



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:32 PM UTC

PDB ID : 3H1K / pdb_00003h1k
Title : Chicken cytochrome BC1 complex with ZN++ and an iodinated derivative of kresoxim-methyl bound
Authors : Berry, E.A.; Zhang, Z.; Bellamy, H.D.; Huang, L.S.
Deposited on : 2009-04-12
Resolution : 3.48 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

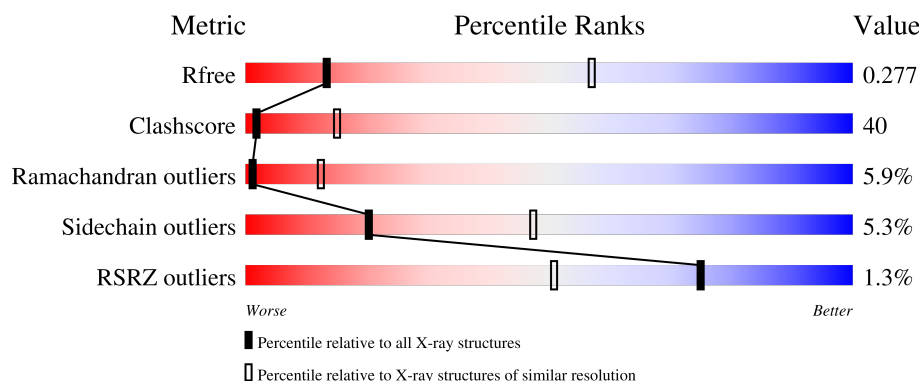
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 Å.

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



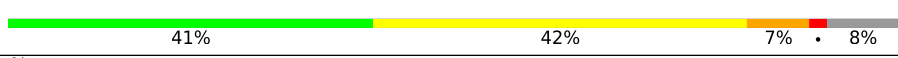
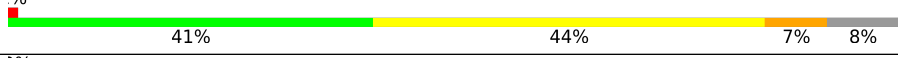
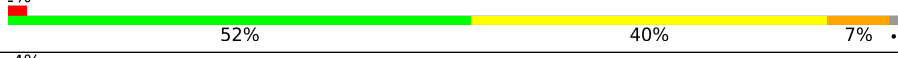
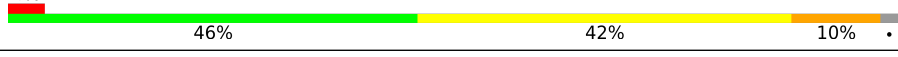
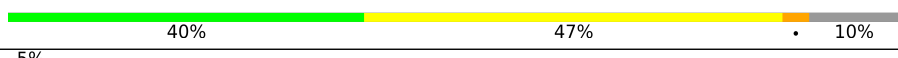
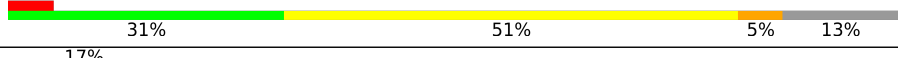
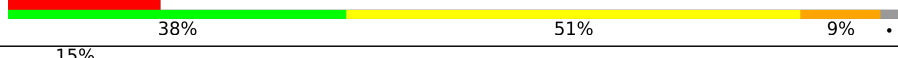
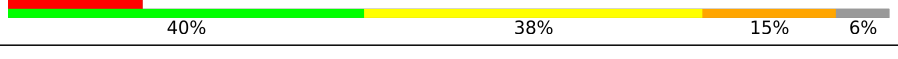
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	39% 53% 7% ..
1	N	446	36% 55% 7% ..
2	B	441	32% 54% 10% ..
2	O	441	30% 54% 12% .
3	C	380	37% 54% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEE	P	3008	-	X	-	-
21	FES	E	501	-	-	X	-
21	FES	R	501	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 32673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3164	1987	551	616	10			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	S	0	0	0
			571	348	105	113	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

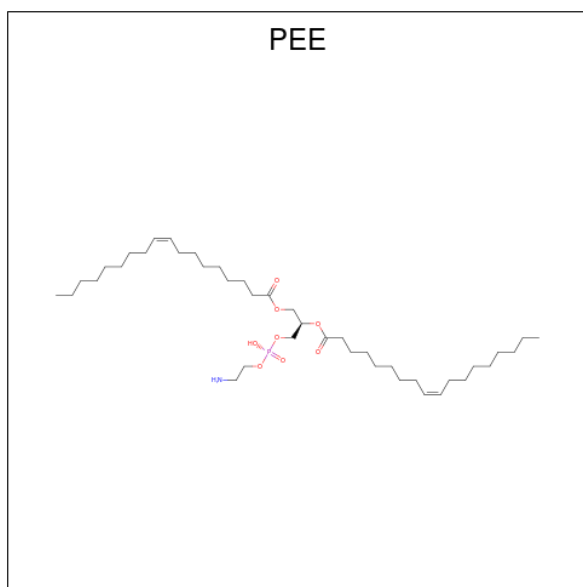
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	O	P		0	0
			18	9	8	1			
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	P	1	Total	O	P			0	0
			5	4	1				
11	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 12 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

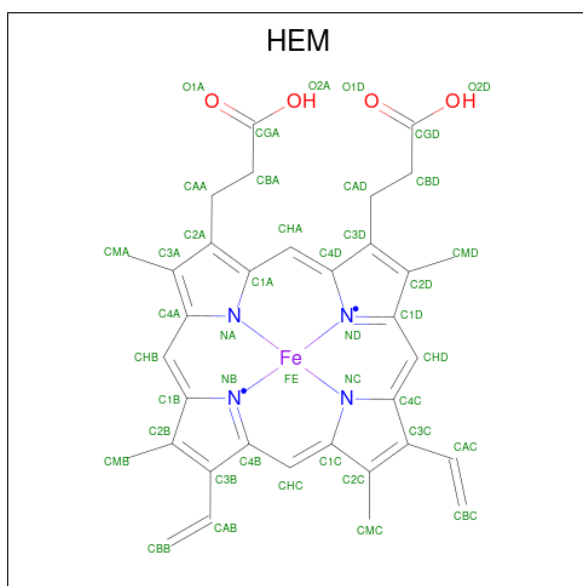
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	O	0	0
			2	2		

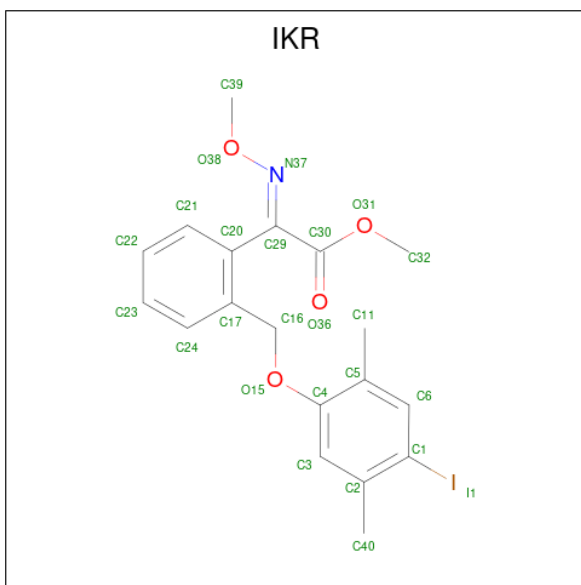
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	O	0	0
			1	1		
12	N	1	Total	O	0	0
			1	1		
12	P	1	Total	O	0	0
			1	1		

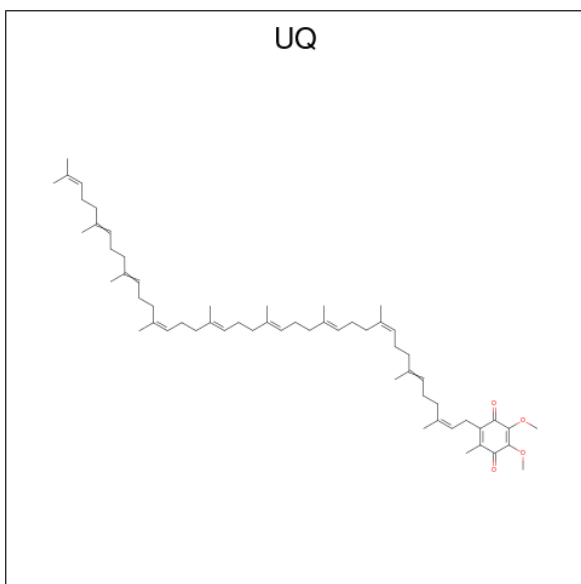
- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
14	P	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

- Molecule 15 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



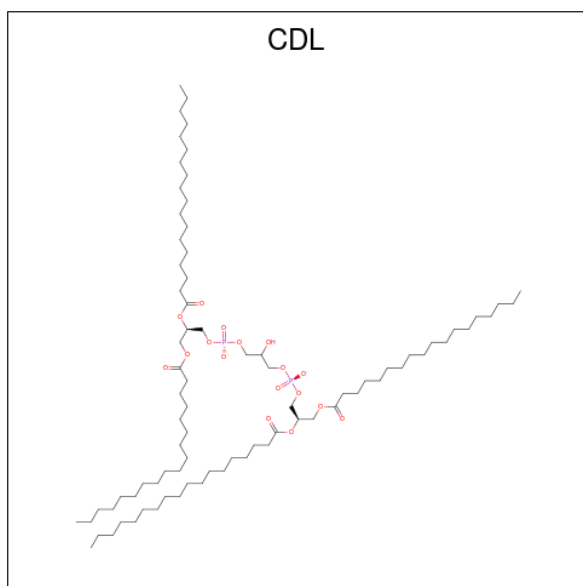
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			19	15	4		

Continued on next page...

Continued from previous page...

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

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

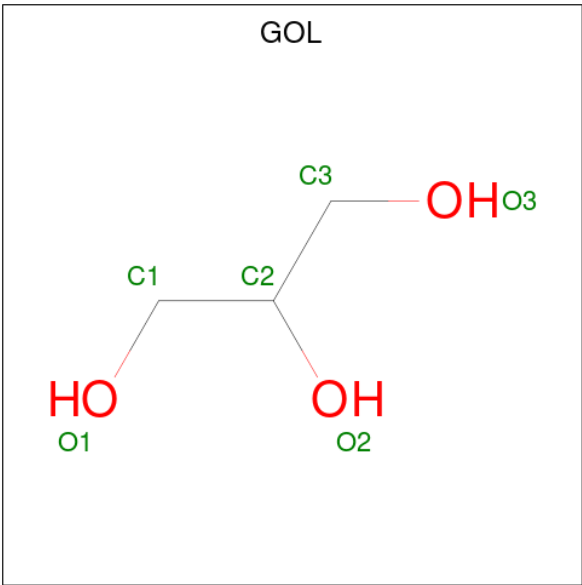


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	O	P	0	0
			40	21	17	2		
16	D	1	Total	C	O	P	0	0
			42	23	17	2		
16	P	1	Total	C	O	P	0	0
			40	21	17	2		
16	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

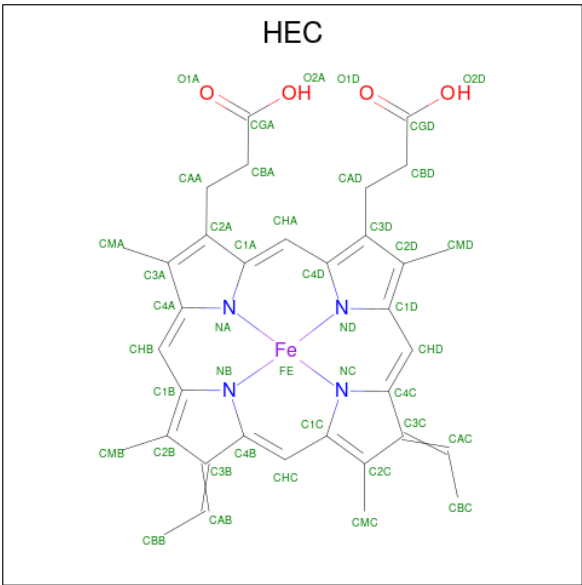
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	1	Total	Zn	0	0
			1	1		
17	P	1	Total	Zn	0	0
			1	1		

- Molecule 18 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

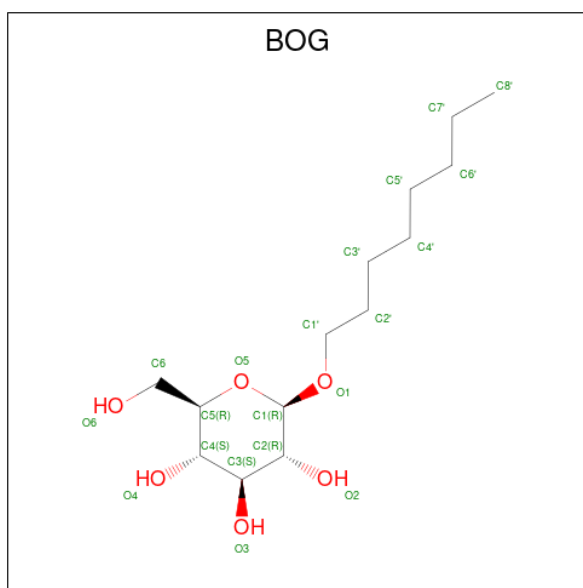


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			6	3	3		
18	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

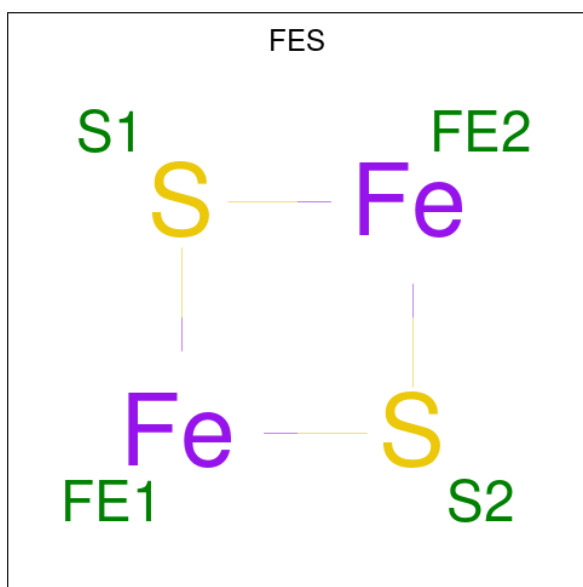


- Molecule 20 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total	C	O	0	0
			20	14	6		
20	D	1	Total	C	O	0	0
			13	7	6		
20	P	1	Total	C	O	0	0
			12	6	6		
20	P	1	Total	C	O	0	0
			13	7	6		
20	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

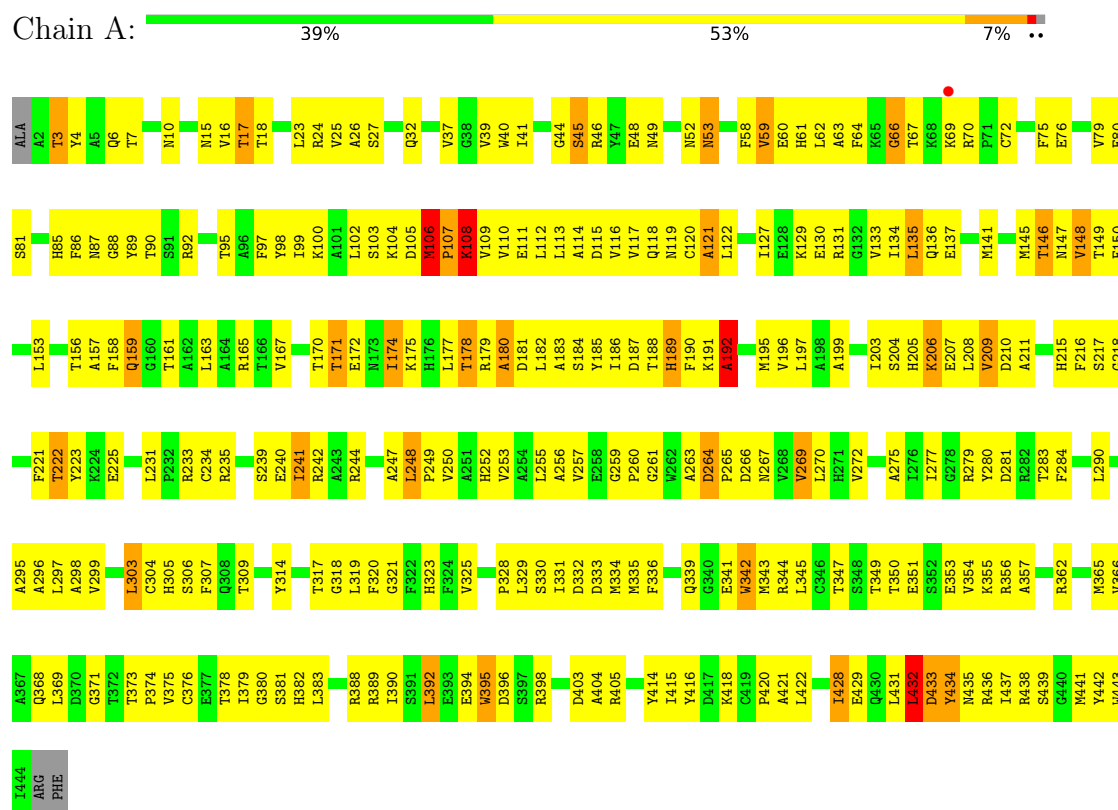
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	O	0	0
			1	1		
22	C	7	Total	O	0	0
			7	7		
22	E	1	Total	O	0	0
			1	1		
22	P	7	Total	O	0	0
			7	7		
22	R	1	Total	O	0	0
			1	1		

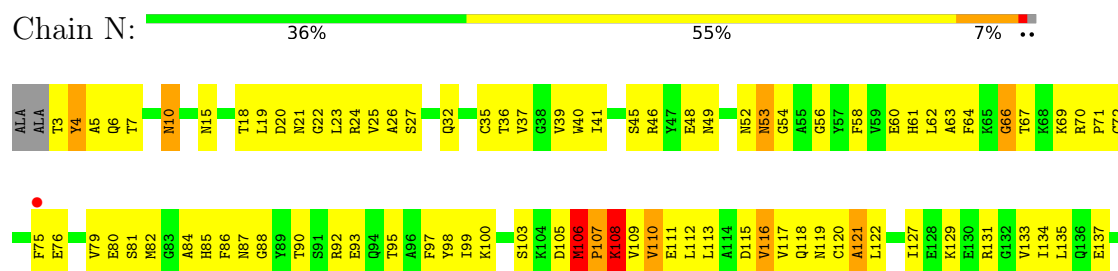
3 Residue-property plots

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

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

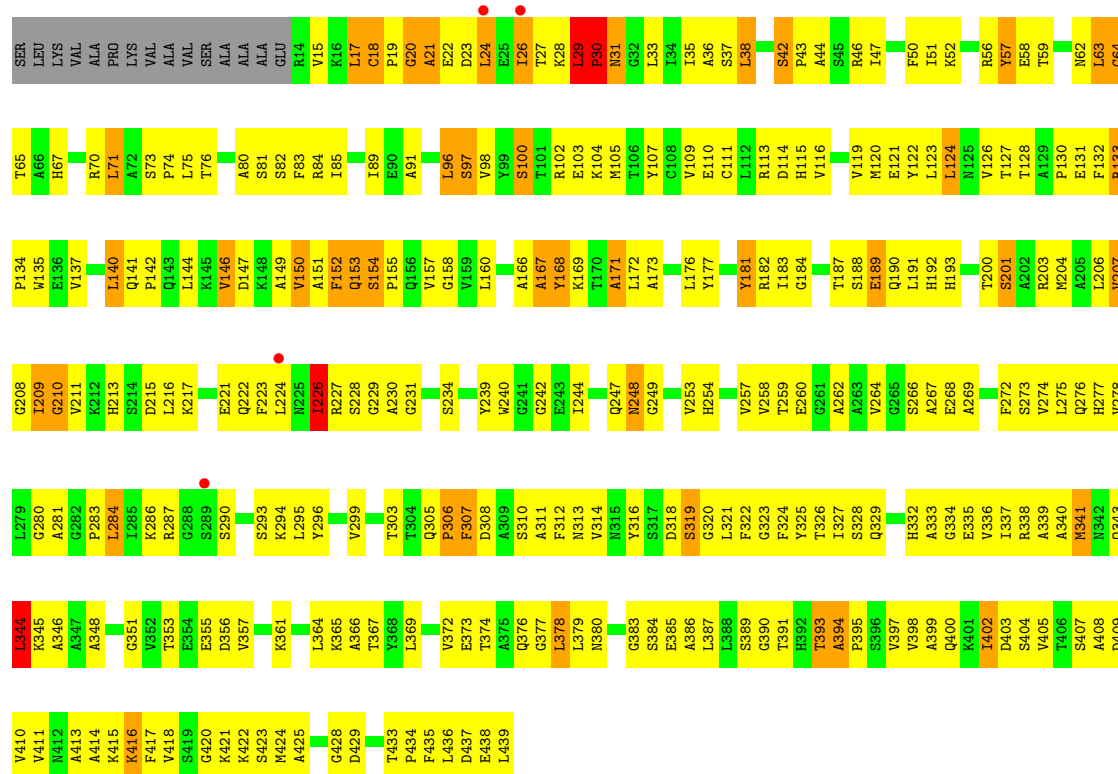


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I



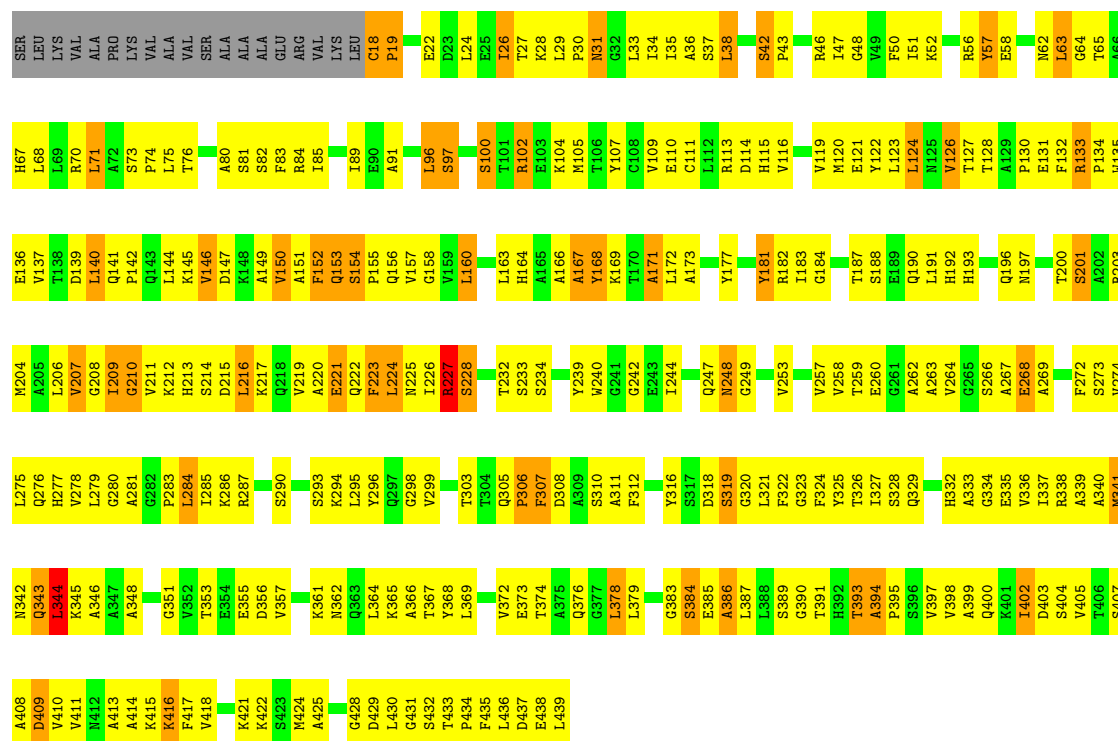


● Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2



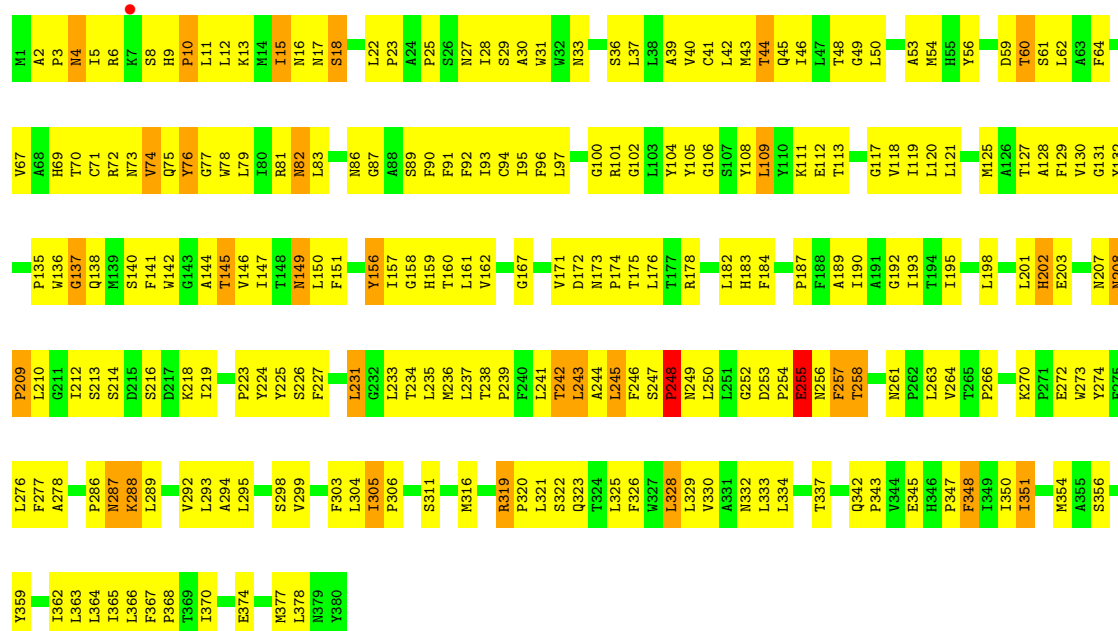
● Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2





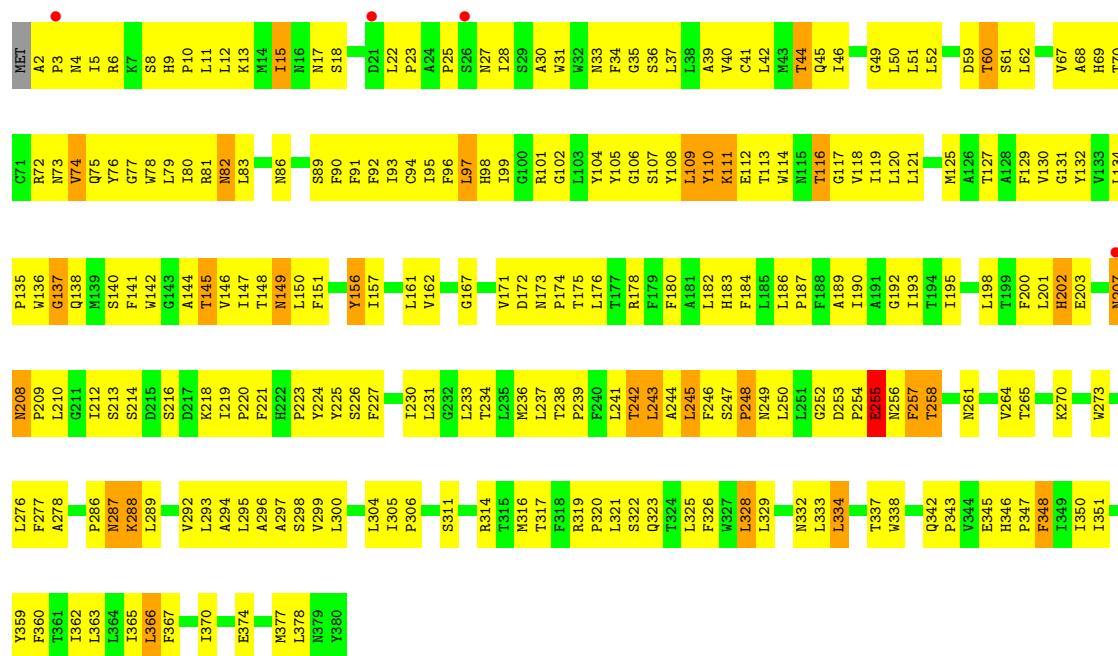
• Molecule 3: Cytochrome b

Chain C: 37% 54% 8%



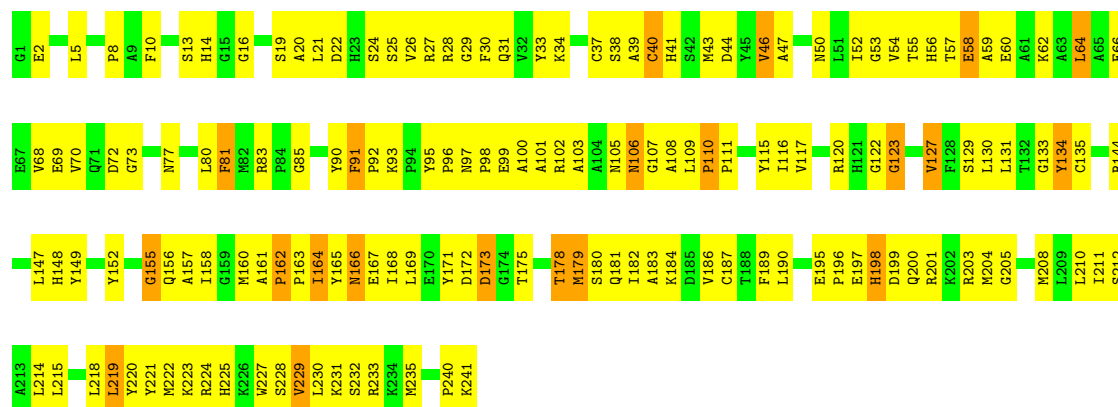
• Molecule 3: Cytochrome b

Chain P: 36% 56% 8%



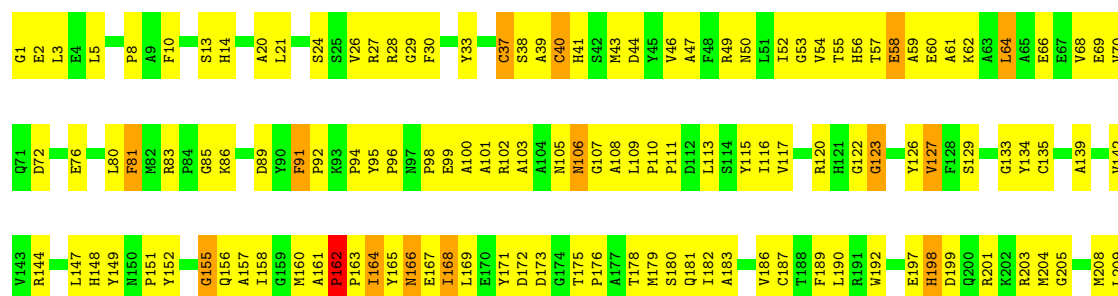
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D: 36% 55% 9%



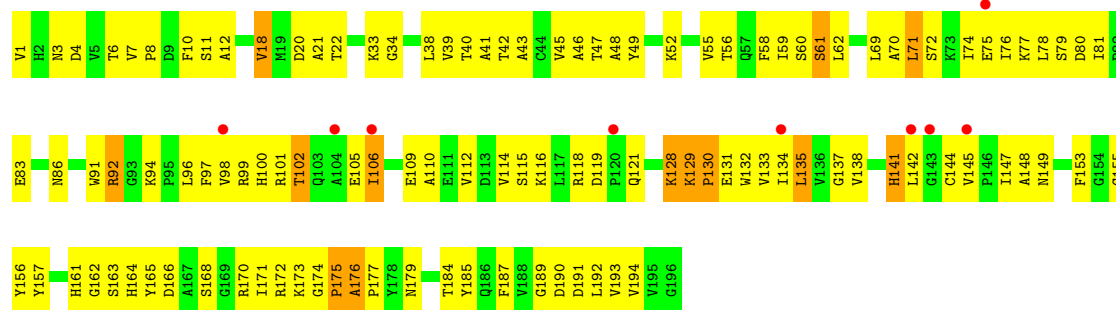
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q: 37% 56% 6%

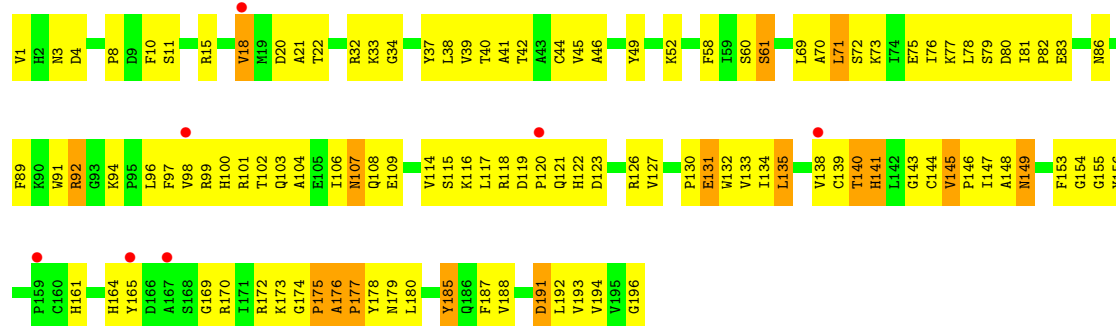
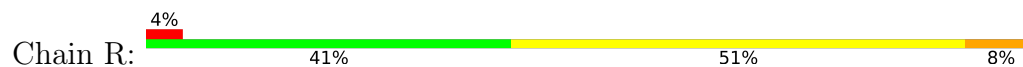




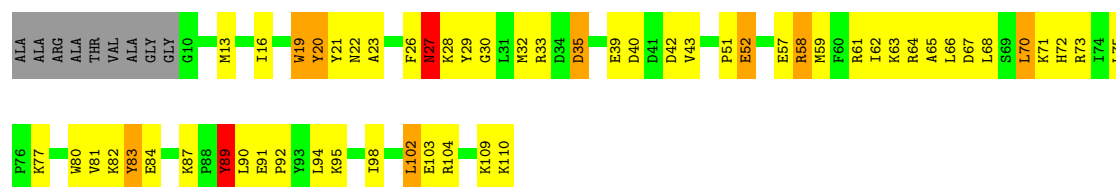
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



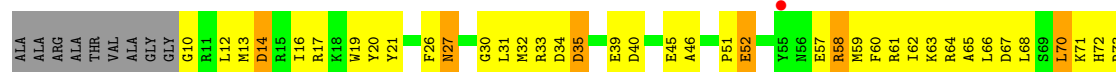
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

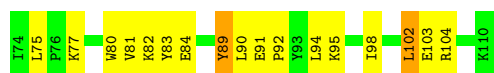


- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



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

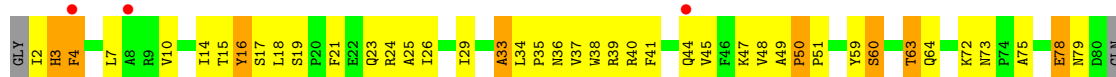




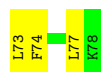
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



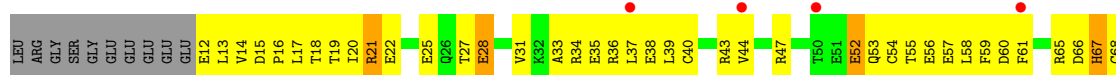
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



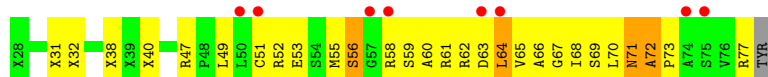
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



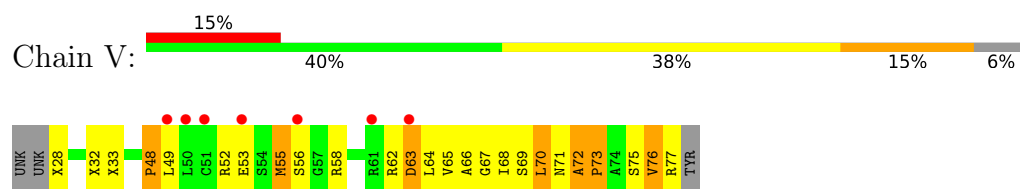
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



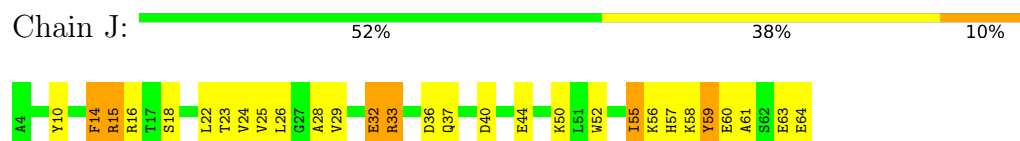
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



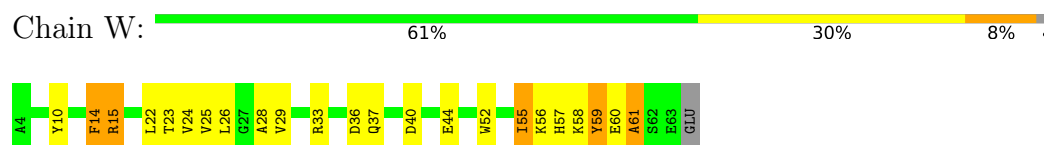
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.72Å 181.30Å 241.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.48 18.00 – 3.48	Depositor EDS
% Data completeness (in resolution range)	89.7 (18.00-3.48) 89.0 (18.00-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.284 0.232 , 0.277	Depositor DCC
R_{free} test set	2570 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	101.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32673	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.57	0/3513	1.04	19/4760 (0.4%)
1	N	0.58	0/3508	1.05	22/4753 (0.5%)
2	B	0.49	0/3219	0.97	15/4364 (0.3%)
2	O	0.54	0/3202	1.01	18/4343 (0.4%)
3	C	0.68	1/3122 (0.0%)	1.08	21/4273 (0.5%)
3	P	0.58	0/3114	1.02	17/4263 (0.4%)
4	D	0.63	0/1956	1.11	16/2658 (0.6%)
4	Q	0.54	0/1956	1.06	13/2658 (0.5%)
5	E	0.47	0/1547	0.90	3/2103 (0.1%)
5	R	0.49	0/1547	0.94	2/2103 (0.1%)
6	F	0.57	0/911	0.98	5/1219 (0.4%)
6	S	0.50	0/911	0.93	4/1219 (0.3%)
7	G	0.64	0/694	1.10	2/941 (0.2%)
7	T	0.57	0/684	1.08	5/929 (0.5%)
8	H	0.56	0/579	0.95	1/775 (0.1%)
8	U	0.44	0/561	0.86	3/751 (0.4%)
9	I	0.54	0/218	1.10	3/293 (1.0%)
9	V	0.62	0/218	0.94	0/293
10	J	0.58	0/508	0.83	0/682
10	W	0.51	0/490	0.84	0/660
All	All	0.56	1/32458 (0.0%)	1.02	169/44040 (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	C	0	2
4	D	0	1
6	F	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	354	MET	SD-CE	5.92	1.94	1.79

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	18	CYS	CA-C-N	8.90	130.96	119.84
2	O	18	CYS	C-N-CA	8.90	130.96	119.84
4	D	110	PRO	CA-C-N	8.51	128.55	119.78
4	D	110	PRO	C-N-CA	8.51	128.55	119.78
4	D	162	PRO	CA-C-N	8.33	128.02	119.19
4	D	162	PRO	C-N-CA	8.33	128.02	119.19
7	T	78	GLU	N-CA-C	-8.19	103.75	114.31
1	A	223	TYR	N-CA-C	-7.54	104.98	114.56
1	N	223	TYR	N-CA-C	-7.52	105.00	114.56
3	P	252	GLY	N-CA-C	7.35	121.32	111.03
3	C	378	LEU	N-CA-C	-7.32	104.33	113.18
1	A	432	LEU	N-CA-C	7.29	126.33	110.80
4	Q	162	PRO	CA-C-N	7.28	126.91	119.19
4	Q	162	PRO	C-N-CA	7.28	126.91	119.19
4	Q	44	ASP	N-CA-C	7.23	121.73	112.34
1	N	415	ILE	CB-CA-C	-7.15	105.64	111.71
1	N	347	THR	N-CA-C	7.11	122.38	112.93
1	N	32	GLN	CA-C-N	7.01	126.49	118.85
1	N	32	GLN	C-N-CA	7.01	126.49	118.85
3	C	365	ILE	N-CA-C	6.97	117.55	111.56
4	D	91	PHE	CA-C-N	6.96	126.93	119.76
4	D	91	PHE	C-N-CA	6.96	126.93	119.76
3	P	365	ILE	N-CA-C	6.96	117.11	111.62
1	A	32	GLN	CA-C-N	6.89	126.36	118.85
1	A	32	GLN	C-N-CA	6.89	126.36	118.85
3	C	15	ILE	N-CA-C	-6.84	104.81	113.22
1	N	156	THR	N-CA-C	-6.81	105.59	114.04
1	N	432	LEU	N-CA-C	6.80	125.30	110.80
4	D	155	GLY	N-CA-C	-6.79	106.39	115.21
2	B	344	LEU	N-CA-C	-6.74	105.59	113.88
3	P	378	LEU	N-CA-C	-6.73	105.07	113.28
3	C	257	PHE	N-CA-C	-6.68	104.26	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	THR	N-CA-C	6.68	121.81	112.93
3	C	252	GLY	N-CA-C	6.65	120.34	111.03
1	A	415	ILE	CB-CA-C	-6.59	106.11	111.71
7	T	26	ILE	CA-C-N	6.57	126.33	119.76
7	T	26	ILE	C-N-CA	6.57	126.33	119.76
7	G	26	ILE	CA-C-N	6.54	126.30	119.76
7	G	26	ILE	C-N-CA	6.54	126.30	119.76
1	A	264	ASP	CA-C-N	6.50	125.93	118.85
1	A	264	ASP	C-N-CA	6.50	125.93	118.85
3	P	226	SER	N-CA-C	-6.46	104.16	111.14
4	Q	85	GLY	N-CA-C	6.41	119.30	111.93
1	A	66	GLY	N-CA-C	6.34	120.00	112.33
4	Q	155	GLY	N-CA-C	-6.33	107.16	114.69
3	C	328	LEU	N-CA-C	-6.31	104.41	111.28
1	N	264	ASP	CA-C-N	6.22	125.95	119.05
1	N	264	ASP	C-N-CA	6.22	125.95	119.05
1	N	305	HIS	N-CA-C	-6.15	105.68	113.43
3	C	167	GLY	N-CA-C	-6.13	106.78	115.30
3	C	226	SER	N-CA-C	-6.11	104.54	111.14
9	I	47	ARG	CA-C-N	6.11	126.08	120.21
9	I	47	ARG	C-N-CA	6.11	126.08	120.21
2	O	344	LEU	N-CA-C	-6.11	106.37	113.88
3	P	137	GLY	N-CA-C	-6.04	103.03	112.58
3	C	109	LEU	N-CA-C	-6.04	105.88	113.18
6	F	26	PHE	N-CA-C	-6.02	105.94	113.28
3	P	257	PHE	N-CA-C	-6.01	105.12	112.88
7	T	24	ARG	N-CA-C	6.00	119.87	110.32
8	H	67	HIS	N-CA-C	-5.99	103.72	111.02
2	O	153	GLN	N-CA-C	-5.97	105.48	112.89
3	P	328	LEU	N-CA-C	-5.96	104.87	111.36
4	Q	58	GLU	N-CA-C	-5.93	105.31	112.54
3	C	266	PRO	CA-C-N	5.92	125.39	119.24
3	C	266	PRO	C-N-CA	5.92	125.39	119.24
4	D	173	ASP	N-CA-C	-5.90	106.12	113.38
4	Q	110	PRO	CA-C-N	5.90	125.91	119.89
4	Q	110	PRO	C-N-CA	5.90	125.91	119.89
2	B	188	SER	N-CA-C	-5.89	104.44	111.69
4	D	40	CYS	N-CA-C	-5.88	105.71	114.64
4	Q	40	CYS	N-CA-C	-5.87	105.72	114.64
6	F	27	ASN	N-CA-C	-5.86	104.97	111.36
3	C	207	ASN	N-CA-C	-5.85	101.82	110.48
1	A	233	ARG	N-CA-C	5.83	118.28	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	110	ALA	N-CA-C	-5.83	105.94	114.39
2	B	100	SER	N-CA-C	5.82	118.26	109.23
1	N	66	GLY	N-CA-C	5.82	119.38	112.33
1	N	415	ILE	N-CA-C	5.81	116.94	111.48
3	C	270	LYS	CA-C-N	5.81	127.10	119.84
3	C	270	LYS	C-N-CA	5.81	127.10	119.84
3	P	231	LEU	N-CA-C	-5.81	104.64	110.97
6	S	26	PHE	N-CA-C	-5.81	106.20	113.28
3	C	97	LEU	N-CA-C	-5.80	104.65	110.97
8	U	67	HIS	N-CA-C	-5.78	103.97	111.02
3	P	167	GLY	N-CA-C	-5.78	107.27	115.30
1	A	45	SER	N-CA-C	-5.75	105.76	112.89
2	B	167	ALA	N-CA-C	-5.74	106.31	113.55
1	N	303	LEU	N-CA-C	5.73	118.26	111.33
3	P	109	LEU	N-CA-C	-5.73	106.06	113.16
1	N	434	TYR	N-CA-C	-5.73	104.94	111.07
5	E	56	THR	N-CA-C	-5.72	104.94	111.07
2	O	133	ARG	CA-C-N	5.72	127.00	119.84
2	O	133	ARG	C-N-CA	5.72	127.00	119.84
1	A	434	TYR	N-CA-C	-5.72	104.95	111.07
2	O	100	SER	N-CA-C	5.71	118.09	109.23
4	D	58	GLU	N-CA-C	-5.69	105.43	112.38
3	P	97	LEU	N-CA-C	-5.67	104.78	110.97
2	O	373	GLU	N-CA-C	-5.67	106.03	113.12
3	C	48	THR	N-CA-C	-5.66	105.25	111.82
2	B	153	GLN	N-CA-C	-5.65	105.89	112.89
4	Q	91	PHE	CA-C-N	5.64	125.57	119.76
4	Q	91	PHE	C-N-CA	5.64	125.57	119.76
2	B	369	LEU	N-CA-C	5.63	118.14	111.33
1	A	231	LEU	N-CA-C	5.61	116.89	109.93
1	A	303	LEU	N-CA-C	5.61	118.12	111.33
3	P	116	THR	N-CA-C	-5.57	105.11	111.07
3	P	270	LYS	CA-C-N	5.56	126.79	119.84
3	P	270	LYS	C-N-CA	5.56	126.79	119.84
6	S	35	ASP	N-CA-C	-5.54	104.64	111.40
3	C	351	ILE	N-CA-C	-5.54	104.97	110.62
3	C	319	ARG	CA-C-N	5.52	124.98	119.24
3	C	319	ARG	C-N-CA	5.52	124.98	119.24
1	N	189	HIS	N-CA-C	5.52	119.99	112.04
3	P	207	ASN	N-CA-C	-5.52	102.31	110.48
3	P	15	ILE	N-CA-C	-5.51	105.52	113.07
2	O	188	SER	N-CA-C	-5.46	104.98	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	42	SER	N-CA-C	-5.45	102.76	110.29
1	N	380	GLY	N-CA-C	-5.44	106.19	112.83
1	A	415	ILE	N-CA-C	5.42	116.57	111.48
1	A	189	HIS	N-CA-C	5.41	119.88	112.68
2	B	310	SER	N-CA-C	5.37	116.43	108.86
2	B	133	ARG	CA-C-N	5.36	126.54	119.84
2	B	133	ARG	C-N-CA	5.36	126.54	119.84
2	O	126	VAL	N-CA-C	5.35	115.98	110.36
7	T	47	LYS	N-CA-C	-5.35	104.80	112.13
2	B	373	GLU	N-CA-C	-5.34	106.44	113.12
8	U	14	VAL	N-CA-C	5.32	115.56	108.11
2	O	167	ALA	N-CA-C	-5.31	106.74	113.43
1	A	305	HIS	N-CA-C	-5.31	106.74	113.43
5	E	106	ILE	N-CA-C	-5.31	106.69	113.22
2	B	305	GLN	CA-C-N	5.29	126.46	119.84
2	B	305	GLN	C-N-CA	5.29	126.46	119.84
2	O	390	GLY	N-CA-C	-5.29	106.40	115.08
4	Q	80	LEU	N-CA-C	-5.29	102.65	110.48
2	B	42	SER	N-CA-C	-5.29	103.41	110.07
5	R	145	VAL	CA-C-N	5.27	126.43	119.84
5	R	145	VAL	C-N-CA	5.27	126.43	119.84
1	N	231	LEU	N-CA-C	5.25	116.44	109.93
6	S	14	ASP	N-CA-C	-5.23	106.85	113.18
2	B	390	GLY	N-CA-C	-5.23	106.51	115.08
6	F	35	ASP	N-CA-C	-5.22	105.04	111.40
3	P	110	TYR	N-CA-C	-5.19	105.66	112.72
1	A	178	THR	N-CA-C	5.18	117.55	109.52
8	U	21	ARG	N-CA-C	-5.17	105.73	111.36
2	O	305	GLN	CA-C-N	5.16	126.28	119.84
2	O	305	GLN	C-N-CA	5.16	126.28	119.84
1	N	248	LEU	CA-C-N	5.14	124.31	118.97
1	N	248	LEU	C-N-CA	5.14	124.31	118.97
4	Q	164	ILE	N-CA-C	5.13	116.75	108.85
9	I	51	CYS	N-CA-C	5.13	116.59	109.31
6	F	39	GLU	N-CA-C	5.12	117.44	108.52
6	F	89	TYR	N-CA-C	5.12	118.31	111.75
1	N	192	ALA	N-CA-C	5.12	121.12	109.81
1	A	192	ALA	N-CA-C	5.08	121.04	109.81
6	S	39	GLU	N-CA-C	5.08	117.47	109.39
4	D	164	ILE	N-CA-C	5.08	116.67	108.85
2	O	369	LEU	N-CA-C	5.07	118.24	111.75
3	C	231	LEU	N-CA-C	-5.07	105.65	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	137	GLY	N-CA-C	-5.06	103.83	112.64
4	D	41	HIS	N-CA-C	5.05	117.21	109.07
4	D	85	GLY	N-CA-C	5.05	118.66	112.14
2	O	310	SER	N-CA-C	5.05	115.71	108.74
2	B	29	LEU	N-CA-C	5.04	120.94	109.81
1	N	171	THR	N-CA-C	-5.03	106.31	112.90
4	D	44	ASP	N-CA-C	5.03	121.50	110.80
4	D	80	LEU	N-CA-C	-5.03	103.04	110.48
4	D	93	LYS	N-CA-C	-5.03	103.70	109.93
1	N	116	VAL	CB-CA-C	-5.02	105.45	111.88
2	O	224	LEU	N-CA-C	5.02	116.94	108.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	56	TYR	Sidechain
3	C	76	TYR	Sidechain
4	D	134	TYR	Sidechain
6	F	20	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	3442	0	3354	281	0
1	N	3437	0	3349	303	0
2	B	3164	0	3158	322	0
2	O	3147	0	3146	356	0
3	C	3020	0	3070	260	0
3	P	3012	0	3058	257	0
4	D	1898	0	1846	184	0
4	Q	1898	0	1846	183	0
5	E	1513	0	1478	120	0
5	R	1513	0	1478	124	0
6	F	891	0	893	57	0
6	S	891	0	893	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	672	0	653	38	0
7	T	662	0	645	44	0
8	H	571	0	547	34	0
8	U	553	0	535	46	0
9	I	285	0	238	40	0
9	V	275	0	238	40	0
10	J	497	0	490	31	0
10	W	479	0	478	34	0
11	A	18	0	11	0	0
11	C	49	0	72	3	0
11	E	50	0	77	0	0
11	P	54	0	72	4	0
11	R	50	0	77	0	0
12	A	2	0	0	0	0
12	C	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
13	C	86	0	60	19	0
13	P	86	0	60	21	0
14	C	25	0	20	5	0
14	P	25	0	20	4	0
15	C	19	0	17	7	0
15	P	19	0	17	4	0
16	C	40	0	24	2	0
16	D	42	0	28	1	0
16	P	40	0	24	2	0
16	Q	42	0	28	3	0
17	C	1	0	0	0	0
17	P	1	0	0	0	0
18	C	6	0	8	1	0
18	P	6	0	8	1	0
19	D	43	0	30	2	0
19	Q	43	0	30	1	0
20	D	33	0	39	1	0
20	P	25	0	22	0	0
20	Q	20	0	28	0	0
21	E	4	0	0	3	0
21	R	4	0	0	2	0
22	A	1	0	0	0	0
22	C	7	0	0	1	0
22	E	1	0	0	0	0
22	P	7	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	R	1	0	0	1	0
All	All	32673	0	32165	2606	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 40.

All (2606) 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:209:ILE:HG22	2:B:210:GLY:H	1.08	1.09
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.31	1.08
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.28	1.07
2:O:209:ILE:HG22	2:O:210:GLY:H	1.09	1.07
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.38	1.06
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.37	1.06
3:C:125:MET:HE2	14:C:2001:IKR:I1	2.31	1.00
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.26	0.99
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.45	0.98
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.43	0.98
3:C:120:LEU:HD13	13:C:502:HEM:HBB2	1.44	0.97
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.47	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	0.97
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.45	0.96
4:D:158:ILE:HG12	4:D:160:MET:H	1.31	0.94
5:R:148:ALA:HA	5:R:156:TYR:HA	1.49	0.94
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.48	0.94
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.48	0.94
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.50	0.93
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.51	0.93
3:P:216:SER:HB3	6:S:59:MET:HE2	1.50	0.92
3:C:216:SER:HB3	6:F:59:MET:HE2	1.48	0.92
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.50	0.91
2:B:207:VAL:HG12	2:B:208:GLY:H	1.35	0.91
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.51	0.91
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.50	0.91
2:O:71:LEU:O	2:O:74:PRO:HD2	1.71	0.91
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.49	0.91
2:O:76:THR:HG22	2:O:82:SER:H	1.35	0.91
5:E:147:ILE:HG22	5:E:148:ALA:H	1.33	0.90
1:A:206:LYS:O	1:A:209:VAL:HG12	1.71	0.90
2:B:327:ILE:HD11	9:I:58:ARG:O	1.71	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.52	0.90
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.52	0.89
4:D:57:THR:HG22	4:D:59:ALA:H	1.36	0.89
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.35	0.89
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.37	0.89
2:O:96:LEU:HB2	2:O:109:VAL:HG12	1.55	0.88
1:A:248:LEU:HD13	1:A:249:PRO:HD2	1.54	0.88
2:B:209:ILE:HG22	2:B:210:GLY:N	1.87	0.88
9:V:49:LEU:HB3	9:V:55:MET:HG2	1.55	0.88
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.88
2:O:209:ILE:HG22	2:O:210:GLY:N	1.87	0.88
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.56	0.88
1:N:328:PRO:HG2	1:N:329:LEU:HD12	1.55	0.88
4:D:47:ALA:H	4:D:50:ASN:HD22	1.19	0.87
9:I:49:LEU:HD13	9:I:55:MET:HE3	1.54	0.87
7:T:29:ILE:O	7:T:33:ALA:HB3	1.73	0.87
2:O:207:VAL:HG12	2:O:208:GLY:H	1.37	0.87
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.37	0.87
9:I:32:UNK:N	9:I:73:PRO:HG2	1.89	0.87
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.09	0.87
5:R:58:PHE:O	5:R:61:SER:HB3	1.75	0.86
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.40	0.86
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.38	0.86
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.55	0.86
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.38	0.86
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.38	0.86
1:N:248:LEU:HD13	1:N:249:PRO:HD2	1.56	0.85
2:B:71:LEU:O	2:B:74:PRO:HD2	1.75	0.85
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.40	0.85
2:O:201:SER:HB3	2:O:227:ARG:HB2	1.56	0.85
2:B:96:LEU:HB2	2:B:109:VAL:HG12	1.57	0.85
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.59	0.85
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.59	0.84
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.60	0.83
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.13	0.83
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.60	0.83
1:N:206:LYS:O	1:N:209:VAL:HG12	1.77	0.83
3:C:253:ASP:OD1	3:C:255:GLU:HG2	1.79	0.82
3:C:125:MET:CE	14:C:2001:IKR:I1	2.96	0.82
2:O:201:SER:H	2:O:227:ARG:HB3	1.41	0.82
2:O:353:THR:HG22	2:O:355:GLU:H	1.43	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:209:ILE:CG2	2:O:210:GLY:H	1.91	0.81
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.63	0.81
2:O:353:THR:HB	2:O:356:ASP:OD1	1.81	0.81
2:B:209:ILE:CG2	2:B:210:GLY:H	1.91	0.81
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.77	0.81
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.15	0.81
2:O:100:SER:HB3	2:O:105:MET:HG2	1.61	0.81
6:S:89:TYR:HD1	6:S:90:LEU:N	1.79	0.81
3:C:118:VAL:N	13:C:502:HEM:HBC2	1.96	0.81
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.46	0.81
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.62	0.81
2:B:353:THR:HG22	2:B:355:GLU:H	1.45	0.80
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.22	0.80
2:O:156:GLN:HE22	9:V:77:ARG:C	1.88	0.80
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.46	0.80
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.63	0.80
2:B:71:LEU:HD11	2:B:144:LEU:HD23	1.62	0.80
1:A:161:THR:HB	1:A:234:CYS:SG	2.22	0.80
1:N:105:ASP:O	1:N:109:VAL:HG23	1.82	0.80
9:V:49:LEU:HD22	9:V:55:MET:HB3	1.62	0.80
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.62	0.80
5:E:116:LYS:H	5:E:116:LYS:HD2	1.46	0.80
1:N:161:THR:HB	1:N:234:CYS:SG	2.21	0.80
1:N:382:HIS:ND1	1:N:389:ARG:HD2	1.98	0.79
3:P:120:LEU:HD13	13:P:502:HEM:HBB2	1.65	0.79
2:B:100:SER:HB3	2:B:105:MET:HG2	1.63	0.79
7:G:29:ILE:O	7:G:33:ALA:HB3	1.81	0.79
3:P:138:GLN:HB2	3:P:255:GLU:O	1.83	0.79
1:N:134:ILE:HG21	1:N:174:ILE:HG12	1.65	0.78
2:B:122:TYR:O	2:B:126:VAL:HG23	1.83	0.78
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.23	0.78
3:P:253:ASP:OD1	3:P:255:GLU:HG2	1.83	0.78
1:A:328:PRO:HG2	1:A:329:LEU:HD12	1.64	0.78
2:O:221:GLU:HG3	2:O:222:GLN:H	1.48	0.78
4:Q:127:VAL:HG12	4:Q:187:CYS:SG	2.23	0.78
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.13	0.78
5:E:114:VAL:HG21	5:E:172:ARG:NH1	1.97	0.78
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.66	0.78
6:F:89:TYR:HD1	6:F:90:LEU:N	1.81	0.78
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.66	0.78
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.49	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:188:VAL:O	5:R:192:LEU:HB2	1.83	0.78
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.67	0.77
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.67	0.77
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.66	0.77
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.66	0.77
3:C:61:SER:O	3:C:62:LEU:HG	1.84	0.77
2:O:102:ARG:HG2	2:O:102:ARG:NH1	1.98	0.77
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.67	0.77
1:N:106:MET:O	1:N:106:MET:HE2	1.84	0.77
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.19	0.77
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.48	0.77
2:O:160:LEU:HB3	9:V:64:LEU:HD22	1.68	0.77
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.16	0.76
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.67	0.76
1:N:277:ILE:HD11	1:N:345:LEU:HD11	1.66	0.76
3:P:12:LEU:HD23	3:P:15:ILE:HD12	1.67	0.76
3:C:120:LEU:CD1	13:C:502:HEM:HBB2	2.15	0.76
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.48	0.76
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.47	0.76
3:P:145:THR:O	3:P:149:ASN:HB2	1.85	0.76
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.50	0.76
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.50	0.76
2:O:37:SER:HB2	2:O:213:HIS:ND1	2.01	0.76
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.01	0.75
3:C:120:LEU:HB3	13:C:502:HEM:CBB	2.16	0.75
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.01	0.75
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.51	0.75
6:S:13:MET:HE2	6:S:17:ARG:NH2	2.02	0.75
1:N:170:THR:HG22	1:N:171:THR:H	1.51	0.75
3:P:118:VAL:N	13:P:502:HEM:HBC2	2.02	0.75
2:B:353:THR:HB	2:B:356:ASP:OD1	1.87	0.74
1:A:362:ARG:O	1:A:365:MET:HG2	1.87	0.74
2:B:341:MET:HE2	2:B:341:MET:HA	1.70	0.74
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.04	0.74
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.52	0.74
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.03	0.74
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.69	0.74
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.52	0.74
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.17	0.74
3:C:59:ASP:O	3:C:61:SER:N	2.20	0.74
1:N:80:GLU:HA	2:O:284:LEU:HD12	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ILE:CD1	2:B:96:LEU:HD23	2.17	0.74
4:D:116:ILE:HG23	4:D:117:VAL:N	2.02	0.74
5:E:58:PHE:O	5:E:61:SER:HB3	1.88	0.74
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.70	0.74
3:P:101:ARG:HD2	3:P:101:ARG:C	2.13	0.74
3:P:173:ASN:N	3:P:174:PRO:HD2	2.03	0.74
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.21	0.74
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.70	0.74
1:N:106:MET:HG2	1:N:203:ILE:HD13	1.70	0.74
5:R:1:VAL:HG23	5:R:3:ASN:H	1.50	0.74
6:S:91:GLU:HB3	6:S:92:PRO:HD3	1.70	0.74
3:P:316:MET:HE2	3:P:322:SER:HB3	1.70	0.73
9:I:49:LEU:HD11	9:I:58:ARG:NH1	2.03	0.73
2:O:225:ASN:O	2:O:227:ARG:HG3	1.87	0.73
1:A:422:LEU:HD21	1:A:431:LEU:HD21	1.69	0.73
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.68	0.73
9:V:49:LEU:HB3	9:V:55:MET:CG	2.17	0.73
2:O:113:ARG:O	2:O:116:VAL:HG23	1.88	0.73
1:A:106:MET:HE2	1:A:106:MET:O	1.88	0.73
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.53	0.73
2:O:374:THR:HG22	2:O:376:GLN:H	1.53	0.73
1:A:106:MET:HG2	1:A:203:ILE:HD13	1.69	0.73
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.52	0.73
2:B:100:SER:CB	2:B:105:MET:HG2	2.19	0.73
19:Q:501:HEC:HMB1	19:Q:501:HEC:HBB3	1.71	0.73
10:W:56:LYS:HG2	10:W:60:GLU:OE1	1.89	0.73
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.71	0.72
2:O:150:VAL:O	2:O:153:GLN:HB2	1.88	0.72
2:O:295:LEU:O	2:O:299:VAL:HG23	1.89	0.72
3:P:214:SER:HB2	3:P:218:LYS:NZ	2.03	0.72
1:A:134:ILE:HG21	1:A:174:ILE:HG12	1.71	0.72
4:D:43:MET:CE	4:D:46:VAL:HG21	2.16	0.72
1:N:58:PHE:HB3	1:N:182:LEU:HD21	1.69	0.72
2:O:71:LEU:N	2:O:71:LEU:HD23	2.04	0.72
3:C:245:LEU:O	4:D:201:ARG:HD3	1.88	0.72
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.53	0.72
2:B:96:LEU:HG	9:I:70:LEU:HD13	1.71	0.72
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.23	0.72
2:O:100:SER:CB	2:O:105:MET:HG2	2.20	0.72
2:O:122:TYR:O	2:O:126:VAL:HG23	1.90	0.72
3:P:127:THR:O	3:P:130:VAL:HG22	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:LEU:CB	4:D:208:MET:HE2	2.18	0.72
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.24	0.72
9:I:49:LEU:HD22	9:I:55:MET:HG2	1.72	0.72
2:B:113:ARG:O	2:B:116:VAL:HG23	1.88	0.72
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.25	0.72
3:P:120:LEU:HB3	13:P:502:HEM:CBB	2.20	0.72
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.25	0.72
5:E:147:ILE:HG22	5:E:148:ALA:N	2.05	0.72
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.71	0.72
2:B:209:ILE:O	2:B:211:VAL:HG22	1.90	0.71
2:B:402:ILE:HG23	2:B:403:ASP:H	1.55	0.71
3:C:214:SER:HB2	3:C:218:LYS:NZ	2.05	0.71
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.53	0.71
2:O:274:VAL:O	2:O:278:VAL:HG23	1.90	0.71
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.24	0.71
5:E:1:VAL:HG23	5:E:3:ASN:H	1.54	0.71
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.25	0.71
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.30	0.71
3:C:92:PHE:O	3:C:95:ILE:HG22	1.90	0.71
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.26	0.71
2:B:226:ILE:HG23	2:B:227:ARG:HD3	1.71	0.71
2:B:374:THR:HG22	2:B:376:GLN:H	1.56	0.71
3:C:236:MET:O	3:C:239:PRO:HD2	1.90	0.71
2:B:18:CYS:HB3	2:B:19:PRO:HD3	1.70	0.71
3:C:173:ASN:N	3:C:174:PRO:HD2	2.05	0.71
1:N:37:VAL:HG12	1:N:199:ALA:HB2	1.73	0.71
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.56	0.71
2:B:295:LEU:O	2:B:299:VAL:HG23	1.91	0.71
2:B:280:GLY:HA3	2:B:293:SER:OG	1.91	0.70
2:O:361:LYS:O	2:O:365:LYS:HG3	1.90	0.70
2:O:154:SER:O	2:O:157:VAL:HG12	1.90	0.70
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.26	0.70
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.27	0.70
3:C:316:MET:HE2	3:C:322:SER:HB3	1.73	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.70
1:N:422:LEU:HD21	1:N:431:LEU:HD21	1.73	0.70
1:N:365:MET:HG3	1:N:366:VAL:N	2.07	0.70
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.71	0.70
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.91	0.70
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.73	0.70
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.06	0.70
5:R:148:ALA:HB2	5:R:156:TYR:CD2	2.27	0.70
3:C:138:GLN:HB2	3:C:255:GLU:O	1.92	0.70
4:D:57:THR:HB	4:D:60:GLU:HG3	1.74	0.70
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.73	0.70
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.73	0.70
1:A:342:TRP:O	1:A:345:LEU:HB2	1.92	0.69
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.07	0.69
2:B:76:THR:CG2	2:B:82:SER:H	2.04	0.69
3:P:247:SER:OG	3:P:250:LEU:HB2	1.92	0.69
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.07	0.69
3:C:238:THR:HB	3:C:239:PRO:HD3	1.74	0.69
2:O:287:ARG:HA	9:V:53:GLU:HG3	1.72	0.69
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.07	0.69
5:R:71:LEU:N	5:R:71:LEU:HD23	2.08	0.69
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.74	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.73	0.69
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.74	0.69
3:P:92:PHE:O	3:P:95:ILE:HG22	1.92	0.69
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.23	0.69
3:C:70:THR:HA	3:C:74:VAL:HG23	1.75	0.69
2:O:89:ILE:CD1	2:O:96:LEU:HD23	2.22	0.69
1:N:239:SER:HB2	7:T:17:SER:O	1.93	0.69
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.26	0.69
2:O:76:THR:CG2	2:O:82:SER:H	2.04	0.69
3:P:61:SER:O	3:P:62:LEU:HG	1.92	0.69
2:O:402:ILE:HG23	2:O:403:ASP:H	1.58	0.68
3:C:101:ARG:HD2	3:C:101:ARG:C	2.17	0.68
1:N:170:THR:HG22	1:N:171:THR:N	2.07	0.68
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.74	0.68
5:E:98:VAL:HG22	5:E:134:ILE:HG12	1.75	0.68
3:C:145:THR:O	3:C:149:ASN:HB2	1.94	0.68
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.28	0.68
3:P:125:MET:HE2	14:P:3001:IKR:I1	2.63	0.68
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.07	0.68
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.75	0.68
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.75	0.68
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.27	0.68
10:W:40:ASP:O	10:W:44:GLU:HG3	1.94	0.68
1:N:369:LEU:HD12	1:N:392:LEU:HD21	1.74	0.68
1:A:433:ASP:OD2	1:A:435:ASN:HB2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.75	0.68
3:C:12:LEU:HD23	3:C:15:ILE:HD12	1.76	0.68
2:O:201:SER:HB3	2:O:227:ARG:CB	2.24	0.68
5:R:98:VAL:HG22	5:R:134:ILE:HG12	1.73	0.68
1:A:45:SER:OG	1:A:92:ARG:HA	1.94	0.68
1:A:170:THR:HG22	1:A:171:THR:H	1.59	0.68
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.59	0.68
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.76	0.68
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.76	0.67
4:D:20:ALA:HB1	4:D:199:ASP:OD2	1.94	0.67
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.24	0.67
1:N:439:SER:HA	1:N:442:TYR:CE2	2.28	0.67
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.28	0.67
2:O:35:ILE:O	2:O:213:HIS:HE1	1.77	0.67
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.88	0.67
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.30	0.67
3:C:79:LEU:HD22	4:D:204:MET:HE1	1.76	0.67
9:I:38:UNK:C	9:I:40:UNK:H	2.06	0.67
1:N:161:THR:HG21	1:N:235:ARG:H	1.58	0.67
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.75	0.67
1:A:117:VAL:HG23	1:A:118:GLN:N	2.09	0.67
3:P:31:TRP:O	3:P:101:ARG:HG3	1.94	0.67
4:Q:52:ILE:O	4:Q:54:VAL:HG23	1.94	0.67
2:O:62:ASN:O	2:O:65:THR:HG22	1.94	0.67
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.25	0.67
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.77	0.67
2:B:274:VAL:O	2:B:278:VAL:HG23	1.95	0.67
2:B:385:GLU:C	2:B:387:LEU:H	2.03	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.10	0.67
2:B:97:SER:HB3	9:I:69:SER:HA	1.76	0.67
1:N:342:TRP:O	1:N:345:LEU:HB2	1.94	0.66
2:O:341:MET:HE2	2:O:341:MET:HA	1.76	0.66
2:B:154:SER:O	2:B:157:VAL:HG12	1.95	0.66
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.31	0.66
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.13	0.66
1:A:80:GLU:HA	2:B:284:LEU:HD12	1.76	0.66
3:C:59:ASP:C	3:C:61:SER:H	2.03	0.66
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.25	0.66
2:B:306:PRO:HB3	9:I:52:ARG:HG3	1.77	0.66
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.24	0.66
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.77	0.66
1:A:249:PRO:HG2	1:A:250:VAL:H	1.60	0.66
2:O:27:THR:HG22	2:O:28:LYS:N	2.08	0.66
3:P:82:ASN:HD22	3:P:82:ASN:N	1.93	0.66
3:P:70:THR:HA	3:P:74:VAL:HG23	1.76	0.66
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.78	0.66
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.09	0.66
3:C:241:LEU:HB3	4:D:208:MET:HE2	1.76	0.66
4:D:52:ILE:O	4:D:54:VAL:HG23	1.96	0.66
19:D:501:HEC:HMB1	19:D:501:HEC:HBB3	1.78	0.66
3:P:241:LEU:HB3	4:Q:208:MET:HE2	1.76	0.66
3:C:137:GLY:H	3:C:140:SER:HB2	1.61	0.66
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.26	0.66
4:D:197:GLU:O	4:D:198:HIS:C	2.39	0.66
1:A:187:ASP:O	1:A:191:LYS:HE3	1.96	0.66
3:C:36:SER:O	3:C:40:VAL:HG23	1.96	0.66
3:P:236:MET:O	3:P:239:PRO:HD2	1.95	0.66
5:R:69:LEU:O	5:R:72:SER:HB3	1.95	0.66
1:N:10:ASN:OD1	2:O:19:PRO:HD2	1.96	0.65
1:N:317:THR:HG23	1:N:318:GLY:N	2.10	0.65
2:O:262:ALA:O	2:O:320:GLY:HA3	1.96	0.65
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	1.78	0.65
1:A:365:MET:HG3	1:A:366:VAL:N	2.10	0.65
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.77	0.65
4:D:37:CYS:C	4:D:39:ALA:H	2.04	0.65
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.11	0.65
2:O:152:PHE:HE1	2:O:177:TYR:HD1	1.44	0.65
2:O:156:GLN:NE2	9:V:77:ARG:C	2.53	0.65
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.35	0.65
1:A:23:LEU:HD23	1:A:24:ARG:N	2.10	0.65
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.25	0.65
1:N:23:LEU:HD23	1:N:24:ARG:N	2.11	0.65
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.77	0.65
3:P:241:LEU:CB	4:Q:208:MET:HE2	2.26	0.65
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.11	0.65
6:S:13:MET:HA	6:S:16:ILE:HD12	1.76	0.65
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.32	0.65
2:O:385:GLU:C	2:O:387:LEU:H	2.03	0.65
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.79	0.65
3:C:247:SER:OG	3:C:250:LEU:HB2	1.97	0.65
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.60	0.65
2:B:19:PRO:O	2:B:22:GLU:N	2.28	0.65
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.77	0.65
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.27	0.65
2:O:402:ILE:HD13	2:O:402:ILE:C	2.21	0.65
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.79	0.65
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.32	0.65
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.31	0.65
5:E:161:HIS:HB2	21:E:501:FES:S1	2.37	0.65
2:O:141:GLN:N	2:O:142:PRO:HD2	2.12	0.65
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.22	0.65
6:F:89:TYR:CD1	6:F:90:LEU:N	2.65	0.65
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.32	0.65
1:A:27:SER:HA	1:A:199:ALA:O	1.97	0.64
6:F:89:TYR:HD1	6:F:90:LEU:H	1.45	0.64
2:O:96:LEU:HG	9:V:70:LEU:HD13	1.78	0.64
4:Q:37:CYS:C	4:Q:39:ALA:H	2.06	0.64
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.79	0.64
2:B:150:VAL:O	2:B:153:GLN:HB2	1.96	0.64
4:D:47:ALA:H	4:D:50:ASN:ND2	1.91	0.64
10:J:14:PHE:CD2	10:J:14:PHE:N	2.64	0.64
2:O:209:ILE:O	2:O:211:VAL:HG22	1.97	0.64
3:P:79:LEU:HD22	4:Q:204:MET:HE1	1.79	0.64
5:E:18:VAL:HG23	5:E:18:VAL:O	1.95	0.64
9:I:63:ASP:CG	9:I:64:LEU:H	2.05	0.64
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.97	0.64
4:Q:197:GLU:O	4:Q:198:HIS:C	2.40	0.64
10:W:26:LEU:O	10:W:29:VAL:HB	1.97	0.64
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.32	0.64
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.27	0.64
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.79	0.64
5:R:161:HIS:HB2	21:R:501:FES:S1	2.38	0.64
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.78	0.64
5:R:78:LEU:HB2	5:R:191:ASP:HA	1.78	0.64
3:C:239:PRO:HA	3:C:242:THR:HB	1.79	0.64
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.26	0.64
2:O:438:GLU:O	2:O:439:LEU:HD23	1.97	0.64
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.80	0.64
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.27	0.64
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	1.79	0.64
3:P:238:THR:HB	3:P:239:PRO:HD3	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.80	0.64
5:E:71:LEU:N	5:E:71:LEU:HD23	2.13	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.31	0.64
7:T:41:PHE:O	7:T:45:VAL:HG23	1.96	0.64
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.80	0.64
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.80	0.64
4:D:186:VAL:O	4:D:190:LEU:HG	1.97	0.64
7:G:77:TYR:HA	7:G:80:ASP:OD2	1.98	0.64
2:O:219:VAL:O	2:O:223:PHE:HB2	1.98	0.64
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.24	0.63
5:E:77:LYS:HE2	5:E:79:SER:OG	1.98	0.63
5:E:78:LEU:HD12	5:E:190:ASP:O	1.97	0.63
1:N:362:ARG:O	1:N:365:MET:HG2	1.97	0.63
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.99	0.63
2:B:160:LEU:HB3	9:I:64:LEU:HD22	1.80	0.63
1:N:199:ALA:HA	1:N:376:CYS:SG	2.38	0.63
2:B:144:LEU:HB2	2:B:183:ILE:CD1	2.28	0.63
2:B:402:ILE:HD13	2:B:402:ILE:C	2.23	0.63
3:C:120:LEU:HD22	13:C:502:HEM:HBB2	1.79	0.63
3:C:323:GLN:O	3:C:326:PHE:HB3	1.98	0.63
5:E:52:LYS:C	5:E:52:LYS:HD3	2.23	0.63
1:N:342:TRP:HA	1:N:345:LEU:HD12	1.79	0.63
3:P:70:THR:HA	3:P:74:VAL:CG2	2.27	0.63
3:P:239:PRO:HA	3:P:242:THR:HB	1.78	0.63
5:R:52:LYS:C	5:R:52:LYS:HD3	2.23	0.63
10:W:14:PHE:N	10:W:14:PHE:CD2	2.63	0.63
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.29	0.63
4:D:33:TYR:HD1	4:D:37:CYS:HB2	1.63	0.63
4:D:102:ARG:NH1	4:D:107:GLY:O	2.32	0.63
4:D:223:LYS:C	4:D:223:LYS:HD3	2.24	0.63
1:N:103:SER:O	1:N:106:MET:HB2	1.99	0.63
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.33	0.63
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.78	0.63
5:R:148:ALA:O	5:R:149:ASN:HB2	1.96	0.63
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.23	0.63
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.97	0.63
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.63
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.78	0.63
3:C:127:THR:O	3:C:130:VAL:HG22	1.99	0.63
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.28	0.63
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:307:PHE:CD1	1:N:307:PHE:C	2.77	0.63
1:N:433:ASP:OD2	1:N:435:ASN:HB2	1.97	0.63
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.80	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.32	0.63
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.80	0.63
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.34	0.63
1:N:45:SER:OG	1:N:92:ARG:HA	1.98	0.63
9:V:49:LEU:HD22	9:V:55:MET:CB	2.27	0.63
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.81	0.62
5:E:69:LEU:O	5:E:72:SER:HB3	1.99	0.62
6:S:89:TYR:CD1	6:S:90:LEU:N	2.65	0.62
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.82	0.62
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.34	0.62
1:N:368:GLN:O	1:N:374:PRO:HB2	1.99	0.62
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.98	0.62
7:G:36:ASN:O	7:G:40:ARG:HG3	2.00	0.62
3:P:323:GLN:O	3:P:326:PHE:HB3	1.99	0.62
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.82	0.62
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.26	0.62
1:N:439:SER:C	1:N:441:MET:H	2.06	0.62
2:O:168:TYR:HB2	2:O:173:ALA:CB	2.27	0.62
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.15	0.62
5:R:126:ARG:HH21	5:R:170:ARG:HG2	1.65	0.62
2:O:31:ASN:HD22	2:O:31:ASN:N	1.98	0.62
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.34	0.62
3:C:82:ASN:HD22	3:C:82:ASN:N	1.97	0.62
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.82	0.62
2:O:96:LEU:C	2:O:96:LEU:HD12	2.25	0.62
3:P:125:MET:CE	14:P:3001:IKR:I1	3.17	0.62
1:A:163:LEU:HD22	1:A:314:TYR:CE1	2.35	0.62
2:B:402:ILE:HG23	2:B:403:ASP:N	2.14	0.62
1:N:112:LEU:O	1:N:116:VAL:HG23	2.00	0.62
4:Q:147:LEU:HD13	4:Q:157:ALA:HB1	1.81	0.62
4:D:232:SER:HB3	7:G:23:GLN:NE2	2.13	0.62
1:N:178:THR:HG22	1:N:179:ARG:N	2.15	0.62
1:A:383:LEU:HD23	1:A:388:ARG:O	2.00	0.61
3:P:59:ASP:C	3:P:61:SER:H	2.08	0.61
3:C:254:PRO:O	3:C:256:ASN:N	2.32	0.61
1:N:270:LEU:HB3	1:N:320:PHE:HE1	1.64	0.61
3:P:234:THR:HG21	4:Q:219:LEU:HD13	1.82	0.61
4:Q:30:PHE:HE2	4:Q:64:LEU:HD11	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:286:PRO:O	3:C:287:ASN:HB2	2.00	0.61
4:D:62:LYS:O	4:D:66:GLU:HG3	1.99	0.61
9:I:65:VAL:HG12	9:I:66:ALA:N	2.15	0.61
1:A:307:PHE:CD1	1:A:307:PHE:C	2.78	0.61
5:E:141:HIS:HB3	21:E:501:FES:S2	2.40	0.61
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.33	0.61
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.61
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.82	0.61
2:O:402:ILE:HG23	2:O:403:ASP:N	2.16	0.61
6:S:89:TYR:HD1	6:S:90:LEU:H	1.46	0.61
5:E:78:LEU:HD13	5:E:129:LYS:HE3	1.82	0.61
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.36	0.61
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.16	0.61
1:N:27:SER:HA	1:N:199:ALA:O	2.00	0.61
1:N:106:MET:HE2	1:N:106:MET:C	2.25	0.61
1:N:106:MET:HB3	1:N:107:PRO:CD	2.30	0.61
5:R:18:VAL:HG23	5:R:18:VAL:O	1.99	0.61
1:A:103:SER:O	1:A:106:MET:HB2	2.01	0.61
2:B:226:ILE:HD13	2:B:227:ARG:NH1	2.16	0.61
2:B:361:LYS:O	2:B:365:LYS:HG3	2.01	0.61
4:D:60:GLU:O	4:D:64:LEU:HB2	2.01	0.61
3:P:370:ILE:O	3:P:374:GLU:HB2	2.01	0.61
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.65	0.61
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.35	0.61
3:C:70:THR:HA	3:C:74:VAL:CG2	2.31	0.61
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.36	0.61
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.47	0.61
1:A:106:MET:HB3	1:A:107:PRO:CD	2.31	0.61
4:D:221:TYR:CD2	5:E:39:VAL:HG21	2.36	0.61
1:A:112:LEU:O	1:A:116:VAL:HG23	2.01	0.60
2:B:24:LEU:O	2:B:24:LEU:HD23	2.01	0.60
5:E:129:LYS:HE2	5:E:187:PHE:HE2	1.65	0.60
8:H:40:CYS:O	8:H:44:VAL:HG23	2.00	0.60
1:N:45:SER:HA	1:N:48:GLU:HG3	1.82	0.60
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.83	0.60
2:O:403:ASP:C	2:O:405:VAL:H	2.08	0.60
3:P:82:ASN:HD22	3:P:82:ASN:H	1.47	0.60
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.33	0.60
8:U:40:CYS:O	8:U:44:VAL:HG23	2.00	0.60
9:V:65:VAL:HG12	9:V:66:ALA:N	2.15	0.60
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLU:O	2:B:387:LEU:N	2.34	0.60
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.24	0.60
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.82	0.60
1:A:161:THR:HG21	1:A:235:ARG:H	1.66	0.60
2:B:141:GLN:N	2:B:142:PRO:HD2	2.16	0.60
2:B:187:THR:OG1	2:B:190:GLN:HG3	2.02	0.60
1:N:63:ALA:O	1:N:116:VAL:HG13	2.00	0.60
4:Q:43:MET:CE	4:Q:46:VAL:HG21	2.19	0.60
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.36	0.60
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.37	0.60
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.37	0.60
1:A:67:THR:HA	1:A:121:ALA:H	1.66	0.60
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.84	0.60
4:D:197:GLU:HG2	4:D:198:HIS:N	2.15	0.60
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.01	0.60
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.34	0.60
13:P:502:HEM:HBD1	22:P:384:HOH:O	2.02	0.60
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.16	0.60
7:G:41:PHE:O	7:G:45:VAL:HG23	2.01	0.60
2:O:402:ILE:O	2:O:405:VAL:HG23	2.00	0.60
4:Q:167:GLU:C	4:Q:169:LEU:H	2.10	0.60
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.01	0.60
2:B:67:HIS:O	2:B:70:ARG:HB3	2.02	0.60
2:B:76:THR:HG22	2:B:82:SER:N	2.14	0.60
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.84	0.60
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.67	0.60
2:O:67:HIS:O	2:O:70:ARG:HB3	2.00	0.60
2:O:76:THR:HG22	2:O:82:SER:N	2.13	0.60
4:Q:95:TYR:CE2	4:Q:101:ALA:HA	2.36	0.60
9:V:52:ARG:O	9:V:56:SER:HB3	2.02	0.60
4:D:158:ILE:CD1	4:D:160:MET:HB3	2.32	0.60
10:W:56:LYS:HE3	10:W:60:GLU:OE1	2.02	0.60
3:C:120:LEU:CG	13:C:502:HEM:HBB2	2.31	0.60
5:E:114:VAL:CG2	5:E:172:ARG:HH12	2.13	0.60
2:O:96:LEU:O	9:V:70:LEU:HD22	2.01	0.60
2:O:144:LEU:HB2	2:O:183:ILE:CD1	2.32	0.60
2:O:385:GLU:O	2:O:387:LEU:N	2.35	0.60
3:P:172:ASP:C	3:P:174:PRO:HD2	2.26	0.60
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.66	0.59
5:E:94:LYS:HD3	5:E:138:VAL:HG21	1.82	0.59
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:C	1:A:195:MET:HE2	2.26	0.59
2:O:187:THR:OG1	2:O:190:GLN:HG3	2.01	0.59
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.32	0.59
8:U:35:GLU:O	8:U:39:LEU:HG	2.02	0.59
1:A:7:THR:HG21	2:B:113:ARG:NE	2.17	0.59
2:B:17:LEU:O	2:B:18:CYS:HB3	2.01	0.59
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.34	0.59
4:D:222:MET:HE3	5:E:40:THR:OG1	2.03	0.59
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.84	0.59
1:A:317:THR:HG23	1:A:318:GLY:N	2.18	0.59
6:F:27:ASN:O	6:F:30:GLY:N	2.30	0.59
6:F:71:LYS:O	6:F:72:HIS:HB2	2.01	0.59
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.83	0.59
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.32	0.59
2:B:71:LEU:N	2:B:71:LEU:HD23	2.16	0.59
2:B:152:PHE:HE1	2:B:177:TYR:HD1	1.50	0.59
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.37	0.59
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.33	0.59
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.18	0.59
1:N:187:ASP:O	1:N:191:LYS:HE3	2.03	0.59
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.28	0.59
3:P:101:ARG:NH2	13:P:502:HEM:HBD2	2.18	0.59
1:A:48:GLU:HB3	1:A:52:ASN:OD1	2.03	0.59
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.37	0.59
3:C:347:PRO:O	3:C:350:ILE:HG22	2.02	0.59
4:D:220:TYR:OH	4:D:224:ARG:HD3	2.02	0.59
9:I:31:UNK:C	9:I:73:PRO:HG2	2.32	0.59
1:N:90:THR:O	1:N:90:THR:HG23	2.02	0.59
2:O:132:PHE:HB2	2:O:192:HIS:CE1	2.38	0.59
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.16	0.59
5:R:169:GLY:O	5:R:179:ASN:HB3	2.02	0.59
1:A:18:THR:HG23	1:A:24:ARG:HG2	1.85	0.59
1:A:105:ASP:O	1:A:109:VAL:HG23	2.02	0.59
2:B:403:ASP:C	2:B:405:VAL:H	2.10	0.59
3:C:184:PHE:CD2	3:P:184:PHE:CD2	2.91	0.59
1:N:261:GLY:HA2	1:N:317:THR:O	2.03	0.59
3:P:294:ALA:O	3:P:298:SER:HB3	2.03	0.59
2:B:438:GLU:O	2:B:439:LEU:HD23	2.03	0.58
5:E:144:CYS:HB2	21:E:501:FES:S2	2.43	0.58
1:N:163:LEU:HD22	1:N:314:TYR:CE1	2.38	0.58
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.03	0.58
2:B:57:TYR:CD1	2:B:57:TYR:N	2.70	0.58
2:B:306:PRO:CB	9:I:52:ARG:HG3	2.33	0.58
3:C:294:ALA:O	3:C:298:SER:HB3	2.03	0.58
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.19	0.58
6:F:51:PRO:O	6:F:52:GLU:C	2.45	0.58
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.18	0.58
2:O:75:LEU:HD11	2:O:140:LEU:CD2	2.32	0.58
3:P:316:MET:HG2	3:P:319:ARG:HH21	1.68	0.58
4:Q:235:MET:HE1	6:S:63:LYS:HG2	1.83	0.58
2:O:156:GLN:NE2	9:V:77:ARG:O	2.36	0.58
1:A:178:THR:HG22	1:A:179:ARG:N	2.17	0.58
2:B:20:GLY:O	2:B:21:ALA:HB3	2.03	0.58
1:N:249:PRO:HG2	1:N:250:VAL:H	1.67	0.58
3:P:286:PRO:O	3:P:287:ASN:HB2	2.03	0.58
3:P:347:PRO:O	3:P:350:ILE:HG22	2.04	0.58
2:B:96:LEU:O	9:I:70:LEU:HD22	2.03	0.58
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.69	0.58
4:D:231:LYS:O	6:F:71:LYS:HE3	2.03	0.58
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.38	0.58
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.33	0.58
1:N:86:PHE:CD2	1:N:99:ILE:HD11	2.37	0.58
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.86	0.58
3:P:137:GLY:H	3:P:140:SER:HB2	1.68	0.58
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.21	0.58
1:A:362:ARG:HA	1:A:365:MET:HE2	1.85	0.58
2:B:281:ALA:HB2	2:B:311:ALA:HB3	1.86	0.58
1:A:90:THR:O	1:A:90:THR:HG23	2.04	0.58
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.18	0.58
1:A:239:SER:HB2	7:G:17:SER:O	2.04	0.58
2:B:307:PHE:CD1	2:B:308:ASP:N	2.72	0.58
2:B:402:ILE:O	2:B:405:VAL:HG23	2.03	0.58
4:D:164:ILE:O	4:D:179:MET:HE2	2.03	0.58
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.34	0.58
1:N:147:ASN:O	1:N:148:VAL:C	2.47	0.58
3:P:243:LEU:C	3:P:243:LEU:HD12	2.27	0.58
1:A:368:GLN:O	1:A:374:PRO:HB2	2.02	0.58
2:B:394:ALA:HB1	2:B:395:PRO:HD2	1.85	0.58
3:C:320:PRO:HG2	3:C:321:LEU:H	1.67	0.58
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.38	0.58
4:Q:180:SER:OG	8:U:77:LEU:HD21	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.39	0.58
3:C:254:PRO:C	3:C:256:ASN:H	2.12	0.58
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.18	0.58
2:O:318:ASP:O	2:O:319:SER:HB2	2.04	0.58
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.38	0.58
6:S:65:ALA:O	6:S:68:LEU:HB2	2.04	0.58
1:A:261:GLY:HA2	1:A:317:THR:O	2.04	0.58
2:B:19:PRO:O	2:B:20:GLY:C	2.45	0.58
3:C:82:ASN:HD22	3:C:82:ASN:H	1.52	0.58
1:N:354:VAL:HG23	1:N:355:LYS:N	2.19	0.58
2:O:124:LEU:HD23	2:O:124:LEU:C	2.29	0.58
2:O:247:GLN:HE21	2:O:249:GLY:H	1.50	0.58
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.19	0.58
1:A:137:GLU:O	1:A:141:MET:HG3	2.04	0.57
2:B:37:SER:HB2	2:B:213:HIS:ND1	2.19	0.57
3:C:362:ILE:HG22	3:C:363:LEU:N	2.19	0.57
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.85	0.57
3:P:2:ALA:CB	3:P:8:SER:HB3	2.33	0.57
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.03	0.57
9:V:49:LEU:HD13	9:V:55:MET:HB3	1.85	0.57
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.39	0.57
3:C:370:ILE:O	3:C:374:GLU:HB2	2.03	0.57
4:D:235:MET:HB3	7:G:15:THR:HG22	1.85	0.57
3:P:101:ARG:HD2	3:P:102:GLY:N	2.18	0.57
6:S:71:LYS:O	6:S:72:HIS:HB2	2.04	0.57
3:C:187:PRO:HG2	13:C:501:HEM:HMC3	1.85	0.57
4:D:57:THR:CB	4:D:60:GLU:HG3	2.35	0.57
1:N:52:ASN:O	1:N:53:ASN:C	2.46	0.57
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.84	0.57
2:O:57:TYR:CE2	2:O:234:SER:HB2	2.38	0.57
2:O:294:LYS:HE3	2:O:356:ASP:OD2	2.05	0.57
4:Q:181:GLN:CA	8:U:77:LEU:HD22	2.34	0.57
8:U:73:LEU:HD12	8:U:73:LEU:O	2.03	0.57
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.33	0.57
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.86	0.57
2:O:399:ALA:O	2:O:402:ILE:HG22	2.05	0.57
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.34	0.57
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.40	0.57
6:S:75:LEU:O	6:S:80:TRP:NE1	2.31	0.57
9:V:72:ALA:HB1	9:V:73:PRO:HD3	1.87	0.57
1:A:439:SER:HA	1:A:442:TYR:CE2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.40	0.57
1:N:307:PHE:HA	1:N:323:HIS:O	2.04	0.57
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.87	0.57
2:O:407:SER:O	2:O:411:VAL:HG23	2.04	0.57
4:Q:5:LEU:HG	4:Q:152:TYR:HE1	1.69	0.57
2:B:262:ALA:O	2:B:320:GLY:HA3	2.05	0.57
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.86	0.57
1:N:19:LEU:C	1:N:21:ASN:H	2.12	0.57
1:N:117:VAL:HG23	1:N:118:GLN:N	2.19	0.57
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.86	0.57
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.04	0.57
1:A:90:THR:O	1:A:167:VAL:HG11	2.04	0.57
3:C:64:PHE:CE1	18:C:2011:GOL:H2	2.39	0.57
3:C:147:ILE:HG13	14:C:2001:IKR:H16A	1.87	0.57
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.87	0.57
5:R:116:LYS:O	5:R:117:LEU:HG	2.05	0.57
1:A:106:MET:HE3	1:A:208:LEU:HD13	1.86	0.57
1:A:332:ASP:O	1:A:333:ASP:C	2.48	0.57
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.39	0.57
5:E:12:ALA:HB1	7:G:28:ASN:HD21	1.70	0.57
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.86	0.57
5:R:107:ASN:C	5:R:109:GLU:H	2.13	0.57
2:B:150:VAL:CG2	2:B:151:ALA:N	2.68	0.57
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.87	0.57
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.85	0.57
2:O:96:LEU:CB	2:O:109:VAL:HG12	2.32	0.57
5:R:140:THR:O	5:R:141:HIS:C	2.48	0.57
3:C:261:ASN:ND2	3:C:264:VAL:H	2.03	0.56
1:N:280:TYR:O	1:N:306:SER:HA	2.04	0.56
2:O:57:TYR:N	2:O:57:TYR:CD1	2.73	0.56
2:O:394:ALA:HB1	2:O:395:PRO:HD2	1.87	0.56
3:P:59:ASP:O	3:P:61:SER:N	2.38	0.56
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	2.88	0.56
1:A:75:PHE:O	1:A:79:VAL:HG23	2.05	0.56
2:B:393:THR:HG22	2:B:397:VAL:HB	1.86	0.56
5:E:94:LYS:HB3	5:E:138:VAL:CG2	2.36	0.56
4:Q:221:TYR:HE1	7:T:25:ALA:CB	2.18	0.56
5:R:94:LYS:HD3	5:R:138:VAL:HG21	1.85	0.56
1:A:7:THR:HG21	2:B:113:ARG:CD	2.35	0.56
1:A:63:ALA:O	1:A:116:VAL:HG13	2.06	0.56
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:O	1:A:306:SER:HA	2.04	0.56
1:A:365:MET:CG	1:A:366:VAL:N	2.68	0.56
2:B:306:PRO:HA	9:I:52:ARG:HE	1.71	0.56
3:C:377:MET:HE2	6:F:20:TYR:CB	2.31	0.56
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.41	0.56
4:D:167:GLU:C	4:D:169:LEU:H	2.13	0.56
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.87	0.56
2:O:264:VAL:HG23	2:O:316:TYR:C	2.30	0.56
2:O:268:GLU:HG2	2:O:268:GLU:O	2.05	0.56
2:O:281:ALA:HB2	2:O:311:ALA:HB3	1.87	0.56
3:P:120:LEU:HD22	13:P:502:HEM:HBB2	1.87	0.56
4:Q:33:TYR:HD1	4:Q:37:CYS:HB2	1.70	0.56
4:Q:43:MET:HG2	4:Q:46:VAL:HG23	1.87	0.56
3:C:129:PHE:HB2	14:C:2001:IKR:H40B	1.88	0.56
3:C:254:PRO:C	3:C:256:ASN:N	2.61	0.56
2:O:424:MET:HG2	2:O:425:ALA:N	2.20	0.56
4:Q:60:GLU:O	4:Q:64:LEU:HB2	2.05	0.56
1:A:266:ASP:HA	1:A:269:VAL:HG23	1.87	0.56
1:A:344:ARG:NH2	1:A:353:GLU:OE2	2.38	0.56
2:B:96:LEU:C	2:B:96:LEU:HD12	2.30	0.56
2:B:168:TYR:N	2:B:168:TYR:CD1	2.72	0.56
3:C:33:ASN:HB3	22:C:1008:HOH:O	2.05	0.56
2:O:437:ASP:OD1	2:O:438:GLU:HG3	2.06	0.56
1:A:270:LEU:HD13	1:A:320:PHE:CD1	2.41	0.56
2:B:168:TYR:N	2:B:168:TYR:HD1	2.04	0.56
2:B:294:LYS:HE3	2:B:356:ASP:OD2	2.05	0.56
10:J:26:LEU:O	10:J:29:VAL:HB	2.06	0.56
2:O:146:VAL:O	2:O:149:ALA:N	2.33	0.56
3:P:95:ILE:CD1	3:P:121:LEU:HD13	2.30	0.56
4:Q:30:PHE:CE2	4:Q:64:LEU:HD11	2.40	0.56
5:R:99:ARG:NH2	5:R:149:ASN:HD22	2.04	0.56
7:T:78:GLU:C	7:T:79:ASN:HD22	2.13	0.56
8:U:44:VAL:HG22	8:U:52:GLU:OE1	2.06	0.56
2:B:247:GLN:HE21	2:B:249:GLY:H	1.53	0.56
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.87	0.56
1:N:365:MET:CG	1:N:366:VAL:N	2.67	0.56
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.72	0.56
2:O:75:LEU:HD11	2:O:140:LEU:HD23	1.88	0.56
2:O:207:VAL:HG12	2:O:208:GLY:N	2.15	0.56
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.88	0.56
1:A:242:ARG:NH2	1:A:432:LEU:HA	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:THR:OG1	1:A:353:GLU:HG3	2.05	0.56
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.36	0.56
10:W:57:HIS:HA	10:W:60:GLU:CG	2.36	0.56
1:N:277:ILE:HB	1:N:309:THR:HG21	1.88	0.56
1:A:16:VAL:O	1:A:17:THR:HG23	2.06	0.56
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.88	0.56
1:A:277:ILE:HB	1:A:309:THR:HG21	1.88	0.56
1:A:381:SER:O	1:A:382:HIS:C	2.49	0.56
2:B:345:LYS:O	2:B:348:ALA:N	2.39	0.56
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.88	0.56
4:D:52:ILE:C	4:D:54:VAL:H	2.13	0.56
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.06	0.56
1:N:253:VAL:HG11	1:N:335:MET:CE	2.35	0.56
2:O:37:SER:CB	2:O:213:HIS:ND1	2.69	0.56
5:R:76:ILE:HG23	5:R:89:PHE:CZ	2.41	0.56
9:V:65:VAL:CG1	9:V:66:ALA:N	2.69	0.56
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.31	0.55
5:E:101:ARG:HB3	5:E:105:GLU:OE1	2.07	0.55
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.21	0.55
10:J:59:TYR:N	10:J:59:TYR:CD1	2.73	0.55
4:Q:40:CYS:HA	4:Q:95:TYR:HE1	1.70	0.55
5:R:100:HIS:CD2	5:R:131:GLU:HB2	2.41	0.55
1:A:180:ALA:O	1:A:183:ALA:HB3	2.06	0.55
1:A:206:LYS:O	1:A:207:GLU:C	2.49	0.55
4:D:100:ALA:O	4:D:103:ALA:HB3	2.06	0.55
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.41	0.55
6:F:75:LEU:O	6:F:80:TRP:NE1	2.32	0.55
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.42	0.55
2:O:280:GLY:HA3	2:O:293:SER:OG	2.06	0.55
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.88	0.55
1:A:199:ALA:HA	1:A:376:CYS:SG	2.46	0.55
1:A:270:LEU:HB3	1:A:320:PHE:HE1	1.71	0.55
1:A:354:VAL:HG23	1:A:355:LYS:N	2.22	0.55
3:C:243:LEU:C	3:C:243:LEU:HD12	2.31	0.55
6:F:61:ARG:HH11	6:F:61:ARG:HG3	1.72	0.55
2:O:259:THR:HG22	2:O:260:GLU:N	2.22	0.55
2:O:283:PRO:C	2:O:284:LEU:HD23	2.32	0.55
5:R:82:PRO:O	5:R:100:HIS:HB3	2.05	0.55
1:A:106:MET:HE2	1:A:106:MET:C	2.30	0.55
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.87	0.55
3:C:89:SER:O	3:C:90:PHE:C	2.49	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:VAL:CG1	9:I:66:ALA:N	2.69	0.55
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.06	0.55
2:O:267:ALA:C	2:O:269:ALA:H	2.13	0.55
3:P:36:SER:O	3:P:40:VAL:HG23	2.06	0.55
4:Q:20:ALA:HB1	4:Q:199:ASP:OD2	2.05	0.55
4:Q:52:ILE:C	4:Q:54:VAL:H	2.15	0.55
4:Q:231:LYS:HA	6:S:71:LYS:HG2	1.88	0.55
1:A:433:ASP:O	1:A:437:ILE:HG13	2.06	0.55
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.89	0.55
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.42	0.55
4:D:24:SER:OG	10:J:55:ILE:HG21	2.07	0.55
2:O:307:PHE:H	9:V:52:ARG:HG2	1.72	0.55
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.86	0.55
9:V:70:LEU:HD23	9:V:71:ASN:N	2.21	0.55
1:A:105:ASP:O	1:A:106:MET:C	2.49	0.55
5:E:55:VAL:O	5:E:59:ILE:HG12	2.06	0.55
2:O:27:THR:HG22	2:O:28:LYS:H	1.72	0.55
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.42	0.55
2:O:225:ASN:C	2:O:227:ARG:H	2.14	0.55
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.89	0.55
8:H:43:ARG:HD2	8:H:47:ARG:CZ	2.37	0.55
8:H:65:ARG:O	8:H:68:CYS:HB3	2.07	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.42	0.55
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.42	0.55
3:C:120:LEU:HB3	13:C:502:HEM:HBB2	1.87	0.55
1:N:67:THR:HA	1:N:121:ALA:H	1.70	0.55
1:N:134:ILE:HG21	1:N:174:ILE:CG1	2.35	0.55
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.35	0.55
2:O:166:ALA:HA	2:O:240:TRP:CZ3	2.42	0.55
1:A:87:ASN:HB3	1:A:98:TYR:CZ	2.42	0.55
1:A:192:ALA:N	1:A:195:MET:HE3	2.22	0.55
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.42	0.55
2:B:424:MET:HG2	2:B:425:ALA:N	2.21	0.55
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.71	0.55
3:C:350:ILE:HG23	3:C:351:ILE:N	2.22	0.55
4:D:171:TYR:HD1	4:D:175:THR:HB	1.72	0.55
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.55
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.42	0.55
9:V:65:VAL:H	9:V:77:ARG:HB2	1.72	0.55
2:B:58:GLU:OE1	2:B:64:GLY:N	2.39	0.55
1:N:107:PRO:O	1:N:108:LYS:C	2.49	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:95:ILE:O	3:P:99:ILE:HG13	2.07	0.55
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.71	0.55
4:Q:100:ALA:O	4:Q:103:ALA:HB3	2.06	0.55
9:V:32:UNK:O	9:V:33:UNK:C	2.54	0.55
2:B:124:LEU:HD23	2:B:124:LEU:C	2.31	0.54
3:C:31:TRP:O	3:C:101:ARG:HG3	2.07	0.54
3:C:137:GLY:N	3:C:140:SER:HB2	2.22	0.54
3:C:214:SER:HB2	3:C:218:LYS:HZ1	1.72	0.54
3:C:287:ASN:O	3:C:288:LYS:C	2.50	0.54
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.36	0.54
1:N:107:PRO:O	1:N:109:VAL:N	2.40	0.54
4:Q:148:HIS:N	4:Q:148:HIS:CD2	2.75	0.54
10:W:59:TYR:N	10:W:59:TYR:CD1	2.74	0.54
1:A:45:SER:HA	1:A:48:GLU:HG3	1.87	0.54
4:D:116:ILE:CG2	4:D:117:VAL:N	2.70	0.54
1:N:105:ASP:O	1:N:106:MET:C	2.50	0.54
1:N:212:ALA:O	1:N:216:PHE:HB2	2.07	0.54
1:N:266:ASP:HA	1:N:269:VAL:HG23	1.89	0.54
1:N:333:ASP:O	1:N:336:PHE:HB3	2.07	0.54
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.72	0.54
2:O:97:SER:HB3	9:V:69:SER:HA	1.88	0.54
3:P:244:ALA:O	3:P:245:LEU:HD23	2.08	0.54
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.42	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.89	0.54
1:N:19:LEU:O	1:N:21:ASN:N	2.40	0.54
1:N:22:GLY:O	1:N:193:PRO:HA	2.08	0.54
1:N:90:THR:O	1:N:167:VAL:HG11	2.07	0.54
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.07	0.54
5:R:118:ARG:NH2	5:R:174:GLY:O	2.41	0.54
2:B:115:HIS:O	2:B:119:VAL:HG23	2.07	0.54
2:B:146:VAL:O	2:B:149:ALA:N	2.35	0.54
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.07	0.54
3:C:141:PHE:O	3:C:144:ALA:HB3	2.07	0.54
1:N:90:THR:HA	1:N:95:THR:HA	1.88	0.54
1:N:106:MET:HE3	1:N:208:LEU:HD13	1.89	0.54
4:Q:10:PHE:HD2	8:U:74:PHE:CE2	2.26	0.54
5:E:20:ASP:C	5:E:22:THR:H	2.16	0.54
1:N:62:LEU:CD1	1:N:127:ILE:HG12	2.37	0.54
1:N:107:PRO:HG2	1:N:108:LYS:H	1.73	0.54
1:N:147:ASN:C	1:N:149:THR:N	2.66	0.54
2:O:107:TYR:CG	2:O:127:THR:HG22	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:374:THR:HG22	2:O:376:GLN:N	2.22	0.54
1:A:304:CYS:HB2	1:A:325:VAL:O	2.08	0.54
2:B:399:ALA:O	2:B:402:ILE:HG22	2.07	0.54
5:E:142:LEU:O	3:P:265:THR:N	2.39	0.54
8:H:20:ILE:HD12	8:H:73:LEU:HA	1.88	0.54
1:N:75:PHE:O	1:N:79:VAL:HG23	2.08	0.54
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.89	0.54
5:R:99:ARG:NH2	5:R:149:ASN:ND2	2.55	0.54
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.37	0.54
2:B:318:ASP:O	2:B:319:SER:HB2	2.08	0.54
2:B:333:ALA:O	2:B:337:ILE:HG13	2.08	0.54
4:D:147:LEU:HD13	4:D:157:ALA:HB1	1.89	0.54
5:E:76:ILE:O	5:E:193:VAL:HG12	2.08	0.54
8:U:25:GLU:HG2	8:U:61:PHE:HZ	1.71	0.54
5:E:116:LYS:HD2	5:E:116:LYS:N	2.19	0.54
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.42	0.54
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.43	0.54
6:S:13:MET:HA	6:S:16:ILE:CD1	2.37	0.54
2:B:283:PRO:C	2:B:284:LEU:HD23	2.33	0.54
4:D:56:HIS:HB3	4:D:60:GLU:HB2	1.90	0.54
6:F:32:MET:CE	6:F:87:LYS:HG2	2.37	0.54
8:H:35:GLU:O	8:H:39:LEU:HG	2.08	0.54
2:O:120:MET:O	2:O:121:GLU:C	2.50	0.54
3:P:189:ALA:O	3:P:193:ILE:HG13	2.08	0.54
1:A:107:PRO:O	1:A:108:LYS:C	2.50	0.54
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.38	0.54
2:B:259:THR:HG22	2:B:260:GLU:N	2.22	0.54
9:I:49:LEU:HB3	9:I:55:MET:SD	2.48	0.54
1:N:25:VAL:HG22	1:N:197:LEU:HB3	1.90	0.54
1:N:343:MET:O	1:N:344:ARG:C	2.50	0.54
2:O:51:ILE:HD11	2:O:204:MET:HE3	1.89	0.54
1:A:3:THR:HG23	1:A:6:GLN:OE1	2.08	0.53
1:A:147:ASN:O	1:A:148:VAL:C	2.51	0.53
1:A:307:PHE:HA	1:A:323:HIS:O	2.09	0.53
2:B:201:SER:OG	2:B:228:SER:HA	2.08	0.53
3:C:9:HIS:HD2	3:C:12:LEU:H	1.56	0.53
3:C:244:ALA:O	3:C:245:LEU:HD23	2.09	0.53
1:N:48:GLU:HB3	1:N:52:ASN:OD1	2.08	0.53
2:O:115:HIS:O	2:O:119:VAL:HG23	2.08	0.53
2:O:393:THR:HG22	2:O:397:VAL:HB	1.89	0.53
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:147:ILE:HG13	14:P:3001:IKR:H16A	1.89	0.53
3:P:214:SER:HB2	3:P:218:LYS:HZ1	1.73	0.53
3:P:287:ASN:O	3:P:288:LYS:C	2.52	0.53
4:Q:5:LEU:HG	4:Q:152:TYR:CE1	2.43	0.53
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.43	0.53
1:A:53:ASN:CG	1:A:165:ARG:HD3	2.33	0.53
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.90	0.53
15:C:2002:UQ:HM51	15:C:2002:UQ:C8	2.39	0.53
4:D:27:ARG:O	4:D:30:PHE:HB3	2.08	0.53
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.89	0.53
2:O:306:PRO:HB3	9:V:52:ARG:N	2.23	0.53
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.35	0.53
5:R:109:GLU:OE1	5:R:123:ASP:HB2	2.08	0.53
6:S:51:PRO:O	6:S:52:GLU:C	2.51	0.53
1:A:52:ASN:O	1:A:53:ASN:C	2.51	0.53
2:B:31:ASN:HD22	2:B:31:ASN:N	2.05	0.53
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.39	0.53
2:B:207:VAL:HG12	2:B:208:GLY:N	2.12	0.53
2:B:227:ARG:HD3	2:B:227:ARG:N	2.23	0.53
3:C:172:ASP:C	3:C:174:PRO:HD2	2.33	0.53
1:N:383:LEU:HD23	1:N:388:ARG:O	2.09	0.53
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.53
4:D:240:PRO:O	4:D:241:LYS:C	2.51	0.53
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.90	0.53
3:P:78:TRP:CD2	3:P:79:LEU:N	2.77	0.53
3:P:316:MET:HE1	3:P:367:PHE:CE2	2.44	0.53
5:R:170:ARG:HG2	5:R:179:ASN:ND2	2.24	0.53
2:B:248:ASN:C	2:B:248:ASN:HD22	2.16	0.53
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.90	0.53
4:D:171:TYR:C	4:D:173:ASP:H	2.17	0.53
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.39	0.53
1:N:158:PHE:O	1:N:159:GLN:O	2.27	0.53
1:N:318:GLY:O	1:N:319:LEU:HD23	2.08	0.53
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.44	0.53
2:O:26:ILE:HG23	2:O:26:ILE:O	2.08	0.53
2:O:201:SER:CB	2:O:227:ARG:HB2	2.32	0.53
2:O:287:ARG:CA	9:V:53:GLU:HG3	2.39	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.44	0.53
1:A:145:MET:HB2	1:A:252:HIS:NE2	2.24	0.53
4:D:28:ARG:O	4:D:31:GLN:N	2.42	0.53
4:D:148:HIS:CE1	4:D:161:ALA:HA	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:73:LEU:HD12	8:H:73:LEU:O	2.09	0.53
1:N:191:LYS:C	1:N:195:MET:HE3	2.34	0.53
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.43	0.53
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.53
3:P:142:TRP:HA	3:P:145:THR:OG1	2.08	0.53
3:P:175:THR:O	3:P:176:LEU:C	2.51	0.53
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.90	0.53
3:P:273:TRP:HA	3:P:276:LEU:HG	1.91	0.53
4:Q:52:ILE:O	4:Q:54:VAL:N	2.41	0.53
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.09	0.53
2:B:81:SER:C	2:B:83:PHE:N	2.64	0.53
1:N:178:THR:C	1:N:180:ALA:N	2.64	0.53
1:N:281:ASP:C	1:N:281:ASP:OD1	2.52	0.53
1:N:433:ASP:O	1:N:437:ILE:HG13	2.07	0.53
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.91	0.53
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.44	0.53
6:S:70:LEU:HG	6:S:71:LYS:N	2.23	0.53
2:B:385:GLU:C	2:B:387:LEU:N	2.66	0.53
3:C:4:ASN:O	3:C:5:ILE:HD13	2.09	0.53
1:N:277:ILE:CD1	1:N:345:LEU:HD11	2.39	0.53
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.44	0.53
16:P:3004:CDL:HA31	7:T:40:ARG:HB3	1.90	0.53
8:U:20:ILE:HD12	8:U:73:LEU:HA	1.91	0.53
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.44	0.53
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.44	0.53
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.91	0.53
3:C:61:SER:C	3:C:62:LEU:HG	2.34	0.53
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.44	0.53
7:G:63:THR:HG22	7:G:64:GLN:N	2.23	0.53
1:N:134:ILE:CG2	1:N:174:ILE:HG12	2.36	0.53
2:O:81:SER:C	2:O:83:PHE:N	2.65	0.53
3:P:9:HIS:HD2	3:P:12:LEU:H	1.57	0.53
4:Q:27:ARG:CZ	10:W:59:TYR:HE2	2.21	0.53
5:R:15:ARG:HD2	7:T:21:PHE:O	2.09	0.53
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.90	0.53
3:C:101:ARG:HD2	3:C:102:GLY:N	2.23	0.53
3:C:350:ILE:CG2	3:C:351:ILE:N	2.72	0.53
4:D:180:SER:OG	8:H:77:LEU:HD21	2.08	0.53
3:P:120:LEU:CD1	13:P:502:HEM:HBB2	2.38	0.53
3:P:201:LEU:C	3:P:203:GLU:H	2.17	0.53
3:P:261:ASN:HD22	3:P:264:VAL:HB	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:24:SER:OG	10:W:55:ILE:HG21	2.09	0.53
5:R:20:ASP:C	5:R:22:THR:H	2.17	0.53
6:S:16:ILE:O	6:S:19:TRP:HB3	2.09	0.53
1:A:117:VAL:CG2	1:A:118:GLN:N	2.72	0.52
2:B:107:TYR:CG	2:B:127:THR:HG22	2.44	0.52
2:B:226:ILE:HD13	2:B:227:ARG:HH12	1.73	0.52
3:C:13:LYS:O	3:C:13:LYS:HG2	2.09	0.52
4:D:27:ARG:CZ	10:J:59:TYR:CE2	2.91	0.52
1:N:192:ALA:N	1:N:195:MET:HE3	2.24	0.52
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.74	0.52
5:R:107:ASN:O	5:R:109:GLU:N	2.39	0.52
10:W:23:THR:O	10:W:24:VAL:C	2.53	0.52
1:A:253:VAL:HG11	1:A:335:MET:CE	2.39	0.52
1:A:277:ILE:HD11	1:A:345:LEU:HD11	1.90	0.52
2:B:437:ASP:OD1	2:B:438:GLU:HG3	2.08	0.52
4:D:43:MET:HG2	4:D:46:VAL:CG2	2.39	0.52
5:E:40:THR:O	5:E:41:ALA:C	2.53	0.52
2:O:258:VAL:HG11	2:O:312:PHE:CD2	2.41	0.52
5:R:79:SER:C	5:R:81:ILE:H	2.18	0.52
1:A:255:LEU:HD13	1:A:422:LEU:CD1	2.39	0.52
2:B:20:GLY:O	2:B:21:ALA:CB	2.57	0.52
2:B:26:ILE:HG23	2:B:26:ILE:O	2.09	0.52
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.40	0.52
2:O:152:PHE:CE1	2:O:177:TYR:HD1	2.26	0.52
2:O:383:GLY:O	2:O:384:SER:C	2.52	0.52
4:Q:165:TYR:O	4:Q:168:ILE:HB	2.09	0.52
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.08	0.52
4:Q:215:LEU:HD13	5:R:46:ALA:CB	2.40	0.52
5:R:141:HIS:HB3	21:R:501:FES:S2	2.49	0.52
1:A:373:THR:N	1:A:374:PRO:HD2	2.25	0.52
3:C:158:GLY:C	3:C:160:THR:N	2.65	0.52
3:C:175:THR:O	3:C:176:LEU:C	2.50	0.52
4:D:165:TYR:O	4:D:168:ILE:HB	2.08	0.52
10:J:40:ASP:O	10:J:44:GLU:HG3	2.08	0.52
1:N:15:ASN:O	1:N:26:ALA:HA	2.09	0.52
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.39	0.52
3:P:75:GLN:C	3:P:77:GLY:H	2.18	0.52
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.74	0.52
4:Q:186:VAL:CG1	4:Q:187:CYS:N	2.72	0.52
6:S:61:ARG:HH11	6:S:61:ARG:HG3	1.74	0.52
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.45	0.52
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.90	0.52
3:C:120:LEU:CD2	13:C:502:HEM:HBB2	2.39	0.52
1:N:147:ASN:O	1:N:149:THR:N	2.43	0.52
1:N:335:MET:HE3	1:N:431:LEU:HD11	1.92	0.52
2:O:168:TYR:N	2:O:168:TYR:CD1	2.75	0.52
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.25	0.52
3:P:326:PHE:O	3:P:329:LEU:HB3	2.09	0.52
2:B:415:LYS:C	2:B:417:PHE:N	2.66	0.52
3:C:208:ASN:C	3:C:208:ASN:OD1	2.53	0.52
4:D:122:GLY:O	4:D:123:GLY:C	2.52	0.52
2:B:43:PRO:O	2:B:113:ARG:HG3	2.09	0.52
2:B:166:ALA:HA	2:B:240:TRP:CE3	2.45	0.52
4:D:57:THR:HG22	4:D:58:GLU:N	2.23	0.52
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.45	0.52
1:N:190:PHE:C	1:N:195:MET:HE2	2.34	0.52
1:N:255:LEU:HD13	1:N:422:LEU:CD1	2.39	0.52
2:O:73:SER:N	2:O:74:PRO:HD2	2.25	0.52
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.45	0.52
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.45	0.52
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.52
7:T:36:ASN:O	7:T:40:ARG:HG3	2.10	0.52
1:A:284:PHE:CD2	9:I:71:ASN:HA	2.45	0.52
2:B:383:GLY:O	2:B:384:SER:C	2.52	0.52
3:C:130:VAL:HG23	3:C:131:GLY:N	2.23	0.52
4:D:81:PHE:H	4:D:81:PHE:HD2	1.57	0.52
2:O:248:ASN:C	2:O:248:ASN:HD22	2.17	0.52
3:P:13:LYS:HG2	3:P:13:LYS:O	2.09	0.52
3:P:120:LEU:HB3	13:P:502:HEM:HBB2	1.90	0.52
3:P:329:LEU:O	3:P:332:ASN:HB3	2.09	0.52
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.44	0.52
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.25	0.52
5:R:170:ARG:HA	5:R:179:ASN:CG	2.35	0.52
1:A:191:LYS:N	1:A:195:MET:HE2	2.24	0.52
2:B:110:GLU:O	2:B:111:CYS:HB3	2.09	0.52
2:B:155:PRO:O	2:B:158:GLY:N	2.40	0.52
4:D:106:ASN:C	4:D:108:ALA:H	2.17	0.52
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.10	0.52
5:E:175:PRO:O	5:E:176:ALA:C	2.53	0.52
6:F:70:LEU:HG	6:F:71:LYS:N	2.25	0.52
1:N:439:SER:C	1:N:441:MET:N	2.68	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:119:VAL:HG12	2:O:119:VAL:O	2.10	0.52
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.92	0.52
2:O:151:ALA:C	2:O:153:GLN:H	2.18	0.52
2:O:215:ASP:C	2:O:217:LYS:N	2.67	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HB2	2.46	0.51
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.45	0.51
4:D:40:CYS:HA	4:D:95:TYR:HE1	1.75	0.51
2:O:290:SER:CB	2:O:293:SER:HB3	2.40	0.51
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.46	0.51
1:N:171:THR:HB	5:R:4:ASP:OD2	2.11	0.51
1:N:332:ASP:O	1:N:333:ASP:C	2.51	0.51
2:O:73:SER:OG	2:O:74:PRO:HD3	2.09	0.51
2:O:168:TYR:N	2:O:168:TYR:HD1	2.08	0.51
2:O:333:ALA:O	2:O:337:ILE:HG13	2.10	0.51
1:A:52:ASN:OD1	1:A:52:ASN:C	2.52	0.51
1:A:242:ARG:HH22	1:A:432:LEU:HA	1.76	0.51
3:C:86:ASN:ND2	3:C:243:LEU:HD11	2.26	0.51
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.91	0.51
4:D:28:ARG:O	4:D:29:GLY:C	2.53	0.51
5:E:142:LEU:HD12	5:E:161:HIS:HE1	1.74	0.51
6:F:32:MET:O	6:F:33:ARG:C	2.52	0.51
6:F:90:LEU:O	6:F:91:GLU:C	2.51	0.51
9:I:59:SER:O	9:I:60:ALA:HB3	2.11	0.51
1:N:394:GLU:O	1:N:395:TRP:C	2.53	0.51
3:P:137:GLY:N	3:P:140:SER:HB2	2.25	0.51
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.75	0.51
2:B:374:THR:HG22	2:B:376:GLN:N	2.25	0.51
4:D:148:HIS:ND1	4:D:161:ALA:HA	2.25	0.51
8:H:57:GLU:O	8:H:60:ASP:HB2	2.10	0.51
2:O:140:LEU:C	2:O:142:PRO:HD2	2.36	0.51
3:P:142:TRP:O	3:P:146:VAL:HG23	2.09	0.51
4:Q:106:ASN:C	4:Q:108:ALA:H	2.18	0.51
1:A:158:PHE:O	1:A:159:GLN:O	2.28	0.51
1:A:255:LEU:HD12	1:A:421:ALA:O	2.10	0.51
1:A:333:ASP:O	1:A:336:PHE:HB3	2.10	0.51
2:B:259:THR:HG23	2:B:421:LYS:O	2.11	0.51
2:B:341:MET:O	2:B:344:LEU:HB2	2.11	0.51
4:D:171:TYR:OH	4:D:182:ILE:HA	2.11	0.51
4:D:235:MET:HE1	6:F:63:LYS:HG2	1.91	0.51
1:N:341:GLU:O	1:N:342:TRP:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:201:SER:H	2:O:227:ARG:CB	2.17	0.51
3:P:129:PHE:HB2	14:P:3001:IKR:H40B	1.91	0.51
3:P:130:VAL:HG23	3:P:131:GLY:N	2.26	0.51
3:P:132:TYR:O	3:P:135:PRO:HD2	2.11	0.51
5:R:76:ILE:O	5:R:193:VAL:HG12	2.10	0.51
9:V:28:UNK:HA	9:V:72:ALA:HB2	1.93	0.51
1:A:163:LEU:HD22	1:A:314:TYR:HE1	1.74	0.51
2:B:287:ARG:C	9:I:53:GLU:HG3	2.35	0.51
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.40	0.51
4:D:168:ILE:O	4:D:168:ILE:HG12	2.10	0.51
6:F:81:VAL:HG12	6:F:82:LYS:N	2.26	0.51
3:P:187:PRO:HG2	13:P:501:HEM:HMC3	1.93	0.51
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.41	0.51
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.45	0.51
1:A:106:MET:HB3	1:A:107:PRO:HD3	1.93	0.51
3:C:78:TRP:CD2	3:C:79:LEU:N	2.79	0.51
4:D:134:TYR:CD2	4:D:162:PRO:HG3	2.45	0.51
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.91	0.51
1:N:53:ASN:CG	1:N:165:ARG:HD3	2.36	0.51
1:N:221:PHE:O	1:N:222:THR:O	2.28	0.51
2:O:415:LYS:O	2:O:417:PHE:N	2.44	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
3:C:92:PHE:O	3:C:93:ILE:C	2.51	0.51
4:D:155:GLY:C	4:D:157:ALA:H	2.19	0.51
6:F:61:ARG:HG3	6:F:61:ARG:NH1	2.26	0.51
8:H:31:VAL:C	8:H:33:ALA:H	2.17	0.51
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.25	0.51
1:N:106:MET:HB3	1:N:107:PRO:HD3	1.93	0.51
1:N:373:THR:N	1:N:374:PRO:HD2	2.24	0.51
2:O:42:SER:O	2:O:113:ARG:HD2	2.10	0.51
4:Q:222:MET:HE3	5:R:40:THR:OG1	2.11	0.51
5:R:101:ARG:NH2	5:R:127:VAL:HG11	2.26	0.51
5:R:101:ARG:HH21	5:R:127:VAL:HG21	1.74	0.51
5:R:133:VAL:O	5:R:133:VAL:HG13	2.11	0.51
1:A:221:PHE:O	1:A:222:THR:O	2.29	0.51
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.26	0.51
1:N:88:GLY:O	2:O:286:LYS:NZ	2.42	0.51
1:N:255:LEU:O	1:N:321:GLY:HA3	2.11	0.51
3:P:89:SER:O	3:P:90:PHE:C	2.52	0.51
6:S:58:ARG:HG3	6:S:89:TYR:OH	2.11	0.51
8:U:52:GLU:HG2	8:U:53:GLN:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:MET:HG2	2:B:425:ALA:H	1.75	0.51
3:C:158:GLY:C	3:C:160:THR:H	2.18	0.51
2:O:102:ARG:NH1	2:O:102:ARG:CG	2.66	0.51
2:O:203:ARG:O	2:O:387:LEU:HD11	2.11	0.51
1:A:191:LYS:C	1:A:195:MET:HE3	2.35	0.50
2:B:24:LEU:HD23	2:B:24:LEU:C	2.36	0.50
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.94	0.50
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.92	0.50
3:C:95:ILE:CG2	3:C:96:PHE:N	2.74	0.50
3:C:198:LEU:HD21	13:C:502:HEM:CMA	2.41	0.50
5:E:129:LYS:HD2	5:E:132:TRP:CD1	2.46	0.50
1:N:180:ALA:O	1:N:183:ALA:HB3	2.10	0.50
2:O:58:GLU:OE1	2:O:64:GLY:N	2.43	0.50
2:O:168:TYR:CE2	2:O:172:LEU:HB2	2.45	0.50
3:P:75:GLN:O	3:P:77:GLY:N	2.44	0.50
5:R:139:CYS:O	5:R:140:THR:C	2.55	0.50
8:U:65:ARG:O	8:U:68:CYS:HB3	2.10	0.50
1:A:64:PHE:HA	1:A:75:PHE:HE2	1.76	0.50
3:C:175:THR:O	3:C:178:ARG:HG2	2.11	0.50
4:D:57:THR:H	4:D:60:GLU:HG3	1.75	0.50
4:D:227:TRP:O	4:D:228:SER:C	2.54	0.50
5:E:81:ILE:HD12	5:E:132:TRP:CZ3	2.46	0.50
10:J:60:GLU:O	10:J:61:ALA:HB3	2.11	0.50
2:O:221:GLU:HG3	2:O:222:GLN:N	2.23	0.50
2:O:341:MET:O	2:O:344:LEU:HB2	2.11	0.50
3:P:320:PRO:HG2	3:P:321:LEU:H	1.76	0.50
4:Q:10:PHE:HD2	8:U:74:PHE:HE2	1.59	0.50
1:A:261:GLY:O	1:A:267:ASN:ND2	2.45	0.50
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.75	0.50
2:B:378:LEU:HD12	2:B:378:LEU:O	2.11	0.50
3:C:377:MET:CE	6:F:20:TYR:HB2	2.37	0.50
4:D:37:CYS:O	4:D:39:ALA:N	2.45	0.50
2:O:109:VAL:HG23	2:O:109:VAL:O	2.11	0.50
2:O:395:PRO:O	2:O:398:VAL:HG12	2.11	0.50
3:P:4:ASN:O	3:P:5:ILE:HD13	2.11	0.50
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.73	0.50
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.92	0.50
1:A:90:THR:HA	1:A:95:THR:HA	1.93	0.50
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.92	0.50
1:A:335:MET:HE3	1:A:431:LEU:HD11	1.93	0.50
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:MET:O	4:D:212:SER:HB2	2.12	0.50
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.40	0.50
4:Q:147:LEU:C	4:Q:148:HIS:HD2	2.19	0.50
4:Q:186:VAL:HG13	4:Q:187:CYS:N	2.25	0.50
6:S:10:GLY:O	6:S:14:ASP:HB2	2.10	0.50
2:B:150:VAL:HG22	2:B:151:ALA:N	2.26	0.50
3:C:29:SER:HB2	16:C:2004:CDL:OB4	2.12	0.50
4:D:165:TYR:O	4:D:166:ASN:C	2.55	0.50
10:J:36:ASP:O	10:J:37:GLN:C	2.54	0.50
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.46	0.50
2:O:152:PHE:HE1	2:O:177:TYR:CD1	2.28	0.50
2:O:341:MET:CE	2:O:417:PHE:HE2	2.23	0.50
2:O:378:LEU:HD12	2:O:378:LEU:O	2.12	0.50
3:P:242:THR:HA	4:Q:208:MET:HE1	1.93	0.50
4:Q:221:TYR:HE1	7:T:25:ALA:HB2	1.75	0.50
5:R:126:ARG:HH21	5:R:179:ASN:ND2	2.10	0.50
1:A:178:THR:C	1:A:180:ALA:N	2.67	0.50
1:A:418:LYS:O	1:A:420:PRO:HD3	2.12	0.50
1:A:439:SER:C	1:A:441:MET:H	2.20	0.50
2:B:96:LEU:CB	2:B:109:VAL:HG12	2.37	0.50
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.18	0.50
2:O:209:ILE:HD11	2:O:378:LEU:HG	1.93	0.50
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.41	0.50
3:P:198:LEU:HD13	15:P:3002:UQ:HM52	1.93	0.50
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.94	0.50
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.11	0.50
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.94	0.50
6:S:40:ASP:C	6:S:40:ASP:OD1	2.54	0.50
8:U:18:THR:O	8:U:22:GLU:HG3	2.12	0.50
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.47	0.50
1:A:344:ARG:HB3	1:A:344:ARG:CZ	2.42	0.50
3:C:247:SER:N	3:C:248:PRO:HD3	2.27	0.50
3:C:316:MET:HG2	3:C:319:ARG:NH2	2.26	0.50
3:C:345:GLU:O	3:C:348:PHE:HB2	2.10	0.50
4:D:210:LEU:O	4:D:211:ILE:C	2.54	0.50
1:N:87:ASN:OD1	1:N:88:GLY:N	2.37	0.50
3:P:75:GLN:C	3:P:77:GLY:N	2.69	0.50
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.94	0.50
16:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.11	0.50
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.92	0.50
6:S:57:GLU:HB3	6:S:61:ARG:HH12	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:57:GLU:O	8:U:60:ASP:HB2	2.12	0.50
8:U:66:ASP:O	8:U:67:HIS:C	2.53	0.50
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.94	0.50
3:C:75:GLN:C	3:C:77:GLY:H	2.20	0.50
3:C:329:LEU:O	3:C:332:ASN:HB3	2.11	0.50
4:D:52:ILE:O	4:D:54:VAL:N	2.45	0.50
8:H:37:LEU:O	8:H:38:GLU:C	2.55	0.50
2:O:259:THR:HG23	2:O:421:LYS:O	2.11	0.50
2:O:345:LYS:O	2:O:348:ALA:N	2.45	0.50
4:Q:148:HIS:CE1	4:Q:161:ALA:HA	2.46	0.50
1:A:429:GLU:O	1:A:429:GLU:HG2	2.11	0.50
3:C:210:LEU:HD12	6:F:66:LEU:HD23	1.92	0.50
5:E:130:PRO:HG2	5:E:131:GLU:H	1.77	0.50
2:O:85:ILE:HA	2:O:122:TYR:CD2	2.47	0.50
2:O:215:ASP:C	2:O:217:LYS:H	2.20	0.50
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.93	0.50
4:Q:171:TYR:C	4:Q:173:ASP:H	2.20	0.50
6:S:12:LEU:C	6:S:14:ASP:H	2.19	0.50
1:A:365:MET:CG	1:A:366:VAL:H	2.25	0.49
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.42	0.49
2:O:263:ALA:O	2:O:266:SER:HB3	2.12	0.49
2:O:385:GLU:C	2:O:387:LEU:N	2.66	0.49
3:P:92:PHE:O	3:P:93:ILE:C	2.53	0.49
4:Q:81:PHE:H	4:Q:81:PHE:HD2	1.60	0.49
7:T:79:ASN:HD22	7:T:79:ASN:N	2.10	0.49
8:U:37:LEU:O	8:U:40:CYS:N	2.44	0.49
9:V:49:LEU:CD2	9:V:55:MET:HB3	2.39	0.49
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.77	0.49
4:D:109:LEU:O	4:D:111:PRO:HD3	2.12	0.49
9:I:63:ASP:O	9:I:64:LEU:HB2	2.12	0.49
2:O:268:GLU:HG2	2:O:272:PHE:HE1	1.77	0.49
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.43	0.49
4:Q:1:GLY:C	4:Q:3:LEU:H	2.20	0.49
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.11	0.49
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.12	0.49
1:A:67:THR:HA	1:A:121:ALA:N	2.27	0.49
1:A:208:LEU:O	1:A:209:VAL:C	2.55	0.49
6:F:27:ASN:O	6:F:28:LYS:C	2.54	0.49
8:H:43:ARG:HD2	8:H:47:ARG:NH2	2.26	0.49
1:N:365:MET:CG	1:N:366:VAL:H	2.23	0.49
2:O:100:SER:HA	2:O:104:LYS:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:124:LEU:O	2:O:128:THR:HG23	2.12	0.49
2:O:290:SER:HB3	2:O:293:SER:HB3	1.94	0.49
3:P:70:THR:O	3:P:74:VAL:HG23	2.12	0.49
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.47	0.49
4:Q:57:THR:H	4:Q:60:GLU:HG3	1.76	0.49
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.37	0.49
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.48	0.49
8:H:18:THR:O	8:H:22:GLU:HG3	2.12	0.49
1:N:253:VAL:O	1:N:323:HIS:HA	2.11	0.49
4:Q:155:GLY:C	4:Q:157:ALA:H	2.19	0.49
4:Q:235:MET:HE1	6:S:63:LYS:C	2.37	0.49
6:S:32:MET:O	6:S:33:ARG:C	2.55	0.49
6:S:61:ARG:HG3	6:S:61:ARG:NH1	2.28	0.49
6:S:94:LEU:O	6:S:95:LYS:C	2.55	0.49
1:A:171:THR:HB	5:E:4:ASP:OD2	2.12	0.49
2:B:313:ASN:O	9:I:62:ARG:O	2.31	0.49
3:C:245:LEU:O	4:D:201:ARG:CD	2.60	0.49
9:I:32:UNK:N	9:I:73:PRO:CG	2.70	0.49
2:O:272:PHE:O	2:O:273:SER:C	2.54	0.49
3:P:86:ASN:ND2	3:P:243:LEU:HD11	2.27	0.49
8:U:31:VAL:C	8:U:33:ALA:H	2.20	0.49
1:A:147:ASN:C	1:A:149:THR:N	2.70	0.49
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.77	0.49
3:C:277:PHE:CG	3:C:278:ALA:N	2.80	0.49
1:N:4:TYR:O	1:N:6:GLN:N	2.46	0.49
2:O:27:THR:CG2	2:O:28:LYS:N	2.74	0.49
5:R:70:ALA:C	5:R:72:SER:H	2.20	0.49
6:S:68:LEU:O	6:S:71:LYS:N	2.46	0.49
3:C:137:GLY:H	3:C:140:SER:CB	2.26	0.49
4:D:10:PHE:CD1	4:D:10:PHE:N	2.81	0.49
4:D:37:CYS:C	4:D:39:ALA:N	2.70	0.49
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.48	0.49
2:O:135:TRP:O	2:O:136:GLU:C	2.55	0.49
2:O:415:LYS:C	2:O:417:PHE:N	2.66	0.49
4:Q:158:ILE:CD1	4:Q:160:MET:HB3	2.42	0.49
5:R:81:ILE:HB	5:R:132:TRP:HH2	1.77	0.49
1:A:40:TRP:CH2	1:A:376:CYS:HB3	2.48	0.49
1:A:122:LEU:HD11	1:A:186:ILE:CD1	2.43	0.49
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.95	0.49
2:B:306:PRO:HB3	9:I:52:ARG:N	2.28	0.49
2:B:395:PRO:O	2:B:398:VAL:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:ASN:O	3:C:83:LEU:C	2.54	0.49
3:C:201:LEU:C	3:C:203:GLU:H	2.21	0.49
4:D:27:ARG:CZ	10:J:59:TYR:HE2	2.25	0.49
6:F:13:MET:HE2	6:F:16:ILE:HD12	1.93	0.49
8:H:25:GLU:HG2	8:H:61:PHE:HZ	1.78	0.49
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.94	0.49
4:Q:126:TYR:CD2	4:Q:126:TYR:C	2.91	0.49
5:R:1:VAL:HG23	5:R:3:ASN:N	2.24	0.49
5:R:15:ARG:HH11	5:R:32:ARG:HB3	1.76	0.49
6:S:90:LEU:O	6:S:91:GLU:C	2.55	0.49
1:A:244:ARG:NE	7:G:10:VAL:HB	2.27	0.49
2:B:326:THR:C	2:B:327:ILE:HG13	2.38	0.49
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.78	0.49
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.49
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.20	0.49
6:F:68:LEU:O	6:F:71:LYS:N	2.46	0.49
7:G:60:SER:O	7:G:64:GLN:HB2	2.13	0.49
7:G:77:TYR:CD1	8:H:52:GLU:HB2	2.48	0.49
1:N:170:THR:HG22	1:N:172:GLU:H	1.78	0.49
1:N:178:THR:CG2	1:N:179:ARG:N	2.76	0.49
1:N:281:ASP:OD1	1:N:281:ASP:O	2.31	0.49
2:O:150:VAL:CG2	2:O:151:ALA:N	2.75	0.49
2:O:415:LYS:O	2:O:416:LYS:C	2.55	0.49
5:R:175:PRO:O	5:R:176:ALA:C	2.56	0.49
1:A:134:ILE:CG2	1:A:174:ILE:HG12	2.42	0.49
1:A:434:TYR:CE2	7:G:19:SER:HB2	2.48	0.49
2:B:51:ILE:HD11	2:B:204:MET:HE3	1.94	0.49
2:B:372:VAL:O	2:B:372:VAL:HG12	2.12	0.49
3:C:75:GLN:C	3:C:77:GLY:N	2.70	0.49
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.94	0.49
3:C:189:ALA:O	3:C:193:ILE:HG13	2.12	0.49
4:D:116:ILE:HG23	4:D:117:VAL:H	1.75	0.49
4:D:117:VAL:HG13	4:D:190:LEU:HB3	1.95	0.49
1:N:52:ASN:OD1	1:N:52:ASN:C	2.56	0.49
1:N:371:GLY:O	1:N:375:VAL:HG23	2.13	0.49
2:O:81:SER:O	2:O:82:SER:C	2.56	0.49
2:O:424:MET:HG2	2:O:425:ALA:H	1.77	0.49
3:P:82:ASN:H	3:P:82:ASN:ND2	2.11	0.49
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.80	0.49
5:R:141:HIS:HB2	5:R:176:ALA:CB	2.43	0.49
10:W:57:HIS:HA	10:W:60:GLU:CD	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:PHE:O	5:E:11:SER:C	2.56	0.48
3:P:104:TYR:HD2	3:P:105:TYR:CE1	2.30	0.48
3:P:254:PRO:C	3:P:256:ASN:N	2.70	0.48
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.13	0.48
4:Q:117:VAL:HG13	4:Q:190:LEU:HB3	1.95	0.48
2:B:415:LYS:O	2:B:417:PHE:N	2.45	0.48
3:C:81:ARG:O	3:C:82:ASN:C	2.56	0.48
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.49	0.48
3:C:273:TRP:HA	3:C:276:LEU:HG	1.94	0.48
5:E:129:LYS:HG2	5:E:187:PHE:CZ	2.48	0.48
6:F:94:LEU:O	6:F:95:LYS:C	2.56	0.48
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.48
1:N:362:ARG:HA	1:N:365:MET:HE2	1.95	0.48
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.95	0.48
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	3.01	0.48
1:A:53:ASN:OD1	1:A:165:ARG:HD3	2.14	0.48
1:A:342:TRP:HA	1:A:345:LEU:HD12	1.94	0.48
1:A:433:ASP:OD2	1:A:435:ASN:N	2.47	0.48
2:B:157:VAL:HG22	2:B:157:VAL:O	2.14	0.48
3:C:241:LEU:HB2	4:D:208:MET:HE2	1.92	0.48
4:D:47:ALA:N	4:D:50:ASN:HD22	2.00	0.48
5:E:52:LYS:C	5:E:52:LYS:CD	2.86	0.48
8:H:27:THR:O	8:H:28:GLU:C	2.56	0.48
9:I:49:LEU:HD13	9:I:55:MET:CE	2.35	0.48
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.91	0.48
1:N:208:LEU:O	1:N:209:VAL:C	2.56	0.48
1:N:271:HIS:NE2	1:N:311:ASN:HB3	2.28	0.48
1:N:434:TYR:O	1:N:435:ASN:C	2.56	0.48
3:P:150:LEU:HB3	3:P:292:VAL:CG2	2.43	0.48
3:P:175:THR:O	3:P:178:ARG:HG2	2.12	0.48
3:P:253:ASP:OD1	3:P:254:PRO:N	2.46	0.48
4:Q:98:PRO:HG2	4:Q:99:GLU:OE1	2.13	0.48
7:T:38:TRP:O	7:T:39:ARG:C	2.56	0.48
1:A:87:ASN:HB3	1:A:98:TYR:CE1	2.48	0.48
1:A:133:VAL:O	1:A:134:ILE:C	2.54	0.48
2:B:203:ARG:O	2:B:387:LEU:HD11	2.14	0.48
2:B:415:LYS:O	2:B:416:LYS:C	2.55	0.48
3:C:41:CYS:SG	3:C:91:PHE:HA	2.54	0.48
4:D:187:CYS:O	4:D:190:LEU:HB2	2.14	0.48
4:D:218:LEU:HD13	5:E:43:ALA:HA	1.94	0.48
5:E:163:SER:HA	5:E:174:GLY:HA3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:58:LYS:C	10:J:59:TYR:CD1	2.91	0.48
1:N:349:THR:HA	1:N:353:GLU:OE1	2.13	0.48
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.93	0.48
3:P:297:ALA:HA	3:P:300:LEU:HB2	1.96	0.48
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.47	0.48
4:Q:37:CYS:C	4:Q:39:ALA:N	2.72	0.48
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.12	0.48
4:Q:204:MET:O	4:Q:205:GLY:C	2.54	0.48
5:R:83:GLU:HA	5:R:100:HIS:O	2.14	0.48
3:C:59:ASP:C	3:C:61:SER:N	2.68	0.48
4:D:164:ILE:HG21	4:D:182:ILE:HG21	1.94	0.48
5:E:129:LYS:HG2	5:E:187:PHE:CE2	2.48	0.48
2:O:166:ALA:O	2:O:242:GLY:N	2.46	0.48
2:O:220:ALA:O	2:O:224:LEU:HB2	2.14	0.48
5:R:118:ARG:O	5:R:120:PRO:HD3	2.13	0.48
1:A:4:TYR:OH	1:A:362:ARG:HD3	2.12	0.48
1:A:356:ARG:HG3	2:B:91:ALA:HA	1.95	0.48
2:B:151:ALA:C	2:B:153:GLN:H	2.21	0.48
2:B:408:ALA:O	2:B:409:ASP:C	2.57	0.48
3:C:132:TYR:O	3:C:135:PRO:HD2	2.13	0.48
4:D:135:CYS:O	4:D:149:TYR:HB3	2.14	0.48
1:N:64:PHE:HA	1:N:75:PHE:HE2	1.79	0.48
1:N:158:PHE:HB3	1:N:161:THR:OG1	2.13	0.48
1:N:242:ARG:NH2	1:N:432:LEU:HA	2.28	0.48
3:P:78:TRP:CG	3:P:79:LEU:N	2.82	0.48
4:Q:28:ARG:O	4:Q:29:GLY:C	2.56	0.48
4:Q:43:MET:HG2	4:Q:46:VAL:CG2	2.44	0.48
2:B:57:TYR:CE2	2:B:234:SER:HB2	2.49	0.48
2:B:76:THR:HG22	2:B:81:SER:HA	1.95	0.48
3:C:60:THR:HG23	3:C:173:ASN:HA	1.96	0.48
3:C:72:ARG:HG2	3:C:72:ARG:NH1	2.29	0.48
15:C:2002:UQ:HM51	15:C:2002:UQ:H8	1.96	0.48
4:D:98:PRO:O	4:D:99:GLU:C	2.56	0.48
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.96	0.48
1:N:270:LEU:HD13	1:N:320:PHE:HD1	1.79	0.48
1:N:317:THR:HG23	1:N:318:GLY:H	1.78	0.48
2:O:43:PRO:O	2:O:113:ARG:HG3	2.13	0.48
2:O:258:VAL:HG21	2:O:321:LEU:HD22	1.95	0.48
3:P:60:THR:HG23	3:P:173:ASN:HA	1.95	0.48
3:P:277:PHE:CG	3:P:278:ALA:N	2.82	0.48
5:R:175:PRO:HG2	5:R:176:ALA:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:10:TYR:CD2	10:W:10:TYR:O	2.67	0.48
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.71	0.48
4:D:218:LEU:CD1	5:E:43:ALA:HA	2.44	0.48
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.35	0.48
8:H:55:THR:O	8:H:56:GLU:C	2.57	0.48
10:J:15:ARG:HG2	10:J:15:ARG:HH11	1.77	0.48
1:N:40:TRP:CH2	1:N:376:CYS:HB3	2.49	0.48
1:N:87:ASN:HB3	1:N:98:TYR:CZ	2.48	0.48
1:N:122:LEU:HD11	1:N:186:ILE:CD1	2.44	0.48
1:N:184:SER:O	1:N:187:ASP:HB2	2.14	0.48
2:O:312:PHE:O	2:O:322:PHE:HA	2.14	0.48
3:P:214:SER:HB2	3:P:218:LYS:HZ3	1.75	0.48
8:U:43:ARG:O	8:U:47:ARG:HG3	2.14	0.48
1:A:134:ILE:HG21	1:A:174:ILE:CG1	2.43	0.48
1:A:178:THR:HG22	1:A:180:ALA:H	1.79	0.48
2:B:47:ILE:HD13	2:B:120:MET:CE	2.43	0.48
2:B:56:ARG:HG2	2:B:234:SER:OG	2.13	0.48
3:C:147:ILE:HA	3:C:150:LEU:HD12	1.96	0.48
5:E:133:VAL:O	5:E:133:VAL:HG13	2.13	0.48
6:F:21:TYR:C	6:F:21:TYR:CD2	2.92	0.48
6:F:67:ASP:HA	6:F:70:LEU:CD2	2.32	0.48
1:N:381:SER:O	1:N:382:HIS:C	2.57	0.48
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.38	0.48
2:O:137:VAL:O	2:O:140:LEU:HB3	2.14	0.48
5:R:15:ARG:NH1	5:R:32:ARG:HB3	2.29	0.48
5:E:116:LYS:H	5:E:116:LYS:CD	2.20	0.48
5:E:147:ILE:CG2	5:E:148:ALA:H	2.15	0.48
8:H:37:LEU:O	8:H:40:CYS:N	2.47	0.48
1:N:277:ILE:O	1:N:277:ILE:HG22	2.12	0.48
2:O:24:LEU:O	2:O:24:LEU:HD23	2.14	0.48
2:O:422:LYS:O	2:O:436:LEU:HD21	2.14	0.48
3:P:141:PHE:O	3:P:144:ALA:HB3	2.13	0.48
3:P:184:PHE:CE2	13:P:501:HEM:HBC1	2.49	0.48
3:P:319:ARG:HB3	3:P:374:GLU:CD	2.39	0.48
4:Q:220:TYR:OH	4:Q:224:ARG:HD3	2.14	0.48
10:W:52:TRP:O	10:W:56:LYS:HB2	2.13	0.48
2:B:109:VAL:HG23	2:B:109:VAL:O	2.14	0.47
2:B:120:MET:O	2:B:121:GLU:C	2.56	0.47
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.49	0.47
3:C:67:VAL:CG2	13:C:501:HEM:HBD2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:ILE:HG23	3:C:96:PHE:N	2.29	0.47
4:Q:56:HIS:HB3	4:Q:60:GLU:HB2	1.96	0.47
5:R:73:LYS:HB3	5:R:196:GLY:HA3	1.95	0.47
5:R:76:ILE:HD13	5:R:89:PHE:CE1	2.49	0.47
5:R:99:ARG:NH2	5:R:148:ALA:HB1	2.28	0.47
5:R:139:CYS:O	5:R:141:HIS:N	2.47	0.47
1:A:182:LEU:O	1:A:186:ILE:HG13	2.14	0.47
1:A:378:THR:O	1:A:382:HIS:N	2.43	0.47
2:B:132:PHE:HB2	2:B:192:HIS:CE1	2.49	0.47
3:C:142:TRP:O	3:C:146:VAL:HG23	2.14	0.47
3:C:316:MET:HG2	3:C:319:ARG:HH21	1.78	0.47
4:D:72:ASP:HB3	4:D:81:PHE:CE2	2.50	0.47
4:D:186:VAL:HG13	4:D:187:CYS:N	2.27	0.47
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.49	0.47
2:O:222:GLN:O	2:O:223:PHE:CG	2.67	0.47
2:O:247:GLN:NE2	2:O:249:GLY:H	2.12	0.47
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.14	0.47
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.79	0.47
7:T:63:THR:HG22	7:T:64:GLN:N	2.28	0.47
1:A:270:LEU:HD13	1:A:320:PHE:HD1	1.77	0.47
3:C:45:GLN:O	3:C:49:GLY:N	2.38	0.47
4:D:167:GLU:C	4:D:169:LEU:N	2.73	0.47
5:E:91:TRP:O	5:E:92:ARG:C	2.57	0.47
6:F:103:GLU:O	6:F:104:ARG:C	2.57	0.47
1:N:404:ALA:O	1:N:405:ARG:C	2.57	0.47
2:O:209:ILE:CG2	2:O:210:GLY:N	2.60	0.47
8:U:52:GLU:CG	8:U:53:GLN:N	2.77	0.47
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.27	0.47
2:B:215:ASP:C	2:B:217:LYS:H	2.23	0.47
2:B:253:VAL:HG11	2:B:433:THR:OG1	2.13	0.47
2:B:407:SER:O	2:B:411:VAL:HG23	2.14	0.47
5:E:96:LEU:HD12	5:E:135:LEU:O	2.14	0.47
6:F:82:LYS:O	6:F:83:TYR:C	2.55	0.47
2:B:215:ASP:C	2:B:217:LYS:N	2.69	0.47
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.47
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.49	0.47
3:C:120:LEU:CB	13:C:502:HEM:HBB2	2.43	0.47
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.79	0.47
2:O:306:PRO:HB3	9:V:52:ARG:H	1.80	0.47
2:O:385:GLU:HB3	2:O:391:THR:O	2.15	0.47
3:P:82:ASN:O	3:P:83:LEU:C	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.78	0.47
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.97	0.47
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.96	0.47
4:Q:167:GLU:C	4:Q:169:LEU:N	2.72	0.47
10:W:60:GLU:O	10:W:61:ALA:HB2	2.15	0.47
1:A:15:ASN:HB2	1:A:205:HIS:ND1	2.30	0.47
1:A:127:ILE:C	1:A:129:LYS:N	2.70	0.47
2:B:266:SER:OG	2:B:267:ALA:N	2.47	0.47
2:B:332:HIS:O	2:B:336:VAL:HG23	2.14	0.47
4:D:186:VAL:CG1	4:D:187:CYS:N	2.77	0.47
5:E:81:ILE:HD12	5:E:132:TRP:CH2	2.50	0.47
1:N:143:ASN:C	1:N:145:MET:HE2	2.40	0.47
2:O:24:LEU:HD23	2:O:24:LEU:C	2.40	0.47
2:O:71:LEU:O	2:O:74:PRO:CD	2.55	0.47
2:O:257:VAL:CG2	2:O:424:MET:HG3	2.42	0.47
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.54	0.47
4:Q:221:TYR:CD2	5:R:39:VAL:HG21	2.50	0.47
6:S:12:LEU:C	6:S:14:ASP:N	2.73	0.47
1:A:23:LEU:HA	1:A:192:ALA:O	2.15	0.47
2:B:152:PHE:CE1	2:B:177:TYR:HD1	2.31	0.47
2:B:209:ILE:O	2:B:211:VAL:N	2.48	0.47
2:B:268:GLU:O	2:B:269:ALA:C	2.58	0.47
3:C:30:ALA:HB1	16:D:2003:CDL:H111	1.95	0.47
1:N:121:ALA:O	1:N:122:LEU:HB2	2.13	0.47
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.15	0.47
1:N:254:ALA:HB3	1:N:423:ALA:HB3	1.96	0.47
1:N:365:MET:HG3	1:N:366:VAL:H	1.80	0.47
1:N:378:THR:O	1:N:382:HIS:N	2.42	0.47
2:O:215:ASP:O	2:O:217:LYS:N	2.47	0.47
2:O:272:PHE:O	2:O:276:GLN:N	2.39	0.47
3:P:30:ALA:HB1	16:Q:3003:CDL:H111	1.96	0.47
3:P:254:PRO:C	3:P:256:ASN:H	2.21	0.47
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.50	0.47
1:A:44:GLY:HA3	1:A:92:ARG:O	2.15	0.47
1:A:204:SER:O	1:A:205:HIS:C	2.58	0.47
2:B:42:SER:C	2:B:44:ALA:H	2.23	0.47
3:C:254:PRO:O	3:C:257:PHE:N	2.47	0.47
5:E:101:ARG:HD2	5:E:105:GLU:HB3	1.96	0.47
1:N:58:PHE:HA	1:N:134:ILE:HD11	1.96	0.47
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.50	0.47
1:N:256:ALA:HA	1:N:320:PHE:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:344:ARG:HG3	1:N:344:ARG:NH1	2.30	0.47
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.50	0.47
1:A:15:ASN:O	1:A:26:ALA:HA	2.15	0.47
2:B:73:SER:N	2:B:74:PRO:HD2	2.29	0.47
2:B:73:SER:OG	2:B:74:PRO:HD3	2.15	0.47
2:B:119:VAL:HG12	2:B:119:VAL:O	2.15	0.47
3:C:160:THR:O	3:C:161:LEU:C	2.58	0.47
3:C:187:PRO:O	3:C:190:ILE:HB	2.14	0.47
4:D:52:ILE:C	4:D:54:VAL:N	2.72	0.47
4:D:73:GLY:N	4:D:81:PHE:HE2	2.13	0.47
4:D:98:PRO:HG2	4:D:99:GLU:OE1	2.15	0.47
6:F:16:ILE:O	6:F:19:TRP:HB3	2.15	0.47
2:O:109:VAL:CG2	2:O:119:VAL:HG12	2.45	0.47
3:P:254:PRO:O	3:P:256:ASN:N	2.48	0.47
5:R:146:PRO:C	5:R:147:ILE:HG13	2.38	0.47
5:R:185:TYR:CD2	5:R:185:TYR:N	2.82	0.47
10:W:22:LEU:C	10:W:22:LEU:HD23	2.40	0.47
1:A:60:GLU:OE2	1:A:89:TYR:C	2.58	0.47
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.79	0.47
3:C:72:ARG:HG2	3:C:72:ARG:HH11	1.78	0.47
4:D:70:VAL:HG23	4:D:83:ARG:HG2	1.97	0.47
3:P:184:PHE:HA	13:P:501:HEM:HBC2	1.97	0.47
5:R:102:THR:C	5:R:104:ALA:N	2.73	0.47
2:B:85:ILE:HA	2:B:122:TYR:CD2	2.51	0.46
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.80	0.46
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.45	0.46
5:E:119:ASP:CG	5:E:179:ASN:ND2	2.74	0.46
1:N:67:THR:HA	1:N:121:ALA:N	2.30	0.46
1:N:178:THR:HG22	1:N:180:ALA:H	1.80	0.46
1:N:295:ALA:O	1:N:298:ALA:HB3	2.15	0.46
1:N:354:VAL:O	1:N:355:LYS:C	2.58	0.46
2:O:34:ILE:HG21	2:O:386:ALA:O	2.15	0.46
2:O:56:ARG:HH22	2:O:318:ASP:CG	2.24	0.46
2:O:272:PHE:HA	2:O:275:LEU:HB3	1.96	0.46
4:Q:2:GLU:H	4:Q:2:GLU:CD	2.23	0.46
4:Q:148:HIS:ND1	4:Q:162:PRO:HD3	2.30	0.46
9:V:32:UNK:N	9:V:73:PRO:HG2	2.31	0.46
10:W:36:ASP:O	10:W:37:GLN:C	2.57	0.46
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.46
1:A:107:PRO:O	1:A:109:VAL:N	2.48	0.46
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PRO:HB3	1:A:414:TYR:CE2	2.51	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.15	0.46
3:C:120:LEU:HD21	3:C:193:ILE:HB	1.96	0.46
4:D:204:MET:O	4:D:205:GLY:C	2.56	0.46
5:E:79:SER:OG	5:E:191:ASP:HB2	2.14	0.46
2:O:258:VAL:HG12	2:O:323:GLY:HA3	1.98	0.46
2:O:366:ALA:O	2:O:367:THR:C	2.58	0.46
16:Q:3003:CDL:HA21	6:S:72:HIS:CD2	2.50	0.46
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.45	0.46
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.80	0.46
1:N:23:LEU:HD23	1:N:23:LEU:C	2.41	0.46
1:N:170:THR:CG2	1:N:171:THR:H	2.25	0.46
1:N:219:VAL:HG12	1:N:220:SER:N	2.30	0.46
3:P:40:VAL:O	3:P:44:THR:OG1	2.32	0.46
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.45	0.46
5:R:44:CYS:HB3	10:W:24:VAL:HG11	1.97	0.46
6:S:67:ASP:O	6:S:71:LYS:HG3	2.15	0.46
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.98	0.46
3:C:39:ALA:O	3:C:40:VAL:C	2.57	0.46
4:D:127:VAL:O	4:D:131:LEU:HG	2.14	0.46
4:D:200:GLN:NE2	20:D:2091:BOG:H3	2.30	0.46
9:I:77:ARG:HE	9:I:77:ARG:HB2	1.56	0.46
1:N:76:GLU:HA	2:O:285:ILE:HD11	1.96	0.46
1:N:163:LEU:HD22	1:N:314:TYR:HE1	1.81	0.46
2:O:337:ILE:O	2:O:340:ALA:HB3	2.16	0.46
3:P:81:ARG:O	3:P:82:ASN:C	2.57	0.46
3:P:82:ASN:N	3:P:82:ASN:ND2	2.63	0.46
3:P:253:ASP:OD1	3:P:254:PRO:CD	2.63	0.46
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.27	0.46
1:A:58:PHE:HA	1:A:134:ILE:HD11	1.97	0.46
1:A:341:GLU:O	1:A:342:TRP:C	2.59	0.46
2:B:18:CYS:CB	2:B:19:PRO:HD3	2.42	0.46
3:C:72:ARG:NE	4:D:115:TYR:OH	2.48	0.46
4:D:218:LEU:HD13	5:E:43:ALA:N	2.31	0.46
4:D:218:LEU:HB3	5:E:43:ALA:HB2	1.96	0.46
7:G:72:LYS:NZ	8:H:52:GLU:HG3	2.30	0.46
1:N:161:THR:HG21	1:N:234:CYS:HA	1.97	0.46
1:N:161:THR:HG21	1:N:235:ARG:N	2.29	0.46
1:N:270:LEU:HB3	1:N:320:PHE:CE1	2.48	0.46
1:N:382:HIS:HB3	1:N:389:ARG:HA	1.97	0.46
2:O:81:SER:O	2:O:83:PHE:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:160:LEU:CB	9:V:64:LEU:HD22	2.42	0.46
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.31	0.46
2:O:408:ALA:O	2:O:409:ASP:C	2.58	0.46
2:O:430:LEU:O	2:O:432:SER:N	2.49	0.46
3:P:261:ASN:ND2	3:P:264:VAL:H	2.14	0.46
4:Q:120:ARG:HG2	4:Q:120:ARG:HH11	1.80	0.46
5:R:52:LYS:C	5:R:52:LYS:CD	2.88	0.46
1:A:23:LEU:HD23	1:A:23:LEU:C	2.41	0.46
1:A:253:VAL:HG11	1:A:335:MET:HE2	1.98	0.46
2:B:81:SER:O	2:B:83:PHE:N	2.48	0.46
2:B:400:GLN:O	2:B:404:SER:HB3	2.16	0.46
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.50	0.46
4:D:158:ILE:HD11	4:D:160:MET:HB3	1.96	0.46
4:D:184:LYS:HG2	8:H:74:PHE:CE1	2.51	0.46
4:D:218:LEU:HD13	5:E:42:THR:HG22	1.96	0.46
6:F:89:TYR:CD1	6:F:89:TYR:C	2.93	0.46
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.79	0.46
1:N:191:LYS:N	1:N:195:MET:HE2	2.30	0.46
1:N:272:VAL:O	1:N:275:ALA:HB3	2.16	0.46
3:P:79:LEU:C	3:P:79:LEU:HD12	2.41	0.46
3:P:147:ILE:HA	3:P:150:LEU:HD12	1.98	0.46
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.98	0.46
5:R:20:ASP:O	5:R:22:THR:N	2.40	0.46
10:W:55:ILE:O	10:W:55:ILE:HG13	2.15	0.46
1:A:127:ILE:C	1:A:129:LYS:H	2.22	0.46
1:A:178:THR:CG2	1:A:179:ARG:N	2.79	0.46
1:A:249:PRO:HG2	1:A:250:VAL:N	2.28	0.46
2:B:410:VAL:O	2:B:413:ALA:N	2.48	0.46
2:B:422:LYS:O	2:B:436:LEU:HD21	2.16	0.46
3:C:5:ILE:O	3:C:5:ILE:HG22	2.16	0.46
3:C:234:THR:HG21	4:D:219:LEU:HD13	1.98	0.46
3:C:276:LEU:O	3:C:277:PHE:C	2.56	0.46
3:C:319:ARG:HB3	3:C:374:GLU:OE1	2.16	0.46
5:E:38:LEU:HB2	10:J:14:PHE:HE1	1.81	0.46
1:N:304:CYS:HB2	1:N:325:VAL:O	2.16	0.46
1:N:335:MET:O	1:N:336:PHE:C	2.59	0.46
2:O:102:ARG:H	2:O:102:ARG:HD2	1.80	0.46
2:O:155:PRO:O	2:O:158:GLY:N	2.46	0.46
2:O:168:TYR:HE2	2:O:172:LEU:HD12	1.80	0.46
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.64	0.46
1:A:272:VAL:O	1:A:275:ALA:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:O	1:A:296:ALA:C	2.59	0.46
1:A:392:LEU:CD2	1:A:392:LEU:N	2.79	0.46
2:B:124:LEU:O	2:B:128:THR:HG23	2.16	0.46
2:B:152:PHE:HE1	2:B:177:TYR:CD1	2.33	0.46
3:C:289:LEU:O	3:C:293:LEU:HG	2.16	0.46
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.80	0.46
4:D:184:LYS:CG	8:H:74:PHE:CE1	2.99	0.46
8:H:58:LEU:HD11	8:H:62:LEU:CD1	2.46	0.46
8:H:66:ASP:O	8:H:67:HIS:C	2.56	0.46
2:O:338:ARG:O	2:O:341:MET:N	2.48	0.46
2:O:415:LYS:O	2:O:418:VAL:N	2.49	0.46
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.46	0.46
5:R:40:THR:O	5:R:41:ALA:C	2.56	0.46
1:A:242:ARG:HH12	1:A:432:LEU:N	2.13	0.46
2:B:81:SER:O	2:B:82:SER:C	2.58	0.46
2:B:131:GLU:O	2:B:132:PHE:C	2.59	0.46
2:B:366:ALA:O	2:B:367:THR:C	2.58	0.46
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.73	0.46
3:C:142:TRP:HA	3:C:145:THR:OG1	2.15	0.46
3:C:238:THR:CB	3:C:239:PRO:HD3	2.44	0.46
3:C:247:SER:HG	3:C:250:LEU:HB2	1.81	0.46
3:C:253:ASP:OD1	3:C:254:PRO:N	2.49	0.46
7:G:44:GLN:O	7:G:45:VAL:C	2.59	0.46
1:N:19:LEU:C	1:N:21:ASN:N	2.74	0.46
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.16	0.46
8:U:21:ARG:HH11	8:U:21:ARG:HG3	1.81	0.46
1:A:178:THR:O	1:A:179:ARG:C	2.59	0.46
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.46
1:A:344:ARG:NH1	1:A:344:ARG:CB	2.79	0.46
2:B:248:ASN:C	2:B:248:ASN:ND2	2.73	0.46
3:C:326:PHE:CD2	3:C:326:PHE:C	2.94	0.46
4:D:148:HIS:CD2	4:D:148:HIS:N	2.82	0.46
5:E:153:PHE:C	5:E:155:GLY:H	2.24	0.46
2:O:50:PHE:C	2:O:51:ILE:HG13	2.41	0.46
3:P:79:LEU:HD12	3:P:79:LEU:O	2.15	0.46
5:R:139:CYS:HB3	5:R:143:GLY:O	2.16	0.46
6:S:81:VAL:HG12	6:S:82:LYS:N	2.31	0.46
8:U:12:GLU:HG2	8:U:13:LEU:N	2.31	0.46
2:B:62:ASN:HD22	2:B:65:THR:HG21	1.81	0.45
2:B:290:SER:CB	2:B:293:SER:HB3	2.46	0.45
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.51	0.45
5:E:128:LYS:HG3	5:E:129:LYS:N	2.32	0.45
5:E:189:GLY:O	5:E:192:LEU:O	2.35	0.45
7:G:38:TRP:O	7:G:39:ARG:C	2.57	0.45
1:N:145:MET:O	1:N:146:THR:C	2.60	0.45
1:N:330:SER:O	1:N:331:ILE:C	2.60	0.45
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.50	0.45
2:O:403:ASP:C	2:O:405:VAL:N	2.74	0.45
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.45	0.45
3:P:366:LEU:HD22	3:P:366:LEU:N	2.31	0.45
4:Q:171:TYR:HD1	4:Q:175:THR:HB	1.81	0.45
5:R:114:VAL:O	5:R:114:VAL:HG12	2.17	0.45
1:A:107:PRO:HG2	1:A:108:LYS:H	1.82	0.45
2:B:42:SER:O	2:B:113:ARG:HD2	2.17	0.45
2:B:107:TYR:CD2	2:B:127:THR:HG22	2.51	0.45
2:B:111:CYS:HB3	2:B:119:VAL:HG21	1.97	0.45
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.51	0.45
3:C:89:SER:O	3:C:92:PHE:N	2.48	0.45
4:D:66:GLU:C	4:D:68:VAL:H	2.23	0.45
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.45
2:O:225:ASN:C	2:O:227:ARG:HG3	2.40	0.45
3:P:208:ASN:OD1	3:P:208:ASN:C	2.58	0.45
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.45
7:T:44:GLN:O	7:T:45:VAL:C	2.60	0.45
7:T:79:ASN:N	7:T:79:ASN:ND2	2.64	0.45
1:A:39:VAL:HG13	1:A:39:VAL:O	2.16	0.45
1:A:64:PHE:C	1:A:66:GLY:H	2.25	0.45
1:A:116:VAL:O	1:A:120:CYS:HB2	2.17	0.45
1:A:403:ASP:O	1:A:404:ALA:C	2.59	0.45
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.50	0.45
2:B:258:VAL:HG11	2:B:312:PHE:CD2	2.41	0.45
2:B:307:PHE:CD1	2:B:307:PHE:C	2.91	0.45
3:C:377:MET:HE2	6:F:20:TYR:CG	2.51	0.45
8:H:43:ARG:HG3	8:H:44:VAL:N	2.30	0.45
3:P:5:ILE:O	3:P:5:ILE:HG22	2.16	0.45
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.52	0.45
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.45
3:P:334:LEU:O	3:P:337:THR:HB	2.17	0.45
4:Q:72:ASP:HB3	4:Q:81:PHE:CE2	2.52	0.45
1:A:259:GLY:N	1:A:318:GLY:O	2.47	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.15	0.45
2:B:70:ARG:NH2	2:B:177:TYR:CE2	2.85	0.45
2:B:102:ARG:H	2:B:102:ARG:HD2	1.81	0.45
2:B:146:VAL:HG12	2:B:147:ASP:N	2.31	0.45
2:B:272:PHE:O	2:B:276:GLN:N	2.39	0.45
2:B:272:PHE:O	2:B:273:SER:C	2.59	0.45
2:B:338:ARG:O	2:B:341:MET:N	2.49	0.45
1:N:429:GLU:O	1:N:429:GLU:HG2	2.16	0.45
2:O:332:HIS:O	2:O:336:VAL:HG23	2.17	0.45
3:P:110:TYR:O	3:P:111:LYS:C	2.60	0.45
1:A:117:VAL:HG23	1:A:118:GLN:H	1.81	0.45
2:B:111:CYS:CB	2:B:119:VAL:HG21	2.46	0.45
3:C:101:ARG:NH2	13:C:502:HEM:HBD2	2.31	0.45
4:D:215:LEU:O	4:D:219:LEU:HD12	2.16	0.45
8:H:58:LEU:HD12	8:H:58:LEU:O	2.16	0.45
2:O:27:THR:CG2	2:O:28:LYS:H	2.29	0.45
2:O:268:GLU:OE1	2:O:416:LYS:NZ	2.48	0.45
2:O:400:GLN:O	2:O:404:SER:HB3	2.16	0.45
3:P:238:THR:CB	3:P:239:PRO:HD3	2.44	0.45
4:Q:98:PRO:O	4:Q:99:GLU:C	2.59	0.45
5:R:38:LEU:O	5:R:39:VAL:C	2.59	0.45
5:R:187:PHE:O	5:R:188:VAL:HG13	2.16	0.45
6:S:58:ARG:HG3	6:S:58:ARG:HH11	1.82	0.45
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.81	0.45
1:A:156:THR:HA	5:E:7:VAL:HG21	1.97	0.45
2:B:51:ILE:HG22	2:B:52:LYS:N	2.30	0.45
2:B:410:VAL:O	2:B:411:VAL:C	2.59	0.45
3:C:4:ASN:C	3:C:5:ILE:HD13	2.41	0.45
3:C:104:TYR:O	3:C:104:TYR:CD2	2.69	0.45
4:D:90:TYR:O	4:D:91:PHE:C	2.60	0.45
1:N:76:GLU:HA	2:O:285:ILE:CD1	2.46	0.45
1:N:127:ILE:C	1:N:129:LYS:N	2.73	0.45
2:O:166:ALA:HB1	2:O:242:GLY:C	2.42	0.45
3:P:120:LEU:HD21	3:P:193:ILE:HB	1.98	0.45
3:P:208:ASN:OD1	3:P:210:LEU:N	2.42	0.45
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.46	0.45
4:Q:227:TRP:O	4:Q:228:SER:C	2.60	0.45
5:R:73:LYS:HG3	22:R:1240:HOH:O	2.17	0.45
5:R:153:PHE:C	5:R:155:GLY:H	2.24	0.45
10:W:57:HIS:HA	10:W:60:GLU:HG2	1.99	0.45
1:A:67:THR:HB	1:A:119:ASN:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:THR:HB	2:B:336:VAL:HG22	1.97	0.45
6:F:40:ASP:OD1	6:F:40:ASP:C	2.58	0.45
6:F:94:LEU:HG	6:F:98:ILE:HD11	1.98	0.45
7:G:4:PHE:HD2	7:G:4:PHE:HA	1.69	0.45
1:N:177:LEU:HD23	1:N:177:LEU:HA	1.80	0.45
1:N:223:TYR:CD1	1:N:223:TYR:C	2.94	0.45
2:O:253:VAL:HG11	2:O:433:THR:OG1	2.17	0.45
3:P:86:ASN:HD21	3:P:243:LEU:HD11	1.82	0.45
3:P:127:THR:O	3:P:130:VAL:CG2	2.64	0.45
3:P:223:PRO:O	3:P:227:PHE:HB2	2.17	0.45
3:P:253:ASP:OD1	3:P:254:PRO:HD2	2.17	0.45
4:Q:37:CYS:O	4:Q:39:ALA:N	2.48	0.45
10:W:15:ARG:HG2	10:W:15:ARG:HH11	1.82	0.45
1:A:46:ARG:C	1:A:48:GLU:H	2.24	0.45
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.83	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.31	0.45
2:B:242:GLY:O	2:B:423:SER:HB2	2.17	0.45
2:B:325:TYR:C	2:B:325:TYR:CD2	2.94	0.45
2:B:328:SER:O	2:B:329:GLN:C	2.59	0.45
3:C:158:GLY:O	3:C:160:THR:N	2.50	0.45
3:C:247:SER:N	3:C:248:PRO:CD	2.79	0.45
5:E:47:THR:O	5:E:48:ALA:C	2.59	0.45
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.64	0.45
10:J:16:ARG:C	10:J:18:SER:H	2.25	0.45
10:J:16:ARG:C	10:J:18:SER:N	2.75	0.45
10:J:52:TRP:O	10:J:56:LYS:HB2	2.16	0.45
2:O:181:TYR:CE1	2:O:182:ARG:CG	2.99	0.45
3:P:28:ILE:CG1	3:P:225:TYR:CE2	3.00	0.45
3:P:39:ALA:O	3:P:40:VAL:C	2.59	0.45
4:Q:57:THR:CB	4:Q:60:GLU:HG3	2.47	0.45
1:A:170:THR:CG2	1:A:171:THR:N	2.80	0.45
1:A:257:VAL:HG23	1:A:320:PHE:HB3	1.99	0.45
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.98	0.45
3:C:39:ALA:O	3:C:42:LEU:N	2.50	0.45
7:G:16:TYR:CD1	7:G:16:TYR:N	2.84	0.45
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.52	0.45
1:N:403:ASP:O	1:N:404:ALA:C	2.59	0.45
2:O:122:TYR:O	2:O:123:LEU:C	2.58	0.45
2:O:227:ARG:HB2	2:O:228:SER:H	1.48	0.45
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.25	0.45
1:A:86:PHE:HE2	1:A:116:VAL:HG21	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:PHE:HD2	9:I:71:ASN:HA	1.80	0.45
2:B:22:GLU:C	2:B:24:LEU:N	2.74	0.45
2:B:141:GLN:CD	2:B:184:GLY:HA2	2.42	0.45
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.98	0.45
2:B:286:LYS:HE2	2:B:287:ARG:NH2	2.32	0.45
3:C:117:GLY:O	3:C:120:LEU:HB2	2.17	0.45
3:C:247:SER:O	3:C:248:PRO:C	2.59	0.45
8:H:40:CYS:O	8:H:41:ASP:C	2.60	0.45
2:O:35:ILE:O	2:O:213:HIS:CE1	2.66	0.45
2:O:264:VAL:C	2:O:266:SER:H	2.25	0.45
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.99	0.45
3:P:221:PHE:HE1	15:P:3002:UQ:O1	2.00	0.45
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.47	0.45
4:Q:76:GLU:H	4:Q:76:GLU:CD	2.24	0.45
4:Q:83:ARG:HH12	4:Q:86:LYS:HG2	1.82	0.45
6:S:98:ILE:O	6:S:102:LEU:HB2	2.17	0.45
8:U:43:ARG:HG3	8:U:44:VAL:N	2.31	0.45
2:B:415:LYS:O	2:B:418:VAL:N	2.50	0.44
1:N:109:VAL:O	1:N:112:LEU:N	2.50	0.44
1:N:137:GLU:O	1:N:141:MET:HG3	2.17	0.44
1:N:356:ARG:HG3	2:O:91:ALA:HA	1.99	0.44
1:N:382:HIS:CG	1:N:389:ARG:HD2	2.51	0.44
3:P:67:VAL:CG2	13:P:501:HEM:HBD2	2.47	0.44
3:P:137:GLY:H	3:P:140:SER:CB	2.29	0.44
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.35	0.44
6:S:70:LEU:C	6:S:70:LEU:HD12	2.42	0.44
2:B:37:SER:O	2:B:38:LEU:CB	2.65	0.44
2:B:385:GLU:HB3	2:B:391:THR:O	2.17	0.44
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.82	0.44
1:N:206:LYS:H	1:N:206:LYS:HD2	1.82	0.44
2:O:408:ALA:O	2:O:410:VAL:N	2.50	0.44
3:P:212:ILE:O	3:P:213:SER:C	2.60	0.44
3:P:236:MET:O	3:P:237:LEU:C	2.59	0.44
9:V:28:UNK:HA	9:V:72:ALA:CB	2.47	0.44
1:A:330:SER:O	1:A:331:ILE:C	2.60	0.44
2:B:98:VAL:O	9:I:67:GLY:HA2	2.18	0.44
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.46	0.44
3:C:83:LEU:O	3:C:87:GLY:N	2.46	0.44
3:C:104:TYR:HA	3:C:316:MET:SD	2.57	0.44
3:C:150:LEU:HB3	3:C:292:VAL:HG22	2.00	0.44
4:D:47:ALA:N	4:D:50:ASN:ND2	2.62	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.48	0.44
2:O:97:SER:HB3	9:V:69:SER:CB	2.47	0.44
2:O:131:GLU:O	2:O:132:PHE:C	2.60	0.44
2:O:146:VAL:O	2:O:147:ASP:C	2.61	0.44
3:P:114:TRP:HE3	13:P:502:HEM:HMD1	1.83	0.44
4:Q:61:ALA:O	4:Q:62:LYS:C	2.59	0.44
1:A:255:LEU:O	1:A:321:GLY:HA3	2.18	0.44
2:B:23:ASP:O	2:B:24:LEU:HB3	2.16	0.44
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.46	0.44
2:B:338:ARG:O	2:B:339:ALA:C	2.61	0.44
3:C:202:HIS:NE2	15:C:2002:UQ:O4	2.49	0.44
4:D:8:PRO:HG2	4:D:10:PHE:HE1	1.81	0.44
8:H:34:ARG:HB2	8:H:61:PHE:CE1	2.52	0.44
1:N:7:THR:HG21	2:O:113:ARG:CD	2.47	0.44
1:N:438:ARG:O	1:N:441:MET:HG2	2.17	0.44
2:O:341:MET:HE1	2:O:417:PHE:CZ	2.49	0.44
3:P:157:ILE:O	3:P:161:LEU:HB3	2.17	0.44
8:U:37:LEU:O	8:U:38:GLU:C	2.60	0.44
1:A:242:ARG:CZ	1:A:432:LEU:HA	2.48	0.44
2:B:259:THR:HG22	2:B:260:GLU:H	1.82	0.44
3:C:212:ILE:O	3:C:213:SER:C	2.59	0.44
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.53	0.44
3:C:236:MET:O	3:C:237:LEU:C	2.60	0.44
4:D:2:GLU:OE1	4:D:2:GLU:HA	2.17	0.44
4:D:68:VAL:HG12	4:D:69:GLU:N	2.32	0.44
5:E:109:GLU:HA	5:E:112:VAL:HG13	1.98	0.44
9:I:67:GLY:O	9:I:68:ILE:HD13	2.18	0.44
1:N:35:CYS:HA	1:N:372:THR:HG21	2.00	0.44
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.82	0.44
1:N:249:PRO:HG2	1:N:250:VAL:N	2.32	0.44
1:N:334:MET:O	1:N:335:MET:C	2.60	0.44
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.86	0.44
2:O:303:THR:HB	2:O:336:VAL:HG22	1.98	0.44
2:O:374:THR:HG22	2:O:376:GLN:HB3	1.99	0.44
3:P:70:THR:CA	3:P:74:VAL:HG23	2.45	0.44
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.33	0.44
5:R:126:ARG:HH22	5:R:179:ASN:HB2	1.82	0.44
7:T:33:ALA:O	7:T:37:VAL:HG23	2.18	0.44
8:U:55:THR:O	8:U:56:GLU:C	2.61	0.44
1:A:295:ALA:O	1:A:298:ALA:N	2.51	0.44
1:A:394:GLU:O	1:A:395:TRP:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:VAL:HG13	1:N:39:VAL:O	2.16	0.44
1:N:56:GLY:HA2	1:N:185:TYR:CE2	2.52	0.44
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.99	0.44
2:O:43:PRO:HA	2:O:113:ARG:HD2	2.00	0.44
2:O:393:THR:O	2:O:394:ALA:O	2.35	0.44
3:P:41:CYS:SG	3:P:91:PHE:HA	2.57	0.44
3:P:156:TYR:N	3:P:156:TYR:CD2	2.85	0.44
4:Q:151:PRO:HB2	8:U:59:PHE:HE1	1.83	0.44
4:Q:165:TYR:O	4:Q:166:ASN:C	2.61	0.44
5:R:127:VAL:HG23	5:R:127:VAL:O	2.18	0.44
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.65	0.44
1:A:349:THR:HA	1:A:353:GLU:OE1	2.17	0.44
2:B:137:VAL:O	2:B:140:LEU:HB3	2.17	0.44
2:B:290:SER:HB3	2:B:293:SER:HB3	1.99	0.44
3:C:135:PRO:HG2	3:C:140:SER:OG	2.18	0.44
3:C:261:ASN:ND2	3:C:264:VAL:N	2.65	0.44
3:C:334:LEU:O	3:C:337:THR:HB	2.18	0.44
4:D:34:LYS:O	4:D:34:LYS:HG2	2.18	0.44
5:E:184:THR:HG22	5:E:185:TYR:N	2.33	0.44
6:F:19:TRP:O	6:F:20:TYR:C	2.61	0.44
6:F:42:ASP:O	6:F:43:VAL:C	2.60	0.44
1:N:36:THR:HG21	1:N:373:THR:HA	2.00	0.44
2:O:193:HIS:O	2:O:197:ASN:ND2	2.51	0.44
3:P:61:SER:C	3:P:62:LEU:HG	2.42	0.44
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.81	0.44
1:A:25:VAL:HG22	1:A:197:LEU:HB3	2.00	0.44
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.44
2:B:29:LEU:CB	2:B:30:PRO:CD	2.96	0.44
9:I:55:MET:O	9:I:56:SER:C	2.60	0.44
1:N:79:VAL:O	1:N:82:MET:HG2	2.18	0.44
1:N:109:VAL:O	1:N:110:VAL:C	2.60	0.44
1:N:182:LEU:O	1:N:186:ILE:HG13	2.16	0.44
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.00	0.44
1:N:370:ASP:OD2	2:O:374:THR:HG23	2.18	0.44
2:O:287:ARG:HB3	9:V:53:GLU:HG2	2.00	0.44
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.53	0.44
3:P:192:GLY:O	3:P:195:ILE:HB	2.18	0.44
6:S:89:TYR:CD1	6:S:89:TYR:C	2.95	0.44
6:S:103:GLU:O	6:S:104:ARG:C	2.61	0.44
7:T:2:ILE:O	7:T:3:HIS:CG	2.71	0.44
1:A:121:ALA:O	1:A:122:LEU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:HB2	2:B:228:SER:HB3	2.00	0.44
2:B:56:ARG:HH22	2:B:318:ASP:CG	2.26	0.44
5:E:33:LYS:HE3	10:J:10:TYR:OH	2.17	0.44
5:E:106:ILE:O	5:E:106:ILE:HG22	2.17	0.44
1:N:133:VAL:O	1:N:134:ILE:C	2.61	0.44
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.99	0.44
2:O:37:SER:OG	2:O:38:LEU:N	2.49	0.44
2:O:326:THR:C	2:O:327:ILE:HG13	2.43	0.44
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.51	0.44
3:P:319:ARG:HA	3:P:320:PRO:HD2	1.84	0.44
3:P:345:GLU:O	3:P:348:PHE:HB2	2.18	0.44
1:A:253:VAL:O	1:A:323:HIS:HA	2.17	0.43
1:A:297:LEU:C	1:A:299:VAL:N	2.74	0.43
2:B:169:LYS:HG3	2:B:240:TRP:HB2	2.00	0.43
2:B:189:GLU:O	2:B:190:GLN:C	2.60	0.43
2:B:312:PHE:N	2:B:323:GLY:O	2.42	0.43
3:C:347:PRO:O	3:C:348:PHE:C	2.61	0.43
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.83	0.43
6:F:20:TYR:O	6:F:23:ALA:HB3	2.18	0.43
1:N:140:GLU:HG2	9:V:48:PRO:HB2	1.99	0.43
1:N:199:ALA:CA	1:N:376:CYS:SG	3.05	0.43
4:Q:70:VAL:HG23	4:Q:83:ARG:HG2	1.98	0.43
5:R:141:HIS:HA	5:R:177:PRO:HD2	1.99	0.43
8:U:73:LEU:HD11	8:U:77:LEU:HD11	2.00	0.43
1:A:335:MET:O	1:A:336:PHE:C	2.61	0.43
2:B:299:VAL:O	2:B:303:THR:HG22	2.18	0.43
3:C:40:VAL:O	3:C:44:THR:OG1	2.35	0.43
3:C:119:ILE:O	3:C:120:LEU:C	2.59	0.43
4:D:165:TYR:O	4:D:166:ASN:O	2.36	0.43
1:N:40:TRP:CG	1:N:380:GLY:HA3	2.53	0.43
1:N:117:VAL:CG2	1:N:118:GLN:N	2.81	0.43
1:N:241:ILE:HG23	1:N:241:ILE:O	2.18	0.43
2:O:337:ILE:HD12	2:O:434:PRO:CD	2.41	0.43
3:P:93:ILE:O	3:P:94:CYS:C	2.60	0.43
4:Q:122:GLY:O	4:Q:123:GLY:C	2.62	0.43
7:T:16:TYR:N	7:T:16:TYR:CD1	2.86	0.43
1:A:90:THR:CB	1:A:95:THR:HG23	2.49	0.43
2:B:100:SER:HA	2:B:104:LYS:O	2.17	0.43
2:B:264:VAL:HG23	2:B:316:TYR:C	2.43	0.43
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.90	0.43
1:N:204:SER:O	1:N:205:HIS:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:253:VAL:HG11	1:N:335:MET:HE1	1.98	0.43
2:O:62:ASN:O	2:O:65:THR:CG2	2.64	0.43
2:O:157:VAL:O	2:O:157:VAL:HG22	2.17	0.43
2:O:328:SER:O	2:O:329:GLN:C	2.59	0.43
8:U:58:LEU:HD12	8:U:58:LEU:O	2.17	0.43
1:A:87:ASN:OD1	1:A:88:GLY:N	2.44	0.43
1:A:106:MET:CG	1:A:203:ILE:HD13	2.46	0.43
1:A:109:VAL:O	1:A:110:VAL:C	2.62	0.43
1:A:117:VAL:CG2	1:A:118:GLN:H	2.32	0.43
1:A:184:SER:HA	1:A:187:ASP:HB2	2.00	0.43
1:A:239:SER:O	1:A:421:ALA:HA	2.17	0.43
1:A:395:TRP:O	1:A:398:ARG:HB2	2.19	0.43
2:B:206:LEU:HG	2:B:206:LEU:O	2.18	0.43
1:N:266:ASP:O	1:N:267:ASN:C	2.60	0.43
2:O:47:ILE:HD13	2:O:120:MET:CE	2.48	0.43
2:O:338:ARG:O	2:O:339:ALA:C	2.61	0.43
2:O:402:ILE:C	2:O:402:ILE:CD1	2.90	0.43
3:P:137:GLY:O	3:P:140:SER:HB2	2.18	0.43
3:P:184:PHE:CD2	13:P:501:HEM:HBC1	2.53	0.43
3:P:333:LEU:O	3:P:334:LEU:C	2.61	0.43
5:R:10:PHE:O	5:R:11:SER:C	2.62	0.43
5:R:141:HIS:HB2	5:R:176:ALA:HB2	2.00	0.43
7:T:4:PHE:HD2	7:T:4:PHE:HA	1.71	0.43
2:B:56:ARG:HD3	2:B:103:GLU:HB3	2.01	0.43
2:B:122:TYR:O	2:B:123:LEU:C	2.62	0.43
2:B:346:ALA:O	2:B:351:GLY:HA3	2.18	0.43
3:C:9:HIS:C	3:C:11:LEU:H	2.26	0.43
3:C:316:MET:HA	3:C:319:ARG:HE	1.84	0.43
4:D:195:GLU:O	4:D:196:PRO:C	2.61	0.43
2:O:34:ILE:HD13	2:O:386:ALA:O	2.19	0.43
2:O:167:ALA:HB3	2:O:168:TYR:HD1	1.83	0.43
3:P:34:PHE:HB2	22:P:381:HOH:O	2.18	0.43
1:A:256:ALA:HA	1:A:320:PHE:O	2.18	0.43
2:B:140:LEU:C	2:B:142:PRO:HD2	2.43	0.43
2:B:254:HIS:ND1	2:B:325:TYR:OH	2.47	0.43
3:C:78:TRP:CG	3:C:79:LEU:N	2.86	0.43
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.53	0.43
5:E:70:ALA:C	5:E:72:SER:H	2.27	0.43
6:F:98:ILE:O	6:F:102:LEU:HB2	2.17	0.43
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.54	0.43
2:O:430:LEU:H	2:O:430:LEU:HG	1.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:101:ARG:CZ	13:P:502:HEM:HBD2	2.49	0.43
9:V:56:SER:C	9:V:58:ARG:H	2.24	0.43
9:V:67:GLY:O	9:V:68:ILE:HD13	2.18	0.43
1:A:247:ALA:HB2	7:G:11:ARG:HD2	2.00	0.43
1:A:318:GLY:O	1:A:319:LEU:HD23	2.19	0.43
1:A:343:MET:O	1:A:344:ARG:C	2.62	0.43
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.81	0.43
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.52	0.43
2:B:244:ILE:O	2:B:425:ALA:HA	2.19	0.43
2:B:403:ASP:C	2:B:405:VAL:N	2.76	0.43
3:C:86:ASN:HD21	3:C:243:LEU:HD11	1.83	0.43
3:C:192:GLY:O	3:C:195:ILE:HB	2.19	0.43
3:C:263:LEU:O	5:R:143:GLY:HA3	2.19	0.43
4:D:179:MET:O	4:D:180:SER:C	2.61	0.43
5:E:147:ILE:HG13	5:E:157:TYR:O	2.18	0.43
1:N:127:ILE:C	1:N:129:LYS:H	2.26	0.43
1:N:159:GLN:O	1:N:159:GLN:HG3	2.18	0.43
1:N:185:TYR:HA	1:N:189:HIS:HD2	1.83	0.43
1:N:206:LYS:HD2	1:N:206:LYS:N	2.32	0.43
2:O:142:PRO:O	2:O:145:LYS:HB2	2.18	0.43
2:O:372:VAL:O	2:O:372:VAL:HG12	2.19	0.43
4:Q:26:VAL:CG1	4:Q:55:THR:HG21	2.45	0.43
4:Q:47:ALA:HB1	4:Q:89:ASP:O	2.18	0.43
4:Q:175:THR:HA	4:Q:176:PRO:HD3	1.84	0.43
6:S:27:ASN:O	6:S:30:GLY:N	2.41	0.43
1:A:76:GLU:O	1:A:80:GLU:HG3	2.19	0.43
1:A:147:ASN:O	1:A:149:THR:N	2.51	0.43
1:A:241:ILE:HG23	1:A:241:ILE:O	2.18	0.43
1:A:242:ARG:NH1	1:A:432:LEU:HA	2.33	0.43
3:C:75:GLN:O	3:C:77:GLY:N	2.52	0.43
3:C:173:ASN:O	3:C:174:PRO:C	2.60	0.43
3:C:272:GLU:O	3:C:273:TRP:C	2.62	0.43
4:D:211:ILE:O	4:D:212:SER:C	2.62	0.43
10:J:63:GLU:O	10:J:64:GLU:HB3	2.19	0.43
1:N:23:LEU:HA	1:N:192:ALA:O	2.18	0.43
1:N:64:PHE:C	1:N:66:GLY:H	2.27	0.43
1:N:76:GLU:HG2	2:O:285:ILE:HD13	2.00	0.43
1:N:112:LEU:H	1:N:112:LEU:HG	1.53	0.43
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.82	0.43
2:O:37:SER:O	2:O:38:LEU:CB	2.67	0.43
2:O:258:VAL:HG12	2:O:323:GLY:CA	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:374:THR:CG2	2:O:376:GLN:HB3	2.48	0.43
3:P:33:ASN:HB3	22:P:385:HOH:O	2.18	0.43
4:Q:41:HIS:HB3	4:Q:113:LEU:HD12	2.00	0.43
8:U:27:THR:O	8:U:28:GLU:C	2.61	0.43
1:A:114:ALA:O	1:A:117:VAL:HG22	2.19	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.77	0.43
3:C:112:GLU:O	3:C:113:THR:C	2.62	0.43
4:D:147:LEU:C	4:D:148:HIS:HD2	2.27	0.43
4:D:171:TYR:C	4:D:173:ASP:N	2.77	0.43
4:D:208:MET:SD	4:D:208:MET:C	3.02	0.43
1:N:163:LEU:HD23	1:N:163:LEU:HA	1.86	0.43
2:O:248:ASN:C	2:O:248:ASN:ND2	2.75	0.43
2:O:275:LEU:O	2:O:279:LEU:HD12	2.19	0.43
3:P:147:ILE:O	3:P:148:THR:C	2.62	0.43
3:P:249:ASN:O	3:P:250:LEU:C	2.62	0.43
3:P:289:LEU:O	3:P:293:LEU:HG	2.17	0.43
6:S:34:ASP:N	6:S:34:ASP:OD1	2.51	0.43
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.99	0.43
1:A:242:ARG:HH12	1:A:432:LEU:H	1.65	0.43
2:B:50:PHE:C	2:B:51:ILE:HG13	2.44	0.43
2:B:166:ALA:O	2:B:242:GLY:N	2.51	0.43
2:B:167:ALA:C	2:B:168:TYR:HD1	2.27	0.43
2:B:191:LEU:O	2:B:192:HIS:C	2.61	0.43
3:C:305:ILE:HA	3:C:305:ILE:HD13	1.83	0.43
5:E:20:ASP:O	5:E:22:THR:N	2.45	0.43
5:E:98:VAL:HG22	5:E:134:ILE:HG23	2.01	0.43
1:N:116:VAL:O	1:N:120:CYS:HB2	2.19	0.43
2:O:70:ARG:NH2	2:O:177:TYR:CE2	2.87	0.43
2:O:141:GLN:CD	2:O:184:GLY:HA2	2.44	0.43
3:P:79:LEU:HD11	3:P:83:LEU:HD11	2.01	0.43
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.37	0.43
4:Q:161:ALA:O	4:Q:162:PRO:C	2.61	0.43
5:R:33:LYS:O	5:R:34:GLY:C	2.62	0.43
5:R:138:VAL:O	5:R:180:LEU:HD22	2.19	0.43
1:A:240:GLU:HB3	1:A:422:LEU:HB3	2.01	0.42
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.81	0.42
2:B:167:ALA:HB3	2:B:168:TYR:HD1	1.84	0.42
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.34	0.42
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.18	0.42
6:F:27:ASN:C	6:F:29:TYR:N	2.77	0.42
6:F:109:LYS:O	6:F:110:LYS:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:THR:HB	1:N:119:ASN:O	2.19	0.42
2:O:51:ILE:N	2:O:105:MET:O	2.51	0.42
2:O:146:VAL:HG12	2:O:147:ASP:N	2.33	0.42
2:O:150:VAL:HG22	2:O:151:ALA:N	2.34	0.42
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.48	0.42
2:O:298:GLY:HA3	2:O:343:GLN:HG3	2.00	0.42
2:O:342:ASN:C	2:O:344:LEU:H	2.25	0.42
2:O:346:ALA:O	2:O:351:GLY:HA3	2.18	0.42
3:P:255:GLU:HG2	3:P:255:GLU:H	1.60	0.42
6:S:13:MET:HB2	6:S:16:ILE:HD12	2.01	0.42
7:T:60:SER:O	7:T:64:GLN:HB2	2.19	0.42
10:W:58:LYS:C	10:W:59:TYR:CD1	2.97	0.42
1:A:210:ASP:O	1:A:211:ALA:C	2.62	0.42
2:B:230:ALA:O	2:B:231:GLY:C	2.62	0.42
3:C:198:LEU:HD13	15:C:2002:UQ:HM53	2.00	0.42
4:D:197:GLU:HG2	4:D:198:HIS:H	1.84	0.42
10:J:23:THR:O	10:J:24:VAL:C	2.62	0.42
2:O:56:ARG:HG2	2:O:234:SER:OG	2.18	0.42
2:O:111:CYS:HB3	2:O:119:VAL:HG21	2.01	0.42
3:P:22:LEU:HA	3:P:23:PRO:HD3	1.88	0.42
3:P:186:LEU:HD23	3:P:186:LEU:HA	1.76	0.42
3:P:346:HIS:CG	3:P:347:PRO:HA	2.54	0.42
4:Q:43:MET:HE2	4:Q:91:PHE:HE2	1.84	0.42
4:Q:221:TYR:CE2	5:R:39:VAL:HG21	2.54	0.42
5:R:77:LYS:C	5:R:79:SER:H	2.27	0.42
5:R:145:VAL:HA	5:R:146:PRO:HD3	1.85	0.42
2:B:176:LEU:HD12	2:B:176:LEU:O	2.19	0.42
3:C:82:ASN:H	3:C:82:ASN:ND2	2.14	0.42
3:C:128:ALA:O	3:C:129:PHE:C	2.62	0.42
4:D:97:ASN:O	4:D:98:PRO:C	2.62	0.42
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.54	0.42
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.43	0.42
1:N:219:VAL:CG1	1:N:220:SER:N	2.82	0.42
1:N:308:GLN:O	1:N:322:PHE:HA	2.19	0.42
1:N:433:ASP:OD2	1:N:433:ASP:C	2.62	0.42
3:P:4:ASN:HD22	3:P:6:ARG:H	1.68	0.42
3:P:68:ALA:HA	18:P:3011:GOL:O3	2.20	0.42
3:P:107:SER:C	3:P:109:LEU:H	2.27	0.42
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.54	0.42
6:S:73:ARG:HE	7:T:36:ASN:CG	2.27	0.42
1:A:156:THR:CG2	1:A:157:ALA:N	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:O	1:A:396:ASP:C	2.63	0.42
2:B:181:TYR:CE1	2:B:182:ARG:CG	3.00	0.42
2:B:215:ASP:O	2:B:217:LYS:N	2.52	0.42
4:D:169:LEU:HD23	4:D:169:LEU:C	2.45	0.42
5:E:1:VAL:HG23	5:E:3:ASN:N	2.27	0.42
5:E:38:LEU:O	5:E:39:VAL:C	2.61	0.42
6:F:58:ARG:HG3	6:F:89:TYR:OH	2.20	0.42
1:N:109:VAL:HA	1:N:112:LEU:CD1	2.47	0.42
1:N:242:ARG:O	7:T:14:ILE:HA	2.19	0.42
1:N:340:GLY:O	1:N:341:GLU:C	2.60	0.42
3:P:59:ASP:C	3:P:61:SER:N	2.74	0.42
3:P:119:ILE:O	3:P:120:LEU:C	2.60	0.42
3:P:207:ASN:ND2	3:P:314:ARG:NH1	2.67	0.42
3:P:230:ILE:O	3:P:233:LEU:HB3	2.19	0.42
3:P:247:SER:O	3:P:248:PRO:C	2.61	0.42
4:Q:148:HIS:ND1	4:Q:161:ALA:HA	2.35	0.42
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.19	0.42
16:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.34	0.42
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.50	0.42
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.48	0.42
2:B:337:ILE:O	2:B:340:ALA:HB3	2.20	0.42
3:C:81:ARG:NH2	13:C:501:HEM:O1A	2.53	0.42
3:C:214:SER:HB2	3:C:218:LYS:HZ3	1.81	0.42
3:C:304:LEU:O	3:C:305:ILE:C	2.63	0.42
4:D:182:ILE:O	4:D:183:ALA:C	2.61	0.42
1:N:46:ARG:C	1:N:48:GLU:H	2.27	0.42
1:N:206:LYS:O	1:N:207:GLU:C	2.61	0.42
1:N:260:PRO:HB3	1:N:414:TYR:CE2	2.54	0.42
1:N:340:GLY:O	1:N:343:MET:HB2	2.19	0.42
1:N:395:TRP:O	1:N:396:ASP:C	2.62	0.42
2:O:68:LEU:HA	2:O:144:LEU:HD21	2.00	0.42
2:O:209:ILE:O	2:O:211:VAL:N	2.53	0.42
2:O:272:PHE:HB3	2:O:322:PHE:CE1	2.55	0.42
3:P:175:THR:HA	3:P:178:ARG:HG2	2.01	0.42
1:A:170:THR:HG22	1:A:172:GLU:H	1.85	0.42
1:A:295:ALA:O	1:A:298:ALA:HB3	2.20	0.42
3:C:231:LEU:O	3:C:235:LEU:HG	2.19	0.42
16:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.20	0.42
5:E:71:LEU:N	5:E:71:LEU:CD2	2.83	0.42
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.55	0.42
1:N:269:VAL:O	1:N:270:LEU:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:273:ALA:O	1:N:274:ASN:C	2.62	0.42
2:O:327:ILE:HD11	9:V:58:ARG:O	2.19	0.42
3:P:35:GLY:C	13:P:502:HEM:HMA3	2.45	0.42
3:P:173:ASN:N	3:P:174:PRO:CD	2.80	0.42
3:P:183:HIS:CE1	13:P:501:HEM:NB	2.87	0.42
5:R:69:LEU:HD23	5:R:69:LEU:HA	1.92	0.42
5:R:156:TYR:HB2	5:R:165:TYR:HB2	2.00	0.42
8:U:34:ARG:HB2	8:U:61:PHE:CE1	2.54	0.42
1:A:109:VAL:O	1:A:112:LEU:N	2.52	0.42
1:A:404:ALA:O	1:A:405:ARG:C	2.62	0.42
3:C:59:ASP:O	3:C:62:LEU:N	2.47	0.42
3:C:93:ILE:O	3:C:94:CYS:C	2.62	0.42
3:C:100:GLY:O	3:C:101:ARG:C	2.63	0.42
3:C:273:TRP:CD2	3:C:274:TYR:N	2.88	0.42
5:E:175:PRO:HG2	5:E:176:ALA:H	1.84	0.42
7:G:73:ASN:HB3	7:G:76:ASP:OD2	2.20	0.42
1:N:41:ILE:HG12	1:N:195:MET:HG2	2.01	0.42
1:N:242:ARG:HH12	1:N:432:LEU:N	2.18	0.42
2:O:80:ALA:HA	2:O:84:ARG:NH2	2.35	0.42
2:O:201:SER:N	2:O:227:ARG:HB3	2.22	0.42
2:O:267:ALA:O	2:O:269:ALA:N	2.52	0.42
3:P:350:ILE:HG23	3:P:351:ILE:N	2.34	0.42
1:A:59:VAL:HG23	1:A:182:LEU:HD23	2.02	0.42
1:A:334:MET:O	1:A:335:MET:C	2.63	0.42
2:B:306:PRO:HA	9:I:52:ARG:CG	2.50	0.42
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.54	0.42
4:D:102:ARG:HG2	4:D:107:GLY:O	2.18	0.42
5:E:137:GLY:O	5:E:145:VAL:HG13	2.20	0.42
1:N:7:THR:HG21	2:O:113:ARG:NE	2.35	0.42
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.44	0.42
1:N:244:ARG:NE	7:T:10:VAL:HB	2.34	0.42
2:O:212:LYS:HG2	2:O:214:SER:OG	2.20	0.42
2:O:272:PHE:HB3	2:O:322:PHE:CD1	2.55	0.42
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.19	0.42
3:P:52:LEU:HD21	3:P:80:ILE:HG22	2.01	0.42
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.54	0.42
5:R:104:ALA:C	5:R:106:ILE:H	2.28	0.42
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.50	0.42
9:V:75:SER:O	9:V:76:VAL:HB	2.20	0.42
1:A:433:ASP:OD2	1:A:433:ASP:C	2.61	0.42
2:B:43:PRO:C	2:B:113:ARG:HG3	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.31	0.42
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.42
3:C:28:ILE:CG1	3:C:225:TYR:CE2	3.03	0.42
3:C:236:MET:O	3:C:238:THR:N	2.53	0.42
5:E:33:LYS:HE3	10:J:10:TYR:CZ	2.55	0.42
5:E:156:TYR:HB2	5:E:165:TYR:HB2	2.01	0.42
1:N:86:PHE:HE2	1:N:116:VAL:HG21	1.85	0.42
1:N:433:ASP:OD2	1:N:435:ASN:N	2.53	0.42
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.19	0.42
2:O:71:LEU:N	2:O:71:LEU:CD2	2.75	0.42
2:O:232:THR:HG22	2:O:233:SER:N	2.35	0.42
3:P:9:HIS:C	3:P:11:LEU:H	2.28	0.42
3:P:362:ILE:HG22	3:P:363:LEU:N	2.35	0.42
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	2.01	0.42
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.55	0.42
2:B:43:PRO:HA	2:B:113:ARG:HD2	2.02	0.42
2:B:100:SER:HB2	2:B:105:MET:HG2	1.99	0.42
2:B:402:ILE:CG2	2:B:403:ASP:H	2.29	0.42
4:D:16:GLY:N	4:D:19:SER:OG	2.52	0.42
5:E:162:GLY:O	5:E:163:SER:C	2.63	0.42
9:I:63:ASP:CG	9:I:64:LEU:N	2.73	0.42
10:J:32:GLU:O	10:J:33:ARG:C	2.62	0.42
1:N:158:PHE:O	1:N:159:GLN:C	2.63	0.42
1:N:280:TYR:HA	1:N:284:PHE:CE1	2.55	0.42
2:O:43:PRO:C	2:O:113:ARG:HG3	2.45	0.42
3:P:134:LEU:HD21	3:P:180:PHE:HA	2.01	0.42
5:R:77:LYS:HE3	5:R:191:ASP:OD2	2.20	0.42
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.68	0.42
7:T:49:ALA:O	7:T:50:PRO:C	2.62	0.42
1:A:102:LEU:C	1:A:104:LYS:N	2.75	0.41
1:A:134:ILE:O	1:A:136:GLN:N	2.53	0.41
2:B:19:PRO:O	2:B:22:GLU:CB	2.68	0.41
2:B:42:SER:C	2:B:44:ALA:N	2.78	0.41
2:B:306:PRO:O	2:B:307:PHE:HB3	2.20	0.41
3:C:326:PHE:O	3:C:330:VAL:HG23	2.20	0.41
4:D:81:PHE:N	4:D:81:PHE:CD2	2.87	0.41
5:E:48:ALA:O	5:E:49:TYR:C	2.62	0.41
5:E:118:ARG:O	5:E:119:ASP:HB2	2.18	0.41
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.20	0.41
9:I:71:ASN:ND2	9:I:71:ASN:C	2.78	0.41
1:N:220:SER:HA	1:N:225:GLU:OE1	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:18:CYS:HA	2:O:19:PRO:HD3	1.84	0.41
2:O:51:ILE:HG22	2:O:52:LYS:N	2.35	0.41
2:O:287:ARG:HA	9:V:53:GLU:CG	2.46	0.41
2:O:295:LEU:O	2:O:296:TYR:C	2.63	0.41
3:P:9:HIS:HD2	3:P:12:LEU:HG	1.80	0.41
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.49	0.41
1:A:172:GLU:O	1:A:175:LYS:HB2	2.20	0.41
2:B:229:GLY:C	2:B:231:GLY:H	2.28	0.41
2:B:402:ILE:CG2	2:B:403:ASP:N	2.83	0.41
3:C:130:VAL:HG23	3:C:183:HIS:HD1	1.85	0.41
3:C:216:SER:O	6:F:63:LYS:HD2	2.19	0.41
4:D:161:ALA:O	4:D:163:PRO:HD3	2.19	0.41
5:E:100:HIS:NE2	5:E:131:GLU:HG3	2.35	0.41
6:F:20:TYR:HA	6:F:23:ALA:HB3	2.02	0.41
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.20	0.41
3:P:202:HIS:NE2	15:P:3002:UQ:O4	2.52	0.41
4:Q:2:GLU:CD	4:Q:2:GLU:N	2.78	0.41
4:Q:81:PHE:N	4:Q:81:PHE:CD2	2.88	0.41
4:Q:198:HIS:O	4:Q:201:ARG:HB3	2.20	0.41
6:S:45:GLU:O	6:S:46:ALA:C	2.62	0.41
1:A:86:PHE:CD2	1:A:99:ILE:HD11	2.55	0.41
2:B:31:ASN:N	2:B:31:ASN:ND2	2.64	0.41
2:B:372:VAL:CG1	2:B:378:LEU:HD13	2.50	0.41
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.02	0.41
2:B:393:THR:O	2:B:394:ALA:O	2.37	0.41
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.89	0.41
3:C:333:LEU:HB3	11:C:2007:PEE:H75	2.02	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.73	0.41
4:D:178:THR:O	4:D:181:GLN:HB3	2.20	0.41
2:O:163:LEU:HD12	2:O:425:ALA:CB	2.50	0.41
2:O:192:HIS:O	2:O:193:HIS:C	2.63	0.41
2:O:290:SER:HB2	2:O:293:SER:HB3	2.02	0.41
3:P:304:LEU:O	3:P:305:ILE:C	2.63	0.41
3:P:316:MET:HA	3:P:319:ARG:HE	1.85	0.41
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.35	0.41
4:Q:66:GLU:C	4:Q:68:VAL:H	2.28	0.41
4:Q:161:ALA:O	4:Q:163:PRO:N	2.54	0.41
5:R:103:GLN:HA	5:R:106:ILE:HD12	2.01	0.41
1:A:99:ILE:HG13	1:A:113:LEU:HD21	2.02	0.41
1:A:240:GLU:CB	1:A:422:LEU:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ILE:HG23	2:B:216:LEU:HG	2.02	0.41
2:B:51:ILE:CG2	2:B:52:LYS:N	2.83	0.41
2:B:146:VAL:O	2:B:147:ASP:C	2.63	0.41
2:B:247:GLN:NE2	2:B:249:GLY:H	2.19	0.41
3:C:127:THR:O	3:C:130:VAL:CG2	2.68	0.41
3:C:311:SER:CB	3:C:319:ARG:NH1	2.82	0.41
4:D:10:PHE:CD2	8:H:74:PHE:HE2	2.38	0.41
4:D:25:SER:O	4:D:26:VAL:C	2.63	0.41
4:D:160:MET:HB2	19:D:501:HEC:C4D	2.50	0.41
4:D:183:ALA:O	4:D:186:VAL:HG12	2.20	0.41
4:D:230:LEU:HD23	4:D:230:LEU:HA	1.87	0.41
5:E:190:ASP:C	5:E:192:LEU:H	2.28	0.41
1:N:39:VAL:HG11	1:N:117:VAL:HG11	2.03	0.41
1:N:210:ASP:O	1:N:213:ARG:N	2.54	0.41
1:N:239:SER:O	1:N:421:ALA:HA	2.21	0.41
1:N:253:VAL:HG11	1:N:335:MET:HE2	2.01	0.41
1:N:417:ASP:OD2	1:N:438:ARG:NH2	2.46	0.41
2:O:299:VAL:O	2:O:303:THR:HG22	2.19	0.41
2:O:410:VAL:O	2:O:411:VAL:C	2.62	0.41
3:P:95:ILE:CG2	3:P:96:PHE:N	2.82	0.41
3:P:97:LEU:O	3:P:98:HIS:C	2.63	0.41
3:P:104:TYR:CD2	11:P:3007:PEE:H14	2.55	0.41
3:P:311:SER:CB	3:P:319:ARG:NH1	2.84	0.41
4:Q:232:SER:CB	7:T:23:GLN:HE22	2.20	0.41
5:R:37:TYR:HB3	10:W:14:PHE:HB3	2.02	0.41
1:A:23:LEU:HB2	1:A:192:ALA:HB1	2.02	0.41
1:A:86:PHE:HD1	1:A:87:ASN:N	2.19	0.41
1:A:158:PHE:O	1:A:159:GLN:C	2.63	0.41
2:B:312:PHE:O	2:B:322:PHE:HA	2.21	0.41
3:C:246:PHE:CZ	4:D:205:GLY:HA3	2.55	0.41
4:D:33:TYR:HA	4:D:37:CYS:SG	2.60	0.41
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.55	0.41
6:F:73:ARG:HE	7:G:36:ASN:CG	2.29	0.41
2:O:157:VAL:HG23	9:V:64:LEU:HD21	2.03	0.41
2:O:191:LEU:O	2:O:192:HIS:C	2.63	0.41
2:O:362:ASN:C	2:O:364:LEU:N	2.77	0.41
4:Q:94:PRO:HB2	4:Q:95:TYR:CD1	2.54	0.41
4:Q:161:ALA:O	4:Q:163:PRO:HD3	2.20	0.41
6:S:58:ARG:HA	6:S:61:ARG:NH2	2.35	0.41
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.34	0.41
1:A:59:VAL:C	1:A:61:HIS:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:H	1:A:428:ILE:HG12	1.57	0.41
2:B:272:PHE:HB3	2:B:322:PHE:CD1	2.55	0.41
2:B:377:GLY:O	2:B:380:ASN:HB3	2.21	0.41
3:C:50:LEU:O	3:C:53:ALA:N	2.54	0.41
4:D:26:VAL:CG1	4:D:55:THR:HG21	2.47	0.41
10:J:22:LEU:HD23	10:J:22:LEU:C	2.46	0.41
10:J:57:HIS:ND1	10:J:58:LYS:HG3	2.36	0.41
1:N:86:PHE:CE2	1:N:116:VAL:HG21	2.55	0.41
1:N:339:GLN:HE22	1:N:437:ILE:HG23	1.86	0.41
2:O:239:TYR:CD2	2:O:240:TRP:N	2.89	0.41
2:O:324:PHE:HD2	2:O:344:LEU:HD12	1.85	0.41
3:P:36:SER:O	3:P:39:ALA:HB3	2.21	0.41
3:P:241:LEU:C	4:Q:208:MET:HE2	2.46	0.41
3:P:366:LEU:N	3:P:366:LEU:CD2	2.83	0.41
4:Q:120:ARG:HG2	4:Q:120:ARG:NH1	2.35	0.41
4:Q:210:LEU:HD23	4:Q:210:LEU:HA	1.88	0.41
8:U:15:ASP:HA	8:U:16:PRO:HD2	1.87	0.41
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.55	0.41
3:C:137:GLY:O	3:C:140:SER:HB2	2.21	0.41
3:C:320:PRO:HG2	3:C:321:LEU:N	2.33	0.41
4:D:22:ASP:HA	10:J:50:LYS:HB3	2.02	0.41
4:D:156:GLN:CD	4:D:156:GLN:N	2.79	0.41
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.84	0.41
1:N:4:TYR:C	1:N:6:GLN:N	2.79	0.41
1:N:48:GLU:CD	1:N:54:GLY:H	2.29	0.41
1:N:85:HIS:CD2	2:O:284:LEU:HB3	2.55	0.41
1:N:184:SER:HA	1:N:187:ASP:HB2	2.02	0.41
1:N:242:ARG:CZ	1:N:432:LEU:HA	2.51	0.41
1:N:354:VAL:CG2	1:N:355:LYS:N	2.82	0.41
1:N:365:MET:SD	1:N:392:LEU:HD13	2.60	0.41
2:O:222:GLN:O	2:O:223:PHE:CB	2.69	0.41
3:P:112:GLU:O	3:P:113:THR:C	2.64	0.41
4:Q:55:THR:C	10:W:52:TRP:CZ3	2.99	0.41
4:Q:224:ARG:O	4:Q:225:HIS:C	2.63	0.41
1:A:90:THR:HB	1:A:95:THR:HG23	2.03	0.41
1:A:127:ILE:O	1:A:130:GLU:N	2.54	0.41
2:B:70:ARG:NH2	2:B:177:TYR:HE2	2.18	0.41
2:B:295:LEU:O	2:B:296:TYR:C	2.63	0.41
3:C:54:MET:SD	5:E:62:LEU:HD21	2.61	0.41
3:C:125:MET:HE1	14:C:2001:IKR:I1	2.85	0.41
4:D:224:ARG:O	4:D:225:HIS:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:VAL:HG23	5:E:112:VAL:O	2.20	0.41
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.56	0.41
1:N:86:PHE:CE1	1:N:97:PHE:HB3	2.55	0.41
1:N:269:VAL:O	1:N:272:VAL:N	2.54	0.41
1:N:398:ARG:NH1	1:N:398:ARG:HG2	2.35	0.41
2:O:111:CYS:CB	2:O:119:VAL:HG21	2.50	0.41
2:O:408:ALA:C	2:O:410:VAL:N	2.76	0.41
3:P:116:THR:O	3:P:117:GLY:C	2.63	0.41
3:P:220:PRO:O	3:P:221:PHE:C	2.63	0.41
3:P:317:THR:HG23	11:P:3007:PEE:H9	2.03	0.41
4:Q:164:ILE:HG21	4:Q:182:ILE:CG2	2.48	0.41
1:A:86:PHE:CE1	1:A:97:PHE:HB3	2.56	0.41
1:A:90:THR:O	1:A:90:THR:CG2	2.69	0.41
1:A:150:PHE:O	1:A:153:LEU:HB3	2.21	0.41
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.41
1:A:339:GLN:NE2	1:A:437:ILE:HG23	2.36	0.41
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.02	0.41
1:A:416:TYR:CE1	1:A:442:TYR:HA	2.56	0.41
2:B:33:LEU:HD21	2:B:224:LEU:HD12	2.02	0.41
2:B:80:ALA:HA	2:B:84:ARG:NH2	2.36	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.90	0.41
2:B:192:HIS:O	2:B:193:HIS:C	2.63	0.41
3:C:42:LEU:O	3:C:43:MET:C	2.64	0.41
3:C:156:TYR:C	3:C:158:GLY:H	2.28	0.41
3:C:184:PHE:CZ	3:P:184:PHE:HB3	2.56	0.41
3:C:249:ASN:O	3:C:250:LEU:C	2.63	0.41
3:C:253:ASP:OD1	3:C:254:PRO:CD	2.68	0.41
13:C:502:HEM:HHA	13:C:502:HEM:HBD1	2.02	0.41
4:D:66:GLU:C	4:D:68:VAL:N	2.78	0.41
4:D:72:ASP:HB2	4:D:83:ARG:HE	1.84	0.41
5:E:128:LYS:O	5:E:129:LYS:C	2.63	0.41
5:E:130:PRO:C	5:E:132:TRP:H	2.28	0.41
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.54	0.41
8:H:31:VAL:C	8:H:33:ALA:N	2.77	0.41
1:N:84:ALA:HA	1:N:100:LYS:O	2.21	0.41
1:N:107:PRO:C	1:N:109:VAL:N	2.77	0.41
1:N:171:THR:O	1:N:175:LYS:HG3	2.20	0.41
1:N:435:ASN:O	1:N:438:ARG:HB3	2.20	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.81	0.41
2:O:26:ILE:HA	2:O:35:ILE:O	2.21	0.41
2:O:47:ILE:HG22	2:O:48:GLY:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:70:ARG:NH2	2:O:177:TYR:HE2	2.19	0.41
2:O:206:LEU:HG	2:O:216:LEU:HD11	2.03	0.41
2:O:367:THR:O	2:O:368:TYR:C	2.64	0.41
3:P:45:GLN:O	3:P:49:GLY:N	2.44	0.41
3:P:52:LEU:HD13	13:P:501:HEM:O2D	2.20	0.41
3:P:347:PRO:O	3:P:348:PHE:C	2.64	0.41
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.34	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.76	0.41
6:S:13:MET:CA	6:S:16:ILE:HD12	2.47	0.41
6:S:13:MET:CB	6:S:16:ILE:HD12	2.51	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.75	0.41
1:A:277:ILE:CD1	1:A:345:LEU:HD11	2.51	0.41
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.83	0.41
2:B:102:ARG:NH1	2:B:172:LEU:O	2.54	0.41
2:B:200:THR:O	2:B:201:SER:C	2.64	0.41
2:B:408:ALA:O	2:B:410:VAL:N	2.54	0.41
2:B:408:ALA:C	2:B:410:VAL:N	2.77	0.41
3:C:70:THR:CA	3:C:74:VAL:HG23	2.49	0.41
1:N:46:ARG:HD3	1:N:231:LEU:HD13	2.02	0.41
1:N:149:THR:HG22	1:N:150:PHE:N	2.35	0.41
1:N:434:TYR:CE2	7:T:19:SER:HB2	2.56	0.41
2:O:206:LEU:HG	2:O:206:LEU:O	2.20	0.41
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.21	0.41
4:Q:179:MET:O	4:Q:182:ILE:HB	2.21	0.41
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.21	0.41
4:Q:209:LEU:HD23	4:Q:209:LEU:HA	1.77	0.41
5:R:96:LEU:HD12	5:R:135:LEU:O	2.20	0.41
1:A:379:ILE:O	1:A:380:GLY:C	2.65	0.40
3:C:316:MET:HE1	3:C:367:PHE:CE2	2.57	0.40
4:D:130:LEU:HD12	4:D:130:LEU:HA	1.92	0.40
4:D:203:ARG:HD3	10:J:40:ASP:OD1	2.21	0.40
6:F:57:GLU:HB3	6:F:61:ARG:HH12	1.85	0.40
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.49	0.40
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.93	0.40
2:O:163:LEU:O	2:O:164:HIS:C	2.64	0.40
2:O:192:HIS:O	2:O:196:GLN:HG3	2.21	0.40
2:O:402:ILE:CG2	2:O:403:ASP:H	2.30	0.40
2:O:410:VAL:O	2:O:413:ALA:N	2.54	0.40
3:P:50:LEU:O	3:P:51:LEU:C	2.64	0.40
3:P:254:PRO:O	3:P:257:PHE:N	2.52	0.40
3:P:350:ILE:CG2	3:P:351:ILE:N	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:21:TYR:CD2	6:S:21:TYR:C	2.98	0.40
1:A:59:VAL:O	1:A:60:GLU:C	2.64	0.40
1:A:135:LEU:HG	1:A:174:ILE:HG21	2.01	0.40
2:B:341:MET:HE1	2:B:417:PHE:CZ	2.52	0.40
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	2.03	0.40
3:C:67:VAL:HG22	13:C:501:HEM:HBD2	2.02	0.40
3:C:364:LEU:O	3:C:368:PRO:HG3	2.21	0.40
4:D:10:PHE:H	4:D:10:PHE:HD1	1.67	0.40
4:D:30:PHE:HE2	4:D:64:LEU:HD11	1.86	0.40
4:D:81:PHE:HD2	4:D:81:PHE:N	2.19	0.40
4:D:164:ILE:O	4:D:179:MET:CE	2.69	0.40
10:J:14:PHE:N	10:J:14:PHE:HD2	2.17	0.40
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.56	0.40
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.77	0.40
2:O:107:TYR:CD2	2:O:127:THR:HG22	2.56	0.40
2:O:163:LEU:CD1	2:O:425:ALA:HB3	2.51	0.40
2:O:167:ALA:C	2:O:168:TYR:HD1	2.29	0.40
2:O:341:MET:HA	2:O:341:MET:CE	2.48	0.40
3:P:36:SER:O	3:P:37:LEU:C	2.64	0.40
3:P:201:LEU:O	3:P:203:GLU:N	2.54	0.40
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.39	0.40
5:R:80:ASP:OD1	5:R:80:ASP:O	2.38	0.40
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.53	0.40
8:U:59:PHE:O	8:U:60:ASP:C	2.65	0.40
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.36	0.40
2:B:280:GLY:HA3	2:B:293:SER:CB	2.52	0.40
3:C:10:PRO:HG2	3:P:200:PHE:CE1	2.56	0.40
3:C:16:ASN:O	3:C:18:SER:N	2.47	0.40
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.52	0.40
3:C:28:ILE:HG12	3:C:225:TYR:CZ	2.56	0.40
3:C:303:PHE:O	3:C:306:PRO:HD2	2.21	0.40
4:D:233:ARG:HG3	7:G:17:SER:OG	2.21	0.40
6:F:65:ALA:O	6:F:68:LEU:HB2	2.21	0.40
7:G:33:ALA:O	7:G:37:VAL:HG23	2.21	0.40
1:N:37:VAL:HA	1:N:198:ALA:O	2.22	0.40
1:N:276:ILE:HG13	1:N:357:ALA:HB2	2.02	0.40
2:O:169:LYS:HE3	2:O:240:TRP:HA	2.02	0.40
2:O:200:THR:O	2:O:201:SER:C	2.64	0.40
2:O:325:TYR:C	2:O:325:TYR:CD2	3.00	0.40
4:Q:238:ARG:HB3	4:Q:238:ARG:NH1	2.37	0.40
5:R:38:LEU:CA	10:W:14:PHE:CE1	3.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:15:ASP:C	8:U:17:LEU:N	2.79	0.40
8:U:25:GLU:HG2	8:U:61:PHE:CZ	2.55	0.40
1:A:86:PHE:CE2	1:A:116:VAL:HG21	2.57	0.40
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.56	0.40
1:A:127:ILE:O	1:A:129:LYS:N	2.54	0.40
3:C:4:ASN:HD22	3:C:6:ARG:H	1.69	0.40
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.61	0.40
6:F:19:TRP:O	6:F:22:ASN:N	2.52	0.40
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.86	0.40
1:N:331:ILE:O	1:N:334:MET:HB3	2.21	0.40
3:P:4:ASN:C	3:P:5:ILE:HD13	2.45	0.40
3:P:42:LEU:CD2	3:P:190:ILE:HG22	2.52	0.40
4:Q:49:ARG:O	4:Q:52:ILE:HG13	2.22	0.40
5:R:70:ALA:C	5:R:72:SER:N	2.80	0.40
5:R:126:ARG:HH22	5:R:179:ASN:CB	2.35	0.40
7:T:34:LEU:HB2	7:T:35:PRO:HD3	2.03	0.40
1:A:185:TYR:HA	1:A:189:HIS:HD2	1.86	0.40
1:A:248:LEU:HA	1:A:248:LEU:HD22	1.89	0.40
1:A:269:VAL:O	1:A:270:LEU:C	2.64	0.40
2:B:324:PHE:HD2	2:B:344:LEU:HD12	1.84	0.40
2:B:341:MET:HA	2:B:341:MET:CE	2.46	0.40
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.45	0.40
3:C:70:THR:O	3:C:74:VAL:HG23	2.22	0.40
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.68	0.40
1:N:295:ALA:O	1:N:298:ALA:N	2.54	0.40
2:O:286:LYS:NZ	2:O:287:ARG:HH22	2.19	0.40
2:O:430:LEU:C	2:O:432:SER:N	2.80	0.40
3:P:362:ILE:HA	3:P:366:LEU:HB2	2.04	0.40
4:Q:28:ARG:HH21	4:Q:181:GLN:NE2	2.19	0.40
4:Q:162:PRO:HA	4:Q:163:PRO:HD2	1.91	0.40
4:Q:168:ILE:HG23	4:Q:169:LEU:HD22	2.04	0.40
4:Q:221:TYR:CE1	7:T:25:ALA:CB	3.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	335 (76%)	84 (19%)	22 (5%)	1	15
1	N	440/446 (99%)	330 (75%)	87 (20%)	23 (5%)	1	14
2	B	424/441 (96%)	315 (74%)	78 (18%)	31 (7%)	1	9
2	O	420/441 (95%)	313 (74%)	78 (19%)	29 (7%)	1	10
3	C	378/380 (100%)	298 (79%)	61 (16%)	19 (5%)	1	15
3	P	377/380 (99%)	294 (78%)	67 (18%)	16 (4%)	2	18
4	D	239/241 (99%)	177 (74%)	51 (21%)	11 (5%)	2	17
4	Q	239/241 (99%)	181 (76%)	47 (20%)	11 (5%)	2	17
5	E	194/196 (99%)	119 (61%)	60 (31%)	15 (8%)	1	8
5	R	194/196 (99%)	122 (63%)	50 (26%)	22 (11%)	0	5
6	F	99/110 (90%)	74 (75%)	21 (21%)	4 (4%)	2	19
6	S	99/110 (90%)	77 (78%)	19 (19%)	3 (3%)	3	25
7	G	78/81 (96%)	59 (76%)	16 (20%)	3 (4%)	2	20
7	T	77/81 (95%)	57 (74%)	15 (20%)	5 (6%)	1	11
8	H	67/77 (87%)	44 (66%)	22 (33%)	1 (2%)	8	37
8	U	65/77 (84%)	43 (66%)	20 (31%)	2 (3%)	3	25
9	I	29/47 (62%)	15 (52%)	10 (34%)	4 (14%)	0	3
9	V	29/47 (62%)	15 (52%)	9 (31%)	5 (17%)	0	2
10	J	59/61 (97%)	38 (64%)	16 (27%)	5 (8%)	0	7
10	W	58/61 (95%)	39 (67%)	14 (24%)	5 (9%)	0	7
All	All	4006/4160 (96%)	2945 (74%)	825 (21%)	236 (6%)	1	12

All (236) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	222	THR
1	A	432	LEU
2	B	15	VAL
2	B	17	LEU
2	B	18	CYS
2	B	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	38	LEU
2	B	201	SER
2	B	210	GLY
2	B	221	GLU
2	B	386	ALA
3	C	18	SER
3	C	60	THR
3	C	111	LYS
3	C	248	PRO
3	C	287	ASN
4	D	166	ASN
4	D	198	HIS
5	E	102	THR
5	E	115	SER
5	E	130	PRO
5	E	177	PRO
7	G	7	LEU
7	G	33	ALA
9	I	56	SER
9	I	61	ARG
1	N	20	ASP
1	N	159	GLN
1	N	222	THR
1	N	432	LEU
2	O	19	PRO
2	O	38	LEU
2	O	201	SER
2	O	223	PHE
2	O	226	ILE
2	O	227	ARG
3	P	18	SER
3	P	60	THR
3	P	111	LYS
3	P	287	ASN
4	Q	166	ASN
4	Q	198	HIS
5	R	8	PRO
5	R	107	ASN
5	R	130	PRO
5	R	140	THR
5	R	141	HIS
5	R	178	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	191	ASP
7	T	3	HIS
7	T	7	LEU
7	T	33	ALA
10	W	61	ALA
1	A	206	LYS
2	B	171	ALA
2	B	226	ILE
3	C	157	ILE
4	D	53	GLY
4	D	77	ASN
5	E	8	PRO
5	E	21	ALA
8	H	28	GLU
1	N	4	TYR
1	N	5	ALA
1	N	81	SER
1	N	108	LYS
1	N	433	ASP
2	O	171	ALA
2	O	210	GLY
2	O	268	GLU
2	O	386	ALA
3	P	76	TYR
3	P	202	HIS
4	Q	53	GLY
4	Q	172	ASP
5	R	21	ALA
5	R	108	GLN
5	R	115	SER
5	R	122	HIS
5	R	131	GLU
5	R	144	CYS
5	R	177	PRO
8	U	52	GLU
9	V	63	ASP
9	V	72	ALA
9	V	76	VAL
10	W	25	VAL
1	A	72	CYS
1	A	81	SER
1	A	107	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	LYS
1	A	135	LEU
1	A	290	LEU
2	B	20	GLY
2	B	26	ILE
2	B	63	LEU
2	B	152	PHE
2	B	207	VAL
2	B	389	SER
3	C	3	PRO
3	C	156	TYR
3	C	202	HIS
3	C	255	GLU
4	D	38	SER
4	D	133	GLY
6	F	52	GLU
6	F	77	LYS
6	F	83	TYR
9	I	64	LEU
10	J	25	VAL
10	J	33	ARG
10	J	55	ILE
1	N	72	CYS
1	N	107	PRO
1	N	121	ALA
1	N	135	LEU
1	N	206	LYS
1	N	218	GLY
1	N	288	LYS
2	O	140	LEU
2	O	389	SER
2	O	431	GLY
3	P	248	PRO
4	Q	38	SER
4	Q	133	GLY
8	U	28	GLU
10	W	15	ARG
10	W	33	ARG
10	W	55	ILE
1	A	121	ALA
1	A	180	ALA
1	A	217	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	218	GLY
1	A	433	ASP
2	B	24	LEU
2	B	140	LEU
2	B	222	GLN
2	B	306	PRO
2	B	393	THR
3	C	288	LYS
3	C	348	PHE
4	D	172	ASP
5	E	92	ARG
5	E	128	LYS
5	E	176	ALA
10	J	15	ARG
2	O	63	LEU
2	O	152	PHE
2	O	221	GLU
2	O	393	THR
2	O	409	ASP
2	O	416	LYS
3	P	3	PRO
3	P	156	TYR
3	P	255	GLU
3	P	288	LYS
3	P	348	PHE
5	R	49	TYR
5	R	149	ASN
5	R	175	PRO
6	S	52	GLU
7	T	50	PRO
9	V	73	PRO
1	A	53	ASN
1	A	106	MET
1	A	192	ALA
2	B	21	ALA
2	B	30	PRO
2	B	307	PHE
2	B	319	SER
2	B	394	ALA
2	B	416	LYS
3	C	4	ASN
3	C	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	76	TYR
3	C	159	HIS
4	D	96	PRO
4	D	123	GLY
5	E	80	ASP
5	E	141	HIS
5	E	149	ASN
6	F	19	TRP
7	G	50	PRO
10	J	32	GLU
1	N	192	ALA
2	O	26	ILE
2	O	207	VAL
2	O	216	LEU
2	O	228	SER
2	O	306	PRO
2	O	307	PHE
2	O	319	SER
2	O	394	ALA
3	P	17	ASN
3	P	296	ALA
3	P	366	LEU
4	Q	106	ASN
5	R	92	ARG
5	R	121	GLN
6	S	77	LYS
6	S	83	TYR
9	V	48	PRO
1	A	263	ALA
4	D	106	ASN
5	E	129	LYS
1	N	53	ASN
1	N	106	MET
1	N	148	VAL
2	O	384	SER
3	P	10	PRO
3	C	10	PRO
5	E	175	PRO
1	N	209	VAL
4	Q	96	PRO
4	Q	162	PRO
5	R	176	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	209	VAL
2	B	209	ILE
2	B	420	GLY
9	I	72	ALA
2	O	209	ILE
5	R	18	VAL
7	T	48	VAL
1	A	148	VAL
2	B	64	GLY
3	C	209	PRO
4	D	229	VAL
1	N	428	ILE
5	E	18	VAL
4	Q	123	GLY
4	Q	168	ILE
5	R	154	GLY
1	A	428	ILE
3	C	305	ILE
1	N	110	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	345 (94%)	20 (6%)	19	46
1	N	365/368 (99%)	345 (94%)	20 (6%)	19	46
2	B	333/347 (96%)	309 (93%)	24 (7%)	13	38
2	O	333/347 (96%)	308 (92%)	25 (8%)	12	38
3	C	329/329 (100%)	314 (95%)	15 (5%)	24	50
3	P	328/329 (100%)	314 (96%)	14 (4%)	26	52
4	D	200/200 (100%)	191 (96%)	9 (4%)	24	51
4	Q	200/200 (100%)	192 (96%)	8 (4%)	28	54
5	E	166/166 (100%)	161 (97%)	5 (3%)	36	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	166/166 (100%)	161 (97%)	5 (3%)	36	60
6	F	93/96 (97%)	86 (92%)	7 (8%)	12	38
6	S	93/96 (97%)	86 (92%)	7 (8%)	12	38
7	G	71/71 (100%)	66 (93%)	5 (7%)	14	40
7	T	70/71 (99%)	66 (94%)	4 (6%)	18	45
8	H	65/71 (92%)	63 (97%)	2 (3%)	35	60
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	70
9	I	23/26 (88%)	22 (96%)	1 (4%)	26	52
9	V	23/26 (88%)	19 (83%)	4 (17%)	2	11
10	J	49/49 (100%)	47 (96%)	2 (4%)	27	53
10	W	47/49 (96%)	45 (96%)	2 (4%)	26	52
All	All	3382/3446 (98%)	3202 (95%)	180 (5%)	20	47

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	10	ASN
1	A	17	THR
1	A	49	ASN
1	A	59	VAL
1	A	106	MET
1	A	108	LYS
1	A	146	THR
1	A	171	THR
1	A	174	ILE
1	A	181	ASP
1	A	188	THR
1	A	241	ILE
1	A	248	LEU
1	A	269	VAL
1	A	279	ARG
1	A	283	THR
1	A	342	TRP
1	A	392	LEU
1	A	395	TRP
2	B	30	PRO
2	B	31	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	57	TYR
2	B	59	THR
2	B	71	LEU
2	B	96	LEU
2	B	97	SER
2	B	114	ASP
2	B	124	LEU
2	B	146	VAL
2	B	150	VAL
2	B	154	SER
2	B	168	TYR
2	B	181	TYR
2	B	189	GLU
2	B	226	ILE
2	B	248	ASN
2	B	284	LEU
2	B	335	GLU
2	B	341	MET
2	B	343	GLN
2	B	344	LEU
2	B	378	LEU
2	B	402	ILE
3	C	44	THR
3	C	74	VAL
3	C	82	ASN
3	C	145	THR
3	C	149	ASN
3	C	182	LEU
3	C	208	ASN
3	C	242	THR
3	C	243	LEU
3	C	245	LEU
3	C	248	PRO
3	C	255	GLU
3	C	258	THR
3	C	299	VAL
3	C	356	SER
4	D	13	SER
4	D	46	VAL
4	D	64	LEU
4	D	81	PHE
4	D	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	178	THR
4	D	179	MET
4	D	214	LEU
4	D	219	LEU
5	E	6	THR
5	E	60	SER
5	E	61	SER
5	E	71	LEU
5	E	135	LEU
6	F	27	ASN
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
6	F	84	GLU
6	F	89	TYR
6	F	102	LEU
7	G	4	PHE
7	G	16	TYR
7	G	60	SER
7	G	63	THR
7	G	65	GLU
8	H	12	GLU
8	H	19	THR
9	I	71	ASN
10	J	14	PHE
10	J	59	TYR
1	N	3	THR
1	N	10	ASN
1	N	49	ASN
1	N	106	MET
1	N	108	LYS
1	N	171	THR
1	N	174	ILE
1	N	181	ASP
1	N	188	THR
1	N	228	VAL
1	N	241	ILE
1	N	248	LEU
1	N	269	VAL
1	N	279	ARG
1	N	283	THR
1	N	307	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	342	TRP
1	N	392	LEU
1	N	395	TRP
1	N	405	ARG
2	O	22	GLU
2	O	31	ASN
2	O	57	TYR
2	O	71	LEU
2	O	96	LEU
2	O	97	SER
2	O	102	ARG
2	O	114	ASP
2	O	124	LEU
2	O	139	ASP
2	O	146	VAL
2	O	150	VAL
2	O	154	SER
2	O	160	LEU
2	O	168	TYR
2	O	181	TYR
2	O	227	ARG
2	O	248	ASN
2	O	284	LEU
2	O	335	GLU
2	O	341	MET
2	O	343	GLN
2	O	344	LEU
2	O	378	LEU
2	O	402	ILE
3	P	44	THR
3	P	74	VAL
3	P	82	ASN
3	P	145	THR
3	P	149	ASN
3	P	182	LEU
3	P	208	ASN
3	P	242	THR
3	P	243	LEU
3	P	245	LEU
3	P	255	GLU
3	P	258	THR
3	P	299	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	334	LEU
4	Q	13	SER
4	Q	37	CYS
4	Q	64	LEU
4	Q	81	PHE
4	Q	127	VAL
4	Q	178	THR
4	Q	214	LEU
4	Q	219	LEU
5	R	60	SER
5	R	61	SER
5	R	71	LEU
5	R	135	LEU
5	R	185	TYR
6	S	27	ASN
6	S	58	ARG
6	S	64	ARG
6	S	70	LEU
6	S	84	GLU
6	S	89	TYR
6	S	102	LEU
7	T	4	PHE
7	T	16	TYR
7	T	60	SER
7	T	63	THR
8	U	19	THR
9	V	55	MET
9	V	62	ARG
9	V	63	ASP
9	V	70	LEU
10	W	14	PHE
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	126	GLN
1	A	173	ASN
1	A	176	HIS
1	A	271	HIS
1	A	274	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	301	HIS
1	A	305	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	40	ASN
2	B	156	GLN
2	B	192	HIS
2	B	197	ASN
2	B	247	GLN
2	B	248	ASN
2	B	250	HIS
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	376	GLN
3	C	9	HIS
3	C	55	HIS
3	C	69	HIS
3	C	82	ASN
3	C	86	ASN
3	C	207	ASN
3	C	261	ASN
3	C	309	HIS
3	C	332	ASN
3	C	342	GLN
4	D	23	HIS
4	D	35	GLN
4	D	50	ASN
4	D	97	ASN
4	D	200	GLN
5	E	57	GLN
5	E	108	GLN
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	28	ASN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	21	ASN
1	N	32	GLN
1	N	94	GLN
1	N	118	GLN
1	N	126	GLN
1	N	173	ASN
1	N	176	HIS
1	N	274	ASN
1	N	305	HIS
1	N	339	GLN
1	N	385	ASN
1	N	435	ASN
2	O	31	ASN
2	O	40	ASN
2	O	156	GLN
2	O	192	HIS
2	O	247	GLN
2	O	248	ASN
2	O	297	GLN
2	O	329	GLN
2	O	332	HIS
2	O	343	GLN
2	O	376	GLN
3	P	9	HIS
3	P	55	HIS
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	115	ASN
3	P	207	ASN
3	P	261	ASN
3	P	309	HIS
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	97	ASN
5	R	57	GLN
5	R	107	ASN
5	R	122	HIS
5	R	149	ASN
5	R	164	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	186	GLN
6	S	108	ASN
7	T	12	HIS
7	T	23	GLN
7	T	28	ASN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	23	HIS
8	U	26	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 5 are unknown and 2 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
20	BOG	Q	3009	-	20,20,20	1.03	2 (10%)	25,25,25	1.01	1 (4%)
16	CDL	D	2003	-	41,41,99	1.16	1 (2%)	47,53,111	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PEE	A	2008	-	16,16,50	1.77	5 (31%)	18,20,55	0.54	0
11	PEE	R	3005	-	49,49,50	1.60	11 (22%)	52,54,55	0.88	3 (5%)
13	HEM	P	502	3	50,50,50	1.58	7 (14%)	67,82,82	1.38	10 (14%)
13	HEM	C	501	3	50,50,50	1.79	9 (18%)	67,82,82	2.00	26 (38%)
11	PEE	P	3007	-	48,48,50	1.35	5 (10%)	51,53,55	0.77	2 (3%)
21	FES	E	501	5	0,4,4	-	-	-	-	-
14	IKR	P	3001	-	26,26,26	1.49	7 (26%)	33,35,35	1.70	6 (18%)
11	PEE	P	3008	-	4,4,50	3.62	4 (100%)	6,6,55	0.66	0
16	CDL	P	3004	-	39,39,99	1.27	5 (12%)	45,51,111	1.16	5 (11%)
16	CDL	C	2004	-	39,39,99	1.31	5 (12%)	45,51,111	1.17	5 (11%)
15	UQ	P	3002	-	19,19,63	2.65	10 (52%)	24,26,79	1.37	3 (12%)
18	GOL	P	3011	-	5,5,5	1.36	0	5,5,5	0.60	0
20	BOG	D	2091	-	13,13,20	1.46	3 (23%)	18,18,25	1.18	2 (11%)
20	BOG	P	3091	-	13,13,20	1.33	2 (15%)	18,18,25	1.12	2 (11%)
20	BOG	D	2009	-	20,20,20	1.09	2 (10%)	25,25,25	0.91	2 (8%)
15	UQ	C	2002	-	19,19,63	2.52	10 (52%)	24,26,79	1.35	3 (12%)
21	FES	R	501	5	0,4,4	-	-	-	-	-
13	HEM	C	502	3	50,50,50	1.88	11 (22%)	67,82,82	2.04	21 (31%)
19	HEC	Q	501	4	46,50,50	1.93	10 (21%)	58,82,82	2.44	12 (20%)
11	PEE	C	2007	-	48,48,50	1.37	5 (10%)	51,53,55	0.80	2 (3%)
19	HEC	D	501	4	46,50,50	1.97	15 (32%)	58,82,82	2.80	14 (24%)
13	HEM	P	501	3	50,50,50	1.71	7 (14%)	67,82,82	1.79	15 (22%)
14	IKR	C	2001	-	26,26,26	1.52	6 (23%)	33,35,35	1.69	7 (21%)
18	GOL	C	2011	-	5,5,5	1.34	0	5,5,5	0.53	0
16	CDL	Q	3003	-	41,41,99	1.17	1 (2%)	47,53,111	1.08	4 (8%)
11	PEE	E	2005	-	49,49,50	1.56	10 (20%)	52,54,55	0.90	3 (5%)
20	BOG	P	2010	-	12,12,20	1.45	2 (16%)	17,17,25	0.63	0

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
20	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
16	CDL	D	2003	-	-	18/51/51/110	-
11	PEE	A	2008	-	-	2/19/19/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEE	R	3005	-	-	26/53/53/54	-
13	HEM	P	502	3	-	9/14/54/54	-
13	HEM	C	501	3	-	6/14/54/54	-
11	PEE	P	3007	-	-	17/52/52/54	-
21	FES	E	501	5	-	-	0/1/1/1
14	IKR	P	3001	-	-	1/18/18/18	0/2/2/2
16	CDL	P	3004	-	-	19/49/49/110	-
16	CDL	C	2004	-	-	19/49/49/110	-
15	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
18	GOL	P	3011	-	-	2/4/4/4	-
20	BOG	D	2091	-	-	1/4/24/31	0/1/1/1
20	BOG	P	3091	-	-	4/4/24/31	0/1/1/1
20	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
15	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
21	FES	R	501	5	-	-	0/1/1/1
13	HEM	C	502	3	-	10/14/54/54	-
19	HEC	Q	501	4	-	6/14/54/54	-
11	PEE	C	2007	-	-	18/52/52/54	-
19	HEC	D	501	4	-	6/14/54/54	-
13	HEM	P	501	3	-	8/14/54/54	-
14	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
18	GOL	C	2011	-	-	4/4/4/4	-
16	CDL	Q	3003	-	-	18/51/51/110	-
11	PEE	E	2005	-	-	24/53/53/54	-
20	BOG	P	2010	-	-	1/2/22/31	0/1/1/1

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	501	HEC	CAC-C3C	6.48	1.56	1.35
13	C	501	HEM	CBC-CAC	6.36	1.60	1.30
19	D	501	HEC	CAB-C3B	5.88	1.54	1.35
19	D	501	HEC	CAC-C3C	5.88	1.54	1.35
15	P	3002	UQ	C7-C6	5.31	1.61	1.51
13	P	501	HEM	CBC-CAC	5.20	1.55	1.30
19	Q	501	HEC	CAB-C3B	5.19	1.51	1.35
15	P	3002	UQ	C6-C5	5.14	1.44	1.35
13	P	502	HEM	CBC-CAC	5.06	1.54	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	CBC-CAC	5.02	1.54	1.30
11	P	3008	PEE	P-O1P	4.83	1.61	1.50
13	P	501	HEM	CBB-CAB	4.79	1.53	1.30
13	C	501	HEM	CBB-CAB	4.78	1.53	1.30
15	C	2002	UQ	C6-C5	4.76	1.43	1.35
15	C	2002	UQ	C7-C6	4.40	1.59	1.51
13	C	502	HEM	CBB-CAB	4.37	1.51	1.30
11	E	2005	PEE	C39-C38	4.11	1.55	1.31
11	P	3007	PEE	C39-C38	4.11	1.55	1.31
11	R	3005	PEE	C39-C38	4.08	1.54	1.31
11	C	2007	PEE	C39-C38	4.07	1.54	1.31
13	P	502	HEM	CBB-CAB	4.07	1.49	1.30
15	C	2002	UQ	C6-C1	3.98	1.57	1.46
13	P	502	HEM	CAB-C3B	-3.85	1.37	1.47
15	P	3002	UQ	C6-C1	3.80	1.57	1.46
19	D	501	HEC	C1D-ND	-3.79	1.32	1.39
11	R	3005	PEE	O2-C10	3.78	1.45	1.34
15	C	2002	UQ	O3-C3	3.59	1.45	1.36
11	R	3005	PEE	O3-C30	3.53	1.43	1.33
13	P	501	HEM	CAB-C3B	-3.51	1.38	1.47
11	R	3005	PEE	P-O1P	3.48	1.62	1.50
13	C	501	HEM	CAB-C3B	-3.48	1.38	1.47
11	E	2005	PEE	O2-C10	3.48	1.44	1.34
11	P	3007	PEE	C21-C22	-3.47	1.34	1.51
14	C	2001	IKR	C40-C2	3.46	1.57	1.51
11	P	3008	PEE	P-O4P	3.46	1.64	1.54
19	Q	501	HEC	C1D-ND	-3.36	1.33	1.39
13	P	501	HEM	CAC-C3C	-3.35	1.38	1.47
13	C	502	HEM	CHB-C4A	-3.34	1.31	1.39
11	E	2005	PEE	C21-C22	-3.30	1.35	1.51
11	C	2007	PEE	C21-C22	-3.30	1.35	1.51
13	P	502	HEM	CAC-C3C	-3.28	1.38	1.47
11	R	3005	PEE	C21-C22	-3.27	1.35	1.51
11	P	3008	PEE	P-O3P	3.26	1.64	1.54
11	E	2005	PEE	O3-C30	3.25	1.42	1.33
11	A	2008	PEE	P-O1P	3.23	1.62	1.50
14	P	3001	IKR	C40-C2	3.20	1.57	1.51
13	C	502	HEM	C1B-C2B	3.17	1.51	1.44
11	E	2005	PEE	P-O1P	3.16	1.61	1.50
15	P	3002	UQ	O3-C3	3.12	1.44	1.36
13	C	502	HEM	CMB-C2B	3.11	1.57	1.50
11	C	2007	PEE	P-O1P	3.10	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	CAB-C3B	-3.06	1.39	1.47
15	P	3002	UQ	C7-C8	3.03	1.55	1.50
19	Q	501	HEC	C3B-C2B	-3.02	1.31	1.41
19	Q	501	HEC	C3B-C4B	-3.01	1.40	1.46
11	P	3007	PEE	O3-C30	2.98	1.42	1.33
11	A	2008	PEE	O2-C10	2.97	1.42	1.34
16	C	2004	CDL	O1-C1	2.96	1.52	1.43
11	C	2007	PEE	O2-C10	2.94	1.42	1.34
20	D	2091	BOG	C4-C5	2.91	1.59	1.53
11	C	2007	PEE	O3-C30	2.85	1.41	1.33
19	Q	501	HEC	CHA-C4D	-2.84	1.33	1.39
11	P	3007	PEE	P-O1P	2.84	1.60	1.50
11	P	3007	PEE	O2-C10	2.81	1.42	1.34
15	P	3002	UQ	C5-C4	2.80	1.56	1.47
15	C	2002	UQ	C5-C4	2.74	1.56	1.47
13	C	502	HEM	FE-ND	-2.74	1.86	1.94
15	P	3002	UQ	CM5-C5	2.74	1.56	1.50
19	Q	501	HEC	C4C-NC	-2.73	1.34	1.39
20	P	2010	BOG	C4-C5	2.72	1.58	1.53
13	P	502	HEM	CHB-C4A	-2.72	1.33	1.39
20	P	2010	BOG	C1-C2	2.72	1.58	1.52
14	P	3001	IKR	C3-C4	2.71	1.43	1.38
13	C	501	HEM	FE-NC	-2.70	1.86	1.95
15	P	3002	UQ	C2-C1	2.68	1.56	1.48
15	C	2002	UQ	CM5-C5	2.68	1.56	1.50
15	C	2002	UQ	C3-C4	2.64	1.56	1.48
14	C	2001	IKR	C3-C4	2.64	1.43	1.38
11	E	2005	PEE	C11-C10	2.64	1.58	1.50
13	C	502	HEM	CAC-C3C	-2.59	1.40	1.47
13	P	501	HEM	CHD-C4C	-2.58	1.33	1.38
13	P	501	HEM	C3B-C2B	-2.58	1.31	1.37
14	C	2001	IKR	C20-C17	2.54	1.44	1.40
14	C	2001	IKR	C24-C17	2.53	1.43	1.39
11	P	3008	PEE	P-O2P	2.52	1.62	1.54
11	E	2005	PEE	O2-C2	2.50	1.52	1.46
11	R	3005	PEE	O2-C2	2.50	1.52	1.46
14	P	3001	IKR	C24-C17	2.48	1.43	1.39
19	D	501	HEC	C3D-C2D	-2.48	1.32	1.38
15	C	2002	UQ	C2-C1	2.47	1.56	1.48
13	C	502	HEM	C4B-NB	-2.47	1.34	1.38
11	R	3005	PEE	C11-C10	2.46	1.57	1.50
16	P	3004	CDL	O1-C1	2.45	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	2009	BOG	O5-C1	2.45	1.48	1.41
11	A	2008	PEE	C3-C2	2.44	1.57	1.51
19	D	501	HEC	CHA-C4D	-2.43	1.34	1.39
20	P	3091	BOG	O5-C1	2.43	1.48	1.41
19	Q	501	HEC	C1B-NB	-2.41	1.35	1.39
16	P	3004	CDL	OA8-CA6	-2.39	1.39	1.45
11	E	2005	PEE	C3-C2	2.39	1.58	1.50
11	R	3005	PEE	C31-C30	2.39	1.57	1.50
19	D	501	HEC	C1C-C2C	2.39	1.48	1.43
19	D	501	HEC	C1B-NB	-2.39	1.35	1.39
20	D	2091	BOG	O5-C1	2.35	1.47	1.41
15	P	3002	UQ	O2-C2	2.35	1.42	1.36
15	P	3002	UQ	C3-C4	2.35	1.55	1.48
19	D	501	HEC	CMC-C2C	2.34	1.55	1.50
14	P	3001	IKR	C20-C17	2.34	1.43	1.40
14	C	2001	IKR	C22-C21	2.34	1.42	1.38
16	C	2004	CDL	CB3-CB4	2.33	1.58	1.50
15	C	2002	UQ	C7-C8	2.33	1.54	1.50
13	C	501	HEM	CAC-C3C	-2.31	1.41	1.47
11	R	3005	PEE	C1-C2	2.30	1.58	1.50
15	C	2002	UQ	O2-C2	2.30	1.42	1.36
20	P	3091	BOG	C4-C5	2.29	1.57	1.53
11	E	2005	PEE	C31-C30	2.29	1.57	1.50
14	C	2001	IKR	C2-C1	2.28	1.42	1.39
19	D	501	HEC	CHC-C4B	-2.28	1.33	1.38
20	Q	3009	BOG	O5-C1	2.27	1.47	1.41
11	A	2008	PEE	C1-C2	2.26	1.57	1.50
19	D	501	HEC	C3C-C2C	-2.25	1.33	1.41
16	C	2004	CDL	OA8-CA6	-2.24	1.40	1.45
13	C	502	HEM	CHC-C1C	-2.23	1.34	1.38
13	C	501	HEM	C1B-C2B	2.23	1.49	1.44
11	R	3005	PEE	C3-C2	2.22	1.57	1.50
19	D	501	HEC	C3B-C2B	-2.22	1.33	1.41
13	C	501	HEM	C4A-NA	-2.20	1.35	1.39
19	Q	501	HEC	CHA-C1A	-2.20	1.34	1.38
19	D	501	HEC	C4A-NA	-2.19	1.35	1.39
13	P	502	HEM	CMA-C3A	2.19	1.55	1.50
16	D	2003	CDL	O1-C1	2.19	1.49	1.43
11	E	2005	PEE	C1-C2	2.19	1.57	1.50
14	P	3001	IKR	C21-C20	2.18	1.43	1.39
13	C	502	HEM	C1C-NC	-2.18	1.35	1.39
16	P	3004	CDL	OB8-CB7	2.16	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	2004	CDL	OA5-CA3	-2.15	1.36	1.44
13	P	502	HEM	CHB-C1B	-2.13	1.34	1.38
19	D	501	HEC	C2A-C3A	-2.11	1.32	1.36
19	D	501	HEC	C4C-NC	-2.11	1.35	1.39
16	Q	3003	CDL	O1-C1	2.11	1.49	1.43
20	D	2009	BOG	C1-C2	2.10	1.58	1.52
13	C	501	HEM	CHC-C4B	-2.10	1.34	1.39
11	A	2008	PEE	C11-C10	2.09	1.56	1.50
20	D	2091	BOG	C1-C2	2.07	1.58	1.52
16	P	3004	CDL	CB3-CB4	2.06	1.57	1.50
20	Q	3009	BOG	C4-C5	2.05	1.57	1.53
14	P	3001	IKR	C2-C1	2.05	1.42	1.39
16	C	2004	CDL	OA6-CA5	2.04	1.40	1.34
11	R	3005	PEE	P-O4P	2.03	1.67	1.59
13	P	501	HEM	CHB-C4A	-2.03	1.34	1.39
19	D	501	HEC	CHD-C1D	-2.02	1.34	1.39
16	P	3004	CDL	OB6-CB5	2.02	1.40	1.34
19	Q	501	HEC	CHC-C4B	-2.02	1.34	1.38
14	P	3001	IKR	C22-C21	2.01	1.42	1.38
13	C	501	HEM	C3D-C2D	-2.00	1.32	1.36

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	501	HEC	CBC-CAC-C3C	-14.32	98.81	127.43
19	Q	501	HEC	CBC-CAC-C3C	-12.60	102.26	127.43
19	D	501	HEC	CBB-CAB-C3B	-6.98	113.48	127.43
13	C	502	HEM	C3B-C2B-C1B	-6.93	101.20	106.41
19	Q	501	HEC	CBB-CAB-C3B	-6.54	114.36	127.43
13	C	501	HEM	C3B-C4B-NB	5.72	113.57	109.47
13	C	502	HEM	CMB-C2B-C1B	5.68	133.91	125.03
14	P	3001	IKR	C40-C2-C1	5.43	127.29	123.40
14	C	2001	IKR	C40-C2-C1	5.13	127.08	123.40
19	D	501	HEC	CMC-C2C-C1C	5.13	133.23	125.42
13	P	501	HEM	CMB-C2B-C1B	4.78	132.50	125.03
19	Q	501	HEC	CBA-CAA-C2A	4.66	125.41	112.53
13	C	501	HEM	CBA-CAA-C2A	-4.64	99.70	112.53
19	D	501	HEC	CBA-CAA-C2A	4.58	125.19	112.53
13	P	501	HEM	C3B-C4B-NB	4.50	112.70	109.47
15	P	3002	UQ	C8-C7-C6	4.44	123.02	112.08
15	C	2002	UQ	C8-C7-C6	4.42	122.96	112.08
19	D	501	HEC	CAA-C2A-C3A	-4.29	119.83	127.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	501	HEC	CMC-C2C-C1C	4.29	131.95	125.42
13	C	502	HEM	C2B-C1B-NB	4.17	114.64	109.84
20	Q	3009	BOG	C1'-O1-C1	4.11	120.70	113.68
13	C	502	HEM	C3B-C4B-NB	4.07	112.39	109.47
13	C	502	HEM	CAD-C3D-C4D	4.07	131.78	124.70
19	D	501	HEC	CAA-C2A-C1A	3.94	132.86	124.85
13	C	501	HEM	CMB-C2B-C1B	3.85	131.05	125.03
13	C	501	HEM	CMA-C3A-C4A	-3.83	119.59	125.42
13	P	502	HEM	C3B-C4B-NB	3.78	112.19	109.47
19	Q	501	HEC	CAA-C2A-C1A	3.64	132.26	124.85
20	P	3091	BOG	C1'-O1-C1	3.58	118.70	113.26
20	D	2091	BOG	C1'-O1-C1	3.56	118.67	113.26
14	P	3001	IKR	C40-C2-C3	-3.56	113.31	119.57
19	Q	501	HEC	CAA-C2A-C3A	-3.46	121.38	127.87
19	D	501	HEC	C3D-C4D-ND	3.44	113.97	110.15
13	P	501	HEM	C3B-C2B-C1B	-3.43	103.84	106.41
13	C	501	HEM	C1A-C2A-C3A	-3.42	101.58	106.87
13	P	502	HEM	CMB-C2B-C1B	3.41	130.37	125.03
13	P	501	HEM	CBA-CAA-C2A	-3.39	103.16	112.53
14	C	2001	IKR	C40-C2-C3	-3.37	113.64	119.57
19	D	501	HEC	C4D-C3D-C2D	-3.36	101.67	106.87
13	C	501	HEM	C3B-C2B-C1B	-3.35	103.90	106.41
15	C	2002	UQ	C7-C6-C1	-3.35	114.63	118.52
15	P	3002	UQ	C7-C6-C1	-3.35	114.63	118.52
13	C	502	HEM	CHD-C4C-NC	-3.34	120.81	124.45
13	P	501	HEM	CAC-C3C-C4C	3.32	132.74	124.82
20	D	2009	BOG	C1'-O1-C1	3.29	119.30	113.68
13	P	501	HEM	C2B-C1B-NB	3.28	113.61	109.84
13	P	501	HEM	CMD-C2D-C1D	3.23	130.07	125.03
14	P	3001	IKR	O31-C30-O36	3.03	129.30	123.50
19	D	501	HEC	CMA-C3A-C4A	3.00	130.01	124.73
14	C	2001	IKR	O31-C30-O36	3.00	129.23	123.50
19	D	501	HEC	C2A-C1A-NA	2.95	113.17	110.32
13	P	501	HEM	C1B-NB-C4B	-2.94	101.73	105.21
16	P	3004	CDL	CB4-OB6-CB5	-2.94	110.77	117.80
13	C	501	HEM	CHC-C1C-C2C	-2.92	119.41	125.49
13	C	501	HEM	C1B-NB-C4B	-2.90	101.77	105.21
13	C	501	HEM	C4A-C3A-C2A	2.90	110.13	106.82
14	C	2001	IKR	O31-C30-C29	-2.89	108.66	111.75
13	C	501	HEM	C2B-C1B-NB	2.89	113.16	109.84
13	C	502	HEM	C3A-C4A-NA	2.88	114.76	110.14
13	C	502	HEM	CAD-C3D-C2D	-2.82	122.59	127.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	3005	PEE	C22-C21-C20	2.80	127.34	113.86
20	D	2091	BOG	O1-C1-C2	2.77	111.33	108.14
13	C	501	HEM	CAA-C2A-C1A	2.76	130.33	124.94
11	E	2005	PEE	C22-C21-C20	2.76	127.12	113.86
16	C	2004	CDL	CB4-OB6-CB5	-2.75	111.20	117.80
13	C	502	HEM	C1B-NB-C4B	-2.72	101.98	105.21
13	C	502	HEM	C4A-NA-C1A	-2.70	101.43	105.82
14	P	3001	IKR	O31-C30-C29	-2.69	108.87	111.75
13	C	501	HEM	CAC-C3C-C4C	2.68	131.22	124.82
19	D	501	HEC	C1D-C2D-C3D	2.67	109.88	106.82
16	P	3004	CDL	CA6-CA4-CA3	-2.67	105.55	111.78
13	C	501	HEM	CMD-C2D-C1D	2.67	129.21	125.03
16	D	2003	CDL	CB4-OB6-CB5	-2.64	111.49	117.80
13	C	502	HEM	C2C-C1C-NC	2.61	114.47	109.64
19	D	501	HEC	CAD-C3D-C4D	2.61	130.03	124.94
11	P	3007	PEE	C22-C21-C20	2.59	126.31	113.86
19	D	501	HEC	CBD-CAD-C3D	2.59	119.69	112.53
11	C	2007	PEE	C22-C21-C20	2.58	126.28	113.86
16	C	2004	CDL	CA6-CA4-CA3	-2.58	105.76	111.78
13	C	502	HEM	C2D-C1D-ND	2.56	112.86	109.90
13	C	501	HEM	C2A-C1A-NA	2.55	112.98	110.15
13	C	501	HEM	C4D-ND-C1D	-2.50	102.25	105.21
13	P	501	HEM	C4D-ND-C1D	-2.50	102.25	105.21
13	P	502	HEM	C2B-C1B-NB	2.49	112.70	109.84
20	P	3091	BOG	O1-C1-C2	2.49	111.01	108.14
11	C	2007	PEE	C21-C22-C23	2.49	126.94	114.37
19	Q	501	HEC	C4D-C3D-C2D	-2.48	103.03	106.87
13	P	502	HEM	CAD-C3D-C2D	-2.47	123.24	127.87
11	P	3007	PEE	C21-C22-C23	2.46	126.78	114.37
13	P	502	HEM	C3B-C2B-C1B	-2.45	104.57	106.41
11	E	2005	PEE	C21-C22-C23	2.44	126.71	114.37
19	Q	501	HEC	C3D-C4D-ND	2.41	112.83	110.15
13	P	501	HEM	CHC-C4B-NB	-2.41	121.83	124.42
11	R	3005	PEE	C21-C22-C23	2.40	126.51	114.37
13	C	502	HEM	CMC-C2C-C1C	2.40	128.96	124.73
16	Q	3003	CDL	CB4-OB6-CB5	-2.39	112.07	117.80
14	C	2001	IKR	C17-C20-C29	2.39	123.57	121.36
13	C	502	HEM	C3C-C2C-C1C	-2.39	104.78	107.05
13	P	501	HEM	CHD-C4C-NC	-2.38	121.86	124.45
13	P	501	HEM	C4C-C3C-C2C	-2.38	104.75	106.81
19	Q	501	HEC	CAD-C3D-C4D	2.37	129.57	124.94
16	P	3004	CDL	OB6-CB4-CB3	2.35	116.77	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	502	HEM	C4A-C3A-C2A	-2.34	104.14	106.82
19	Q	501	HEC	CBD-CAD-C3D	2.31	118.91	112.53
14	P	3001	IKR	C17-C20-C29	2.29	123.48	121.36
16	C	2004	CDL	OB6-CB4-CB3	2.29	116.56	108.34
13	C	502	HEM	CAB-C3B-C2B	-2.28	121.01	128.43
13	P	502	HEM	CAD-C3D-C4D	2.28	128.66	124.70
15	C	2002	UQ	C10-C9-C8	-2.26	117.83	123.63
16	D	2003	CDL	CA6-CA4-CA3	-2.25	106.54	111.78
19	D	501	HEC	CMC-C2C-C3C	-2.25	121.26	126.55
14	P	3001	IKR	C6-C1-C2	-2.24	120.52	122.20
13	C	502	HEM	C4C-NC-C1C	-2.23	102.18	105.82
13	C	501	HEM	CHB-C4A-C3A	-2.23	120.96	127.43
11	E	2005	PEE	O3-C3-C2	2.22	114.80	108.40
13	P	502	HEM	CHB-C4A-C3A	-2.22	120.98	127.43
13	C	501	HEM	CHC-C1C-NC	2.21	126.86	124.45
13	P	501	HEM	CHB-C1B-NB	-2.20	121.64	124.37
15	P	3002	UQ	C10-C9-C8	-2.19	117.99	123.63
13	C	501	HEM	C4A-NA-C1A	-2.19	102.25	105.82
13	P	502	HEM	C3A-C4A-NA	2.19	113.65	110.14
16	Q	3003	CDL	CA4-OA6-CA5	-2.18	112.58	117.80
16	C	2004	CDL	CA4-OA6-CA5	-2.17	112.60	117.80
13	C	502	HEM	CAC-C3C-C4C	2.16	129.98	124.82
13	C	501	HEM	CAD-C3D-C2D	-2.15	123.84	127.87
16	Q	3003	CDL	CA6-CA4-CA3	-2.14	106.79	111.78
13	P	502	HEM	C4A-C3A-C2A	-2.12	104.39	106.82
11	R	3005	PEE	O3-C3-C2	2.12	114.50	108.40
13	C	501	HEM	C2C-C1C-NC	2.11	113.53	109.64
14	C	2001	IKR	C6-C1-C2	-2.11	120.62	122.20
19	Q	501	HEC	CMA-C3A-C4A	2.10	128.43	124.73
16	P	3004	CDL	CA6-OA8-CA7	-2.10	111.91	117.08
16	Q	3003	CDL	CA6-OA8-CA7	-2.10	111.91	117.08
19	Q	501	HEC	CMC-C2C-C3C	-2.09	121.62	126.55
16	P	3004	CDL	CA4-OA6-CA5	-2.08	112.81	117.80
13	C	501	HEM	CHD-C1D-ND	-2.08	122.18	124.42
20	D	2009	BOG	O1-C1-C2	2.08	111.43	108.27
13	P	501	HEM	CMA-C3A-C2A	2.07	130.02	125.62
13	P	501	HEM	CHB-C4A-C3A	-2.07	121.42	127.43
13	C	501	HEM	CMA-C3A-C2A	2.07	130.01	125.62
13	C	501	HEM	CAD-C3D-C4D	2.06	128.28	124.70
13	P	502	HEM	CBA-CAA-C2A	2.06	118.22	112.53
13	C	501	HEM	CBB-CAB-C3B	-2.05	117.26	127.53
13	C	502	HEM	CHC-C1C-NC	-2.05	122.23	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	2001	IKR	C20-C29-C30	-2.04	116.37	119.54
13	C	501	HEM	CHC-C4B-NB	-2.04	122.23	124.42
13	C	502	HEM	CHB-C4A-C3A	-2.04	121.50	127.43
16	C	2004	CDL	CA6-OA8-CA7	-2.03	112.07	117.08
13	C	502	HEM	C2A-C1A-NA	2.01	112.39	110.15
13	C	501	HEM	C2D-C1D-ND	2.01	112.23	109.90
16	D	2003	CDL	CA4-OA6-CA5	-2.00	113.01	117.80

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O3P
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	O4P-C4-C5-N
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C4-O4P-P-O1P
11	R	3005	PEE	O4P-C4-C5-N
13	C	501	HEM	C2B-C3B-CAB-CBB
13	C	501	HEM	C4B-C3B-CAB-CBB
13	C	502	HEM	C2B-C3B-CAB-CBB
13	C	502	HEM	C4B-C3B-CAB-CBB
13	C	502	HEM	C2C-C3C-CAC-CBC
13	P	501	HEM	C2B-C3B-CAB-CBB
13	P	501	HEM	C4B-C3B-CAB-CBB
13	P	502	HEM	C2B-C3B-CAB-CBB
13	P	502	HEM	C4B-C3B-CAB-CBB
13	P	502	HEM	C2C-C3C-CAC-CBC
13	P	502	HEM	C4C-C3C-CAC-CBC
15	C	2002	UQ	C1-C6-C7-C8
15	C	2002	UQ	C5-C6-C7-C8
15	C	2002	UQ	C12-C11-C9-C8
15	C	2002	UQ	C12-C11-C9-C10
15	P	3002	UQ	C1-C6-C7-C8
15	P	3002	UQ	C5-C6-C7-C8
15	P	3002	UQ	C12-C11-C9-C8
15	P	3002	UQ	C12-C11-C9-C10
16	C	2004	CDL	CA2-OA2-PA1-OA4
16	C	2004	CDL	CB2-OB2-PB2-OB3
16	C	2004	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	C	2004	CDL	CB2-OB2-PB2-OB5
16	C	2004	CDL	C51-CB5-OB6-CB4
16	D	2003	CDL	CB2-OB2-PB2-OB4
16	D	2003	CDL	CB2-OB2-PB2-OB5
16	P	3004	CDL	CA2-OA2-PA1-OA4
16	P	3004	CDL	CA2-OA2-PA1-OA5
16	P	3004	CDL	CB2-OB2-PB2-OB3
16	P	3004	CDL	CB2-OB2-PB2-OB4
16	P	3004	CDL	CB2-OB2-PB2-OB5
16	P	3004	CDL	C51-CB5-OB6-CB4
16	Q	3003	CDL	CB2-OB2-PB2-OB4
16	Q	3003	CDL	CB2-OB2-PB2-OB5
18	C	2011	GOL	O1-C1-C2-C3
18	P	3011	GOL	C1-C2-C3-O3
19	D	501	HEC	C3A-C2A-CAA-CBA
19	D	501	HEC	C2B-C3B-CAB-CBB
19	D	501	HEC	C4B-C3B-CAB-CBB
19	D	501	HEC	C4C-C3C-CAC-CBC
19	Q	501	HEC	C3A-C2A-CAA-CBA
19	Q	501	HEC	C2B-C3B-CAB-CBB
19	Q	501	HEC	C4B-C3B-CAB-CBB
19	Q	501	HEC	C2C-C3C-CAC-CBC
19	Q	501	HEC	C4C-C3C-CAC-CBC
20	P	3091	BOG	C2-C1-O1-C1'
20	P	3091	BOG	O5-C1-O1-C1'
16	C	2004	CDL	C31-CA7-OA8-CA6
16	P	3004	CDL	C31-CA7-OA8-CA6
16	C	2004	CDL	OA9-CA7-OA8-CA6
16	P	3004	CDL	OA9-CA7-OA8-CA6
11	E	2005	PEE	O5-C30-O3-C3
11	R	3005	PEE	O5-C30-O3-C3
16	C	2004	CDL	OB9-CB7-OB8-CB6
16	P	3004	CDL	OB9-CB7-OB8-CB6
16	D	2003	CDL	C31-CA7-OA8-CA6
11	A	2008	PEE	O4-C10-O2-C2
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	O4-C10-O2-C2
16	C	2004	CDL	OB7-CB5-OB6-CB4
16	P	3004	CDL	OB7-CB5-OB6-CB4
11	E	2005	PEE	C31-C30-O3-C3
11	R	3005	PEE	C31-C30-O3-C3
16	Q	3003	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C11-C10-O2-C2
16	C	2004	CDL	C71-CB7-OB8-CB6
16	P	3004	CDL	C71-CB7-OB8-CB6
19	Q	501	HEC	C1A-C2A-CAA-CBA
20	P	3091	BOG	O5-C5-C6-O6
16	D	2003	CDL	OA9-CA7-OA8-CA6
20	P	3091	BOG	C4-C5-C6-O6
20	D	2009	BOG	O5-C1-O1-C1'
20	Q	3009	BOG	O5-C1-O1-C1'
16	D	2003	CDL	C71-CB7-OB8-CB6
16	Q	3003	CDL	C71-CB7-OB8-CB6
16	Q	3003	CDL	OA9-CA7-OA8-CA6
16	D	2003	CDL	OB9-CB7-OB8-CB6
16	Q	3003	CDL	OB9-CB7-OB8-CB6
20	D	2009	BOG	C2-C1-O1-C1'
20	Q	3009	BOG	C2-C1-O1-C1'
11	E	2005	PEE	C30-C31-C32-C33
11	R	3005	PEE	C30-C31-C32-C33
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
20	D	2009	BOG	O1-C1'-C2'-C3'
20	Q	3009	BOG	O1-C1'-C2'-C3'
11	P	3007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C10-C11-C12-C13
18	C	2011	GOL	C1-C2-C3-O3
11	P	3007	PEE	C12-C13-C14-C15
11	R	3005	PEE	C42-C43-C44-C45
18	C	2011	GOL	O1-C1-C2-O2
11	C	2007	PEE	C12-C13-C14-C15
11	E	2005	PEE	C42-C43-C44-C45
16	D	2003	CDL	CB5-C51-C52-C53
16	Q	3003	CDL	CB5-C51-C52-C53
11	C	2007	PEE	C15-C16-C17-C18
11	R	3005	PEE	C10-C11-C12-C13
11	E	2005	PEE	C34-C35-C36-C37
11	R	3005	PEE	C34-C35-C36-C37
11	C	2007	PEE	C11-C10-O2-C2
16	D	2003	CDL	CB7-C71-C72-C73
19	D	501	HEC	C1A-C2A-CAA-CBA
11	P	3007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C20-C21-C22-C23
11	R	3005	PEE	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C10-C11-C12-C13
11	P	3007	PEE	C20-C21-C22-C23
16	C	2004	CDL	OB5-CB3-CB4-OB6
13	C	502	HEM	C4C-C3C-CAC-CBC
11	E	2005	PEE	C21-C22-C23-C24
16	Q	3003	CDL	CB7-C71-C72-C73
18	C	2011	GOL	O2-C2-C3-O3
18	P	3011	GOL	O2-C2-C3-O3
11	E	2005	PEE	C19-C20-C21-C22
11	E	2005	PEE	C35-C36-C37-C38
16	C	2004	CDL	OA5-CA3-CA4-CA6
16	P	3004	CDL	OA5-CA3-CA4-CA6
13	C	502	HEM	C4D-C3D-CAD-CBD
16	C	2004	CDL	CA3-CA4-CA6-OA8
16	P	3004	CDL	CA3-CA4-CA6-OA8
11	R	3005	PEE	C19-C20-C21-C22
11	R	3005	PEE	C35-C36-C37-C38
11	P	3007	PEE	C14-C15-C16-C17
16	P	3004	CDL	OB5-CB3-CB4-OB6
11	C	2007	PEE	C11-C12-C13-C14
11	C	2007	PEE	O2-C2-C3-O3
11	P	3007	PEE	O2-C2-C3-O3
11	P	3007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C14-C15-C16-C17
11	C	2007	PEE	C41-C42-C43-C44
11	E	2005	PEE	O3P-C1-C2-C3
11	R	3005	PEE	O3P-C1-C2-C3
16	C	2004	CDL	OB5-CB3-CB4-CB6
16	D	2003	CDL	OA5-CA3-CA4-CA6
16	P	3004	CDL	OB5-CB3-CB4-CB6
16	Q	3003	CDL	OA5-CA3-CA4-CA6
16	Q	3003	CDL	C71-C72-C73-C74
16	D	2003	CDL	C71-C72-C73-C74
11	C	2007	PEE	O4-C10-O2-C2
11	E	2005	PEE	O3P-C1-C2-O2
11	R	3005	PEE	O3P-C1-C2-O2
11	P	3007	PEE	C41-C42-C43-C44
11	E	2005	PEE	C43-C44-C45-C46
11	P	3007	PEE	C11-C10-O2-C2
11	R	3005	PEE	C43-C44-C45-C46
20	D	2091	BOG	O5-C5-C6-O6
13	P	501	HEM	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C35-C36-C37-C38
16	Q	3003	CDL	OA5-CA3-CA4-OA6
20	D	2009	BOG	C2'-C3'-C4'-C5'
13	C	502	HEM	C2D-C3D-CAD-CBD
11	R	3005	PEE	C14-C15-C16-C17
11	P	3007	PEE	C40-C41-C42-C43
11	P	3007	PEE	C32-C33-C34-C35
11	P	3007	PEE	O4-C10-O2-C2
16	D	2003	CDL	OA5-CA3-CA4-OA6
16	P	3004	CDL	OA5-CA3-CA4-OA6
11	E	2005	PEE	C39-C40-C41-C42
11	E	2005	PEE	C11-C12-C13-C14
11	E	2005	PEE	C14-C15-C16-C17
16	C	2004	CDL	OA6-CA4-CA6-OA8
16	P	3004	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C1-C2-C3-O3
11	C	2007	PEE	C40-C41-C42-C43
11	E	2005	PEE	C4-O4P-P-O2P
11	R	3005	PEE	C4-O4P-P-O2P
16	C	2004	CDL	CA2-OA2-PA1-OA5
16	D	2003	CDL	CA3-OA5-PA1-OA3
16	Q	3003	CDL	CA3-OA5-PA1-OA3
19	D	501	HEC	C2C-C3C-CAC-CBC
16	C	2004	CDL	C1-CB2-OB2-PB2
16	P	3004	CDL	C1-CB2-OB2-PB2
20	Q	3009	BOG	C2'-C3'-C4'-C5'
16	C	2004	CDL	OA5-CA3-CA4-OA6
11	C	2007	PEE	C32-C33-C34-C35
11	R	3005	PEE	C11-C12-C13-C14
13	P	501	HEM	CAA-CBA-CGA-O2A
16	D	2003	CDL	O1-C1-CB2-OB2
11	R	3005	PEE	C39-C40-C41-C42
11	P	3007	PEE	C42-C43-C44-C45
13	P	502	HEM	CAD-CBD-CGD-O2D
13	C	501	HEM	CAA-CBA-CGA-O1A
13	P	501	HEM	CAA-CBA-CGA-O1A
11	P	3007	PEE	C1-C2-C3-O3
11	E	2005	PEE	C1-C2-O2-C10
11	R	3005	PEE	C1-C2-O2-C10
13	C	501	HEM	CAA-CBA-CGA-O2A
16	D	2003	CDL	C1-CA2-OA2-PA1

Continued on next page...

Continued from previous page...

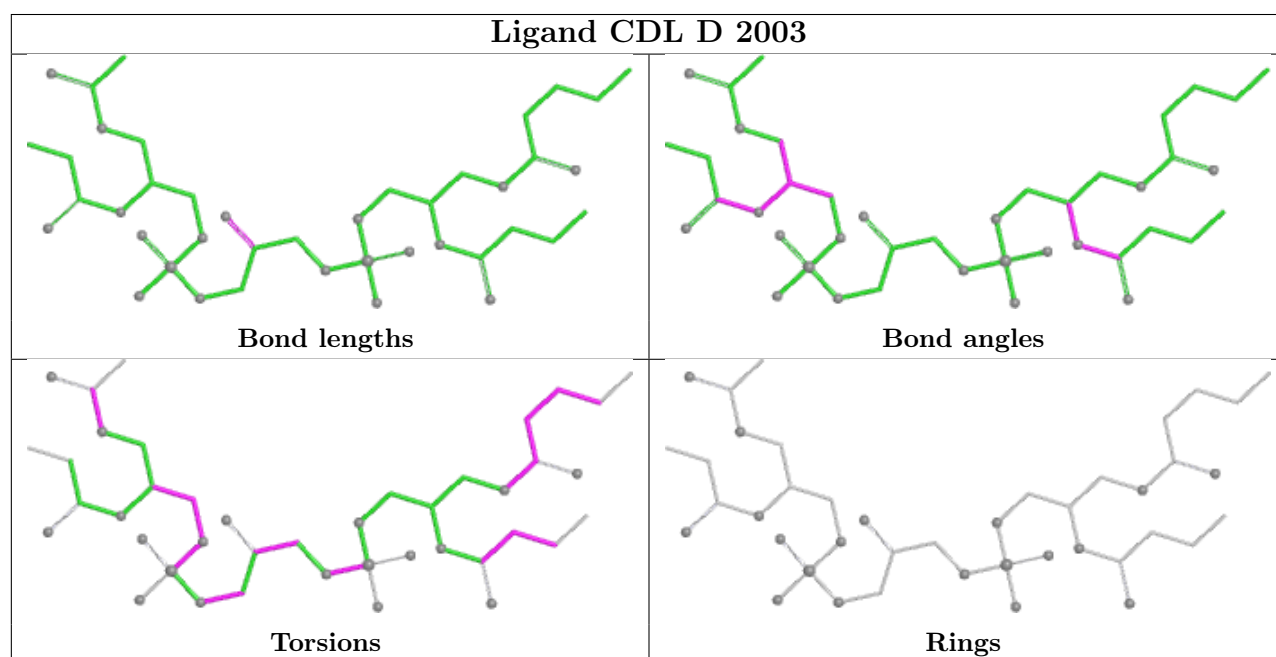
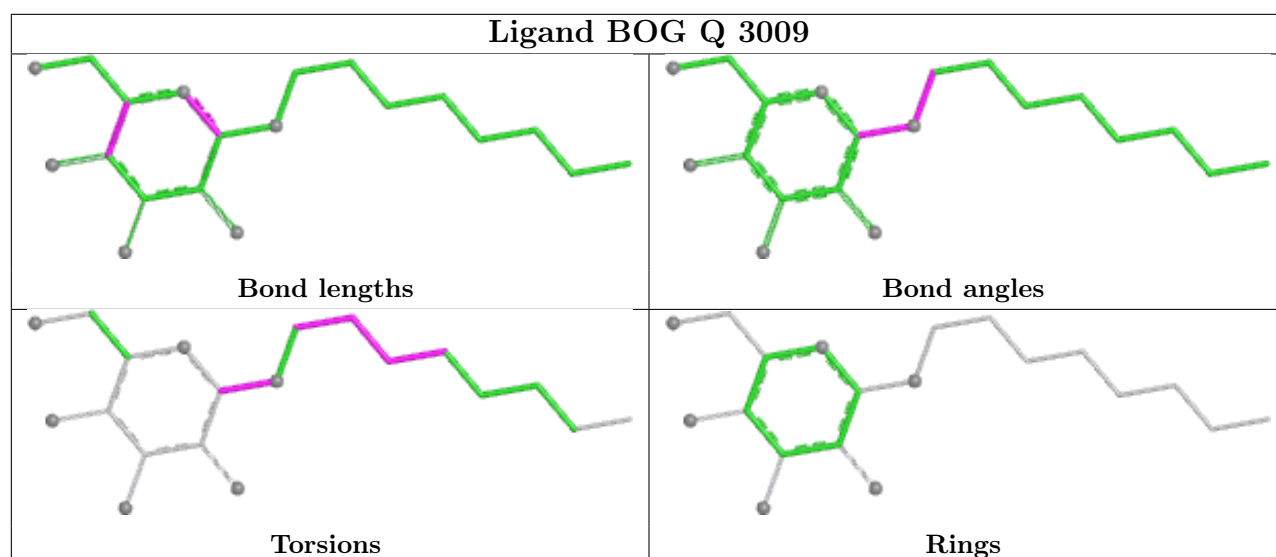
Mol	Chain	Res	Type	Atoms
16	Q	3003	CDL	C1-CA2-OA2-PA1
13	P	502	HEM	CAD-CBD-CGD-O1D
20	P	2010	BOG	C4-C5-C6-O6
11	C	2007	PEE	C42-C43-C44-C45
13	C	502	HEM	CAD-CBD-CGD-O2D
11	P	3007	PEE	C34-C35-C36-C37
13	P	501	HEM	CAD-CBD-CGD-O2D
13	C	502	HEM	CAD-CBD-CGD-O1D
16	Q	3003	CDL	O1-C1-CB2-OB2
13	C	501	HEM	CAD-CBD-CGD-O2D
13	C	502	HEM	CAA-CBA-CGA-O2A
13	P	502	HEM	CAA-CBA-CGA-O1A
13	C	502	HEM	CAA-CBA-CGA-O1A
11	R	3005	PEE	C38-C39-C40-C41
11	R	3005	PEE	C17-C18-C19-C20
13	P	502	HEM	CAA-CBA-CGA-O2A
11	E	2005	PEE	C38-C39-C40-C41
13	C	501	HEM	CAD-CBD-CGD-O1D
13	P	501	HEM	CAD-CBD-CGD-O1D
13	P	501	HEM	C4C-C3C-CAC-CBC
14	P	3001	IKR	O15-C16-C17-C20
20	Q	3009	BOG	C1'-C2'-C3'-C4'
16	D	2003	CDL	C72-C71-CB7-OB8
16	Q	3003	CDL	C72-C71-CB7-OB8
11	R	3005	PEE	C23-C24-C25-C26
13	P	502	HEM	C4D-C3D-CAD-CBD
16	P	3004	CDL	OA7-CA5-OA6-CA4
11	C	2007	PEE	C31-C32-C33-C34
16	Q	3003	CDL	C12-C11-CA5-OA6
16	Q	3003	CDL	C72-C71-CB7-OB9
16	Q	3003	CDL	C52-C51-CB5-OB6
16	D	2003	CDL	C72-C71-CB7-OB9
16	C	2004	CDL	OA7-CA5-OA6-CA4
11	R	3005	PEE	C33-C34-C35-C36
16	D	2003	CDL	CA4-CA3-OA5-PA1
11	C	2007	PEE	C34-C35-C36-C37
16	D	2003	CDL	C52-C51-CB5-OB6
11	E	2005	PEE	C17-C18-C19-C20

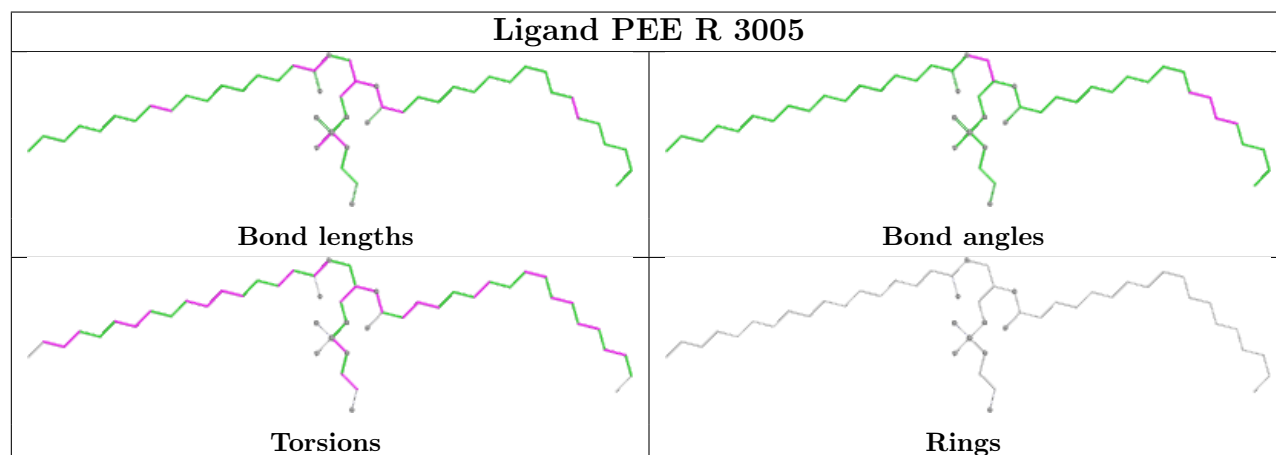
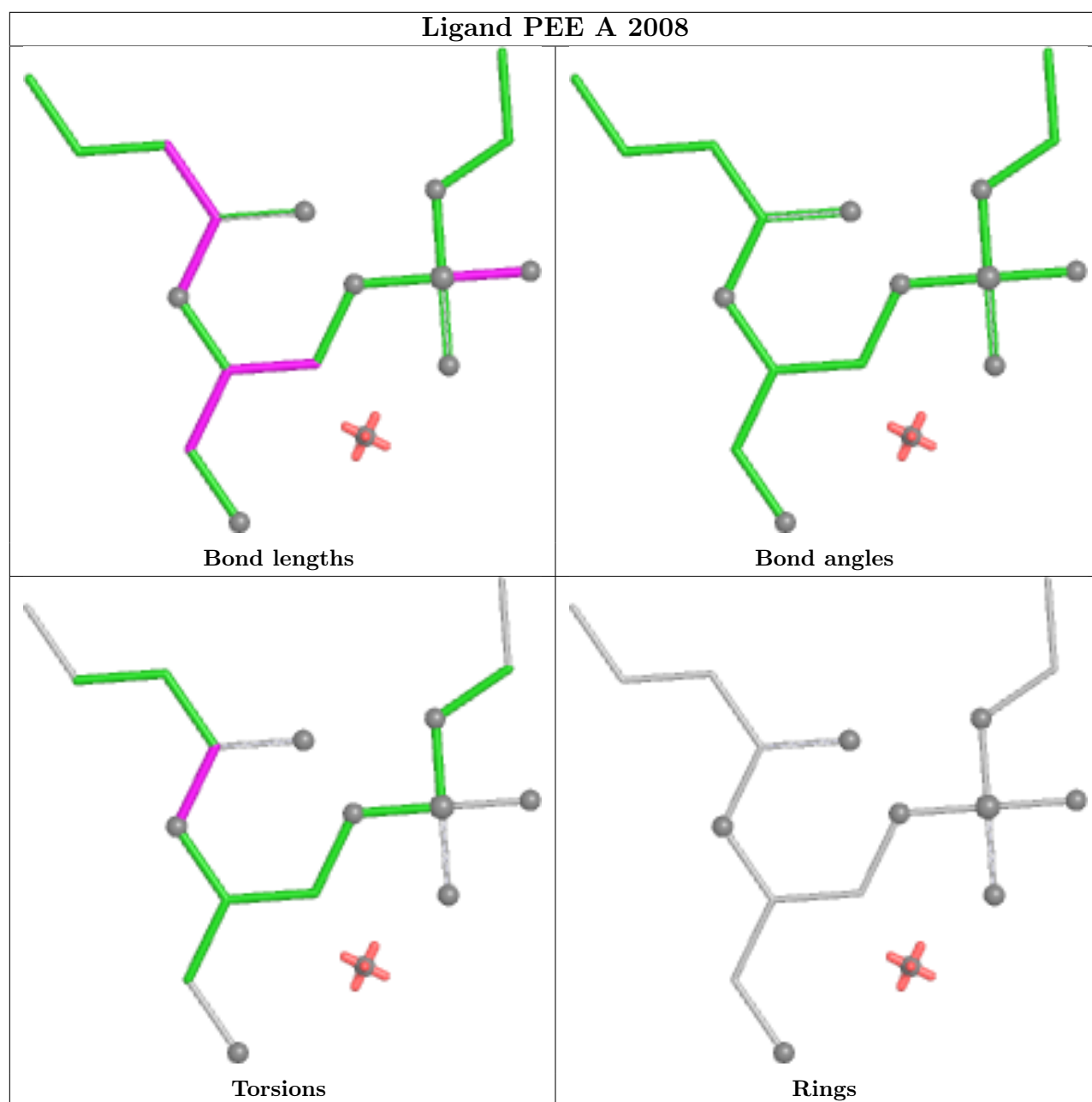
There are no ring outliers.

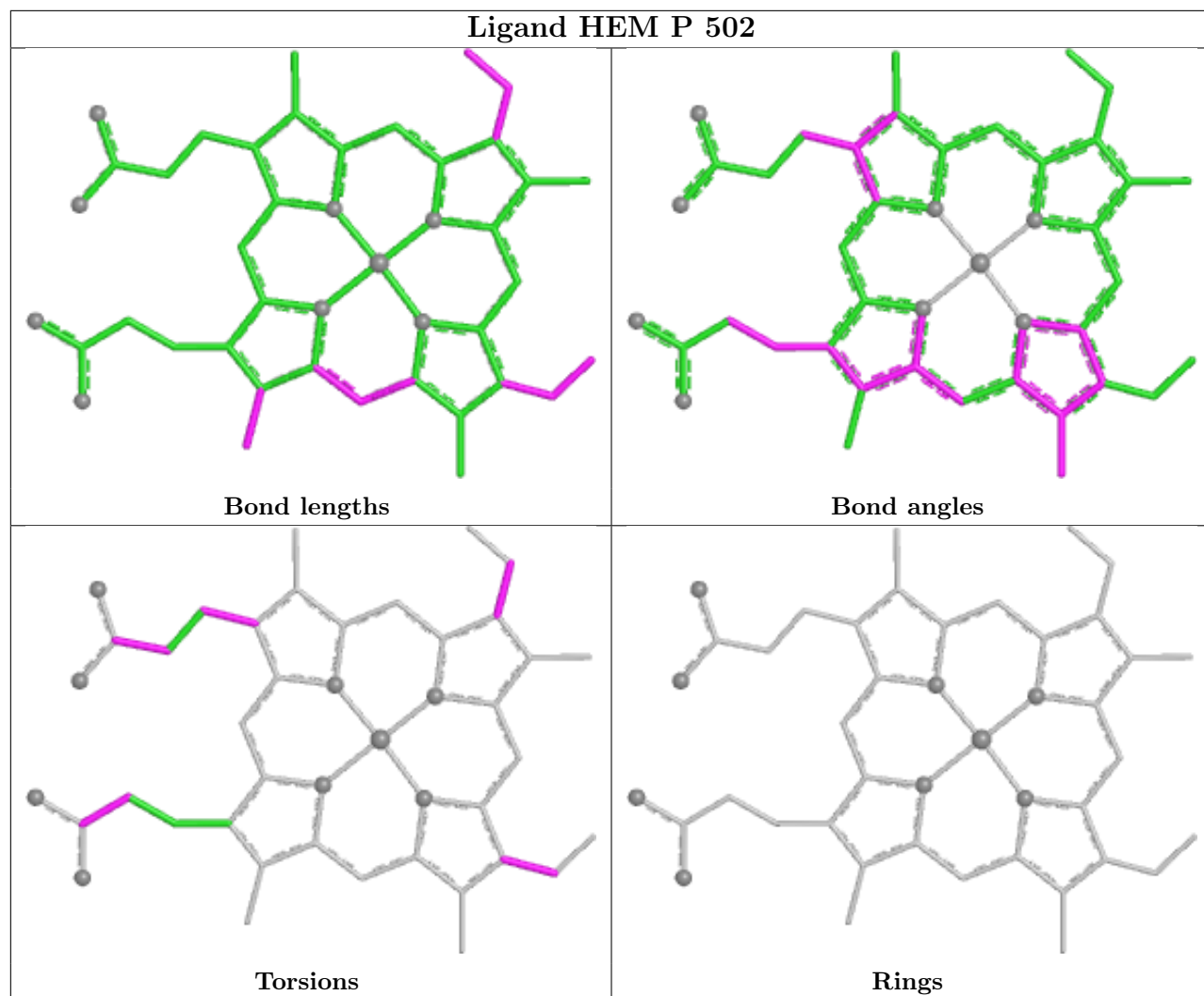
21 monomers are involved in 86 short contacts:

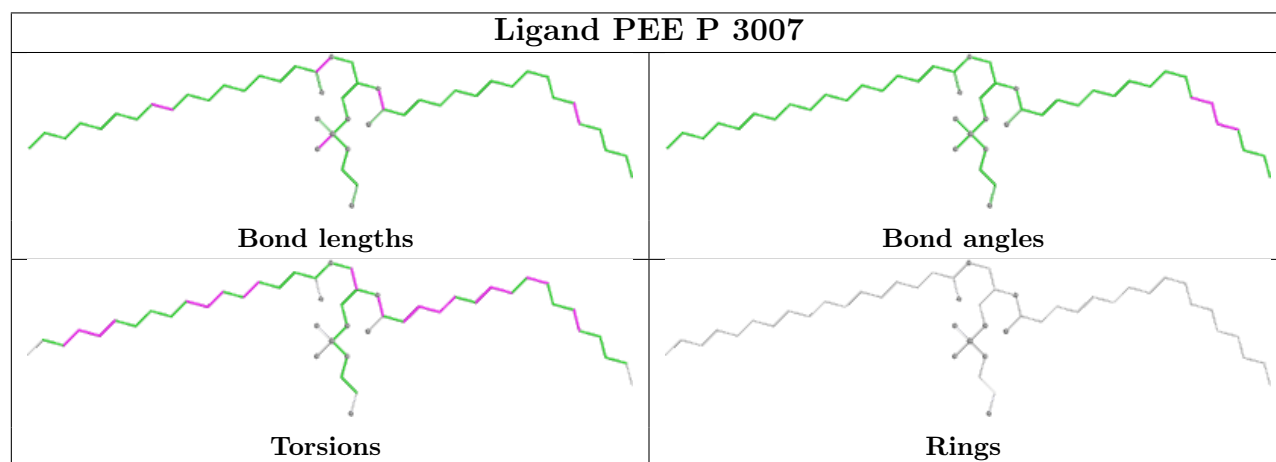
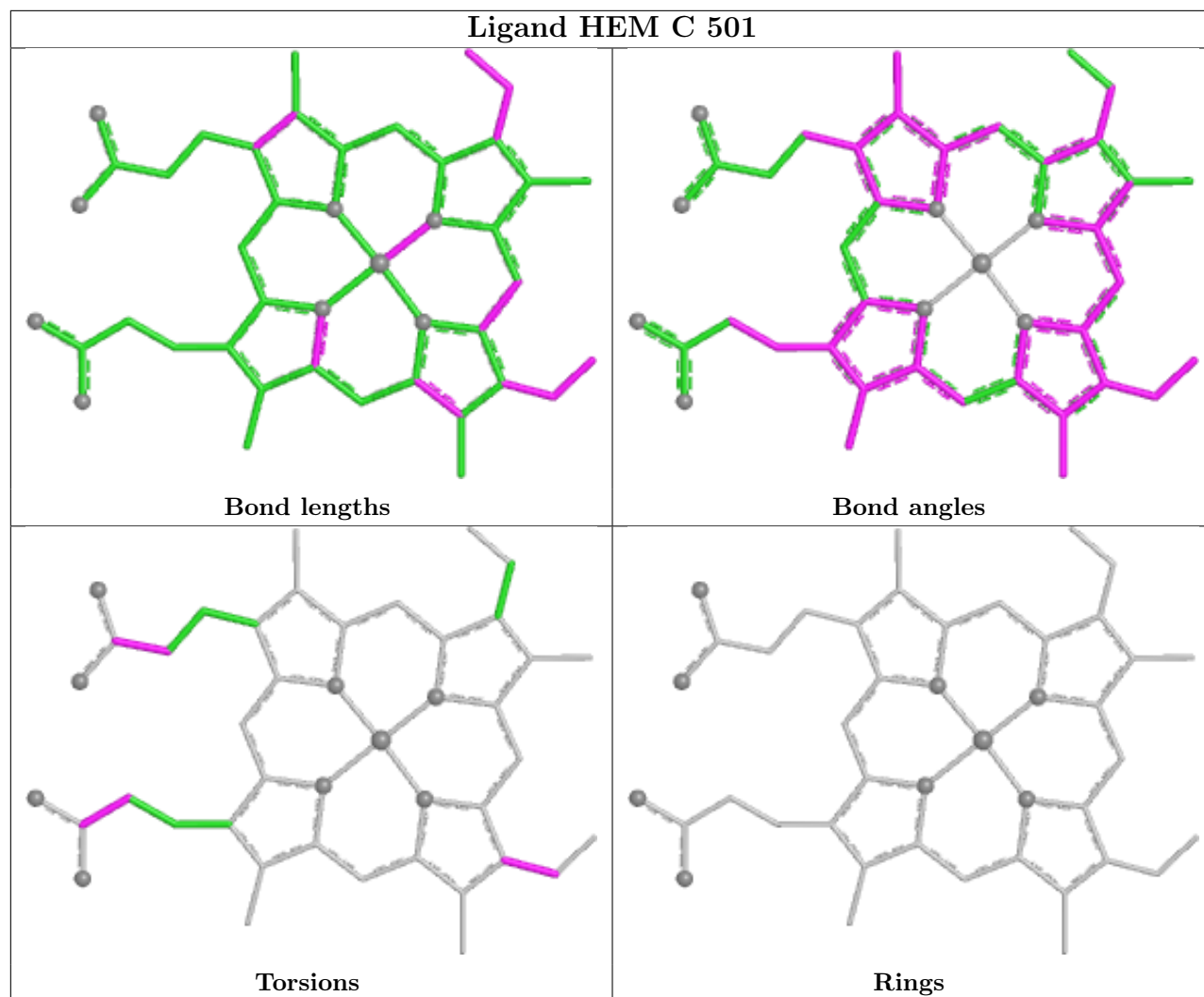
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	2003	CDL	1	0
13	P	502	HEM	12	0
13	C	501	HEM	6	0
11	P	3007	PEE	4	0
21	E	501	FES	3	0
14	P	3001	IKR	4	0
16	P	3004	CDL	2	0
16	C	2004	CDL	2	0
15	P	3002	UQ	4	0
18	P	3011	GOL	1	0
20	D	2091	BOG	1	0
15	C	2002	UQ	7	0
21	R	501	FES	2	0
13	C	502	HEM	13	0
19	Q	501	HEC	1	0
11	C	2007	PEE	3	0
19	D	501	HEC	2	0
13	P	501	HEM	9	0
14	C	2001	IKR	5	0
18	C	2011	GOL	1	0
16	Q	3003	CDL	3	0

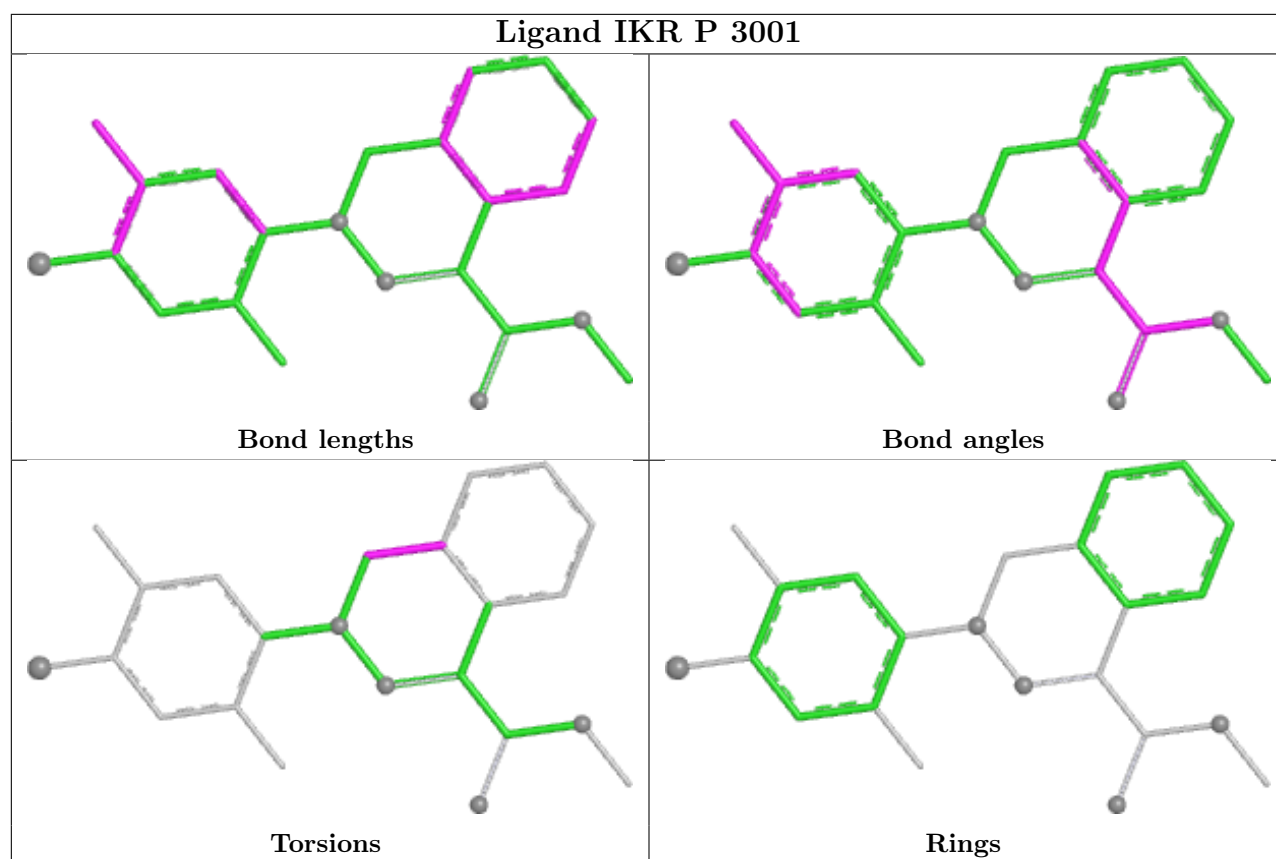
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

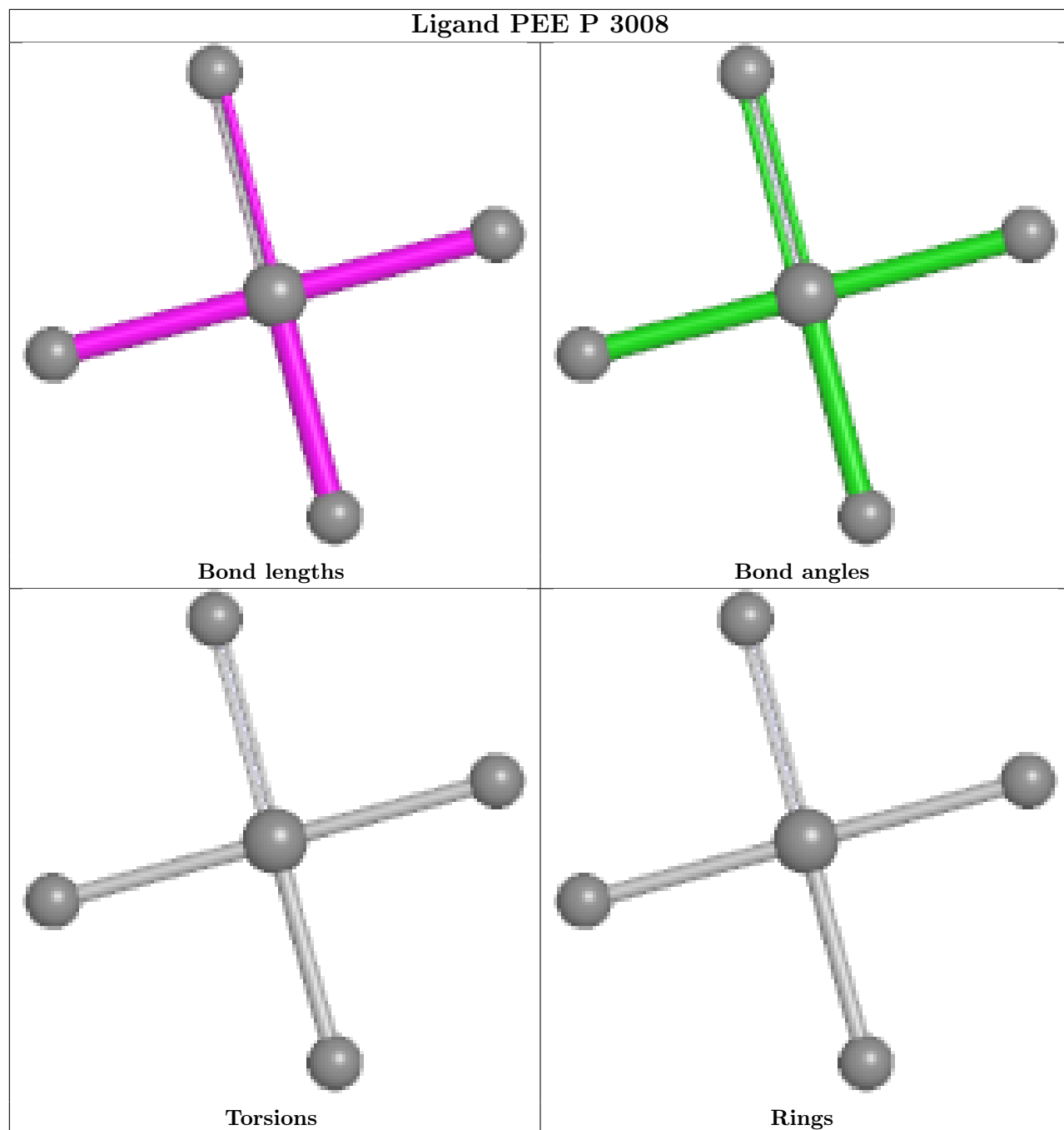


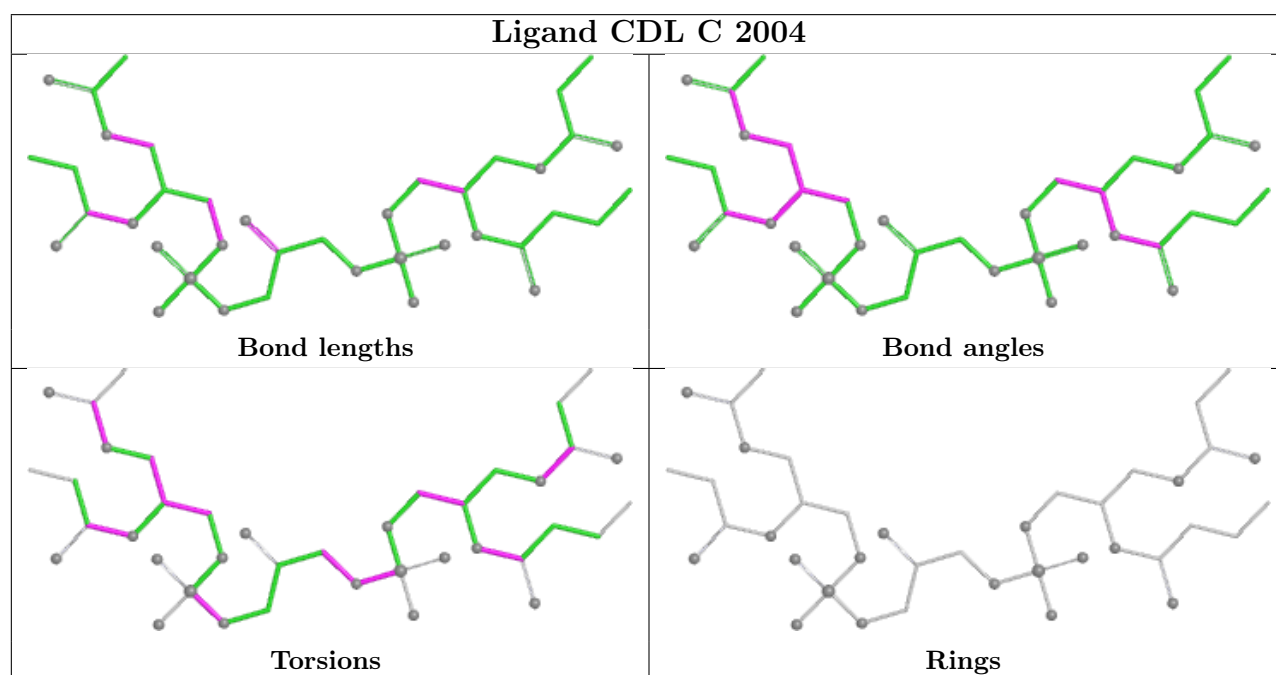
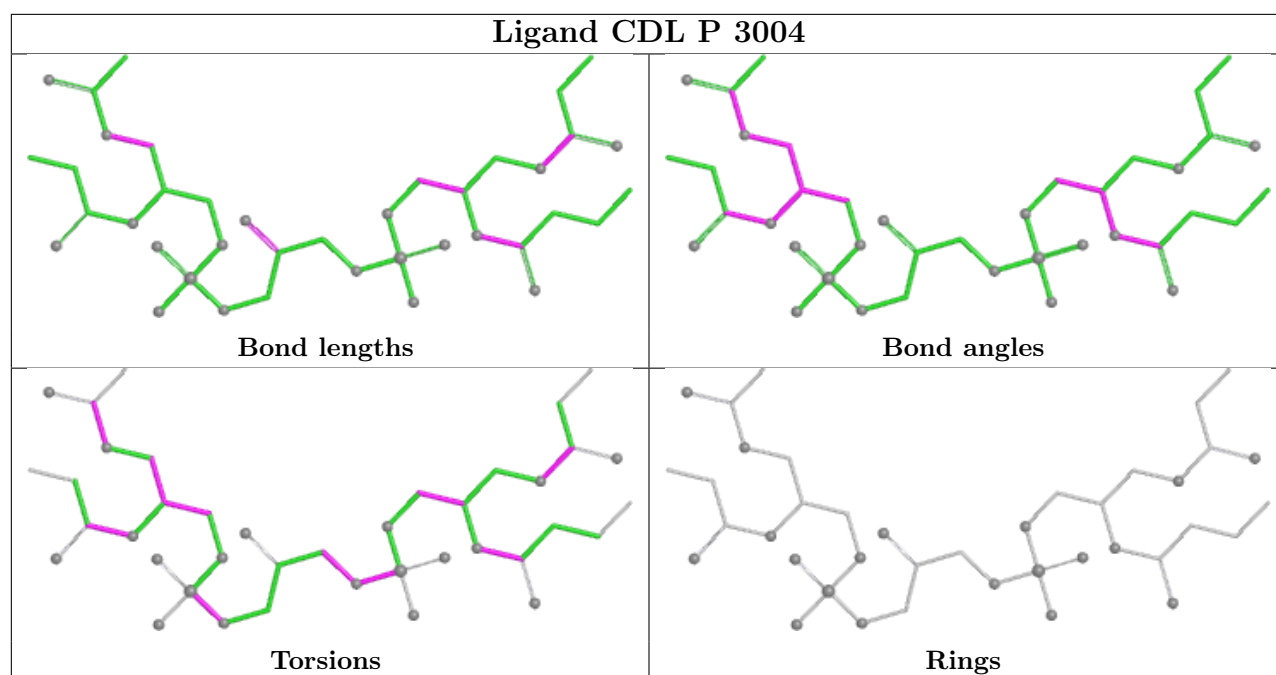


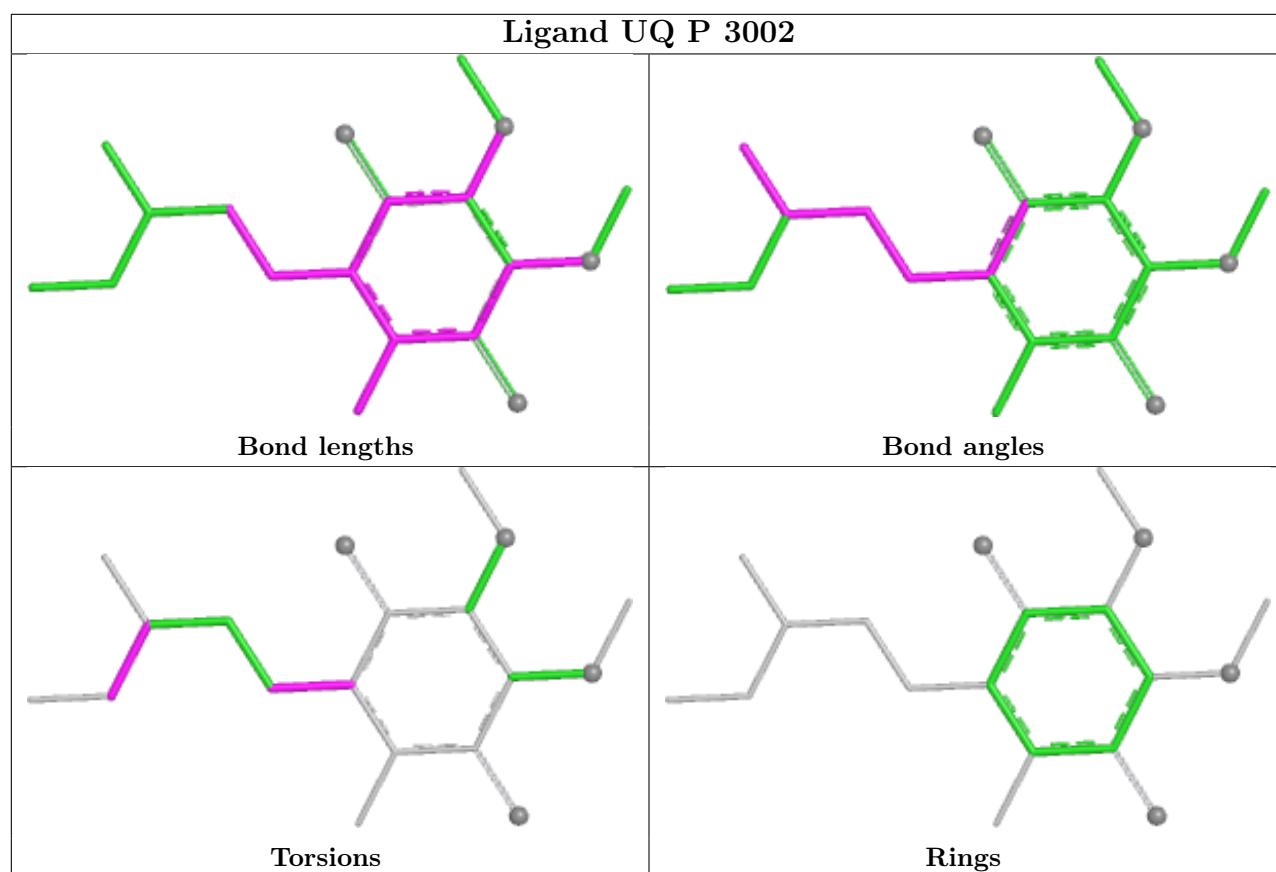




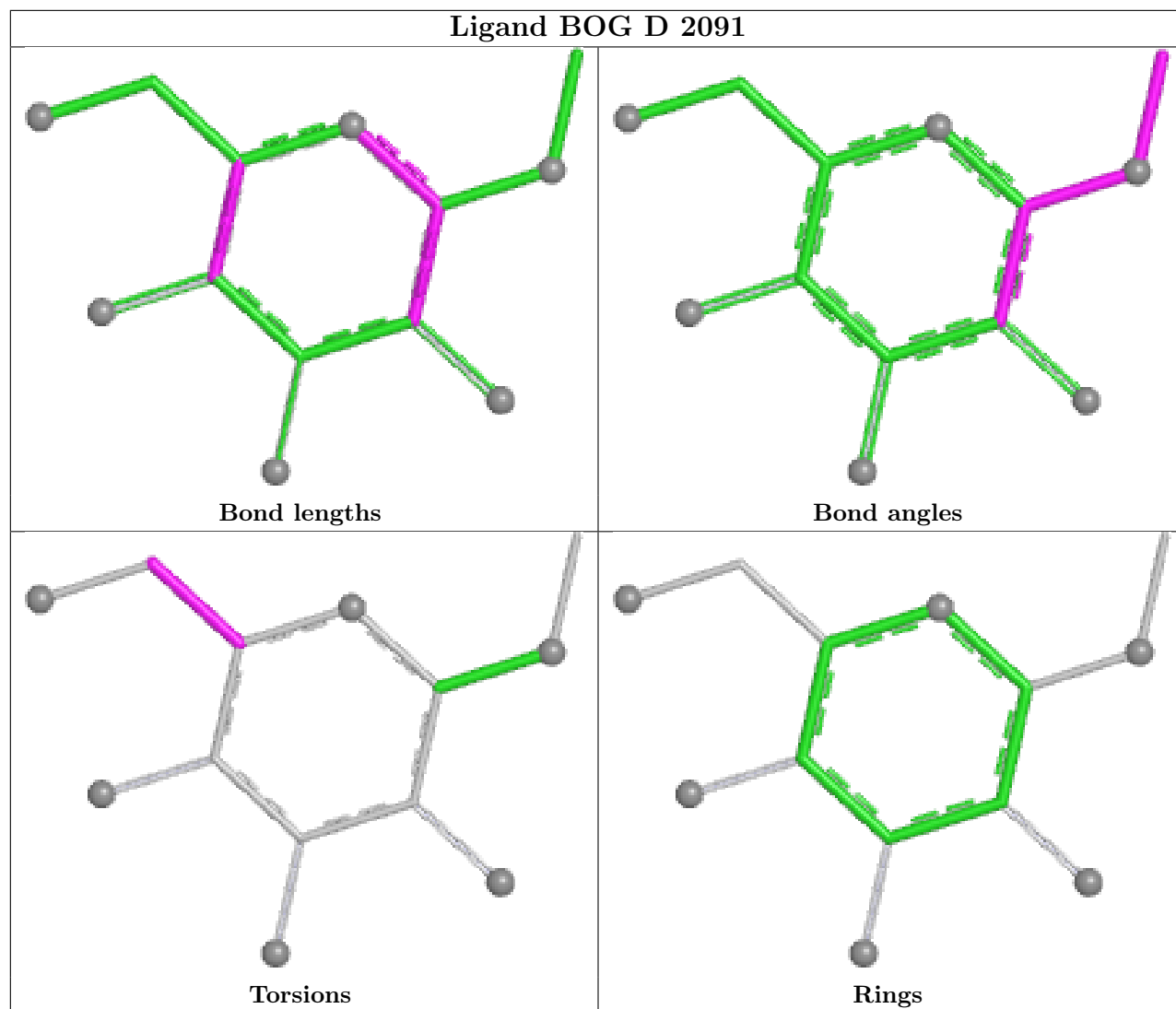




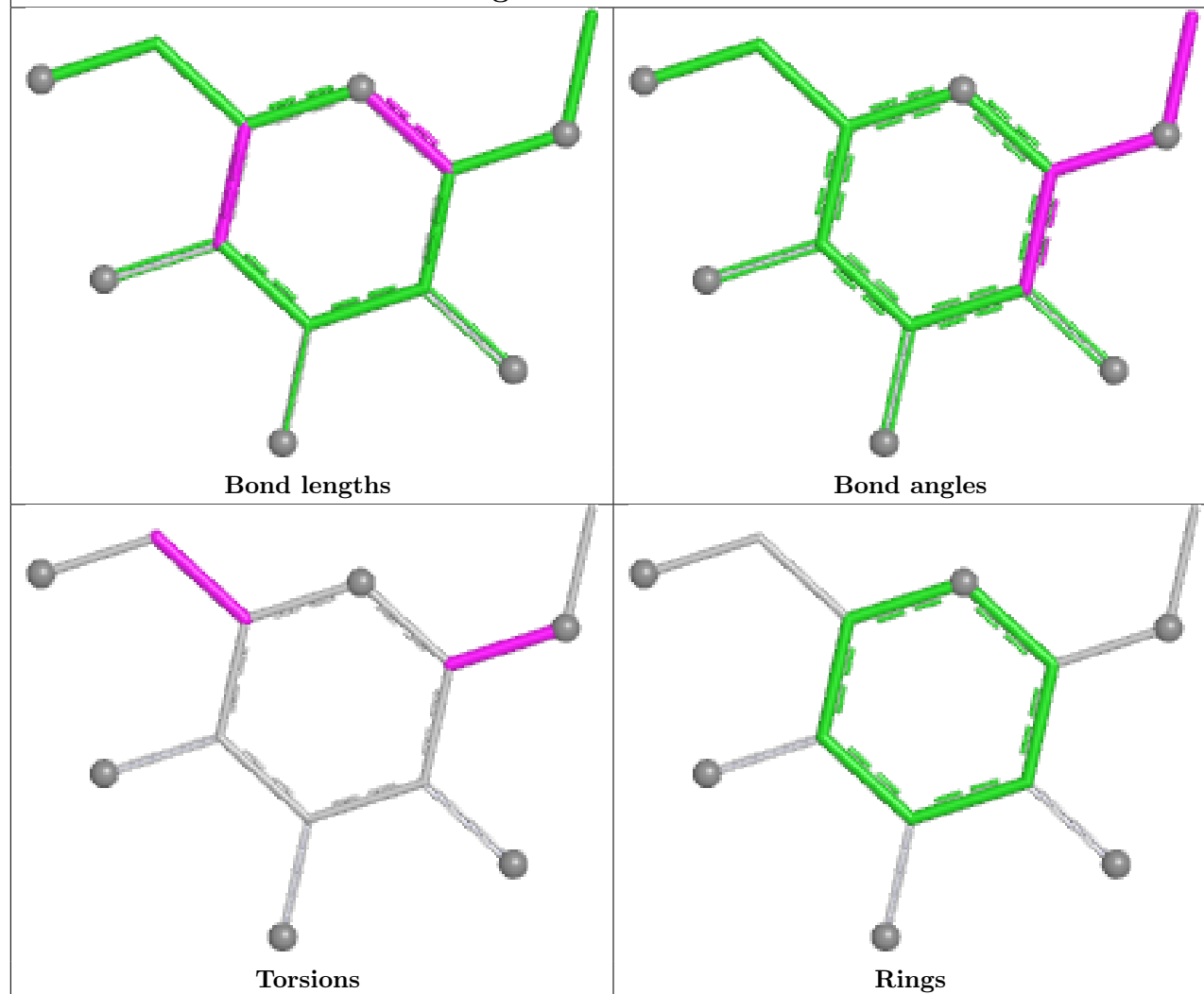




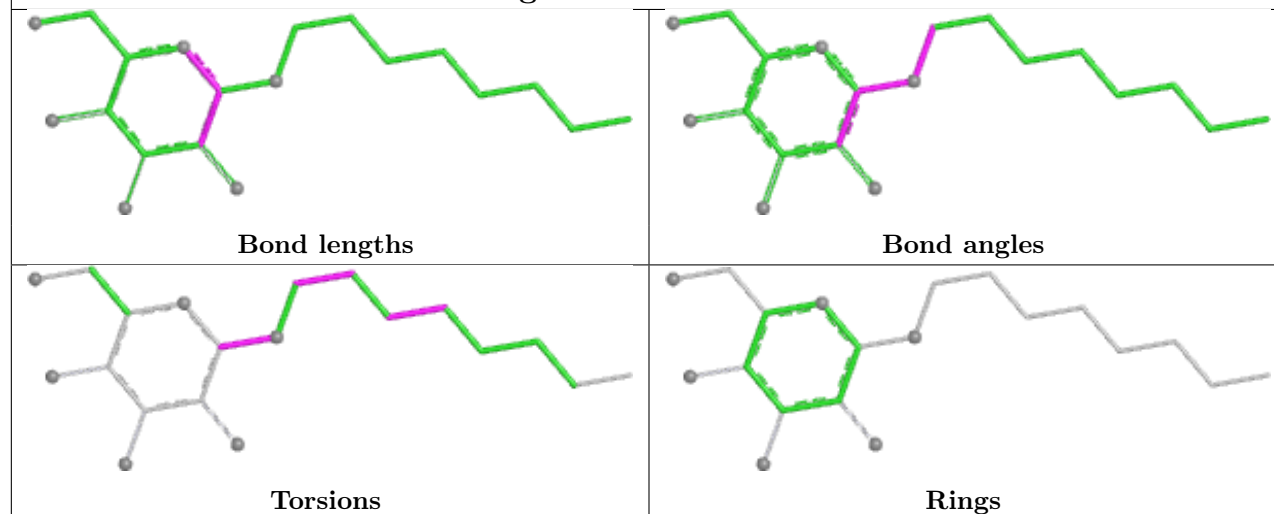
Ligand BOG D 2091

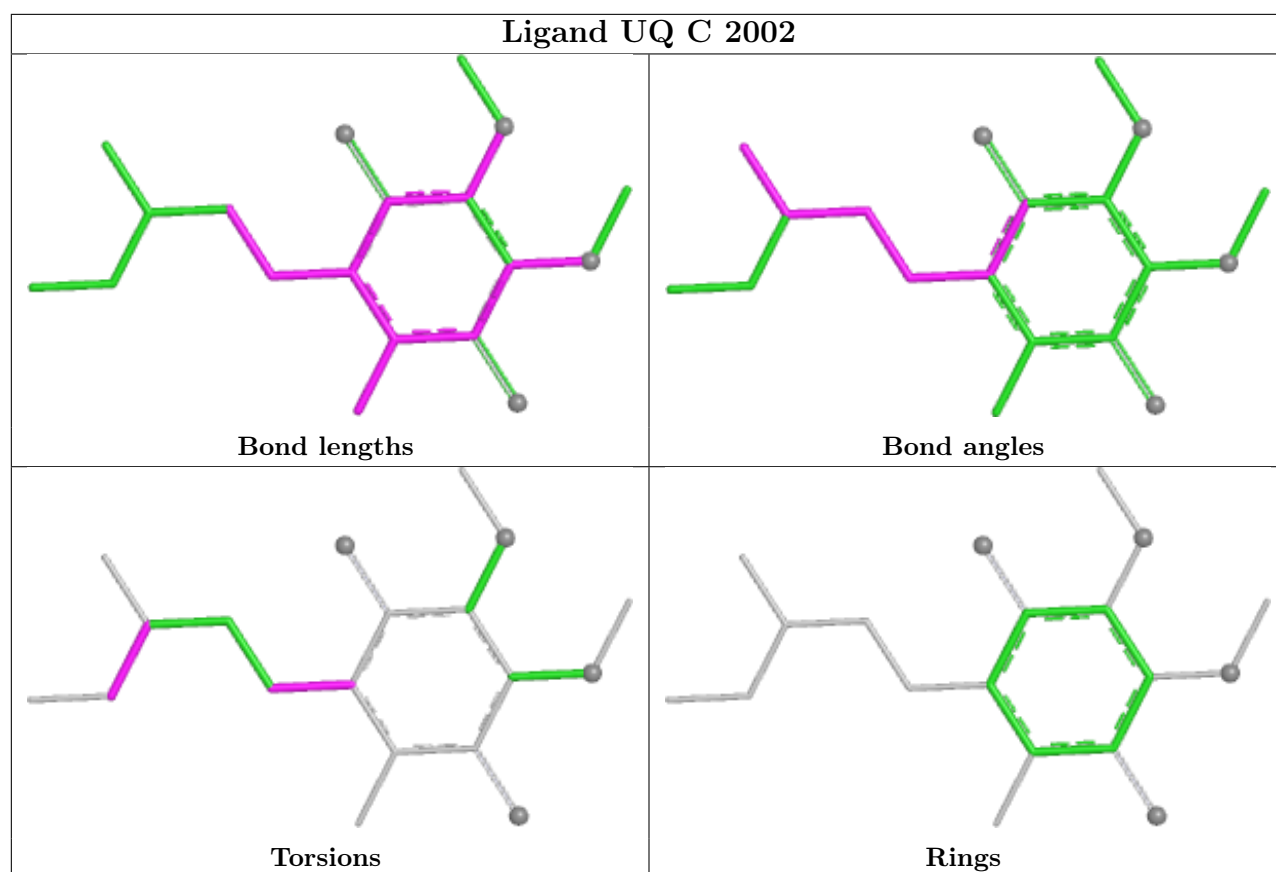


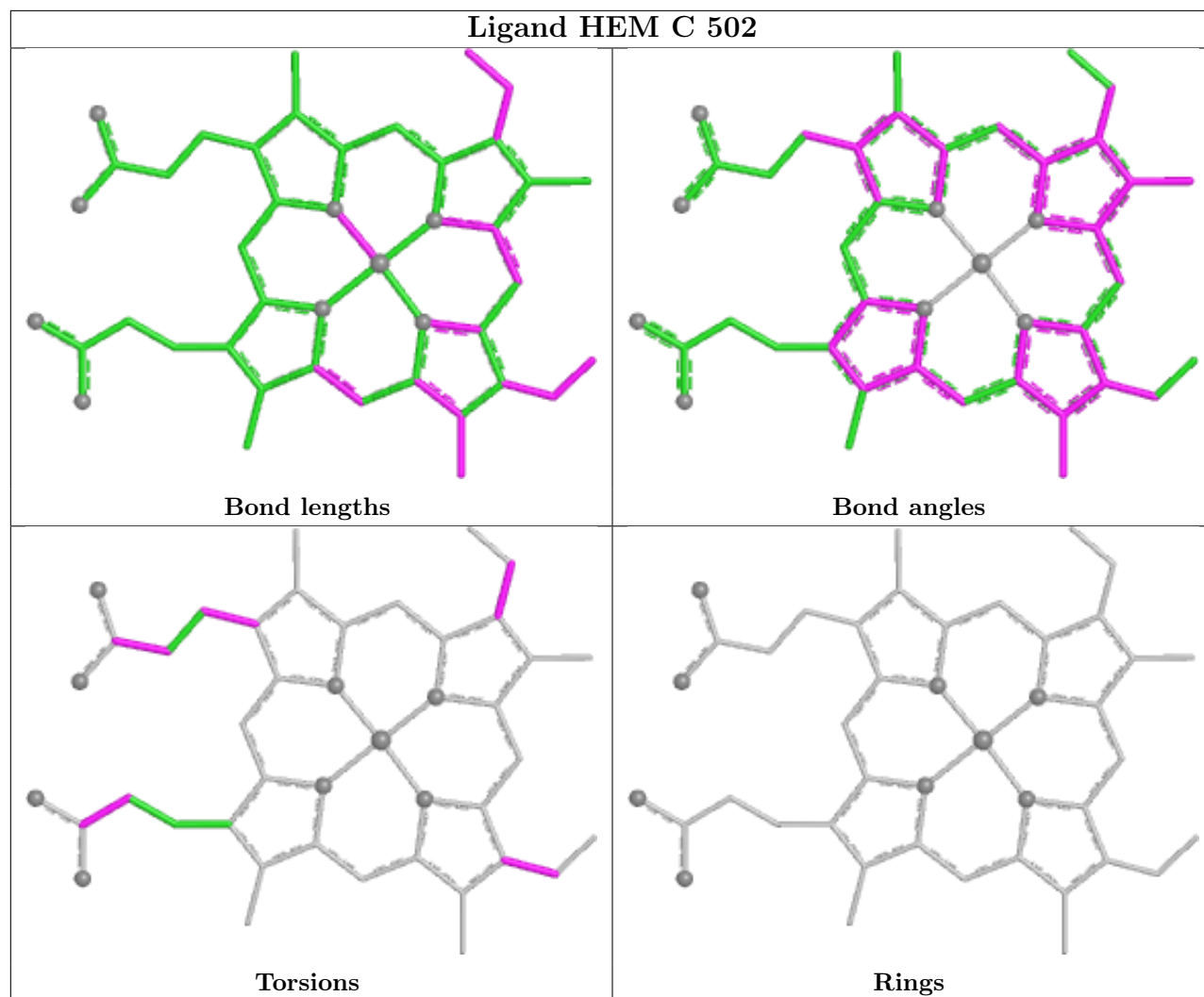
Ligand BOG P 3091



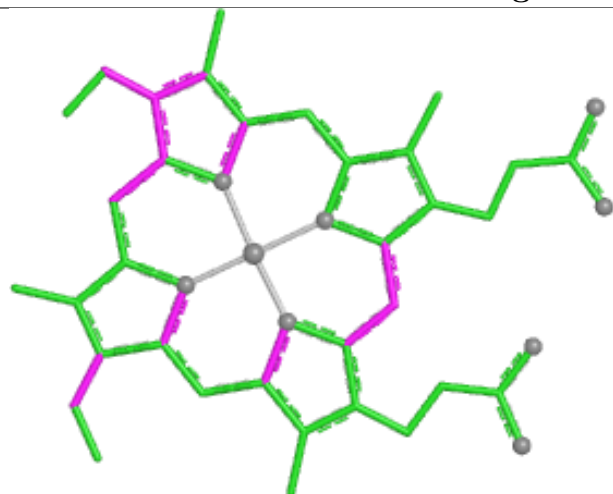
Ligand BOG D 2009



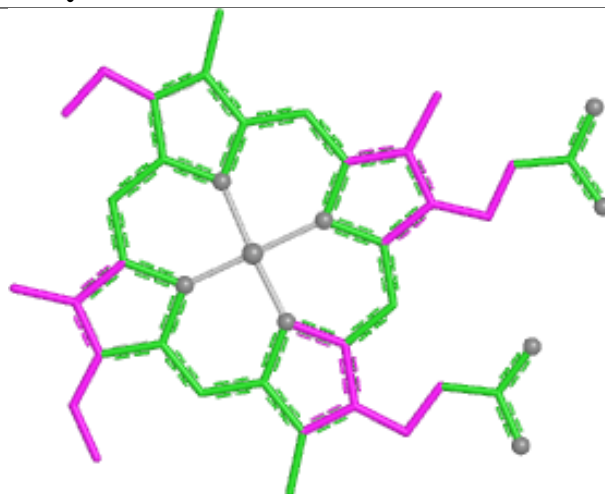




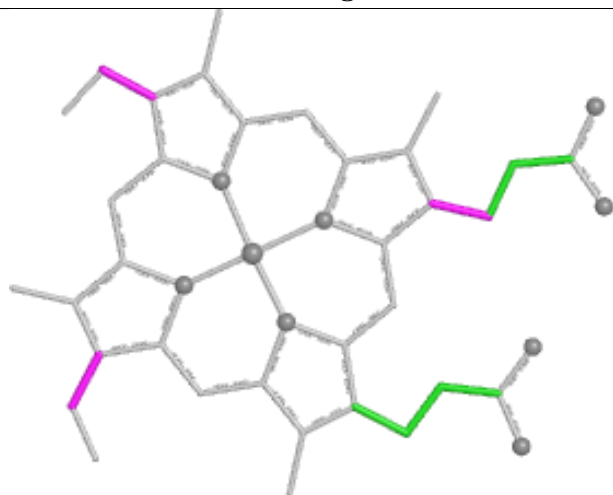
Ligand HEC Q 501



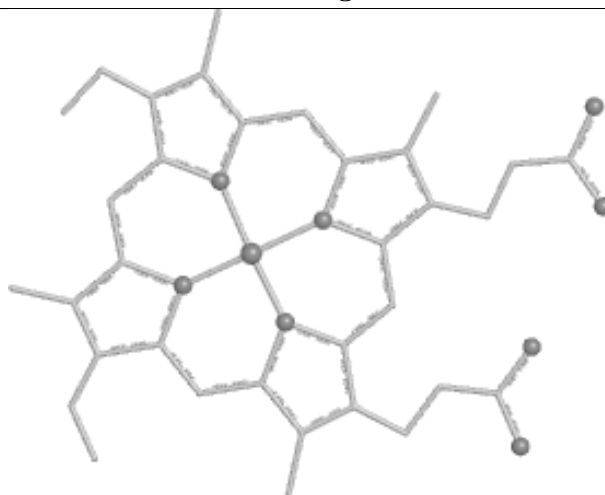
Bond lengths



Bond angles



Torsions



Rings

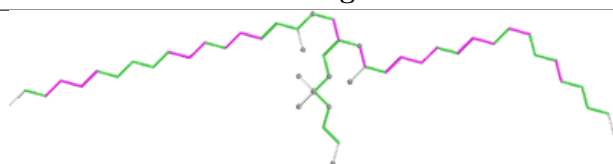
Ligand PEE C 2007



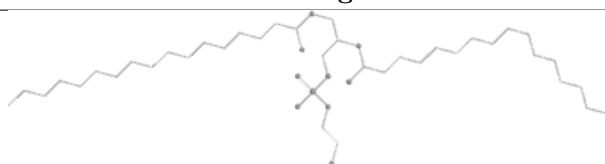
Bond lengths



Bond angles

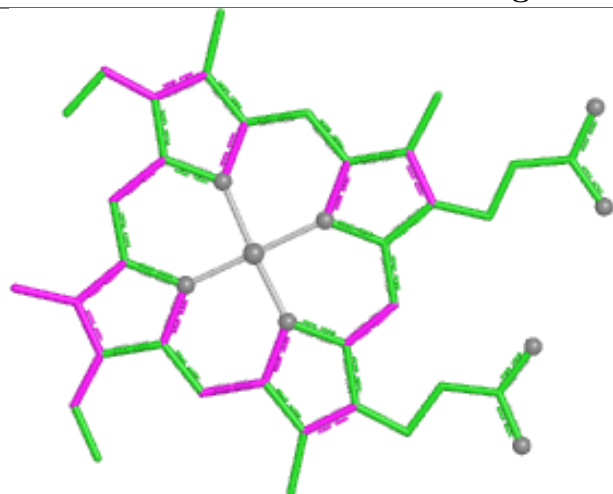


Torsions

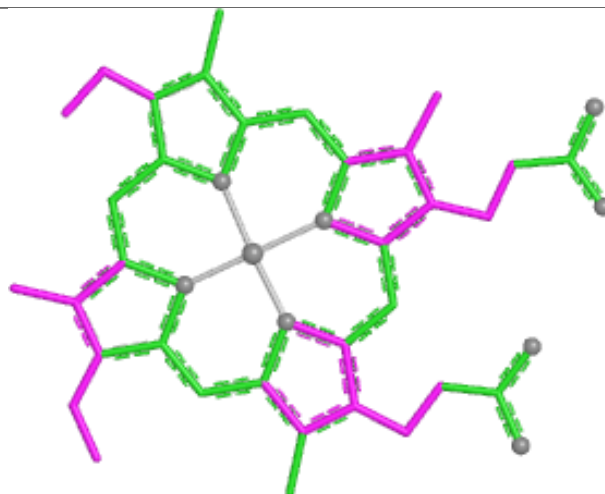


Rings

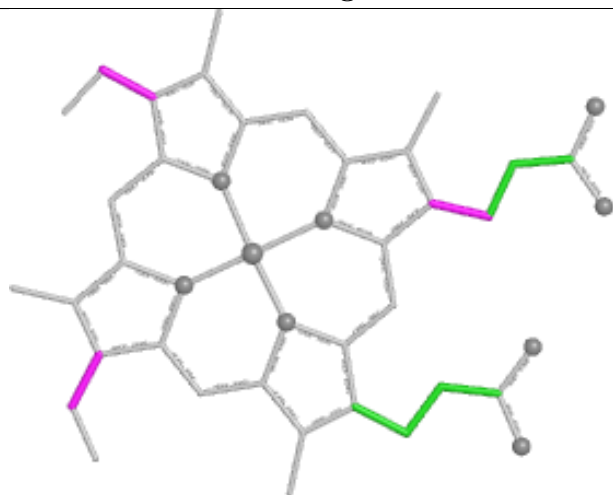
Ligand HEC D 501



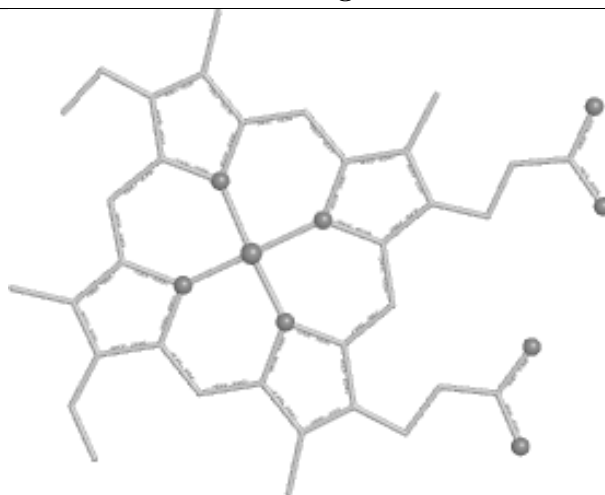
Bond lengths



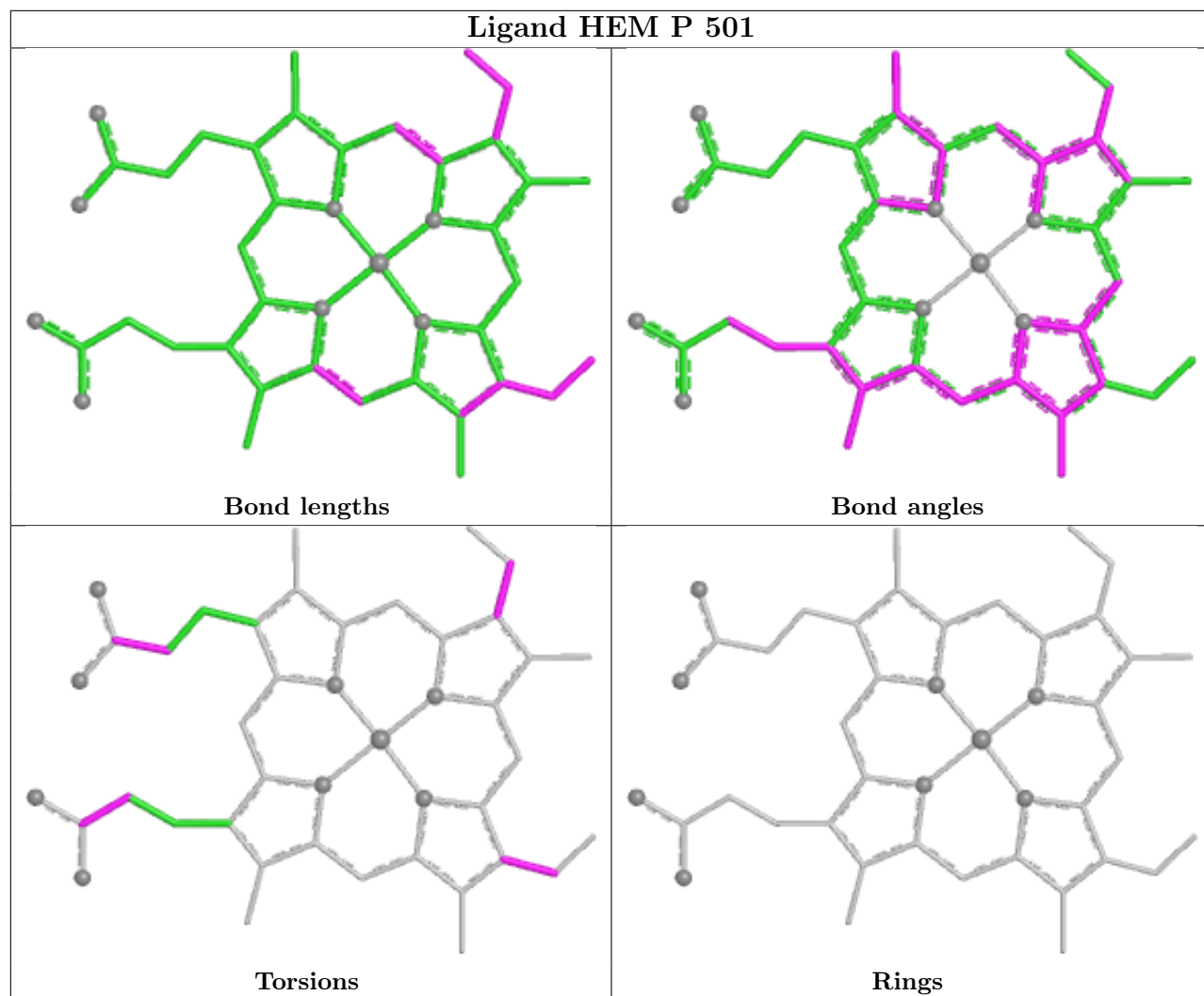
Bond angles

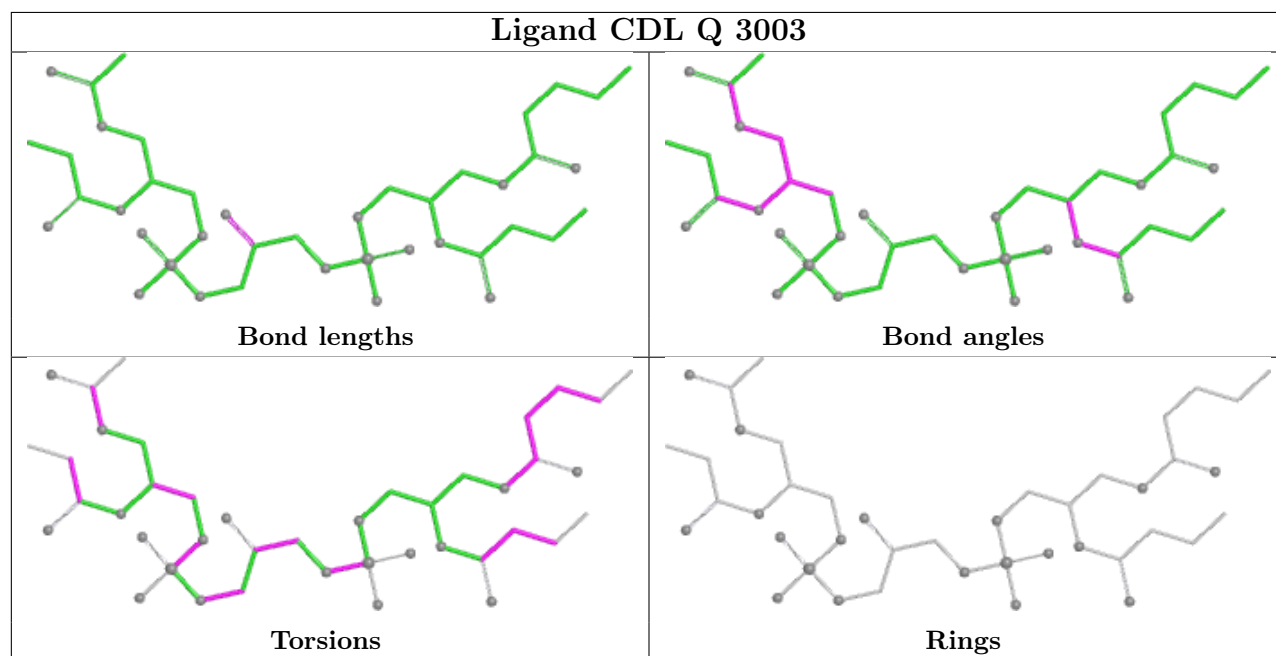
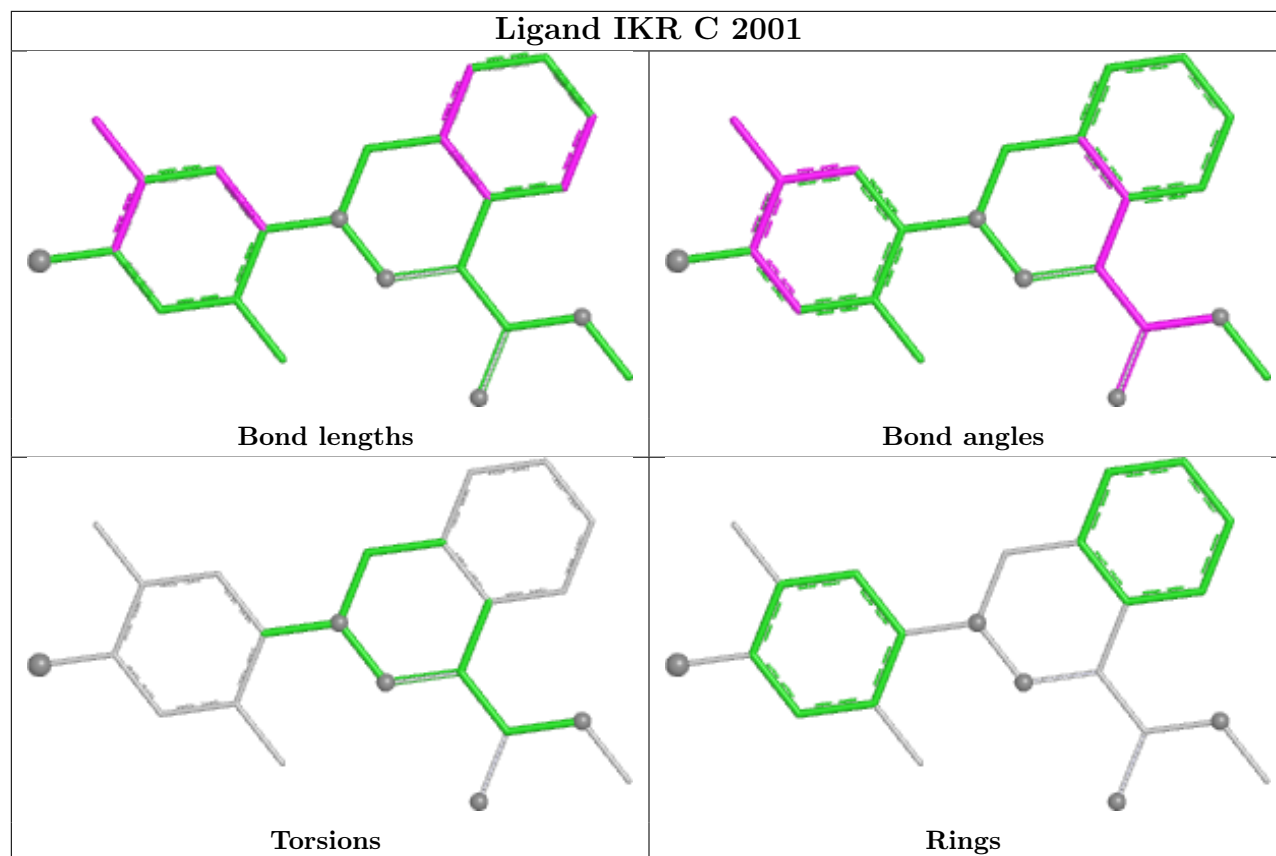


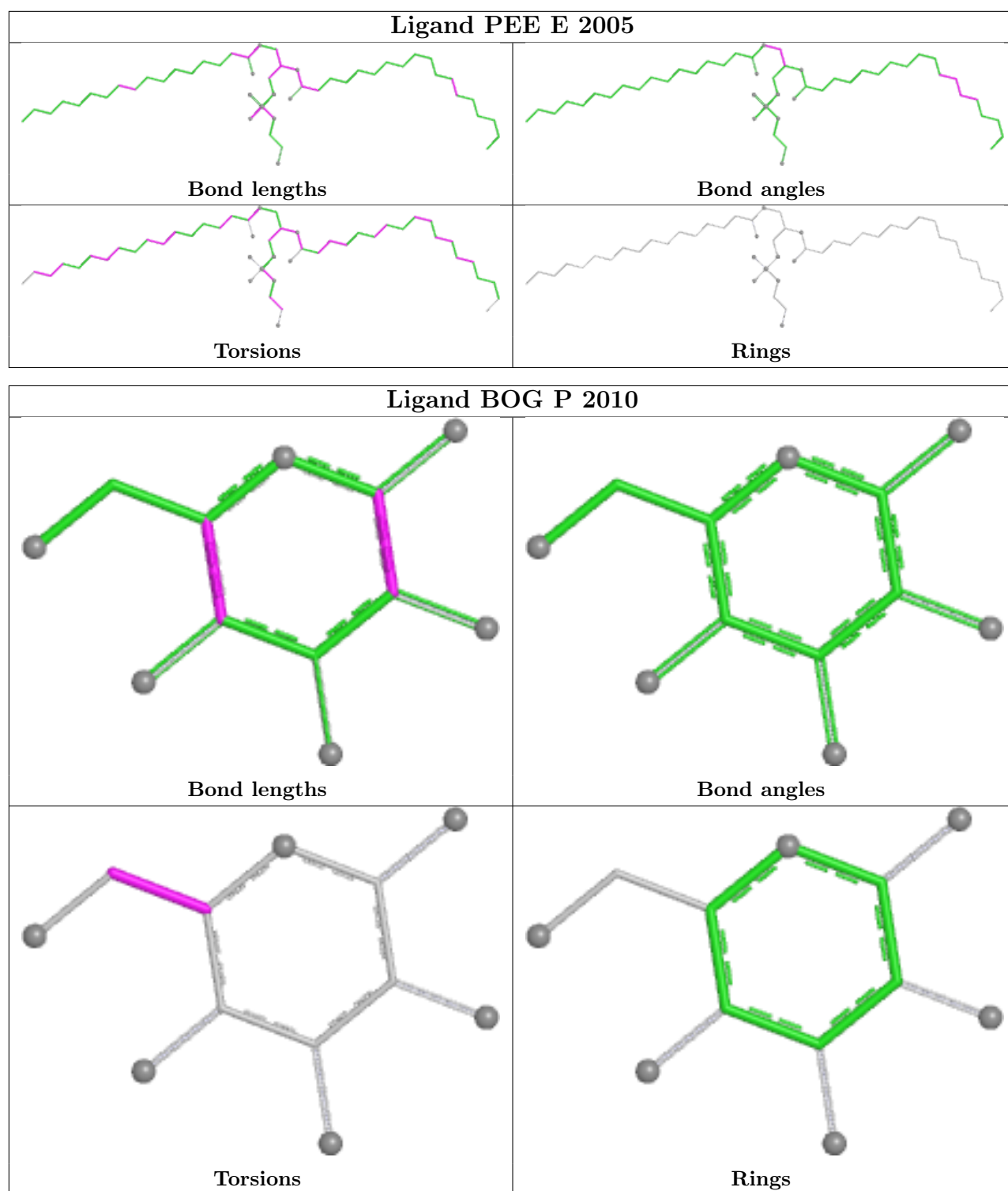
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	-0.40	1 (0%) 91 82	56, 103, 147, 160	0
1	N	442/446 (99%)	-0.29	2 (0%) 87 69	65, 100, 132, 147	0
2	B	426/441 (96%)	-0.19	4 (0%) 81 58	85, 126, 182, 218	0
2	O	422/441 (95%)	-0.29	0 100 100	70, 108, 147, 161	0
3	C	380/380 (100%)	-0.65	1 (0%) 90 77	40, 64, 131, 204	0
3	P	379/380 (99%)	-0.32	4 (1%) 78 54	52, 97, 148, 187	0
4	D	241/241 (100%)	-0.64	0 100 100	48, 72, 121, 138	0
4	Q	241/241 (100%)	-0.17	0 100 100	74, 108, 149, 167	0
5	E	196/196 (100%)	0.31	9 (4%) 37 21	57, 169, 205, 207	125 (63%)
5	R	196/196 (100%)	0.15	7 (3%) 46 26	64, 172, 215, 220	1 (0%)
6	F	101/110 (91%)	-0.66	0 100 100	56, 75, 97, 116	0
6	S	101/110 (91%)	-0.26	1 (0%) 79 57	87, 124, 174, 190	0
7	G	80/81 (98%)	-0.41	2 (2%) 58 35	58, 86, 158, 166	0
7	T	79/81 (97%)	0.22	3 (3%) 44 25	81, 126, 222, 227	0
8	H	69/77 (89%)	-0.42	0 100 100	70, 98, 119, 154	0
8	U	67/77 (87%)	0.20	4 (5%) 27 17	133, 165, 209, 211	0
9	I	31/47 (65%)	1.74	8 (25%) 1 2	147, 185, 257, 259	0
9	V	31/47 (65%)	1.21	7 (22%) 2 2	121, 163, 242, 244	0
10	J	61/61 (100%)	-0.48	0 100 100	75, 93, 139, 177	0
10	W	60/61 (98%)	-0.37	0 100 100	84, 108, 157, 165	0
All	All	4046/4160 (97%)	-0.26	53 (1%) 75 51	40, 104, 189, 259	126 (3%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	63	ASP	5.0
9	I	51	CYS	5.0
9	I	50	LEU	4.9
5	E	142	LEU	4.1
8	U	50	THR	3.6
9	I	74	ALA	3.4
9	V	51	CYS	3.3
1	A	69	LYS	3.2
9	I	64	LEU	3.0
1	N	376	CYS	3.0
5	E	106	ILE	2.9
5	E	134	ILE	2.9
9	V	49	LEU	2.9
7	T	44	GLN	2.9
7	G	5	GLY	2.8
5	R	98	VAL	2.7
1	N	75	PHE	2.7
9	V	63	ASP	2.7
5	R	18	VAL	2.6
3	C	7	LYS	2.6
5	R	167	ALA	2.6
9	I	57	GLY	2.5
9	I	58	ARG	2.5
2	B	26	ILE	2.5
3	P	3	PRO	2.5
5	E	145	VAL	2.4
7	T	4	PHE	2.4
3	P	21	ASP	2.4
8	U	61	PHE	2.4
2	B	224	LEU	2.4
9	V	50	LEU	2.4
5	R	165	TYR	2.3
6	S	55	TYR	2.3
2	B	24	LEU	2.3
5	E	120	PRO	2.3
9	I	75	SER	2.3
8	U	44	VAL	2.3
3	P	26	SER	2.3
5	R	159	PRO	2.3
5	E	143	GLY	2.3
2	B	289	SER	2.3
5	R	138	VAL	2.2
9	V	53	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	104	ALA	2.2
3	P	207	ASN	2.2
7	T	8	ALA	2.1
9	V	56	SER	2.1
7	G	2	ILE	2.1
9	V	61	ARG	2.1
5	R	120	PRO	2.0
5	E	75	GLU	2.0
5	E	98	VAL	2.0
8	U	37	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	BOG	P	3091	13/20	0.42	0.17	298,299,299,300	0
11	PEE	P	3008	5/51	0.59	0.10	184,184,184,185	0
11	PEE	A	2008	18/51	0.69	0.20	89,197,198,199	0
16	CDL	Q	3003	42/100	0.73	0.20	183,193,208,208	0
20	BOG	P	2010	12/20	0.73	0.18	248,249,250,250	0
16	CDL	P	3004	40/100	0.73	0.16	147,157,162,162	0
21	FES	R	501	4/4	0.84	0.11	201,201,201,202	0
21	FES	E	501	4/4	0.85	0.12	257,257,257,257	4
11	PEE	R	3005	50/51	0.86	0.19	114,131,139,141	0
16	CDL	D	2003	42/100	0.87	0.17	134,141,153,153	0
12	UNL	A	3231	1/-	0.87	0.08	45,45,45,45	0
20	BOG	Q	3009	20/20	0.87	0.14	103,118,120,121	0
16	CDL	C	2004	40/100	0.87	0.12	103,110,126,128	0

Continued on next page...

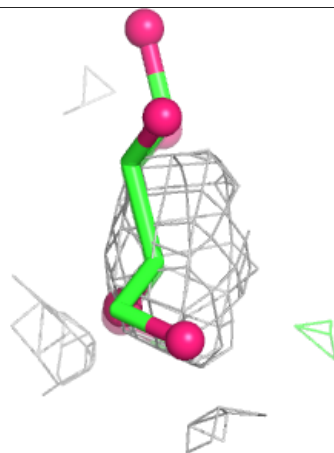
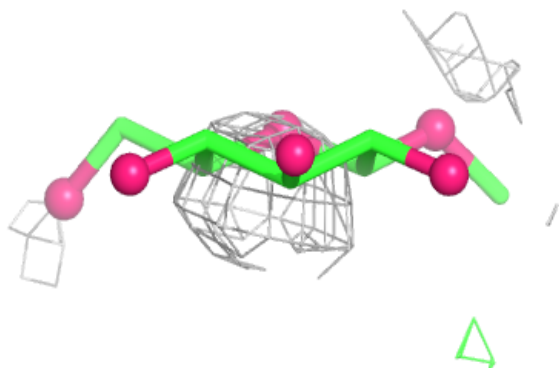
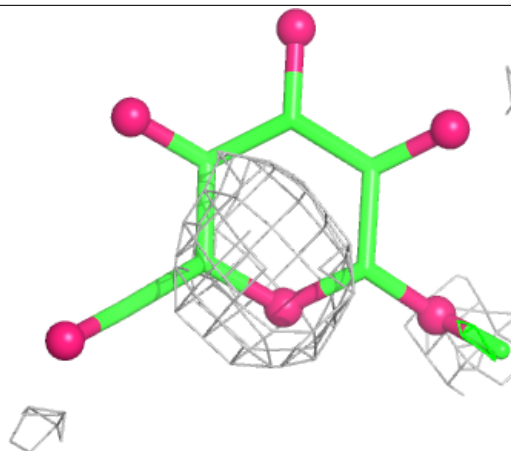
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	BOG	D	2091	13/20	0.87	0.15	191,192,193,193	0
12	UNL	P	4236	1/-	0.88	0.07	94,94,94,94	0
11	PEE	E	2005	50/51	0.89	0.16	113,127,137,139	0
11	PEE	P	3007	49/51	0.89	0.13	102,116,140,141	0
15	UQ	P	3002	19/63	0.91	0.22	134,146,148,149	0
11	PEE	C	2007	49/51	0.92	0.12	68,80,102,104	0
20	BOG	D	2009	20/20	0.93	0.11	93,104,108,108	0
12	UNL	C	4234	1/-	0.94	0.09	58,58,58,58	0
12	UNL	A	3284	1/-	0.94	0.12	31,31,31,31	0
12	UNL	N	4231	1/-	0.95	0.13	90,90,90,90	0
18	GOL	P	3011	6/6	0.95	0.14	103,108,109,110	0
15	UQ	C	2002	19/63	0.95	0.15	107,111,115,115	0
18	GOL	C	2011	6/6	0.96	0.12	69,72,75,78	0
19	HEC	Q	501	43/43	0.97	0.09	87,91,97,99	0
14	IKR	P	3001	25/25	0.97	0.11	86,89,108,116	0
17	ZN	C	2012	1/1	0.98	0.03	104,104,104,104	0
13	HEM	P	502	43/43	0.98	0.09	68,73,82,82	0
13	HEM	P	501	43/43	0.98	0.08	65,72,79,81	0
19	HEC	D	501	43/43	0.98	0.07	57,60,68,70	0
17	ZN	P	3012	1/1	0.99	0.04	121,121,121,121	0
14	IKR	C	2001	25/25	0.99	0.08	65,67,75,79	0
13	HEM	C	501	43/43	0.99	0.06	48,52,62,66	0
13	HEM	C	502	43/43	0.99	0.07	41,46,56,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

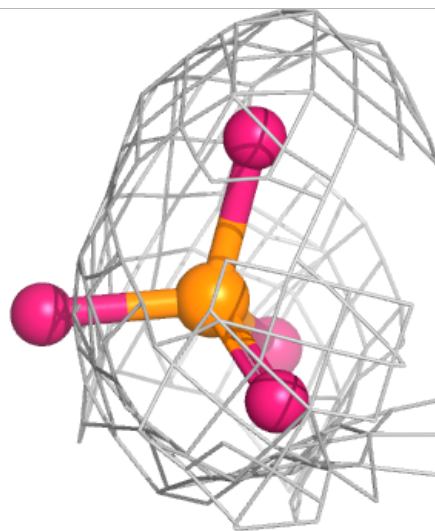
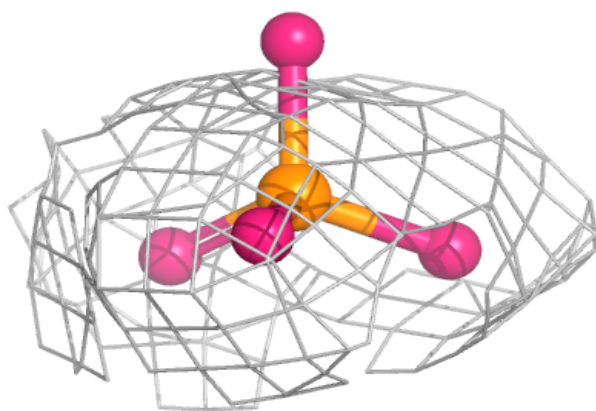
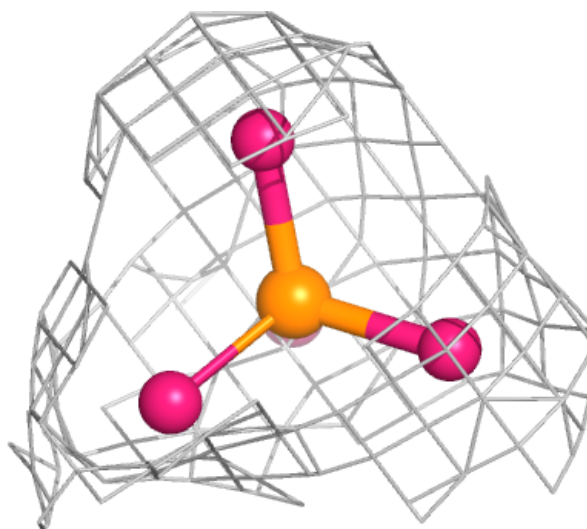
Electron density around BOG P 3091:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



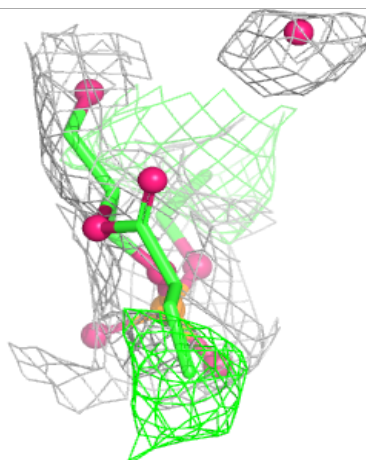
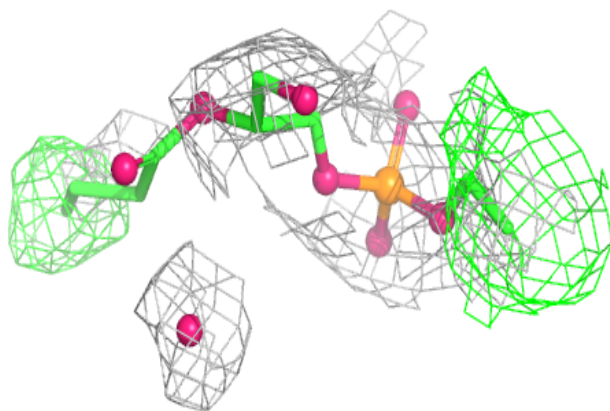
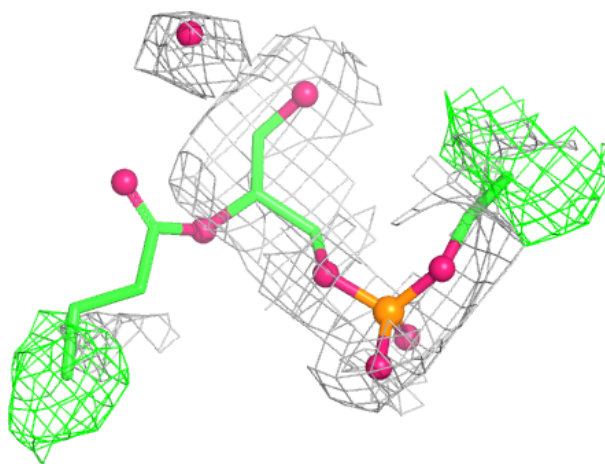
Electron density around PEE P 3008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



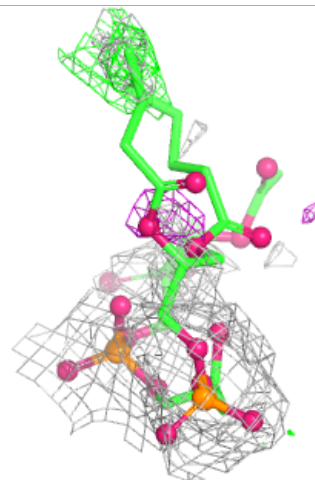
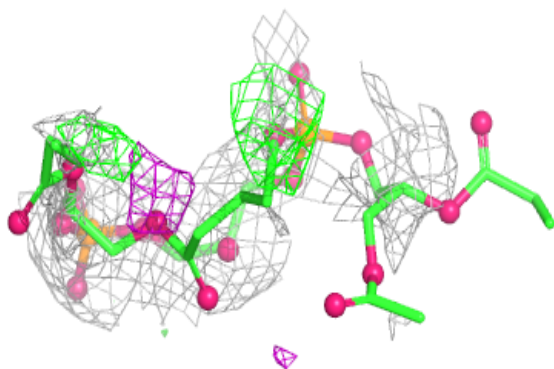
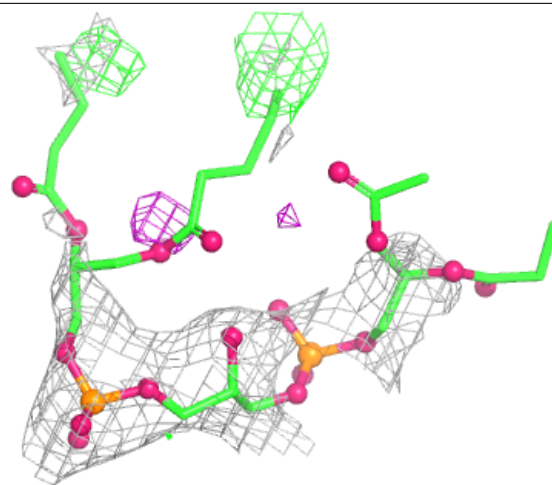
Electron density around PEE A 2008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



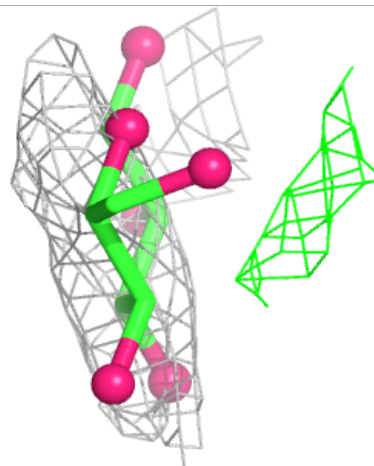
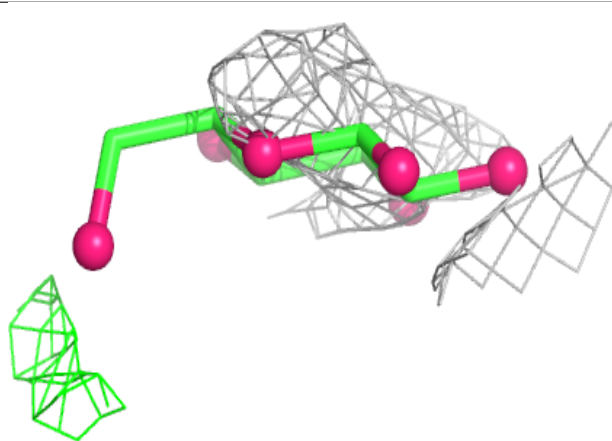
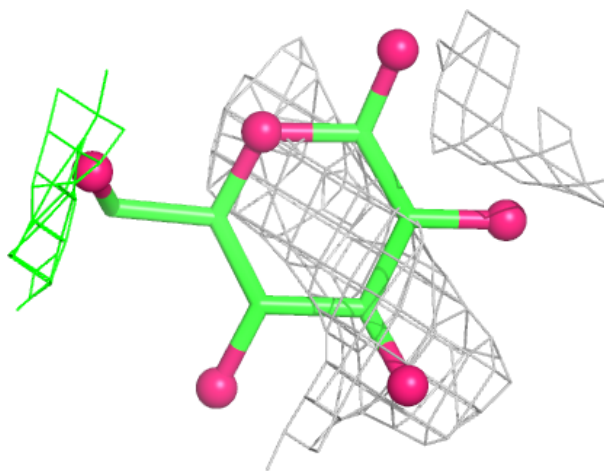
Electron density around CDL Q 3003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



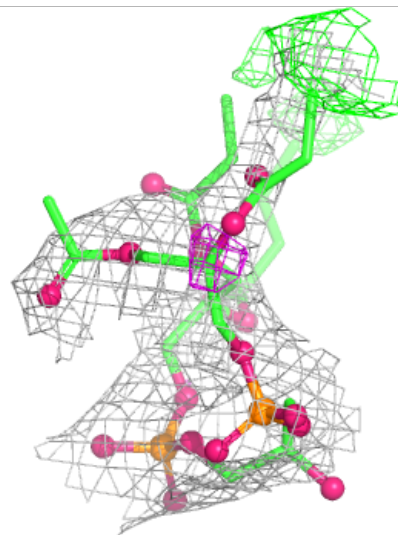
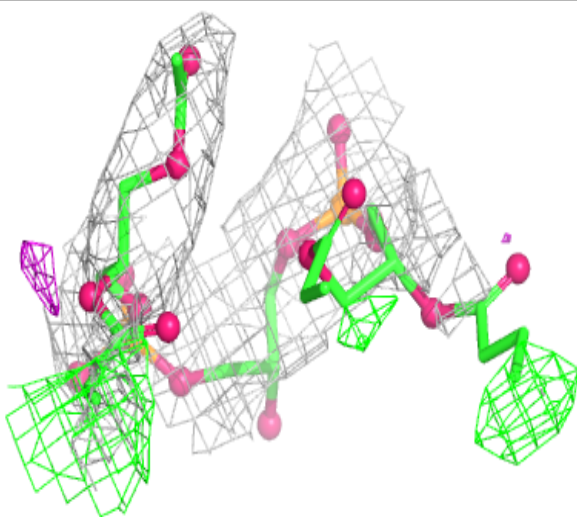
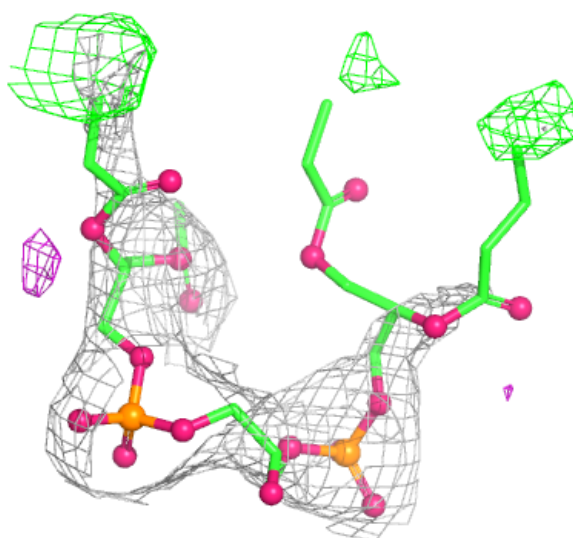
Electron density around BOG P 2010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



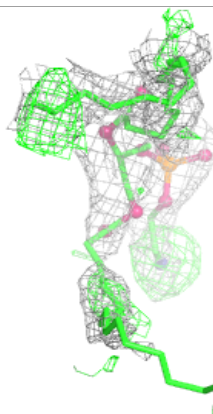
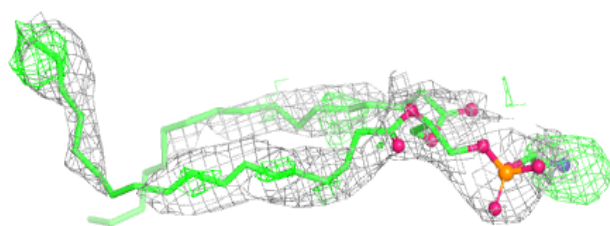
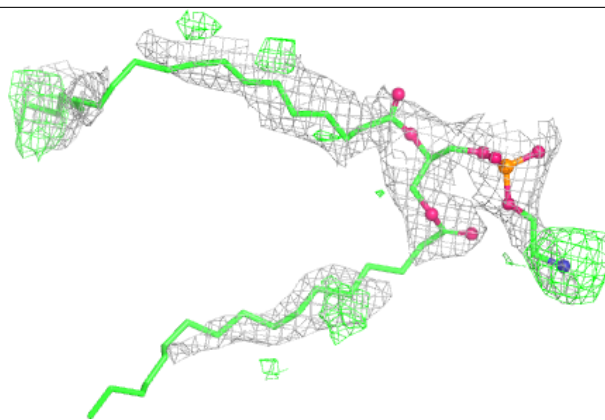
Electron density around CDL P 3004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



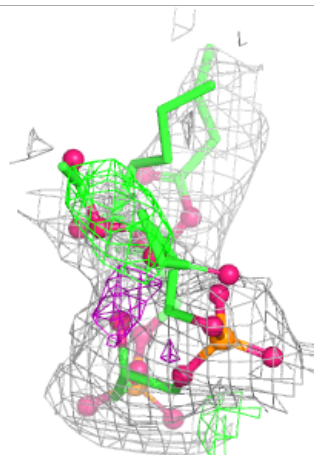
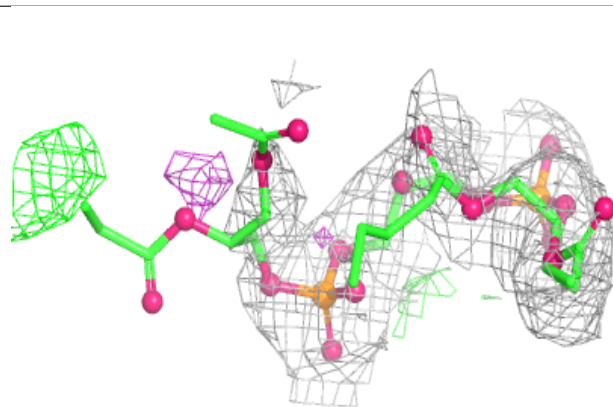
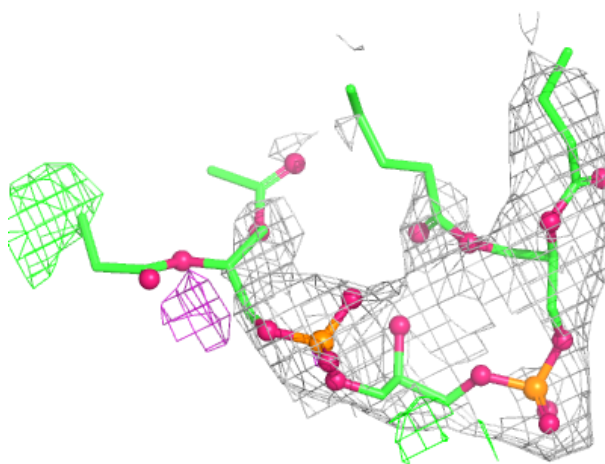
Electron density around PEE R 3005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



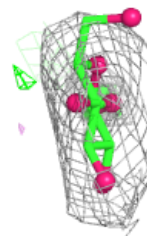
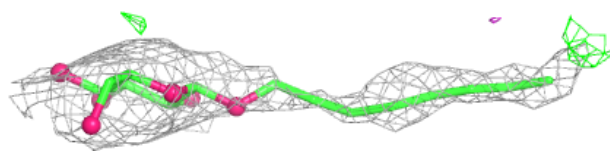
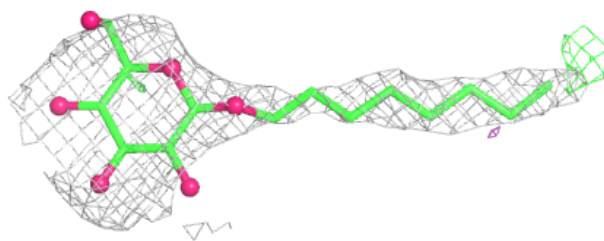
Electron density around CDL D 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



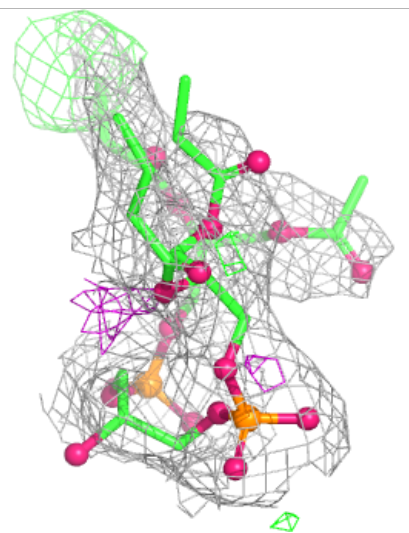
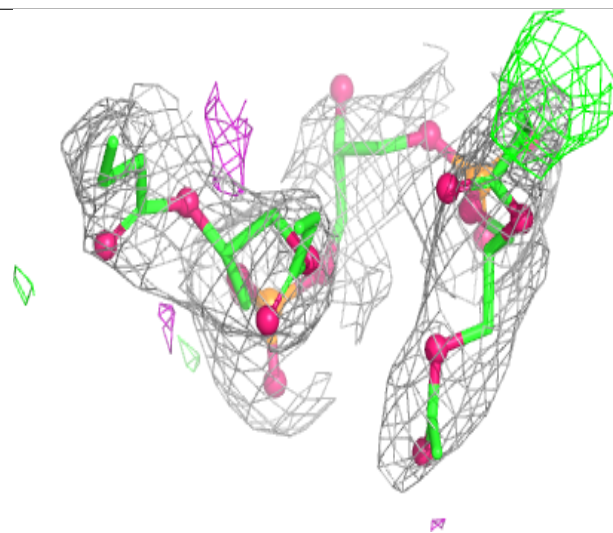
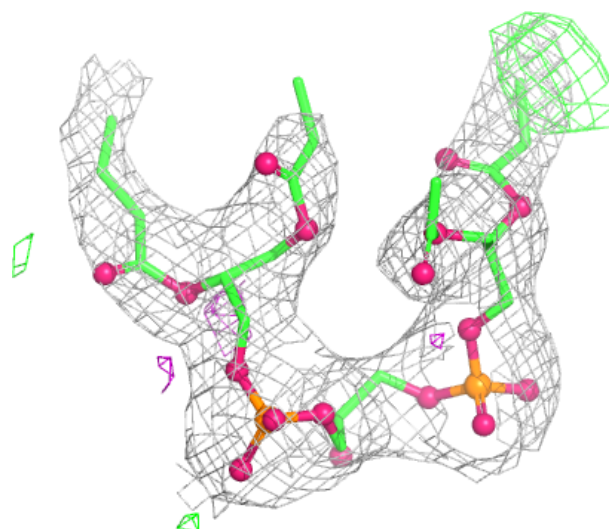
Electron density around BOG Q 3009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



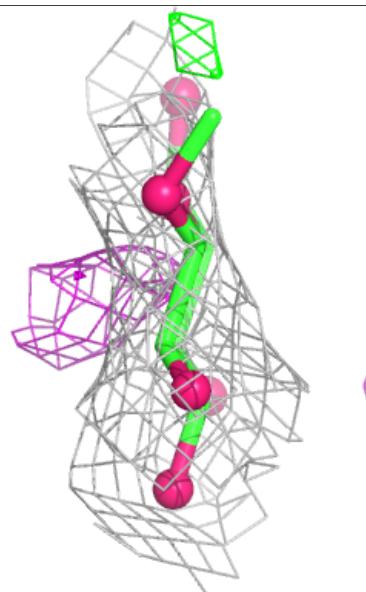
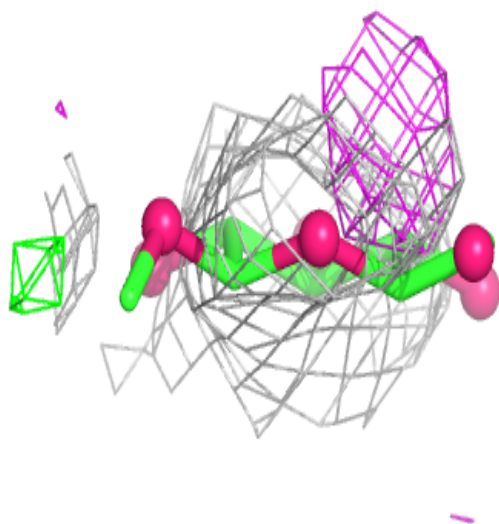
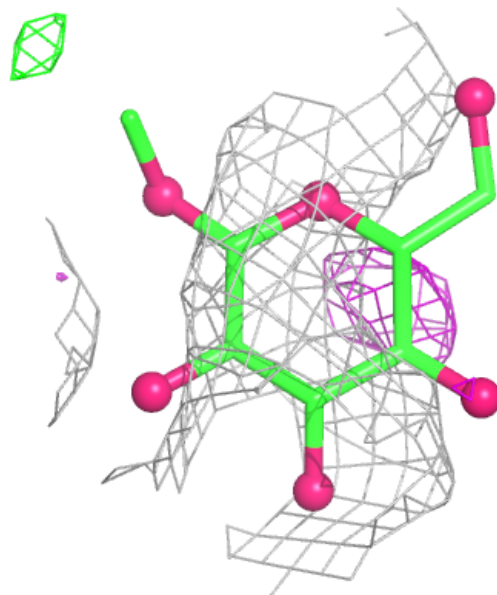
Electron density around CDL C 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



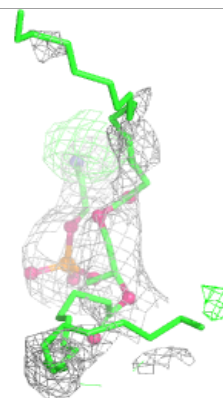
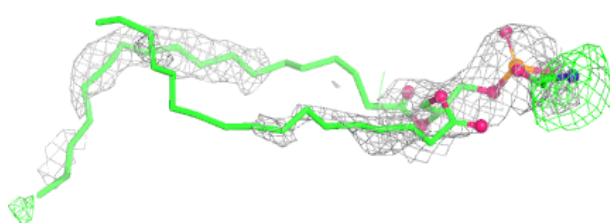
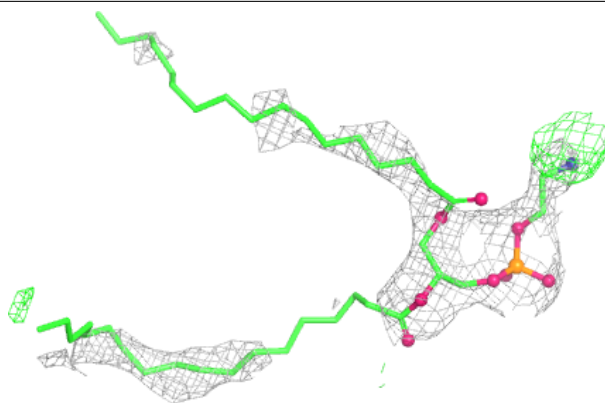
Electron density around BOG D 2091:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

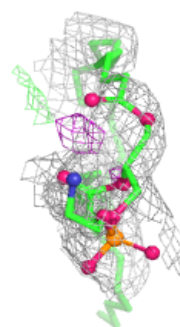
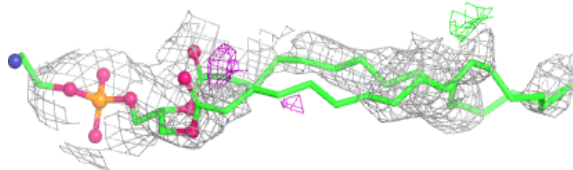
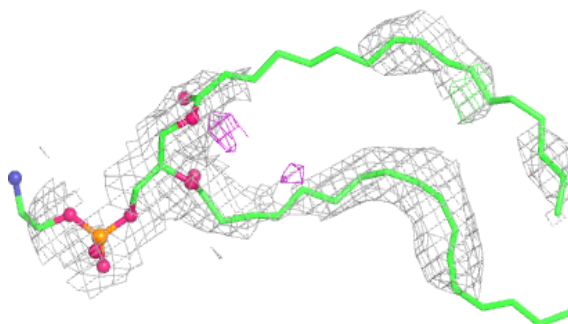


Electron density around PEE E 2005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

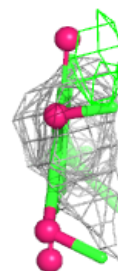
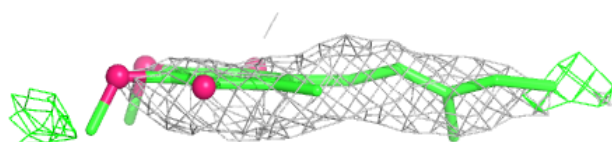
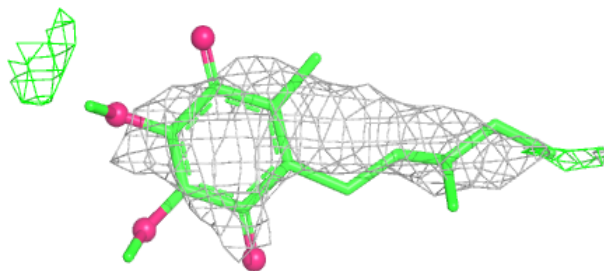
**Electron density around PEE P 3007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

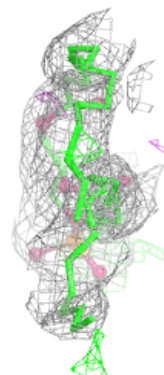
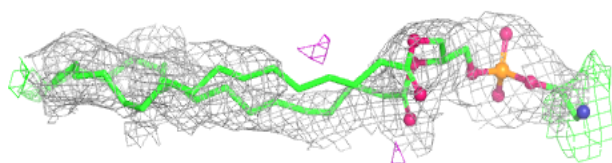
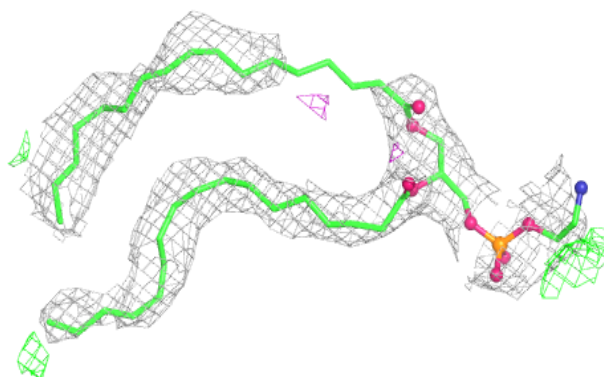


Electron density around UQ P 3002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

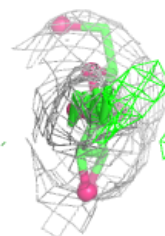
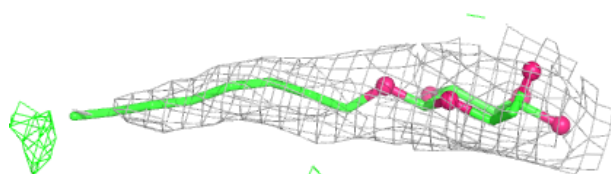
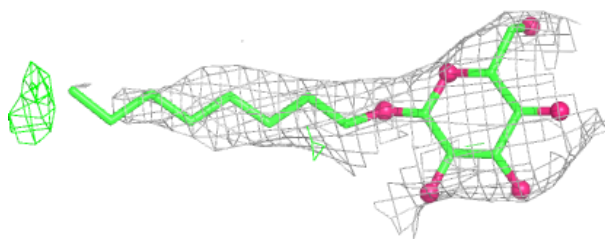
**Electron density around PEE C 2007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

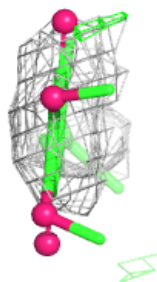
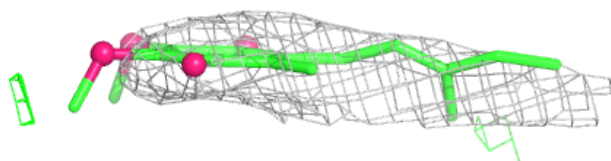
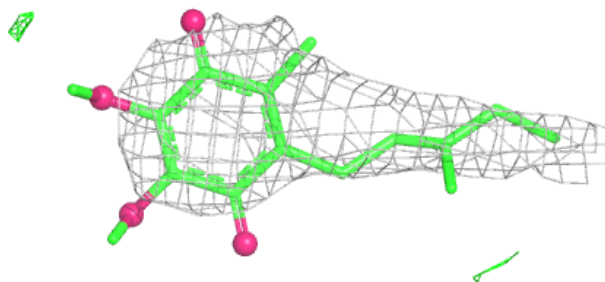


Electron density around BOG D 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

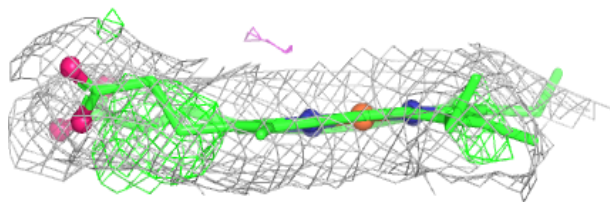
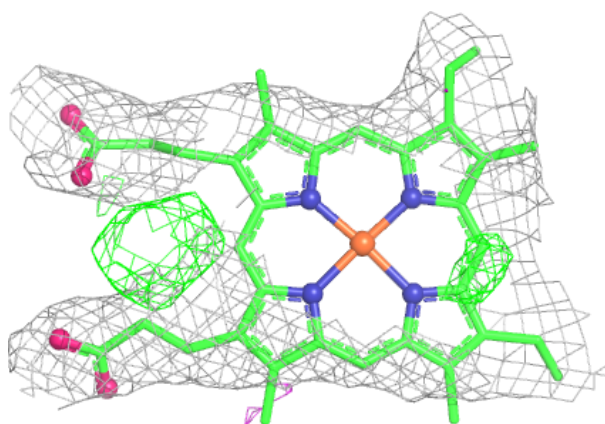
**Electron density around UQ C 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

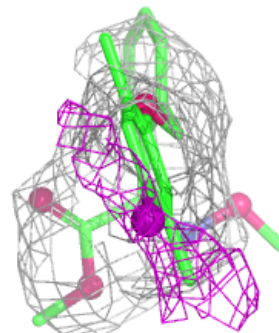
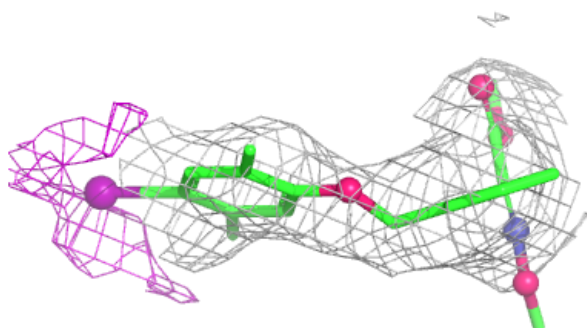
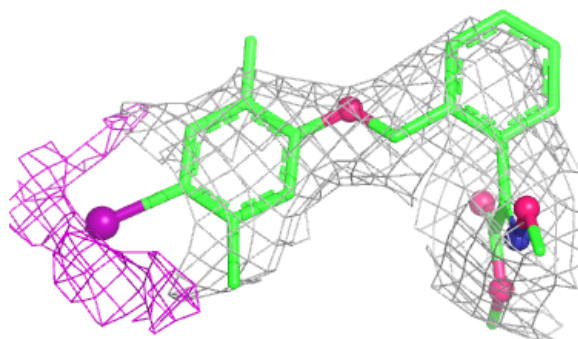


Electron density around HEC Q 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

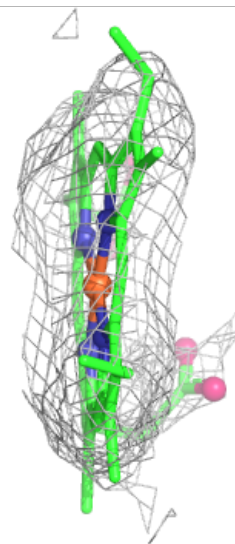
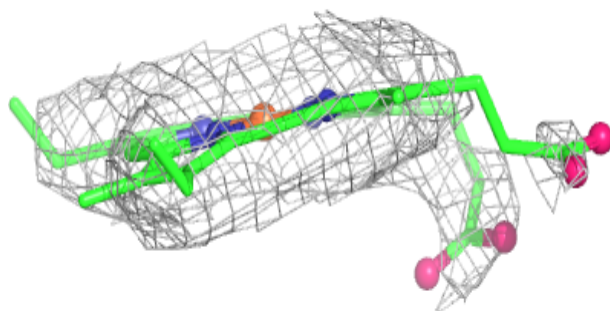
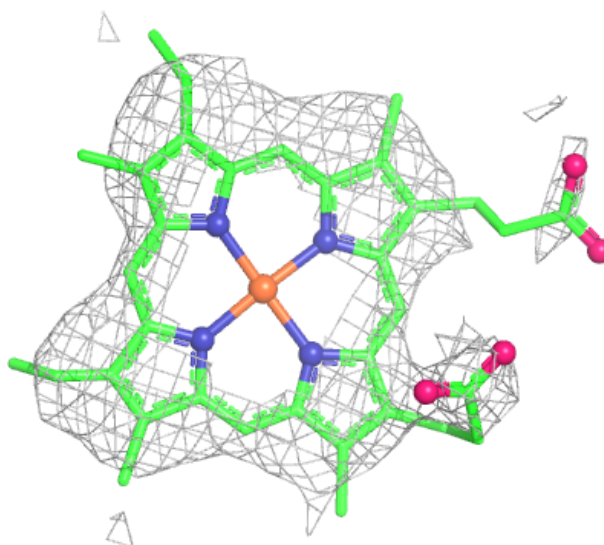
**Electron density around IKR P 3001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



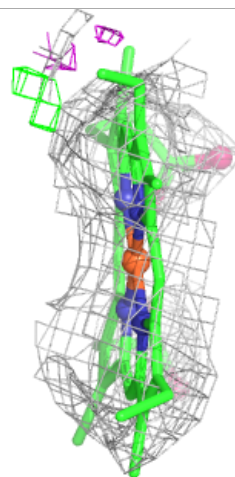
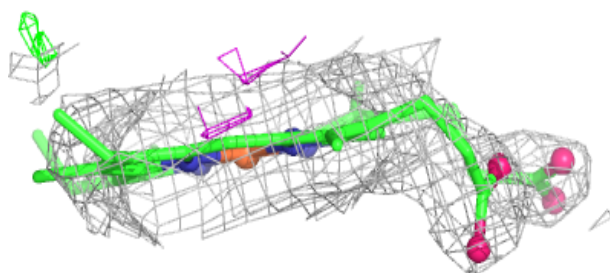
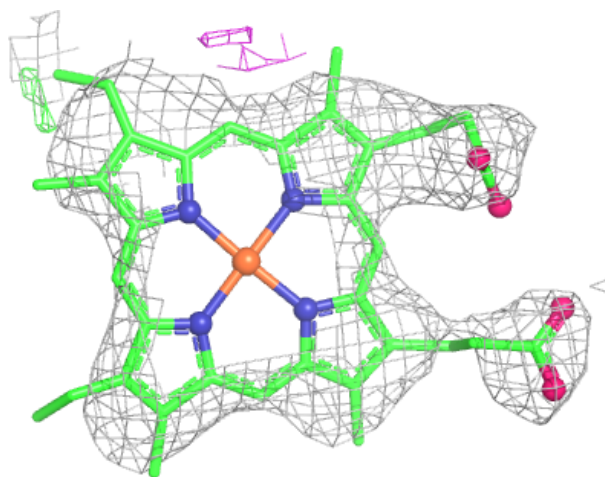
Electron density around HEM P 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



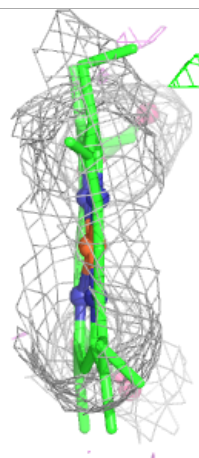
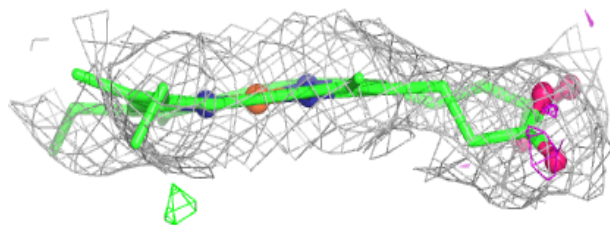
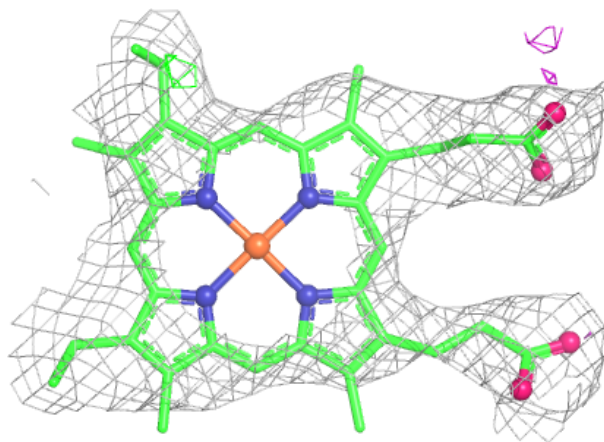
Electron density around HEM P 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



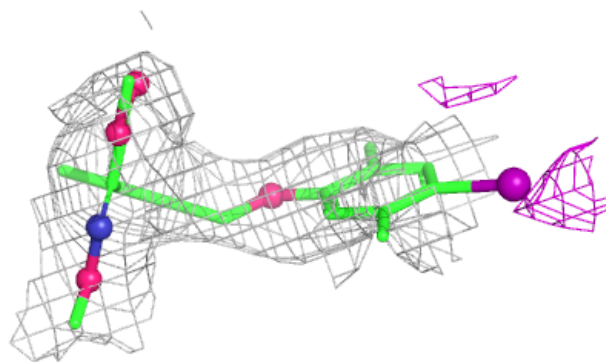
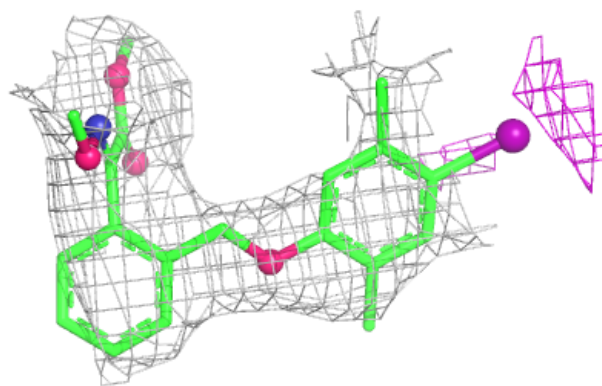
Electron density around HEC D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



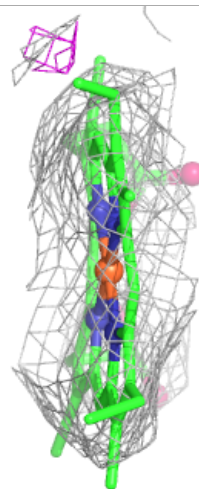
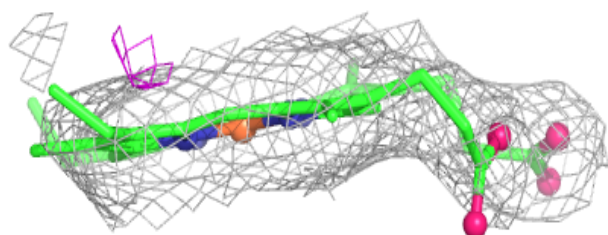
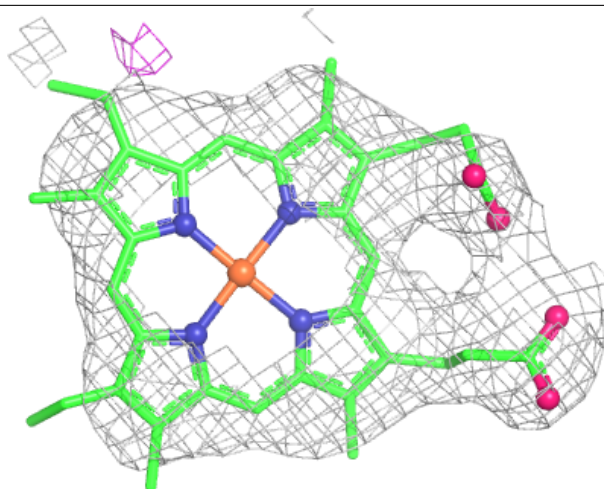
Electron density around IKR C 2001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



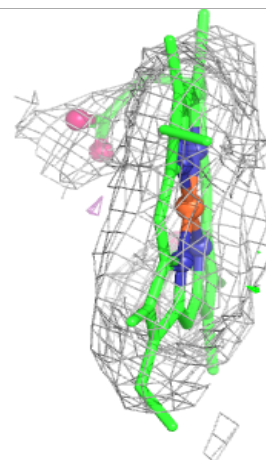
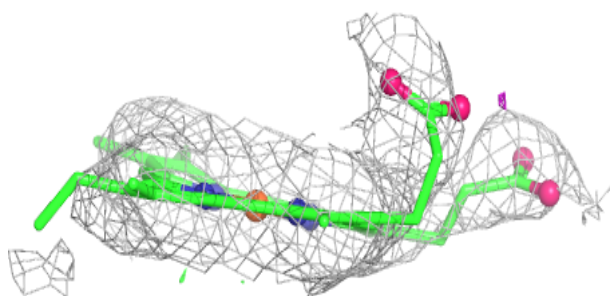
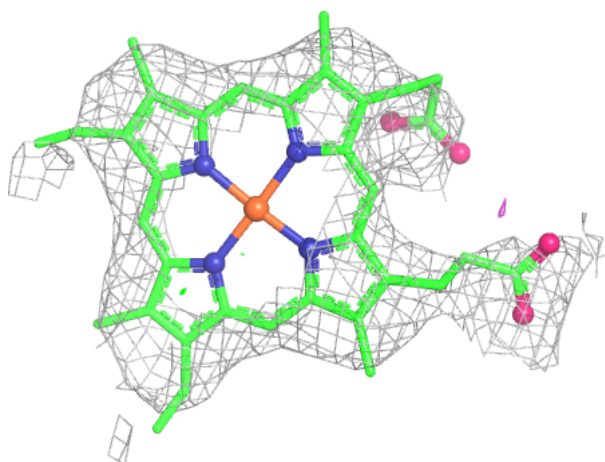
Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.