



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:02 PM EDT

PDB ID : 1KYO / pdb_00001kyo
Title : YEAST CYTOCHROME BC1 COMPLEX WITH BOUND SUBSTRATE
CYTOCHROME C
Authors : Lange, C.; Hunte, C.
Deposited on : 2002-02-05
Resolution : 2.97 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

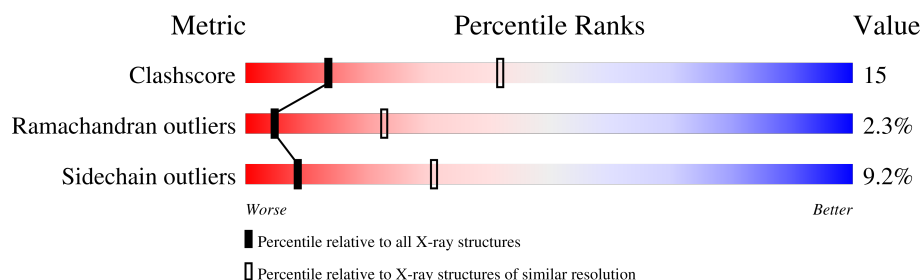
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)

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	430	66% 30% .
1	L	430	61% 33% 6%
2	B	352	55% 36% 9% .
2	M	352	55% 35% 8% .
3	C	385	67% 28% 5%
3	N	385	68% 27% . .
4	D	248	77% 20% . .
4	O	248	73% 25% . .

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Mol	Chain	Length	Quality of chain
5	E	185	
5	P	185	
6	F	74	
6	Q	74	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	57	
9	T	57	
10	J	127	
10	U	127	
11	K	107	
11	V	107	
12	W	108	

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
13	HEC	C	501	X	-	-	-
13	HEC	C	502	X	-	-	-
13	HEC	D	503	X	-	-	-
13	HEC	N	521	X	-	-	-
13	HEC	N	522	X	-	-	-
13	HEC	O	523	X	-	-	-
13	HEC	W	526	X	-	-	-
14	SMA	C	505	X	-	-	-
14	SMA	N	525	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 35643 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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			
1	L	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P07256
A	152	ASP	GLU	conflict	UNP P07256
L	?	-	SER	deletion	UNP P07256
L	152	ASP	GLU	conflict	UNP P07256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			
2	M	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			
3	N	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	270	VAL	ASP	SEE REMARK 999	UNP P00163
N	270	VAL	ASP	SEE REMARK 999	UNP P00163

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1929	1229	332	359	9			
4	O	245	Total	C	N	O	S	0	0	0
			1929	1229	332	359	9			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			
5	P	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			625	390	108	125	2			
6	Q	74	Total	C	N	O	S	0	0	0
			625	390	108	125	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	74	ASP	VAL	conflict	UNP P00127
Q	74	ASP	VAL	conflict	UNP P00127

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			
7	R	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	53	Total	C	N	O	0	0	0
			436	292	71	73			
9	T	53	Total	C	N	O	0	0	0
			436	292	71	73			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	55	LYS	ARG	conflict	UNP P22289
T	55	LYS	ARG	conflict	UNP P22289

- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			
10	U	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			
11	V	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

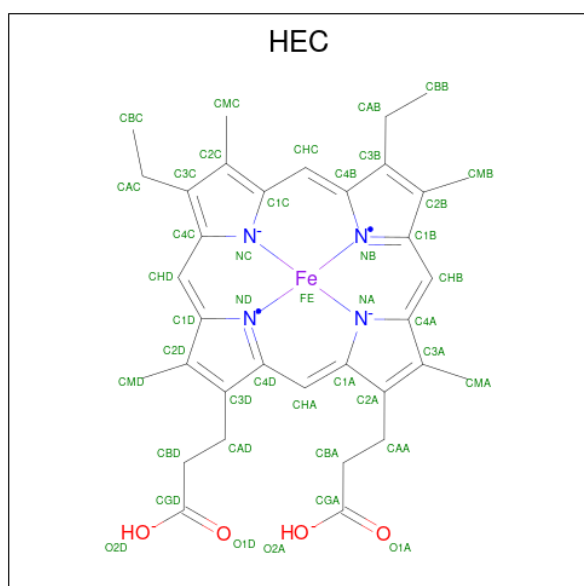
- Molecule 12 is a protein called CYTOCHROME C, ISO-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	0	0
			850	537	151	157	5			

There is a discrepancy between the modelled and reference sequences:

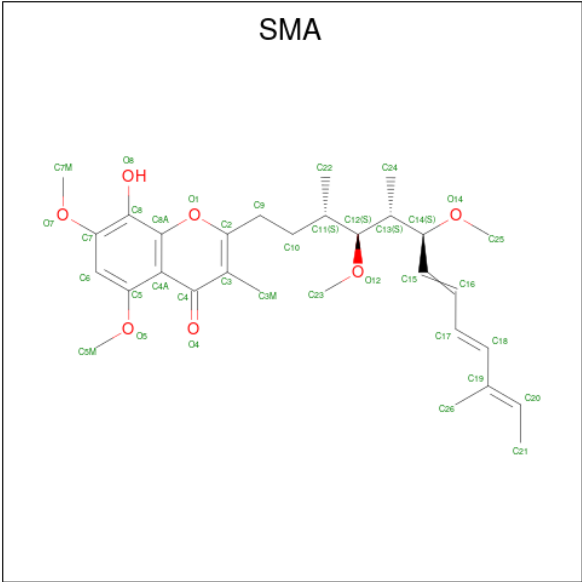
Chain	Residue	Modelled	Actual	Comment	Reference
W	77	M3L	LYS	modified residue	UNP P00044

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



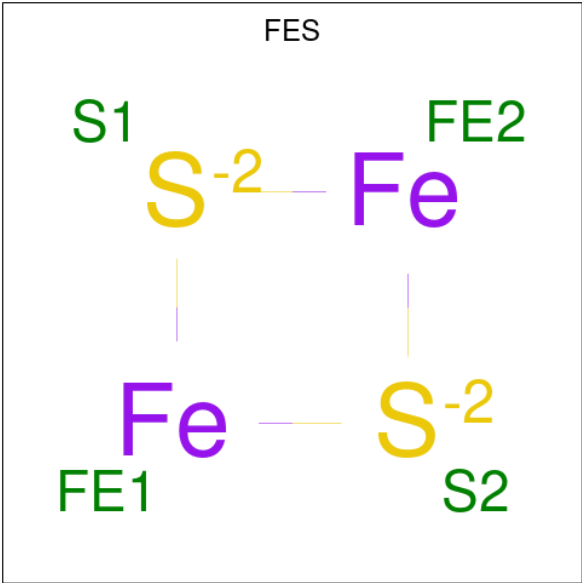
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4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

- Molecule 14 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			37	30	7		
14	N	1	Total	C	O	0	0
			37	30	7		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



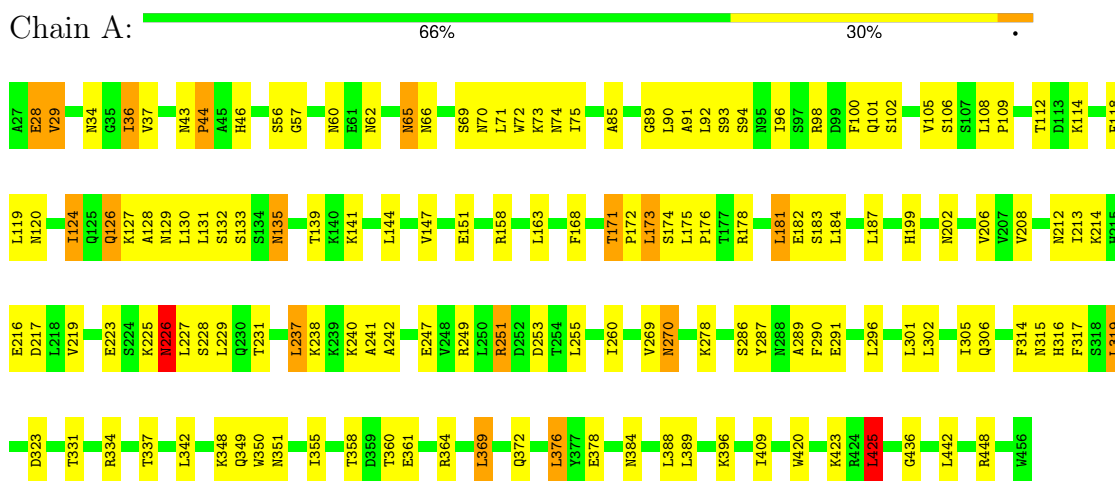
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	E	1	Total	Fe	S	0	0
			4	2	2		
15	P	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots

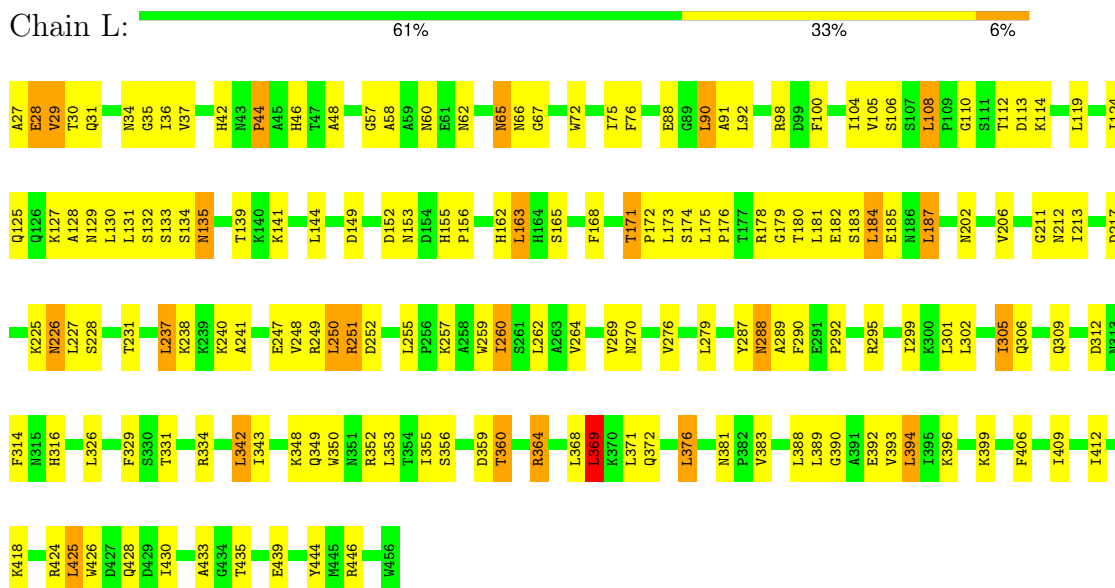
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

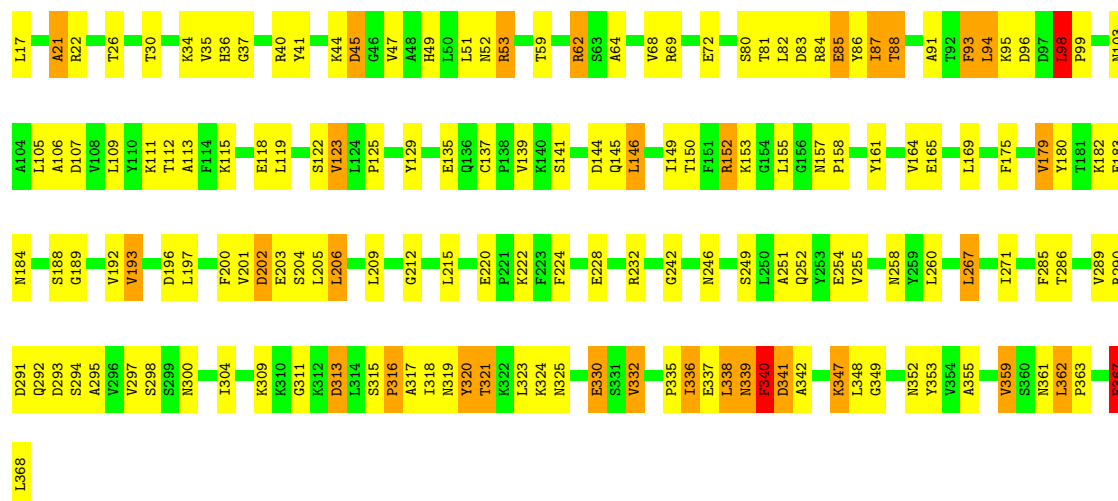


- Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I



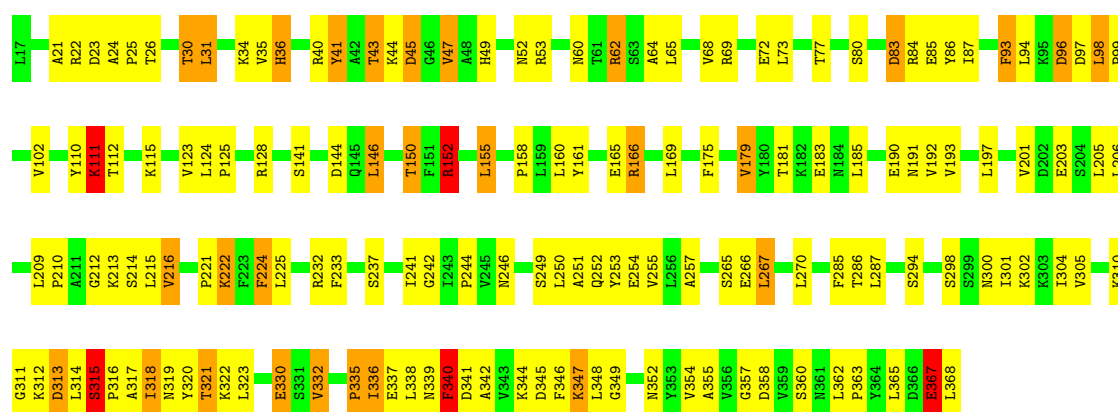
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN
2

Chain B: 



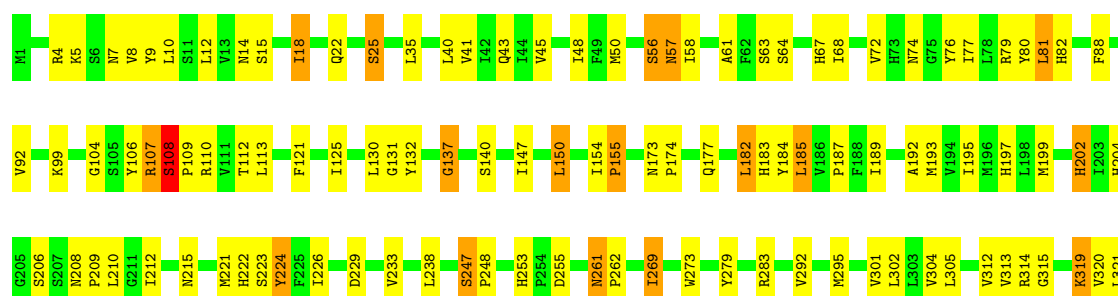
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN
2

Chain M: 



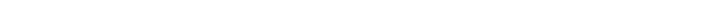
• Molecule 3: CYTOCHROME B

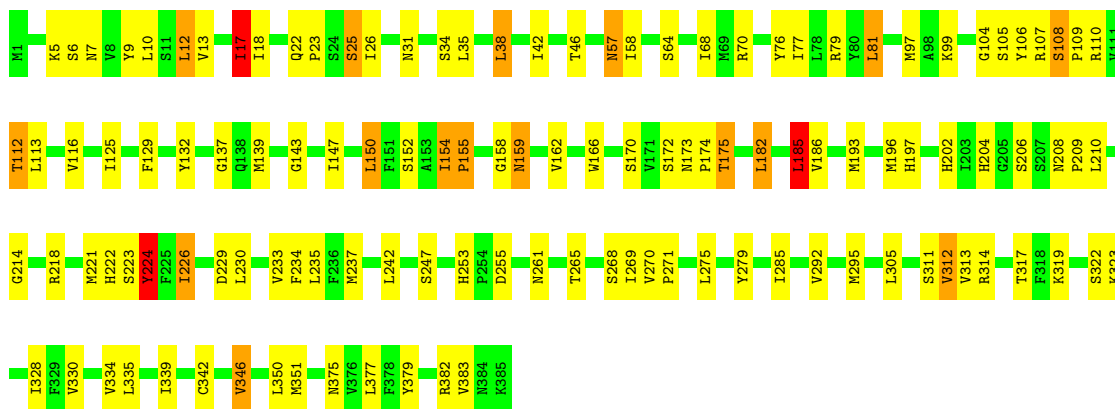
Chain C: 



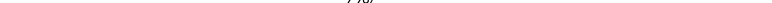


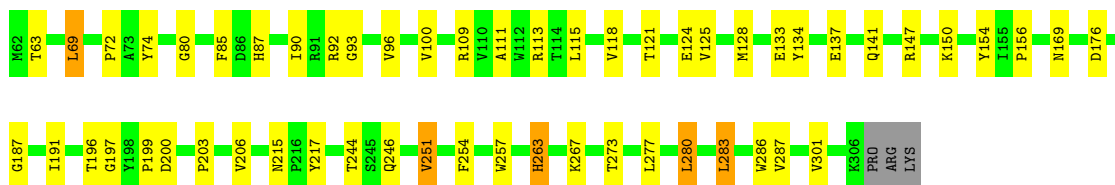
- Molecule 3: CYTOCHROME B

Chain N:  68% 27% .

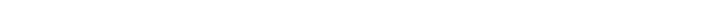


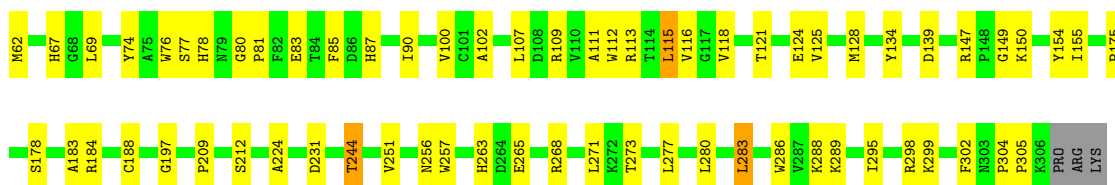
- Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain D:  77% 20% 3%



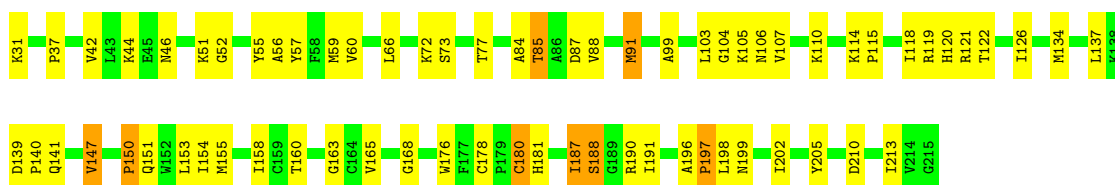
- Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain O:  73% 25%

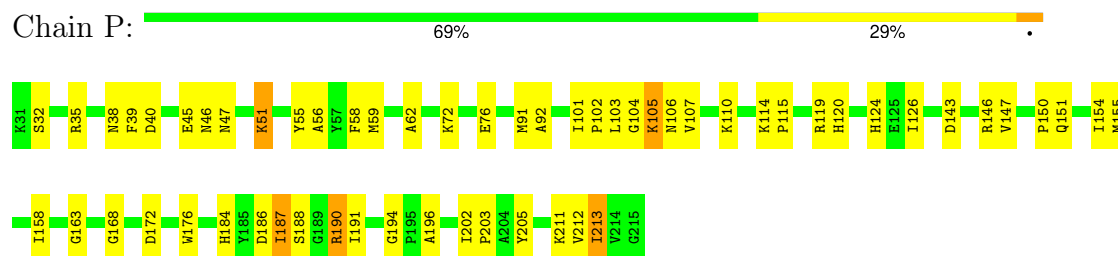


- Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

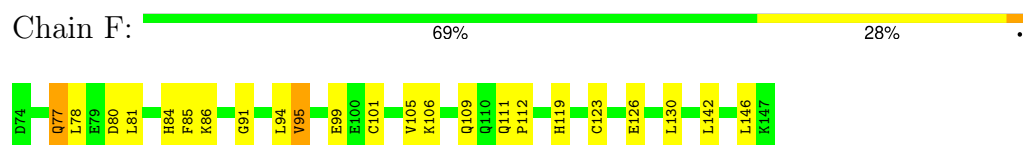
Chain E:  63% 32% .



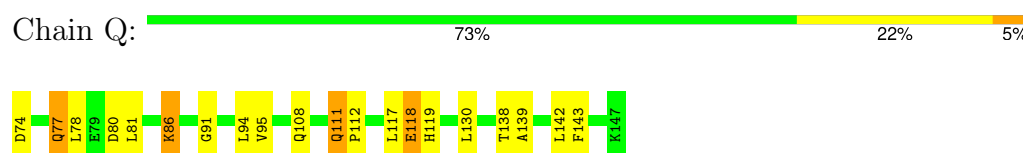
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT



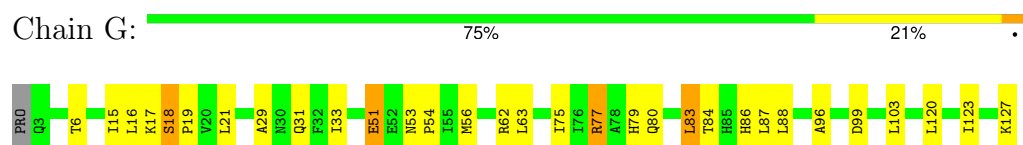
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN



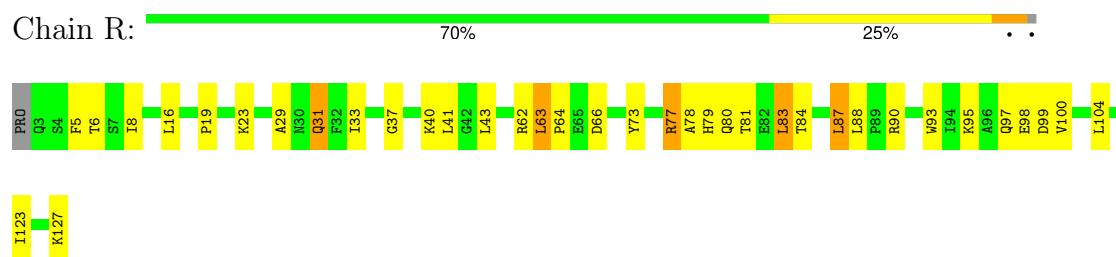
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN



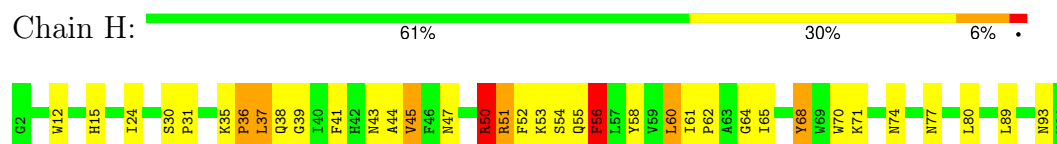
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN



• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

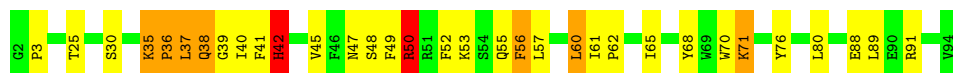


• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



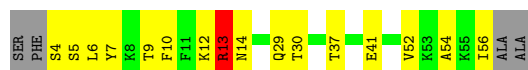
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain S: 



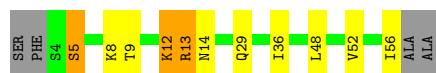
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I: 



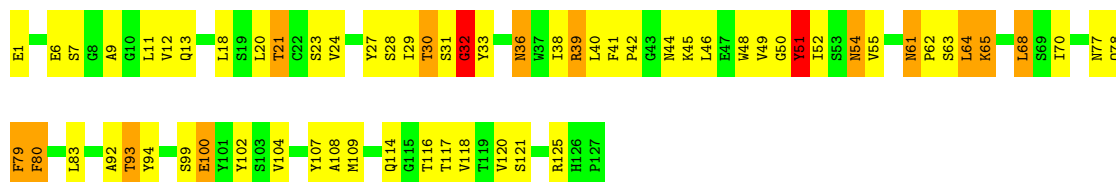
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain T: 



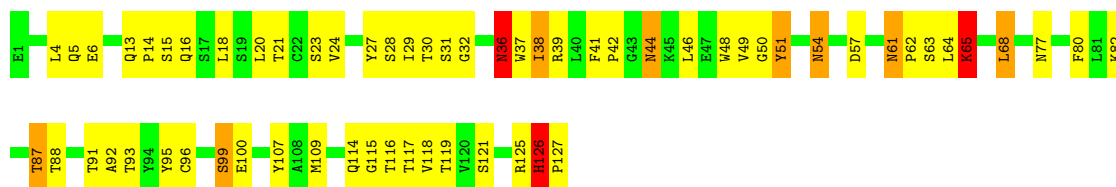
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J: 



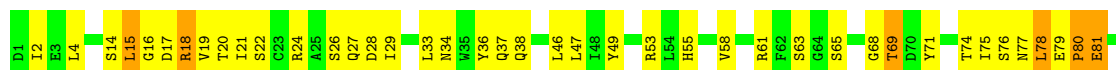
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain U: 



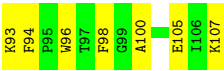
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K: 

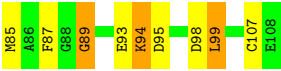
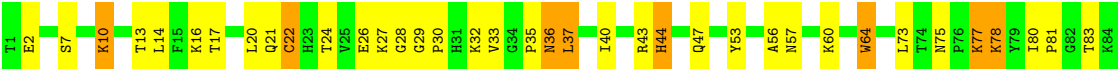




● Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



● Molecule 12: CYTOCHROME C, ISO-1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.22Å 165.53Å 195.89Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	29.64 – 2.97	Depositor
% Data completeness (in resolution range)	93.7 (29.64-2.97)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35643	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: M3L, HEC, FES, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/3399	0.97	13/4606 (0.3%)
1	L	0.49	0/3399	1.00	13/4606 (0.3%)
2	B	0.45	0/2781	1.10	24/3764 (0.6%)
2	M	0.46	0/2781	1.08	18/3764 (0.5%)
3	C	0.60	1/3191 (0.0%)	1.10	19/4353 (0.4%)
3	N	0.60	0/3191	1.12	22/4353 (0.5%)
4	D	0.50	0/1989	1.05	10/2710 (0.4%)
4	O	0.50	0/1989	1.04	5/2710 (0.2%)
5	E	0.52	0/1444	1.11	14/1957 (0.7%)
5	P	0.50	0/1444	1.12	11/1957 (0.6%)
6	F	0.41	0/639	0.94	1/859 (0.1%)
6	Q	0.42	0/639	1.02	2/859 (0.2%)
7	G	0.49	0/1032	1.09	5/1397 (0.4%)
7	R	0.51	0/1032	1.05	5/1397 (0.4%)
8	H	0.53	0/804	1.09	5/1088 (0.5%)
8	S	0.54	0/804	1.09	5/1088 (0.5%)
9	I	0.42	0/449	0.92	1/605 (0.2%)
9	T	0.45	0/449	0.95	1/605 (0.2%)
10	J	0.42	0/1043	0.98	5/1422 (0.4%)
10	U	0.43	0/1043	0.94	4/1422 (0.3%)
11	K	0.44	0/863	0.89	2/1172 (0.2%)
11	V	0.43	0/863	0.89	0/1172
12	W	0.62	0/856	1.11	5/1145 (0.4%)
All	All	0.50	1/36124 (0.0%)	1.05	190/49011 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	367	VAL	CA-CB	5.01	1.56	1.54

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	53	LYS	N-CA-C	-11.72	99.19	114.31
8	S	50	ARG	N-CA-C	-9.62	101.53	113.18
8	S	53	LYS	N-CA-C	-9.16	102.61	113.88
1	L	424	ARG	N-CA-C	9.08	121.26	111.36
10	U	32	GLY	N-CA-C	8.69	133.77	113.18
2	B	340	PHE	N-CA-C	-8.33	93.80	108.13
2	M	111	LYS	N-CA-C	8.25	120.34	110.44
8	H	50	ARG	N-CA-C	-8.25	102.66	112.89
3	C	261	ASN	CA-C-N	8.19	127.91	119.56
3	C	261	ASN	C-N-CA	8.19	127.91	119.56
2	B	123	VAL	N-CA-C	8.15	118.21	110.30
2	B	84	ARG	N-CA-C	-8.12	103.38	113.28
2	B	111	LYS	N-CA-C	8.10	122.89	111.30
2	B	323	LEU	N-CA-C	-8.09	103.54	113.41
1	A	135	ASN	N-CA-C	-8.06	103.40	113.55
2	B	341	ASP	N-CA-C	-8.04	101.58	113.40
4	D	100	VAL	N-CA-C	8.00	117.94	111.62
2	M	340	PHE	N-CA-C	-7.95	93.87	110.80
5	E	139	ASP	CA-C-N	7.79	127.78	119.76
5	E	139	ASP	C-N-CA	7.79	127.78	119.76
1	A	128	ALA	N-CA-C	-7.76	104.42	114.04
2	M	84	ARG	N-CA-C	-7.67	103.38	112.89
5	E	163	GLY	N-CA-C	7.66	126.66	115.32
3	N	17	ILE	CB-CA-C	-7.59	102.58	110.93
3	N	154	ILE	CA-C-N	7.53	129.25	119.84
3	N	154	ILE	C-N-CA	7.53	129.25	119.84
5	P	46	ASN	N-CA-C	7.49	121.60	110.52
2	B	220	GLU	CA-C-N	7.42	129.11	119.84
2	B	220	GLU	C-N-CA	7.42	129.11	119.84
2	B	179	VAL	N-CA-C	7.36	119.02	111.00
4	O	100	VAL	N-CA-C	7.33	117.41	111.62
10	J	32	GLY	N-CA-C	7.33	130.55	113.18
5	P	194	GLY	CA-C-N	7.32	126.95	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	194	GLY	C-N-CA	7.32	126.95	119.56
1	L	153	ASN	N-CA-C	7.18	121.91	112.72
3	N	261	ASN	CA-C-N	7.16	126.83	119.82
3	N	261	ASN	C-N-CA	7.16	126.83	119.82
2	B	113	ALA	N-CA-C	7.08	120.03	111.82
2	M	155	LEU	N-CA-C	-7.07	104.62	113.18
1	A	355	ILE	N-CA-C	7.04	120.00	112.96
2	M	141	SER	N-CA-C	-6.98	104.92	113.50
5	E	188	SER	N-CA-C	-6.97	104.43	114.12
5	E	121	ARG	N-CA-C	6.91	119.98	110.24
1	L	356	SER	N-CA-C	6.83	121.59	112.30
2	M	96	ASP	N-CA-C	6.83	118.72	111.28
1	L	128	ALA	N-CA-C	-6.82	105.59	114.04
3	C	346	VAL	N-CA-C	6.77	123.51	108.88
2	B	202	ASP	N-CA-C	-6.76	101.81	110.53
3	C	25	SER	N-CA-C	6.72	121.09	113.02
3	N	346	VAL	N-CA-C	6.69	123.34	108.88
5	E	165	VAL	CA-C-N	6.64	126.62	119.78
5	E	165	VAL	C-N-CA	6.64	126.62	119.78
5	P	105	LYS	N-CA-C	6.60	119.75	109.52
3	C	137	GLY	N-CA-C	-6.54	102.25	112.58
3	C	348	TYR	N-CA-C	6.53	120.46	112.23
5	P	163	GLY	N-CA-C	6.53	124.99	115.32
7	G	6	THR	N-CA-C	-6.44	104.26	111.28
3	N	202	HIS	N-CA-C	6.43	120.71	112.34
1	L	355	ILE	N-CA-C	6.43	117.52	112.12
12	W	64	TRP	N-CA-C	6.42	119.08	109.25
1	A	442	LEU	N-CA-C	6.39	118.27	110.41
6	F	86	LYS	N-CA-C	-6.38	104.42	111.82
3	C	154	ILE	CA-C-N	6.36	127.79	119.84
3	C	154	ILE	C-N-CA	6.36	127.79	119.84
3	N	265	THR	N-CA-C	-6.36	101.78	109.72
3	N	25	SER	N-CA-C	6.34	120.87	113.20
10	J	104	VAL	N-CA-C	6.32	117.88	111.00
3	N	226	ILE	N-CA-C	-6.31	104.35	110.72
8	S	35	LYS	CA-C-N	6.30	127.72	119.84
8	S	35	LYS	C-N-CA	6.30	127.72	119.84
9	T	5	SER	N-CA-C	-6.29	105.25	113.17
7	G	51	GLU	N-CA-C	6.27	121.07	113.17
3	C	226	ILE	N-CA-C	-6.26	104.39	110.72
1	A	306	GLN	N-CA-C	6.25	120.64	112.89
3	N	185	LEU	N-CA-C	6.23	117.87	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	18	ILE	N-CA-C	6.23	117.34	111.48
3	N	143	GLY	N-CA-C	-6.22	104.80	112.77
2	M	160	LEU	N-CA-C	6.22	119.78	110.14
3	C	202	HIS	N-CA-C	6.21	119.96	112.38
4	D	169	ASN	N-CA-C	6.21	118.37	110.61
2	B	93	PHE	N-CA-C	6.20	116.27	108.45
10	U	65	LYS	N-CA-C	6.20	124.01	110.80
3	N	247	SER	CA-C-N	6.20	126.66	119.47
3	N	247	SER	C-N-CA	6.20	126.66	119.47
2	B	359	VAL	N-CA-C	6.17	116.34	110.42
11	K	65	SER	N-CA-C	6.11	116.15	108.45
2	B	316	PRO	N-CA-C	-6.08	106.55	114.03
12	W	56	ALA	N-CA-C	6.05	117.87	111.28
7	R	87	LEU	N-CA-C	-6.00	100.64	109.81
2	M	166	ARG	N-CA-C	5.99	118.68	110.24
1	L	100	PHE	N-CA-C	5.95	116.13	108.34
3	C	273	TRP	N-CA-C	5.94	118.23	111.11
4	D	215	ASN	CA-C-N	5.91	126.33	119.47
4	D	215	ASN	C-N-CA	5.91	126.33	119.47
3	N	137	GLY	N-CA-C	-5.91	103.25	112.58
1	L	369	LEU	N-CA-C	-5.91	104.48	111.03
1	A	199	HIS	N-CA-C	5.90	120.27	112.72
5	P	45	GLU	N-CA-C	-5.89	98.25	110.80
5	E	46	ASN	N-CA-C	5.89	118.88	110.10
5	E	180	CYS	N-CA-C	5.89	117.37	111.07
4	D	196	THR	N-CA-C	5.87	118.91	111.69
7	G	18	SER	CA-C-N	5.82	127.11	119.84
7	G	18	SER	C-N-CA	5.82	127.11	119.84
3	C	305	LEU	N-CA-C	5.81	121.41	113.16
2	B	87	ILE	N-CA-C	-5.79	97.30	109.34
12	W	37	LEU	N-CA-C	5.79	120.12	112.25
8	H	54	SER	N-CA-C	-5.77	105.00	112.68
7	R	63	LEU	CA-C-N	5.74	125.75	119.90
7	R	63	LEU	C-N-CA	5.74	125.75	119.90
3	C	328	ILE	N-CA-C	-5.74	104.93	110.72
6	Q	143	PHE	N-CA-C	5.72	119.36	112.38
2	B	129	TYR	N-CA-C	-5.70	104.70	111.03
7	R	37	GLY	N-CA-C	5.70	123.18	115.32
4	D	85	PHE	N-CA-C	-5.67	103.43	110.41
5	E	155	MET	N-CA-C	5.67	116.04	108.38
1	A	334	ARG	N-CA-C	-5.66	106.36	113.72
2	B	336	ILE	N-CA-C	5.65	121.10	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	LYS	N-CA-C	5.65	117.89	111.11
2	M	332	VAL	N-CA-C	5.63	121.05	109.34
1	L	35	GLY	N-CA-C	-5.63	99.84	113.18
2	M	87	ILE	N-CA-C	-5.62	97.64	109.34
9	I	13	ARG	N-CA-C	5.61	119.43	112.47
4	O	178	SER	N-CA-C	5.61	118.93	111.75
3	N	197	HIS	N-CA-C	-5.60	105.17	111.28
5	P	101	ILE	N-CA-C	5.60	113.09	107.55
3	N	70	ARG	N-CA-C	5.59	120.23	112.90
5	P	188	SER	N-CA-C	-5.59	106.45	113.72
3	C	68	ILE	N-CA-C	-5.58	105.08	110.72
3	C	247	SER	CA-C-N	5.58	125.94	119.47
3	C	247	SER	C-N-CA	5.58	125.94	119.47
5	E	87	ASP	N-CA-C	5.54	119.51	112.87
2	M	102	VAL	N-CA-C	-5.54	106.30	111.45
1	A	425	LEU	N-CA-C	5.53	119.75	111.96
3	N	305	LEU	N-CA-C	5.52	122.02	109.81
8	S	60	LEU	N-CA-C	5.52	117.73	111.11
2	B	309	LYS	N-CA-C	-5.49	105.45	111.82
3	C	185	LEU	N-CA-C	5.49	116.95	110.97
10	U	44	ASN	N-CA-C	5.46	118.87	111.17
1	L	342	LEU	N-CA-C	-5.46	105.23	111.07
5	E	84	ALA	N-CA-C	5.45	118.38	110.42
8	H	45	VAL	N-CA-C	-5.44	107.13	111.81
4	O	107	LEU	N-CA-C	-5.43	103.82	110.61
1	L	135	ASN	N-CA-C	-5.39	106.75	113.55
2	M	315	SER	N-CA-C	5.38	121.69	109.81
8	H	51	ARG	N-CA-C	-5.31	101.04	109.96
1	L	425	LEU	N-CA-C	5.30	119.73	112.68
5	P	101	ILE	CA-C-N	5.29	126.45	119.84
5	P	101	ILE	C-N-CA	5.29	126.45	119.84
2	M	30	THR	N-CA-C	5.28	116.18	107.20
1	A	331	THR	N-CA-C	5.28	116.55	108.52
4	D	80	GLY	CA-C-N	5.27	126.43	119.84
4	D	80	GLY	C-N-CA	5.27	126.43	119.84
2	M	93	PHE	N-CA-C	5.26	116.00	108.74
1	L	104	ILE	N-CA-C	5.26	116.05	108.48
5	P	47	ASN	N-CA-C	-5.26	106.65	114.64
11	K	53	ARG	N-CA-C	5.24	117.76	109.96
4	D	176	ASP	N-CA-C	-5.23	102.11	109.96
6	Q	86	LYS	N-CA-C	-5.23	106.40	112.89
1	A	102	SER	N-CA-C	5.23	117.13	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	178	CYS	CA-C-N	5.20	124.81	119.56
5	E	178	CYS	C-N-CA	5.20	124.81	119.56
12	W	17	THR	N-CA-C	5.19	117.02	111.36
7	G	87	LEU	N-CA-C	-5.19	101.65	109.85
1	A	70	ASN	N-CA-C	-5.19	105.75	111.71
10	U	36	ASN	N-CA-C	5.19	117.76	110.14
2	B	321	THR	N-CA-C	-5.19	106.79	113.01
2	B	59	THR	N-CA-C	-5.18	102.10	110.14
2	M	310	LYS	N-CA-C	-5.18	103.48	110.68
1	A	208	VAL	N-CA-C	5.18	116.04	108.53
2	M	330	GLU	N-CA-C	-5.17	106.78	114.64
2	M	179	VAL	N-CA-C	5.17	116.64	111.00
4	O	155	ILE	CA-C-N	5.16	125.31	119.90
4	O	155	ILE	C-N-CA	5.16	125.31	119.90
10	J	80	PHE	N-CA-C	5.15	117.11	109.69
1	L	426	TRP	N-CA-C	5.14	117.62	109.96
2	M	321	THR	N-CA-C	-5.14	106.70	112.87
7	R	104	LEU	N-CA-C	5.14	120.56	113.77
3	N	6	SER	N-CA-C	5.14	117.78	111.82
2	B	98	LEU	N-CA-C	5.13	120.54	113.77
3	N	328	ILE	N-CA-C	-5.13	105.39	110.62
10	J	55	VAL	N-CA-C	-5.10	106.71	111.45
3	C	197	HIS	N-CA-C	-5.07	105.64	111.07
2	B	141	SER	N-CA-C	-5.07	106.27	112.90
12	W	89	GLY	N-CA-C	5.06	117.20	112.04
2	B	94	LEU	N-CA-C	5.05	117.02	110.65
10	J	51	TYR	N-CA-C	5.05	114.96	108.34
4	D	118	VAL	CB-CA-C	-5.04	106.57	111.05
1	A	290	PHE	N-CA-C	5.03	119.27	113.18
3	N	285	ILE	CA-C-N	5.01	126.11	119.84
3	N	285	ILE	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	224	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3338	0	3316	94	0
1	L	3338	0	3316	105	0
2	B	2735	0	2774	104	0
2	M	2735	0	2774	110	0
3	C	3089	0	3125	90	0
3	N	3089	0	3125	91	0
4	D	1929	0	1844	26	0
4	O	1929	0	1844	44	0
5	E	1411	0	1386	48	0
5	P	1411	0	1386	41	0
6	F	625	0	576	11	0
6	Q	625	0	576	9	0
7	G	1012	0	1026	19	0
7	R	1012	0	1026	21	0
8	H	773	0	736	29	0
8	S	773	0	736	30	0
9	I	436	0	435	9	0
9	T	436	0	435	12	0
10	J	1015	0	959	51	0
10	U	1015	0	959	47	0
11	K	842	0	820	42	0
11	V	842	0	820	42	0
12	W	850	0	855	27	0
13	C	86	0	64	6	0
13	D	43	0	30	0	0
13	N	86	0	64	6	0
13	O	43	0	30	3	0
13	W	43	0	30	3	0
14	C	37	0	40	5	0
14	N	37	0	40	5	0
15	E	4	0	0	1	0
15	P	4	0	0	0	0
All	All	35643	0	35147	1031	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 15.

All (1031) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:HIS:HD2	2:B:161:TYR:H	1.08	0.97
2:M:49:HIS:HD2	2:M:161:TYR:H	1.13	0.96
7:R:31:GLN:HE21	7:R:31:GLN:HA	1.31	0.96
1:L:62:ASN:H	1:L:65:ASN:HD21	1.13	0.95
1:A:62:ASN:HB2	1:A:65:ASN:HD21	1.31	0.95
3:N:58:ILE:H	3:N:173:ASN:ND2	1.64	0.95
1:L:62:ASN:H	1:L:65:ASN:ND2	1.65	0.94
3:N:7:ASN:HD22	3:N:10:LEU:H	0.99	0.93
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.32	0.93
2:B:98:LEU:HD11	2:B:192:VAL:HG13	1.49	0.92
2:B:83:ASP:HB2	2:B:86:TYR:H	1.35	0.92
6:F:77:GLN:H	6:F:77:GLN:NE2	1.67	0.91
2:M:98:LEU:HD11	2:M:192:VAL:HG13	1.53	0.91
2:B:347:LYS:H	2:B:347:LYS:HD3	1.37	0.90
6:F:77:GLN:H	6:F:77:GLN:HE21	0.97	0.89
2:B:49:HIS:CD2	2:B:161:TYR:H	1.89	0.89
10:U:29:ILE:H	10:U:77:ASN:HD21	1.21	0.88
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.40	0.87
1:A:62:ASN:HB2	1:A:65:ASN:ND2	1.91	0.85
1:L:57:GLY:H	1:L:60:ASN:HD22	1.24	0.85
3:C:295:MET:HE3	14:C:505:SMA:H33	1.58	0.85
6:F:77:GLN:HE21	6:F:77:GLN:N	1.75	0.84
2:M:49:HIS:CD2	2:M:161:TYR:H	1.96	0.84
2:M:300:ASN:O	2:M:304:ILE:HG12	1.78	0.83
5:P:172:ASP:H	5:P:184:HIS:HD2	1.24	0.82
1:L:237:LEU:H	1:L:237:LEU:HD23	1.43	0.82
5:E:187:ILE:HD12	5:E:187:ILE:H	1.45	0.81
2:M:110:TYR:HD2	2:M:205:LEU:HD23	1.46	0.81
5:P:72:LYS:NZ	9:T:29:GLN:HE22	1.77	0.81
10:U:54:ASN:H	10:U:54:ASN:HD22	1.27	0.81
3:C:193:MET:HA	3:C:193:MET:HE2	1.60	0.80
3:N:7:ASN:ND2	3:N:10:LEU:H	1.79	0.80
1:A:120:ASN:HD21	1:A:124:ILE:HD12	1.46	0.80
8:H:35:LYS:HE2	8:H:36:PRO:HD2	1.64	0.80
3:C:253:HIS:HD2	3:C:255:ASP:H	1.30	0.79
10:J:61:ASN:HD22	10:J:63:SER:H	1.28	0.79
10:J:54:ASN:HD22	10:J:54:ASN:H	1.27	0.79
4:O:125:VAL:HA	4:O:128:MET:HE3	1.64	0.78
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.64	0.78
8:H:80:LEU:HB3	8:H:89:LEU:HD23	1.64	0.78
1:A:65:ASN:HA	1:A:187:LEU:HD11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:41:PHE:HA	8:H:45:VAL:HB	1.65	0.77
3:N:159:ASN:HD22	3:N:159:ASN:H	1.33	0.77
1:L:57:GLY:H	1:L:60:ASN:ND2	1.81	0.77
10:U:6:GLU:H	10:U:114:GLN:HE21	1.33	0.77
4:O:62:MET:HB3	4:O:67:HIS:CE1	2.20	0.77
3:N:108:SER:CB	3:N:109:PRO:HD3	2.15	0.76
3:C:4:ARG:HE	3:C:14:ASN:ND2	1.84	0.76
5:E:191:ILE:HD13	5:E:196:ALA:HB3	1.67	0.76
3:C:125:ILE:HG22	14:C:505:SMA:H37	1.67	0.75
1:L:295:ARG:HD2	1:L:306:GLN:OE1	1.85	0.75
10:U:36:ASN:HD21	10:U:99:SER:HB3	1.52	0.75
4:D:197:GLY:O	4:D:199:PRO:HD3	1.86	0.75
2:M:60:ASN:HD22	2:M:111:LYS:HB2	1.52	0.75
3:N:13:VAL:HG13	3:N:17:ILE:HD12	1.67	0.75
11:V:36:TYR:CE2	11:V:89:GLN:HG2	2.21	0.74
1:L:316:HIS:HE1	1:L:350:TRP:HE1	1.36	0.74
5:P:172:ASP:H	5:P:184:HIS:CD2	2.05	0.74
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.69	0.73
4:O:111:ALA:HA	4:O:154:TYR:HA	1.68	0.73
2:B:318:ILE:HA	2:B:321:THR:HG22	1.70	0.73
1:L:260:ILE:HD11	1:L:343:ILE:HD11	1.71	0.73
3:C:56:SER:HB2	3:C:177:GLN:HG2	1.71	0.73
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.29	0.72
1:A:126:GLN:HG2	1:A:129:ASN:HB2	1.69	0.72
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.72	0.72
3:C:7:ASN:ND2	3:C:10:LEU:H	1.86	0.72
3:N:253:HIS:HD2	3:N:255:ASP:H	1.35	0.72
4:O:271:LEU:HD23	9:T:36:ILE:HG23	1.72	0.72
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.71	0.71
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.05	0.71
10:U:100:GLU:O	10:U:107:TYR:HA	1.91	0.71
10:U:41:PHE:HD2	10:U:92:ALA:HB2	1.56	0.71
5:E:72:LYS:NZ	9:I:29:GLN:HE21	1.89	0.71
1:A:72:TRP:CE3	1:A:75:ILE:HD11	2.26	0.71
1:A:316:HIS:HE1	1:A:350:TRP:HE1	1.38	0.71
4:O:289:LYS:NZ	8:S:40:ILE:HD11	2.06	0.71
11:V:34:ASN:HD22	11:V:49:TYR:HA	1.55	0.70
3:N:7:ASN:ND2	3:N:9:TYR:H	1.89	0.70
1:A:62:ASN:CB	1:A:65:ASN:HD21	2.04	0.70
5:E:44:LYS:NZ	5:E:52:GLY:H	1.89	0.70
5:E:72:LYS:HZ2	9:I:29:GLN:HE21	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:103:LEU:HA	5:P:120:HIS:ND1	2.07	0.70
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.72	0.70
3:C:335:LEU:O	3:C:339:ILE:HG12	1.92	0.70
3:N:208:ASN:HD22	3:N:210:LEU:H	1.40	0.70
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.40	0.70
3:N:107:ARG:HD3	3:N:314:ARG:HG3	1.73	0.70
2:M:347:LYS:HG2	2:M:348:LEU:H	1.57	0.69
10:J:99:SER:HB3	10:J:109:MET:HG2	1.74	0.69
1:A:369:LEU:HD13	1:A:409:ILE:HD13	1.75	0.69
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.57	0.69
2:B:197:LEU:O	2:B:201:VAL:HG23	1.93	0.69
2:M:183:GLU:HB2	2:M:212:GLY:O	1.94	0.68
2:M:62:ARG:HH21	2:M:62:ARG:HB2	1.58	0.68
10:U:61:ASN:HD22	10:U:63:SER:H	1.41	0.68
3:C:108:SER:OG	3:C:109:PRO:HD2	1.93	0.68
11:K:2:ILE:HD12	11:K:2:ILE:H	1.58	0.68
2:B:318:ILE:HD13	2:B:341:ASP:H	1.58	0.67
3:N:108:SER:HB3	3:N:109:PRO:HD3	1.75	0.67
2:B:34:LYS:HG3	2:B:88:THR:HG23	1.76	0.67
4:O:147:ARG:HH21	4:O:150:LYS:HE3	1.57	0.67
3:C:301:VAL:O	3:C:304:VAL:HG12	1.93	0.67
10:J:107:TYR:H	11:K:91:HIS:CD2	2.12	0.67
5:E:134:MET:HG2	10:J:31:SER:HB3	1.77	0.67
2:B:337:GLU:O	2:B:339:ASN:N	2.28	0.67
8:S:38:GLN:O	8:S:40:ILE:HD12	1.95	0.67
7:G:123:ILE:O	1:L:360:THR:HG21	1.95	0.66
2:B:340:PHE:O	2:B:341:ASP:HB2	1.95	0.66
10:J:41:PHE:HD1	10:J:45:LYS:HG3	1.60	0.66
2:M:40:ARG:HD3	2:M:155:LEU:HG	1.77	0.66
3:N:108:SER:OG	3:N:109:PRO:HD3	1.96	0.66
10:U:54:ASN:HD22	10:U:54:ASN:N	1.94	0.66
2:M:340:PHE:C	2:M:342:ALA:H	2.02	0.66
3:C:173:ASN:HB3	3:C:174:PRO:HD3	1.78	0.66
7:R:31:GLN:HA	7:R:31:GLN:NE2	2.07	0.66
1:L:376:LEU:HD22	1:L:388:LEU:HD11	1.78	0.66
2:B:62:ARG:CB	2:B:62:ARG:HH21	2.09	0.66
5:P:72:LYS:HZ1	9:T:29:GLN:HE22	1.44	0.66
1:A:348:LYS:HD3	1:A:351:ASN:OD1	1.95	0.66
3:C:279:TYR:CE1	14:C:505:SMA:H5	2.30	0.65
3:N:17:ILE:HG22	3:N:226:ILE:HD11	1.78	0.65
12:W:33:VAL:O	13:W:526:HEC:HMD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:HIS:CD2	3:C:255:ASP:H	2.14	0.65
1:L:108:LEU:HD22	2:M:323:LEU:HD23	1.78	0.65
1:L:288:ASN:C	1:L:288:ASN:HD22	2.03	0.65
3:N:58:ILE:H	3:N:173:ASN:HD22	1.45	0.65
3:C:7:ASN:HD22	3:C:10:LEU:H	1.43	0.65
3:N:7:ASN:HD22	3:N:10:LEU:N	1.83	0.65
11:V:2:ILE:HD12	11:V:2:ILE:H	1.62	0.65
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.93	0.65
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.78	0.64
2:M:69:ARG:O	2:M:73:LEU:HD23	1.97	0.64
3:N:104:GLY:HA2	3:N:106:TYR:CE2	2.31	0.64
3:C:58:ILE:H	3:C:173:ASN:ND2	1.95	0.64
10:U:29:ILE:H	10:U:77:ASN:ND2	1.93	0.64
11:V:32:PHE:HB2	11:V:92:ILE:HG22	1.78	0.64
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.79	0.64
1:A:147:VAL:HG22	1:A:178:ARG:HB3	1.79	0.64
10:J:29:ILE:H	10:J:77:ASN:HD21	1.46	0.64
3:N:147:ILE:O	3:N:150:LEU:HB2	1.98	0.64
11:V:74:THR:HG22	11:V:75:ILE:H	1.63	0.64
2:B:44:LYS:O	2:B:47:VAL:HG23	1.98	0.63
1:L:228:SER:HB3	1:L:231:THR:HB	1.81	0.63
2:M:347:LYS:HD3	2:M:347:LYS:H	1.62	0.63
3:N:25:SER:OG	7:R:79:HIS:HD2	1.82	0.63
10:U:29:ILE:HG12	10:U:77:ASN:ND2	2.13	0.63
2:M:365:LEU:HD12	2:M:368:LEU:HD12	1.80	0.63
3:N:147:ILE:HA	3:N:150:LEU:HD22	1.80	0.63
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.81	0.63
5:P:32:SER:HB3	5:P:35:ARG:HG3	1.81	0.63
3:C:108:SER:CB	3:C:109:PRO:HD2	2.28	0.63
1:A:296:LEU:O	2:B:69:ARG:NH2	2.31	0.62
3:N:379:TYR:CE1	3:N:383:VAL:HG21	2.33	0.62
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.81	0.62
2:B:49:HIS:HD2	2:B:161:TYR:N	1.91	0.62
1:A:66:ASN:ND2	1:A:175:LEU:HD12	2.13	0.62
2:M:347:LYS:HG2	2:M:348:LEU:N	2.13	0.62
2:M:355:ALA:HB1	2:M:362:LEU:HD23	1.82	0.62
7:R:80:GLN:O	7:R:84:THR:HG23	1.98	0.62
2:M:337:GLU:O	2:M:339:ASN:N	2.33	0.62
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.35	0.62
5:E:181:HIS:HB2	15:E:504:FES:S1	2.40	0.61
1:L:67:GLY:HA3	1:L:184:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:GLY:HA3	1:L:184:LEU:CD1	2.29	0.61
9:T:12:LYS:O	9:T:13:ARG:HG3	2.01	0.61
3:C:208:ASN:HD22	3:C:210:LEU:H	1.46	0.61
7:R:87:LEU:HG	8:S:50:ARG:HH11	1.65	0.61
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.81	0.61
1:L:62:ASN:N	1:L:65:ASN:HD21	1.92	0.61
10:U:28:SER:HB3	10:U:30:THR:HG22	1.82	0.61
5:P:106:ASN:ND2	5:P:119:ARG:HH21	1.99	0.61
11:V:38:GLN:O	11:V:84:ALA:HB1	2.01	0.61
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.30	0.61
10:U:93:THR:HG22	10:U:117:THR:HG23	1.82	0.61
2:B:164:VAL:HG21	2:M:232:ARG:NH1	2.16	0.60
12:W:13:THR:HA	12:W:16:LYS:HE2	1.83	0.60
1:A:316:HIS:CE1	1:A:350:TRP:HE1	2.19	0.60
3:C:132:TYR:HA	13:C:501:HEC:HAA2	1.84	0.60
2:M:340:PHE:O	2:M:341:ASP:HB2	2.00	0.60
12:W:29:GLY:HA2	12:W:36:ASN:OD1	2.01	0.60
2:M:257:ALA:HB2	2:M:285:PHE:HE1	1.66	0.60
5:E:107:VAL:CG1	5:E:118:ILE:HB	2.31	0.60
1:L:288:ASN:ND2	1:L:290:PHE:H	2.00	0.60
2:M:44:LYS:O	2:M:47:VAL:HG23	2.02	0.60
11:K:17:ASP:HB2	11:K:18:ARG:HH22	1.66	0.60
3:N:275:LEU:HD13	14:N:525:SMA:H14	1.83	0.60
11:V:75:ILE:HG22	11:V:76:SER:N	2.16	0.60
2:B:45:ASP:HB2	2:B:165:GLU:HG2	1.84	0.60
3:N:58:ILE:H	3:N:173:ASN:HD21	1.49	0.60
3:N:64:SER:O	3:N:68:ILE:HG13	2.02	0.60
3:N:166:TRP:HA	3:N:175:THR:HG23	1.84	0.60
8:S:40:ILE:HD12	8:S:40:ILE:H	1.66	0.60
6:F:91:GLY:O	6:F:95:VAL:HG13	2.01	0.59
5:P:72:LYS:HZ2	9:T:29:GLN:HE22	1.47	0.59
10:U:91:THR:HG23	10:U:119:THR:HA	1.84	0.59
12:W:13:THR:HG22	12:W:16:LYS:HE2	1.83	0.59
3:C:347:PRO:HG3	8:H:77:ASN:HB2	1.84	0.59
1:L:264:VAL:HG12	1:L:430:ILE:HG22	1.83	0.59
2:M:312:LYS:O	2:M:313:ASP:HB2	2.02	0.59
4:O:147:ARG:NH2	4:O:150:LYS:HE3	2.16	0.59
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.84	0.59
8:S:48:SER:C	8:S:50:ARG:H	2.10	0.59
2:B:152:ARG:HH21	2:B:152:ARG:HG3	1.67	0.59
8:H:61:ILE:O	8:H:65:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:LEU:HG	1:L:228:SER:H	1.67	0.59
1:L:287:TYR:HB3	1:L:314:PHE:CE2	2.38	0.59
10:J:49:VAL:HG13	10:J:64:LEU:HD12	1.85	0.59
10:U:16:GLN:HE21	10:U:16:GLN:HA	1.68	0.59
1:A:168:PHE:O	1:A:174:SER:HB3	2.03	0.58
1:A:214:LYS:HB2	1:A:217:ASP:HB2	1.84	0.58
1:A:227:LEU:HG	1:A:228:SER:H	1.68	0.58
11:K:17:ASP:O	11:K:78:LEU:HD13	2.03	0.58
11:V:17:ASP:HB2	11:V:18:ARG:NH2	2.18	0.58
1:A:75:ILE:HG23	1:A:139:THR:HG21	1.85	0.58
8:S:80:LEU:HB3	8:S:89:LEU:HD23	1.84	0.58
5:E:99:ALA:HB2	5:E:210:ASP:HB3	1.85	0.58
5:E:187:ILE:HD12	5:E:187:ILE:N	2.17	0.58
11:K:55:HIS:O	11:K:58:VAL:HG22	2.04	0.58
2:M:62:ARG:HH21	2:M:62:ARG:CB	2.15	0.58
5:P:102:PRO:HB2	5:P:105:LYS:HG2	1.85	0.58
1:A:171:THR:HG23	1:A:172:PRO:HD2	1.85	0.58
11:K:63:SER:HB2	11:K:74:THR:HB	1.85	0.58
1:L:171:THR:HG23	1:L:172:PRO:HD2	1.85	0.58
3:N:208:ASN:HD22	3:N:210:LEU:N	2.00	0.58
2:M:155:LEU:N	2:M:155:LEU:HD12	2.19	0.58
12:W:57:ASN:HD21	13:W:526:HEC:HAA2	1.67	0.58
2:B:313:ASP:C	2:B:315:SER:H	2.12	0.58
8:H:52:PHE:O	8:H:56:PHE:HB3	2.03	0.58
10:J:61:ASN:ND2	10:J:63:SER:H	1.99	0.58
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.38	0.58
1:A:237:LEU:HD23	1:A:237:LEU:H	1.68	0.58
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.44	0.58
3:C:7:ASN:HD22	3:C:10:LEU:N	2.02	0.57
1:L:250:LEU:HD23	8:S:25:THR:HG23	1.86	0.57
10:U:29:ILE:N	10:U:77:ASN:HD21	1.98	0.57
2:B:105:LEU:O	2:B:109:LEU:HD12	2.04	0.57
1:L:36:ILE:HG12	1:L:202:ASN:OD1	2.05	0.57
1:L:316:HIS:CE1	1:L:350:TRP:HE1	2.20	0.57
12:W:35:PRO:HG3	12:W:53:TYR:CE1	2.40	0.57
2:B:146:LEU:HD23	2:B:286:THR:HG22	1.86	0.57
2:M:252:GLN:O	2:M:255:VAL:HG22	2.03	0.57
12:W:27:LYS:HD2	12:W:28:GLY:N	2.20	0.57
1:A:37:VAL:HG13	1:A:206:VAL:HG22	1.87	0.57
1:A:65:ASN:N	1:A:65:ASN:HD22	2.01	0.57
1:A:216:GLU:HA	1:A:219:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.85	0.57
7:R:29:ALA:O	7:R:33:ILE:HG13	2.05	0.57
1:A:183:SER:O	1:A:187:LEU:HD13	2.05	0.57
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.20	0.57
4:O:121:THR:OG1	4:O:124:GLU:HG3	2.05	0.57
5:P:154:ILE:HB	5:P:205:TYR:CE1	2.40	0.57
8:S:41:PHE:H	8:S:45:VAL:HB	1.69	0.57
12:W:27:LYS:HD2	12:W:28:GLY:H	1.69	0.57
3:C:4:ARG:NE	3:C:14:ASN:ND2	2.53	0.56
3:C:109:PRO:HB2	3:C:204:HIS:CE1	2.40	0.56
5:E:197:PRO:O	5:E:198:LEU:HD23	2.05	0.56
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.87	0.56
1:L:91:ALA:HB3	1:L:106:SER:HB2	1.86	0.56
1:L:390:GLY:O	1:L:394:LEU:HB2	2.05	0.56
7:R:43:LEU:HD21	7:R:78:ALA:HB2	1.87	0.56
2:B:367:GLU:O	2:B:368:LEU:HB2	2.04	0.56
10:J:38:ILE:HD12	10:J:46:LEU:HD22	1.87	0.56
1:L:48:ALA:HA	1:L:211:GLY:HA3	1.87	0.56
3:N:335:LEU:O	3:N:339:ILE:HG12	2.05	0.56
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.87	0.56
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.87	0.56
10:J:39:ARG:NH2	10:J:41:PHE:HZ	2.03	0.56
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.87	0.56
2:M:347:LYS:HD3	2:M:347:LYS:N	2.20	0.56
4:D:125:VAL:HA	4:D:128:MET:HE3	1.87	0.56
4:O:118:VAL:HG11	4:O:257:TRP:CE2	2.40	0.56
12:W:24:THR:HG23	12:W:32:LYS:HE2	1.88	0.56
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.86	0.56
5:E:147:VAL:HG21	5:E:150:PRO:HA	1.87	0.56
10:J:62:PRO:O	10:J:65:LYS:HG2	2.06	0.56
3:N:132:TYR:HA	13:N:521:HEC:HAA2	1.87	0.56
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.86	0.56
7:G:80:GLN:O	7:G:84:THR:HG23	2.06	0.56
1:L:381:ASN:OD1	1:L:383:VAL:HG22	2.05	0.56
6:Q:91:GLY:O	6:Q:95:VAL:HG13	2.06	0.56
10:J:6:GLU:H	10:J:114:GLN:HE21	1.52	0.56
1:L:37:VAL:HG13	1:L:206:VAL:HG22	1.87	0.56
1:A:72:TRP:CH2	1:A:131:LEU:HD21	2.41	0.55
1:A:301:LEU:HB2	1:A:349:GLN:HG3	1.88	0.55
1:L:29:VAL:HG11	1:L:399:LYS:HB3	1.87	0.55
5:P:187:ILE:HD12	5:P:187:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:THR:HG22	11:K:75:ILE:N	2.21	0.55
3:N:193:MET:HE1	3:N:196:MET:SD	2.46	0.55
3:C:58:ILE:H	3:C:173:ASN:HD22	1.52	0.55
2:B:52:ASN:HD21	2:B:80:SER:C	2.15	0.55
1:A:36:ILE:HG22	1:A:37:VAL:H	1.70	0.55
1:L:75:ILE:HG22	1:L:139:THR:HG21	1.89	0.55
4:O:295:ILE:O	4:O:298:ARG:HB2	2.05	0.55
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.40	0.55
3:C:77:ILE:O	3:C:81:LEU:HB2	2.06	0.55
1:L:183:SER:O	1:L:187:LEU:HD13	2.07	0.55
5:E:190:ARG:HA	5:E:199:ASN:HB3	1.88	0.55
10:J:36:ASN:H	10:J:36:ASN:HD22	1.55	0.55
2:M:335:PRO:HG2	2:M:336:ILE:HG13	1.88	0.55
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.41	0.55
1:L:75:ILE:HG13	1:L:76:PHE:N	2.21	0.55
2:B:150:THR:HG22	2:B:352:ASN:HD22	1.69	0.54
3:C:15:SER:O	3:C:202:HIS:HE1	1.90	0.54
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.90	0.54
5:E:122:THR:O	5:E:126:ILE:HG13	2.07	0.54
5:P:155:MET:HA	5:P:203:PRO:HD2	1.88	0.54
6:Q:111:GLN:HB3	6:Q:112:PRO:HD2	1.89	0.54
1:A:287:TYR:CD2	1:A:302:LEU:HD21	2.43	0.54
2:B:271:ILE:HG22	2:B:289:VAL:HG22	1.89	0.54
11:V:75:ILE:HG22	11:V:76:SER:H	1.71	0.54
10:U:13:GLN:HA	10:U:121:SER:O	2.07	0.54
2:B:40:ARG:HH11	2:B:85:GLU:HG3	1.73	0.54
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.07	0.54
2:B:146:LEU:O	2:B:150:THR:HG23	2.07	0.54
2:B:202:ASP:O	2:B:203:GLU:HG2	2.08	0.54
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.22	0.54
3:C:108:SER:OG	3:C:314:ARG:NH2	2.41	0.54
1:A:98:ARG:HD3	1:A:173:LEU:HD12	1.89	0.54
3:C:253:HIS:HD2	3:C:255:ASP:N	2.01	0.54
1:A:228:SER:HB3	1:A:231:THR:HB	1.90	0.54
10:J:42:PRO:C	10:J:44:ASN:H	2.15	0.54
1:L:42:HIS:HB3	1:L:213:ILE:O	2.08	0.54
1:L:162:HIS:HA	1:L:165:SER:HB3	1.90	0.54
8:S:76:TYR:O	8:S:80:LEU:HG	2.08	0.54
5:E:56:ALA:O	5:E:60:VAL:HG23	2.07	0.53
10:J:18:LEU:HD11	10:J:118:VAL:HG11	1.89	0.53
11:K:107:LYS:HE3	11:K:107:LYS:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:6:GLU:N	10:U:114:GLN:HE21	2.05	0.53
1:A:57:GLY:H	1:A:60:ASN:HD22	1.56	0.53
1:A:147:VAL:HG12	1:A:181:LEU:HD23	1.90	0.53
2:B:36:HIS:HB3	2:B:41:TYR:CE1	2.43	0.53
3:C:187:PRO:HG3	13:C:501:HEC:HBB3	1.90	0.53
1:L:72:TRP:CZ3	1:L:75:ILE:HD11	2.43	0.53
1:A:129:ASN:C	1:A:131:LEU:H	2.16	0.53
2:B:246:ASN:HD22	2:B:249:SER:HB2	1.73	0.53
10:J:28:SER:HB2	10:J:31:SER:OG	2.08	0.53
11:K:27:GLN:HG2	11:K:28:ASP:H	1.73	0.53
3:N:223:SER:O	3:N:224:TYR:CG	2.62	0.53
2:M:246:ASN:HD22	2:M:249:SER:HB3	1.73	0.53
3:N:108:SER:CB	3:N:109:PRO:CD	2.86	0.53
1:A:37:VAL:CG1	1:A:206:VAL:HG22	2.39	0.53
2:M:52:ASN:ND2	2:M:80:SER:OG	2.41	0.53
3:N:323:LYS:HE3	8:S:55:GLN:HE22	1.73	0.53
2:M:237:SER:HA	2:M:357:GLY:HA3	1.90	0.53
2:B:51:LEU:HD11	2:B:180:TYR:HE1	1.74	0.53
1:L:44:PRO:HA	1:L:212:ASN:HB2	1.90	0.53
3:C:76:TYR:CE1	3:C:77:ILE:HG13	2.43	0.53
3:N:109:PRO:HB2	3:N:204:HIS:CE1	2.44	0.53
11:V:47:LEU:HA	11:V:58:VAL:HG11	1.90	0.53
10:J:33:TYR:N	10:J:33:TYR:CD2	2.77	0.53
1:L:31:GLN:HE22	1:L:393:VAL:HB	1.74	0.53
2:M:205:LEU:HD12	2:M:205:LEU:N	2.23	0.52
13:N:521:HEC:HBC3	13:N:521:HEC:HHH	1.90	0.52
5:P:186:ASP:OD2	5:P:190:ARG:NH2	2.42	0.52
7:G:120:LEU:HD13	2:M:69:ARG:HG3	1.90	0.52
2:M:146:LEU:HD23	2:M:286:THR:HG22	1.92	0.52
3:N:268:SER:O	3:N:270:VAL:HG23	2.09	0.52
12:W:7:SER:OG	12:W:10:LYS:HB2	2.10	0.52
1:A:65:ASN:HD22	1:A:65:ASN:H	1.56	0.52
7:G:63:LEU:HD13	7:G:103:LEU:CD1	2.40	0.52
2:M:250:LEU:HD23	2:M:251:ALA:H	1.75	0.52
8:S:35:LYS:O	8:S:37:LEU:N	2.42	0.52
10:U:61:ASN:ND2	10:U:63:SER:H	2.07	0.52
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.09	0.52
4:O:289:LYS:HZ3	8:S:40:ILE:HD11	1.73	0.52
2:B:339:ASN:HA	2:B:342:ALA:HB3	1.90	0.52
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.53	0.52
2:M:41:TYR:O	2:M:175:PHE:HE1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:77:ILE:O	3:N:81:LEU:HB2	2.09	0.52
1:L:178:ARG:HG2	1:L:178:ARG:HH21	1.75	0.52
1:A:75:ILE:CG2	1:A:139:THR:HG21	2.40	0.52
10:U:54:ASN:H	10:U:54:ASN:ND2	2.03	0.52
8:H:12:TRP:NE1	8:S:3:PRO:HB3	2.25	0.52
4:O:224:ALA:HB3	13:O:523:HEC:HBD2	1.92	0.52
1:A:66:ASN:HD21	1:A:176:PRO:HD2	1.75	0.52
2:M:34:LYS:HB3	2:M:86:TYR:CD1	2.45	0.52
3:N:193:MET:HE2	3:N:193:MET:HA	1.92	0.52
1:A:151:GLU:HA	1:A:158:ARG:HD2	1.92	0.52
2:B:317:ALA:O	2:B:320:TYR:HB3	2.10	0.52
1:L:178:ARG:H	1:L:178:ARG:HD2	1.74	0.52
1:L:349:GLN:HE22	1:L:352:ARG:HH21	1.57	0.52
3:N:105:SER:CB	13:N:522:HEC:HBD2	2.40	0.52
7:R:98:GLU:O	7:R:100:VAL:HG23	2.09	0.52
11:V:17:ASP:O	11:V:78:LEU:HD13	2.10	0.52
11:K:103:LYS:HG3	11:K:104:LEU:N	2.25	0.51
3:N:110:ARG:O	3:N:113:LEU:HB3	2.10	0.51
11:V:15:LEU:HD12	11:V:15:LEU:H	1.75	0.51
8:H:50:ARG:HE	8:H:51:ARG:HH21	1.58	0.51
11:K:74:THR:HG22	11:K:75:ILE:H	1.74	0.51
2:M:315:SER:HB3	2:M:344:LYS:HB2	1.91	0.51
4:O:289:LYS:HZ2	8:S:40:ILE:HD11	1.72	0.51
10:J:40:LEU:HB3	10:J:93:THR:HG23	1.90	0.51
2:M:318:ILE:O	2:M:319:ASN:HB2	2.09	0.51
3:N:105:SER:HB3	13:N:522:HEC:HBD2	1.91	0.51
3:N:311:SER:CB	3:N:319:LYS:HZ1	2.23	0.51
8:S:38:GLN:CD	8:S:39:GLY:H	2.19	0.51
3:C:22:GLN:HE21	3:C:221:MET:HE2	1.75	0.51
1:L:163:LEU:HD12	1:L:326:LEU:HD13	1.93	0.51
10:U:4:LEU:HG	10:U:24:VAL:HG22	1.93	0.51
3:C:22:GLN:NE2	3:C:221:MET:HE2	2.26	0.51
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.91	0.51
7:G:18:SER:HB3	7:G:21:LEU:HD23	1.93	0.51
10:J:36:ASN:N	10:J:36:ASN:ND2	2.59	0.51
1:L:252:ASP:HB3	1:L:255:LEU:HD12	1.91	0.51
2:M:35:VAL:HG12	2:M:179:VAL:HG12	1.91	0.51
2:B:205:LEU:HD12	2:B:205:LEU:H	1.76	0.51
3:C:104:GLY:O	3:C:107:ARG:HG3	2.11	0.51
3:C:189:ILE:O	3:C:192:ALA:HB3	2.11	0.51
9:I:54:ALA:C	9:I:56:ILE:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:LEU:N	11:K:15:LEU:HD12	2.25	0.51
3:N:253:HIS:CD2	3:N:255:ASP:HB2	2.45	0.51
2:B:202:ASP:C	2:B:204:SER:H	2.19	0.51
2:M:225:LEU:HD21	2:M:244:PRO:HD2	1.93	0.51
3:N:152:SER:HB3	3:N:162:VAL:HG21	1.92	0.51
4:O:289:LYS:HB2	8:S:37:LEU:HD13	1.93	0.51
10:U:28:SER:HB2	10:U:31:SER:OG	2.11	0.51
1:L:288:ASN:C	1:L:288:ASN:ND2	2.69	0.51
2:M:155:LEU:HD12	2:M:155:LEU:H	1.76	0.51
5:P:172:ASP:N	5:P:184:HIS:HD2	2.03	0.51
7:R:19:PRO:O	7:R:23:LYS:HG3	2.11	0.51
3:C:195:ILE:O	3:C:199:MET:HG3	2.11	0.51
1:L:250:LEU:O	1:L:435:THR:HA	2.10	0.51
1:L:444:TYR:CE2	8:S:30:SER:HB2	2.46	0.51
5:P:38:ASN:HD21	5:P:40:ASP:CG	2.19	0.51
6:Q:117:LEU:O	6:Q:118:GLU:HG3	2.10	0.51
3:N:22:GLN:NE2	3:N:221:MET:HE2	2.26	0.50
1:A:36:ILE:HG23	1:A:202:ASN:OD1	2.12	0.50
2:B:139:VAL:HG13	2:B:290:ARG:HD2	1.93	0.50
1:L:301:LEU:HB2	1:L:349:GLN:HG3	1.92	0.50
3:N:125:ILE:CG2	14:N:525:SMA:H37	2.42	0.50
4:O:273:THR:HG22	4:O:277:LEU:HD12	1.92	0.50
5:P:51:LYS:HE2	5:P:55:TYR:HE2	1.75	0.50
1:A:255:LEU:HD12	1:A:436:GLY:HA2	1.93	0.50
9:I:5:SER:O	9:I:9:THR:HG23	2.12	0.50
3:N:125:ILE:HG22	14:N:525:SMA:H37	1.94	0.50
11:K:19:VAL:HG22	11:K:20:THR:N	2.27	0.50
2:M:146:LEU:HD13	2:M:354:VAL:CG2	2.42	0.50
4:O:134:TYR:CE2	4:O:149:GLY:HA3	2.47	0.50
11:V:11:LEU:HG	11:V:12:ALA:H	1.77	0.50
11:V:12:ALA:HB1	11:V:105:GLU:O	2.11	0.50
2:B:300:ASN:O	2:B:304:ILE:HG12	2.12	0.50
8:S:41:PHE:O	8:S:42:HIS:HB2	2.10	0.50
11:V:29:ILE:HD11	11:V:71:TYR:CE1	2.47	0.50
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.00	0.50
2:M:65:LEU:O	2:M:69:ARG:HG2	2.12	0.50
3:N:182:LEU:O	3:N:186:VAL:HG23	2.12	0.50
10:U:51:TYR:C	10:U:51:TYR:CD2	2.89	0.50
2:B:103:ASN:O	2:B:107:ASP:HB2	2.12	0.50
7:R:40:LYS:HD3	7:R:93:TRP:CH2	2.47	0.50
1:A:65:ASN:ND2	1:A:65:ASN:H	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:GLY:O	3:C:319:LYS:HD2	2.11	0.49
13:C:501:HEC:HBC3	13:C:501:HEC:HHD	1.93	0.49
2:B:255:VAL:HA	2:B:321:THR:OG1	2.12	0.49
4:D:280:LEU:HD11	5:E:66:LEU:HB2	1.92	0.49
2:B:21:ALA:HA	2:B:189:GLY:O	2.12	0.49
2:B:62:ARG:HH21	2:B:62:ARG:HB3	1.76	0.49
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.46	0.49
2:M:98:LEU:N	2:M:99:PRO:HD2	2.27	0.49
5:P:58:PHE:HD2	5:P:59:MET:HE2	1.78	0.49
1:A:65:ASN:ND2	1:A:65:ASN:N	2.60	0.49
1:A:378:GLU:OE1	2:B:26:THR:HB	2.12	0.49
3:C:8:VAL:HG13	3:C:9:TYR:N	2.27	0.49
2:M:83:ASP:HB2	2:M:86:TYR:H	1.77	0.49
2:M:152:ARG:HG3	2:M:152:ARG:HH21	1.77	0.49
5:P:106:ASN:HD21	5:P:119:ARG:HD2	1.77	0.49
1:A:112:THR:HB	1:A:213:ILE:HG21	1.93	0.49
7:G:53:ASN:HB2	7:G:54:PRO:HD2	1.93	0.49
1:L:65:ASN:HA	1:L:187:LEU:HD11	1.94	0.49
2:M:36:HIS:HB3	2:M:41:TYR:CE1	2.48	0.49
1:A:120:ASN:ND2	1:A:124:ILE:HD12	2.21	0.49
3:N:129:PHE:CD1	3:N:147:ILE:HD12	2.48	0.49
3:N:295:MET:HE3	14:N:525:SMA:C23	2.41	0.49
11:V:29:ILE:HA	11:V:92:ILE:HG21	1.95	0.49
1:A:376:LEU:HD22	1:A:388:LEU:HD11	1.94	0.49
5:E:44:LYS:HB2	8:H:35:LYS:HE3	1.94	0.49
2:M:146:LEU:O	2:M:150:THR:HG23	2.12	0.49
2:M:205:LEU:HD12	2:M:205:LEU:H	1.78	0.49
12:W:94:LYS:HG3	12:W:95:ASP:N	2.27	0.49
10:U:37:TRP:CZ3	10:U:96:CYS:HB3	2.47	0.49
2:B:193:VAL:HG23	2:B:196:ASP:HB2	1.94	0.49
10:J:51:TYR:C	10:J:51:TYR:CD2	2.90	0.49
1:A:130:LEU:C	1:A:132:SER:H	2.20	0.49
11:K:61:ARG:HB2	11:K:76:SER:HB3	1.94	0.49
9:T:48:LEU:O	9:T:52:VAL:HG23	2.13	0.49
11:V:17:ASP:HB2	11:V:18:ARG:HH22	1.76	0.49
1:A:85:ALA:HB2	1:A:118:PHE:CE1	2.47	0.48
3:C:80:TYR:CE1	3:C:248:PRO:HB2	2.47	0.48
3:C:108:SER:CB	3:C:109:PRO:CD	2.91	0.48
10:J:23:SER:HA	10:J:78:GLN:HB3	1.94	0.48
3:N:7:ASN:ND2	3:N:9:TYR:N	2.57	0.48
2:B:252:GLN:O	2:B:255:VAL:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.41	0.48
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.44	0.48
8:H:44:ALA:HA	8:H:47:ASN:HB3	1.94	0.48
10:J:109:MET:HE1	11:K:98:PHE:HZ	1.78	0.48
11:K:4:LEU:HD22	11:K:88:CYS:SG	2.53	0.48
1:L:312:ASP:OD1	1:L:334:ARG:HD3	2.13	0.48
3:N:172:SER:OG	3:N:174:PRO:HD2	2.14	0.48
3:N:214:GLY:O	3:N:218:ARG:HD3	2.13	0.48
8:S:56:PHE:CE2	8:S:57:LEU:HG	2.48	0.48
2:M:340:PHE:C	2:M:342:ALA:N	2.71	0.48
13:N:521:HEC:HMB1	13:N:521:HEC:HBB3	1.95	0.48
11:V:6:GLN:OE1	11:V:87:PHE:HA	2.12	0.48
1:A:92:LEU:HD21	1:A:118:PHE:CE2	2.48	0.48
3:C:362:TYR:HA	3:C:366:ILE:HB	1.95	0.48
5:E:44:LYS:HZ3	5:E:52:GLY:H	1.62	0.48
7:G:29:ALA:O	7:G:33:ILE:HG13	2.12	0.48
9:I:12:LYS:O	9:I:13:ARG:HG3	2.13	0.48
2:M:22:ARG:HB3	2:M:191:ASN:H	1.79	0.48
10:U:87:THR:HG22	10:U:88:THR:H	1.79	0.48
2:B:145:GLN:O	2:B:149:ILE:HG12	2.13	0.48
3:C:320:VAL:HG13	8:H:58:TYR:HE2	1.78	0.48
10:J:24:VAL:CG2	10:J:29:ILE:HD11	2.43	0.48
1:L:287:TYR:HE2	1:L:295:ARG:HG2	1.79	0.48
2:M:45:ASP:HB2	2:M:165:GLU:HG2	1.96	0.48
3:N:22:GLN:O	3:N:218:ARG:HD2	2.13	0.48
3:C:18:ILE:HA	3:C:222:HIS:HB2	1.95	0.48
11:V:19:VAL:HG22	11:V:20:THR:N	2.29	0.48
1:A:133:SER:C	1:A:135:ASN:H	2.22	0.48
4:D:286:TRP:CZ3	5:E:59:MET:HG3	2.48	0.48
8:H:35:LYS:O	8:H:37:LEU:N	2.47	0.48
2:M:43:THR:HG22	2:M:175:PHE:HD1	1.78	0.48
4:O:288:LYS:HD3	4:O:288:LYS:C	2.39	0.48
12:W:16:LYS:O	12:W:20:LEU:HB3	2.14	0.48
2:B:119:LEU:HA	2:B:123:VAL:HB	1.94	0.48
2:B:347:LYS:H	2:B:347:LYS:CD	2.19	0.48
2:M:30:THR:HG23	2:M:190:GLU:HB3	1.96	0.48
8:S:88:GLU:O	8:S:91:ARG:HB3	2.13	0.48
2:B:122:SER:C	2:B:125:PRO:HD2	2.39	0.47
3:C:7:ASN:ND2	3:C:9:TYR:N	2.61	0.47
3:N:229:ASP:O	3:N:233:VAL:HG23	2.14	0.47
2:B:242:GLY:HA2	2:B:285:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:LEU:O	9:I:10:PHE:HD2	1.97	0.47
10:J:11:LEU:HD13	10:J:125:ARG:HD2	1.96	0.47
10:J:27:TYR:HE2	10:J:32:GLY:N	2.13	0.47
2:M:225:LEU:HD21	2:M:244:PRO:CD	2.44	0.47
3:N:342:CYS:SG	8:S:70:TRP:HH2	2.36	0.47
5:P:91:MET:HE3	5:P:92:ALA:O	2.14	0.47
10:U:18:LEU:HD11	10:U:118:VAL:HG11	1.95	0.47
11:V:37:GLN:HB2	11:V:47:LEU:HD11	1.95	0.47
2:B:175:PHE:CE2	2:B:179:VAL:HG21	2.49	0.47
4:D:280:LEU:HD11	5:E:66:LEU:CB	2.43	0.47
10:J:54:ASN:H	10:J:54:ASN:ND2	2.03	0.47
10:U:4:LEU:N	10:U:4:LEU:HD12	2.30	0.47
12:W:75:ASN:CG	12:W:78:LYS:HB3	2.39	0.47
5:E:91:MET:O	5:E:91:MET:HG3	2.14	0.47
8:H:58:TYR:O	8:H:62:PRO:HG2	2.14	0.47
1:L:58:ALA:HB3	1:L:98:ARG:HA	1.97	0.47
1:A:72:TRP:CZ3	1:A:75:ILE:HD11	2.49	0.47
2:B:183:GLU:HB2	2:B:212:GLY:O	2.15	0.47
11:K:75:ILE:HG22	11:K:76:SER:N	2.30	0.47
2:M:146:LEU:HD13	2:M:354:VAL:HG22	1.95	0.47
2:M:298:SER:OG	2:M:363:PRO:HD3	2.14	0.47
2:B:106:ALA:HB2	2:B:206:LEU:HD22	1.97	0.47
4:D:69:LEU:HD12	4:D:217:TYR:CE2	2.49	0.47
5:E:187:ILE:H	5:E:187:ILE:CD1	2.13	0.47
1:L:133:SER:O	1:L:134:SER:HB2	2.15	0.47
2:M:305:VAL:HG11	2:M:368:LEU:HB3	1.95	0.47
10:U:42:PRO:C	10:U:44:ASN:H	2.21	0.47
10:U:61:ASN:HD22	10:U:61:ASN:C	2.23	0.47
2:B:94:LEU:O	2:B:96:ASP:N	2.48	0.47
2:B:109:LEU:HD23	2:B:180:TYR:CD2	2.50	0.47
2:B:135:GLU:O	2:B:135:GLU:HG2	2.15	0.47
3:C:64:SER:O	3:C:67:HIS:HB3	2.15	0.47
3:C:121:PHE:CZ	3:C:125:ILE:HD11	2.50	0.47
3:C:193:MET:HA	3:C:193:MET:CE	2.39	0.47
3:C:295:MET:HE3	14:C:505:SMA:C23	2.35	0.47
4:D:246:GLN:HA	6:F:146:LEU:HD22	1.97	0.47
5:E:188:SER:HB3	5:E:190:ARG:HG3	1.96	0.47
11:K:21:ILE:HG22	11:K:22:SER:N	2.29	0.47
1:L:171:THR:HG23	1:L:241:ALA:HA	1.97	0.47
2:M:315:SER:HB3	2:M:344:LYS:CB	2.45	0.47
4:O:76:TRP:CE2	4:O:188:CYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:LEU:C	2:B:340:PHE:H	2.22	0.47
2:M:320:TYR:C	2:M:322:LYS:N	2.71	0.47
5:P:120:HIS:HD2	5:P:151:GLN:HG2	1.80	0.47
7:R:95:LYS:HB2	7:R:98:GLU:HG3	1.97	0.47
3:C:88:PHE:O	3:C:92:VAL:HG23	2.15	0.47
1:L:66:ASN:HD22	1:L:180:THR:HG23	1.80	0.47
2:M:320:TYR:C	2:M:322:LYS:H	2.23	0.47
4:O:134:TYR:HE2	4:O:149:GLY:HA3	1.80	0.47
10:U:21:THR:HG22	10:U:80:PHE:CD2	2.49	0.47
12:W:22:CYS:O	12:W:32:LYS:HB2	2.15	0.47
2:M:24:ALA:HB1	2:M:25:PRO:HD2	1.97	0.47
7:R:98:GLU:O	7:R:100:VAL:N	2.45	0.47
3:C:80:TYR:CD1	3:C:248:PRO:HB2	2.50	0.46
4:D:93:GLY:HA3	4:D:254:PHE:HB2	1.97	0.46
11:K:29:ILE:CA	11:K:92:ILE:HG21	2.46	0.46
10:U:38:ILE:HD11	10:U:46:LEU:HD22	1.97	0.46
11:V:88:CYS:O	11:V:98:PHE:HA	2.15	0.46
2:B:251:ALA:HB1	2:B:339:ASN:HB3	1.97	0.46
1:L:262:LEU:C	1:L:262:LEU:HD23	2.40	0.46
3:N:110:ARG:HH11	3:N:314:ARG:NH2	2.14	0.46
12:W:40:ILE:O	12:W:64:TRP:HB2	2.15	0.46
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.27	0.46
5:E:191:ILE:HG22	5:E:199:ASN:OD1	2.14	0.46
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.51	0.46
1:L:144:LEU:HD21	1:L:185:GLU:HB3	1.97	0.46
1:L:260:ILE:CD1	1:L:343:ILE:HD11	2.42	0.46
5:P:187:ILE:HD12	5:P:187:ILE:N	2.31	0.46
10:U:51:TYR:C	10:U:51:TYR:HD2	2.22	0.46
3:C:56:SER:HB2	3:C:177:GLN:HA	1.96	0.46
4:D:87:HIS:HA	4:D:90:ILE:HD12	1.98	0.46
1:L:129:ASN:O	1:L:131:LEU:N	2.46	0.46
7:R:90:ARG:HG2	7:R:93:TRP:CZ2	2.51	0.46
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.97	0.46
10:J:99:SER:HB3	10:J:109:MET:CG	2.44	0.46
1:L:66:ASN:HD21	1:L:176:PRO:HG2	1.80	0.46
1:L:369:LEU:HD13	1:L:409:ILE:HD13	1.97	0.46
10:U:49:VAL:CG1	10:U:68:LEU:HD23	2.46	0.46
3:C:212:ILE:CD1	7:G:75:ILE:HG23	2.46	0.46
2:M:35:VAL:CG1	2:M:179:VAL:HG12	2.46	0.46
1:A:270:ASN:OD1	1:A:396:LYS:HD2	2.16	0.46
2:B:91:ALA:O	2:B:93:PHE:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:VAL:O	3:C:45:VAL:HG23	2.16	0.46
2:M:313:ASP:O	2:M:314:LEU:HB2	2.15	0.46
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.96	0.46
1:A:34:ASN:HD21	1:A:223:GLU:CD	2.24	0.46
3:C:7:ASN:ND2	3:C:9:TYR:H	2.13	0.46
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.50	0.46
2:B:355:ALA:HB1	2:B:362:LEU:HD23	1.97	0.46
3:C:131:GLY:HA3	3:C:183:HIS:CE1	2.51	0.46
5:E:85:THR:O	5:E:88:VAL:HG22	2.16	0.46
1:L:62:ASN:N	1:L:65:ASN:ND2	2.47	0.46
1:L:371:LEU:HD21	2:M:77:THR:HG23	1.98	0.46
2:M:31:LEU:HB2	2:M:93:PHE:HE2	1.81	0.46
3:N:31:ASN:ND2	3:N:229:ASP:HA	2.30	0.46
3:N:107:ARG:HB3	3:N:108:SER:H	1.54	0.46
8:S:76:TYR:CE2	8:S:80:LEU:HD11	2.51	0.46
1:A:337:THR:HG22	8:H:15:HIS:HD2	1.81	0.46
2:B:339:ASN:HA	2:B:342:ALA:CB	2.46	0.46
6:F:111:GLN:HB3	6:F:112:PRO:HD2	1.96	0.46
1:L:287:TYR:CE1	1:L:305:ILE:HD11	2.51	0.46
2:M:197:LEU:O	2:M:201:VAL:HG23	2.15	0.46
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.97	0.46
5:P:146:ARG:O	5:P:202:ILE:HD13	2.16	0.46
5:P:187:ILE:H	5:P:187:ILE:CD1	2.27	0.46
7:R:83:LEU:C	7:R:83:LEU:HD12	2.41	0.46
1:A:69:SER:HB3	1:A:96:ILE:HD12	1.97	0.45
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.51	0.45
11:K:2:ILE:HD12	11:K:2:ILE:N	2.29	0.45
1:L:381:ASN:CG	1:L:383:VAL:HG22	2.41	0.45
2:M:83:ASP:CB	2:M:86:TYR:H	2.29	0.45
3:N:312:VAL:HG21	7:R:5:PHE:CE1	2.51	0.45
3:N:375:ASN:HB3	7:R:8:ILE:CD1	2.47	0.45
2:B:315:SER:N	2:B:316:PRO:HD3	2.32	0.45
6:F:106:LYS:HA	6:F:109:GLN:HE21	1.81	0.45
10:J:79:PHE:H	10:J:79:PHE:HD2	1.63	0.45
1:L:237:LEU:C	1:L:238:LYS:HG3	2.42	0.45
3:N:42:ILE:O	3:N:46:THR:HG23	2.16	0.45
5:P:126:ILE:HG21	5:P:150:PRO:HB2	1.98	0.45
11:V:6:GLN:HB2	11:V:100:ALA:HB3	1.97	0.45
2:B:98:LEU:N	2:B:99:PRO:HD2	2.31	0.45
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.45
1:L:168:PHE:O	1:L:174:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:237:LEU:H	1:L:237:LEU:CD2	2.22	0.45
2:M:34:LYS:HB3	2:M:86:TYR:HD1	1.81	0.45
10:U:95:TYR:CE1	10:U:115:GLY:HA3	2.51	0.45
2:B:200:PHE:O	2:B:204:SER:HB3	2.16	0.45
2:B:258:ASN:ND2	2:B:324:LYS:HB3	2.32	0.45
1:L:248:VAL:O	1:L:433:ALA:HA	2.16	0.45
3:N:76:TYR:CE1	3:N:77:ILE:HG13	2.51	0.45
9:T:5:SER:O	9:T:9:THR:HG23	2.17	0.45
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.16	0.45
4:D:72:PRO:HG2	4:D:74:TYR:CE2	2.51	0.45
2:M:315:SER:N	2:M:316:PRO:HD3	2.31	0.45
3:N:57:ASN:HA	3:N:173:ASN:HD21	1.82	0.45
9:T:52:VAL:O	9:T:56:ILE:HG12	2.16	0.45
1:A:171:THR:CG2	1:A:241:ALA:HA	2.46	0.45
3:C:74:ASN:OD1	5:E:77:THR:HG23	2.17	0.45
3:C:222:HIS:CD2	3:C:223:SER:H	2.34	0.45
4:D:121:THR:O	4:D:125:VAL:HG23	2.17	0.45
4:D:187:GLY:O	4:D:191:ILE:HG12	2.17	0.45
2:M:318:ILE:CG2	2:M:319:ASN:HD22	2.29	0.45
3:N:159:ASN:HD22	3:N:159:ASN:N	2.06	0.45
7:R:63:LEU:HA	7:R:64:PRO:HD2	1.77	0.45
1:A:89:GLY:HA3	2:B:319:ASN:O	2.17	0.45
1:A:129:ASN:C	1:A:131:LEU:N	2.74	0.45
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.98	0.45
5:E:44:LYS:CB	8:H:35:LYS:HE3	2.47	0.45
4:O:302:PHE:HB2	7:R:73:TYR:CD1	2.51	0.45
4:O:304:PRO:HA	4:O:305:PRO:HD2	1.81	0.45
5:P:155:MET:HE1	5:P:176:TRP:CZ3	2.52	0.45
10:J:54:ASN:HD22	10:J:54:ASN:N	2.05	0.45
10:J:70:ILE:HG23	10:J:80:PHE:O	2.16	0.45
1:L:302:LEU:O	1:L:306:GLN:HG3	2.16	0.45
3:N:125:ILE:HG22	14:N:525:SMA:H40	1.97	0.45
5:P:104:GLY:O	5:P:105:LYS:HD2	2.16	0.45
10:U:41:PHE:CD2	10:U:92:ALA:HB2	2.44	0.45
1:A:225:LYS:H	1:A:225:LYS:HD2	1.82	0.45
3:C:107:ARG:HB2	3:C:108:SER:H	1.64	0.45
3:C:208:ASN:HD22	3:C:210:LEU:N	2.14	0.45
1:L:348:LYS:HE2	1:L:348:LYS:HA	1.98	0.45
13:W:526:HEC:HMC1	13:W:526:HEC:HBC3	1.97	0.45
3:C:223:SER:O	3:C:224:TYR:CG	2.70	0.45
4:D:283:LEU:O	4:D:287:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:LEU:C	1:L:132:SER:H	2.24	0.45
1:A:57:GLY:H	1:A:60:ASN:ND2	2.15	0.44
1:A:91:ALA:HB3	1:A:106:SER:HB2	1.99	0.44
3:C:212:ILE:HD12	7:G:75:ILE:HG23	1.99	0.44
6:F:123:CYS:HA	6:F:126:GLU:OE1	2.17	0.44
1:L:257:LYS:HB2	1:L:259:TRP:CH2	2.51	0.44
1:L:353:LEU:O	1:L:418:LYS:HA	2.16	0.44
4:O:256:ASN:C	4:O:256:ASN:HD22	2.25	0.44
6:Q:108:GLN:HA	6:Q:111:GLN:HG3	1.98	0.44
3:C:130:LEU:HD13	3:C:182:LEU:HB3	1.98	0.44
5:E:180:CYS:SG	3:N:269:ILE:HD13	2.58	0.44
7:G:83:LEU:C	7:G:83:LEU:HD12	2.43	0.44
11:K:77:ASN:C	11:K:79:GLU:H	2.25	0.44
2:M:252:GLN:HG3	2:M:253:TYR:N	2.31	0.44
5:P:120:HIS:CD2	5:P:151:GLN:HG2	2.51	0.44
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.98	0.44
9:T:8:LYS:O	9:T:12:LYS:HG2	2.17	0.44
10:U:14:PRO:O	10:U:15:SER:HB3	2.17	0.44
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.47	0.44
2:B:293:ASP:OD2	2:B:295:ALA:HB3	2.17	0.44
3:C:137:GLY:O	3:C:140:SER:HB2	2.18	0.44
3:C:269:ILE:HG23	3:C:269:ILE:O	2.18	0.44
4:D:115:LEU:HD12	4:D:257:TRP:CH2	2.52	0.44
1:L:31:GLN:NE2	1:L:393:VAL:HB	2.32	0.44
2:B:188:SER:OG	2:B:332:VAL:HG21	2.17	0.44
3:C:147:ILE:O	3:C:150:LEU:HB2	2.17	0.44
4:D:111:ALA:HA	4:D:154:TYR:HA	2.00	0.44
5:P:190:ARG:HH21	5:P:190:ARG:HB2	1.83	0.44
2:B:35:VAL:HG12	2:B:179:VAL:HG12	2.00	0.44
2:M:314:LEU:C	2:M:316:PRO:HD3	2.42	0.44
2:M:340:PHE:O	2:M:341:ASP:CB	2.66	0.44
3:N:242:LEU:HD23	3:N:242:LEU:HA	1.85	0.44
1:A:291:GLU:CD	2:B:53:ARG:HH12	2.24	0.44
3:C:323:LYS:HD3	8:H:55:GLN:HE22	1.82	0.44
1:L:247:GLU:CD	1:L:249:ARG:HH21	2.26	0.44
4:O:74:TYR:CE1	6:Q:139:ALA:HA	2.53	0.44
10:U:68:LEU:HA	10:U:82:LYS:O	2.17	0.44
11:V:2:ILE:HD12	11:V:2:ILE:N	2.30	0.44
12:W:95:ASP:O	12:W:99:LEU:HB2	2.18	0.44
1:A:92:LEU:HD23	1:A:105:VAL:HG22	2.00	0.44
1:A:129:ASN:O	1:A:130:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:SER:HA	1:A:315:ASN:HA	1.99	0.44
2:B:69:ARG:HG2	2:B:69:ARG:HH21	1.83	0.44
2:B:232:ARG:NH1	2:M:158:PRO:HG2	2.33	0.44
3:C:58:ILE:HB	3:C:173:ASN:HA	2.00	0.44
2:M:250:LEU:HD23	2:M:251:ALA:N	2.32	0.44
4:O:87:HIS:HA	4:O:90:ILE:HD12	2.00	0.44
7:R:123:ILE:O	7:R:123:ILE:HG13	2.18	0.44
10:U:54:ASN:N	10:U:54:ASN:ND2	2.60	0.44
12:W:43:ARG:HD2	12:W:47:GLN:HB2	1.99	0.44
2:M:242:GLY:HA2	2:M:285:PHE:O	2.18	0.44
3:N:97:MET:HG2	13:N:522:HEC:HBC2	1.99	0.44
12:W:44:HIS:O	12:W:47:GLN:HG2	2.17	0.44
1:A:127:LYS:HD2	1:A:127:LYS:HA	1.76	0.44
2:B:367:GLU:H	2:B:367:GLU:HG2	1.42	0.44
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.82	0.44
3:C:320:VAL:HG13	8:H:58:TYR:CE2	2.52	0.44
5:E:106:ASN:HD22	5:E:119:ARG:HB2	1.82	0.44
5:E:134:MET:CG	10:J:31:SER:HB3	2.47	0.44
2:M:146:LEU:HD23	2:M:286:THR:CG2	2.47	0.44
3:N:330:VAL:O	3:N:334:VAL:HG23	2.17	0.44
7:G:86:HIS:HE1	8:H:47:ASN:HD21	1.65	0.43
4:O:271:LEU:HD23	9:T:36:ILE:CG2	2.46	0.43
10:U:49:VAL:HG12	10:U:68:LEU:HD23	2.00	0.43
11:V:15:LEU:HD12	11:V:15:LEU:N	2.33	0.43
12:W:29:GLY:N	12:W:30:PRO:CD	2.81	0.43
2:B:157:ASN:HA	2:B:158:PRO:HD3	1.90	0.43
3:C:72:VAL:HA	5:E:85:THR:HG22	1.99	0.43
3:C:229:ASP:O	3:C:233:VAL:HG23	2.17	0.43
5:E:137:LEU:HD13	5:E:190:ARG:HD3	2.00	0.43
7:G:86:HIS:HE1	8:H:47:ASN:ND2	2.17	0.43
3:C:348:TYR:OH	8:H:74:ASN:OD1	2.36	0.43
1:A:85:ALA:HB1	1:A:90:LEU:HB2	2.01	0.43
1:A:237:LEU:HD23	1:A:237:LEU:N	2.33	0.43
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.53	0.43
3:C:110:ARG:O	3:C:113:LEU:HB3	2.18	0.43
1:L:127:LYS:HD2	1:L:127:LYS:HA	1.85	0.43
2:M:205:LEU:O	2:M:209:LEU:HG	2.18	0.43
4:O:78:HIS:HB3	4:O:85:PHE:HA	2.01	0.43
5:P:103:LEU:O	5:P:120:HIS:O	2.36	0.43
1:A:90:LEU:HD23	1:A:105:VAL:HG11	2.00	0.43
1:A:109:PRO:HB3	1:A:212:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:263:HIS:CE1	4:D:267:LYS:HE3	2.53	0.43
7:G:15:ILE:HG23	7:G:21:LEU:HB3	2.00	0.43
2:M:65:LEU:HD11	2:M:69:ARG:NH2	2.34	0.43
2:M:222:LYS:HB3	2:M:224:PHE:CE1	2.53	0.43
2:M:265:SER:OG	2:M:267:LEU:HD12	2.19	0.43
3:N:17:ILE:HG22	3:N:17:ILE:O	2.18	0.43
3:N:139:MET:HE3	3:N:255:ASP:CB	2.49	0.43
2:B:291:ASP:CG	2:B:292:GLN:N	2.77	0.43
4:D:273:THR:HG22	4:D:277:LEU:HD12	2.00	0.43
9:I:52:VAL:O	9:I:56:ILE:HG12	2.19	0.43
11:K:79:GLU:HA	11:K:80:PRO:HA	1.68	0.43
2:M:93:PHE:HD1	2:M:94:LEU:O	2.01	0.43
2:M:181:THR:HB	2:M:212:GLY:H	1.84	0.43
3:N:38:LEU:CD1	3:N:233:VAL:HG13	2.49	0.43
13:O:523:HEC:HBA2	13:O:523:HEC:HHA	2.00	0.43
5:P:191:ILE:HD13	5:P:196:ALA:HB3	2.00	0.43
1:A:358:THR:HG1	1:A:361:GLU:HG3	1.83	0.43
3:C:48:ILE:HD13	3:N:185:LEU:HG	2.00	0.43
7:G:17:LYS:O	7:G:19:PRO:HD3	2.19	0.43
8:H:30:SER:HA	8:H:31:PRO:HD3	1.91	0.43
10:J:7:SER:OG	10:J:21:THR:HG23	2.19	0.43
10:J:94:TYR:N	10:J:94:TYR:CD1	2.86	0.43
10:J:100:GLU:O	10:J:107:TYR:HA	2.18	0.43
1:L:168:PHE:O	1:L:171:THR:HB	2.18	0.43
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.53	0.43
1:L:67:GLY:CA	1:L:179:GLY:HA3	2.48	0.43
1:L:257:LYS:HB2	1:L:259:TRP:CZ2	2.54	0.43
2:M:270:LEU:HA	2:M:300:ASN:HD22	1.84	0.43
4:O:80:GLY:HA2	4:O:81:PRO:HD2	1.81	0.43
10:U:126:HIS:HA	10:U:127:PRO:HD2	1.90	0.43
1:A:171:THR:HG23	1:A:241:ALA:HA	2.00	0.43
2:B:298:SER:OG	2:B:363:PRO:HD3	2.18	0.43
3:C:43:GLN:CB	13:C:501:HEC:HAB	2.49	0.43
3:C:184:TYR:CE1	13:C:501:HEC:HBC1	2.54	0.43
11:K:34:ASN:ND2	11:K:49:TYR:HA	2.30	0.43
3:N:271:PRO:HG2	3:N:279:TYR:CG	2.54	0.43
4:O:115:LEU:N	4:O:115:LEU:HD22	2.34	0.43
1:A:226:ASN:HB3	1:A:227:LEU:H	1.47	0.43
2:M:346:PHE:CE1	2:M:347:LYS:O	2.72	0.43
3:N:154:ILE:HA	3:N:155:PRO:HD2	1.77	0.43
4:O:188:CYS:SG	4:O:256:ASN:OD1	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:28:SER:O	10:U:31:SER:HB2	2.19	0.43
1:A:89:GLY:HA2	2:B:320:TYR:HB2	2.01	0.42
2:B:64:ALA:O	2:B:68:VAL:HG23	2.18	0.42
3:C:43:GLN:HB3	13:C:501:HEC:HAB	2.01	0.42
3:C:125:ILE:CG2	14:C:505:SMA:H37	2.44	0.42
3:C:222:HIS:CG	3:C:223:SER:N	2.87	0.42
3:C:365:ILE:O	3:C:369:VAL:HG23	2.19	0.42
5:E:104:GLY:O	5:E:105:LYS:HD2	2.18	0.42
10:J:12:VAL:O	10:J:120:VAL:HA	2.19	0.42
1:A:56:SER:O	1:A:101:GLN:HG2	2.19	0.42
2:B:206:LEU:O	2:B:209:LEU:HB2	2.19	0.42
10:J:51:TYR:C	10:J:51:TYR:HD2	2.27	0.42
1:L:349:GLN:NE2	1:L:352:ARG:HD3	2.35	0.42
2:M:53:ARG:HB3	2:M:123:VAL:HG13	2.00	0.42
11:V:74:THR:HG22	11:V:75:ILE:N	2.33	0.42
11:V:94:PHE:HE1	11:V:96:TRP:CZ2	2.37	0.42
1:A:168:PHE:C	1:A:174:SER:HB3	2.44	0.42
2:B:260:LEU:O	2:B:271:ILE:HD11	2.18	0.42
10:J:6:GLU:H	10:J:114:GLN:NE2	2.15	0.42
1:L:181:LEU:HD23	1:L:181:LEU:O	2.19	0.42
3:N:166:TRP:CE3	3:N:170:SER:HA	2.53	0.42
3:N:193:MET:CE	3:N:196:MET:SD	3.07	0.42
11:V:80:PRO:HD2	11:V:81:GLU:CD	2.44	0.42
12:W:13:THR:HG22	12:W:16:LYS:CE	2.46	0.42
5:E:57:TYR:N	5:E:57:TYR:CD1	2.86	0.42
1:L:27:ALA:O	1:L:28:GLU:HB2	2.19	0.42
1:L:225:LYS:HD2	1:L:225:LYS:H	1.84	0.42
2:M:43:THR:HG22	2:M:175:PHE:CD1	2.54	0.42
4:O:116:VAL:HG22	4:O:125:VAL:HG21	2.02	0.42
4:O:283:LEU:HD21	5:P:62:ALA:HB3	2.02	0.42
10:U:4:LEU:HA	10:U:23:SER:O	2.19	0.42
10:U:13:GLN:O	10:U:16:GLN:HB2	2.19	0.42
8:H:39:GLY:O	8:H:44:ALA:HB3	2.20	0.42
10:J:30:THR:O	10:J:54:ASN:HB2	2.20	0.42
2:M:315:SER:C	2:M:317:ALA:N	2.77	0.42
3:N:23:PRO:HB2	3:N:26:ILE:HG23	2.02	0.42
10:U:20:LEU:HD21	10:U:116:THR:HG21	2.00	0.42
11:V:8:PRO:HG3	11:V:11:LEU:HD22	2.02	0.42
2:B:153:LYS:NZ	2:B:153:LYS:HB3	2.34	0.42
5:E:197:PRO:HG2	5:E:198:LEU:HG	2.01	0.42
11:K:24:ARG:HA	11:K:69:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:238:LYS:HB2	1:L:238:LYS:HE3	1.75	0.42
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	2.02	0.42
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.80	0.42
5:E:106:ASN:HD21	5:E:119:ARG:HD2	1.84	0.42
1:L:269:VAL:O	1:L:270:ASN:CB	2.68	0.42
1:L:364:ARG:NH2	2:M:72:GLU:OE1	2.53	0.42
3:C:25:SER:OG	7:G:79:HIS:CD2	2.73	0.42
4:D:133:GLU:HA	4:D:147:ARG:O	2.20	0.42
8:H:64:GLY:O	8:H:68:TYR:HB2	2.20	0.42
10:J:13:GLN:HA	10:J:121:SER:O	2.20	0.42
11:K:38:GLN:HB3	11:K:85:THR:HB	2.02	0.42
1:L:295:ARG:HB3	1:L:306:GLN:HE22	1.84	0.42
2:M:40:ARG:HD3	2:M:155:LEU:CG	2.47	0.42
2:M:209:LEU:HA	2:M:210:PRO:HD3	1.92	0.42
4:O:302:PHE:HB2	7:R:73:TYR:CE1	2.55	0.42
11:V:33:LEU:HD13	11:V:71:TYR:CD1	2.55	0.42
12:W:16:LYS:HA	12:W:20:LEU:HB2	2.01	0.42
12:W:60:LYS:HD2	12:W:60:LYS:HA	1.78	0.42
5:E:150:PRO:HD3	10:J:102:TYR:CG	2.55	0.42
3:N:38:LEU:HD11	3:N:233:VAL:HG13	2.02	0.42
4:O:299:LYS:HD2	5:P:39:PHE:CE2	2.54	0.42
5:P:55:TYR:O	5:P:59:MET:HG2	2.19	0.42
5:P:143:ASP:O	5:P:147:VAL:HG22	2.19	0.42
10:U:62:PRO:O	10:U:65:LYS:HG2	2.19	0.42
1:A:57:GLY:N	1:A:60:ASN:HD22	2.17	0.42
1:A:420:TRP:CZ3	1:A:425:LEU:HD22	2.55	0.42
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.55	0.42
1:L:133:SER:C	1:L:135:ASN:H	2.28	0.42
1:L:288:ASN:HD22	1:L:289:ALA:N	2.18	0.42
2:M:214:SER:OG	2:M:216:VAL:HG23	2.20	0.42
12:W:37:LEU:O	12:W:107:CYS:HB2	2.20	0.42
1:A:89:GLY:CA	2:B:319:ASN:O	2.68	0.41
1:A:247:GLU:CD	1:A:249:ARG:HH21	2.28	0.41
1:A:358:THR:OG1	1:A:361:GLU:HG3	2.20	0.41
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.54	0.41
5:E:160:THR:OG1	5:E:197:PRO:HD2	2.20	0.41
11:K:18:ARG:HD2	11:K:18:ARG:O	2.20	0.41
3:N:18:ILE:HA	3:N:222:HIS:HB2	2.02	0.41
3:N:159:ASN:H	3:N:159:ASN:ND2	2.07	0.41
5:P:103:LEU:HA	5:P:120:HIS:CE1	2.55	0.41
1:A:314:PHE:CD1	1:A:314:PHE:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:CYS:SG	8:H:70:TRP:HH2	2.43	0.41
2:M:68:VAL:O	2:M:72:GLU:HG3	2.20	0.41
3:N:12:LEU:HD23	3:N:12:LEU:HA	1.67	0.41
4:O:209:PRO:O	4:O:212:SER:HB2	2.20	0.41
9:T:14:ASN:HD22	9:T:14:ASN:HA	1.68	0.41
1:A:171:THR:HG21	1:A:242:ALA:H	1.85	0.41
7:G:31:GLN:HA	7:G:31:GLN:NE2	2.34	0.41
10:J:65:LYS:HB2	10:J:65:LYS:HE3	1.87	0.41
3:N:108:SER:OG	3:N:109:PRO:CD	2.67	0.41
11:V:32:PHE:CD2	11:V:92:ILE:HG22	2.56	0.41
12:W:87:PHE:CE1	12:W:89:GLY:HA2	2.56	0.41
2:B:315:SER:C	2:B:317:ALA:N	2.75	0.41
10:J:93:THR:HB	10:J:117:THR:HG23	2.02	0.41
1:L:250:LEU:HD23	8:S:25:THR:CG2	2.50	0.41
1:L:392:GLU:O	1:L:396:LYS:HG2	2.20	0.41
2:M:26:THR:OG1	2:M:191:ASN:ND2	2.52	0.41
3:N:319:LYS:HB2	3:N:322:SER:HB2	2.02	0.41
11:V:4:LEU:CD2	11:V:88:CYS:SG	3.09	0.41
7:G:86:HIS:CE1	8:H:47:ASN:ND2	2.89	0.41
4:O:283:LEU:HD12	4:O:283:LEU:HA	1.90	0.41
8:S:48:SER:O	8:S:50:ARG:N	2.53	0.41
2:B:109:LEU:HD23	2:B:180:TYR:HD2	1.86	0.41
3:C:347:PRO:HG3	8:H:77:ASN:CB	2.49	0.41
3:N:112:THR:O	3:N:116:VAL:HG23	2.21	0.41
3:N:226:ILE:HD13	3:N:226:ILE:HA	1.92	0.41
8:S:35:LYS:HA	8:S:36:PRO:HD2	1.77	0.41
11:V:4:LEU:HD22	11:V:88:CYS:SG	2.61	0.41
1:A:251:ARG:HH21	1:A:253:ASP:CG	2.29	0.41
2:B:291:ASP:HB3	2:B:297:VAL:HG22	2.02	0.41
4:D:134:TYR:OH	4:D:156:PRO:HD3	2.20	0.41
2:M:294:SER:HB3	2:M:358:ASP:HB3	2.02	0.41
4:O:231:ASP:OD2	4:O:244:THR:HG22	2.20	0.41
10:U:48:TRP:CZ2	10:U:50:GLY:HA2	2.56	0.41
1:A:28:GLU:HB3	1:A:29:VAL:H	1.55	0.41
1:A:100:PHE:CD1	1:A:101:GLN:N	2.89	0.41
1:A:129:ASN:O	1:A:131:LEU:N	2.45	0.41
2:B:91:ALA:O	2:B:93:PHE:CD2	2.74	0.41
2:B:315:SER:C	2:B:317:ALA:H	2.29	0.41
6:F:101:CYS:O	6:F:105:VAL:HG23	2.21	0.41
10:J:42:PRO:C	10:J:44:ASN:N	2.78	0.41
11:K:21:ILE:HG22	11:K:22:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:ILE:HG22	1:L:37:VAL:H	1.86	0.41
1:L:92:LEU:HD23	1:L:105:VAL:HG22	2.02	0.41
1:L:155:HIS:N	1:L:156:PRO:HD2	2.36	0.41
2:M:64:ALA:O	2:M:68:VAL:HG23	2.21	0.41
11:V:79:GLU:HA	11:V:80:PRO:HA	1.73	0.41
12:W:77:M3L:HM12	12:W:83:THR:O	2.20	0.41
12:W:94:LYS:HD2	12:W:98:ASP:OD2	2.20	0.41
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.90	0.41
1:A:73:LYS:HG3	1:A:94:SER:HB3	2.01	0.41
1:A:364:ARG:HH21	2:B:72:GLU:CD	2.27	0.41
2:B:82:LEU:HD12	2:B:87:ILE:HG12	2.03	0.41
3:C:50:MET:HE1	3:C:82:HIS:CB	2.51	0.41
4:D:92:ARG:O	4:D:96:VAL:HG23	2.21	0.41
7:G:53:ASN:ND2	7:G:56:MET:H	2.19	0.41
8:H:24:ILE:HD12	8:H:24:ILE:H	1.85	0.41
10:J:41:PHE:CD2	10:J:92:ALA:HB2	2.56	0.41
11:K:2:ILE:HG23	11:K:26:SER:OG	2.21	0.41
11:K:14:SER:HB3	11:K:15:LEU:H	1.74	0.41
1:L:88:GLU:HB3	1:L:90:LEU:HD22	2.02	0.41
1:L:251:ARG:NH1	1:L:439:GLU:HB2	2.36	0.41
1:L:287:TYR:CE2	1:L:295:ARG:HG2	2.56	0.41
1:L:299:ILE:HB	1:L:302:LEU:HD12	2.03	0.41
2:M:146:LEU:HD12	2:M:146:LEU:HA	1.85	0.41
2:M:367:GLU:H	2:M:367:GLU:HG2	1.49	0.41
4:O:85:PHE:CE1	4:O:257:TRP:HA	2.56	0.41
4:O:265:GLU:CD	4:O:268:ARG:HH22	2.29	0.41
12:W:73:LEU:HD13	12:W:99:LEU:HD12	2.03	0.41
1:A:317:PHE:HB2	1:A:319:LEU:HD13	2.03	0.41
2:B:83:ASP:HB2	2:B:86:TYR:N	2.18	0.41
2:B:202:ASP:C	2:B:204:SER:N	2.79	0.41
2:B:315:SER:HB2	2:B:318:ILE:HG13	2.03	0.41
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.92	0.41
3:C:253:HIS:CD2	3:C:255:ASP:HB2	2.56	0.41
5:E:118:ILE:HA	5:E:153:LEU:O	2.21	0.41
10:J:68:LEU:HB3	10:J:83:LEU:HD13	2.02	0.40
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.61	0.40
1:L:368:LEU:HD23	1:L:368:LEU:HA	1.89	0.40
1:L:428:GLN:HE22	9:T:13:ARG:CZ	2.33	0.40
2:M:124:LEU:HB2	2:M:125:PRO:HD3	2.03	0.40
2:M:241:ILE:HA	2:M:352:ASN:O	2.22	0.40
3:N:351:MET:HE1	8:S:70:TRP:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:LEU:HD12	3:C:40:LEU:HA	1.82	0.40
3:C:261:ASN:HA	3:C:262:PRO:HD3	1.85	0.40
6:F:81:LEU:O	6:F:85:PHE:HD1	2.05	0.40
8:H:56:PHE:O	8:H:60:LEU:HB2	2.21	0.40
9:I:37:THR:O	9:I:41:GLU:HG3	2.20	0.40
1:L:276:VAL:HA	1:L:412:ILE:HD13	2.04	0.40
2:M:165:GLU:O	2:M:165:GLU:HG3	2.19	0.40
3:N:159:ASN:N	3:N:159:ASN:ND2	2.69	0.40
4:O:175:PRO:HG3	13:O:523:HEC:HAA1	2.03	0.40
8:S:71:LYS:HB3	8:S:71:LYS:HE3	1.91	0.40
11:V:75:ILE:CG2	11:V:76:SER:H	2.33	0.40
11:V:89:GLN:HB3	11:V:98:PHE:CD1	2.56	0.40
1:A:91:ALA:O	1:A:105:VAL:HA	2.21	0.40
1:A:120:ASN:O	1:A:124:ILE:HB	2.21	0.40
4:D:147:ARG:NH2	4:D:150:LYS:HE3	2.37	0.40
5:E:140:PRO:O	5:E:141:GLN:HG3	2.21	0.40
10:J:52:ILE:O	10:J:52:ILE:HG23	2.21	0.40
11:K:17:ASP:HB2	11:K:18:ARG:NH2	2.33	0.40
1:L:75:ILE:CG2	1:L:139:THR:HG21	2.51	0.40
1:L:406:PHE:N	1:L:406:PHE:CD1	2.90	0.40
2:M:301:ILE:HG23	2:M:302:LYS:N	2.36	0.40
3:N:233:VAL:O	3:N:237:MET:HG3	2.22	0.40
3:N:253:HIS:CD2	3:N:255:ASP:H	2.25	0.40
4:O:112:TRP:O	4:O:115:LEU:HD23	2.21	0.40
8:S:61:ILE:O	8:S:65:ILE:HG13	2.22	0.40
11:V:4:LEU:HD12	11:V:4:LEU:N	2.36	0.40
11:K:29:ILE:HD11	11:K:71:TYR:CE1	2.56	0.40
2:M:35:VAL:HG13	2:M:185:LEU:HB3	2.03	0.40
2:M:115:LYS:HD2	2:M:115:LYS:HA	1.77	0.40
3:N:58:ILE:HB	3:N:173:ASN:HD22	1.87	0.40
4:O:183:ALA:O	4:O:184:ARG:HD3	2.21	0.40
4:O:286:TRP:CD2	8:S:37:LEU:HD12	2.56	0.40
10:U:99:SER:HA	10:U:109:MET:HA	2.02	0.40
11:V:75:ILE:CG2	11:V:76:SER:N	2.82	0.40
2:B:152:ARG:HG3	2:B:152:ARG:NH2	2.36	0.40
3:C:349:VAL:O	3:C:353:GLN:HG3	2.21	0.40
11:K:38:GLN:O	11:K:84:ALA:HB1	2.21	0.40
1:L:110:GLY:C	1:L:112:THR:H	2.29	0.40
1:L:288:ASN:HD22	1:L:290:PHE:H	1.69	0.40
2:M:21:ALA:HB1	2:M:192:VAL:O	2.21	0.40
2:M:96:ASP:C	2:M:98:LEU:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:234:PHE:O	3:N:235:LEU:C	2.64	0.40
5:P:126:ILE:CG2	5:P:150:PRO:HB2	2.50	0.40
5:P:212:VAL:HG22	5:P:213:ILE:N	2.37	0.40
10:U:49:VAL:HG12	10:U:68:LEU:CD2	2.51	0.40
11:V:21:ILE:HG22	11:V:22:SER:N	2.37	0.40
11:V:29:ILE:HG22	11:V:92:ILE:HD12	2.02	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	428/430 (100%)	374 (87%)	47 (11%)	7 (2%)	7	31
1	L	428/430 (100%)	384 (90%)	37 (9%)	7 (2%)	7	31
2	B	350/352 (99%)	286 (82%)	47 (13%)	17 (5%)	1	9
2	M	350/352 (99%)	283 (81%)	48 (14%)	19 (5%)	1	7
3	C	383/385 (100%)	357 (93%)	21 (6%)	5 (1%)	9	36
3	N	383/385 (100%)	354 (92%)	24 (6%)	5 (1%)	9	36
4	D	243/248 (98%)	222 (91%)	20 (8%)	1 (0%)	30	62
4	O	243/248 (98%)	225 (93%)	14 (6%)	4 (2%)	7	31
5	E	183/185 (99%)	161 (88%)	19 (10%)	3 (2%)	7	31
5	P	183/185 (99%)	163 (89%)	20 (11%)	0	100	100
6	F	72/74 (97%)	65 (90%)	7 (10%)	0	100	100
6	Q	72/74 (97%)	62 (86%)	10 (14%)	0	100	100
7	G	123/126 (98%)	113 (92%)	8 (6%)	2 (2%)	7	31
7	R	123/126 (98%)	120 (98%)	2 (2%)	1 (1%)	16	47
8	H	91/93 (98%)	79 (87%)	8 (9%)	4 (4%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	91/93 (98%)	73 (80%)	13 (14%)	5 (6%)	1	7
9	I	51/57 (90%)	45 (88%)	6 (12%)	0	100	100
9	T	51/57 (90%)	45 (88%)	5 (10%)	1 (2%)	6	26
10	J	125/127 (98%)	110 (88%)	11 (9%)	4 (3%)	3	16
10	U	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	4	22
11	K	105/107 (98%)	85 (81%)	14 (13%)	6 (6%)	1	7
11	V	105/107 (98%)	83 (79%)	17 (16%)	5 (5%)	2	9
12	W	105/108 (97%)	89 (85%)	14 (13%)	2 (2%)	6	27
All	All	4413/4476 (99%)	3885 (88%)	427 (10%)	101 (2%)	5	23

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
2	B	95	LYS
2	B	152	ARG
2	B	335	PRO
2	B	336	ILE
3	C	108	SER
4	D	263	HIS
8	H	93	ASN
11	K	80	PRO
1	L	34	ASN
1	L	226	ASN
2	M	203	GLU
2	M	222	LYS
2	M	311	GLY
2	M	313	ASP
2	M	338	LEU
3	N	108	SER
3	N	346	VAL
4	O	263	HIS
8	S	36	PRO
8	S	52	PHE
1	A	29	VAL
2	B	45	ASP
2	B	320	TYR
2	B	338	LEU
3	C	215	ASN

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Mol	Chain	Res	Type
7	G	96	ALA
8	H	37	LEU
10	J	32	GLY
10	J	65	LYS
1	L	28	GLU
2	M	36	HIS
2	M	45	ASP
2	M	335	PRO
2	M	336	ILE
2	M	340	PHE
2	M	367	GLU
3	N	158	GLY
3	N	224	TYR
4	O	139	ASP
4	O	197	GLY
10	U	65	LYS
11	V	68	GLY
1	A	28	GLU
1	A	44	PRO
1	A	238	LYS
2	B	22	ARG
2	B	330	GLU
2	B	367	GLU
3	C	61	ALA
3	C	155	PRO
5	E	103	LEU
8	H	36	PRO
10	J	9	ALA
10	J	108	ALA
11	K	16	GLY
11	K	81	GLU
1	L	44	PRO
2	M	23	ASP
2	M	152	ARG
2	M	315	SER
4	O	102	ALA
8	S	42	HIS
9	T	12	LYS
11	V	30	ASN
12	W	22	CYS
2	B	222	LYS
2	B	224	PHE

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Mol	Chain	Res	Type
2	B	349	GLY
7	G	99	ASP
11	K	78	LEU
11	K	91	HIS
2	M	224	PHE
8	S	37	LEU
10	U	27	TYR
10	U	126	HIS
11	V	80	PRO
1	A	289	ALA
2	B	313	ASP
1	L	309	GLN
2	M	97	ASP
3	N	155	PRO
7	R	99	ASP
8	S	49	PHE
11	V	73	LEU
2	B	21	ALA
2	B	311	GLY
3	C	224	TYR
8	H	56	PHE
1	L	29	VAL
2	M	221	PRO
11	V	16	GLY
5	E	150	PRO
11	K	68	GLY
2	M	332	VAL
1	A	36	ILE
5	E	37	PRO
12	W	81	PRO
2	M	349	GLY
2	B	332	VAL
1	L	124	ILE

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	369/369 (100%)	329 (89%)	40 (11%)	6	24
1	L	369/369 (100%)	326 (88%)	43 (12%)	5	21
2	B	301/301 (100%)	273 (91%)	28 (9%)	8	30
2	M	301/301 (100%)	269 (89%)	32 (11%)	6	25
3	C	338/338 (100%)	308 (91%)	30 (9%)	9	32
3	N	338/338 (100%)	313 (93%)	25 (7%)	13	40
4	D	202/206 (98%)	190 (94%)	12 (6%)	18	48
4	O	202/206 (98%)	192 (95%)	10 (5%)	22	54
5	E	151/151 (100%)	137 (91%)	14 (9%)	8	30
5	P	151/151 (100%)	141 (93%)	10 (7%)	15	44
6	F	67/67 (100%)	59 (88%)	8 (12%)	5	20
6	Q	67/67 (100%)	58 (87%)	9 (13%)	4	16
7	G	109/110 (99%)	103 (94%)	6 (6%)	19	51
7	R	109/110 (99%)	98 (90%)	11 (10%)	7	27
8	H	77/77 (100%)	70 (91%)	7 (9%)	9	31
8	S	77/77 (100%)	69 (90%)	8 (10%)	7	26
9	I	45/47 (96%)	41 (91%)	4 (9%)	9	32
9	T	45/47 (96%)	44 (98%)	1 (2%)	45	73
10	J	112/112 (100%)	99 (88%)	13 (12%)	5	21
10	U	112/112 (100%)	98 (88%)	14 (12%)	4	19
11	K	93/93 (100%)	85 (91%)	8 (9%)	10	34
11	V	93/93 (100%)	88 (95%)	5 (5%)	20	51
12	W	88/88 (100%)	75 (85%)	13 (15%)	3	13
All	All	3816/3830 (100%)	3465 (91%)	351 (9%)	8	31

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	65	ASN
1	A	71	LEU
1	A	74	ASN
1	A	93	SER
1	A	108	LEU
1	A	114	LYS

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	124	ILE
1	A	126	GLN
1	A	141	LYS
1	A	144	LEU
1	A	163	LEU
1	A	171	THR
1	A	173	LEU
1	A	181	LEU
1	A	182	GLU
1	A	184	LEU
1	A	226	ASN
1	A	229	LEU
1	A	237	LEU
1	A	240	LYS
1	A	251	ARG
1	A	260	ILE
1	A	269	VAL
1	A	270	ASN
1	A	278	LYS
1	A	305	ILE
1	A	319	LEU
1	A	323	ASP
1	A	342	LEU
1	A	360	THR
1	A	369	LEU
1	A	372	GLN
1	A	376	LEU
1	A	384	ASN
1	A	389	LEU
1	A	423	LYS
1	A	425	LEU
1	A	448	ARG
2	B	17	LEU
2	B	30	THR
2	B	53	ARG
2	B	62	ARG
2	B	81	THR
2	B	85	GLU
2	B	88	THR
2	B	98	LEU
2	B	112	THR

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Mol	Chain	Res	Type
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	193	VAL
2	B	206	LEU
2	B	215	LEU
2	B	254	GLU
2	B	267	LEU
2	B	294	SER
2	B	325	ASN
2	B	330	GLU
2	B	339	ASN
2	B	340	PHE
2	B	347	LYS
2	B	348	LEU
2	B	359	VAL
2	B	361	ASN
2	B	362	LEU
2	B	367	GLU
3	C	5	LYS
3	C	12	LEU
3	C	35	LEU
3	C	56	SER
3	C	57	ASN
3	C	63	SER
3	C	79	ARG
3	C	81	LEU
3	C	99	LYS
3	C	107	ARG
3	C	108	SER
3	C	112	THR
3	C	150	LEU
3	C	155	PRO
3	C	182	LEU
3	C	185	LEU
3	C	206	SER
3	C	238	LEU
3	C	247	SER
3	C	269	ILE
3	C	283	ARG
3	C	292	VAL
3	C	302	LEU

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Mol	Chain	Res	Type
3	C	312	VAL
3	C	313	VAL
3	C	319	LYS
3	C	321	LEU
3	C	335	LEU
3	C	342	CYS
3	C	377	LEU
4	D	63	THR
4	D	69	LEU
4	D	109	ARG
4	D	113	ARG
4	D	137	GLU
4	D	141	GLN
4	D	200	ASP
4	D	244	THR
4	D	251	VAL
4	D	280	LEU
4	D	283	LEU
4	D	301	VAL
5	E	31	LYS
5	E	42	VAL
5	E	51	LYS
5	E	55	TYR
5	E	73	SER
5	E	85	THR
5	E	91	MET
5	E	110	LYS
5	E	114	LYS
5	E	147	VAL
5	E	187	ILE
5	E	197	PRO
5	E	202	ILE
5	E	213	ILE
6	F	77	GLN
6	F	80	ASP
6	F	84	HIS
6	F	94	LEU
6	F	95	VAL
6	F	99	GLU
6	F	119	HIS
6	F	130	LEU
7	G	16	LEU

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Mol	Chain	Res	Type
7	G	51	GLU
7	G	62	ARG
7	G	77	ARG
7	G	83	LEU
7	G	127	LYS
8	H	38	GLN
8	H	43	ASN
8	H	50	ARG
8	H	56	PHE
8	H	60	LEU
8	H	68	TYR
8	H	71	LYS
9	I	4	SER
9	I	13	ARG
9	I	14	ASN
9	I	30	THR
10	J	1	GLU
10	J	21	THR
10	J	30	THR
10	J	36	ASN
10	J	39	ARG
10	J	51	TYR
10	J	54	ASN
10	J	61	ASN
10	J	64	LEU
10	J	68	LEU
10	J	79	PHE
10	J	93	THR
10	J	100	GLU
11	K	15	LEU
11	K	18	ARG
11	K	33	LEU
11	K	69	THR
11	K	81	GLU
11	K	92	ILE
11	K	104	LEU
11	K	107	LYS
1	L	30	THR
1	L	46	HIS
1	L	65	ASN
1	L	90	LEU
1	L	108	LEU

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Mol	Chain	Res	Type
1	L	113	ASP
1	L	114	LYS
1	L	119	LEU
1	L	125	GLN
1	L	141	LYS
1	L	149	ASP
1	L	152	ASP
1	L	163	LEU
1	L	171	THR
1	L	173	LEU
1	L	175	LEU
1	L	182	GLU
1	L	184	LEU
1	L	187	LEU
1	L	217	ASP
1	L	226	ASN
1	L	237	LEU
1	L	240	LYS
1	L	250	LEU
1	L	251	ARG
1	L	260	ILE
1	L	279	LEU
1	L	288	ASN
1	L	292	PRO
1	L	305	ILE
1	L	329	PHE
1	L	331	THR
1	L	342	LEU
1	L	359	ASP
1	L	360	THR
1	L	364	ARG
1	L	369	LEU
1	L	372	GLN
1	L	376	LEU
1	L	389	LEU
1	L	394	LEU
1	L	425	LEU
1	L	446	ARG
2	M	31	LEU
2	M	41	TYR
2	M	43	THR
2	M	47	VAL

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Mol	Chain	Res	Type
2	M	62	ARG
2	M	83	ASP
2	M	85	GLU
2	M	98	LEU
2	M	111	LYS
2	M	112	THR
2	M	128	ARG
2	M	144	ASP
2	M	146	LEU
2	M	150	THR
2	M	152	ARG
2	M	166	ARG
2	M	169	LEU
2	M	193	VAL
2	M	206	LEU
2	M	213	LYS
2	M	215	LEU
2	M	216	VAL
2	M	254	GLU
2	M	266	GLU
2	M	267	LEU
2	M	287	LEU
2	M	318	ILE
2	M	330	GLU
2	M	345	ASP
2	M	347	LYS
2	M	360	SER
2	M	367	GLU
3	N	5	LYS
3	N	12	LEU
3	N	17	ILE
3	N	34	SER
3	N	35	LEU
3	N	38	LEU
3	N	57	ASN
3	N	79	ARG
3	N	81	LEU
3	N	99	LYS
3	N	112	THR
3	N	150	LEU
3	N	159	ASN
3	N	175	THR

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Mol	Chain	Res	Type
3	N	182	LEU
3	N	185	LEU
3	N	206	SER
3	N	230	LEU
3	N	292	VAL
3	N	312	VAL
3	N	313	VAL
3	N	317	THR
3	N	350	LEU
3	N	377	LEU
3	N	382	ARG
4	O	69	LEU
4	O	77	SER
4	O	83	GLU
4	O	109	ARG
4	O	113	ARG
4	O	115	LEU
4	O	244	THR
4	O	251	VAL
4	O	280	LEU
4	O	283	LEU
5	P	51	LYS
5	P	76	GLU
5	P	107	VAL
5	P	110	LYS
5	P	114	LYS
5	P	124	HIS
5	P	187	ILE
5	P	190	ARG
5	P	211	LYS
5	P	213	ILE
6	Q	74	ASP
6	Q	77	GLN
6	Q	80	ASP
6	Q	86	LYS
6	Q	94	LEU
6	Q	111	GLN
6	Q	118	GLU
6	Q	119	HIS
6	Q	130	LEU
7	R	6	THR
7	R	16	LEU

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Mol	Chain	Res	Type
7	R	31	GLN
7	R	41	LEU
7	R	62	ARG
7	R	66	ASP
7	R	77	ARG
7	R	81	THR
7	R	83	LEU
7	R	97	GLN
7	R	127	LYS
8	S	38	GLN
8	S	42	HIS
8	S	47	ASN
8	S	50	ARG
8	S	56	PHE
8	S	60	LEU
8	S	68	TYR
8	S	71	LYS
9	T	13	ARG
10	U	5	GLN
10	U	36	ASN
10	U	38	ILE
10	U	39	ARG
10	U	51	TYR
10	U	54	ASN
10	U	57	ASP
10	U	61	ASN
10	U	64	LEU
10	U	68	LEU
10	U	87	THR
10	U	99	SER
10	U	125	ARG
10	U	126	HIS
11	V	18	ARG
11	V	74	THR
11	V	92	ILE
11	V	93	LYS
11	V	107	LYS
12	W	2	GLU
12	W	10	LYS
12	W	14	LEU
12	W	21	GLN
12	W	26	GLU

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Mol	Chain	Res	Type
12	W	36	ASN
12	W	44	HIS
12	W	78	LYS
12	W	80	ILE
12	W	85	MET
12	W	93	GLU
12	W	94	LYS
12	W	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	62	ASN
1	A	65	ASN
1	A	66	ASN
1	A	101	GLN
1	A	120	ASN
1	A	121	GLN
1	A	126	GLN
1	A	129	ASN
1	A	155	HIS
1	A	169	GLN
1	A	170	ASN
1	A	198	ASN
1	A	199	HIS
1	A	204	ASN
1	A	282	GLN
1	A	304	ASN
1	A	309	GLN
1	A	316	HIS
1	A	335	ASN
1	A	344	HIS
1	A	375	GLN
2	B	49	HIS
2	B	52	ASN
2	B	191	ASN
2	B	246	ASN
2	B	252	GLN
2	B	325	ASN
2	B	339	ASN
3	C	7	ASN

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Mol	Chain	Res	Type
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	173	ASN
3	C	202	HIS
3	C	208	ASN
3	C	222	HIS
3	C	253	HIS
3	C	256	ASN
3	C	332	ASN
4	D	70	HIS
4	D	122	ASN
4	D	213	ASN
5	E	38	ASN
5	E	106	ASN
6	F	77	GLN
6	F	109	GLN
6	F	111	GLN
7	G	31	GLN
7	G	53	ASN
7	G	57	GLN
7	G	79	HIS
7	G	86	HIS
8	H	15	HIS
8	H	42	HIS
9	I	14	ASN
9	I	29	GLN
10	J	36	ASN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	31	ASN
11	K	34	ASN
11	K	55	HIS
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS
1	L	31	GLN
1	L	60	ASN

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Mol	Chain	Res	Type
1	L	62	ASN
1	L	65	ASN
1	L	66	ASN
1	L	95	ASN
1	L	101	GLN
1	L	120	ASN
1	L	121	GLN
1	L	155	HIS
1	L	170	ASN
1	L	199	HIS
1	L	204	ASN
1	L	288	ASN
1	L	313	ASN
1	L	316	HIS
1	L	335	ASN
1	L	349	GLN
1	L	384	ASN
1	L	387	ASN
1	L	428	GLN
2	M	49	HIS
2	M	52	ASN
2	M	55	ASN
2	M	60	ASN
2	M	145	GLN
2	M	191	ASN
2	M	246	ASN
2	M	252	GLN
2	M	319	ASN
2	M	328	GLN
2	M	339	ASN
3	N	7	ASN
3	N	14	ASN
3	N	22	GLN
3	N	31	ASN
3	N	74	ASN
3	N	159	ASN
3	N	173	ASN
3	N	202	HIS
3	N	208	ASN
3	N	222	HIS
3	N	253	HIS
3	N	332	ASN

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Mol	Chain	Res	Type
4	O	67	HIS
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	143	ASN
4	O	256	ASN
4	O	303	ASN
5	P	38	ASN
5	P	106	ASN
5	P	127	GLN
5	P	151	GLN
5	P	184	HIS
6	Q	77	GLN
7	R	31	GLN
7	R	34	ASN
7	R	79	HIS
7	R	122	ASN
8	S	15	HIS
9	T	14	ASN
9	T	29	GLN
10	U	16	GLN
10	U	36	ASN
10	U	54	ASN
10	U	59	ASN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
10	U	114	GLN
11	V	31	ASN
11	V	34	ASN
11	V	91	HIS
12	W	57	ASN
12	W	67	ASN
12	W	75	ASN
12	W	97	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
12	M3L	W	77	12	10,11,12	0.64	0	9,14,16	1.24	1 (11%)

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
12	M3L	W	77	12	-	1/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	W	77	M3L	CM3-NZ-CM2	-2.80	101.61	108.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	W	77	M3L	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	W	77	M3L	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEC	C	502	3	50,50,50	1.27	3 (6%)	68,82,82	1.31	6 (8%)
13	HEC	W	526	12	50,50,50	1.19	5 (10%)	68,82,82	1.70	6 (8%)
15	FES	E	504	5	0,4,4	-	-	-		
13	HEC	N	521	3	50,50,50	1.51	5 (10%)	68,82,82	1.55	9 (13%)
13	HEC	D	503	4	50,50,50	1.04	2 (4%)	68,82,82	1.43	6 (8%)
13	HEC	C	501	3	50,50,50	1.50	5 (10%)	68,82,82	1.38	5 (7%)
15	FES	P	524	5	0,4,4	-	-	-		
14	SMA	N	525	-	38,38,38	1.63	7 (18%)	47,52,52	2.22	10 (21%)
14	SMA	C	505	-	38,38,38	1.59	6 (15%)	47,52,52	2.15	11 (23%)
13	HEC	O	523	4	50,50,50	1.04	4 (8%)	68,82,82	1.06	5 (7%)
13	HEC	N	522	3	50,50,50	1.26	4 (8%)	68,82,82	1.40	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEC	C	502	3	1/1/3/7	6/14/54/54	-
13	HEC	W	526	12	1/1/3/7	5/14/54/54	-
15	FES	E	504	5	-	-	0/1/1/1
13	HEC	N	521	3	1/1/3/7	9/14/54/54	-
13	HEC	D	503	4	1/1/3/7	7/14/54/54	-
13	HEC	C	501	3	1/1/3/7	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FES	P	524	5	-	-	0/1/1/1
14	SMA	N	525	-	2/2/5/10	18/34/34/34	0/2/2/2
14	SMA	C	505	-	2/2/5/10	23/34/34/34	0/2/2/2
13	HEC	O	523	4	1/1/3/7	6/14/54/54	-
13	HEC	N	522	3	1/1/3/7	8/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEC	CAB-C3B	-5.86	1.36	1.51
13	N	521	HEC	CAC-C3C	-5.46	1.37	1.51
13	N	521	HEC	CAB-C3B	-5.08	1.38	1.51
13	C	502	HEC	CAC-C3C	-4.91	1.38	1.51
13	C	501	HEC	CAC-C3C	-4.70	1.39	1.51
14	C	505	SMA	C20-C19	4.59	1.36	1.33
14	N	525	SMA	C20-C19	4.57	1.36	1.33
13	N	522	HEC	CAC-C3C	-4.28	1.40	1.51
13	C	502	HEC	CAB-C3B	-4.21	1.40	1.51
13	W	526	HEC	FE-NC	3.70	2.07	1.95
14	N	525	SMA	O1-C2	3.63	1.40	1.36
13	N	521	HEC	FE-NB	3.59	2.06	1.94
13	W	526	HEC	FE-NB	3.58	2.05	1.94
13	N	522	HEC	CAB-C3B	-3.57	1.42	1.51
14	N	525	SMA	C13-C12	3.45	1.62	1.54
14	C	505	SMA	C13-C12	3.40	1.62	1.54
13	D	503	HEC	FE-ND	3.27	2.05	1.94
14	N	525	SMA	C4A-C8A	3.24	1.47	1.40
14	C	505	SMA	C4A-C8A	3.21	1.47	1.40
13	C	501	HEC	FE-NB	3.16	2.04	1.94
14	C	505	SMA	C4A-C5	3.16	1.46	1.40
13	D	503	HEC	FE-NA	3.08	2.05	1.95
13	C	501	HEC	CMC-C2C	3.05	1.57	1.50
14	C	505	SMA	O1-C2	3.05	1.40	1.36
13	O	523	HEC	FE-ND	2.87	2.03	1.94
13	N	521	HEC	CMC-C2C	2.72	1.56	1.50
13	N	522	HEC	CMC-C2C	2.72	1.56	1.50
14	N	525	SMA	C4A-C5	2.51	1.45	1.40
13	W	526	HEC	FE-NA	2.48	2.03	1.95
13	N	521	HEC	CBC-CAC	-2.44	1.41	1.51
14	N	525	SMA	O1-C8A	2.41	1.41	1.38
13	N	522	HEC	FE-NB	2.23	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	525	SMA	O7-C7	2.19	1.40	1.37
13	C	502	HEC	FE-NB	2.19	2.01	1.94
14	C	505	SMA	O7-C7	2.16	1.40	1.37
13	O	523	HEC	CAA-C2A	-2.15	1.45	1.51
13	O	523	HEC	FE-NA	2.15	2.02	1.95
13	W	526	HEC	FE-ND	2.13	2.01	1.94
13	W	526	HEC	CAB-C3B	2.10	1.56	1.51
13	C	501	HEC	FE-NA	2.02	2.01	1.95
13	O	523	HEC	FE-NC	2.00	2.01	1.95

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	525	SMA	C26-C19-C18	-6.85	107.62	118.09
13	D	503	HEC	CAC-C3C-C4C	-6.61	115.81	124.91
14	C	505	SMA	C26-C19-C18	-6.59	108.02	118.09
13	W	526	HEC	CAC-C3C-C4C	-6.47	116.00	124.91
13	W	526	HEC	CAC-C3C-C2C	6.33	136.91	126.89
13	C	501	HEC	CAC-C3C-C4C	6.24	133.49	124.91
13	D	503	HEC	CAC-C3C-C2C	6.23	136.74	126.89
14	N	525	SMA	O14-C14-C15	6.20	129.06	111.05
14	C	505	SMA	O14-C14-C15	5.96	128.38	111.05
13	W	526	HEC	CAB-C3B-C4B	-5.76	117.29	124.79
13	N	521	HEC	CMC-C2C-C1C	5.56	133.89	125.42
14	C	505	SMA	O14-C14-C13	5.56	119.46	107.97
13	N	522	HEC	CBB-CAB-C3B	5.47	127.25	112.42
13	C	502	HEC	CBB-CAB-C3B	5.43	127.15	112.42
13	N	521	HEC	CAC-C3C-C4C	5.40	132.33	124.91
14	N	525	SMA	O14-C14-C13	5.34	119.00	107.97
13	W	526	HEC	CAB-C3B-C2B	5.16	137.05	127.56
13	N	522	HEC	CBC-CAC-C3C	4.84	125.54	112.42
13	C	501	HEC	CAC-C3C-C2C	-4.70	119.46	126.89
13	N	521	HEC	CBB-CAB-C3B	4.45	124.49	112.42
13	N	521	HEC	CAC-C3C-C2C	-4.15	120.33	126.89
14	N	525	SMA	O7-C7-C8	4.05	118.77	114.53
13	N	522	HEC	CAC-C3C-C2C	4.05	133.31	126.89
14	C	505	SMA	O12-C12-C13	4.03	113.91	107.97
13	C	502	HEC	CBC-CAC-C3C	3.98	123.21	112.42
13	C	502	HEC	CAA-C2A-C3A	-3.70	120.93	127.87
13	C	501	HEC	CBC-CAC-C3C	3.53	121.98	112.42
14	N	525	SMA	O12-C12-C13	3.51	113.15	107.97
13	O	523	HEC	CMA-C3A-C4A	3.45	130.81	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	505	SMA	O1-C2-C9	3.45	117.45	110.12
13	C	502	HEC	CAA-C2A-C1A	3.45	131.87	124.85
13	N	522	HEC	CAC-C3C-C4C	-3.44	120.18	124.91
14	N	525	SMA	O1-C2-C9	3.32	117.17	110.12
14	C	505	SMA	O7-C7-C8	3.17	117.85	114.53
14	N	525	SMA	O1-C8A-C8	3.16	122.54	116.28
14	N	525	SMA	C18-C19-C20	3.08	126.74	118.55
14	N	525	SMA	O7-C7-C6	-2.99	118.93	124.08
13	C	502	HEC	CAB-C3B-C4B	-2.98	120.92	124.79
13	C	501	HEC	CMB-C2B-C1B	2.94	129.62	125.03
13	D	503	HEC	CAB-C3B-C4B	-2.91	121.00	124.79
13	C	501	HEC	CMC-C2C-C1C	2.91	129.85	125.42
14	C	505	SMA	O1-C8A-C8	2.86	121.94	116.28
13	N	521	HEC	CMC-C2C-C3C	-2.81	119.67	125.62
13	O	523	HEC	CAB-C3B-C4B	-2.80	121.15	124.79
14	C	505	SMA	C18-C19-C20	2.80	125.99	118.55
13	O	523	HEC	CAA-C2A-C3A	-2.61	122.98	127.87
13	N	521	HEC	CAD-C3D-C4D	2.55	129.14	124.70
13	D	503	HEC	CAB-C3B-C2B	2.53	132.20	127.56
13	N	521	HEC	CBC-CAC-C3C	2.50	119.20	112.42
14	C	505	SMA	O7-C7-C6	-2.49	119.79	124.08
13	C	502	HEC	CAB-C3B-C2B	2.48	132.11	127.56
13	O	523	HEC	CAA-C2A-C1A	2.45	129.83	124.85
13	W	526	HEC	C2B-C1B-NB	-2.37	107.16	109.90
13	O	523	HEC	CAB-C3B-C2B	2.31	131.81	127.56
13	N	522	HEC	CAA-C2A-C1A	2.26	129.45	124.85
14	C	505	SMA	C11-C12-C13	-2.17	108.51	114.29
13	N	521	HEC	O1A-CGA-CBA	-2.16	116.24	123.09
13	N	521	HEC	CAD-C3D-C2D	-2.14	123.86	127.87
13	N	522	HEC	CMC-C2C-C3C	2.11	130.10	125.62
13	N	522	HEC	CAA-C2A-C3A	-2.09	123.95	127.87
14	C	505	SMA	C3M-C3-C2	-2.09	120.18	123.28
13	W	526	HEC	CHB-C1B-NB	2.08	126.66	124.42
13	D	503	HEC	CMD-C2D-C1D	2.06	128.25	125.03
14	N	525	SMA	C11-C12-C13	-2.03	108.87	114.29
13	D	503	HEC	CBC-CAC-C3C	-2.00	106.99	112.42

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	501	HEC	NA
13	C	502	HEC	NA

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Mol	Chain	Res	Type	Atom
13	D	503	HEC	NA
13	N	521	HEC	NA
13	N	522	HEC	NA
13	O	523	HEC	NA
13	W	526	HEC	NA
14	C	505	SMA	C12
14	C	505	SMA	C14
14	N	525	SMA	C12
14	N	525	SMA	C14

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	505	SMA	C11-C12-C13-C24
14	C	505	SMA	O12-C12-C13-C24
14	C	505	SMA	C13-C14-O14-C25
14	C	505	SMA	C14-C15-C16-C17
14	C	505	SMA	C16-C17-C18-C19
14	N	525	SMA	C11-C12-C13-C24
14	N	525	SMA	O12-C12-C13-C14
14	N	525	SMA	O12-C12-C13-C24
14	N	525	SMA	C12-C13-C14-C15
14	N	525	SMA	C24-C13-C14-C15
14	N	525	SMA	O14-C14-C15-C16
14	N	525	SMA	C13-C14-O14-C25
14	N	525	SMA	C14-C15-C16-C17
14	N	525	SMA	C16-C17-C18-C19
13	C	501	HEC	C4C-C3C-CAC-CBC
13	N	521	HEC	C4B-C3B-CAB-CBB
13	N	522	HEC	C4B-C3B-CAB-CBB
13	N	521	HEC	C2B-C3B-CAB-CBB
13	N	522	HEC	C2B-C3B-CAB-CBB
13	C	501	HEC	C2C-C3C-CAC-CBC
13	N	522	HEC	C4C-C3C-CAC-CBC
13	N	522	HEC	C2C-C3C-CAC-CBC
13	C	502	HEC	C4B-C3B-CAB-CBB
13	C	502	HEC	C2B-C3B-CAB-CBB
14	C	505	SMA	C9-C10-C11-C22
13	N	521	HEC	C2C-C3C-CAC-CBC
14	C	505	SMA	C15-C16-C17-C18
14	N	525	SMA	C15-C16-C17-C18
13	N	521	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	C	505	SMA	C6-C5-O5-C5M
13	N	521	HEC	C4C-C3C-CAC-CBC
13	W	526	HEC	C2C-C3C-CAC-CBC
14	C	505	SMA	O12-C12-C13-C14
14	C	505	SMA	C4A-C5-O5-C5M
14	N	525	SMA	C17-C18-C19-C26
14	N	525	SMA	C17-C18-C19-C20
13	O	523	HEC	C2B-C3B-CAB-CBB
13	W	526	HEC	C4C-C3C-CAC-CBC
14	C	505	SMA	C17-C18-C19-C26
14	C	505	SMA	C24-C13-C14-O14
13	C	501	HEC	C2A-CAA-CBA-CGA
14	C	505	SMA	C12-C13-C14-C15
14	C	505	SMA	C22-C11-C12-O12
14	N	525	SMA	C22-C11-C12-O12
14	C	505	SMA	C17-C18-C19-C20
13	O	523	HEC	C4C-C3C-CAC-CBC
14	C	505	SMA	O14-C14-C15-C16
14	C	505	SMA	C9-C10-C11-C12
14	N	525	SMA	C11-C12-C13-C14
13	O	523	HEC	C4B-C3B-CAB-CBB
14	C	505	SMA	C24-C13-C14-C15
14	N	525	SMA	C24-C13-C14-O14
13	D	503	HEC	C4D-C3D-CAD-CBD
13	O	523	HEC	C2C-C3C-CAC-CBC
13	D	503	HEC	CAD-CBD-CGD-O2D
13	D	503	HEC	CAD-CBD-CGD-O1D
13	C	501	HEC	CAD-CBD-CGD-O1D
13	C	502	HEC	CAD-CBD-CGD-O1D
13	C	501	HEC	CAD-CBD-CGD-O2D
13	C	502	HEC	CAD-CBD-CGD-O2D
13	C	502	HEC	CAA-CBA-CGA-O1A
13	O	523	HEC	CAA-CBA-CGA-O2A
14	C	505	SMA	C11-C12-C13-C14
13	N	522	HEC	CAA-CBA-CGA-O1A
13	O	523	HEC	CAA-CBA-CGA-O1A
13	C	502	HEC	CAA-CBA-CGA-O2A
13	N	521	HEC	CAD-CBD-CGD-O2D
13	N	522	HEC	CAA-CBA-CGA-O2A
13	D	503	HEC	CAA-CBA-CGA-O2A
13	N	522	HEC	CAD-CBD-CGD-O2D
13	N	521	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	W	526	HEC	CAA-CBA-CGA-O2A
13	N	521	HEC	CAA-CBA-CGA-O2A
13	N	521	HEC	CAD-CBD-CGD-O1D
13	N	522	HEC	CAD-CBD-CGD-O1D
13	D	503	HEC	CAA-CBA-CGA-O1A
14	C	505	SMA	C10-C11-C12-O12
14	N	525	SMA	O1-C2-C9-C10
14	N	525	SMA	C10-C11-C12-O12
14	N	525	SMA	C9-C10-C11-C22
13	C	501	HEC	CAA-CBA-CGA-O1A
13	C	501	HEC	CAA-CBA-CGA-O2A
13	W	526	HEC	CAA-CBA-CGA-O1A
14	C	505	SMA	C3-C2-C9-C10
14	C	505	SMA	C13-C14-C15-C16
14	C	505	SMA	C12-C13-C14-O14
13	W	526	HEC	C2B-C3B-CAB-CBB
13	D	503	HEC	C2B-C3B-CAB-CBB
13	D	503	HEC	C4B-C3B-CAB-CBB

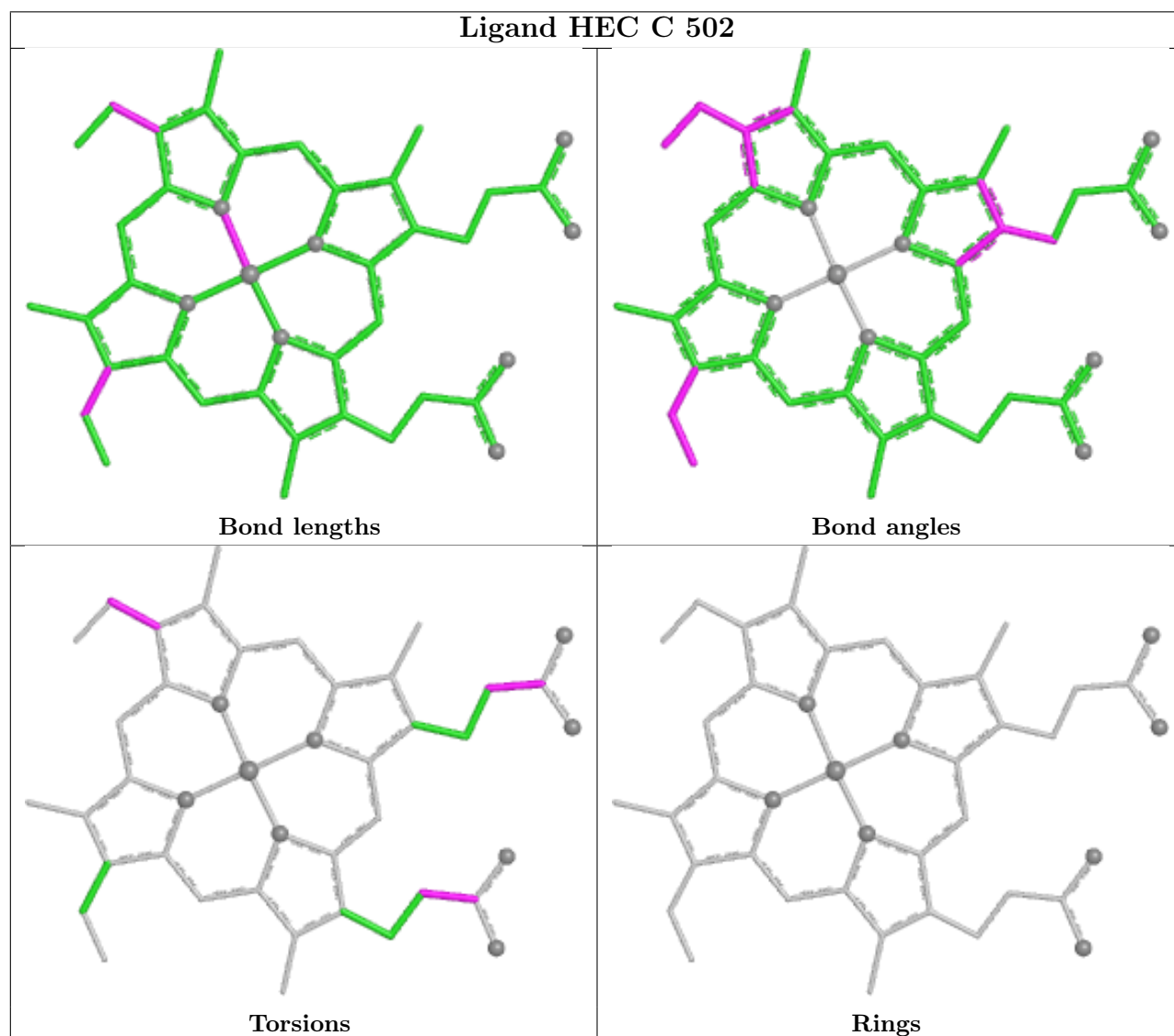
There are no ring outliers.

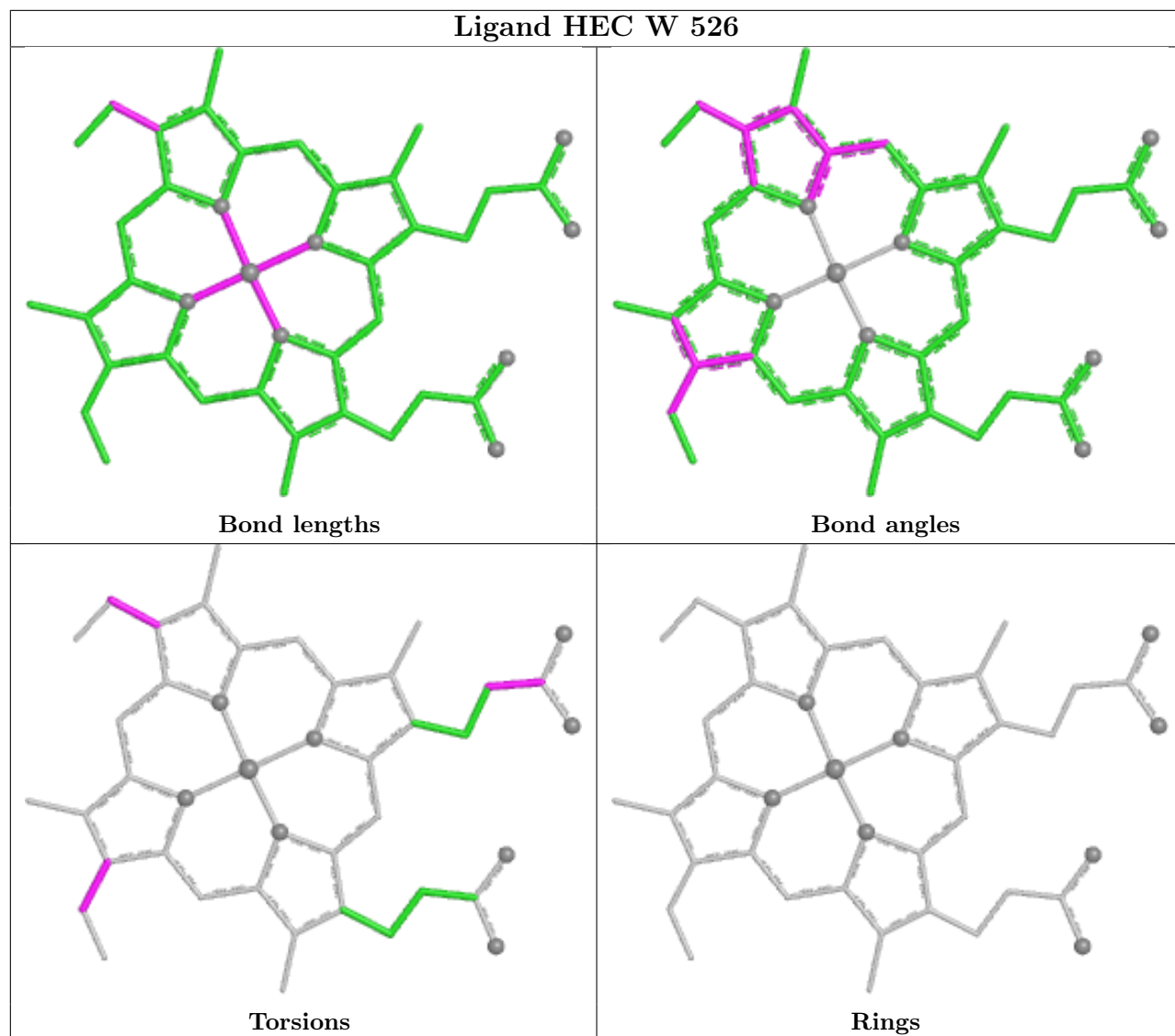
8 monomers are involved in 29 short contacts:

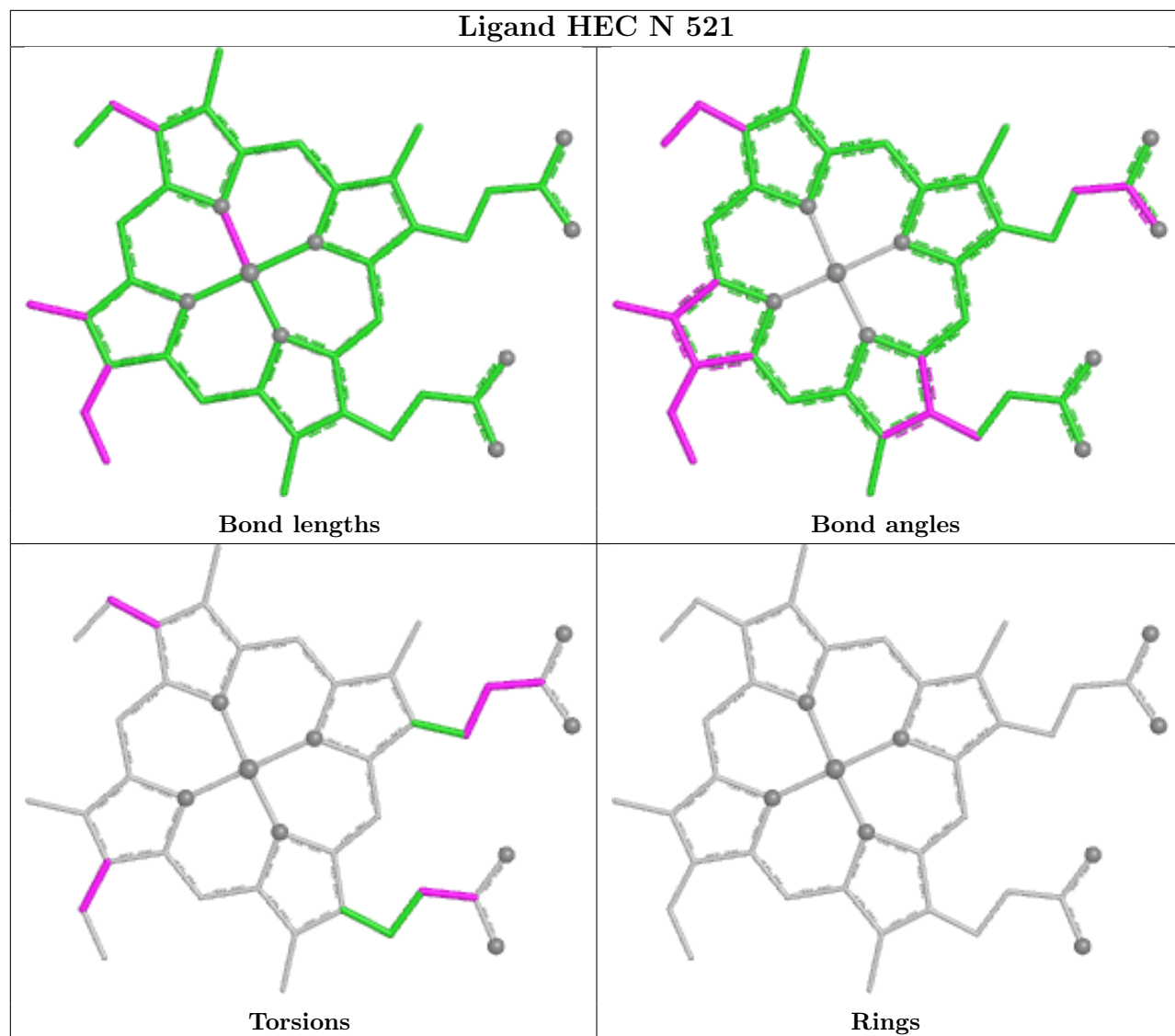
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	526	HEC	3	0
15	E	504	FES	1	0
13	N	521	HEC	3	0
13	C	501	HEC	6	0
14	N	525	SMA	5	0
14	C	505	SMA	5	0
13	O	523	HEC	3	0
13	N	522	HEC	3	0

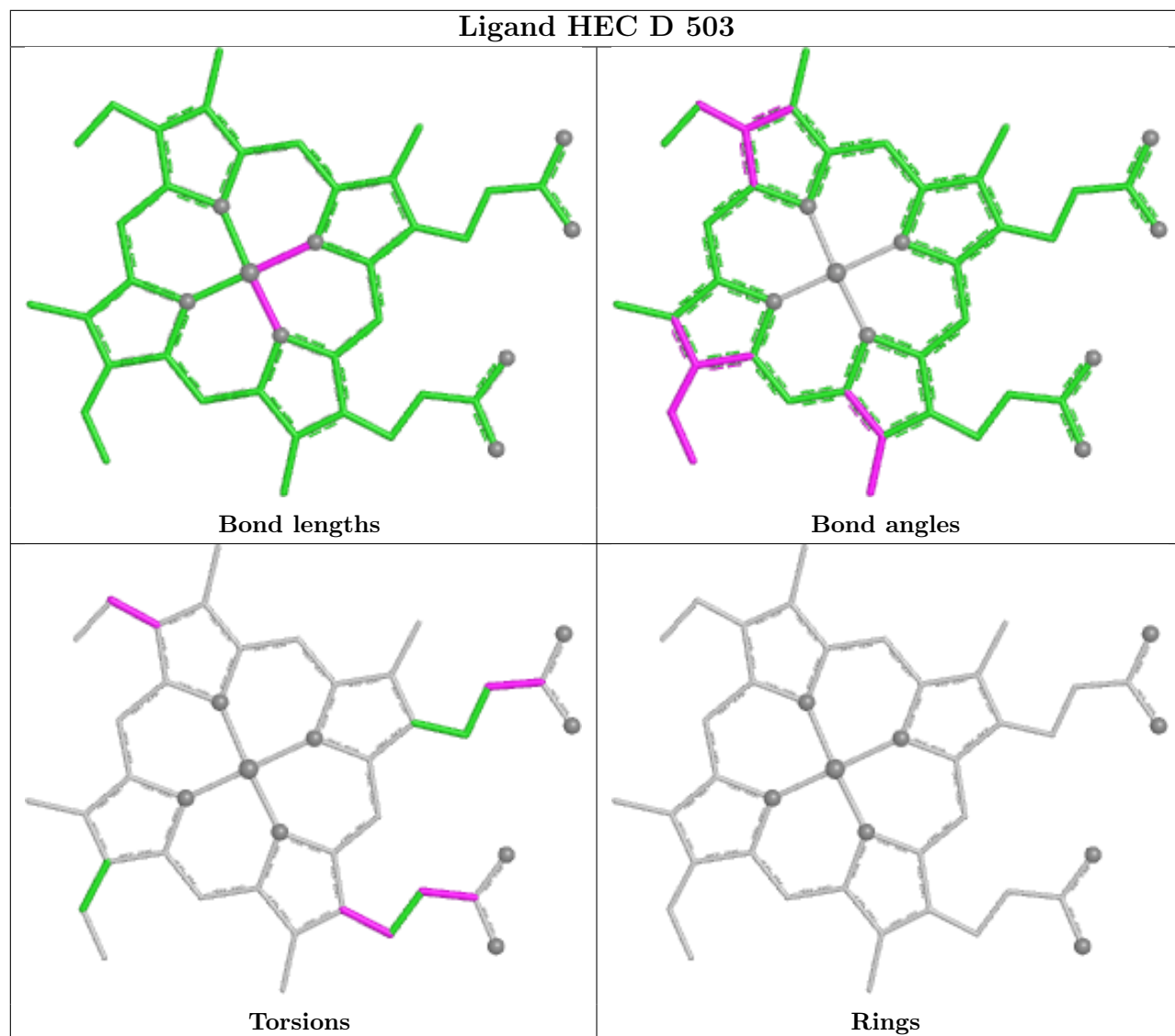
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

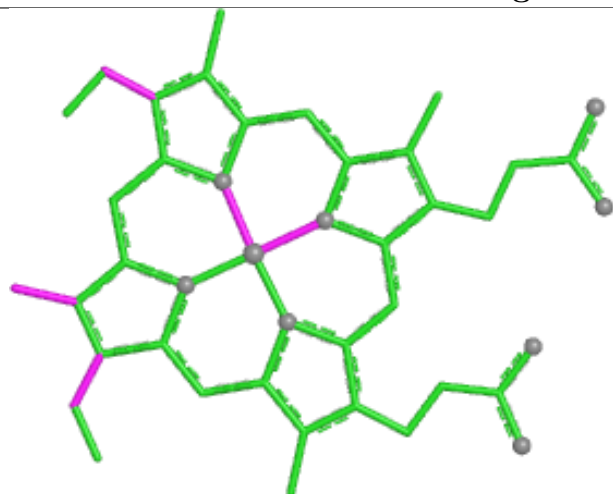




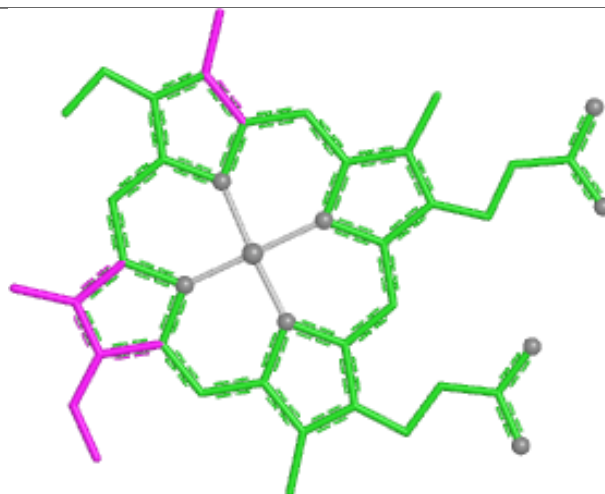




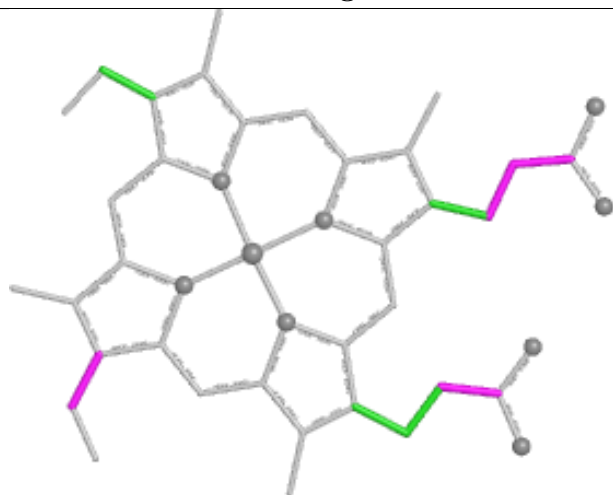
Ligand HEC C 501



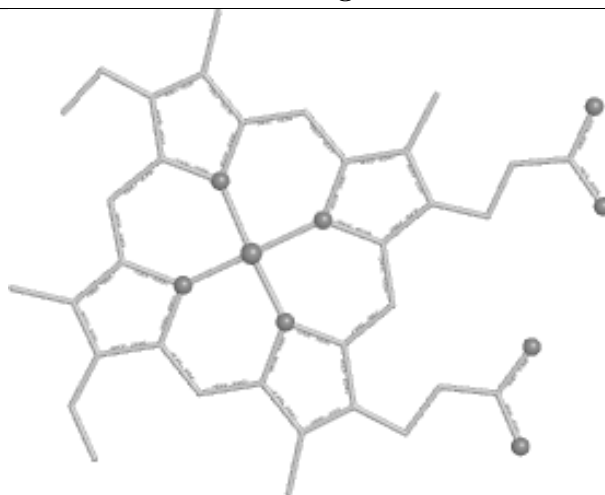
Bond lengths



Bond angles

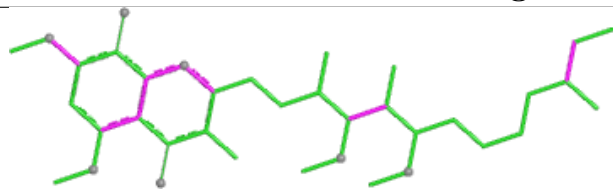


Torsions

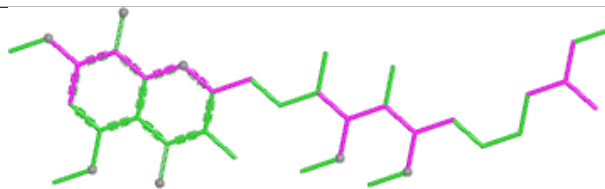


Rings

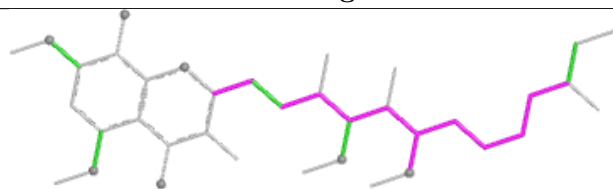
Ligand SMA N 525



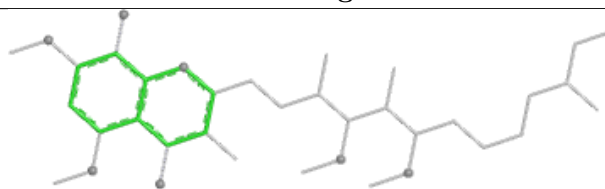
Bond lengths



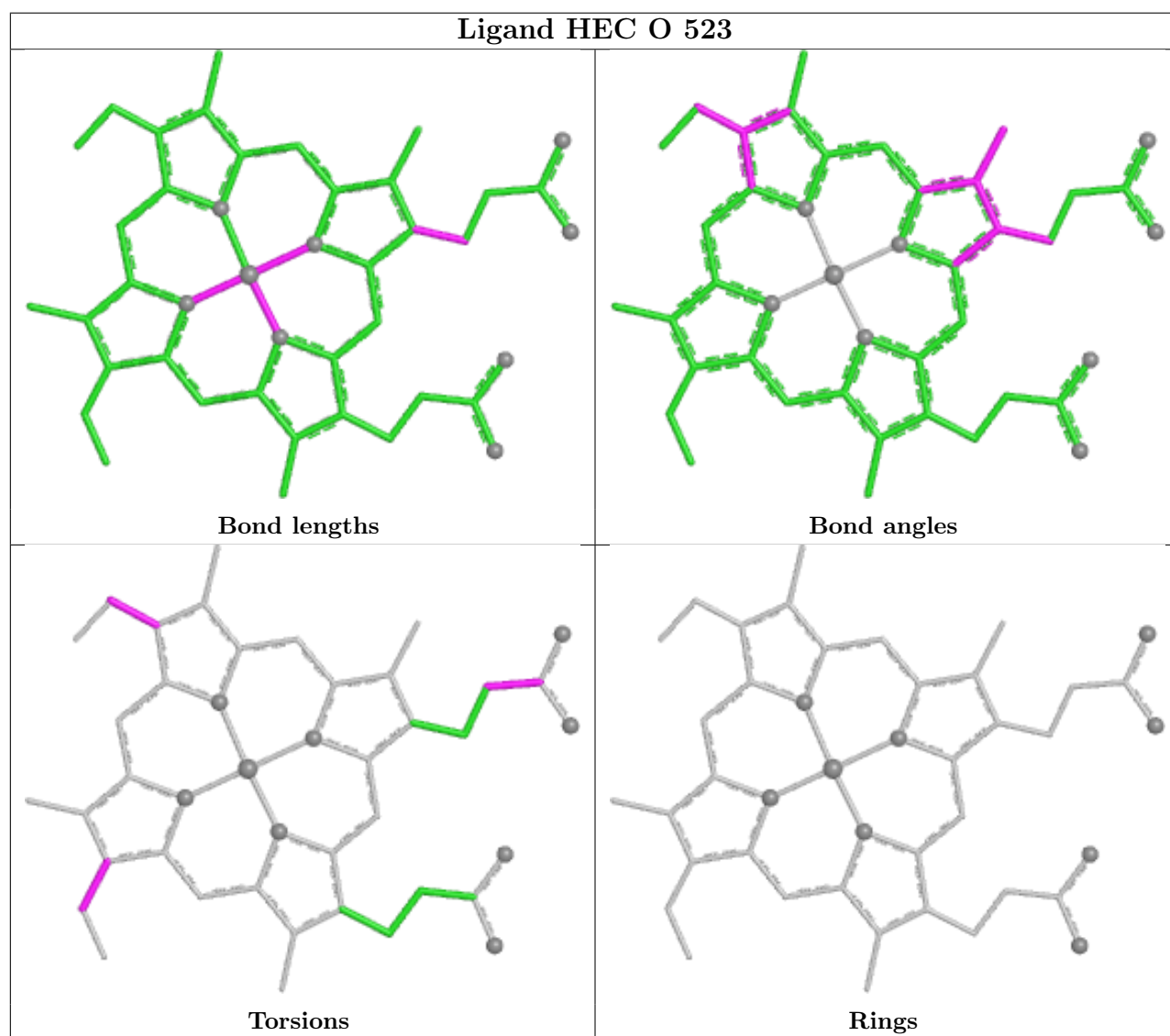
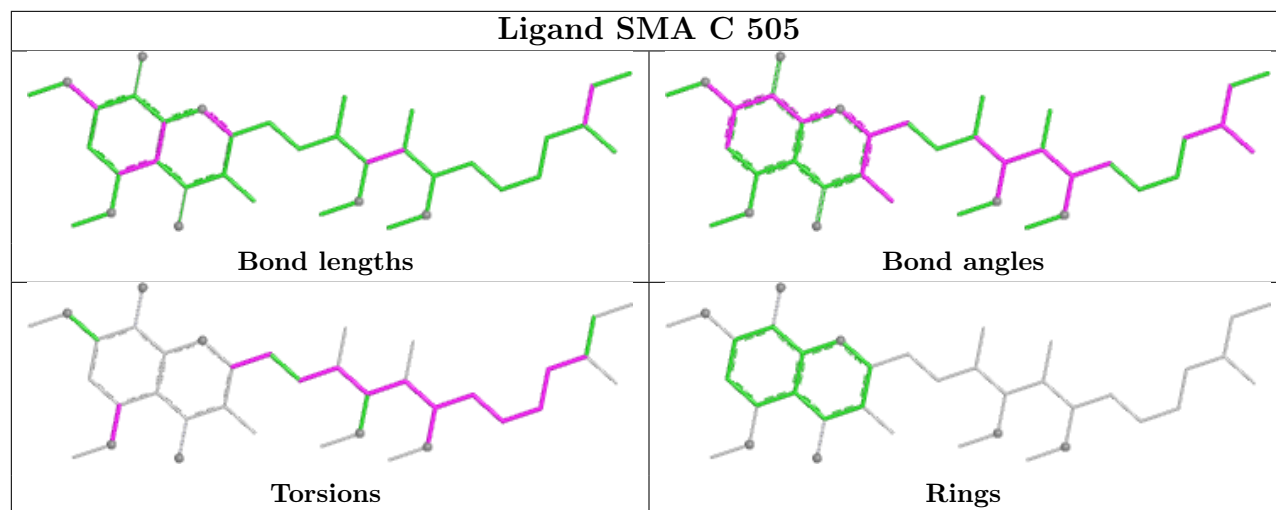
Bond angles

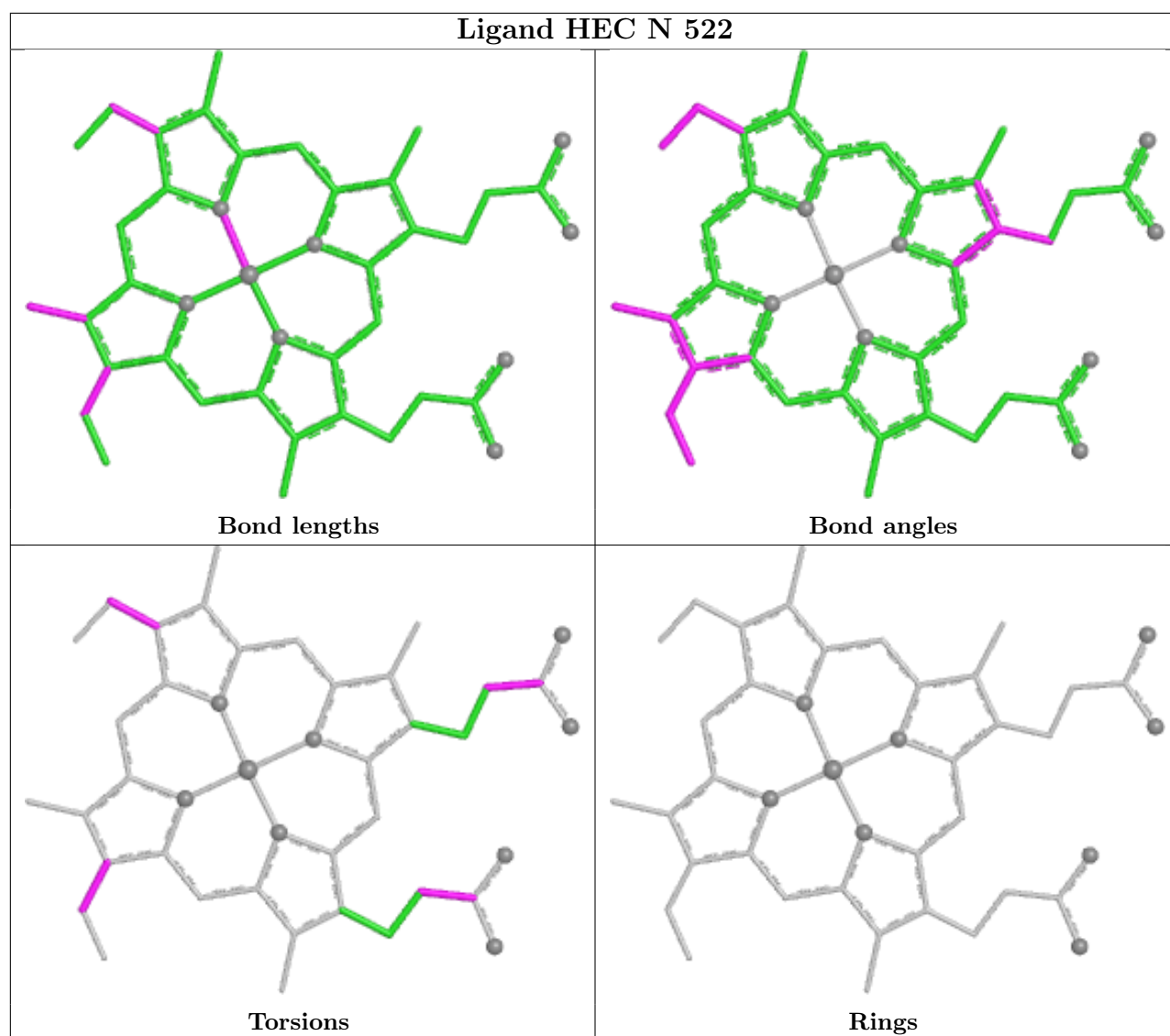


Torsions



Rings





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.