



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:53 PM EDT

PDB ID : 3H1I / pdb_00003h1i
Title : Stigmatellin and antimycin bound cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.;
Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on : 2009-04-12
Resolution : 3.53 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:

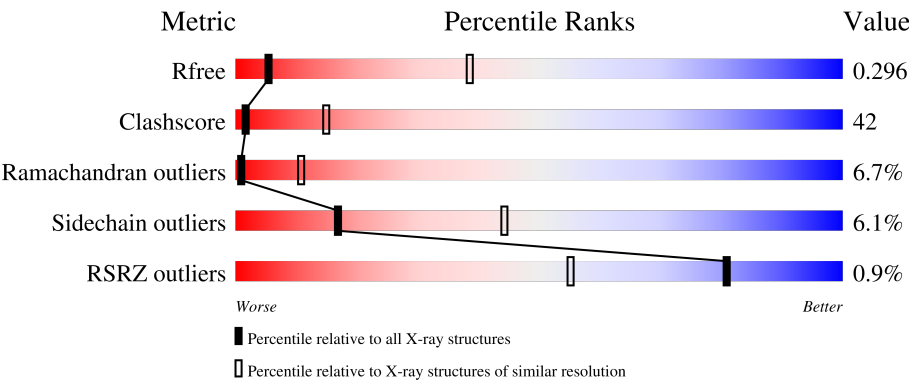
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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.



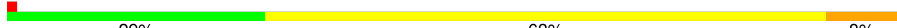
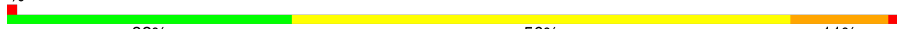
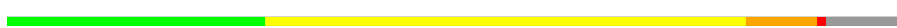
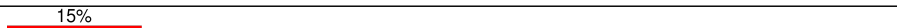
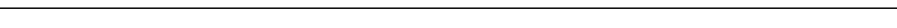
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	36%54%9%..
1	N	446	% 34%55%9%..
2	B	441	% 34%51%10%5%
2	O	441	% 36%49%10%.
3	C	380	32%58%10%.

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	N	3008	-	X	-	-
15	ANY	C	2002	X	-	-	-
15	ANY	P	3002	X	-	-	-
18	HEC	D	501	X	-	-	-
18	HEC	Q	501	X	-	-	-
19	FES	E	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	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 UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
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 CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

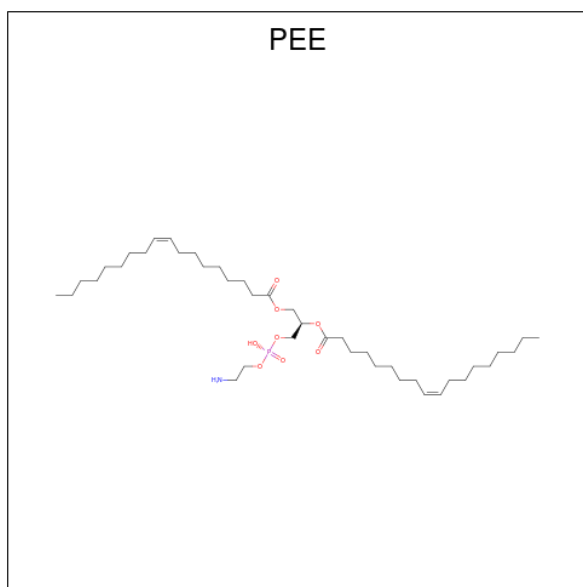
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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	59	Total	C	N	O	0	0	0
			478	311	85	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
			21	12	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	N	1	Total	O	P			0	0
			5	4	1				
11	P	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		

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

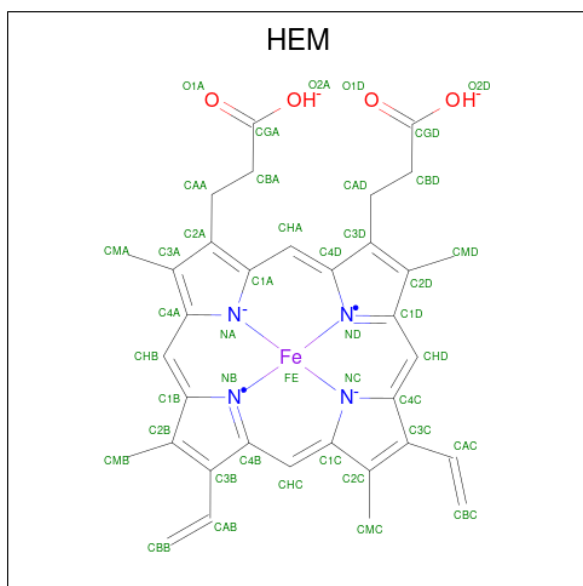
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total 1 O 1	0	0

Continued on next page...

Continued from previous page...

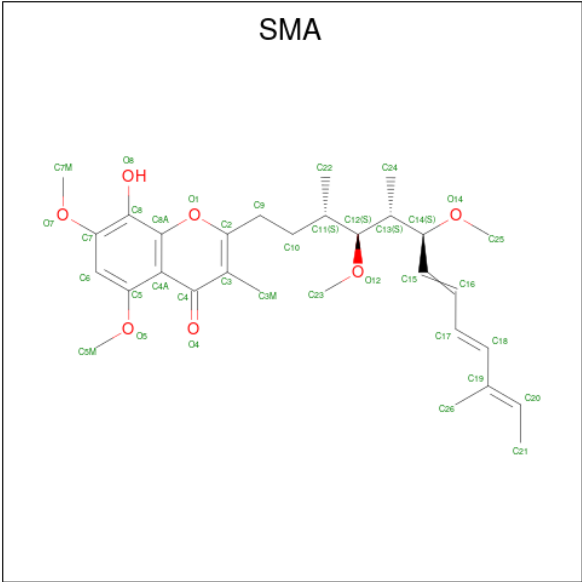
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	3	Total	O	0	0
			3	3		
12	E	2	Total	O	0	0
			2	2		
12	P	3	Total	O	0	0
			3	3		
12	R	1	Total	O	0	0
			1	1		

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



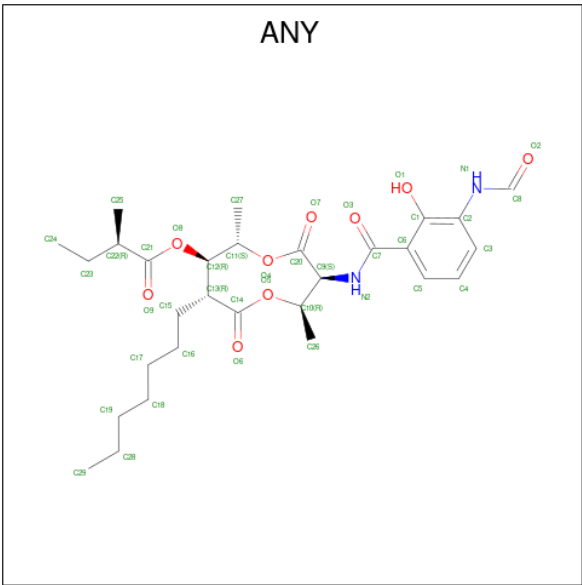
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 15 is 2-METHYL-BUTYRIC ACID 3-(3-FORMYLAMINO-2-HYDROXY-BENZ OYLAMINO)-8-HEPTYL-2,6-DIMETHYL-4,9-DIOXO-[1,5]DIOXONAN-7-YL ESTER (CCD ID: ANY) (formula: C₂₉H₄₂N₂O₉).



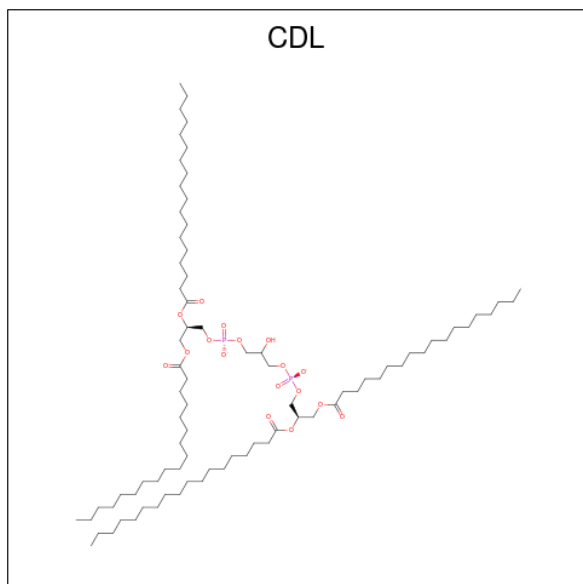
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	N	O	0	0
			37	26	2	9		

Continued on next page...

Continued from previous page...

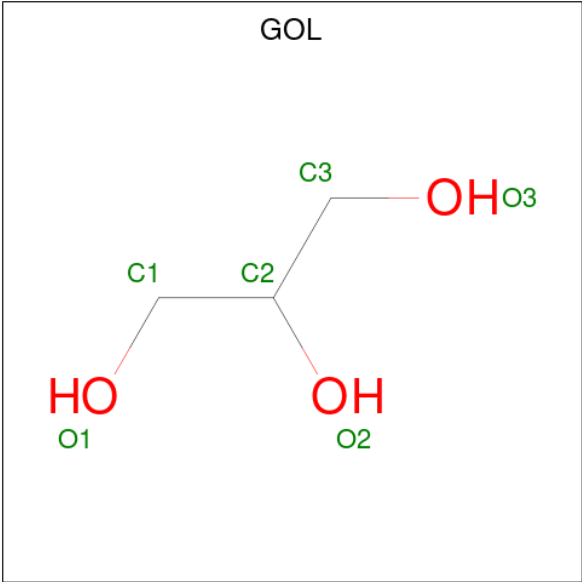
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	P	1	Total	C	N	O	0	0
			37	26	2	9		

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



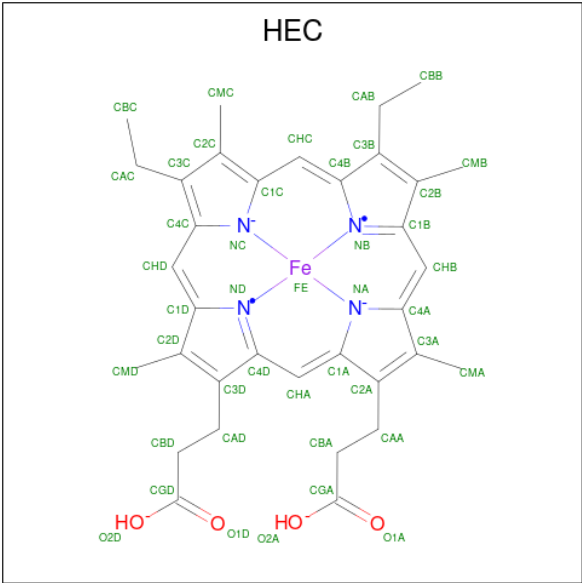
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	O	P	0	0
			40	21	17	2		
16	D	1	Total	C	O	P	0	0
			50	31	17	2		
16	P	1	Total	C	O	P	0	0
			40	21	17	2		
16	Q	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 17 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



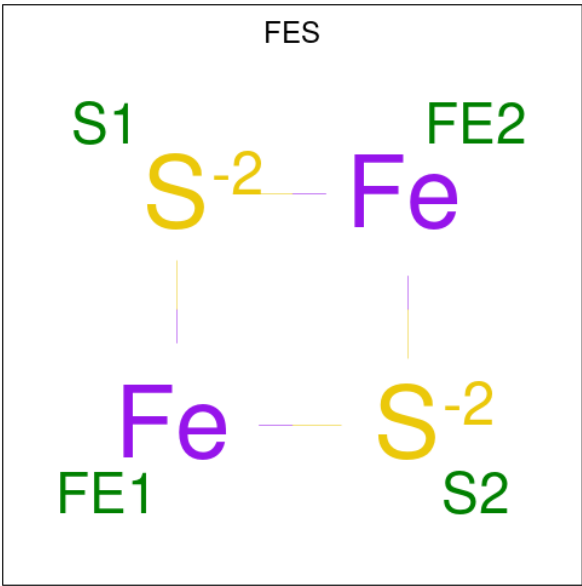
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			6	3	3		
17	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



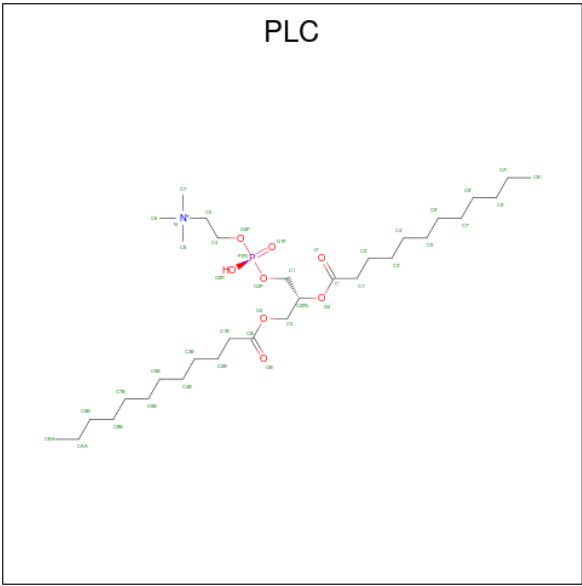
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
18	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

Continued on next page...

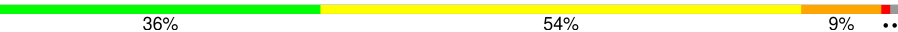
Continued from previous page...

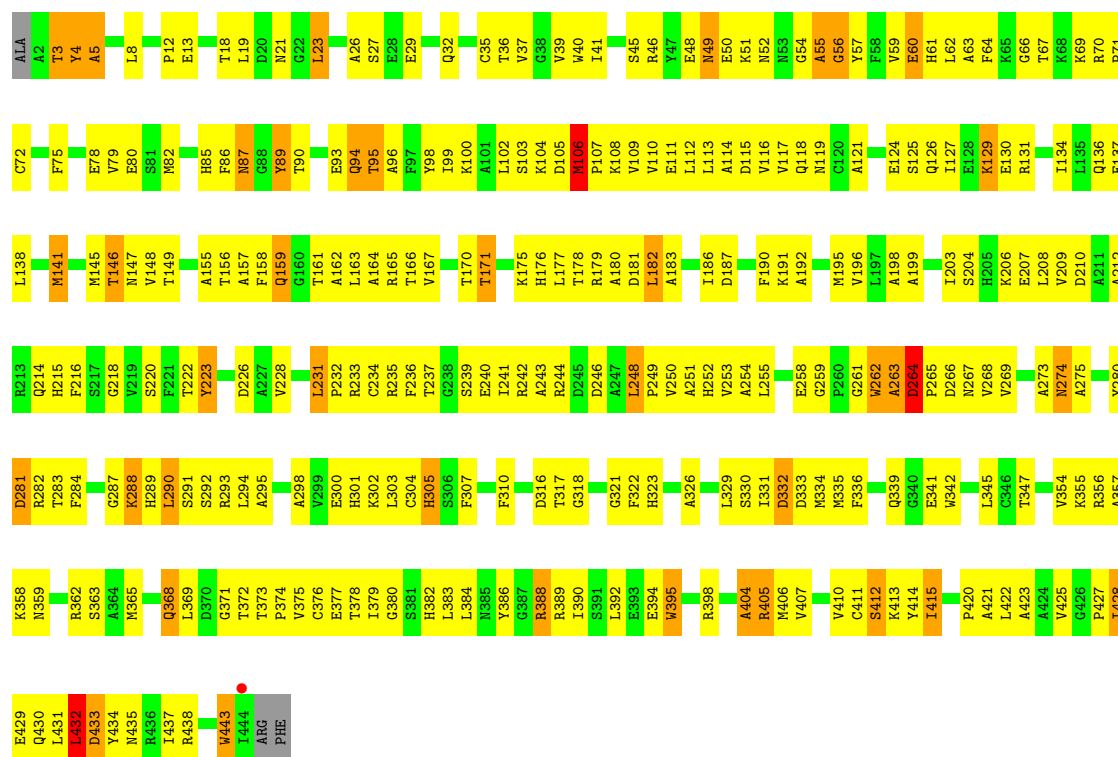
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

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.

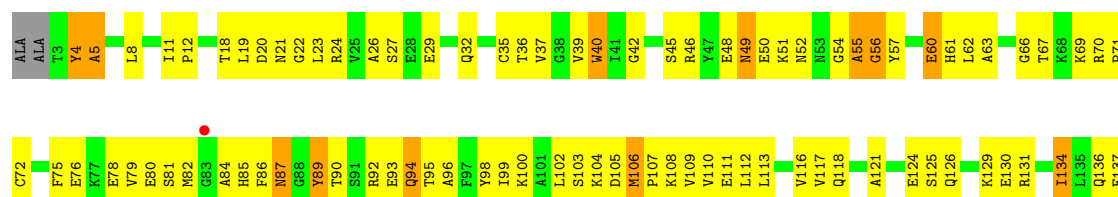
• Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

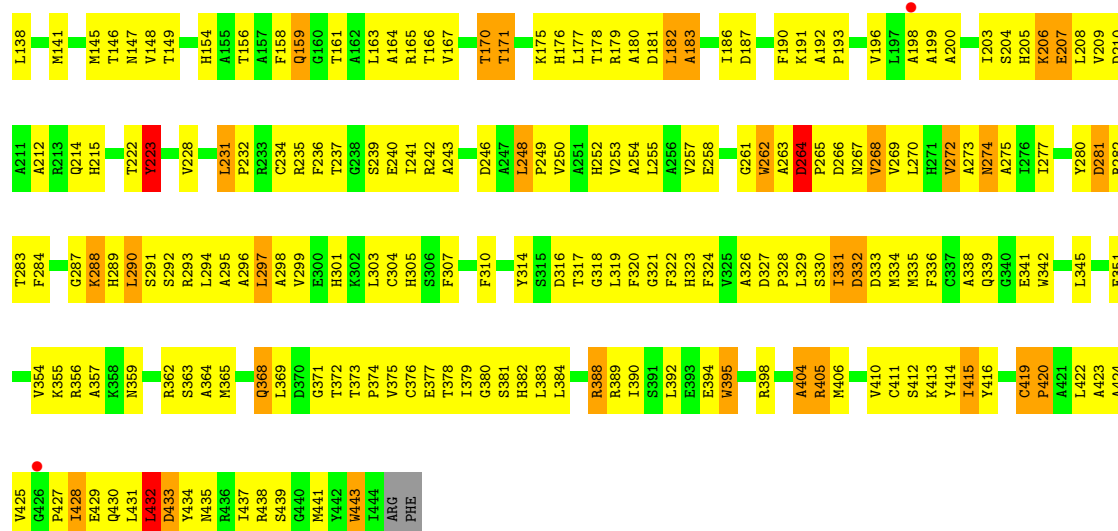
Chain A: 



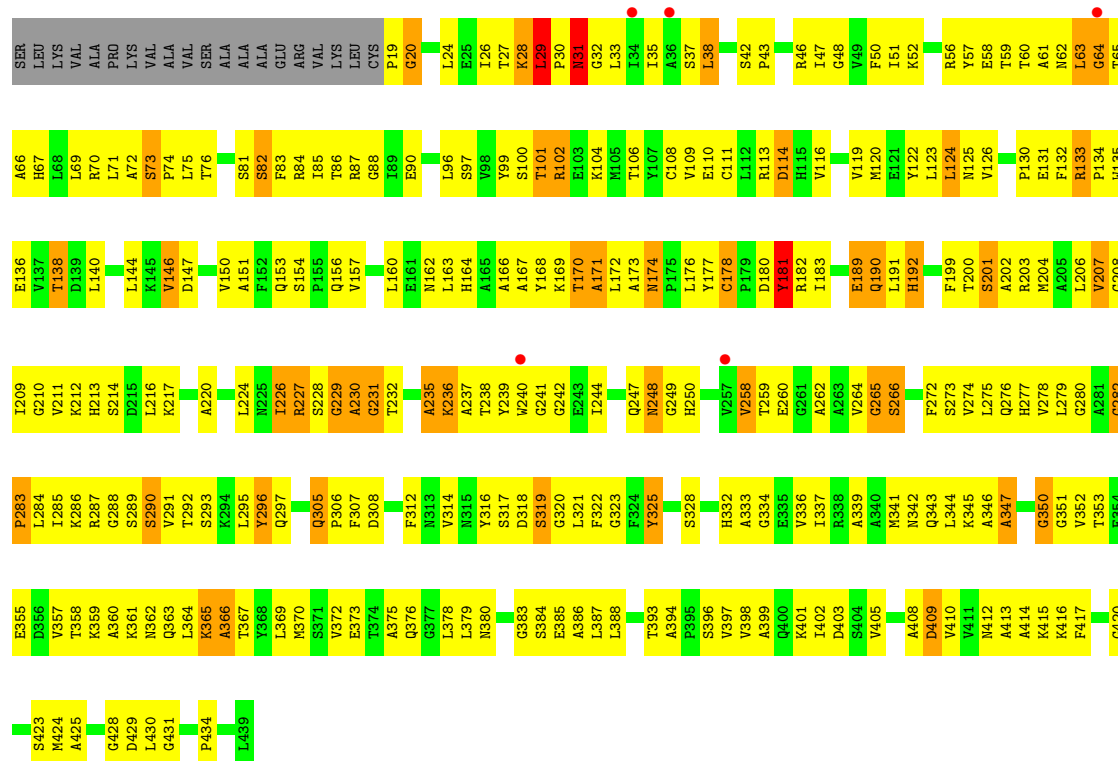
• Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

Chain N: 



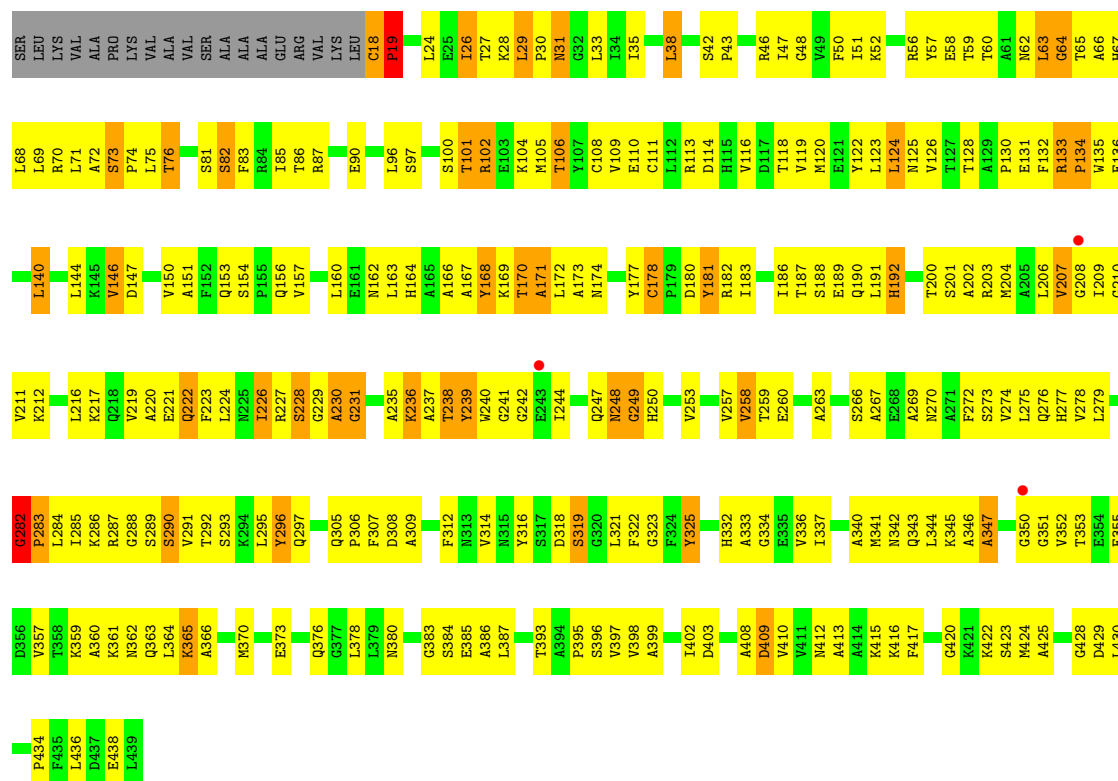


• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL



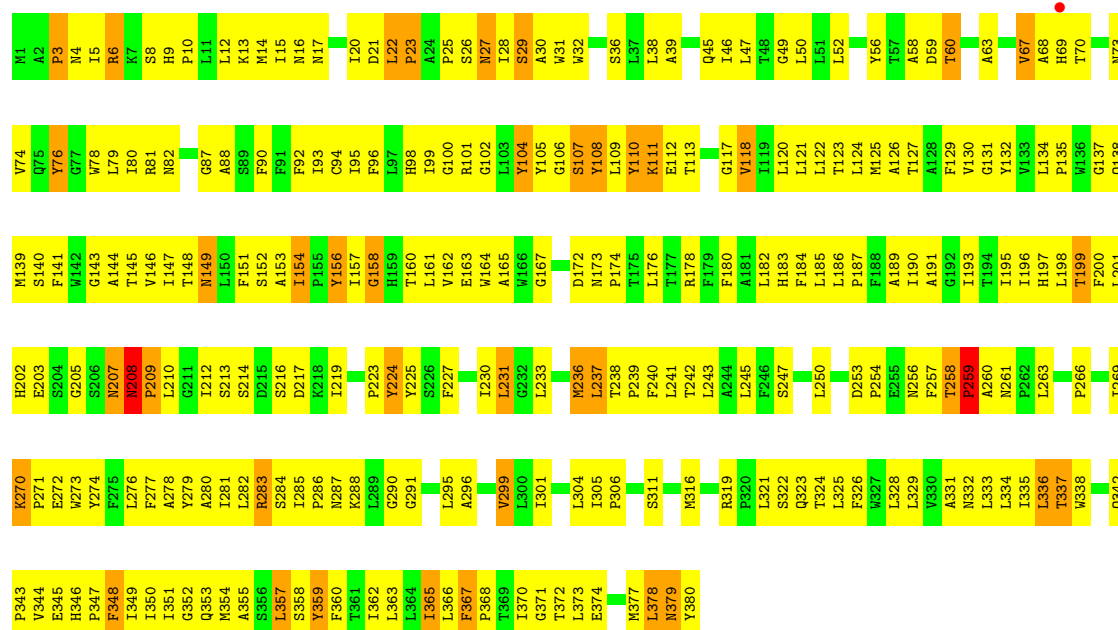
• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL





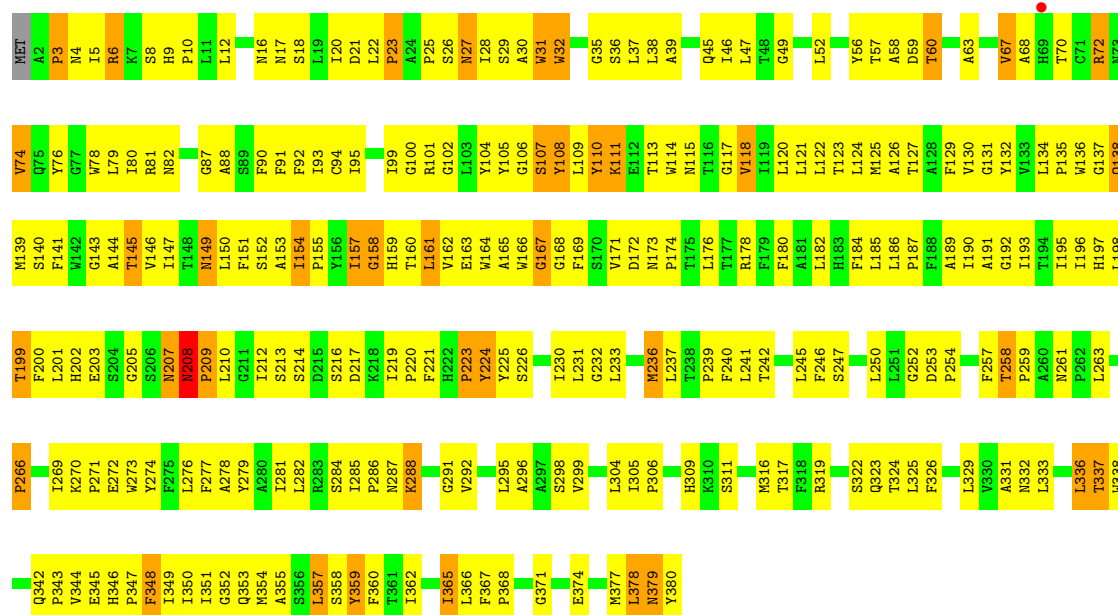
• Molecule 3: Cytochrome b

Chain C: 32% 58% 10%

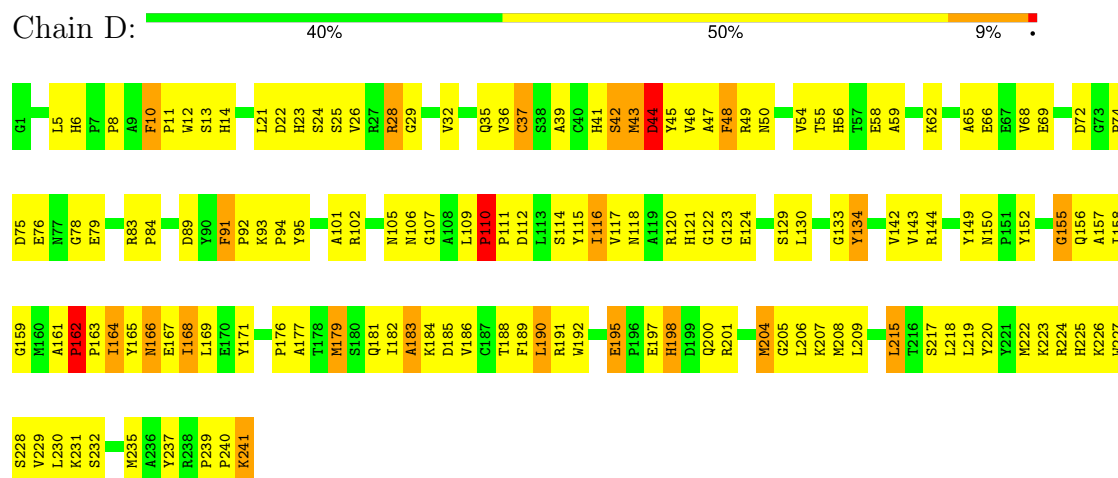


• Molecule 3: Cytochrome b

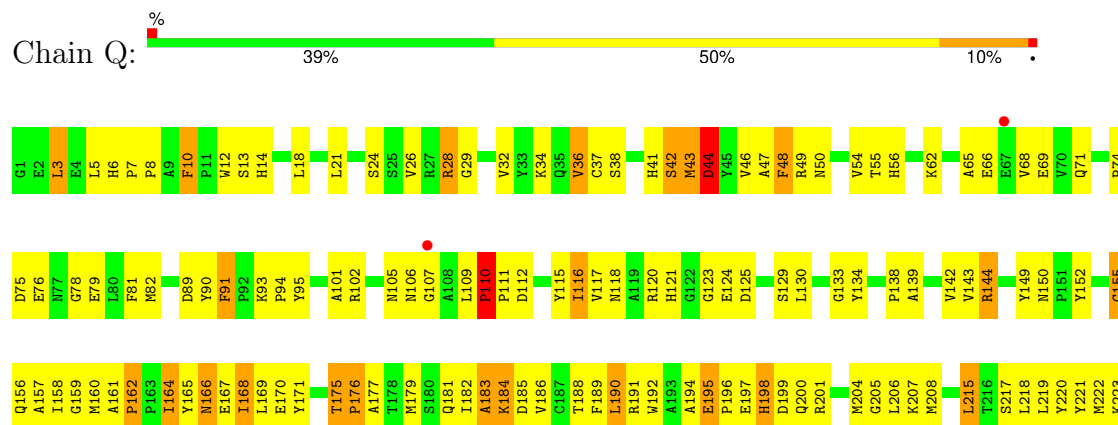
Chain P: 32% 57% 11%

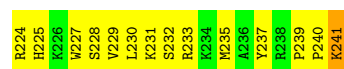


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

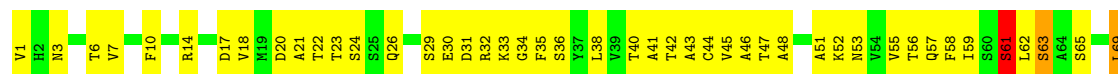


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL





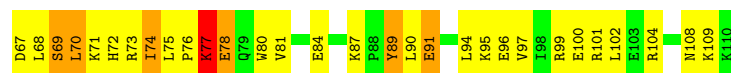
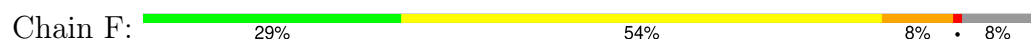
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



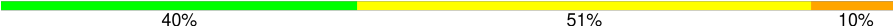
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN



• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN

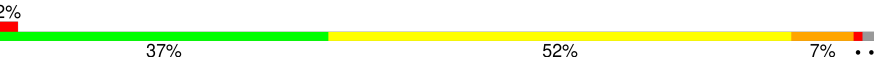


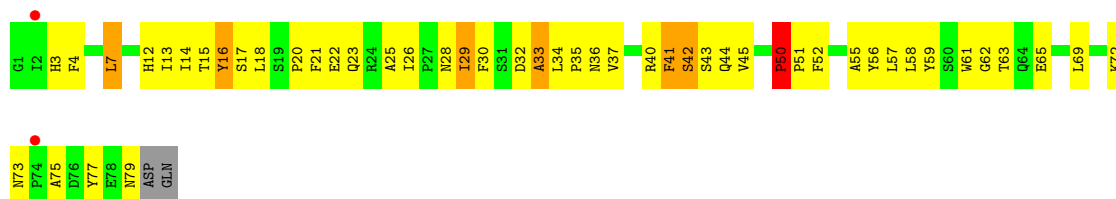
● Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



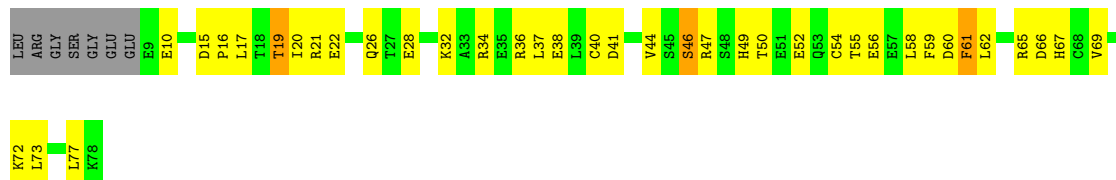
● Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain T: 



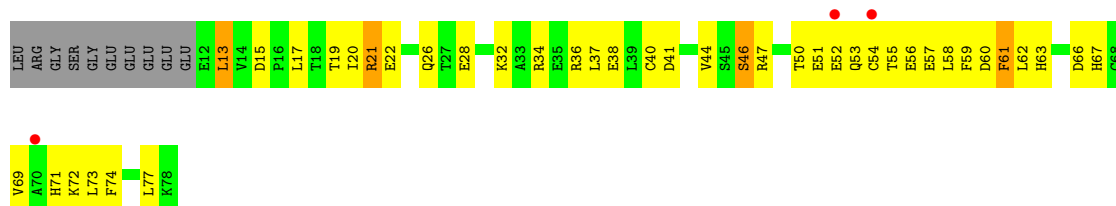
● Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN

Chain H: 

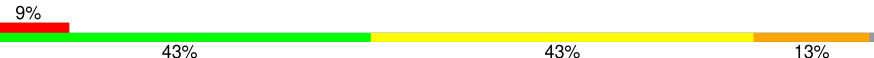


● Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN

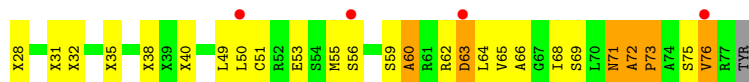
Chain U: 



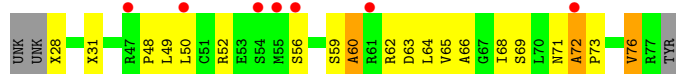
● Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 

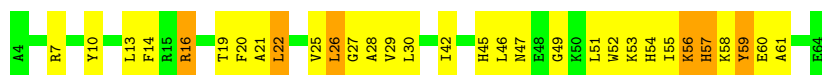




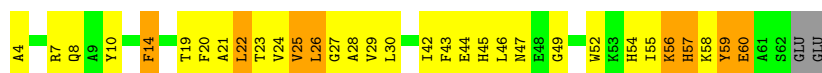
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



- Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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	174.69Å 181.67Å 240.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.53 19.99 – 3.53	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.99-3.53) 90.1 (19.99-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.306 0.253 , 0.296	Depositor DCC
R_{free} test set	2560 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32701	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: SMA, CDL, PEE, HEC, FES, GOL, ANY, PLC, HEM, UNL

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	0.58	0/3511	1.07	26/4757 (0.5%)
1	N	0.58	0/3508	1.06	30/4753 (0.6%)
2	B	0.52	0/3196	1.04	19/4334 (0.4%)
2	O	0.55	0/3202	1.03	15/4343 (0.3%)
3	C	0.74	0/3122	1.11	23/4273 (0.5%)
3	P	0.64	0/3114	1.09	21/4263 (0.5%)
4	D	0.64	0/1956	1.13	21/2658 (0.8%)
4	Q	0.56	0/1956	1.12	21/2658 (0.8%)
5	E	0.51	0/1547	1.08	12/2103 (0.6%)
5	R	0.56	0/1547	1.05	11/2103 (0.5%)
6	F	0.64	0/911	0.99	5/1219 (0.4%)
6	S	0.55	0/911	0.99	4/1219 (0.3%)
7	G	0.65	0/698	1.03	0/946
7	T	0.57	0/680	0.97	1/923 (0.1%)
8	H	0.54	0/582	0.85	1/779 (0.1%)
8	U	0.44	0/561	0.84	1/751 (0.1%)
9	I	0.65	0/218	1.06	2/293 (0.7%)
9	V	0.65	0/218	0.93	0/293
10	J	0.58	0/508	0.89	0/682
10	W	0.54	0/489	0.89	0/658
All	All	0.59	0/32435	1.06	213/44008 (0.5%)

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

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

There are no bond length outliers.

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	LEU	N-CA-C	12.09	127.03	110.35
5	E	71	LEU	N-CA-C	11.95	126.84	110.35
4	Q	36	VAL	N-CA-C	9.27	118.94	111.62
1	N	415	ILE	N-CA-C	8.18	118.53	111.90
1	N	66	GLY	N-CA-C	7.99	123.36	112.17
3	P	252	GLY	N-CA-C	7.96	122.89	110.71
2	O	133	ARG	CA-C-N	7.86	129.66	119.84
2	O	133	ARG	C-N-CA	7.86	129.66	119.84
1	A	66	GLY	N-CA-C	7.85	123.16	112.17
2	O	18	CYS	CA-C-N	7.81	129.60	119.84
2	O	18	CYS	C-N-CA	7.81	129.60	119.84
2	B	133	ARG	CA-C-N	7.67	129.42	119.84
2	B	133	ARG	C-N-CA	7.67	129.42	119.84
4	D	195	GLU	CA-C-N	7.56	127.94	119.32
4	D	195	GLU	C-N-CA	7.56	127.94	119.32
3	P	27	ASN	N-CA-C	7.53	122.18	112.92
1	N	329	LEU	N-CA-C	7.50	121.33	112.93
4	D	36	VAL	N-CA-C	7.46	117.51	111.62
1	N	412	SER	N-CA-C	-7.27	103.29	111.07
6	S	15	ARG	N-CA-C	-7.25	104.69	113.97
4	D	155	GLY	N-CA-C	-7.24	105.24	114.37
3	P	107	SER	N-CA-C	-7.23	103.72	112.54
1	A	248	LEU	CA-C-N	7.21	126.74	119.24
1	A	248	LEU	C-N-CA	7.21	126.74	119.24
3	C	107	SER	N-CA-C	-7.13	103.84	112.54
4	Q	7	PRO	N-CA-C	7.13	117.31	110.47
4	Q	155	GLY	N-CA-C	-7.08	105.45	114.37
1	A	329	LEU	N-CA-C	6.96	120.66	112.72
3	C	270	LYS	CA-C-N	6.94	128.52	119.84
3	C	270	LYS	C-N-CA	6.94	128.52	119.84
5	R	17	ASP	N-CA-C	6.94	121.33	113.01
3	C	357	LEU	N-CA-C	-6.93	103.73	111.28
1	N	214	GLN	N-CA-C	6.92	118.91	111.36
3	C	27	ASN	N-CA-C	6.91	121.42	112.92
1	A	3	THR	N-CA-C	6.88	119.19	110.24
4	Q	6	HIS	CA-C-N	6.88	124.68	119.66
4	Q	6	HIS	C-N-CA	6.88	124.68	119.66
1	A	305	HIS	N-CA-C	-6.81	104.44	112.89
1	N	432	LEU	N-CA-C	6.74	119.00	108.96
5	E	105	GLU	N-CA-C	-6.72	104.11	112.72
1	A	214	GLN	N-CA-C	6.69	118.65	111.36
1	A	415	ILE	N-CA-C	6.66	117.29	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	GLN	N-CA-C	6.64	119.36	111.33
1	A	412	SER	N-CA-C	-6.63	103.98	111.07
1	A	432	LEU	N-CA-C	6.62	118.82	108.96
2	B	365	LYS	N-CA-C	-6.58	104.03	111.07
1	A	129	LYS	N-CA-C	-6.56	104.20	112.93
4	Q	116	ILE	N-CA-C	6.56	116.72	110.42
1	N	125	SER	N-CA-C	-6.56	105.09	113.23
5	E	118	ARG	N-CA-C	-6.49	103.89	110.97
3	C	208	ASN	CA-C-N	6.45	127.91	119.84
3	C	208	ASN	C-N-CA	6.45	127.91	119.84
1	A	231	LEU	N-CA-C	6.43	117.76	109.72
2	O	188	SER	N-CA-C	-6.42	105.30	113.01
4	D	110	PRO	CA-C-N	6.41	126.36	119.76
4	D	110	PRO	C-N-CA	6.41	126.36	119.76
4	D	28	ARG	N-CA-C	-6.36	103.64	111.40
5	R	143	GLY	N-CA-C	6.35	125.50	115.08
1	A	264	ASP	CA-C-N	6.34	126.47	119.87
1	A	264	ASP	C-N-CA	6.34	126.47	119.87
2	B	31	ASN	N-CA-C	6.32	117.86	110.97
3	C	205	GLY	N-CA-C	-6.30	101.24	112.58
5	E	70	ALA	N-CA-C	-6.29	97.40	110.80
4	D	116	ILE	N-CA-C	6.28	116.39	110.30
1	N	129	LYS	N-CA-C	-6.27	104.34	112.68
4	D	91	PHE	CA-C-N	6.27	127.68	119.84
4	D	91	PHE	C-N-CA	6.27	127.68	119.84
4	Q	36	VAL	CB-CA-C	-6.23	105.51	111.05
3	P	378	LEU	N-CA-C	-6.19	105.56	113.23
1	N	305	HIS	N-CA-C	-6.18	105.23	112.89
5	E	143	GLY	N-CA-C	6.17	127.80	113.18
1	A	125	SER	N-CA-C	-6.16	105.60	113.23
4	D	36	VAL	CB-CA-C	-6.14	105.58	111.05
3	C	272	GLU	N-CA-C	-6.11	102.05	110.35
9	I	72	ALA	CA-C-N	6.11	127.47	119.84
9	I	72	ALA	C-N-CA	6.11	127.47	119.84
2	O	347	ALA	N-CA-C	-6.09	106.17	113.97
3	P	272	GLU	N-CA-C	-6.05	102.12	110.35
2	B	28	LYS	N-CA-C	6.03	117.52	110.41
5	R	102	THR	N-CA-C	-6.03	101.08	110.42
5	R	70	ALA	N-CA-C	-6.02	97.97	110.80
6	F	39	GLU	N-CA-C	6.00	119.50	108.58
5	R	121	GLN	N-CA-C	-5.99	98.05	110.80
3	P	152	SER	N-CA-C	-5.97	105.84	113.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	378	LEU	N-CA-C	-5.97	106.00	113.28
5	E	17	ASP	N-CA-C	5.97	120.29	113.19
4	D	41	HIS	N-CA-C	5.96	118.24	108.52
3	P	67	VAL	N-CA-C	-5.96	104.70	110.42
3	P	205	GLY	N-CA-C	-5.96	101.86	112.58
2	O	170	THR	N-CA-C	5.92	116.05	108.24
1	A	347	THR	N-CA-C	5.91	121.03	113.18
5	E	129	LYS	CA-C-N	5.90	127.22	119.84
5	E	129	LYS	C-N-CA	5.90	127.22	119.84
6	F	109	LYS	N-CA-C	-5.86	105.23	112.90
1	N	416	TYR	N-CA-C	5.85	118.68	109.96
1	N	60	GLU	N-CA-C	-5.82	105.01	111.71
4	Q	41	HIS	N-CA-C	5.82	118.01	108.52
4	Q	164	ILE	N-CA-C	5.82	117.12	108.46
3	P	185	LEU	N-CA-C	5.78	117.45	111.03
1	N	248	LEU	CA-C-N	5.78	125.25	119.24
1	N	248	LEU	C-N-CA	5.78	125.25	119.24
2	O	282	GLY	CA-C-N	5.77	127.06	119.84
2	O	282	GLY	C-N-CA	5.77	127.06	119.84
2	B	282	GLY	CA-C-N	5.77	127.05	119.84
2	B	282	GLY	C-N-CA	5.77	127.05	119.84
3	C	152	SER	N-CA-C	-5.75	106.11	113.01
2	B	347	ALA	N-CA-C	-5.74	106.91	114.31
6	F	26	PHE	N-CA-C	-5.73	105.78	112.89
1	N	415	ILE	CB-CA-C	-5.71	105.81	111.30
3	P	72	ARG	N-CA-C	5.69	117.28	111.14
3	C	154	ILE	CB-CA-C	-5.67	105.66	110.94
4	Q	91	PHE	CA-C-N	5.67	126.93	119.84
4	Q	91	PHE	C-N-CA	5.67	126.93	119.84
4	Q	195	GLU	CA-C-N	5.67	126.92	119.84
4	Q	195	GLU	C-N-CA	5.67	126.92	119.84
3	P	257	PHE	N-CA-C	-5.66	105.95	112.92
2	B	108	CYS	N-CA-C	5.65	118.32	108.76
1	N	231	LEU	N-CA-C	5.64	117.17	110.07
5	E	104	ALA	N-CA-C	-5.63	106.25	113.01
3	P	143	GLY	N-CA-C	-5.63	105.97	112.50
3	C	50	LEU	N-CA-C	-5.62	105.05	111.07
1	N	419	CYS	N-CA-C	-5.62	102.57	109.65
5	R	131	GLU	N-CA-C	-5.62	106.47	113.38
2	B	29	LEU	CA-C-N	5.62	125.08	119.24
2	B	29	LEU	C-N-CA	5.62	125.08	119.24
6	S	39	GLU	N-CA-C	5.62	118.80	108.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	368	GLN	N-CA-C	-5.61	105.94	112.89
5	E	61	SER	N-CA-C	-5.58	105.29	111.71
4	D	204	MET	N-CA-C	-5.58	104.89	110.97
4	D	162	PRO	CA-C-N	5.55	125.17	119.56
4	D	162	PRO	C-N-CA	5.55	125.17	119.56
1	A	89	TYR	N-CA-C	5.55	115.57	108.24
2	O	365	LYS	N-CA-C	-5.54	105.14	111.07
3	C	365	ILE	N-CA-C	5.53	120.85	109.34
5	R	190	ASP	N-CA-C	-5.53	106.58	113.55
2	B	170	THR	N-CA-C	5.52	115.13	107.73
2	B	305	GLN	CA-C-N	5.52	125.83	119.92
2	B	305	GLN	C-N-CA	5.52	125.83	119.92
6	F	52	GLU	N-CA-C	5.51	118.00	111.33
3	C	67	VAL	N-CA-C	-5.48	104.98	110.30
4	D	164	ILE	N-CA-C	5.48	116.62	108.46
3	C	29	SER	N-CA-C	5.47	117.58	110.53
4	Q	184	LYS	N-CA-C	-5.47	104.19	111.24
3	P	357	LEU	N-CA-C	-5.46	105.33	111.28
1	A	368	GLN	N-CA-C	-5.46	106.12	112.89
2	B	174	ASN	CA-C-N	5.46	125.45	119.89
2	B	174	ASN	C-N-CA	5.46	125.45	119.89
4	Q	110	PRO	CA-C-N	5.45	125.38	119.76
4	Q	110	PRO	C-N-CA	5.45	125.38	119.76
2	B	29	LEU	N-CA-C	5.45	121.86	109.81
3	C	143	GLY	N-CA-C	-5.45	106.18	112.50
1	N	134	ILE	N-CA-C	-5.44	105.41	110.53
3	C	22	LEU	CA-C-N	5.44	126.92	120.23
3	C	22	LEU	C-N-CA	5.44	126.92	120.23
1	N	414	TYR	N-CA-C	5.44	120.19	113.50
1	A	60	GLU	N-CA-C	-5.43	105.75	112.38
1	N	430	GLN	N-CA-C	5.43	117.62	111.11
3	C	328	LEU	N-CA-C	-5.43	105.36	111.28
1	N	264	ASP	CA-C-N	5.41	125.50	119.87
1	N	264	ASP	C-N-CA	5.41	125.50	119.87
1	N	32	GLN	CA-C-N	5.41	125.08	119.56
1	N	32	GLN	C-N-CA	5.41	125.08	119.56
5	R	61	SER	N-CA-C	-5.41	105.49	111.71
4	D	93	LYS	N-CA-C	-5.40	102.97	109.83
8	U	21	ARG	N-CA-C	-5.40	105.43	112.23
3	P	167	GLY	N-CA-C	-5.39	108.40	115.47
3	C	167	GLY	N-CA-C	-5.39	108.41	115.47
1	A	95	THR	N-CA-C	-5.39	102.22	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	TYR	N-CA-C	5.38	120.00	113.38
3	C	110	TYR	N-CA-C	-5.36	105.44	112.72
1	A	415	ILE	CB-CA-C	-5.33	106.18	111.30
8	H	21	ARG	N-CA-C	-5.33	105.51	112.23
1	A	32	GLN	CA-C-N	5.32	124.98	119.56
1	A	32	GLN	C-N-CA	5.32	124.98	119.56
1	N	272	VAL	N-CA-C	-5.32	105.32	110.42
3	P	365	ILE	N-CA-C	5.31	120.38	109.34
2	O	168	TYR	N-CA-C	5.30	116.33	108.86
2	B	237	ALA	N-CA-C	5.29	117.37	109.59
1	A	428	ILE	N-CA-C	5.29	120.34	109.34
3	P	208	ASN	CA-C-N	5.28	126.44	119.84
3	P	208	ASN	C-N-CA	5.28	126.44	119.84
3	C	185	LEU	N-CA-C	5.26	116.88	111.03
2	O	29	LEU	N-CA-C	5.26	117.78	110.20
2	O	238	THR	N-CA-C	-5.25	101.97	110.32
6	F	51	PRO	N-CA-C	-5.23	102.89	111.21
3	P	87	GLY	N-CA-C	-5.22	106.32	112.64
3	P	154	ILE	CA-C-N	5.22	125.12	119.85
3	P	154	ILE	C-N-CA	5.22	125.12	119.85
4	Q	28	ARG	N-CA-C	-5.21	104.54	112.04
4	Q	233	ARG	N-CA-C	5.21	117.58	110.24
6	S	52	GLU	N-CA-C	5.21	117.63	111.33
3	P	110	TYR	N-CA-C	-5.19	105.66	112.72
5	E	110	ALA	N-CA-C	-5.18	107.34	113.97
2	B	350	GLY	N-CA-C	5.18	121.99	115.42
2	O	140	LEU	N-CA-C	5.17	118.06	111.69
5	R	129	LYS	CA-C-N	5.17	126.30	119.84
5	R	129	LYS	C-N-CA	5.17	126.30	119.84
5	E	168	SER	N-CA-C	-5.16	107.03	113.38
1	N	89	TYR	N-CA-C	5.16	115.05	108.24
1	N	428	ILE	N-CA-C	5.14	120.03	109.34
7	T	50	PRO	N-CA-C	5.09	116.91	110.70
1	N	223	TYR	N-CA-C	-5.08	106.24	112.90
4	D	134	TYR	N-CA-C	5.08	117.47	110.35
2	O	438	GLU	N-CA-C	-5.08	105.17	113.19
4	Q	93	LYS	N-CA-C	-5.06	103.40	109.83
4	Q	175	THR	CA-C-N	5.05	126.15	119.84
4	Q	175	THR	C-N-CA	5.05	126.15	119.84
6	S	26	PHE	N-CA-C	-5.05	106.63	112.89
4	D	35	GLN	N-CA-C	5.04	119.28	113.18
1	N	183	ALA	N-CA-C	-5.04	104.87	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	HIS	CA-C-N	5.02	125.55	120.38
4	D	6	HIS	C-N-CA	5.02	125.55	120.38
1	N	364	ALA	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	104	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	293	0
1	N	3437	0	3349	298	0
2	B	3141	0	3142	300	0
2	O	3147	0	3146	319	0
3	C	3020	0	3070	287	0
3	P	3012	0	3058	311	0
4	D	1898	0	1846	166	0
4	Q	1898	0	1846	178	0
5	E	1513	0	1478	144	0
5	R	1513	0	1478	129	0
6	F	891	0	893	74	0
6	S	891	0	893	78	0
7	G	676	0	659	61	0
7	T	658	0	647	67	0
8	H	574	0	548	30	0
8	U	553	0	535	43	0
9	I	285	0	239	30	0
9	V	275	0	238	30	0
10	J	497	0	490	31	0
10	W	478	0	478	38	0
11	A	21	0	13	0	0
11	C	49	0	72	2	0
11	E	50	0	77	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	N	5	0	0	0	0
11	P	99	0	149	6	0
12	A	1	0	0	0	0
12	C	3	0	0	0	0
12	E	2	0	0	0	0
12	P	3	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	20	0
13	P	86	0	60	22	0
14	C	37	0	42	3	0
14	P	37	0	42	4	0
15	C	37	0	28	3	0
15	P	37	0	29	1	0
16	C	40	0	24	2	0
16	D	50	0	44	1	0
16	P	40	0	24	2	0
16	Q	50	0	44	5	0
17	C	6	0	8	1	0
17	P	6	0	8	0	0
18	D	43	0	30	6	0
18	Q	43	0	30	5	0
19	E	4	0	0	2	0
19	R	4	0	0	1	0
20	E	32	0	38	2	0
20	R	32	0	38	3	0
All	All	32701	0	32246	2697	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 42.

All (2697) 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)
3:P:157:ILE:HG13	3:P:158:GLY:H	1.04	1.15
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.19	1.12
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.16	1.12
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.29	1.07
5:E:119:ASP:HB3	5:E:179:ASN:ND2	1.67	1.07
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.36	1.04
1:A:294:LEU:HD11	1:A:334:MET:HE1	1.38	1.03
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.38	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:ILE:H	7:T:29:ILE:HD12	1.25	1.01
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.43	1.00
3:P:271:PRO:HA	14:P:3001:SMA:H10	1.42	1.00
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.41	0.99
3:P:46:ILE:HA	13:P:501:HEM:HMC3	1.46	0.98
4:D:47:ALA:H	4:D:50:ASN:HD22	1.07	0.97
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.43	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.97
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.31	0.95
2:B:207:VAL:HG12	2:B:208:GLY:H	1.29	0.95
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.33	0.94
7:G:29:ILE:H	7:G:29:ILE:HD12	1.30	0.93
5:E:103:GLN:HA	5:E:106:ILE:HB	1.49	0.93
8:U:13:LEU:HD23	8:U:13:LEU:H	1.34	0.93
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.16	0.92
2:O:207:VAL:HG12	2:O:208:GLY:H	1.34	0.92
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.52	0.91
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.31	0.91
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.52	0.91
2:O:76:THR:HG22	2:O:82:SER:H	1.34	0.90
3:P:157:ILE:HG13	3:P:158:GLY:N	1.81	0.90
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.54	0.90
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.50	0.90
1:A:137:GLU:O	1:A:141:MET:HG3	1.73	0.89
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.08	0.89
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.53	0.89
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.53	0.88
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.53	0.88
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.55	0.88
4:D:32:VAL:HG11	4:D:186:VAL:HB	1.56	0.88
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.56	0.87
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.37	0.87
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.56	0.87
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.21	0.86
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.38	0.86
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.40	0.86
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.38	0.86
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.11	0.85
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.58	0.85
1:N:137:GLU:O	1:N:141:MET:HG3	1.77	0.85
3:C:101:ARG:HD2	3:C:101:ARG:C	2.01	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.59	0.84
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.07	0.84
1:N:388:ARG:HH21	1:N:388:ARG:HG3	1.41	0.84
2:O:361:LYS:O	2:O:365:LYS:HG3	1.77	0.84
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.24	0.84
4:Q:215:LEU:HD22	5:R:46:ALA:HB1	1.60	0.84
3:P:101:ARG:HD2	3:P:101:ARG:C	2.02	0.84
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.58	0.84
5:R:128:LYS:O	5:R:130:PRO:HD3	1.78	0.83
4:D:235:MET:HB3	7:G:15:THR:HG22	1.61	0.83
2:B:76:THR:HG22	2:B:82:SER:H	1.43	0.83
3:C:46:ILE:HA	13:C:501:HEM:CMC	2.07	0.83
1:A:206:LYS:O	1:A:209:VAL:HG12	1.78	0.83
2:B:274:VAL:O	2:B:278:VAL:HG23	1.78	0.83
10:J:16:ARG:HB3	10:J:19:THR:HG23	1.60	0.83
2:O:398:VAL:O	2:O:402:ILE:HG13	1.79	0.83
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.77	0.83
2:O:274:VAL:O	2:O:278:VAL:HG23	1.78	0.83
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.13	0.82
4:D:47:ALA:N	4:D:50:ASN:HD22	1.75	0.82
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.61	0.82
1:A:130:GLU:O	1:A:134:ILE:HG13	1.80	0.82
3:C:101:ARG:HD2	3:C:102:GLY:N	1.94	0.81
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.80	0.81
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.62	0.81
18:D:501:HEC:HMB3	18:D:501:HEC:HBB3	1.60	0.81
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.44	0.81
3:C:247:SER:OG	3:C:250:LEU:HB2	1.81	0.81
3:P:101:ARG:HD2	3:P:102:GLY:N	1.96	0.81
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.45	0.80
4:Q:32:VAL:HG11	4:Q:186:VAL:HB	1.63	0.80
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.64	0.80
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.11	0.80
2:O:128:THR:HA	2:O:226:ILE:HD11	1.63	0.80
3:C:146:VAL:HG21	14:C:2001:SMA:H6	1.63	0.80
2:O:150:VAL:HG23	2:O:151:ALA:H	1.47	0.80
3:P:46:ILE:HA	13:P:501:HEM:CMC	2.11	0.80
5:E:73:LYS:HB3	5:E:195:VAL:O	1.80	0.80
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.62	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.47	0.79
2:O:150:VAL:HG23	2:O:151:ALA:N	1.97	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.62	0.79
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.17	0.79
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.65	0.79
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.64	0.78
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.65	0.78
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.84	0.78
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.17	0.78
2:B:150:VAL:HG23	2:B:151:ALA:N	1.98	0.78
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.18	0.78
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.47	0.78
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.49	0.78
3:C:241:LEU:HB2	4:D:208:MET:HE2	1.66	0.78
4:Q:200:GLN:HE21	20:R:3009:PLC:H51	1.48	0.78
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.64	0.78
2:B:361:LYS:O	2:B:365:LYS:HG3	1.83	0.78
1:A:362:ARG:O	1:A:365:MET:HB3	1.84	0.78
1:N:390:ILE:HG23	1:N:394:GLU:OE1	1.84	0.78
3:C:132:TYR:O	3:C:135:PRO:HD2	1.84	0.78
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.48	0.77
2:O:248:ASN:C	2:O:248:ASN:HD22	1.92	0.77
2:O:345:LYS:C	2:O:347:ALA:H	1.92	0.77
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.13	0.77
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.64	0.77
1:A:4:TYR:HA	2:B:113:ARG:HD3	1.66	0.77
2:B:398:VAL:O	2:B:402:ILE:HG13	1.84	0.77
3:C:113:THR:HG21	3:C:201:LEU:HD13	1.67	0.77
7:T:29:ILE:O	7:T:33:ALA:HB3	1.84	0.77
2:B:43:PRO:O	2:B:113:ARG:HG3	1.85	0.77
1:N:90:THR:O	1:N:167:VAL:HG11	1.84	0.77
2:O:76:THR:CG2	2:O:82:SER:H	1.97	0.77
3:P:118:VAL:N	13:P:502:HEM:HBC2	1.99	0.77
2:B:46:ARG:NH2	2:B:376:GLN:HG3	1.99	0.77
2:B:227:ARG:HA	2:B:227:ARG:HE	1.49	0.77
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.66	0.77
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.65	0.76
1:N:49:ASN:ND2	1:N:52:ASN:H	1.83	0.76
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.49	0.76
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.15	0.76
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.68	0.76
2:O:56:ARG:HB2	2:O:171:ALA:HB1	1.67	0.76
2:B:248:ASN:C	2:B:248:ASN:HD22	1.92	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:34:ARG:O	8:H:38:GLU:HG2	1.84	0.76
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.68	0.75
3:C:355:ALA:O	3:C:358:SER:HB3	1.86	0.75
6:F:32:MET:CE	6:F:87:LYS:H	1.98	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.66	0.75
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.69	0.75
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.01	0.75
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.01	0.75
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.22	0.75
1:N:429:GLU:OE1	7:T:7:LEU:HB2	1.87	0.74
4:Q:120:ARG:HG2	4:Q:120:ARG:HH11	1.51	0.74
6:F:89:TYR:HD1	6:F:90:LEU:N	1.84	0.74
1:N:362:ARG:O	1:N:365:MET:HB3	1.86	0.74
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.70	0.74
3:P:132:TYR:O	3:P:135:PRO:HD2	1.88	0.74
1:A:106:MET:HE2	1:A:106:MET:O	1.87	0.74
3:C:271:PRO:HA	14:C:2001:SMA:H10	1.69	0.74
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.23	0.74
2:O:325:TYR:HD1	9:V:60:ALA:HB2	1.50	0.74
18:Q:501:HEC:HMB3	18:Q:501:HEC:HBB3	1.70	0.74
7:G:41:PHE:C	7:G:41:PHE:CD2	2.66	0.73
5:R:58:PHE:O	5:R:61:SER:HB3	1.87	0.73
1:N:49:ASN:C	1:N:49:ASN:HD22	1.95	0.73
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.89	0.73
2:B:199:PHE:O	2:B:226:ILE:HG12	1.88	0.73
7:G:41:PHE:C	7:G:41:PHE:HD2	1.96	0.73
1:A:390:ILE:HG23	1:A:394:GLU:OE1	1.88	0.73
2:B:207:VAL:HG12	2:B:208:GLY:N	2.02	0.73
1:N:19:LEU:HB3	1:N:21:ASN:OD1	1.88	0.73
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.54	0.73
1:N:45:SER:HA	1:N:48:GLU:HG3	1.69	0.73
2:B:169:LYS:O	2:B:170:THR:HG23	1.88	0.73
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.04	0.73
5:E:102:THR:O	5:E:106:ILE:HG13	1.88	0.73
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.19	0.73
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.70	0.73
8:U:34:ARG:O	8:U:38:GLU:HG2	1.89	0.73
3:C:332:ASN:HD21	3:C:359:TYR:N	1.86	0.73
2:B:76:THR:CG2	2:B:82:SER:H	2.02	0.73
2:O:221:GLU:HG3	2:O:222:GLN:H	1.54	0.73
4:Q:222:MET:HE3	5:R:40:THR:OG1	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.04	0.73
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.71	0.72
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.18	0.72
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.71	0.72
1:A:49:ASN:C	1:A:49:ASN:HD22	1.97	0.72
2:B:47:ILE:HG12	2:B:120:MET:CE	2.08	0.72
2:B:357:VAL:O	2:B:361:LYS:HG3	1.89	0.72
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.52	0.72
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.71	0.72
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.23	0.72
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.25	0.72
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.89	0.72
2:B:162:ASN:O	2:B:244:ILE:HD12	1.90	0.72
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.24	0.72
3:C:241:LEU:CB	4:D:208:MET:HE2	2.19	0.72
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.05	0.72
1:N:223:TYR:H	1:N:223:TYR:HD2	1.37	0.72
6:S:89:TYR:HD1	6:S:90:LEU:N	1.88	0.72
2:O:71:LEU:O	2:O:74:PRO:HD2	1.90	0.72
1:N:69:LYS:CE	1:N:70:ARG:HH21	2.02	0.72
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.20	0.72
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.24	0.72
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.53	0.72
5:R:53:ASN:O	5:R:57:GLN:HG3	1.90	0.72
1:A:90:THR:O	1:A:167:VAL:HG11	1.89	0.72
2:B:345:LYS:C	2:B:347:ALA:H	1.95	0.72
2:B:227:ARG:HA	2:B:227:ARG:NE	2.05	0.71
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.53	0.71
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.71	0.71
3:P:277:PHE:CD1	3:P:278:ALA:N	2.58	0.71
4:Q:223:LYS:O	4:Q:223:LYS:HD3	1.90	0.71
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.89	0.71
9:I:71:ASN:HD22	9:I:71:ASN:H	1.36	0.71
7:T:41:PHE:HD2	7:T:41:PHE:C	1.99	0.71
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.24	0.71
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.71	0.71
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.52	0.71
8:H:40:CYS:O	8:H:44:VAL:HG23	1.89	0.71
1:N:130:GLU:O	1:N:134:ILE:HG13	1.90	0.71
3:P:184:PHE:CD2	13:P:501:HEM:HBC1	2.26	0.71
7:T:41:PHE:C	7:T:41:PHE:CD2	2.67	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:CYS:HB3	2:B:119:VAL:HG11	1.72	0.71
5:R:113:ASP:C	5:R:115:SER:H	1.99	0.71
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.72	0.71
5:E:141:HIS:O	5:E:142:LEU:HD23	1.91	0.71
1:A:45:SER:HA	1:A:48:GLU:HG3	1.71	0.70
3:C:189:ALA:O	3:C:193:ILE:HG13	1.90	0.70
4:D:46:VAL:HG12	4:D:47:ALA:N	2.06	0.70
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.71	0.70
1:A:49:ASN:ND2	1:A:52:ASN:H	1.89	0.70
1:A:269:VAL:HG11	1:A:410:VAL:HG21	1.73	0.70
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.27	0.70
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.73	0.70
5:E:53:ASN:O	5:E:57:GLN:HG3	1.91	0.70
1:N:373:THR:HB	1:N:374:PRO:HD3	1.71	0.70
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.31	0.70
1:A:373:THR:HB	1:A:374:PRO:HD3	1.73	0.70
4:D:231:LYS:O	6:F:71:LYS:HE3	1.91	0.70
18:Q:501:HEC:HBC3	18:Q:501:HEC:HMC3	1.74	0.70
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.74	0.70
7:G:29:ILE:O	7:G:33:ALA:HB3	1.92	0.70
2:O:219:VAL:O	2:O:223:PHE:HB2	1.92	0.70
4:Q:171:TYR:OH	4:Q:182:ILE:HA	1.91	0.70
4:Q:215:LEU:HD22	5:R:46:ALA:CB	2.21	0.70
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.25	0.70
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.74	0.70
2:O:24:LEU:HD13	2:O:38:LEU:HB2	1.72	0.70
2:B:47:ILE:CG1	2:B:120:MET:HE1	2.09	0.70
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.74	0.70
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.73	0.70
3:C:92:PHE:O	3:C:95:ILE:HG22	1.92	0.70
3:C:134:LEU:HB2	3:C:135:PRO:HD3	1.73	0.70
3:P:189:ALA:O	3:P:193:ILE:HG13	1.91	0.70
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.73	0.70
8:U:73:LEU:HD12	8:U:73:LEU:O	1.92	0.70
1:A:223:TYR:H	1:A:223:TYR:HD2	1.38	0.69
5:E:58:PHE:O	5:E:61:SER:HB3	1.92	0.69
6:F:61:ARG:NH2	6:F:89:TYR:HE2	1.89	0.69
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.27	0.69
3:P:126:ALA:O	3:P:129:PHE:HB3	1.92	0.69
3:P:241:LEU:HB2	4:Q:208:MET:HE2	1.74	0.69
3:P:247:SER:OG	3:P:250:LEU:HB2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG23	2:B:151:ALA:H	1.56	0.69
4:D:215:LEU:HD22	5:E:46:ALA:HB1	1.74	0.69
1:N:206:LYS:O	1:N:209:VAL:HG12	1.92	0.69
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.58	0.69
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.22	0.69
16:C:2004:CDL:OA4	7:G:40:ARG:HD2	1.92	0.69
4:D:47:ALA:N	4:D:50:ASN:ND2	2.41	0.69
2:O:150:VAL:CG2	2:O:151:ALA:H	2.06	0.69
2:O:154:SER:O	2:O:157:VAL:HG12	1.92	0.69
1:A:429:GLU:OE1	7:G:7:LEU:HB2	1.92	0.69
2:O:43:PRO:O	2:O:113:ARG:HG3	1.93	0.69
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.08	0.69
2:O:226:ILE:HG22	2:O:227:ARG:N	2.07	0.69
2:O:357:VAL:O	2:O:361:LYS:HG3	1.93	0.69
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.28	0.69
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.17	0.69
1:N:161:THR:HG21	1:N:235:ARG:H	1.57	0.69
3:P:92:PHE:O	3:P:95:ILE:HG22	1.93	0.69
3:P:146:VAL:HG21	14:P:3001:SMA:H6	1.74	0.69
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.22	0.69
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.27	0.68
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.74	0.68
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.56	0.68
4:D:164:ILE:O	4:D:179:MET:HE2	1.93	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
3:C:282:LEU:O	3:C:282:LEU:HD23	1.94	0.68
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.28	0.68
2:O:207:VAL:HG12	2:O:208:GLY:N	2.07	0.68
2:B:312:PHE:N	2:B:323:GLY:O	2.22	0.68
4:D:223:LYS:O	4:D:223:LYS:HD3	1.94	0.68
8:H:73:LEU:HD12	8:H:73:LEU:O	1.93	0.68
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.76	0.68
3:P:113:THR:HG21	3:P:201:LEU:HD13	1.74	0.68
3:P:135:PRO:HG3	13:P:501:HEM:O1D	1.94	0.68
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.08	0.68
2:B:341:MET:O	2:B:344:LEU:N	2.26	0.68
1:A:209:VAL:O	1:A:212:ALA:HB3	1.94	0.68
3:C:319:ARG:HB3	3:C:374:GLU:OE1	1.93	0.68
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.75	0.68
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.75	0.68
1:N:246:ASP:HA	1:N:427:PRO:HB3	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:32:ARG:HH12	7:T:22:GLU:CD	2.01	0.67
4:D:46:VAL:HG12	4:D:47:ALA:H	1.59	0.67
2:B:353:THR:HG22	2:B:355:GLU:H	1.58	0.67
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.58	0.67
3:P:104:TYR:HD2	3:P:105:TYR:CE1	2.11	0.67
1:A:106:MET:HE3	1:A:208:LEU:HD13	1.76	0.67
1:A:136:GLN:HG2	9:I:51:CYS:HB3	1.77	0.67
3:C:269:ILE:HG23	3:C:269:ILE:O	1.93	0.67
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.75	0.67
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	1.77	0.67
4:Q:94:PRO:HG2	4:Q:95:TYR:HD1	1.60	0.67
2:B:359:LYS:HA	2:B:362:ASN:ND2	2.10	0.67
3:C:118:VAL:N	13:C:502:HEM:HBC2	2.10	0.67
8:U:32:LYS:O	8:U:36:ARG:HG3	1.94	0.67
1:A:69:LYS:CE	1:A:70:ARG:HH21	2.03	0.67
2:O:75:LEU:CD2	2:O:136:GLU:HB3	2.24	0.67
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.60	0.67
5:R:77:LYS:HE2	5:R:79:SER:CB	2.24	0.67
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.75	0.67
2:B:62:ASN:O	2:B:65:THR:HG22	1.95	0.67
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.77	0.67
2:O:248:ASN:ND2	2:O:250:HIS:H	1.93	0.67
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.42	0.67
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.60	0.67
3:C:236:MET:O	3:C:239:PRO:HD2	1.93	0.67
5:E:40:THR:HG21	11:E:2005:PEE:O2P	1.96	0.67
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.76	0.67
3:P:241:LEU:CB	4:Q:208:MET:HE2	2.25	0.67
4:D:94:PRO:HG2	4:D:95:TYR:CD1	2.30	0.66
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.77	0.66
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.30	0.66
1:A:136:GLN:NE2	9:I:50:LEU:HB2	2.09	0.66
4:D:223:LYS:HD3	4:D:223:LYS:C	2.20	0.66
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.31	0.66
4:D:47:ALA:H	4:D:50:ASN:ND2	1.86	0.66
2:B:212:LYS:HD2	2:B:214:SER:OG	1.94	0.66
2:O:293:SER:OG	2:O:296:TYR:HB2	1.96	0.66
3:P:254:PRO:HB2	4:Q:118:ASN:O	1.96	0.66
3:P:332:ASN:HD21	3:P:359:TYR:N	1.94	0.66
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.20	0.66
1:N:294:LEU:HD11	1:N:334:MET:CE	2.21	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:33:ARG:O	6:F:36:THR:HG23	1.96	0.66
3:P:282:LEU:HD23	3:P:282:LEU:C	2.20	0.66
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.31	0.66
9:V:72:ALA:HB1	9:V:73:PRO:HD3	1.77	0.66
1:A:182:LEU:N	1:A:182:LEU:HD23	2.11	0.66
3:C:316:MET:HE2	3:C:322:SER:HB3	1.77	0.66
2:O:29:LEU:HD12	2:O:33:LEU:HD23	1.78	0.66
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.26	0.66
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.96	0.66
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.10	0.66
2:O:47:ILE:HD12	2:O:47:ILE:N	2.08	0.66
3:P:355:ALA:O	3:P:358:SER:HB3	1.96	0.66
2:O:111:CYS:HB3	2:O:119:VAL:HG11	1.78	0.65
4:Q:94:PRO:HG2	4:Q:95:TYR:CD1	2.30	0.65
4:Q:198:HIS:O	4:Q:201:ARG:HB3	1.95	0.65
4:D:198:HIS:O	4:D:201:ARG:HB3	1.96	0.65
1:N:307:PHE:CD1	1:N:307:PHE:C	2.74	0.65
3:C:30:ALA:C	3:C:32:TRP:H	2.04	0.65
3:C:282:LEU:HD23	3:C:282:LEU:C	2.21	0.65
3:C:316:MET:HG2	3:C:319:ARG:HH21	1.61	0.65
4:D:155:GLY:C	4:D:157:ALA:H	2.04	0.65
1:N:49:ASN:ND2	1:N:49:ASN:C	2.51	0.65
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.78	0.65
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.11	0.65
3:C:135:PRO:HG3	13:C:501:HEM:O1D	1.97	0.65
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.43	0.65
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.26	0.65
3:C:254:PRO:HB2	4:D:118:ASN:O	1.95	0.65
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.78	0.65
1:N:295:ALA:O	1:N:298:ALA:HB3	1.96	0.65
2:O:72:ALA:CB	2:O:75:LEU:HD12	2.25	0.65
4:Q:46:VAL:HG12	4:Q:47:ALA:N	2.12	0.65
1:A:161:THR:HG21	1:A:234:CYS:HA	1.77	0.65
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.77	0.65
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.88	0.65
1:A:246:ASP:HA	1:A:427:PRO:HB3	1.78	0.65
2:B:47:ILE:HD12	2:B:47:ILE:N	2.11	0.65
1:N:335:MET:HG3	1:N:339:GLN:HE21	1.60	0.65
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.79	0.65
6:S:50:LEU:HD21	6:S:90:LEU:HD12	1.79	0.65
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.43	0.65
8:U:13:LEU:HD23	8:U:13:LEU:N	2.08	0.65
1:A:5:ALA:O	1:A:8:LEU:HB2	1.97	0.65
3:C:277:PHE:CD1	3:C:278:ALA:N	2.64	0.65
3:P:157:ILE:HD12	3:P:161:LEU:HD12	1.79	0.65
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.64	0.65
1:A:388:ARG:HG3	1:A:388:ARG:NH2	2.12	0.64
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.27	0.64
18:D:501:HEC:HBC3	18:D:501:HEC:HMC1	1.79	0.64
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.63	0.64
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.79	0.64
2:O:29:LEU:CD2	2:O:30:PRO:HD2	2.27	0.64
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.31	0.64
5:R:91:TRP:CE3	5:R:96:LEU:HD22	2.33	0.64
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.62	0.64
3:P:6:ARG:HD3	3:P:16:ASN:OD1	1.97	0.64
5:R:166:ASP:HB3	5:R:172:ARG:HH11	1.61	0.64
6:S:13:MET:HA	6:S:16:ILE:HB	1.79	0.64
6:S:63:LYS:HD3	7:T:13:ILE:HG21	1.79	0.64
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.80	0.64
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.33	0.64
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.13	0.64
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.32	0.64
1:A:35:CYS:HA	1:A:372:THR:HG21	1.78	0.64
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.32	0.64
2:O:353:THR:HG22	2:O:355:GLU:H	1.62	0.64
2:O:359:LYS:HA	2:O:362:ASN:ND2	2.12	0.64
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.28	0.64
1:N:23:LEU:HA	1:N:192:ALA:O	1.98	0.64
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.33	0.64
4:Q:46:VAL:HG12	4:Q:47:ALA:H	1.63	0.64
1:N:379:ILE:HG12	1:N:389:ARG:HE	1.64	0.64
3:P:157:ILE:O	3:P:159:HIS:N	2.31	0.64
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.66	0.64
4:D:218:LEU:HD13	5:E:43:ALA:HA	1.80	0.63
1:N:145:MET:HE2	1:N:145:MET:HA	1.80	0.63
1:N:432:LEU:HD23	1:N:433:ASP:H	1.62	0.63
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.25	0.63
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.80	0.63
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.34	0.63
6:S:13:MET:O	6:S:17:ARG:HG3	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:PHE:CD1	4:D:10:PHE:N	2.66	0.63
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.34	0.63
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.38	0.63
6:F:31:LEU:HD21	6:F:65:ALA:HB2	1.79	0.63
9:I:32:UNK:N	9:I:73:PRO:HG2	2.14	0.63
7:T:41:PHE:HD2	7:T:41:PHE:O	1.80	0.63
2:B:71:LEU:O	2:B:74:PRO:HD2	1.98	0.63
2:B:72:ALA:CB	2:B:75:LEU:HD12	2.29	0.63
2:B:248:ASN:C	2:B:248:ASN:ND2	2.56	0.63
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.80	0.63
4:D:171:TYR:OH	4:D:182:ILE:HA	1.99	0.63
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.63	0.63
1:N:5:ALA:O	1:N:8:LEU:HB2	1.98	0.63
2:O:62:ASN:O	2:O:65:THR:HG22	1.98	0.63
1:A:294:LEU:HD11	1:A:334:MET:CE	2.20	0.63
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.79	0.63
1:N:35:CYS:HA	1:N:372:THR:HG21	1.81	0.63
1:N:49:ASN:ND2	1:N:51:LYS:H	1.96	0.63
2:O:248:ASN:C	2:O:248:ASN:ND2	2.54	0.63
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.62	0.63
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.63	0.63
5:R:73:LYS:HB3	5:R:195:VAL:O	1.98	0.63
5:R:165:TYR:CE2	5:R:180:LEU:HG	2.33	0.63
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.28	0.63
1:A:49:ASN:C	1:A:49:ASN:ND2	2.56	0.63
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.81	0.63
7:G:58:LEU:HD12	7:G:58:LEU:O	1.99	0.63
2:O:341:MET:O	2:O:344:LEU:N	2.30	0.63
3:P:123:THR:HG21	3:P:190:ILE:HG13	1.79	0.63
3:C:30:ALA:O	3:C:32:TRP:N	2.31	0.62
4:D:235:MET:HE3	6:F:60:PHE:CE1	2.32	0.62
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.12	0.62
2:O:147:ASP:OD1	9:V:68:ILE:HD11	1.98	0.62
2:B:24:LEU:HD13	2:B:38:LEU:HB2	1.79	0.62
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.14	0.62
3:C:207:ASN:O	3:C:208:ASN:HB3	1.98	0.62
4:D:164:ILE:HG21	4:D:182:ILE:HG21	1.81	0.62
6:S:68:LEU:O	6:S:71:LYS:N	2.26	0.62
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.82	0.62
1:A:182:LEU:O	1:A:186:ILE:HG13	1.98	0.62
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.14	0.62
3:C:36:SER:O	3:C:39:ALA:HB3	1.99	0.62
3:C:316:MET:HG2	3:C:319:ARG:NH2	2.14	0.62
4:D:167:GLU:C	4:D:169:LEU:H	2.06	0.62
1:N:105:ASP:O	1:N:109:VAL:HG23	1.99	0.62
3:P:70:THR:HA	3:P:74:VAL:CG2	2.29	0.62
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.34	0.62
2:B:220:ALA:O	2:B:224:LEU:HB2	1.98	0.62
9:I:65:VAL:HG12	9:I:66:ALA:N	2.15	0.62
1:A:406:MET:O	1:A:410:VAL:HG23	1.99	0.62
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.24	0.62
1:N:49:ASN:HD21	1:N:52:ASN:H	1.46	0.62
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.35	0.62
6:S:67:ASP:OD1	6:S:71:LYS:HD2	1.99	0.62
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.64	0.62
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.82	0.62
6:F:68:LEU:O	6:F:71:LYS:N	2.30	0.62
1:N:61:HIS:CE1	1:N:137:GLU:OE1	2.53	0.62
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.15	0.62
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.64	0.62
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.80	0.62
2:O:226:ILE:HG22	2:O:227:ARG:H	1.63	0.62
5:R:109:GLU:O	5:R:123:ASP:HB2	1.99	0.62
6:S:21:TYR:C	6:S:21:TYR:CD2	2.78	0.62
10:W:56:LYS:HE2	10:W:60:GLU:CD	2.25	0.62
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.35	0.62
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.34	0.62
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.35	0.62
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.15	0.61
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.15	0.61
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.81	0.61
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.34	0.61
4:D:116:ILE:HG23	4:D:117:VAL:N	2.14	0.61
8:H:58:LEU:HG	8:H:62:LEU:HD12	1.82	0.61
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.25	0.61
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.82	0.61
3:P:95:ILE:CD1	3:P:121:LEU:HD13	2.29	0.61
5:R:109:GLU:OE1	5:R:166:ASP:HB2	2.00	0.61
1:A:161:THR:HG21	1:A:235:ARG:H	1.65	0.61
1:A:240:GLU:OE1	1:A:434:TYR:HB2	1.99	0.61
2:B:58:GLU:OE1	2:B:64:GLY:N	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:227:TRP:O	4:D:228:SER:C	2.41	0.61
2:B:109:VAL:CG1	2:B:123:LEU:HB2	2.30	0.61
3:C:63:ALA:HB2	3:C:176:LEU:HD21	1.80	0.61
4:D:8:PRO:HG2	4:D:10:PHE:HE1	1.63	0.61
1:N:406:MET:O	1:N:410:VAL:HG23	2.00	0.61
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.66	0.61
2:B:150:VAL:CG2	2:B:151:ALA:H	2.13	0.61
1:N:394:GLU:O	1:N:395:TRP:C	2.44	0.61
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.30	0.61
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.35	0.61
3:C:345:GLU:O	3:C:349:ILE:HG13	2.01	0.61
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.16	0.61
2:B:150:VAL:CG2	2:B:151:ALA:N	2.63	0.61
2:O:150:VAL:CG2	2:O:151:ALA:N	2.62	0.61
4:D:94:PRO:HG2	4:D:95:TYR:HD1	1.66	0.61
3:P:30:ALA:C	3:P:32:TRP:H	2.09	0.61
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.66	0.61
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.30	0.61
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.81	0.61
4:D:167:GLU:O	4:D:169:LEU:N	2.34	0.61
2:O:312:PHE:N	2:O:323:GLY:O	2.32	0.61
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.15	0.61
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.36	0.61
1:A:156:THR:HA	5:E:7:VAL:HG21	1.83	0.61
1:A:335:MET:CG	1:A:339:GLN:HE21	2.13	0.61
3:C:70:THR:HA	3:C:74:VAL:HG23	1.82	0.61
4:D:222:MET:HE3	5:E:40:THR:OG1	2.01	0.61
4:Q:155:GLY:C	4:Q:157:ALA:H	2.08	0.61
1:A:332:ASP:O	1:A:333:ASP:C	2.43	0.61
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.31	0.61
1:N:281:ASP:O	1:N:284:PHE:HD1	1.84	0.61
5:R:34:GLY:HA2	10:W:10:TYR:HB2	1.83	0.61
1:N:106:MET:O	1:N:106:MET:HE2	2.01	0.60
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.01	0.60
6:S:32:MET:CE	6:S:87:LYS:H	2.13	0.60
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.83	0.60
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.31	0.60
3:C:173:ASN:N	3:C:174:PRO:HD2	2.16	0.60
3:C:184:PHE:CD2	13:C:501:HEM:HBC1	2.35	0.60
1:N:240:GLU:OE1	1:N:434:TYR:HB2	2.02	0.60
6:S:11:ARG:HG2	6:S:11:ARG:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:HB2	1:A:199:ALA:O	2.01	0.60
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.35	0.60
6:F:32:MET:HE3	6:F:87:LYS:H	1.64	0.60
2:O:312:PHE:HE1	9:V:62:ARG:O	1.84	0.60
3:P:70:THR:HA	3:P:74:VAL:HG23	1.83	0.60
3:P:342:GLN:HA	3:P:342:GLN:NE2	2.15	0.60
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.83	0.60
1:N:388:ARG:HG3	1:N:388:ARG:NH2	2.15	0.60
1:A:89:TYR:O	1:A:95:THR:HG23	2.01	0.60
5:E:128:LYS:O	5:E:130:PRO:HD3	2.02	0.60
1:N:182:LEU:N	1:N:182:LEU:HD23	2.17	0.60
3:P:123:THR:HG22	3:P:190:ILE:HD11	1.83	0.60
6:S:32:MET:HE3	6:S:87:LYS:HB2	1.82	0.60
1:N:182:LEU:O	1:N:186:ILE:HG13	2.00	0.60
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.37	0.60
3:P:134:LEU:HB2	3:P:135:PRO:HD3	1.82	0.60
4:Q:167:GLU:C	4:Q:169:LEU:H	2.10	0.60
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.65	0.60
2:B:396:SER:O	2:B:399:ALA:HB3	2.01	0.60
4:D:102:ARG:HH11	4:D:102:ARG:HG2	1.67	0.60
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.84	0.60
1:N:86:PHE:CD2	1:N:99:ILE:HD11	2.36	0.60
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.37	0.60
2:B:109:VAL:HG13	2:B:123:LEU:HB2	1.84	0.60
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.83	0.60
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.02	0.60
2:O:219:VAL:HG13	2:O:223:PHE:CD1	2.37	0.60
3:P:117:GLY:C	13:P:502:HEM:HBC2	2.27	0.60
2:B:230:ALA:O	2:B:232:THR:N	2.35	0.59
1:N:86:PHE:HB3	2:O:285:ILE:HG22	1.83	0.59
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.84	0.59
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.82	0.59
3:P:325:LEU:HD21	3:P:366:LEU:CB	2.32	0.59
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.36	0.59
2:B:140:LEU:HD12	2:B:140:LEU:O	2.02	0.59
2:B:332:HIS:O	2:B:336:VAL:HG23	2.02	0.59
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.84	0.59
1:N:255:LEU:HD13	1:N:422:LEU:CD1	2.31	0.59
2:O:332:HIS:O	2:O:336:VAL:HG23	2.02	0.59
4:Q:235:MET:HE3	6:S:60:PHE:CE1	2.36	0.59
2:B:248:ASN:ND2	2:B:250:HIS:H	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.84	0.59
2:O:76:THR:HG22	2:O:82:SER:N	2.13	0.59
3:P:27:ASN:ND2	3:P:209:PRO:HD2	2.16	0.59
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.36	0.59
10:J:25:VAL:O	10:J:29:VAL:HG23	2.01	0.59
1:N:161:THR:HG21	1:N:234:CYS:HA	1.83	0.59
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.84	0.59
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.03	0.59
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.37	0.59
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.37	0.59
2:O:73:SER:N	2:O:74:PRO:HD2	2.17	0.59
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.84	0.59
3:P:27:ASN:HD21	3:P:208:ASN:CG	2.10	0.59
3:C:21:ASP:O	3:C:23:PRO:HD3	2.03	0.59
3:P:21:ASP:O	3:P:23:PRO:HD3	2.01	0.59
4:Q:167:GLU:O	4:Q:169:LEU:N	2.36	0.59
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.32	0.59
1:A:310:PHE:HE1	1:A:322:PHE:N	2.00	0.59
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.66	0.59
3:C:139:MET:HE2	3:C:253:ASP:OD2	2.02	0.59
9:V:65:VAL:HG12	9:V:66:ALA:N	2.17	0.59
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.38	0.59
2:B:295:LEU:HA	2:B:343:GLN:HG2	1.85	0.59
3:C:162:VAL:O	3:C:163:GLU:C	2.45	0.59
4:D:215:LEU:HD22	5:E:46:ALA:CB	2.31	0.59
5:E:171:ILE:HG12	5:E:176:ALA:O	2.02	0.59
2:O:220:ALA:O	2:O:224:LEU:HB2	2.01	0.59
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.21	0.59
1:A:242:ARG:O	7:G:14:ILE:HA	2.03	0.59
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.83	0.59
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.84	0.59
16:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.03	0.59
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.36	0.59
4:Q:71:GLN:HG3	4:Q:82:MET:HE1	1.85	0.59
3:C:104:TYR:HD2	3:C:105:TYR:CE1	2.21	0.58
4:D:191:ARG:O	4:D:192:TRP:C	2.45	0.58
3:P:154:ILE:HG23	3:P:155:PRO:HD2	1.84	0.58
3:P:173:ASN:N	3:P:174:PRO:HD2	2.17	0.58
5:R:134:ILE:HB	5:R:185:TYR:CE2	2.38	0.58
1:A:241:ILE:HG23	1:A:241:ILE:O	2.03	0.58
4:D:130:LEU:HD12	4:D:150:ASN:ND2	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:38:LEU:HA	10:J:14:PHE:CE1	2.38	0.58
7:G:41:PHE:HD2	7:G:41:PHE:O	1.85	0.58
1:N:45:SER:HA	1:N:48:GLU:CG	2.33	0.58
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.17	0.58
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.85	0.58
2:B:75:LEU:CD2	2:B:136:GLU:HB3	2.33	0.58
3:C:76:TYR:CE1	5:E:57:GLN:HG2	2.39	0.58
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.19	0.58
1:N:253:VAL:HG11	1:N:335:MET:CE	2.33	0.58
2:O:58:GLU:OE1	2:O:64:GLY:N	2.36	0.58
2:O:162:ASN:O	2:O:244:ILE:HD12	2.03	0.58
4:Q:191:ARG:O	4:Q:192:TRP:C	2.45	0.58
6:S:61:ARG:NH2	6:S:89:TYR:HE2	1.95	0.58
1:A:45:SER:HA	1:A:48:GLU:CG	2.34	0.58
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.38	0.58
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.85	0.58
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.38	0.58
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.86	0.58
2:O:206:LEU:HG	2:O:216:LEU:HD11	1.85	0.58
2:O:207:VAL:O	2:O:216:LEU:HD21	2.03	0.58
3:P:26:SER:HA	3:P:219:ILE:CD1	2.33	0.58
3:P:36:SER:O	3:P:39:ALA:HB3	2.03	0.58
3:C:311:SER:HB2	3:C:319:ARG:HH11	1.68	0.58
5:E:185:TYR:O	5:E:186:GLN:HB2	2.04	0.58
2:O:227:ARG:HG3	2:O:228:SER:N	2.17	0.58
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.38	0.58
3:P:52:LEU:HD13	13:P:501:HEM:HBD1	1.85	0.58
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.03	0.58
3:P:365:ILE:HG22	3:P:366:LEU:HD23	1.85	0.58
1:A:310:PHE:CE1	1:A:322:PHE:N	2.71	0.58
2:B:102:ARG:CZ	2:B:164:HIS:CD2	2.87	0.58
3:P:120:LEU:HD22	13:P:502:HEM:HBB1	1.84	0.58
9:V:65:VAL:O	9:V:76:VAL:HG23	2.04	0.58
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.68	0.58
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.33	0.58
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.38	0.58
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.58
1:A:379:ILE:HG12	1:A:389:ARG:HE	1.69	0.58
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.31	0.58
3:P:141:PHE:O	3:P:144:ALA:HB3	2.04	0.58
3:P:333:LEU:HD11	11:P:3007:PEE:H38	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:69:LEU:HD13	5:R:71:LEU:HD11	1.85	0.58
1:A:307:PHE:CD1	1:A:307:PHE:C	2.82	0.58
1:N:410:VAL:O	1:N:413:LYS:HB3	2.03	0.58
2:O:109:VAL:HG13	2:O:123:LEU:HB2	1.86	0.58
3:P:130:VAL:HG23	3:P:131:GLY:N	2.19	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.38	0.58
5:R:51:ALA:O	5:R:52:LYS:C	2.47	0.58
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.85	0.58
2:B:189:GLU:O	2:B:191:LEU:N	2.36	0.58
2:B:203:ARG:O	2:B:387:LEU:HD11	2.04	0.58
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.38	0.58
5:R:57:GLN:OE1	20:R:3009:PLC:H12	2.03	0.58
6:S:71:LYS:O	6:S:72:HIS:HB2	2.04	0.58
1:N:330:SER:O	1:N:331:ILE:C	2.46	0.57
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.39	0.57
1:A:40:TRP:O	1:A:384:LEU:HD22	2.04	0.57
4:D:116:ILE:HG23	4:D:117:VAL:H	1.69	0.57
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.85	0.57
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.39	0.57
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.38	0.57
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.57
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.34	0.57
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.22	0.57
4:D:76:GLU:CD	4:D:76:GLU:H	2.12	0.57
3:P:166:TRP:CD1	3:P:171:VAL:HG22	2.40	0.57
4:Q:224:ARG:HH12	16:Q:3003:CDL:HB21	1.69	0.57
1:A:61:HIS:CE1	1:A:137:GLU:OE1	2.57	0.57
2:B:67:HIS:O	2:B:70:ARG:HB3	2.04	0.57
2:B:189:GLU:O	2:B:192:HIS:N	2.37	0.57
2:B:293:SER:OG	2:B:296:TYR:HB2	2.05	0.57
3:P:76:TYR:CE1	5:R:57:GLN:HG2	2.40	0.57
3:P:282:LEU:HD23	3:P:282:LEU:O	2.04	0.57
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.39	0.57
8:U:40:CYS:O	8:U:44:VAL:HG23	2.04	0.57
1:A:86:PHE:HB3	2:B:285:ILE:HG22	1.86	0.57
1:A:178:THR:HB	1:A:181:ASP:OD1	2.05	0.57
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.40	0.57
2:O:27:THR:HG22	2:O:28:LYS:N	2.17	0.57
7:T:42:SER:O	7:T:45:VAL:HG12	2.05	0.57
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.40	0.57
1:N:254:ALA:HB3	1:N:423:ALA:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:137:GLY:N	3:P:140:SER:HB2	2.20	0.57
3:P:139:MET:HE2	3:P:253:ASP:OD2	2.05	0.57
3:P:184:PHE:HA	13:P:501:HEM:CBC	2.34	0.57
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.87	0.57
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.03	0.57
2:B:258:VAL:HB	2:B:322:PHE:O	2.05	0.57
4:D:42:SER:HB2	4:D:112:ASP:OD2	2.04	0.57
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.40	0.57
1:N:239:SER:HB2	7:T:17:SER:O	2.04	0.57
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.19	0.57
3:P:5:ILE:HG22	3:P:12:LEU:HD12	1.86	0.57
5:R:108:GLN:C	5:R:110:ALA:H	2.13	0.57
1:N:356:ARG:O	1:N:357:ALA:C	2.47	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.87	0.57
3:P:162:VAL:O	3:P:163:GLU:C	2.47	0.57
3:P:207:ASN:O	3:P:208:ASN:HB3	2.03	0.57
3:P:269:ILE:HG23	3:P:269:ILE:O	2.05	0.57
4:D:10:PHE:H	4:D:10:PHE:HD1	1.52	0.57
5:E:108:GLN:O	5:E:112:VAL:HG23	2.04	0.57
6:F:27:ASN:HB2	6:F:81:VAL:HB	1.86	0.57
2:O:42:SER:OG	2:O:43:PRO:HD2	2.05	0.57
2:O:146:VAL:HG12	2:O:147:ASP:N	2.19	0.57
2:O:209:ILE:HG22	2:O:210:GLY:N	2.19	0.57
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	1.87	0.57
1:A:49:ASN:HD21	1:A:52:ASN:H	1.53	0.57
4:D:168:ILE:O	4:D:168:ILE:HG12	2.05	0.57
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.40	0.57
5:R:135:LEU:CD2	5:R:169:GLY:HA3	2.35	0.57
1:A:45:SER:HA	1:A:48:GLU:CD	2.30	0.56
2:B:86:THR:O	2:B:90:GLU:HG3	2.05	0.56
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.87	0.56
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.35	0.56
3:C:126:ALA:O	3:C:129:PHE:HB3	2.04	0.56
4:D:232:SER:HB3	7:G:23:GLN:NE2	2.19	0.56
5:E:35:PHE:O	5:E:38:LEU:N	2.38	0.56
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.86	0.56
1:N:333:ASP:O	1:N:336:PHE:HB3	2.05	0.56
10:W:14:PHE:N	10:W:14:PHE:CD2	2.70	0.56
10:W:22:LEU:N	10:W:22:LEU:HD23	2.20	0.56
2:B:272:PHE:O	2:B:275:LEU:N	2.38	0.56
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ASP:O	2:B:319:SER:HB2	2.04	0.56
6:F:72:HIS:O	6:F:73:ARG:HD3	2.05	0.56
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.40	0.56
3:P:107:SER:C	3:P:109:LEU:H	2.13	0.56
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.34	0.56
1:A:46:ARG:HD3	1:A:231:LEU:HD13	1.88	0.56
1:A:180:ALA:O	1:A:183:ALA:HB3	2.05	0.56
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.35	0.56
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.40	0.56
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.05	0.56
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.38	0.56
3:P:186:LEU:O	3:P:187:PRO:C	2.46	0.56
3:P:230:ILE:HG23	11:P:3005:PEE:H25	1.88	0.56
6:S:68:LEU:O	6:S:70:LEU:N	2.38	0.56
6:S:73:ARG:HH11	6:S:73:ARG:HG3	1.70	0.56
7:T:58:LEU:HD12	7:T:58:LEU:O	2.06	0.56
1:A:404:ALA:O	1:A:405:ARG:C	2.48	0.56
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.87	0.56
2:B:229:GLY:C	2:B:231:GLY:H	2.13	0.56
2:B:345:LYS:C	2:B:347:ALA:N	2.63	0.56
5:E:103:GLN:HA	5:E:106:ILE:CB	2.30	0.56
2:O:135:TRP:O	2:O:136:GLU:C	2.46	0.56
2:O:308:ASP:OD1	9:V:56:SER:HA	2.06	0.56
3:P:106:GLY:HA2	3:P:108:TYR:CD2	2.39	0.56
4:Q:218:LEU:HD13	5:R:43:ALA:HA	1.87	0.56
1:A:23:LEU:HA	1:A:192:ALA:O	2.06	0.56
3:C:22:LEU:HD12	3:C:23:PRO:N	2.20	0.56
3:C:134:LEU:HD21	3:C:180:PHE:HA	1.86	0.56
3:C:208:ASN:C	3:C:208:ASN:OD1	2.48	0.56
5:R:44:CYS:HB3	10:W:24:VAL:HG11	1.87	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.56
5:R:62:LEU:O	5:R:63:SER:O	2.23	0.56
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.39	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.41	0.56
3:C:70:THR:HA	3:C:74:VAL:CG2	2.36	0.56
5:E:148:ALA:HA	5:E:156:TYR:CD2	2.41	0.56
8:H:37:LEU:O	8:H:38:GLU:C	2.48	0.56
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.06	0.56
1:A:356:ARG:O	1:A:357:ALA:C	2.47	0.56
2:B:177:TYR:O	2:B:178:CYS:C	2.49	0.56
2:B:333:ALA:O	2:B:337:ILE:HG13	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:SER:HG	3:C:250:LEU:HB2	1.71	0.56
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.41	0.56
6:F:32:MET:O	6:F:35:ASP:HB2	2.06	0.56
10:J:22:LEU:N	10:J:22:LEU:HD23	2.20	0.56
1:N:106:MET:HE3	1:N:208:LEU:HD13	1.86	0.56
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.41	0.56
2:O:385:GLU:C	2:O:387:LEU:H	2.13	0.56
3:P:139:MET:O	3:P:140:SER:C	2.49	0.56
4:Q:47:ALA:HB1	4:Q:89:ASP:O	2.05	0.56
1:A:394:GLU:O	1:A:395:TRP:C	2.49	0.56
3:C:45:GLN:CB	13:C:501:HEM:HAB	2.36	0.56
3:C:285:ILE:HD12	3:C:285:ILE:N	2.21	0.56
7:G:42:SER:O	7:G:45:VAL:HG12	2.06	0.56
1:N:335:MET:CG	1:N:339:GLN:HE21	2.18	0.56
2:O:396:SER:O	2:O:399:ALA:HB3	2.06	0.56
2:B:239:TYR:HE1	2:B:260:GLU:N	2.04	0.56
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.71	0.56
5:E:29:SER:HA	5:E:32:ARG:HH21	1.71	0.56
1:N:209:VAL:O	1:N:212:ALA:HB3	2.05	0.56
2:O:47:ILE:N	2:O:47:ILE:CD1	2.68	0.56
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.42	0.56
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.06	0.56
6:S:27:ASN:HB2	6:S:81:VAL:HB	1.87	0.56
1:A:186:ILE:O	1:A:190:PHE:HB2	2.06	0.55
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.70	0.55
2:B:146:VAL:HG12	2:B:147:ASP:N	2.22	0.55
3:C:304:LEU:O	3:C:305:ILE:C	2.50	0.55
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.41	0.55
4:D:235:MET:HE3	6:F:60:PHE:HE1	1.70	0.55
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.36	0.55
10:J:14:PHE:CD2	10:J:14:PHE:N	2.71	0.55
3:P:45:GLN:CB	13:P:501:HEM:HAB	2.36	0.55
3:P:231:LEU:HD11	4:Q:220:TYR:HA	1.88	0.55
4:Q:227:TRP:O	4:Q:228:SER:C	2.49	0.55
5:R:1:VAL:HG23	5:R:3:ASN:H	1.70	0.55
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.32	0.55
1:A:49:ASN:ND2	1:A:51:LYS:H	2.04	0.55
1:A:106:MET:O	1:A:110:VAL:HG23	2.06	0.55
3:C:9:HIS:ND1	3:C:10:PRO:HD2	2.21	0.55
7:G:55:ALA:O	7:G:56:TYR:C	2.48	0.55
1:N:318:GLY:O	1:N:319:LEU:HD23	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.15	0.55
3:P:27:ASN:ND2	3:P:208:ASN:OD1	2.35	0.55
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.88	0.55
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.87	0.55
1:A:342:TRP:O	1:A:345:LEU:HB2	2.06	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.88	0.55
5:E:171:ILE:N	5:E:179:ASN:OD1	2.37	0.55
1:N:45:SER:HA	1:N:48:GLU:CD	2.31	0.55
1:N:332:ASP:O	1:N:333:ASP:C	2.50	0.55
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.22	0.55
3:P:276:LEU:O	3:P:279:TYR:HB3	2.06	0.55
7:T:29:ILE:O	7:T:34:LEU:HG	2.07	0.55
2:B:27:THR:HG22	2:B:28:LYS:H	1.71	0.55
2:B:385:GLU:C	2:B:387:LEU:H	2.14	0.55
3:C:365:ILE:HG22	3:C:366:LEU:HD23	1.86	0.55
5:E:136:VAL:O	5:E:138:VAL:N	2.37	0.55
5:E:157:TYR:HE1	5:E:162:GLY:HA2	1.69	0.55
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.06	0.55
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.41	0.55
2:O:273:SER:O	2:O:276:GLN:HB3	2.07	0.55
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.41	0.55
18:D:501:HEC:HMB3	18:D:501:HEC:CBB	2.34	0.55
6:F:63:LYS:HD3	7:G:13:ILE:HG21	1.88	0.55
6:F:71:LYS:O	6:F:72:HIS:HB2	2.04	0.55
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.72	0.55
2:O:170:THR:O	2:O:172:LEU:N	2.40	0.55
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.41	0.55
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.41	0.55
5:R:35:PHE:O	5:R:36:SER:C	2.50	0.55
2:B:47:ILE:N	2:B:47:ILE:CD1	2.70	0.55
2:B:292:THR:O	2:B:292:THR:HG22	2.06	0.55
3:P:316:MET:HG2	3:P:319:ARG:HH21	1.70	0.55
1:A:75:PHE:O	1:A:79:VAL:HG23	2.07	0.55
2:B:229:GLY:O	2:B:231:GLY:N	2.39	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.55
3:C:79:LEU:O	3:C:79:LEU:HD12	2.06	0.55
1:N:19:LEU:O	1:N:21:ASN:N	2.40	0.55
1:N:54:GLY:O	1:N:55:ALA:C	2.49	0.55
1:N:86:PHE:O	2:O:285:ILE:HA	2.06	0.55
3:P:137:GLY:H	3:P:140:SER:HB2	1.72	0.55
6:S:32:MET:O	6:S:35:ASP:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:THR:CG2	2:B:397:VAL:HB	2.37	0.55
1:N:4:TYR:HA	2:O:113:ARG:HD3	1.89	0.55
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.42	0.55
1:N:281:ASP:HB3	1:N:284:PHE:HE1	1.71	0.55
2:O:122:TYR:O	2:O:126:VAL:HG23	2.07	0.55
4:Q:220:TYR:CE2	16:Q:3003:CDL:H722	2.42	0.55
5:R:113:ASP:C	5:R:115:SER:N	2.65	0.55
6:S:13:MET:HB2	6:S:17:ARG:NH1	2.21	0.55
10:W:59:TYR:O	10:W:60:GLU:O	2.24	0.55
3:C:139:MET:O	3:C:140:SER:C	2.50	0.55
6:F:21:TYR:C	6:F:21:TYR:CD2	2.84	0.55
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.88	0.55
2:O:272:PHE:O	2:O:276:GLN:N	2.40	0.55
4:Q:120:ARG:HG2	4:Q:120:ARG:NH1	2.18	0.55
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.42	0.54
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.42	0.54
2:B:170:THR:O	2:B:172:LEU:N	2.40	0.54
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.88	0.54
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.42	0.54
5:E:152:ASP:C	5:E:153:PHE:CD1	2.85	0.54
1:N:124:GLU:O	1:N:124:GLU:HG2	2.08	0.54
2:O:81:SER:O	2:O:83:PHE:N	2.40	0.54
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.07	0.54
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.07	0.54
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.42	0.54
1:A:410:VAL:O	1:A:413:LYS:HB3	2.08	0.54
3:C:156:TYR:CD2	3:C:156:TYR:N	2.74	0.54
5:E:136:VAL:HB	5:E:181:GLU:HB3	1.88	0.54
2:O:239:TYR:CD2	2:O:240:TRP:N	2.75	0.54
3:P:231:LEU:CD1	4:Q:220:TYR:HA	2.37	0.54
5:R:83:GLU:CG	5:R:102:THR:HG22	2.28	0.54
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.43	0.54
1:A:176:HIS:O	1:A:177:LEU:C	2.50	0.54
2:B:272:PHE:O	2:B:276:GLN:N	2.37	0.54
3:C:286:PRO:HA	5:R:175:PRO:HB3	1.90	0.54
2:O:258:VAL:HB	2:O:322:PHE:O	2.06	0.54
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.42	0.54
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.07	0.54
1:A:4:TYR:O	1:A:5:ALA:C	2.51	0.54
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.88	0.54
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.16	0.54
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.88	0.54
2:O:169:LYS:O	2:O:170:THR:HG23	2.07	0.54
3:P:37:LEU:HD21	3:P:232:GLY:O	2.07	0.54
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.54
8:U:37:LEU:O	8:U:38:GLU:C	2.51	0.54
1:A:339:GLN:HE22	1:A:437:ILE:HG23	1.71	0.54
3:C:186:LEU:O	3:C:187:PRO:C	2.51	0.54
3:C:278:ALA:HB1	3:C:295:LEU:HD13	1.87	0.54
3:C:347:PRO:O	3:C:350:ILE:HG22	2.08	0.54
3:C:380:TYR:OH	6:F:34:ASP:HA	2.08	0.54
1:N:206:LYS:O	1:N:208:LEU:N	2.40	0.54
5:R:188:VAL:HG23	5:R:188:VAL:O	2.06	0.54
8:U:13:LEU:H	8:U:13:LEU:CD2	2.15	0.54
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.69	0.54
1:A:269:VAL:HG11	1:A:410:VAL:CG2	2.38	0.54
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.07	0.54
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.88	0.54
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.43	0.54
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.89	0.54
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.89	0.54
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.88	0.54
1:N:253:VAL:HG11	1:N:335:MET:HE1	1.89	0.54
2:O:81:SER:C	2:O:83:PHE:N	2.64	0.54
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.88	0.54
3:P:80:ILE:O	3:P:81:ARG:C	2.51	0.54
3:P:101:ARG:HH22	13:P:502:HEM:CGA	2.21	0.54
3:P:273:TRP:CE3	3:P:274:TYR:HA	2.43	0.54
5:R:140:THR:HG21	5:R:178:TYR:HB2	1.89	0.54
1:A:295:ALA:O	1:A:298:ALA:HB3	2.08	0.54
2:B:31:ASN:HD22	2:B:32:GLY:H	1.56	0.54
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.90	0.54
2:B:273:SER:O	2:B:276:GLN:HB3	2.08	0.54
3:C:92:PHE:C	3:C:95:ILE:HG22	2.32	0.54
5:E:51:ALA:O	5:E:52:LYS:C	2.50	0.54
5:E:113:ASP:C	5:E:115:SER:H	2.16	0.54
6:F:52:GLU:HG2	6:F:56:ASN:ND2	2.22	0.54
2:O:63:LEU:O	2:O:65:THR:N	2.38	0.54
2:O:350:GLY:O	2:O:352:VAL:N	2.32	0.54
3:P:95:ILE:HD13	3:P:121:LEU:HD12	1.90	0.54
3:P:236:MET:O	3:P:239:PRO:HD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:72:HIS:O	6:S:73:ARG:HD3	2.07	0.54
1:A:248:LEU:HB3	1:A:249:PRO:HD2	1.90	0.54
3:C:6:ARG:HD3	3:C:16:ASN:OD1	2.07	0.54
4:D:142:VAL:HG23	4:D:142:VAL:O	2.08	0.54
5:E:83:GLU:HA	5:E:100:HIS:CG	2.43	0.54
6:F:74:ILE:HG13	6:F:75:LEU:N	2.22	0.54
1:N:158:PHE:O	1:N:159:GLN:O	2.26	0.54
1:N:371:GLY:O	1:N:375:VAL:HG23	2.08	0.54
4:Q:54:VAL:HG11	4:Q:192:TRP:CE2	2.43	0.54
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.89	0.54
2:B:312:PHE:HE1	9:I:62:ARG:O	1.91	0.54
1:N:433:ASP:O	1:N:437:ILE:HG13	2.08	0.54
3:P:366:LEU:HD23	3:P:366:LEU:N	2.23	0.54
1:A:145:MET:HE2	1:A:145:MET:HA	1.90	0.53
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.89	0.53
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.39	0.53
2:O:97:SER:HA	9:V:69:SER:HA	1.90	0.53
3:P:104:TYR:HD2	3:P:105:TYR:CD1	2.27	0.53
5:R:136:VAL:O	5:R:138:VAL:N	2.35	0.53
3:C:160:THR:O	3:C:163:GLU:HB3	2.09	0.53
3:C:172:ASP:C	3:C:174:PRO:HD2	2.33	0.53
4:D:167:GLU:C	4:D:169:LEU:N	2.62	0.53
5:E:177:PRO:O	5:E:178:TYR:HD1	1.91	0.53
2:O:318:ASP:O	2:O:319:SER:HB2	2.08	0.53
3:P:172:ASP:C	3:P:174:PRO:HD2	2.33	0.53
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.23	0.53
1:A:334:MET:O	1:A:335:MET:C	2.51	0.53
3:C:365:ILE:C	3:C:368:PRO:HD2	2.33	0.53
6:F:50:LEU:HD21	6:F:90:LEU:HD12	1.89	0.53
7:G:81:GLN:O	8:H:47:ARG:HA	2.08	0.53
2:O:81:SER:O	2:O:82:SER:C	2.52	0.53
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.71	0.53
2:O:350:GLY:C	2:O:352:VAL:H	2.17	0.53
3:P:113:THR:HG21	3:P:201:LEU:CD1	2.39	0.53
3:P:287:ASN:O	3:P:288:LYS:C	2.50	0.53
4:Q:164:ILE:HD11	4:Q:183:ALA:HB2	1.89	0.53
8:U:61:PHE:O	8:U:62:LEU:C	2.50	0.53
2:B:239:TYR:HE1	2:B:260:GLU:H	1.56	0.53
2:B:325:TYR:C	2:B:325:TYR:CD2	2.87	0.53
3:C:325:LEU:HD21	3:C:366:LEU:CB	2.38	0.53
6:F:67:ASP:OD1	6:F:71:LYS:HD2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.49	0.53
1:N:304:CYS:HA	1:N:326:ALA:HB2	1.91	0.53
2:O:428:GLY:O	2:O:430:LEU:HG	2.08	0.53
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.89	0.53
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.08	0.53
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.08	0.53
8:U:59:PHE:O	8:U:60:ASP:C	2.52	0.53
2:B:135:TRP:O	2:B:136:GLU:C	2.51	0.53
3:C:287:ASN:O	3:C:288:LYS:C	2.52	0.53
5:E:62:LEU:O	5:E:63:SER:O	2.27	0.53
1:N:40:TRP:HZ3	1:N:376:CYS:SG	2.27	0.53
1:N:334:MET:O	1:N:335:MET:C	2.52	0.53
1:N:404:ALA:O	1:N:405:ARG:C	2.52	0.53
1:N:411:CYS:O	1:N:415:ILE:HG13	2.09	0.53
4:Q:235:MET:HE1	6:S:63:LYS:C	2.34	0.53
2:B:122:TYR:O	2:B:126:VAL:HG23	2.08	0.53
3:C:148:THR:O	3:C:151:PHE:HD1	1.92	0.53
4:D:44:ASP:OD1	4:D:44:ASP:N	2.42	0.53
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.74	0.53
2:O:109:VAL:CG1	2:O:123:LEU:HB2	2.38	0.53
2:O:207:VAL:CG1	2:O:208:GLY:H	2.16	0.53
3:P:157:ILE:O	3:P:158:GLY:C	2.52	0.53
3:P:273:TRP:CE3	3:P:274:TYR:N	2.77	0.53
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.48	0.53
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.90	0.53
3:C:30:ALA:C	3:C:32:TRP:N	2.67	0.53
3:C:113:THR:HG21	3:C:201:LEU:CD1	2.37	0.53
3:C:120:LEU:HB3	13:C:502:HEM:HAB	1.90	0.53
3:C:123:THR:HG21	3:C:190:ILE:HG13	1.89	0.53
9:I:71:ASN:HD22	9:I:71:ASN:N	1.97	0.53
1:N:4:TYR:O	1:N:5:ALA:C	2.52	0.53
2:O:67:HIS:O	2:O:70:ARG:HB3	2.09	0.53
4:Q:44:ASP:N	4:Q:44:ASP:OD1	2.40	0.53
2:B:350:GLY:O	2:B:352:VAL:N	2.39	0.53
4:D:158:ILE:HG12	4:D:159:GLY:H	1.74	0.53
4:D:197:GLU:HG2	4:D:198:HIS:N	2.24	0.53
1:N:26:ALA:O	1:N:198:ALA:HA	2.09	0.53
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.89	0.53
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.44	0.53
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.43	0.53
8:U:13:LEU:N	8:U:13:LEU:CD2	2.71	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:58:LEU:HG	8:U:62:LEU:HD12	1.91	0.53
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.44	0.53
1:A:432:LEU:HD23	1:A:433:ASP:H	1.72	0.53
2:B:28:LYS:O	2:B:29:LEU:O	2.27	0.53
2:B:312:PHE:CD1	9:I:60:ALA:HB1	2.44	0.53
10:J:59:TYR:N	10:J:59:TYR:CD1	2.77	0.53
2:O:147:ASP:O	2:O:150:VAL:HG22	2.08	0.53
2:O:239:TYR:HD2	2:O:240:TRP:N	2.07	0.53
3:P:78:TRP:CD2	3:P:79:LEU:N	2.77	0.53
1:A:255:LEU:HD12	1:A:421:ALA:O	2.08	0.53
2:B:200:THR:O	2:B:202:ALA:N	2.42	0.53
2:B:207:VAL:CG1	2:B:208:GLY:H	2.12	0.53
2:B:209:ILE:HG22	2:B:210:GLY:N	2.24	0.53
2:B:307:PHE:CD1	2:B:308:ASP:N	2.77	0.53
3:C:164:TRP:O	3:C:165:ALA:C	2.50	0.53
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.24	0.53
4:D:28:ARG:O	4:D:29:GLY:C	2.52	0.53
4:D:68:VAL:HG12	4:D:69:GLU:N	2.23	0.53
4:D:102:ARG:HG2	4:D:102:ARG:NH1	2.24	0.53
5:E:55:VAL:O	5:E:56:THR:C	2.52	0.53
1:N:281:ASP:O	1:N:284:PHE:CD1	2.61	0.53
1:N:433:ASP:OD1	1:N:435:ASN:HB2	2.08	0.53
2:O:177:TYR:O	2:O:178:CYS:C	2.51	0.53
3:P:245:LEU:O	4:Q:201:ARG:CG	2.57	0.53
6:S:77:LYS:HA	6:S:80:TRP:NE1	2.23	0.53
2:B:167:ALA:C	2:B:168:TYR:CD1	2.87	0.52
3:C:344:VAL:HG12	3:C:349:ILE:HD11	1.90	0.52
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.39	0.52
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.52
1:N:22:GLY:O	1:N:193:PRO:HA	2.09	0.52
5:R:35:PHE:O	5:R:38:LEU:N	2.42	0.52
5:R:134:ILE:C	5:R:135:LEU:HG	2.33	0.52
6:S:104:ARG:O	6:S:108:ASN:ND2	2.42	0.52
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.75	0.52
3:P:285:ILE:N	3:P:285:ILE:HD12	2.24	0.52
3:P:304:LEU:O	3:P:305:ILE:C	2.52	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.76	0.52
1:A:244:ARG:HH22	1:A:429:GLU:CD	2.17	0.52
3:C:49:GLY:HA3	13:C:501:HEM:C2C	2.44	0.52
4:D:161:ALA:O	4:D:162:PRO:C	2.53	0.52
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:THR:HG22	1:N:171:THR:H	1.73	0.52
1:N:170:THR:HG22	1:N:171:THR:N	2.25	0.52
3:P:246:PHE:CZ	4:Q:205:GLY:C	2.87	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.90	0.52
3:C:326:PHE:O	3:C:329:LEU:HB3	2.08	0.52
1:N:40:TRP:O	1:N:384:LEU:HD22	2.09	0.52
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.44	0.52
1:N:145:MET:O	1:N:146:THR:C	2.52	0.52
1:N:180:ALA:O	1:N:183:ALA:HB3	2.09	0.52
1:N:186:ILE:O	1:N:190:PHE:HB2	2.08	0.52
2:O:226:ILE:CG2	2:O:227:ARG:H	2.23	0.52
2:B:97:SER:HA	9:I:69:SER:HA	1.92	0.52
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.22	0.52
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.69	0.52
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.09	0.52
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.92	0.52
2:B:182:ARG:NH2	2:B:190:GLN:OE1	2.43	0.52
3:C:52:LEU:HD11	3:C:81:ARG:HA	1.92	0.52
8:H:19:THR:O	8:H:22:GLU:HB2	2.09	0.52
2:O:307:PHE:CD1	2:O:308:ASP:N	2.78	0.52
3:P:326:PHE:O	3:P:329:LEU:HB3	2.08	0.52
5:R:148:ALA:O	5:R:149:ASN:HB2	2.10	0.52
2:B:81:SER:C	2:B:83:PHE:N	2.65	0.52
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.44	0.52
3:C:279:TYR:CZ	3:C:283:ARG:HD3	2.45	0.52
1:N:342:TRP:O	1:N:345:LEU:HB2	2.10	0.52
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.91	0.52
2:O:259:THR:O	2:O:260:GLU:C	2.51	0.52
3:P:347:PRO:HG3	7:T:62:GLY:HA2	1.90	0.52
4:Q:167:GLU:C	4:Q:169:LEU:N	2.65	0.52
9:V:31:UNK:C	9:V:73:PRO:HG2	2.39	0.52
1:A:239:SER:HB2	7:G:17:SER:O	2.09	0.52
1:A:287:GLY:O	1:A:289:HIS:N	2.43	0.52
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.74	0.52
3:C:245:LEU:HD13	4:D:205:GLY:HA2	1.92	0.52
3:C:276:LEU:O	3:C:279:TYR:HB3	2.10	0.52
4:D:186:VAL:O	4:D:190:LEU:HG	2.10	0.52
6:F:58:ARG:HA	6:F:61:ARG:NH2	2.25	0.52
1:N:176:HIS:O	1:N:177:LEU:C	2.53	0.52
6:S:90:LEU:O	6:S:91:GLU:C	2.53	0.52
3:C:183:HIS:O	3:C:187:PRO:HD3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:GLY:HA2	10:J:10:TYR:HB2	1.92	0.52
5:E:41:ALA:O	5:E:44:CYS:HB2	2.09	0.52
7:G:65:GLU:O	7:G:69:LEU:HG	2.10	0.52
3:P:277:PHE:CD1	3:P:277:PHE:C	2.88	0.52
4:Q:55:THR:HG1	4:Q:56:HIS:CE1	2.23	0.52
5:R:157:TYR:HE1	5:R:162:GLY:HA2	1.72	0.52
10:W:42:ILE:O	10:W:46:LEU:HG	2.10	0.52
2:B:28:LYS:O	2:B:28:LYS:HG2	2.10	0.52
2:B:31:ASN:HD22	2:B:31:ASN:N	2.08	0.52
3:C:3:PRO:HG2	3:C:4:ASN:H	1.75	0.52
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.52
11:P:3005:PEE:O2P	5:R:40:THR:HG21	2.10	0.52
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.33	0.51
2:B:428:GLY:O	2:B:430:LEU:N	2.43	0.51
3:C:101:ARG:CD	3:C:102:GLY:N	2.71	0.51
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.92	0.51
8:H:15:ASP:O	8:H:17:LEU:N	2.43	0.51
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.19	0.51
1:A:159:GLN:NE2	1:A:237:THR:HG21	2.25	0.51
2:B:428:GLY:O	2:B:430:LEU:HG	2.10	0.51
3:C:201:LEU:O	3:C:203:GLU:N	2.44	0.51
6:F:58:ARG:HA	6:F:61:ARG:CZ	2.41	0.51
2:O:272:PHE:O	2:O:275:LEU:N	2.42	0.51
3:P:201:LEU:O	3:P:203:GLU:N	2.43	0.51
1:A:54:GLY:O	1:A:55:ALA:C	2.54	0.51
6:F:32:MET:CE	6:F:87:LYS:HG2	2.32	0.51
8:H:61:PHE:O	8:H:62:LEU:C	2.53	0.51
1:N:105:ASP:O	1:N:106:MET:C	2.54	0.51
2:O:29:LEU:CD1	2:O:33:LEU:HD23	2.41	0.51
3:P:9:HIS:ND1	3:P:10:PRO:HD2	2.25	0.51
3:P:284:SER:O	3:P:286:PRO:HD3	2.11	0.51
1:A:239:SER:HB2	7:G:18:LEU:HA	1.91	0.51
2:B:50:PHE:N	2:B:50:PHE:CD1	2.78	0.51
2:B:63:LEU:O	2:B:65:THR:N	2.43	0.51
2:B:239:TYR:CD2	2:B:240:TRP:N	2.78	0.51
3:C:210:LEU:HD11	6:F:69:SER:HB2	1.91	0.51
3:C:332:ASN:O	3:C:336:LEU:HD12	2.11	0.51
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.46	0.51
6:F:68:LEU:O	6:F:70:LEU:N	2.44	0.51
6:F:104:ARG:O	6:F:108:ASN:ND2	2.44	0.51
1:N:49:ASN:ND2	1:N:51:LYS:N	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:89:TYR:O	1:N:95:THR:HG23	2.11	0.51
2:O:101:THR:OG1	2:O:104:LYS:HB3	2.11	0.51
3:P:26:SER:HA	3:P:219:ILE:HD11	1.92	0.51
5:R:38:LEU:CA	10:W:14:PHE:CE1	2.94	0.51
6:S:32:MET:HE3	6:S:87:LYS:H	1.74	0.51
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.58	0.51
2:B:102:ARG:NH1	2:B:172:LEU:O	2.44	0.51
2:B:181:TYR:CE1	2:O:249:GLY:HA3	2.45	0.51
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.40	0.51
1:N:19:LEU:C	1:N:21:ASN:H	2.18	0.51
2:O:187:THR:OG1	2:O:189:GLU:HB2	2.10	0.51
2:O:226:ILE:CG2	2:O:227:ARG:N	2.73	0.51
2:O:345:LYS:C	2:O:347:ALA:N	2.59	0.51
3:P:237:LEU:O	3:P:241:LEU:HG	2.10	0.51
5:R:47:THR:O	5:R:48:ALA:C	2.52	0.51
1:A:106:MET:HE2	1:A:106:MET:C	2.35	0.51
1:A:180:ALA:O	1:A:183:ALA:N	2.44	0.51
1:A:330:SER:O	1:A:331:ILE:C	2.53	0.51
1:A:372:THR:O	1:A:373:THR:C	2.54	0.51
3:C:5:ILE:HG22	3:C:12:LEU:HD12	1.93	0.51
2:O:86:THR:O	2:O:90:GLU:HG3	2.11	0.51
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.75	0.51
4:Q:46:VAL:HB	4:Q:91:PHE:CE2	2.45	0.51
1:A:86:PHE:O	2:B:285:ILE:HA	2.10	0.51
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.92	0.51
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.45	0.51
1:N:61:HIS:ND1	1:N:134:ILE:HG12	2.25	0.51
1:N:171:THR:O	1:N:175:LYS:HG3	2.11	0.51
3:P:59:ASP:O	3:P:60:THR:C	2.54	0.51
3:P:365:ILE:C	3:P:368:PRO:HD2	2.36	0.51
4:Q:183:ALA:HA	4:Q:186:VAL:HG12	1.93	0.51
6:S:16:ILE:O	6:S:19:TRP:HB3	2.10	0.51
1:A:114:ALA:HA	1:A:216:PHE:HE2	1.76	0.51
2:B:239:TYR:CD2	2:B:239:TYR:C	2.89	0.51
3:C:231:LEU:CD1	4:D:220:TYR:HA	2.41	0.51
3:C:277:PHE:CD1	3:C:277:PHE:C	2.88	0.51
4:D:43:MET:HG2	4:D:91:PHE:HD2	1.76	0.51
5:E:186:GLN:HE21	5:E:188:VAL:HG12	1.75	0.51
6:F:36:THR:O	6:F:37:LEU:C	2.54	0.51
6:F:87:LYS:O	6:F:89:TYR:N	2.44	0.51
7:G:29:ILE:H	7:G:29:ILE:CD1	2.01	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:ILE:O	7:G:34:LEU:HG	2.11	0.51
7:G:33:ALA:O	7:G:34:LEU:C	2.54	0.51
10:J:42:ILE:O	10:J:46:LEU:HG	2.11	0.51
1:N:388:ARG:HD3	1:N:388:ARG:H	1.76	0.51
2:O:221:GLU:O	2:O:223:PHE:N	2.43	0.51
2:O:308:ASP:OD2	9:V:59:SER:HB2	2.11	0.51
3:P:107:SER:HB2	13:P:502:HEM:HMD3	1.93	0.51
3:P:245:LEU:HD13	4:Q:205:GLY:HA2	1.91	0.51
3:P:345:GLU:O	3:P:349:ILE:HG13	2.11	0.51
5:R:31:ASP:OD2	10:W:7:ARG:HG3	2.11	0.51
2:B:189:GLU:C	2:B:191:LEU:N	2.67	0.51
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.10	0.51
3:C:245:LEU:O	4:D:201:ARG:CG	2.58	0.51
3:C:335:ILE:O	3:C:336:LEU:C	2.53	0.51
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.92	0.51
4:Q:121:HIS:C	4:Q:123:GLY:H	2.18	0.51
5:R:41:ALA:O	5:R:44:CYS:HB2	2.11	0.51
5:R:108:GLN:O	5:R:110:ALA:N	2.44	0.51
4:D:54:VAL:HG11	4:D:192:TRP:CE2	2.45	0.51
6:F:40:ASP:O	6:F:44:LYS:HG3	2.11	0.51
1:N:22:GLY:C	1:N:193:PRO:HA	2.35	0.51
1:N:107:PRO:HG2	1:N:108:LYS:H	1.75	0.51
3:P:230:ILE:O	3:P:233:LEU:HB3	2.11	0.51
3:P:295:LEU:O	3:P:296:ALA:C	2.54	0.51
7:T:55:ALA:O	7:T:58:LEU:N	2.44	0.51
2:B:370:MET:O	2:B:373:GLU:HG3	2.11	0.50
3:C:92:PHE:CA	3:C:95:ILE:HG22	2.38	0.50
3:C:230:ILE:O	3:C:233:LEU:HB3	2.11	0.50
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.26	0.50
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.41	0.50
8:H:40:CYS:O	8:H:41:ASP:C	2.54	0.50
2:O:272:PHE:HB3	2:O:322:PHE:CE1	2.46	0.50
4:Q:134:TYR:CD1	4:Q:162:PRO:HG3	2.46	0.50
7:T:56:TYR:O	7:T:59:TYR:HB3	2.11	0.50
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.76	0.50
2:B:100:SER:HA	2:B:104:LYS:O	2.11	0.50
2:B:275:LEU:O	2:B:279:LEU:HD12	2.12	0.50
4:D:232:SER:CB	7:G:23:GLN:HE22	2.23	0.50
5:E:29:SER:CB	5:E:32:ARG:HH21	2.25	0.50
7:G:34:LEU:O	7:G:37:VAL:N	2.45	0.50
1:N:27:SER:HB2	1:N:199:ALA:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:MET:HE2	1:N:106:MET:C	2.36	0.50
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.47	0.50
2:O:263:ALA:HA	2:O:319:SER:O	2.11	0.50
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.26	0.50
2:O:393:THR:CG2	2:O:397:VAL:HB	2.42	0.50
3:P:134:LEU:HD21	3:P:180:PHE:HA	1.92	0.50
3:P:332:ASN:ND2	3:P:359:TYR:HA	2.26	0.50
5:R:74:ILE:HG23	5:R:74:ILE:O	2.11	0.50
3:C:273:TRP:CE3	3:C:274:TYR:N	2.79	0.50
2:O:63:LEU:C	2:O:65:THR:H	2.20	0.50
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.93	0.50
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.46	0.50
1:A:55:ALA:O	1:A:57:TYR:N	2.44	0.50
1:A:124:GLU:O	1:A:124:GLU:HG2	2.11	0.50
1:A:147:ASN:O	1:A:148:VAL:C	2.55	0.50
1:A:253:VAL:HG11	1:A:335:MET:CE	2.40	0.50
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.41	0.50
2:B:81:SER:O	2:B:83:PHE:N	2.45	0.50
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.92	0.50
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.92	0.50
3:C:104:TYR:HD2	3:C:105:TYR:CD1	2.29	0.50
4:D:102:ARG:NH1	4:D:107:GLY:O	2.44	0.50
2:O:227:ARG:HG3	2:O:228:SER:H	1.77	0.50
2:O:275:LEU:HD12	2:O:275:LEU:O	2.11	0.50
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.46	0.50
1:A:138:LEU:HD22	5:E:3:ASN:ND2	2.26	0.50
2:B:393:THR:HG23	2:B:397:VAL:HB	1.94	0.50
3:C:284:SER:O	3:C:286:PRO:HD3	2.12	0.50
3:C:295:LEU:O	3:C:296:ALA:C	2.51	0.50
4:D:26:VAL:HG13	4:D:189:PHE:HD1	1.76	0.50
4:D:47:ALA:HB1	4:D:89:ASP:O	2.12	0.50
6:F:32:MET:HE3	6:F:87:LYS:CG	2.32	0.50
8:H:59:PHE:O	8:H:60:ASP:C	2.54	0.50
1:N:269:VAL:HG11	1:N:410:VAL:CG2	2.39	0.50
1:N:335:MET:O	1:N:338:ALA:HB3	2.11	0.50
3:P:198:LEU:HD11	15:P:3002:ANY:O4	2.12	0.50
3:P:208:ASN:OD1	3:P:208:ASN:C	2.54	0.50
3:P:354:MET:O	3:P:357:LEU:N	2.45	0.50
8:U:66:ASP:O	8:U:69:VAL:HB	2.11	0.50
1:A:206:LYS:O	1:A:209:VAL:CG1	2.56	0.50
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.92	0.50
3:C:273:TRP:HA	3:C:276:LEU:HG	1.93	0.50
5:E:45:VAL:O	5:E:48:ALA:HB3	2.11	0.50
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.93	0.50
1:N:206:LYS:O	1:N:207:GLU:C	2.55	0.50
4:Q:102:ARG:HG2	4:Q:102:ARG:HH11	1.77	0.50
10:W:22:LEU:HD23	10:W:22:LEU:H	1.75	0.50
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.47	0.50
3:C:273:TRP:CE3	3:C:274:TYR:HA	2.47	0.50
3:C:354:MET:O	3:C:357:LEU:N	2.45	0.50
5:E:29:SER:OG	5:E:30:GLU:N	2.44	0.50
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.94	0.50
6:F:73:ARG:HH11	6:F:73:ARG:HG3	1.75	0.50
1:N:55:ALA:O	1:N:57:TYR:N	2.45	0.50
1:N:180:ALA:O	1:N:183:ALA:N	2.45	0.50
4:Q:28:ARG:O	4:Q:29:GLY:C	2.53	0.50
6:S:89:TYR:CD1	6:S:90:LEU:N	2.75	0.50
1:A:333:ASP:O	1:A:336:PHE:HB3	2.12	0.50
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.50
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.39	0.50
6:F:32:MET:O	6:F:33:ARG:C	2.53	0.50
2:O:235:ALA:O	2:O:236:LYS:C	2.54	0.50
4:Q:215:LEU:HD12	4:Q:215:LEU:O	2.12	0.50
5:R:55:VAL:O	5:R:56:THR:C	2.54	0.50
5:R:78:LEU:HD21	5:R:193:VAL:HG11	1.92	0.50
1:A:161:THR:HB	1:A:234:CYS:SG	2.51	0.50
1:A:261:GLY:O	1:A:262:TRP:C	2.55	0.50
1:A:289:HIS:O	1:A:290:LEU:C	2.55	0.50
2:B:272:PHE:HB3	2:B:322:PHE:CE1	2.47	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.12	0.50
1:N:310:PHE:HE1	1:N:322:PHE:N	2.10	0.50
2:O:66:ALA:O	2:O:69:LEU:HB3	2.12	0.50
3:P:92:PHE:C	3:P:95:ILE:HG22	2.37	0.50
3:P:100:GLY:O	3:P:101:ARG:C	2.54	0.50
4:Q:167:GLU:HG3	8:U:13:LEU:HD11	1.94	0.50
6:S:32:MET:HE1	6:S:87:LYS:HG2	1.92	0.50
7:T:41:PHE:CE2	7:T:45:VAL:HB	2.47	0.50
1:A:233:ARG:HG3	1:A:233:ARG:NH1	2.27	0.49
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.41	0.49
1:A:411:CYS:O	1:A:415:ILE:HG13	2.11	0.49
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:LEU:HG	2:B:206:LEU:O	2.11	0.49
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.47	0.49
8:H:32:LYS:O	8:H:36:ARG:HG3	2.12	0.49
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.47	0.49
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.94	0.49
3:P:242:THR:N	4:Q:208:MET:CE	2.75	0.49
4:Q:232:SER:CB	7:T:23:GLN:HE22	2.25	0.49
1:A:107:PRO:HG2	1:A:108:LYS:H	1.76	0.49
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.94	0.49
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.77	0.49
2:B:412:ASN:O	2:B:413:ALA:C	2.56	0.49
1:N:40:TRP:CD1	1:N:96:ALA:CB	2.95	0.49
2:O:345:LYS:O	2:O:347:ALA:N	2.46	0.49
6:S:36:THR:O	6:S:37:LEU:C	2.54	0.49
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.42	0.49
1:A:21:ASN:HD22	1:A:192:ALA:CB	2.25	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
1:A:266:ASP:O	1:A:267:ASN:C	2.54	0.49
3:C:173:ASN:O	3:C:174:PRO:C	2.53	0.49
4:D:105:ASN:O	4:D:106:ASN:HB2	2.11	0.49
8:H:58:LEU:HG	8:H:62:LEU:CD1	2.43	0.49
8:H:66:ASP:O	8:H:69:VAL:HB	2.12	0.49
10:J:60:GLU:O	10:J:61:ALA:HB3	2.12	0.49
1:N:45:SER:CA	1:N:48:GLU:HG3	2.41	0.49
1:N:356:ARG:O	1:N:359:ASN:N	2.46	0.49
3:P:129:PHE:CD1	3:P:129:PHE:C	2.89	0.49
3:P:164:TRP:O	3:P:165:ALA:C	2.54	0.49
3:P:316:MET:HE2	3:P:322:SER:HB3	1.94	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB2	1.95	0.49
6:S:63:LYS:O	6:S:63:LYS:HG2	2.12	0.49
6:S:96:GLU:O	6:S:97:VAL:C	2.55	0.49
1:A:220:SER:HB2	1:A:226:ASP:OD1	2.12	0.49
2:B:272:PHE:HZ	2:B:416:LYS:HD3	1.78	0.49
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.48	0.49
6:F:16:ILE:O	6:F:19:TRP:HB3	2.13	0.49
1:N:104:LYS:O	1:N:107:PRO:HD2	2.13	0.49
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.94	0.49
3:P:130:VAL:O	3:P:131:GLY:C	2.56	0.49
4:Q:222:MET:HE3	5:R:40:THR:CB	2.41	0.49
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.95	0.49
2:B:325:TYR:C	2:B:325:TYR:HD2	2.19	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.47	0.49
3:P:92:PHE:CA	3:P:95:ILE:HG22	2.42	0.49
3:P:192:GLY:O	3:P:195:ILE:HB	2.12	0.49
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.12	0.49
2:B:408:ALA:O	2:B:410:VAL:N	2.46	0.49
3:C:26:SER:HA	3:C:219:ILE:CD1	2.43	0.49
3:C:366:LEU:HD23	3:C:366:LEU:N	2.28	0.49
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.94	0.49
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.13	0.49
2:O:239:TYR:HE1	2:O:260:GLU:N	2.11	0.49
3:P:79:LEU:HD12	3:P:79:LEU:O	2.12	0.49
3:P:151:PHE:C	3:P:153:ALA:N	2.70	0.49
4:Q:116:ILE:HG23	4:Q:117:VAL:H	1.76	0.49
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.95	0.49
2:B:259:THR:O	2:B:260:GLU:C	2.56	0.49
3:C:78:TRP:CD2	3:C:79:LEU:N	2.80	0.49
3:C:109:LEU:C	3:C:111:LYS:H	2.21	0.49
4:D:55:THR:HG1	4:D:56:HIS:CE1	2.30	0.49
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.94	0.49
4:Q:208:MET:SD	4:Q:208:MET:C	2.96	0.49
4:Q:224:ARG:O	4:Q:225:HIS:C	2.55	0.49
2:B:31:ASN:ND2	2:B:32:GLY:H	2.11	0.49
2:B:235:ALA:O	2:B:236:LYS:C	2.54	0.49
3:C:100:GLY:O	3:C:101:ARG:C	2.54	0.49
5:E:171:ILE:HG23	5:E:171:ILE:O	2.12	0.49
7:G:45:VAL:HG13	7:G:46:PHE:N	2.28	0.49
1:N:40:TRP:CZ3	1:N:376:CYS:SG	3.02	0.49
1:N:429:GLU:CD	7:T:7:LEU:HB2	2.37	0.49
2:O:292:THR:O	2:O:292:THR:HG22	2.12	0.49
3:P:30:ALA:O	3:P:32:TRP:N	2.45	0.49
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.13	0.49
5:R:29:SER:OG	5:R:30:GLU:N	2.46	0.49
5:R:114:VAL:O	5:R:114:VAL:HG12	2.12	0.49
2:B:72:ALA:O	2:B:75:LEU:HB2	2.12	0.49
2:B:209:ILE:HD11	2:B:378:LEU:HG	1.94	0.49
4:D:24:SER:OG	10:J:55:ILE:HD11	2.13	0.49
5:E:29:SER:HA	5:E:32:ARG:HE	1.78	0.49
1:N:45:SER:HG	1:N:92:ARG:HA	1.77	0.49
1:N:191:LYS:C	1:N:193:PRO:HD2	2.38	0.49
1:N:241:ILE:HG23	1:N:241:ILE:O	2.11	0.49
1:N:420:PRO:HD2	1:N:434:TYR:OH	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.47	0.49
1:A:105:ASP:O	1:A:106:MET:C	2.55	0.49
4:D:109:LEU:O	4:D:111:PRO:HD3	2.12	0.49
4:D:112:ASP:OD1	4:D:114:SER:OG	2.30	0.49
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.48	0.49
5:E:29:SER:O	5:E:30:GLU:C	2.56	0.49
1:N:255:LEU:O	1:N:321:GLY:HA3	2.13	0.49
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.14	0.49
3:P:292:VAL:O	3:P:295:LEU:HB3	2.12	0.49
4:Q:47:ALA:O	4:Q:49:ARG:N	2.46	0.49
8:U:40:CYS:O	8:U:41:ASP:C	2.55	0.49
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.48	0.48
4:D:215:LEU:HD12	4:D:215:LEU:O	2.13	0.48
5:E:113:ASP:HB3	5:E:116:LYS:HB2	1.95	0.48
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.26	0.48
1:N:310:PHE:CE1	1:N:322:PHE:N	2.81	0.48
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.28	0.48
2:O:269:ALA:O	2:O:270:ASN:C	2.56	0.48
5:R:165:TYR:HA	5:R:170:ARG:O	2.13	0.48
10:W:25:VAL:O	10:W:29:VAL:HG23	2.13	0.48
2:B:189:GLU:O	2:B:190:GLN:C	2.55	0.48
2:B:239:TYR:HD2	2:B:240:TRP:N	2.12	0.48
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.95	0.48
2:B:350:GLY:C	2:B:352:VAL:H	2.21	0.48
7:G:29:ILE:HD12	7:G:29:ILE:N	2.13	0.48
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.76	0.48
3:P:146:VAL:O	3:P:147:ILE:C	2.56	0.48
1:A:36:THR:OG1	1:A:100:LYS:HG2	2.13	0.48
1:A:206:LYS:C	1:A:209:VAL:HG12	2.37	0.48
3:C:123:THR:O	3:C:124:LEU:C	2.56	0.48
3:C:129:PHE:C	3:C:129:PHE:CD1	2.88	0.48
1:N:55:ALA:C	1:N:57:TYR:N	2.71	0.48
1:N:63:ALA:O	1:N:116:VAL:HG11	2.13	0.48
1:N:266:ASP:O	1:N:267:ASN:C	2.56	0.48
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.94	0.48
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.13	0.48
1:A:170:THR:HG22	1:A:171:THR:N	2.29	0.48
1:A:239:SER:CB	7:G:18:LEU:HA	2.43	0.48
3:C:106:GLY:HA2	3:C:108:TYR:CD2	2.49	0.48
8:H:66:ASP:O	8:H:67:HIS:C	2.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:307:PHE:H	9:V:52:ARG:HG2	1.78	0.48
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.13	0.48
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.95	0.48
2:B:31:ASN:N	2:B:31:ASN:ND2	2.61	0.48
2:B:81:SER:O	2:B:82:SER:C	2.57	0.48
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.96	0.48
4:D:204:MET:O	4:D:205:GLY:C	2.56	0.48
5:E:69:LEU:HD13	5:E:71:LEU:HD11	1.96	0.48
7:G:34:LEU:O	7:G:35:PRO:C	2.56	0.48
2:O:296:TYR:O	2:O:297:GLN:C	2.57	0.48
2:O:408:ALA:O	2:O:409:ASP:C	2.56	0.48
3:P:184:PHE:CG	13:P:501:HEM:HBC1	2.49	0.48
3:P:311:SER:HB2	3:P:319:ARG:HH11	1.79	0.48
5:R:163:SER:HA	5:R:174:GLY:HA3	1.94	0.48
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.95	0.48
1:A:21:ASN:HB3	1:A:218:GLY:O	2.12	0.48
3:C:93:ILE:O	3:C:94:CYS:C	2.56	0.48
5:E:142:LEU:HD22	3:P:149:ASN:HB3	1.96	0.48
1:N:46:ARG:HD3	1:N:231:LEU:HD13	1.95	0.48
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.44	0.48
2:O:75:LEU:HD21	2:O:136:GLU:HB3	1.95	0.48
2:O:167:ALA:C	2:O:168:TYR:CD1	2.92	0.48
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.44	0.48
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.94	0.48
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.96	0.48
3:C:245:LEU:O	4:D:201:ARG:HG2	2.14	0.48
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.95	0.48
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.14	0.48
5:E:122:HIS:C	5:E:124:LEU:N	2.71	0.48
7:G:49:ALA:O	7:G:50:PRO:C	2.53	0.48
2:O:272:PHE:HZ	2:O:416:LYS:HD3	1.79	0.48
3:P:127:THR:O	3:P:130:VAL:HG22	2.14	0.48
3:P:158:GLY:O	3:P:161:LEU:N	2.47	0.48
1:A:292:SER:O	1:A:293:ARG:C	2.55	0.48
2:B:66:ALA:O	2:B:69:LEU:HB3	2.14	0.48
4:D:155:GLY:C	4:D:157:ALA:N	2.71	0.48
4:D:206:LEU:O	4:D:207:LYS:C	2.57	0.48
6:F:42:ASP:O	6:F:43:VAL:C	2.55	0.48
1:N:85:HIS:CD2	2:O:284:LEU:HB3	2.48	0.48
2:O:253:VAL:HG13	2:O:430:LEU:CD2	2.44	0.48
3:P:123:THR:O	3:P:124:LEU:C	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:273:TRP:CE3	3:P:274:TYR:CA	2.97	0.48
1:A:191:LYS:O	1:A:195:MET:HG3	2.13	0.48
1:N:93:GLU:O	1:N:93:GLU:HG3	2.14	0.48
1:N:93:GLU:O	1:N:94:GLN:HB2	2.14	0.48
1:N:372:THR:O	1:N:373:THR:C	2.56	0.48
2:O:29:LEU:HD23	2:O:30:PRO:HD2	1.95	0.48
3:P:191:ALA:O	3:P:195:ILE:HG12	2.13	0.48
5:R:29:SER:O	5:R:30:GLU:C	2.56	0.48
5:R:52:LYS:C	5:R:52:LYS:HD3	2.39	0.48
1:A:63:ALA:O	1:A:116:VAL:HG11	2.14	0.48
1:A:287:GLY:C	1:A:289:HIS:H	2.22	0.48
2:B:147:ASP:O	2:B:150:VAL:HG22	2.14	0.48
3:C:125:MET:HE1	3:C:299:VAL:HG21	1.95	0.48
4:D:26:VAL:CG1	4:D:189:PHE:HD1	2.27	0.48
4:D:218:LEU:HD13	5:E:43:ALA:N	2.28	0.48
1:N:178:THR:HG22	1:N:180:ALA:H	1.79	0.48
2:O:163:LEU:HD13	2:O:425:ALA:CB	2.44	0.48
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.48
3:C:196:ILE:O	3:C:199:THR:N	2.46	0.47
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.29	0.47
4:D:130:LEU:HD12	4:D:150:ASN:CG	2.39	0.47
7:G:61:TRP:CE3	7:G:62:GLY:N	2.82	0.47
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.79	0.47
9:I:59:SER:O	9:I:60:ALA:C	2.56	0.47
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.49	0.47
2:O:59:THR:HG22	2:O:60:THR:N	2.28	0.47
3:P:3:PRO:HG2	3:P:4:ASN:H	1.78	0.47
1:A:171:THR:O	1:A:175:LYS:HG3	2.14	0.47
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.96	0.47
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.28	0.47
2:B:163:LEU:HD13	2:B:425:ALA:CB	2.43	0.47
2:B:166:ALA:O	2:B:242:GLY:N	2.37	0.47
2:B:402:ILE:O	2:B:405:VAL:HG23	2.14	0.47
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.44	0.47
4:D:165:TYR:O	4:D:166:ASN:C	2.57	0.47
5:E:52:LYS:HD3	5:E:56:THR:OG1	2.13	0.47
5:E:113:ASP:C	5:E:115:SER:N	2.72	0.47
7:G:57:LEU:C	7:G:59:TYR:N	2.70	0.47
1:N:35:CYS:HB2	1:N:200:ALA:O	2.14	0.47
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.49	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:287:GLY:O	1:N:289:HIS:N	2.47	0.47
1:N:438:ARG:HH11	1:N:438:ARG:HG3	1.80	0.47
2:O:182:ARG:NH2	2:O:190:GLN:OE1	2.47	0.47
2:O:206:LEU:HG	2:O:206:LEU:O	2.14	0.47
3:P:107:SER:O	3:P:109:LEU:N	2.47	0.47
3:P:120:LEU:HB3	13:P:502:HEM:HAB	1.96	0.47
3:P:154:ILE:CG2	3:P:155:PRO:HD2	2.43	0.47
3:P:201:LEU:HD11	13:P:502:HEM:HAD2	1.95	0.47
7:T:4:PHE:CD2	7:T:7:LEU:HD11	2.49	0.47
9:V:49:LEU:O	9:V:50:LEU:HG	2.14	0.47
1:A:55:ALA:C	1:A:57:TYR:N	2.72	0.47
3:C:165:ALA:O	3:C:178:ARG:HD2	2.14	0.47
4:D:200:GLN:HE21	20:E:2009:PLC:H51	1.79	0.47
5:E:152:ASP:O	5:E:153:PHE:CD1	2.67	0.47
1:N:45:SER:OG	1:N:92:ARG:HA	2.13	0.47
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.50	0.47
4:Q:26:VAL:CG1	4:Q:189:PHE:HD1	2.27	0.47
4:Q:26:VAL:HG13	4:Q:189:PHE:HD1	1.79	0.47
4:Q:47:ALA:O	4:Q:48:PHE:C	2.56	0.47
6:S:58:ARG:HA	6:S:61:ARG:CZ	2.44	0.47
7:T:33:ALA:O	7:T:34:LEU:C	2.57	0.47
7:T:55:ALA:O	7:T:56:TYR:C	2.57	0.47
3:C:123:THR:HG22	3:C:190:ILE:HD11	1.95	0.47
5:E:35:PHE:O	5:E:36:SER:C	2.56	0.47
6:F:19:TRP:O	6:F:22:ASN:N	2.47	0.47
8:H:37:LEU:O	8:H:40:CYS:N	2.47	0.47
1:N:261:GLY:O	1:N:262:TRP:C	2.57	0.47
2:O:230:ALA:O	2:O:231:GLY:C	2.57	0.47
3:P:31:TRP:O	3:P:101:ARG:HG3	2.13	0.47
4:Q:12:TRP:CZ2	4:Q:124:GLU:HB2	2.49	0.47
7:T:16:TYR:N	7:T:16:TYR:CD1	2.82	0.47
1:A:69:LYS:HE3	1:A:70:ARG:NH2	2.14	0.47
2:B:343:GLN:O	2:B:347:ALA:HB2	2.15	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.28	0.47
3:C:371:GLY:O	3:C:374:GLU:HB2	2.14	0.47
5:E:85:LYS:HG2	5:E:86:ASN:N	2.29	0.47
6:F:52:GLU:HG2	6:F:56:ASN:HD21	1.78	0.47
7:G:56:TYR:O	7:G:59:TYR:HB3	2.15	0.47
9:I:38:UNK:C	9:I:40:UNK:N	2.76	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.13	0.47
2:O:412:ASN:O	2:O:413:ALA:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:117:GLY:HA3	13:P:502:HEM:HBC2	1.97	0.47
3:P:184:PHE:CD2	3:P:184:PHE:C	2.92	0.47
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.47	0.47
4:Q:130:LEU:HD12	4:Q:150:ASN:ND2	2.30	0.47
10:W:26:LEU:O	10:W:30:LEU:HG	2.14	0.47
1:A:29:GLU:HG3	1:A:203:ILE:O	2.15	0.47
2:B:239:TYR:HD1	2:B:260:GLU:HB2	1.76	0.47
3:C:95:ILE:HD13	3:C:121:LEU:HD12	1.96	0.47
3:C:101:ARG:C	3:C:101:ARG:CD	2.77	0.47
3:C:117:GLY:C	13:C:502:HEM:HBC2	2.39	0.47
1:N:422:LEU:HD22	1:N:437:ILE:HD12	1.96	0.47
2:O:67:HIS:ND1	2:O:177:TYR:HA	2.30	0.47
2:O:239:TYR:CD2	2:O:239:TYR:C	2.91	0.47
3:P:347:PRO:O	3:P:350:ILE:HG22	2.14	0.47
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.29	0.47
7:T:34:LEU:O	7:T:37:VAL:N	2.47	0.47
8:U:15:ASP:O	8:U:17:LEU:N	2.48	0.47
1:A:27:SER:CB	1:A:199:ALA:O	2.62	0.47
1:A:45:SER:CA	1:A:48:GLU:HG3	2.42	0.47
3:C:14:MET:O	3:C:15:ILE:C	2.57	0.47
3:C:92:PHE:HA	3:C:95:ILE:CG2	2.41	0.47
3:C:213:SER:HB2	6:F:39:GLU:OE2	2.15	0.47
4:D:47:ALA:O	4:D:50:ASN:N	2.38	0.47
4:D:121:HIS:C	4:D:123:GLY:H	2.22	0.47
4:D:182:ILE:O	4:D:184:LYS:N	2.48	0.47
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.95	0.47
5:E:126:ARG:O	5:E:182:VAL:HG11	2.15	0.47
5:E:177:PRO:C	5:E:178:TYR:HD1	2.22	0.47
6:F:32:MET:HE1	6:F:87:LYS:H	1.78	0.47
6:F:77:LYS:HA	6:F:80:TRP:NE1	2.30	0.47
8:H:44:VAL:HG22	8:H:52:GLU:HG2	1.97	0.47
9:I:65:VAL:HG12	9:I:66:ALA:H	1.79	0.47
1:N:103:SER:O	1:N:106:MET:HB2	2.15	0.47
2:O:378:LEU:C	2:O:380:ASN:N	2.70	0.47
3:P:122:LEU:O	3:P:125:MET:HB2	2.13	0.47
3:P:196:ILE:O	3:P:197:HIS:C	2.57	0.47
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.96	0.47
4:Q:158:ILE:HG12	4:Q:159:GLY:H	1.80	0.47
2:B:258:VAL:HB	2:B:322:PHE:C	2.40	0.47
5:E:32:ARG:HH12	7:G:22:GLU:CD	2.23	0.47
1:N:67:THR:HA	1:N:121:ALA:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:439:SER:C	1:N:441:MET:H	2.23	0.47
2:O:29:LEU:HD22	2:O:30:PRO:HD2	1.96	0.47
2:O:200:THR:O	2:O:202:ALA:N	2.47	0.47
2:O:209:ILE:HD11	2:O:378:LEU:HG	1.97	0.47
2:O:275:LEU:O	2:O:279:LEU:HD12	2.15	0.47
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.50	0.47
6:S:76:PRO:O	6:S:78:GLU:N	2.48	0.47
1:A:281:ASP:HB3	1:A:284:PHE:CE1	2.50	0.47
2:B:412:ASN:O	2:B:415:LYS:N	2.47	0.47
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.62	0.47
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.33	0.47
1:N:42:GLY:HA2	1:N:384:LEU:HD21	1.97	0.47
1:N:388:ARG:NH2	1:N:388:ARG:CG	2.78	0.47
2:O:309:ALA:HA	2:O:325:TYR:O	2.15	0.47
3:P:130:VAL:HG23	3:P:131:GLY:H	1.80	0.47
3:P:151:PHE:C	3:P:153:ALA:H	2.21	0.47
3:P:380:TYR:OH	6:S:34:ASP:HA	2.15	0.47
4:Q:191:ARG:O	4:Q:194:ALA:N	2.46	0.47
4:Q:220:TYR:HE2	16:Q:3003:CDL:H722	1.79	0.47
4:Q:230:LEU:O	6:S:70:LEU:HD11	2.15	0.47
6:S:89:TYR:CD1	6:S:89:TYR:C	2.93	0.47
10:W:45:HIS:C	10:W:47:ASN:H	2.23	0.47
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.50	0.47
1:A:178:THR:O	1:A:179:ARG:C	2.57	0.47
2:B:176:LEU:HD12	2:B:176:LEU:O	2.15	0.47
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.45	0.47
3:C:121:LEU:HG	3:C:125:MET:HE3	1.96	0.47
3:C:199:THR:HG22	3:C:200:PHE:N	2.30	0.47
4:D:46:VAL:CG1	4:D:47:ALA:N	2.76	0.47
6:F:49:ARG:HH22	6:F:100:GLU:CD	2.23	0.47
1:N:106:MET:O	1:N:110:VAL:HG23	2.14	0.47
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.96	0.47
1:N:280:TYR:CG	1:N:281:ASP:N	2.83	0.47
2:O:100:SER:HB3	2:O:105:MET:HA	1.97	0.47
3:P:29:SER:O	3:P:32:TRP:HB2	2.15	0.47
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.50	0.47
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.55	0.47
1:A:235:ARG:NH2	5:E:14:ARG:NH2	2.63	0.46
1:A:305:HIS:ND1	9:I:35:UNK:CB	2.79	0.46
3:C:101:ARG:HD2	3:C:102:GLY:CA	2.45	0.46
4:D:62:LYS:O	4:D:66:GLU:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:393:THR:HG23	2:O:397:VAL:HB	1.96	0.46
2:O:428:GLY:O	2:O:430:LEU:N	2.47	0.46
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.29	0.46
5:R:108:GLN:C	5:R:110:ALA:N	2.73	0.46
10:W:52:TRP:O	10:W:56:LYS:HB2	2.15	0.46
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.80	0.46
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.30	0.46
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.81	0.46
3:C:107:SER:C	3:C:109:LEU:H	2.23	0.46
5:E:148:ALA:O	5:E:149:ASN:HB2	2.15	0.46
1:N:50:GLU:HB2	1:N:165:ARG:NH2	2.30	0.46
1:N:112:LEU:O	1:N:113:LEU:C	2.57	0.46
1:N:435:ASN:O	1:N:438:ARG:HB3	2.15	0.46
3:P:63:ALA:CB	3:P:176:LEU:HD21	2.44	0.46
3:P:93:ILE:O	3:P:94:CYS:C	2.57	0.46
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.30	0.46
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.46
10:W:49:GLY:N	10:W:54:HIS:ND1	2.63	0.46
1:A:21:ASN:HD22	1:A:192:ALA:HB1	1.79	0.46
1:A:86:PHE:CD2	1:A:99:ILE:HD11	2.50	0.46
3:C:4:ASN:O	3:C:4:ASN:OD1	2.33	0.46
3:C:80:ILE:O	3:C:81:ARG:C	2.56	0.46
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.78	0.46
4:D:143:VAL:O	4:D:144:ARG:C	2.57	0.46
1:N:19:LEU:C	1:N:21:ASN:N	2.72	0.46
1:N:307:PHE:HA	1:N:324:PHE:HA	1.97	0.46
2:O:314:VAL:HG11	2:O:316:TYR:CZ	2.50	0.46
5:R:136:VAL:HB	5:R:181:GLU:HB3	1.97	0.46
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.30	0.46
2:B:101:THR:OG1	2:B:104:LYS:HB3	2.16	0.46
2:B:280:GLY:HA3	2:B:293:SER:OG	2.16	0.46
3:C:59:ASP:O	3:C:60:THR:C	2.58	0.46
3:C:122:LEU:O	3:C:125:MET:HB2	2.15	0.46
3:C:172:ASP:OD1	3:C:173:ASN:N	2.43	0.46
3:C:285:ILE:HG21	3:C:290:GLY:HA3	1.98	0.46
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.81	0.46
3:P:104:TYR:CD2	3:P:105:TYR:CE1	2.97	0.46
3:P:107:SER:C	3:P:109:LEU:N	2.72	0.46
3:P:281:ILE:O	3:P:285:ILE:HD13	2.16	0.46
3:P:352:GLY:O	3:P:353:GLN:C	2.58	0.46
5:R:38:LEU:CA	10:W:14:PHE:HE1	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:CD	2:B:290:SER:HA	2.41	0.46
3:C:338:TRP:CE2	7:G:59:TYR:HD1	2.32	0.46
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.41	0.46
6:F:89:TYR:CD1	6:F:90:LEU:N	2.73	0.46
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.50	0.46
3:P:350:ILE:HG23	3:P:351:ILE:N	2.30	0.46
4:Q:182:ILE:O	4:Q:184:LYS:N	2.49	0.46
5:R:20:ASP:C	5:R:22:THR:H	2.23	0.46
1:A:104:LYS:O	1:A:107:PRO:HD2	2.16	0.46
1:A:388:ARG:NH2	1:A:388:ARG:CG	2.77	0.46
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.50	0.46
2:B:378:LEU:C	2:B:380:ASN:N	2.72	0.46
3:C:78:TRP:CG	3:C:79:LEU:N	2.83	0.46
3:C:270:LYS:HA	3:C:271:PRO:HD3	1.77	0.46
4:D:10:PHE:N	4:D:10:PHE:HD1	2.07	0.46
8:H:15:ASP:C	8:H:17:LEU:N	2.72	0.46
1:N:284:PHE:CE2	9:V:71:ASN:O	2.69	0.46
2:O:113:ARG:O	2:O:116:VAL:HG23	2.16	0.46
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.46	0.46
2:O:417:PHE:C	2:O:417:PHE:CD2	2.94	0.46
3:P:277:PHE:HD2	11:P:3007:PEE:H77	1.79	0.46
3:P:332:ASN:HD21	3:P:359:TYR:CA	2.29	0.46
5:R:171:ILE:O	5:R:171:ILE:HG23	2.16	0.46
8:U:15:ASP:C	8:U:17:LEU:N	2.73	0.46
10:W:55:ILE:O	10:W:56:LYS:C	2.58	0.46
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.98	0.46
2:B:408:ALA:O	2:B:409:ASP:C	2.58	0.46
3:C:219:ILE:HD11	3:C:225:TYR:CE1	2.51	0.46
3:C:258:THR:HG22	3:C:258:THR:O	2.15	0.46
3:C:357:LEU:HD12	3:C:357:LEU:HA	1.68	0.46
10:J:52:TRP:O	10:J:56:LYS:HB2	2.15	0.46
10:J:55:ILE:O	10:J:56:LYS:C	2.59	0.46
1:N:112:LEU:H	1:N:112:LEU:HG	1.48	0.46
2:O:168:TYR:CD2	2:O:237:ALA:HB1	2.51	0.46
2:O:307:PHE:HE2	9:V:52:ARG:HE	1.64	0.46
6:S:18:LYS:HA	6:S:83:TYR:CD1	2.50	0.46
7:T:77:TYR:C	7:T:79:ASN:H	2.23	0.46
10:W:14:PHE:N	10:W:14:PHE:HD2	2.13	0.46
2:B:67:HIS:ND1	2:B:177:TYR:HA	2.31	0.46
2:B:239:TYR:HE2	2:B:241:GLY:CA	2.29	0.46
3:C:344:VAL:CG1	3:C:349:ILE:HD11	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:SER:C	4:D:112:ASP:OD2	2.59	0.46
8:H:65:ARG:O	8:H:69:VAL:HG23	2.15	0.46
1:N:147:ASN:O	1:N:148:VAL:C	2.59	0.46
2:O:128:THR:CA	2:O:226:ILE:HD11	2.41	0.46
2:O:241:GLY:HA2	2:O:423:SER:OG	2.16	0.46
3:P:25:PRO:HG2	3:P:207:ASN:O	2.16	0.46
3:P:56:TYR:OH	3:P:176:LEU:HD11	2.16	0.46
3:P:199:THR:HG22	3:P:200:PHE:N	2.31	0.46
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.34	0.46
4:Q:29:GLY:HA3	4:Q:185:ASP:O	2.16	0.46
6:S:76:PRO:O	6:S:77:LYS:C	2.59	0.46
1:A:93:GLU:O	1:A:94:GLN:HB2	2.16	0.46
1:A:243:ALA:O	1:A:425:VAL:HA	2.16	0.46
2:B:72:ALA:CA	2:B:75:LEU:HD12	2.46	0.46
2:B:113:ARG:O	2:B:116:VAL:HG23	2.15	0.46
3:C:70:THR:O	3:C:70:THR:HG22	2.15	0.46
3:C:99:ILE:O	3:C:100:GLY:C	2.58	0.46
4:D:109:LEU:O	4:D:109:LEU:HG	2.15	0.46
5:E:20:ASP:C	5:E:22:THR:H	2.24	0.46
5:E:29:SER:CA	5:E:32:ARG:HH21	2.29	0.46
5:E:122:HIS:O	5:E:124:LEU:N	2.49	0.46
5:E:134:ILE:C	5:E:135:LEU:HG	2.40	0.46
6:F:90:LEU:O	6:F:91:GLU:C	2.59	0.46
1:N:80:GLU:CD	2:O:290:SER:HA	2.41	0.46
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.46
1:N:434:TYR:O	1:N:435:ASN:C	2.58	0.46
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.97	0.46
3:P:166:TRP:NE1	3:P:171:VAL:HG22	2.31	0.46
3:P:198:LEU:HA	3:P:198:LEU:HD23	1.64	0.46
3:P:355:ALA:HA	3:P:358:SER:HB3	1.97	0.46
5:R:29:SER:HA	5:R:32:ARG:HE	1.81	0.46
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.81	0.46
8:U:46:SER:OG	8:U:47:ARG:N	2.48	0.46
1:A:103:SER:O	1:A:106:MET:HB2	2.15	0.46
3:C:104:TYR:CD2	3:C:105:TYR:CE1	3.04	0.46
3:C:117:GLY:HA3	13:C:502:HEM:HBC2	1.97	0.46
3:C:183:HIS:O	3:C:187:PRO:CD	2.64	0.46
3:C:378:LEU:O	3:C:379:ASN:CB	2.63	0.46
5:E:140:THR:HG21	5:E:178:TYR:HB2	1.97	0.46
7:G:81:GLN:OXT	8:H:49:HIS:HB3	2.16	0.46
3:P:242:THR:CA	4:Q:208:MET:HE1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:5:LEU:HG	4:Q:152:TYR:HE1	1.81	0.46
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.96	0.46
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.46	0.46
6:S:58:ARG:HA	6:S:61:ARG:NH2	2.30	0.46
6:S:74:ILE:HG13	6:S:75:LEU:N	2.30	0.46
1:A:411:CYS:HB3	1:A:415:ILE:HD12	1.98	0.45
2:B:76:THR:HG22	2:B:82:SER:N	2.21	0.45
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.51	0.45
2:B:366:ALA:O	2:B:367:THR:C	2.59	0.45
3:C:269:ILE:O	3:C:269:ILE:CG2	2.63	0.45
4:D:208:MET:SD	4:D:208:MET:C	2.99	0.45
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.45
6:F:89:TYR:HD1	6:F:89:TYR:C	2.24	0.45
1:N:79:VAL:O	1:N:82:MET:HG2	2.16	0.45
1:N:159:GLN:NE2	1:N:237:THR:HG21	2.31	0.45
3:P:99:ILE:O	3:P:100:GLY:C	2.58	0.45
3:P:201:LEU:C	3:P:203:GLU:H	2.24	0.45
3:P:332:ASN:O	3:P:336:LEU:HD12	2.16	0.45
3:P:338:TRP:CE2	7:T:59:TYR:CD1	3.02	0.45
4:Q:5:LEU:HG	4:Q:152:TYR:CE1	2.51	0.45
5:R:18:VAL:HG23	5:R:18:VAL:O	2.15	0.45
5:R:150:SER:OG	5:R:157:TYR:HB3	2.16	0.45
6:S:42:ASP:O	6:S:43:VAL:C	2.59	0.45
7:T:40:ARG:O	7:T:41:PHE:C	2.59	0.45
2:B:57:TYR:CD1	2:B:57:TYR:N	2.84	0.45
2:B:289:SER:O	2:B:290:SER:C	2.58	0.45
3:C:141:PHE:O	3:C:144:ALA:HB3	2.16	0.45
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.46	0.45
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.50	0.45
1:N:235:ARG:NH2	5:R:14:ARG:NH2	2.65	0.45
1:N:242:ARG:O	7:T:14:ILE:HA	2.15	0.45
1:N:301:HIS:HB2	1:N:303:LEU:HD21	1.97	0.45
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.46	0.45
4:Q:42:SER:HB2	4:Q:112:ASP:OD2	2.16	0.45
7:T:41:PHE:HE2	7:T:45:VAL:HB	1.81	0.45
1:A:21:ASN:ND2	1:A:192:ALA:HB1	2.30	0.45
2:B:42:SER:OG	2:B:43:PRO:HD2	2.16	0.45
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.97	0.45
3:C:38:LEU:HB3	13:C:502:HEM:CMB	2.46	0.45
3:C:154:ILE:O	3:C:158:GLY:HA3	2.16	0.45
3:C:273:TRP:CE3	3:C:274:TYR:CA	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:PHE:O	5:E:38:LEU:HB3	2.17	0.45
10:J:51:LEU:C	10:J:53:LYS:N	2.74	0.45
1:N:49:ASN:HD21	1:N:52:ASN:N	2.13	0.45
1:N:178:THR:HG22	1:N:179:ARG:N	2.30	0.45
1:N:178:THR:HB	1:N:181:ASP:OD1	2.16	0.45
1:N:354:VAL:HG23	1:N:355:LYS:N	2.31	0.45
2:O:422:LYS:O	2:O:436:LEU:HD21	2.16	0.45
3:P:27:ASN:HD22	3:P:209:PRO:HD2	1.82	0.45
3:P:117:GLY:CA	13:P:502:HEM:HBC2	2.46	0.45
5:R:46:ALA:O	5:R:47:THR:C	2.58	0.45
1:A:433:ASP:O	1:A:437:ILE:HG13	2.16	0.45
2:B:99:TYR:HA	9:I:66:ALA:O	2.16	0.45
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.16	0.45
3:C:52:LEU:HD13	13:C:501:HEM:HBD1	1.97	0.45
3:C:316:MET:HA	3:C:319:ARG:HE	1.81	0.45
4:D:46:VAL:HB	4:D:91:PHE:CD2	2.51	0.45
4:D:48:PHE:CE2	4:D:65:ALA:HA	2.51	0.45
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.77	0.45
2:O:131:GLU:O	2:O:132:PHE:C	2.59	0.45
2:O:209:ILE:CG2	2:O:210:GLY:N	2.80	0.45
2:O:221:GLU:C	2:O:223:PHE:H	2.25	0.45
2:O:295:LEU:O	2:O:296:TYR:C	2.60	0.45
2:O:325:TYR:C	2:O:325:TYR:CD2	2.94	0.45
2:O:408:ALA:O	2:O:410:VAL:N	2.48	0.45
6:S:32:MET:HE3	6:S:87:LYS:CB	2.45	0.45
7:T:29:ILE:H	7:T:29:ILE:CD1	2.00	0.45
1:A:287:GLY:C	1:A:289:HIS:N	2.74	0.45
2:B:275:LEU:O	2:B:275:LEU:HD12	2.16	0.45
3:C:29:SER:O	3:C:30:ALA:C	2.59	0.45
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.34	0.45
5:E:119:ASP:CB	5:E:179:ASN:ND2	2.59	0.45
2:O:209:ILE:O	2:O:211:VAL:HG22	2.16	0.45
3:P:67:VAL:O	3:P:68:ALA:C	2.59	0.45
3:P:157:ILE:CG1	3:P:158:GLY:H	1.96	0.45
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.52	0.45
4:Q:204:MET:O	4:Q:205:GLY:C	2.59	0.45
5:R:135:LEU:HA	5:R:183:PRO:HD3	1.98	0.45
6:S:52:GLU:HG2	6:S:56:ASN:ND2	2.31	0.45
8:U:19:THR:O	8:U:22:GLU:HB2	2.16	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.51	0.45
1:A:87:ASN:ND2	1:A:98:TYR:OH	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:GLN:HB3	13:C:501:HEM:HAB	1.99	0.45
3:C:231:LEU:HD11	4:D:220:TYR:HA	1.98	0.45
3:C:285:ILE:N	3:C:285:ILE:CD1	2.79	0.45
3:C:325:LEU:HD22	3:C:370:ILE:HG13	1.97	0.45
5:E:122:HIS:C	5:E:124:LEU:H	2.24	0.45
1:N:187:ASP:O	1:N:191:LYS:HE3	2.16	0.45
3:P:95:ILE:O	3:P:99:ILE:HG13	2.16	0.45
3:P:109:LEU:C	3:P:111:LYS:H	2.25	0.45
3:P:182:LEU:HD23	14:P:3001:SMA:H26	1.98	0.45
10:W:20:PHE:O	10:W:23:THR:HB	2.17	0.45
2:B:73:SER:N	2:B:74:PRO:HD2	2.31	0.45
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.97	0.45
3:C:280:ALA:O	3:C:281:ILE:C	2.59	0.45
5:E:91:TRP:O	5:E:92:ARG:C	2.59	0.45
5:E:161:HIS:HB2	19:E:501:FES:S1	2.56	0.45
7:G:40:ARG:O	7:G:41:PHE:C	2.59	0.45
1:N:84:ALA:HB1	1:N:99:ILE:CG2	2.47	0.45
2:O:259:THR:HG22	2:O:260:GLU:N	2.31	0.45
6:S:40:ASP:O	6:S:44:LYS:HG3	2.15	0.45
1:A:357:ALA:O	1:A:358:LYS:C	2.59	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
3:C:184:PHE:CD2	3:C:184:PHE:C	2.95	0.45
3:C:331:ALA:HB2	7:G:52:PHE:CD2	2.52	0.45
5:E:52:LYS:C	5:E:52:LYS:HD3	2.41	0.45
6:F:94:LEU:O	6:F:95:LYS:C	2.60	0.45
1:N:158:PHE:O	1:N:159:GLN:C	2.59	0.45
1:N:283:THR:O	1:N:284:PHE:C	2.59	0.45
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.95	0.45
3:P:271:PRO:CA	14:P:3001:SMA:H10	2.31	0.45
4:Q:76:GLU:H	4:Q:76:GLU:CD	2.24	0.45
4:Q:221:TYR:CE1	7:T:25:ALA:HB2	2.51	0.45
6:S:19:TRP:O	6:S:20:TYR:C	2.60	0.45
6:S:77:LYS:HA	6:S:80:TRP:CD1	2.51	0.45
6:S:89:TYR:HD1	6:S:89:TYR:C	2.23	0.45
10:W:21:ALA:O	10:W:24:VAL:N	2.50	0.45
1:A:50:GLU:HB2	1:A:165:ARG:NH2	2.32	0.45
1:A:249:PRO:HG2	1:A:250:VAL:H	1.81	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.67	0.45
2:B:67:HIS:ND1	2:B:178:CYS:N	2.65	0.45
3:C:365:ILE:O	3:C:368:PRO:HD2	2.17	0.45
6:F:11:ARG:O	6:F:12:LEU:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:28:ASN:HB2	7:G:32:ASP:HB3	1.99	0.45
1:N:261:GLY:HA2	1:N:317:THR:O	2.17	0.45
1:N:288:LYS:HE3	1:N:289:HIS:NE2	2.31	0.45
1:N:379:ILE:O	1:N:380:GLY:C	2.60	0.45
3:P:35:GLY:O	3:P:38:LEU:HB2	2.16	0.45
3:P:166:TRP:C	3:P:168:GLY:H	2.24	0.45
4:Q:206:LEU:O	4:Q:207:LYS:C	2.59	0.45
6:S:19:TRP:O	6:S:22:ASN:N	2.50	0.45
6:S:65:ALA:O	6:S:68:LEU:HB2	2.17	0.45
1:A:61:HIS:ND1	1:A:134:ILE:HG12	2.32	0.45
2:B:84:ARG:O	2:B:88:GLY:N	2.47	0.45
5:E:165:TYR:HA	5:E:170:ARG:O	2.17	0.45
2:O:203:ARG:O	2:O:387:LEU:HD11	2.17	0.45
2:O:239:TYR:HE2	2:O:241:GLY:CA	2.30	0.45
2:O:279:LEU:O	2:O:295:LEU:HB3	2.17	0.45
3:P:121:LEU:O	3:P:122:LEU:C	2.60	0.45
3:P:186:LEU:HD23	3:P:186:LEU:HA	1.71	0.45
5:R:152:ASP:C	5:R:153:PHE:CD1	2.95	0.45
2:B:379:LEU:HG	2:B:379:LEU:O	2.15	0.44
3:C:49:GLY:HA3	13:C:501:HEM:C3C	2.52	0.44
3:C:63:ALA:CB	3:C:176:LEU:HD21	2.46	0.44
6:F:19:TRP:O	6:F:20:TYR:C	2.60	0.44
8:H:15:ASP:O	8:H:16:PRO:C	2.59	0.44
2:O:47:ILE:HG22	2:O:48:GLY:N	2.31	0.44
2:O:171:ALA:O	2:O:174:ASN:HB2	2.16	0.44
3:P:125:MET:HE1	3:P:299:VAL:HG21	1.99	0.44
7:T:57:LEU:C	7:T:59:TYR:N	2.73	0.44
1:A:49:ASN:ND2	1:A:51:LYS:N	2.65	0.44
1:A:62:LEU:HD21	1:A:126:GLN:HG3	1.99	0.44
1:A:289:HIS:O	1:A:290:LEU:O	2.34	0.44
1:A:300:GLU:HG2	1:A:301:HIS:CE1	2.52	0.44
2:B:59:THR:HG22	2:B:60:THR:N	2.31	0.44
2:B:63:LEU:C	2:B:65:THR:H	2.25	0.44
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.98	0.44
2:B:265:GLY:O	2:B:266:SER:C	2.60	0.44
3:C:316:MET:CG	3:C:319:ARG:HH21	2.29	0.44
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.52	0.44
5:E:87:VAL:HG12	5:E:88:ALA:N	2.31	0.44
8:H:56:GLU:O	8:H:59:PHE:HB2	2.16	0.44
9:I:49:LEU:O	9:I:50:LEU:HG	2.17	0.44
9:I:49:LEU:HB3	9:I:55:MET:CG	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ASP:C	1:N:109:VAL:HG23	2.42	0.44
1:N:289:HIS:O	1:N:290:LEU:C	2.60	0.44
1:N:368:GLN:O	1:N:374:PRO:HB3	2.18	0.44
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.82	0.44
3:P:38:LEU:HD21	3:P:95:ILE:N	2.32	0.44
3:P:117:GLY:O	3:P:118:VAL:C	2.60	0.44
3:P:199:THR:O	3:P:200:PHE:C	2.60	0.44
3:P:323:GLN:O	3:P:326:PHE:HB3	2.17	0.44
7:T:28:ASN:HB2	7:T:32:ASP:HB3	1.99	0.44
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.30	0.44
10:W:4:ALA:N	10:W:8:GLN:HE21	2.16	0.44
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.48	0.44
2:B:229:GLY:C	2:B:231:GLY:N	2.75	0.44
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.85	0.44
3:C:156:TYR:N	3:C:156:TYR:HD2	2.16	0.44
5:E:135:LEU:HA	5:E:183:PRO:HD3	1.99	0.44
5:E:141:HIS:HB3	19:E:501:FES:S2	2.57	0.44
6:F:89:TYR:CD1	6:F:89:TYR:C	2.94	0.44
7:G:30:PHE:O	7:G:35:PRO:CD	2.65	0.44
10:J:45:HIS:C	10:J:47:ASN:H	2.25	0.44
2:O:279:LEU:O	2:O:295:LEU:CB	2.66	0.44
5:R:87:VAL:HG12	5:R:88:ALA:N	2.32	0.44
6:S:45:GLU:O	6:S:46:ALA:C	2.61	0.44
6:S:73:ARG:NH1	7:T:32:ASP:OD1	2.49	0.44
1:A:3:THR:O	1:A:4:TYR:C	2.60	0.44
1:A:67:THR:HB	1:A:119:ASN:O	2.17	0.44
1:A:105:ASP:C	1:A:107:PRO:HD2	2.43	0.44
1:A:170:THR:HG22	1:A:171:THR:H	1.82	0.44
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.53	0.44
3:C:332:ASN:ND2	3:C:359:TYR:CA	2.81	0.44
4:D:22:ASP:O	4:D:25:SER:N	2.51	0.44
4:D:47:ALA:O	4:D:48:PHE:C	2.60	0.44
4:D:183:ALA:HA	4:D:186:VAL:HG12	2.00	0.44
1:N:136:GLN:C	1:N:138:LEU:N	2.73	0.44
1:N:294:LEU:O	1:N:298:ALA:HB2	2.17	0.44
2:O:239:TYR:HD2	2:O:239:TYR:C	2.25	0.44
2:O:277:HIS:HB2	2:O:360:ALA:HB1	1.98	0.44
2:O:289:SER:O	2:O:290:SER:C	2.61	0.44
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.98	0.44
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.52	0.44
5:R:85:LYS:HG2	5:R:86:ASN:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.50	0.44
3:C:29:SER:HB2	16:C:2004:CDL:HB21	2.00	0.44
3:C:201:LEU:C	3:C:203:GLU:H	2.26	0.44
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.85	0.44
5:E:57:GLN:OE1	20:E:2009:PLC:H12	2.18	0.44
5:E:160:CYS:HB3	5:E:161:HIS:CE1	2.53	0.44
1:N:36:THR:OG1	1:N:100:LYS:HG2	2.18	0.44
1:N:253:VAL:O	1:N:323:HIS:HA	2.17	0.44
3:P:81:ARG:O	3:P:82:ASN:C	2.60	0.44
4:Q:26:VAL:HG13	4:Q:189:PHE:HA	2.00	0.44
4:Q:143:VAL:O	4:Q:144:ARG:C	2.59	0.44
7:T:34:LEU:O	7:T:35:PRO:C	2.59	0.44
8:U:66:ASP:O	8:U:67:HIS:C	2.61	0.44
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.18	0.44
3:C:184:PHE:HA	13:C:501:HEM:CBC	2.48	0.44
6:F:77:LYS:HA	6:F:80:TRP:CD1	2.53	0.44
7:G:73:ASN:O	7:G:75:ALA:N	2.50	0.44
1:N:86:PHE:CE2	1:N:99:ILE:HD11	2.53	0.44
1:N:248:LEU:HB3	1:N:249:PRO:HD2	1.99	0.44
1:N:419:CYS:SG	7:T:21:PHE:HB2	2.58	0.44
2:O:50:PHE:CD2	2:O:106:THR:HG23	2.53	0.44
2:O:181:TYR:CD1	2:O:181:TYR:C	2.96	0.44
2:O:333:ALA:O	2:O:337:ILE:HG13	2.17	0.44
3:P:108:TYR:HE1	3:P:309:HIS:HB2	1.81	0.44
3:P:145:THR:O	3:P:149:ASN:HB2	2.17	0.44
3:P:295:LEU:O	3:P:298:SER:OG	2.29	0.44
3:P:358:SER:O	3:P:362:ILE:HG13	2.18	0.44
4:Q:55:THR:OG1	4:Q:56:HIS:CE1	2.69	0.44
5:R:179:ASN:O	5:R:180:LEU:C	2.60	0.44
2:B:59:THR:C	2:B:61:ALA:H	2.25	0.44
2:B:96:LEU:HD13	2:B:109:VAL:HG12	2.00	0.44
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.82	0.44
3:C:355:ALA:C	3:C:358:SER:HB3	2.43	0.44
6:F:16:ILE:O	6:F:19:TRP:N	2.48	0.44
6:F:72:HIS:C	6:F:73:ARG:HD3	2.43	0.44
9:I:65:VAL:CG1	9:I:66:ALA:N	2.81	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.72	0.44
1:N:277:ILE:O	1:N:277:ILE:HG22	2.17	0.44
2:O:253:VAL:HG13	2:O:430:LEU:HD22	1.99	0.44
2:O:306:PRO:HB3	9:V:52:ARG:N	2.32	0.44
4:Q:102:ARG:HG2	4:Q:102:ARG:NH1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:75:LEU:O	6:S:80:TRP:NE1	2.39	0.44
7:T:29:ILE:C	7:T:33:ALA:HB3	2.43	0.44
1:A:57:TYR:O	1:A:60:GLU:N	2.51	0.44
1:A:304:CYS:HA	1:A:326:ALA:HB2	2.00	0.44
1:A:428:ILE:O	1:A:429:GLU:C	2.60	0.44
2:B:56:ARG:NH1	2:B:172:LEU:HD21	2.33	0.44
2:B:264:VAL:HG11	2:B:388:LEU:CD1	2.41	0.44
3:C:198:LEU:HD11	15:C:2002:ANY:O4	2.17	0.44
3:C:352:GLY:O	3:C:353:GLN:C	2.61	0.44
13:C:502:HEM:CMB	13:C:502:HEM:HBB2	2.48	0.44
18:D:501:HEC:HBB3	18:D:501:HEC:CMB	2.40	0.44
2:O:229:GLY:O	2:O:231:GLY:N	2.49	0.44
3:P:30:ALA:C	3:P:32:TRP:N	2.72	0.44
3:P:151:PHE:N	3:P:151:PHE:CD1	2.85	0.44
4:Q:29:GLY:O	4:Q:32:VAL:HB	2.18	0.44
4:Q:197:GLU:O	4:Q:198:HIS:C	2.60	0.44
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.53	0.44
5:R:29:SER:HA	5:R:32:ARG:HH21	1.82	0.44
5:R:112:VAL:HG12	5:R:113:ASP:N	2.32	0.44
7:T:36:ASN:O	7:T:40:ARG:HG3	2.17	0.44
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.51	0.44
1:A:207:GLU:O	1:A:210:ASP:HB2	2.17	0.44
1:A:210:ASP:C	1:A:212:ALA:N	2.73	0.44
1:A:254:ALA:HB3	1:A:423:ALA:HB3	2.00	0.44
2:B:163:LEU:HD13	2:B:425:ALA:HB2	1.99	0.44
3:C:107:SER:HB2	13:C:502:HEM:HMD3	2.00	0.44
5:E:1:VAL:HG23	5:E:3:ASN:H	1.83	0.44
1:N:81:SER:HB2	2:O:359:LYS:HE2	1.99	0.44
1:N:192:ALA:N	1:N:193:PRO:HD2	2.33	0.44
2:O:163:LEU:CD1	2:O:425:ALA:HB2	2.47	0.44
2:O:325:TYR:C	2:O:325:TYR:HD2	2.25	0.44
2:O:370:MET:O	2:O:373:GLU:HG3	2.18	0.44
3:P:95:ILE:CD1	3:P:121:LEU:CD1	2.89	0.44
3:P:354:MET:O	3:P:358:SER:N	2.41	0.44
4:Q:235:MET:CE	6:S:64:ARG:HA	2.48	0.44
1:A:291:SER:OG	2:B:87:ARG:HD3	2.18	0.43
1:A:341:GLU:O	1:A:342:TRP:C	2.59	0.43
2:B:169:LYS:HD2	2:B:238:THR:HG21	2.00	0.43
2:B:415:LYS:C	2:B:417:PHE:N	2.76	0.43
4:D:227:TRP:O	4:D:230:LEU:N	2.50	0.43
1:N:388:ARG:HD3	1:N:388:ARG:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:100:SER:HA	2:O:104:LYS:O	2.18	0.43
2:O:221:GLU:C	2:O:223:PHE:N	2.76	0.43
2:B:19:PRO:O	2:B:20:GLY:C	2.61	0.43
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.99	0.43
2:B:171:ALA:O	2:B:174:ASN:HB2	2.17	0.43
2:B:239:TYR:C	2:B:239:TYR:HD2	2.25	0.43
2:B:344:LEU:HD12	2:B:344:LEU:HA	1.89	0.43
3:C:172:ASP:O	3:C:173:ASN:C	2.61	0.43
3:C:212:ILE:O	3:C:213:SER:C	2.60	0.43
4:D:182:ILE:C	4:D:184:LYS:N	2.76	0.43
4:D:189:PHE:O	4:D:191:ARG:N	2.50	0.43
7:G:48:VAL:O	7:G:51:PRO:HD2	2.18	0.43
10:J:10:TYR:CD2	10:J:10:TYR:C	2.96	0.43
1:N:296:ALA:O	1:N:297:LEU:C	2.58	0.43
2:O:166:ALA:O	2:O:242:GLY:N	2.35	0.43
2:O:286:LYS:O	2:O:287:ARG:HB2	2.17	0.43
3:P:60:THR:HG23	3:P:173:ASN:HA	2.00	0.43
3:P:111:LYS:O	3:P:114:TRP:HB3	2.18	0.43
4:Q:197:GLU:O	4:Q:199:ASP:N	2.51	0.43
4:Q:225:HIS:CE1	7:T:20:PRO:HB2	2.53	0.43
1:A:108:LYS:O	1:A:112:LEU:HG	2.19	0.43
1:A:301:HIS:HB2	1:A:303:LEU:HD21	1.99	0.43
2:B:131:GLU:O	2:B:132:PHE:C	2.61	0.43
3:C:87:GLY:O	3:C:88:ALA:C	2.61	0.43
3:C:92:PHE:O	3:C:96:PHE:CD2	2.71	0.43
3:C:242:THR:N	4:D:208:MET:CE	2.80	0.43
5:E:135:LEU:HD22	5:E:180:LEU:HD12	1.99	0.43
6:F:31:LEU:HD21	6:F:65:ALA:CB	2.48	0.43
1:N:94:GLN:NE2	1:N:381:SER:OG	2.44	0.43
1:N:334:MET:O	1:N:334:MET:HE3	2.18	0.43
2:O:124:LEU:HG	2:O:125:ASN:N	2.34	0.43
2:O:160:LEU:HD12	9:V:64:LEU:HB2	1.99	0.43
2:O:235:ALA:O	2:O:236:LYS:O	2.36	0.43
2:O:341:MET:O	2:O:342:ASN:C	2.62	0.43
2:O:353:THR:C	2:O:355:GLU:H	2.27	0.43
2:O:395:PRO:O	2:O:398:VAL:HG12	2.19	0.43
3:P:78:TRP:CG	3:P:79:LEU:N	2.86	0.43
3:P:355:ALA:C	3:P:358:SER:HB3	2.43	0.43
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.84	0.43
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.82	0.43
6:S:67:ASP:HA	6:S:70:LEU:CD2	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:46:SER:O	8:U:47:ARG:C	2.60	0.43
1:A:155:ALA:O	5:E:7:VAL:HG23	2.19	0.43
1:A:191:LYS:C	1:A:195:MET:HG3	2.42	0.43
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.54	0.43
4:D:223:LYS:C	4:D:223:LYS:CD	2.89	0.43
5:E:74:ILE:HG23	5:E:74:ILE:O	2.17	0.43
10:J:22:LEU:HD23	10:J:22:LEU:H	1.82	0.43
2:O:31:ASN:ND2	2:O:31:ASN:H	2.17	0.43
2:O:50:PHE:N	2:O:50:PHE:CD1	2.86	0.43
2:O:207:VAL:CG1	2:O:208:GLY:N	2.79	0.43
2:O:385:GLU:C	2:O:387:LEU:N	2.75	0.43
3:P:29:SER:HB2	16:P:3004:CDL:HB21	2.00	0.43
3:P:371:GLY:O	3:P:374:GLU:HB2	2.18	0.43
4:Q:171:TYR:HH	4:Q:182:ILE:HA	1.81	0.43
4:Q:227:TRP:O	4:Q:230:LEU:N	2.50	0.43
5:R:32:ARG:HD2	7:T:21:PHE:O	2.18	0.43
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.32	0.43
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.18	0.43
1:A:85:HIS:CD2	2:B:284:LEU:HB3	2.54	0.43
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.53	0.43
1:A:262:TRP:O	1:A:263:ALA:C	2.61	0.43
2:B:135:TRP:O	2:B:138:THR:N	2.51	0.43
3:C:151:PHE:C	3:C:153:ALA:N	2.76	0.43
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.53	0.43
3:C:285:ILE:HG21	3:C:290:GLY:C	2.43	0.43
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.31	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.62	0.43
5:E:179:ASN:O	5:E:180:LEU:C	2.60	0.43
10:J:26:LEU:O	10:J:30:LEU:HG	2.18	0.43
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.54	0.43
1:N:204:SER:O	1:N:205:HIS:C	2.60	0.43
1:N:294:LEU:HD23	1:N:307:PHE:CE1	2.53	0.43
2:O:72:ALA:O	2:O:75:LEU:HB2	2.18	0.43
2:O:306:PRO:HA	9:V:52:ARG:HG3	2.00	0.43
3:P:22:LEU:HD12	3:P:23:PRO:CD	2.49	0.43
3:P:241:LEU:O	3:P:242:THR:C	2.61	0.43
4:Q:109:LEU:HA	4:Q:110:PRO:HD2	1.91	0.43
4:Q:165:TYR:O	4:Q:166:ASN:C	2.62	0.43
5:R:94:LYS:O	5:R:95:PRO:O	2.37	0.43
8:U:37:LEU:O	8:U:40:CYS:N	2.50	0.43
1:A:86:PHE:CG	1:A:99:ILE:HG12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:ILE:HD12	15:C:2002:ANY:H3	2.00	0.43
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.25	0.43
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.49	0.43
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.83	0.43
6:F:43:VAL:O	6:F:44:LYS:C	2.60	0.43
1:N:317:THR:HG23	1:N:318:GLY:N	2.33	0.43
1:N:351:GLU:OE2	1:N:404:ALA:HB3	2.19	0.43
2:O:96:LEU:HD13	2:O:109:VAL:HG12	2.00	0.43
3:P:101:ARG:HD2	3:P:102:GLY:CA	2.48	0.43
3:P:232:GLY:HA2	16:Q:3003:CDL:H121	2.00	0.43
5:R:141:HIS:HB3	19:R:501:FES:S2	2.58	0.43
1:A:145:MET:O	1:A:146:THR:C	2.61	0.43
1:A:259:GLY:HA3	1:A:318:GLY:HA3	1.99	0.43
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.48	0.43
2:B:163:LEU:O	2:B:167:ALA:N	2.52	0.43
2:B:181:TYR:CD1	2:B:181:TYR:C	2.96	0.43
3:C:95:ILE:CD1	3:C:121:LEU:HD13	2.49	0.43
3:C:104:TYR:HB2	3:C:326:PHE:CE1	2.53	0.43
3:C:149:ASN:HD22	3:C:149:ASN:HA	1.54	0.43
4:D:72:ASP:CG	4:D:83:ARG:HE	2.27	0.43
4:D:116:ILE:CG2	4:D:117:VAL:N	2.82	0.43
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.54	0.43
8:H:20:ILE:O	8:H:20:ILE:HG22	2.18	0.43
1:N:382:HIS:HE1	1:N:390:ILE:O	2.02	0.43
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.49	0.43
3:P:88:ALA:O	3:P:91:PHE:HB3	2.19	0.43
3:P:138:GLN:NE2	3:P:266:PRO:HD3	2.34	0.43
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.81	0.43
7:T:73:ASN:C	7:T:75:ALA:H	2.27	0.43
1:A:57:TYR:C	1:A:59:VAL:N	2.74	0.43
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.43
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.54	0.43
1:A:368:GLN:O	1:A:374:PRO:HB3	2.18	0.43
2:B:241:GLY:HA2	2:B:423:SER:OG	2.19	0.43
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.83	0.43
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.54	0.43
2:B:353:THR:C	2:B:355:GLU:N	2.77	0.43
3:C:130:VAL:HG23	3:C:131:GLY:N	2.33	0.43
4:D:46:VAL:CG1	4:D:47:ALA:H	2.30	0.43
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.47	0.43
5:E:114:VAL:O	5:E:114:VAL:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:67:ASP:HA	6:F:70:LEU:CD2	2.47	0.43
1:N:261:GLY:HA2	1:N:314:TYR:O	2.19	0.43
1:N:269:VAL:O	1:N:270:LEU:C	2.62	0.43
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.75	0.43
2:O:344:LEU:HD12	2:O:344:LEU:HA	1.92	0.43
3:P:169:PHE:HD2	3:P:169:PHE:HA	1.77	0.43
4:Q:10:PHE:HB3	8:U:74:PHE:CE1	2.54	0.43
5:R:42:THR:O	5:R:43:ALA:C	2.61	0.43
5:R:49:TYR:O	5:R:50:ALA:C	2.60	0.43
5:R:78:LEU:HG	5:R:193:VAL:HG12	2.00	0.43
9:V:65:VAL:HG12	9:V:66:ALA:H	1.82	0.43
3:C:81:ARG:HH22	17:C:2011:GOL:H2	1.83	0.43
3:C:241:LEU:O	3:C:245:LEU:N	2.51	0.43
4:D:209:LEU:HD23	4:D:209:LEU:HA	1.82	0.43
10:J:14:PHE:N	10:J:14:PHE:HD2	2.15	0.43
10:J:19:THR:O	10:J:20:PHE:C	2.61	0.43
1:N:63:ALA:O	1:N:116:VAL:CG1	2.67	0.43
2:O:182:ARG:HH11	2:O:182:ARG:HG2	1.84	0.43
4:Q:47:ALA:O	4:Q:50:ASN:N	2.39	0.43
4:Q:182:ILE:C	4:Q:184:LYS:N	2.74	0.43
4:Q:189:PHE:O	4:Q:191:ARG:N	2.52	0.43
1:A:255:LEU:HA	1:A:421:ALA:O	2.19	0.43
2:B:47:ILE:HG22	2:B:48:GLY:N	2.32	0.43
3:C:22:LEU:HD12	3:C:23:PRO:HD2	2.01	0.43
3:C:137:GLY:N	3:C:140:SER:HB2	2.33	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB1	1.84	0.43
7:G:28:ASN:HB3	7:G:31:SER:OG	2.18	0.43
7:G:57:LEU:O	7:G:59:TYR:N	2.52	0.43
2:O:102:ARG:CZ	2:O:164:HIS:CD2	3.02	0.43
2:O:258:VAL:HG21	2:O:321:LEU:HD22	2.01	0.43
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.01	0.43
2:O:337:ILE:O	2:O:340:ALA:HB3	2.18	0.43
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.18	0.43
4:Q:130:LEU:HD12	4:Q:150:ASN:CG	2.44	0.43
5:R:29:SER:C	5:R:31:ASP:N	2.76	0.43
5:R:122:HIS:O	5:R:123:ASP:C	2.62	0.43
6:S:43:VAL:O	6:S:44:LYS:C	2.61	0.43
8:U:58:LEU:HG	8:U:62:LEU:CD1	2.49	0.43
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.49	0.42
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.02	0.42
1:A:147:ASN:C	1:A:149:THR:N	2.75	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG23	1:A:355:LYS:N	2.33	0.42
1:A:422:LEU:HD22	1:A:437:ILE:HD12	2.00	0.42
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.42
2:B:383:GLY:O	2:B:384:SER:C	2.62	0.42
2:B:385:GLU:C	2:B:387:LEU:N	2.77	0.42
3:C:8:SER:O	3:C:9:HIS:C	2.62	0.42
3:C:25:PRO:HG2	3:C:207:ASN:O	2.18	0.42
3:C:29:SER:O	3:C:32:TRP:HB2	2.18	0.42
3:C:82:ASN:HD22	3:C:82:ASN:N	2.16	0.42
3:C:117:GLY:O	3:C:118:VAL:C	2.60	0.42
3:C:237:LEU:O	3:C:241:LEU:HG	2.19	0.42
3:C:258:THR:O	3:C:259:PRO:C	2.61	0.42
4:D:134:TYR:CD1	4:D:162:PRO:HG3	2.54	0.42
6:F:96:GLU:O	6:F:97:VAL:C	2.62	0.42
7:G:55:ALA:O	7:G:58:LEU:N	2.52	0.42
1:N:273:ALA:O	1:N:275:ALA:N	2.52	0.42
1:N:277:ILE:CD1	1:N:345:LEU:HD11	2.49	0.42
1:N:319:LEU:HD23	1:N:319:LEU:HA	1.73	0.42
2:O:47:ILE:CG2	2:O:48:GLY:N	2.81	0.42
2:O:144:LEU:CB	2:O:183:ILE:CD1	2.97	0.42
2:O:248:ASN:HD22	2:O:250:HIS:H	1.65	0.42
2:O:399:ALA:HA	2:O:402:ILE:HD12	2.00	0.42
3:P:220:PRO:O	3:P:221:PHE:C	2.60	0.42
4:Q:36:VAL:O	18:Q:501:HEC:HMC1	2.18	0.42
5:R:97:PHE:O	5:R:134:ILE:HA	2.19	0.42
6:S:49:ARG:HH22	6:S:100:GLU:CD	2.27	0.42
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.49	0.42
2:B:295:LEU:O	2:B:296:TYR:C	2.61	0.42
3:C:28:ILE:HG13	3:C:225:TYR:HE2	1.82	0.42
3:C:67:VAL:O	3:C:68:ALA:C	2.61	0.42
4:D:237:TYR:CD2	4:D:239:PRO:HD3	2.54	0.42
6:F:20:TYR:O	6:F:23:ALA:HB3	2.19	0.42
1:N:54:GLY:O	1:N:56:GLY:N	2.52	0.42
1:N:284:PHE:HD1	1:N:284:PHE:H	1.66	0.42
3:P:337:THR:O	3:P:338:TRP:C	2.62	0.42
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.20	0.42
1:A:354:VAL:O	1:A:355:LYS:C	2.62	0.42
2:B:169:LYS:HB2	2:B:238:THR:HB	2.00	0.42
2:B:358:THR:HA	2:B:361:LYS:HD2	2.02	0.42
3:C:141:PHE:HB2	3:C:260:ALA:HB1	2.02	0.42
3:C:154:ILE:HG21	3:C:157:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:378:LEU:O	3:C:379:ASN:HB3	2.19	0.42
4:D:22:ASP:O	4:D:24:SER:N	2.52	0.42
5:E:113:ASP:CB	5:E:116:LYS:HB2	2.49	0.42
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.49	0.42
1:N:90:THR:HB	1:N:95:THR:HG23	2.02	0.42
1:N:292:SER:O	1:N:293:ARG:C	2.61	0.42
2:O:118:THR:C	2:O:120:MET:N	2.77	0.42
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.46	0.42
3:P:99:ILE:HD11	3:P:121:LEU:HD22	2.01	0.42
3:P:134:LEU:C	3:P:136:TRP:N	2.76	0.42
5:R:103:GLN:C	5:R:105:GLU:N	2.76	0.42
1:A:78:GLU:OE1	1:A:108:LYS:CE	2.67	0.42
4:D:189:PHE:C	4:D:191:ARG:N	2.78	0.42
6:F:76:PRO:O	6:F:77:LYS:C	2.61	0.42
1:N:145:MET:HE2	1:N:145:MET:CA	2.48	0.42
1:N:262:TRP:O	1:N:263:ALA:C	2.62	0.42
2:O:239:TYR:HE1	2:O:260:GLU:H	1.65	0.42
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.80	0.42
5:R:109:GLU:CD	5:R:167:ALA:HB3	2.44	0.42
5:R:186:GLN:HE21	5:R:188:VAL:HG12	1.84	0.42
10:W:19:THR:O	10:W:20:PHE:C	2.62	0.42
1:A:261:GLY:HA2	1:A:317:THR:O	2.20	0.42
1:A:301:HIS:HB2	1:A:303:LEU:CD2	2.50	0.42
2:B:317:SER:OG	2:B:318:ASP:N	2.52	0.42
3:C:241:LEU:HB3	4:D:208:MET:HE2	2.01	0.42
5:E:47:THR:O	5:E:48:ALA:C	2.63	0.42
8:H:49:HIS:CG	8:H:49:HIS:O	2.71	0.42
10:J:13:LEU:O	10:J:19:THR:OG1	2.36	0.42
2:O:168:TYR:HD2	2:O:237:ALA:HB1	1.83	0.42
2:O:189:GLU:O	2:O:190:GLN:C	2.62	0.42
2:O:247:GLN:HE21	2:O:249:GLY:H	1.68	0.42
3:P:70:THR:HA	3:P:74:VAL:HG21	2.01	0.42
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.27	0.42
4:Q:46:VAL:CG1	4:Q:47:ALA:N	2.81	0.42
4:Q:155:GLY:C	4:Q:157:ALA:N	2.74	0.42
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.42
5:R:29:SER:O	5:R:31:ASP:N	2.52	0.42
6:S:16:ILE:O	6:S:19:TRP:N	2.52	0.42
2:B:209:ILE:O	2:B:211:VAL:HG22	2.19	0.42
3:C:107:SER:C	3:C:109:LEU:N	2.78	0.42
3:C:193:ILE:HG13	3:C:193:ILE:H	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:LEU:HD12	3:C:243:LEU:HA	1.76	0.42
3:C:285:ILE:HB	3:C:291:GLY:HA2	2.01	0.42
5:E:185:TYR:HB2	5:E:186:GLN:H	1.63	0.42
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.50	0.42
2:O:57:TYR:N	2:O:57:TYR:CD1	2.87	0.42
4:Q:217:SER:O	4:Q:218:LEU:C	2.62	0.42
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.54	0.42
6:S:50:LEU:HA	6:S:51:PRO:HD3	1.83	0.42
7:T:30:PHE:O	7:T:35:PRO:CD	2.67	0.42
1:A:127:ILE:C	1:A:129:LYS:H	2.27	0.42
1:A:283:THR:O	1:A:284:PHE:C	2.61	0.42
1:A:284:PHE:H	1:A:284:PHE:HD1	1.66	0.42
1:A:429:GLU:CD	7:G:7:LEU:HB2	2.45	0.42
3:C:36:SER:HA	15:C:2002:ANY:O7	2.20	0.42
3:C:191:ALA:O	3:C:195:ILE:HG12	2.20	0.42
3:C:273:TRP:CD2	3:C:274:TYR:N	2.88	0.42
3:C:301:ILE:HD13	3:C:363:LEU:HD13	2.02	0.42
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.01	0.42
6:F:62:ILE:C	6:F:64:ARG:N	2.77	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.19	0.42
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.19	0.42
1:N:257:VAL:HG23	1:N:320:PHE:HB3	2.01	0.42
1:N:378:THR:O	1:N:382:HIS:N	2.50	0.42
2:O:76:THR:HG23	2:O:82:SER:HB2	2.02	0.42
3:P:49:GLY:HA3	13:P:501:HEM:C2C	2.55	0.42
5:R:83:GLU:HA	5:R:100:HIS:CG	2.54	0.42
7:T:73:ASN:O	7:T:75:ALA:N	2.53	0.42
8:U:50:THR:OG1	8:U:51:GLU:N	2.52	0.42
10:W:45:HIS:C	10:W:47:ASN:N	2.76	0.42
1:A:187:ASP:O	1:A:191:LYS:HE3	2.20	0.42
1:A:236:PHE:HB2	1:A:258:GLU:OE1	2.19	0.42
2:B:163:LEU:CD1	2:B:425:ALA:HB2	2.50	0.42
3:C:162:VAL:O	3:C:165:ALA:N	2.52	0.42
5:E:94:LYS:O	5:E:95:PRO:O	2.37	0.42
6:F:16:ILE:O	6:F:17:ARG:C	2.61	0.42
8:H:50:THR:C	8:H:52:GLU:H	2.27	0.42
1:N:29:GLU:OE1	1:N:204:SER:HA	2.19	0.42
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.60	0.42
1:N:301:HIS:HB2	1:N:303:LEU:CD2	2.50	0.42
2:O:353:THR:C	2:O:355:GLU:N	2.77	0.42
3:P:273:TRP:CD2	3:P:274:TYR:N	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:10:GLY:C	6:S:12:LEU:H	2.26	0.42
6:S:82:LYS:O	6:S:83:TYR:C	2.62	0.42
7:T:12:HIS:O	7:T:13:ILE:HG13	2.19	0.42
1:A:112:LEU:O	1:A:113:LEU:C	2.62	0.42
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.33	0.42
1:A:379:ILE:O	1:A:380:GLY:C	2.63	0.42
2:B:50:PHE:HD1	2:B:50:PHE:H	1.68	0.42
3:C:38:LEU:HD21	3:C:95:ILE:N	2.35	0.42
5:E:29:SER:O	5:E:31:ASP:N	2.53	0.42
5:E:103:GLN:O	5:E:107:ASN:ND2	2.53	0.42
5:E:127:VAL:HG11	5:E:133:VAL:HG23	2.02	0.42
5:E:149:ASN:O	5:E:150:SER:HB3	2.19	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HB	2.55	0.42
1:N:78:GLU:OE1	1:N:108:LYS:CE	2.67	0.42
1:N:297:LEU:O	1:N:298:ALA:C	2.63	0.42
2:O:47:ILE:O	2:O:108:CYS:HB2	2.20	0.42
3:P:201:LEU:C	3:P:203:GLU:N	2.77	0.42
3:P:223:PRO:HA	3:P:226:SER:OG	2.20	0.42
3:P:246:PHE:HZ	4:Q:205:GLY:C	2.28	0.42
4:Q:18:LEU:HD22	4:Q:206:LEU:HD13	2.02	0.42
4:Q:44:ASP:O	4:Q:90:TYR:HD2	2.03	0.42
6:S:73:ARG:HG3	6:S:73:ARG:NH1	2.33	0.42
1:A:40:TRP:CD1	1:A:96:ALA:CB	3.03	0.42
1:A:89:TYR:O	1:A:95:THR:CG2	2.65	0.42
1:A:90:THR:HB	1:A:95:THR:HG23	2.01	0.42
1:A:138:LEU:HD22	5:E:3:ASN:HD21	1.84	0.42
1:A:182:LEU:HD23	1:A:182:LEU:H	1.85	0.42
1:A:251:ALA:HB1	1:A:428:ILE:HG22	2.02	0.42
2:B:62:ASN:HD22	2:B:65:THR:HG21	1.85	0.42
2:B:296:TYR:O	2:B:297:GLN:C	2.62	0.42
2:B:408:ALA:C	2:B:410:VAL:N	2.76	0.42
4:D:186:VAL:HG21	18:D:501:HEC:HBB3	2.02	0.42
5:E:78:LEU:HD21	5:E:193:VAL:HG11	2.02	0.42
5:E:141:HIS:HB3	5:E:142:LEU:H	1.66	0.42
1:N:273:ALA:C	1:N:275:ALA:N	2.78	0.42
1:N:433:ASP:OD2	1:N:435:ASN:N	2.53	0.42
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.50	0.42
2:O:191:LEU:O	2:O:192:HIS:C	2.63	0.42
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.20	0.42
7:T:73:ASN:C	7:T:75:ALA:N	2.78	0.42
1:A:239:SER:O	1:A:421:ALA:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:O	1:A:359:ASN:N	2.53	0.41
2:B:35:ILE:O	2:B:213:HIS:HE1	2.03	0.41
2:B:209:ILE:CG2	2:B:210:GLY:N	2.82	0.41
2:B:424:MET:HE1	2:B:434:PRO:O	2.20	0.41
14:C:2001:SMA:H4	5:R:161:HIS:CE1	2.55	0.41
4:D:11:PRO:O	4:D:12:TRP:C	2.63	0.41
4:D:182:ILE:O	4:D:185:ASP:N	2.53	0.41
18:D:501:HEC:HBC3	18:D:501:HEC:CMC	2.44	0.41
5:E:78:LEU:HD22	5:E:132:TRP:CD2	2.54	0.41
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.55	0.41
9:I:49:LEU:HB3	9:I:55:MET:HG2	2.02	0.41
1:N:268:VAL:O	1:N:269:VAL:C	2.63	0.41
1:N:317:THR:OG1	1:N:318:GLY:N	2.51	0.41
1:N:341:GLU:O	1:N:342:TRP:C	2.63	0.41
2:O:163:LEU:O	2:O:166:ALA:N	2.52	0.41
2:O:189:GLU:C	2:O:191:LEU:N	2.77	0.41
3:P:101:ARG:C	3:P:101:ARG:CD	2.79	0.41
4:Q:160:MET:HB2	18:Q:501:HEC:C1D	2.50	0.41
4:Q:215:LEU:HD12	4:Q:219:LEU:HG	2.02	0.41
4:Q:225:HIS:O	4:Q:228:SER:OG	2.35	0.41
1:A:158:PHE:O	1:A:159:GLN:O	2.37	0.41
3:C:145:THR:O	3:C:149:ASN:HB2	2.20	0.41
3:C:254:PRO:C	3:C:256:ASN:N	2.78	0.41
3:C:269:ILE:O	3:C:270:LYS:HD3	2.20	0.41
10:J:21:ALA:O	10:J:22:LEU:C	2.62	0.41
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.55	0.41
2:O:169:LYS:HB2	2:O:238:THR:HB	2.01	0.41
2:O:183:ILE:HD13	2:O:183:ILE:HA	1.88	0.41
2:O:189:GLU:O	2:O:191:LEU:N	2.53	0.41
3:P:6:ARG:CD	3:P:16:ASN:OD1	2.65	0.41
4:Q:3:LEU:HD23	4:Q:3:LEU:H	1.85	0.41
4:Q:218:LEU:HD13	5:R:43:ALA:CA	2.50	0.41
4:Q:223:LYS:C	4:Q:223:LYS:CD	2.88	0.41
1:A:178:THR:HG22	1:A:179:ARG:N	2.36	0.41
1:A:233:ARG:NH2	1:A:316:ASP:HB2	2.35	0.41
2:B:201:SER:N	2:B:227:ARG:O	2.53	0.41
2:B:431:GLY:HA3	2:O:60:THR:HG21	2.01	0.41
3:C:236:MET:O	3:C:238:THR:N	2.53	0.41
3:C:337:THR:O	3:C:338:TRP:C	2.63	0.41
5:E:18:VAL:O	5:E:18:VAL:HG23	2.20	0.41
1:N:76:GLU:HG2	2:O:285:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.41
1:N:249:PRO:HG2	1:N:250:VAL:H	1.85	0.41
1:N:262:TRP:CD1	1:N:314:TYR:C	2.99	0.41
1:N:288:LYS:N	1:N:299:VAL:HG11	2.34	0.41
1:N:354:VAL:O	1:N:355:LYS:C	2.61	0.41
2:O:26:ILE:HG23	2:O:26:ILE:O	2.20	0.41
2:O:151:ALA:C	2:O:153:GLN:H	2.28	0.41
2:O:408:ALA:C	2:O:410:VAL:N	2.76	0.41
3:P:184:PHE:C	3:P:184:PHE:HD2	2.27	0.41
5:R:45:VAL:O	5:R:48:ALA:HB3	2.21	0.41
1:A:55:ALA:O	1:A:56:GLY:C	2.61	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.38	0.41
2:B:353:THR:C	2:B:355:GLU:H	2.28	0.41
2:B:366:ALA:O	2:B:369:LEU:N	2.53	0.41
3:C:95:ILE:O	3:C:99:ILE:HG13	2.21	0.41
3:C:201:LEU:C	3:C:203:GLU:N	2.78	0.41
3:C:261:ASN:C	3:C:263:LEU:H	2.28	0.41
4:D:37:CYS:C	4:D:39:ALA:N	2.78	0.41
4:D:197:GLU:HG2	4:D:198:HIS:H	1.83	0.41
5:E:24:SER:OG	5:E:26:GLN:HB2	2.21	0.41
5:E:38:LEU:CA	10:J:14:PHE:CE1	3.01	0.41
10:J:45:HIS:C	10:J:47:ASN:N	2.78	0.41
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.36	0.41
3:P:57:THR:O	3:P:57:THR:HG22	2.20	0.41
3:P:134:LEU:C	3:P:136:TRP:H	2.28	0.41
3:P:160:THR:O	3:P:163:GLU:HB3	2.21	0.41
3:P:261:ASN:C	3:P:263:LEU:H	2.28	0.41
3:P:331:ALA:HB2	7:T:52:PHE:CD2	2.55	0.41
3:P:350:ILE:O	3:P:351:ILE:C	2.62	0.41
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.01	0.41
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.37	0.41
8:U:52:GLU:C	8:U:53:GLN:HG3	2.45	0.41
1:A:40:TRP:CD2	1:A:380:GLY:HA3	2.56	0.41
1:A:86:PHE:HD1	1:A:87:ASN:N	2.18	0.41
1:A:166:THR:HG21	5:E:3:ASN:OD1	2.20	0.41
2:B:111:CYS:SG	2:B:119:VAL:HG21	2.60	0.41
2:B:259:THR:HG22	2:B:260:GLU:N	2.34	0.41
3:C:12:LEU:O	3:C:13:LYS:C	2.63	0.41
4:D:195:GLU:HG3	4:D:195:GLU:O	2.20	0.41
7:G:73:ASN:C	7:G:75:ALA:H	2.29	0.41
8:H:55:THR:O	8:H:58:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:LYS:HE3	1:N:70:ARG:NH2	2.15	0.41
1:N:291:SER:OG	2:O:87:ARG:HD3	2.20	0.41
2:O:144:LEU:HB3	2:O:183:ILE:CD1	2.51	0.41
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.85	0.41
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.56	0.41
8:U:20:ILE:O	8:U:20:ILE:HG22	2.20	0.41
1:A:281:ASP:O	1:A:284:PHE:HD1	2.03	0.41
3:C:196:ILE:O	3:C:197:HIS:C	2.63	0.41
3:C:321:LEU:O	3:C:322:SER:C	2.63	0.41
4:D:241:LYS:HA	4:D:241:LYS:CE	2.42	0.41
5:E:33:LYS:HG2	7:G:21:PHE:CD1	2.56	0.41
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.56	0.41
9:I:75:SER:O	9:I:76:VAL:HB	2.20	0.41
2:O:283:PRO:CG	9:V:56:SER:HB2	2.47	0.41
2:O:362:ASN:HA	2:O:365:LYS:HD2	2.01	0.41
3:P:38:LEU:HB3	13:P:502:HEM:CMB	2.51	0.41
3:P:60:THR:N	3:P:176:LEU:HD23	2.36	0.41
4:Q:48:PHE:CE2	4:Q:65:ALA:HA	2.56	0.41
4:Q:195:GLU:N	4:Q:196:PRO:HD3	2.36	0.41
6:S:18:LYS:HA	6:S:83:TYR:CE1	2.55	0.41
6:S:53:ASP:O	6:S:57:GLU:HG3	2.21	0.41
9:V:65:VAL:CG1	9:V:66:ALA:N	2.83	0.41
10:W:10:TYR:CD2	10:W:10:TYR:C	2.98	0.41
1:A:29:GLU:OE1	1:A:204:SER:HA	2.21	0.41
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.56	0.41
1:A:162:ALA:O	1:A:163:LEU:C	2.64	0.41
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.83	0.41
1:A:206:LYS:CA	1:A:209:VAL:HG12	2.50	0.41
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.21	0.41
3:C:238:THR:O	3:C:239:PRO:C	2.62	0.41
4:D:217:SER:O	4:D:218:LEU:C	2.63	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41
6:F:63:LYS:HD3	7:G:13:ILE:HD13	2.01	0.41
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.55	0.41
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.01	0.41
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.02	0.41
2:O:31:ASN:N	2:O:31:ASN:HD22	2.18	0.41
2:O:144:LEU:HB3	2:O:183:ILE:HD11	2.02	0.41
2:O:166:ALA:HB1	2:O:242:GLY:O	2.20	0.41
2:O:227:ARG:NH1	2:O:228:SER:H	2.17	0.41
2:O:248:ASN:HD21	2:O:250:HIS:CB	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:8:SER:O	3:P:9:HIS:C	2.63	0.41
3:P:22:LEU:HD12	3:P:23:PRO:N	2.35	0.41
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.56	0.41
3:P:285:ILE:HB	3:P:291:GLY:HA2	2.03	0.41
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.36	0.41
3:P:332:ASN:ND2	3:P:359:TYR:CA	2.82	0.41
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.55	0.41
1:A:67:THR:HA	1:A:121:ALA:H	1.85	0.41
1:A:95:THR:HG22	1:A:96:ALA:N	2.36	0.41
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.55	0.41
2:B:235:ALA:O	2:B:236:LYS:O	2.38	0.41
3:C:110:TYR:O	3:C:111:LYS:C	2.63	0.41
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.55	0.41
3:C:186:LEU:HD23	3:C:186:LEU:HA	1.71	0.41
3:C:372:THR:O	3:C:373:LEU:C	2.63	0.41
4:D:22:ASP:C	4:D:24:SER:N	2.78	0.41
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.46	0.41
5:E:29:SER:C	5:E:31:ASP:N	2.78	0.41
5:E:140:THR:O	5:E:141:HIS:C	2.64	0.41
6:F:53:ASP:O	6:F:55:TYR:N	2.53	0.41
6:F:87:LYS:O	6:F:87:LYS:CG	2.69	0.41
8:H:46:SER:O	8:H:47:ARG:C	2.63	0.41
1:N:272:VAL:O	1:N:275:ALA:HB3	2.21	0.41
2:O:75:LEU:HD11	2:O:140:LEU:HD23	2.03	0.41
2:O:154:SER:C	2:O:156:GLN:N	2.77	0.41
3:P:92:PHE:HA	3:P:95:ILE:CG2	2.45	0.41
3:P:241:LEU:O	3:P:245:LEU:N	2.54	0.41
3:P:378:LEU:O	3:P:379:ASN:CB	2.68	0.41
4:Q:34:LYS:O	4:Q:38:SER:OG	2.34	0.41
4:Q:182:ILE:C	4:Q:184:LYS:H	2.28	0.41
4:Q:220:TYR:CE1	4:Q:224:ARG:HG3	2.56	0.41
6:S:52:GLU:HG2	6:S:56:ASN:HD21	1.86	0.41
1:A:235:ARG:CZ	5:E:14:ARG:NH2	2.84	0.41
1:A:273:ALA:C	1:A:275:ALA:N	2.78	0.41
1:A:288:LYS:HE3	1:A:289:HIS:NE2	2.36	0.41
2:B:47:ILE:CG2	2:B:48:GLY:N	2.83	0.41
2:B:59:THR:C	2:B:61:ALA:N	2.76	0.41
2:B:124:LEU:HG	2:B:125:ASN:N	2.36	0.41
2:B:412:ASN:C	2:B:414:ALA:N	2.78	0.41
3:C:199:THR:O	3:C:200:PHE:C	2.63	0.41
3:C:227:PHE:CD2	4:D:226:LYS:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:358:SER:O	3:C:362:ILE:HG13	2.21	0.41
3:C:367:PHE:HD2	3:C:367:PHE:HA	1.73	0.41
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.02	0.41
4:D:215:LEU:HD12	4:D:219:LEU:HG	2.03	0.41
4:D:224:ARG:HH12	16:D:2003:CDL:HB21	1.86	0.41
6:F:43:VAL:O	6:F:46:ALA:N	2.54	0.41
10:J:27:GLY:O	10:J:28:ALA:C	2.64	0.41
1:N:29:GLU:HG3	1:N:203:ILE:O	2.21	0.41
1:N:62:LEU:HD21	1:N:126:GLN:HG3	2.01	0.41
1:N:210:ASP:C	1:N:212:ALA:N	2.79	0.41
1:N:223:TYR:N	1:N:223:TYR:CD2	2.81	0.41
1:N:411:CYS:HB3	1:N:415:ILE:HD12	2.02	0.41
2:O:72:ALA:CA	2:O:75:LEU:HD12	2.50	0.41
2:O:130:PRO:CB	2:O:132:PHE:CE2	2.95	0.41
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.56	0.41
2:O:207:VAL:HG21	2:O:383:GLY:HA3	2.03	0.41
2:O:412:ASN:O	2:O:415:LYS:N	2.53	0.41
2:O:415:LYS:C	2:O:417:PHE:N	2.77	0.41
3:P:16:ASN:C	3:P:18:SER:H	2.28	0.41
3:P:28:ILE:HG13	3:P:225:TYR:HE2	1.84	0.41
3:P:104:TYR:CD1	3:P:316:MET:SD	3.14	0.41
3:P:165:ALA:O	3:P:178:ARG:HD2	2.20	0.41
3:P:172:ASP:O	3:P:173:ASN:C	2.63	0.41
3:P:212:ILE:O	3:P:213:SER:C	2.64	0.41
3:P:230:ILE:CG2	11:P:3005:PEE:H25	2.50	0.41
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.89	0.41
4:Q:43:MET:HG2	4:Q:91:PHE:HD2	1.85	0.41
4:Q:237:TYR:CD2	4:Q:239:PRO:HD3	2.56	0.41
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	2.03	0.41
5:R:50:ALA:HA	20:R:3009:PLC:OB	2.21	0.41
8:U:62:LEU:O	8:U:63:HIS:C	2.64	0.41
10:W:27:GLY:O	10:W:28:ALA:C	2.63	0.41
1:A:46:ARG:NH1	1:A:316:ASP:OD1	2.36	0.41
1:A:157:ALA:HB1	1:A:236:PHE:HE1	1.86	0.41
1:A:182:LEU:O	1:A:183:ALA:C	2.64	0.41
1:A:373:THR:HB	1:A:374:PRO:CD	2.46	0.41
1:A:412:SER:O	1:A:413:LYS:C	2.63	0.41
2:B:154:SER:C	2:B:156:GLN:N	2.79	0.41
2:B:417:PHE:CD2	2:B:417:PHE:C	2.99	0.41
3:C:190:ILE:O	3:C:191:ALA:C	2.64	0.41
3:C:323:GLN:O	3:C:326:PHE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:O	4:D:45:TYR:N	2.54	0.41
4:D:47:ALA:O	4:D:49:ARG:N	2.54	0.41
1:N:177:LEU:HA	1:N:177:LEU:HD23	1.86	0.41
2:O:71:LEU:C	2:O:73:SER:H	2.29	0.41
2:O:312:PHE:CE1	9:V:62:ARG:O	2.69	0.41
2:O:383:GLY:O	2:O:384:SER:C	2.63	0.41
3:P:245:LEU:O	4:Q:201:ARG:HG2	2.20	0.41
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.97	0.41
3:P:365:ILE:O	3:P:368:PRO:HD2	2.21	0.41
5:R:57:GLN:O	5:R:58:PHE:C	2.63	0.41
1:A:158:PHE:O	1:A:159:GLN:C	2.64	0.40
2:B:328:SER:OG	2:B:333:ALA:HA	2.21	0.40
2:B:339:ALA:HA	2:B:342:ASN:ND2	2.36	0.40
2:B:369:LEU:O	2:B:372:VAL:HG22	2.21	0.40
4:D:158:ILE:HG12	4:D:159:GLY:N	2.34	0.40
6:F:40:ASP:OD1	6:F:40:ASP:C	2.64	0.40
1:N:147:ASN:C	1:N:149:THR:N	2.78	0.40
2:O:56:ARG:C	2:O:58:GLU:H	2.29	0.40
2:O:62:ASN:O	2:O:65:THR:CG2	2.67	0.40
3:P:78:TRP:CE3	3:P:79:LEU:N	2.89	0.40
3:P:164:TRP:O	3:P:167:GLY:N	2.54	0.40
4:Q:81:PHE:C	4:Q:82:MET:HE2	2.46	0.40
5:R:29:SER:CB	5:R:32:ARG:HH21	2.34	0.40
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.36	0.40
1:A:12:PRO:O	1:A:13:GLU:C	2.65	0.40
2:B:130:PRO:HB2	2:B:132:PHE:CD2	2.56	0.40
3:C:333:LEU:O	3:C:334:LEU:C	2.64	0.40
1:N:11:ILE:HA	1:N:12:PRO:HD2	1.86	0.40
1:N:106:MET:HB3	1:N:107:PRO:CD	2.51	0.40
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.40
1:N:296:ALA:O	1:N:299:VAL:HB	2.22	0.40
2:O:266:SER:O	2:O:267:ALA:C	2.65	0.40
3:P:38:LEU:HD23	3:P:38:LEU:HA	1.85	0.40
3:P:110:TYR:O	3:P:111:LYS:C	2.64	0.40
3:P:200:PHE:O	3:P:203:GLU:HB2	2.21	0.40
3:P:273:TRP:HA	3:P:276:LEU:HG	2.02	0.40
3:P:357:LEU:HD12	3:P:357:LEU:HA	1.69	0.40
3:P:378:LEU:O	3:P:379:ASN:HB3	2.22	0.40
3:P:378:LEU:HD23	3:P:378:LEU:HA	1.94	0.40
10:W:43:PHE:O	10:W:44:GLU:C	2.63	0.40
2:B:151:ALA:C	2:B:153:GLN:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:LEU:O	2:B:192:HIS:C	2.64	0.40
2:B:394:ALA:HB3	2:B:397:VAL:HG23	2.03	0.40
3:C:27:ASN:ND2	3:C:209:PRO:HD2	2.36	0.40
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.87	0.40
3:C:346:HIS:CG	3:C:347:PRO:HA	2.56	0.40
4:D:164:ILE:HD11	4:D:183:ALA:HB2	2.02	0.40
4:D:224:ARG:O	4:D:225:HIS:C	2.63	0.40
5:E:10:PHE:O	5:E:14:ARG:HG3	2.22	0.40
5:E:52:LYS:C	5:E:52:LYS:CD	2.95	0.40
5:E:55:VAL:C	5:E:57:GLN:N	2.80	0.40
6:F:101:ARG:O	6:F:102:LEU:C	2.62	0.40
1:N:61:HIS:NE2	1:N:137:GLU:OE1	2.53	0.40
1:N:86:PHE:HD1	1:N:87:ASN:N	2.19	0.40
2:O:68:LEU:HD22	2:O:186:ILE:HD12	2.02	0.40
2:O:73:SER:N	2:O:74:PRO:CD	2.84	0.40
3:P:115:ASN:O	3:P:118:VAL:HG23	2.21	0.40
3:P:146:VAL:O	3:P:149:ASN:N	2.54	0.40
4:Q:175:THR:HA	4:Q:176:PRO:HD3	1.85	0.40
18:Q:501:HEC:HMB3	18:Q:501:HEC:CBB	2.43	0.40
16:Q:3003:CDL:H732	16:Q:3003:CDL:HA61	2.04	0.40
5:R:113:ASP:O	5:R:115:SER:N	2.53	0.40
1:A:67:THR:HG21	1:A:115:ASP:CG	2.47	0.40
1:A:112:LEU:HG	1:A:112:LEU:H	1.49	0.40
1:A:241:ILE:O	1:A:241:ILE:CG2	2.70	0.40
1:A:339:GLN:NE2	1:A:437:ILE:HG23	2.37	0.40
3:C:112:GLU:O	3:C:113:THR:C	2.64	0.40
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.21	0.40
4:D:58:GLU:O	4:D:59:ALA:C	2.64	0.40
1:N:246:ASP:HA	1:N:427:PRO:CB	2.48	0.40
2:O:24:LEU:CD1	2:O:38:LEU:HB2	2.46	0.40
2:O:163:LEU:HD12	2:O:163:LEU:HA	1.83	0.40
3:P:242:THR:HA	4:Q:208:MET:HE1	2.03	0.40
3:P:285:ILE:N	3:P:285:ILE:CD1	2.85	0.40
3:P:338:TRP:CZ2	7:T:59:TYR:HD1	2.39	0.40
3:P:346:HIS:CG	3:P:347:PRO:HA	2.57	0.40
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.21	0.40
5:R:186:GLN:O	5:R:193:VAL:HG23	2.21	0.40
6:S:40:ASP:OD1	6:S:40:ASP:C	2.65	0.40
7:T:61:TRP:CE3	7:T:62:GLY:N	2.89	0.40
8:U:56:GLU:O	8:U:59:PHE:HB2	2.22	0.40
8:U:57:GLU:O	8:U:58:LEU:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.57	0.40
1:A:262:TRP:HE3	1:A:386:TYR:CZ	2.39	0.40
1:A:273:ALA:O	1:A:275:ALA:N	2.55	0.40
1:A:378:THR:O	1:A:382:HIS:N	2.52	0.40
1:A:406:MET:O	1:A:407:VAL:C	2.65	0.40
2:B:345:LYS:O	2:B:347:ALA:N	2.54	0.40
3:C:56:TYR:OH	3:C:176:LEU:HD11	2.21	0.40
3:C:241:LEU:O	3:C:242:THR:C	2.65	0.40
3:C:311:SER:OG	3:C:319:ARG:HD3	2.21	0.40
3:C:333:LEU:HD11	11:C:2007:PEE:H38	2.04	0.40
5:E:77:LYS:C	5:E:79:SER:H	2.29	0.40
5:E:170:ARG:HA	5:E:179:ASN:CB	2.51	0.40
6:F:55:TYR:O	6:F:56:ASN:C	2.64	0.40
6:F:76:PRO:O	6:F:78:GLU:N	2.54	0.40
7:G:41:PHE:HE2	7:G:45:VAL:HB	1.87	0.40
1:N:51:LYS:HE3	1:N:51:LYS:HB2	1.94	0.40
1:N:55:ALA:C	1:N:57:TYR:H	2.29	0.40
1:N:110:VAL:HA	1:N:113:LEU:HD12	2.03	0.40
1:N:163:LEU:C	1:N:165:ARG:H	2.30	0.40
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.37	0.40
3:P:149:ASN:O	3:P:150:LEU:C	2.64	0.40
3:P:184:PHE:CE2	13:P:501:HEM:HBC1	2.57	0.40
3:P:270:LYS:HA	3:P:271:PRO:HD3	1.94	0.40
4:Q:46:VAL:HB	4:Q:91:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	441/446 (99%)	323 (73%)	94 (21%)	24 (5%)	1 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	440/446 (99%)	320 (73%)	95 (22%)	25 (6%)	1	13
2	B	419/441 (95%)	302 (72%)	77 (18%)	40 (10%)	0	6
2	O	420/441 (95%)	302 (72%)	85 (20%)	33 (8%)	1	8
3	C	378/380 (100%)	284 (75%)	72 (19%)	22 (6%)	1	12
3	P	377/380 (99%)	284 (75%)	73 (19%)	20 (5%)	1	14
4	D	239/241 (99%)	188 (79%)	37 (16%)	14 (6%)	1	12
4	Q	239/241 (99%)	186 (78%)	40 (17%)	13 (5%)	1	13
5	E	194/196 (99%)	136 (70%)	42 (22%)	16 (8%)	0	8
5	R	194/196 (99%)	136 (70%)	36 (19%)	22 (11%)	0	4
6	F	99/110 (90%)	73 (74%)	24 (24%)	2 (2%)	6	32
6	S	99/110 (90%)	73 (74%)	23 (23%)	3 (3%)	3	25
7	G	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	1	9
7	T	77/81 (95%)	52 (68%)	20 (26%)	5 (6%)	1	11
8	H	68/77 (88%)	46 (68%)	18 (26%)	4 (6%)	1	12
8	U	65/77 (84%)	41 (63%)	20 (31%)	4 (6%)	1	12
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0	3
9	V	29/47 (62%)	21 (72%)	4 (14%)	4 (14%)	0	3
10	J	59/61 (97%)	41 (70%)	16 (27%)	2 (3%)	3	23
10	W	57/61 (93%)	36 (63%)	17 (30%)	4 (7%)	1	10
All	All	4002/4160 (96%)	2919 (73%)	816 (20%)	267 (7%)	1	11

All (267) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	72	CYS
1	A	94	GLN
1	A	159	GLN
1	A	282	ARG
1	A	290	LEU
2	B	29	LEU
2	B	171	ALA
2	B	201	SER
2	B	226	ILE
2	B	230	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	236	LYS
2	B	283	PRO
3	C	31	TRP
3	C	58	ALA
3	C	111	LYS
3	C	224	TYR
3	C	348	PHE
4	D	44	ASP
4	D	198	HIS
5	E	63	SER
5	E	95	PRO
5	E	113	ASP
5	E	141	HIS
6	F	69	SER
7	G	7	LEU
7	G	33	ALA
9	I	63	ASP
10	J	56	LYS
1	N	4	TYR
1	N	55	ALA
1	N	72	CYS
1	N	159	GLN
1	N	206	LYS
1	N	282	ARG
1	N	433	ASP
2	O	171	ALA
2	O	201	SER
2	O	226	ILE
2	O	230	ALA
2	O	236	LYS
2	O	283	PRO
3	P	58	ALA
3	P	111	LYS
3	P	224	TYR
4	Q	198	HIS
5	R	63	SER
5	R	95	PRO
5	R	141	HIS
6	S	69	SER
7	T	7	LEU
7	T	33	ALA
10	W	56	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	W	60	GLU
1	A	288	LYS
1	A	404	ALA
1	A	433	ASP
2	B	20	GLY
2	B	26	ILE
2	B	64	GLY
2	B	110	GLU
2	B	190	GLN
2	B	231	GLY
2	B	249	GLY
2	B	290	SER
2	B	319	SER
2	B	366	ALA
2	B	386	ALA
2	B	420	GLY
3	C	6	ARG
3	C	17	ASN
3	C	202	HIS
4	D	133	GLY
4	D	168	ILE
4	D	177	ALA
4	D	183	ALA
5	E	92	ARG
5	E	137	GLY
5	E	154	GLY
5	E	180	LEU
5	E	188	VAL
6	F	77	LYS
9	I	60	ALA
9	I	73	PRO
9	I	76	VAL
10	J	57	HIS
1	N	20	ASP
1	N	94	GLN
1	N	207	GLU
1	N	288	LYS
1	N	290	LEU
1	N	404	ALA
2	O	19	PRO
2	O	26	ILE
2	O	64	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	222	GLN
2	O	231	GLY
2	O	290	SER
2	O	351	GLY
2	O	420	GLY
3	P	6	ARG
3	P	17	ASN
3	P	31	TRP
3	P	108	TYR
3	P	158	GLY
3	P	202	HIS
3	P	217	ASP
3	P	348	PHE
4	Q	44	ASP
4	Q	48	PHE
4	Q	133	GLY
4	Q	168	ILE
4	Q	177	ALA
4	Q	183	ALA
5	R	8	PRO
5	R	92	ARG
5	R	109	GLU
5	R	113	ASP
5	R	137	GLY
5	R	180	LEU
6	S	77	LYS
7	T	42	SER
8	U	46	SER
10	W	57	HIS
1	A	4	TYR
1	A	5	ALA
1	A	164	ALA
1	A	222	THR
1	A	274	ASN
2	B	114	ASP
2	B	180	ASP
2	B	265	GLY
2	B	334	GLY
2	B	409	ASP
3	C	3	PRO
3	C	158	GLY
3	C	207	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	217	ASP
3	C	359	TYR
4	D	48	PHE
4	D	166	ASN
4	D	190	LEU
5	E	69	LEU
5	E	70	ALA
5	E	72	SER
5	E	123	ASP
5	E	150	SER
7	G	42	SER
8	H	28	GLU
1	N	222	THR
1	N	262	TRP
1	N	274	ASN
1	N	405	ARG
2	O	110	GLU
2	O	249	GLY
2	O	319	SER
2	O	334	GLY
2	O	346	ALA
2	O	366	ALA
2	O	386	ALA
2	O	409	ASP
3	P	207	ASN
4	Q	162	PRO
4	Q	190	LEU
5	R	21	ALA
5	R	70	ALA
5	R	72	SER
8	U	28	GLU
9	V	48	PRO
1	A	23	LEU
1	A	56	GLY
1	A	71	PRO
1	A	262	TRP
1	A	332	ASP
1	A	405	ARG
2	B	82	SER
2	B	227	ARG
2	B	346	ALA
2	B	351	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	60	THR
3	C	108	TYR
3	C	156	TYR
3	C	379	ASN
4	D	23	HIS
5	E	186	GLN
8	H	72	LYS
1	N	56	GLY
1	N	164	ALA
1	N	332	ASP
2	O	76	THR
2	O	82	SER
2	O	180	ASP
2	O	296	TYR
3	P	3	PRO
3	P	60	THR
3	P	288	LYS
3	P	359	TYR
3	P	379	ASN
4	Q	144	ARG
4	Q	166	ASN
5	R	114	VAL
5	R	121	GLN
8	U	61	PHE
8	U	72	LYS
9	V	72	ALA
9	V	76	VAL
1	A	141	MET
2	B	63	LEU
2	B	235	ALA
2	B	296	TYR
2	B	375	ALA
2	B	401	LYS
3	C	208	ASN
3	C	209	PRO
3	C	237	LEU
4	D	162	PRO
4	D	176	PRO
5	E	21	ALA
7	G	50	PRO
7	G	61	TRP
8	H	46	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	61	PHE
1	N	71	PRO
1	N	170	THR
2	O	114	ASP
3	P	157	ILE
3	P	209	PRO
5	R	30	GLU
5	R	46	ALA
5	R	57	GLN
5	R	69	LEU
5	R	130	PRO
5	R	154	GLY
5	R	188	VAL
6	S	68	LEU
7	T	43	SER
9	V	60	ALA
1	A	106	MET
1	A	263	ALA
1	A	268	VAL
2	B	181	TYR
2	B	207	VAL
2	B	229	GLY
2	B	266	SER
3	C	76	TYR
4	D	110	PRO
1	N	5	ALA
2	O	63	LEU
2	O	178	CYS
3	P	208	ASN
4	Q	176	PRO
5	R	149	ASN
7	T	50	PRO
2	O	134	PRO
2	O	207	VAL
4	Q	110	PRO
3	C	259	PRO
7	G	74	PRO
1	N	268	VAL
1	N	331	ILE
10	W	25	VAL
2	O	85	ILE
2	B	85	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	178	CYS
2	B	282	GLY
2	O	282	GLY
4	D	122	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	344 (94%)	21 (6%)	18	45
1	N	365/368 (99%)	343 (94%)	22 (6%)	17	44
2	B	332/347 (96%)	316 (95%)	16 (5%)	23	49
2	O	333/347 (96%)	315 (95%)	18 (5%)	20	47
3	C	329/329 (100%)	307 (93%)	22 (7%)	15	41
3	P	328/329 (100%)	305 (93%)	23 (7%)	14	40
4	D	200/200 (100%)	191 (96%)	9 (4%)	24	51
4	Q	200/200 (100%)	191 (96%)	9 (4%)	24	51
5	E	166/166 (100%)	156 (94%)	10 (6%)	17	44
5	R	166/166 (100%)	156 (94%)	10 (6%)	17	44
6	F	93/96 (97%)	83 (89%)	10 (11%)	6	28
6	S	93/96 (97%)	83 (89%)	10 (11%)	6	28
7	G	71/71 (100%)	65 (92%)	6 (8%)	10	34
7	T	69/71 (97%)	64 (93%)	5 (7%)	13	39
8	H	65/71 (92%)	62 (95%)	3 (5%)	24	50
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	49
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	34
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	45 (92%)	4 (8%)	10	35
10	W	47/49 (96%)	43 (92%)	4 (8%)	10	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3380/3446 (98%)	3173 (94%)	207 (6%)	17	44

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	49	ASN
1	A	87	ASN
1	A	102	LEU
1	A	106	MET
1	A	146	THR
1	A	171	THR
1	A	182	LEU
1	A	223	TYR
1	A	228	VAL
1	A	264	ASP
1	A	274	ASN
1	A	281	ASP
1	A	302	LYS
1	A	363	SER
1	A	388	ARG
1	A	395	TRP
1	A	420	PRO
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	38	LEU
2	B	73	SER
2	B	101	THR
2	B	102	ARG
2	B	106	THR
2	B	124	LEU
2	B	138	THR
2	B	146	VAL
2	B	181	TYR
2	B	189	GLU
2	B	192	HIS
2	B	248	ASN
2	B	258	VAL
2	B	325	TYR
2	B	403	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	23	PRO
3	C	47	LEU
3	C	118	VAL
3	C	149	ASN
3	C	161	LEU
3	C	182	LEU
3	C	199	THR
3	C	208	ASN
3	C	214	SER
3	C	216	SER
3	C	223	PRO
3	C	231	LEU
3	C	236	MET
3	C	258	THR
3	C	259	PRO
3	C	266	PRO
3	C	283	ARG
3	C	299	VAL
3	C	324	THR
3	C	336	LEU
3	C	337	THR
3	C	367	PHE
4	D	10	PHE
4	D	13	SER
4	D	37	CYS
4	D	42	SER
4	D	43	MET
4	D	44	ASP
4	D	179	MET
4	D	215	LEU
4	D	241	LYS
5	E	6	THR
5	E	23	THR
5	E	59	ILE
5	E	61	SER
5	E	65	SER
5	E	123	ASP
5	E	125	ASP
5	E	131	GLU
5	E	135	LEU
5	E	190	ASP
6	F	36	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	59	MET
6	F	70	LEU
6	F	74	ILE
6	F	77	LYS
6	F	78	GLU
6	F	84	GLU
6	F	89	TYR
6	F	91	GLU
6	F	99	ARG
7	G	16	TYR
7	G	26	ILE
7	G	29	ILE
7	G	41	PHE
7	G	63	THR
7	G	81	GLN
8	H	10	GLU
8	H	19	THR
8	H	26	GLN
9	I	63	ASP
9	I	71	ASN
10	J	16	ARG
10	J	22	LEU
10	J	26	LEU
10	J	59	TYR
1	N	40	TRP
1	N	49	ASN
1	N	87	ASN
1	N	102	LEU
1	N	106	MET
1	N	154	HIS
1	N	166	THR
1	N	171	THR
1	N	182	LEU
1	N	223	TYR
1	N	228	VAL
1	N	264	ASP
1	N	274	ASN
1	N	281	ASP
1	N	297	LEU
1	N	363	SER
1	N	388	ARG
1	N	395	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	420	PRO
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	38	LEU
2	O	73	SER
2	O	101	THR
2	O	102	ARG
2	O	106	THR
2	O	124	LEU
2	O	146	VAL
2	O	181	TYR
2	O	192	HIS
2	O	212	LYS
2	O	228	SER
2	O	239	TYR
2	O	248	ASN
2	O	258	VAL
2	O	325	TYR
2	O	403	ASP
3	P	23	PRO
3	P	32	TRP
3	P	47	LEU
3	P	74	VAL
3	P	118	VAL
3	P	138	GLN
3	P	145	THR
3	P	149	ASN
3	P	161	LEU
3	P	199	THR
3	P	208	ASN
3	P	214	SER
3	P	216	SER
3	P	223	PRO
3	P	236	MET
3	P	258	THR
3	P	259	PRO
3	P	266	PRO
3	P	317	THR
3	P	324	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	336	LEU
3	P	337	THR
3	P	367	PHE
4	Q	3	LEU
4	Q	10	PHE
4	Q	13	SER
4	Q	37	CYS
4	Q	42	SER
4	Q	43	MET
4	Q	44	ASP
4	Q	215	LEU
4	Q	241	LYS
5	R	6	THR
5	R	23	THR
5	R	59	ILE
5	R	61	SER
5	R	65	SER
5	R	69	LEU
5	R	131	GLU
5	R	135	LEU
5	R	147	ILE
5	R	190	ASP
6	S	13	MET
6	S	16	ILE
6	S	36	THR
6	S	59	MET
6	S	70	LEU
6	S	77	LYS
6	S	78	GLU
6	S	84	GLU
6	S	89	TYR
6	S	91	GLU
7	T	16	TYR
7	T	26	ILE
7	T	29	ILE
7	T	41	PHE
7	T	63	THR
8	U	13	LEU
8	U	26	GLN
8	U	71	HIS
10	W	14	PHE
10	W	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	W	26	LEU
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	87	ASN
1	A	118	GLN
1	A	136	GLN
1	A	159	GLN
1	A	205	HIS
1	A	271	HIS
1	A	274	ASN
1	A	301	HIS
1	A	308	GLN
1	A	339	GLN
1	A	385	ASN
2	B	31	ASN
2	B	153	GLN
2	B	196	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	297	GLN
2	B	329	GLN
2	B	332	HIS
2	B	362	ASN
2	B	363	GLN
2	B	376	GLN
2	B	380	ASN
2	B	400	GLN
3	C	69	HIS
3	C	73	ASN
3	C	75	GLN
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	35	GLN
4	D	50	ASN
4	D	121	HIS
4	D	200	GLN
4	D	225	HIS
5	E	86	ASN
5	E	107	ASN
5	E	122	HIS
5	E	164	HIS
5	E	186	GLN
6	F	56	ASN
7	G	23	GLN
7	G	28	ASN
7	G	73	ASN
7	G	79	ASN
7	G	81	GLN
8	H	26	GLN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	87	ASN
1	N	118	GLN
1	N	136	GLN
1	N	159	GLN
1	N	274	ASN
1	N	305	HIS
1	N	308	GLN
1	N	339	GLN
1	N	435	ASN
2	O	31	ASN
2	O	143	GLN
2	O	153	GLN
2	O	156	GLN
2	O	193	HIS
2	O	196	GLN
2	O	222	GLN
2	O	225	ASN
2	O	247	GLN
2	O	248	ASN
2	O	315	ASN
2	O	329	GLN
2	O	332	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	362	ASN
2	O	363	GLN
2	O	376	GLN
2	O	400	GLN
3	P	69	HIS
3	P	82	ASN
3	P	149	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
3	P	379	ASN
4	Q	35	GLN
4	Q	50	ASN
4	Q	200	GLN
4	Q	225	HIS
5	R	122	HIS
5	R	164	HIS
5	R	186	GLN
6	S	56	ASN
6	S	79	GLN
7	T	12	HIS
7	T	23	GLN
7	T	28	ASN
7	T	44	GLN
7	T	73	ASN

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, 10 are unknown - leaving 26 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
13	HEM	C	501	3	50,50,50	1.73	9 (18%)	67,82,82	1.87	17 (25%)
16	CDL	Q	3003	-	49,49,99	1.16	3 (6%)	55,61,111	0.96	2 (3%)
20	PLC	E	2009	-	31,31,41	1.74	6 (19%)	37,39,49	0.73	1 (2%)
15	ANY	C	2002	-	38,38,41	1.58	5 (13%)	32,52,55	2.27	8 (25%)
18	HEC	D	501	4	50,50,50	1.25	6 (12%)	68,82,82	1.68	11 (16%)
16	CDL	D	2003	-	49,49,99	1.20	4 (8%)	55,61,111	0.94	1 (1%)
11	PEE	A	2008	-	20,20,50	1.82	6 (30%)	23,25,55	0.73	1 (4%)
11	PEE	P	3007	-	48,48,50	1.46	7 (14%)	51,53,55	0.83	3 (5%)
13	HEM	C	502	3	50,50,50	1.83	13 (26%)	67,82,82	1.87	13 (19%)
15	ANY	P	3002	-	38,38,41	1.87	8 (21%)	32,52,55	2.29	7 (21%)
14	SMA	P	3001	-	38,38,38	1.57	8 (21%)	47,52,52	0.80	1 (2%)
16	CDL	C	2004	-	39,39,99	1.27	5 (12%)	45,51,111	1.16	3 (6%)
11	PEE	N	3008	-	4,4,50	3.72	4 (100%)	6,6,55	0.70	0
13	HEM	P	502	3	50,50,50	1.61	8 (16%)	67,82,82	1.53	11 (16%)
17	GOL	C	2011	-	5,5,5	1.29	0	5,5,5	0.62	0
11	PEE	E	2005	-	49,49,50	1.46	8 (16%)	52,54,55	0.87	3 (5%)
17	GOL	P	3011	-	5,5,5	1.25	0	5,5,5	0.60	0
13	HEM	P	501	3	50,50,50	1.73	9 (18%)	67,82,82	1.74	17 (25%)
16	CDL	P	3004	-	39,39,99	1.26	5 (12%)	45,51,111	1.16	2 (4%)
14	SMA	C	2001	-	38,38,38	1.34	4 (10%)	47,52,52	0.82	3 (6%)
11	PEE	C	2007	-	48,48,50	1.48	9 (18%)	51,53,55	0.84	3 (5%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
11	PEE	P	3005	-	49,49,50	1.57	10 (20%)	52,54,55	0.87	3 (5%)
18	HEC	Q	501	4	50,50,50	1.31	6 (12%)	68,82,82	1.60	10 (14%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
20	PLC	R	3009	-	31,31,41	1.65	9 (29%)	37,39,49	0.61	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
13	HEM	C	501	3	-	8/14/54/54	-
16	CDL	Q	3003	-	-	28/59/59/110	-
20	PLC	E	2009	-	-	13/35/35/45	-
15	ANY	C	2002	-	1/1/10/13	1/37/52/56	0/1/2/2
18	HEC	D	501	4	1/1/3/7	7/14/54/54	-
16	CDL	D	2003	-	-	29/59/59/110	-
11	PEE	A	2008	-	-	14/24/24/54	-
11	PEE	P	3007	-	-	28/52/52/54	-
13	HEM	C	502	3	-	7/14/54/54	-
15	ANY	P	3002	-	1/1/10/13	1/37/52/56	0/1/2/2
14	SMA	P	3001	-	-	15/34/34/34	0/2/2/2
16	CDL	C	2004	-	-	23/49/49/110	-
13	HEM	P	502	3	-	6/14/54/54	-
17	GOL	C	2011	-	-	1/4/4/4	-
11	PEE	E	2005	-	-	28/53/53/54	-
17	GOL	P	3011	-	-	2/4/4/4	-
13	HEM	P	501	3	-	8/14/54/54	-
16	CDL	P	3004	-	-	22/49/49/110	-
14	SMA	C	2001	-	-	15/34/34/34	0/2/2/2
11	PEE	C	2007	-	-	29/52/52/54	-
19	FES	E	501	5	-	-	0/1/1/1
18	HEC	Q	501	4	1/1/3/7	10/14/54/54	-
11	PEE	P	3005	-	-	27/53/53/54	-
19	FES	R	501	5	-	-	0/1/1/1
20	PLC	R	3009	-	-	12/35/35/45	-

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	3002	ANY	C8-N1	5.85	1.42	1.34
15	C	2002	ANY	C8-N1	5.60	1.41	1.34
13	C	501	HEM	CBC-CAC	5.29	1.55	1.30
13	C	502	HEM	CBB-CAB	5.18	1.55	1.30
14	C	2001	SMA	C7-C8	4.83	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	501	HEM	CBC-CAC	4.80	1.53	1.30
13	P	501	HEM	CBB-CAB	4.79	1.53	1.30
11	N	3008	PEE	P-O1P	4.66	1.61	1.50
13	P	502	HEM	CBC-CAC	4.43	1.51	1.30
20	E	2009	PLC	O2-C'	4.42	1.46	1.34
13	C	502	HEM	CAC-C3C	-4.37	1.35	1.47
11	E	2005	PEE	C39-C38	4.27	1.55	1.31
11	P	3005	PEE	C39-C38	4.24	1.55	1.31
11	C	2007	PEE	C39-C38	4.22	1.55	1.31
13	C	502	HEM	C4A-NA	-4.19	1.31	1.39
11	P	3007	PEE	C39-C38	4.17	1.55	1.31
14	P	3001	SMA	C20-C19	4.14	1.36	1.33
14	P	3001	SMA	O1-C2	4.08	1.41	1.36
15	P	3002	ANY	C2-C1	4.01	1.46	1.40
13	P	502	HEM	CBB-CAB	3.99	1.49	1.30
13	C	501	HEM	CAB-C3B	-3.97	1.36	1.47
20	R	3009	PLC	O2-C'	3.81	1.45	1.34
11	N	3008	PEE	P-O3P	3.78	1.65	1.54
13	P	502	HEM	CAB-C3B	-3.76	1.37	1.47
13	C	502	HEM	CBC-CAC	3.72	1.48	1.30
13	C	501	HEM	CBB-CAB	3.67	1.48	1.30
11	N	3008	PEE	P-O4P	3.66	1.65	1.54
11	C	2007	PEE	O2-C10	3.63	1.44	1.34
11	P	3007	PEE	O2-C10	3.53	1.44	1.34
11	P	3005	PEE	P-O1P	3.51	1.63	1.50
20	E	2009	PLC	O2-C2	3.45	1.54	1.46
13	P	502	HEM	CAC-C3C	-3.42	1.38	1.47
20	E	2009	PLC	P-O1P	3.41	1.62	1.50
11	P	3007	PEE	C21-C22	-3.41	1.34	1.51
18	D	501	HEC	CHC-C4B	-3.38	1.31	1.38
11	P	3005	PEE	O2-C10	3.35	1.43	1.34
11	C	2007	PEE	C21-C22	-3.34	1.35	1.51
11	E	2005	PEE	C21-C22	-3.33	1.35	1.51
13	P	501	HEM	CAC-C3C	-3.30	1.38	1.47
11	A	2008	PEE	O2-C10	3.30	1.43	1.34
18	D	501	HEC	C1D-ND	-3.30	1.34	1.40
11	P	3005	PEE	O3-C30	3.26	1.42	1.33
13	P	501	HEM	CAB-C3B	-3.23	1.38	1.47
15	P	3002	ANY	O8-C21	3.21	1.41	1.34
11	C	2007	PEE	P-O1P	3.21	1.61	1.50
11	P	3005	PEE	C21-C22	-3.17	1.36	1.51
20	R	3009	PLC	P-O1P	3.17	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2008	PEE	P-O1P	3.16	1.61	1.50
11	E	2005	PEE	P-O1P	3.13	1.61	1.50
15	C	2002	ANY	C2-C1	3.11	1.44	1.40
15	P	3002	ANY	C12-C11	3.10	1.59	1.52
13	C	501	HEM	CAC-C3C	-3.10	1.39	1.47
11	E	2005	PEE	O3-C30	3.08	1.42	1.33
15	C	2002	ANY	C12-C11	3.06	1.59	1.52
13	C	501	HEM	C4A-NA	-3.06	1.33	1.39
14	P	3001	SMA	C7-C8	3.04	1.44	1.40
20	E	2009	PLC	O3-CB	3.03	1.42	1.33
14	P	3001	SMA	C6-C5	3.02	1.44	1.38
11	E	2005	PEE	O2-C10	3.01	1.42	1.34
11	A	2008	PEE	O3-C30	3.00	1.42	1.33
11	P	3005	PEE	C31-C30	2.95	1.59	1.50
20	R	3009	PLC	O3-CB	2.95	1.41	1.33
11	P	3007	PEE	P-O1P	2.93	1.61	1.50
20	E	2009	PLC	C1-C2	2.84	1.59	1.50
11	P	3007	PEE	O3-C30	2.84	1.41	1.33
13	C	502	HEM	C1B-C2B	2.81	1.50	1.44
13	P	501	HEM	FE-NC	-2.80	1.85	1.95
13	P	501	HEM	C3D-C2D	-2.78	1.30	1.36
13	P	502	HEM	C4C-NC	-2.77	1.34	1.39
15	P	3002	ANY	C13-C12	2.76	1.58	1.53
14	C	2001	SMA	C6-C5	2.68	1.43	1.38
16	D	2003	CDL	O1-C1	2.66	1.51	1.43
18	Q	501	HEC	CHC-C1C	-2.63	1.33	1.39
14	P	3001	SMA	C3-C2	2.63	1.39	1.34
15	C	2002	ANY	O8-C21	2.62	1.40	1.34
13	C	501	HEM	C2A-C3A	-2.61	1.32	1.38
11	A	2008	PEE	C1-C2	2.61	1.59	1.50
11	P	3005	PEE	C11-C10	2.60	1.58	1.50
16	D	2003	CDL	CA6-CA4	2.60	1.58	1.50
11	C	2007	PEE	O3-C30	2.59	1.40	1.33
13	C	502	HEM	C3D-C2D	-2.59	1.31	1.36
18	Q	501	HEC	CHC-C4B	-2.56	1.33	1.38
20	R	3009	PLC	C1-C2	2.53	1.58	1.50
13	C	502	HEM	C2A-C3A	-2.52	1.32	1.38
15	P	3002	ANY	C6-C1	2.52	1.45	1.41
13	C	502	HEM	CAB-C3B	-2.50	1.40	1.47
14	P	3001	SMA	C8-C8A	2.50	1.43	1.39
20	R	3009	PLC	O2-C2	2.46	1.52	1.46
13	C	501	HEM	CHA-C4D	-2.45	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	3002	ANY	C3-C2	2.43	1.43	1.39
11	N	3008	PEE	P-O2P	2.43	1.61	1.54
13	P	502	HEM	C4D-C3D	2.42	1.49	1.45
11	E	2005	PEE	C31-C30	2.42	1.57	1.50
13	C	501	HEM	C3B-C2B	-2.41	1.32	1.37
16	P	3004	CDL	CA3-CA4	2.41	1.58	1.50
18	Q	501	HEC	C1D-ND	-2.39	1.36	1.40
16	C	2004	CDL	OA6-CA5	2.38	1.41	1.34
13	C	502	HEM	CHC-C1C	-2.36	1.33	1.38
16	P	3004	CDL	O1-C1	2.35	1.50	1.43
18	Q	501	HEC	C3B-C2B	-2.34	1.31	1.36
13	C	502	HEM	C1C-C2C	-2.32	1.40	1.45
16	Q	3003	CDL	O1-C1	2.31	1.50	1.43
13	C	502	HEM	C3C-C4C	-2.31	1.42	1.46
13	C	502	HEM	C4D-ND	-2.30	1.36	1.40
13	P	501	HEM	CHA-C1A	-2.30	1.34	1.39
16	C	2004	CDL	CA3-CA4	2.30	1.58	1.50
16	D	2003	CDL	CA3-CA4	2.30	1.58	1.50
13	C	501	HEM	CMD-C2D	2.28	1.55	1.50
16	C	2004	CDL	CB3-CB4	2.28	1.57	1.50
14	C	2001	SMA	C4A-C5	2.27	1.44	1.40
14	P	3001	SMA	C4A-C5	2.26	1.44	1.40
11	E	2005	PEE	C11-C10	2.26	1.57	1.50
18	Q	501	HEC	C3C-C2C	-2.25	1.33	1.38
20	R	3009	PLC	C5-C4	2.24	1.58	1.51
20	R	3009	PLC	C1B-CB	2.24	1.57	1.50
20	E	2009	PLC	C3-C2	2.24	1.57	1.50
16	Q	3003	CDL	CA3-CA4	2.23	1.57	1.50
18	D	501	HEC	C3C-C2C	-2.22	1.33	1.38
18	D	501	HEC	C2A-C3A	-2.22	1.32	1.36
15	P	3002	ANY	O5-C14	2.21	1.39	1.34
16	C	2004	CDL	OB8-CB7	2.21	1.39	1.33
11	P	3007	PEE	C3-C2	2.19	1.57	1.50
14	C	2001	SMA	O1-C2	2.19	1.39	1.36
13	C	502	HEM	C3B-C4B	2.19	1.49	1.44
13	P	501	HEM	C2A-C3A	-2.19	1.33	1.38
16	D	2003	CDL	OB8-CB7	2.18	1.39	1.33
11	P	3005	PEE	P-O4P	2.17	1.67	1.59
16	C	2004	CDL	O1-C1	2.15	1.49	1.43
18	Q	501	HEC	C1B-NB	-2.14	1.34	1.38
11	E	2005	PEE	P-O4P	2.14	1.67	1.59
20	R	3009	PLC	C1'-C'	2.12	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3005	PEE	C3-C2	2.12	1.57	1.50
15	C	2002	ANY	C10-C9	2.11	1.58	1.53
13	P	502	HEM	C1C-NC	-2.11	1.35	1.39
11	C	2007	PEE	O2-C2	2.10	1.51	1.46
14	P	3001	SMA	C6-C7	2.10	1.42	1.38
11	C	2007	PEE	C3-C2	2.09	1.57	1.50
16	Q	3003	CDL	CA6-CA4	2.09	1.57	1.50
13	P	501	HEM	C3B-C2B	-2.07	1.33	1.37
11	A	2008	PEE	C3-C2	2.06	1.57	1.50
11	C	2007	PEE	P-O4P	2.06	1.67	1.59
16	P	3004	CDL	OB8-CB7	2.05	1.39	1.33
11	C	2007	PEE	C1-C2	2.04	1.57	1.50
18	D	501	HEC	C3B-C2B	-2.04	1.32	1.36
16	P	3004	CDL	OA8-CA6	-2.03	1.40	1.45
16	P	3004	CDL	OA6-CA5	2.03	1.40	1.34
11	P	3005	PEE	C1-C2	2.02	1.57	1.50
13	P	502	HEM	C1C-C2C	-2.02	1.41	1.45
11	P	3007	PEE	O2-C2	2.01	1.51	1.46
11	A	2008	PEE	C11-C10	2.01	1.56	1.50
20	R	3009	PLC	C3-C2	2.01	1.57	1.50
18	D	501	HEC	FE-NB	2.00	2.01	1.94

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	3002	ANY	C25-C22-C21	8.07	135.38	110.94
15	C	2002	ANY	C25-C22-C21	7.87	134.77	110.94
13	C	502	HEM	C3B-C2B-C1B	-6.91	101.22	106.41
13	C	502	HEM	CMB-C2B-C1B	5.90	134.25	125.03
15	P	3002	ANY	C25-C22-C23	-5.61	89.40	111.60
15	C	2002	ANY	O5-C14-O6	-5.55	117.22	124.10
13	C	501	HEM	CAD-C3D-C4D	5.47	134.24	124.70
15	C	2002	ANY	C25-C22-C23	-4.82	92.54	111.60
13	P	501	HEM	C3B-C4B-NB	4.55	112.73	109.47
15	P	3002	ANY	O5-C14-O6	-4.52	118.50	124.10
18	D	501	HEC	CBC-CAC-C3C	-4.47	100.31	112.42
18	D	501	HEC	CAA-C2A-C1A	4.32	133.64	124.85
18	Q	501	HEC	CAA-C2A-C1A	4.29	133.58	124.85
13	C	501	HEM	C4C-C3C-C2C	-4.27	103.11	106.81
18	D	501	HEC	CAA-C2A-C3A	-4.14	120.12	127.87
13	C	502	HEM	C4A-C3A-C2A	4.11	111.52	106.82
13	C	501	HEM	CMB-C2B-C1B	4.06	131.38	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	501	HEC	CAA-C2A-C3A	-4.06	120.27	127.87
13	P	501	HEM	CAD-C3D-C4D	4.04	131.73	124.70
13	C	501	HEM	C3D-C4D-ND	3.94	114.50	110.17
13	C	502	HEM	CAD-C3D-C4D	3.92	131.53	124.70
18	Q	501	HEC	CBC-CAC-C3C	-3.88	101.91	112.42
16	P	3004	CDL	CB4-OB6-CB5	-3.86	108.55	117.80
18	D	501	HEC	CAD-C3D-C4D	3.83	131.38	124.70
13	P	502	HEM	C3B-C2B-C1B	-3.83	103.53	106.41
13	C	502	HEM	C1A-C2A-C3A	-3.78	101.01	106.87
13	P	502	HEM	CBD-CAD-C3D	-3.68	102.36	112.53
18	Q	501	HEC	CMC-C2C-C1C	3.68	131.02	125.42
16	C	2004	CDL	CB4-OB6-CB5	-3.67	109.00	117.80
13	P	502	HEM	CAD-C3D-C4D	3.65	131.05	124.70
13	C	502	HEM	CAA-C2A-C1A	3.63	132.04	124.94
13	C	502	HEM	CHB-C1B-NB	-3.51	120.03	124.37
13	C	501	HEM	C3B-C4B-NB	3.40	111.91	109.47
15	P	3002	ANY	O4-C20-O7	-3.35	119.95	124.10
13	C	501	HEM	C2A-C1A-NA	3.34	113.86	110.15
13	P	501	HEM	C4C-C3C-C2C	-3.32	103.93	106.81
18	Q	501	HEC	CBA-CAA-C2A	3.31	121.67	112.53
13	P	501	HEM	CAC-C3C-C4C	3.28	132.65	124.82
15	C	2002	ANY	O4-C20-O7	-3.24	120.08	124.10
13	C	501	HEM	CBA-CAA-C2A	-3.22	103.62	112.53
18	D	501	HEC	CBA-CAA-C2A	3.20	121.37	112.53
13	P	501	HEM	C2A-C1A-NA	3.12	113.61	110.15
13	C	501	HEM	CAC-C3C-C4C	3.10	132.22	124.82
18	D	501	HEC	CHA-C1A-NA	-3.08	121.10	124.45
13	P	501	HEM	C4D-ND-C1D	-3.07	101.57	105.21
18	Q	501	HEC	CAD-C3D-C4D	3.07	130.04	124.70
18	D	501	HEC	CMC-C2C-C1C	3.05	130.07	125.42
18	D	501	HEC	C3B-C4B-NB	3.04	113.51	110.17
18	D	501	HEC	CMB-C2B-C1B	3.02	129.75	125.03
13	P	501	HEM	CMB-C2B-C1B	3.00	129.72	125.03
18	Q	501	HEC	CAC-C3C-C4C	-3.00	120.79	124.91
13	C	501	HEM	CAD-C3D-C2D	-2.94	122.37	127.87
13	P	502	HEM	C3B-C4B-NB	2.94	111.58	109.47
13	P	501	HEM	CMD-C2D-C1D	2.91	129.58	125.03
13	C	502	HEM	CAD-C3D-C2D	-2.90	122.44	127.87
11	P	3005	PEE	C22-C21-C20	2.87	127.64	113.86
11	E	2005	PEE	C22-C21-C20	2.83	127.45	113.86
15	P	3002	ANY	C12-O8-C21	2.82	122.45	117.76
18	Q	501	HEC	CAC-C3C-C2C	2.81	131.33	126.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	3007	PEE	C22-C21-C20	2.73	126.98	113.86
13	C	502	HEM	C2B-C1B-NB	2.69	112.94	109.84
13	P	501	HEM	CAD-C3D-C2D	-2.69	122.83	127.87
13	P	502	HEM	C1A-C2A-C3A	-2.69	102.71	106.87
13	P	502	HEM	C4A-C3A-C2A	2.68	109.89	106.82
11	C	2007	PEE	C22-C21-C20	2.67	126.69	113.86
14	C	2001	SMA	O7-C7-C8	2.66	117.31	114.53
16	D	2003	CDL	CB4-OB6-CB5	-2.64	111.47	117.80
13	P	501	HEM	C2D-C1D-ND	2.62	112.93	109.90
15	C	2002	ANY	C23-C22-C21	2.61	118.85	110.94
13	P	501	HEM	C1B-NB-C4B	-2.59	102.14	105.21
11	P	3005	PEE	C21-C22-C23	2.58	127.43	114.37
13	P	502	HEM	CAD-C3D-C2D	-2.58	123.04	127.87
11	C	2007	PEE	C21-C22-C23	2.56	127.33	114.37
13	C	502	HEM	C2A-C1A-NA	2.56	112.99	110.15
13	P	501	HEM	C3D-C4D-ND	2.54	112.95	110.17
13	C	501	HEM	C1A-C2A-C3A	-2.53	102.94	106.87
13	P	502	HEM	C1B-NB-C4B	-2.53	102.21	105.21
18	Q	501	HEC	CAB-C3B-C2B	2.53	132.21	127.56
11	E	2005	PEE	C21-C22-C23	2.53	127.15	114.37
13	C	501	HEM	C4C-NC-C1C	-2.52	101.71	105.82
13	P	502	HEM	CAA-C2A-C1A	2.51	129.85	124.94
13	P	501	HEM	C4A-NA-C1A	-2.49	101.77	105.82
11	P	3007	PEE	C21-C22-C23	2.45	126.74	114.37
15	C	2002	ANY	C12-O8-C21	2.45	121.83	117.76
14	P	3001	SMA	C4A-C4-C3	-2.44	115.18	118.78
13	P	502	HEM	CMB-C2B-C1B	2.42	128.82	125.03
13	C	502	HEM	CBD-CAD-C3D	-2.42	105.85	112.53
18	D	501	HEC	C4B-NB-C1B	-2.42	102.35	105.21
13	C	501	HEM	C4D-C3D-C2D	-2.41	103.38	106.89
16	Q	3003	CDL	CB4-OB6-CB5	-2.41	112.03	117.80
13	C	501	HEM	CAA-C2A-C1A	2.39	129.60	124.94
15	C	2002	ANY	O8-C21-O9	-2.38	119.65	123.95
13	P	501	HEM	C3B-C2B-C1B	-2.37	104.63	106.41
13	P	501	HEM	CBA-CAA-C2A	-2.37	105.98	112.53
11	E	2005	PEE	O3-C3-C2	2.32	115.08	108.40
13	C	501	HEM	C4A-C3A-C2A	2.31	109.46	106.82
13	C	501	HEM	C4D-ND-C1D	-2.30	102.49	105.21
14	C	2001	SMA	C4A-C4-C3	-2.29	115.41	118.78
18	D	501	HEC	CHC-C4B-NB	-2.25	121.59	124.37
15	C	2002	ANY	O1-C1-C6	2.24	125.11	121.11
14	C	2001	SMA	C9-C10-C11	-2.21	110.33	114.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	3002	ANY	C23-C22-C21	2.21	117.62	110.94
11	C	2007	PEE	O3-C3-C2	2.19	114.72	108.40
13	C	501	HEM	CMB-C2B-C3B	-2.17	123.17	128.43
11	A	2008	PEE	O3-C3-C2	2.17	114.65	108.40
11	P	3007	PEE	O3-C3-C2	2.17	114.65	108.40
16	C	2004	CDL	OB6-CB4-CB3	2.17	116.12	108.34
13	C	501	HEM	C1B-NB-C4B	-2.16	102.65	105.21
11	P	3005	PEE	O3-C3-C2	2.16	114.62	108.40
13	P	501	HEM	C2B-C1B-NB	2.14	112.30	109.84
13	C	502	HEM	C1B-NB-C4B	-2.14	102.67	105.21
15	P	3002	ANY	O1-C1-C6	2.14	124.92	121.11
13	P	502	HEM	C2A-C1A-NA	2.10	112.49	110.15
16	P	3004	CDL	CA6-CA4-CA3	-2.10	106.89	111.78
13	C	502	HEM	CBC-CAC-C3C	-2.08	117.12	127.53
18	Q	501	HEC	CMB-C2B-C1B	2.05	128.23	125.03
16	C	2004	CDL	CA4-OA6-CA5	-2.02	112.95	117.80
13	P	501	HEM	CBC-CAC-C3C	-2.01	117.47	127.53
20	E	2009	PLC	O3-C3-C2	2.01	114.19	108.40
16	Q	3003	CDL	CA6-CA4-CA3	-2.01	107.10	111.78

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	2002	ANY	C22
15	P	3002	ANY	C22
18	D	501	HEC	NA
18	Q	501	HEC	NA

All (334) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	O3P-C1-C2-O2
11	C	2007	PEE	C1-O3P-P-O2P
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C1-O3P-P-O1P
11	E	2005	PEE	C1-O3P-P-O4P
11	E	2005	PEE	C4-O4P-P-O3P
11	E	2005	PEE	C4-O4P-P-O2P
11	E	2005	PEE	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	O4P-C4-C5-N
11	P	3005	PEE	C11-C10-O2-C2
11	P	3005	PEE	C1-O3P-P-O1P
11	P	3005	PEE	C1-O3P-P-O4P
11	P	3005	PEE	C4-O4P-P-O3P
11	P	3005	PEE	C4-O4P-P-O2P
11	P	3005	PEE	C4-O4P-P-O1P
11	P	3005	PEE	O4P-C4-C5-N
11	P	3007	PEE	O3P-C1-C2-O2
11	P	3007	PEE	C1-O3P-P-O2P
11	P	3007	PEE	C4-O4P-P-O3P
11	P	3007	PEE	C4-O4P-P-O2P
11	P	3007	PEE	C4-O4P-P-O1P
13	C	501	HEM	C2B-C3B-CAB-CBB
13	C	502	HEM	C2C-C3C-CAC-CBC
13	P	501	HEM	C2B-C3B-CAB-CBB
13	P	502	HEM	C2C-C3C-CAC-CBC
13	P	502	HEM	C4C-C3C-CAC-CBC
14	C	2001	SMA	C3-C2-C9-C10
14	C	2001	SMA	O1-C2-C9-C10
14	C	2001	SMA	C24-C13-C14-O14
14	C	2001	SMA	C13-C14-C15-C16
14	C	2001	SMA	C13-C14-O14-C25
14	C	2001	SMA	C15-C14-O14-C25
14	C	2001	SMA	C14-C15-C16-C17
14	P	3001	SMA	C3-C2-C9-C10
14	P	3001	SMA	O1-C2-C9-C10
14	P	3001	SMA	C13-C14-O14-C25
14	P	3001	SMA	C15-C14-O14-C25
14	P	3001	SMA	C14-C15-C16-C17
16	C	2004	CDL	O1-C1-CA2-OA2
16	C	2004	CDL	CA2-OA2-PA1-OA4
16	C	2004	CDL	CA2-OA2-PA1-OA5
16	C	2004	CDL	CA3-OA5-PA1-OA2
16	C	2004	CDL	CA3-OA5-PA1-OA3
16	C	2004	CDL	CA3-OA5-PA1-OA4
16	C	2004	CDL	OB5-CB3-CB4-OB6
16	D	2003	CDL	O1-C1-CB2-OB2
16	D	2003	CDL	CB2-OB2-PB2-OB3
16	D	2003	CDL	CB2-OB2-PB2-OB4
16	D	2003	CDL	CB2-OB2-PB2-OB5
16	P	3004	CDL	O1-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	P	3004	CDL	CA2-OA2-PA1-OA4
16	P	3004	CDL	CA2-OA2-PA1-OA5
16	P	3004	CDL	CA3-OA5-PA1-OA2
16	P	3004	CDL	CA3-OA5-PA1-OA3
16	P	3004	CDL	CA3-OA5-PA1-OA4
16	P	3004	CDL	OB5-CB3-CB4-OB6
16	Q	3003	CDL	CA2-OA2-PA1-OA5
16	Q	3003	CDL	CB2-OB2-PB2-OB3
16	Q	3003	CDL	CB2-OB2-PB2-OB4
16	Q	3003	CDL	CB2-OB2-PB2-OB5
18	D	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C4B-C3B-CAB-CBB
18	D	501	HEC	C4B-C3B-CAB-CBB
11	E	2005	PEE	O5-C30-O3-C3
11	P	3005	PEE	O5-C30-O3-C3
11	E	2005	PEE	O4-C10-O2-C2
11	P	3005	PEE	O4-C10-O2-C2
11	E	2005	PEE	C31-C30-O3-C3
18	D	501	HEC	C2B-C3B-CAB-CBB
18	Q	501	HEC	C2B-C3B-CAB-CBB
11	P	3005	PEE	C31-C30-O3-C3
18	D	501	HEC	C1A-C2A-CAA-CBA
14	C	2001	SMA	C8-C7-O7-C7M
14	P	3001	SMA	C8-C7-O7-C7M
16	Q	3003	CDL	O1-C1-CB2-OB2
11	A	2008	PEE	C31-C30-O3-C3
16	P	3004	CDL	C51-CB5-OB6-CB4
16	Q	3003	CDL	C31-CA7-OA8-CA6
11	A	2008	PEE	O5-C30-O3-C3
16	D	2003	CDL	C31-CA7-OA8-CA6
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
16	C	2004	CDL	C51-CB5-OB6-CB4
20	E	2009	PLC	C1'-C'-O2-C2
16	Q	3003	CDL	CA2-C1-CB2-OB2
16	D	2003	CDL	C71-CB7-OB8-CB6
16	Q	3003	CDL	C71-CB7-OB8-CB6
14	P	3001	SMA	C6-C7-O7-C7M
14	C	2001	SMA	C17-C18-C19-C26
14	P	3001	SMA	C17-C18-C19-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	C	2001	SMA	C17-C18-C19-C20
14	P	3001	SMA	C17-C18-C19-C20
18	D	501	HEC	C4C-C3C-CAC-CBC
14	C	2001	SMA	C6-C7-O7-C7M
20	E	2009	PLC	O'-C'-O2-C2
16	P	3004	CDL	C31-CA7-OA8-CA6
20	R	3009	PLC	C1'-C'-O2-C2
11	E	2005	PEE	C37-C38-C39-C40
11	P	3005	PEE	C37-C38-C39-C40
16	P	3004	CDL	OB7-CB5-OB6-CB4
16	D	2003	CDL	OA9-CA7-OA8-CA6
16	Q	3003	CDL	OA9-CA7-OA8-CA6
16	D	2003	CDL	CA5-C11-C12-C13
16	Q	3003	CDL	CA5-C11-C12-C13
16	Q	3003	CDL	OB9-CB7-OB8-CB6
11	E	2005	PEE	C10-C11-C12-C13
11	P	3005	PEE	C10-C11-C12-C13
16	P	3004	CDL	C71-CB7-OB8-CB6
16	D	2003	CDL	OB9-CB7-OB8-CB6
16	C	2004	CDL	OB7-CB5-OB6-CB4
20	R	3009	PLC	O'-C'-O2-C2
11	P	3007	PEE	C17-C18-C19-C20
16	C	2004	CDL	C71-CB7-OB8-CB6
16	C	2004	CDL	CB2-C1-CA2-OA2
16	D	2003	CDL	CA2-C1-CB2-OB2
16	P	3004	CDL	CB2-C1-CA2-OA2
18	Q	501	HEC	C4C-C3C-CAC-CBC
16	C	2004	CDL	C31-CA7-OA8-CA6
20	E	2009	PLC	C'-C1'-C2'-C3'
17	P	3011	GOL	C1-C2-C3-O3
16	C	2004	CDL	OB9-CB7-OB8-CB6
11	C	2007	PEE	C21-C22-C23-C24
11	E	2005	PEE	C40-C41-C42-C43
11	P	3005	PEE	C40-C41-C42-C43
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C21-C22-C23-C24
16	P	3004	CDL	OB9-CB7-OB8-CB6
11	C	2007	PEE	C32-C33-C34-C35
11	C	2007	PEE	C34-C35-C36-C37
11	P	3007	PEE	C34-C35-C36-C37
11	P	3007	PEE	C32-C33-C34-C35
16	Q	3003	CDL	CB7-C71-C72-C73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	R	3009	PLC	C'-C1'-C2'-C3'
16	C	2004	CDL	CB5-C51-C52-C53
16	P	3004	CDL	CB5-C51-C52-C53
11	P	3007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C41-C42-C43-C44
16	P	3004	CDL	OA9-CA7-OA8-CA6
11	P	3007	PEE	C41-C42-C43-C44
20	E	2009	PLC	C1B-CB-O3-C3
20	R	3009	PLC	C1B-CB-O3-C3
16	D	2003	CDL	C14-C15-C16-C17
16	C	2004	CDL	C11-CA5-OA6-CA4
16	P	3004	CDL	C11-CA5-OA6-CA4
16	C	2004	CDL	OA7-CA5-OA6-CA4
11	P	3005	PEE	C39-C40-C41-C42
11	P	3007	PEE	C15-C16-C17-C18
16	D	2003	CDL	C12-C13-C14-C15
16	D	2003	CDL	CB7-C71-C72-C73
13	C	501	HEM	C4B-C3B-CAB-CBB
13	C	502	HEM	C4C-C3C-CAC-CBC
13	P	501	HEM	C4B-C3B-CAB-CBB
16	Q	3003	CDL	C14-C15-C16-C17
11	E	2005	PEE	C39-C40-C41-C42
11	E	2005	PEE	C14-C15-C16-C17
16	Q	3003	CDL	C12-C13-C14-C15
14	P	3001	SMA	C24-C13-C14-C15
14	P	3001	SMA	C24-C13-C14-O14
16	C	2004	CDL	OA9-CA7-OA8-CA6
16	P	3004	CDL	OA7-CA5-OA6-CA4
14	C	2001	SMA	C12-C13-C14-C15
14	C	2001	SMA	C12-C13-C14-O14
14	P	3001	SMA	C12-C13-C14-C15
14	P	3001	SMA	C12-C13-C14-O14
11	P	3005	PEE	C14-C15-C16-C17
11	E	2005	PEE	C2-C3-O3-C30
11	P	3005	PEE	C13-C14-C15-C16
17	P	3011	GOL	O2-C2-C3-O3
11	E	2005	PEE	C13-C14-C15-C16
11	P	3005	PEE	C33-C34-C35-C36
11	C	2007	PEE	O3P-C1-C2-C3
11	P	3007	PEE	O3P-C1-C2-C3
16	C	2004	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	P	3004	CDL	OB5-CB3-CB4-CB6
20	E	2009	PLC	OB-CB-O3-C3
20	R	3009	PLC	OB-CB-O3-C3
11	A	2008	PEE	C10-C11-C12-C13
11	E	2005	PEE	C33-C34-C35-C36
11	E	2005	PEE	C30-C31-C32-C33
11	P	3005	PEE	C23-C24-C25-C26
11	P	3007	PEE	C12-C13-C14-C15
14	C	2001	SMA	C16-C17-C18-C19
14	P	3001	SMA	C16-C17-C18-C19
11	C	2007	PEE	C15-C16-C17-C18
16	Q	3003	CDL	C71-C72-C73-C74
16	D	2003	CDL	C71-C72-C73-C74
11	E	2005	PEE	C23-C24-C25-C26
15	P	3002	ANY	C16-C17-C18-C19
15	C	2002	ANY	C16-C17-C18-C19
11	C	2007	PEE	C12-C13-C14-C15
20	E	2009	PLC	C4'-C5'-C6'-C7'
20	R	3009	PLC	C4'-C5'-C6'-C7'
11	P	3005	PEE	C2-C3-O3-C30
11	C	2007	PEE	C40-C41-C42-C43
11	P	3007	PEE	C40-C41-C42-C43
11	P	3007	PEE	C43-C44-C45-C46
11	C	2007	PEE	C43-C44-C45-C46
16	C	2004	CDL	OA6-CA4-CA6-OA8
16	D	2003	CDL	OA6-CA4-CA6-OA8
16	Q	3003	CDL	OA6-CA4-CA6-OA8
20	E	2009	PLC	C2'-C3'-C4'-C5'
11	P	3005	PEE	C30-C31-C32-C33
11	C	2007	PEE	C10-C11-C12-C13
16	D	2003	CDL	C16-C17-C18-C19
20	R	3009	PLC	C2'-C3'-C4'-C5'
11	C	2007	PEE	C23-C24-C25-C26
13	P	501	HEM	C2C-C3C-CAC-CBC
11	P	3007	PEE	C23-C24-C25-C26
20	E	2009	PLC	O3P-C1-C2-O2
16	P	3004	CDL	CA3-CA4-CA6-OA8
16	P	3004	CDL	CB3-CB4-CB6-OB8
16	C	2004	CDL	OB6-CB4-CB6-OB8
16	P	3004	CDL	OB6-CB4-CB6-OB8
16	Q	3003	CDL	C16-C17-C18-C19
14	C	2001	SMA	C24-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	P	3001	SMA	C13-C14-C15-C16
20	E	2009	PLC	O4P-C4-C5-N
20	R	3009	PLC	O4P-C4-C5-N
13	C	502	HEM	C4D-C3D-CAD-CBD
20	E	2009	PLC	C1B-C2B-C3B-C4B
11	A	2008	PEE	C11-C10-O2-C2
11	A	2008	PEE	O4-C10-O2-C2
20	R	3009	PLC	O3P-C1-C2-O2
11	A	2008	PEE	O2-C2-C3-O3
16	P	3004	CDL	OA6-CA4-CA6-OA8
16	C	2004	CDL	CA3-CA4-CA6-OA8
16	C	2004	CDL	CB3-CB4-CB6-OB8
16	Q	3003	CDL	CA3-CA4-CA6-OA8
11	A	2008	PEE	C1-O3P-P-O1P
11	A	2008	PEE	C1-O3P-P-O4P
11	C	2007	PEE	C1-O3P-P-O1P
11	C	2007	PEE	C1-O3P-P-O4P
11	P	3007	PEE	C1-O3P-P-O1P
11	P	3007	PEE	C1-O3P-P-O4P
16	D	2003	CDL	CA2-OA2-PA1-OA5
16	D	2003	CDL	CA3-OA5-PA1-OA2
16	D	2003	CDL	CA3-OA5-PA1-OA3
16	Q	3003	CDL	CA3-OA5-PA1-OA3
20	E	2009	PLC	C1-O3P-P-O4P
16	D	2003	CDL	C1-CA2-OA2-PA1
16	Q	3003	CDL	C1-CA2-OA2-PA1
11	C	2007	PEE	C31-C32-C33-C34
11	P	3007	PEE	C10-C11-C12-C13
11	E	2005	PEE	C1-C2-O2-C10
11	P	3005	PEE	C1-C2-O2-C10
11	P	3007	PEE	C31-C32-C33-C34
11	E	2005	PEE	C12-C13-C14-C15
11	P	3005	PEE	C36-C37-C38-C39
13	C	501	HEM	C2C-C3C-CAC-CBC
11	P	3007	PEE	C11-C12-C13-C14
11	E	2005	PEE	C36-C37-C38-C39
11	P	3007	PEE	C42-C43-C44-C45
16	Q	3003	CDL	C15-C16-C17-C18
18	Q	501	HEC	C2C-C3C-CAC-CBC
16	D	2003	CDL	C15-C16-C17-C18
13	C	502	HEM	CAA-CBA-CGA-O1A
11	A	2008	PEE	O3-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	P	502	HEM	CAA-CBA-CGA-O1A
13	C	501	HEM	CAA-CBA-CGA-O1A
13	C	502	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAD-CBD-CGD-O2D
11	A	2008	PEE	O3P-C1-C2-C3
13	P	501	HEM	CAA-CBA-CGA-O1A
13	P	501	HEM	CAA-CBA-CGA-O2A
11	P	3005	PEE	C32-C33-C34-C35
11	P	3007	PEE	C13-C14-C15-C16
20	R	3009	PLC	C1B-C2B-C3B-C4B
13	C	501	HEM	CAA-CBA-CGA-O2A
13	C	502	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C13-C14-C15-C16
13	C	502	HEM	CAD-CBD-CGD-O1D
11	C	2007	PEE	C11-C12-C13-C14
11	A	2008	PEE	O5-C30-C31-C32
16	D	2003	CDL	CA3-CA4-CA6-OA8
13	P	502	HEM	CAD-CBD-CGD-O1D
13	C	501	HEM	CAD-CBD-CGD-O2D
17	C	2011	GOL	O1-C1-C2-O2
13	P	501	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAA-CBA-CGA-O2A
20	E	2009	PLC	O3P-C1-C2-C3
11	P	3005	PEE	O2-C2-C3-O3
16	Q	3003	CDL	C13-C14-C15-C16
11	E	2005	PEE	C32-C33-C34-C35
11	P	3005	PEE	C12-C13-C14-C15
16	D	2003	CDL	C13-C14-C15-C16
11	E	2005	PEE	C38-C39-C40-C41
13	C	501	HEM	CAD-CBD-CGD-O1D
11	C	2007	PEE	C42-C43-C44-C45
11	P	3005	PEE	C38-C39-C40-C41
16	C	2004	CDL	C1-CB2-OB2-PB2
11	A	2008	PEE	C1-C2-C3-O3
13	C	501	HEM	C4C-C3C-CAC-CBC
13	P	501	HEM	C4C-C3C-CAC-CBC
13	P	501	HEM	CAD-CBD-CGD-O1D
11	P	3005	PEE	C42-C43-C44-C45
11	E	2005	PEE	O2-C2-C3-O3
18	Q	501	HEC	CAA-CBA-CGA-O2A
16	Q	3003	CDL	C72-C71-CB7-OB8
20	R	3009	PLC	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	D	2003	CDL	C72-C71-CB7-OB8
18	Q	501	HEC	CAD-CBD-CGD-O2D
16	D	2003	CDL	C12-C11-CA5-OA6
16	Q	3003	CDL	C12-C11-CA5-OA6
16	Q	3003	CDL	C52-C51-CB5-OB6
16	D	2003	CDL	C52-C51-CB5-OB6
11	C	2007	PEE	O2-C2-C3-O3
11	P	3007	PEE	O2-C2-C3-O3
20	E	2009	PLC	O2-C2-C3-O3
20	R	3009	PLC	O2-C2-C3-O3
11	A	2008	PEE	O2-C10-C11-C12
18	Q	501	HEC	CAA-CBA-CGA-O1A
11	P	3007	PEE	O2-C10-C11-C12
11	C	2007	PEE	O2-C10-C11-C12
18	D	501	HEC	CAA-CBA-CGA-O2A
18	Q	501	HEC	CAD-CBD-CGD-O1D
11	E	2005	PEE	C42-C43-C44-C45
11	C	2007	PEE	C20-C21-C22-C23
11	E	2005	PEE	C22-C23-C24-C25
16	D	2003	CDL	C52-C51-CB5-OB7
16	D	2003	CDL	C72-C71-CB7-OB9
16	Q	3003	CDL	C52-C51-CB5-OB7
16	Q	3003	CDL	C72-C71-CB7-OB9
16	Q	3003	CDL	C12-C11-CA5-OA7
16	D	2003	CDL	C12-C11-CA5-OA7
18	D	501	HEC	CAA-CBA-CGA-O1A
11	P	3007	PEE	O4-C10-C11-C12
11	C	2007	PEE	O4-C10-C11-C12
11	A	2008	PEE	O4-C10-C11-C12

There are no ring outliers.

23 monomers are involved in 92 short contacts:

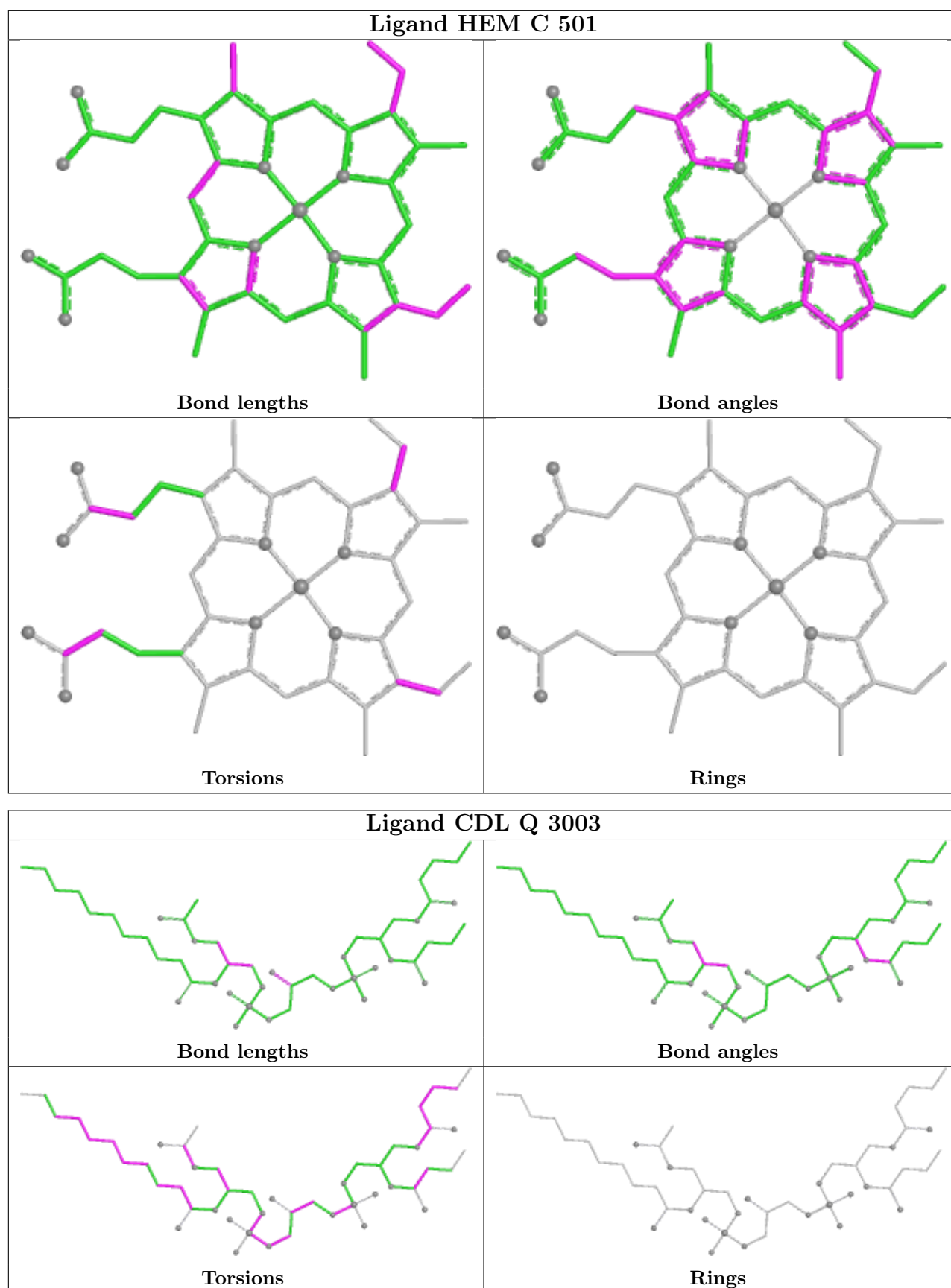
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	501	HEM	11	0
16	Q	3003	CDL	5	0
20	E	2009	PLC	2	0
15	C	2002	ANY	3	0
18	D	501	HEC	6	0
16	D	2003	CDL	1	0
11	P	3007	PEE	3	0
13	C	502	HEM	9	0

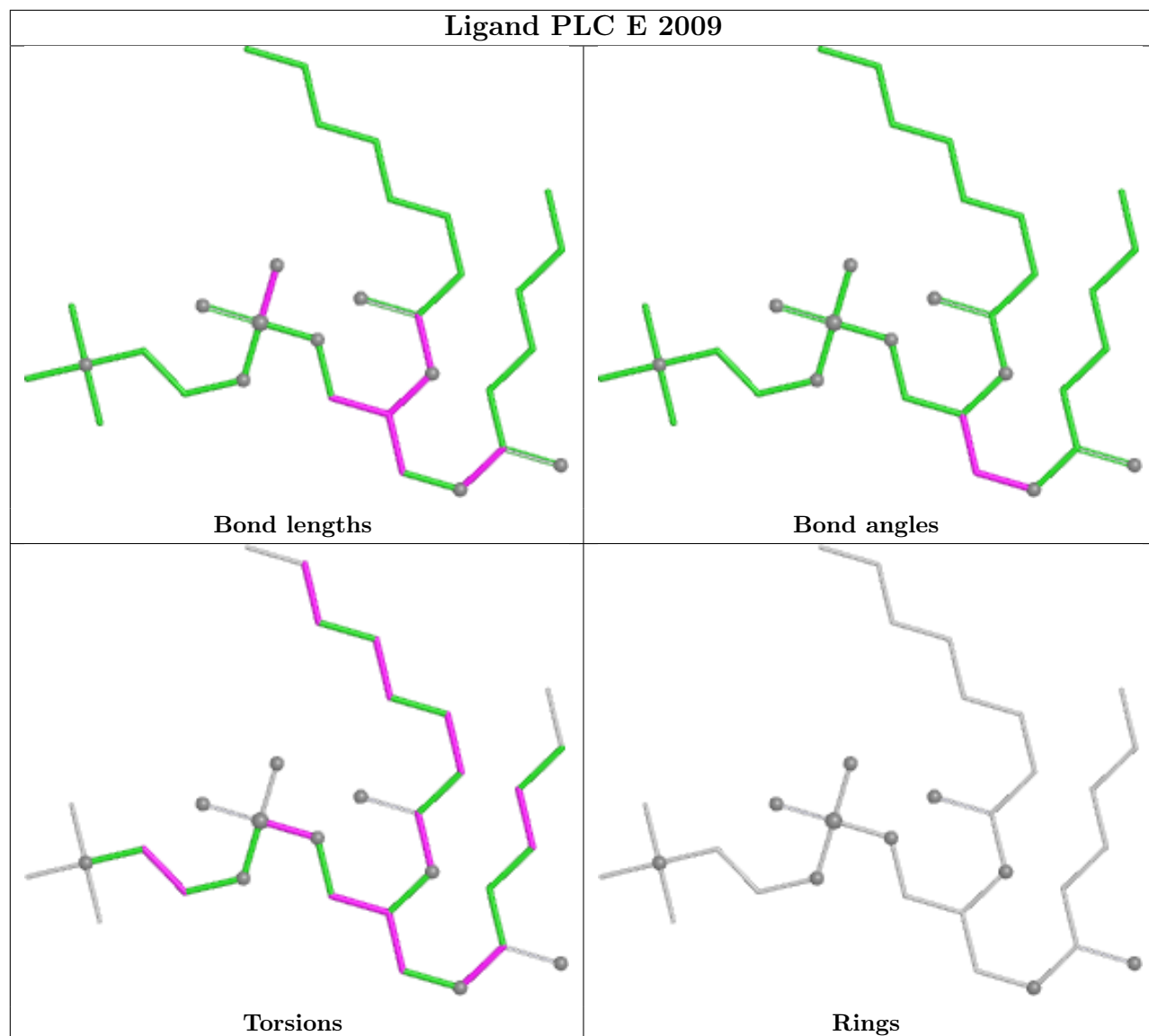
Continued on next page...

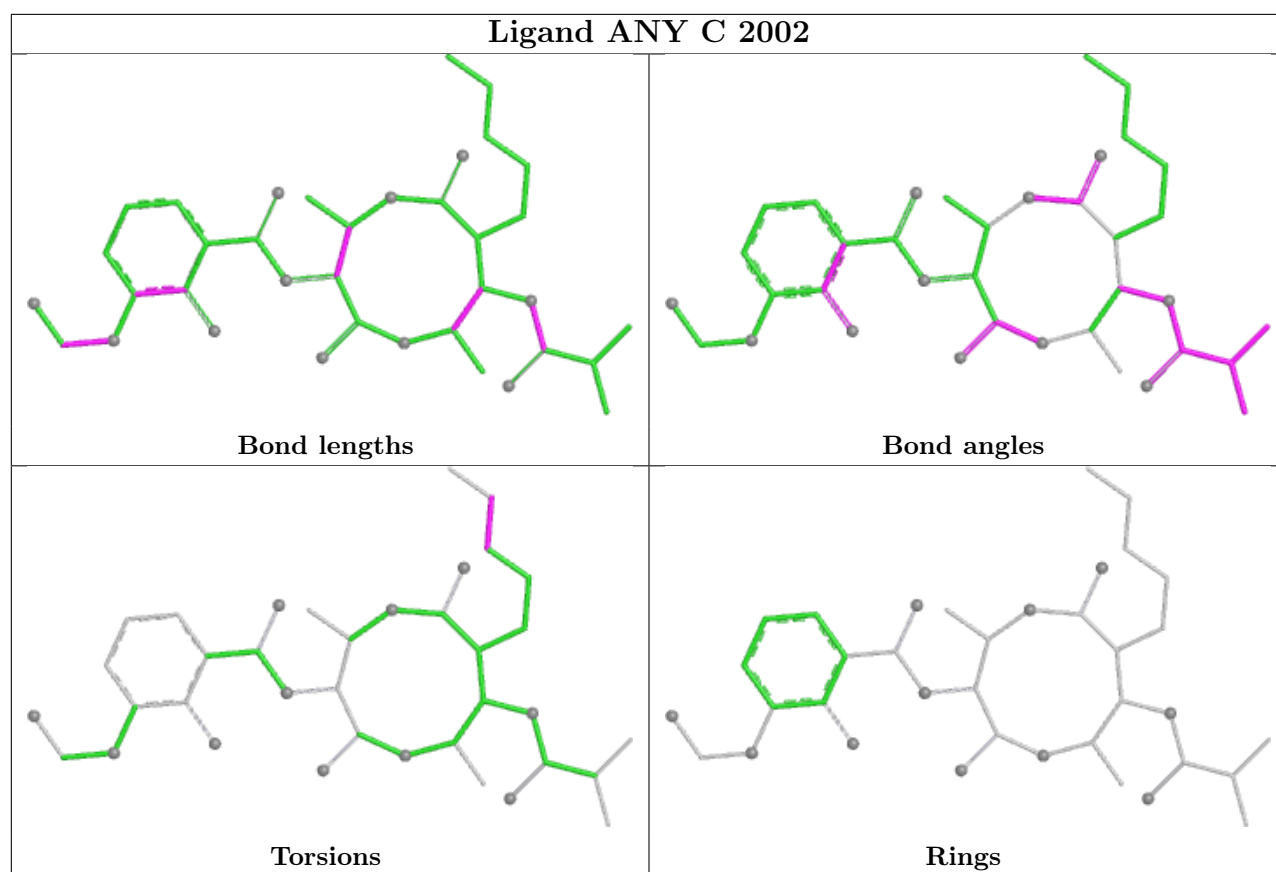
Continued from previous page...

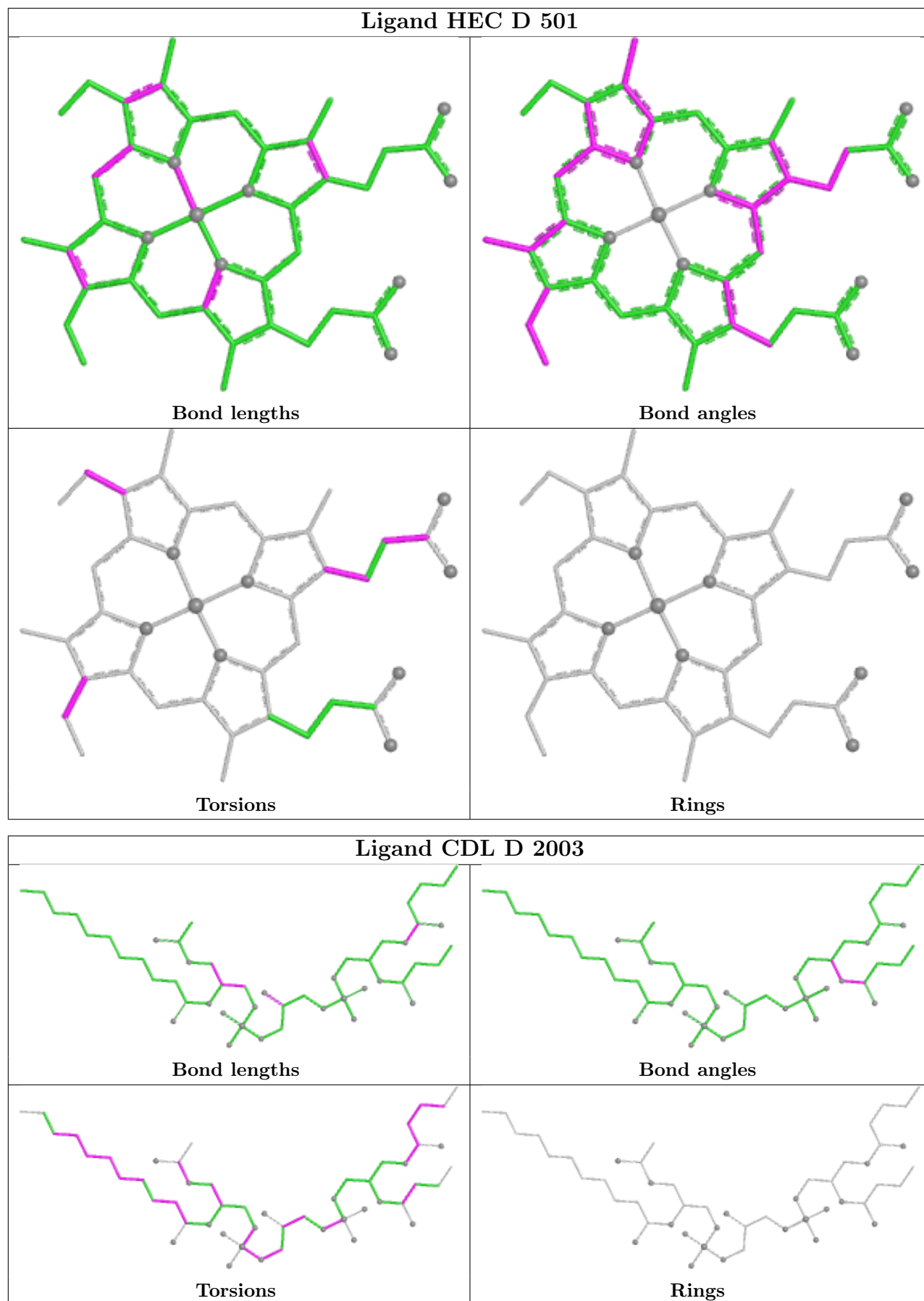
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	3002	ANY	1	0
14	P	3001	SMA	4	0
16	C	2004	CDL	2	0
13	P	502	HEM	11	0
17	C	2011	GOL	1	0
11	E	2005	PEE	1	0
13	P	501	HEM	11	0
16	P	3004	CDL	2	0
14	C	2001	SMA	3	0
11	C	2007	PEE	2	0
19	E	501	FES	2	0
11	P	3005	PEE	3	0
18	Q	501	HEC	5	0
19	R	501	FES	1	0
20	R	3009	PLC	3	0

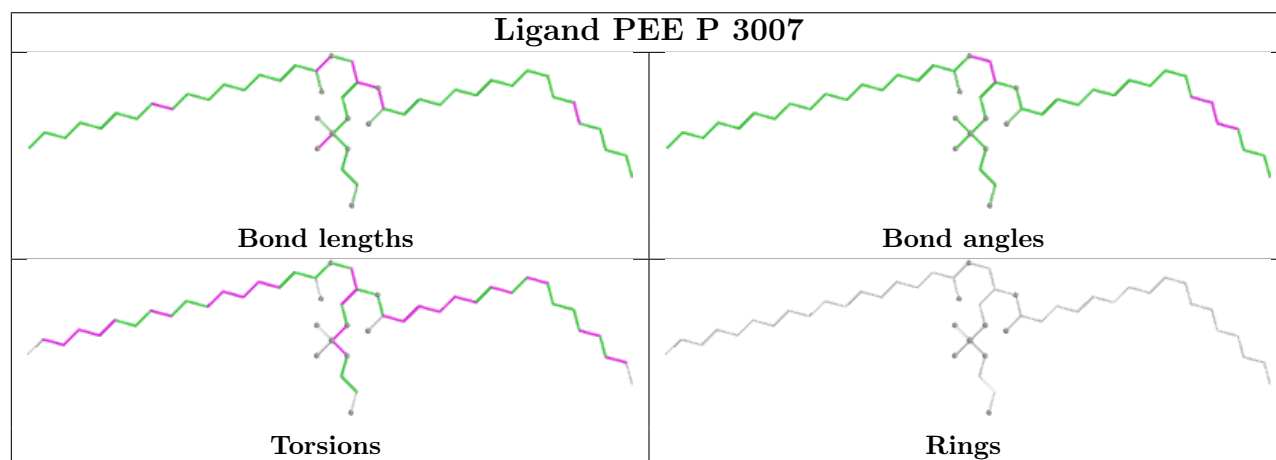
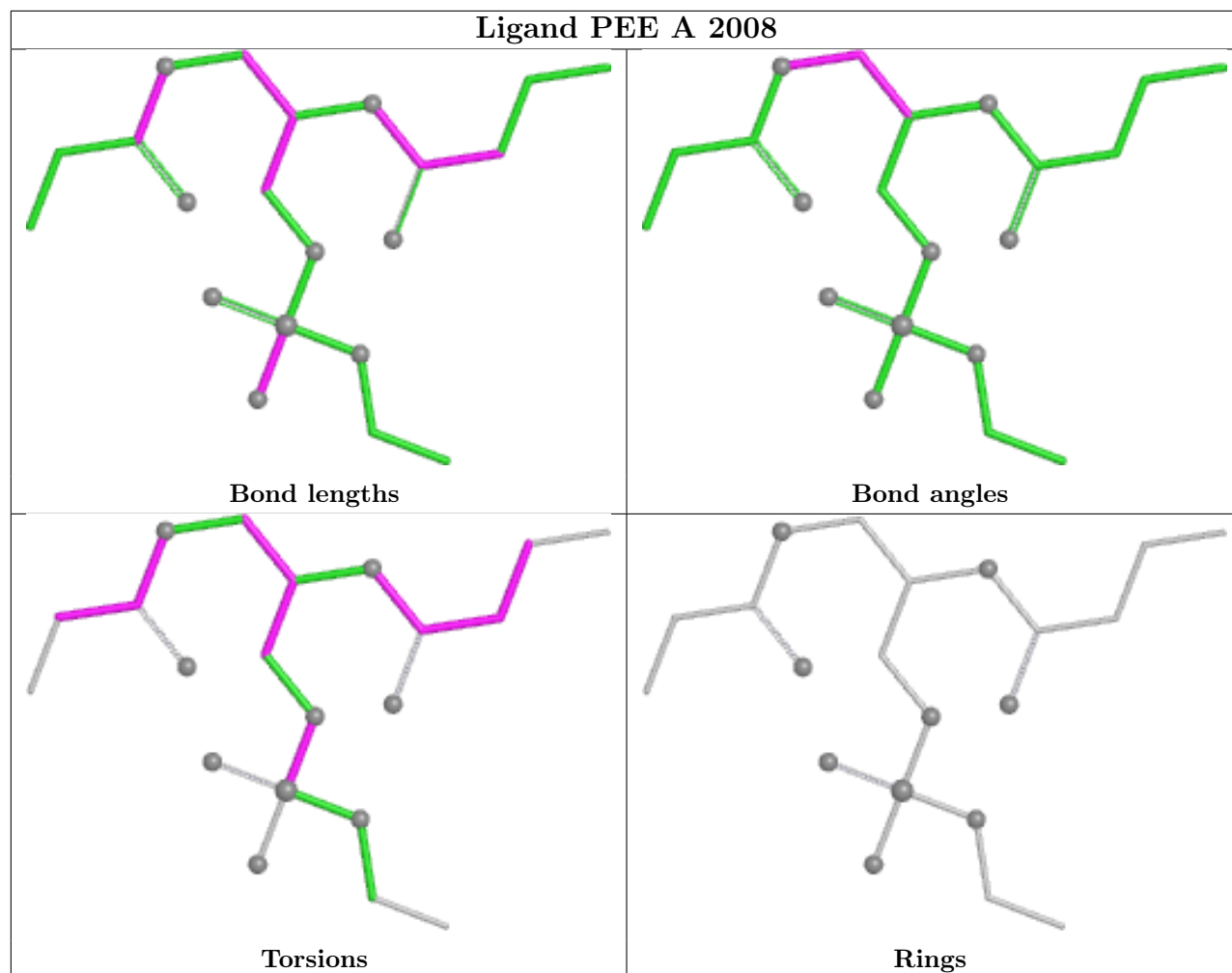
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

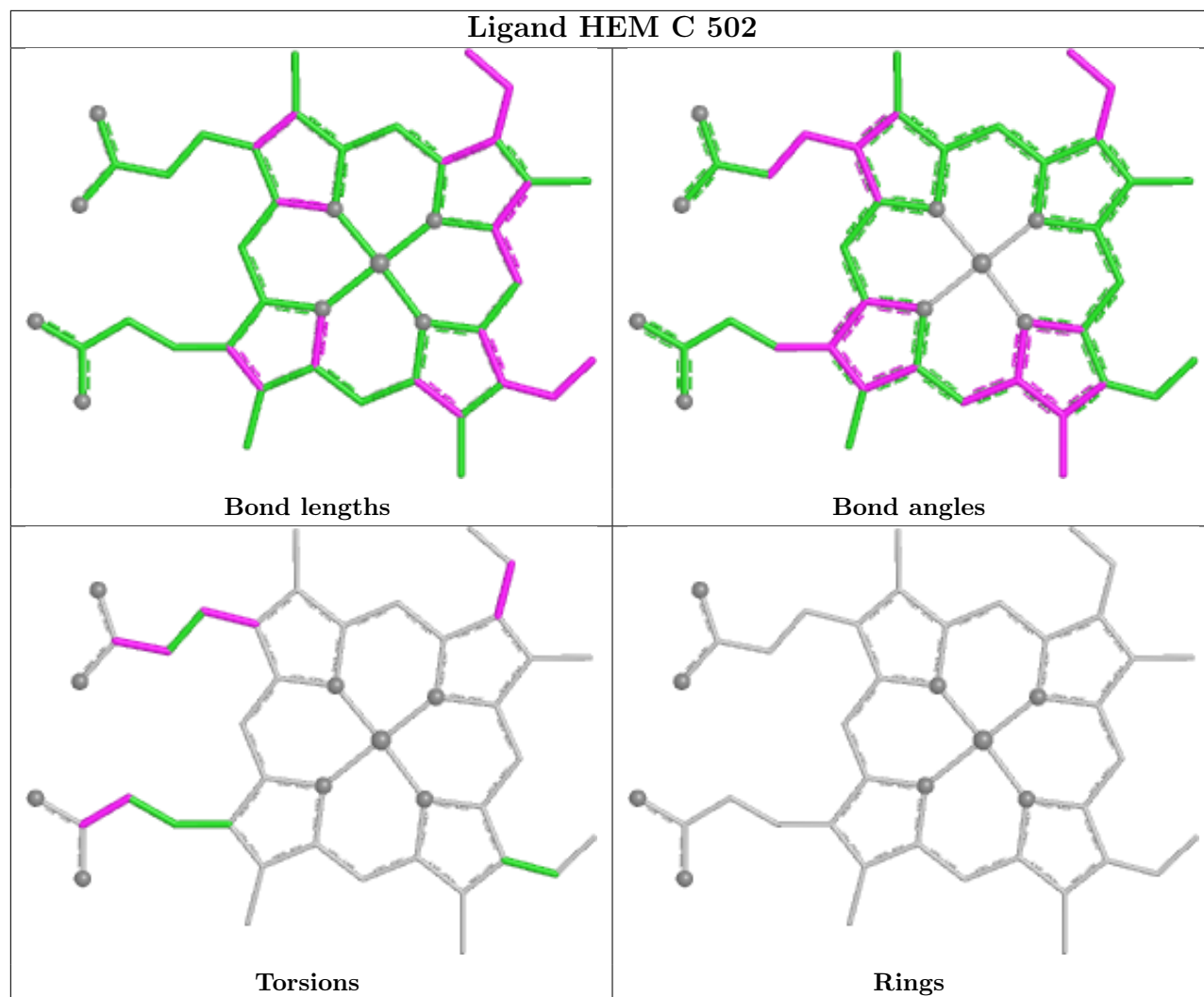




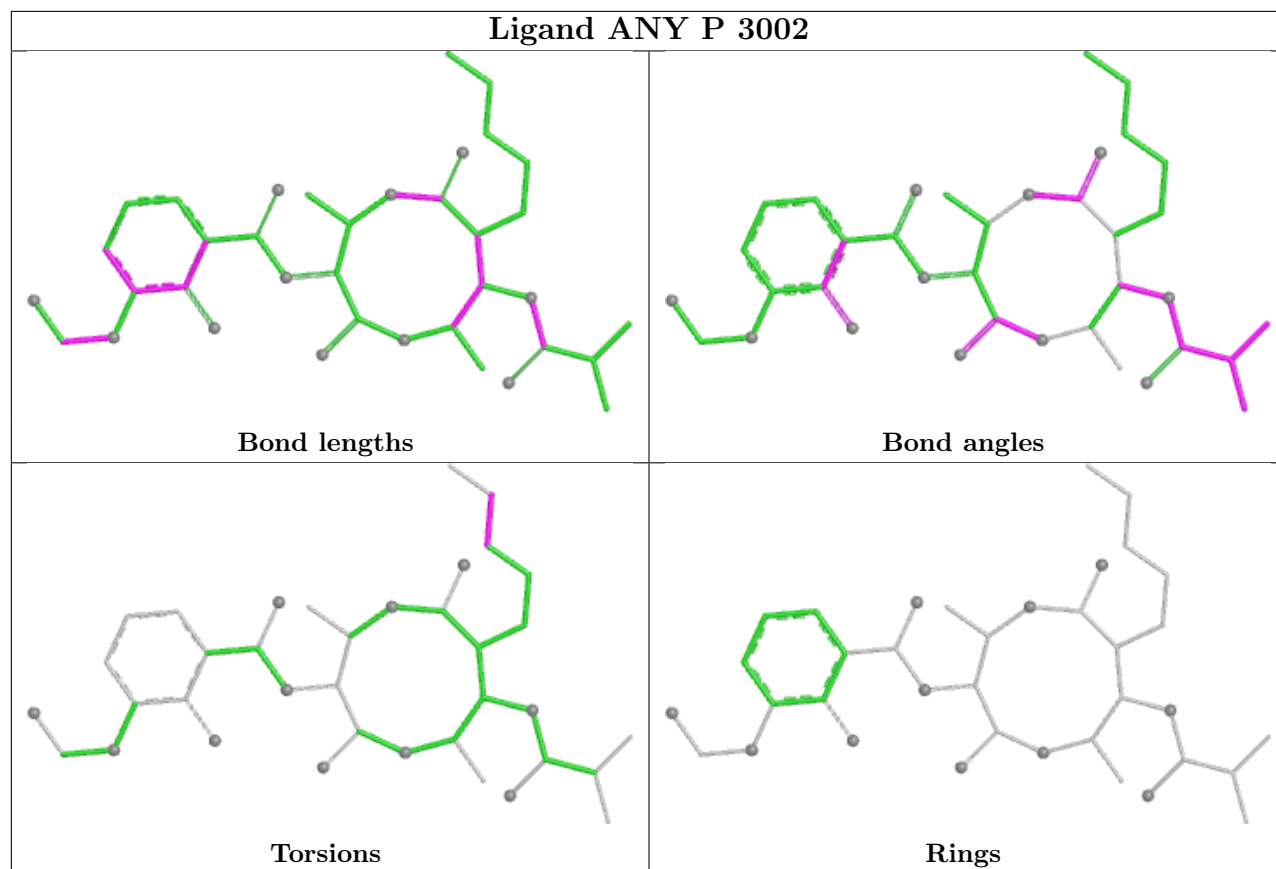




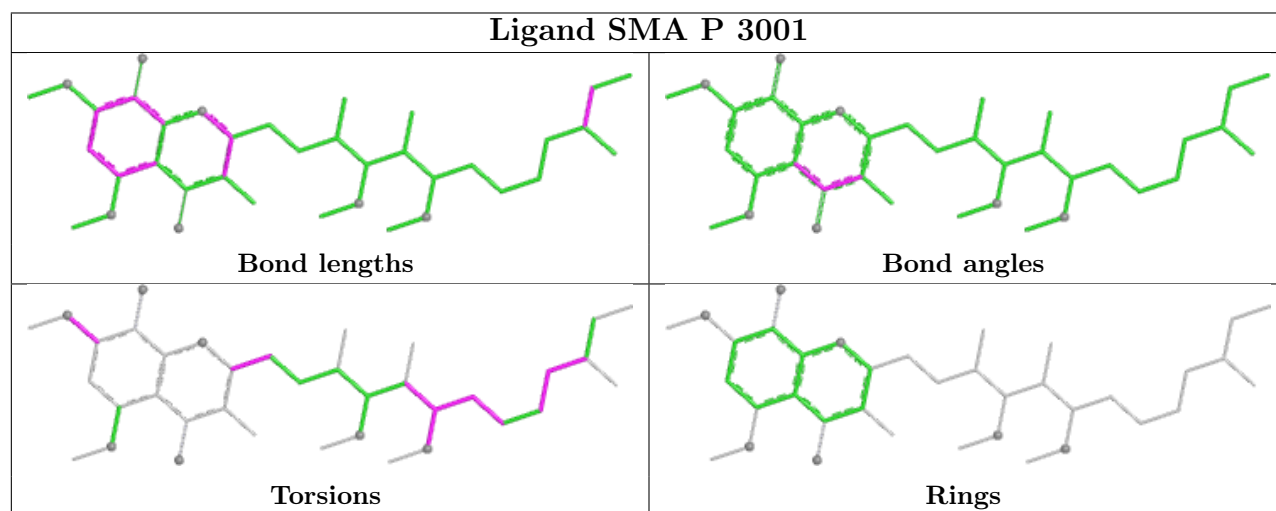


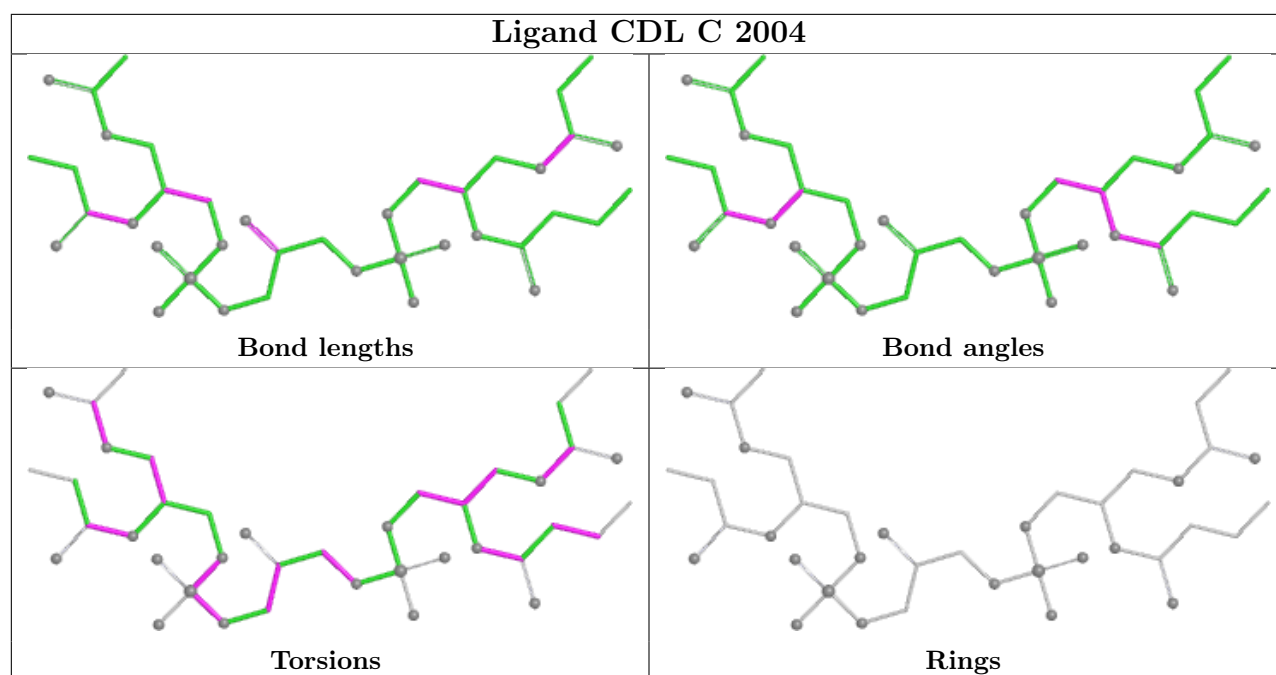


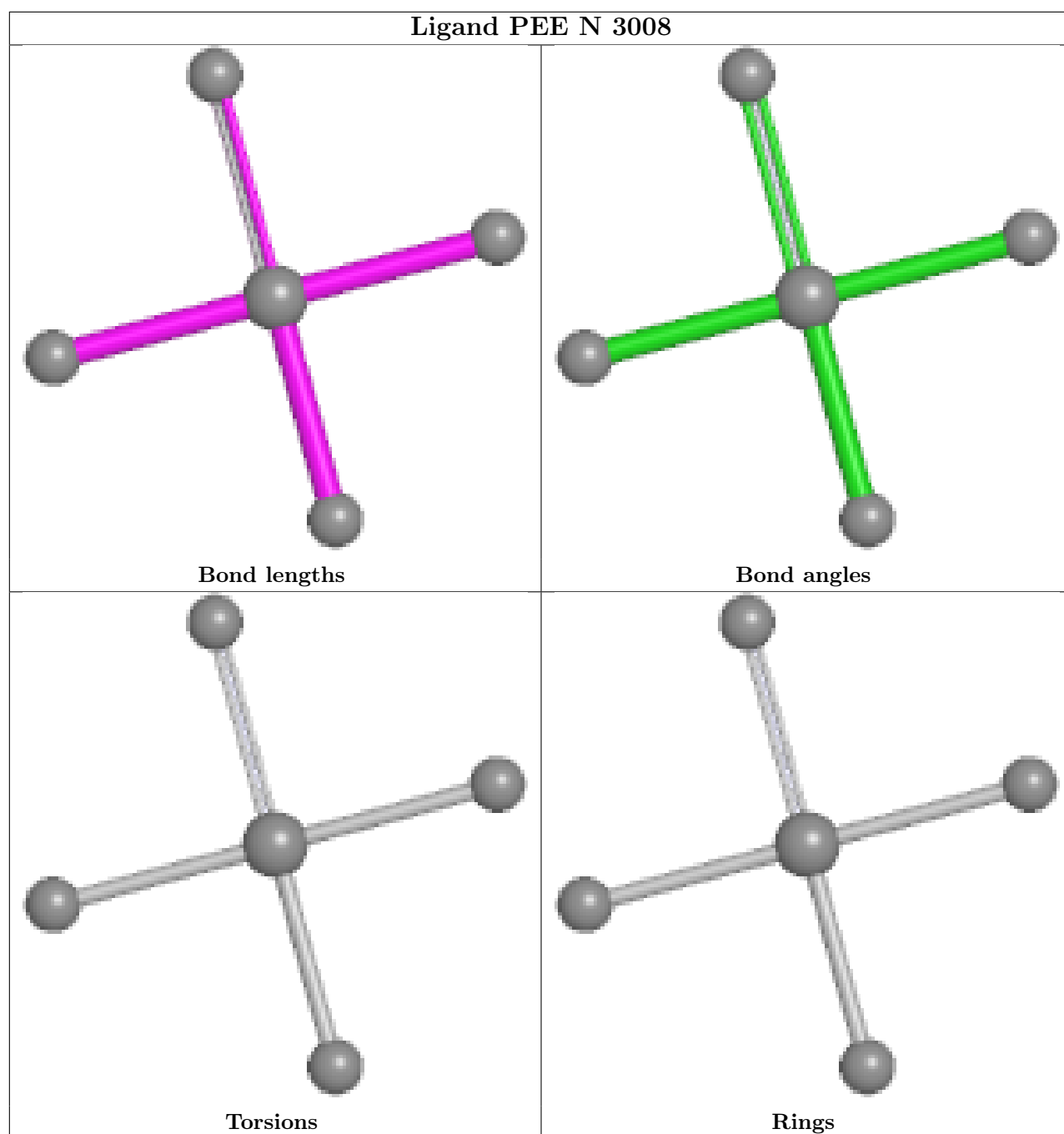
Ligand ANY P 3002

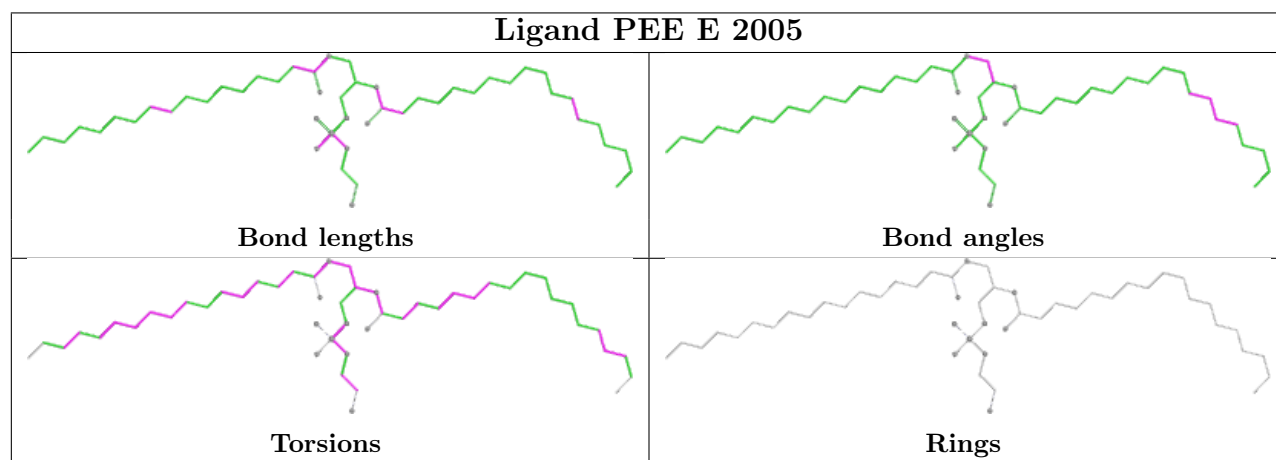
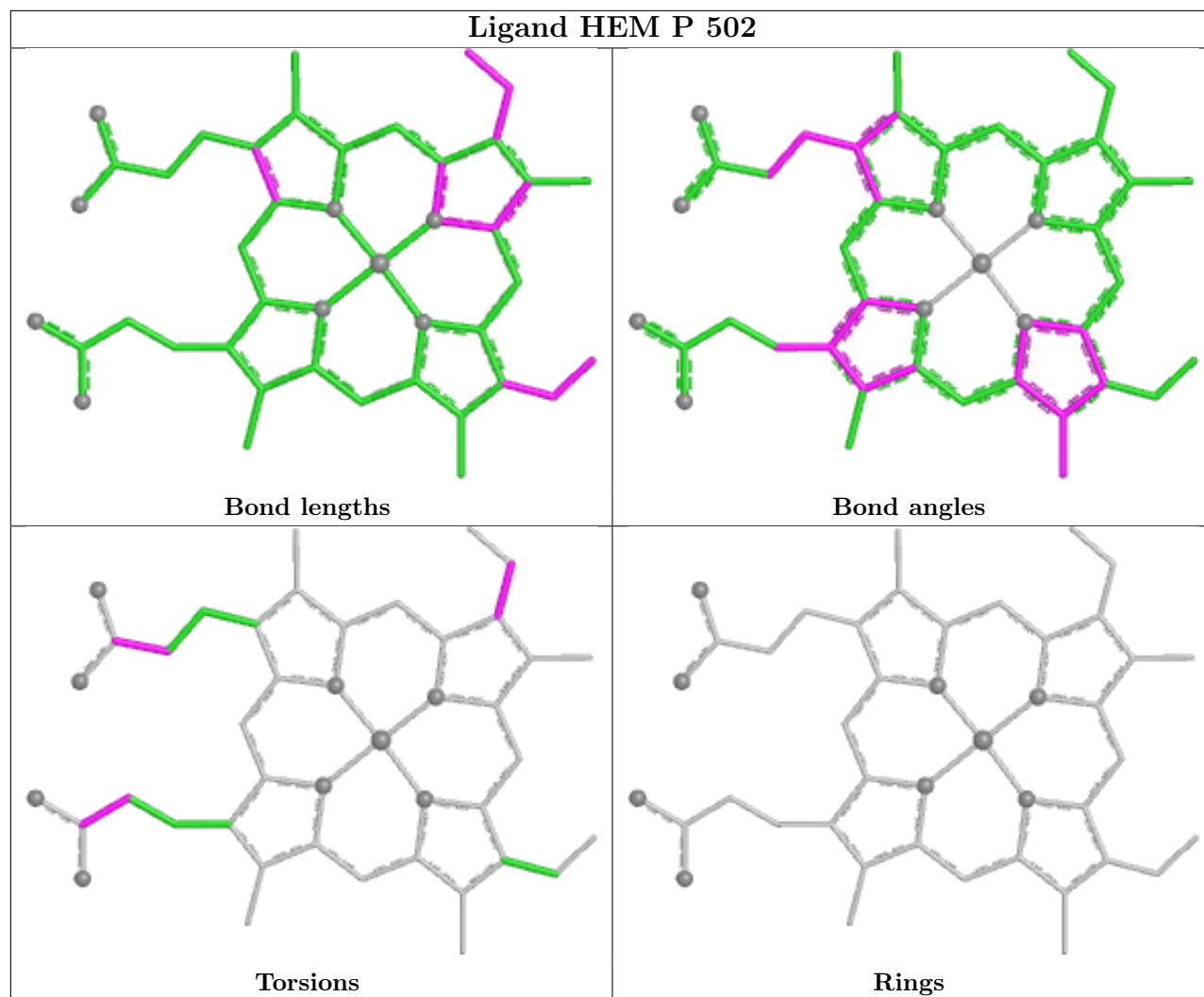


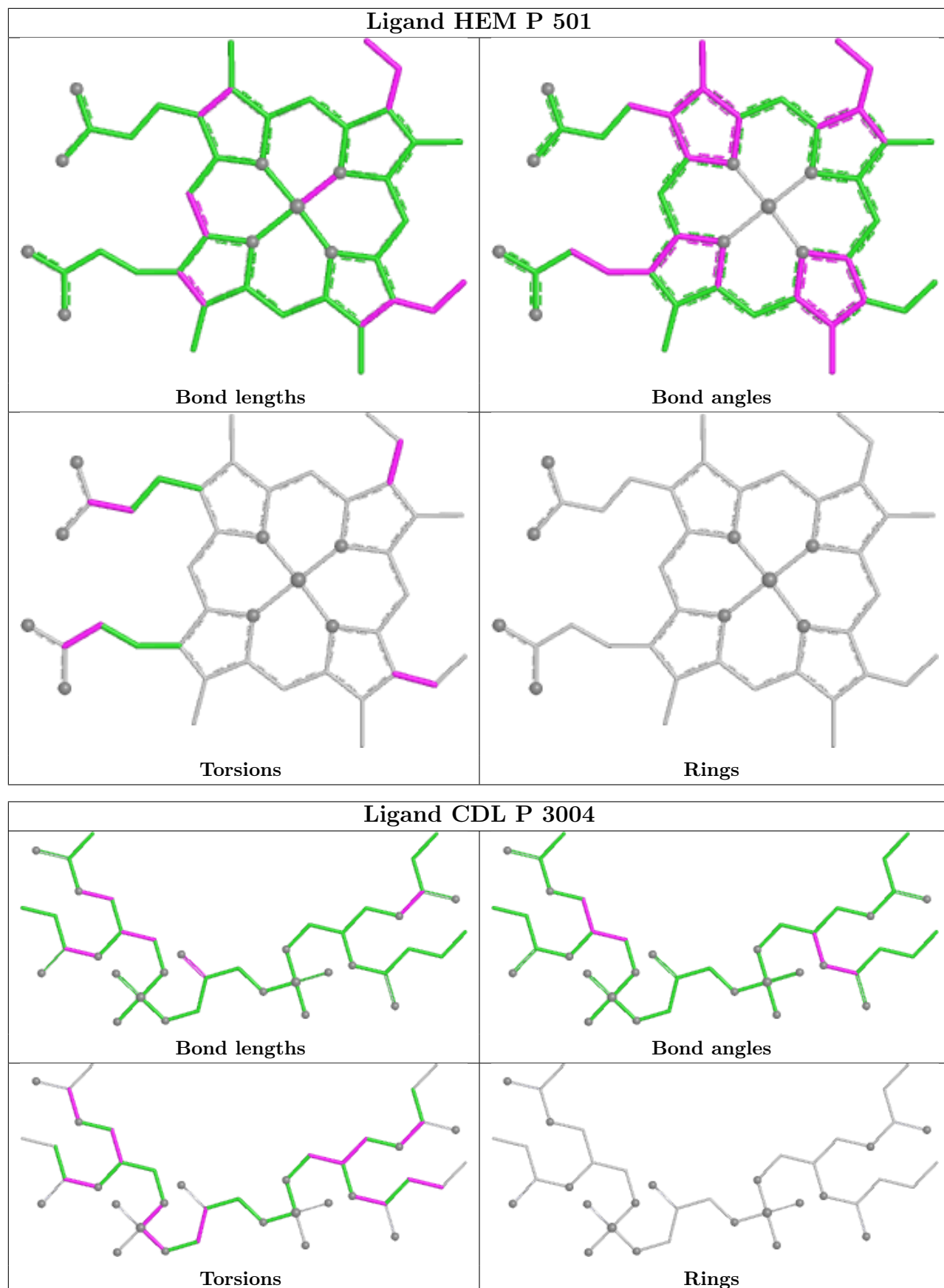
Ligand SMA P 3001

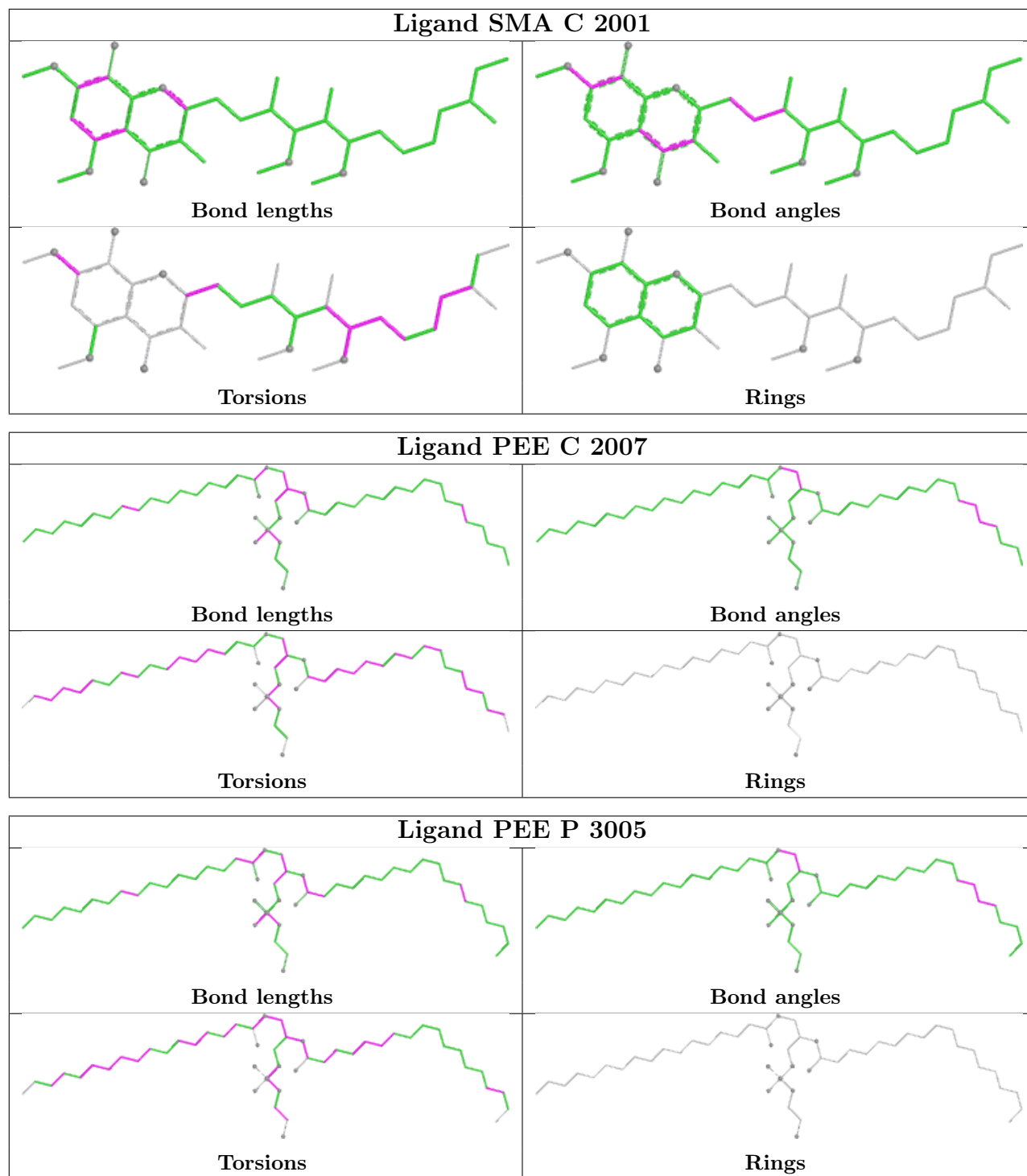




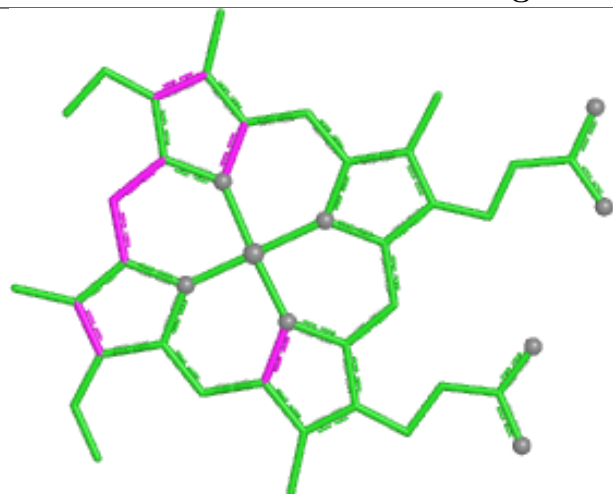




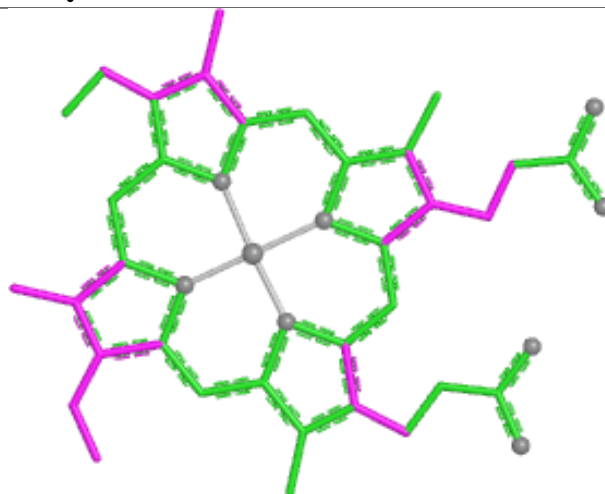




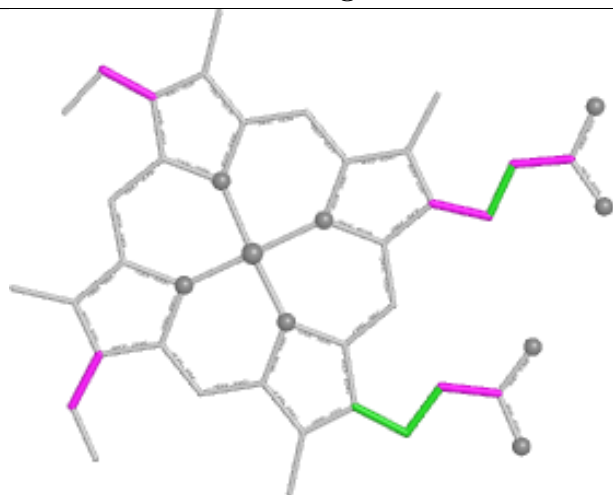
Ligand HEC Q 501



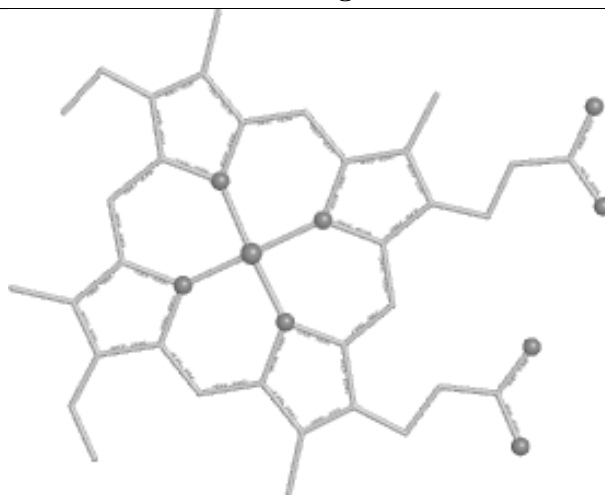
Bond lengths



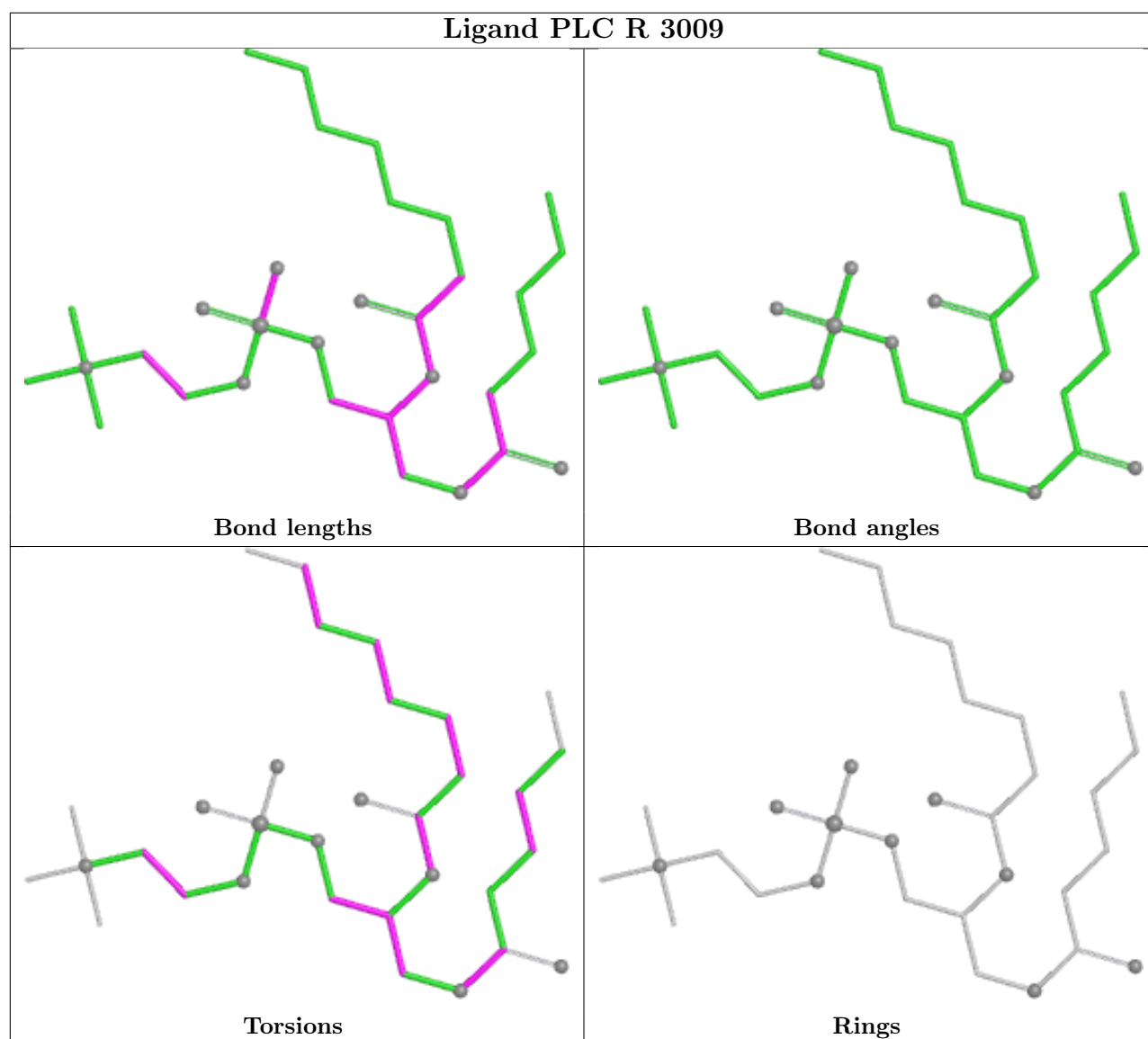
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.01	1 (0%) 91 80	40, 85, 131, 143	0
1	N	442/446 (99%)	0.17	3 (0%) 84 60	42, 91, 131, 143	0
2	B	421/441 (95%)	0.25	5 (1%) 76 49	63, 107, 145, 173	0
2	O	422/441 (95%)	0.14	3 (0%) 84 60	50, 97, 140, 150	0
3	C	380/380 (100%)	-0.64	1 (0%) 90 74	17, 40, 73, 122	0
3	P	379/380 (99%)	-0.25	1 (0%) 90 74	20, 71, 106, 136	0
4	D	241/241 (100%)	-0.44	0 100 100	28, 55, 105, 118	0
4	Q	241/241 (100%)	0.01	2 (0%) 82 57	51, 93, 136, 148	0
5	E	196/196 (100%)	0.23	1 (0%) 87 66	36, 123, 175, 180	0
5	R	196/196 (100%)	0.15	1 (0%) 87 66	50, 97, 152, 159	0
6	F	101/110 (91%)	-0.58	0 100 100	32, 57, 80, 112	0
6	S	101/110 (91%)	0.09	1 (0%) 79 53	67, 103, 138, 161	0
7	G	81/81 (100%)	-0.14	0 100 100	38, 66, 112, 123	0
7	T	79/81 (97%)	0.49	2 (2%) 58 32	62, 112, 176, 184	0
8	H	70/77 (90%)	-0.11	0 100 100	50, 90, 109, 132	0
8	U	67/77 (87%)	0.66	3 (4%) 38 19	129, 151, 171, 173	0
9	I	31/47 (65%)	1.05	4 (12%) 7 5	100, 143, 177, 178	0
9	V	31/47 (65%)	1.46	7 (22%) 2 2	107, 152, 194, 197	0
10	J	61/61 (100%)	-0.23	0 100 100	57, 72, 124, 165	0
10	W	59/61 (96%)	-0.10	0 100 100	62, 89, 125, 148	0
All	All	4042/4160 (97%)	-0.01	35 (0%) 81 55	17, 87, 148, 197	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	2	ILE	4.1
9	V	54	SER	4.0
1	A	444	ILE	3.9
9	V	72	ALA	3.7
9	V	56	SER	3.5
2	O	208	GLY	3.4
1	N	83	GLY	3.3
2	O	243	GLU	3.3
1	N	198	ALA	3.1
9	V	55	MET	2.9
2	B	64	GLY	2.8
2	B	34	ILE	2.5
5	E	132	TRP	2.5
2	O	350	GLY	2.5
2	B	36	ALA	2.5
8	U	54	CYS	2.5
9	I	63	ASP	2.5
4	Q	67	GLU	2.5
3	C	69	HIS	2.4
9	V	47	ARG	2.4
8	U	70	ALA	2.3
7	T	74	PRO	2.3
6	S	10	GLY	2.3
9	I	50	LEU	2.2
5	R	72	SER	2.2
3	P	69	HIS	2.2
9	V	61	ARG	2.1
2	B	240	TRP	2.1
9	I	56	SER	2.1
9	I	76	VAL	2.0
4	Q	107	GLY	2.0
2	B	257	VAL	2.0
1	N	426	GLY	2.0
8	U	52	GLU	2.0
9	V	50	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
11	PEE	A	2008	21/51	0.60	0.18	121,125,130,130	0
12	UNL	A	3016	1/-	0.75	0.09	10,10,10,10	0
16	CDL	Q	3003	50/100	0.79	0.26	116,149,158,158	0
16	CDL	D	2003	50/100	0.80	0.19	63,103,110,111	0
12	UNL	C	2010	1/-	0.80	0.13	24,24,24,24	0
11	PEE	N	3008	5/51	0.81	0.11	105,105,106,106	0
11	PEE	P	3005	50/51	0.81	0.25	75,97,113,115	0
16	CDL	P	3004	40/100	0.83	0.15	101,108,110,110	0
20	PLC	E	2009	32/42	0.84	0.19	37,60,94,95	0
20	PLC	R	3009	32/42	0.84	0.23	74,93,118,118	0
11	PEE	P	3007	49/51	0.85	0.17	63,96,134,135	0
16	CDL	C	2004	40/100	0.86	0.14	50,72,90,92	0
12	UNL	P	3104	1/-	0.86	0.10	42,42,42,42	0
12	UNL	R	2103	1/-	0.86	0.12	12,12,12,12	0
11	PEE	E	2005	50/51	0.87	0.19	66,86,100,101	0
12	UNL	P	3010	1/-	0.89	0.12	24,24,24,24	0
11	PEE	C	2007	49/51	0.90	0.14	44,56,90,91	0
12	UNL	E	2105	1/-	0.92	0.08	35,35,35,35	0
12	UNL	P	2015	1/-	0.93	0.07	25,25,25,25	0
12	UNL	E	3103	1/-	0.93	0.10	32,32,32,32	0
14	SMA	P	3001	37/37	0.93	0.12	64,69,74,75	0
12	UNL	C	3015	1/-	0.95	0.13	32,32,32,32	0
12	UNL	C	2104	1/-	0.95	0.22	36,36,36,36	0
15	ANY	P	3002	37/40	0.95	0.12	65,69,82,82	0
15	ANY	C	2002	37/40	0.96	0.08	27,36,48,50	0
18	HEC	Q	501	43/43	0.97	0.09	64,68,72,76	0
13	HEM	P	502	43/43	0.97	0.10	49,52,70,77	0
17	GOL	P	3011	6/6	0.97	0.15	46,48,50,50	0
13	HEM	C	502	43/43	0.98	0.07	21,28,43,49	0
18	HEC	D	501	43/43	0.98	0.07	34,39,48,55	0
14	SMA	C	2001	37/37	0.98	0.06	20,30,37,39	0
19	FES	E	501	4/4	0.98	0.04	87,88,89,90	0

Continued on next page...

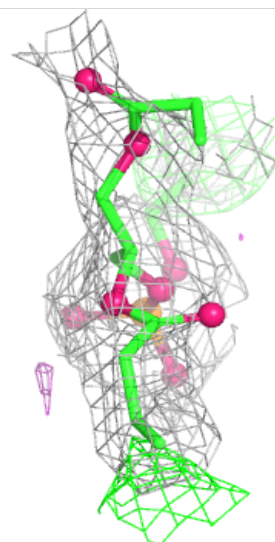
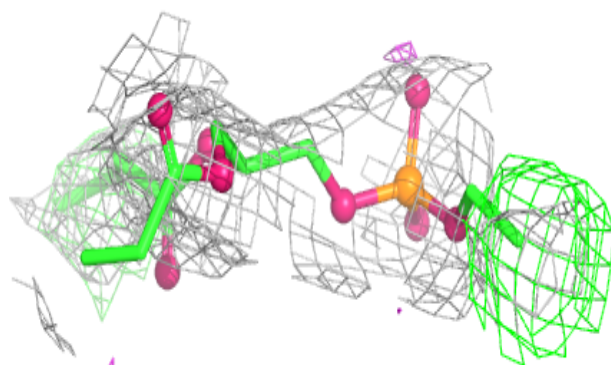
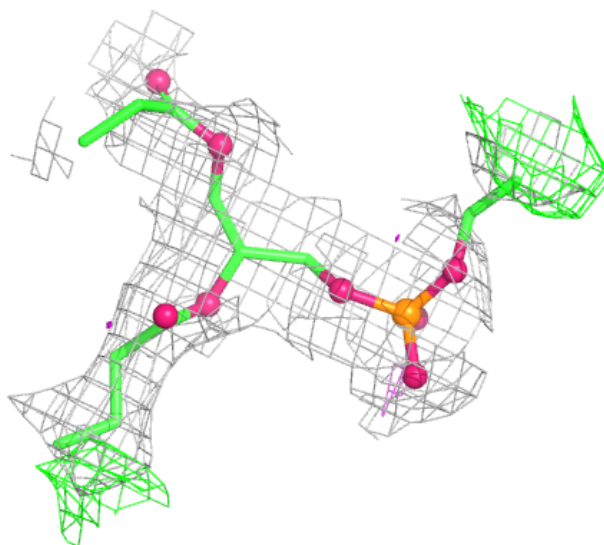
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	HEM	P	501	43/43	0.98	0.07	44,49,55,56	0
17	GOL	C	2011	6/6	0.98	0.14	67,70,71,73	0
13	HEM	C	501	43/43	0.99	0.07	24,32,36,39	0
19	FES	R	501	4/4	0.99	0.04	55,56,58,58	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.

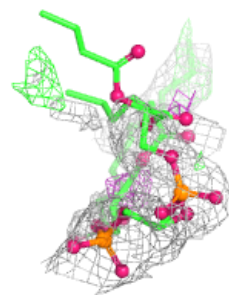
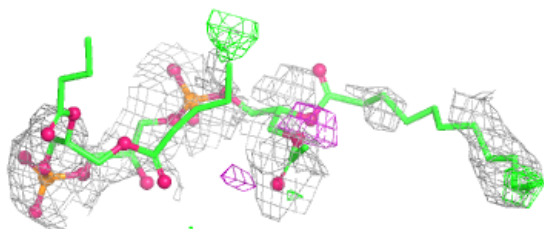
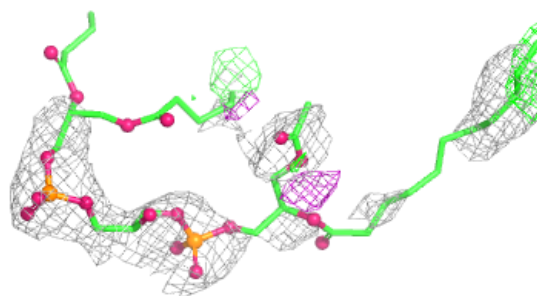
Electron density around PEE A 2008:

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

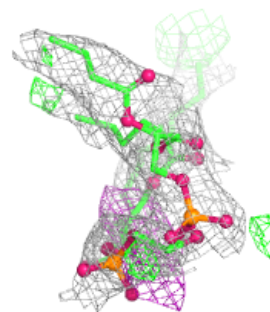
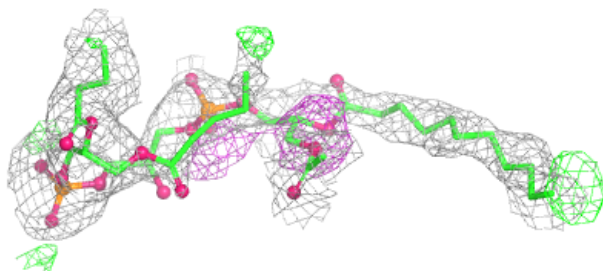
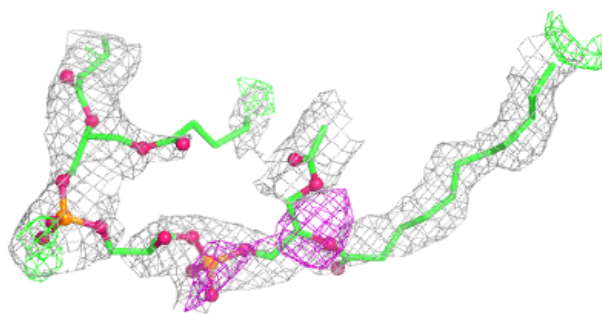


Electron density around CDL Q 3003:

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

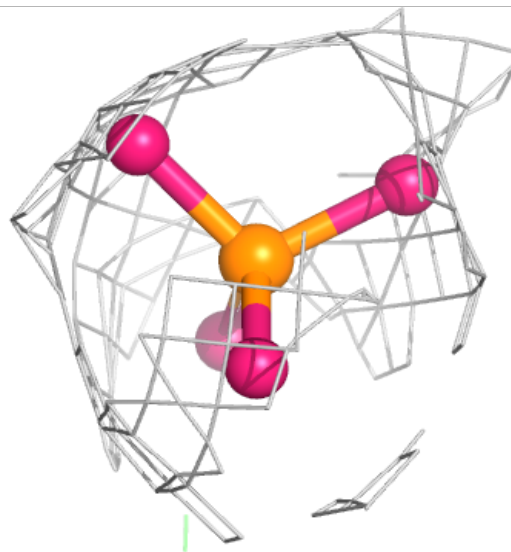
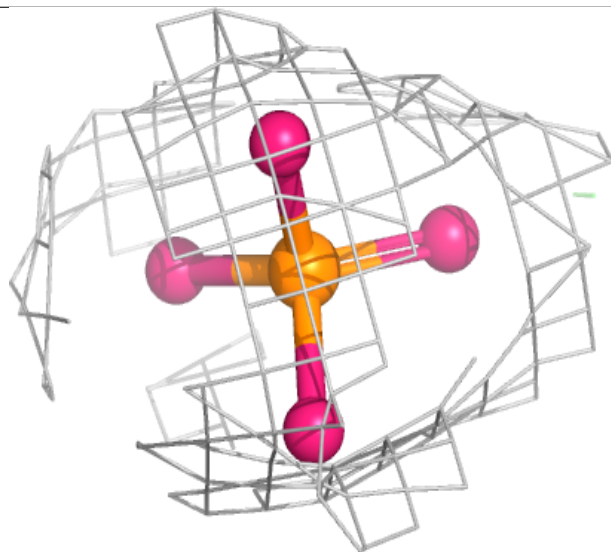
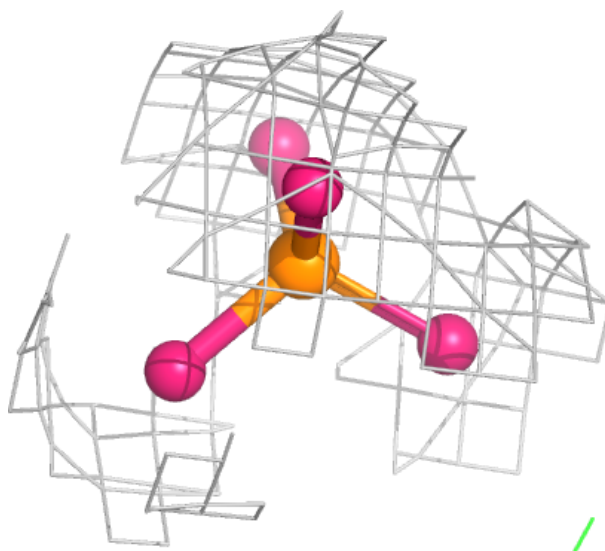
**Electron density around CDL D 2003:**

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



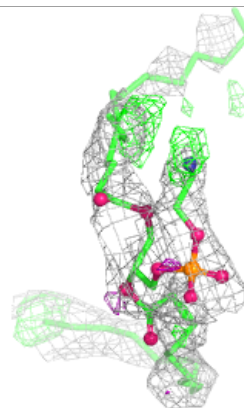
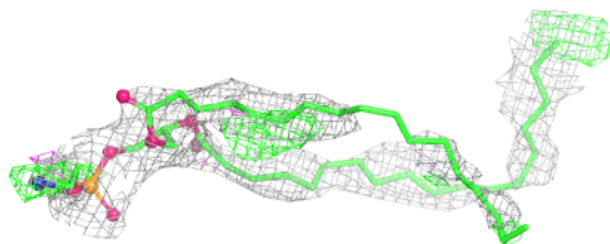
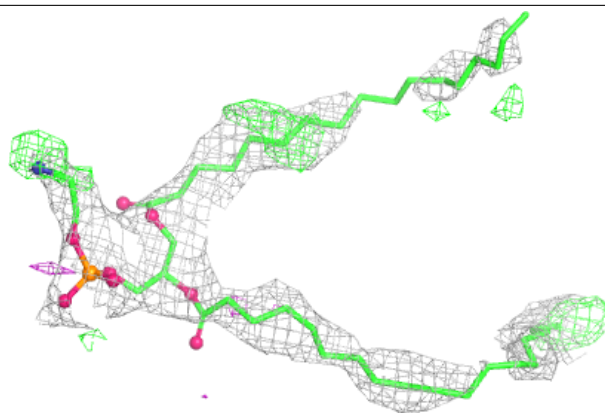
Electron density around PEE N 3008:

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



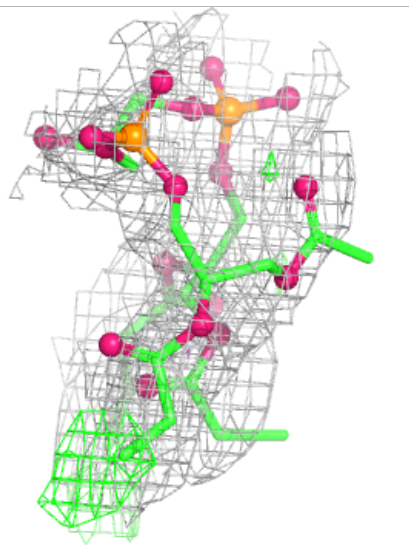
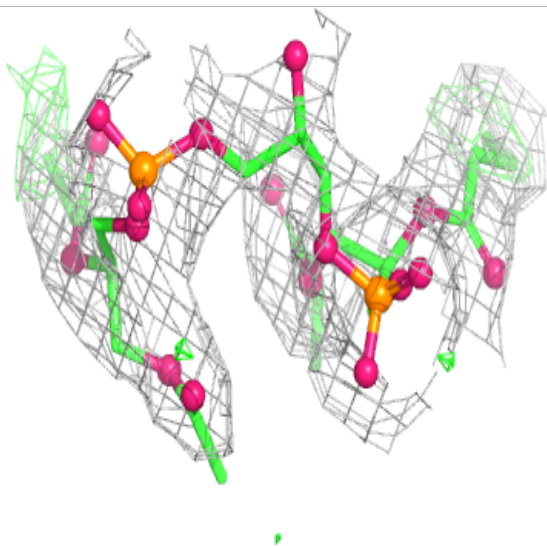
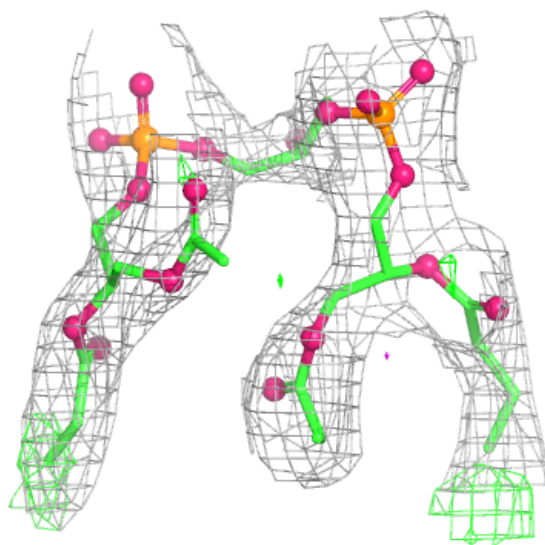
Electron density around PEE P 3005:

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



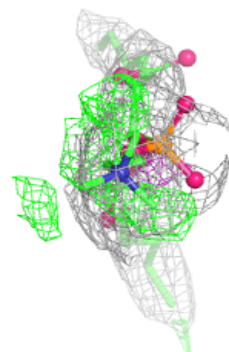
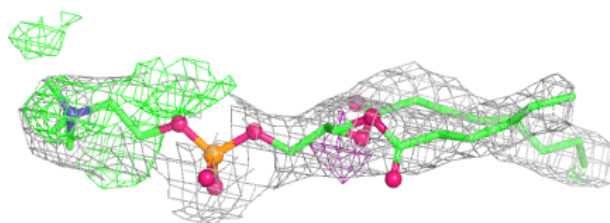
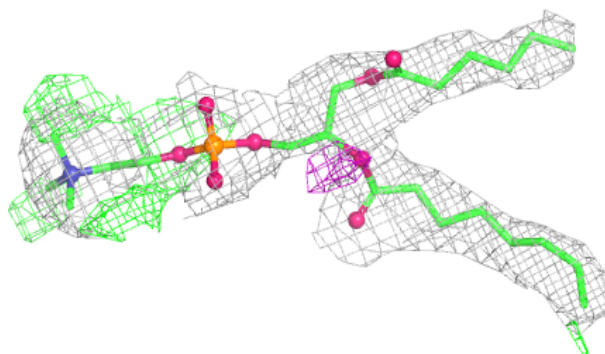
Electron density around CDL P 3004:

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

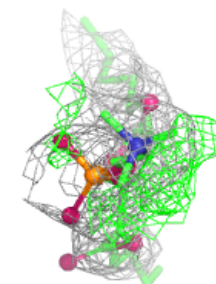
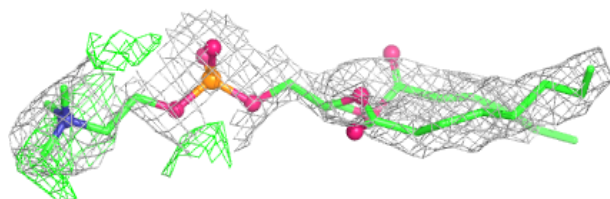
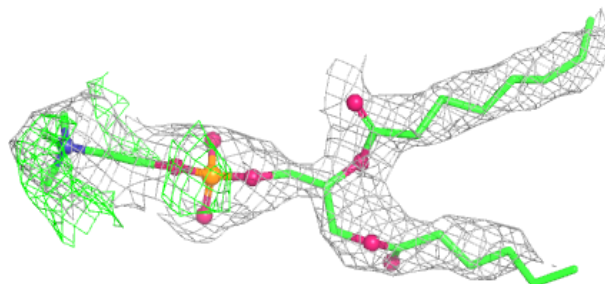


Electron density around PLC E 2009:

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

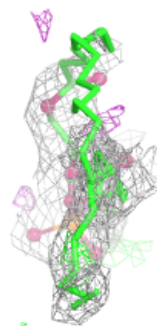
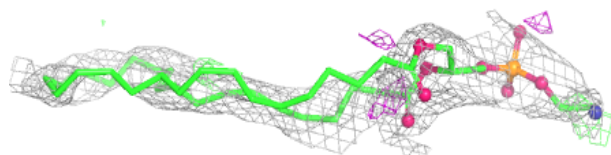
**Electron density around PLC R 3009:**

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



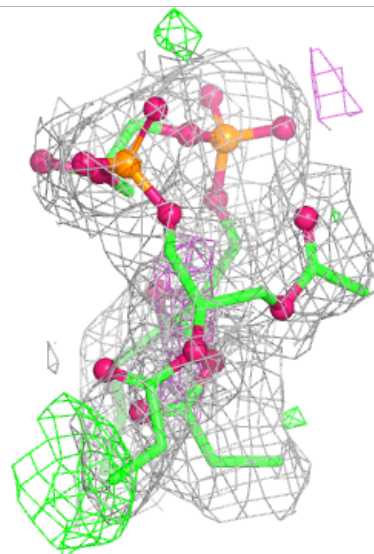
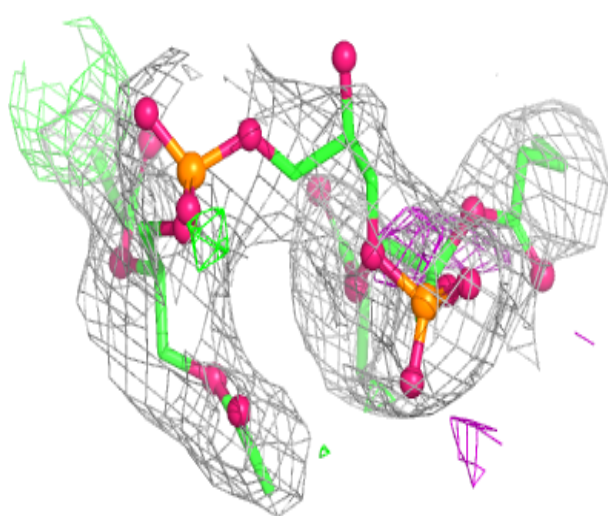
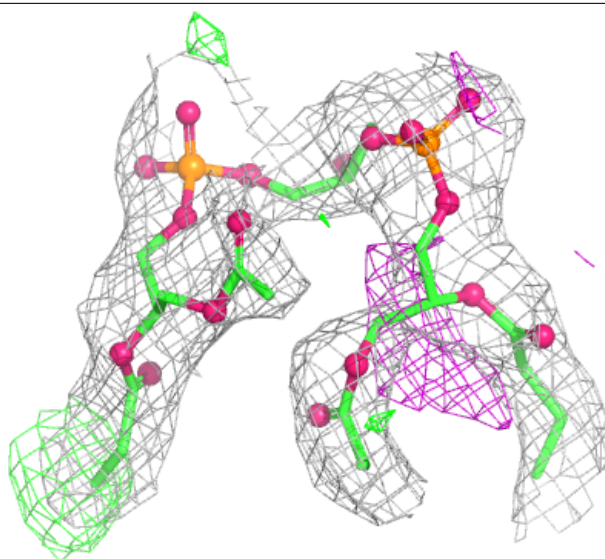
Electron density around PEE P 3007:

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



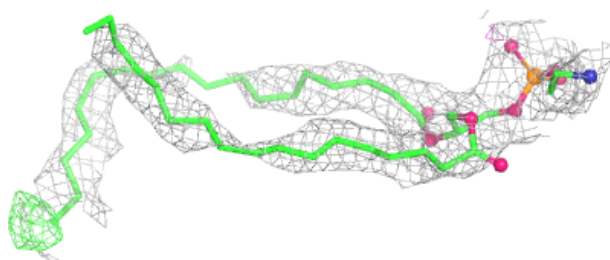
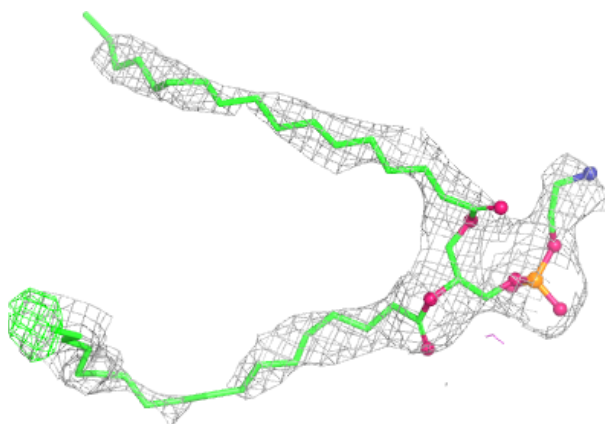
Electron density around CDL C 2004:

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

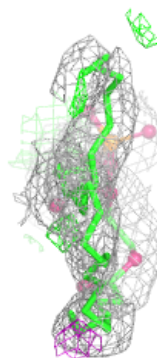
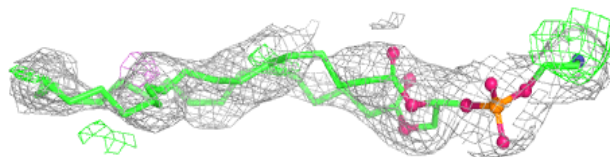
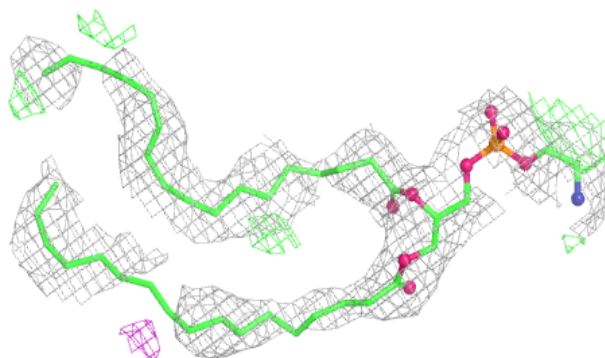


Electron density around PEE E 2005:

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

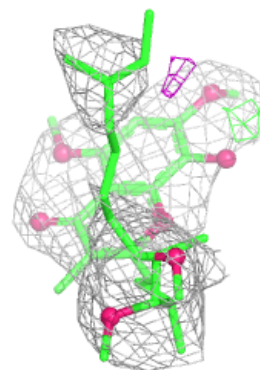
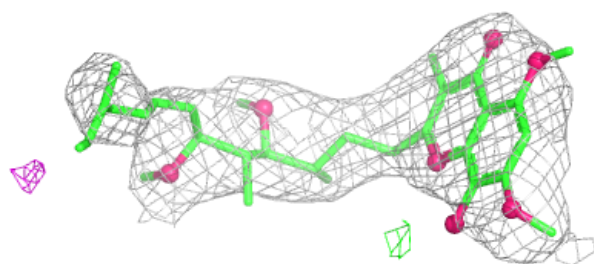
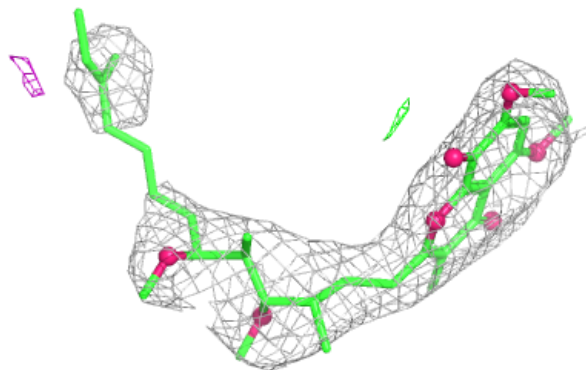
**Electron density around PEE C 2007:**

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

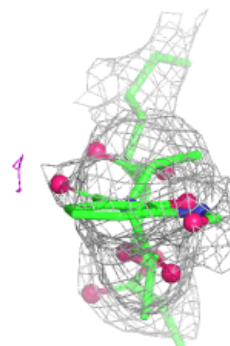
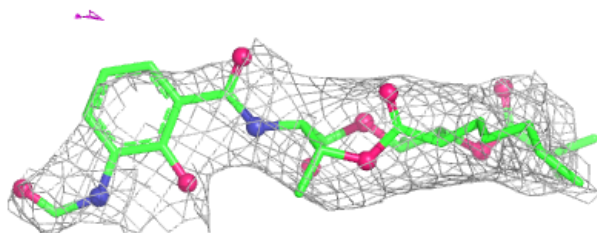
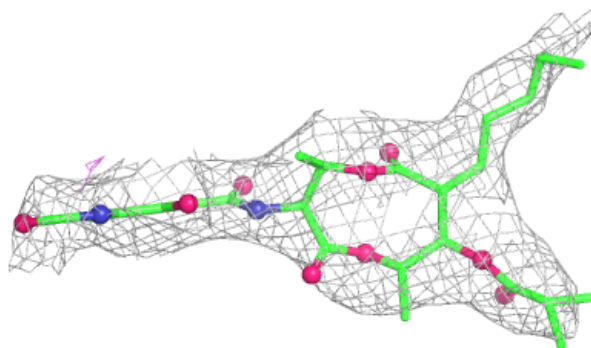


Electron density around SMA P 3001:

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

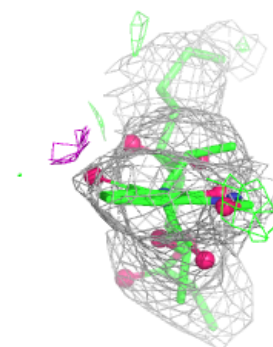
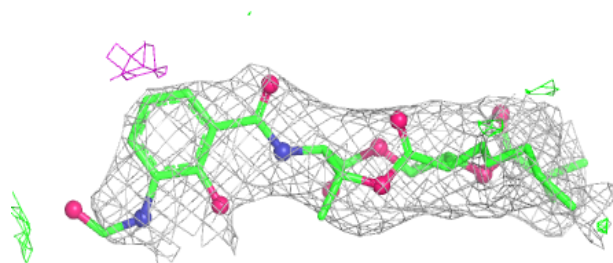
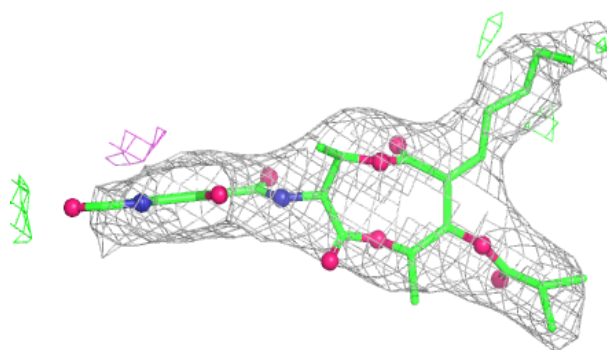
**Electron density around ANY P 3002:**

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

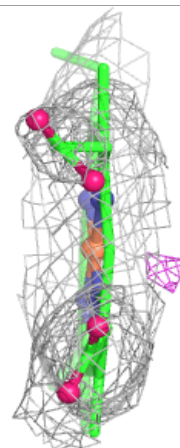
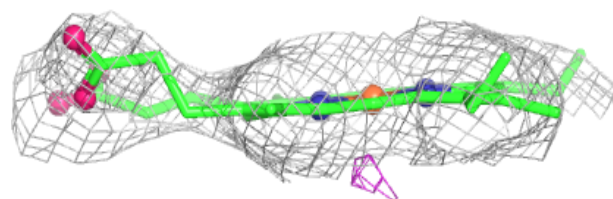
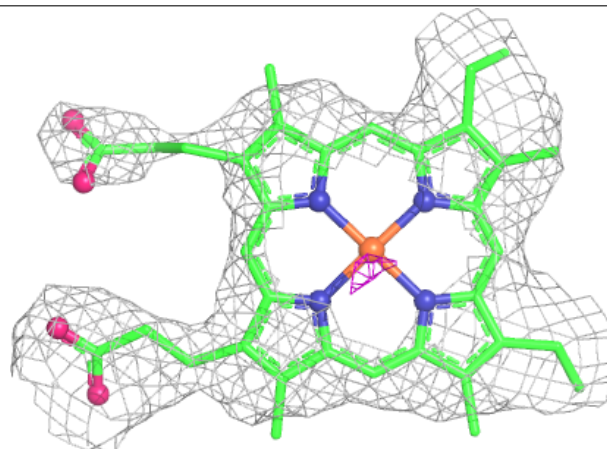


Electron density around ANY C 2002:

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

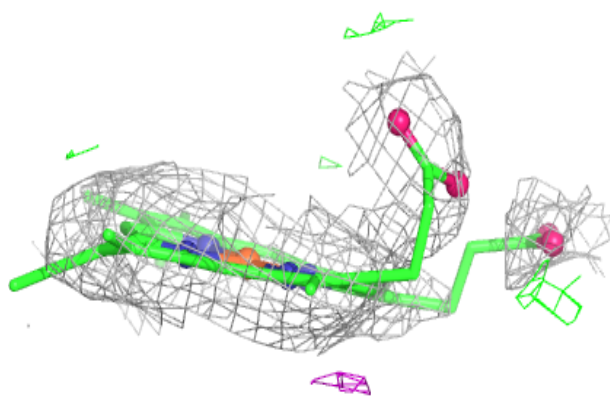
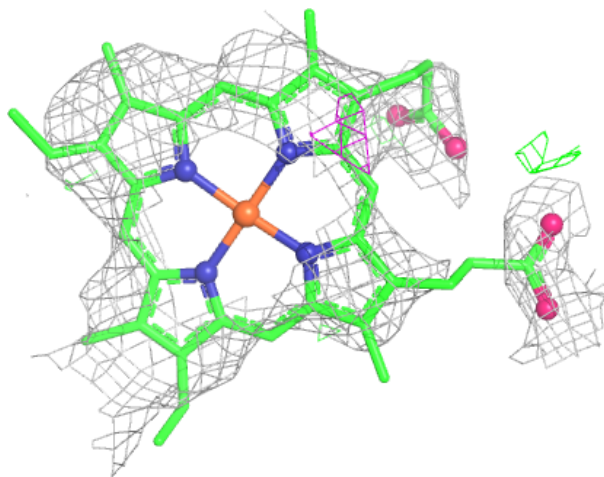
**Electron density around HEC Q 501:**

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



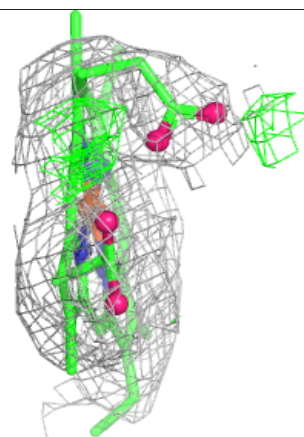
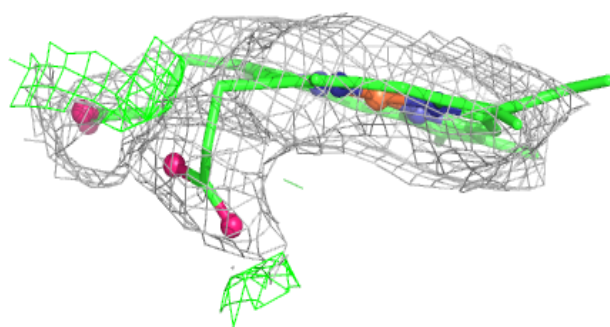
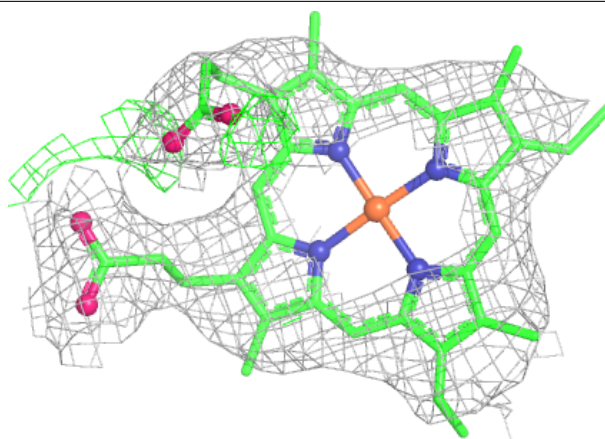
Electron density around HEM P 502:

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



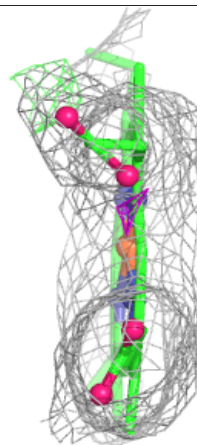
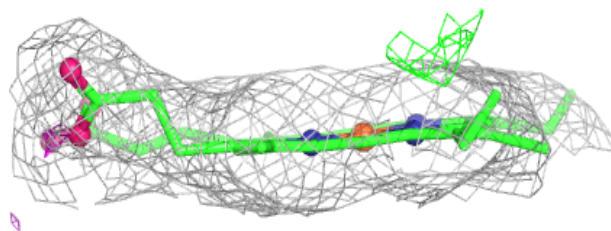
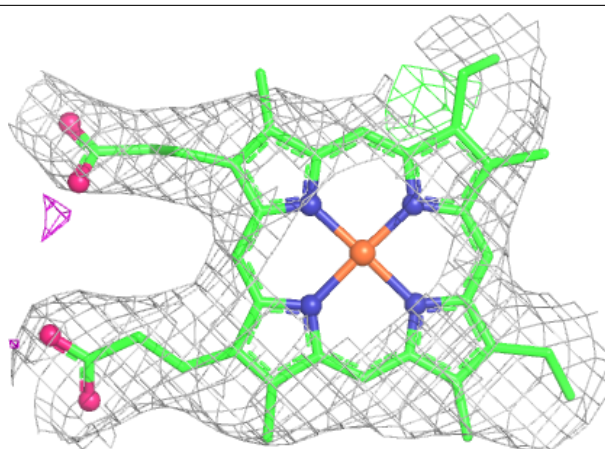
Electron density around HEM C 502:

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



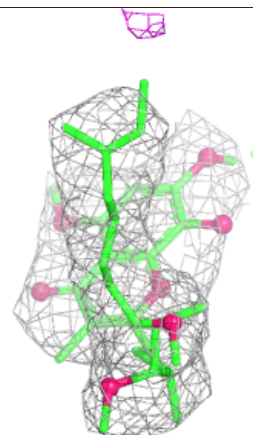
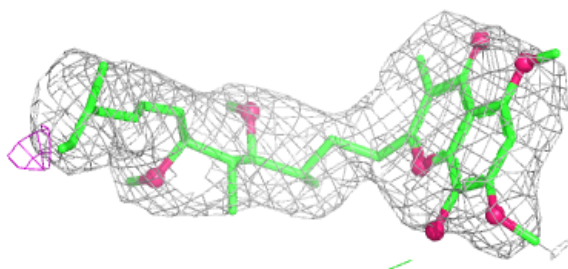
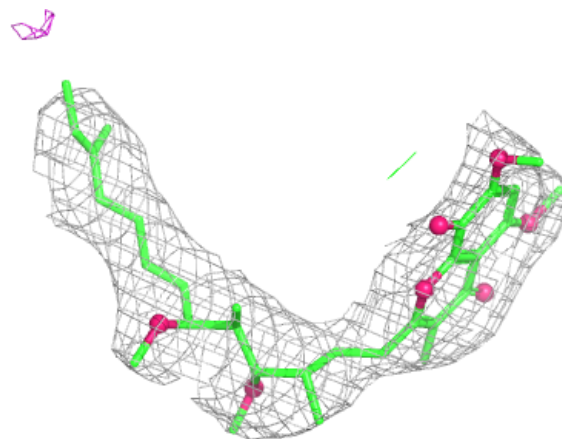
Electron density around HEC D 501:

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



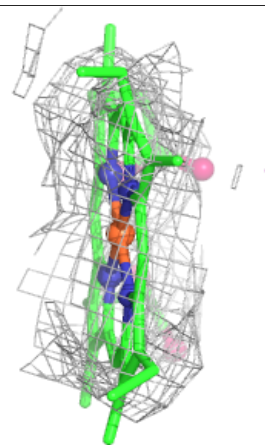
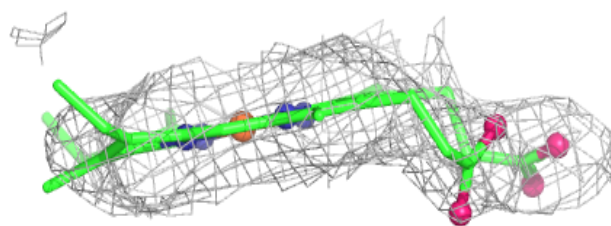
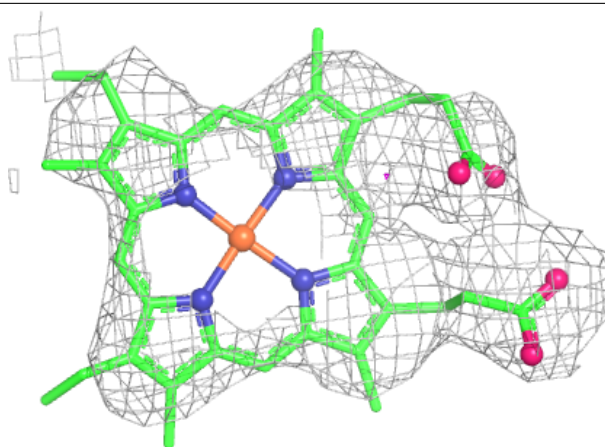
Electron density around SMA C 2001:

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



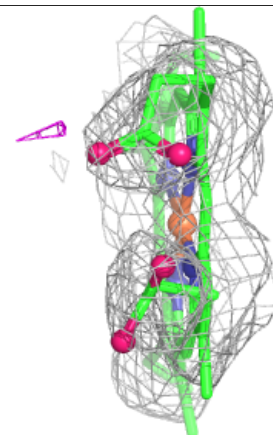
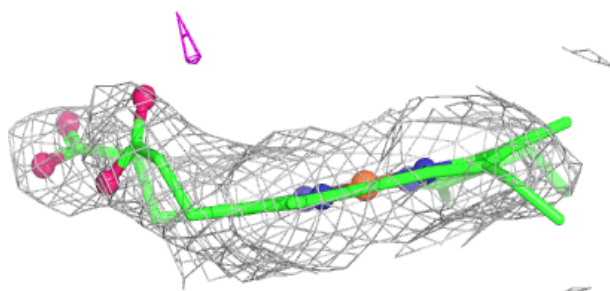
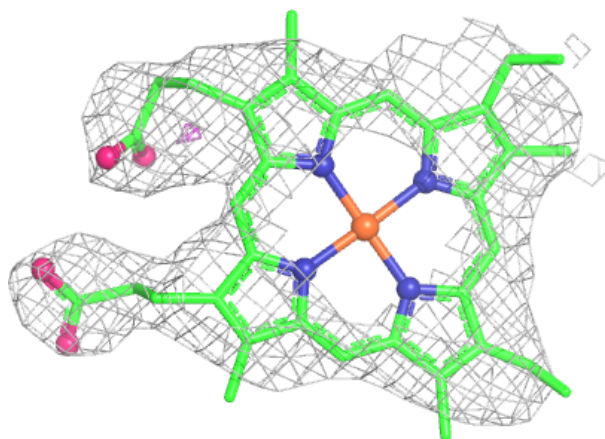
Electron density around HEM P 501:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.