0.41
3:P:154:GLY:HA2	6:S:6:VAL:CG1	2.50	0.41
1:A:105:LEU:HA	1:A:105:LEU:HD12	1.76	0.41
1:A:159:LEU:HA	1:A:159:LEU:HD12	1.78	0.41
2:B:108:TYR:N	2:B:108:TYR:CD1	2.89	0.41
2:B:188:ARG:HD3	9:I:51:TYR:HE1	1.85	0.41
3:C:40:MET:O	3:C:44:MET:HG2	2.20	0.41
4:D:48:TRP:NE1	5:E:56:ARG:NH2	2.69	0.41
5:E:44:GLU:OE1	5:E:45:PRO:HD2	2.20	0.41
7:G:4:ALA:HB3	1:N:285:PHE:CE2	2.56	0.41
7:G:37:LEU:C	7:G:38:HIS:HD1	2.29	0.41
9:I:60:PHE:HE1	9:I:69:PHE:CE2	2.38	0.41
10:J:3:ASN:ND2	10:J:3:ASN:O	2.53	0.41
1:N:321:PHE:HB3	2:O:65:TRP:CE3	2.55	0.41
2:O:113:TYR:OH	8:U:12:GLN:HA	2.21	0.41
7:G:7:ASP:CB	1:N:189:MET:SD	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:132:LEU:HD13	3:P:176:LEU:CD1	2.51	0.41
1:A:8:PHE:N	1:A:8:PHE:CD1	2.89	0.41
2:B:108:TYR:CE2	2:B:142:VAL:HG11	2.56	0.41
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.95	0.41
2:B:184:LEU:HD23	2:B:185:MET:N	2.35	0.41
5:E:79:LYS:HB2	5:E:79:LYS:HE2	1.76	0.41
5:E:93:LEU:HD23	5:E:93:LEU:HA	1.77	0.41
7:G:2:SER:O	7:G:3:ALA:HB2	2.20	0.41
7:G:69:PHE:HD2	7:G:70:PHE:CE1	2.38	0.41
8:H:81:PHE:CE2	8:H:85:ILE:HD11	2.56	0.41
10:J:14:GLU:O	10:J:23:LYS:HE3	2.21	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.56	0.41
1:N:506:GLU:OE1	3:P:1:MET:HB3	2.20	0.41
2:O:100:MET:HE3	2:O:100:MET:HB3	1.81	0.41
6:S:9:ASP:C	6:S:11:GLU:N	2.77	0.41
10:W:29:ASN:HD21	10:W:33:ARG:HD2	1.86	0.41
1:A:128:VAL:HG22	1:A:128:VAL:O	2.21	0.41
1:A:443:TYR:HE2	1:A:448:THR:HA	1.85	0.41
1:N:260:TYR:CE1	1:N:487:LEU:HD12	2.56	0.41
1:N:349:THR:O	1:N:353:LEU:HB2	2.21	0.41
1:N:506:GLU:HB3	3:P:1:MET:CG	2.51	0.41
2:O:162:SER:HB3	2:O:197:SER:O	2.20	0.41
5:E:52:LEU:O	5:E:55:CYS:HB2	2.21	0.40
7:G:23:LEU:O	7:G:24:ALA:C	2.64	0.40
8:H:17:ASP:OD2	8:H:19:ARG:NH1	2.53	0.40
9:I:37:PHE:HA	9:I:41:GLU:HB2	2.03	0.40
11:K:22:ALA:O	11:K:26:VAL:HG12	2.21	0.40
1:N:85:LEU:O	1:N:492:LEU:HD13	2.21	0.40
2:O:87:MET:C	2:O:89[B]:GLU:N	2.77	0.40
6:S:9:ASP:C	6:S:11:GLU:H	2.29	0.40
9:V:60:PHE:HE1	9:V:69:PHE:CE2	2.39	0.40
4:D:118:LYS:HA	11:K:51:LYS:O	2.22	0.40
4:D:132:GLN:HE21	9:I:42:LYS:HE3	1.85	0.40
2:O:20:LEU:CD2	2:O:83:ILE:HG21	2.52	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.22	0.40
3:P:132:LEU:O	3:P:136:VAL:HG23	2.21	0.40
4:Q:138:TRP:HD1	4:Q:140:TYR:CD1	2.38	0.40
8:U:38:ARG:NH1	8:U:84:LYS:O	2.51	0.40
1:A:270:TYR:CD1	1:A:270:TYR:C	2.99	0.40
1:A:302:ARG:HH11	1:A:302:ARG:HD3	1.73	0.40
1:A:436:MET:HA	1:A:437:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:36:TRP:HD1	7:G:36:TRP:O	2.04	0.40
8:H:51:SER:HB3	8:U:48:GLY:C	2.46	0.40
10:J:2:GLU:HG3	10:J:3:ASN:H	1.85	0.40
1:N:19:TYR:O	1:N:20:LEU:C	2.64	0.40
1:N:98:ASN:HB2	1:N:163:ASN:HD21	1.85	0.40
1:N:376:HIS:CD2	18:N:516:HEA:ND	2.89	0.40
1:N:377:PHE:HB3	18:N:516:HEA:C1D	2.51	0.40
1:N:443:TYR:CD1	1:N:443:TYR:N	2.87	0.40
2:O:68:LEU:HD12	2:O:68:LEU:HA	1.94	0.40
4:Q:59:LEU:HD12	4:Q:59:LEU:HA	1.95	0.40
4:Q:139:ASP:O	4:Q:143:ASN:N	2.54	0.40
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.71	0.40
4:D:119:GLN:O	4:D:123:MET:HG3	2.21	0.40
4:D:130:PRO:HG2	4:D:131:ILE:N	2.34	0.40
4:D:131:ILE:HG13	4:D:131:ILE:H	1.68	0.40
5:E:20:ASN:O	5:E:21:LYS:C	2.64	0.40
1:N:8:PHE:N	1:N:8:PHE:CD1	2.89	0.40
1:N:33:LEU:O	1:N:37:ILE:HG13	2.21	0.40
1:N:360:ASN:O	1:N:364:ASP:N	2.51	0.40
1:N:400:PHE:O	1:N:499:PRO:HB3	2.20	0.40
2:O:7:LEU:HD12	2:O:7:LEU:HA	1.79	0.40
6:S:49:VAL:O	6:S:91:LEU:HD12	2.21	0.40
1:A:340:TRP:HH2	1:A:417:MET:HG2	1.86	0.40
2:B:144:LEU:HD22	2:B:150:ILE:HD13	2.04	0.40
3:C:75:VAL:O	3:C:79:LEU:HD12	2.22	0.40
5:E:26:ALA:O	5:E:27:TRP:C	2.62	0.40
7:G:56:ARG:HG2	7:G:56:ARG:NH1	2.36	0.40
1:N:92:MET:HE2	1:N:167:THR:CG2	2.51	0.40
3:P:104:SER:CB	3:P:192:VAL:HG11	2.50	0.40
3:P:106:LEU:HD23	3:P:106:LEU:HA	1.92	0.40
5:R:26:ALA:O	5:R:27:TRP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	469 (92%)	39 (8%)	4 (1%)	16	44
1	N	512/514 (100%)	470 (92%)	38 (7%)	4 (1%)	16	44
2	B	230/227 (101%)	197 (86%)	27 (12%)	6 (3%)	4	17
2	O	230/227 (101%)	197 (86%)	27 (12%)	6 (3%)	4	17
3	C	259/261 (99%)	249 (96%)	7 (3%)	3 (1%)	10	34
3	P	259/261 (99%)	248 (96%)	8 (3%)	3 (1%)	10	34
4	D	142/147 (97%)	131 (92%)	10 (7%)	1 (1%)	18	48
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	18	48
5	E	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
5	R	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	82 (85%)	7 (7%)	7 (7%)	1	2
6	S	96/98 (98%)	79 (82%)	10 (10%)	7 (7%)	1	2
7	G	82/84 (98%)	64 (78%)	13 (16%)	5 (6%)	1	4
7	T	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	1	4
8	H	73/85 (86%)	61 (84%)	10 (14%)	2 (3%)	4	16
8	U	73/85 (86%)	61 (84%)	10 (14%)	2 (3%)	4	16
9	I	71/73 (97%)	67 (94%)	3 (4%)	1 (1%)	9	30
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	54/59 (92%)	47 (87%)	5 (9%)	2 (4%)	2	11
10	W	54/59 (92%)	47 (87%)	5 (9%)	2 (4%)	2	11
11	K	47/56 (84%)	35 (74%)	12 (26%)	0	100	100
11	X	47/56 (84%)	36 (77%)	11 (23%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3518/3612 (97%)	3169 (90%)	288 (8%)	61 (2%)	7	26

All (61) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains ⓘ

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%)	388 (91%)	39 (9%)	9	28
1	N	427/427 (100%)	384 (90%)	43 (10%)	7	24
2	B	216/211 (102%)	195 (90%)	21 (10%)	8	25
2	O	216/211 (102%)	194 (90%)	22 (10%)	7	23
3	C	226/226 (100%)	199 (88%)	27 (12%)	5	16
3	P	226/226 (100%)	199 (88%)	27 (12%)	5	16
4	D	128/129 (99%)	117 (91%)	11 (9%)	10	30
4	Q	128/129 (99%)	117 (91%)	11 (9%)	10	30
5	E	95/95 (100%)	89 (94%)	6 (6%)	16	45
5	R	95/95 (100%)	89 (94%)	6 (6%)	16	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	81/81 (100%)	67 (83%)	14 (17%)	2	7
6	S	81/81 (100%)	69 (85%)	12 (15%)	3	10
7	G	68/68 (100%)	56 (82%)	12 (18%)	2	6
7	T	68/68 (100%)	55 (81%)	13 (19%)	1	5
8	H	67/75 (89%)	55 (82%)	12 (18%)	2	6
8	U	67/75 (89%)	57 (85%)	10 (15%)	3	10
9	I	58/58 (100%)	50 (86%)	8 (14%)	3	12
9	V	58/58 (100%)	50 (86%)	8 (14%)	3	12
10	J	47/50 (94%)	40 (85%)	7 (15%)	3	10
10	W	47/50 (94%)	40 (85%)	7 (15%)	3	10
11	K	39/46 (85%)	35 (90%)	4 (10%)	7	23
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	23
12	L	40/40 (100%)	36 (90%)	4 (10%)	7	24
12	Y	40/40 (100%)	36 (90%)	4 (10%)	7	24
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	21
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	21
All	All	3058/3088 (99%)	2718 (89%)	340 (11%)	6	20

All (340) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	35	LEU
1	A	56	VAL
1	A	92	MET
1	A	96	ARG
1	A	105	LEU
1	A	136	LEU
1	A	138	HIS
1	A	146	THR
1	A	150	LEU
1	A	156	SER
1	A	158	ILE
1	A	159	LEU
1	A	169	ILE
1	A	172	LYS

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Mol	Chain	Res	Type
1	A	189	MET
1	A	194	LEU
1	A	213	ARG
1	A	215	LEU
1	A	278	MET
1	A	295	VAL
1	A	301	THR
1	A	312	ILE
1	A	318	VAL
1	A	336	PRO
1	A	347	LEU
1	A	354	THR
1	A	365	ILE
1	A	366	VAL
1	A	369	ASP
1	A	373	VAL
1	A	383	MET
1	A	452	THR
1	A	465	VAL
1	A	467	LEU
1	A	474	GLU
1	A	482	VAL
1	A	492	LEU
1	A	508	PRO
2	B	3	TYR
2	B	7	LEU
2	B	31	VAL
2	B	55	THR
2	B	60	GLU
2	B	66	THR
2	B	67	ILE
2	B	81	LEU
2	B	88[A]	ASP
2	B	88[B]	ASP
2	B	90[A]	ILE
2	B	90[B]	ILE
2	B	126	SER
2	B	130	PRO
2	B	142	VAL
2	B	170	LEU
2	B	171	LYS
2	B	185	MET

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Mol	Chain	Res	Type
2	B	188	ARG
2	B	205	SER
2	B	216	LEU
3	C	11	VAL
3	C	12	ASN
3	C	13	PRO
3	C	14	SER
3	C	18	LEU
3	C	22	LEU
3	C	26	LEU
3	C	41	THR
3	C	85	LEU
3	C	112	LEU
3	C	128	GLU
3	C	131	LEU
3	C	132	LEU
3	C	137	LEU
3	C	142	VAL
3	C	159	MET
3	C	160	LEU
3	C	163	LEU
3	C	168	THR
3	C	179	SER
3	C	188	ILE
3	C	196	THR
3	C	199	VAL
3	C	213	THR
3	C	222	GLN
3	C	245	VAL
3	C	258	TRP
4	D	9	GLU
4	D	40	LEU
4	D	52	SER
4	D	53	ILE
4	D	59	LEU
4	D	62	LEU
4	D	99	GLU
4	D	107	ILE
4	D	110	THR
4	D	116	VAL
4	D	147	LYS
5	E	29	LEU

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Mol	Chain	Res	Type
5	E	41	LEU
5	E	70	VAL
5	E	79	LYS
5	E	80	GLU
5	E	109	VAL
6	F	6	VAL
6	F	10	GLU
6	F	19	GLU
6	F	20	VAL
6	F	33	ILE
6	F	37	LYS
6	F	44	GLU
6	F	46	PRO
6	F	52	ILE
6	F	58	VAL
6	F	65	ASP
6	F	74	LEU
6	F	95	GLN
6	F	98	HIS
7	G	5	LYS
7	G	14	ARG
7	G	17	ARG
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	41	HIS
7	G	42	ARG
7	G	48	ILE
7	G	55	ILE
7	G	68	THR
7	G	78	LEU
8	H	19	ARG
8	H	21	PRO
8	H	29	CYS
8	H	41	LYS
8	H	51	SER
8	H	52	VAL
8	H	53	CYS
8	H	57	ARG
8	H	60	TYR
8	H	67	SER
8	H	69	VAL

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Mol	Chain	Res	Type
8	H	82	PRO
9	I	2	THR
9	I	8	GLN
9	I	21	ILE
9	I	26	MET
9	I	41	GLU
9	I	42	LYS
9	I	44	LYS
9	I	64	ARG
10	J	2	GLU
10	J	5	VAL
10	J	8	LYS
10	J	10	LYS
10	J	27	THR
10	J	30	ILE
10	J	47	LEU
11	K	7	PRO
11	K	26	VAL
11	K	30	VAL
11	K	45	VAL
12	L	7	PRO
12	L	15	VAL
12	L	22	LEU
12	L	26	THR
13	M	13	LYS
13	M	24	LEU
13	M	34	LEU
13	M	42	LYS
1	N	18	LEU
1	N	35	LEU
1	N	56	VAL
1	N	92	MET
1	N	96	ARG
1	N	105	LEU
1	N	130	PRO
1	N	136	LEU
1	N	138	HIS
1	N	146	THR
1	N	150	LEU
1	N	156	SER
1	N	158	ILE
1	N	159	LEU

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Mol	Chain	Res	Type
1	N	172	LYS
1	N	174	PRO
1	N	189	MET
1	N	199	LEU
1	N	213	ARG
1	N	215	LEU
1	N	278	MET
1	N	295	VAL
1	N	301	THR
1	N	312	ILE
1	N	318	VAL
1	N	324	LEU
1	N	336	PRO
1	N	347	LEU
1	N	354	THR
1	N	365	ILE
1	N	366	VAL
1	N	369	ASP
1	N	373	VAL
1	N	383	MET
1	N	389	ILE
1	N	444	PRO
1	N	452	THR
1	N	465	VAL
1	N	467	LEU
1	N	471	ILE
1	N	474	GLU
1	N	482	VAL
1	N	492	LEU
2	O	3	TYR
2	O	7	LEU
2	O	31	VAL
2	O	55	THR
2	O	60	GLU
2	O	66	THR
2	O	67	ILE
2	O	81	LEU
2	O	88[A]	ASP
2	O	88[B]	ASP
2	O	90[A]	ILE
2	O	90[B]	ILE
2	O	126	SER

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Mol	Chain	Res	Type
2	O	130	PRO
2	O	142	VAL
2	O	146	MET
2	O	170	LEU
2	O	171	LYS
2	O	185	MET
2	O	188	ARG
2	O	205	SER
2	O	216	LEU
3	P	11	VAL
3	P	12	ASN
3	P	13	PRO
3	P	14	SER
3	P	18	LEU
3	P	22	LEU
3	P	26	LEU
3	P	41	THR
3	P	85	LEU
3	P	112	LEU
3	P	128	GLU
3	P	131	LEU
3	P	132	LEU
3	P	137	LEU
3	P	142	VAL
3	P	159	MET
3	P	160	LEU
3	P	163	LEU
3	P	168	THR
3	P	179	SER
3	P	188	ILE
3	P	196	THR
3	P	199	VAL
3	P	213	THR
3	P	222	GLN
3	P	245	VAL
3	P	258	TRP
4	Q	9	GLU
4	Q	40	LEU
4	Q	52	SER
4	Q	53	ILE
4	Q	59	LEU
4	Q	62	LEU

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Mol	Chain	Res	Type
4	Q	99	GLU
4	Q	107	ILE
4	Q	110	THR
4	Q	116	VAL
4	Q	147	LYS
5	R	2	HIS
5	R	29	LEU
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	109	VAL
6	S	6	VAL
6	S	10	GLU
6	S	19	GLU
6	S	20	VAL
6	S	33	ILE
6	S	37	LYS
6	S	52	ILE
6	S	58	VAL
6	S	65	ASP
6	S	74	LEU
6	S	95	GLN
6	S	98	HIS
7	T	5	LYS
7	T	14	ARG
7	T	17	ARG
7	T	26	PRO
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	41	HIS
7	T	42	ARG
7	T	48	ILE
7	T	55	ILE
7	T	68	THR
7	T	78	LEU
8	U	19	ARG
8	U	29	CYS
8	U	41	LYS
8	U	51	SER
8	U	52	VAL
8	U	57	ARG

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Mol	Chain	Res	Type
8	U	60	TYR
8	U	67	SER
8	U	69	VAL
8	U	82	PRO
9	V	2	THR
9	V	8	GLN
9	V	21	ILE
9	V	26	MET
9	V	41	GLU
9	V	42	LYS
9	V	44	LYS
9	V	64	ARG
10	W	2	GLU
10	W	5	VAL
10	W	8	LYS
10	W	10	LYS
10	W	27	THR
10	W	30	ILE
10	W	47	LEU
11	X	7	PRO
11	X	26	VAL
11	X	30	VAL
11	X	45	VAL
12	Y	7	PRO
12	Y	15	VAL
12	Y	22	LEU
12	Y	26	THR
13	Z	13	LYS
13	Z	24	LEU
13	Z	34	LEU
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	61	HIS
1	A	232	GLN
1	A	368	HIS
1	A	512	ASN
2	B	103	GLN
2	B	195	GLN

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Mol	Chain	Res	Type
3	C	3	HIS
3	C	4	GLN
3	C	12	ASN
3	C	38	ASN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	133	ASN
3	C	149	HIS
3	C	222	GLN
4	D	119	GLN
4	D	132	GLN
5	E	5	HIS
7	G	67	HIS
9	I	53	ASN
10	J	3	ASN
1	N	12	HIS
1	N	61	HIS
1	N	232	GLN
1	N	368	HIS
2	O	103	GLN
3	P	3	HIS
3	P	4	GLN
3	P	12	ASN
3	P	38	ASN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	103	HIS
3	P	133	ASN
3	P	149	HIS
3	P	222	GLN
4	Q	119	GLN
4	Q	132	GLN
5	R	5	HIS
7	T	67	HIS
9	V	53	ASN
9	V	70	GLN
10	W	3	ASN
10	W	21	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	AZI	N	520	14,18	2,2,2	1.03	0	0,1,1	-	-
17	AZI	N	521	-	2,2,2	0.72	0	0,1,1	-	-
18	HEA	N	516	17,1	67,67,67	1.38	10 (14%)	81,103,103	1.42	14 (17%)
17	AZI	A	521	-	2,2,2	2.84	2 (100%)	0,1,1	-	-
18	HEA	A	515	1	67,67,67	1.12	5 (7%)	81,103,103	1.73	17 (20%)
18	HEA	A	516	17,1	67,67,67	1.50	12 (17%)	81,103,103	1.60	17 (20%)
17	AZI	A	520	14,18	2,2,2	2.92	2 (100%)	0,1,1	-	-
18	HEA	N	515	1	67,67,67	1.22	6 (8%)	81,103,103	1.50	11 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HEA	A	516	17,1	-	13/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HEA	N	515	1	-	11/36/76/76	-
18	HEA	N	516	17,1	-	13/36/76/76	-
18	HEA	A	515	1	-	11/36/76/76	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	CAA-C2A	3.82	1.61	1.51
18	N	515	HEA	C11-C3B	-3.80	1.46	1.51
18	A	516	HEA	FE-NA	3.64	2.07	1.95
18	A	516	HEA	C1D-ND	-3.48	1.34	1.40
17	A	520	AZI	N1-N2	-3.33	1.16	1.23
18	A	516	HEA	C1B-NB	-3.33	1.32	1.38
18	N	515	HEA	C1D-ND	-3.10	1.34	1.40
18	A	515	HEA	C11-C3B	-3.03	1.47	1.51
17	A	521	AZI	N3-N2	-3.02	1.17	1.23
18	N	516	HEA	C1B-NB	-3.02	1.32	1.38
18	N	516	HEA	C4B-NB	-2.96	1.35	1.40
18	A	516	HEA	CMA-C3A	-2.93	1.38	1.45
18	A	516	HEA	C1A-NA	-2.89	1.34	1.39
18	A	515	HEA	CMA-C3A	-2.87	1.39	1.45
18	A	516	HEA	CHB-C4A	2.72	1.43	1.38
18	N	516	HEA	FE-ND	2.65	2.03	1.94
17	A	521	AZI	N1-N2	-2.65	1.17	1.23
18	A	516	HEA	C3C-C2C	-2.59	1.32	1.41
18	A	516	HEA	C17-C18	2.54	1.58	1.50
18	N	515	HEA	CAD-C3D	2.51	1.57	1.51
18	N	516	HEA	C11-C3B	-2.49	1.48	1.51
18	N	516	HEA	CMD-C2D	2.45	1.55	1.50
18	N	516	HEA	FE-NA	2.44	2.03	1.95
18	A	516	HEA	C4C-NC	-2.44	1.35	1.39
17	A	520	AZI	N3-N2	-2.43	1.18	1.23
18	N	516	HEA	CMA-C3A	-2.39	1.40	1.45
18	N	516	HEA	C3C-C2C	-2.36	1.33	1.41
18	N	515	HEA	CHB-C1B	-2.36	1.33	1.39
18	A	515	HEA	C1A-C2A	-2.31	1.41	1.45
18	N	516	HEA	CAA-C2A	2.27	1.57	1.51
18	N	515	HEA	CAC-C3C	2.26	1.53	1.47
18	N	516	HEA	C1A-NA	-2.24	1.35	1.39
18	A	515	HEA	CHB-C1B	-2.21	1.34	1.39
18	N	515	HEA	CMA-C3A	-2.19	1.40	1.45
18	A	516	HEA	C4A-NA	-2.05	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C4B-C3B	2.04	1.48	1.44
18	A	516	HEA	O2D-CGD	-2.02	1.24	1.30

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C13-C14-C15	-4.72	116.81	127.62
18	A	515	HEA	C13-C14-C15	-4.53	117.25	127.62
18	N	515	HEA	C17-C18-C19	-4.40	117.55	127.62
18	A	515	HEA	C3C-C4C-NC	4.34	113.46	109.80
18	A	515	HEA	C17-C18-C19	-3.91	118.68	127.62
18	A	516	HEA	CHA-C1A-NA	-3.69	120.43	124.45
18	A	516	HEA	CHD-C4C-NC	-3.64	117.26	123.86
18	A	516	HEA	C3A-C2A-C1A	-3.64	103.61	107.05
18	A	515	HEA	C1B-C2B-C3B	3.56	110.91	106.80
18	A	515	HEA	C4B-C3B-C2B	-3.51	101.53	107.44
18	A	515	HEA	C27-C19-C20	3.51	121.32	115.23
18	A	515	HEA	C27-C19-C18	-3.42	114.85	123.63
18	A	516	HEA	CBD-CAD-C3D	3.38	121.87	112.53
18	N	515	HEA	C3C-C4C-NC	3.37	112.64	109.80
18	A	515	HEA	C17-C16-C15	-3.22	102.50	113.19
18	N	515	HEA	C17-C16-C15	-3.17	102.68	113.19
18	A	516	HEA	C2A-C1A-NA	3.15	113.36	110.32
18	N	516	HEA	C17-C18-C19	-2.96	120.86	127.62
18	N	515	HEA	C27-C19-C18	-2.95	116.05	123.63
18	A	516	HEA	O11-C11-C12	-2.92	101.40	109.14
18	N	515	HEA	C27-C19-C20	2.90	120.25	115.23
18	N	516	HEA	O11-C11-C12	-2.84	101.62	109.14
18	A	516	HEA	CMB-C2B-C3B	-2.79	124.88	130.28
18	N	516	HEA	C2A-C1A-NA	2.78	113.01	110.32
18	N	516	HEA	C25-C23-C24	2.78	120.99	114.59
18	A	516	HEA	CHB-C4A-NA	-2.75	121.46	124.45
18	N	516	HEA	C4B-C3B-C2B	-2.74	102.83	107.44
18	N	516	HEA	CMB-C2B-C3B	-2.73	124.99	130.28
18	A	515	HEA	O11-C11-C12	-2.65	102.12	109.14
18	A	516	HEA	C25-C23-C24	2.62	120.62	114.59
18	N	515	HEA	C4D-C3D-C2D	-2.60	103.10	106.89
18	N	515	HEA	C1B-C2B-C3B	2.58	109.78	106.80
18	A	516	HEA	C17-C18-C19	-2.55	121.80	127.62
18	N	516	HEA	CHB-C4A-NA	-2.54	121.68	124.45
18	N	516	HEA	CMC-C2C-C1C	2.52	129.25	125.42
18	A	516	HEA	CHB-C1B-NB	-2.51	121.72	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C2D-C1D-ND	2.50	112.72	109.84
18	A	516	HEA	CMC-C2C-C1C	2.48	129.20	125.42
18	N	515	HEA	C12-C13-C14	-2.42	105.80	112.16
18	N	516	HEA	C3B-C4B-NB	2.41	112.61	109.84
18	N	516	HEA	C3A-C2A-C1A	-2.39	104.78	107.05
18	A	515	HEA	CMB-C2B-C3B	-2.37	125.68	130.28
18	N	515	HEA	CHC-C4B-NB	-2.35	121.46	124.37
18	N	516	HEA	C1D-C2D-C3D	-2.33	104.53	106.98
18	A	516	HEA	C2D-C1D-ND	2.32	112.51	109.84
18	A	516	HEA	C4B-C3B-C2B	-2.31	103.55	107.44
18	A	515	HEA	C3D-C4D-ND	2.30	112.58	110.35
18	A	515	HEA	C3B-C4B-NB	2.28	112.46	109.84
18	N	516	HEA	CBA-CAA-C2A	2.26	118.77	112.53
18	A	516	HEA	C1B-C2B-C3B	2.22	109.36	106.80
18	A	516	HEA	C12-C11-C3B	2.15	115.48	112.12
18	N	515	HEA	CMB-C2B-C3B	-2.15	126.12	130.28
18	N	516	HEA	CHD-C4C-NC	-2.15	119.97	123.86
18	A	515	HEA	C26-C15-C16	2.14	118.94	115.23
18	N	516	HEA	C1B-C2B-C3B	2.13	109.26	106.80
18	A	515	HEA	CHC-C4B-NB	-2.13	121.73	124.37
18	A	515	HEA	CBA-CAA-C2A	2.11	118.38	112.53
18	A	515	HEA	C12-C13-C14	-2.07	106.71	112.16
18	A	516	HEA	C26-C15-C14	-2.02	118.45	123.63

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C2A-C3A-CMA-OMA
18	A	515	HEA	C4A-C3A-CMA-OMA
18	A	515	HEA	C12-C11-C3B-C2B
18	A	516	HEA	C2A-C3A-CMA-OMA
18	A	516	HEA	C4A-C3A-CMA-OMA
18	A	516	HEA	C2D-C3D-CAD-CBD
18	A	516	HEA	C4D-C3D-CAD-CBD
18	N	515	HEA	C2A-C3A-CMA-OMA
18	N	515	HEA	C4A-C3A-CMA-OMA
18	N	515	HEA	C12-C11-C3B-C2B
18	N	516	HEA	C2A-C3A-CMA-OMA
18	N	516	HEA	C4A-C3A-CMA-OMA
18	N	516	HEA	C2D-C3D-CAD-CBD
18	N	516	HEA	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
18	A	516	HEA	C21-C22-C23-C25
18	N	516	HEA	C21-C22-C23-C25
18	N	515	HEA	C21-C22-C23-C25
18	N	516	HEA	C21-C22-C23-C24
18	A	516	HEA	C21-C22-C23-C24
18	A	515	HEA	C15-C16-C17-C18
18	N	515	HEA	C15-C16-C17-C18
18	A	515	HEA	C21-C22-C23-C25
18	N	515	HEA	C21-C22-C23-C24
18	A	516	HEA	C4C-C3C-CAC-CBC
18	A	516	HEA	C2C-C3C-CAC-CBC
18	A	515	HEA	C21-C22-C23-C24
18	N	515	HEA	C13-C14-C15-C26
18	N	516	HEA	C4C-C3C-CAC-CBC
18	N	516	HEA	C2C-C3C-CAC-CBC
18	A	515	HEA	C13-C14-C15-C26
18	A	516	HEA	CAA-CBA-CGA-O2A
18	A	516	HEA	CAA-CBA-CGA-O1A
18	N	516	HEA	CAA-CBA-CGA-O2A
18	A	515	HEA	CAA-CBA-CGA-O1A
18	N	516	HEA	CAA-CBA-CGA-O1A
18	N	515	HEA	CAA-CBA-CGA-O1A
18	A	515	HEA	CAD-CBD-CGD-O1D
18	N	515	HEA	CAD-CBD-CGD-O1D
18	A	515	HEA	CAD-CBD-CGD-O2D
18	N	515	HEA	CAD-CBD-CGD-O2D
18	N	515	HEA	CAA-CBA-CGA-O2A
18	A	515	HEA	CAA-CBA-CGA-O2A
18	A	516	HEA	CAD-CBD-CGD-O2D
18	N	516	HEA	CAD-CBD-CGD-O2D
18	N	516	HEA	CAD-CBD-CGD-O1D
18	A	516	HEA	CAD-CBD-CGD-O1D
18	A	516	HEA	C26-C15-C16-C17
18	N	516	HEA	C26-C15-C16-C17

There are no ring outliers.

6 monomers are involved in 32 short contacts:

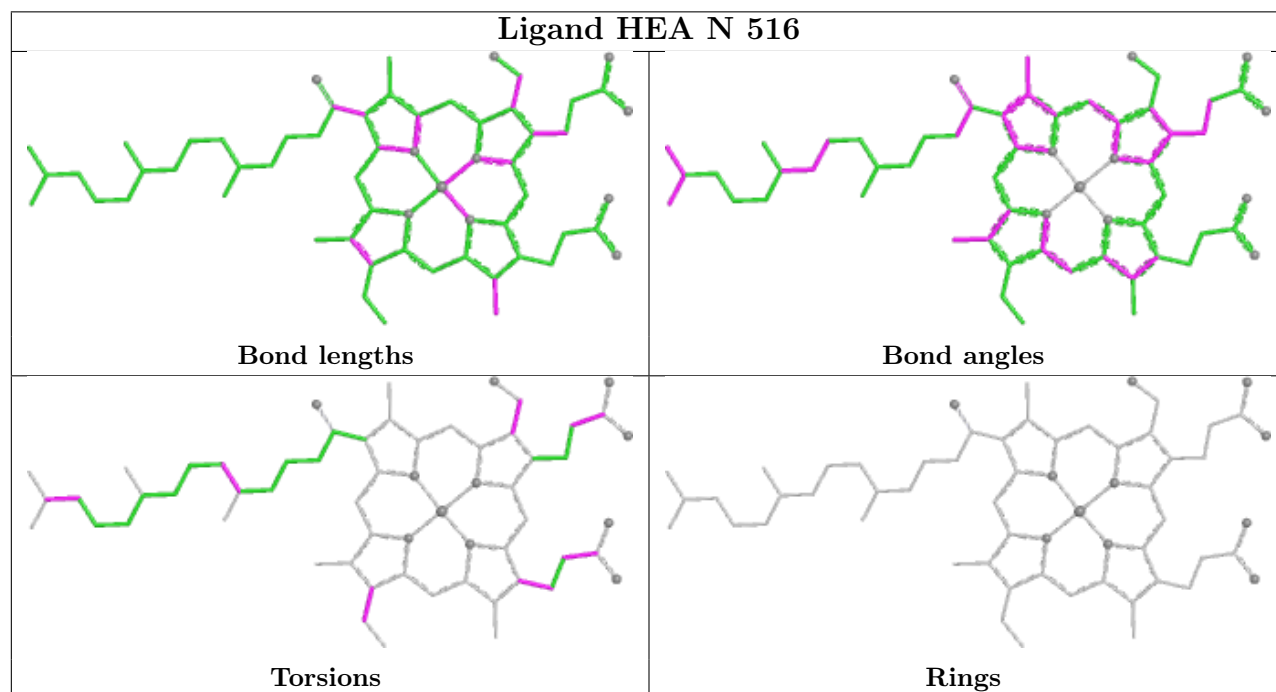
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	521	AZI	4	0
18	N	516	HEA	9	0
18	A	515	HEA	7	0

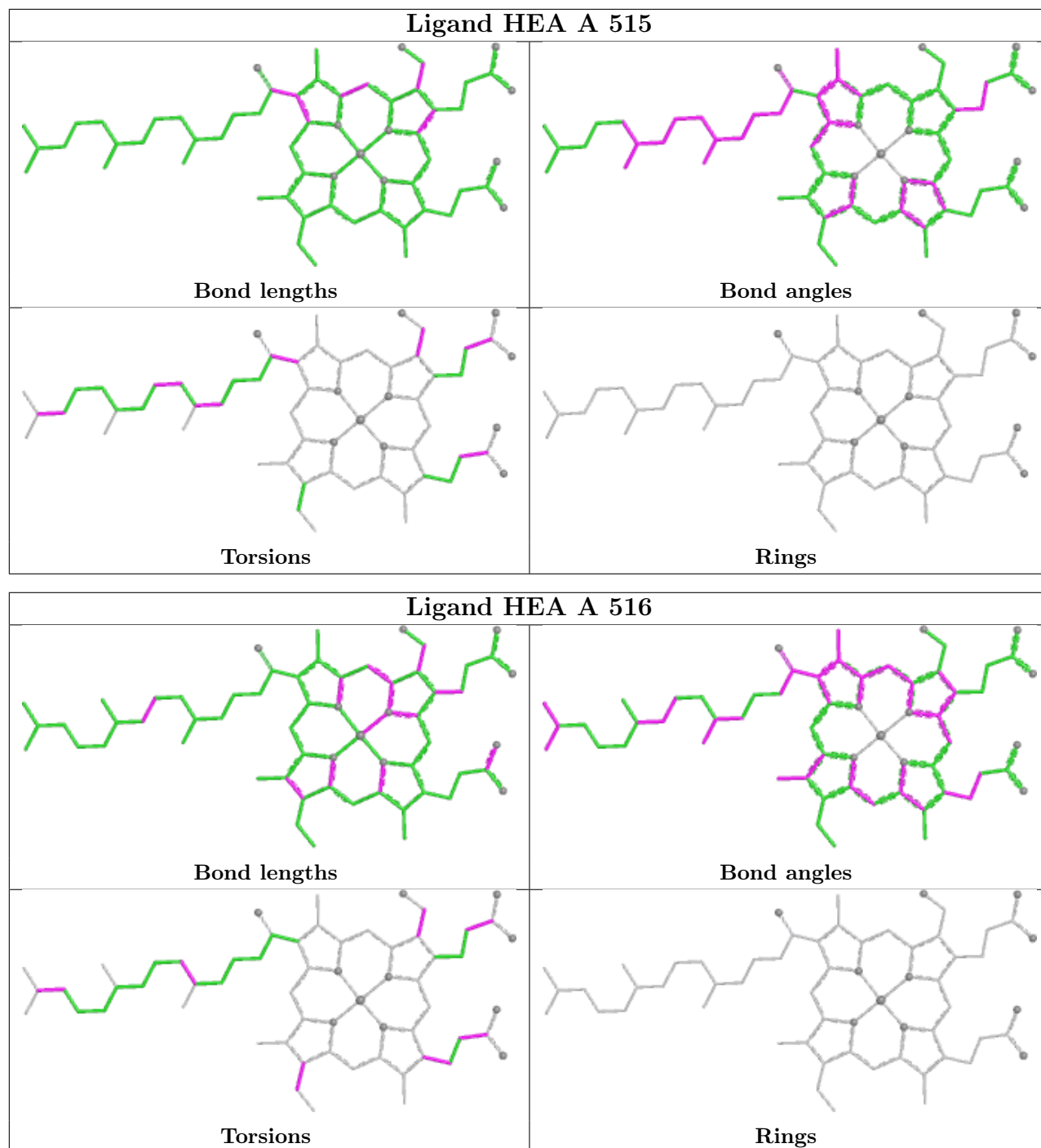
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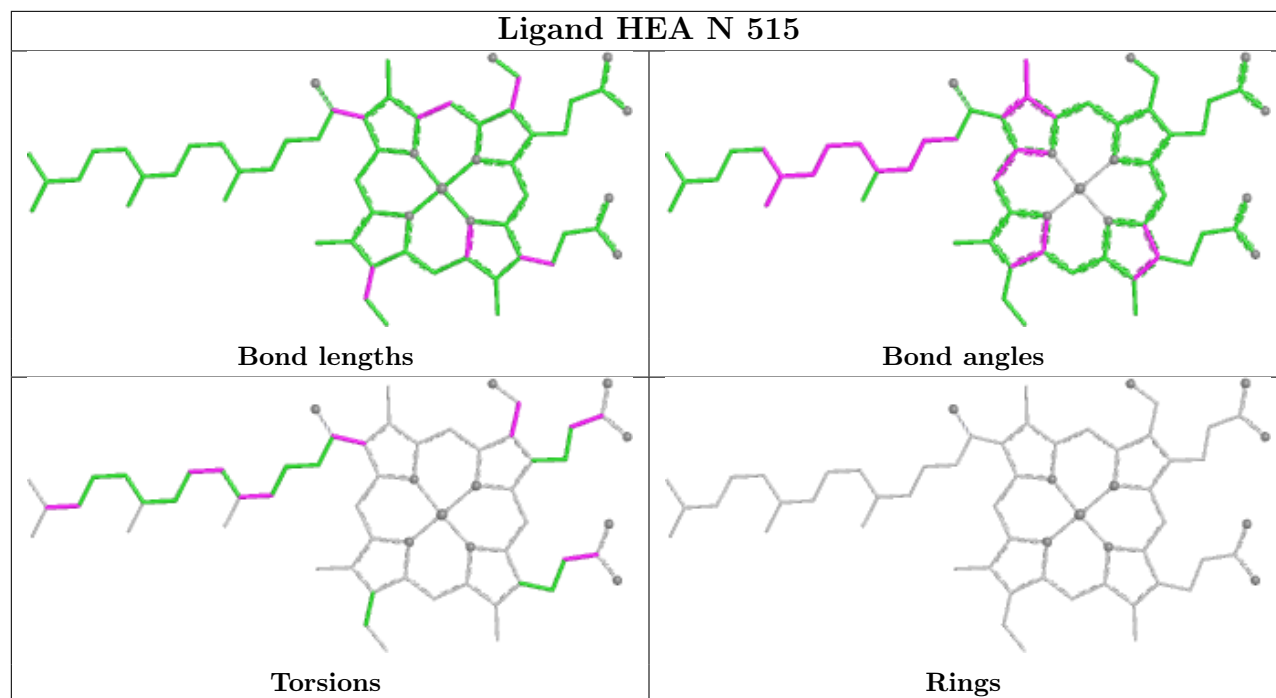
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	516	HEA	7	0
17	A	520	AZI	1	0
18	N	515	HEA	4	0

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.