



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:58 PM BST

PDB ID : 3CWB
Title : Chicken Cytochrome BC1 Complex inhibited by an iodinated analogue of the polyketide Crocacin-D
Authors : Huang, L.; Cromartie, T.; Viner, R.; Crowley, P.J.; Berry, E.A.
Deposited on : 2008-04-21
Resolution : 3.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

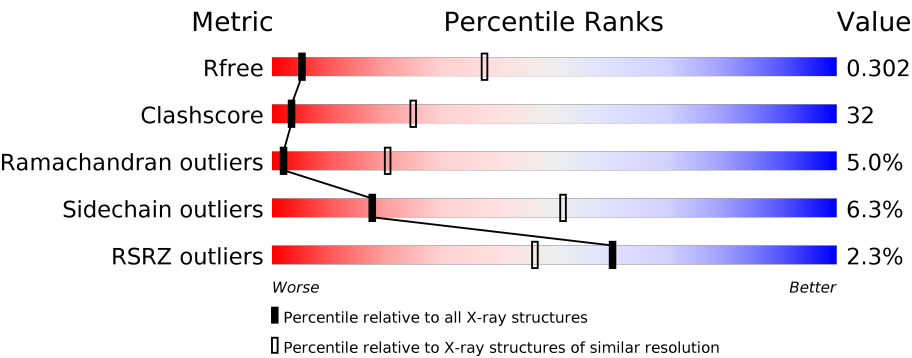
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div><div>%</div><div><div></div><div>48%</div><div>44%</div><div>7%</div><div></div></div><div></div></div>
1	N	446	<div><div>2%</div><div><div></div><div>46%</div><div>46%</div><div>7%</div><div></div></div><div></div></div>
2	B	441	<div><div>%</div><div><div></div><div>40%</div><div>49%</div><div>6%</div><div>5%</div><div></div></div><div></div></div>
2	O	441	<div><div>2%</div><div><div></div><div>39%</div><div>50%</div><div>6%</div><div></div></div><div></div></div>
3	C	380	<div><div>%</div><div><div></div><div>43%</div><div>50%</div><div>7%</div><div></div></div><div></div></div>
3	P	380	<div><div>2%</div><div><div></div><div>44%</div><div>48%</div><div>7%</div><div></div></div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	52	
9	V	52	
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	A	2008	-	-	-	X
11	PEE	C	2005	-	-	-	X
11	PEE	P	3008	-	X	-	X
11	PEE	W	3005	-	-	-	X
12	BOG	D	2091	-	-	-	X
12	BOG	P	2010	-	-	-	X
12	BOG	Q	3091	-	-	-	X
18	CDL	P	3003	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32696 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

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 MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

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

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

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
			1508	948	262	292	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			
6	S	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

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			

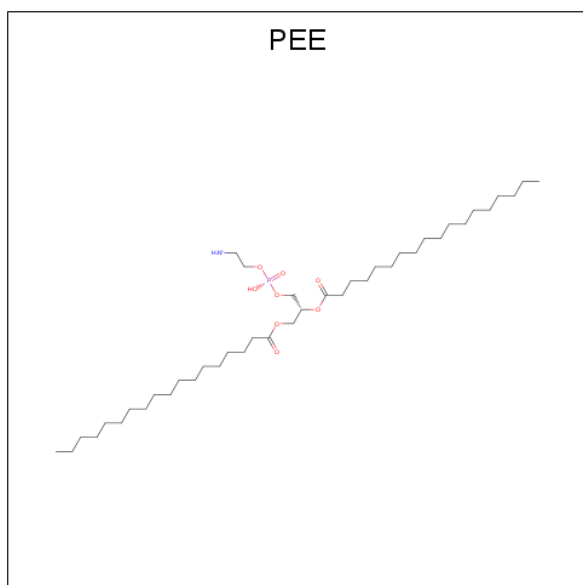
- Molecule 9 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	51	Total	C	N	O	S	0	0	2
			302	181	61	58	2			
9	V	49	Total	C	N	O	S	0	0	3
			292	176	59	55	2			

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

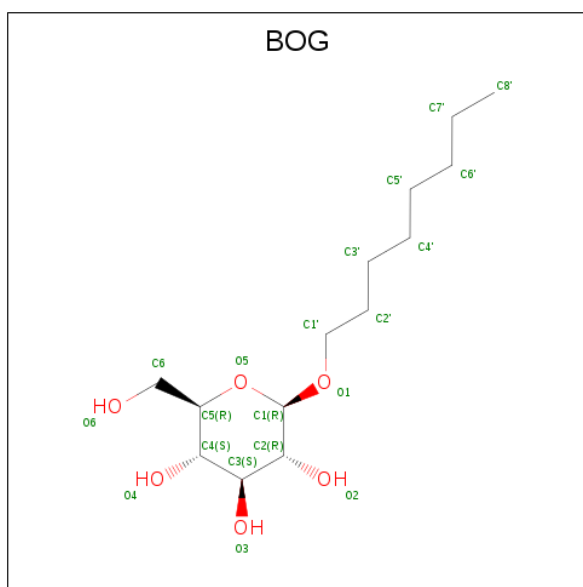
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

- Molecule 11 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



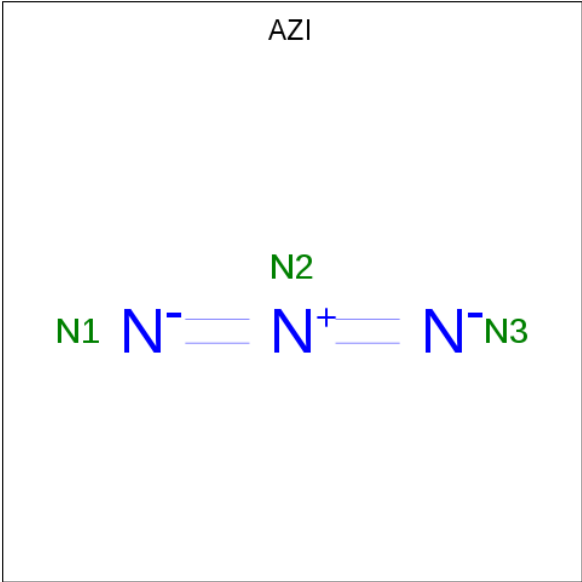
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	P	0	0
			21	12	8	1		
11	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	P	1	Total	O	P		0	0
			5	4	1			
11	W	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 12 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



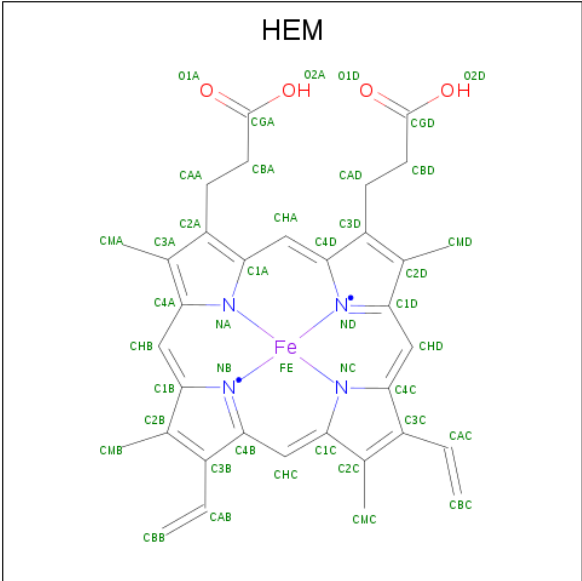
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			12	10	2		
12	D	1	Total	C	O	0	0
			20	14	6		
12	E	1	Total	C	O	0	0
			20	14	6		
12	P	1	Total	C	O	0	0
			19	13	6		
12	Q	1	Total	C	O	0	0
			20	14	6		
12	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	N			0	0
			3	3				
13	P	1	Total	N			0	0
			3	3				

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



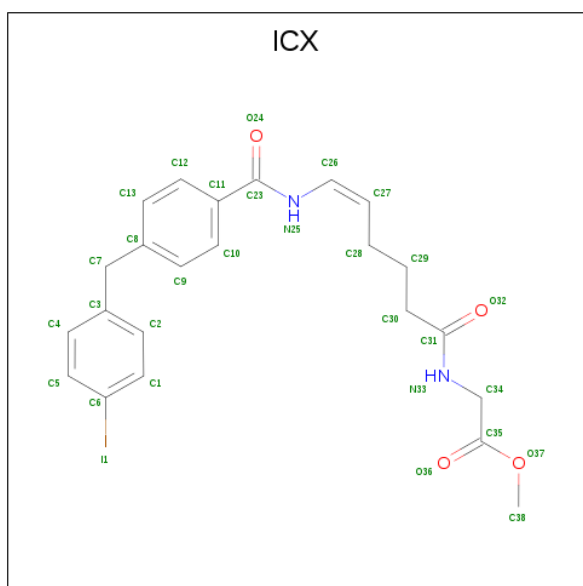
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

Continued on next page...

Continued from previous page...

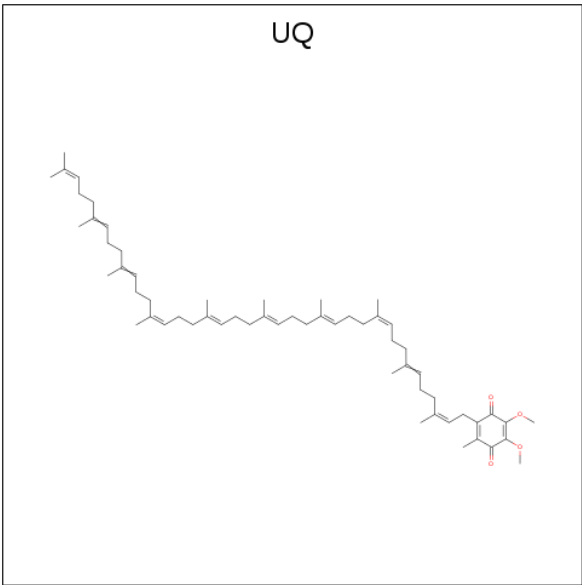
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
14	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
14	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 15 is methyl N-[(5Z)-6-({[4-(4-iodobenzyl)phenyl]carbonyl}amino)hex-5-enoyl]glycinate (three-letter code: ICX) (formula: C₂₃H₂₅IN₂O₄).



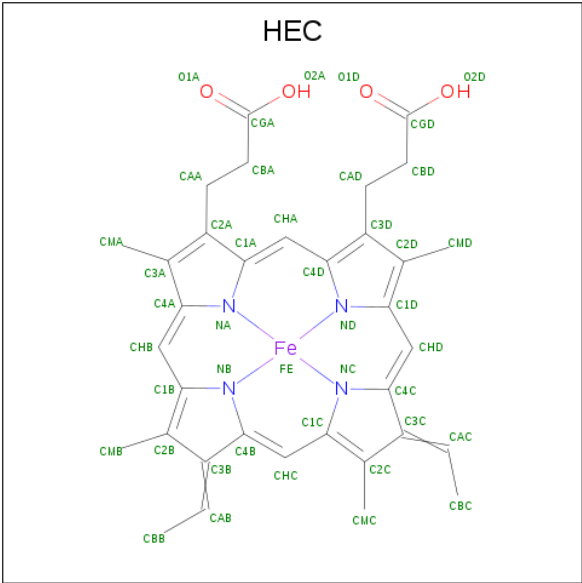
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	I	N	O	
			30	23	1	2	4	
15	P	1	Total	C	I	N	O	
			30	23	1	2	4	

- Molecule 16 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



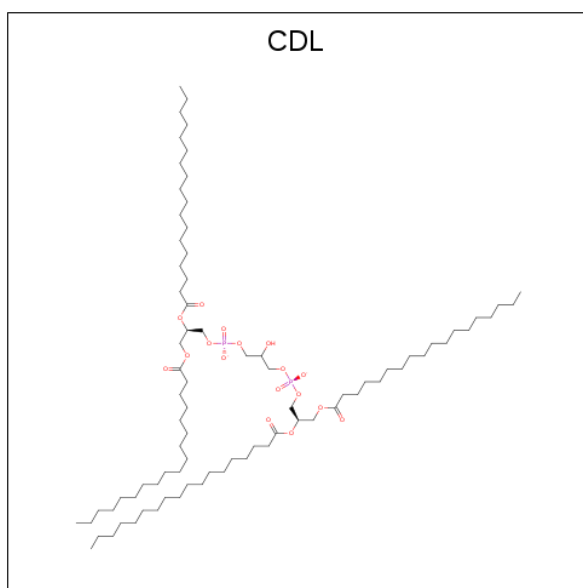
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			19	15	4		
16	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



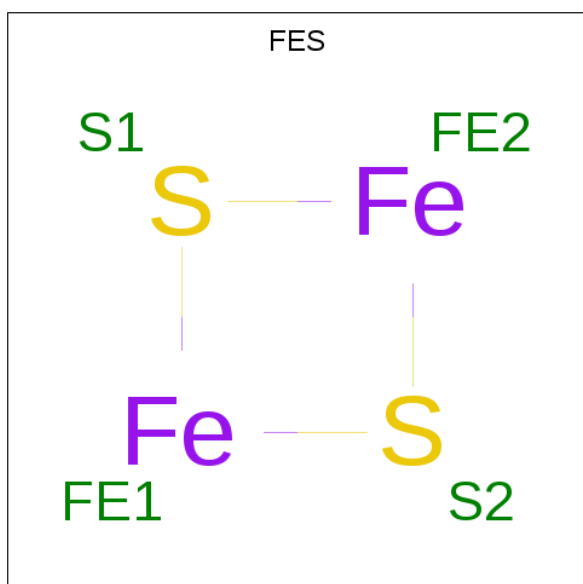
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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 UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	P	2	Total	O	0	0
			2	2		
20	Q	1	Total	O	0	0
			1	1		
20	E	1	Total	O	0	0
			2	2		

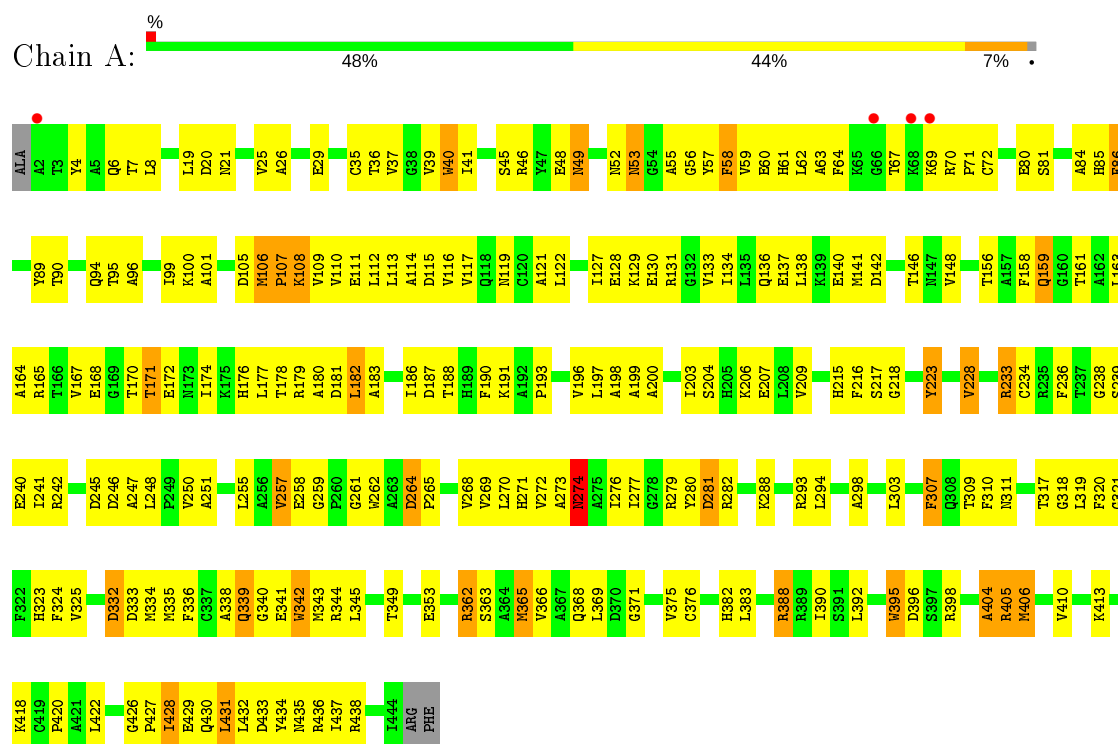
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	C	8	Total	O	0	0
			8	8		
21	P	7	Total	O	0	0
			7	7		
21	U	1	Total	O	0	0
			1	1		

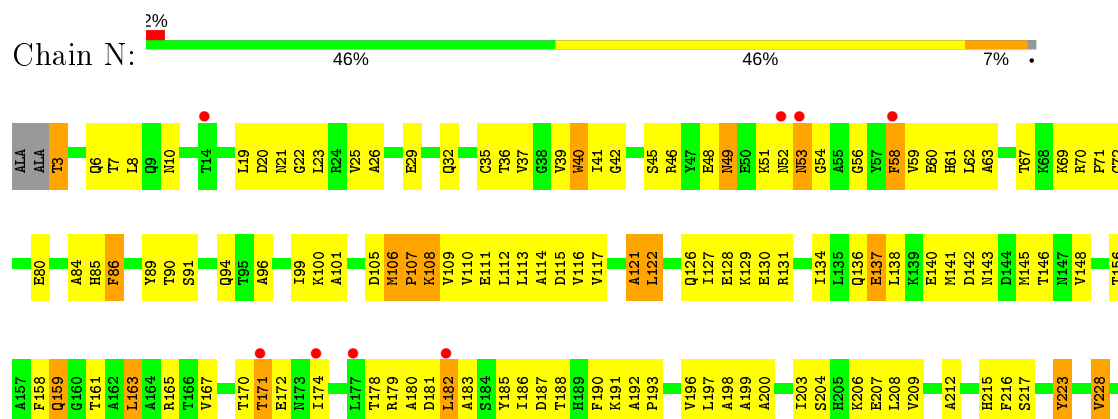
3 Residue-property plots

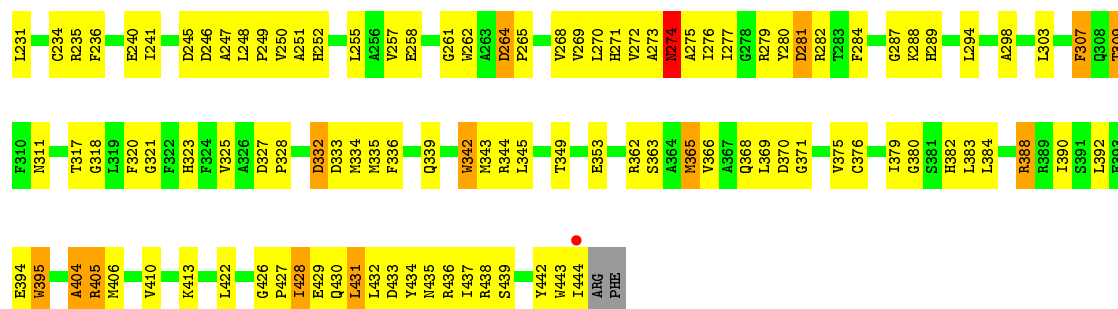
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

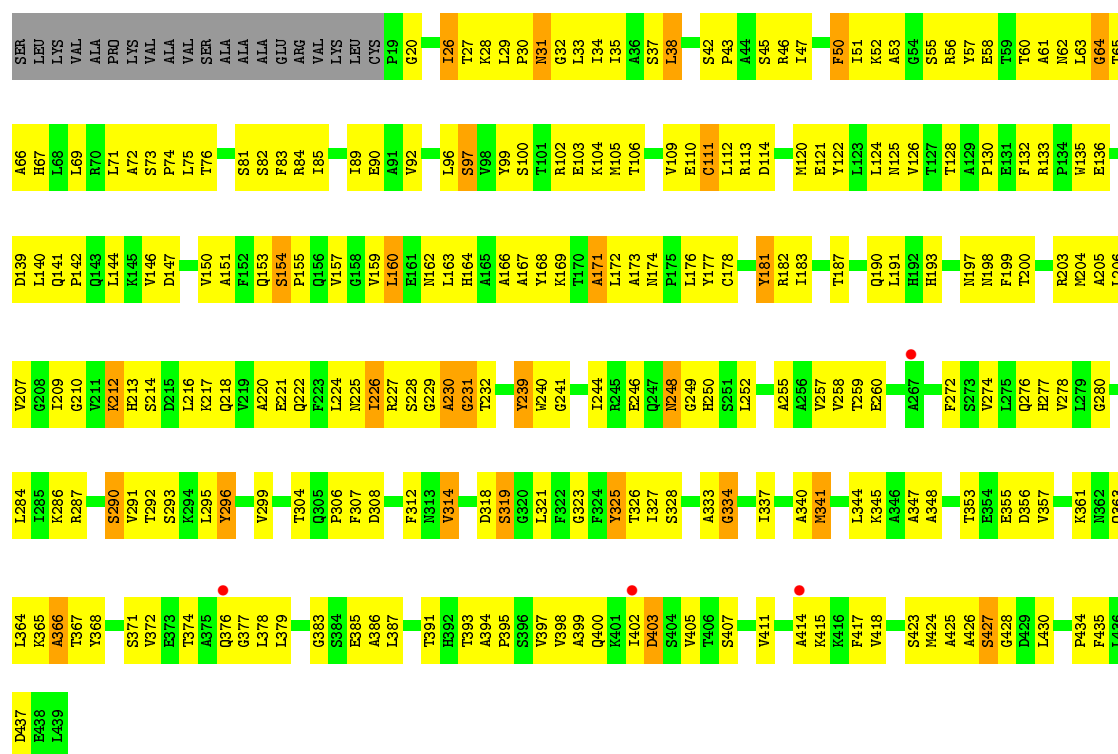
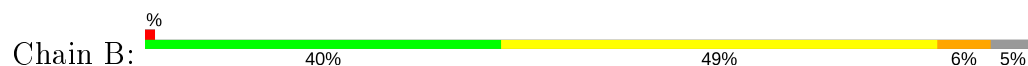


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

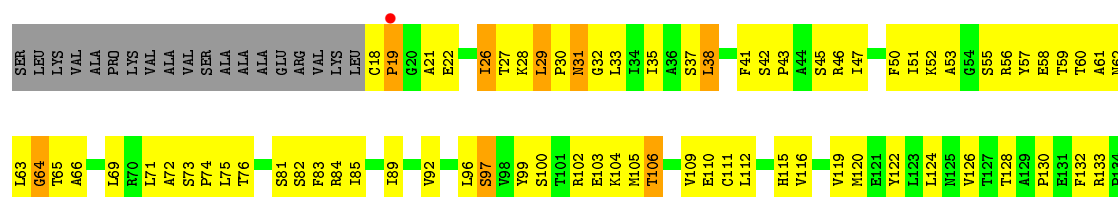


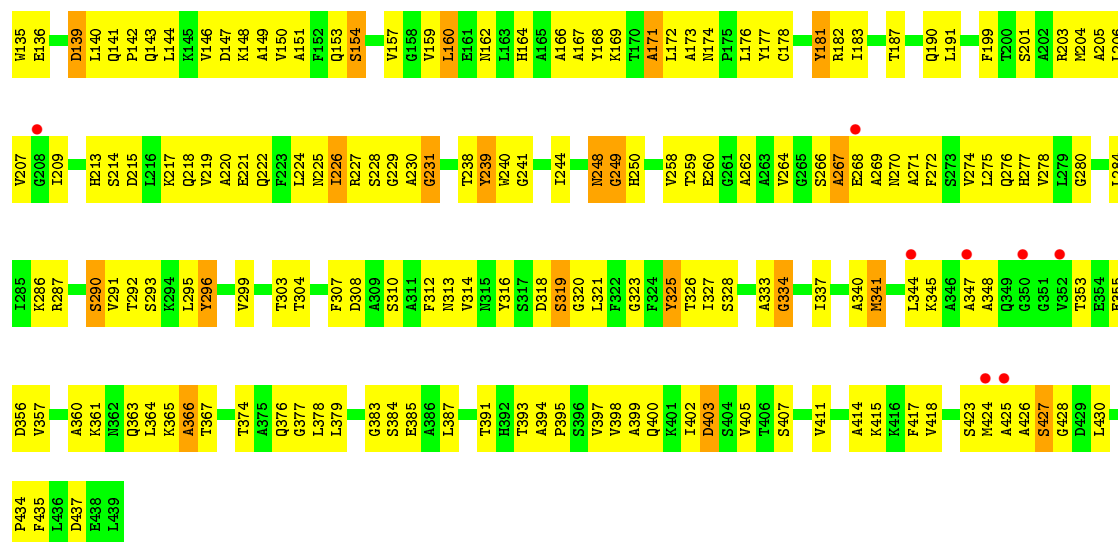


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

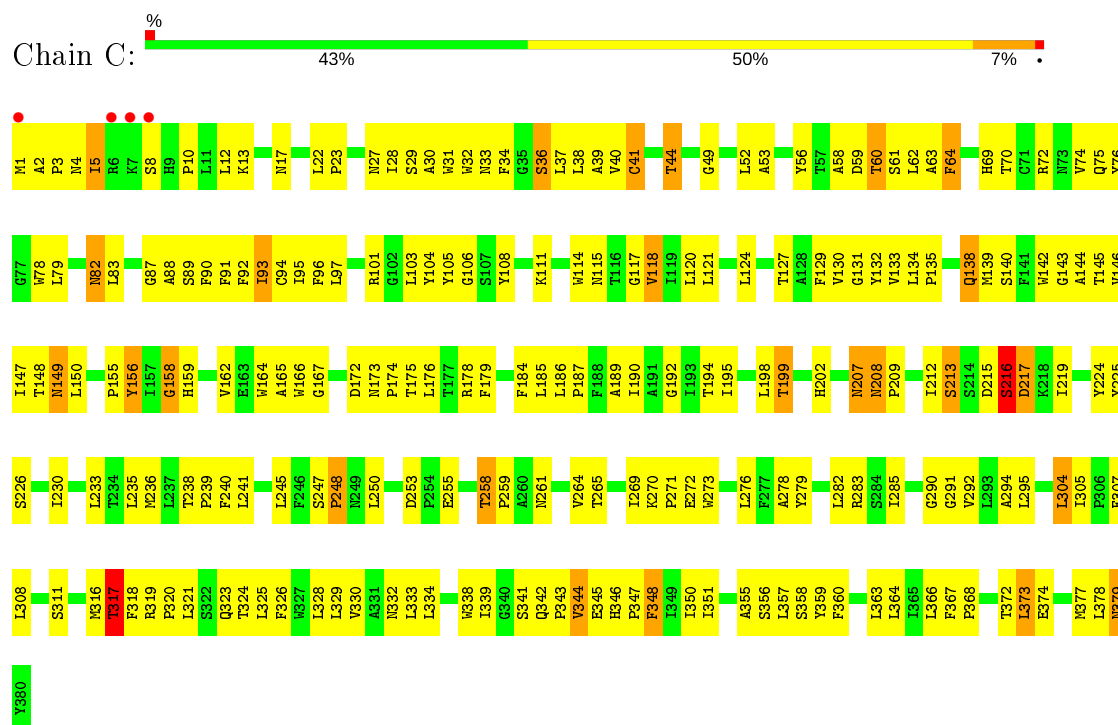


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

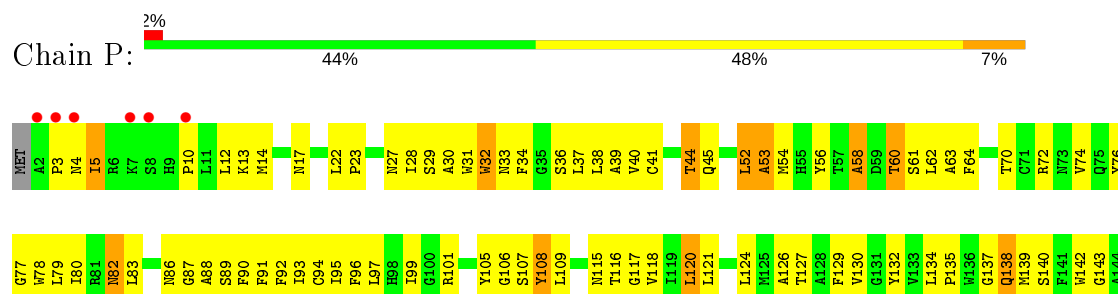


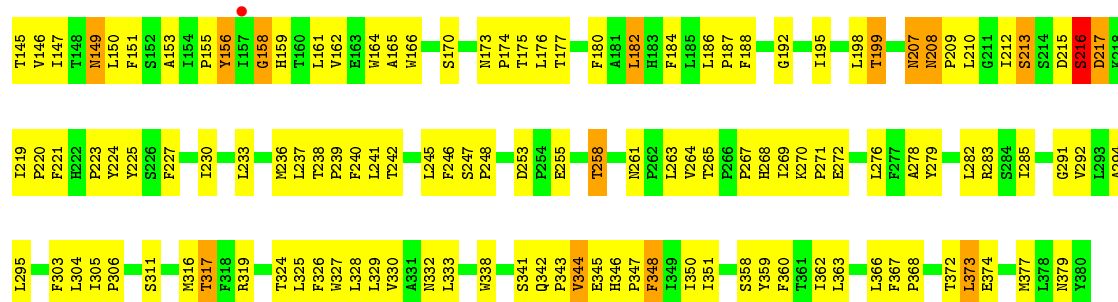


• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b





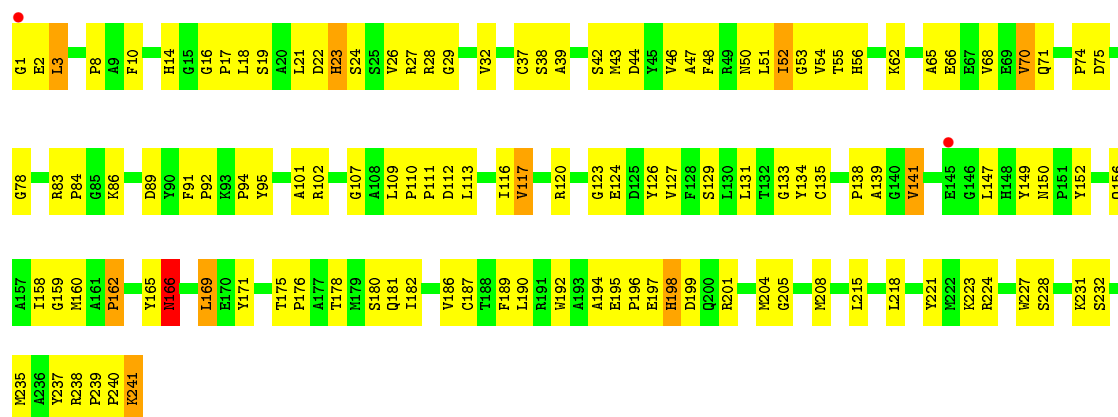
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D: 51% 46% .



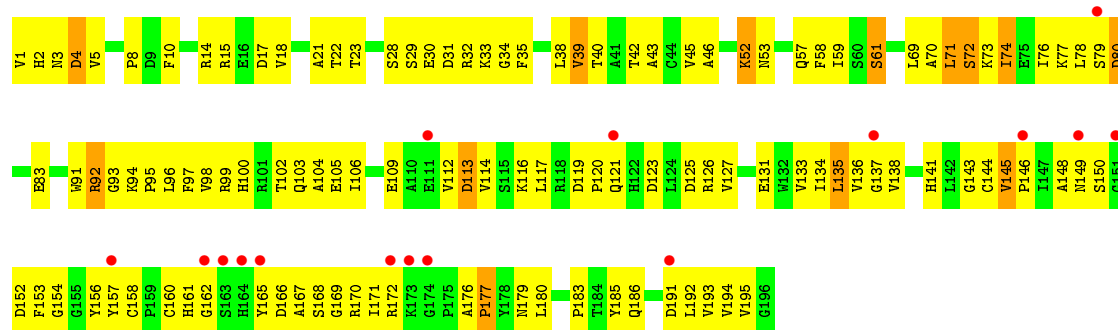
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q: 49% 47% .

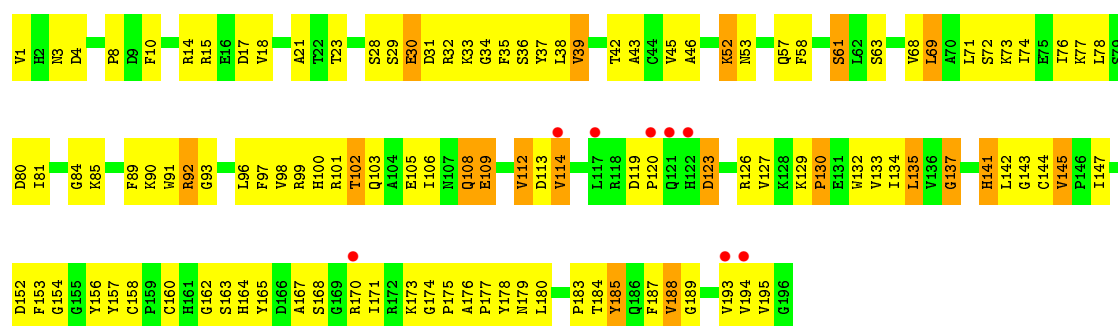


• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN

Chain E: 8% 39% 54% 7%



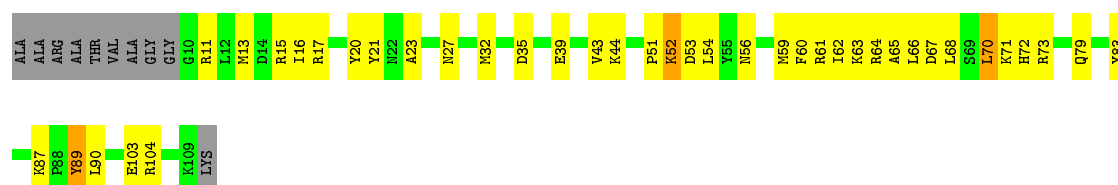
• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN



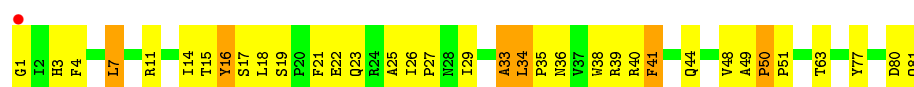
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



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



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



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



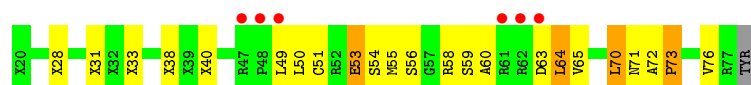
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



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

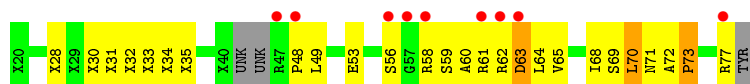


- Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence



- Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence

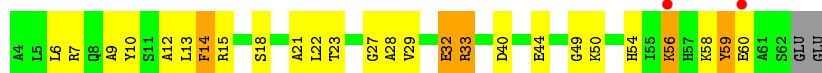




- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.78Å 182.66Å 242.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 3.51 44.88 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.8 (21.98-3.51) 98.9 (44.88-3.51)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.285 , 0.319 0.263 , 0.302	Depositor DCC
R_{free} test set	4918 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32696	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: AZI, CDL, UQ, ICX, FES, HEC, PEE, UNL, HEM, BOG

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	0.52	0/3511	0.72	0/4757
1	N	0.53	0/3508	0.72	0/4753
2	B	0.47	0/3196	0.66	0/4334
2	O	0.48	0/3202	0.67	0/4343
3	C	0.63	0/3122	0.76	0/4273
3	P	0.53	0/3114	0.72	0/4263
4	D	0.58	0/1956	0.72	0/2658
4	Q	0.47	0/1956	0.67	0/2658
5	E	0.42	0/1547	0.69	1/2103 (0.0%)
5	R	0.47	0/1542	0.73	1/2097 (0.0%)
6	F	0.66	0/901	0.72	0/1207
6	S	0.50	0/901	0.64	0/1207
7	G	0.58	0/698	0.70	0/946
7	T	0.49	0/680	0.65	0/923
8	H	0.53	0/582	0.67	0/779
8	U	0.37	0/561	0.68	1/751 (0.1%)
9	I	0.47	0/218	0.71	0/293
9	V	0.46	0/218	0.69	0/293
10	J	0.52	0/508	0.65	0/682
10	W	0.47	0/489	0.61	0/658
All	All	0.52	0/32410	0.70	3/43978 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	143	GLY	N-CA-C	7.12	130.89	113.10
5	E	143	GLY	N-CA-C	6.33	128.92	113.10
8	U	49	HIS	N-CA-C	-5.70	95.61	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	227	0
1	N	3437	0	3349	220	0
2	B	3141	0	3142	275	0
2	O	3147	0	3146	259	0
3	C	3020	0	3070	211	0
3	P	3012	0	3058	216	0
4	D	1898	0	1846	123	0
4	Q	1898	0	1846	135	0
5	E	1513	0	1478	128	0
5	R	1508	0	1466	131	0
6	F	881	0	887	42	0
6	S	881	0	887	48	0
7	G	676	0	659	42	0
7	T	658	0	647	48	0
8	H	574	0	548	37	0
8	U	553	0	535	40	0
9	I	302	0	251	36	0
9	V	292	0	251	29	0
10	J	497	0	490	19	0
10	W	478	0	478	29	0
11	A	21	0	13	0	0
11	C	99	0	149	5	0
11	P	54	0	72	2	0
11	W	50	0	77	1	0
12	C	12	0	18	0	0
12	D	20	0	28	5	0
12	E	20	0	28	1	0
12	P	19	0	24	1	0
12	Q	40	0	56	0	0
13	C	3	0	0	0	0
13	P	3	0	0	0	0
14	C	86	0	60	19	0
14	P	86	0	60	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	30	0	25	2	0
15	P	30	0	25	2	0
16	C	19	0	17	5	0
16	P	19	0	17	6	0
17	D	43	0	30	3	0
17	Q	43	0	30	3	0
18	D	42	0	28	3	0
18	G	40	0	24	1	0
18	P	82	0	52	5	0
19	E	4	0	0	1	0
19	R	4	0	0	0	0
20	E	2	0	0	0	0
20	P	2	0	0	0	0
20	Q	1	0	0	0	0
21	C	8	0	0	2	0
21	P	7	0	0	2	0
21	U	1	0	0	0	0
All	All	32696	0	32220	2098	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 32.

All (2098) 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:C:17:ASN:HD21	7:G:1:GLY:HA3	1.15	1.08
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.37	1.04
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.42	1.01
5:E:73:LYS:O	5:E:74:ILE:HG13	1.60	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	1.00
2:B:353:THR:HG22	2:B:355:GLU:H	1.26	0.98
5:E:74:ILE:HD12	5:E:195:VAL:HB	1.45	0.97
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.47	0.96
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	1.45	0.96
3:P:17:ASN:HD21	7:T:1:GLY:HA3	1.28	0.96
1:A:233:ARG:HB3	1:A:233:ARG:HH11	1.30	0.95
5:R:72:SER:HB3	5:R:92:ARG:HD3	1.49	0.95
1:A:336:PHE:HE2	3:C:4:ASN:HB3	1.29	0.95
2:B:76:THR:HG22	2:B:81:SER:HA	1.49	0.94
4:Q:224:ARG:HH21	7:T:26:ILE:HG23	1.27	0.94
4:D:224:ARG:HH21	7:G:26:ILE:HG23	1.32	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:THR:HG22	2:O:355:GLU:H	1.31	0.94
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.04	0.92
2:O:310:SER:HB2	9:V:59:SER:HB2	1.53	0.91
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.53	0.90
2:O:341:MET:HE2	2:O:341:MET:HA	1.55	0.88
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.74	0.88
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.88
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.09	0.88
2:B:248:ASN:ND2	2:B:428:GLY:HA2	1.89	0.88
2:O:76:THR:HG22	2:O:81:SER:HA	1.54	0.88
2:O:274:VAL:O	2:O:278:VAL:HG23	1.73	0.87
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.56	0.87
2:B:150:VAL:O	2:B:153:GLN:HG3	1.73	0.87
2:B:53:ALA:HB3	2:B:105:MET:HG3	1.54	0.87
2:O:361:LYS:O	2:O:365:LYS:HG3	1.75	0.85
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.41	0.84
5:R:98:VAL:HA	5:R:134:ILE:HG12	1.58	0.84
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.13	0.83
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.58	0.83
3:P:184:PHE:HA	14:P:501:HEM:HBC2	1.59	0.83
5:E:119:ASP:HB3	5:E:179:ASN:ND2	1.95	0.82
2:O:150:VAL:O	2:O:153:GLN:HG3	1.79	0.82
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.14	0.82
1:N:336:PHE:HE2	3:P:4:ASN:HB3	1.45	0.82
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.44	0.81
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.14	0.81
2:B:274:VAL:O	2:B:278:VAL:HG23	1.80	0.81
5:E:98:VAL:HA	5:E:134:ILE:HG12	1.61	0.81
6:S:89:TYR:HD1	6:S:90:LEU:N	1.79	0.81
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.16	0.81
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.63	0.80
6:F:89:TYR:HD1	6:F:90:LEU:N	1.78	0.80
2:O:53:ALA:HB3	2:O:105:MET:HG3	1.63	0.80
6:F:61:ARG:NH2	6:F:89:TYR:HE2	1.80	0.80
2:O:220:ALA:O	2:O:224:LEU:HB2	1.81	0.80
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.25	0.80
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.47	0.80
2:B:361:LYS:O	2:B:365:LYS:HG3	1.81	0.80
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.64	0.80
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.64	0.79
1:A:130:GLU:O	1:A:134:ILE:HG13	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLN:HE22	1:A:437:ILE:HG23	1.47	0.79
2:B:160:LEU:HD12	9:I:63:ASP:O	1.82	0.79
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.62	0.79
5:R:98:VAL:HG13	5:R:134:ILE:HD11	1.64	0.79
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.18	0.79
3:C:129:PHE:CZ	3:C:147:ILE:HB	2.17	0.79
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.64	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.79	0.79
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.47	0.78
1:N:105:ASP:O	1:N:109:VAL:HG23	1.82	0.78
5:R:58:PHE:O	5:R:61:SER:HB3	1.82	0.78
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.13	0.78
4:Q:239:PRO:HB2	4:Q:240:PRO:HD2	1.65	0.78
2:B:341:MET:HE2	2:B:341:MET:HA	1.64	0.78
9:I:63:ASP:O	9:I:64:LEU:HB2	1.84	0.78
2:B:327:ILE:HD11	9:I:58:ARG:O	1.84	0.78
1:A:339:GLN:NE2	1:A:437:ILE:HG23	1.99	0.78
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.64	0.78
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.66	0.77
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.77
1:A:277:ILE:HD11	1:A:345:LEU:HD11	1.66	0.77
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.49	0.77
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.19	0.77
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.19	0.77
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.48	0.77
2:O:248:ASN:ND2	2:O:428:GLY:HA2	1.98	0.77
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.20	0.77
3:P:347:PRO:O	3:P:350:ILE:HG22	1.85	0.77
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.05	0.77
5:E:76:ILE:O	5:E:192:LEU:HD12	1.85	0.76
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.50	0.76
3:P:127:THR:HG21	14:P:501:HEM:HBB2	1.66	0.76
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.33	0.76
5:R:102:THR:HG23	5:R:105:GLU:HG2	1.68	0.76
6:F:32:MET:CE	6:F:87:LYS:HG2	2.15	0.76
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.22	0.75
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.68	0.75
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.68	0.75
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.34	0.75
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.69	0.75
5:E:160:CYS:SG	3:P:269:ILE:HD13	2.27	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.50	0.75
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.87	0.75
2:O:248:ASN:HD22	2:O:248:ASN:C	1.86	0.75
5:R:71:LEU:HD22	5:R:92:ARG:NH1	2.02	0.74
6:S:61:ARG:NH2	6:S:89:TYR:HE2	1.85	0.74
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.69	0.74
2:O:47:ILE:HD12	2:O:47:ILE:N	2.02	0.74
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.22	0.74
3:C:17:ASN:ND2	7:G:1:GLY:HA3	1.98	0.74
1:N:342:TRP:HA	1:N:345:LEU:HD12	1.69	0.74
3:C:33:ASN:ND2	18:D:2003:CDL:H112	2.02	0.74
5:R:38:LEU:HD13	10:W:14:PHE:HZ	1.51	0.74
2:B:248:ASN:HD22	2:B:248:ASN:C	1.91	0.74
3:C:347:PRO:O	3:C:350:ILE:HG22	1.87	0.74
3:C:127:THR:HG21	14:C:501:HEM:HBB2	1.68	0.74
8:H:34:ARG:O	8:H:38:GLU:HG2	1.88	0.74
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.69	0.74
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.70	0.74
2:O:76:THR:CG2	2:O:82:SER:H	2.01	0.73
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.70	0.73
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.17	0.73
4:D:200:GLN:NE2	12:D:2091:BOG:H5	2.04	0.73
1:N:433:ASP:OD1	1:N:435:ASN:HB2	1.87	0.73
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.18	0.73
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.71	0.73
2:B:76:THR:CG2	2:B:82:SER:H	2.02	0.73
5:E:71:LEU:HB3	5:E:92:ARG:HD2	1.70	0.73
7:G:77:TYR:HA	7:G:80:ASP:OD1	1.89	0.73
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.04	0.73
2:O:154:SER:O	2:O:157:VAL:HG12	1.89	0.73
3:P:31:TRP:O	3:P:101:ARG:HG3	1.89	0.73
6:F:32:MET:HE1	6:F:87:LYS:HG2	1.70	0.73
2:B:47:ILE:HD12	2:B:47:ILE:N	2.03	0.73
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.71	0.73
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.53	0.73
1:N:339:GLN:NE2	1:N:437:ILE:HG23	2.04	0.73
3:P:129:PHE:CZ	3:P:147:ILE:HB	2.24	0.73
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.03	0.73
2:O:150:VAL:HG23	2:O:151:ALA:N	2.03	0.72
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.69	0.72
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:339:GLN:HE22	1:N:437:ILE:HG23	1.54	0.72
3:C:184:PHE:HA	14:C:501:HEM:HBC2	1.72	0.72
1:A:433:ASP:OD1	1:A:435:ASN:HB2	1.90	0.72
1:A:178:THR:HB	1:A:181:ASP:OD1	1.89	0.72
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.25	0.72
3:C:269:ILE:O	3:C:270:LYS:HD3	1.89	0.71
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.72	0.71
1:N:29:GLU:OE2	1:N:204:SER:HA	1.89	0.71
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.71	0.71
4:Q:117:VAL:HG21	4:Q:190:LEU:O	1.91	0.71
2:O:248:ASN:ND2	2:O:250:HIS:H	1.86	0.71
2:O:62:ASN:O	2:O:65:THR:HG22	1.91	0.71
5:E:98:VAL:HG13	5:E:134:ILE:HD11	1.73	0.71
1:N:130:GLU:O	1:N:134:ILE:HG13	1.90	0.71
2:O:327:ILE:HD11	9:V:58:ARG:O	1.88	0.71
1:N:3:THR:HG23	1:N:6:GLN:OE1	1.91	0.71
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.71	0.71
4:D:47:ALA:H	4:D:50:ASN:ND2	1.87	0.71
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.19	0.71
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.30	0.71
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.26	0.71
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.73	0.71
2:B:33:LEU:HD21	2:B:224:LEU:HD22	1.73	0.71
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.72	0.71
2:B:248:ASN:ND2	2:B:250:HIS:H	1.88	0.71
3:C:265:THR:HB	5:R:145:VAL:HG12	1.73	0.70
1:N:294:LEU:HD11	1:N:334:MET:CE	2.21	0.70
4:D:223:LYS:HD3	4:D:223:LYS:C	2.11	0.70
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.73	0.70
4:D:120:ARG:HH11	4:D:120:ARG:HG2	1.54	0.70
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.72	0.70
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.73	0.70
1:N:371:GLY:O	1:N:375:VAL:HG23	1.92	0.70
4:Q:120:ARG:HH11	4:Q:120:ARG:HG2	1.55	0.70
1:A:251:ALA:HB1	1:A:428:ILE:HG22	1.72	0.70
3:C:269:ILE:HD13	5:R:160:CYS:SG	2.32	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.70
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.26	0.70
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.74	0.70
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.74	0.70
1:N:298:ALA:HA	1:N:303:LEU:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TRP:HA	1:A:345:LEU:HD12	1.72	0.69
2:B:241:GLY:HA2	2:B:423:SER:OG	1.92	0.69
5:R:102:THR:O	5:R:106:ILE:HG13	1.92	0.69
3:C:344:VAL:HG21	5:R:162:GLY:HA3	1.73	0.69
3:C:265:THR:H	5:R:145:VAL:CG1	2.05	0.69
3:P:70:THR:HA	3:P:74:VAL:HG23	1.74	0.69
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.07	0.69
5:R:71:LEU:HD22	5:R:92:ARG:HH11	1.55	0.69
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.75	0.69
4:D:138:PRO:O	4:D:141:VAL:HG23	1.92	0.69
1:N:342:TRP:O	1:N:345:LEU:HB2	1.93	0.69
1:N:49:ASN:ND2	1:N:52:ASN:H	1.90	0.69
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.75	0.68
2:O:37:SER:HB3	2:O:213:HIS:ND1	2.08	0.68
2:B:258:VAL:HG11	2:B:312:PHE:CD2	2.28	0.68
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.68
1:A:140:GLU:OE2	9:I:50:LEU:HB2	1.92	0.68
1:N:277:ILE:HD11	1:N:345:LEU:HD11	1.74	0.68
2:B:150:VAL:HG23	2:B:151:ALA:N	2.07	0.68
1:A:294:LEU:HD11	1:A:334:MET:CE	2.24	0.68
1:N:251:ALA:HB1	1:N:428:ILE:HG22	1.76	0.68
2:O:407:SER:O	2:O:411:VAL:HG23	1.94	0.68
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.28	0.68
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.27	0.68
3:C:238:THR:HB	3:C:239:PRO:HD3	1.76	0.68
14:C:502:HEM:HMB1	14:C:502:HEM:HBB2	1.74	0.68
5:E:58:PHE:O	5:E:61:SER:HB3	1.94	0.68
3:P:359:TYR:HD2	3:P:360:PHE:HD1	1.41	0.68
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.74	0.68
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.77	0.67
3:C:187:PRO:HG2	14:C:501:HEM:HMC3	1.75	0.67
5:E:1:VAL:HG23	5:E:3:ASN:H	1.57	0.67
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.24	0.67
5:E:73:LYS:O	5:E:74:ILE:CG1	2.40	0.67
5:E:72:SER:H	5:E:92:ARG:HD3	1.58	0.67
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.29	0.67
8:U:34:ARG:O	8:U:38:GLU:HG2	1.93	0.67
1:A:105:ASP:O	1:A:109:VAL:HG23	1.94	0.67
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.28	0.67
1:A:29:GLU:OE2	1:A:204:SER:HA	1.95	0.67
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:56:LYS:HG2	10:W:60:GLU:HG3	1.77	0.67
5:R:72:SER:HB2	5:R:91:TRP:HE1	1.59	0.67
4:D:28:ARG:HD2	4:D:171:TYR:CE1	2.30	0.67
1:N:431:LEU:HD12	1:N:432:LEU:N	2.10	0.67
1:N:29:GLU:HG3	1:N:203:ILE:O	1.95	0.67
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.77	0.67
2:B:220:ALA:O	2:B:224:LEU:HB2	1.95	0.67
3:C:359:TYR:HD2	3:C:360:PHE:HD1	1.43	0.67
2:B:33:LEU:CD2	2:B:224:LEU:HD22	2.25	0.67
8:H:58:LEU:HG	8:H:62:LEU:HD12	1.76	0.67
1:A:294:LEU:HD11	1:A:334:MET:HE1	1.76	0.66
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.13	0.66
4:D:54:VAL:CG2	12:D:2091:BOG:H7'1	2.25	0.66
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.76	0.66
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.10	0.66
5:R:171:ILE:N	5:R:179:ASN:OD1	2.26	0.66
2:B:259:THR:HG22	2:B:260:GLU:N	2.10	0.66
4:D:43:MET:O	4:D:43:MET:HG3	1.96	0.66
7:G:40:ARG:HD2	18:G:2004:CDL:OA4	1.95	0.66
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.78	0.66
2:O:33:LEU:HD21	2:O:220:ALA:HB1	1.78	0.66
3:P:238:THR:HB	3:P:239:PRO:HD3	1.78	0.66
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.77	0.66
5:E:117:LEU:HD12	5:E:120:PRO:HA	1.78	0.66
4:Q:171:TYR:OH	4:Q:182:ILE:HA	1.96	0.66
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.76	0.66
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.76	0.66
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.78	0.66
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.26	0.66
2:O:241:GLY:HA2	2:O:423:SER:OG	1.95	0.66
5:R:168:SER:HB3	5:R:170:ARG:HG3	1.78	0.66
5:E:102:THR:O	5:E:106:ILE:HG13	1.96	0.66
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.77	0.66
3:P:41:CYS:O	3:P:44:THR:HG22	1.96	0.66
5:R:1:VAL:HG23	5:R:3:ASN:H	1.59	0.66
1:A:29:GLU:HG3	1:A:203:ILE:O	1.96	0.65
1:A:371:GLY:O	1:A:375:VAL:HG23	1.95	0.65
3:C:269:ILE:HG23	3:C:269:ILE:O	1.95	0.65
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.79	0.65
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.30	0.65
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:SER:HB2	2:B:213:HIS:HD1	1.60	0.65
5:E:83:GLU:HA	5:E:100:HIS:CG	2.31	0.65
5:E:38:LEU:HD13	10:J:14:PHE:HZ	1.60	0.65
5:R:185:TYR:HD2	5:R:185:TYR:H	1.43	0.65
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.26	0.65
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.78	0.65
1:N:49:ASN:C	1:N:49:ASN:HD22	1.99	0.65
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.61	0.65
1:N:156:THR:HA	1:N:159:GLN:HB3	1.77	0.65
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.61	0.65
1:A:431:LEU:HD12	1:A:432:LEU:N	2.11	0.65
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.31	0.65
1:N:107:PRO:HG2	1:N:108:LYS:H	1.60	0.65
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.77	0.65
5:E:83:GLU:HA	5:E:100:HIS:ND1	2.11	0.65
3:P:92:PHE:O	3:P:95:ILE:HG22	1.96	0.65
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.78	0.65
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.39	0.65
4:Q:117:VAL:HG23	4:Q:194:ALA:HB2	1.79	0.65
8:U:73:LEU:O	8:U:73:LEU:HD12	1.97	0.65
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.77	0.65
1:N:37:VAL:HG12	1:N:199:ALA:HB2	1.79	0.65
3:C:120:LEU:HD22	14:C:502:HEM:CAB	2.27	0.65
8:H:15:ASP:O	8:H:17:LEU:N	2.30	0.65
2:B:333:ALA:O	2:B:337:ILE:HG13	1.97	0.64
2:B:62:ASN:O	2:B:65:THR:HG22	1.97	0.64
1:A:298:ALA:HA	1:A:303:LEU:HD12	1.79	0.64
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.62	0.64
3:C:70:THR:HA	3:C:74:VAL:HG23	1.79	0.64
4:Q:95:TYR:CE2	4:Q:101:ALA:HA	2.32	0.64
3:C:271:PRO:HG2	3:C:276:LEU:HD23	1.79	0.64
3:C:127:THR:O	3:C:130:VAL:HG22	1.97	0.64
1:N:48:GLU:OE1	1:N:53:ASN:HA	1.98	0.64
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.13	0.64
1:A:170:THR:HG22	1:A:171:THR:N	2.11	0.64
2:B:212:LYS:HD3	2:B:213:HIS:N	2.13	0.64
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.79	0.64
1:N:35:CYS:HB2	1:N:200:ALA:O	1.97	0.64
3:P:79:LEU:HD11	3:P:83:LEU:HD11	1.80	0.64
4:Q:138:PRO:O	4:Q:141:VAL:HG23	1.98	0.64
3:C:198:LEU:HD21	14:C:502:HEM:CMA	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:VAL:HG23	4:D:194:ALA:HB2	1.80	0.64
5:E:94:LYS:HE2	3:P:170:SER:HB2	1.80	0.64
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.80	0.64
1:A:156:THR:HA	1:A:159:GLN:HB3	1.78	0.64
1:A:67:THR:HG21	1:A:115:ASP:OD2	1.98	0.64
6:F:52:LYS:CE	7:G:11:ARG:HH11	2.11	0.64
4:D:235:MET:HB3	7:G:15:THR:HG22	1.78	0.64
9:I:53:GLU:C	9:I:55:MET:H	2.02	0.64
2:O:337:ILE:O	2:O:340:ALA:HB3	1.98	0.63
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.81	0.63
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.80	0.63
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.34	0.63
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.63	0.63
4:Q:235:MET:HE1	6:S:63:LYS:C	2.19	0.63
1:A:245:ASP:OD1	1:A:247:ALA:HB3	1.98	0.63
2:O:71:LEU:O	2:O:74:PRO:HD2	1.98	0.63
5:R:18:VAL:HG23	5:R:18:VAL:O	1.97	0.63
3:C:13:LYS:O	3:C:17:ASN:HB2	1.97	0.63
3:C:120:LEU:HD22	14:C:502:HEM:CBB	2.28	0.63
1:N:170:THR:HG22	1:N:171:THR:N	2.14	0.63
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.89	0.63
4:Q:43:MET:HG2	4:Q:91:PHE:CD2	2.34	0.63
5:R:15:ARG:HD2	7:T:21:PHE:O	1.99	0.63
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.34	0.63
2:B:154:SER:O	2:B:157:VAL:HG12	1.98	0.63
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.34	0.63
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.39	0.63
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.81	0.63
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.29	0.63
1:A:433:ASP:O	1:A:437:ILE:HG13	1.99	0.63
1:A:69:LYS:CE	1:A:70:ARG:HH21	2.12	0.63
6:F:71:LYS:O	6:F:72:HIS:HB2	1.97	0.63
1:N:69:LYS:CE	1:N:70:ARG:HH21	2.12	0.63
3:P:32:TRP:HA	3:P:101:ARG:NH1	2.14	0.63
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.98	0.63
1:N:46:ARG:HH11	1:N:46:ARG:HG2	1.64	0.62
2:B:407:SER:O	2:B:411:VAL:HG23	1.99	0.62
1:N:284:PHE:CE2	9:V:71:ASN:O	2.52	0.62
2:B:110:GLU:O	2:B:111:CYS:HB3	1.99	0.62
2:O:150:VAL:CG2	2:O:151:ALA:N	2.61	0.62
2:O:76:THR:HG22	2:O:82:SER:H	1.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.29	0.62
1:A:107:PRO:HG2	1:A:108:LYS:H	1.64	0.62
2:B:424:MET:HG2	2:B:425:ALA:N	2.14	0.62
3:C:32:TRP:HA	3:C:101:ARG:NH1	2.15	0.62
4:D:218:LEU:HD13	5:E:43:ALA:N	2.14	0.62
5:E:77:LYS:HB2	5:E:80:ASP:OD2	2.00	0.62
2:O:166:ALA:HB2	2:O:244:ILE:HD12	1.82	0.62
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	1.82	0.62
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.80	0.62
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.35	0.62
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.64	0.62
3:P:70:THR:HA	3:P:74:VAL:CG2	2.29	0.62
4:Q:238:ARG:HB3	4:Q:238:ARG:NH1	2.15	0.62
2:B:60:THR:HG23	2:B:61:ALA:N	2.15	0.62
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.17	0.62
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.81	0.62
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.82	0.62
5:R:15:ARG:HG3	7:T:22:GLU:O	2.00	0.62
3:C:202:HIS:NE2	16:C:2002:UQ:O4	2.32	0.62
5:E:52:LYS:O	5:E:52:LYS:HD3	1.99	0.62
6:S:73:ARG:HG3	6:S:73:ARG:HH11	1.65	0.62
1:A:137:GLU:O	1:A:141:MET:HG3	1.99	0.61
3:C:32:TRP:HA	3:C:101:ARG:HH12	1.65	0.61
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.35	0.61
5:E:95:PRO:HG2	5:E:145:VAL:HG21	1.80	0.61
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.30	0.61
2:O:248:ASN:C	2:O:248:ASN:ND2	2.54	0.61
3:P:173:ASN:N	3:P:174:PRO:HD2	2.15	0.61
5:R:72:SER:HB3	5:R:92:ARG:CD	2.26	0.61
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.15	0.61
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.30	0.61
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.34	0.61
2:O:141:GLN:N	2:O:142:PRO:HD2	2.15	0.61
2:B:141:GLN:N	2:B:142:PRO:HD2	2.15	0.61
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.82	0.61
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.35	0.61
1:N:49:ASN:C	1:N:49:ASN:ND2	2.50	0.61
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.17	0.61
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.82	0.61
5:E:15:ARG:HD2	7:G:21:PHE:O	2.01	0.61
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:13:LYS:O	3:P:17:ASN:HB2	2.01	0.61
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.31	0.61
2:B:307:PHE:CD1	2:B:308:ASP:N	2.69	0.61
2:B:76:THR:HG22	2:B:82:SER:H	1.66	0.61
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.82	0.61
5:R:163:SER:OG	5:R:175:PRO:HD2	1.99	0.61
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.82	0.61
1:N:36:THR:OG1	1:N:100:LYS:HG2	2.01	0.61
1:A:178:THR:HG22	1:A:180:ALA:H	1.65	0.61
3:C:1:MET:HG2	3:C:2:ALA:H	1.65	0.61
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.30	0.61
14:C:502:HEM:HBB2	14:C:502:HEM:CMB	2.30	0.61
4:D:158:ILE:HG12	4:D:160:MET:H	1.63	0.61
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.36	0.61
4:Q:113:LEU:HD22	4:Q:116:ILE:HG21	1.82	0.61
4:Q:43:MET:HG3	4:Q:43:MET:O	2.00	0.61
9:V:70:LEU:O	9:V:70:LEU:HG	2.01	0.61
2:B:218:GLN:O	2:B:222:GLN:HG3	2.01	0.61
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.83	0.61
4:D:171:TYR:OH	4:D:182:ILE:HA	2.01	0.61
5:E:117:LEU:HD12	5:E:121:GLN:H	1.65	0.61
6:F:52:LYS:HE2	7:G:11:ARG:HH11	1.64	0.61
2:O:357:VAL:O	2:O:361:LYS:HG3	2.01	0.61
3:P:36:SER:O	3:P:39:ALA:N	2.33	0.61
5:R:177:PRO:C	5:R:178:TYR:HD2	2.03	0.61
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.36	0.61
4:D:117:VAL:HG21	4:D:190:LEU:O	2.00	0.61
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.30	0.61
1:A:369:LEU:HD11	1:A:392:LEU:HD21	1.83	0.60
1:A:49:ASN:ND2	1:A:52:ASN:H	1.99	0.60
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.83	0.60
4:D:197:GLU:HG2	4:D:198:HIS:N	2.16	0.60
4:D:224:ARG:HH12	4:D:231:LYS:HE2	1.66	0.60
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.82	0.60
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.60
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.36	0.60
1:A:40:TRP:HZ3	1:A:376:CYS:SG	2.24	0.60
5:E:52:LYS:C	5:E:52:LYS:HD3	2.22	0.60
5:R:188:VAL:HG12	5:R:189:GLY:N	2.16	0.60
1:A:233:ARG:HH11	1:A:233:ARG:CB	2.11	0.60
10:W:40:ASP:O	10:W:44:GLU:HG3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.83	0.60
9:I:70:LEU:HD23	9:I:71:ASN:HB2	1.81	0.60
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.66	0.60
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.35	0.60
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.16	0.60
3:C:173:ASN:N	3:C:174:PRO:HD2	2.17	0.60
3:C:265:THR:H	5:R:145:VAL:HG12	1.64	0.60
1:N:268:VAL:O	1:N:272:VAL:HG23	2.02	0.60
2:O:140:LEU:HD12	2:O:140:LEU:O	2.02	0.60
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.66	0.60
1:N:140:GLU:HG2	9:V:48:PRO:O	2.00	0.60
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.36	0.60
2:O:424:MET:HG2	2:O:425:ALA:N	2.16	0.60
5:R:52:LYS:HD3	5:R:52:LYS:C	2.22	0.60
3:P:198:LEU:HD21	14:P:502:HEM:CMA	2.32	0.60
5:R:96:LEU:HD12	5:R:135:LEU:O	2.02	0.60
4:Q:224:ARG:NH2	7:T:26:ILE:HG23	2.08	0.60
7:T:41:PHE:C	7:T:41:PHE:HD2	2.05	0.60
2:B:295:LEU:O	2:B:299:VAL:HG23	2.02	0.60
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.32	0.60
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.31	0.60
3:C:92:PHE:O	3:C:95:ILE:HG22	2.01	0.60
1:N:178:THR:HG22	1:N:180:ALA:H	1.65	0.60
1:N:433:ASP:O	1:N:437:ILE:HG13	2.02	0.60
3:P:271:PRO:HG2	3:P:276:LEU:HD23	1.84	0.60
1:A:46:ARG:HH11	1:A:46:ARG:HG2	1.67	0.59
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.83	0.59
4:D:109:LEU:O	4:D:111:PRO:HD3	2.02	0.59
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.84	0.59
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.17	0.59
1:N:80:GLU:OE2	2:O:290:SER:HA	2.02	0.59
6:S:52:LYS:HE2	7:T:11:ARG:HH11	1.67	0.59
3:P:79:LEU:O	3:P:79:LEU:HD12	2.02	0.59
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.66	0.59
3:C:30:ALA:HB1	18:D:2003:CDL:H111	1.84	0.59
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.84	0.59
3:P:30:ALA:HB1	18:P:3003:CDL:H111	1.84	0.59
3:P:33:ASN:HB3	21:P:3020:HOH:O	2.02	0.59
5:R:52:LYS:HD3	5:R:52:LYS:O	2.03	0.59
2:B:150:VAL:CG2	2:B:151:ALA:N	2.65	0.59
3:C:253:ASP:OD1	3:C:255:GLU:N	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.84	0.59
3:C:41:CYS:O	3:C:44:THR:HG22	2.03	0.59
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.38	0.59
2:B:46:ARG:HG3	2:B:110:GLU:HG2	1.84	0.59
4:D:186:VAL:O	4:D:190:LEU:HG	2.02	0.59
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.33	0.59
4:D:62:LYS:O	4:D:66:GLU:HG3	2.01	0.59
1:N:84:ALA:HB2	1:N:101:ALA:HB2	1.85	0.59
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.83	0.59
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.85	0.59
3:P:101:ARG:C	3:P:101:ARG:HD2	2.22	0.59
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.30	0.59
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.37	0.59
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.02	0.59
9:I:33:UNK:HB2	9:I:73:PRO:HB3	1.85	0.59
2:O:29:LEU:HD22	2:O:30:PRO:HD2	1.83	0.59
5:R:114:VAL:HG12	5:R:114:VAL:O	2.02	0.59
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.85	0.59
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.18	0.59
8:H:65:ARG:O	8:H:68:CYS:HB3	2.03	0.59
3:P:32:TRP:HA	3:P:101:ARG:HH12	1.68	0.59
1:N:90:THR:O	1:N:167:VAL:HG11	2.03	0.58
2:B:181:TYR:CE1	2:O:249:GLY:HA3	2.38	0.58
2:O:259:THR:HG22	2:O:260:GLU:N	2.18	0.58
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.18	0.58
8:U:15:ASP:O	8:U:17:LEU:N	2.36	0.58
1:A:106:MET:O	1:A:110:VAL:HG23	2.04	0.58
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.68	0.58
2:B:140:LEU:HD12	2:B:140:LEU:O	2.04	0.58
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.33	0.58
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.84	0.58
2:B:280:GLY:HA3	2:B:293:SER:OG	2.02	0.58
2:B:353:THR:HG22	2:B:355:GLU:N	2.09	0.58
5:E:117:LEU:CD1	5:E:121:GLN:H	2.15	0.58
1:A:161:THR:HG21	1:A:234:CYS:HA	1.85	0.58
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.19	0.58
2:B:199:PHE:O	2:B:226:ILE:HD13	2.04	0.58
3:C:195:ILE:O	3:C:199:THR:HB	2.03	0.58
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.58
2:O:60:THR:HG23	2:O:61:ALA:N	2.18	0.58
1:N:84:ALA:CB	1:N:101:ALA:HB2	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:30:UNK:HG3	9:V:31:UNK:N	2.19	0.58
2:B:76:THR:HG23	2:B:82:SER:H	1.67	0.58
4:D:43:MET:HG2	4:D:91:PHE:CD2	2.39	0.58
5:E:83:GLU:CG	5:E:102:THR:HG22	2.26	0.58
5:E:144:CYS:HB3	3:P:265:THR:HG21	1.85	0.58
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.33	0.58
4:D:200:GLN:HE21	12:D:2091:BOG:H5	1.69	0.58
5:E:109:GLU:OE2	5:E:166:ASP:HB2	2.03	0.58
6:F:73:ARG:HG3	6:F:73:ARG:HH11	1.68	0.58
2:O:75:LEU:HD11	2:O:140:LEU:HD23	1.86	0.58
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.85	0.58
8:U:65:ARG:O	8:U:68:CYS:HB3	2.04	0.58
4:Q:10:PHE:HD2	8:U:74:PHE:CE2	2.21	0.58
9:V:34:UNK:N	9:V:35:UNK:N	2.51	0.58
2:B:403:ASP:C	2:B:405:VAL:H	2.07	0.58
2:B:58:GLU:OE1	2:B:64:GLY:N	2.36	0.58
2:O:272:PHE:O	2:O:276:GLN:N	2.34	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.39	0.58
2:B:31:ASN:HB3	2:B:227:ARG:NH1	2.19	0.58
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.84	0.58
8:H:43:ARG:O	8:H:47:ARG:HG3	2.04	0.58
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.33	0.57
7:G:49:ALA:O	7:G:50:PRO:C	2.42	0.57
4:Q:10:PHE:HB3	8:U:74:PHE:CE2	2.39	0.57
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.86	0.57
6:F:53:ASP:OD1	6:F:54:LEU:N	2.37	0.57
2:O:307:PHE:CD1	2:O:308:ASP:N	2.71	0.57
3:P:142:TRP:O	3:P:146:VAL:HG23	2.04	0.57
5:R:33:LYS:HG2	7:T:21:PHE:CE1	2.38	0.57
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.38	0.57
1:A:269:VAL:HG11	1:A:410:VAL:HG21	1.86	0.57
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.86	0.57
4:D:37:CYS:C	4:D:39:ALA:H	2.07	0.57
4:Q:224:ARG:HH12	4:Q:231:LYS:HE2	1.66	0.57
6:S:13:MET:O	6:S:17:ARG:HG3	2.04	0.57
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.69	0.57
4:D:22:ASP:O	4:D:24:SER:N	2.37	0.57
2:O:146:VAL:HG12	2:O:147:ASP:N	2.18	0.57
4:Q:117:VAL:HG22	4:Q:190:LEU:HB3	1.85	0.57
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.69	0.57
1:A:49:ASN:ND2	1:A:49:ASN:C	2.56	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LYS:O	2:B:221:GLU:HG2	2.04	0.57
2:B:258:VAL:HG23	2:B:321:LEU:HD22	1.86	0.57
3:C:142:TRP:O	3:C:146:VAL:HG23	2.05	0.57
7:G:41:PHE:CD2	7:G:41:PHE:C	2.78	0.57
3:P:292:VAL:O	3:P:295:LEU:HB3	2.05	0.57
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.68	0.57
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.86	0.57
3:P:101:ARG:NH2	14:P:502:HEM:HBD2	2.20	0.57
4:Q:28:ARG:HD2	4:Q:171:TYR:CE1	2.40	0.57
3:C:33:ASN:HB3	21:C:3017:HOH:O	2.05	0.57
4:D:120:ARG:NH1	4:D:120:ARG:HG2	2.20	0.57
5:E:28:SER:O	5:E:32:ARG:HG3	2.04	0.57
2:B:50:PHE:CD1	2:B:50:PHE:N	2.72	0.57
4:D:102:ARG:NH1	4:D:107:GLY:O	2.38	0.57
7:G:41:PHE:HD2	7:G:41:PHE:C	2.07	0.57
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.87	0.57
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.86	0.57
1:A:268:VAL:O	1:A:272:VAL:HG23	2.05	0.57
3:C:292:VAL:O	3:C:295:LEU:HB3	2.05	0.57
1:N:182:LEU:O	1:N:186:ILE:HG13	2.05	0.57
1:A:114:ALA:HA	1:A:216:PHE:HE2	1.70	0.56
1:A:182:LEU:O	1:A:186:ILE:HG13	2.05	0.56
1:A:433:ASP:HB3	1:A:436:ARG:HB2	1.87	0.56
2:B:248:ASN:HD21	2:B:250:HIS:CB	2.18	0.56
2:B:71:LEU:O	2:B:74:PRO:HD2	2.04	0.56
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.20	0.56
5:E:145:VAL:O	5:E:145:VAL:HG12	2.04	0.56
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.87	0.56
5:E:71:LEU:HB3	5:E:92:ARG:CD	2.35	0.56
10:J:60:GLU:O	10:J:61:ALA:HB3	2.05	0.56
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.38	0.56
1:A:240:GLU:HA	1:A:422:LEU:O	2.05	0.56
2:B:314:VAL:HG11	9:I:63:ASP:HB3	1.86	0.56
1:N:136:GLN:C	1:N:138:LEU:H	2.07	0.56
2:O:258:VAL:HG11	2:O:312:PHE:CD2	2.40	0.56
3:P:269:ILE:HG23	3:P:269:ILE:O	2.04	0.56
5:R:38:LEU:HD13	10:W:14:PHE:CZ	2.37	0.56
7:T:41:PHE:CD2	7:T:41:PHE:C	2.76	0.56
1:A:342:TRP:O	1:A:345:LEU:HB2	2.04	0.56
1:N:178:THR:HB	1:N:181:ASP:OD1	2.04	0.56
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:37:SER:CB	2:O:213:HIS:ND1	2.68	0.56
2:B:248:ASN:ND2	2:B:248:ASN:C	2.57	0.56
3:C:88:ALA:O	3:C:91:PHE:HB3	2.05	0.56
4:D:54:VAL:HG21	12:D:2091:BOG:H7'1	1.87	0.56
1:N:429:GLU:OE1	7:T:7:LEU:HB2	2.06	0.56
1:A:170:THR:HG22	1:A:172:GLU:H	1.71	0.56
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.87	0.56
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.35	0.56
1:A:49:ASN:C	1:A:49:ASN:HD22	2.08	0.56
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.40	0.56
6:F:52:LYS:HE2	7:G:11:ARG:NH1	2.19	0.56
1:N:255:LEU:CD1	1:N:422:LEU:HD13	2.35	0.56
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.69	0.56
5:R:91:TRP:O	5:R:93:GLY:N	2.38	0.56
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.20	0.56
3:C:111:LYS:HE2	3:C:307:PHE:HE1	1.70	0.56
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.40	0.56
4:D:83:ARG:HB2	4:D:84:PRO:HD2	1.88	0.56
5:E:96:LEU:HD12	5:E:135:LEU:O	2.06	0.56
6:F:59:MET:HA	6:F:59:MET:CE	2.36	0.56
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.87	0.56
4:Q:43:MET:HG2	4:Q:91:PHE:HD2	1.69	0.56
8:U:58:LEU:HG	8:U:62:LEU:HD12	1.88	0.56
3:C:187:PRO:HG3	14:C:501:HEM:HBB2	1.87	0.56
1:N:45:SER:HA	1:N:48:GLU:CG	2.36	0.56
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.34	0.56
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.41	0.56
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.88	0.56
4:D:23:HIS:HB2	10:J:50:LYS:O	2.05	0.56
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.88	0.56
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.88	0.56
4:Q:117:VAL:HG21	4:Q:190:LEU:C	2.25	0.56
4:Q:43:MET:HE1	4:Q:189:PHE:HE2	1.71	0.56
2:B:318:ASP:O	2:B:319:SER:HB2	2.05	0.55
2:B:205:ALA:HB2	2:B:387:LEU:HD13	1.87	0.55
3:C:279:TYR:CZ	3:C:283:ARG:HD3	2.41	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.86	0.55
2:O:333:ALA:O	2:O:337:ILE:HG13	2.05	0.55
2:O:42:SER:OG	2:O:43:PRO:HD2	2.06	0.55
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.35	0.55
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:32:MET:CE	6:S:87:LYS:HG2	2.36	0.55
6:S:51:PRO:O	6:S:52:LYS:C	2.45	0.55
4:D:117:VAL:HG22	4:D:190:LEU:HB3	1.88	0.55
1:A:178:THR:O	1:A:179:ARG:C	2.45	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.07	0.55
5:E:185:TYR:CB	5:E:195:VAL:HG22	2.37	0.55
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.87	0.55
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.06	0.55
3:P:182:LEU:HD12	3:P:186:LEU:HD11	1.88	0.55
8:U:50:THR:OG1	8:U:51:GLU:N	2.39	0.55
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.21	0.55
3:C:101:ARG:C	3:C:101:ARG:HD2	2.27	0.55
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.41	0.55
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.55	0.55
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.88	0.55
2:B:124:LEU:HD12	2:B:128:THR:HG21	1.87	0.55
2:B:272:PHE:O	2:B:276:GLN:N	2.38	0.55
6:F:89:TYR:HD1	6:F:89:TYR:C	2.10	0.55
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.06	0.55
1:N:240:GLU:HA	1:N:422:LEU:O	2.06	0.55
2:O:205:ALA:HB2	2:O:387:LEU:HD13	1.87	0.55
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.40	0.55
2:B:230:ALA:O	2:B:232:THR:N	2.40	0.55
2:O:280:GLY:HA3	2:O:293:SER:OG	2.07	0.55
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.89	0.55
1:A:251:ALA:HB2	1:A:427:PRO:HD2	1.89	0.55
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.42	0.55
3:C:64:PHE:CD1	3:C:259:PRO:HG3	2.42	0.55
3:C:72:ARG:HG2	3:C:72:ARG:HH11	1.72	0.55
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.22	0.55
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.89	0.55
3:P:127:THR:O	3:P:130:VAL:HG22	2.06	0.55
1:A:277:ILE:CD1	1:A:345:LEU:HD11	2.35	0.55
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.22	0.55
16:C:2002:UQ:HM51	16:C:2002:UQ:C8	2.37	0.55
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.72	0.55
1:N:49:ASN:HD21	1:N:52:ASN:H	1.53	0.55
2:O:248:ASN:HD21	2:O:250:HIS:CB	2.19	0.55
2:O:76:THR:HG23	2:O:82:SER:H	1.69	0.55
2:B:402:ILE:O	2:B:405:VAL:HG23	2.07	0.55
3:C:187:PRO:HG3	14:C:501:HEM:CBB	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:PHE:HB2	21:C:3011:HOH:O	2.06	0.55
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.36	0.55
4:Q:120:ARG:NH1	4:Q:120:ARG:HG2	2.22	0.55
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.89	0.55
1:A:106:MET:CE	1:A:110:VAL:HG21	2.36	0.55
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.89	0.55
3:C:33:ASN:HD22	18:D:2003:CDL:H112	1.71	0.55
5:E:72:SER:C	5:E:73:LYS:HG3	2.27	0.55
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.87	0.55
8:H:73:LEU:HD12	8:H:73:LEU:O	2.07	0.55
3:P:132:TYR:HA	14:P:501:HEM:HAA2	1.89	0.55
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.88	0.55
6:S:89:TYR:HD1	6:S:89:TYR:C	2.10	0.55
6:S:52:LYS:CE	7:T:11:ARG:HH11	2.18	0.55
9:V:64:LEU:HD12	9:V:77:ARG:C	2.27	0.55
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.72	0.54
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.22	0.54
2:O:323:GLY:HA2	2:O:417:PHE:HE1	1.72	0.54
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.41	0.54
8:U:35:GLU:HA	8:U:38:GLU:HG3	1.89	0.54
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.40	0.54
10:J:6:LEU:O	10:J:9:ALA:HB3	2.08	0.54
2:B:286:LYS:HG2	2:B:287:ARG:HG3	1.90	0.54
2:O:402:ILE:O	2:O:405:VAL:HG23	2.07	0.54
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.07	0.54
2:B:220:ALA:HA	2:B:224:LEU:HD13	1.89	0.54
1:N:106:MET:O	1:N:110:VAL:HG23	2.08	0.54
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.23	0.54
1:A:36:THR:OG1	1:A:100:LYS:HG2	2.06	0.54
1:A:365:MET:O	1:A:368:GLN:HB2	2.08	0.54
2:B:252:LEU:CD1	9:I:49:LEU:HB2	2.37	0.54
3:C:56:TYR:OH	3:C:176:LEU:HD11	2.08	0.54
1:N:45:SER:HA	1:N:48:GLU:HG3	1.88	0.54
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.38	0.54
5:R:78:LEU:HD22	5:R:132:TRP:CD2	2.43	0.54
3:C:31:TRP:O	3:C:101:ARG:HG3	2.08	0.54
3:C:22:LEU:HD21	16:C:2002:UQ:O4	2.08	0.54
5:E:102:THR:OG1	5:E:104:ALA:HB3	2.08	0.54
9:I:70:LEU:C	9:I:70:LEU:HD23	2.28	0.54
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.38	0.54
4:D:169:LEU:HD23	4:D:169:LEU:C	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:THR:HG22	2:O:355:GLU:N	2.13	0.54
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.07	0.54
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.38	0.54
1:N:206:LYS:O	1:N:209:VAL:HG12	2.08	0.54
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.42	0.54
3:P:37:LEU:O	3:P:41:CYS:HB2	2.08	0.54
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.08	0.54
5:R:193:VAL:HG22	5:R:194:VAL:N	2.23	0.54
1:A:307:PHE:C	1:A:307:PHE:CD1	2.81	0.54
2:B:47:ILE:HG12	2:B:120:MET:CE	2.38	0.54
8:H:24:CYS:C	8:H:26:GLN:H	2.11	0.54
1:N:40:TRP:HZ3	1:N:376:CYS:SG	2.30	0.54
6:S:21:TYR:C	6:S:21:TYR:CD2	2.82	0.54
2:B:323:GLY:HA2	2:B:417:PHE:HE1	1.73	0.54
4:D:43:MET:HE1	4:D:189:PHE:HE2	1.72	0.54
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.90	0.54
2:O:266:SER:O	2:O:268:GLU:N	2.41	0.54
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.90	0.54
3:P:198:LEU:HD21	14:P:502:HEM:HMA1	1.88	0.54
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.43	0.54
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.23	0.53
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.38	0.53
2:B:357:VAL:O	2:B:361:LYS:HG3	2.08	0.53
3:C:198:LEU:HD21	14:C:502:HEM:HMA1	1.89	0.53
1:N:127:ILE:C	1:N:129:LYS:H	2.10	0.53
2:O:47:ILE:CD1	2:O:47:ILE:N	2.71	0.53
3:P:253:ASP:OD1	3:P:255:GLU:N	2.40	0.53
3:P:282:LEU:HD12	3:P:291:GLY:C	2.29	0.53
3:P:31:TRP:HE1	18:P:3004:CDL:H1	1.73	0.53
3:P:118:VAL:HG11	3:P:303:PHE:CE1	2.43	0.53
6:S:89:TYR:CD1	6:S:89:TYR:C	2.81	0.53
1:A:48:GLU:OE1	1:A:53:ASN:HA	2.06	0.53
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.71	0.53
4:D:171:TYR:HD1	4:D:175:THR:HB	1.73	0.53
4:D:224:ARG:NH2	7:G:26:ILE:HG23	2.13	0.53
2:O:225:ASN:O	2:O:226:ILE:C	2.45	0.53
8:U:73:LEU:HD12	8:U:73:LEU:C	2.28	0.53
1:A:250:VAL:HG21	1:A:325:VAL:CG1	2.39	0.53
1:A:362:ARG:HG3	1:A:365:MET:HE1	1.90	0.53
1:A:95:THR:HG22	1:A:96:ALA:N	2.23	0.53
2:B:428:GLY:O	2:B:430:LEU:HG	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:MET:O	3:C:140:SER:C	2.47	0.53
3:C:38:LEU:HB3	14:C:502:HEM:CMB	2.39	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.24	0.53
6:F:89:TYR:C	6:F:89:TYR:CD1	2.80	0.53
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.43	0.53
1:A:45:SER:HA	1:A:48:GLU:CG	2.38	0.53
1:N:271:HIS:NE2	1:N:311:ASN:HB3	2.23	0.53
2:O:150:VAL:CG2	2:O:151:ALA:H	2.21	0.53
2:O:393:THR:CG2	2:O:397:VAL:HB	2.39	0.53
3:P:72:ARG:HH11	3:P:72:ARG:HG2	1.72	0.53
4:D:37:CYS:O	4:D:39:ALA:N	2.40	0.53
5:E:114:VAL:O	5:E:114:VAL:HG12	2.08	0.53
5:E:126:ARG:HH11	5:E:126:ARG:HG2	1.73	0.53
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.44	0.53
1:N:137:GLU:O	1:N:141:MET:HG3	2.08	0.53
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.44	0.53
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.43	0.53
4:Q:94:PRO:HB2	4:Q:95:TYR:CE1	2.43	0.53
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.24	0.53
5:R:177:PRO:C	5:R:178:TYR:CD2	2.82	0.53
5:E:79:SER:HB3	5:E:191:ASP:HB2	1.90	0.53
2:O:57:TYR:N	2:O:57:TYR:CD1	2.76	0.53
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.43	0.53
5:R:147:ILE:N	5:R:157:TYR:O	2.40	0.53
1:A:90:THR:O	1:A:167:VAL:HG11	2.09	0.53
3:C:118:VAL:N	14:C:502:HEM:HBC2	2.24	0.53
3:C:70:THR:HA	3:C:74:VAL:CG2	2.38	0.53
4:D:10:PHE:N	4:D:10:PHE:CD1	2.76	0.53
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	2.94	0.53
3:C:344:VAL:HG21	5:R:162:GLY:CA	2.39	0.53
6:S:70:LEU:HD12	6:S:70:LEU:O	2.09	0.53
2:O:229:GLY:C	2:O:231:GLY:H	2.12	0.53
2:O:258:VAL:HG23	2:O:321:LEU:HD22	1.91	0.53
1:A:247:ALA:HB2	7:G:11:ARG:HD2	1.90	0.53
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.38	0.53
2:B:398:VAL:HG13	2:B:399:ALA:N	2.22	0.53
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.08	0.53
6:F:20:TYR:O	6:F:23:ALA:HB3	2.09	0.53
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.14	0.53
6:F:51:PRO:O	6:F:52:LYS:C	2.48	0.53
1:N:156:THR:HG21	1:N:241:ILE:HG22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.44	0.53
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.90	0.53
2:O:97:SER:HB3	9:V:69:SER:OG	2.08	0.53
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.16	0.53
1:A:259:GLY:N	1:A:318:GLY:O	2.31	0.53
3:C:56:TYR:OH	3:C:134:LEU:O	2.25	0.53
5:E:168:SER:HB3	5:E:170:ARG:HG3	1.90	0.53
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.44	0.53
6:F:89:TYR:CD1	6:F:90:LEU:N	2.69	0.53
8:H:35:GLU:HA	8:H:38:GLU:HG3	1.91	0.53
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.08	0.53
3:P:279:TYR:CZ	3:P:283:ARG:HD3	2.44	0.53
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.91	0.53
2:B:306:PRO:CB	9:I:51:CYS:HA	2.40	0.52
3:C:330:VAL:O	3:C:333:LEU:HB2	2.08	0.52
3:C:37:LEU:O	3:C:41:CYS:HB2	2.08	0.52
3:C:120:LEU:HB3	14:C:502:HEM:HAB	1.91	0.52
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.69	0.52
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.90	0.52
1:N:85:HIS:HD2	2:O:284:LEU:HB3	1.74	0.52
3:P:326:PHE:O	3:P:330:VAL:HG23	2.09	0.52
5:E:162:GLY:HA3	3:P:344:VAL:HG21	1.90	0.52
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.74	0.52
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.44	0.52
3:C:28:ILE:CD1	16:C:2002:UQ:HM21	2.38	0.52
5:E:91:TRP:O	5:E:93:GLY:N	2.42	0.52
7:G:80:ASP:O	7:G:81:GLN:HG3	2.10	0.52
8:H:26:GLN:HA	8:H:26:GLN:OE1	2.09	0.52
3:P:34:PHE:HB2	21:P:3015:HOH:O	2.09	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG2	1.91	0.52
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.42	0.52
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.91	0.52
5:R:38:LEU:O	5:R:38:LEU:HD12	2.10	0.52
3:C:338:TRP:O	3:C:341:SER:HB3	2.08	0.52
2:O:403:ASP:C	2:O:405:VAL:H	2.11	0.52
2:O:50:PHE:C	2:O:51:ILE:HG13	2.29	0.52
2:O:58:GLU:OE1	2:O:64:GLY:N	2.42	0.52
3:P:270:LYS:O	3:P:270:LYS:HG3	2.08	0.52
6:S:67:ASP:OD1	6:S:71:LYS:HD2	2.09	0.52
8:U:31:VAL:HA	8:U:34:ARG:HB3	1.91	0.52
4:Q:180:SER:OG	8:U:77:LEU:HD21	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:LEU:HD22	2:B:30:PRO:HD2	1.91	0.52
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.44	0.52
5:E:18:VAL:O	5:E:18:VAL:HG23	2.10	0.52
7:G:38:TRP:O	7:G:39:ARG:C	2.47	0.52
1:N:22:GLY:O	1:N:193:PRO:HA	2.10	0.52
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.25	0.52
16:P:3002:UQ:C8	16:P:3002:UQ:HM51	2.39	0.52
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.25	0.52
5:R:33:LYS:O	5:R:34:GLY:C	2.48	0.52
1:A:61:HIS:ND1	1:A:134:ILE:HG12	2.25	0.52
2:B:102:ARG:CZ	2:B:164:HIS:CD2	2.92	0.52
2:B:212:LYS:HD2	2:B:214:SER:OG	2.10	0.52
2:B:393:THR:CG2	2:B:397:VAL:HB	2.39	0.52
1:N:307:PHE:CD1	1:N:307:PHE:C	2.82	0.52
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.40	0.52
2:O:215:ASP:C	2:O:217:LYS:N	2.62	0.52
2:O:286:LYS:HG2	2:O:287:ARG:HG3	1.92	0.52
3:P:147:ILE:O	3:P:150:LEU:HB2	2.10	0.52
4:Q:29:GLY:O	4:Q:32:VAL:HB	2.08	0.52
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.91	0.52
3:C:162:VAL:O	3:C:165:ALA:HB3	2.09	0.52
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.10	0.52
3:P:72:ARG:NH1	3:P:72:ARG:HG2	2.24	0.52
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.73	0.52
2:B:176:LEU:O	2:B:176:LEU:HD12	2.10	0.52
4:D:113:LEU:HD22	4:D:116:ILE:HG21	1.92	0.52
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.37	0.52
4:Q:126:TYR:CD2	4:Q:126:TYR:C	2.82	0.52
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.91	0.52
1:A:280:TYR:CG	1:A:281:ASP:N	2.78	0.52
2:B:187:THR:OG1	2:B:190:GLN:HG3	2.09	0.52
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.39	0.52
3:C:367:PHE:N	3:C:368:PRO:HD2	2.25	0.52
3:C:36:SER:O	3:C:39:ALA:N	2.43	0.52
4:D:134:TYR:OH	4:D:160:MET:O	2.11	0.52
4:D:32:VAL:HG21	4:D:182:ILE:HG23	1.92	0.52
5:E:160:CYS:HA	3:P:269:ILE:HG21	1.92	0.52
2:O:110:GLU:O	2:O:111:CYS:HB3	2.10	0.52
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.75	0.52
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.45	0.52
2:B:37:SER:HB2	2:B:213:HIS:ND1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:GLY:N	3:C:240:PHE:HE2	2.08	0.52
1:N:161:THR:HG21	1:N:234:CYS:HA	1.92	0.52
3:P:271:PRO:HB3	15:P:3001:ICX:O32	2.10	0.52
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.75	0.52
3:P:78:TRP:CD2	3:P:79:LEU:N	2.78	0.52
5:R:165:TYR:CE2	5:R:180:LEU:HG	2.45	0.52
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.91	0.51
2:B:55:SER:O	2:B:174:ASN:HB2	2.10	0.51
3:C:155:PRO:O	3:C:156:TYR:HB2	2.11	0.51
2:O:428:GLY:O	2:O:430:LEU:HG	2.11	0.51
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.45	0.51
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.53	0.51
10:W:59:TYR:N	10:W:59:TYR:CD1	2.77	0.51
1:A:338:ALA:O	1:A:341:GLU:N	2.43	0.51
1:A:45:SER:HA	1:A:48:GLU:HG3	1.92	0.51
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.91	0.51
1:N:140:GLU:OE2	9:V:49:LEU:HA	2.09	0.51
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.46	0.51
2:O:21:ALA:O	2:O:22:GLU:HG2	2.09	0.51
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.93	0.51
5:R:179:ASN:O	5:R:180:LEU:C	2.48	0.51
5:R:84:GLY:O	5:R:85:LYS:HD3	2.11	0.51
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.74	0.51
3:P:82:ASN:N	3:P:82:ASN:HD22	2.09	0.51
4:Q:197:GLU:O	4:Q:199:ASP:N	2.43	0.51
17:Q:501:HEC:CBB	17:Q:501:HEC:HMB1	2.25	0.51
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.91	0.51
5:R:15:ARG:HH11	5:R:32:ARG:HB3	1.75	0.51
8:U:13:LEU:HD23	8:U:13:LEU:H	1.75	0.51
2:B:47:ILE:CD1	2:B:47:ILE:N	2.70	0.51
3:C:91:PHE:CE1	3:C:124:LEU:HD22	2.45	0.51
5:E:74:ILE:HD12	5:E:195:VAL:CB	2.31	0.51
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.40	0.51
1:N:69:LYS:NZ	1:N:70:ARG:HH21	2.08	0.51
3:P:40:VAL:O	3:P:44:THR:HB	2.11	0.51
3:P:58:ALA:O	3:P:177:THR:HG22	2.11	0.51
1:A:251:ALA:HB1	1:A:428:ILE:CG2	2.40	0.51
3:C:265:THR:H	5:R:145:VAL:HG11	1.75	0.51
4:D:10:PHE:HD1	4:D:10:PHE:H	1.57	0.51
4:D:218:LEU:HD22	5:E:39:VAL:HG12	1.93	0.51
6:F:21:TYR:C	6:F:21:TYR:CD2	2.83	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:22:LEU:HD21	16:P:3002:UQ:O4	2.11	0.51
2:B:162:ASN:O	2:B:244:ILE:HD12	2.10	0.51
3:C:127:THR:HG21	14:C:501:HEM:CBB	2.39	0.51
3:C:319:ARG:HB3	3:C:374:GLU:OE1	2.10	0.51
4:D:83:ARG:HH11	4:D:83:ARG:HG3	1.76	0.51
9:I:59:SER:O	9:I:60:ALA:HB3	2.10	0.51
1:N:433:ASP:HB3	1:N:436:ARG:HB2	1.93	0.51
2:O:295:LEU:O	2:O:299:VAL:HG23	2.11	0.51
2:O:81:SER:O	2:O:85:ILE:HG13	2.11	0.51
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.78	0.51
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.10	0.51
1:A:363:SER:HB3	2:B:112:LEU:HD21	1.93	0.51
2:B:255:ALA:O	2:B:325:TYR:HA	2.11	0.51
2:B:337:ILE:O	2:B:340:ALA:HB3	2.11	0.51
9:I:38:UNK:C	9:I:40:UNK:N	2.72	0.51
1:N:191:LYS:C	1:N:193:PRO:HD2	2.31	0.51
2:O:46:ARG:HG3	2:O:110:GLU:HG2	1.92	0.51
2:O:220:ALA:HA	2:O:224:LEU:HD13	1.91	0.51
2:O:275:LEU:O	2:O:275:LEU:HD12	2.11	0.51
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.36	0.51
4:Q:240:PRO:HG2	4:Q:241:LYS:H	1.76	0.51
4:Q:83:ARG:HG3	4:Q:83:ARG:HH11	1.75	0.51
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.76	0.51
10:W:12:ALA:O	10:W:13:LEU:HD23	2.11	0.51
2:O:56:ARG:HH22	2:O:318:ASP:CG	2.14	0.51
10:W:49:GLY:N	10:W:54:HIS:ND1	2.59	0.51
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.45	0.51
5:E:100:HIS:HA	5:E:131:GLU:O	2.11	0.51
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.45	0.51
1:N:127:ILE:O	1:N:129:LYS:N	2.43	0.51
1:N:369:LEU:HD11	1:N:392:LEU:HD21	1.93	0.51
1:N:49:ASN:ND2	1:N:51:LYS:H	2.08	0.51
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.10	0.51
5:R:28:SER:O	5:R:32:ARG:HG3	2.10	0.51
1:A:85:HIS:O	1:A:99:ILE:HA	2.11	0.51
2:O:55:SER:O	2:O:174:ASN:HB2	2.11	0.51
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.11	0.51
1:N:171:THR:HB	5:R:4:ASP:OD2	2.10	0.51
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.74	0.51
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.46	0.51
2:B:181:TYR:CZ	2:O:249:GLY:HA3	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ILE:O	2:B:92:VAL:HG22	2.11	0.50
5:E:152:ASP:C	5:E:153:PHE:CD1	2.85	0.50
8:H:66:ASP:HA	8:H:69:VAL:HG23	1.93	0.50
3:P:120:LEU:HD22	14:P:502:HEM:CBB	2.41	0.50
14:P:502:HEM:HMB1	14:P:502:HEM:HBB2	1.93	0.50
3:P:95:ILE:O	3:P:99:ILE:HG13	2.11	0.50
4:Q:14:HIS:HA	4:Q:19:SER:HB3	1.93	0.50
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.39	0.50
2:B:259:THR:HG22	2:B:260:GLU:H	1.73	0.50
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.11	0.50
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.46	0.50
10:J:40:ASP:O	10:J:44:GLU:HG3	2.12	0.50
10:J:49:GLY:N	10:J:54:HIS:ND1	2.59	0.50
1:N:158:PHE:O	1:N:159:GLN:O	2.29	0.50
1:N:161:THR:HG21	1:N:235:ARG:H	1.75	0.50
1:N:334:MET:O	1:N:335:MET:C	2.49	0.50
2:O:398:VAL:O	2:O:402:ILE:HG13	2.12	0.50
3:P:53:ALA:N	14:P:501:HEM:HMD2	2.26	0.50
4:Q:10:PHE:HD2	8:U:74:PHE:HE2	1.54	0.50
9:V:59:SER:O	9:V:60:ALA:HB3	2.12	0.50
1:A:236:PHE:HB2	1:A:258:GLU:OE1	2.10	0.50
4:D:227:TRP:O	4:D:228:SER:C	2.49	0.50
1:N:108:LYS:O	1:N:112:LEU:HG	2.12	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.50
2:O:318:ASP:O	2:O:319:SER:HB2	2.10	0.50
2:B:229:GLY:C	2:B:231:GLY:H	2.14	0.50
3:C:166:TRP:HA	3:C:175:THR:HG23	1.92	0.50
3:C:329:LEU:O	3:C:332:ASN:HB3	2.12	0.50
5:E:38:LEU:HD13	10:J:14:PHE:CZ	2.45	0.50
1:N:178:THR:O	1:N:179:ARG:C	2.49	0.50
2:O:248:ASN:ND2	2:O:250:HIS:CB	2.74	0.50
3:P:14:MET:HG2	12:P:2010:BOG:O3	2.12	0.50
4:Q:23:HIS:HB2	10:W:50:LYS:O	2.10	0.50
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.76	0.50
2:O:201:SER:OG	2:O:228:SER:HB3	2.12	0.50
3:P:305:ILE:HD11	3:P:363:LEU:HD22	1.94	0.50
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.92	0.50
1:A:35:CYS:HB2	1:A:200:ALA:O	2.11	0.50
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.25	0.50
4:D:117:VAL:HG21	4:D:190:LEU:C	2.32	0.50
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HB2	5:E:22:THR:O	2.12	0.50
5:E:95:PRO:HG2	5:E:145:VAL:CG2	2.41	0.50
6:F:72:HIS:C	6:F:73:ARG:HD3	2.31	0.50
2:O:264:VAL:HG23	2:O:316:TYR:C	2.31	0.50
3:P:139:MET:O	3:P:140:SER:C	2.50	0.50
3:P:158:GLY:O	3:P:159:HIS:C	2.49	0.50
5:R:102:THR:HG23	5:R:105:GLU:CG	2.39	0.50
1:A:136:GLN:C	1:A:138:LEU:H	2.15	0.50
1:A:69:LYS:NZ	1:A:70:ARG:HH21	2.10	0.50
1:A:7:THR:HG21	2:B:113:ARG:CD	2.42	0.50
1:N:121:ALA:O	1:N:122:LEU:HB2	2.12	0.50
1:N:178:THR:HG22	1:N:179:ARG:N	2.25	0.50
3:P:37:LEU:CD2	3:P:233:LEU:HA	2.41	0.50
3:C:372:THR:O	3:C:373:LEU:C	2.50	0.50
5:E:148:ALA:HB2	5:E:156:TYR:CE2	2.47	0.50
1:N:136:GLN:C	1:N:138:LEU:N	2.64	0.50
3:P:36:SER:O	3:P:37:LEU:C	2.50	0.50
5:R:145:VAL:CG1	5:R:145:VAL:O	2.59	0.50
1:A:58:PHE:HB3	1:A:182:LEU:HD11	1.94	0.50
1:A:45:SER:HA	1:A:48:GLU:CD	2.32	0.50
2:B:415:LYS:C	2:B:417:PHE:N	2.66	0.50
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.47	0.50
2:B:306:PRO:HB3	9:I:51:CYS:HA	1.93	0.50
1:N:143:ASN:ND2	9:V:48:PRO:HD2	2.26	0.50
1:N:280:TYR:CG	1:N:281:ASP:N	2.80	0.50
2:O:162:ASN:O	2:O:244:ILE:HD12	2.12	0.50
2:O:385:GLU:HG2	2:O:391:THR:O	2.12	0.50
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.12	0.50
3:P:92:PHE:O	3:P:96:PHE:CD2	2.65	0.50
6:S:71:LYS:O	6:S:72:HIS:HB2	2.11	0.50
9:V:65:VAL:HB	9:V:77:ARG:HD2	1.94	0.50
1:A:279:ARG:HA	1:A:307:PHE:CE1	2.47	0.49
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.49
3:C:72:ARG:HG2	3:C:72:ARG:NH1	2.25	0.49
5:E:53:ASN:O	5:E:57:GLN:HG3	2.11	0.49
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.90	0.49
1:N:106:MET:CE	1:N:110:VAL:HG21	2.42	0.49
1:N:294:LEU:HG	1:N:307:PHE:CE2	2.46	0.49
1:N:317:THR:OG1	1:N:318:GLY:N	2.44	0.49
1:N:269:VAL:HG11	1:N:410:VAL:CG2	2.42	0.49
3:P:187:PRO:HG2	14:P:501:HEM:HMC3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:22:ASP:O	4:Q:24:SER:N	2.45	0.49
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	2.95	0.49
4:Q:28:ARG:O	4:Q:29:GLY:C	2.51	0.49
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.77	0.49
5:E:183:PRO:HG2	5:E:185:TYR:HD2	1.76	0.49
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.40	0.49
8:H:40:CYS:O	8:H:44:VAL:HG23	2.12	0.49
1:N:410:VAL:O	1:N:413:LYS:HB3	2.11	0.49
1:N:251:ALA:HB1	1:N:428:ILE:CG2	2.41	0.49
5:R:29:SER:O	5:R:30:GLU:C	2.50	0.49
5:R:42:THR:O	5:R:45:VAL:N	2.44	0.49
6:S:32:MET:HE1	6:S:87:LYS:HG2	1.92	0.49
3:C:133:VAL:CG2	3:C:144:ALA:HB2	2.42	0.49
3:C:79:LEU:HD11	3:C:83:LEU:HD11	1.93	0.49
4:D:238:ARG:HB3	4:D:238:ARG:NH1	2.27	0.49
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.42	0.49
1:N:61:HIS:ND1	1:N:134:ILE:HG12	2.26	0.49
2:O:398:VAL:HG13	2:O:399:ALA:N	2.27	0.49
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.27	0.49
18:P:3003:CDL:HB22	6:S:72:HIS:HD2	1.77	0.49
5:R:114:VAL:O	5:R:120:PRO:HB3	2.13	0.49
2:B:50:PHE:HD1	2:B:50:PHE:H	1.59	0.49
3:C:82:ASN:HD22	3:C:82:ASN:N	2.10	0.49
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.95	0.49
2:O:259:THR:O	2:O:260:GLU:C	2.50	0.49
3:P:137:GLY:H	3:P:140:SER:CB	2.26	0.49
5:R:177:PRO:O	5:R:178:TYR:HD2	1.95	0.49
1:A:170:THR:CG2	1:A:171:THR:N	2.75	0.49
2:B:53:ALA:CB	2:B:105:MET:HG3	2.36	0.49
2:B:146:VAL:HG12	2:B:147:ASP:N	2.28	0.49
2:B:50:PHE:CE1	2:B:207:VAL:HB	2.47	0.49
2:B:248:ASN:ND2	2:B:250:HIS:CB	2.75	0.49
2:B:81:SER:O	2:B:85:ILE:HG13	2.12	0.49
3:C:117:GLY:O	3:C:120:LEU:HB2	2.12	0.49
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.49
2:O:73:SER:N	2:O:74:PRO:HD2	2.28	0.49
3:P:134:LEU:HD21	3:P:180:PHE:HA	1.95	0.49
4:Q:223:LYS:O	4:Q:223:LYS:HD3	2.11	0.49
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.94	0.49
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.47	0.49
2:O:147:ASP:O	2:O:150:VAL:HG22	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:127:THR:HG21	14:P:501:HEM:CBB	2.40	0.49
3:P:166:TRP:HA	3:P:175:THR:HG23	1.94	0.49
1:A:106:MET:N	1:A:107:PRO:HD2	2.28	0.49
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.47	0.49
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.48	0.49
1:N:61:HIS:CD2	2:O:287:ARG:CZ	2.95	0.49
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.43	0.49
2:O:50:PHE:CE1	2:O:207:VAL:HB	2.48	0.49
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.47	0.49
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.26	0.49
5:R:32:ARG:HH12	7:T:22:GLU:CD	2.16	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.12	0.49
1:A:362:ARG:HD2	1:A:396:ASP:OD2	2.13	0.49
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.43	0.49
5:E:10:PHE:O	5:E:14:ARG:HG3	2.12	0.49
2:O:374:THR:O	2:O:377:GLY:N	2.45	0.49
4:Q:48:PHE:CE2	4:Q:65:ALA:HA	2.47	0.49
1:A:277:ILE:HD11	1:A:345:LEU:CD1	2.39	0.49
1:N:187:ASP:O	1:N:191:LYS:HE3	2.13	0.49
1:N:261:GLY:HA2	1:N:317:THR:O	2.13	0.49
2:O:50:PHE:CD1	2:O:50:PHE:N	2.80	0.49
5:R:31:ASP:OD1	10:W:7:ARG:HG3	2.12	0.49
2:O:325:TYR:HB3	9:V:59:SER:HB3	1.93	0.49
1:A:255:LEU:CD1	1:A:422:LEU:HD13	2.42	0.49
3:C:316:MET:O	3:C:317:THR:C	2.50	0.49
4:D:138:PRO:HG2	4:D:141:VAL:HG21	1.93	0.49
4:D:48:PHE:CE2	4:D:65:ALA:HA	2.47	0.49
1:N:223:TYR:CD2	1:N:223:TYR:N	2.80	0.49
2:O:100:SER:HA	2:O:104:LYS:O	2.13	0.49
2:O:66:ALA:O	2:O:69:LEU:HB3	2.12	0.49
3:P:187:PRO:HG3	14:P:501:HEM:HBB2	1.94	0.49
3:P:325:LEU:HD21	3:P:366:LEU:CB	2.42	0.49
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.95	0.49
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.47	0.48
2:B:291:VAL:C	2:B:293:SER:H	2.16	0.48
4:D:197:GLU:O	4:D:199:ASP:N	2.45	0.48
4:D:43:MET:CE	4:D:189:PHE:HE2	2.25	0.48
8:H:73:LEU:HD12	8:H:73:LEU:C	2.34	0.48
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.48	0.48
1:N:365:MET:O	1:N:368:GLN:HB2	2.12	0.48
3:P:195:ILE:O	3:P:199:THR:HB	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:261:ASN:ND2	3:P:264:VAL:HG23	2.28	0.48
3:P:345:GLU:O	3:P:348:PHE:HB2	2.13	0.48
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.95	0.48
2:B:84:ARG:NH1	2:B:122:TYR:HE2	2.10	0.48
4:D:180:SER:OG	8:H:77:LEU:HD21	2.13	0.48
3:C:247:SER:N	3:C:248:PRO:HD3	2.28	0.48
2:O:143:GLN:O	2:O:146:VAL:N	2.45	0.48
7:T:29:ILE:HA	7:T:33:ALA:HB3	1.95	0.48
10:W:21:ALA:O	10:W:23:THR:N	2.47	0.48
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
2:B:47:ILE:HG21	2:B:120:MET:HE3	1.96	0.48
3:C:23:PRO:HG2	7:G:3:HIS:CB	2.43	0.48
4:D:54:VAL:HG12	4:D:55:THR:N	2.27	0.48
7:T:38:TRP:O	7:T:39:ARG:C	2.51	0.48
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.47	0.48
1:A:273:ALA:O	1:A:276:ILE:N	2.45	0.48
1:A:434:TYR:CE2	7:G:19:SER:HA	2.48	0.48
4:D:110:PRO:HB3	17:D:501:HEC:C1D	2.44	0.48
5:E:32:ARG:HH12	7:G:22:GLU:CD	2.17	0.48
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.76	0.48
2:O:47:ILE:HG12	2:O:120:MET:CE	2.43	0.48
4:Q:127:VAL:O	4:Q:131:LEU:HG	2.13	0.48
5:R:10:PHE:O	5:R:14:ARG:HG3	2.14	0.48
18:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.13	0.48
1:A:180:ALA:O	1:A:183:ALA:HB3	2.14	0.48
2:B:57:TYR:CD1	2:B:57:TYR:N	2.81	0.48
3:C:111:LYS:HE2	3:C:307:PHE:CE1	2.47	0.48
3:C:147:ILE:O	3:C:150:LEU:HB2	2.13	0.48
3:C:207:ASN:ND2	3:C:208:ASN:H	2.11	0.48
5:E:70:ALA:O	5:E:71:LEU:CB	2.61	0.48
6:F:43:VAL:O	6:F:44:LYS:C	2.52	0.48
2:O:167:ALA:O	2:O:168:TYR:CD1	2.66	0.48
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.95	0.48
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.96	0.48
5:R:35:PHE:O	5:R:38:LEU:N	2.47	0.48
1:A:410:VAL:O	1:A:413:LYS:HB3	2.13	0.48
4:D:158:ILE:HG23	4:D:158:ILE:O	2.13	0.48
4:D:47:ALA:HB1	4:D:89:ASP:O	2.13	0.48
5:E:185:TYR:HB2	5:E:195:VAL:HG22	1.96	0.48
5:E:35:PHE:O	5:E:38:LEU:N	2.45	0.48
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:28:ILE:CD1	16:P:3002:UQ:HM21	2.44	0.48
3:P:358:SER:O	3:P:362:ILE:HG13	2.13	0.48
4:Q:221:TYR:CE1	7:T:25:ALA:CB	2.97	0.48
7:T:34:LEU:N	7:T:35:PRO:HD2	2.29	0.48
8:U:24:CYS:C	8:U:26:GLN:H	2.17	0.48
2:B:31:ASN:O	2:B:228:SER:HB3	2.14	0.48
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.96	0.48
5:E:185:TYR:HB3	5:E:195:VAL:HG22	1.95	0.48
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.44	0.48
1:N:3:THR:O	1:N:7:THR:HG23	2.14	0.48
2:O:116:VAL:O	2:O:119:VAL:HG22	2.13	0.48
2:O:248:ASN:ND2	2:O:250:HIS:HB2	2.29	0.48
2:O:73:SER:OG	2:O:74:PRO:HD3	2.13	0.48
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.22	0.48
1:A:223:TYR:N	1:A:223:TYR:HD2	2.12	0.48
1:A:338:ALA:O	1:A:340:GLY:N	2.46	0.48
8:H:21:ARG:O	8:H:25:GLU:HG3	2.13	0.48
4:Q:169:LEU:C	4:Q:169:LEU:HD23	2.34	0.48
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.95	0.48
5:R:194:VAL:HG12	5:R:195:VAL:N	2.28	0.48
9:V:28:UNK:H	9:V:71:ASN:HD21	1.61	0.48
1:A:108:LYS:O	1:A:112:LEU:HG	2.14	0.48
2:B:76:THR:HG22	2:B:82:SER:N	2.29	0.48
5:E:112:VAL:HG11	5:E:172:ARG:NH2	2.28	0.48
2:O:169:LYS:HD2	2:O:238:THR:HG21	1.96	0.48
3:P:215:ASP:C	3:P:217:ASP:H	2.18	0.48
4:Q:239:PRO:CB	4:Q:240:PRO:HD2	2.41	0.48
4:Q:94:PRO:HB2	4:Q:95:TYR:CD1	2.49	0.48
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.96	0.48
1:A:241:ILE:HG23	1:A:241:ILE:O	2.14	0.47
2:B:150:VAL:CG2	2:B:151:ALA:H	2.26	0.47
4:D:28:ARG:NH1	4:D:173:ASP:OD2	2.47	0.47
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.44	0.47
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.95	0.47
10:J:59:TYR:CD1	10:J:59:TYR:N	2.82	0.47
1:N:45:SER:HA	1:N:48:GLU:CD	2.34	0.47
1:N:56:GLY:HA2	1:N:185:TYR:CE2	2.49	0.47
3:P:207:ASN:ND2	3:P:208:ASN:H	2.11	0.47
3:P:346:HIS:CG	3:P:347:PRO:HA	2.49	0.47
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	1.96	0.47
8:U:37:LEU:O	8:U:38:GLU:C	2.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:H	1:A:223:TYR:HD2	1.63	0.47
2:B:398:VAL:O	2:B:402:ILE:HG13	2.14	0.47
4:D:235:MET:HE1	6:F:63:LYS:C	2.35	0.47
3:P:38:LEU:HB3	14:P:502:HEM:CMB	2.44	0.47
4:Q:127:VAL:HG12	4:Q:187:CYS:SG	2.54	0.47
4:Q:1:GLY:O	4:Q:3:LEU:N	2.47	0.47
6:S:59:MET:HA	6:S:59:MET:CE	2.44	0.47
5:R:38:LEU:HB2	10:W:14:PHE:CE1	2.48	0.47
1:A:127:ILE:C	1:A:129:LYS:H	2.17	0.47
2:B:206:LEU:HG	2:B:206:LEU:O	2.13	0.47
2:B:248:ASN:ND2	2:B:250:HIS:HB2	2.29	0.47
3:C:78:TRP:CD2	3:C:79:LEU:N	2.82	0.47
4:D:135:CYS:O	4:D:149:TYR:HB3	2.14	0.47
12:D:2091:BOG:H3	12:E:2009:BOG:O4	2.14	0.47
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.96	0.47
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.96	0.47
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.14	0.47
2:O:75:LEU:HD11	2:O:140:LEU:CD2	2.45	0.47
5:R:101:ARG:O	5:R:106:ILE:HD11	2.14	0.47
1:A:223:TYR:CD2	1:A:223:TYR:N	2.81	0.47
3:C:269:ILE:CG2	3:C:269:ILE:O	2.62	0.47
3:C:27:ASN:HD22	3:C:209:PRO:HG2	1.79	0.47
8:H:24:CYS:C	8:H:26:GLN:N	2.68	0.47
8:H:37:LEU:O	8:H:38:GLU:C	2.52	0.47
9:I:53:GLU:O	9:I:55:MET:N	2.47	0.47
2:O:299:VAL:O	2:O:303:THR:HG22	2.14	0.47
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.97	0.47
2:B:84:ARG:HG2	2:B:84:ARG:NH1	2.28	0.47
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.95	0.47
4:D:29:GLY:O	4:D:32:VAL:HB	2.14	0.47
4:D:75:ASP:OD1	4:D:78:GLY:N	2.46	0.47
8:H:24:CYS:O	8:H:26:GLN:N	2.47	0.47
2:O:239:TYR:CD2	2:O:240:TRP:N	2.82	0.47
3:P:116:THR:O	3:P:117:GLY:C	2.53	0.47
3:P:238:THR:CB	3:P:239:PRO:HD3	2.45	0.47
3:P:247:SER:N	3:P:248:PRO:HD3	2.29	0.47
4:Q:138:PRO:HG2	4:Q:141:VAL:HG21	1.97	0.47
5:R:145:VAL:HG13	5:R:145:VAL:O	2.14	0.47
1:A:168:GLU:H	1:A:168:GLU:CD	2.18	0.47
2:B:73:SER:OG	2:B:74:PRO:HD3	2.15	0.47
3:C:40:VAL:HG11	3:C:233:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:ARG:NH1	7:G:22:GLU:HA	2.29	0.47
7:G:48:VAL:HG12	7:G:49:ALA:N	2.29	0.47
1:N:40:TRP:CZ3	1:N:376:CYS:SG	3.00	0.47
1:N:443:TRP:O	1:N:444:ILE:CB	2.63	0.47
5:R:153:PHE:CD1	5:R:153:PHE:N	2.83	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.97	0.47
2:B:50:PHE:C	2:B:51:ILE:HG13	2.34	0.47
2:B:60:THR:HG23	2:B:61:ALA:H	1.79	0.47
3:C:87:GLY:HA2	3:C:240:PHE:CE2	2.49	0.47
4:D:14:HIS:HA	4:D:19:SER:HB3	1.96	0.47
6:F:103:GLU:O	6:F:104:ARG:C	2.53	0.47
1:N:178:THR:CG2	1:N:179:ARG:N	2.77	0.47
2:O:37:SER:OG	2:O:38:LEU:N	2.47	0.47
2:O:47:ILE:HD12	2:O:47:ILE:H	1.78	0.47
3:P:134:LEU:N	3:P:135:PRO:HD2	2.30	0.47
3:P:372:THR:O	3:P:373:LEU:C	2.53	0.47
4:Q:238:ARG:HB3	4:Q:238:ARG:HH11	1.80	0.47
5:R:36:SER:O	5:R:39:VAL:HG23	2.15	0.47
1:A:148:VAL:HG13	5:E:2:HIS:CB	2.44	0.47
3:C:28:ILE:HD11	16:C:2002:UQ:HM21	1.97	0.47
3:C:238:THR:CB	3:C:239:PRO:HD3	2.44	0.47
5:E:144:CYS:O	5:E:146:PRO:HD3	2.15	0.47
1:N:63:ALA:O	1:N:116:VAL:CG1	2.63	0.47
2:O:269:ALA:O	2:O:272:PHE:N	2.47	0.47
2:O:345:LYS:C	2:O:347:ALA:H	2.17	0.47
3:P:162:VAL:O	3:P:165:ALA:HB3	2.14	0.47
4:Q:147:LEU:HD23	4:Q:159:GLY:HA2	1.95	0.47
4:Q:227:TRP:O	4:Q:228:SER:C	2.53	0.47
1:A:343:MET:O	1:A:344:ARG:C	2.52	0.47
1:A:332:ASP:HB2	1:A:430:GLN:HG2	1.96	0.47
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.30	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.30	0.47
3:C:93:ILE:O	3:C:94:CYS:C	2.50	0.47
1:N:180:ALA:O	1:N:183:ALA:HB3	2.14	0.47
1:N:382:HIS:HB3	1:N:388:ARG:O	2.14	0.47
1:N:41:ILE:HG21	1:N:190:PHE:CD2	2.49	0.47
2:O:27:THR:HG22	2:O:28:LYS:N	2.29	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.96	0.47
5:R:168:SER:CB	5:R:170:ARG:HG3	2.43	0.47
6:S:11:ARG:O	6:S:15:ARG:HG2	2.15	0.47
10:W:32:GLU:O	10:W:33:ARG:C	2.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ALA:HB2	1:A:101:ALA:HB2	1.97	0.47
3:C:186:LEU:HB2	3:C:187:PRO:HD3	1.97	0.47
1:N:223:TYR:HD2	1:N:223:TYR:N	2.11	0.47
2:O:176:LEU:O	2:O:176:LEU:HD12	2.15	0.47
2:O:366:ALA:O	2:O:367:THR:C	2.52	0.47
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.29	0.47
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.45	0.47
1:A:142:ASP:OD1	5:E:2:HIS:N	2.38	0.47
1:A:206:LYS:O	1:A:207:GLU:C	2.53	0.47
2:B:76:THR:HG22	2:B:81:SER:CA	2.32	0.47
3:C:133:VAL:HG21	3:C:144:ALA:HB2	1.97	0.47
11:C:2005:PEE:O2P	5:E:40:THR:HG21	2.15	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.50	0.47
5:E:148:ALA:O	5:E:149:ASN:HB2	2.14	0.47
6:F:16:ILE:HG22	6:F:17:ARG:N	2.29	0.47
8:H:31:VAL:HA	8:H:34:ARG:HB3	1.95	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.50	0.47
1:N:6:GLN:C	1:N:8:LEU:N	2.67	0.47
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.50	0.47
2:O:291:VAL:C	2:O:293:SER:H	2.18	0.47
3:P:311:SER:HB2	3:P:319:ARG:HH11	1.79	0.47
3:P:367:PHE:N	3:P:368:PRO:HD2	2.30	0.47
6:S:73:ARG:HG3	6:S:73:ARG:NH1	2.29	0.47
8:U:58:LEU:O	8:U:61:PHE:HB3	2.15	0.47
1:A:178:THR:HG22	1:A:179:ARG:N	2.30	0.46
1:A:261:GLY:HA2	1:A:317:THR:O	2.16	0.46
1:A:84:ALA:CB	1:A:101:ALA:HB2	2.45	0.46
2:B:146:VAL:O	2:B:147:ASP:C	2.53	0.46
5:E:3:ASN:C	5:E:5:VAL:H	2.18	0.46
2:O:26:ILE:HA	2:O:35:ILE:O	2.15	0.46
2:O:76:THR:HG22	2:O:82:SER:N	2.28	0.46
3:P:155:PRO:O	3:P:156:TYR:HB2	2.15	0.46
3:C:265:THR:CB	5:R:145:VAL:HG12	2.41	0.46
2:B:246:GLU:O	2:B:427:SER:HA	2.15	0.46
2:B:259:THR:CG2	2:B:260:GLU:N	2.77	0.46
1:N:85:HIS:O	1:N:99:ILE:HA	2.15	0.46
2:O:46:ARG:NH1	2:O:110:GLU:OE2	2.48	0.46
3:P:198:LEU:HD22	16:P:3002:UQ:HM53	1.96	0.46
3:P:216:SER:O	3:P:217:ASP:HB2	2.15	0.46
3:P:28:ILE:HD11	16:P:3002:UQ:HM21	1.98	0.46
4:Q:43:MET:CE	4:Q:189:PHE:HE2	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:20:TYR:O	6:S:23:ALA:HB3	2.15	0.46
1:A:294:LEU:HB2	1:A:341:GLU:HG3	1.98	0.46
1:A:6:GLN:C	1:A:8:LEU:N	2.67	0.46
2:B:209:ILE:CD1	2:B:378:LEU:HD23	2.42	0.46
5:E:126:ARG:NH1	5:E:126:ARG:HG2	2.30	0.46
5:E:186:GLN:O	5:E:193:VAL:HG23	2.16	0.46
1:N:223:TYR:HD2	1:N:223:TYR:H	1.63	0.46
2:O:169:LYS:HD2	2:O:238:THR:CG2	2.46	0.46
3:P:325:LEU:HD11	3:P:362:ILE:HG23	1.96	0.46
5:R:178:TYR:CD2	5:R:178:TYR:N	2.82	0.46
6:S:68:LEU:O	6:S:71:LYS:N	2.48	0.46
2:B:198:ASN:OD1	2:B:203:ARG:NH2	2.48	0.46
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.97	0.46
1:N:349:THR:HA	1:N:353:GLU:OE1	2.16	0.46
2:O:124:LEU:HD12	2:O:128:THR:HG21	1.97	0.46
2:O:146:VAL:O	2:O:149:ALA:N	2.48	0.46
2:O:217:LYS:O	2:O:219:VAL:N	2.48	0.46
14:P:502:HEM:HBB2	14:P:502:HEM:CMB	2.45	0.46
1:A:90:THR:HB	1:A:95:THR:HG23	1.96	0.46
2:B:167:ALA:O	2:B:168:TYR:CD1	2.68	0.46
9:I:28:UNK:N	9:I:72:ALA:HB2	2.25	0.46
5:E:30:GLU:CB	10:J:7:ARG:HG2	2.43	0.46
3:P:90:PHE:HB2	3:P:240:PHE:CD2	2.50	0.46
3:P:86:ASN:O	3:P:89:SER:N	2.49	0.46
4:Q:95:TYR:CD2	4:Q:101:ALA:CA	2.97	0.46
1:A:317:THR:OG1	1:A:318:GLY:N	2.48	0.46
2:B:426:ALA:O	2:B:427:SER:HB3	2.14	0.46
2:B:42:SER:OG	2:B:43:PRO:HD2	2.15	0.46
7:G:16:TYR:N	7:G:16:TYR:CD1	2.83	0.46
1:N:122:LEU:HD11	1:N:186:ILE:CD1	2.46	0.46
1:N:394:GLU:O	1:N:395:TRP:C	2.53	0.46
2:O:29:LEU:CD2	2:O:30:PRO:HD2	2.46	0.46
3:P:117:GLY:O	3:P:120:LEU:HB2	2.16	0.46
3:P:311:SER:CB	3:P:319:ARG:NH1	2.78	0.46
4:Q:197:GLU:O	4:Q:198:HIS:C	2.54	0.46
4:Q:46:VAL:HG12	4:Q:47:ALA:N	2.31	0.46
5:R:109:GLU:CD	5:R:167:ALA:HB3	2.35	0.46
5:R:134:ILE:C	5:R:135:LEU:HG	2.33	0.46
6:S:89:TYR:CD1	6:S:90:LEU:N	2.70	0.46
1:A:388:ARG:HH21	1:A:388:ARG:HG3	1.80	0.46
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:LYS:O	2:B:203:ARG:NH2	2.48	0.46
2:B:73:SER:N	2:B:74:PRO:HD2	2.31	0.46
3:C:64:PHE:CE1	3:C:259:PRO:HG3	2.51	0.46
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.80	0.46
3:C:82:ASN:H	3:C:82:ASN:HD22	1.64	0.46
4:D:221:TYR:CE2	5:E:39:VAL:HG21	2.51	0.46
4:D:43:MET:CE	4:D:189:PHE:CE2	2.97	0.46
1:N:343:MET:O	1:N:344:ARG:C	2.51	0.46
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.45	0.46
3:P:115:ASN:HA	3:P:118:VAL:HG23	1.96	0.46
4:Q:239:PRO:HB2	4:Q:240:PRO:CD	2.42	0.46
4:Q:54:VAL:HG12	4:Q:55:THR:N	2.30	0.46
5:R:109:GLU:O	5:R:123:ASP:HB2	2.15	0.46
1:A:136:GLN:C	1:A:138:LEU:N	2.69	0.46
3:C:215:ASP:C	3:C:217:ASP:H	2.17	0.46
8:H:66:ASP:O	8:H:67:HIS:C	2.53	0.46
9:I:65:VAL:O	9:I:76:VAL:HA	2.16	0.46
1:N:136:GLN:O	1:N:138:LEU:N	2.49	0.46
1:N:245:ASP:OD1	1:N:247:ALA:HB3	2.15	0.46
2:O:89:ILE:O	2:O:92:VAL:HG22	2.16	0.46
5:R:53:ASN:O	5:R:57:GLN:HG3	2.16	0.46
1:A:334:MET:O	1:A:335:MET:C	2.54	0.46
2:B:374:THR:O	2:B:377:GLY:N	2.49	0.46
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.51	0.46
3:C:158:GLY:O	3:C:159:HIS:C	2.55	0.46
1:N:25:VAL:HG22	1:N:197:LEU:HB3	1.98	0.46
2:O:239:TYR:HE1	2:O:260:GLU:N	2.13	0.46
3:P:242:THR:O	3:P:246:PHE:HB2	2.16	0.46
3:P:338:TRP:O	3:P:341:SER:HB3	2.16	0.46
3:P:362:ILE:HA	3:P:366:LEU:HB2	1.96	0.46
3:P:34:PHE:CE1	3:P:97:LEU:HD12	2.51	0.46
5:R:32:ARG:NH1	7:T:22:GLU:HA	2.31	0.46
2:B:31:ASN:HD22	2:B:32:GLY:N	2.14	0.46
2:B:37:SER:OG	2:B:38:LEU:N	2.48	0.46
2:B:415:LYS:C	2:B:417:PHE:H	2.19	0.46
3:C:316:MET:O	3:C:318:PHE:N	2.49	0.46
3:C:325:LEU:HD21	3:C:366:LEU:CB	2.44	0.46
3:C:79:LEU:HD12	3:C:79:LEU:O	2.16	0.46
6:F:12:LEU:O	6:F:13:MET:C	2.52	0.46
1:N:332:ASP:O	1:N:333:ASP:C	2.54	0.46
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:221:GLU:HG3	2:O:222:GLN:N	2.27	0.46
3:P:147:ILE:HD11	15:P:3001:ICX:H34	1.97	0.46
3:P:350:ILE:HG23	3:P:351:ILE:N	2.31	0.46
4:Q:37:CYS:C	4:Q:39:ALA:H	2.19	0.46
1:A:122:LEU:HD11	1:A:186:ILE:CD1	2.46	0.45
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.97	0.45
3:C:320:PRO:HG2	3:C:321:LEU:H	1.81	0.45
4:D:150:ASN:O	4:D:156:GLN:HA	2.16	0.45
4:D:43:MET:HE3	4:D:189:PHE:CE2	2.51	0.45
5:E:103:GLN:C	5:E:105:GLU:H	2.20	0.45
9:I:70:LEU:O	9:I:70:LEU:HG	2.14	0.45
1:N:170:THR:HG22	1:N:172:GLU:H	1.80	0.45
1:N:365:MET:HG2	1:N:366:VAL:N	2.30	0.45
2:B:249:GLY:HA3	2:O:181:TYR:CE1	2.51	0.45
3:P:139:MET:O	3:P:143:GLY:N	2.38	0.45
4:Q:32:VAL:HG21	4:Q:182:ILE:HG23	1.98	0.45
3:P:245:LEU:O	4:Q:201:ARG:CD	2.64	0.45
2:B:418:VAL:O	2:B:418:VAL:HG12	2.16	0.45
5:E:153:PHE:N	5:E:153:PHE:CD1	2.84	0.45
1:A:127:ILE:O	1:A:129:LYS:N	2.50	0.45
4:D:197:GLU:O	4:D:198:HIS:C	2.55	0.45
8:H:58:LEU:O	8:H:58:LEU:HD12	2.17	0.45
3:P:118:VAL:N	14:P:502:HEM:HBC2	2.31	0.45
3:P:5:ILE:O	3:P:12:LEU:HD23	2.17	0.45
5:R:29:SER:O	5:R:31:ASP:N	2.49	0.45
4:Q:215:LEU:HD13	5:R:46:ALA:CB	2.46	0.45
8:U:59:PHE:O	8:U:60:ASP:C	2.55	0.45
5:R:38:LEU:HA	10:W:14:PHE:CZ	2.51	0.45
4:D:117:VAL:O	4:D:123:GLY:HA2	2.16	0.45
6:F:79:GLN:HB3	6:F:79:GLN:HE21	1.63	0.45
7:G:29:ILE:HA	7:G:33:ALA:HB3	1.97	0.45
2:O:135:TRP:O	2:O:136:GLU:C	2.53	0.45
2:O:353:THR:HB	2:O:356:ASP:OD2	2.16	0.45
3:P:87:GLY:HA2	3:P:240:PHE:CE2	2.51	0.45
5:R:126:ARG:HD3	5:R:168:SER:OG	2.16	0.45
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.82	0.45
6:S:72:HIS:C	6:S:73:ARG:HD3	2.37	0.45
1:A:53:ASN:OD1	1:A:165:ARG:HD3	2.16	0.45
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.76	0.45
2:B:257:VAL:O	2:B:323:GLY:HA3	2.16	0.45
4:D:215:LEU:HD13	5:E:46:ALA:CB	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:HG2	4:D:91:PHE:HD2	1.80	0.45
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.56	0.45
5:E:70:ALA:O	5:E:71:LEU:HB2	2.17	0.45
1:N:206:LYS:O	1:N:208:LEU:N	2.49	0.45
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.52	0.45
2:O:146:VAL:O	2:O:147:ASP:C	2.54	0.45
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.51	0.45
9:V:63:ASP:OD1	9:V:63:ASP:N	2.49	0.45
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.52	0.45
1:A:80:GLU:OE2	2:B:290:SER:HA	2.17	0.45
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.99	0.45
2:B:56:ARG:HH22	2:B:318:ASP:CG	2.20	0.45
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.32	0.45
7:G:80:ASP:OD2	8:H:50:THR:HA	2.17	0.45
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.44	0.45
1:N:287:GLY:O	1:N:289:HIS:N	2.49	0.45
2:O:266:SER:O	2:O:267:ALA:C	2.55	0.45
3:P:220:PRO:O	3:P:221:PHE:C	2.54	0.45
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.98	0.45
3:P:61:SER:C	3:P:62:LEU:HD12	2.37	0.45
3:P:246:PHE:CE2	4:Q:205:GLY:HA3	2.52	0.45
6:S:52:LYS:HE2	7:T:11:ARG:NH1	2.29	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.69	0.45
2:B:385:GLU:HG2	2:B:391:THR:O	2.17	0.45
1:N:106:MET:N	1:N:107:PRO:HD2	2.32	0.45
1:N:39:VAL:HG11	1:N:117:VAL:CG1	2.47	0.45
1:N:439:SER:HA	1:N:442:TYR:CE2	2.52	0.45
2:O:325:TYR:HD2	2:O:326:THR:N	2.15	0.45
2:O:47:ILE:HG21	2:O:120:MET:CE	2.46	0.45
5:R:14:ARG:HG2	5:R:14:ARG:HH11	1.80	0.45
3:P:213:SER:HB2	6:S:39:GLU:OE2	2.16	0.45
1:N:279:ARG:NH2	9:V:30:UNK:C	2.80	0.45
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.47	0.45
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.51	0.45
2:B:248:ASN:HD22	2:B:249:GLY:N	2.14	0.45
3:C:175:THR:HG22	3:C:179:PHE:CE1	2.51	0.45
4:D:165:TYR:O	4:D:166:ASN:C	2.55	0.45
5:E:70:ALA:C	5:E:71:LEU:HG	2.37	0.45
6:F:100:GLU:OE1	2:O:133:ARG:NH1	2.50	0.45
7:G:34:LEU:N	7:G:35:PRO:HD2	2.32	0.45
1:N:127:ILE:C	1:N:129:LYS:N	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:269:ALA:O	2:O:271:ALA:N	2.50	0.45
2:O:341:MET:CE	2:O:344:LEU:HD23	2.47	0.45
2:O:63:LEU:C	2:O:65:THR:H	2.20	0.45
7:T:16:TYR:N	7:T:16:TYR:CD1	2.85	0.45
7:T:48:VAL:HG12	7:T:49:ALA:N	2.31	0.45
10:W:6:LEU:O	10:W:9:ALA:HB3	2.16	0.45
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.45
1:A:245:ASP:C	1:A:247:ALA:H	2.20	0.45
3:C:134:LEU:N	3:C:135:PRO:HD2	2.32	0.45
3:C:36:SER:O	3:C:37:LEU:C	2.55	0.45
1:N:23:LEU:HA	1:N:192:ALA:O	2.17	0.45
4:Q:158:ILE:HG23	4:Q:158:ILE:O	2.15	0.45
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.99	0.45
6:S:52:LYS:HE3	6:S:56:ASN:HD21	1.82	0.45
1:A:242:ARG:O	7:G:14:ILE:HA	2.17	0.45
1:A:265:PRO:O	1:A:268:VAL:HG23	2.17	0.45
1:A:418:LYS:O	1:A:420:PRO:HD3	2.17	0.45
2:B:207:VAL:HG12	2:B:379:LEU:CD1	2.47	0.45
2:B:258:VAL:HG12	2:B:323:GLY:HA3	1.99	0.45
2:B:397:VAL:O	2:B:400:GLN:HB3	2.17	0.45
3:C:104:TYR:O	3:C:316:MET:HG3	2.17	0.45
4:D:28:ARG:O	4:D:29:GLY:C	2.55	0.45
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.99	0.45
1:N:332:ASP:HB2	1:N:430:GLN:HG2	1.98	0.45
2:O:353:THR:C	2:O:355:GLU:N	2.69	0.45
2:O:63:LEU:O	2:O:65:THR:N	2.49	0.45
5:R:42:THR:O	5:R:43:ALA:C	2.55	0.45
1:A:238:GLY:O	1:A:239:SER:HB3	2.17	0.44
1:A:362:ARG:HA	1:A:365:MET:HE1	1.99	0.44
2:B:26:ILE:O	2:B:26:ILE:HG12	2.17	0.44
3:C:282:LEU:HD12	3:C:291:GLY:C	2.37	0.44
4:Q:186:VAL:CG1	4:Q:187:CYS:N	2.79	0.44
2:B:220:ALA:O	2:B:224:LEU:HD13	2.18	0.44
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.52	0.44
2:O:18:CYS:HA	2:O:19:PRO:HD3	1.78	0.44
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.51	0.44
2:B:157:VAL:O	2:B:157:VAL:HG22	2.17	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.53	0.44
2:B:292:THR:O	2:B:292:THR:HG22	2.17	0.44
3:C:164:TRP:O	3:C:165:ALA:C	2.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:GLY:O	3:C:195:ILE:HB	2.17	0.44
3:C:95:ILE:CG2	3:C:96:PHE:N	2.80	0.44
1:N:39:VAL:O	1:N:39:VAL:HG13	2.17	0.44
2:O:292:THR:HG22	2:O:292:THR:O	2.18	0.44
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.99	0.44
3:P:56:TYR:OH	3:P:134:LEU:O	2.23	0.44
3:P:245:LEU:HD23	3:P:245:LEU:HA	1.64	0.44
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.47	0.44
18:P:3003:CDL:HB22	6:S:72:HIS:CD2	2.53	0.44
3:P:56:TYR:OH	3:P:176:LEU:HD11	2.17	0.44
4:Q:16:GLY:C	4:Q:18:LEU:H	2.20	0.44
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.17	0.44
5:R:76:ILE:HG12	5:R:89:PHE:CE2	2.52	0.44
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.82	0.44
1:A:106:MET:CE	1:A:110:VAL:CG2	2.95	0.44
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.17	0.44
2:B:130:PRO:CB	2:B:132:PHE:CE2	2.96	0.44
2:B:353:THR:HB	2:B:356:ASP:OD2	2.18	0.44
2:B:53:ALA:O	2:B:103:GLU:C	2.55	0.44
3:C:245:LEU:O	4:D:201:ARG:HD2	2.17	0.44
1:N:270:LEU:HB3	1:N:311:ASN:ND2	2.33	0.44
2:O:206:LEU:O	2:O:206:LEU:HG	2.17	0.44
2:O:19:PRO:HG3	2:O:41:PHE:CE2	2.53	0.44
2:O:99:TYR:O	2:O:106:THR:N	2.50	0.44
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.50	0.44
4:Q:223:LYS:C	4:Q:223:LYS:CD	2.83	0.44
6:S:43:VAL:O	6:S:44:LYS:C	2.54	0.44
2:B:37:SER:O	2:B:38:LEU:CB	2.66	0.44
2:B:99:TYR:O	2:B:106:THR:N	2.49	0.44
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.23	0.44
4:D:168:ILE:HG12	4:D:168:ILE:O	2.17	0.44
5:E:72:SER:C	5:E:73:LYS:CG	2.85	0.44
8:H:58:LEU:HD11	8:H:62:LEU:CD1	2.47	0.44
4:Q:117:VAL:CG2	4:Q:194:ALA:HB2	2.45	0.44
7:T:29:ILE:O	7:T:33:ALA:HB3	2.17	0.44
1:A:64:PHE:HE2	1:A:86:PHE:CE2	2.36	0.44
2:B:84:ARG:NH1	2:B:122:TYR:CE2	2.85	0.44
2:B:226:ILE:O	2:B:226:ILE:HG23	2.18	0.44
2:B:34:ILE:HG21	2:B:386:ALA:O	2.18	0.44
3:C:13:LYS:O	3:C:17:ASN:N	2.51	0.44
6:F:73:ARG:HG3	6:F:73:ARG:NH1	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.46	0.44
10:J:32:GLU:O	10:J:33:ARG:C	2.55	0.44
2:O:248:ASN:HD22	2:O:249:GLY:N	2.14	0.44
2:O:394:ALA:HB3	2:O:397:VAL:HG23	2.00	0.44
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.52	0.44
5:R:68:VAL:O	5:R:69:LEU:O	2.35	0.44
1:A:349:THR:HA	1:A:353:GLU:OE1	2.18	0.44
1:A:58:PHE:CD2	1:A:134:ILE:HD11	2.53	0.44
1:A:59:VAL:C	1:A:61:HIS:N	2.71	0.44
2:O:418:VAL:O	2:O:418:VAL:HG12	2.18	0.44
3:P:359:TYR:CD2	3:P:360:PHE:CD1	3.03	0.44
3:P:89:SER:O	3:P:90:PHE:C	2.56	0.44
5:R:15:ARG:HG3	7:T:22:GLU:C	2.38	0.44
1:A:365:MET:HG2	1:A:366:VAL:N	2.33	0.44
1:A:63:ALA:O	1:A:116:VAL:CG1	2.66	0.44
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.53	0.44
3:C:167:GLY:HA3	3:C:178:ARG:NH2	2.32	0.44
3:C:304:LEU:O	3:C:305:ILE:C	2.56	0.44
3:C:345:GLU:O	3:C:348:PHE:HB2	2.18	0.44
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.53	0.44
5:E:10:PHE:CB	7:G:18:LEU:HD11	2.48	0.44
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.75	0.44
3:P:329:LEU:O	3:P:332:ASN:HB3	2.18	0.44
3:P:44:THR:CG2	3:P:45:GLN:N	2.81	0.44
1:A:159:GLN:O	1:A:159:GLN:HG3	2.17	0.44
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.48	0.44
3:C:359:TYR:CD2	3:C:360:PHE:CD1	3.03	0.44
1:N:170:THR:CG2	1:N:171:THR:N	2.79	0.44
1:N:26:ALA:O	1:N:198:ALA:HA	2.18	0.44
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.52	0.44
2:O:310:SER:HB2	9:V:59:SER:CB	2.35	0.44
2:O:415:LYS:C	2:O:417:PHE:N	2.69	0.44
3:P:330:VAL:O	3:P:333:LEU:HB2	2.18	0.44
4:Q:178:THR:HG21	8:U:16:PRO:HD2	1.99	0.44
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.59	0.43
2:B:100:SER:HA	2:B:104:LYS:O	2.18	0.43
2:B:193:HIS:O	2:B:197:ASN:HB2	2.18	0.43
1:A:61:HIS:CD2	2:B:287:ARG:CZ	3.00	0.43
3:C:132:TYR:HA	14:C:501:HEM:HAA2	2.00	0.43
3:C:245:LEU:O	4:D:201:ARG:CD	2.66	0.43
4:D:169:LEU:HD23	4:D:169:LEU:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:VAL:CG2	4:D:194:ALA:HB2	2.47	0.43
9:I:51:CYS:O	9:I:55:MET:SD	2.76	0.43
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.70	0.43
1:N:279:ARG:HA	1:N:307:PHE:CE1	2.53	0.43
2:O:81:SER:C	2:O:83:PHE:N	2.71	0.43
4:Q:43:MET:CE	4:Q:189:PHE:CE2	3.00	0.43
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.48	0.43
1:A:90:THR:HA	1:A:95:THR:HA	1.99	0.43
3:C:187:PRO:O	3:C:190:ILE:HB	2.18	0.43
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.46	0.43
3:P:63:ALA:HB2	3:P:176:LEU:HD21	2.01	0.43
3:P:192:GLY:O	3:P:195:ILE:HB	2.17	0.43
3:P:78:TRP:CG	3:P:79:LEU:N	2.85	0.43
5:R:32:ARG:HH11	7:T:22:GLU:HA	1.84	0.43
8:U:50:THR:O	8:U:51:GLU:HB2	2.18	0.43
1:A:338:ALA:C	1:A:340:GLY:N	2.72	0.43
1:A:404:ALA:O	1:A:405:ARG:C	2.57	0.43
4:D:223:LYS:HD3	4:D:223:LYS:O	2.18	0.43
8:H:55:THR:O	8:H:56:GLU:C	2.56	0.43
1:N:303:LEU:HB3	1:N:334:MET:SD	2.58	0.43
2:O:345:LYS:C	2:O:347:ALA:N	2.70	0.43
2:O:353:THR:C	2:O:355:GLU:H	2.21	0.43
2:O:84:ARG:HG2	2:O:84:ARG:NH1	2.33	0.43
3:P:105:TYR:HD2	3:P:209:PRO:HA	1.78	0.43
3:P:79:LEU:HD12	3:P:79:LEU:C	2.36	0.43
9:V:61:ARG:O	9:V:62:ARG:HG3	2.18	0.43
1:A:294:LEU:HD11	1:A:334:MET:HE3	1.99	0.43
1:A:431:LEU:HD12	1:A:431:LEU:C	2.39	0.43
2:B:258:VAL:CG1	2:B:312:PHE:HD2	2.24	0.43
2:B:252:LEU:HD12	9:I:49:LEU:HD12	2.01	0.43
1:N:134:ILE:HG21	1:N:174:ILE:CD1	2.49	0.43
2:O:116:VAL:HA	2:O:119:VAL:HG22	1.99	0.43
2:O:102:ARG:CZ	2:O:164:HIS:CD2	3.02	0.43
3:P:151:PHE:C	3:P:153:ALA:H	2.22	0.43
8:U:15:ASP:C	8:U:17:LEU:N	2.72	0.43
1:A:158:PHE:CE1	1:A:319:LEU:HD21	2.54	0.43
1:A:362:ARG:O	1:A:365:MET:HE2	2.18	0.43
2:B:239:TYR:CD2	2:B:240:TRP:N	2.86	0.43
2:B:353:THR:C	2:B:355:GLU:N	2.71	0.43
3:C:346:HIS:CG	3:C:347:PRO:HA	2.53	0.43
5:E:33:LYS:O	5:E:34:GLY:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.53	0.43
1:N:197:LEU:HA	1:N:197:LEU:HD12	1.79	0.43
2:O:76:THR:HG22	2:O:81:SER:CA	2.37	0.43
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.17	0.43
7:T:49:ALA:O	7:T:50:PRO:C	2.57	0.43
8:U:21:ARG:O	8:U:25:GLU:HG3	2.18	0.43
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.01	0.43
1:A:228:VAL:HG22	1:A:228:VAL:O	2.17	0.43
1:A:310:PHE:CE2	1:A:321:GLY:N	2.87	0.43
2:B:307:PHE:CG	2:B:308:ASP:N	2.86	0.43
2:B:60:THR:CG2	2:B:61:ALA:N	2.82	0.43
2:B:81:SER:C	2:B:83:PHE:N	2.70	0.43
2:B:84:ARG:HG2	2:B:84:ARG:HH11	1.83	0.43
3:C:127:THR:O	3:C:130:VAL:CG2	2.66	0.43
3:C:226:SER:O	3:C:230:ILE:HG12	2.19	0.43
3:C:230:ILE:HG23	11:C:2005:PEE:H25	2.01	0.43
3:C:75:GLN:O	3:C:76:TYR:HB2	2.19	0.43
4:D:147:LEU:HD23	4:D:159:GLY:HA2	2.01	0.43
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.53	0.43
5:E:192:LEU:HG	5:E:193:VAL:N	2.34	0.43
1:N:58:PHE:HB3	1:N:182:LEU:HD11	1.99	0.43
1:N:255:LEU:O	1:N:321:GLY:HA3	2.18	0.43
1:N:429:GLU:O	1:N:432:LEU:HD13	2.19	0.43
2:O:277:HIS:HB2	2:O:360:ALA:HB1	1.99	0.43
2:O:397:VAL:O	2:O:400:GLN:HB3	2.18	0.43
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.18	0.43
3:P:241:LEU:HB3	4:Q:208:MET:HE2	2.00	0.43
4:Q:218:LEU:HD22	5:R:39:VAL:HG12	2.01	0.43
4:Q:221:TYR:CE1	7:T:25:ALA:HB1	2.52	0.43
10:W:27:GLY:O	10:W:28:ALA:C	2.56	0.43
2:B:366:ALA:O	2:B:367:THR:C	2.56	0.43
2:B:379:LEU:O	2:B:379:LEU:HG	2.18	0.43
2:B:50:PHE:HZ	2:B:379:LEU:HG	1.84	0.43
2:B:52:LYS:HD2	2:B:203:ARG:HG2	2.01	0.43
4:D:175:THR:HA	4:D:176:PRO:HD3	1.90	0.43
5:E:52:LYS:CD	5:E:52:LYS:C	2.87	0.43
1:N:62:LEU:CD1	1:N:127:ILE:HG12	2.48	0.43
1:N:158:PHE:O	1:N:159:GLN:C	2.57	0.43
2:O:75:LEU:CD2	2:O:136:GLU:HB3	2.45	0.43
4:Q:134:TYR:OH	4:Q:160:MET:O	2.29	0.43
8:U:40:CYS:O	8:U:44:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG11	1:A:117:VAL:HG11	2.01	0.43
3:C:212:ILE:O	3:C:213:SER:C	2.57	0.43
3:C:89:SER:O	3:C:92:PHE:N	2.52	0.43
5:E:59:ILE:HA	5:E:59:ILE:HD13	1.82	0.43
1:N:435:ASN:O	1:N:438:ARG:N	2.52	0.43
2:O:417:PHE:C	2:O:417:PHE:CD2	2.92	0.43
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.83	0.43
3:P:87:GLY:N	3:P:240:PHE:HE2	2.17	0.43
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	2.01	0.43
7:T:55:ALA:O	7:T:56:TYR:C	2.56	0.43
3:P:215:ASP:HB3	7:T:7:LEU:HB3	2.00	0.43
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.34	0.43
1:A:187:ASP:O	1:A:191:LYS:HE3	2.19	0.43
1:A:438:ARG:NH1	1:A:438:ARG:HG3	2.34	0.43
1:A:55:ALA:O	1:A:56:GLY:C	2.57	0.43
2:B:162:ASN:HB3	2:B:244:ILE:HG21	2.01	0.43
2:B:325:TYR:HD2	2:B:326:THR:N	2.15	0.43
3:C:28:ILE:CG1	3:C:225:TYR:CE2	3.00	0.43
3:C:247:SER:OG	3:C:250:LEU:HB2	2.19	0.43
3:C:5:ILE:O	3:C:12:LEU:HD23	2.18	0.43
4:D:10:PHE:HB3	8:H:74:PHE:CE2	2.54	0.43
5:E:106:ILE:HD11	5:E:131:GLU:HA	2.00	0.43
1:A:171:THR:HB	5:E:4:ASP:OD2	2.19	0.43
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.99	0.43
9:I:53:GLU:C	9:I:55:MET:N	2.70	0.43
1:N:246:ASP:HA	1:N:427:PRO:HB3	2.01	0.43
1:N:404:ALA:O	1:N:405:ARG:C	2.56	0.43
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.74	0.43
5:R:97:PHE:CE2	5:R:137:GLY:HA3	2.54	0.43
1:A:176:HIS:O	1:A:177:LEU:C	2.55	0.43
1:A:246:ASP:HA	1:A:427:PRO:HB3	2.00	0.43
1:A:25:VAL:HG22	1:A:197:LEU:HB3	2.00	0.43
1:A:392:LEU:N	1:A:392:LEU:HD23	2.33	0.43
2:B:345:LYS:C	2:B:347:ALA:H	2.20	0.43
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.43
8:H:15:ASP:C	8:H:17:LEU:N	2.71	0.43
2:O:27:THR:HG22	2:O:28:LYS:H	1.83	0.43
3:P:107:SER:C	3:P:109:LEU:H	2.22	0.43
3:P:13:LYS:O	3:P:17:ASN:N	2.51	0.43
3:P:93:ILE:O	3:P:94:CYS:C	2.56	0.43
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:91:TRP:O	5:R:92:ARG:C	2.57	0.43
6:S:67:ASP:HA	6:S:70:LEU:HD23	2.01	0.43
2:B:121:GLU:HG3	2:B:125:ASN:ND2	2.34	0.42
2:B:63:LEU:O	2:B:65:THR:N	2.52	0.42
4:D:43:MET:HE3	4:D:189:PHE:CZ	2.53	0.42
6:F:68:LEU:O	6:F:71:LYS:N	2.51	0.42
1:N:19:LEU:C	1:N:21:ASN:H	2.21	0.42
1:N:274:ASN:CG	1:N:309:THR:HB	2.38	0.42
2:O:205:ALA:CB	2:O:387:LEU:HD13	2.48	0.42
4:Q:186:VAL:HG13	4:Q:187:CYS:N	2.33	0.42
5:R:141:HIS:CE1	5:R:142:LEU:HD12	2.54	0.42
5:R:14:ARG:NH1	5:R:14:ARG:HG2	2.34	0.42
6:S:103:GLU:O	6:S:104:ARG:C	2.58	0.42
6:S:64:ARG:O	6:S:68:LEU:HG	2.18	0.42
8:U:66:ASP:O	8:U:67:HIS:C	2.57	0.42
1:A:109:VAL:O	1:A:112:LEU:N	2.52	0.42
5:E:168:SER:CB	5:E:170:ARG:HG3	2.49	0.42
6:F:67:ASP:OD1	6:F:71:LYS:HD2	2.19	0.42
2:O:84:ARG:HH11	2:O:84:ARG:HG2	1.84	0.42
4:Q:16:GLY:O	4:Q:18:LEU:N	2.52	0.42
4:Q:218:LEU:HD13	5:R:43:ALA:N	2.34	0.42
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.48	0.42
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.83	0.42
1:A:388:ARG:NH2	1:A:388:ARG:HG3	2.34	0.42
3:C:339:ILE:HA	3:C:339:ILE:HD13	1.83	0.42
4:D:127:VAL:O	4:D:131:LEU:HG	2.18	0.42
10:J:14:PHE:CD2	10:J:14:PHE:N	2.85	0.42
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.83	0.42
2:O:46:ARG:HH11	2:O:110:GLU:CD	2.22	0.42
3:P:56:TYR:CZ	3:P:134:LEU:HB3	2.54	0.42
4:Q:1:GLY:C	4:Q:3:LEU:H	2.23	0.42
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.20	0.42
2:B:225:ASN:O	2:B:226:ILE:C	2.57	0.42
3:C:114:TRP:O	3:C:115:ASN:C	2.57	0.42
3:C:186:LEU:O	3:C:189:ALA:HB3	2.19	0.42
4:D:54:VAL:CG1	4:D:55:THR:HG23	2.49	0.42
5:E:78:LEU:HD21	5:E:193:VAL:HG11	2.01	0.42
5:E:79:SER:HB3	5:E:191:ASP:CB	2.50	0.42
5:E:33:LYS:HG2	7:G:21:PHE:CE1	2.55	0.42
8:H:15:ASP:O	8:H:16:PRO:C	2.58	0.42
1:N:42:GLY:HA2	1:N:384:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.20	0.42
3:P:86:ASN:O	3:P:87:GLY:C	2.58	0.42
4:Q:165:TYR:O	4:Q:166:ASN:C	2.57	0.42
6:S:65:ALA:O	6:S:68:LEU:HB2	2.19	0.42
7:T:38:TRP:O	7:T:41:PHE:N	2.52	0.42
2:B:130:PRO:HB2	2:B:132:PHE:CD2	2.53	0.42
2:B:147:ASP:O	2:B:150:VAL:HG22	2.20	0.42
3:C:114:TRP:O	3:C:117:GLY:N	2.53	0.42
3:C:326:PHE:C	3:C:326:PHE:CD2	2.92	0.42
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.77	0.42
3:C:213:SER:HB2	6:F:39:GLU:OE2	2.20	0.42
1:N:248:LEU:HB3	1:N:249:PRO:HD2	2.00	0.42
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.50	0.42
4:Q:54:VAL:CG1	4:Q:55:THR:HG23	2.50	0.42
5:R:135:LEU:HA	5:R:183:PRO:HD3	2.01	0.42
1:A:178:THR:CG2	1:A:179:ARG:N	2.82	0.42
1:A:191:LYS:C	1:A:193:PRO:HD2	2.39	0.42
1:A:49:ASN:HD21	1:A:52:ASN:H	1.65	0.42
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.54	0.42
2:B:200:THR:HB	2:B:227:ARG:O	2.19	0.42
3:C:145:THR:O	3:C:149:ASN:HB2	2.20	0.42
3:C:273:TRP:HA	3:C:276:LEU:HG	2.00	0.42
3:C:49:GLY:C	14:C:501:HEM:HAC	2.40	0.42
5:E:113:ASP:HB3	5:E:116:LYS:HG2	2.00	0.42
5:E:135:LEU:HD22	5:E:169:GLY:HA3	2.02	0.42
5:E:136:VAL:O	5:E:138:VAL:N	2.52	0.42
8:H:58:LEU:O	8:H:61:PHE:HB3	2.19	0.42
1:N:163:LEU:HB2	1:N:234:CYS:SG	2.60	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.83	0.42
2:O:348:ALA:HA	2:O:414:ALA:CB	2.49	0.42
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.83	0.42
4:Q:171:TYR:HD1	4:Q:175:THR:HB	1.84	0.42
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	2.01	0.42
7:T:29:ILE:HA	7:T:33:ALA:CB	2.50	0.42
2:B:341:MET:CE	2:B:344:LEU:HD23	2.50	0.42
3:C:356:SER:O	3:C:357:LEU:C	2.57	0.42
4:D:210:LEU:HD23	4:D:210:LEU:HA	1.81	0.42
5:E:31:ASP:O	5:E:32:ARG:C	2.56	0.42
2:B:325:TYR:HB3	9:I:59:SER:HB3	2.00	0.42
1:N:142:ASP:O	1:N:148:VAL:HG21	2.19	0.42
1:N:434:TYR:O	1:N:435:ASN:C	2.56	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:48:GLU:OE1	1:N:54:GLY:N	2.47	0.42
2:O:259:THR:CG2	2:O:260:GLU:N	2.83	0.42
3:P:77:GLY:O	3:P:78:TRP:C	2.58	0.42
5:R:170:ARG:HA	5:R:179:ASN:HB3	2.02	0.42
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.49	0.42
1:A:332:ASP:O	1:A:333:ASP:C	2.58	0.42
2:B:47:ILE:HG21	2:B:120:MET:CE	2.49	0.42
2:B:52:LYS:HB2	2:B:203:ARG:HB3	2.01	0.42
3:C:103:LEU:HA	3:C:103:LEU:HD12	1.65	0.42
3:C:184:PHE:CD2	3:P:184:PHE:CD2	3.08	0.42
3:C:216:SER:O	3:C:217:ASP:HB2	2.19	0.42
6:F:53:ASP:O	6:F:54:LEU:C	2.57	0.42
1:N:209:VAL:O	1:N:212:ALA:HB3	2.18	0.42
1:N:63:ALA:O	1:N:116:VAL:HG11	2.20	0.42
2:O:229:GLY:C	2:O:231:GLY:N	2.73	0.42
3:P:120:LEU:HB3	14:P:502:HEM:HAB	2.02	0.42
3:P:276:LEU:O	3:P:279:TYR:HB3	2.19	0.42
3:P:89:SER:O	3:P:92:PHE:N	2.53	0.42
6:S:79:GLN:HE21	6:S:79:GLN:HB3	1.65	0.42
3:P:347:PRO:HG3	7:T:62:GLY:HA2	2.02	0.42
1:A:86:PHE:CG	1:A:99:ILE:HG12	2.55	0.42
2:B:163:LEU:O	2:B:166:ALA:N	2.51	0.42
2:B:177:TYR:O	2:B:178:CYS:C	2.58	0.42
2:B:368:TYR:O	2:B:371:SER:HB2	2.20	0.42
3:C:101:ARG:HD2	3:C:101:ARG:O	2.20	0.42
3:C:186:LEU:HA	3:C:186:LEU:HD23	1.77	0.42
3:C:355:ALA:HA	3:C:358:SER:OG	2.20	0.42
3:C:53:ALA:N	14:C:501:HEM:HMD2	2.35	0.42
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.60	0.42
5:E:31:ASP:OD1	10:J:7:ARG:HG3	2.19	0.42
1:A:429:GLU:OE1	7:G:7:LEU:HB2	2.19	0.42
1:A:140:GLU:OE2	9:I:50:LEU:N	2.53	0.42
9:I:31:UNK:C	9:I:73:PRO:HG2	2.50	0.42
1:N:112:LEU:HG	1:N:112:LEU:H	1.59	0.42
1:N:307:PHE:HA	1:N:323:HIS:O	2.20	0.42
2:O:31:ASN:HD22	2:O:32:GLY:N	2.18	0.42
2:O:393:THR:HG23	2:O:397:VAL:HB	2.00	0.42
2:O:53:ALA:O	2:O:103:GLU:C	2.59	0.42
3:P:316:MET:O	3:P:317:THR:C	2.58	0.42
1:A:271:HIS:NE2	1:A:311:ASN:HB3	2.34	0.42
2:B:153:GLN:O	2:B:155:PRO:HD3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HD13	2:B:199:PHE:CD2	2.55	0.42
3:C:276:LEU:O	3:C:279:TYR:HB3	2.20	0.42
3:C:285:ILE:CD1	3:C:294:ALA:HB2	2.50	0.42
3:C:60:THR:N	3:C:176:LEU:HD23	2.35	0.42
5:E:112:VAL:O	5:E:114:VAL:N	2.53	0.42
5:E:72:SER:O	5:E:73:LYS:CG	2.68	0.42
2:O:141:GLN:N	2:O:142:PRO:CD	2.83	0.42
2:O:239:TYR:HD2	2:O:240:TRP:N	2.18	0.42
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.55	0.42
2:O:59:THR:HG22	2:O:60:THR:N	2.35	0.42
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.54	0.42
3:P:88:ALA:O	3:P:91:PHE:HB3	2.20	0.42
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	2.01	0.42
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.91	0.42
1:A:138:LEU:C	1:A:140:GLU:N	2.71	0.41
1:A:206:LYS:O	1:A:209:VAL:HG12	2.20	0.41
3:C:130:VAL:HG23	3:C:131:GLY:N	2.34	0.41
3:C:378:LEU:O	3:C:379:ASN:HB3	2.20	0.41
3:C:89:SER:O	3:C:90:PHE:C	2.57	0.41
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.55	0.41
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.50	0.41
1:N:39:VAL:HG11	1:N:117:VAL:HG11	2.01	0.41
1:N:46:ARG:HD3	1:N:231:LEU:HD13	2.02	0.41
1:N:273:ALA:O	1:N:275:ALA:N	2.53	0.41
2:O:177:TYR:O	2:O:178:CYS:C	2.58	0.41
1:A:203:ILE:HG22	1:A:204:SER:N	2.34	0.41
3:C:147:ILE:HD11	15:C:2001:ICX:H34	2.01	0.41
3:C:285:ILE:HG21	3:C:290:GLY:HA3	2.01	0.41
5:E:29:SER:O	5:E:30:GLU:C	2.59	0.41
8:H:28:GLU:O	8:H:29:LYS:C	2.58	0.41
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.01	0.41
1:N:53:ASN:OD1	1:N:165:ARG:HD3	2.19	0.41
3:P:120:LEU:HD22	14:P:502:HEM:CAB	2.49	0.41
5:R:185:TYR:HB2	5:R:194:VAL:O	2.20	0.41
6:S:70:LEU:HD12	6:S:70:LEU:C	2.40	0.41
4:Q:221:TYR:CE1	7:T:25:ALA:HB2	2.56	0.41
8:U:55:THR:O	8:U:58:LEU:HB3	2.19	0.41
10:W:14:PHE:CD2	10:W:14:PHE:N	2.88	0.41
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.51	0.41
2:B:56:ARG:CG	2:B:171:ALA:HB1	2.40	0.41
4:D:27:ARG:O	4:D:30:PHE:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:TRP:O	5:E:92:ARG:C	2.58	0.41
6:F:89:TYR:CD1	6:F:90:LEU:HB2	2.55	0.41
1:N:109:VAL:O	1:N:112:LEU:N	2.52	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.90	0.41
2:O:187:THR:OG1	2:O:190:GLN:HG3	2.19	0.41
2:O:312:PHE:N	2:O:323:GLY:O	2.41	0.41
3:P:12:LEU:HA	3:P:12:LEU:HD12	1.91	0.41
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	2.01	0.41
2:B:206:LEU:O	2:B:216:LEU:HD21	2.20	0.41
3:C:143:GLY:HA2	15:C:2001:ICX:H28	2.03	0.41
3:C:34:PHE:CE1	3:C:97:LEU:HD12	2.56	0.41
4:D:16:GLY:C	4:D:18:LEU:H	2.24	0.41
5:E:123:ASP:O	5:E:127:VAL:HG22	2.21	0.41
1:N:138:LEU:C	1:N:140:GLU:N	2.73	0.41
1:N:58:PHE:CD2	1:N:134:ILE:HD11	2.55	0.41
3:P:164:TRP:O	3:P:165:ALA:C	2.58	0.41
5:R:152:ASP:C	5:R:153:PHE:CD1	2.93	0.41
9:V:28:UNK:O	9:V:71:ASN:ND2	2.53	0.41
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.83	0.41
3:C:63:ALA:HB2	3:C:176:LEU:HD21	2.03	0.41
6:F:102:LEU:HD23	6:F:102:LEU:HA	1.87	0.41
6:F:19:TRP:O	6:F:20:TYR:C	2.58	0.41
2:B:90:GLU:HG2	9:I:71:ASN:ND2	2.34	0.41
1:N:126:GLN:O	1:N:129:LYS:HB3	2.20	0.41
3:P:241:LEU:HB3	4:Q:208:MET:CE	2.50	0.41
3:P:311:SER:OG	3:P:319:ARG:HD3	2.20	0.41
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.35	0.41
3:P:107:SER:HB2	14:P:502:HEM:HMD3	2.02	0.41
4:Q:195:GLU:N	4:Q:196:PRO:HD3	2.35	0.41
4:Q:55:THR:OG1	4:Q:56:HIS:ND1	2.41	0.41
4:Q:70:VAL:HG12	4:Q:71:GLN:H	1.85	0.41
5:R:98:VAL:HG13	5:R:134:ILE:CD1	2.43	0.41
10:W:10:TYR:C	10:W:10:TYR:CD2	2.94	0.41
1:A:324:PHE:CD1	1:A:334:MET:HG2	2.55	0.41
2:B:403:ASP:C	2:B:405:VAL:N	2.74	0.41
2:B:63:LEU:C	2:B:65:THR:H	2.24	0.41
6:F:32:MET:O	6:F:33:ARG:C	2.57	0.41
1:N:59:VAL:C	1:N:61:HIS:N	2.73	0.41
2:O:313:ASN:O	9:V:62:ARG:HG2	2.19	0.41
2:O:62:ASN:O	2:O:65:THR:CG2	2.63	0.41
3:P:52:LEU:O	3:P:54:MET:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:79:LEU:HD22	4:Q:204:MET:HE1	2.02	0.41
7:T:41:PHE:O	7:T:41:PHE:HD2	2.03	0.41
8:U:24:CYS:C	8:U:26:GLN:N	2.74	0.41
1:A:106:MET:HG3	1:A:203:ILE:HD13	2.03	0.41
3:C:31:TRP:CH2	11:C:2007:PEE:H20	2.56	0.41
3:C:235:LEU:HA	3:C:235:LEU:HD23	1.78	0.41
17:D:501:HEC:HMB1	17:D:501:HEC:CBB	2.25	0.41
5:E:103:GLN:C	5:E:105:GLU:N	2.73	0.41
1:N:145:MET:O	1:N:146:THR:C	2.59	0.41
4:Q:109:LEU:HA	4:Q:110:PRO:HD2	1.94	0.41
6:S:53:ASP:OD1	6:S:54:LEU:N	2.54	0.41
8:U:66:ASP:HA	8:U:69:VAL:HG23	2.02	0.41
1:A:55:ALA:O	1:A:57:TYR:N	2.53	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.39	0.41
2:B:372:VAL:O	2:B:372:VAL:HG12	2.21	0.41
3:C:148:THR:HG1	3:C:166:TRP:HE1	1.68	0.41
3:C:308:LEU:HD11	3:C:364:LEU:HD23	2.03	0.41
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.91	0.41
6:F:40:ASP:C	6:F:40:ASP:OD1	2.59	0.41
2:O:415:LYS:C	2:O:417:PHE:H	2.22	0.41
3:P:126:ALA:O	3:P:129:PHE:HB3	2.20	0.41
3:P:261:ASN:C	3:P:263:LEU:H	2.23	0.41
4:Q:235:MET:HE1	6:S:64:ARG:N	2.35	0.41
5:R:74:ILE:HG12	5:R:195:VAL:HB	2.02	0.41
6:S:89:TYR:CD1	6:S:90:LEU:HB2	2.56	0.41
9:V:32:UNK:O	9:V:33:UNK:C	2.68	0.41
1:A:109:VAL:O	1:A:110:VAL:C	2.59	0.41
2:B:209:ILE:HG22	2:B:210:GLY:N	2.36	0.41
2:B:393:THR:HG23	2:B:397:VAL:HB	2.02	0.41
3:C:320:PRO:O	3:C:323:GLN:HB2	2.20	0.41
3:C:38:LEU:HB3	14:C:502:HEM:HMB1	2.01	0.41
4:D:37:CYS:C	4:D:39:ALA:N	2.73	0.41
4:D:95:TYR:CD2	4:D:101:ALA:CA	3.00	0.41
5:E:161:HIS:HB2	19:E:501:FES:S1	2.61	0.41
5:E:95:PRO:HG3	3:P:263:LEU:CD2	2.50	0.41
10:J:6:LEU:HD23	10:J:6:LEU:HA	1.90	0.41
1:N:273:ALA:O	1:N:276:ILE:N	2.52	0.41
2:O:51:ILE:HD13	2:O:199:PHE:CD2	2.56	0.41
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.50	0.41
3:P:184:PHE:HA	14:P:501:HEM:CBC	2.42	0.41
3:P:267:PRO:HG2	3:P:268:HIS:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.03	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.51	0.41
6:S:16:ILE:HG22	6:S:17:ARG:N	2.35	0.41
8:U:24:CYS:O	8:U:26:GLN:N	2.54	0.41
1:A:67:THR:HB	1:A:119:ASN:O	2.21	0.41
2:B:46:ARG:HH11	2:B:110:GLU:CD	2.24	0.41
2:B:141:GLN:N	2:B:142:PRO:CD	2.84	0.41
2:B:183:ILE:HD13	2:B:183:ILE:HA	1.89	0.41
2:B:395:PRO:O	2:B:398:VAL:HG12	2.20	0.41
2:B:66:ALA:O	2:B:69:LEU:HB3	2.21	0.41
3:C:59:ASP:O	3:C:60:THR:C	2.59	0.41
4:D:28:ARG:O	4:D:31:GLN:N	2.54	0.41
4:D:52:ILE:HG22	4:D:53:GLY:N	2.36	0.41
5:E:150:SER:OG	5:E:157:TYR:HB3	2.21	0.41
4:D:10:PHE:CD2	8:H:74:PHE:HE2	2.39	0.41
2:O:248:ASN:ND2	2:O:250:HIS:N	2.63	0.41
2:O:383:GLY:O	2:O:384:SER:C	2.59	0.41
3:P:145:THR:O	3:P:149:ASN:HB2	2.21	0.41
3:P:28:ILE:CG1	3:P:225:TYR:CE2	3.01	0.41
3:P:230:ILE:HG23	11:W:3005:PEE:H25	2.03	0.41
3:P:342:GLN:HE21	3:P:343:PRO:CD	2.27	0.41
3:P:79:LEU:HD11	3:P:83:LEU:CD1	2.49	0.41
4:Q:51:LEU:O	4:Q:52:ILE:C	2.60	0.41
8:U:32:LYS:O	8:U:36:ARG:HG3	2.21	0.41
9:V:28:UNK:H	9:V:71:ASN:ND2	2.17	0.41
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.56	0.41
1:A:293:ARG:HD3	1:A:344:ARG:HD2	2.02	0.41
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.86	0.41
1:A:406:MET:O	1:A:410:VAL:HG23	2.21	0.41
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.41
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.56	0.41
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.56	0.41
5:R:52:LYS:CD	5:R:52:LYS:C	2.89	0.41
5:R:53:ASN:HA	5:R:53:ASN:HD22	1.67	0.41
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.51	0.41
9:V:68:ILE:HD13	9:V:68:ILE:HA	1.76	0.41
5:R:37:TYR:HB3	10:W:14:PHE:HB3	2.03	0.41
1:A:240:GLU:CD	1:A:242:ARG:HE	2.24	0.40
1:A:382:HIS:HB3	1:A:388:ARG:O	2.20	0.40
2:B:345:LYS:C	2:B:347:ALA:N	2.74	0.40
2:B:67:HIS:ND1	2:B:178:CYS:N	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ASP:OD1	3:C:173:ASN:N	2.49	0.40
3:C:278:ALA:HB1	3:C:295:LEU:HD11	2.01	0.40
3:C:326:PHE:HA	3:C:367:PHE:HZ	1.85	0.40
8:H:72:LYS:O	8:H:73:LEU:C	2.60	0.40
2:O:135:TRP:O	2:O:139:ASP:HB2	2.20	0.40
2:O:262:ALA:O	2:O:320:GLY:HA3	2.21	0.40
2:O:395:PRO:O	2:O:398:VAL:HG12	2.21	0.40
4:Q:169:LEU:O	4:Q:169:LEU:HD23	2.21	0.40
4:Q:86:LYS:N	4:Q:89:ASP:OD2	2.47	0.40
5:R:126:ARG:NE	5:R:168:SER:O	2.45	0.40
8:U:28:GLU:O	8:U:29:LYS:C	2.60	0.40
1:A:142:ASP:O	1:A:148:VAL:HG21	2.21	0.40
2:B:198:ASN:O	2:B:203:ARG:NE	2.54	0.40
2:B:212:LYS:HD2	2:B:214:SER:H	1.86	0.40
2:B:229:GLY:C	2:B:231:GLY:N	2.74	0.40
2:B:248:ASN:HD22	2:B:250:HIS:H	1.65	0.40
2:B:90:GLU:HG2	9:I:71:ASN:HD21	1.86	0.40
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.50	0.40
5:E:91:TRP:NE1	5:E:92:ARG:HG3	2.36	0.40
1:N:363:SER:HB3	2:O:112:LEU:HD21	2.04	0.40
2:O:183:ILE:HG23	2:O:183:ILE:HD12	1.90	0.40
2:O:426:ALA:O	2:O:427:SER:HB3	2.21	0.40
3:P:60:THR:N	3:P:176:LEU:HD23	2.37	0.40
3:P:326:PHE:C	3:P:326:PHE:CD2	2.94	0.40
4:Q:37:CYS:O	4:Q:39:ALA:N	2.54	0.40
8:U:55:THR:O	8:U:56:GLU:C	2.60	0.40
8:U:67:HIS:O	8:U:70:ALA:HB3	2.21	0.40
10:W:21:ALA:C	10:W:23:THR:N	2.75	0.40
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.51	0.40
1:A:257:VAL:HG23	1:A:320:PHE:HB3	2.03	0.40
1:A:269:VAL:HG11	1:A:410:VAL:CG2	2.51	0.40
2:B:248:ASN:ND2	2:B:428:GLY:CA	2.74	0.40
2:B:258:VAL:HG21	2:B:321:LEU:HD22	2.03	0.40
3:C:185:LEU:HD13	3:P:188:PHE:CZ	2.56	0.40
4:D:184:LYS:HG3	8:H:74:PHE:CE1	2.56	0.40
1:N:228:VAL:O	1:N:228:VAL:HG22	2.20	0.40
1:N:379:ILE:O	1:N:380:GLY:C	2.58	0.40
2:O:115:HIS:O	2:O:116:VAL:C	2.60	0.40
2:O:148:LYS:HG3	2:O:177:TYR:HB3	2.03	0.40
2:O:248:ASN:HD22	2:O:250:HIS:H	1.61	0.40
3:P:223:PRO:O	3:P:227:PHE:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:76:TYR:O	3:P:80:ILE:HG13	2.22	0.40
5:R:112:VAL:HG13	5:R:113:ASP:N	2.37	0.40
1:A:133:VAL:O	1:A:134:ILE:C	2.56	0.40
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.56	0.40
2:B:341:MET:CE	2:B:417:PHE:CE2	3.04	0.40
3:C:241:LEU:HB3	4:D:208:MET:CE	2.51	0.40
7:G:19:SER:HB3	7:G:22:GLU:HG2	2.04	0.40
1:N:106:MET:CE	1:N:110:VAL:CG2	3.00	0.40
2:O:130:PRO:CB	2:O:132:PHE:CE2	2.93	0.40
3:P:109:LEU:HA	3:P:109:LEU:HD23	1.88	0.40
3:P:237:LEU:HD12	3:P:237:LEU:HA	1.89	0.40
5:R:77:LYS:HB2	5:R:80:ASP:OD2	2.22	0.40
2:B:124:LEU:HD12	2:B:128:THR:CG2	2.50	0.40
2:B:167:ALA:C	2:B:168:TYR:CD1	2.95	0.40
2:B:205:ALA:CB	2:B:387:LEU:HD13	2.51	0.40
2:B:398:VAL:CG1	2:B:399:ALA:N	2.84	0.40
2:B:97:SER:HB2	2:B:99:TYR:CE1	2.56	0.40
3:C:56:TYR:CZ	3:C:134:LEU:HB3	2.57	0.40
3:C:350:ILE:CG2	3:C:351:ILE:N	2.84	0.40
3:C:61:SER:OG	3:C:62:LEU:HD12	2.21	0.40
4:D:144:ARG:HB3	4:D:147:LEU:HD12	2.04	0.40
4:D:200:GLN:O	4:D:204:MET:HG3	2.22	0.40
5:E:126:ARG:HD3	5:E:168:SER:OG	2.22	0.40
5:E:74:ILE:O	5:E:194:VAL:HG13	2.22	0.40
2:O:144:LEU:HB3	2:O:183:ILE:CD1	2.51	0.40
2:O:269:ALA:C	2:O:271:ALA:N	2.71	0.40
3:P:241:LEU:O	3:P:245:LEU:HB2	2.21	0.40
3:P:221:PHE:HE1	16:P:3002:UQ:C1	2.35	0.40
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.94	0.40
5:R:126:ARG:HG2	5:R:126:ARG:HH11	1.87	0.40
5:R:36:SER:HA	5:R:39:VAL:CG2	2.52	0.40
7:T:28:ASN:HB2	7:T:32:ASP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	345 (78%)	75 (17%)	21 (5%)	2	21
1	N	440/446 (99%)	344 (78%)	75 (17%)	21 (5%)	2	21
2	B	419/441 (95%)	342 (82%)	62 (15%)	15 (4%)	3	28
2	O	420/441 (95%)	333 (79%)	67 (16%)	20 (5%)	2	21
3	C	378/380 (100%)	300 (79%)	62 (16%)	16 (4%)	3	24
3	P	377/380 (99%)	302 (80%)	60 (16%)	15 (4%)	3	25
4	D	239/241 (99%)	195 (82%)	35 (15%)	9 (4%)	3	27
4	Q	239/241 (99%)	190 (80%)	36 (15%)	13 (5%)	2	19
5	E	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	15
5	R	194/196 (99%)	146 (75%)	31 (16%)	17 (9%)	1	9
6	F	98/110 (89%)	73 (74%)	22 (22%)	3 (3%)	4	32
6	S	98/110 (89%)	74 (76%)	22 (22%)	2 (2%)	7	41
7	G	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	2	20
7	T	77/81 (95%)	61 (79%)	11 (14%)	5 (6%)	1	15
8	H	68/77 (88%)	49 (72%)	16 (24%)	3 (4%)	2	23
8	U	65/77 (84%)	42 (65%)	17 (26%)	6 (9%)	1	8
9	I	29/52 (56%)	14 (48%)	10 (34%)	5 (17%)	0	2
9	V	29/52 (56%)	18 (62%)	8 (28%)	3 (10%)	0	7
10	J	59/61 (97%)	42 (71%)	15 (25%)	2 (3%)	3	30
10	W	57/61 (93%)	42 (74%)	9 (16%)	6 (10%)	0	7
All	All	4000/4170 (96%)	3120 (78%)	681 (17%)	199 (5%)	2	20

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	159	GLN
2	B	26	ILE
2	B	38	LEU
2	B	171	ALA
2	B	226	ILE
3	C	217	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	38	SER
4	D	198	HIS
5	E	69	LEU
5	E	92	ARG
5	E	177	PRO
7	G	7	LEU
9	I	56	SER
9	I	64	LEU
9	I	73	PRO
1	N	72	CYS
1	N	159	GLN
1	N	262	TRP
1	N	282	ARG
2	O	26	ILE
2	O	38	LEU
2	O	171	ALA
2	O	226	ILE
2	O	267	ALA
4	Q	198	HIS
5	R	69	LEU
5	R	92	ARG
5	R	188	VAL
7	T	7	LEU
8	U	49	HIS
8	U	51	GLU
9	V	56	SER
1	A	71	PRO
1	A	128	GLU
1	A	217	SER
1	A	262	TRP
1	A	282	ARG
2	B	20	GLY
2	B	64	GLY
2	B	231	GLY
2	B	427	SER
3	C	60	THR
3	C	213	SER
3	C	348	PHE
4	D	23	HIS
4	D	44	ASP
4	D	166	ASN
5	E	21	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	72	SER
5	E	113	ASP
5	E	137	GLY
5	E	141	HIS
9	I	54	SER
1	N	20	ASP
1	N	128	GLU
1	N	207	GLU
1	N	217	SER
1	N	288	LYS
1	N	332	ASP
2	O	19	PRO
2	O	64	GLY
2	O	218	GLN
2	O	231	GLY
2	O	427	SER
3	P	60	THR
3	P	217	ASP
4	Q	2	GLU
4	Q	23	HIS
4	Q	38	SER
4	Q	44	ASP
4	Q	166	ASN
5	R	21	ALA
5	R	73	LYS
5	R	109	GLU
5	R	137	GLY
6	S	83	TYR
9	V	63	ASP
10	W	22	LEU
1	A	218	GLY
1	A	274	ASN
1	A	288	LYS
1	A	332	ASP
1	A	339	GLN
1	A	404	ALA
2	B	319	SER
3	C	3	PRO
3	C	29	SER
3	C	58	ALA
3	C	158	GLY
3	C	216	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	71	LEU
6	F	52	LYS
7	G	33	ALA
7	G	50	PRO
8	H	25	GLU
8	H	65	ARG
9	I	53	GLU
10	J	32	GLU
10	J	56	LYS
1	N	121	ALA
1	N	274	ASN
1	N	404	ALA
2	O	227	ARG
2	O	290	SER
3	P	108	TYR
3	P	156	TYR
3	P	216	SER
3	P	348	PHE
5	R	63	SER
6	S	52	LYS
10	W	32	GLU
1	A	20	ASP
1	A	121	ALA
1	A	388	ARG
2	B	290	SER
2	B	296	TYR
3	C	156	TYR
3	C	317	THR
5	E	4	ASP
6	F	83	TYR
8	H	16	PRO
1	N	71	PRO
1	N	107	PRO
1	N	388	ARG
1	N	428	ILE
2	O	230	ALA
2	O	270	ASN
2	O	296	TYR
3	P	3	PRO
3	P	29	SER
3	P	58	ALA
3	P	158	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	213	SER
3	P	379	ASN
4	Q	17	PRO
4	Q	75	ASP
5	R	8	PRO
5	R	30	GLU
5	R	123	ASP
5	R	130	PRO
5	R	141	HIS
7	T	25	ALA
7	T	33	ALA
8	U	25	GLU
8	U	65	ARG
1	A	94	GLN
1	A	107	PRO
1	A	164	ALA
1	A	428	ILE
2	B	111	CYS
2	B	230	ALA
2	B	366	ALA
3	C	10	PRO
3	C	379	ASN
4	D	75	ASP
4	D	133	GLY
5	E	74	ILE
6	F	11	ARG
1	N	91	SER
1	N	94	GLN
1	N	122	LEU
2	O	319	SER
2	O	366	ALA
3	P	10	PRO
3	P	53	ALA
4	Q	176	PRO
5	R	90	LYS
7	T	50	PRO
7	T	75	ALA
8	U	16	PRO
8	U	47	ARG
10	W	14	PHE
10	W	33	ARG
1	A	81	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	25	ALA
1	N	137	GLU
4	Q	133	GLY
5	R	108	GLN
10	W	56	LYS
2	B	334	GLY
3	C	5	ILE
4	D	176	PRO
2	O	29	LEU
3	P	5	ILE
3	C	248	PRO
5	E	154	GLY
4	Q	52	ILE
4	Q	162	PRO
5	R	114	VAL
9	V	73	PRO
10	W	29	VAL
2	O	334	GLY
4	Q	53	GLY
3	C	93	ILE
4	D	17	PRO
5	E	8	PRO
2	O	249	GLY
5	R	154	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	338 (93%)	27 (7%)	13	45
1	N	365/368 (99%)	336 (92%)	29 (8%)	12	42
2	B	332/347 (96%)	313 (94%)	19 (6%)	20	54
2	O	333/347 (96%)	314 (94%)	19 (6%)	20	54
3	C	329/329 (100%)	306 (93%)	23 (7%)	15	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	328/329 (100%)	307 (94%)	21 (6%)	17	51
4	D	200/200 (100%)	190 (95%)	10 (5%)	24	58
4	Q	200/200 (100%)	190 (95%)	10 (5%)	24	58
5	E	166/166 (100%)	156 (94%)	10 (6%)	19	53
5	R	165/166 (99%)	153 (93%)	12 (7%)	14	45
6	F	92/96 (96%)	89 (97%)	3 (3%)	38	68
6	S	92/96 (96%)	89 (97%)	3 (3%)	38	68
7	G	71/71 (100%)	64 (90%)	7 (10%)	8	34
7	T	69/71 (97%)	63 (91%)	6 (9%)	10	39
8	H	65/71 (92%)	62 (95%)	3 (5%)	27	61
8	U	63/71 (89%)	59 (94%)	4 (6%)	18	51
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	62
9	V	23/26 (88%)	22 (96%)	1 (4%)	29	62
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	64
10	W	47/49 (96%)	45 (96%)	2 (4%)	29	62
All	All	3377/3446 (98%)	3165 (94%)	212 (6%)	18	51

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	TRP
1	A	49	ASN
1	A	53	ASN
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	108	LYS
1	A	163	LEU
1	A	171	THR
1	A	182	LEU
1	A	188	THR
1	A	223	TYR
1	A	228	VAL
1	A	233	ARG
1	A	257	VAL
1	A	264	ASP
1	A	274	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	ASP
1	A	307	PHE
1	A	309	THR
1	A	342	TRP
1	A	362	ARG
1	A	365	MET
1	A	395	TRP
1	A	405	ARG
1	A	406	MET
1	A	431	LEU
2	B	31	ASN
2	B	45	SER
2	B	50	PHE
2	B	97	SER
2	B	139	ASP
2	B	154	SER
2	B	160	LEU
2	B	181	TYR
2	B	212	LYS
2	B	239	TYR
2	B	248	ASN
2	B	296	TYR
2	B	304	THR
2	B	314	VAL
2	B	325	TYR
2	B	328	SER
2	B	341	MET
2	B	403	ASP
2	B	437	ASP
3	C	36	SER
3	C	41	CYS
3	C	44	THR
3	C	52	LEU
3	C	64	PHE
3	C	69	HIS
3	C	82	ASN
3	C	118	VAL
3	C	138	GLN
3	C	149	ASN
3	C	194	THR
3	C	199	THR
3	C	207	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	208	ASN
3	C	216	SER
3	C	258	THR
3	C	272	GLU
3	C	304	LEU
3	C	317	THR
3	C	324	THR
3	C	334	LEU
3	C	344	VAL
3	C	373	LEU
4	D	2	GLU
4	D	3	LEU
4	D	42	SER
4	D	70	VAL
4	D	76	GLU
4	D	112	ASP
4	D	117	VAL
4	D	141	VAL
4	D	145	GLU
4	D	169	LEU
5	E	17	ASP
5	E	23	THR
5	E	39	VAL
5	E	52	LYS
5	E	61	SER
5	E	80	ASP
5	E	125	ASP
5	E	135	LEU
5	E	145	VAL
5	E	177	PRO
6	F	27	ASN
6	F	70	LEU
6	F	89	TYR
7	G	4	PHE
7	G	16	TYR
7	G	17	SER
7	G	27	PRO
7	G	34	LEU
7	G	41	PHE
7	G	63	THR
8	H	19	THR
8	H	71	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	73	LEU
9	I	70	LEU
10	J	18	SER
10	J	59	TYR
1	N	3	THR
1	N	32	GLN
1	N	40	TRP
1	N	49	ASN
1	N	53	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	108	LYS
1	N	163	LEU
1	N	171	THR
1	N	182	LEU
1	N	188	THR
1	N	223	TYR
1	N	228	VAL
1	N	257	VAL
1	N	264	ASP
1	N	274	ASN
1	N	281	ASP
1	N	307	PHE
1	N	309	THR
1	N	342	TRP
1	N	362	ARG
1	N	365	MET
1	N	370	ASP
1	N	395	TRP
1	N	405	ARG
1	N	406	MET
1	N	431	LEU
2	O	31	ASN
2	O	45	SER
2	O	97	SER
2	O	106	THR
2	O	139	ASP
2	O	154	SER
2	O	160	LEU
2	O	181	TYR
2	O	214	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	239	TYR
2	O	248	ASN
2	O	296	TYR
2	O	304	THR
2	O	314	VAL
2	O	325	TYR
2	O	328	SER
2	O	341	MET
2	O	403	ASP
2	O	437	ASP
3	P	32	TRP
3	P	44	THR
3	P	52	LEU
3	P	64	PHE
3	P	82	ASN
3	P	120	LEU
3	P	138	GLN
3	P	149	ASN
3	P	161	LEU
3	P	182	LEU
3	P	199	THR
3	P	207	ASN
3	P	208	ASN
3	P	216	SER
3	P	258	THR
3	P	272	GLU
3	P	304	LEU
3	P	317	THR
3	P	324	THR
3	P	344	VAL
3	P	373	LEU
4	Q	3	LEU
4	Q	42	SER
4	Q	70	VAL
4	Q	112	ASP
4	Q	117	VAL
4	Q	124	GLU
4	Q	141	VAL
4	Q	166	ASN
4	Q	169	LEU
4	Q	241	LYS
5	R	17	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	23	THR
5	R	39	VAL
5	R	52	LYS
5	R	61	SER
5	R	102	THR
5	R	108	GLN
5	R	112	VAL
5	R	135	LEU
5	R	145	VAL
5	R	184	THR
5	R	185	TYR
6	S	27	ASN
6	S	70	LEU
6	S	89	TYR
7	T	4	PHE
7	T	16	TYR
7	T	17	SER
7	T	34	LEU
7	T	41	PHE
7	T	63	THR
8	U	13	LEU
8	U	19	THR
8	U	48	SER
8	U	73	LEU
9	V	70	LEU
10	W	18	SER
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	118	GLN
1	A	159	GLN
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	125	ASN
2	B	156	GLN
2	B	248	ASN
2	B	329	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	363	GLN
3	C	17	ASN
3	C	82	ASN
3	C	115	ASN
3	C	149	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	105	ASN
4	D	200	GLN
5	E	53	ASN
5	E	57	GLN
5	E	103	GLN
5	E	122	HIS
5	E	164	HIS
6	F	22	ASN
6	F	79	GLN
6	F	108	ASN
7	G	23	GLN
7	G	44	GLN
7	G	79	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	136	GLN
1	N	143	ASN
1	N	159	GLN
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	125	ASN
2	O	156	GLN
2	O	248	ASN
2	O	329	GLN
2	O	363	GLN
2	O	376	GLN
3	P	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	82	ASN
3	P	115	ASN
3	P	149	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	31	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	105	ASN
4	Q	200	GLN
5	R	53	ASN
5	R	57	GLN
5	R	164	HIS
6	S	22	ASN
6	S	56	ASN
6	S	72	HIS
6	S	79	GLN
6	S	108	ASN
7	T	23	GLN
7	T	44	GLN
7	T	79	ASN
8	U	75	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are unknown - leaving 30 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
12	BOG	Q	3091	-	20,20,20	1.16	3 (15%)	25,25,25	0.95	1 (4%)
15	ICX	P	3001	-	31,31,31	1.38	6 (19%)	36,39,39	0.91	1 (2%)
11	PEE	P	3008	-	4,4,50	3.44	4 (100%)	6,6,55	0.57	0
18	CDL	D	2003	-	41,41,99	1.18	1 (2%)	47,53,111	1.05	2 (4%)
11	PEE	C	2007	-	48,48,50	1.29	7 (14%)	51,53,55	0.91	5 (9%)
12	BOG	E	2009	-	20,20,20	1.15	2 (10%)	25,25,25	0.92	1 (4%)
11	PEE	W	3005	-	49,49,50	1.49	10 (20%)	52,54,55	0.95	5 (9%)
18	CDL	G	2004	-	39,39,99	1.29	5 (12%)	45,51,111	1.08	3 (6%)
14	HEM	P	502	3	27,50,50	1.98	8 (29%)	17,82,82	1.65	4 (23%)
18	CDL	P	3004	-	39,39,99	1.25	3 (7%)	45,51,111	1.07	3 (6%)
11	PEE	P	3007	-	48,48,50	1.31	6 (12%)	51,53,55	0.91	4 (7%)
14	HEM	P	501	3	27,50,50	2.54	9 (33%)	17,82,82	2.18	4 (23%)
14	HEM	C	502	3	27,50,50	2.55	9 (33%)	17,82,82	2.15	5 (29%)
16	UQ	P	3002	-	19,19,63	2.57	10 (52%)	23,26,79	1.27	2 (8%)
17	HEC	Q	501	4	26,50,50	2.53	3 (11%)	18,82,82	1.91	3 (16%)
13	AZI	P	3011	-	0,2,2	0.00	-	0,1,1	0.00	-
17	HEC	D	501	4	26,50,50	2.71	7 (26%)	18,82,82	2.05	6 (33%)
18	CDL	P	3003	-	41,41,99	1.18	2 (4%)	47,53,111	1.07	2 (4%)
13	AZI	C	2011	-	0,2,2	0.00	-	0,1,1	0.00	-
16	UQ	C	2002	-	19,19,63	2.49	9 (47%)	23,26,79	1.25	2 (8%)
12	BOG	Q	3009	-	20,20,20	1.21	3 (15%)	25,25,25	1.14	1 (4%)
11	PEE	A	2008	-	20,20,50	1.80	5 (25%)	23,25,55	0.74	1 (4%)
11	PEE	C	2005	-	49,49,50	1.41	10 (20%)	52,54,55	0.95	5 (9%)
15	ICX	C	2001	-	31,31,31	1.32	4 (12%)	36,39,39	1.04	2 (5%)
12	BOG	D	2091	-	20,20,20	1.12	2 (10%)	25,25,25	0.97	1 (4%)
19	FES	R	501	5	0,4,4	0.00	-	-	-	-
12	BOG	C	3010	-	11,11,20	1.03	2 (18%)	10,11,25	0.91	1 (10%)
12	BOG	P	2010	-	18,18,20	1.11	3 (16%)	22,22,25	0.55	0
14	HEM	C	501	3	27,50,50	2.61	12 (44%)	17,82,82	2.45	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	FES	E	501	5	0,4,4	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BOG	Q	3091	-	-	6/11/31/31	0/1/1/1
15	ICX	P	3001	-	-	2/24/24/24	0/2/2/2
18	CDL	D	2003	-	-	23/51/51/110	-
12	BOG	E	2009	-	-	6/11/31/31	0/1/1/1
18	CDL	G	2004	-	-	21/49/49/110	-
14	HEM	P	502	3	-	2/6/54/54	-
15	ICX	C	2001	-	-	2/24/24/24	0/2/2/2
18	CDL	P	3004	-	-	21/49/49/110	-
11	PEE	P	3007	-	-	29/52/52/54	-
14	HEM	P	501	3	-	0/6/54/54	-
14	HEM	C	502	3	-	2/6/54/54	-
16	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
17	HEC	Q	501	4	-	2/6/54/54	-
11	PEE	A	2008	-	-	12/24/24/54	-
17	HEC	D	501	4	-	2/6/54/54	-
18	CDL	P	3003	-	-	24/51/51/110	-
11	PEE	W	3005	-	-	29/53/53/54	-
16	UQ	C	2002	-	-	2/11/35/87	0/1/1/1
12	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
11	PEE	C	2005	-	-	28/53/53/54	-
11	PEE	C	2007	-	-	28/52/52/54	-
12	BOG	D	2091	-	-	4/11/31/31	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
12	BOG	C	3010	-	-	4/9/9/31	-
12	BOG	P	2010	-	-	2/6/26/31	0/1/1/1
14	HEM	C	501	3	-	0/6/54/54	-
19	FES	E	501	5	-	-	0/1/1/1

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3B-C2B	-11.00	1.29	1.40
17	D	501	HEC	C3B-C2B	-10.50	1.29	1.40
14	P	501	HEM	C3B-C2B	-6.40	1.31	1.40
14	C	502	HEM	C3C-C2C	-6.24	1.31	1.40
14	C	501	HEM	C3B-CAB	-5.99	1.35	1.47
16	P	3002	UQ	C7-C6	5.96	1.61	1.51
17	D	501	HEC	C3C-C2C	-5.95	1.34	1.40
14	P	501	HEM	C3B-CAB	-5.75	1.36	1.47
14	C	502	HEM	C3C-CAC	-5.62	1.36	1.47
14	C	502	HEM	C3B-CAB	-5.54	1.36	1.47
14	C	501	HEM	C3C-CAC	-5.33	1.36	1.47
16	C	2002	UQ	C7-C6	5.24	1.60	1.51
14	P	502	HEM	C3B-CAB	-5.19	1.37	1.47
14	P	501	HEM	C3C-CAC	-5.18	1.37	1.47
16	P	3002	UQ	C6-C5	4.83	1.44	1.35
11	P	3008	PEE	P-O1P	4.70	1.61	1.50
16	C	2002	UQ	C6-C5	4.50	1.43	1.35
14	C	501	HEM	C3B-C2B	-4.42	1.34	1.40
14	C	501	HEM	C3C-C2C	-4.33	1.34	1.40
14	C	502	HEM	C1B-C2B	4.22	1.52	1.42
14	C	501	HEM	C1B-C2B	4.18	1.52	1.42
14	P	502	HEM	CBC-CAC	3.83	1.54	1.29
11	W	3005	PEE	O3-C30	3.76	1.44	1.33
14	C	501	HEM	CBC-CAC	3.72	1.54	1.29
16	C	2002	UQ	C6-C1	3.72	1.57	1.46
16	P	3002	UQ	C6-C1	3.72	1.57	1.46
14	P	501	HEM	CBC-CAC	3.68	1.53	1.29
14	C	502	HEM	CBC-CAC	3.65	1.53	1.29
11	W	3005	PEE	O2-C10	3.58	1.44	1.34
14	P	501	HEM	CBB-CAB	3.58	1.53	1.29
14	P	502	HEM	C3C-CAC	-3.53	1.40	1.47
11	C	2005	PEE	O3-C30	3.53	1.43	1.33
14	P	501	HEM	C1B-C2B	3.53	1.50	1.42
14	P	501	HEM	C3C-C2C	-3.39	1.35	1.40
11	P	3008	PEE	P-O4P	3.33	1.64	1.54
17	D	501	HEC	C3C-C4C	3.32	1.49	1.43
11	P	3007	PEE	O2-C10	3.31	1.43	1.34
17	Q	501	HEC	C3C-C2C	-3.30	1.37	1.40
11	C	2005	PEE	O2-C10	3.26	1.43	1.34
14	C	501	HEM	CBB-CAB	3.22	1.50	1.29
11	A	2008	PEE	O2-C10	3.21	1.43	1.34
11	A	2008	PEE	P-O1P	3.17	1.62	1.50
14	C	502	HEM	C2A-C3A	-3.13	1.28	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	2002	UQ	O3-C3	3.11	1.44	1.36
11	W	3005	PEE	P-O1P	3.11	1.61	1.50
11	W	3005	PEE	C19-C18	-3.05	1.34	1.51
11	C	2005	PEE	P-O1P	3.05	1.61	1.50
11	A	2008	PEE	O3-C30	3.04	1.42	1.33
14	P	502	HEM	C1B-C2B	3.01	1.49	1.42
15	P	3001	ICX	C12-C11	3.00	1.44	1.39
11	P	3007	PEE	O3-C30	2.99	1.42	1.33
11	C	2005	PEE	C19-C18	-2.99	1.34	1.51
11	P	3008	PEE	P-O3P	2.98	1.63	1.54
11	C	2005	PEE	C22-C21	-2.97	1.34	1.51
11	W	3005	PEE	C22-C21	-2.96	1.35	1.51
11	C	2007	PEE	C19-C18	-2.91	1.35	1.51
11	P	3007	PEE	P-O1P	2.91	1.61	1.50
11	C	2007	PEE	C22-C21	-2.89	1.35	1.51
11	C	2007	PEE	O2-C10	2.84	1.42	1.34
11	P	3007	PEE	C22-C21	-2.83	1.35	1.51
16	C	2002	UQ	C5-C4	2.78	1.57	1.47
16	P	3002	UQ	CM5-C5	2.77	1.56	1.50
16	C	2002	UQ	CM5-C5	2.77	1.56	1.50
16	P	3002	UQ	O3-C3	2.75	1.43	1.36
11	P	3007	PEE	C19-C18	-2.73	1.36	1.51
14	P	502	HEM	CBB-CAB	2.72	1.47	1.29
11	C	2007	PEE	P-O1P	2.72	1.60	1.50
12	E	2009	BOG	O5-C1	2.69	1.48	1.41
15	P	3001	ICX	C13-C12	2.68	1.43	1.38
16	C	2002	UQ	O2-C2	2.65	1.43	1.36
17	Q	501	HEC	C4D-CHA	-2.63	1.33	1.41
16	C	2002	UQ	C2-C1	2.61	1.56	1.48
17	D	501	HEC	C2A-C3A	-2.61	1.29	1.37
11	W	3005	PEE	C11-C10	2.59	1.58	1.50
15	P	3001	ICX	C10-C9	2.58	1.43	1.38
16	C	2002	UQ	C3-C4	2.58	1.56	1.48
16	P	3002	UQ	C5-C4	2.57	1.56	1.47
12	Q	3091	BOG	O5-C1	2.56	1.48	1.41
11	C	2007	PEE	O3-C30	2.55	1.40	1.33
12	Q	3009	BOG	O5-C1	2.55	1.48	1.41
12	D	2091	BOG	O5-C1	2.55	1.48	1.41
14	C	501	HEM	C3D-C2D	-2.52	1.30	1.37
14	P	501	HEM	C4A-NA	2.52	1.41	1.36
11	W	3005	PEE	C3-C2	2.48	1.58	1.50
14	C	502	HEM	CBB-CAB	2.47	1.45	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	3002	UQ	C7-C8	2.46	1.54	1.50
12	C	3010	BOG	C2-C1	2.46	1.57	1.50
15	C	2001	ICX	C12-C11	2.44	1.43	1.39
11	A	2008	PEE	C3-C2	2.43	1.58	1.50
12	P	2010	BOG	C4-C5	2.42	1.58	1.53
18	P	3004	CDL	CA3-CA4	2.41	1.58	1.50
11	C	2005	PEE	C31-C30	2.41	1.57	1.50
11	A	2008	PEE	C1-C2	2.41	1.58	1.50
15	C	2001	ICX	C13-C12	2.40	1.43	1.38
18	D	2003	CDL	O1-C1	2.40	1.50	1.43
11	W	3005	PEE	C31-C30	2.37	1.57	1.50
16	P	3002	UQ	C2-C1	2.34	1.55	1.48
16	P	3002	UQ	O2-C2	2.34	1.42	1.36
18	G	2004	CDL	CA3-CA4	2.34	1.57	1.50
12	D	2091	BOG	C4-C5	2.33	1.58	1.53
15	C	2001	ICX	C10-C9	2.32	1.43	1.38
18	G	2004	CDL	O1-C1	2.32	1.50	1.43
11	C	2007	PEE	C3-C2	2.32	1.57	1.50
14	C	501	HEM	C4B-NB	2.31	1.40	1.36
18	P	3003	CDL	O1-C1	2.30	1.50	1.43
11	P	3008	PEE	P-O2P	2.29	1.61	1.54
15	P	3001	ICX	C9-C8	2.28	1.43	1.38
16	P	3002	UQ	C3-C4	2.28	1.55	1.48
11	W	3005	PEE	C1-C2	2.28	1.57	1.50
15	C	2001	ICX	C10-C11	2.27	1.43	1.39
11	C	2005	PEE	C1-C2	2.27	1.57	1.50
12	Q	3091	BOG	C4-C5	2.26	1.57	1.53
17	D	501	HEC	C1C-NC	2.26	1.40	1.36
12	Q	3009	BOG	C4-C5	2.25	1.57	1.53
18	P	3004	CDL	O1-C1	2.24	1.50	1.43
14	C	501	HEM	C1D-CHD	-2.24	1.34	1.41
12	E	2009	BOG	O5-C5	2.23	1.49	1.44
14	P	502	HEM	C3C-C2C	-2.17	1.37	1.40
11	C	2005	PEE	P-O4P	2.17	1.68	1.59
12	Q	3009	BOG	C1-C2	2.16	1.58	1.52
17	D	501	HEC	C4D-CHA	-2.16	1.35	1.41
11	C	2005	PEE	C3-C2	2.15	1.57	1.50
12	P	2010	BOG	C1-C2	2.15	1.57	1.52
12	C	3010	BOG	O5-C1	2.15	1.45	1.40
18	P	3003	CDL	CA3-CA4	2.15	1.57	1.50
11	C	2005	PEE	C11-C10	2.15	1.57	1.50
15	P	3001	ICX	C1-C2	2.14	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	502	HEM	C1A-CHA	-2.13	1.35	1.41
14	C	502	HEM	CAA-C2A	-2.13	1.48	1.52
11	C	2007	PEE	C11-C10	2.11	1.56	1.50
17	D	501	HEC	C1D-CHD	-2.09	1.35	1.41
11	P	3007	PEE	C31-C30	2.07	1.56	1.50
18	G	2004	CDL	OA6-CA5	2.05	1.40	1.34
14	P	501	HEM	C3D-C2D	-2.04	1.31	1.37
14	C	501	HEM	C1A-CHA	-2.03	1.35	1.41
14	C	502	HEM	C3B-C2B	-2.03	1.37	1.40
18	G	2004	CDL	CB3-CB4	2.03	1.56	1.50
18	G	2004	CDL	C51-CB5	2.02	1.56	1.50
14	P	502	HEM	C4B-CHC	-2.02	1.35	1.41
18	P	3004	CDL	OB8-CB7	2.02	1.39	1.33
12	P	2010	BOG	O5-C1	2.02	1.47	1.42
15	P	3001	ICX	C10-C11	2.02	1.42	1.39
11	W	3005	PEE	O2-C2	2.01	1.51	1.46
12	Q	3091	BOG	O5-C5	2.01	1.49	1.44
14	C	501	HEM	CAA-C2A	-2.00	1.49	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	501	HEM	CBA-CAA-C2A	-6.48	100.53	112.49
14	C	502	HEM	C1D-C2D-C3D	6.22	111.32	107.00
14	C	501	HEM	CBA-CAA-C2A	-6.17	101.11	112.49
17	D	501	HEC	CBA-CAA-C2A	5.32	122.28	112.48
17	Q	501	HEC	CBA-CAA-C2A	4.94	121.58	112.48
12	Q	3009	BOG	C1'-O1-C1	4.89	121.96	113.84
15	C	2001	ICX	C30-C31-N33	-4.36	109.09	116.42
12	D	2091	BOG	C1'-O1-C1	4.04	120.54	113.84
17	Q	501	HEC	CMB-C2B-C3B	-4.02	121.09	125.82
14	C	501	HEM	CMC-C2C-C3C	3.97	132.11	124.68
14	P	501	HEM	C4A-C3A-C2A	-3.93	104.26	107.00
16	P	3002	UQ	C8-C7-C6	3.90	122.57	112.05
12	Q	3091	BOG	C1'-O1-C1	3.84	120.20	113.84
16	C	2002	UQ	C8-C7-C6	3.82	122.33	112.05
15	P	3001	ICX	C30-C31-N33	-3.69	110.21	116.42
12	E	2009	BOG	C1'-O1-C1	3.46	119.58	113.84
14	C	501	HEM	C3B-C4B-NB	3.27	113.44	109.21
14	P	502	HEM	CMB-C2B-C3B	3.24	130.75	124.68
14	C	502	HEM	CBA-CAA-C2A	3.24	118.45	112.49
16	P	3002	UQ	C7-C6-C1	-3.14	114.70	118.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	3004	CDL	CB4-OB6-CB5	-3.11	110.13	117.79
16	C	2002	UQ	C7-C6-C1	-3.11	114.74	118.48
14	P	502	HEM	C3B-C4B-NB	3.05	113.16	109.21
18	G	2004	CDL	CB4-OB6-CB5	-3.04	110.32	117.79
14	C	502	HEM	C3B-C4B-NB	2.95	113.02	109.21
14	C	502	HEM	CMD-C2D-C1D	-2.87	124.05	128.46
11	P	3007	PEE	C20-C19-C18	2.80	128.66	114.42
11	C	2007	PEE	C20-C19-C18	2.79	128.60	114.42
17	D	501	HEC	C4C-C3C-C2C	2.78	109.35	106.35
14	C	501	HEM	CMD-C2D-C1D	2.73	132.65	128.46
14	C	501	HEM	CBD-CAD-C3D	2.72	117.50	112.48
11	W	3005	PEE	C20-C19-C18	2.71	128.19	114.42
11	C	2005	PEE	C20-C19-C18	2.71	128.19	114.42
17	D	501	HEC	CMB-C2B-C3B	-2.70	122.65	125.82
11	P	3007	PEE	C19-C18-C17	2.66	127.91	114.42
11	C	2005	PEE	C19-C18-C17	2.60	127.63	114.42
11	C	2007	PEE	C19-C18-C17	2.59	127.59	114.42
17	Q	501	HEC	C4C-C3C-C2C	2.57	109.13	106.35
11	P	3007	PEE	C22-C21-C20	2.55	127.36	114.42
11	W	3005	PEE	C19-C18-C17	2.54	127.32	114.42
14	C	502	HEM	CMC-C2C-C3C	2.54	129.43	124.68
18	D	2003	CDL	CB4-OB6-CB5	-2.52	111.60	117.79
11	W	3005	PEE	C22-C21-C20	2.49	127.07	114.42
11	P	3007	PEE	C23-C22-C21	2.47	126.99	114.42
11	C	2007	PEE	C23-C22-C21	2.47	126.95	114.42
11	C	2005	PEE	C22-C21-C20	2.46	126.89	114.42
17	D	501	HEC	CAA-C2A-C3A	-2.44	120.22	127.25
14	P	501	HEM	CMC-C2C-C3C	2.44	129.24	124.68
18	P	3003	CDL	CB4-OB6-CB5	-2.42	111.83	117.79
11	C	2007	PEE	C22-C21-C20	2.42	126.70	114.42
11	W	3005	PEE	O3-C3-C2	2.39	115.39	108.43
11	W	3005	PEE	C23-C22-C21	2.38	126.50	114.42
11	C	2005	PEE	C23-C22-C21	2.35	126.37	114.42
14	P	502	HEM	CBA-CAA-C2A	2.35	116.81	112.49
11	C	2005	PEE	O3-C3-C2	2.34	115.25	108.43
18	D	2003	CDL	CA6-CA4-CA3	-2.32	106.30	111.79
14	P	502	HEM	CMC-C2C-C3C	2.31	129.00	124.68
11	C	2007	PEE	O3-C3-C2	2.29	115.10	108.43
14	C	501	HEM	CMD-C2D-C3D	-2.25	120.71	124.94
18	P	3003	CDL	CA6-CA4-CA3	-2.24	106.48	111.79
14	C	501	HEM	CAD-C3D-C2D	-2.22	120.86	127.25
17	D	501	HEC	CMD-C2D-C3D	-2.22	120.76	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	2004	CDL	CA4-OA6-CA5	-2.22	112.33	117.79
17	D	501	HEC	CMA-C3A-C2A	-2.17	120.85	124.94
12	C	3010	BOG	C1'-O1-C1	2.12	118.65	114.00
18	P	3004	CDL	CA4-OA6-CA5	-2.11	112.60	117.79
14	P	501	HEM	C3B-C4B-NB	2.10	111.93	109.21
11	A	2008	PEE	O3-C3-C2	2.10	114.55	108.43
18	G	2004	CDL	OB6-CB4-CB3	2.08	115.93	108.40
15	C	2001	ICX	O32-C31-C30	2.06	125.78	122.02
18	P	3004	CDL	OB6-CB4-CB3	2.03	115.75	108.40
14	C	501	HEM	CMB-C2B-C3B	-2.02	120.90	124.68

There are no chirality outliers.

All (257) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	Q	3091	BOG	C2-C1-O1-C1'
12	Q	3091	BOG	O5-C1-O1-C1'
18	D	2003	CDL	O1-C1-CB2-OB2
18	D	2003	CDL	CA2-OA2-PA1-OA5
18	D	2003	CDL	CB2-OB2-PB2-OB3
18	D	2003	CDL	CB2-OB2-PB2-OB4
11	W	3005	PEE	C11-C10-O2-C2
11	W	3005	PEE	C1-O3P-P-O1P
11	W	3005	PEE	C1-O3P-P-O2P
11	W	3005	PEE	C4-O4P-P-O1P
11	W	3005	PEE	C4-O4P-P-O2P
18	G	2004	CDL	O1-C1-CA2-OA2
18	G	2004	CDL	CA3-OA5-PA1-OA3
18	G	2004	CDL	CB3-OB5-PB2-OB3
18	G	2004	CDL	C51-CB5-OB6-CB4
14	P	502	HEM	C4D-C3D-CAD-CBD
18	P	3004	CDL	O1-C1-CA2-OA2
18	P	3004	CDL	CA3-OA5-PA1-OA3
18	P	3004	CDL	CB3-OB5-PB2-OB3
18	P	3004	CDL	C51-CB5-OB6-CB4
11	P	3007	PEE	C4-O4P-P-O1P
11	P	3007	PEE	C4-O4P-P-O2P
11	P	3007	PEE	C4-O4P-P-O3P
14	C	502	HEM	C2D-C3D-CAD-CBD
14	C	502	HEM	C4D-C3D-CAD-CBD
16	P	3002	UQ	C1-C6-C7-C8
16	P	3002	UQ	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	Q	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
17	D	501	HEC	C1A-C2A-CAA-CBA
17	D	501	HEC	C3A-C2A-CAA-CBA
18	P	3003	CDL	O1-C1-CB2-OB2
18	P	3003	CDL	CA2-OA2-PA1-OA5
18	P	3003	CDL	CB2-OB2-PB2-OB3
18	P	3003	CDL	CB2-OB2-PB2-OB4
16	C	2002	UQ	C1-C6-C7-C8
16	C	2002	UQ	C5-C6-C7-C8
11	A	2008	PEE	C1-O3P-P-O1P
11	A	2008	PEE	C1-O3P-P-O2P
11	C	2005	PEE	C11-C10-O2-C2
11	C	2005	PEE	C1-O3P-P-O1P
11	C	2005	PEE	C1-O3P-P-O2P
11	C	2005	PEE	C4-O4P-P-O1P
11	C	2005	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O3P
11	W	3005	PEE	O5-C30-O3-C3
11	C	2005	PEE	O5-C30-O3-C3
11	W	3005	PEE	C31-C30-O3-C3
11	C	2005	PEE	C31-C30-O3-C3
18	D	2003	CDL	C31-CA7-OA8-CA6
18	P	3003	CDL	C31-CA7-OA8-CA6
11	W	3005	PEE	O4-C10-O2-C2
18	G	2004	CDL	OB7-CB5-OB6-CB4
18	P	3004	CDL	OB7-CB5-OB6-CB4
11	C	2005	PEE	O4-C10-O2-C2
18	G	2004	CDL	OB9-CB7-OB8-CB6
18	P	3004	CDL	OB9-CB7-OB8-CB6
18	D	2003	CDL	C71-CB7-OB8-CB6
18	G	2004	CDL	C71-CB7-OB8-CB6
18	P	3004	CDL	C71-CB7-OB8-CB6
18	P	3003	CDL	C71-CB7-OB8-CB6
18	D	2003	CDL	OA9-CA7-OA8-CA6
18	P	3003	CDL	OA9-CA7-OA8-CA6
12	Q	3091	BOG	O5-C5-C6-O6
12	D	2091	BOG	O5-C5-C6-O6
18	D	2003	CDL	OB9-CB7-OB8-CB6
18	P	3003	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C31-C30-O3-C3
12	D	2091	BOG	C4-C5-C6-O6
11	W	3005	PEE	C30-C31-C32-C33
11	A	2008	PEE	C10-C11-C12-C13
11	C	2005	PEE	C30-C31-C32-C33
11	A	2008	PEE	O5-C30-O3-C3
12	E	2009	BOG	O1-C1'-C2'-C3'
12	Q	3009	BOG	O5-C1-O1-C1'
12	Q	3009	BOG	O1-C1'-C2'-C3'
12	C	3010	BOG	O1-C1'-C2'-C3'
18	G	2004	CDL	C11-CA5-OA6-CA4
18	P	3004	CDL	C11-CA5-OA6-CA4
18	D	2003	CDL	CB2-OB2-PB2-OB5
11	W	3005	PEE	C1-O3P-P-O4P
11	W	3005	PEE	C4-O4P-P-O3P
18	G	2004	CDL	CA3-OA5-PA1-OA2
18	P	3004	CDL	CA3-OA5-PA1-OA2
18	P	3003	CDL	CB2-OB2-PB2-OB5
11	A	2008	PEE	C1-O3P-P-O4P
11	C	2005	PEE	C1-O3P-P-O4P
11	C	2005	PEE	C4-O4P-P-O3P
18	G	2004	CDL	C31-CA7-OA8-CA6
18	P	3004	CDL	C31-CA7-OA8-CA6
18	D	2003	CDL	CA2-C1-CB2-OB2
18	G	2004	CDL	CB2-C1-CA2-OA2
18	P	3004	CDL	CB2-C1-CA2-OA2
18	P	3003	CDL	CA2-C1-CB2-OB2
18	G	2004	CDL	OA7-CA5-OA6-CA4
18	P	3004	CDL	OA7-CA5-OA6-CA4
11	P	3007	PEE	C12-C13-C14-C15
11	C	2007	PEE	C17-C18-C19-C20
11	C	2007	PEE	C18-C19-C20-C21
12	C	3010	BOG	C2'-C3'-C4'-C5'
11	C	2005	PEE	C16-C17-C18-C19
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C18-C19-C20-C21
11	P	3007	PEE	C17-C18-C19-C20
11	W	3005	PEE	C16-C17-C18-C19
11	C	2007	PEE	C12-C13-C14-C15
12	Q	3009	BOG	C2-C1-O1-C1'
11	W	3005	PEE	C18-C19-C20-C21
11	P	3007	PEE	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	2005	PEE	C18-C19-C20-C21
11	P	3007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C10-C11-C12-C13
11	P	3007	PEE	C36-C37-C38-C39
12	Q	3091	BOG	C4-C5-C6-O6
11	W	3005	PEE	C11-C12-C13-C14
11	P	3007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C34-C35-C36-C37
11	C	2007	PEE	C36-C37-C38-C39
11	W	3005	PEE	C40-C41-C42-C43
11	C	2005	PEE	C40-C41-C42-C43
11	P	3007	PEE	C14-C15-C16-C17
11	C	2005	PEE	C11-C12-C13-C14
11	C	2007	PEE	C15-C16-C17-C18
12	C	3010	BOG	C3'-C4'-C5'-C6'
11	W	3005	PEE	O4P-C4-C5-N
11	C	2005	PEE	C14-C15-C16-C17
11	C	2005	PEE	C33-C34-C35-C36
11	C	2007	PEE	C37-C38-C39-C40
11	W	3005	PEE	C33-C34-C35-C36
11	P	3007	PEE	C37-C38-C39-C40
11	C	2007	PEE	C14-C15-C16-C17
11	W	3005	PEE	C14-C15-C16-C17
11	W	3005	PEE	C35-C36-C37-C38
11	C	2005	PEE	C35-C36-C37-C38
12	P	2010	BOG	C3'-C4'-C5'-C6'
12	Q	3091	BOG	O1-C1'-C2'-C3'
11	C	2005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C40-C41-C42-C43
11	C	2007	PEE	C41-C42-C43-C44
12	E	2009	BOG	C2-C1-O1-C1'
18	D	2003	CDL	OA6-CA4-CA6-OA8
18	P	3003	CDL	OA6-CA4-CA6-OA8
18	G	2004	CDL	OA9-CA7-OA8-CA6
18	P	3004	CDL	OA9-CA7-OA8-CA6
11	P	3007	PEE	C41-C42-C43-C44
11	W	3005	PEE	C19-C20-C21-C22
12	Q	3091	BOG	C1'-C2'-C3'-C4'
18	P	3004	CDL	CB3-OB5-PB2-OB2
11	A	2008	PEE	C4-O4P-P-O3P
11	A	2008	PEE	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C40-C41-C42-C43
11	C	2007	PEE	C11-C12-C13-C14
12	P	2010	BOG	C2'-C3'-C4'-C5'
11	P	3007	PEE	C16-C17-C18-C19
11	P	3007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C16-C17-C18-C19
11	P	3007	PEE	C20-C21-C22-C23
12	E	2009	BOG	C2'-C3'-C4'-C5'
11	C	2005	PEE	C38-C39-C40-C41
11	C	2007	PEE	C20-C21-C22-C23
11	C	2007	PEE	C38-C39-C40-C41
15	P	3001	ICX	N33-C34-C35-O37
18	P	3003	CDL	C71-C72-C73-C74
11	C	2007	PEE	C39-C40-C41-C42
18	D	2003	CDL	OA5-CA3-CA4-CA6
18	P	3003	CDL	OA5-CA3-CA4-CA6
11	C	2005	PEE	O4P-C4-C5-N
18	D	2003	CDL	C71-C72-C73-C74
11	C	2005	PEE	C20-C21-C22-C23
11	P	3007	PEE	C38-C39-C40-C41
12	D	2091	BOG	C2'-C1'-O1-C1
12	C	3010	BOG	C2'-C1'-O1-C1
18	D	2003	CDL	CA3-CA4-CA6-OA8
18	G	2004	CDL	CA3-CA4-CA6-OA8
18	P	3004	CDL	CA3-CA4-CA6-OA8
18	P	3003	CDL	CA3-CA4-CA6-OA8
11	W	3005	PEE	C20-C21-C22-C23
11	C	2005	PEE	C37-C38-C39-C40
18	G	2004	CDL	OB5-CB3-CB4-OB6
18	P	3003	CDL	OA5-CA3-CA4-OA6
11	W	3005	PEE	C37-C38-C39-C40
11	W	3005	PEE	C38-C39-C40-C41
18	G	2004	CDL	C1-CB2-OB2-PB2
18	P	3004	CDL	C1-CB2-OB2-PB2
11	P	3007	PEE	C39-C40-C41-C42
15	C	2001	ICX	N33-C34-C35-O37
11	C	2007	PEE	C31-C32-C33-C34
15	P	3001	ICX	N33-C34-C35-O36
11	P	3007	PEE	C32-C33-C34-C35
12	E	2009	BOG	O5-C1-O1-C1'
12	D	2091	BOG	O5-C1-O1-C1'
18	D	2003	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	P	3004	CDL	OB5-CB3-CB4-OB6
12	Q	3009	BOG	C2'-C3'-C4'-C5'
11	C	2005	PEE	C15-C16-C17-C18
11	P	3007	PEE	C31-C32-C33-C34
18	G	2004	CDL	CB3-OB5-PB2-OB2
18	G	2004	CDL	CA3-OA5-PA1-OA4
18	G	2004	CDL	CB3-OB5-PB2-OB4
18	P	3004	CDL	CA3-OA5-PA1-OA4
18	P	3004	CDL	CB3-OB5-PB2-OB4
11	A	2008	PEE	C4-O4P-P-O2P
11	A	2008	PEE	O3P-C1-C2-O2
11	C	2005	PEE	O3P-C1-C2-O2
11	W	3005	PEE	C15-C16-C17-C18
11	C	2007	PEE	C32-C33-C34-C35
14	P	502	HEM	C2D-C3D-CAD-CBD
18	G	2004	CDL	OA6-CA4-CA6-OA8
18	P	3004	CDL	OA6-CA4-CA6-OA8
18	D	2003	CDL	CB7-C71-C72-C73
18	P	3003	CDL	CB7-C71-C72-C73
11	W	3005	PEE	C1-C2-O2-C10
11	C	2005	PEE	C1-C2-O2-C10
15	C	2001	ICX	N33-C34-C35-O36
11	W	3005	PEE	C21-C22-C23-C24
18	P	3003	CDL	C1-CA2-OA2-PA1
11	P	3007	PEE	C21-C22-C23-C24
11	P	3007	PEE	C43-C44-C45-C46
18	D	2003	CDL	C1-CA2-OA2-PA1
11	C	2007	PEE	C43-C44-C45-C46
11	C	2007	PEE	C21-C22-C23-C24
12	E	2009	BOG	C1'-C2'-C3'-C4'
11	W	3005	PEE	O3P-C1-C2-O2
18	G	2004	CDL	OB5-CB3-CB4-CB6
18	P	3004	CDL	OB5-CB3-CB4-CB6
11	C	2005	PEE	C21-C22-C23-C24
18	P	3003	CDL	C12-C11-CA5-OA6
11	W	3005	PEE	C2-C1-O3P-P
11	C	2005	PEE	C2-C1-O3P-P
18	D	2003	CDL	OB6-CB4-CB6-OB8
11	P	3007	PEE	O2-C10-C11-C12
11	C	2007	PEE	O2-C10-C11-C12
11	A	2008	PEE	O2-C10-C11-C12
18	D	2003	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O3-C30-C31-C32
18	P	3003	CDL	C72-C71-CB7-OB8
11	C	2007	PEE	O3-C30-C31-C32
18	P	3003	CDL	OB6-CB4-CB6-OB8
12	E	2009	BOG	C4'-C5'-C6'-C7'
11	C	2007	PEE	O4-C10-C11-C12
11	A	2008	PEE	O4-C10-C11-C12
18	D	2003	CDL	C12-C11-CA5-OA7
18	D	2003	CDL	C72-C71-CB7-OB9
11	P	3007	PEE	O4-C10-C11-C12
11	P	3007	PEE	O5-C30-C31-C32
18	P	3003	CDL	CA2-OA2-PA1-OA4
18	P	3003	CDL	C72-C71-CB7-OB9
11	C	2007	PEE	O5-C30-C31-C32
18	D	2003	CDL	C52-C51-CB5-OB6
18	P	3003	CDL	C52-C51-CB5-OB6
11	W	3005	PEE	C2-C3-O3-C30
11	P	3007	PEE	C42-C43-C44-C45
18	D	2003	CDL	C12-C11-CA5-OA6
18	P	3003	CDL	C52-C51-CB5-OB7

There are no ring outliers.

22 monomers are involved in 83 short contacts:

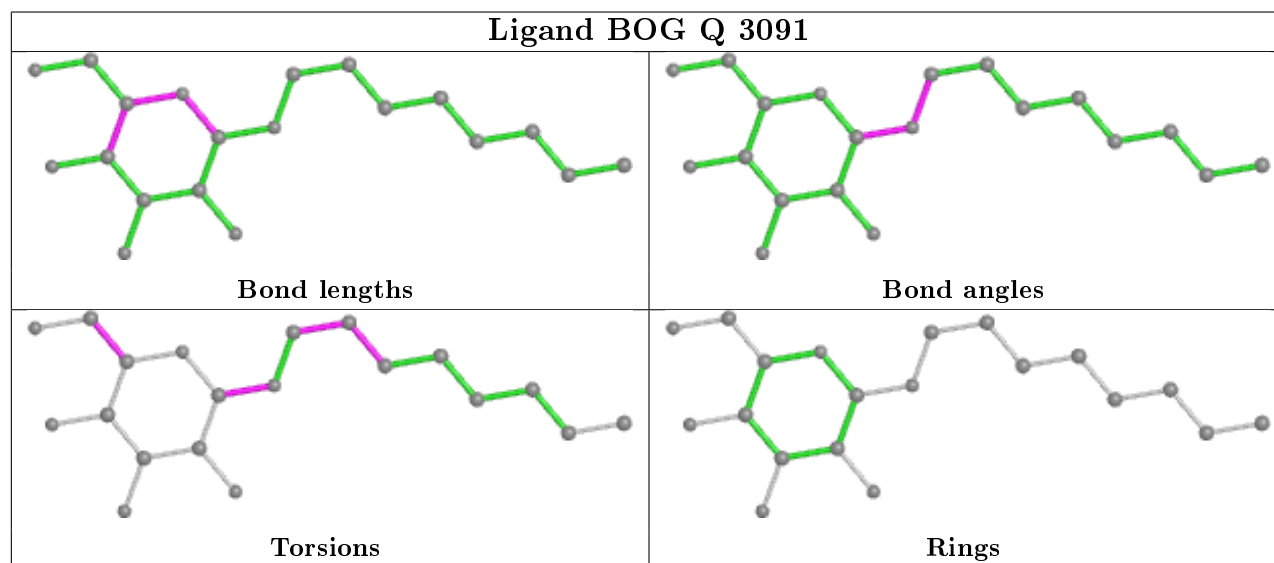
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	3001	ICX	2	0
18	D	2003	CDL	3	0
11	C	2007	PEE	3	0
12	E	2009	BOG	1	0
11	W	3005	PEE	1	0
18	G	2004	CDL	1	0
14	P	502	HEM	11	0
18	P	3004	CDL	2	0
11	P	3007	PEE	2	0
14	P	501	HEM	8	0
14	C	502	HEM	10	0
16	P	3002	UQ	6	0
17	Q	501	HEC	3	0
17	D	501	HEC	3	0
18	P	3003	CDL	3	0
16	C	2002	UQ	5	0
11	C	2005	PEE	2	0

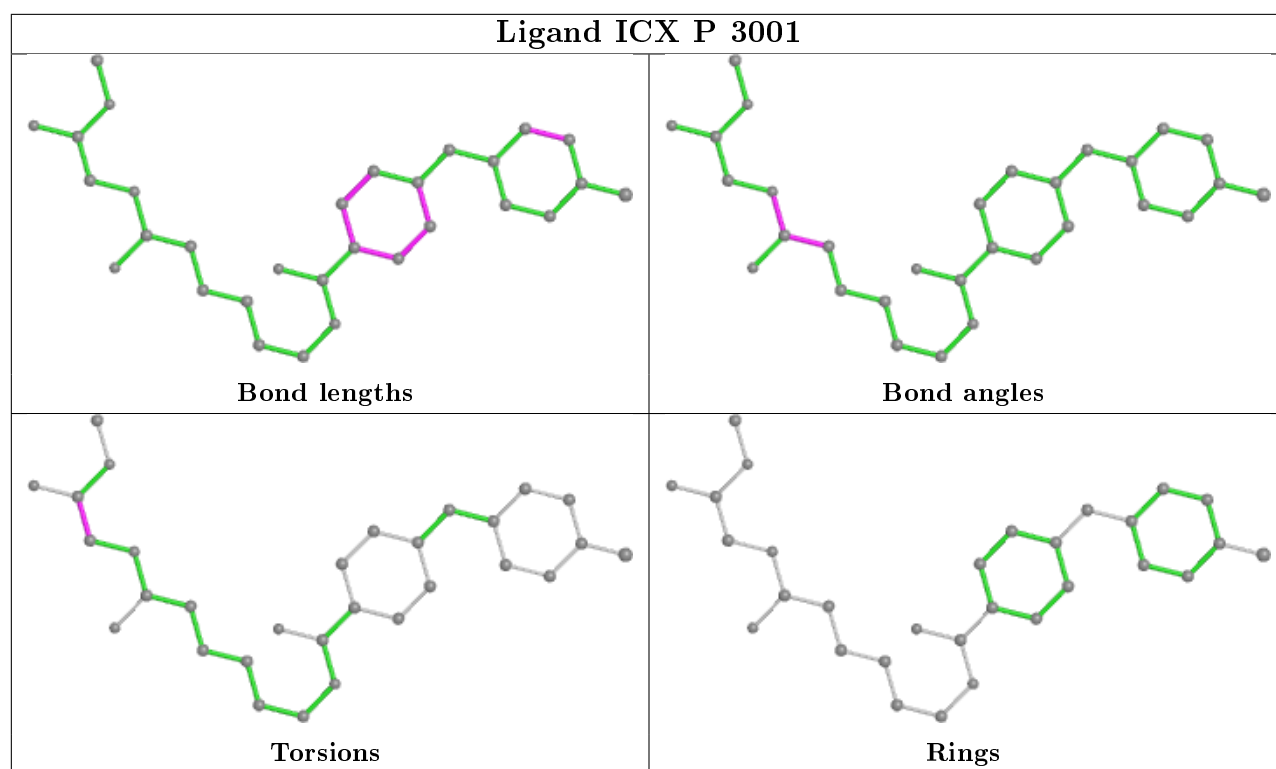
Continued on next page...

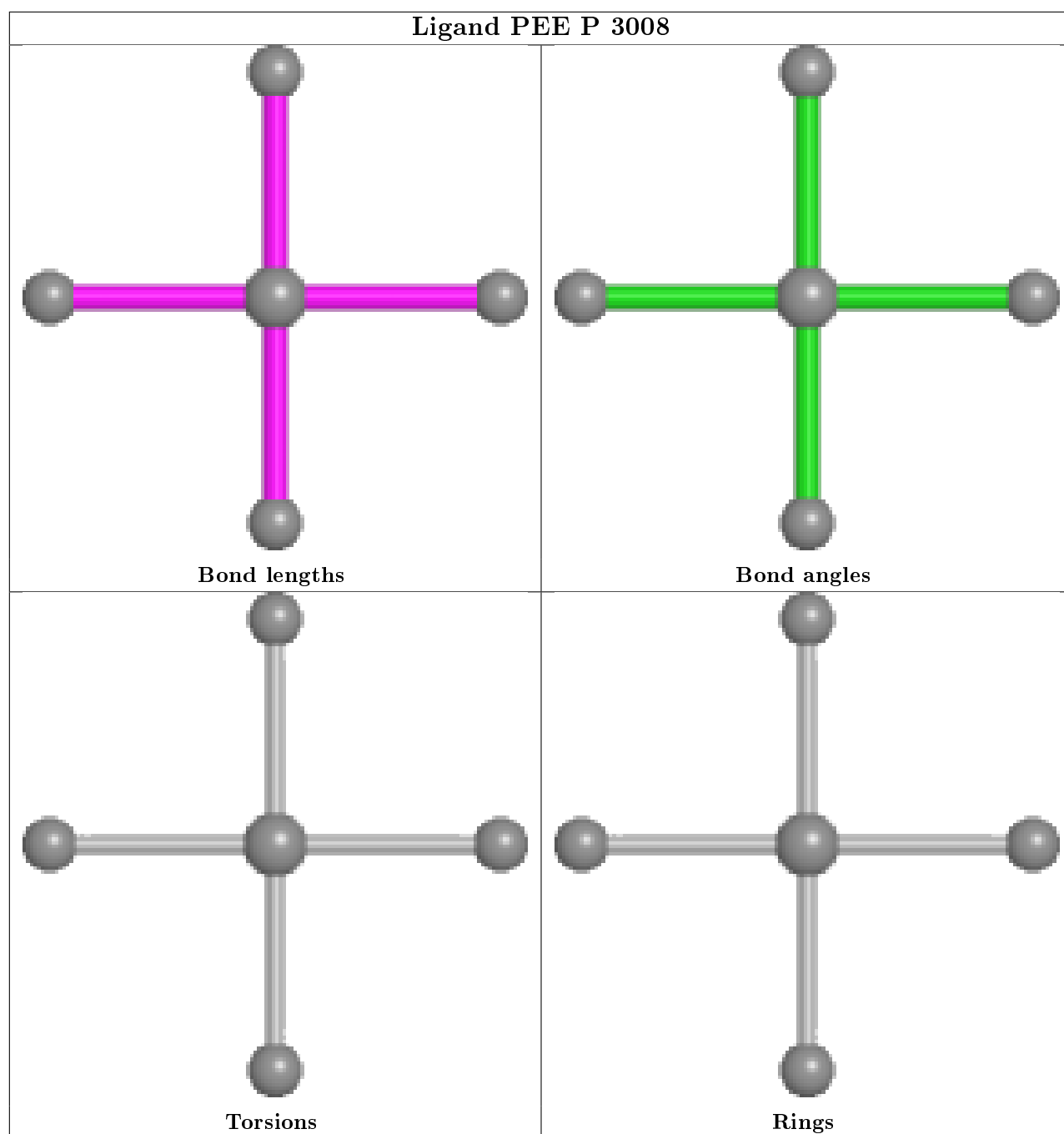
Continued from previous page...

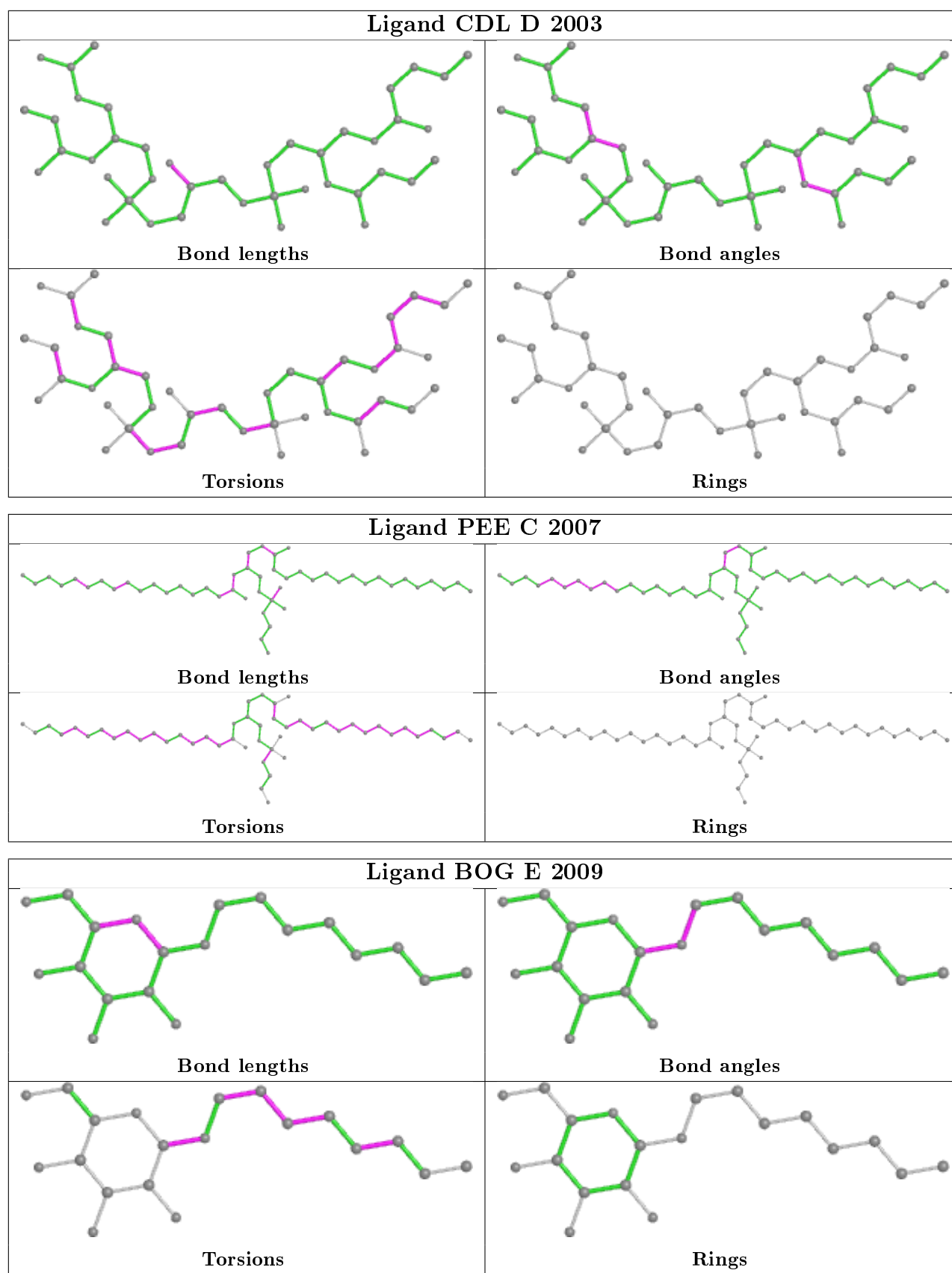
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	2001	ICX	2	0
12	D	2091	BOG	5	0
12	P	2010	BOG	1	0
14	C	501	HEM	9	0
19	E	501	FES	1	0

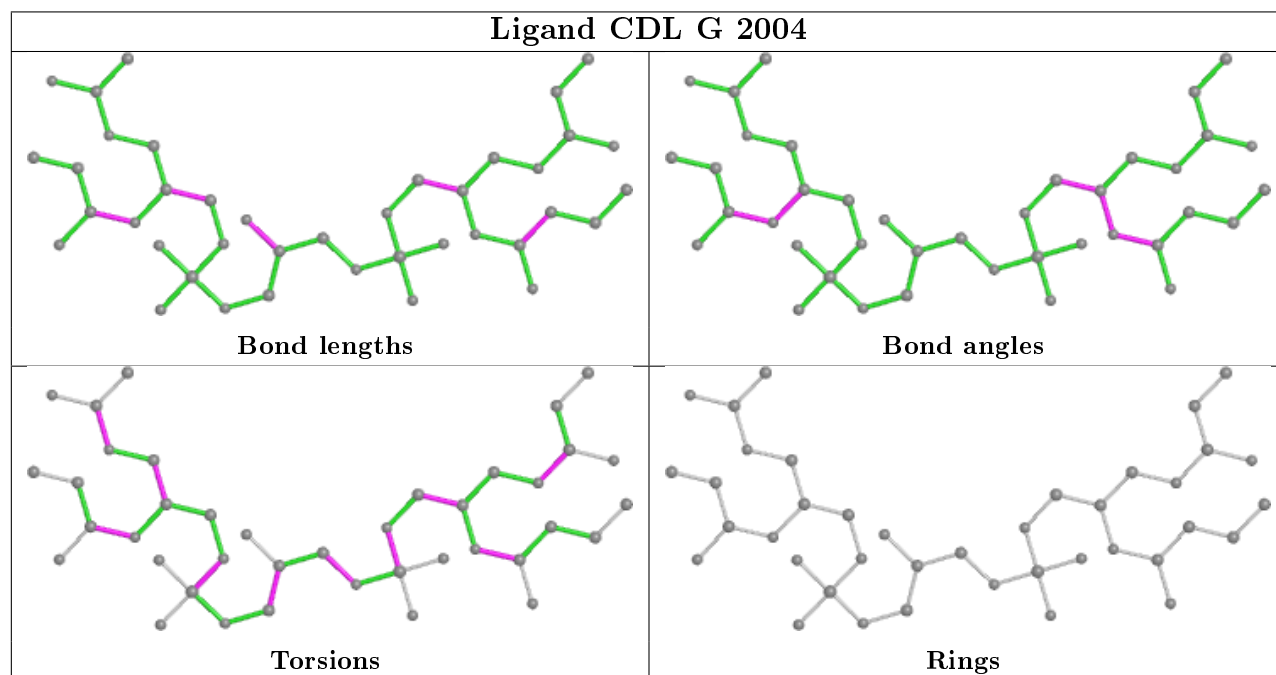
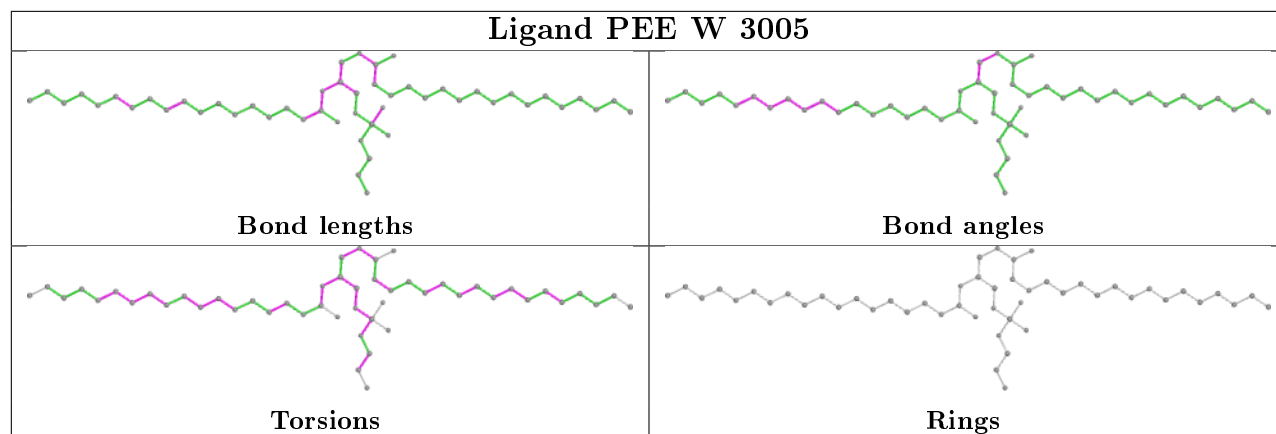
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

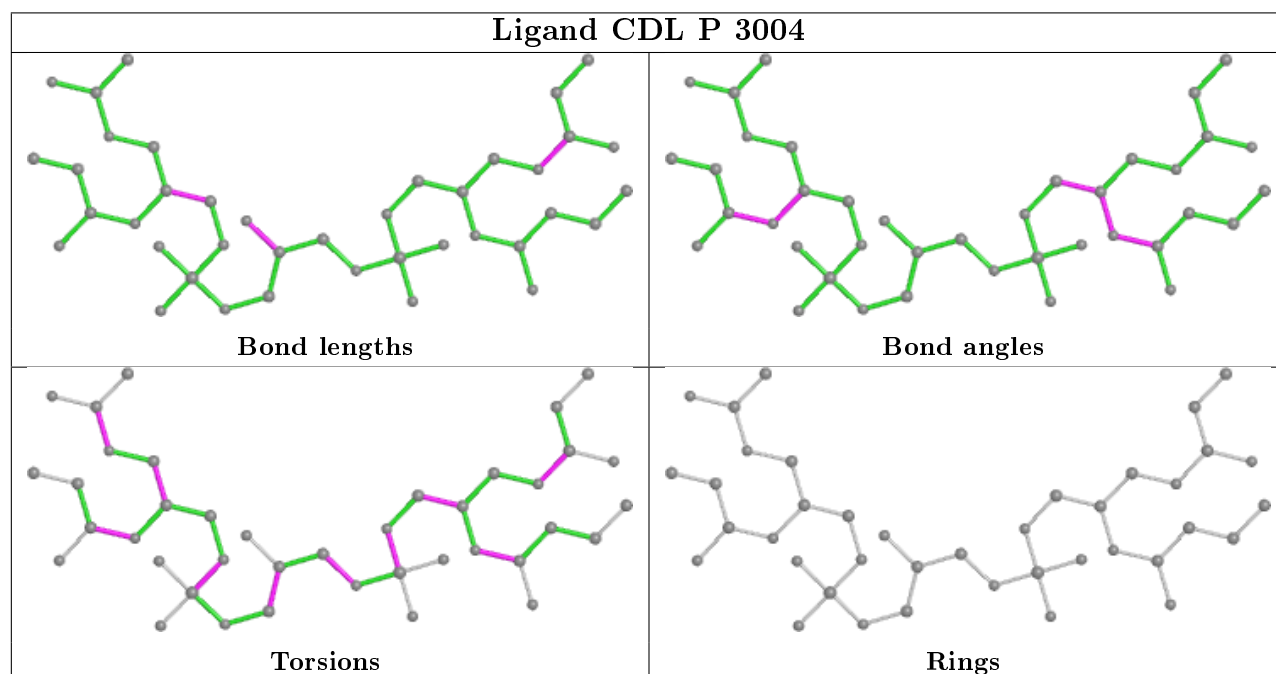
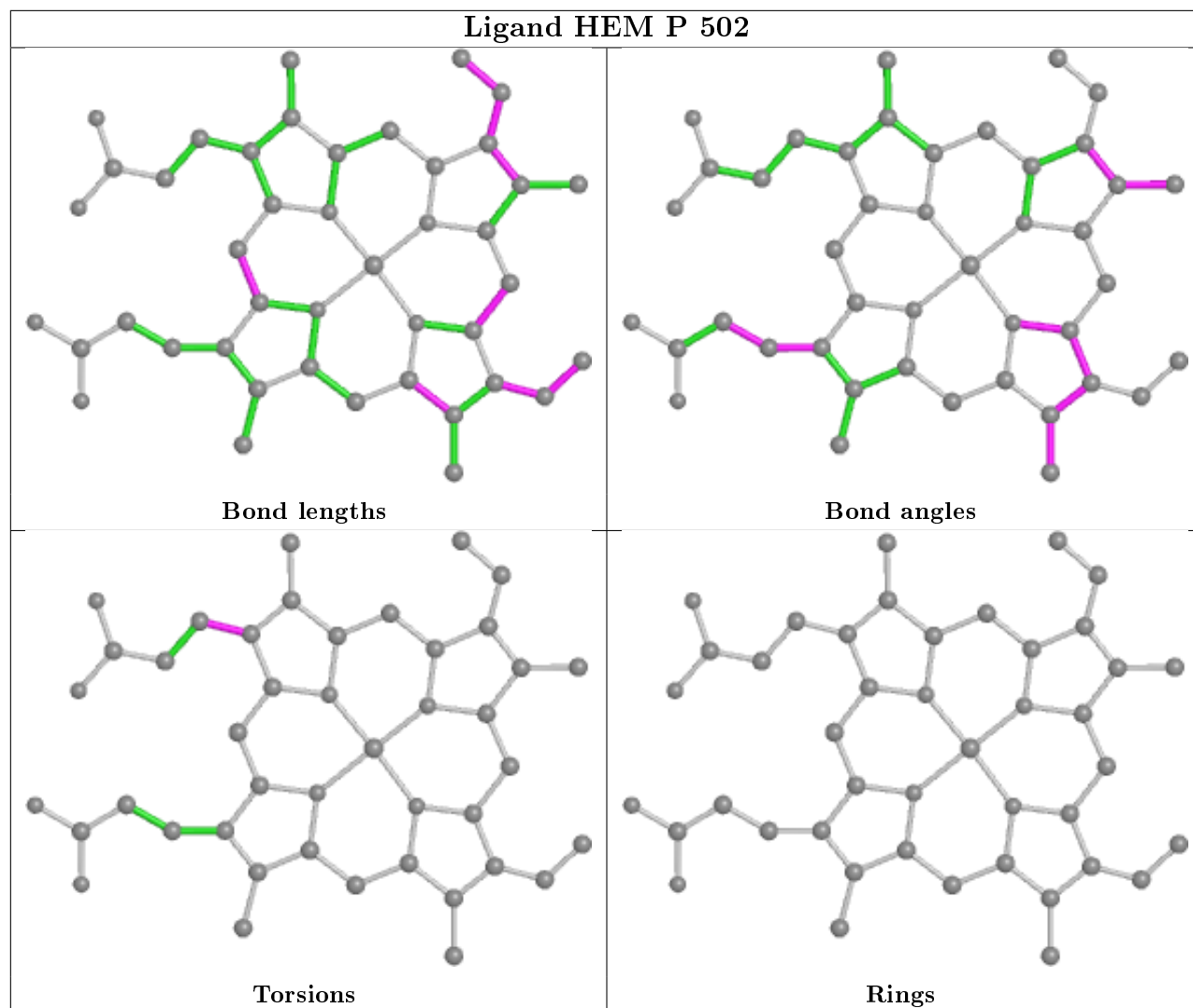


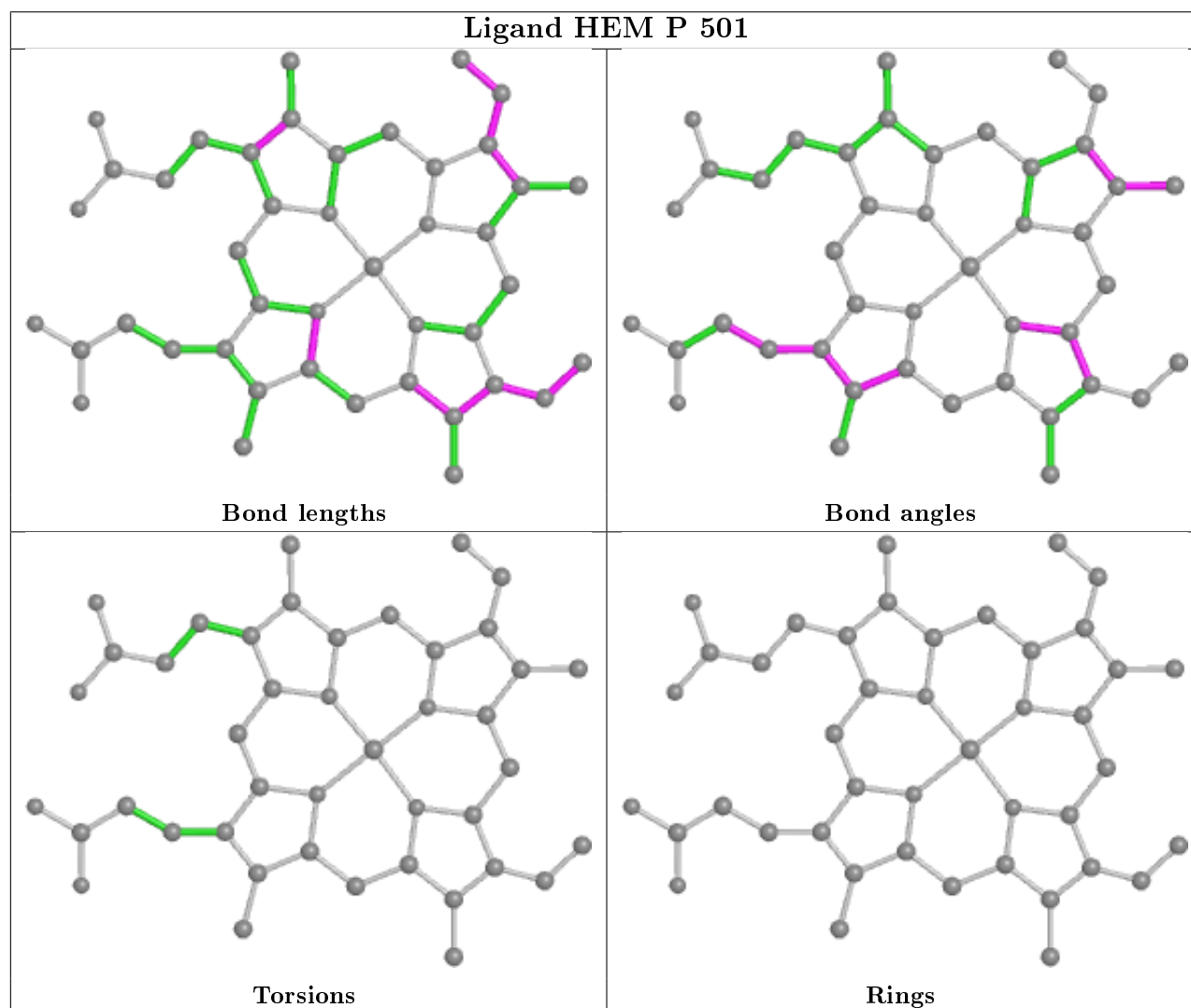
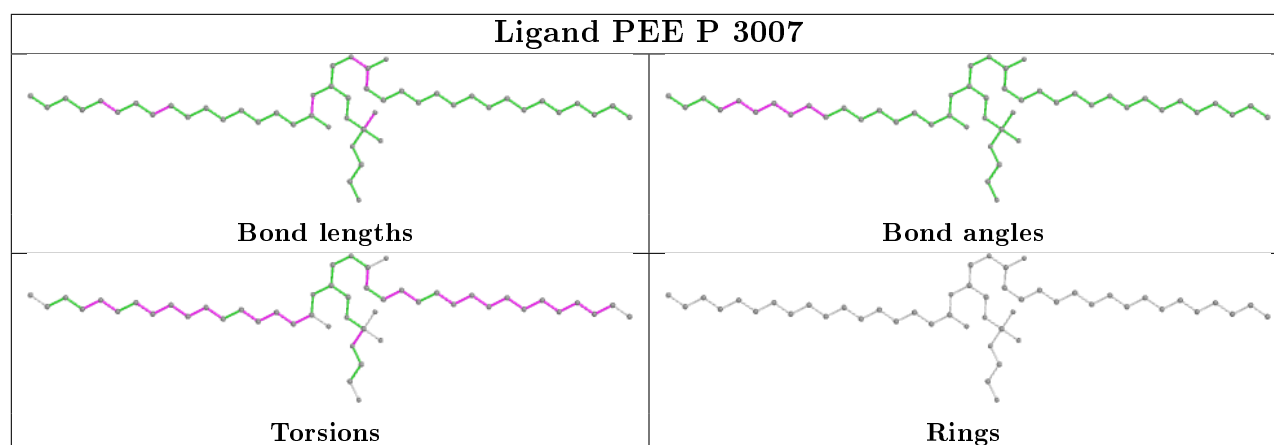


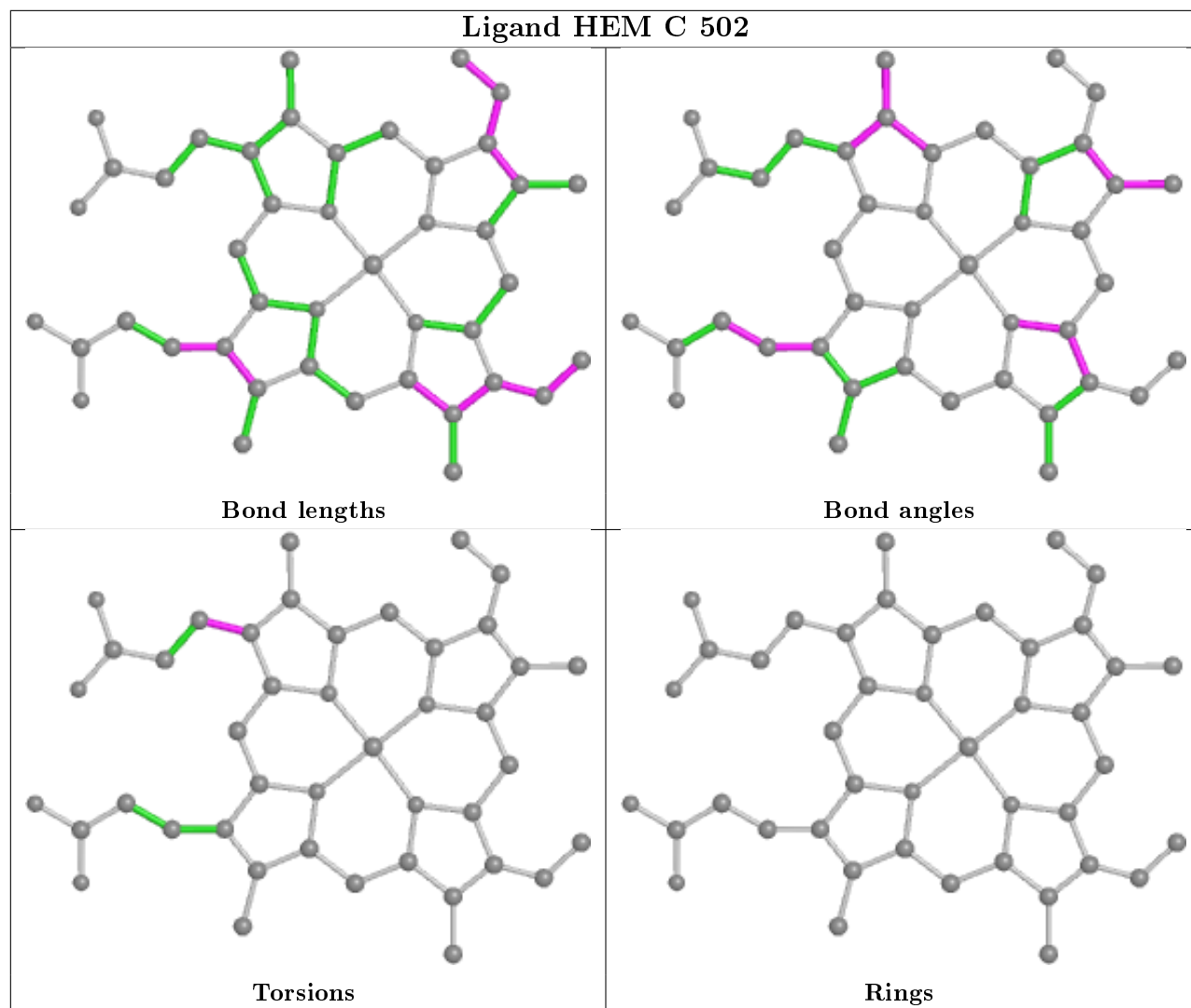


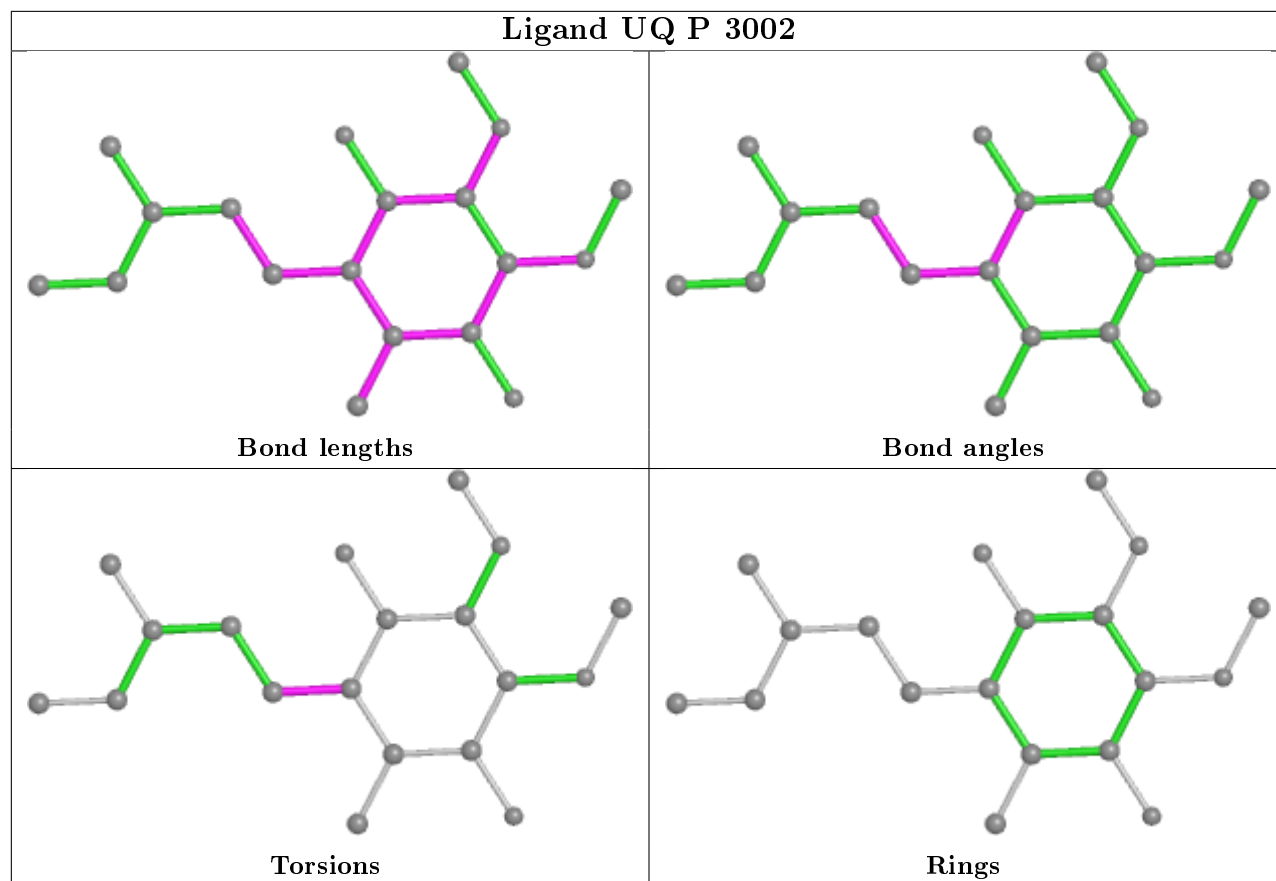


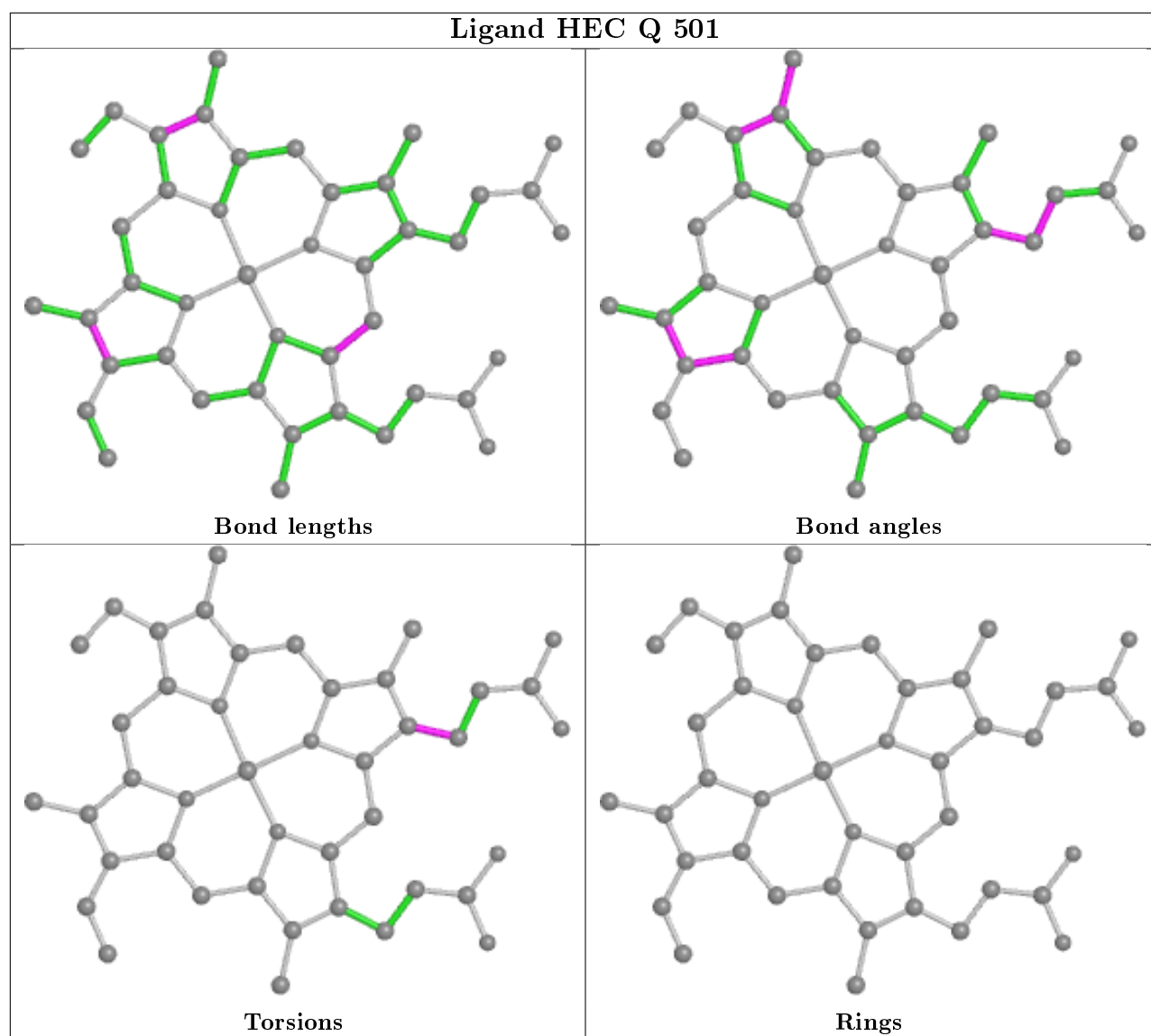


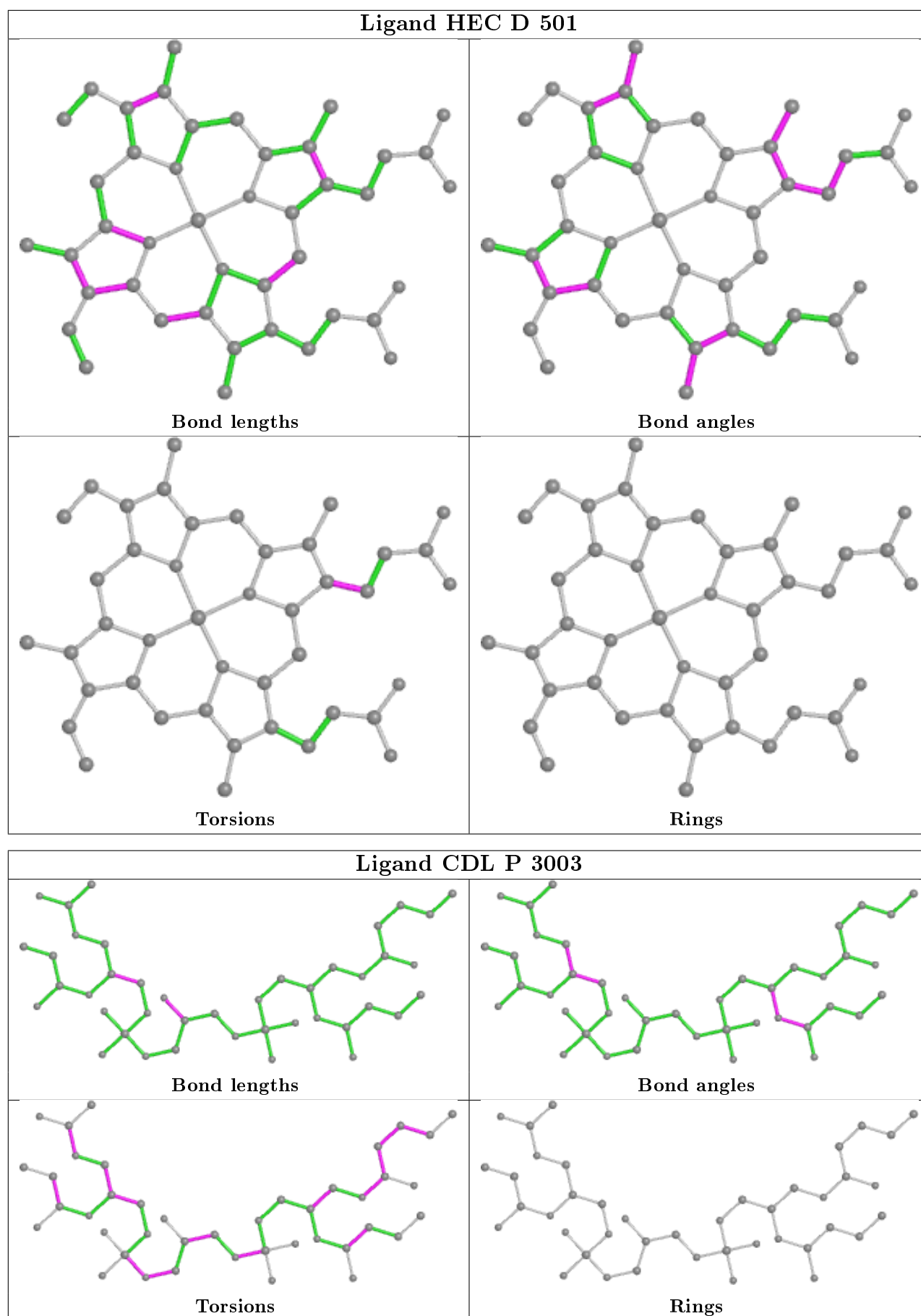


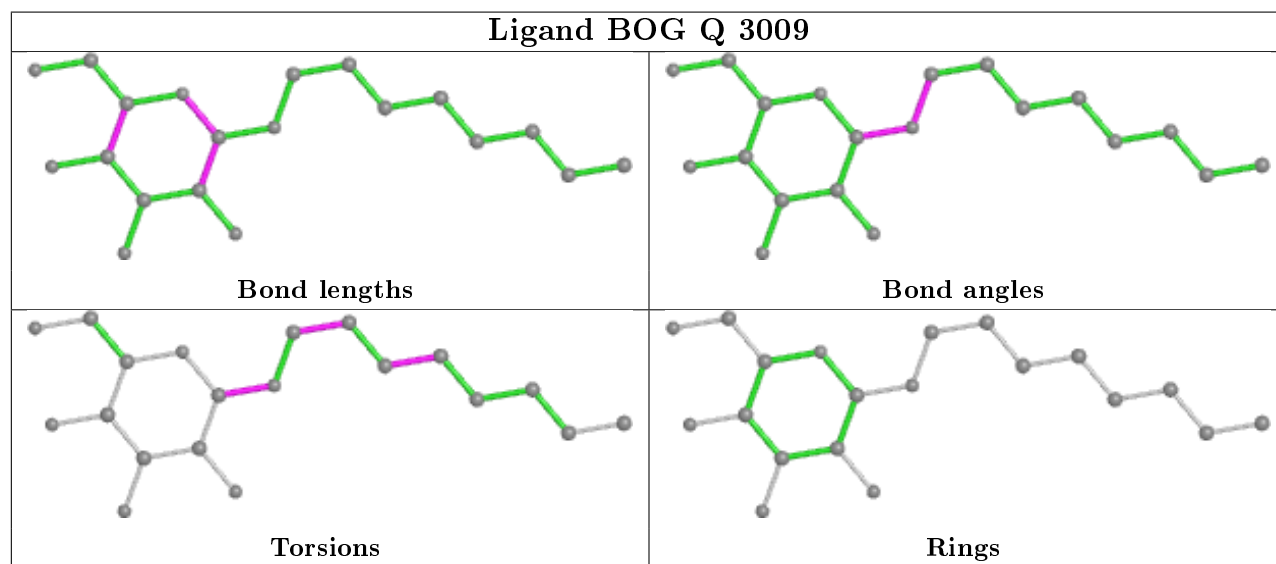
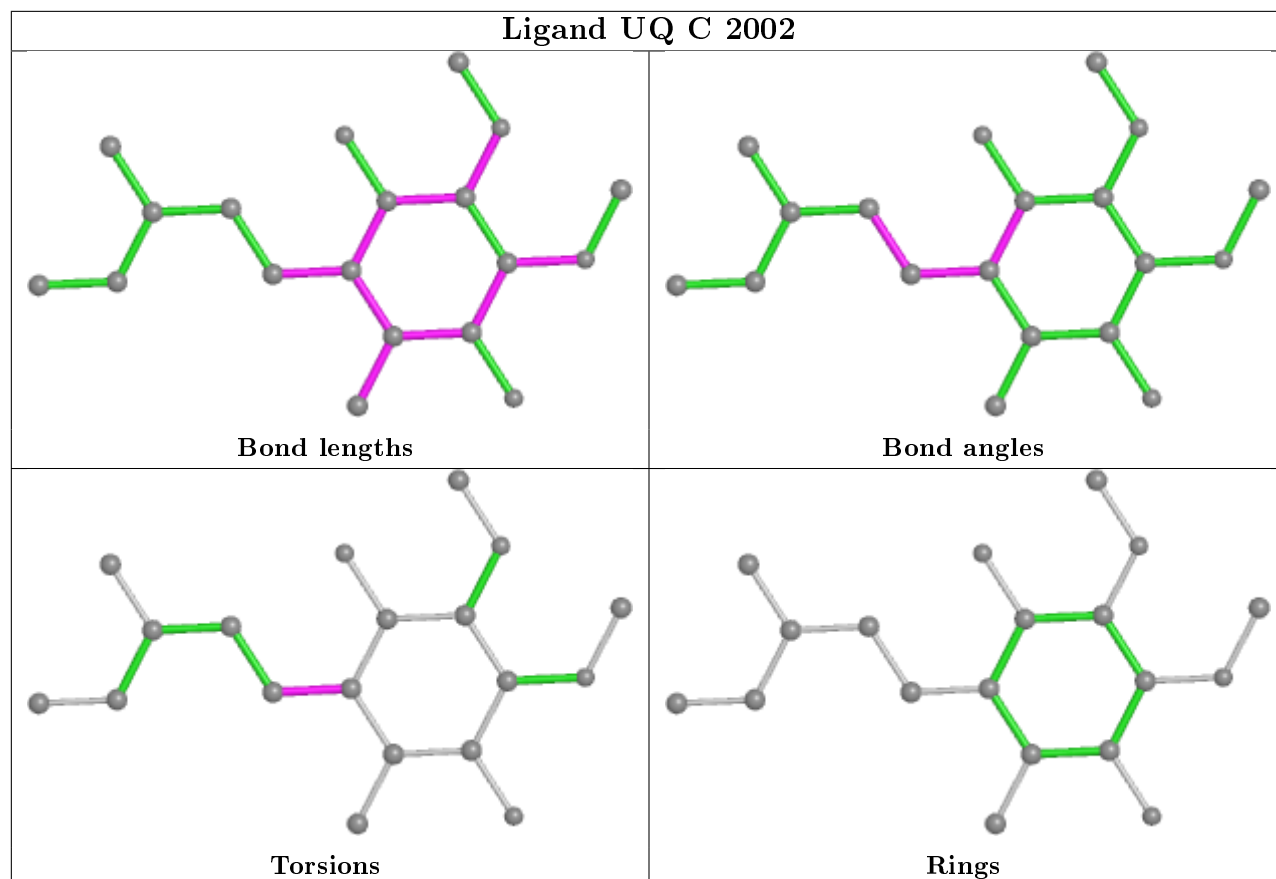


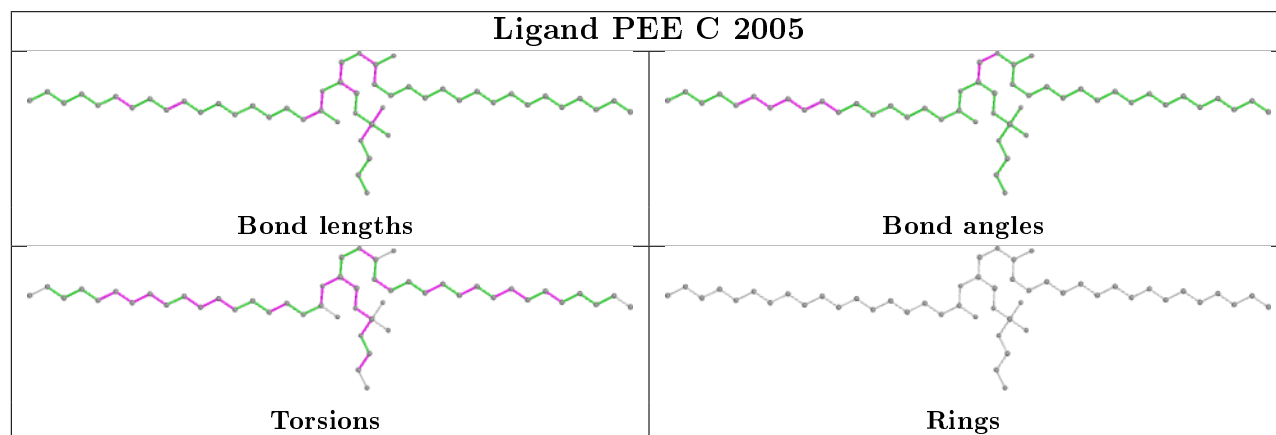
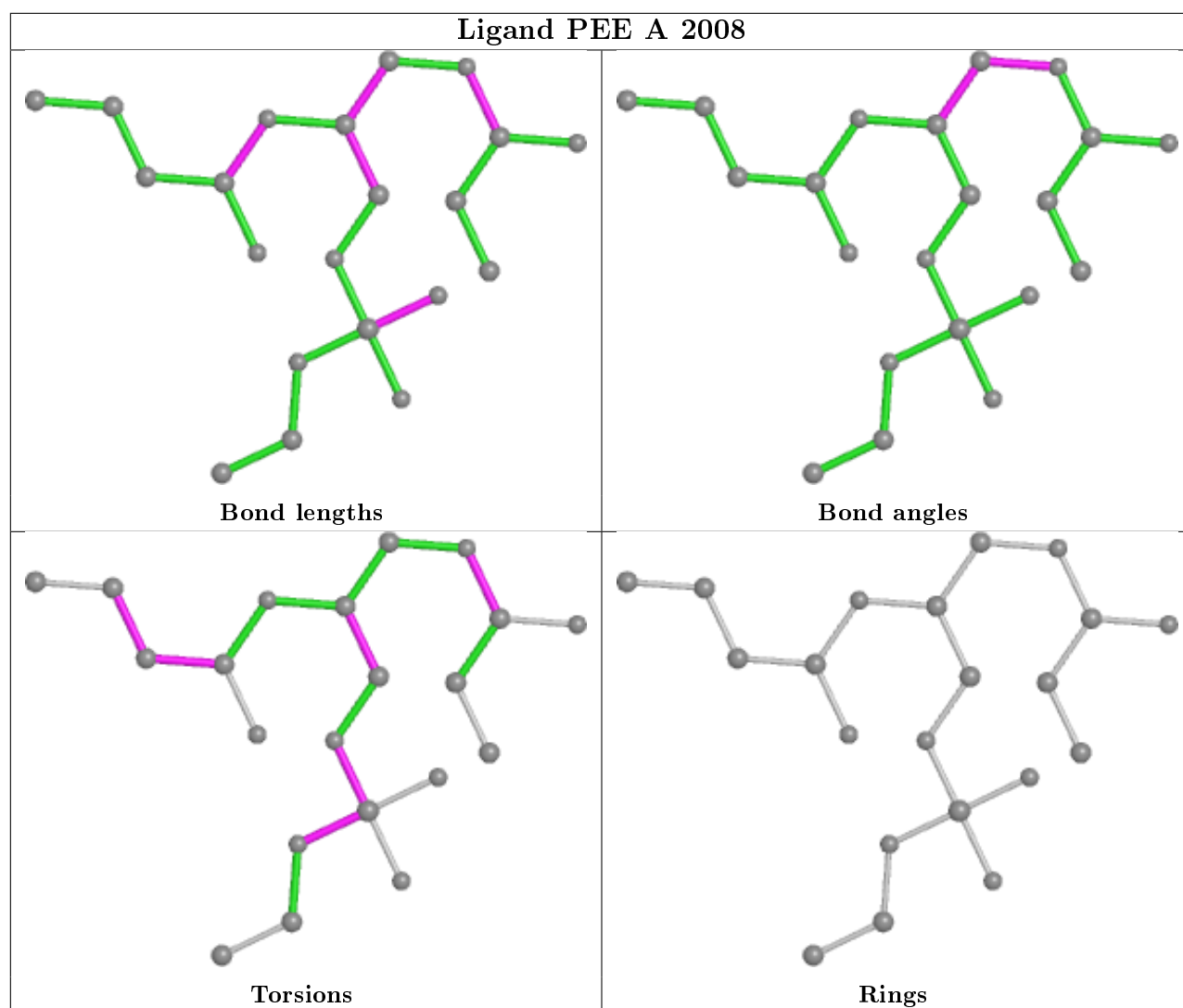


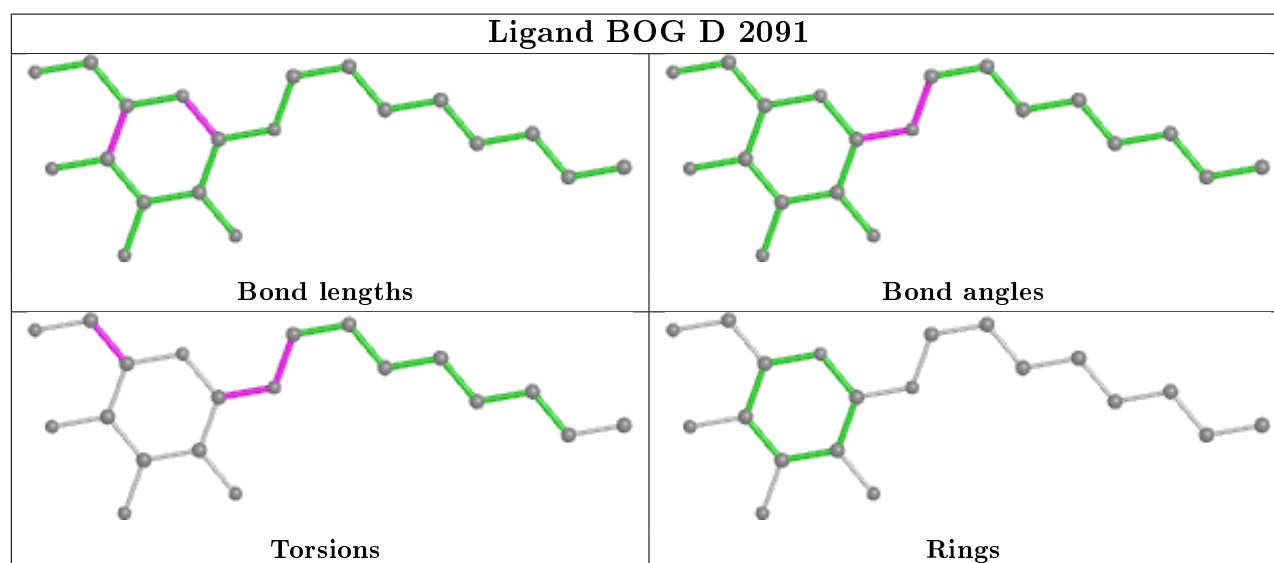
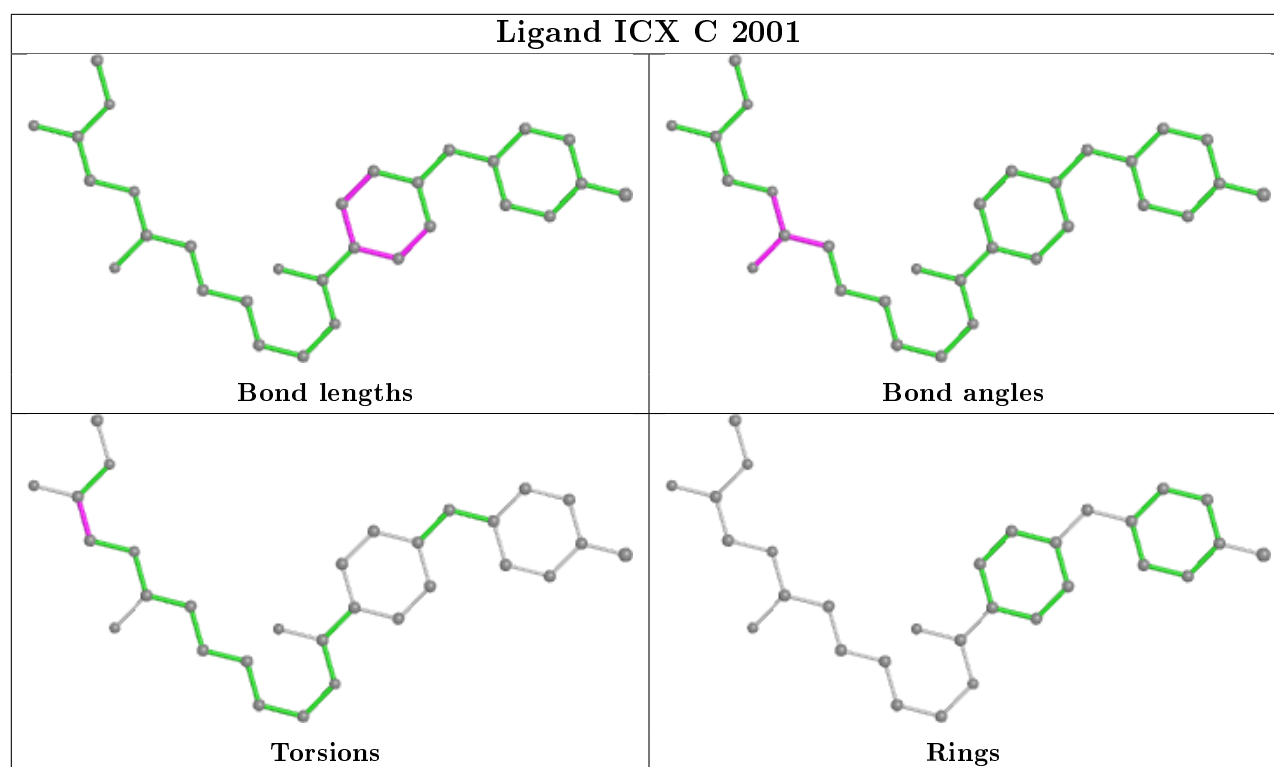


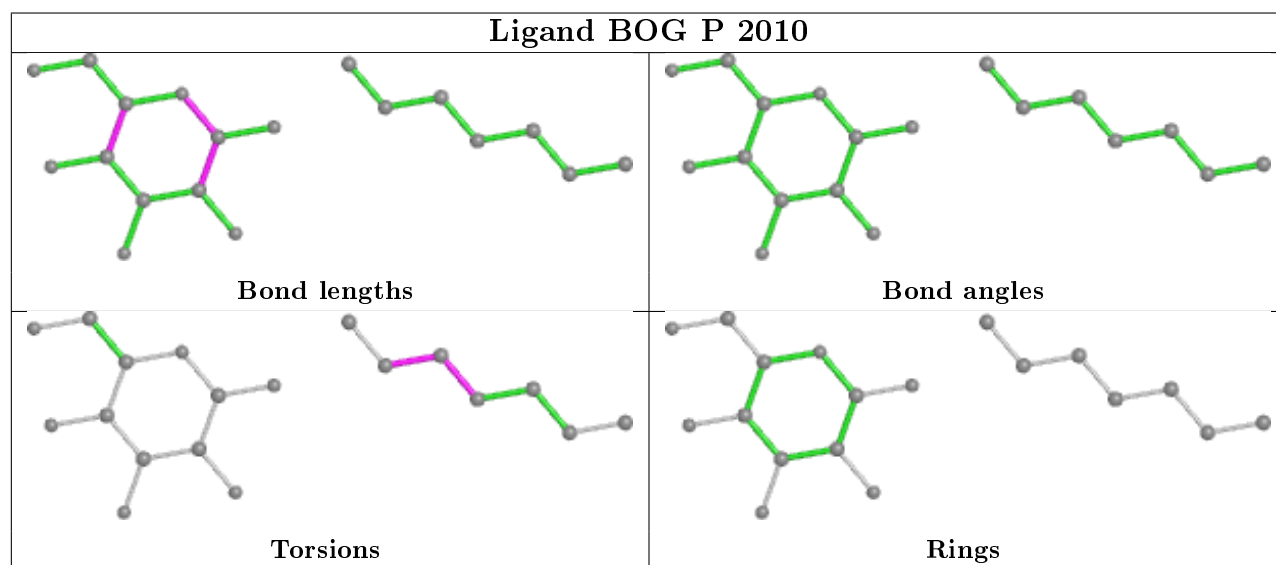
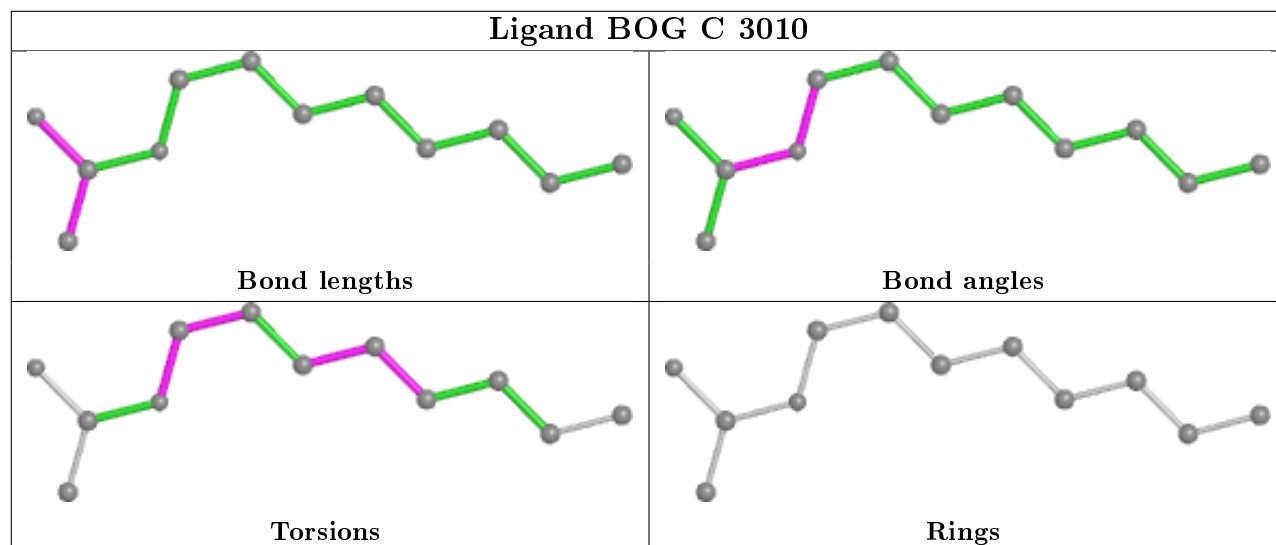


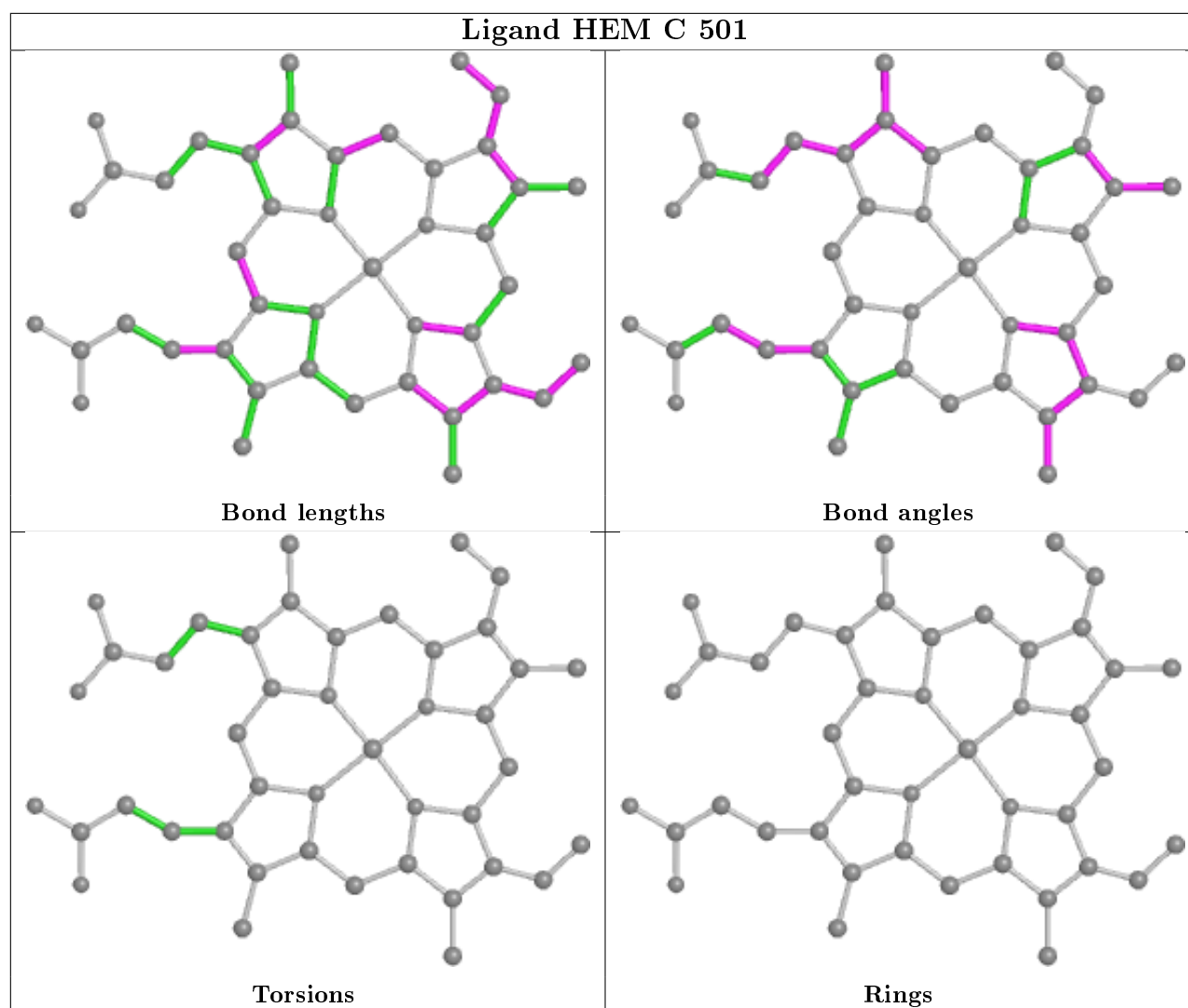












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	-0.31	4 (0%) 84 73	36, 89, 137, 150	0
1	N	442/446 (99%)	-0.28	9 (2%) 65 52	54, 91, 136, 153	0
2	B	421/441 (95%)	-0.16	4 (0%) 82 71	60, 113, 170, 193	0
2	O	422/441 (95%)	-0.14	9 (2%) 63 50	51, 100, 146, 172	0
3	C	380/380 (100%)	-0.66	4 (1%) 80 69	19, 50, 104, 192	0
3	P	379/380 (99%)	-0.45	7 (1%) 68 55	29, 89, 132, 186	0
4	D	241/241 (100%)	-0.50	1 (0%) 92 87	30, 58, 109, 133	0
4	Q	241/241 (100%)	-0.33	2 (0%) 86 75	65, 105, 150, 165	0
5	E	196/196 (100%)	0.32	16 (8%) 11 10	45, 137, 184, 198	127 (64%)
5	R	196/196 (100%)	0.02	8 (4%) 37 27	53, 101, 166, 184	0
6	F	100/110 (90%)	-0.74	0 100 100	31, 61, 87, 102	0
6	S	100/110 (90%)	-0.12	0 100 100	77, 117, 167, 188	0
7	G	81/81 (100%)	-0.32	1 (1%) 79 67	43, 77, 129, 156	0
7	T	79/81 (97%)	0.10	7 (8%) 9 8	71, 137, 202, 211	0
8	H	70/77 (90%)	-0.38	0 100 100	51, 94, 117, 153	0
8	U	67/77 (87%)	-0.06	0 100 100	141, 175, 213, 219	0
9	I	31/52 (59%)	1.10	6 (19%) 1 1	109, 158, 223, 229	0
9	V	31/52 (59%)	1.21	9 (29%) 0 0	109, 157, 222, 224	0
10	J	61/61 (100%)	-0.38	2 (3%) 46 35	65, 82, 144, 187	0
10	W	59/61 (96%)	0.01	2 (3%) 45 34	75, 107, 139, 154	0
All	All	4040/4170 (96%)	-0.25	91 (2%) 60 46	19, 93, 168, 229	127 (3%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	163	SER	10.8
7	T	1	GLY	6.8
3	P	8	SER	6.2
5	E	162	GLY	5.5
9	V	61	ARG	5.5
5	R	121	GLN	5.2
3	P	2	ALA	5.0
9	I	48	PRO	5.0
5	E	164	HIS	5.0
5	E	173	LYS	4.7
9	I	61	ARG	4.7
5	E	174	GLY	4.4
9	V	57	GLY	4.4
1	A	69	LYS	4.3
3	C	1	MET	4.1
9	V	48	PRO	4.1
10	J	64	GLU	3.9
9	I	47	ARG	3.8
3	P	10	PRO	3.7
7	G	1	GLY	3.7
3	C	7	LYS	3.6
9	V	62	ARG	3.5
7	T	2	ILE	3.5
9	I	62	ARG	3.5
2	O	268	GLU	3.5
5	E	111	GLU	3.4
5	E	165	TYR	3.4
4	Q	1	GLY	3.4
5	R	120	PRO	3.4
2	O	208	GLY	3.3
7	T	6	ASN	3.2
2	O	344	LEU	3.1
3	C	8	SER	3.0
5	E	172	ARG	3.0
3	P	3	PRO	3.0
4	D	241	LYS	3.0
3	P	4	ASN	2.9
1	N	444	ILE	2.8
5	R	122	HIS	2.8
5	E	137	GLY	2.7
5	R	114	VAL	2.7
10	W	56	LYS	2.7
7	T	78	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	414	ALA	2.6
9	V	47	ARG	2.6
4	Q	145	GLU	2.5
5	E	157	TYR	2.5
5	E	146	PRO	2.5
5	E	79	SER	2.5
1	N	177	LEU	2.5
9	V	56	SER	2.5
3	P	7	LYS	2.5
2	O	350	GLY	2.5
1	A	2	ALA	2.5
3	P	157	ILE	2.5
5	E	191	ASP	2.4
1	N	174	ILE	2.4
9	V	58	ARG	2.4
9	V	63	ASP	2.4
2	B	402	ILE	2.4
1	A	68	LYS	2.4
2	O	352	VAL	2.3
2	B	267	ALA	2.3
9	I	63	ASP	2.3
5	R	117	LEU	2.3
2	O	425	ALA	2.3
9	I	49	LEU	2.3
9	V	77	ARG	2.3
10	J	63	GLU	2.3
2	O	424	MET	2.3
2	O	19	PRO	2.2
7	T	74	PRO	2.2
5	R	194	VAL	2.2
2	B	376	GLN	2.2
7	T	73	ASN	2.2
1	N	58	PHE	2.2
10	W	60	GLU	2.2
5	R	170	ARG	2.1
5	E	151	GLY	2.1
1	A	66	GLY	2.1
7	T	5	GLY	2.1
1	N	171	THR	2.1
5	E	149	ASN	2.1
3	C	6	ARG	2.1
1	N	14	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	182	LEU	2.1
5	R	193	VAL	2.1
2	O	347	ALA	2.1
1	N	53	ASN	2.0
1	N	52	ASN	2.0
5	E	121	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	BOG	Q	3091	20/20	0.32	0.90	242,249,250,251	0
12	BOG	P	2010	19/20	0.55	0.41	102,248,249,249	0
11	PEE	A	2008	21/51	0.57	0.56	225,229,230,230	0
11	PEE	W	3005	50/51	0.66	0.51	129,146,150,152	0
18	CDL	P	3003	42/100	0.67	0.46	203,214,224,225	0
11	PEE	P	3008	5/51	0.68	0.82	213,213,214,214	0
18	CDL	P	3004	40/100	0.69	0.39	164,168,173,174	0
12	BOG	C	3010	12/20	0.74	0.39	168,168,170,170	0
12	BOG	D	2091	20/20	0.74	0.46	178,180,180,180	0
18	CDL	D	2003	42/100	0.77	0.38	144,158,180,181	0
11	PEE	C	2005	50/51	0.78	0.41	122,134,139,141	0
20	UNL	P	3014	1/-	0.80	0.33	33,33,33,33	0
16	UQ	P	3002	19/63	0.80	0.36	163,166,168,168	0
13	AZI	C	2011	3/3	0.83	0.33	46,46,47,49	0
11	PEE	P	3007	49/51	0.83	0.39	107,122,143,144	0
16	UQ	C	2002	19/63	0.88	0.41	123,126,128,129	0
13	AZI	P	3011	3/3	0.88	0.37	54,54,55,56	0

Continued on next page...

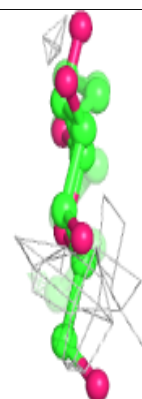
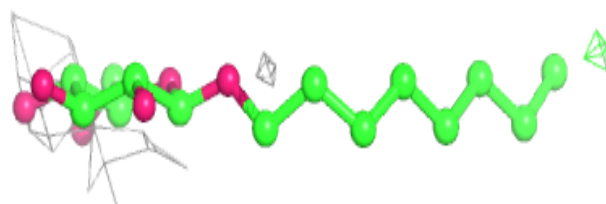
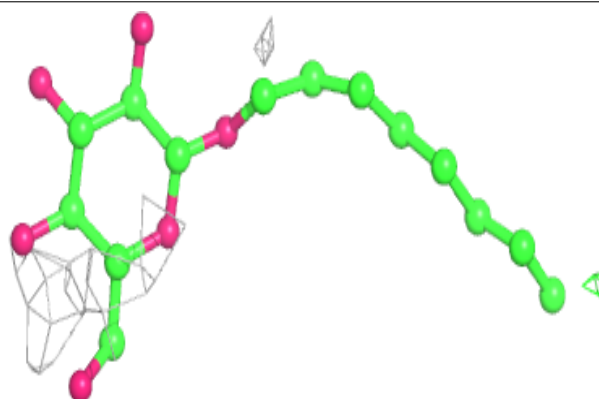
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PEE	C	2007	49/51	0.90	0.28	63,76,100,101	0
20	UNL	E	2012	2/-	0.90	0.20	36,36,36,38	0
20	UNL	Q	3012	1/-	0.90	0.20	8,8,8,8	0
18	CDL	G	2004	40/100	0.91	0.23	92,97,116,117	0
12	BOG	Q	3009	20/20	0.92	0.28	87,110,112,112	0
15	ICX	P	3001	30/30	0.93	0.30	101,117,133,136	0
12	BOG	E	2009	20/20	0.93	0.25	71,73,77,77	0
20	UNL	P	3013	1/-	0.95	0.49	40,40,40,40	0
17	HEC	Q	501	43/43	0.95	0.19	76,84,88,90	0
14	HEM	P	501	43/43	0.96	0.22	53,59,72,77	0
14	HEM	P	502	43/43	0.97	0.21	58,62,69,70	0
14	HEM	C	501	43/43	0.97	0.22	30,35,50,57	0
14	HEM	C	502	43/43	0.98	0.18	25,30,40,43	0
15	ICX	C	2001	30/30	0.98	0.19	43,56,65,66	0
17	HEC	D	501	43/43	0.98	0.17	25,36,45,53	0
19	FES	E	501	4/4	0.98	0.12	105,105,107,107	4
19	FES	R	501	4/4	0.99	0.08	60,61,62,63	0

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

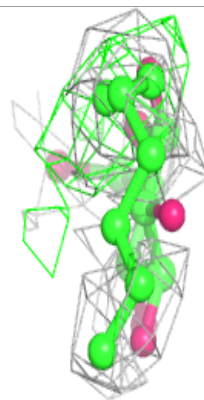
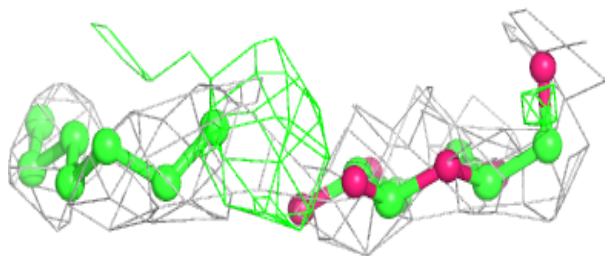
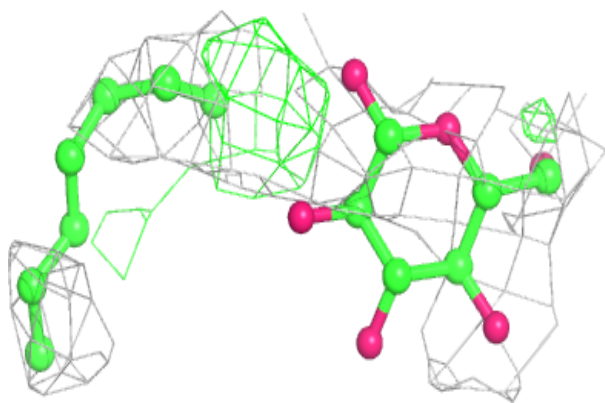
Electron density around BOG Q 3091:

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

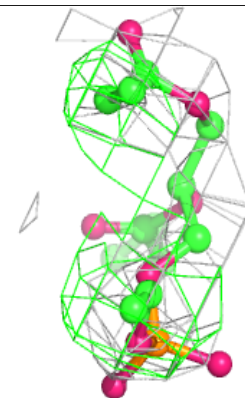
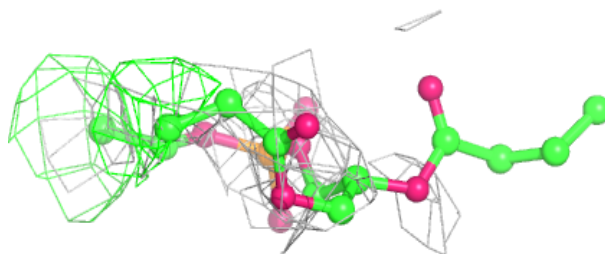
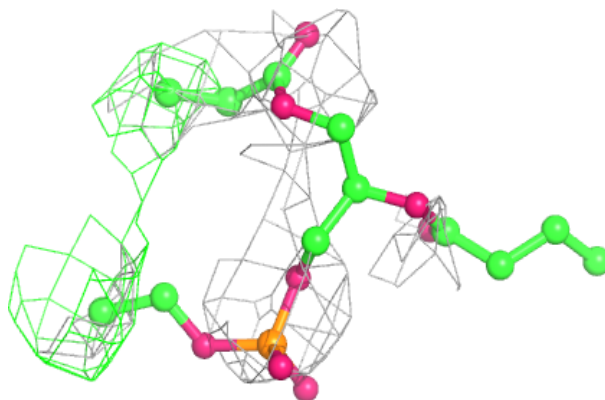


Electron density around BOG P 2010:

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

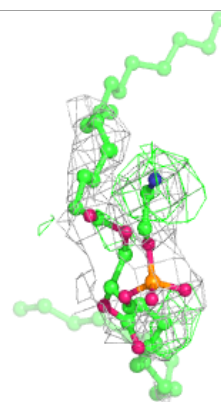
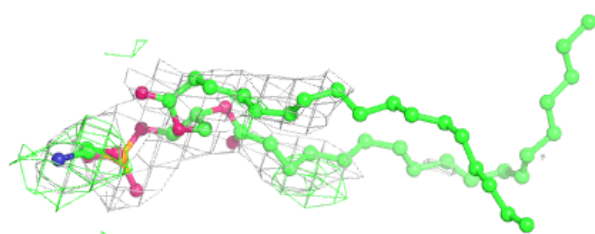
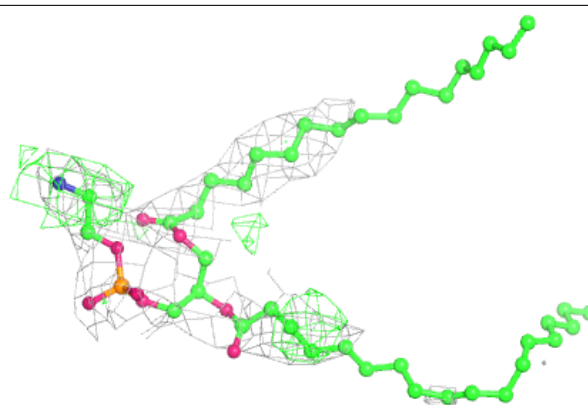
**Electron density around PEE A 2008:**

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

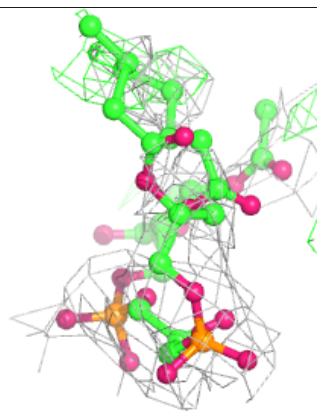
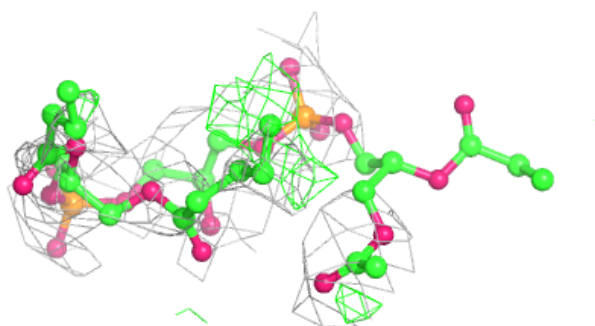
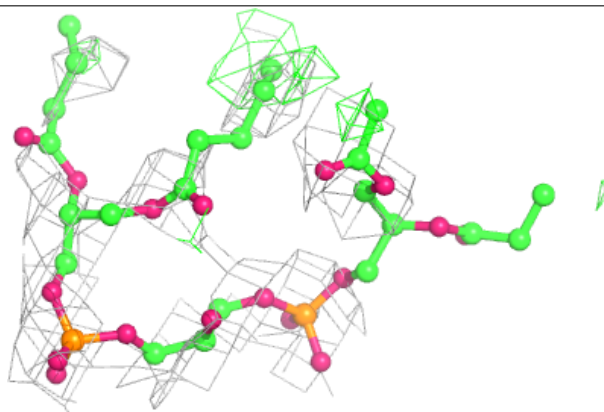


Electron density around PEE W 3005:

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

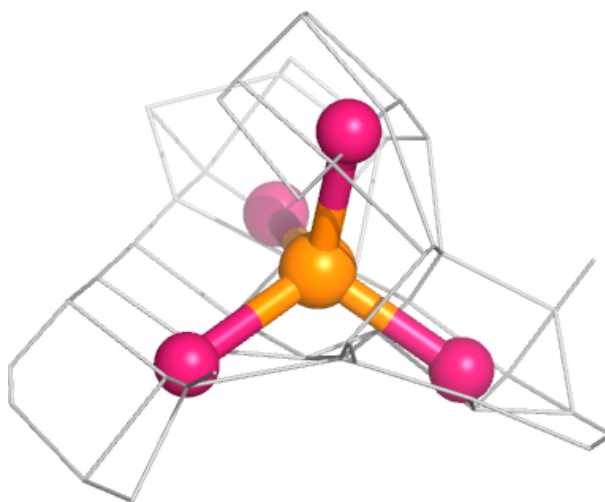
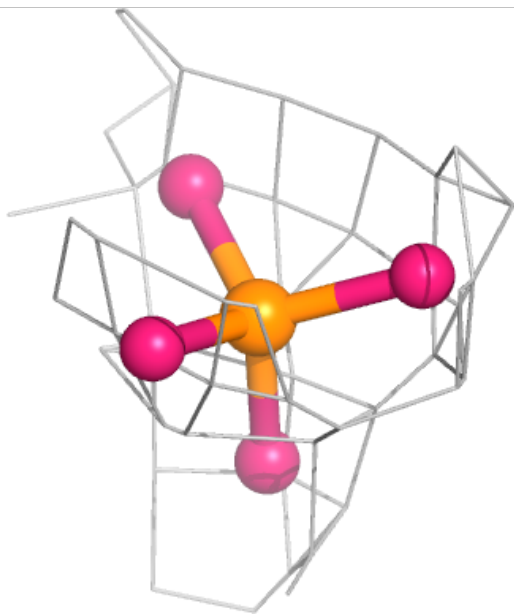
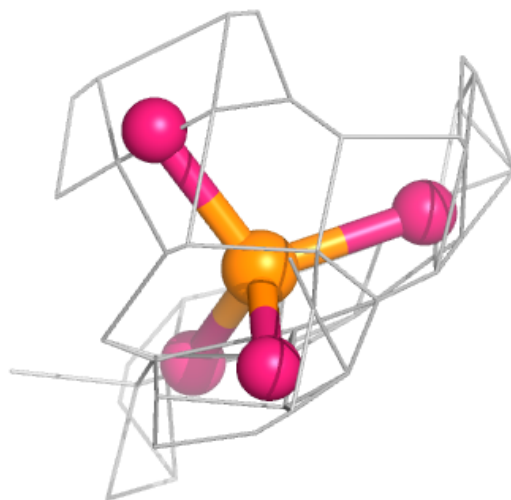
**Electron density around CDL P 3003:**

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



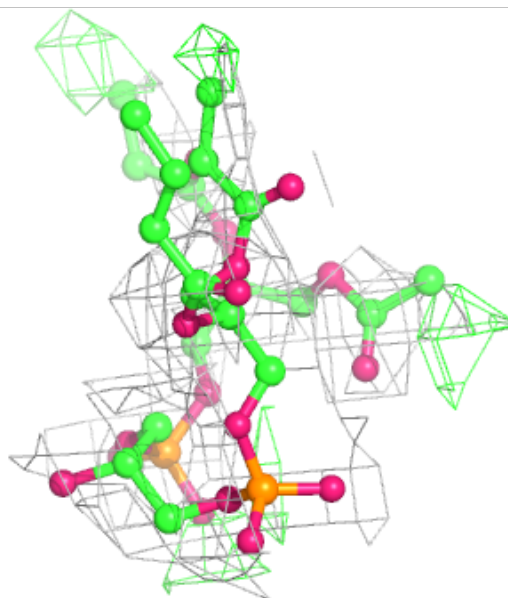
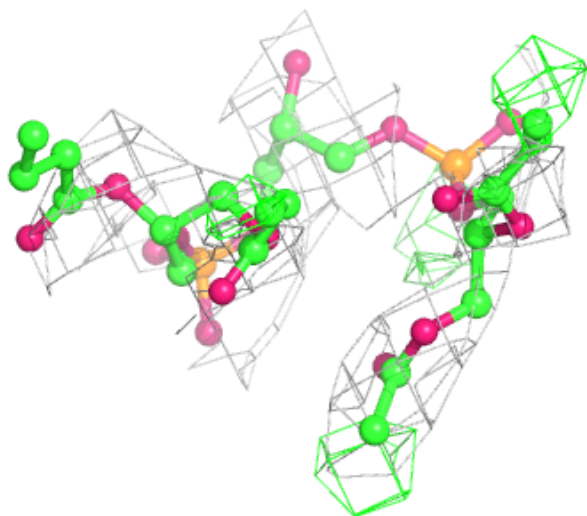
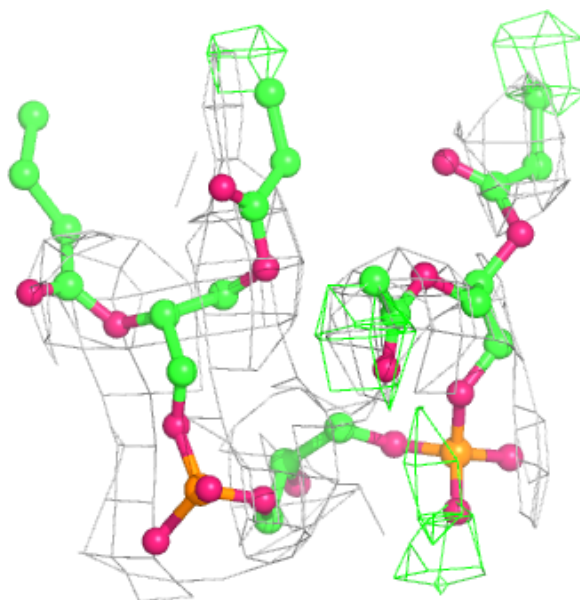
Electron density around PEE P 3008:

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



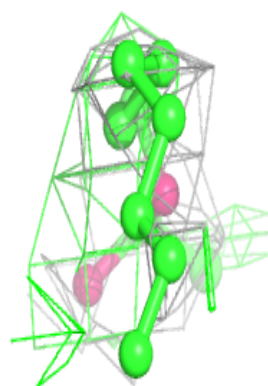
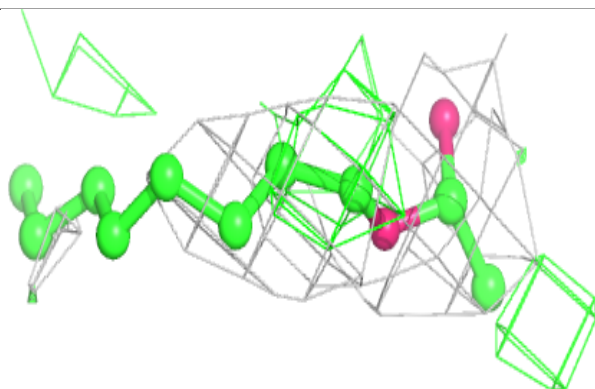
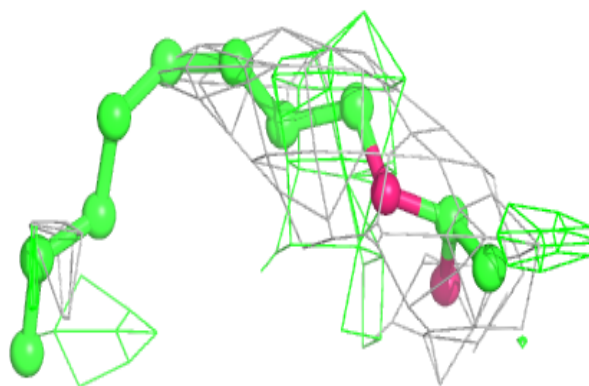
Electron density around CDL P 3004:

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

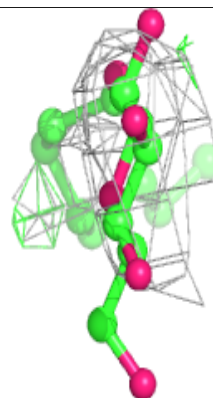
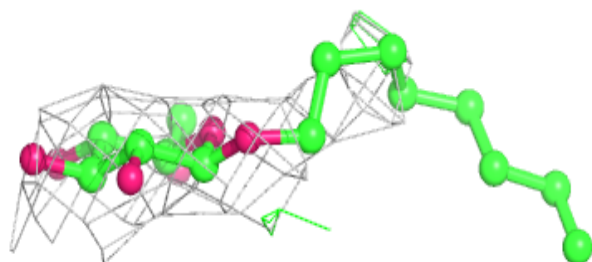
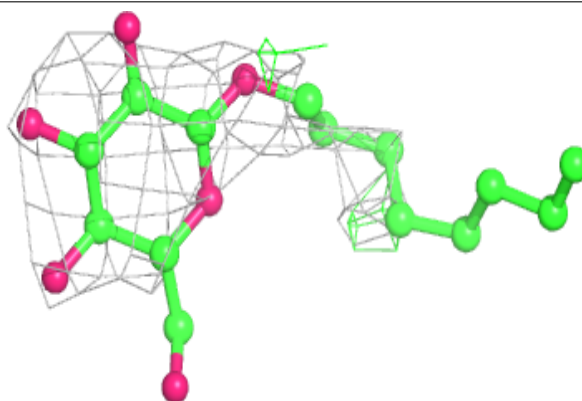


Electron density around BOG C 3010:

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

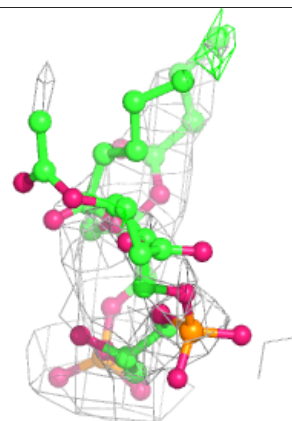
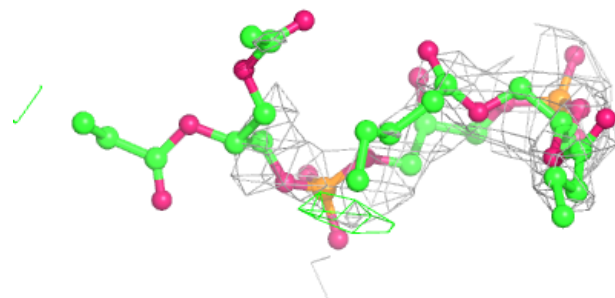
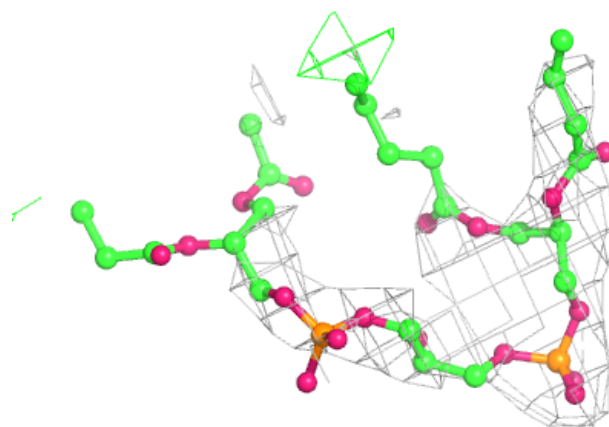
**Electron density around BOG D 2091:**

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

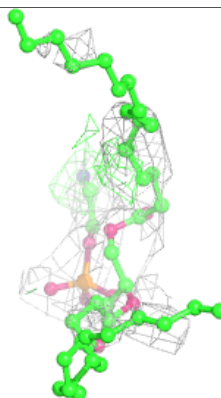
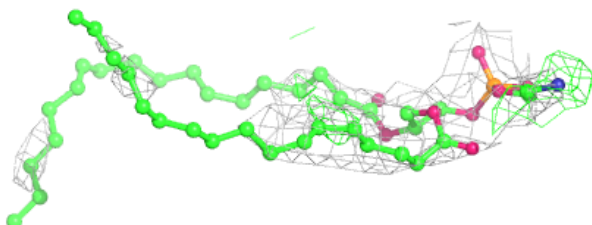
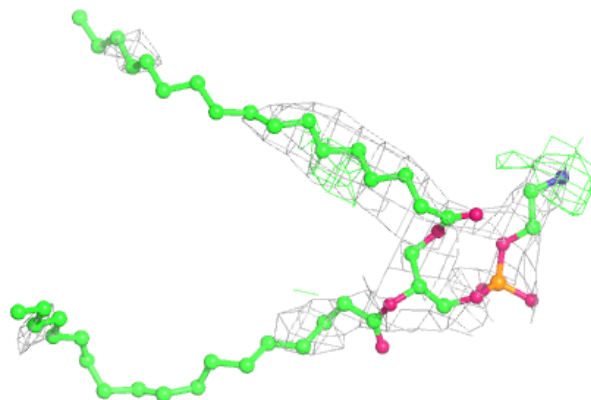


Electron density around CDL D 2003:

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

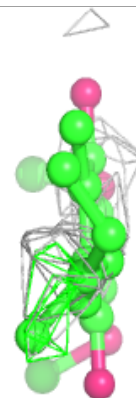
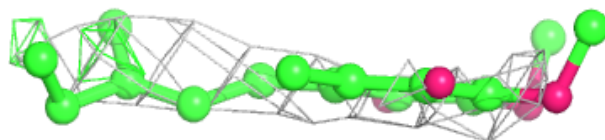
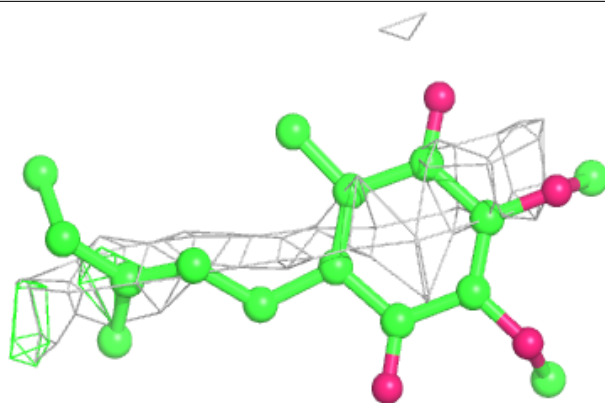
**Electron density around PEE C 2005:**

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

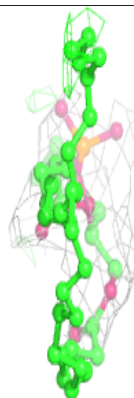
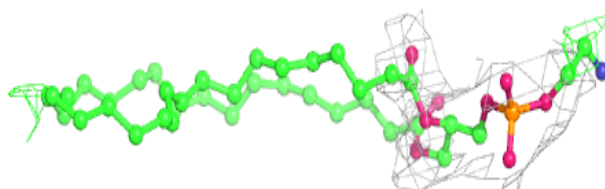
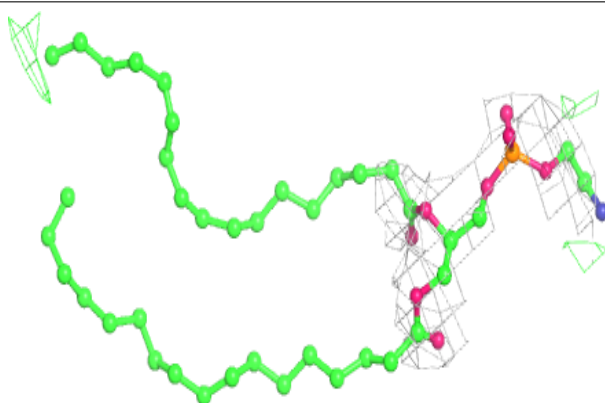


Electron density around UQ P 3002:

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

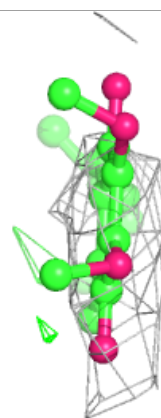
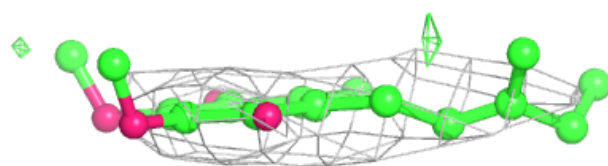
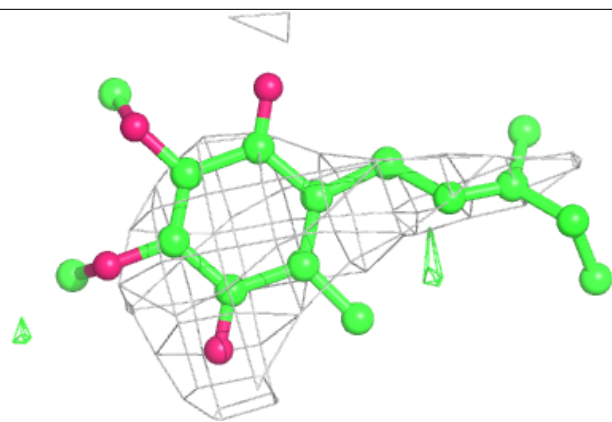
**Electron density around PEE P 3007:**

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

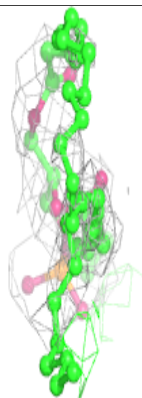
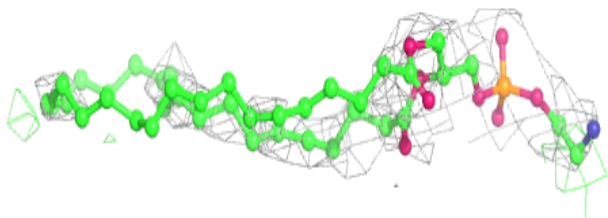
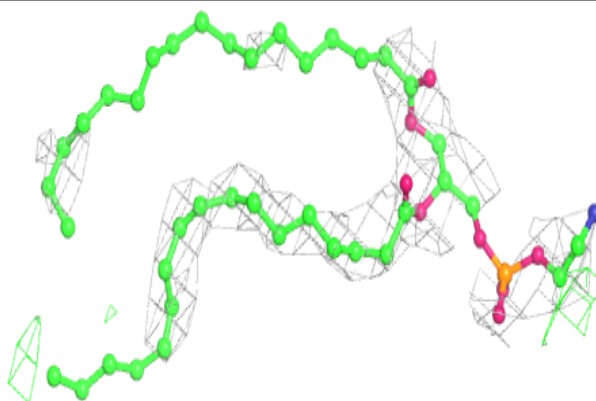


Electron density around UQ C 2002:

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

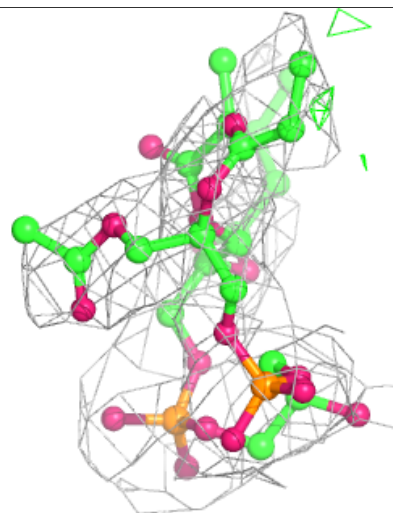
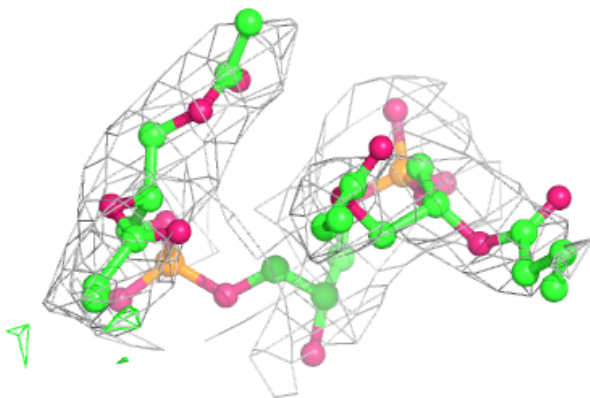
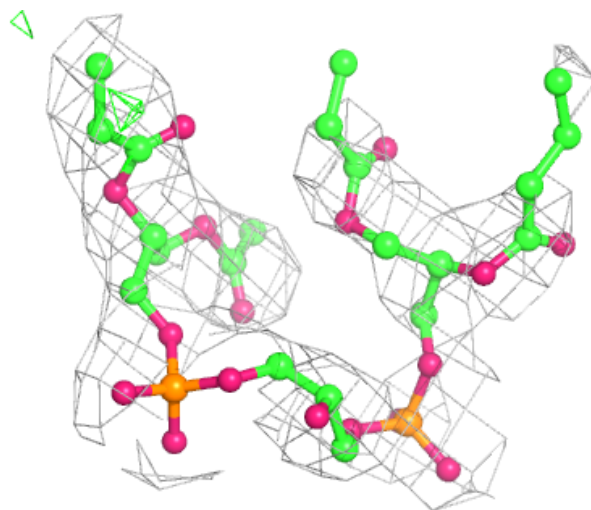
**Electron density around PEE C 2007:**

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



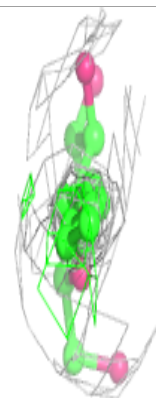
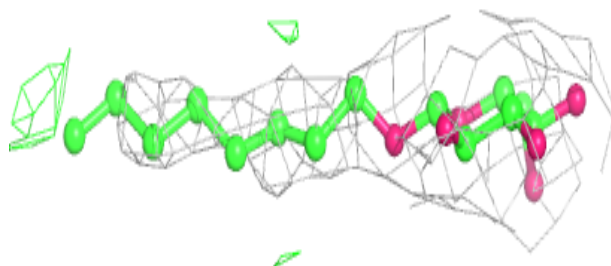
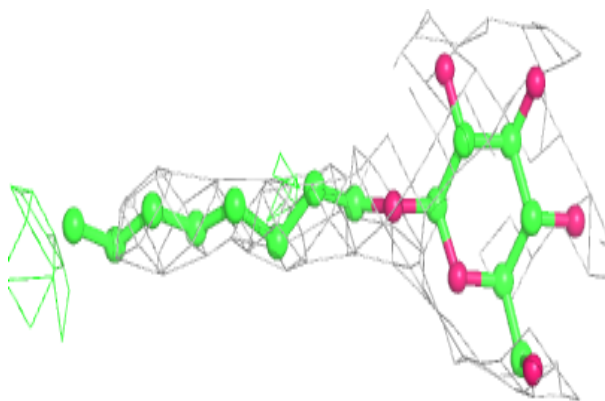
Electron density around CDL G 2004:

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



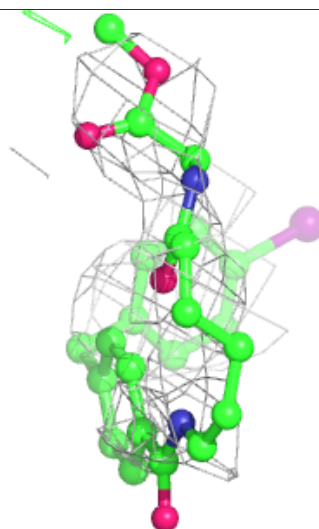
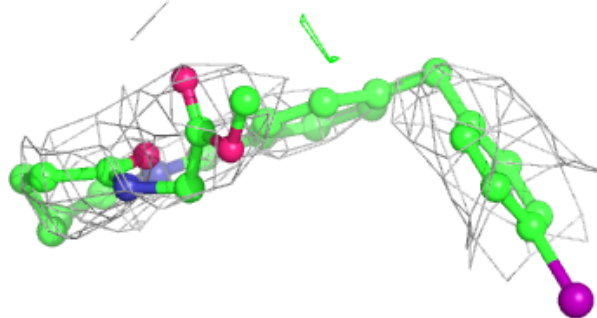
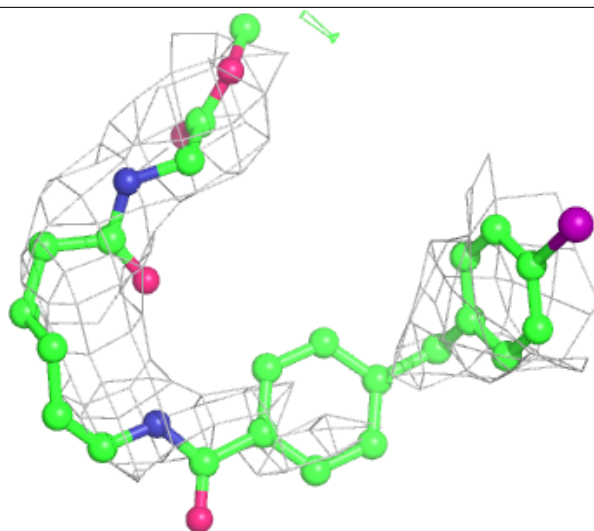
Electron density around BOG Q 3009:

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



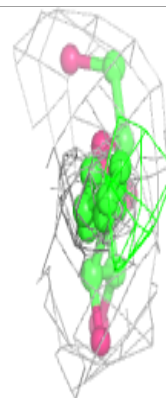
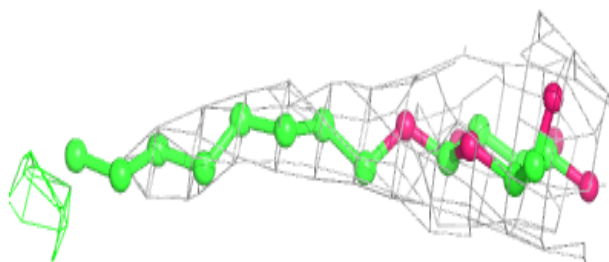
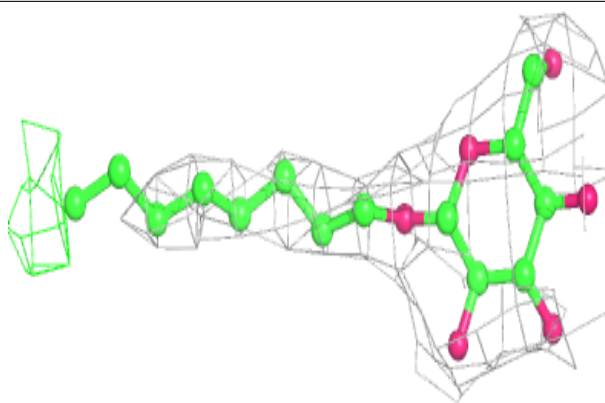
Electron density around ICX P 3001:

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

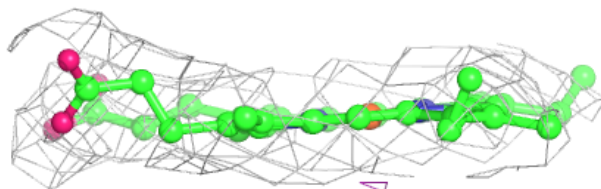
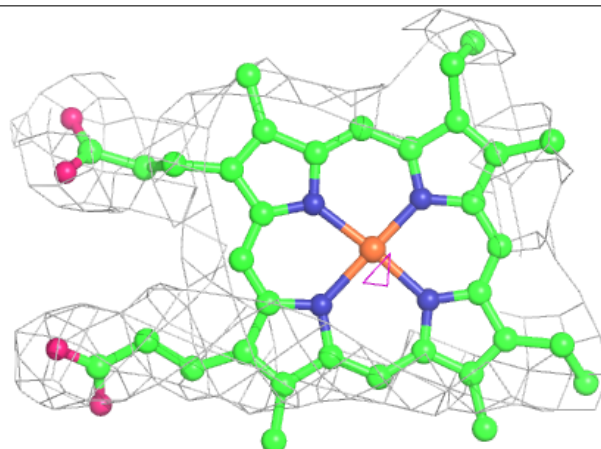


Electron density around BOG E 2009:

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

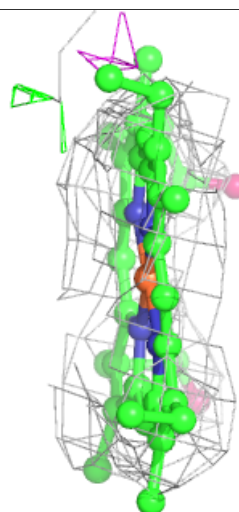
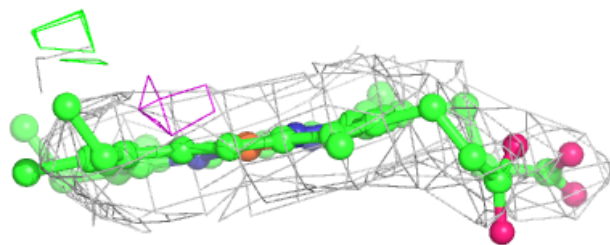
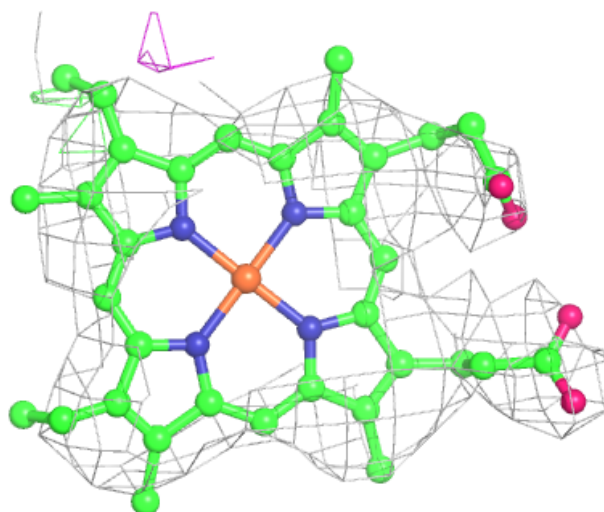
**Electron density around HEC Q 501:**

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



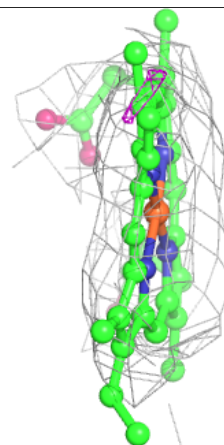
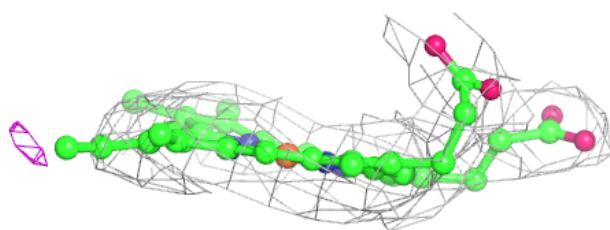
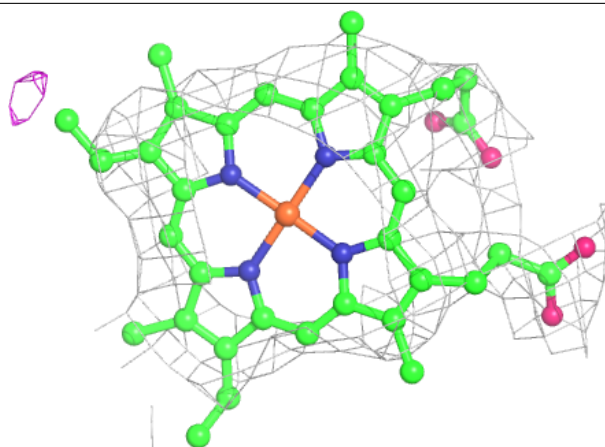
Electron density around HEM P 501:

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



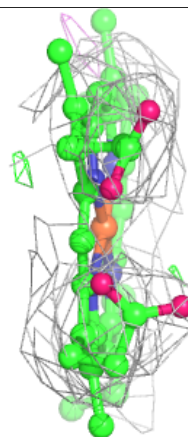
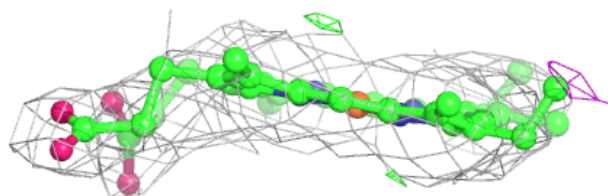
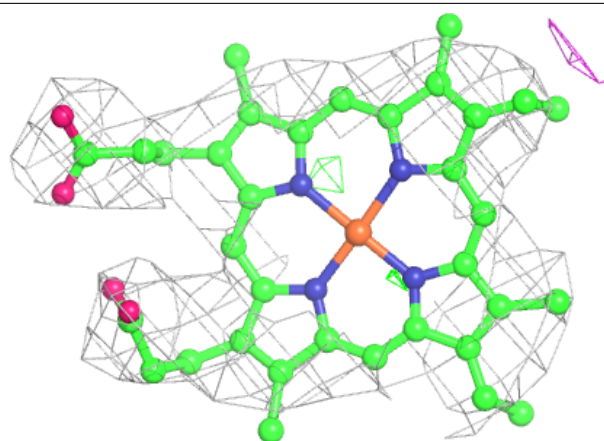
Electron density around HEM P 502:

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



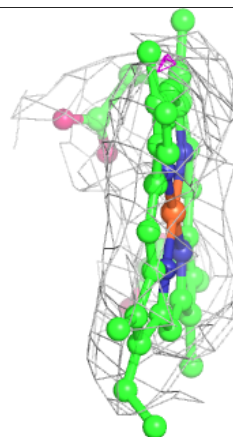
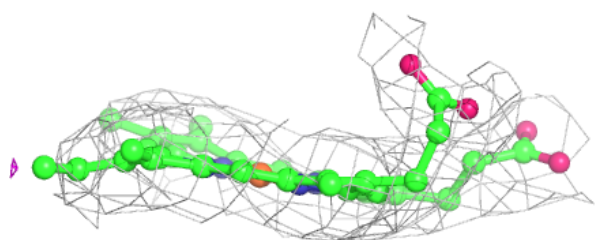
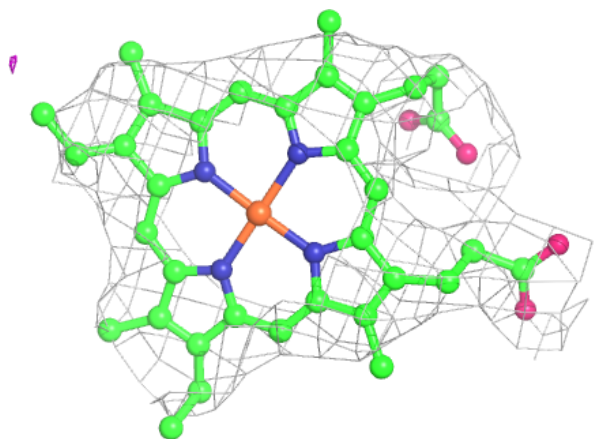
Electron density around HEM C 501:

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



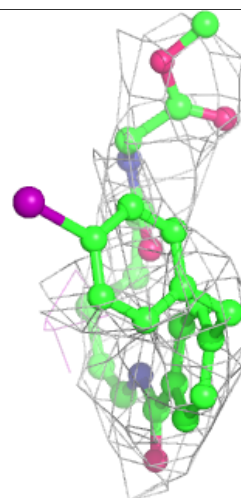
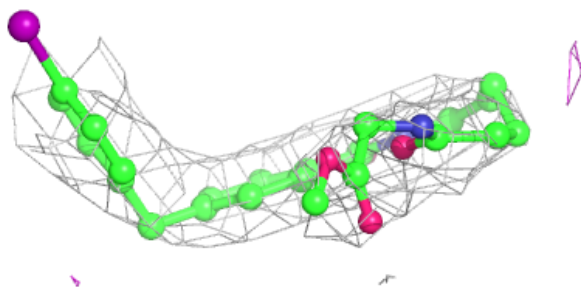
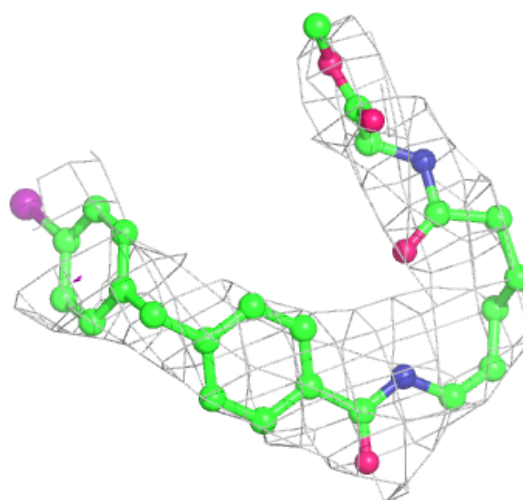
Electron density around HEM C 502:

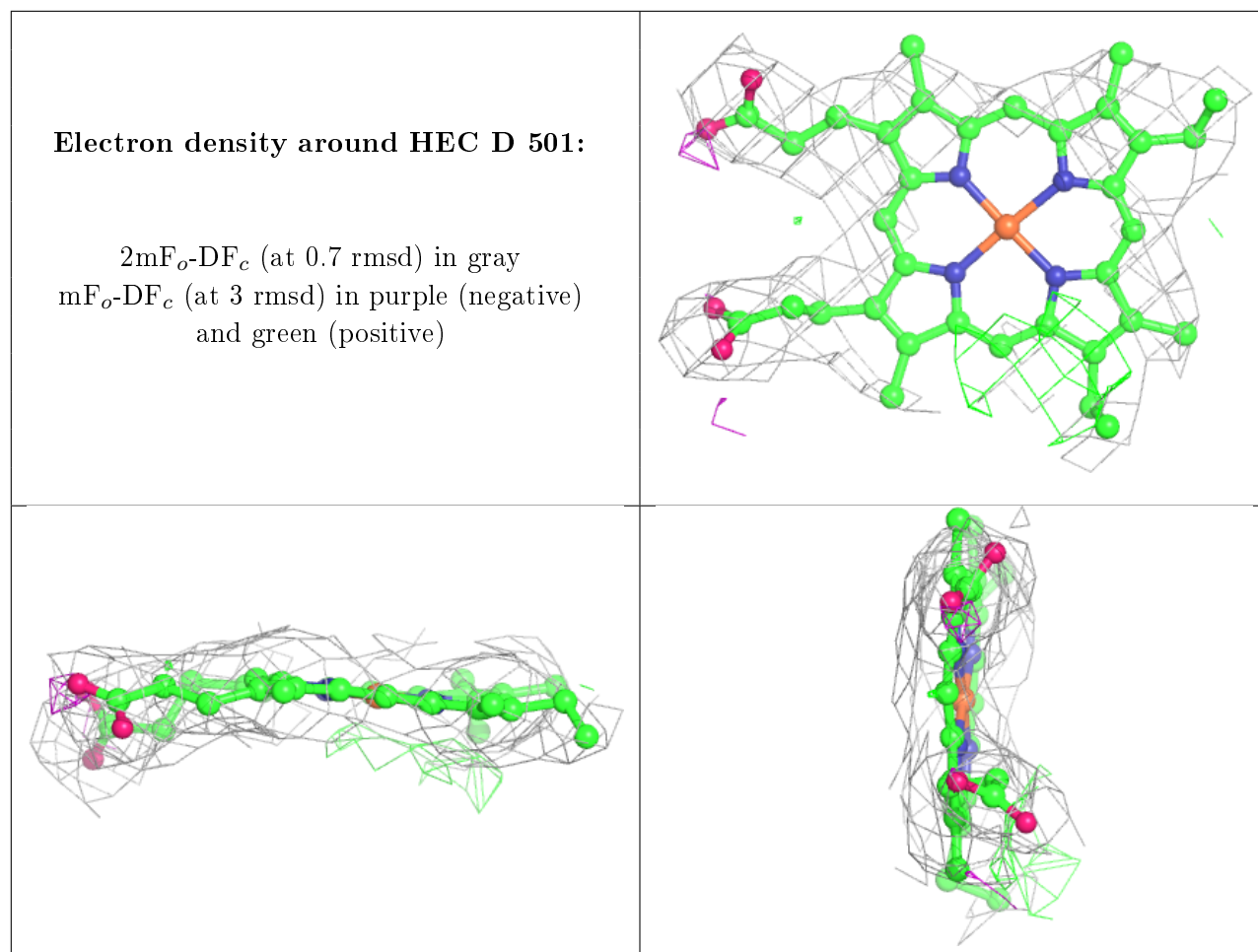
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ICX 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.