



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 01:29 AM EDT

PDB ID : 3L72
Title : Chicken cytochrome BC1 complex with kresoxim-I-dimethyl bound
Authors : Huang, L.; Zhang, Z.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

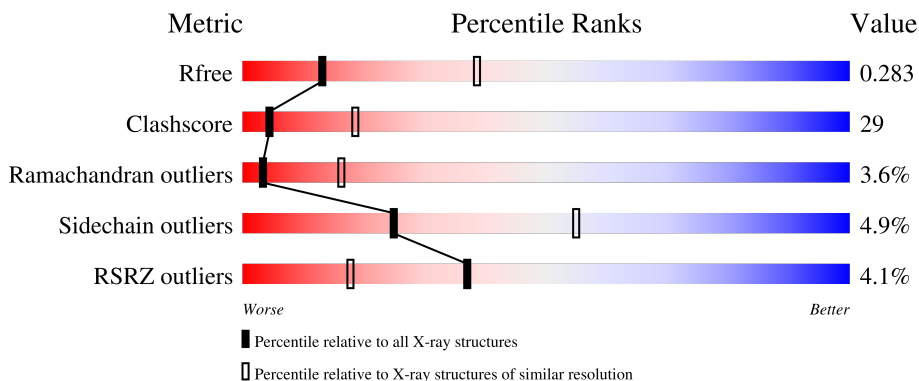
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	
1	N	446	
2	B	441	
2	O	441	
3	C	380	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PEE	P	3008	-	X	-	-
18	BOG	D	2091	-	-	-	X
18	BOG	P	2010	-	-	-	X
18	BOG	Q	3091	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	Total 3447	C 2160	N 607	O 659	S 21	0	0	0
1	N	442	Total 3437	C 2154	N 605	O 657	S 21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	421	Total 3137	C 1970	N 545	O 613	S 9	0	0	0
2	O	422	Total 3147	C 1977	N 546	O 614	S 10	0	0	0

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	380	Total 3017	C 2022	N 478	O 505	S 12	0	0	0
3	P	379	Total 3012	C 2019	N 477	O 504	S 12	0	0	0

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

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

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

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

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

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

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

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

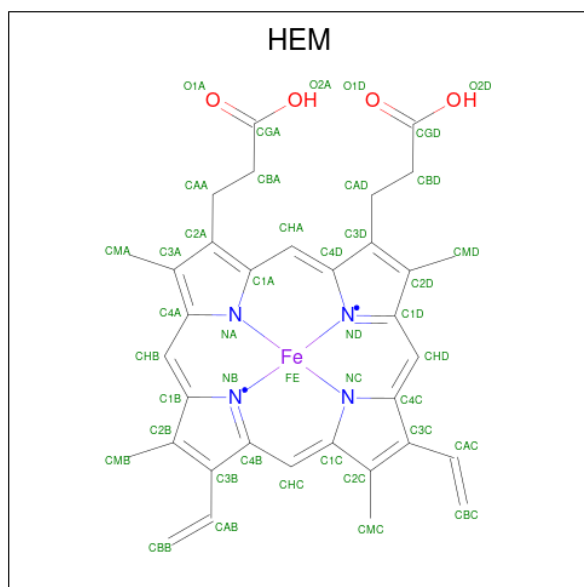
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

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

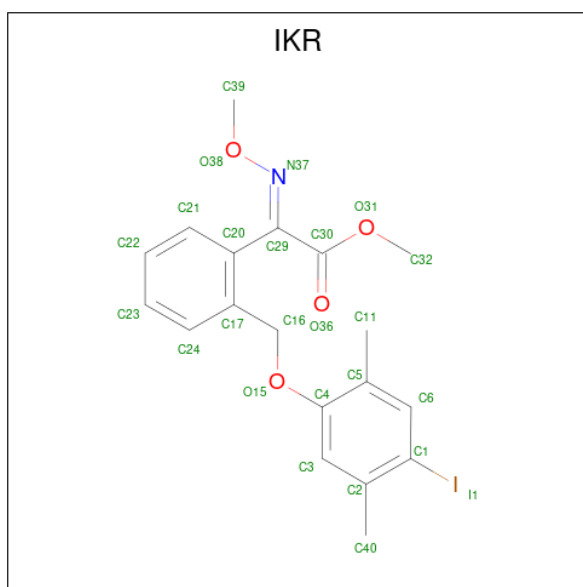
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



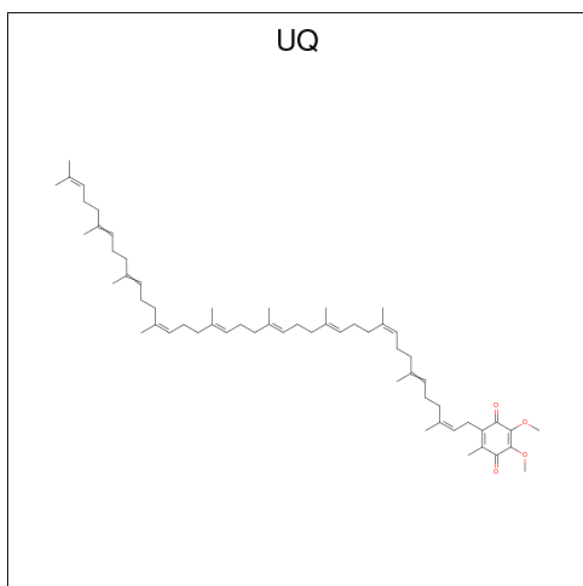
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is methyl (2E)-{2-[(4-iodo-2,5-dimethylphenoxy)methyl]phenyl}(methoxyimino)ethanoate (three-letter code: IKR) (formula: $C_{19}H_{20}INO_4$).



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

- Molecule 13 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



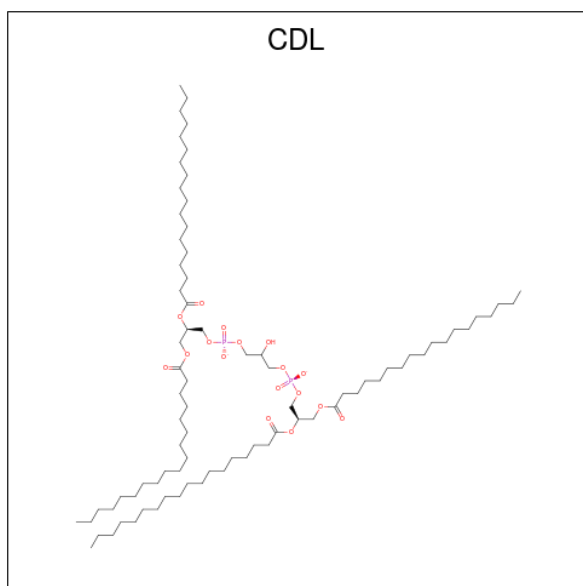
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	C			O
13	C	1	19	15	4	0	0

Continued on next page...

Continued from previous page...

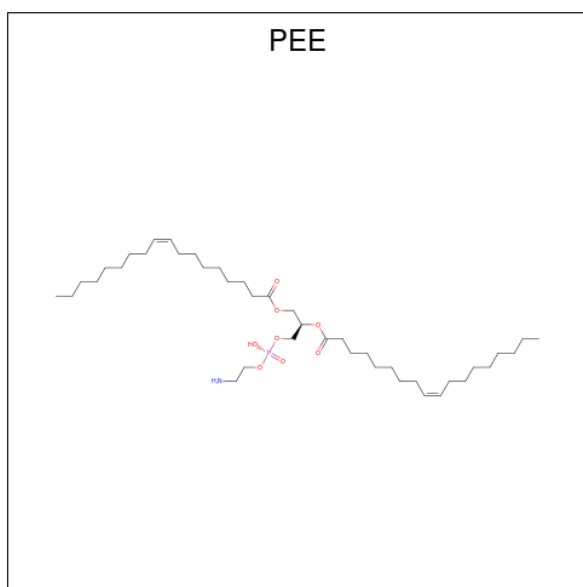
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	P	1	19	15	4	0	0

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



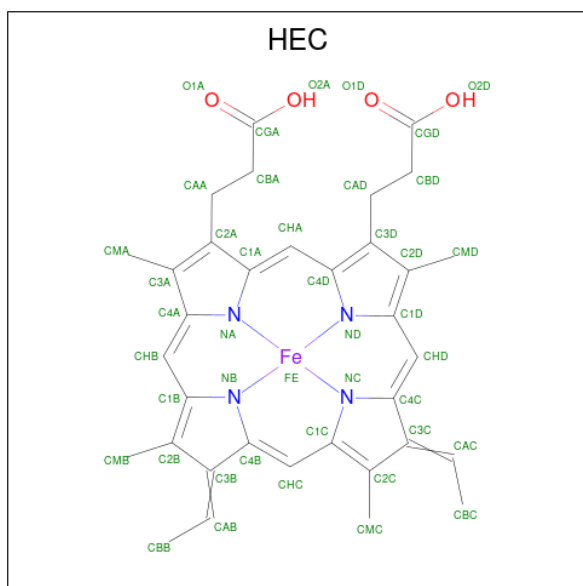
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	P	1	Total	O	P			0	0
			5	4	1				
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



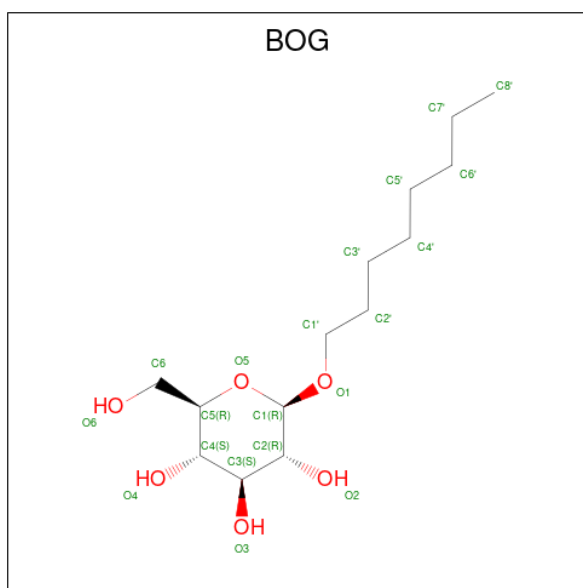
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	O			
			6	3	3	0	0	
16	P	1	Total	C	O			
			6	3	3	0	0	

- 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		
			43	34	1	4	4	0	0
17	Q	1	Total	C	Fe	N	O		
			43	34	1	4	4	0	0

- Molecule 18 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- 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		

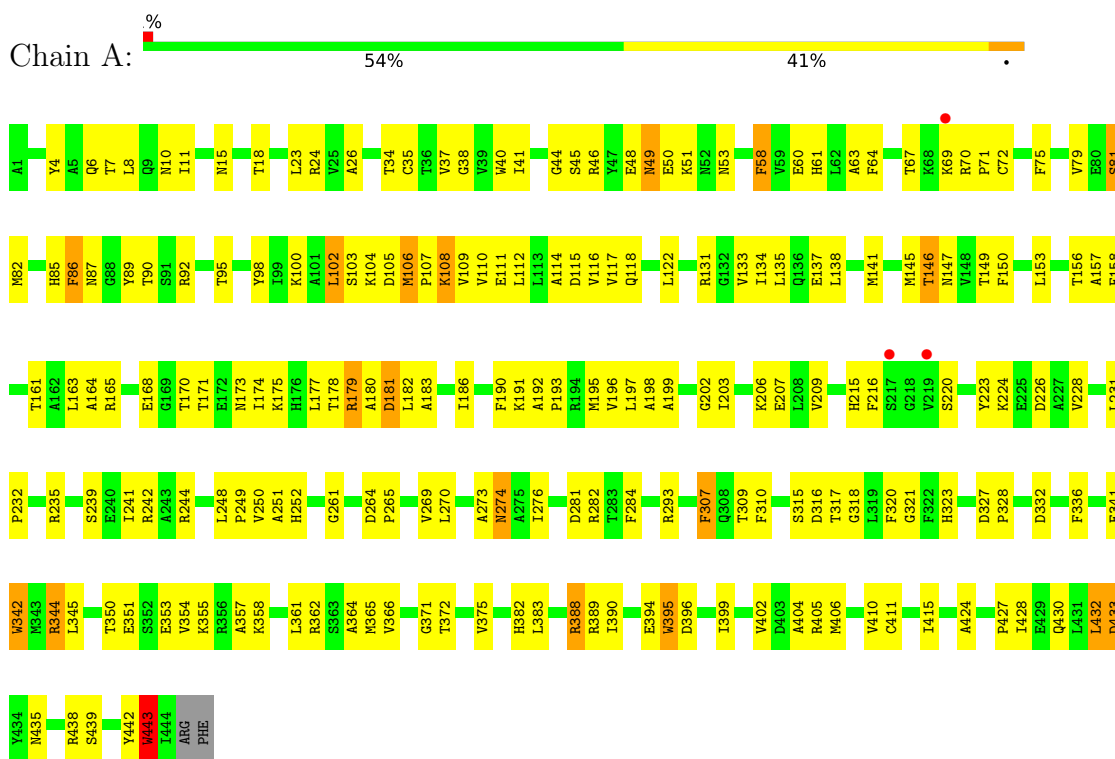
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	8	Total	O	0	0
			8	8		
20	E	1	Total	O	0	0
			1	1		
20	P	8	Total	O	0	0
			8	8		
20	R	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

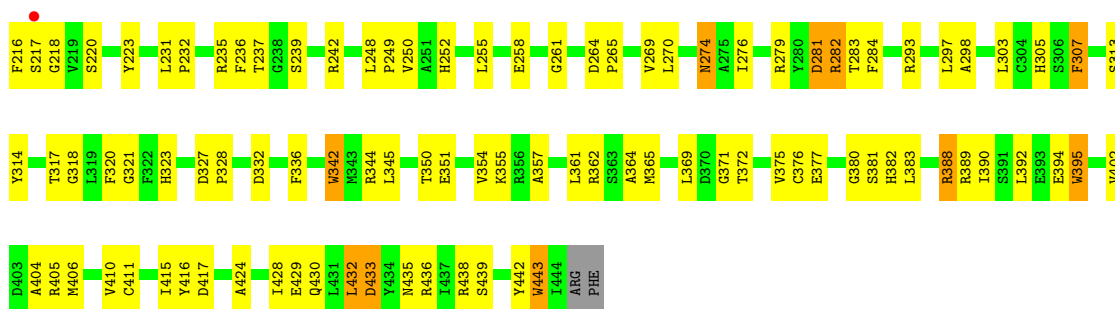
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

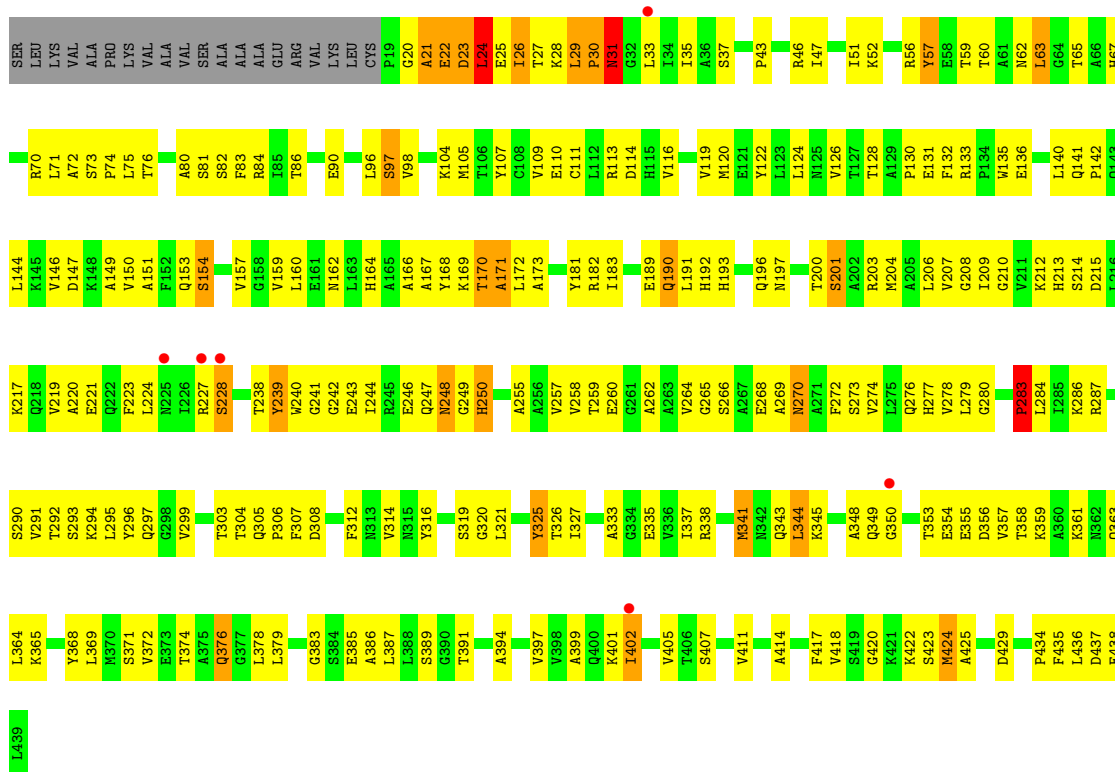


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

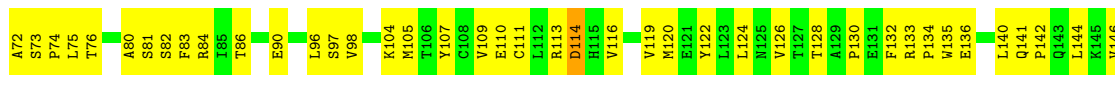
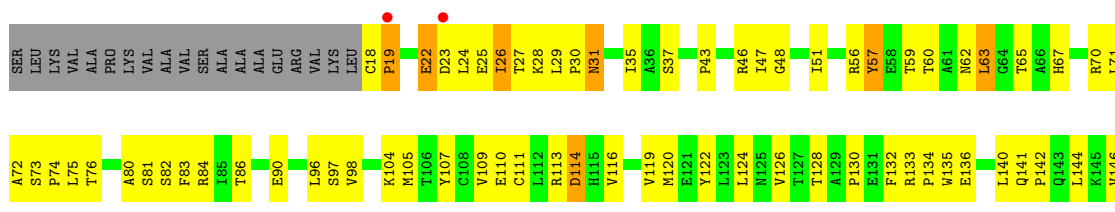


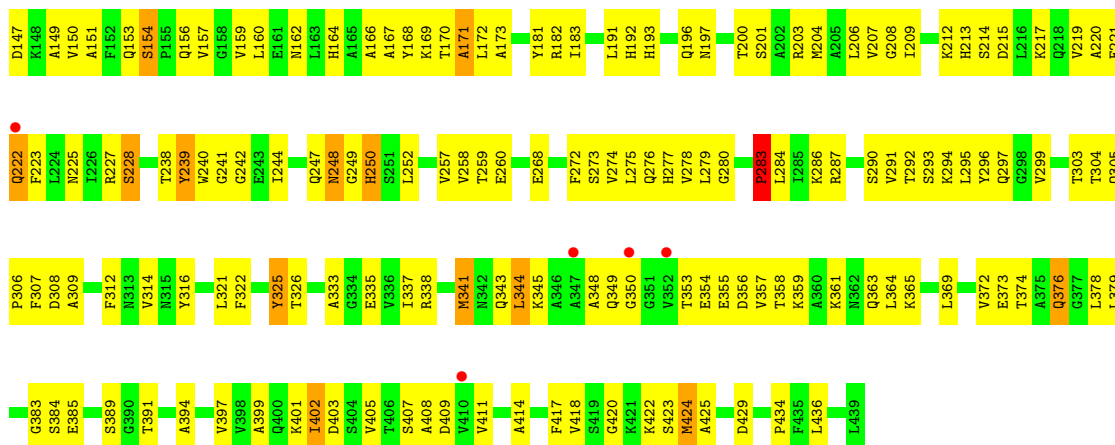


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

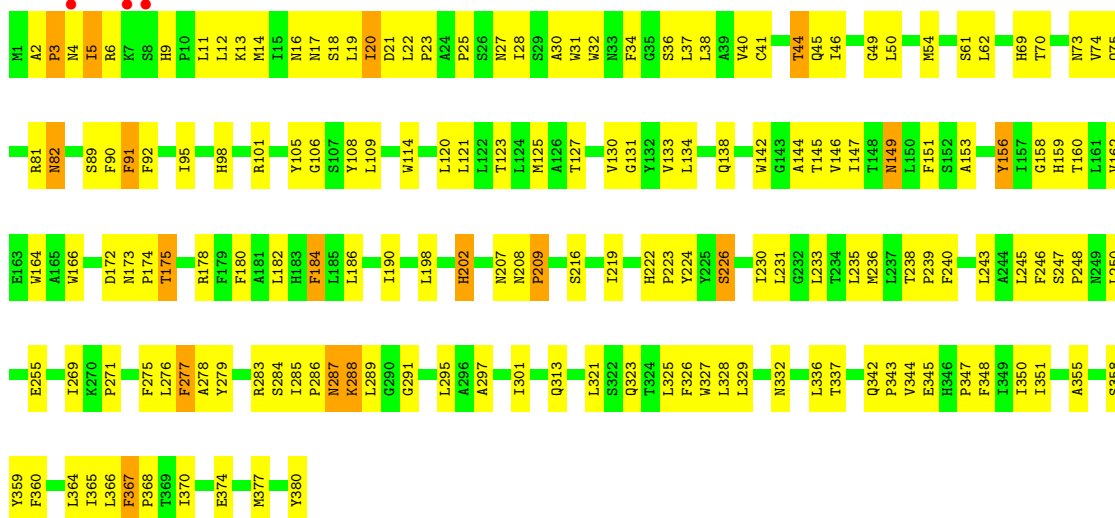


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

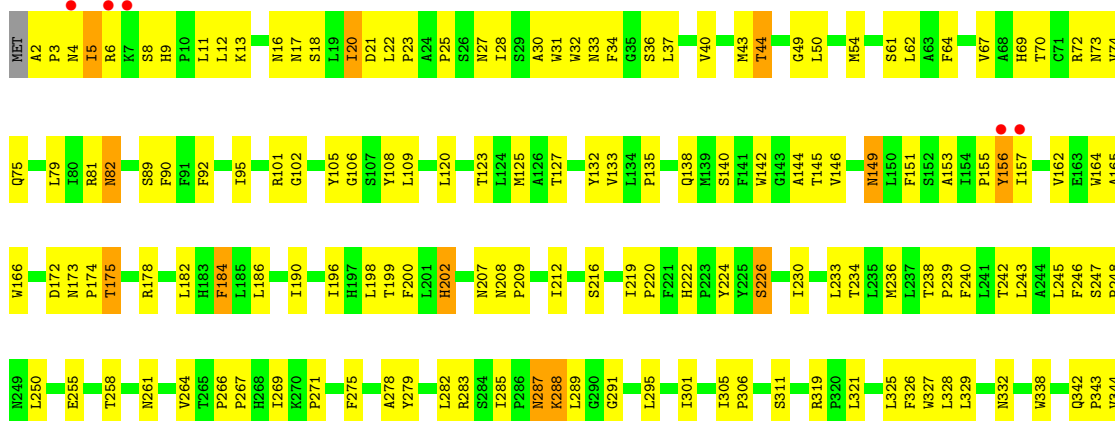




• Molecule 3: CYTOCHROME B



• Molecule 3: CYTOCHROME B

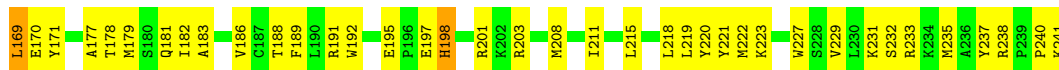




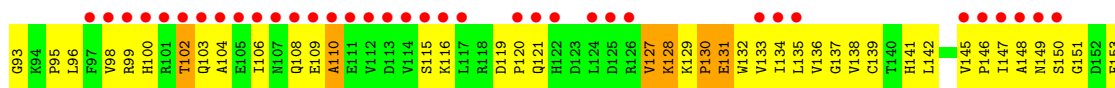
- Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



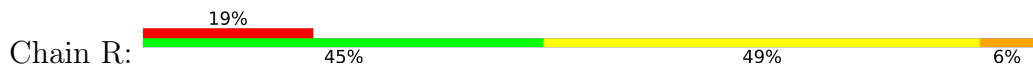
- Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

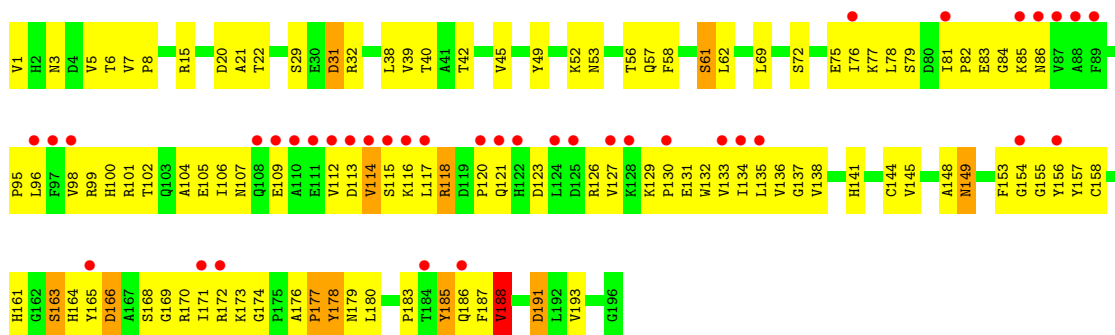


- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



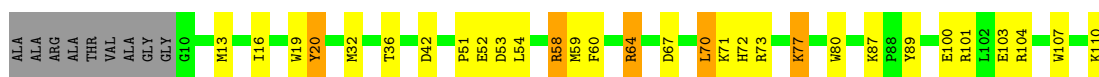
- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL





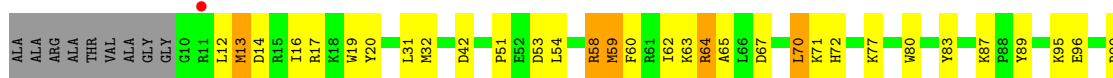
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain F: 65% 23% 5% 8%



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

Chain S: 59% 28% 5% 8%



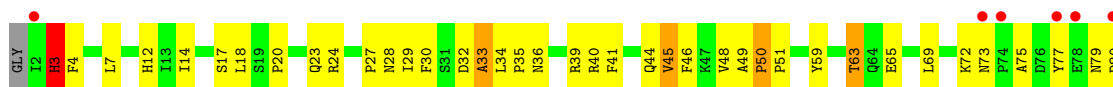
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 49% 40% 10%



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

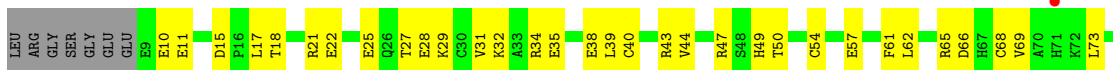
Chain T: 49% 42% 5% 7%



GLN

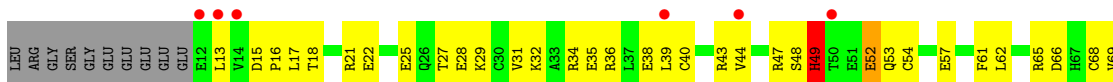
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H: 48% 43% 9%



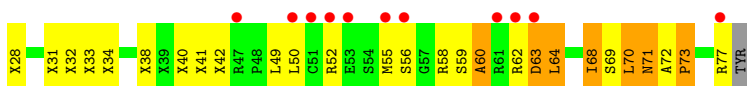
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U: 8% 36% 47% 13%



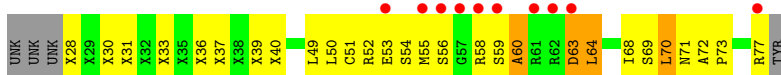
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I: 23% 40% 43% 15%



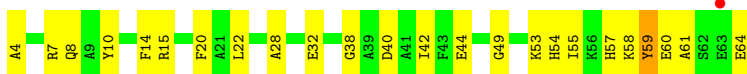
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain V: 21% 32% 51% 9%

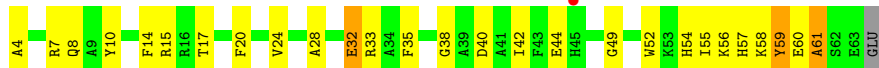


- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J: 2% 61% 38%



- 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	172.61Å 181.55Å 241.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.93 – 3.06 49.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (28.93-3.06) 93.1 (49.92-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.294 0.252 , 0.283	Depositor DCC
R_{free} test set	2766 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32648	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/3518	0.66	0/4767
1	N	0.45	0/3508	0.66	0/4753
2	B	0.40	0/3191	0.67	0/4326
2	O	0.42	0/3202	0.68	0/4343
3	C	0.51	0/3119	0.68	0/4270
3	P	0.48	0/3114	0.66	0/4263
4	D	0.46	0/1956	0.66	0/2658
4	Q	0.40	0/1956	0.63	0/2658
5	E	0.39	0/1547	0.61	0/2103
5	R	0.40	0/1543	0.62	0/2098
6	F	0.51	0/911	0.70	0/1219
6	S	0.43	0/911	0.64	0/1219
7	G	0.53	0/694	0.70	1/941 (0.1%)
7	T	0.50	0/684	0.71	1/929 (0.1%)
8	H	0.45	0/582	0.66	0/779
8	U	0.37	0/561	0.60	0/751
9	I	0.43	0/218	0.68	0/293
9	V	0.43	0/218	0.67	0/293
10	J	0.45	0/508	0.65	0/682
10	W	0.42	0/490	0.65	0/660
All	All	0.45	0/32431	0.66	2/44005 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	18	LEU	CA-CB-CG	5.17	127.19	115.30
7	G	18	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	20	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3362	181	0
1	N	3437	0	3349	204	0
2	B	3137	0	3131	262	0
2	O	3147	0	3146	254	0
3	C	3017	0	3063	148	0
3	P	3012	0	3058	166	0
4	D	1898	0	1846	93	0
4	Q	1898	0	1846	115	0
5	E	1513	0	1478	123	0
5	R	1509	0	1474	126	0
6	F	891	0	893	32	0
6	S	891	0	893	40	0
7	G	672	0	653	48	0
7	T	662	0	645	42	0
8	H	574	0	548	35	0
8	U	553	0	535	42	0
9	I	287	0	251	46	0
9	V	277	0	251	45	0
10	J	497	0	490	20	0
10	W	479	0	478	27	0
11	C	86	0	60	7	0
11	P	86	0	60	5	0
12	C	25	0	20	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	P	25	0	20	3	0
13	C	19	0	17	6	0
13	P	19	0	17	5	0
14	C	40	0	24	1	0
14	D	42	0	28	0	0
14	P	40	0	24	2	0
14	Q	42	0	28	2	0
15	C	70	0	85	1	0
15	E	50	0	77	0	0
15	P	54	0	72	2	0
15	R	50	0	77	1	0
16	C	6	0	8	0	0
16	P	6	0	8	2	0
17	D	43	0	30	2	0
17	Q	43	0	30	2	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	8	0	0	1	0
20	R	1	0	0	0	0
All	All	32648	0	32164	1865	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 29.

All (1865) 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.26	1.14
5:E:127:VAL:HG12	5:E:128:LYS:H	1.15	1.09
2:O:76:THR:HG22	2:O:82:SER:H	1.14	1.04
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.36	1.04
2:B:76:THR:HG22	2:B:82:SER:H	1.17	1.03
2:O:353:THR:HG22	2:O:355:GLU:H	1.24	1.02
2:B:353:THR:HG22	2:B:355:GLU:H	1.24	1.00
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.41	1.00
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.45	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:THR:HG22	1:N:180:ALA:H	1.26	0.97
1:N:102:LEU:H	1:N:102:LEU:HD12	1.31	0.95
4:D:222:MET:HE1	5:E:40:THR:HG23	1.46	0.95
2:B:270:ASN:HD22	2:B:270:ASN:H	1.01	0.94
7:G:41:PHE:O	7:G:45:VAL:HG23	1.68	0.94
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.47	0.94
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.33	0.93
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.50	0.93
1:A:102:LEU:HD12	1:A:102:LEU:H	1.33	0.93
7:T:41:PHE:O	7:T:45:VAL:HG23	1.69	0.93
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.32	0.92
1:A:178:THR:HG22	1:A:180:ALA:H	1.31	0.92
4:D:57:THR:HG22	4:D:59:ALA:H	1.34	0.91
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.52	0.91
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.52	0.90
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.53	0.90
2:O:76:THR:CG2	2:O:82:SER:H	1.85	0.90
2:B:76:THR:CG2	2:B:82:SER:H	1.85	0.89
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.03	0.89
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.73	0.89
1:N:170:THR:HG22	1:N:171:THR:H	1.37	0.89
4:D:2:GLU:HB3	7:G:70:LYS:HE2	1.54	0.88
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.22	0.88
5:R:118:ARG:O	5:R:120:PRO:HD3	1.74	0.87
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.38	0.87
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.74	0.86
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.56	0.86
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.57	0.86
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.58	0.86
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.57	0.85
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.93	0.84
6:F:32:MET:CE	6:F:87:LYS:HG2	2.07	0.84
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.59	0.84
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.60	0.83
5:E:83:GLU:HG2	5:E:102:THR:HA	1.59	0.83
4:D:231:LYS:O	6:F:71:LYS:HE3	1.78	0.83
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.59	0.83
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.13	0.83
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.59	0.83
4:D:47:ALA:H	4:D:50:ASN:HD22	1.22	0.82
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:MET:CE	12:C:2001:IKR:I1	2.97	0.82
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.79	0.82
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.45	0.82
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.44	0.82
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.62	0.81
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.46	0.81
3:C:125:MET:HE2	12:C:2001:IKR:I1	2.50	0.81
8:U:32:LYS:O	8:U:36:ARG:HG3	1.79	0.81
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.46	0.81
2:O:150:VAL:O	2:O:153:GLN:HG3	1.81	0.80
3:P:125:MET:HE2	12:P:3001:IKR:I1	2.51	0.80
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.46	0.80
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.63	0.80
5:E:127:VAL:HG12	5:E:128:LYS:N	1.96	0.80
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.64	0.79
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.65	0.79
2:B:150:VAL:O	2:B:153:GLN:HG3	1.81	0.79
2:O:76:THR:HG22	2:O:82:SER:N	1.94	0.79
5:R:112:VAL:HG21	5:R:170:ARG:NH2	1.97	0.79
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.63	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.63	0.78
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.83	0.78
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.65	0.78
5:R:117:LEU:HD11	5:R:172:ARG:NH1	1.98	0.78
1:N:105:ASP:O	1:N:109:VAL:HG23	1.84	0.78
2:O:207:VAL:HG12	2:O:208:GLY:H	1.49	0.78
2:O:341:MET:HE2	2:O:341:MET:HA	1.64	0.78
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.66	0.78
2:O:222:GLN:O	2:O:222:GLN:HG2	1.84	0.78
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.64	0.77
2:O:62:ASN:O	2:O:65:THR:HG22	1.84	0.77
2:B:207:VAL:HG12	2:B:208:GLY:H	1.49	0.77
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.63	0.77
2:B:57:TYR:HE2	2:B:203:ARG:HH22	1.29	0.77
2:B:76:THR:HG22	2:B:82:SER:N	1.96	0.77
5:E:78:LEU:HD12	5:E:190:ASP:O	1.85	0.77
1:A:112:LEU:O	1:A:116:VAL:HG23	1.84	0.77
9:I:64:LEU:HD12	9:I:77:ARG:C	2.05	0.77
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.50	0.77
3:C:120:LEU:HD13	11:C:502:HEM:HAB	1.65	0.76
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.50	0.76
1:N:182:LEU:O	1:N:186:ILE:HG13	1.86	0.76
8:U:43:ARG:HD2	8:U:47:ARG:NH2	1.99	0.76
1:A:170:THR:HG22	1:A:171:THR:H	1.49	0.76
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.67	0.76
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.68	0.76
1:A:50:GLU:HB2	1:A:165:ARG:NH2	2.00	0.76
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.68	0.76
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.21	0.76
2:O:57:TYR:HE2	2:O:203:ARG:HH22	1.32	0.76
2:O:192:HIS:O	2:O:196:GLN:HG3	1.85	0.76
3:P:125:MET:CE	12:P:3001:IKR:I1	3.04	0.76
3:P:9:HIS:O	3:P:13:LYS:HB3	1.86	0.75
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.47	0.75
2:O:248:ASN:C	2:O:248:ASN:HD22	1.89	0.75
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.66	0.75
2:O:283:PRO:HG2	9:V:56:SER:HB2	1.67	0.75
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.02	0.75
2:B:270:ASN:H	2:B:270:ASN:ND2	1.78	0.75
1:N:170:THR:HG22	1:N:171:THR:N	2.01	0.75
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.22	0.75
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.69	0.75
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.69	0.75
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.68	0.75
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.69	0.75
7:G:81:GLN:HA	8:H:47:ARG:HG2	1.68	0.74
2:O:221:GLU:HG3	2:O:222:GLN:H	1.52	0.74
9:I:70:LEU:HD23	9:I:71:ASN:N	2.02	0.74
3:P:138:GLN:HB2	3:P:255:GLU:O	1.87	0.74
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.53	0.74
1:N:35:CYS:HA	1:N:372:THR:HG21	1.69	0.74
2:O:397:VAL:O	2:O:401:LYS:HG2	1.87	0.74
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.52	0.74
2:B:169:LYS:O	2:B:170:THR:HG23	1.87	0.74
6:F:107:TRP:O	6:F:110:LYS:HB3	1.88	0.74
10:W:57:HIS:HA	10:W:60:GLU:HG2	1.69	0.74
1:A:182:LEU:O	1:A:186:ILE:HG13	1.88	0.73
3:C:22:LEU:HD21	13:C:2002:UQ:HM32	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.70	0.73
1:A:206:LYS:O	1:A:209:VAL:HG12	1.88	0.73
2:B:270:ASN:HD22	2:B:270:ASN:N	1.82	0.73
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.22	0.73
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.73
2:O:47:ILE:HD13	2:O:120:MET:CE	2.19	0.73
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.19	0.73
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.71	0.73
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.24	0.73
7:G:65:GLU:O	7:G:69:LEU:HG	1.87	0.73
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.69	0.73
7:T:29:ILE:O	7:T:33:ALA:HB3	1.88	0.73
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.70	0.72
3:C:9:HIS:O	3:C:13:LYS:HB3	1.89	0.72
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.54	0.72
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.14	0.72
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.71	0.72
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.04	0.72
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.03	0.72
3:C:50:LEU:O	3:C:54:MET:HG3	1.90	0.72
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.55	0.72
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.05	0.72
1:N:206:LYS:O	1:N:209:VAL:HG12	1.89	0.72
1:N:112:LEU:O	1:N:116:VAL:HG23	1.89	0.72
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.25	0.72
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.25	0.71
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.55	0.71
3:C:125:MET:HE1	12:C:2001:IKR:I1	2.60	0.71
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.72	0.71
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.58	0.71
2:B:306:PRO:HA	9:I:52:ARG:CG	2.19	0.71
5:E:106:ILE:O	5:E:110:ALA:HB3	1.90	0.71
7:G:80:ASP:HB3	8:H:50:THR:HA	1.72	0.71
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.71	0.71
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.90	0.71
14:P:3004:CDL:OA4	7:T:40:ARG:HD2	1.89	0.71
2:B:341:MET:HE2	2:B:341:MET:HA	1.71	0.71
15:C:2007:PEE:H7	7:G:44:GLN:HE21	1.54	0.71
7:G:29:ILE:O	7:G:33:ALA:HB3	1.91	0.71
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.56	0.71
6:S:13:MET:HA	6:S:16:ILE:HB	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HD13	2:B:120:MET:CE	2.21	0.71
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.73	0.71
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.06	0.71
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.73	0.71
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.05	0.71
6:F:32:MET:HE3	6:F:87:LYS:CG	2.21	0.70
3:P:101:ARG:HD2	3:P:101:ARG:C	2.12	0.70
5:R:120:PRO:O	5:R:121:GLN:HG3	1.90	0.70
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.57	0.70
2:O:422:LYS:O	2:O:436:LEU:HD21	1.91	0.70
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.26	0.70
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.73	0.70
5:R:112:VAL:HG21	5:R:170:ARG:HH22	1.54	0.70
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.54	0.70
3:P:245:LEU:O	4:Q:201:ARG:HD3	1.91	0.70
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.73	0.70
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.57	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.22	0.70
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.72	0.70
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.21	0.70
5:R:77:LYS:HA	5:R:191:ASP:O	1.92	0.70
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.25	0.69
3:P:238:THR:HB	3:P:239:PRO:HD3	1.74	0.69
1:A:178:THR:HB	1:A:181:ASP:OD1	1.92	0.69
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.73	0.69
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.59	0.69
2:B:248:ASN:C	2:B:248:ASN:HD22	1.94	0.69
2:B:397:VAL:O	2:B:401:LYS:HG2	1.91	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.73	0.69
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.07	0.69
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.75	0.69
4:D:47:ALA:H	4:D:50:ASN:ND2	1.90	0.69
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.75	0.69
1:N:50:GLU:HB2	1:N:165:ARG:NH2	2.08	0.69
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.08	0.69
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.27	0.69
2:O:238:THR:HG22	2:O:239:TYR:N	2.09	0.68
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.56	0.68
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.58	0.68
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.75	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:248:ASN:ND2	2:O:250:HIS:H	1.92	0.68
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.58	0.68
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.22	0.68
2:O:96:LEU:HB3	9:V:70:LEU:HD22	1.76	0.68
2:O:154:SER:O	2:O:157:VAL:HG12	1.94	0.68
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.27	0.68
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.28	0.68
2:B:238:THR:HG22	2:B:239:TYR:H	1.59	0.68
1:A:170:THR:HG22	1:A:171:THR:N	2.08	0.68
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.59	0.67
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.24	0.67
2:O:27:THR:HG22	2:O:28:LYS:N	2.09	0.67
6:S:95:LYS:O	6:S:99:ARG:HG3	1.95	0.67
1:A:50:GLU:HB2	1:A:165:ARG:HH21	1.56	0.67
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.23	0.67
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.76	0.67
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.76	0.67
15:P:3007:PEE:H7	7:T:44:GLN:HE21	1.59	0.67
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.23	0.67
3:C:138:GLN:HB2	3:C:255:GLU:O	1.95	0.67
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.76	0.67
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.29	0.67
9:V:64:LEU:HD12	9:V:77:ARG:C	2.15	0.67
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.77	0.67
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.30	0.67
5:R:117:LEU:HD11	5:R:172:ARG:HH11	1.58	0.67
3:P:50:LEU:O	3:P:54:MET:HG3	1.96	0.66
5:R:177:PRO:HG2	5:R:178:TYR:H	1.59	0.66
10:J:38:GLY:O	10:J:42:ILE:HG13	1.95	0.66
2:O:361:LYS:O	2:O:365:LYS:HG3	1.94	0.66
10:W:49:GLY:N	10:W:54:HIS:ND1	2.44	0.66
2:B:374:THR:HG22	2:B:376:GLN:H	1.61	0.66
3:C:101:ARG:HD2	3:C:101:ARG:C	2.15	0.66
8:U:27:THR:O	8:U:31:VAL:HG23	1.96	0.66
4:D:57:THR:HG22	4:D:59:ALA:N	2.10	0.66
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.77	0.66
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.78	0.66
7:T:65:GLU:O	7:T:69:LEU:HG	1.95	0.66
2:O:169:LYS:O	2:O:170:THR:HG23	1.96	0.66
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.13	0.66
3:C:238:THR:HB	3:C:239:PRO:HD3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.31	0.66
2:O:31:ASN:HD22	2:O:31:ASN:N	1.93	0.66
2:B:283:PRO:HG2	9:I:56:SER:HB2	1.77	0.65
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.76	0.65
2:O:325:TYR:HD1	9:V:60:ALA:CB	2.09	0.65
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.79	0.65
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.61	0.65
5:E:165:TYR:HA	5:E:170:ARG:O	1.96	0.65
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.78	0.65
2:O:238:THR:HG22	2:O:239:TYR:H	1.60	0.65
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.77	0.65
10:J:49:GLY:N	10:J:54:HIS:ND1	2.45	0.65
2:O:166:ALA:HB1	2:O:242:GLY:O	1.97	0.65
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.10	0.65
1:A:35:CYS:HA	1:A:372:THR:HG21	1.77	0.65
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.32	0.65
1:N:371:GLY:O	1:N:375:VAL:HG23	1.95	0.65
5:E:116:LYS:H	5:E:116:LYS:HD2	1.62	0.65
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.79	0.65
3:P:173:ASN:N	3:P:174:PRO:HD2	2.12	0.65
2:B:264:VAL:HG23	2:B:316:TYR:C	2.18	0.64
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.11	0.64
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.61	0.64
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.33	0.64
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.80	0.64
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.77	0.64
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.31	0.64
2:B:238:THR:HG22	2:B:239:TYR:N	2.11	0.64
3:C:173:ASN:N	3:C:174:PRO:HD2	2.12	0.64
9:I:71:ASN:HD22	9:I:71:ASN:H	1.44	0.64
2:B:325:TYR:HD1	9:I:60:ALA:HB3	1.61	0.64
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.79	0.64
1:A:117:VAL:HG23	1:A:118:GLN:N	2.12	0.64
2:B:192:HIS:O	2:B:196:GLN:HG3	1.98	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.97	0.64
10:W:38:GLY:O	10:W:42:ILE:HG13	1.97	0.64
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.32	0.64
5:E:69:LEU:O	5:E:72:SER:HB3	1.97	0.64
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.97	0.64
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.79	0.64
1:N:178:THR:HB	1:N:181:ASP:OD1	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.21	0.64
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.80	0.64
4:D:102:ARG:NH1	4:D:107:GLY:O	2.31	0.64
17:D:501:HEC:HMB1	17:D:501:HEC:HBB3	1.78	0.64
5:E:190:ASP:C	5:E:192:LEU:H	2.00	0.64
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.28	0.64
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.79	0.64
1:N:49:ASN:ND2	1:N:51:LYS:H	1.95	0.63
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.63	0.63
2:O:325:TYR:HD2	2:O:326:THR:N	1.96	0.63
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.26	0.63
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.63	0.63
1:N:332:ASP:HB2	1:N:430:GLN:HG2	1.81	0.63
2:O:56:ARG:HA	2:O:171:ALA:O	1.97	0.63
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.81	0.63
2:B:295:LEU:O	2:B:299:VAL:HG23	1.98	0.63
5:E:106:ILE:C	5:E:110:ALA:HB3	2.19	0.63
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.27	0.63
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.28	0.63
5:E:96:LEU:HD12	5:E:135:LEU:O	1.99	0.63
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.13	0.63
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.80	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.32	0.63
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.64	0.63
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.61	0.63
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.34	0.63
1:A:249:PRO:HG2	1:A:250:VAL:H	1.64	0.63
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.33	0.63
2:B:422:LYS:O	2:B:436:LEU:HD21	1.97	0.63
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.64	0.63
2:O:56:ARG:HH11	2:O:56:ARG:HG3	1.64	0.63
2:O:359:LYS:O	2:O:363:GLN:HG3	1.99	0.63
2:B:57:TYR:CD1	2:B:57:TYR:N	2.67	0.63
1:N:161:THR:HG21	1:N:235:ARG:H	1.62	0.63
3:C:198:LEU:HD13	13:C:2002:UQ:HM53	1.81	0.62
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.34	0.62
2:O:399:ALA:O	2:O:402:ILE:HG22	1.99	0.62
9:I:32:UNK:N	9:I:73:PRO:HG2	2.14	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.34	0.62
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.81	0.62
2:B:166:ALA:HB1	2:B:242:GLY:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.81	0.62
9:V:70:LEU:HD23	9:V:71:ASN:N	2.13	0.62
2:O:417:PHE:O	2:O:422:LYS:HE3	1.99	0.62
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.81	0.62
1:N:249:PRO:HG2	1:N:250:VAL:H	1.62	0.62
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.64	0.62
8:H:40:CYS:O	8:H:44:VAL:HG23	2.00	0.62
3:P:67:VAL:HG12	16:P:3011:GOL:H31	1.82	0.62
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.35	0.62
5:R:96:LEU:HD12	5:R:135:LEU:O	2.00	0.62
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.81	0.62
2:B:417:PHE:O	2:B:422:LYS:HE3	1.99	0.61
2:O:424:MET:HG2	2:O:425:ALA:N	2.15	0.61
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.22	0.61
2:B:21:ALA:O	2:B:22:GLU:HB2	1.99	0.61
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.82	0.61
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.30	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.35	0.61
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.82	0.61
5:R:165:TYR:HA	5:R:170:ARG:O	2.00	0.61
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.61
2:O:219:VAL:O	2:O:223:PHE:HB2	1.99	0.61
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.00	0.61
1:A:191:LYS:O	1:A:195:MET:HG3	1.99	0.61
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.83	0.61
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.15	0.61
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.65	0.61
3:P:70:THR:HA	3:P:74:VAL:HG23	1.82	0.61
5:R:129:LYS:HB3	5:R:131:GLU:OE1	1.99	0.61
3:C:347:PRO:O	3:C:350:ILE:HG22	2.01	0.61
14:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.01	0.61
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.40	0.61
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.30	0.61
2:O:374:THR:HG22	2:O:376:GLN:H	1.65	0.61
3:P:49:GLY:C	11:P:501:HEM:HAC	2.21	0.61
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.66	0.61
2:O:338:ARG:HG3	2:O:338:ARG:NH1	2.16	0.61
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.36	0.61
5:R:69:LEU:O	5:R:72:SER:HB3	2.00	0.61
3:P:199:THR:HA	18:P:2010:BOG:O1	2.01	0.61
3:C:127:THR:HG21	11:C:501:HEM:HBB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.83	0.61
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.83	0.61
2:O:325:TYR:HD1	9:V:60:ALA:HB3	1.64	0.61
7:T:77:TYR:C	7:T:79:ASN:H	2.04	0.61
1:A:178:THR:HG22	1:A:179:ARG:N	2.14	0.60
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.36	0.60
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.16	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.36	0.60
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.83	0.60
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.82	0.60
3:P:9:HIS:HD2	3:P:12:LEU:H	1.49	0.60
5:R:148:ALA:HB2	5:R:156:TYR:CD2	2.36	0.60
2:B:292:THR:O	2:B:292:THR:HG22	2.02	0.60
2:B:341:MET:HE3	2:B:417:PHE:HE2	1.65	0.60
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.84	0.60
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.37	0.60
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.84	0.60
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.04	0.60
2:B:399:ALA:O	2:B:402:ILE:HG22	2.01	0.60
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.36	0.60
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.37	0.60
2:B:325:TYR:HD2	2:B:326:THR:N	1.99	0.60
2:O:295:LEU:O	2:O:299:VAL:HG23	2.02	0.60
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.16	0.60
1:A:406:MET:O	1:A:410:VAL:HG23	2.01	0.60
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.82	0.60
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.37	0.60
2:B:201:SER:OG	2:B:228:SER:HA	2.00	0.60
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.67	0.60
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.28	0.59
8:H:18:THR:O	8:H:22:GLU:HG3	2.02	0.59
2:B:31:ASN:HD22	2:B:31:ASN:N	2.00	0.59
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.02	0.59
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.84	0.59
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.36	0.59
2:O:341:MET:HE3	2:O:417:PHE:CE2	2.37	0.59
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.67	0.59
6:S:32:MET:HE3	6:S:87:LYS:HB2	1.83	0.59
9:V:30:UNK:HG3	9:V:31:UNK:N	2.17	0.59
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.33	0.59
8:H:27:THR:HG22	8:H:29:LYS:H	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.41	0.59
1:N:178:THR:HG22	1:N:179:ARG:N	2.17	0.59
8:U:62:LEU:O	8:U:66:ASP:HB2	2.02	0.59
1:A:156:THR:HA	5:E:7:VAL:HG21	1.84	0.59
1:A:371:GLY:O	1:A:375:VAL:HG23	2.02	0.59
1:A:332:ASP:HB2	1:A:430:GLN:HG2	1.83	0.59
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.37	0.59
2:O:341:MET:CE	2:O:417:PHE:HE2	2.15	0.59
2:O:402:ILE:HD13	2:O:402:ILE:C	2.23	0.59
3:P:22:LEU:HD21	13:P:3002:UQ:HM32	1.84	0.59
2:B:248:ASN:ND2	2:B:250:HIS:H	2.01	0.59
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.36	0.59
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.17	0.59
2:B:424:MET:HG2	2:B:425:ALA:N	2.17	0.59
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.33	0.59
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.37	0.59
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.50	0.59
2:B:341:MET:CE	2:B:417:PHE:HE2	2.16	0.59
3:C:9:HIS:HD2	3:C:12:LEU:H	1.50	0.59
1:N:317:THR:HG23	1:N:318:GLY:N	2.18	0.59
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.03	0.59
5:R:187:PHE:O	5:R:188:VAL:HG13	2.03	0.59
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.67	0.59
2:O:248:ASN:HD22	2:O:249:GLY:N	2.00	0.59
10:W:14:PHE:N	10:W:14:PHE:CD2	2.69	0.59
2:B:97:SER:HB3	9:I:69:SER:HA	1.85	0.58
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.38	0.58
2:O:239:TYR:HE2	2:O:241:GLY:CA	2.16	0.58
13:P:3002:UQ:HM51	13:P:3002:UQ:C8	2.33	0.58
1:A:64:PHE:HA	1:A:75:PHE:HE2	1.68	0.58
2:B:327:ILE:HD11	9:I:58:ARG:O	2.04	0.58
2:O:71:LEU:O	2:O:74:PRO:HD2	2.02	0.58
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.03	0.58
5:R:82:PRO:O	5:R:100:HIS:HB3	2.03	0.58
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.84	0.58
13:C:2002:UQ:HM51	13:C:2002:UQ:C8	2.33	0.58
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.18	0.58
3:P:31:TRP:O	3:P:101:ARG:HG3	2.03	0.58
3:C:245:LEU:O	4:D:201:ARG:HD3	2.03	0.58
1:N:406:MET:O	1:N:410:VAL:HG23	2.03	0.58
1:N:439:SER:HA	1:N:442:TYR:CE2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:28:GLU:O	8:U:32:LYS:HG3	2.04	0.58
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.32	0.58
1:A:362:ARG:O	1:A:365:MET:HG2	2.03	0.58
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.86	0.58
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.33	0.58
8:H:27:THR:O	8:H:31:VAL:HG23	2.02	0.58
2:O:207:VAL:HG12	2:O:208:GLY:N	2.18	0.58
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.85	0.58
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.18	0.58
2:B:207:VAL:HG12	2:B:208:GLY:N	2.18	0.58
2:B:262:ALA:O	2:B:320:GLY:HA3	2.03	0.58
4:Q:24:SER:OG	10:W:55:ILE:HG21	2.04	0.58
5:E:102:THR:HB	5:E:103:GLN:OE1	2.03	0.58
1:N:38:GLY:HA3	1:N:98:TYR:HA	1.86	0.58
3:P:142:TRP:O	3:P:146:VAL:HG23	2.03	0.58
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.39	0.58
2:O:292:THR:O	2:O:292:THR:HG22	2.02	0.58
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.38	0.58
10:W:56:LYS:HG2	10:W:60:GLU:OE1	2.03	0.58
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.85	0.57
3:P:127:THR:HG21	11:P:501:HEM:HBB2	1.85	0.57
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.85	0.57
8:U:40:CYS:O	8:U:44:VAL:HG23	2.03	0.57
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.69	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.85	0.57
2:B:26:ILE:HG12	2:B:26:ILE:O	2.03	0.57
8:H:34:ARG:HD2	8:H:38:GLU:OE2	2.05	0.57
9:I:31:UNK:C	9:I:73:PRO:HG2	2.33	0.57
1:N:342:TRP:O	1:N:345:LEU:HB2	2.03	0.57
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.70	0.57
3:P:145:THR:O	3:P:149:ASN:HB2	2.04	0.57
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.67	0.57
2:B:259:THR:HG22	2:B:260:GLU:N	2.19	0.57
2:B:407:SER:O	2:B:411:VAL:HG23	2.04	0.57
5:E:29:SER:HA	5:E:32:ARG:NH2	2.19	0.57
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.35	0.57
1:N:117:VAL:HG23	1:N:118:GLN:N	2.20	0.57
3:P:40:VAL:HA	3:P:43:MET:HE3	1.87	0.57
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.87	0.57
5:E:136:VAL:O	5:E:138:VAL:N	2.36	0.57
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:O	1:A:109:VAL:HG23	2.04	0.57
8:H:10:GLU:O	8:H:11:GLU:HG3	2.04	0.57
1:N:50:GLU:HB2	1:N:165:ARG:HH21	1.67	0.57
2:O:57:TYR:N	2:O:57:TYR:CD1	2.73	0.57
2:O:97:SER:HB3	9:V:69:SER:HA	1.85	0.57
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.40	0.57
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.33	0.57
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.69	0.57
2:B:46:ARG:HG3	2:B:379:LEU:HD22	1.87	0.57
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.40	0.57
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.86	0.57
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.40	0.57
5:R:29:SER:HA	5:R:32:ARG:NH2	2.19	0.57
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.20	0.57
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.19	0.57
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.53	0.57
7:T:80:ASP:HB3	8:U:47:ARG:NH1	2.14	0.57
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.34	0.56
2:O:259:THR:HG22	2:O:260:GLU:N	2.20	0.56
5:R:118:ARG:NH2	5:R:174:GLY:O	2.38	0.56
2:B:71:LEU:O	2:B:74:PRO:HD2	2.05	0.56
2:B:76:THR:HG22	2:B:81:SER:HA	1.87	0.56
8:H:62:LEU:O	8:H:66:ASP:HB2	2.05	0.56
3:P:236:MET:O	3:P:239:PRO:HD2	2.05	0.56
3:P:347:PRO:O	3:P:350:ILE:HG22	2.04	0.56
5:R:78:LEU:HB3	5:R:132:TRP:HZ2	1.65	0.56
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.40	0.56
1:A:402:VAL:HG22	1:A:406:MET:CE	2.34	0.56
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.86	0.56
2:B:239:TYR:HE2	2:B:241:GLY:CA	2.18	0.56
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.88	0.56
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.88	0.56
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.87	0.56
3:C:70:THR:HA	3:C:74:VAL:HG23	1.87	0.56
3:C:329:LEU:O	3:C:332:ASN:HB3	2.05	0.56
7:G:81:GLN:HA	8:H:47:ARG:CG	2.34	0.56
3:P:329:LEU:O	3:P:332:ASN:HB3	2.04	0.56
8:U:18:THR:O	8:U:22:GLU:HG3	2.04	0.56
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.87	0.56
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.71	0.56
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
3:C:247:SER:OG	3:C:250:LEU:HB2	2.06	0.56
1:A:137:GLU:O	1:A:141:MET:HG3	2.05	0.56
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.40	0.56
5:R:136:VAL:O	5:R:138:VAL:N	2.38	0.56
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.41	0.56
1:N:307:PHE:CD1	1:N:307:PHE:C	2.78	0.56
10:W:60:GLU:O	10:W:61:ALA:HB2	2.06	0.56
3:C:350:ILE:HG23	3:C:351:ILE:N	2.21	0.56
5:E:178:TYR:H	5:E:178:TYR:HD1	1.54	0.56
5:E:187:PHE:C	5:E:189:GLY:H	2.07	0.56
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.05	0.56
10:W:40:ASP:O	10:W:44:GLU:HG3	2.05	0.56
3:C:222:HIS:HA	3:C:226:SER:OG	2.06	0.56
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.20	0.56
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.40	0.56
1:N:137:GLU:O	1:N:141:MET:HG3	2.06	0.56
1:N:402:VAL:HG22	1:N:406:MET:CE	2.36	0.56
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.88	0.56
2:O:357:VAL:O	2:O:361:LYS:HG3	2.06	0.56
2:O:414:ALA:O	2:O:418:VAL:HG23	2.06	0.56
9:V:59:SER:O	9:V:60:ALA:C	2.43	0.56
2:B:23:ASP:OD1	2:B:24:LEU:N	2.39	0.56
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.21	0.56
1:N:64:PHE:HA	1:N:75:PHE:HE2	1.71	0.56
1:N:170:THR:CG2	1:N:171:THR:H	2.15	0.56
2:O:27:THR:CG2	2:O:28:LYS:N	2.69	0.56
3:P:61:SER:O	3:P:62:LEU:HD23	2.06	0.56
6:S:100:GLU:O	6:S:103:GLU:HB3	2.05	0.56
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.41	0.55
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.88	0.55
5:E:131:GLU:H	5:E:131:GLU:CD	2.09	0.55
2:O:407:SER:O	2:O:411:VAL:HG23	2.06	0.55
5:R:29:SER:HA	5:R:32:ARG:HH21	1.71	0.55
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.22	0.55
6:S:58:ARG:HG3	6:S:89:TYR:OH	2.06	0.55
2:B:306:PRO:HB3	9:I:52:ARG:N	2.21	0.55
6:F:104:ARG:HA	2:O:83:PHE:CE2	2.41	0.55
1:N:281:ASP:OD2	9:V:33:UNK:HB1	2.07	0.55
8:U:21:ARG:HH11	8:U:21:ARG:HG3	1.71	0.55
1:A:327:ASP:HB3	1:A:328:PRO:HD2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.89	0.55
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.88	0.55
5:E:133:VAL:O	5:E:133:VAL:HG13	2.06	0.55
3:P:198:LEU:HD21	11:P:502:HEM:HMA3	1.88	0.55
3:P:247:SER:OG	3:P:250:LEU:HB2	2.07	0.55
4:D:62:LYS:O	4:D:66:GLU:HG3	2.05	0.55
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.06	0.55
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.21	0.55
2:O:325:TYR:CD1	9:V:60:ALA:N	2.75	0.55
3:P:125:MET:HE1	12:P:3001:IKR:I1	2.75	0.55
1:A:49:ASN:ND2	1:A:51:LYS:H	2.05	0.55
1:A:117:VAL:HG23	1:A:118:GLN:H	1.70	0.55
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.89	0.55
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.41	0.55
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.42	0.55
2:O:306:PRO:CG	9:V:51:CYS:HA	2.37	0.55
3:C:377:MET:CE	6:F:20:TYR:HB2	2.32	0.55
5:E:147:ILE:O	5:E:156:TYR:HA	2.06	0.55
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.37	0.55
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.07	0.55
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.89	0.55
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.88	0.55
4:Q:211:ILE:HG12	10:W:35:PHE:CZ	2.42	0.55
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.37	0.55
3:C:236:MET:O	3:C:239:PRO:HD2	2.06	0.55
5:E:52:LYS:C	5:E:52:LYS:HD3	2.27	0.55
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.89	0.55
8:U:43:ARG:O	8:U:47:ARG:HG3	2.06	0.55
3:C:49:GLY:C	11:C:501:HEM:HAC	2.26	0.55
4:D:97:ASN:HB2	4:D:99:GLU:OE1	2.06	0.55
2:O:402:ILE:HD13	2:O:402:ILE:O	2.06	0.55
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.37	0.55
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.07	0.55
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.07	0.55
7:T:29:ILE:O	7:T:34:LEU:HG	2.07	0.55
1:A:40:TRP:CZ3	1:A:198:ALA:HB3	2.43	0.55
1:A:178:THR:CG2	1:A:179:ARG:N	2.69	0.55
3:C:377:MET:HE2	6:F:20:TYR:CB	2.33	0.55
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.07	0.55
2:O:56:ARG:NH1	2:O:56:ARG:HG3	2.22	0.55
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:OD2	1:A:284:PHE:HE1	1.90	0.54
2:B:357:VAL:O	2:B:361:LYS:HG3	2.06	0.54
8:H:28:GLU:O	8:H:32:LYS:HG3	2.07	0.54
10:J:14:PHE:CD2	10:J:14:PHE:N	2.71	0.54
1:N:63:ALA:O	1:N:116:VAL:HG13	2.07	0.54
5:R:133:VAL:O	5:R:133:VAL:HG13	2.07	0.54
1:A:106:MET:HE2	1:A:107:PRO:HA	1.87	0.54
2:B:28:LYS:O	2:B:29:LEU:O	2.25	0.54
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.89	0.54
1:N:61:HIS:NE2	2:O:287:ARG:NE	2.55	0.54
3:P:222:HIS:HA	3:P:226:SER:OG	2.06	0.54
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.39	0.54
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.47	0.54
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.71	0.54
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.42	0.54
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.28	0.54
2:B:402:ILE:HD13	2:B:402:ILE:C	2.27	0.54
5:E:127:VAL:CG1	5:E:128:LYS:H	1.99	0.54
7:G:59:TYR:O	7:G:63:THR:HB	2.07	0.54
1:N:58:PHE:HB3	1:N:182:LEU:HD21	1.88	0.54
2:B:140:LEU:C	2:B:142:PRO:HD2	2.28	0.54
4:D:65:ALA:O	4:D:85:GLY:HA3	2.07	0.54
5:E:155:GLY:HA3	5:E:166:ASP:O	2.08	0.54
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.71	0.54
1:N:417:ASP:O	1:N:438:ARG:NH2	2.40	0.54
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.88	0.54
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.23	0.54
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.72	0.54
5:E:109:GLU:HB2	5:E:167:ALA:HB3	1.89	0.54
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.90	0.54
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.72	0.54
4:D:37:CYS:C	4:D:39:ALA:H	2.09	0.54
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.88	0.54
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.89	0.54
2:O:181:TYR:CE1	2:O:182:ARG:CG	2.90	0.54
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.90	0.54
3:C:120:LEU:HD13	11:C:502:HEM:CAB	2.35	0.54
3:C:142:TRP:O	3:C:146:VAL:HG23	2.08	0.54
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.56	0.54
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.08	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:THR:CG2	1:N:179:ARG:N	2.70	0.54
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.23	0.54
8:H:35:GLU:O	8:H:39:LEU:HG	2.08	0.54
2:O:162:ASN:O	2:O:244:ILE:HD12	2.08	0.54
3:P:23:PRO:HG3	7:T:4:PHE:CD1	2.43	0.54
3:P:155:PRO:O	3:P:156:TYR:HB2	2.08	0.54
5:R:141:HIS:HB3	19:R:501:FES:S2	2.48	0.54
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.22	0.54
2:B:365:LYS:O	2:B:369:LEU:HG	2.08	0.54
3:C:332:ASN:ND2	3:C:358:SER:OG	2.41	0.54
1:N:362:ARG:O	1:N:365:MET:HG2	2.07	0.54
5:R:178:TYR:N	5:R:178:TYR:CD1	2.75	0.54
8:U:27:THR:HG22	8:U:29:LYS:H	1.73	0.54
1:A:342:TRP:O	1:A:345:LEU:HB2	2.08	0.54
5:E:130:PRO:HG2	5:E:131:GLU:H	1.73	0.54
9:I:63:ASP:CG	9:I:64:LEU:H	2.12	0.54
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.89	0.54
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.43	0.54
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.72	0.54
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.89	0.54
1:A:242:ARG:O	7:G:14:ILE:HA	2.07	0.53
2:B:31:ASN:N	2:B:31:ASN:ND2	2.54	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.22	0.53
9:I:63:ASP:O	9:I:64:LEU:HB2	2.07	0.53
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.38	0.53
2:B:312:PHE:HE1	9:I:62:ARG:O	1.91	0.53
9:I:49:LEU:O	9:I:50:LEU:HD23	2.09	0.53
9:I:55:MET:O	9:I:58:ARG:HB2	2.07	0.53
2:O:46:ARG:HG3	2:O:46:ARG:O	2.07	0.53
5:R:148:ALA:O	5:R:149:ASN:HB2	2.09	0.53
8:U:34:ARG:HD2	8:U:38:GLU:OE2	2.09	0.53
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.37	0.53
5:E:29:SER:HA	5:E:32:ARG:HH21	1.74	0.53
1:N:351:GLU:O	1:N:354:VAL:HG22	2.08	0.53
1:A:307:PHE:CD1	1:A:307:PHE:C	2.81	0.53
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.11	0.53
1:N:239:SER:HB2	7:T:17:SER:O	2.08	0.53
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.43	0.53
3:P:40:VAL:HA	3:P:43:MET:CE	2.38	0.53
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.90	0.53
2:B:312:PHE:CE1	9:I:62:ARG:O	2.61	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.23	0.53
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.72	0.53
5:R:78:LEU:HB2	5:R:191:ASP:HA	1.91	0.53
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.09	0.53
1:A:102:LEU:HD13	1:A:105:ASP:OD2	2.09	0.53
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.43	0.53
2:B:110:GLU:O	2:B:111:CYS:HB3	2.09	0.53
2:B:248:ASN:HD22	2:B:249:GLY:N	2.06	0.53
2:B:359:LYS:O	2:B:363:GLN:HG3	2.07	0.53
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.43	0.53
1:N:32:GLN:OE1	2:O:373:GLU:HG2	2.08	0.53
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.90	0.53
5:R:76:ILE:O	5:R:193:VAL:HG12	2.08	0.53
5:R:126:ARG:NH2	5:R:169:GLY:O	2.40	0.53
8:U:52:GLU:HG3	8:U:53:GLN:N	2.24	0.53
1:A:7:THR:O	1:A:11:ILE:HG13	2.09	0.53
3:C:23:PRO:HG3	7:G:4:PHE:CE1	2.44	0.53
3:C:34:PHE:HB2	20:C:381:HOH:O	2.08	0.53
6:F:53:ASP:OD1	6:F:54:LEU:N	2.42	0.53
2:O:140:LEU:C	2:O:142:PRO:HD2	2.29	0.53
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.44	0.53
4:Q:235:MET:CE	6:S:64:ARG:HA	2.39	0.53
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.88	0.53
4:Q:147:LEU:C	4:Q:148:HIS:HD2	2.13	0.53
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.44	0.53
5:E:163:SER:HA	5:E:174:GLY:HA3	1.90	0.53
2:O:221:GLU:HG3	2:O:222:GLN:N	2.24	0.53
2:O:248:ASN:C	2:O:248:ASN:ND2	2.59	0.53
5:R:98:VAL:HG22	5:R:134:ILE:HG12	1.90	0.53
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.90	0.52
2:B:70:ARG:HG3	2:B:98:VAL:CG1	2.39	0.52
4:Q:220:TYR:CE2	14:Q:3003:CDL:H722	2.44	0.52
5:R:79:SER:OG	5:R:191:ASP:HB2	2.08	0.52
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.24	0.52
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.91	0.52
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.44	0.52
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.52
1:N:276:ILE:HG12	1:N:357:ALA:HB2	1.90	0.52
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.52
2:B:239:TYR:HD1	2:B:260:GLU:OE1	1.91	0.52
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:VAL:C	3:C:164:TRP:H	2.12	0.52
3:C:285:ILE:HB	3:C:291:GLY:HA2	1.90	0.52
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.43	0.52
4:Q:16:GLY:CA	4:Q:19:SER:OG	2.57	0.52
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.91	0.52
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.74	0.52
2:B:333:ALA:O	2:B:337:ILE:HG13	2.09	0.52
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.09	0.52
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.44	0.52
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.45	0.52
3:C:9:HIS:CD2	3:C:11:LEU:H	2.27	0.52
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.90	0.52
2:B:303:THR:HA	2:B:335:GLU:OE1	2.08	0.52
3:C:279:TYR:O	3:C:283:ARG:HG3	2.09	0.52
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.44	0.52
2:O:274:VAL:O	2:O:278:VAL:HG23	2.10	0.52
3:P:287:ASN:O	3:P:288:LYS:C	2.46	0.52
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.34	0.52
6:S:12:LEU:C	6:S:14:ASP:H	2.12	0.52
7:T:28:ASN:HB2	7:T:32:ASP:HB3	1.91	0.52
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.24	0.52
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.40	0.52
3:C:287:ASN:O	3:C:288:LYS:C	2.48	0.52
5:E:58:PHE:O	5:E:61:SER:HB3	2.09	0.52
5:E:95:PRO:HG2	5:E:145:VAL:HG11	1.90	0.52
1:N:7:THR:O	1:N:11:ILE:HG13	2.10	0.52
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.38	0.52
2:O:303:THR:HA	2:O:335:GLU:OE1	2.09	0.52
3:P:9:HIS:CD2	3:P:12:LEU:H	2.27	0.52
5:E:84:GLY:CA	5:E:102:THR:HG23	2.39	0.52
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.31	0.52
1:N:117:VAL:HG23	1:N:118:GLN:H	1.74	0.52
1:N:133:VAL:O	1:N:137:GLU:HG3	2.10	0.52
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.92	0.52
2:O:76:THR:HG22	2:O:81:SER:HA	1.92	0.52
2:O:105:MET:HE2	2:O:107:TYR:HE1	1.75	0.52
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.91	0.52
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.40	0.52
1:A:317:THR:HG23	1:A:318:GLY:N	2.25	0.52
2:B:274:VAL:O	2:B:278:VAL:HG23	2.10	0.52
3:C:9:HIS:CD2	3:C:12:LEU:H	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:PRO:HG3	7:G:4:PHE:CD1	2.45	0.52
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.45	0.52
1:N:45:SER:HA	1:N:48:GLU:HG3	1.92	0.52
2:O:96:LEU:HD12	2:O:97:SER:N	2.25	0.52
2:O:156:GLN:NE2	9:V:77:ARG:C	2.63	0.52
3:C:92:PHE:O	3:C:95:ILE:HG22	2.10	0.52
8:H:21:ARG:O	8:H:25:GLU:HG3	2.10	0.52
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.91	0.52
1:N:23:LEU:HA	1:N:192:ALA:O	2.10	0.52
3:P:198:LEU:HD13	13:P:3002:UQ:HM53	1.92	0.52
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.44	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.52
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.39	0.51
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.22	0.51
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.40	0.51
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.45	0.51
2:O:305:GLN:HB3	2:O:306:PRO:HD2	1.92	0.51
8:U:35:GLU:O	8:U:39:LEU:HG	2.09	0.51
3:C:246:PHE:C	3:C:248:PRO:HD3	2.30	0.51
1:N:81:SER:HB3	2:O:359:LYS:HD3	1.93	0.51
1:N:281:ASP:HB3	9:V:33:UNK:HB2	1.91	0.51
3:P:120:LEU:HD13	11:P:502:HEM:HAB	1.91	0.51
3:C:365:ILE:O	3:C:368:PRO:HG2	2.09	0.51
1:N:4:TYR:HB2	2:O:114:ASP:OD1	2.11	0.51
5:R:169:GLY:O	5:R:179:ASN:HB3	2.11	0.51
6:S:58:ARG:HG3	6:S:58:ARG:HH11	1.76	0.51
2:B:46:ARG:HG3	2:B:46:ARG:O	2.10	0.51
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.51
2:O:170:THR:O	2:O:172:LEU:N	2.43	0.51
3:P:182:LEU:O	3:P:186:LEU:HG	2.10	0.51
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.91	0.51
5:E:189:GLY:O	5:E:192:LEU:O	2.28	0.51
6:F:58:ARG:HG3	6:F:89:TYR:OH	2.11	0.51
1:N:354:VAL:HG23	1:N:355:LYS:N	2.26	0.51
3:P:246:PHE:C	3:P:248:PRO:HD3	2.31	0.51
5:E:76:ILE:O	5:E:193:VAL:HG12	2.11	0.51
5:E:139:CYS:SG	5:E:176:ALA:HB2	2.50	0.51
8:H:43:ARG:HD2	8:H:47:ARG:NH2	2.26	0.51
2:O:46:ARG:HG3	2:O:379:LEU:HD22	1.91	0.51
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.93	0.51
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:O	1:A:137:GLU:HG3	2.10	0.51
2:B:215:ASP:O	2:B:219:VAL:HG23	2.11	0.51
1:N:106:MET:CG	1:N:203:ILE:HD13	2.39	0.51
1:A:61:HIS:NE2	2:B:287:ARG:NE	2.59	0.51
1:A:108:LYS:O	1:A:108:LYS:HG3	2.11	0.51
1:A:281:ASP:OD2	9:I:33:UNK:HG2	2.11	0.51
4:D:57:THR:HG22	4:D:58:GLU:N	2.26	0.51
3:P:23:PRO:HG3	7:T:4:PHE:CE1	2.46	0.51
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.45	0.51
5:R:52:LYS:C	5:R:52:LYS:HD3	2.30	0.51
1:A:23:LEU:HD23	1:A:24:ARG:N	2.26	0.51
2:B:56:ARG:HA	2:B:171:ALA:O	2.11	0.51
2:B:124:LEU:O	2:B:128:THR:HG23	2.10	0.51
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.93	0.51
2:B:270:ASN:ND2	2:B:270:ASN:N	2.49	0.51
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.75	0.51
3:C:5:ILE:O	3:C:5:ILE:HG22	2.11	0.51
5:E:109:GLU:CB	5:E:167:ALA:HB3	2.41	0.51
5:E:171:ILE:HG12	5:E:176:ALA:O	2.10	0.51
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.93	0.51
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.22	0.51
9:V:55:MET:HA	9:V:58:ARG:HG3	1.92	0.51
2:B:372:VAL:O	2:B:372:VAL:HG12	2.11	0.51
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.92	0.51
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.46	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.46	0.51
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.26	0.51
1:A:75:PHE:O	1:A:79:VAL:HG23	2.11	0.50
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.47	0.50
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.46	0.50
2:O:268:GLU:HG2	2:O:268:GLU:O	2.10	0.50
2:O:279:LEU:O	2:O:295:LEU:HB3	2.11	0.50
2:O:308:ASP:CG	9:V:56:SER:HA	2.31	0.50
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.44	0.50
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.92	0.50
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.46	0.50
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.47	0.50
2:B:21:ALA:O	2:B:22:GLU:CB	2.60	0.50
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.47	0.50
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.50
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.93	0.50
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.46	0.50
1:N:87:ASN:CG	1:N:88:GLY:H	2.14	0.50
2:O:26:ILE:O	2:O:26:ILE:HG12	2.10	0.50
4:Q:26:VAL:CG2	4:Q:188:THR:HG22	2.41	0.50
4:Q:197:GLU:O	4:Q:198:HIS:C	2.50	0.50
4:Q:235:MET:HE1	6:S:64:ARG:N	2.27	0.50
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.29	0.50
8:U:21:ARG:O	8:U:25:GLU:HG3	2.12	0.50
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.77	0.50
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.41	0.50
4:D:197:GLU:O	4:D:198:HIS:C	2.50	0.50
4:Q:148:HIS:N	4:Q:148:HIS:CD2	2.79	0.50
6:S:32:MET:CE	6:S:87:LYS:H	2.23	0.50
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.93	0.50
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.46	0.50
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.74	0.50
4:D:143:VAL:HG21	4:D:149:TYR:HB2	1.94	0.50
5:E:185:TYR:O	5:E:186:GLN:HB3	2.12	0.50
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.93	0.50
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.93	0.50
4:D:26:VAL:CG2	4:D:188:THR:HG22	2.42	0.50
5:R:53:ASN:O	5:R:56:THR:HB	2.10	0.50
6:S:13:MET:CA	6:S:16:ILE:HB	2.41	0.50
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.14	0.50
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.93	0.50
7:G:36:ASN:O	7:G:40:ARG:HG3	2.12	0.50
1:N:102:LEU:HD13	1:N:105:ASP:OD2	2.11	0.50
1:N:436:ARG:NH1	3:P:220:PRO:HB2	2.26	0.50
2:O:62:ASN:O	2:O:65:THR:CG2	2.57	0.50
3:P:162:VAL:C	3:P:164:TRP:H	2.14	0.50
4:Q:221:TYR:CE2	5:R:39:VAL:HG21	2.47	0.50
5:R:114:VAL:O	5:R:114:VAL:HG12	2.12	0.50
5:R:155:GLY:HA3	5:R:166:ASP:O	2.11	0.50
6:S:16:ILE:O	6:S:19:TRP:HB3	2.12	0.50
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.50
3:C:271:PRO:HB2	3:C:275:PHE:HB2	1.94	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.50
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.27	0.50
1:N:106:MET:HE2	1:N:107:PRO:HA	1.92	0.50
4:Q:34:LYS:O	4:Q:34:LYS:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.11	0.50
2:B:146:VAL:HG12	2:B:147:ASP:N	2.27	0.50
3:C:145:THR:O	3:C:149:ASN:HB2	2.12	0.50
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.10	0.50
4:D:148:HIS:CD2	4:D:148:HIS:N	2.80	0.50
4:D:223:LYS:C	4:D:223:LYS:HD3	2.32	0.50
5:E:84:GLY:N	5:E:102:THR:HG23	2.26	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.50
1:N:158:PHE:O	1:N:164:ALA:HB2	2.12	0.50
3:P:184:PHE:O	3:P:184:PHE:HD2	1.95	0.50
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.47	0.50
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.12	0.49
9:I:32:UNK:N	9:I:73:PRO:CG	2.75	0.49
3:P:142:TRP:HB3	3:P:269:ILE:HD13	1.94	0.49
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.12	0.49
4:Q:203:ARG:HD3	18:Q:3009:BOG:O6	2.12	0.49
1:A:103:SER:HB3	1:A:202:GLY:O	2.12	0.49
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.49
2:O:31:ASN:N	2:O:31:ASN:ND2	2.60	0.49
2:O:67:HIS:O	2:O:70:ARG:HB3	2.13	0.49
3:P:9:HIS:CD2	3:P:11:LEU:H	2.31	0.49
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.32	0.49
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.94	0.49
2:B:96:LEU:HB3	9:I:70:LEU:HD22	1.94	0.49
2:B:181:TYR:CE1	2:B:182:ARG:CG	2.95	0.49
4:D:148:HIS:CE1	4:D:161:ALA:HB2	2.48	0.49
5:E:187:PHE:C	5:E:189:GLY:N	2.66	0.49
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.12	0.49
2:O:333:ALA:O	2:O:337:ILE:HG13	2.12	0.49
3:P:332:ASN:ND2	3:P:358:SER:OG	2.43	0.49
6:S:13:MET:HA	6:S:16:ILE:HD12	1.93	0.49
1:A:23:LEU:HA	1:A:192:ALA:O	2.13	0.49
2:B:248:ASN:C	2:B:248:ASN:ND2	2.62	0.49
1:N:242:ARG:O	7:T:14:ILE:HA	2.12	0.49
1:N:361:LEU:O	1:N:364:ALA:HB3	2.12	0.49
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.30	0.49
4:Q:70:VAL:CG2	4:Q:83:ARG:CZ	2.90	0.49
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.12	0.49
5:E:84:GLY:N	5:E:100:HIS:O	2.40	0.49
5:E:98:VAL:HG22	5:E:134:ILE:HG12	1.95	0.49
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:PHE:O	7:G:35:PRO:HD3	2.11	0.49
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.28	0.49
1:N:37:VAL:HG12	1:N:199:ALA:HA	1.95	0.49
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.48	0.49
2:O:272:PHE:O	2:O:276:GLN:N	2.44	0.49
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.95	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.95	0.49
4:Q:181:GLN:CA	8:U:77:LEU:HD22	2.42	0.49
7:T:30:PHE:CD2	7:T:34:LEU:HD12	2.47	0.49
8:U:73:LEU:HD12	8:U:73:LEU:O	2.12	0.49
1:A:63:ALA:O	1:A:116:VAL:HG13	2.12	0.49
1:A:293:ARG:HD3	1:A:344:ARG:NH1	2.27	0.49
1:N:212:ALA:O	1:N:216:PHE:HB2	2.13	0.49
1:N:293:ARG:O	1:N:297:LEU:HG	2.13	0.49
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.95	0.49
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.77	0.49
1:A:37:VAL:HG12	1:A:199:ALA:HA	1.93	0.49
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.93	0.49
2:O:306:PRO:HB3	9:V:52:ARG:N	2.27	0.49
10:W:60:GLU:O	10:W:60:GLU:HG3	2.12	0.49
1:A:161:THR:HG21	1:A:235:ARG:H	1.78	0.49
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.93	0.49
2:B:62:ASN:O	2:B:65:THR:CG2	2.60	0.49
2:B:325:TYR:HD1	9:I:60:ALA:CB	2.26	0.49
3:C:172:ASP:C	3:C:174:PRO:HD2	2.32	0.49
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.77	0.49
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.43	0.49
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.49
2:O:341:MET:CE	2:O:417:PHE:CE2	2.95	0.49
2:B:73:SER:OG	2:B:74:PRO:HD3	2.13	0.49
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.78	0.49
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.77	0.49
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.95	0.49
4:D:235:MET:HE2	6:F:64:ARG:HA	1.94	0.49
1:N:10:ASN:OD1	2:O:19:PRO:HD2	2.13	0.49
1:N:223:TYR:H	1:N:223:TYR:HD2	1.61	0.49
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.42	0.49
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.95	0.49
1:A:23:LEU:HB2	1:A:192:ALA:HB1	1.94	0.48
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.94	0.48
1:A:223:TYR:H	1:A:223:TYR:HD2	1.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:CG2	2:B:151:ALA:N	2.76	0.48
3:P:285:ILE:HB	3:P:291:GLY:HA2	1.95	0.48
6:S:96:GLU:OE1	6:S:99:ARG:NH2	2.46	0.48
1:A:15:ASN:O	1:A:26:ALA:HA	2.13	0.48
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.95	0.48
2:B:46:ARG:CD	2:B:110:GLU:HG2	2.44	0.48
2:B:147:ASP:O	2:B:150:VAL:HG22	2.13	0.48
4:D:57:THR:HB	4:D:60:GLU:HG3	1.93	0.48
4:D:70:VAL:CG2	4:D:83:ARG:CZ	2.91	0.48
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.28	0.48
7:T:59:TYR:O	7:T:63:THR:HB	2.14	0.48
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.53	0.48
1:A:354:VAL:HG23	1:A:355:LYS:N	2.28	0.48
3:C:2:ALA:HB1	3:C:3:PRO:HD2	1.96	0.48
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.48
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.48	0.48
8:H:10:GLU:C	8:H:11:GLU:HG3	2.34	0.48
3:P:70:THR:HA	3:P:74:VAL:CG2	2.43	0.48
3:P:125:MET:HE2	3:P:275:PHE:HE2	1.79	0.48
4:Q:35:GLN:NE2	4:Q:169:LEU:HD12	2.28	0.48
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.43	0.48
2:B:24:LEU:HG	2:B:24:LEU:O	2.13	0.48
3:C:207:ASN:ND2	3:C:208:ASN:H	2.11	0.48
4:Q:37:CYS:C	4:Q:39:ALA:H	2.17	0.48
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.45	0.48
7:T:46:PHE:O	7:T:50:PRO:HG2	2.13	0.48
8:U:34:ARG:HB2	8:U:61:PHE:CE1	2.48	0.48
1:N:108:LYS:HG3	1:N:108:LYS:O	2.12	0.48
2:O:345:LYS:O	2:O:349:GLN:HG3	2.13	0.48
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.28	0.48
8:U:48:SER:O	8:U:49:HIS:ND1	2.45	0.48
1:A:18:THR:HG23	1:A:24:ARG:HG3	1.94	0.48
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.14	0.48
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.48	0.48
2:O:46:ARG:CD	2:O:110:GLU:HG2	2.44	0.48
2:O:287:ARG:HA	9:V:53:GLU:HG3	1.95	0.48
3:P:5:ILE:O	3:P:5:ILE:HG22	2.14	0.48
3:P:271:PRO:HD2	3:P:279:TYR:CD2	2.48	0.48
1:A:38:GLY:HA3	1:A:98:TYR:HA	1.95	0.48
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.77	0.48
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.96	0.48
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.48	0.48
3:C:166:TRP:HA	3:C:175:THR:HG23	1.96	0.48
4:D:34:LYS:O	4:D:34:LYS:HG2	2.12	0.48
5:E:77:LYS:HE2	5:E:79:SER:OG	2.14	0.48
6:F:58:ARG:HG3	6:F:58:ARG:HH11	1.77	0.48
10:J:40:ASP:O	10:J:44:GLU:HG3	2.13	0.48
4:Q:97:ASN:HB2	4:Q:99:GLU:OE1	2.13	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:B:290:SER:O	2:B:297:GLN:HG2	2.14	0.48
4:D:47:ALA:N	4:D:50:ASN:HD22	2.03	0.48
5:E:161:HIS:HB2	19:E:501:FES:S1	2.54	0.48
2:O:166:ALA:HB1	2:O:242:GLY:C	2.34	0.48
2:O:193:HIS:O	2:O:197:ASN:ND2	2.46	0.48
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.78	0.48
1:A:53:ASN:N	1:A:173:ASN:HD22	2.11	0.48
1:A:170:THR:CG2	1:A:171:THR:H	2.23	0.48
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.49	0.48
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.96	0.48
3:C:142:TRP:HB3	3:C:269:ILE:HD13	1.95	0.48
4:D:37:CYS:C	4:D:39:ALA:N	2.67	0.48
1:N:15:ASN:O	1:N:26:ALA:HA	2.14	0.48
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.49	0.48
2:O:37:SER:HB3	2:O:213:HIS:CG	2.48	0.48
5:R:178:TYR:N	5:R:178:TYR:HD1	2.11	0.48
6:S:53:ASP:OD1	6:S:54:LEU:N	2.46	0.48
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.29	0.48
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.23	0.48
3:C:9:HIS:HB3	3:C:12:LEU:HB2	1.95	0.48
8:H:34:ARG:HB2	8:H:61:PHE:CE1	2.49	0.48
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.39	0.47
3:C:350:ILE:CG2	3:C:351:ILE:N	2.77	0.47
4:D:16:GLY:CA	4:D:19:SER:OG	2.62	0.47
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.18	0.47
1:N:94:GLN:NE2	1:N:381:SER:OG	2.37	0.47
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.44	0.47
3:P:132:TYR:O	3:P:135:PRO:HD2	2.14	0.47
3:P:138:GLN:O	3:P:142:TRP:HD1	1.97	0.47
7:T:30:PHE:O	7:T:35:PRO:HD3	2.14	0.47
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.96	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:TYR:N	5:E:178:TYR:CD1	2.82	0.47
6:F:71:LYS:O	6:F:72:HIS:HB2	2.14	0.47
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.13	0.47
1:N:53:ASN:N	1:N:173:ASN:HD22	2.12	0.47
1:N:382:HIS:HB3	1:N:388:ARG:O	2.13	0.47
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.48	0.47
2:O:150:VAL:CG2	2:O:151:ALA:N	2.77	0.47
3:P:261:ASN:HD21	3:P:264:VAL:HG23	1.78	0.47
5:R:78:LEU:HD13	5:R:132:TRP:HE1	1.76	0.47
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.96	0.47
2:O:146:VAL:HG12	2:O:147:ASP:N	2.28	0.47
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.95	0.47
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.44	0.47
1:A:170:THR:CG2	1:A:171:THR:N	2.78	0.47
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.96	0.47
2:B:279:LEU:O	2:B:295:LEU:HB3	2.13	0.47
3:C:31:TRP:O	3:C:101:ARG:HG3	2.14	0.47
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.95	0.47
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.49	0.47
5:E:82:PRO:O	5:E:100:HIS:HB3	2.14	0.47
2:O:122:TYR:O	2:O:126:VAL:HG23	2.15	0.47
2:O:156:GLN:HE22	9:V:77:ARG:C	2.18	0.47
2:O:225:ASN:O	2:O:227:ARG:HG2	2.15	0.47
4:Q:2:GLU:O	4:Q:3:LEU:O	2.31	0.47
4:Q:65:ALA:O	4:Q:85:GLY:HA3	2.14	0.47
1:A:102:LEU:H	1:A:102:LEU:CD1	2.10	0.47
2:B:157:VAL:HG22	2:B:157:VAL:O	2.14	0.47
10:J:44:GLU:OE2	10:J:53:LYS:NZ	2.42	0.47
2:O:341:MET:HE3	2:O:417:PHE:HE2	1.74	0.47
3:P:182:LEU:HA	3:P:182:LEU:HD23	1.58	0.47
5:R:95:PRO:HG2	5:R:145:VAL:CG1	2.45	0.47
2:B:57:TYR:N	2:B:57:TYR:HD1	2.11	0.47
2:B:122:TYR:O	2:B:126:VAL:HG23	2.15	0.47
2:B:162:ASN:O	2:B:244:ILE:HD12	2.15	0.47
2:B:243:GLU:OE1	2:B:436:LEU:HB3	2.14	0.47
2:B:286:LYS:HE2	2:B:287:ARG:NH2	2.29	0.47
4:D:109:LEU:O	4:D:111:PRO:HD3	2.14	0.47
1:N:87:ASN:CG	1:N:88:GLY:N	2.68	0.47
2:O:43:PRO:O	2:O:113:ARG:HG3	2.13	0.47
2:O:259:THR:OG1	2:O:422:LYS:HG3	2.14	0.47
3:P:350:ILE:HG23	3:P:351:ILE:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.14	0.47
2:B:83:PHE:CE2	6:S:104:ARG:HA	2.49	0.47
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.97	0.47
4:D:203:ARG:HD3	18:D:2009:BOG:O6	2.15	0.47
8:H:44:VAL:HG13	8:H:50:THR:HG21	1.95	0.47
1:N:23:LEU:HB2	1:N:192:ALA:HB1	1.97	0.47
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.40	0.47
2:O:110:GLU:O	2:O:111:CYS:HB3	2.13	0.47
2:O:290:SER:O	2:O:297:GLN:HG2	2.15	0.47
2:O:372:VAL:O	2:O:372:VAL:HG12	2.14	0.47
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.15	0.47
5:R:101:ARG:HA	5:R:105:GLU:OE1	2.15	0.47
6:S:71:LYS:O	6:S:72:HIS:HB2	2.14	0.47
1:A:147:ASN:C	1:A:149:THR:N	2.68	0.47
1:N:10:ASN:OD1	2:O:18:CYS:N	2.47	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.14	0.47
3:P:16:ASN:OD1	3:P:21:ASP:OD1	2.32	0.47
3:P:30:ALA:HB1	14:Q:3003:CDL:H111	1.97	0.47
1:A:244:ARG:NE	7:G:10:VAL:HB	2.29	0.47
1:A:439:SER:HA	1:A:442:TYR:CE2	2.49	0.47
3:C:151:PHE:HB2	3:C:162:VAL:CG2	2.44	0.47
3:C:182:LEU:O	3:C:186:LEU:HG	2.15	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.50	0.47
1:N:46:ARG:HD3	1:N:231:LEU:HD13	1.95	0.47
2:O:73:SER:OG	2:O:74:PRO:HD3	2.15	0.47
3:P:133:VAL:HG22	3:P:144:ALA:HB2	1.96	0.47
5:R:185:TYR:N	5:R:185:TYR:CD2	2.83	0.47
1:A:180:ALA:O	1:A:183:ALA:HB3	2.15	0.47
2:B:86:THR:O	2:B:90:GLU:HG3	2.14	0.47
2:B:345:LYS:O	2:B:349:GLN:HG3	2.15	0.47
3:C:164:TRP:CZ2	5:R:62:LEU:HD12	2.50	0.47
3:C:202:HIS:NE2	13:C:2002:UQ:O4	2.44	0.47
4:D:240:PRO:O	4:D:241:LYS:C	2.53	0.47
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.22	0.47
5:R:185:TYR:N	5:R:185:TYR:HD2	2.12	0.47
7:T:48:VAL:HG12	7:T:49:ALA:N	2.30	0.47
9:V:63:ASP:OD1	9:V:63:ASP:N	2.48	0.47
10:W:20:PHE:O	10:W:24:VAL:HG23	2.15	0.47
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.30	0.46
2:B:353:THR:HB	2:B:356:ASP:CG	2.35	0.46
1:N:180:ALA:O	1:N:183:ALA:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:239:TYR:HE2	2:O:241:GLY:HA2	1.79	0.46
2:O:290:SER:C	2:O:297:GLN:HE21	2.19	0.46
3:P:9:HIS:HB3	3:P:12:LEU:HB2	1.98	0.46
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.97	0.46
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.97	0.46
5:R:100:HIS:CD2	5:R:131:GLU:HB2	2.50	0.46
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.29	0.46
1:A:7:THR:HG21	2:B:113:ARG:CD	2.43	0.46
3:C:198:LEU:HD21	11:C:502:HEM:CMA	2.45	0.46
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.33	0.46
4:D:43:MET:CE	4:D:189:PHE:CZ	2.98	0.46
4:D:235:MET:CE	6:F:64:ARG:HA	2.45	0.46
5:E:163:SER:H	5:E:175:PRO:HD2	1.79	0.46
1:N:140:GLU:OE2	9:V:50:LEU:N	2.45	0.46
1:N:146:THR:O	1:N:150:PHE:HD1	1.98	0.46
2:O:424:MET:HG2	2:O:425:ALA:H	1.79	0.46
3:P:40:VAL:O	3:P:44:THR:OG1	2.33	0.46
3:P:172:ASP:C	3:P:174:PRO:HD2	2.36	0.46
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.45	0.46
5:R:83:GLU:HG2	5:R:100:HIS:CD2	2.51	0.46
2:B:239:TYR:C	2:B:239:TYR:CD2	2.88	0.46
7:G:48:VAL:HG12	7:G:49:ALA:N	2.31	0.46
1:N:249:PRO:HG2	1:N:250:VAL:N	2.31	0.46
2:O:47:ILE:HG22	2:O:48:GLY:N	2.29	0.46
2:O:227:ARG:O	2:O:228:SER:O	2.33	0.46
2:O:353:THR:HB	2:O:356:ASP:OD1	2.15	0.46
2:O:385:GLU:HB3	2:O:391:THR:O	2.15	0.46
3:P:6:ARG:HG2	3:P:16:ASN:CB	2.45	0.46
4:Q:235:MET:HE1	6:S:63:LYS:C	2.36	0.46
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.98	0.46
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.45	0.46
2:B:307:PHE:CD1	2:B:308:ASP:N	2.83	0.46
3:C:121:LEU:O	3:C:125:MET:HG3	2.16	0.46
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.38	0.46
5:E:62:LEU:HD12	3:P:164:TRP:CZ2	2.51	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
1:N:344:ARG:HG3	1:N:344:ARG:NH1	2.26	0.46
2:O:239:TYR:C	2:O:239:TYR:CD2	2.89	0.46
2:O:325:TYR:C	2:O:325:TYR:CD2	2.89	0.46
3:P:13:LYS:O	3:P:17:ASN:HB2	2.15	0.46
3:P:123:THR:CG2	3:P:190:ILE:HG13	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:32:VAL:HG11	4:Q:186:VAL:HB	1.98	0.46
4:Q:167:GLU:HG3	8:U:13:LEU:HD12	1.97	0.46
10:W:52:TRP:O	10:W:56:LYS:HB2	2.15	0.46
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.50	0.46
1:A:192:ALA:N	1:A:193:PRO:HD2	2.30	0.46
4:D:148:HIS:ND1	4:D:161:ALA:HA	2.30	0.46
6:F:100:GLU:O	6:F:104:ARG:HG3	2.16	0.46
8:H:15:ASP:O	8:H:17:LEU:N	2.49	0.46
1:N:269:VAL:HG21	1:N:410:VAL:HG21	1.98	0.46
1:N:281:ASP:OD2	1:N:284:PHE:HE1	1.99	0.46
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.50	0.46
3:P:364:LEU:O	3:P:368:PRO:HG3	2.15	0.46
4:Q:186:VAL:O	4:Q:189:PHE:HB3	2.14	0.46
5:R:58:PHE:O	5:R:61:SER:HB3	2.15	0.46
6:S:51:PRO:HD2	6:S:54:LEU:HD12	1.98	0.46
1:A:146:THR:O	1:A:150:PHE:HD1	1.99	0.46
2:B:385:GLU:HB3	2:B:391:THR:O	2.16	0.46
2:B:402:ILE:HD13	2:B:402:ILE:O	2.16	0.46
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.51	0.46
4:D:150:ASN:O	4:D:156:GLN:HA	2.15	0.46
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.15	0.46
6:F:59:MET:HA	6:F:59:MET:CE	2.46	0.46
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.51	0.46
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.98	0.46
5:R:100:HIS:HB2	5:R:132:TRP:CZ3	2.51	0.46
5:R:120:PRO:O	5:R:121:GLN:CG	2.62	0.46
2:B:290:SER:C	2:B:297:GLN:HE21	2.19	0.46
2:B:325:TYR:C	2:B:325:TYR:CD2	2.88	0.46
5:E:188:VAL:HG12	5:E:188:VAL:O	2.16	0.46
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.75	0.46
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.36	0.46
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.42	0.46
3:P:123:THR:HG21	3:P:190:ILE:HG13	1.97	0.46
5:R:163:SER:OG	5:R:176:ALA:HB2	2.16	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.15	0.46
2:B:206:LEU:O	2:B:206:LEU:HG	2.16	0.46
2:B:368:TYR:O	2:B:371:SER:HB2	2.16	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.98	0.46
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.98	0.46
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.83	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:LEU:HD21	3:C:180:PHE:HA	1.98	0.46
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.30	0.46
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.36	0.46
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.51	0.46
1:N:106:MET:CE	1:N:110:VAL:CG2	2.94	0.46
1:N:145:MET:CB	1:N:252:HIS:CD2	2.99	0.46
2:O:124:LEU:O	2:O:128:THR:HG23	2.16	0.46
5:R:118:ARG:O	5:R:120:PRO:CD	2.56	0.46
9:V:63:ASP:O	9:V:64:LEU:HB2	2.16	0.46
1:A:351:GLU:O	1:A:354:VAL:HG22	2.16	0.45
2:B:170:THR:O	2:B:172:LEU:N	2.49	0.45
3:C:13:LYS:O	3:C:17:ASN:HB2	2.16	0.45
3:C:22:LEU:CD2	13:C:2002:UQ:HM32	2.43	0.45
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.45
1:N:191:LYS:O	1:N:195:MET:HG3	2.16	0.45
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.51	0.45
2:O:252:LEU:HD11	9:V:49:LEU:HB2	1.97	0.45
3:P:92:PHE:O	3:P:95:ILE:HG22	2.16	0.45
3:P:271:PRO:HB2	3:P:275:PHE:HB2	1.97	0.45
4:Q:99:GLU:H	4:Q:99:GLU:CD	2.19	0.45
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.16	0.45
5:R:109:GLU:OE2	5:R:168:SER:HB2	2.17	0.45
5:R:171:ILE:HG21	5:R:177:PRO:O	2.16	0.45
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.99	0.45
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.79	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.45
3:C:6:ARG:HG2	3:C:16:ASN:CB	2.46	0.45
3:C:98:HIS:CD2	11:C:502:HEM:NC	2.83	0.45
3:C:231:LEU:O	3:C:235:LEU:HG	2.16	0.45
4:D:117:VAL:O	4:D:123:GLY:HA2	2.16	0.45
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	0.45
1:N:281:ASP:C	1:N:281:ASP:OD1	2.55	0.45
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.16	0.45
3:P:6:ARG:O	3:P:13:LYS:HA	2.16	0.45
3:P:151:PHE:HB2	3:P:162:VAL:CG2	2.46	0.45
5:R:77:LYS:HE3	5:R:191:ASP:OD2	2.16	0.45
5:R:100:HIS:HA	5:R:131:GLU:O	2.16	0.45
5:R:116:LYS:O	5:R:117:LEU:HD23	2.16	0.45
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.45	0.45
2:B:71:LEU:HD22	9:I:68:ILE:HG13	1.98	0.45
2:B:189:GLU:O	2:B:190:GLN:C	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:ASN:OD1	3:C:21:ASP:OD1	2.34	0.45
3:C:82:ASN:HD22	3:C:82:ASN:N	2.14	0.45
9:I:38:UNK:C	9:I:40:UNK:N	2.76	0.45
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.34	0.45
1:N:79:VAL:O	1:N:82:MET:HG2	2.16	0.45
2:O:157:VAL:O	2:O:157:VAL:HG22	2.16	0.45
3:P:166:TRP:HA	3:P:175:THR:HG23	1.99	0.45
6:S:100:GLU:O	6:S:104:ARG:HG3	2.17	0.45
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.99	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.32	0.45
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.99	0.45
9:I:33:UNK:O	9:I:34:UNK:O	2.34	0.45
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.17	0.45
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.98	0.45
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.51	0.45
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.52	0.45
3:P:344:VAL:O	3:P:345:GLU:HG3	2.16	0.45
5:R:161:HIS:HB2	19:R:501:FES:S1	2.57	0.45
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.15	0.45
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.85	0.45
1:N:112:LEU:O	1:N:113:LEU:C	2.55	0.45
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.47	0.45
8:U:65:ARG:O	8:U:69:VAL:HG23	2.17	0.45
10:W:10:TYR:HE2	10:W:15:ARG:HD2	1.81	0.45
1:A:274:ASN:ND2	1:A:309:THR:HB	2.32	0.45
4:D:99:GLU:CD	4:D:99:GLU:H	2.20	0.45
5:E:171:ILE:HG21	5:E:177:PRO:O	2.16	0.45
9:I:71:ASN:N	9:I:71:ASN:HD22	2.09	0.45
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.30	0.45
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.52	0.45
1:N:90:THR:O	1:N:167:VAL:HG11	2.15	0.45
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.44	0.45
1:N:354:VAL:HG11	1:N:404:ALA:HA	1.99	0.45
2:O:31:ASN:HD22	2:O:31:ASN:H	1.62	0.45
2:O:70:ARG:HG3	2:O:98:VAL:CG1	2.47	0.45
4:Q:47:ALA:N	4:Q:50:ASN:HD22	2.02	0.45
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.99	0.45
2:B:424:MET:HG2	2:B:425:ALA:H	1.81	0.45
1:N:30:SER:O	1:N:202:GLY:HA2	2.15	0.45
1:N:106:MET:CE	1:N:110:VAL:HG21	2.47	0.45
1:N:131:ARG:NH2	1:N:177:LEU:O	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:89:SER:O	3:P:90:PHE:C	2.55	0.45
3:P:338:TRP:NE1	7:T:59:TYR:HE1	2.15	0.45
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.47	0.45
1:A:106:MET:CG	1:A:203:ILE:HD13	2.46	0.45
1:A:251:ALA:HB2	1:A:427:PRO:HG2	1.99	0.45
1:A:269:VAL:HG21	1:A:410:VAL:HG21	1.98	0.45
3:C:147:ILE:HG13	12:C:2001:IKR:H16A	1.99	0.45
5:E:191:ASP:OD2	5:E:191:ASP:N	2.49	0.45
7:G:68:ARG:NH2	7:G:69:LEU:HD21	2.31	0.45
1:N:19:LEU:O	1:N:21:ASN:N	2.50	0.45
1:N:147:ASN:O	1:N:149:THR:N	2.50	0.45
2:O:294:LYS:NZ	2:O:356:ASP:OD2	2.41	0.45
2:O:307:PHE:CD1	2:O:308:ASP:N	2.85	0.45
3:P:101:ARG:HD2	3:P:102:GLY:N	2.32	0.45
3:P:207:ASN:ND2	3:P:208:ASN:H	2.15	0.45
5:R:102:THR:O	5:R:106:ILE:HG13	2.16	0.45
1:A:249:PRO:HG2	1:A:250:VAL:N	2.29	0.45
2:B:146:VAL:O	2:B:149:ALA:N	2.50	0.45
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.99	0.45
5:E:78:LEU:HD11	5:E:187:PHE:HE2	1.80	0.45
2:O:325:TYR:HD2	2:O:325:TYR:C	2.20	0.45
2:O:353:THR:HB	2:O:356:ASP:CG	2.38	0.45
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.52	0.44
2:B:325:TYR:HD2	2:B:325:TYR:C	2.21	0.44
3:C:75:GLN:HA	3:C:75:GLN:OE1	2.17	0.44
13:C:2002:UQ:HM51	13:C:2002:UQ:H8	1.99	0.44
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.76	0.44
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.52	0.44
1:N:282:ARG:NH2	9:V:37:UNK:N	2.65	0.44
2:O:86:THR:O	2:O:90:GLU:HG3	2.17	0.44
2:O:168:TYR:HE2	2:O:172:LEU:HD12	1.82	0.44
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.77	0.44
3:P:261:ASN:ND2	3:P:264:VAL:HG23	2.32	0.44
4:Q:54:VAL:HG11	4:Q:192:TRP:HE1	1.82	0.44
7:T:36:ASN:O	7:T:40:ARG:HG3	2.15	0.44
2:B:27:THR:HG22	2:B:28:LYS:N	2.32	0.44
2:B:150:VAL:HG23	2:B:151:ALA:N	2.32	0.44
3:C:158:GLY:O	3:C:160:THR:N	2.50	0.44
4:D:147:LEU:C	4:D:148:HIS:HD2	2.21	0.44
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.27	0.44
2:O:25:GLU:HB2	2:O:213:HIS:ND1	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:26:ILE:HA	2:O:35:ILE:O	2.17	0.44
3:P:278:ALA:HB1	3:P:295:LEU:HD13	1.98	0.44
13:P:3002:UQ:HM51	13:P:3002:UQ:H8	1.98	0.44
4:Q:46:VAL:HB	4:Q:91:PHE:CE2	2.53	0.44
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.47	0.44
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.52	0.44
4:D:24:SER:OG	10:J:55:ILE:HG21	2.17	0.44
5:E:75:GLU:HG3	5:E:75:GLU:O	2.17	0.44
1:N:58:PHE:HA	1:N:134:ILE:HD11	1.98	0.44
1:N:134:ILE:HG21	1:N:174:ILE:CG1	2.47	0.44
2:O:286:LYS:HE2	2:O:287:ARG:NH2	2.33	0.44
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	2.00	0.44
1:A:106:MET:CE	1:A:110:VAL:CG2	2.95	0.44
2:B:43:PRO:O	2:B:113:ARG:HG3	2.17	0.44
2:B:72:ALA:HB1	2:B:75:LEU:HD12	2.00	0.44
2:B:105:MET:HE2	2:B:107:TYR:CE1	2.53	0.44
2:B:268:GLU:HG2	2:B:272:PHE:HE1	1.81	0.44
5:E:175:PRO:O	5:E:176:ALA:C	2.55	0.44
1:N:82:MET:CE	1:N:105:ASP:HB3	2.48	0.44
2:O:31:ASN:ND2	2:O:31:ASN:H	2.15	0.44
2:O:374:THR:HG22	2:O:376:GLN:HB3	1.99	0.44
3:P:151:PHE:C	3:P:153:ALA:H	2.21	0.44
3:P:175:THR:O	3:P:178:ARG:HG2	2.17	0.44
3:P:319:ARG:HB3	3:P:374:GLU:OE1	2.17	0.44
9:V:64:LEU:CD1	9:V:77:ARG:C	2.85	0.44
1:A:45:SER:OG	1:A:92:ARG:HA	2.18	0.44
4:D:164:ILE:O	4:D:179:MET:CE	2.65	0.44
1:N:19:LEU:C	1:N:21:ASN:H	2.21	0.44
1:N:147:ASN:C	1:N:149:THR:N	2.68	0.44
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.98	0.44
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.99	0.44
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.17	0.44
5:R:79:SER:OG	5:R:191:ASP:CB	2.65	0.44
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.44
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.98	0.44
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.38	0.44
3:C:278:ALA:HB1	3:C:295:LEU:HD13	1.99	0.44
4:D:17:PRO:O	4:D:202:LYS:HD3	2.17	0.44
17:D:501:HEC:HHA	17:D:501:HEC:HBA1	2.00	0.44
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.52	0.44
5:R:53:ASN:O	5:R:57:GLN:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:12:LEU:C	6:S:14:ASP:N	2.71	0.44
10:W:60:GLU:O	10:W:61:ALA:CB	2.65	0.44
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.17	0.44
4:D:43:MET:HG3	4:D:46:VAL:HG23	1.99	0.44
4:D:43:MET:HE3	4:D:91:PHE:HE2	1.82	0.44
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.33	0.44
1:N:192:ALA:N	1:N:193:PRO:HD2	2.32	0.44
3:P:33:ASN:HB3	20:P:386:HOH:O	2.16	0.44
3:P:279:TYR:O	3:P:282:LEU:HB3	2.18	0.44
1:A:177:LEU:HD22	1:A:181:ASP:HB2	2.00	0.44
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.33	0.44
4:D:2:GLU:CB	7:G:70:LYS:HE2	2.39	0.44
4:D:218:LEU:HD13	5:E:43:ALA:N	2.33	0.44
5:E:53:ASN:O	5:E:57:GLN:HG3	2.18	0.44
7:G:28:ASN:HB2	7:G:32:ASP:HB3	1.98	0.44
2:O:275:LEU:HD12	2:O:275:LEU:O	2.18	0.44
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.52	0.44
5:R:113:ASP:O	5:R:115:SER:N	2.51	0.44
5:R:136:VAL:HG23	5:R:183:PRO:HD3	2.00	0.44
6:S:13:MET:O	6:S:17:ARG:HG3	2.18	0.44
9:V:39:UNK:O	9:V:40:UNK:C	2.66	0.44
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.23	0.44
2:B:238:THR:CG2	2:B:239:TYR:N	2.80	0.44
3:C:184:PHE:HD2	3:C:184:PHE:O	2.01	0.44
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.27	0.44
1:N:45:SER:HA	1:N:48:GLU:CD	2.38	0.44
3:P:31:TRP:NE1	15:P:3007:PEE:O4	2.51	0.44
3:P:75:GLN:OE1	3:P:75:GLN:HA	2.18	0.44
8:U:34:ARG:O	8:U:34:ARG:HD3	2.17	0.44
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.53	0.43
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.99	0.43
2:B:46:ARG:HD3	2:B:110:GLU:HG2	1.99	0.43
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.33	0.43
1:N:206:LYS:O	1:N:208:LEU:N	2.51	0.43
2:O:59:THR:HG22	2:O:60:THR:N	2.33	0.43
2:O:306:PRO:HB3	9:V:51:CYS:C	2.39	0.43
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.18	0.43
5:R:75:GLU:HG3	5:R:75:GLU:O	2.18	0.43
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.58	0.43
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.36	0.43
1:A:411:CYS:HB3	1:A:415:ILE:HD12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:GLY:H	2:B:411:VAL:HG11	1.82	0.43
3:C:18:SER:HB2	3:C:202:HIS:CE1	2.48	0.43
5:E:106:ILE:O	5:E:106:ILE:HG22	2.18	0.43
7:G:46:PHE:O	7:G:50:PRO:HG2	2.18	0.43
9:I:59:SER:O	9:I:60:ALA:C	2.56	0.43
1:N:135:LEU:CD2	1:N:174:ILE:HG21	2.48	0.43
2:O:306:PRO:HB3	9:V:51:CYS:HA	1.99	0.43
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.53	0.43
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.92	0.43
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	2.00	0.43
5:R:15:ARG:NH1	5:R:32:ARG:HB3	2.33	0.43
8:U:72:LYS:O	8:U:74:PHE:N	2.51	0.43
2:B:338:ARG:O	2:B:341:MET:HB2	2.18	0.43
3:C:6:ARG:O	3:C:13:LYS:HA	2.19	0.43
3:C:364:LEU:O	3:C:368:PRO:HG3	2.19	0.43
4:D:16:GLY:N	4:D:19:SER:OG	2.50	0.43
4:D:238:ARG:CZ	5:E:5:VAL:HG22	2.49	0.43
9:I:28:UNK:N	9:I:72:ALA:HB2	2.33	0.43
1:N:281:ASP:CB	9:V:33:UNK:HB2	2.49	0.43
2:O:168:TYR:HB2	2:O:173:ALA:CB	2.43	0.43
2:O:225:ASN:O	2:O:227:ARG:CG	2.65	0.43
3:P:34:PHE:CD1	3:P:37:LEU:HD12	2.54	0.43
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.33	0.43
4:Q:178:THR:HG21	8:U:16:PRO:HD2	2.01	0.43
4:Q:231:LYS:HD3	6:S:71:LYS:HA	2.00	0.43
2:B:167:ALA:C	2:B:168:TYR:CD1	2.92	0.43
2:B:435:PHE:O	2:B:438:GLU:N	2.52	0.43
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.48	0.43
5:E:100:HIS:CD2	5:E:131:GLU:HB2	2.53	0.43
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.53	0.43
9:I:33:UNK:HG2	9:I:73:PRO:HB3	2.00	0.43
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.99	0.43
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.18	0.43
2:O:164:HIS:O	2:O:173:ALA:HA	2.19	0.43
2:O:365:LYS:O	2:O:369:LEU:HG	2.17	0.43
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.99	0.43
3:P:261:ASN:ND2	3:P:264:VAL:CG2	2.81	0.43
5:R:69:LEU:O	5:R:72:SER:CB	2.67	0.43
9:V:49:LEU:O	9:V:50:LEU:HD23	2.19	0.43
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.43
1:A:87:ASN:OD1	2:B:286:LYS:HD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:SER:HB2	7:G:17:SER:O	2.18	0.43
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.48	0.43
2:B:353:THR:HB	2:B:356:ASP:OD1	2.18	0.43
3:C:41:CYS:SG	3:C:91:PHE:HA	2.58	0.43
3:C:133:VAL:HG22	3:C:144:ALA:HB2	2.01	0.43
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.82	0.43
5:E:119:ASP:O	5:E:121:GLN:N	2.52	0.43
5:E:141:HIS:HB2	5:E:176:ALA:CA	2.49	0.43
1:N:23:LEU:HD23	1:N:24:ARG:N	2.33	0.43
1:N:159:GLN:NE2	1:N:237:THR:HG21	2.33	0.43
2:O:312:PHE:O	2:O:322:PHE:HA	2.18	0.43
1:A:131:ARG:NH2	1:A:177:LEU:O	2.52	0.43
2:B:28:LYS:O	2:B:28:LYS:HG2	2.18	0.43
2:B:70:ARG:HG3	2:B:98:VAL:HG12	1.99	0.43
4:D:27:ARG:O	4:D:30:PHE:HB3	2.18	0.43
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.89	0.43
9:I:33:UNK:HG3	9:I:73:PRO:HB3	2.01	0.43
1:N:236:PHE:CB	1:N:258:GLU:OE1	2.66	0.43
2:O:306:PRO:HB3	9:V:51:CYS:CA	2.49	0.43
2:O:309:ALA:HA	2:O:325:TYR:O	2.18	0.43
4:Q:76:GLU:H	4:Q:76:GLU:CD	2.21	0.43
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.47	0.43
5:R:148:ALA:O	5:R:149:ASN:CB	2.66	0.43
1:A:103:SER:O	1:A:106:MET:HB2	2.18	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.83	0.43
1:A:241:ILE:O	1:A:241:ILE:HG23	2.19	0.43
2:B:385:GLU:O	2:B:387:LEU:N	2.51	0.43
3:C:36:SER:O	3:C:40:VAL:HG23	2.18	0.43
5:E:59:ILE:HD13	5:E:59:ILE:HA	1.82	0.43
8:H:43:ARG:HG3	8:H:44:VAL:N	2.33	0.43
1:N:50:GLU:O	1:N:50:GLU:HG2	2.18	0.43
3:P:64:PHE:CE1	16:P:3011:GOL:H12	2.53	0.43
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.52	0.43
5:R:20:ASP:C	5:R:22:THR:H	2.22	0.43
1:A:6:GLN:C	1:A:8:LEU:N	2.72	0.43
1:A:147:ASN:O	1:A:149:THR:N	2.52	0.43
3:C:151:PHE:C	3:C:153:ALA:H	2.22	0.43
3:C:156:TYR:C	3:C:158:GLY:H	2.22	0.43
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.84	0.43
6:F:16:ILE:O	6:F:19:TRP:HB3	2.19	0.43
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:80:ASP:O	7:G:81:GLN:C	2.57	0.43
2:O:76:THR:HG23	2:O:82:SER:HB2	2.00	0.43
2:O:109:VAL:CG2	2:O:119:VAL:HG12	2.47	0.43
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.18	0.43
4:Q:222:MET:HE3	5:R:40:THR:CG2	2.43	0.43
5:R:135:LEU:HD13	5:R:180:LEU:HD12	2.00	0.43
2:B:255:ALA:O	2:B:325:TYR:HA	2.19	0.43
3:C:19:LEU:O	3:C:20:ILE:HG13	2.18	0.43
1:N:49:ASN:CG	1:N:51:LYS:H	2.22	0.43
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.53	0.43
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.31	0.43
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.54	0.43
5:R:148:ALA:HB2	5:R:156:TYR:CE2	2.53	0.43
5:R:153:PHE:CE2	5:R:172:ARG:NE	2.87	0.43
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.49	0.43
2:B:166:ALA:HB1	2:B:242:GLY:C	2.39	0.43
2:B:209:ILE:HG22	2:B:210:GLY:N	2.33	0.43
2:B:325:TYR:CD1	9:I:60:ALA:CB	3.02	0.43
3:C:175:THR:O	3:C:178:ARG:HG2	2.18	0.43
3:C:367:PHE:N	3:C:368:PRO:HD2	2.34	0.43
1:N:411:CYS:HB3	1:N:415:ILE:HD12	2.01	0.43
2:O:258:VAL:HG21	2:O:321:LEU:HD22	2.01	0.43
3:P:43:MET:HE1	13:P:3002:UQ:C12	2.49	0.43
5:R:29:SER:CA	5:R:32:ARG:HH21	2.32	0.43
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.49	0.43
2:B:26:ILE:HA	2:B:35:ILE:O	2.18	0.42
2:B:59:THR:HG22	2:B:60:THR:N	2.33	0.42
2:B:355:GLU:O	2:B:358:THR:HB	2.19	0.42
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.01	0.42
3:C:37:LEU:O	3:C:41:CYS:HB2	2.18	0.42
5:E:75:GLU:HA	5:E:193:VAL:O	2.18	0.42
5:E:156:TYR:CD1	5:E:156:TYR:N	2.87	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.41	0.42
1:N:45:SER:OG	1:N:92:ARG:HA	2.19	0.42
3:P:82:ASN:HD22	3:P:82:ASN:N	2.15	0.42
3:P:133:VAL:HA	3:P:140:SER:HB3	2.01	0.42
3:P:266:PRO:HA	3:P:267:PRO:HD3	1.84	0.42
4:Q:167:GLU:C	4:Q:169:LEU:N	2.71	0.42
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.84	0.42
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.52	0.42
1:A:341:GLU:HA	1:A:344:ARG:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HG22	2:B:52:LYS:N	2.35	0.42
3:C:19:LEU:C	3:C:20:ILE:HG13	2.39	0.42
5:E:100:HIS:HD2	5:E:131:GLU:HB2	1.84	0.42
2:O:350:GLY:H	2:O:411:VAL:HG11	1.84	0.42
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.19	0.42
4:Q:143:VAL:HG21	4:Q:149:TYR:HB2	2.01	0.42
8:U:43:ARG:HG3	8:U:44:VAL:N	2.34	0.42
2:B:246:GLU:O	2:B:246:GLU:HG2	2.19	0.42
2:B:424:MET:HB2	2:B:436:LEU:HD13	2.01	0.42
2:O:150:VAL:HG23	2:O:151:ALA:N	2.34	0.42
2:O:353:THR:HG22	2:O:354:GLU:N	2.34	0.42
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.01	0.42
3:P:379:ASN:HA	6:S:17:ARG:HH12	1.85	0.42
4:Q:66:GLU:C	4:Q:68:VAL:H	2.23	0.42
1:A:153:LEU:O	1:A:156:THR:HG22	2.18	0.42
1:N:44:GLY:HA3	1:N:92:ARG:O	2.19	0.42
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.42
1:N:135:LEU:HD23	1:N:135:LEU:HA	1.86	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.42
2:O:325:TYR:HB3	9:V:59:SER:HB3	2.01	0.42
3:P:172:ASP:OD1	3:P:173:ASN:N	2.40	0.42
11:P:502:HEM:HBB2	11:P:502:HEM:HMB1	2.00	0.42
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.34	0.42
7:T:77:TYR:C	7:T:79:ASN:N	2.72	0.42
1:A:90:THR:HB	1:A:95:THR:HG23	2.01	0.42
1:A:315:SER:OG	1:A:316:ASP:N	2.52	0.42
5:E:20:ASP:C	5:E:22:THR:H	2.23	0.42
5:E:147:ILE:HD11	5:E:159:PRO:HG3	2.01	0.42
7:G:30:PHE:O	7:G:35:PRO:CD	2.68	0.42
9:I:41:UNK:O	9:I:42:UNK:C	2.67	0.42
3:P:365:ILE:HG22	3:P:366:LEU:N	2.35	0.42
5:R:83:GLU:HA	5:R:100:HIS:O	2.19	0.42
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.33	0.42
8:U:15:ASP:C	8:U:17:LEU:N	2.73	0.42
8:U:15:ASP:O	8:U:17:LEU:N	2.52	0.42
1:A:310:PHE:C	1:A:310:PHE:CD2	2.93	0.42
2:B:124:LEU:HD23	2:B:124:LEU:C	2.39	0.42
2:B:193:HIS:O	2:B:197:ASN:ND2	2.53	0.42
3:C:284:SER:O	3:C:286:PRO:HD3	2.18	0.42
4:D:167:GLU:C	4:D:169:LEU:N	2.73	0.42
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:313:SER:O	1:N:314:TYR:CD2	2.72	0.42
2:O:46:ARG:HD3	2:O:110:GLU:HG2	2.02	0.42
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.55	0.42
3:P:224:TYR:HB3	4:Q:227:TRP:CZ2	2.54	0.42
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.55	0.42
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	2.01	0.42
5:R:39:VAL:O	5:R:42:THR:HB	2.20	0.42
6:S:80:TRP:N	6:S:80:TRP:CD1	2.86	0.42
1:A:171:THR:O	1:A:175:LYS:HG3	2.20	0.42
2:B:141:GLN:N	2:B:142:PRO:HD2	2.33	0.42
2:B:189:GLU:O	2:B:191:LEU:N	2.53	0.42
3:C:30:ALA:C	3:C:32:TRP:H	2.22	0.42
3:C:123:THR:CG2	3:C:190:ILE:HG13	2.49	0.42
4:D:76:GLU:O	4:Q:99:GLU:HB3	2.20	0.42
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.01	0.42
1:N:24:ARG:NH2	1:N:193:PRO:O	2.53	0.42
1:N:383:LEU:HD23	1:N:388:ARG:HA	2.02	0.42
2:O:22:GLU:HG3	2:O:23:ASP:H	1.84	0.42
2:O:280:GLY:HA3	2:O:293:SER:OG	2.20	0.42
3:P:287:ASN:O	3:P:289:LEU:N	2.53	0.42
3:P:346:HIS:CG	3:P:347:PRO:HA	2.54	0.42
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.50	0.42
4:Q:16:GLY:HA3	4:Q:19:SER:OG	2.19	0.42
4:Q:16:GLY:N	4:Q:19:SER:OG	2.53	0.42
6:S:31:LEU:HD21	6:S:65:ALA:HB2	2.01	0.42
8:U:65:ARG:O	8:U:68:CYS:HB3	2.19	0.42
10:W:4:ALA:O	10:W:8:GLN:HG3	2.19	0.42
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.52	0.42
1:A:206:LYS:O	1:A:207:GLU:C	2.57	0.42
1:A:365:MET:HG3	1:A:366:VAL:N	2.33	0.42
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.54	0.42
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.47	0.42
1:N:136:GLN:OE1	9:V:50:LEU:HD13	2.20	0.42
2:O:146:VAL:O	2:O:149:ALA:N	2.53	0.42
5:R:157:TYR:HD1	5:R:164:HIS:HD1	1.68	0.42
10:W:59:TYR:CD1	10:W:59:TYR:N	2.87	0.42
1:A:24:ARG:NH2	1:A:193:PRO:O	2.53	0.42
2:B:220:ALA:O	2:B:224:LEU:HB2	2.20	0.42
4:D:32:VAL:HG11	4:D:186:VAL:HB	2.01	0.42
8:H:34:ARG:O	8:H:38:GLU:HG3	2.20	0.42
1:N:6:GLN:C	1:N:8:LEU:N	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:LYS:CA	1:N:195:MET:HE2	2.50	0.42
1:N:298:ALA:HA	1:N:303:LEU:HD12	2.02	0.42
2:O:124:LEU:HD23	2:O:124:LEU:C	2.39	0.42
2:O:167:ALA:C	2:O:168:TYR:CD1	2.93	0.42
2:O:355:GLU:O	2:O:358:THR:HB	2.20	0.42
4:Q:179:MET:O	4:Q:182:ILE:HB	2.19	0.42
1:A:106:MET:CE	1:A:110:VAL:HG21	2.49	0.42
1:A:310:PHE:CD2	1:A:310:PHE:O	2.73	0.42
3:C:38:LEU:HA	3:C:38:LEU:HD23	1.83	0.42
3:C:61:SER:O	3:C:62:LEU:HD23	2.20	0.42
3:C:276:LEU:HB2	3:C:337:THR:HG23	2.02	0.42
3:C:297:ALA:O	3:C:301:ILE:HB	2.20	0.42
4:D:234:LYS:HD2	5:E:8:PRO:HB2	2.01	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.55	0.42
1:N:156:THR:HG23	1:N:157:ALA:N	2.35	0.42
1:N:279:ARG:HA	1:N:307:PHE:CE1	2.55	0.42
2:O:215:ASP:O	2:O:219:VAL:HG23	2.19	0.42
3:P:165:ALA:O	3:P:178:ARG:HD2	2.19	0.42
5:R:78:LEU:N	5:R:191:ASP:O	2.53	0.42
5:R:102:THR:OG1	5:R:105:GLU:HG3	2.20	0.42
3:C:40:VAL:O	3:C:44:THR:OG1	2.38	0.41
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.02	0.41
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.95	0.41
5:E:104:ALA:O	5:E:108:GLN:HB3	2.19	0.41
7:G:80:ASP:HB3	8:H:50:THR:CA	2.46	0.41
8:H:15:ASP:C	8:H:17:LEU:N	2.73	0.41
2:O:239:TYR:C	2:O:239:TYR:HD2	2.23	0.41
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	2.01	0.41
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.55	0.41
1:A:117:VAL:CG2	1:A:118:GLN:N	2.80	0.41
1:A:156:THR:HG23	1:A:157:ALA:N	2.34	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.54	0.41
5:E:189:GLY:O	5:E:192:LEU:N	2.53	0.41
1:N:255:LEU:O	1:N:321:GLY:HA3	2.21	0.41
1:N:261:GLY:HA2	1:N:317:THR:O	2.19	0.41
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.41
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.41
4:Q:167:GLU:C	4:Q:169:LEU:H	2.22	0.41
1:A:104:LYS:O	1:A:107:PRO:HD2	2.20	0.41
1:A:106:MET:HB3	1:A:107:PRO:HD3	2.01	0.41
1:A:186:ILE:HG13	1:A:186:ILE:H	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TYR:HE2	2:B:241:GLY:HA2	1.84	0.41
3:C:70:THR:HA	3:C:74:VAL:CG2	2.49	0.41
3:C:89:SER:O	3:C:90:PHE:C	2.58	0.41
3:C:162:VAL:C	3:C:164:TRP:N	2.74	0.41
3:C:277:PHE:CG	3:C:278:ALA:N	2.88	0.41
5:E:82:PRO:HG2	5:E:85:LYS:HB2	2.01	0.41
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.19	0.41
8:H:65:ARG:O	8:H:68:CYS:HB3	2.21	0.41
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.41
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.34	0.41
1:N:39:VAL:HG13	1:N:39:VAL:O	2.20	0.41
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.02	0.41
2:O:259:THR:O	2:O:260:GLU:C	2.59	0.41
3:P:365:ILE:O	3:P:368:PRO:HG2	2.20	0.41
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.36	0.41
1:A:90:THR:HA	1:A:95:THR:HA	2.02	0.41
2:B:319:SER:OG	2:B:320:GLY:N	2.53	0.41
2:B:355:GLU:O	2:B:358:THR:N	2.53	0.41
2:B:372:VAL:HG13	2:B:378:LEU:CA	2.42	0.41
3:C:336:LEU:HG	3:C:355:ALA:HB1	2.02	0.41
5:E:30:GLU:HB2	10:J:7:ARG:HG2	2.01	0.41
1:N:136:GLN:O	1:N:140:GLU:HG3	2.21	0.41
1:N:153:LEU:O	1:N:156:THR:HG22	2.20	0.41
1:N:307:PHE:HA	1:N:323:HIS:O	2.20	0.41
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.47	0.41
2:O:238:THR:CG2	2:O:239:TYR:H	2.31	0.41
2:O:291:VAL:C	2:O:293:SER:H	2.24	0.41
3:P:30:ALA:C	3:P:32:TRP:H	2.23	0.41
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.35	0.41
5:R:156:TYR:CD1	5:R:156:TYR:N	2.87	0.41
1:A:44:GLY:HA3	1:A:92:ARG:O	2.20	0.41
1:A:58:PHE:HA	1:A:134:ILE:HD11	2.01	0.41
2:B:71:LEU:HD11	2:B:144:LEU:HD23	2.02	0.41
2:B:131:GLU:O	2:B:132:PHE:C	2.57	0.41
2:B:209:ILE:CG2	2:B:210:GLY:N	2.83	0.41
2:B:239:TYR:C	2:B:239:TYR:HD2	2.24	0.41
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.55	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.86	0.41
4:D:37:CYS:O	4:D:39:ALA:N	2.52	0.41
1:N:106:MET:HB3	1:N:107:PRO:CD	2.50	0.41
1:N:171:THR:O	1:N:175:LYS:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:27:THR:CG2	2:O:28:LYS:H	2.32	0.41
2:O:338:ARG:O	2:O:341:MET:HB2	2.21	0.41
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.54	0.41
3:P:242:THR:N	4:Q:208:MET:HE1	2.35	0.41
3:P:350:ILE:O	3:P:354:MET:HG2	2.21	0.41
1:A:81:SER:HB3	2:B:359:LYS:HD3	2.02	0.41
1:A:191:LYS:CA	1:A:195:MET:HE2	2.51	0.41
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.20	0.41
2:B:278:VAL:O	2:B:294:LYS:HG3	2.20	0.41
3:C:130:VAL:HG23	3:C:131:GLY:N	2.35	0.41
3:C:287:ASN:O	3:C:289:LEU:N	2.53	0.41
2:O:97:SER:HB3	9:V:69:SER:CB	2.51	0.41
3:P:79:LEU:CD2	5:R:57:GLN:NE2	2.84	0.41
3:P:138:GLN:HG2	3:P:258:THR:HG22	2.03	0.41
3:P:230:ILE:HG21	15:R:3005:PEE:H22	2.02	0.41
5:R:84:GLY:N	5:R:102:THR:HG23	2.36	0.41
1:A:382:HIS:HB3	1:A:388:ARG:O	2.20	0.41
2:B:37:SER:HB3	2:B:213:HIS:CG	2.55	0.41
2:B:238:THR:CG2	2:B:239:TYR:H	2.31	0.41
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.36	0.41
3:C:11:LEU:HA	3:C:14:MET:HG3	2.02	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CG	2.55	0.41
5:E:53:ASN:O	5:E:56:THR:HB	2.19	0.41
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.85	0.41
1:N:45:SER:HA	1:N:48:GLU:CG	2.50	0.41
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.55	0.41
3:P:162:VAL:C	3:P:164:TRP:N	2.74	0.41
1:A:358:LYS:HE3	1:A:399:ILE:O	2.21	0.41
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.38	0.41
2:B:259:THR:CG2	2:B:260:GLU:N	2.82	0.41
2:B:265:GLY:O	2:B:266:SER:C	2.58	0.41
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.20	0.41
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.35	0.41
1:N:269:VAL:HG22	1:N:406:MET:CE	2.51	0.41
1:N:274:ASN:HD22	1:N:274:ASN:HA	1.59	0.41
2:O:212:LYS:HG2	2:O:214:SER:OG	2.20	0.41
2:O:287:ARG:NH1	2:O:287:ARG:HG3	2.36	0.41
3:P:151:PHE:C	3:P:153:ALA:N	2.73	0.41
3:P:326:PHE:O	3:P:329:LEU:HB3	2.21	0.41
1:A:228:VAL:HG13	1:A:228:VAL:O	2.21	0.41
1:A:270:LEU:O	1:A:273:ALA:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:HIS:O	2:B:173:ALA:HA	2.21	0.41
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.68	0.41
3:C:151:PHE:C	3:C:153:ALA:N	2.74	0.41
3:C:173:ASN:N	3:C:174:PRO:CD	2.83	0.41
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.35	0.41
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.56	0.41
4:D:208:MET:O	4:D:212:SER:HB2	2.21	0.41
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.86	0.41
6:F:51:PRO:O	6:F:52:GLU:C	2.58	0.41
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.95	0.41
7:G:30:PHE:CD2	7:G:34:LEU:HD12	2.56	0.41
7:G:72:LYS:CE	8:H:57:GLU:OE1	2.69	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.96	0.41
2:O:141:GLN:N	2:O:142:PRO:HD2	2.36	0.41
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.51	0.41
3:P:120:LEU:HD23	3:P:120:LEU:HA	1.95	0.41
3:P:196:ILE:HG22	3:P:200:PHE:CE2	2.56	0.41
3:P:357:LEU:HD12	3:P:357:LEU:HA	1.92	0.41
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.89	0.41
4:Q:148:HIS:CE1	4:Q:161:ALA:HB2	2.56	0.41
4:Q:161:ALA:O	4:Q:163:PRO:N	2.53	0.41
4:Q:165:TYR:O	4:Q:166:ASN:C	2.60	0.41
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.91	0.41
6:S:59:MET:HA	6:S:59:MET:CE	2.51	0.41
1:A:45:SER:HA	1:A:48:GLU:HG3	2.02	0.41
1:A:46:ARG:HD3	1:A:231:LEU:HD13	2.03	0.41
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.20	0.41
2:B:385:GLU:C	2:B:387:LEU:H	2.25	0.41
2:B:402:ILE:O	2:B:405:VAL:HG23	2.21	0.41
7:G:53:LEU:O	7:G:57:LEU:HG	2.21	0.41
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.50	0.41
1:N:104:LYS:O	1:N:107:PRO:HD2	2.21	0.41
2:O:206:LEU:HG	2:O:206:LEU:O	2.21	0.41
2:O:408:ALA:O	2:O:409:ASP:C	2.59	0.41
5:R:109:GLU:CD	5:R:123:ASP:HB2	2.41	0.41
1:A:106:MET:HB3	1:A:107:PRO:CD	2.52	0.40
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.87	0.40
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.56	0.40
2:B:212:LYS:HG2	2:B:214:SER:OG	2.21	0.40
3:C:46:ILE:HA	11:C:501:HEM:HMC2	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:323:GLN:O	3:C:326:PHE:HB3	2.21	0.40
3:C:344:VAL:O	3:C:345:GLU:HG3	2.22	0.40
4:D:148:HIS:CE1	4:D:161:ALA:CB	3.04	0.40
5:E:29:SER:CA	5:E:32:ARG:HH21	2.34	0.40
5:E:157:TYR:O	5:E:159:PRO:HD3	2.21	0.40
1:N:191:LYS:C	1:N:193:PRO:HD2	2.41	0.40
2:O:306:PRO:CB	9:V:51:CYS:HA	2.51	0.40
3:P:198:LEU:HD23	3:P:198:LEU:HA	1.90	0.40
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.84	0.40
4:Q:147:LEU:C	4:Q:148:HIS:CD2	2.92	0.40
9:V:49:LEU:HD22	9:V:54:SER:O	2.21	0.40
4:D:66:GLU:C	4:D:68:VAL:H	2.24	0.40
4:D:167:GLU:C	4:D:169:LEU:H	2.25	0.40
6:F:100:GLU:O	6:F:103:GLU:HB3	2.21	0.40
8:H:65:ARG:O	8:H:69:VAL:HG23	2.21	0.40
1:N:159:GLN:HE21	1:N:237:THR:HB	1.87	0.40
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.35	0.40
3:P:31:TRP:HE1	14:P:3004:CDL:H1	1.86	0.40
3:P:238:THR:CB	3:P:239:PRO:HD3	2.48	0.40
4:Q:161:ALA:O	4:Q:162:PRO:C	2.59	0.40
4:Q:238:ARG:NH1	5:R:5:VAL:HG22	2.36	0.40
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.61	0.40
5:R:166:ASP:OD1	5:R:168:SER:N	2.47	0.40
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.02	0.40
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.03	0.40
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.51	0.40
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.49	0.40
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.85	0.40
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.87	0.40
3:P:36:SER:O	3:P:40:VAL:HG23	2.21	0.40
7:T:30:PHE:O	7:T:35:PRO:CD	2.69	0.40
1:A:156:THR:CG2	1:A:157:ALA:N	2.84	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.94	0.40
1:A:261:GLY:HA2	1:A:317:THR:O	2.21	0.40
1:A:361:LEU:O	1:A:364:ALA:HB3	2.22	0.40
2:B:353:THR:HG22	2:B:354:GLU:N	2.36	0.40
2:B:437:ASP:O	2:B:437:ASP:OD1	2.39	0.40
3:C:123:THR:HG21	3:C:190:ILE:HG13	2.03	0.40
5:E:136:VAL:HG21	5:E:181:GLU:HG2	2.04	0.40
1:N:39:VAL:HA	1:N:196:VAL:O	2.22	0.40
1:N:177:LEU:HD22	1:N:181:ASP:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:403:ASP:C	2:O:405:VAL:H	2.25	0.40
3:P:245:LEU:HA	3:P:245:LEU:HD23	1.80	0.40
3:P:350:ILE:CG2	3:P:351:ILE:N	2.84	0.40
4:Q:105:ASN:O	4:Q:106:ASN:CB	2.69	0.40
1:A:4:TYR:OH	1:A:396:ASP:OD2	2.31	0.40
2:B:280:GLY:HA3	2:B:293:SER:OG	2.21	0.40
4:D:116:ILE:CG2	4:D:117:VAL:N	2.85	0.40
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.57	0.40
10:J:20:PHE:CD1	10:J:20:PHE:C	2.94	0.40
1:N:35:CYS:HB2	1:N:200:ALA:O	2.21	0.40
9:V:70:LEU:HD23	9:V:70:LEU:C	2.42	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	442/446 (99%)	391 (88%)	44 (10%)	7 (2%)	9	33
1	N	440/446 (99%)	380 (86%)	49 (11%)	11 (2%)	5	22
2	B	419/441 (95%)	337 (80%)	62 (15%)	20 (5%)	2	11
2	O	420/441 (95%)	351 (84%)	57 (14%)	12 (3%)	4	20
3	C	378/380 (100%)	332 (88%)	37 (10%)	9 (2%)	6	23
3	P	377/380 (99%)	322 (85%)	47 (12%)	8 (2%)	7	26
4	D	239/241 (99%)	212 (89%)	19 (8%)	8 (3%)	4	17
4	Q	239/241 (99%)	213 (89%)	15 (6%)	11 (5%)	2	12
5	E	194/196 (99%)	142 (73%)	32 (16%)	20 (10%)	0	2
5	R	194/196 (99%)	158 (81%)	23 (12%)	13 (7%)	1	6
6	F	99/110 (90%)	89 (90%)	9 (9%)	1 (1%)	15	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	99/110 (90%)	88 (89%)	10 (10%)	1 (1%)	15	45
7	G	78/81 (96%)	63 (81%)	11 (14%)	4 (5%)	2	10
7	T	77/81 (95%)	60 (78%)	13 (17%)	4 (5%)	2	10
8	H	68/77 (88%)	57 (84%)	10 (15%)	1 (2%)	10	35
8	U	65/77 (84%)	48 (74%)	14 (22%)	3 (5%)	2	12
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0	1
9	V	29/47 (62%)	23 (79%)	3 (10%)	3 (10%)	0	2
10	J	59/61 (97%)	46 (78%)	12 (20%)	1 (2%)	9	32
10	W	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1	5
All	All	4003/4160 (96%)	3377 (84%)	481 (12%)	145 (4%)	3	16

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA
2	B	22	GLU
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	227	ARG
2	B	228	SER
2	B	283	PRO
3	C	287	ASN
5	E	102	THR
5	E	115	SER
5	E	127	VAL
5	E	128	LYS
5	E	149	ASN
5	E	150	SER
5	E	177	PRO
7	G	79	ASN
9	I	63	ASP
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
2	O	283	PRO
3	P	287	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	3	LEU
5	R	118	ARG
5	R	137	GLY
5	R	177	PRO
8	U	49	HIS
9	V	63	ASP
10	W	61	ALA
1	A	433	ASP
2	B	31	ASN
2	B	63	LEU
2	B	201	SER
2	B	221	GLU
2	B	269	ALA
2	B	420	GLY
5	E	130	PRO
5	E	137	GLY
5	E	151	GLY
5	E	163	SER
5	E	166	ASP
7	G	45	VAL
8	H	73	LEU
1	N	20	ASP
1	N	206	LYS
1	N	207	GLU
1	N	218	GLY
1	N	282	ARG
2	O	201	SER
4	Q	198	HIS
5	R	8	PRO
5	R	21	ALA
5	R	154	GLY
5	R	163	SER
5	R	166	ASP
5	R	188	VAL
6	S	83	TYR
7	T	3	HIS
7	T	33	ALA
7	T	45	VAL
8	U	73	LEU
1	A	282	ARG
1	A	388	ARG
2	B	30	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	386	ALA
3	C	159	HIS
3	C	288	LYS
4	D	166	ASN
4	D	198	HIS
4	D	233	ARG
5	E	21	ALA
5	E	146	PRO
7	G	33	ALA
9	I	64	LEU
1	N	5	ALA
2	O	24	LEU
2	O	63	LEU
2	O	222	GLN
3	P	288	LYS
4	Q	2	GLU
4	Q	20	ALA
5	R	114	VAL
5	R	149	ASN
5	R	191	ASP
8	U	52	GLU
9	V	60	ALA
9	V	64	LEU
10	W	17	THR
2	B	389	SER
3	C	202	HIS
4	D	106	ASN
4	D	133	GLY
4	D	156	GLN
5	E	120	PRO
5	E	191	ASP
6	F	77	LYS
9	I	73	PRO
10	J	32	GLU
1	N	72	CYS
1	N	81	SER
1	N	388	ARG
3	P	156	TYR
3	P	202	HIS
4	Q	156	GLN
4	Q	162	PRO
4	Q	166	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	233	ARG
10	W	32	GLU
10	W	33	ARG
1	A	72	CYS
3	C	156	TYR
4	D	162	PRO
5	E	154	GLY
7	G	50	PRO
9	I	60	ALA
2	O	384	SER
2	O	389	SER
3	P	5	ILE
4	Q	133	GLY
4	Q	177	ALA
5	R	127	VAL
7	T	50	PRO
1	A	71	PRO
1	A	81	SER
1	A	443	TRP
2	B	190	GLN
3	C	3	PRO
4	D	38	SER
5	E	80	ASP
5	E	110	ALA
1	N	217	SER
3	P	157	ILE
4	Q	106	ASN
3	C	5	ILE
5	E	8	PRO
2	O	19	PRO
3	C	20	ILE
3	P	20	ILE
3	P	3	PRO
2	B	20	GLY
3	C	209	PRO
2	O	420	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%)	341 (93%)	24 (7%)	16	43
1	N	365/368 (99%)	341 (93%)	24 (7%)	16	43
2	B	331/347 (95%)	308 (93%)	23 (7%)	15	42
2	O	333/347 (96%)	314 (94%)	19 (6%)	20	49
3	C	328/329 (100%)	313 (95%)	15 (5%)	27	57
3	P	328/329 (100%)	314 (96%)	14 (4%)	29	59
4	D	200/200 (100%)	196 (98%)	4 (2%)	55	78
4	Q	200/200 (100%)	196 (98%)	4 (2%)	55	78
5	E	166/166 (100%)	158 (95%)	8 (5%)	25	55
5	R	165/166 (99%)	159 (96%)	6 (4%)	35	65
6	F	93/96 (97%)	90 (97%)	3 (3%)	39	68
6	S	93/96 (97%)	88 (95%)	5 (5%)	22	51
7	G	71/71 (100%)	67 (94%)	4 (6%)	21	49
7	T	70/71 (99%)	68 (97%)	2 (3%)	42	70
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	83
8	U	63/71 (89%)	61 (97%)	2 (3%)	39	68
9	I	23/26 (88%)	20 (87%)	3 (13%)	4	15
9	V	23/26 (88%)	21 (91%)	2 (9%)	10	33
10	J	49/49 (100%)	46 (94%)	3 (6%)	18	46
10	W	47/49 (96%)	46 (98%)	1 (2%)	53	77
All	All	3378/3446 (98%)	3211 (95%)	167 (5%)	25	55

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	34	THR
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	102	LEU
1	A	106	MET
1	A	108	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	THR
1	A	174	ILE
1	A	179	ARG
1	A	181	ASP
1	A	220	SER
1	A	226	ASP
1	A	248	LEU
1	A	274	ASN
1	A	307	PHE
1	A	342	TRP
1	A	344	ARG
1	A	350	THR
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	24	LEU
2	B	31	ASN
2	B	57	TYR
2	B	97	SER
2	B	104	LYS
2	B	114	ASP
2	B	154	SER
2	B	170	THR
2	B	239	TYR
2	B	248	ASN
2	B	250	HIS
2	B	270	ASN
2	B	283	PRO
2	B	296	TYR
2	B	304	THR
2	B	325	TYR
2	B	341	MET
2	B	343	GLN
2	B	344	LEU
2	B	376	GLN
2	B	402	ILE
2	B	424	MET
3	C	44	THR
3	C	81	ARG
3	C	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	91	PHE
3	C	149	ASN
3	C	175	THR
3	C	184	PHE
3	C	216	SER
3	C	223	PRO
3	C	226	SER
3	C	240	PHE
3	C	243	LEU
3	C	277	PHE
3	C	367	PHE
3	C	380	TYR
4	D	43	MET
4	D	169	LEU
4	D	173	ASP
4	D	215	LEU
5	E	6	THR
5	E	31	ASP
5	E	52	LYS
5	E	61	SER
5	E	80	ASP
5	E	131	GLU
5	E	178	TYR
5	E	185	TYR
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
7	G	3	HIS
7	G	63	THR
7	G	79	ASN
7	G	80	ASP
8	H	49	HIS
9	I	68	ILE
9	I	70	LEU
9	I	71	ASN
10	J	22	LEU
10	J	59	TYR
10	J	64	GLU
1	N	3	THR
1	N	10	ASN
1	N	18	THR
1	N	49	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	58	PHE
1	N	86	PHE
1	N	102	LEU
1	N	106	MET
1	N	108	LYS
1	N	174	ILE
1	N	179	ARG
1	N	181	ASP
1	N	220	SER
1	N	248	LEU
1	N	274	ASN
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	350	THR
1	N	376	CYS
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	22	GLU
2	O	31	ASN
2	O	57	TYR
2	O	104	LYS
2	O	114	ASP
2	O	154	SER
2	O	239	TYR
2	O	248	ASN
2	O	250	HIS
2	O	283	PRO
2	O	296	TYR
2	O	304	THR
2	O	325	TYR
2	O	341	MET
2	O	343	GLN
2	O	344	LEU
2	O	376	GLN
2	O	402	ILE
2	O	424	MET
3	P	44	THR
3	P	81	ARG
3	P	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	149	ASN
3	P	175	THR
3	P	184	PHE
3	P	216	SER
3	P	226	SER
3	P	240	PHE
3	P	243	LEU
3	P	283	ARG
3	P	367	PHE
3	P	374	GLU
3	P	380	TYR
4	Q	43	MET
4	Q	76	GLU
4	Q	169	LEU
4	Q	215	LEU
5	R	6	THR
5	R	31	ASP
5	R	61	SER
5	R	178	TYR
5	R	185	TYR
5	R	188	VAL
6	S	13	MET
6	S	58	ARG
6	S	59	MET
6	S	64	ARG
6	S	70	LEU
7	T	3	HIS
7	T	63	THR
8	U	49	HIS
8	U	71	HIS
9	V	68	ILE
9	V	70	LEU
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	159	GLN
1	A	173	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	197	ASN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
8	H	71	HIS
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	159	GLN
1	N	173	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
1	N	435	ASN
2	O	31	ASN
2	O	156	GLN
2	O	197	ASN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	105	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	164	HIS
5	R	186	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	75	ASN

5.3.3 RNA ⓘ

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](#)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEE	C	2007	-	48,48,50	1.40	7 (14%)	51,53,55	0.82	2 (3%)
14	CDL	P	3004	-	39,39,99	1.25	3 (7%)	45,51,111	1.11	4 (8%)
19	FES	E	501	5	0,4,4	-	-	-		
14	CDL	C	2004	-	39,39,99	1.22	2 (5%)	45,51,111	1.10	4 (8%)
11	HEM	P	502	3	41,50,50	1.72	8 (19%)	45,82,82	1.86	10 (22%)
13	UQ	P	3002	-	19,19,63	2.60	10 (52%)	23,26,79	1.42	4 (17%)
15	PEE	C	2008	-	20,20,50	1.85	6 (30%)	23,25,55	0.65	0
17	HEC	Q	501	4	32,50,50	2.05	3 (9%)	24,82,82	1.53	4 (16%)
16	GOL	P	3011	-	5,5,5	1.34	0	5,5,5	0.61	0
15	PEE	P	3008	-	4,4,50	3.56	4 (100%)	6,6,55	0.59	0
17	HEC	D	501	4	32,50,50	2.54	6 (18%)	24,82,82	1.71	6 (25%)
18	BOG	Q	3091	-	13,13,20	1.58	3 (23%)	18,18,25	1.11	2 (11%)
19	FES	R	501	5	0,4,4	-	-	-		
15	PEE	P	3007	-	48,48,50	1.38	6 (12%)	51,53,55	0.79	2 (3%)
18	BOG	D	2009	-	20,20,20	1.09	1 (5%)	25,25,25	0.92	1 (4%)
16	GOL	C	2011	-	5,5,5	1.58	1 (20%)	5,5,5	0.77	0
14	CDL	D	2003	-	41,41,99	1.21	2 (4%)	47,53,111	1.06	2 (4%)
15	PEE	E	2005	-	49,49,50	1.51	10 (20%)	52,54,55	0.88	3 (5%)
11	HEM	C	501	3	41,50,50	1.46	5 (12%)	45,82,82	1.70	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	UQ	C	2002	-	19,19,63	2.67	10 (52%)	23,26,79	1.43	4 (17%)
18	BOG	Q	3009	-	20,20,20	1.14	3 (15%)	25,25,25	1.00	1 (4%)
11	HEM	P	501	3	41,50,50	1.58	7 (17%)	45,82,82	1.69	9 (20%)
18	BOG	P	2010	-	12,12,20	1.44	4 (33%)	17,17,25	0.59	0
11	HEM	C	502	3	41,50,50	1.80	8 (19%)	45,82,82	2.01	11 (24%)
14	CDL	Q	3003	-	41,41,99	1.21	3 (7%)	47,53,111	1.04	2 (4%)
12	IKR	C	2001	-	25,26,26	1.65	6 (24%)	31,35,35	1.27	5 (16%)
12	IKR	P	3001	-	25,26,26	1.46	5 (20%)	31,35,35	1.33	5 (16%)
15	PEE	R	3005	-	49,49,50	1.59	10 (20%)	52,54,55	0.89	3 (5%)
18	BOG	D	2091	-	13,13,20	1.49	4 (30%)	18,18,25	1.17	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEE	C	2007	-	-	26/52/52/54	-
14	CDL	P	3004	-	-	21/49/49/110	-
19	FES	E	501	5	-	-	0/1/1/1
14	CDL	C	2004	-	-	22/49/49/110	-
11	HEM	P	502	3	-	7/12/54/54	-
13	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
15	PEE	C	2008	-	-	9/24/24/54	-
17	HEC	Q	501	4	-	6/10/54/54	-
16	GOL	P	3011	-	-	4/4/4/4	-
17	HEC	D	501	4	-	6/10/54/54	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
15	PEE	P	3007	-	-	26/52/52/54	-
18	BOG	D	2009	-	-	5/11/31/31	0/1/1/1
16	GOL	C	2011	-	-	3/4/4/4	-
14	CDL	D	2003	-	-	18/51/51/110	-
15	PEE	E	2005	-	-	27/53/53/54	-
11	HEM	C	501	3	-	7/12/54/54	-
13	UQ	C	2002	-	-	4/11/35/87	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
11	HEM	P	501	3	-	7/12/54/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
11	HEM	C	502	3	-	7/12/54/54	-
14	CDL	Q	3003	-	-	20/51/51/110	-
12	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
12	IKR	P	3001	-	-	0/18/18/18	0/2/2/2
15	PEE	R	3005	-	-	22/53/53/54	-
18	BOG	D	2091	-	-	3/4/24/31	0/1/1/1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C2B-C3B	-9.85	1.30	1.40
17	Q	501	HEC	C2B-C3B	-8.26	1.32	1.40
17	D	501	HEC	C3C-C2C	-7.60	1.32	1.40
13	P	3002	UQ	C7-C6	5.56	1.60	1.51
11	C	502	HEM	C3C-C2C	-5.40	1.32	1.40
17	Q	501	HEC	C3C-C2C	-5.36	1.35	1.40
13	C	2002	UQ	C7-C6	5.18	1.59	1.51
15	P	3008	PEE	P-O1P	4.82	1.62	1.50
13	P	3002	UQ	C6-C5	4.81	1.44	1.35
13	C	2002	UQ	C6-C5	4.53	1.43	1.35
11	P	502	HEM	CBB-CAB	4.45	1.52	1.30
11	P	501	HEM	CBB-CAB	4.43	1.52	1.30
11	C	502	HEM	CBB-CAB	4.29	1.51	1.30
11	P	502	HEM	C3C-CAC	-4.29	1.39	1.47
15	C	2007	PEE	C39-C38	4.12	1.55	1.31
15	P	3007	PEE	C39-C38	4.10	1.55	1.31
15	R	3005	PEE	C39-C38	4.05	1.55	1.31
15	E	2005	PEE	C39-C38	4.04	1.55	1.31
11	P	501	HEM	C3C-CAC	-4.03	1.39	1.47
13	C	2002	UQ	C6-C1	3.97	1.57	1.46
15	R	3005	PEE	O2-C10	3.84	1.45	1.34
13	C	2002	UQ	O3-C3	3.78	1.46	1.36
11	C	501	HEM	C3C-CAC	-3.70	1.40	1.47
11	C	502	HEM	C3C-CAC	-3.68	1.40	1.47
13	P	3002	UQ	C6-C1	3.64	1.56	1.46
11	P	501	HEM	CBC-CAC	3.50	1.52	1.29
11	C	501	HEM	CBB-CAB	3.49	1.47	1.30
11	C	501	HEM	CBC-CAC	3.48	1.52	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2008	PEE	O2-C10	3.46	1.44	1.34
12	C	2001	IKR	C40-C2	3.45	1.57	1.51
15	E	2005	PEE	O2-C10	3.40	1.43	1.34
13	P	3002	UQ	O3-C3	3.37	1.45	1.36
15	E	2005	PEE	O3-C30	3.30	1.43	1.33
15	P	3008	PEE	P-O3P	3.30	1.64	1.54
15	P	3008	PEE	P-O4P	3.26	1.64	1.54
15	R	3005	PEE	C11-C10	3.24	1.60	1.50
15	R	3005	PEE	O3-C30	3.24	1.42	1.33
11	C	501	HEM	CAB-C3B	-3.23	1.38	1.47
15	C	2007	PEE	O3-C30	3.23	1.42	1.33
15	P	3007	PEE	O3-C30	3.19	1.42	1.33
11	C	502	HEM	CBC-CAC	3.16	1.50	1.29
15	C	2008	PEE	O3-C30	3.14	1.42	1.33
15	R	3005	PEE	P-O1P	3.13	1.62	1.50
15	C	2008	PEE	P-O1P	3.12	1.62	1.50
11	P	502	HEM	CBC-CAC	3.10	1.49	1.29
11	P	502	HEM	CAB-C3B	-3.09	1.39	1.47
11	C	502	HEM	CAB-C3B	-3.08	1.39	1.47
15	C	2007	PEE	P-O1P	3.05	1.61	1.50
12	C	2001	IKR	C24-C17	3.02	1.44	1.39
15	E	2005	PEE	P-O1P	3.00	1.61	1.50
13	C	2002	UQ	C3-C4	2.99	1.57	1.48
12	C	2001	IKR	C21-C20	2.98	1.44	1.39
15	P	3007	PEE	C21-C22	-2.96	1.35	1.51
15	P	3007	PEE	O2-C10	2.93	1.42	1.34
15	E	2005	PEE	C11-C10	2.92	1.59	1.50
12	P	3001	IKR	C40-C2	2.89	1.56	1.51
15	P	3007	PEE	P-O1P	2.88	1.61	1.50
13	C	2002	UQ	C2-C1	2.87	1.57	1.48
13	C	2002	UQ	O2-C2	2.86	1.43	1.36
15	C	2007	PEE	O2-C10	2.86	1.42	1.34
11	P	501	HEM	CAB-C3B	-2.86	1.39	1.47
12	C	2001	IKR	C3-C4	2.85	1.44	1.38
15	R	3005	PEE	C21-C22	-2.80	1.35	1.51
18	Q	3091	BOG	O5-C1	2.79	1.48	1.41
11	C	502	HEM	C3B-C4B	2.74	1.50	1.44
15	E	2005	PEE	C21-C22	-2.73	1.36	1.51
13	C	2002	UQ	C7-C8	2.72	1.54	1.50
12	P	3001	IKR	C3-C4	2.71	1.43	1.38
18	Q	3091	BOG	C4-C5	2.71	1.58	1.53
15	C	2007	PEE	C21-C22	-2.69	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3002	UQ	C2-C1	2.69	1.56	1.48
12	P	3001	IKR	C24-C17	2.68	1.44	1.39
13	P	3002	UQ	C7-C8	2.68	1.54	1.50
17	D	501	HEC	C2A-C1A	2.67	1.48	1.42
11	P	502	HEM	C1B-C2B	2.66	1.49	1.44
13	P	3002	UQ	C5-C4	2.65	1.56	1.47
18	D	2091	BOG	O5-C1	2.63	1.48	1.41
13	P	3002	UQ	C3-C4	2.62	1.56	1.48
15	E	2005	PEE	C31-C30	2.59	1.58	1.50
12	P	3001	IKR	C21-C20	2.48	1.43	1.39
12	C	2001	IKR	C1-I1	-2.48	2.04	2.10
13	C	2002	UQ	C5-C4	2.48	1.56	1.47
18	Q	3009	BOG	O5-C1	2.45	1.48	1.41
18	D	2091	BOG	C4-C5	2.44	1.58	1.53
15	P	3008	PEE	P-O2P	2.44	1.61	1.54
15	R	3005	PEE	C31-C30	2.42	1.57	1.50
11	P	502	HEM	CAA-C2A	2.42	1.55	1.52
14	C	2004	CDL	CB3-CB4	2.42	1.58	1.50
15	C	2008	PEE	C11-C10	2.41	1.57	1.50
15	C	2008	PEE	C1-C2	2.40	1.58	1.50
11	C	502	HEM	C1B-C2B	2.37	1.49	1.44
17	D	501	HEC	C1D-CHD	-2.37	1.34	1.41
13	P	3002	UQ	CM5-C5	2.35	1.55	1.50
13	C	2002	UQ	CM5-C5	2.34	1.55	1.50
15	R	3005	PEE	C3-C2	2.34	1.57	1.50
14	P	3004	CDL	CB3-CB4	2.34	1.57	1.50
13	P	3002	UQ	O2-C2	2.33	1.42	1.36
14	P	3004	CDL	O1-C1	2.33	1.50	1.43
18	Q	3091	BOG	O5-C5	2.32	1.50	1.44
14	C	2004	CDL	O1-C1	2.31	1.50	1.43
11	C	502	HEM	C4D-C3D	2.30	1.49	1.45
18	P	2010	BOG	C4-C5	2.27	1.57	1.53
14	D	2003	CDL	OA6-CA5	2.27	1.40	1.34
14	D	2003	CDL	O1-C1	2.25	1.50	1.43
16	C	2011	GOL	O2-C2	2.25	1.50	1.43
18	D	2009	BOG	O5-C1	2.24	1.47	1.41
17	D	501	HEC	C3A-C4A	2.23	1.47	1.42
15	R	3005	PEE	C1-C2	2.22	1.57	1.50
15	C	2008	PEE	C3-C2	2.21	1.57	1.50
12	C	2001	IKR	C20-C17	2.21	1.43	1.40
11	P	502	HEM	C3B-C4B	2.20	1.49	1.44
11	P	502	HEM	CMB-C2B	2.20	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	2010	BOG	C4-C3	2.20	1.57	1.52
18	P	2010	BOG	O5-C1	2.20	1.48	1.42
11	P	501	HEM	C2C-C1C	2.19	1.47	1.42
18	Q	3009	BOG	C1-C2	2.17	1.58	1.52
15	R	3005	PEE	P-O4P	2.17	1.68	1.59
14	Q	3003	CDL	O1-C1	2.16	1.49	1.43
11	C	501	HEM	C2C-C1C	2.14	1.47	1.42
18	Q	3009	BOG	C4-C5	2.13	1.57	1.53
18	P	2010	BOG	C1-C2	2.13	1.57	1.52
18	D	2091	BOG	C1-C2	2.12	1.58	1.52
12	P	3001	IKR	C20-C17	2.12	1.43	1.40
14	Q	3003	CDL	OA6-CA5	2.12	1.40	1.34
15	E	2005	PEE	P-O4P	2.12	1.67	1.59
15	E	2005	PEE	C3-C2	2.11	1.57	1.50
17	D	501	HEC	C4B-C3B	2.08	1.46	1.43
15	E	2005	PEE	C1-C2	2.08	1.57	1.50
15	C	2007	PEE	C31-C30	2.08	1.56	1.50
11	P	501	HEM	CHD-C1D	-2.07	1.35	1.41
18	D	2091	BOG	C4-C3	2.05	1.57	1.52
11	P	501	HEM	CMD-C2D	2.02	1.55	1.50
15	P	3007	PEE	C3-C2	2.02	1.56	1.50
17	Q	501	HEC	C4D-CHA	-2.01	1.35	1.41
15	C	2007	PEE	C3-C2	2.01	1.56	1.50
14	P	3004	CDL	OB8-CB7	2.01	1.39	1.33
14	Q	3003	CDL	OB5-CB3	-2.00	1.37	1.44

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	502	HEM	C3B-C2B-C1B	-6.68	101.53	106.49
11	P	502	HEM	C3B-C2B-C1B	-6.39	101.75	106.49
11	C	501	HEM	CBA-CAA-C2A	-5.91	102.54	112.62
11	C	502	HEM	CMB-C2B-C1B	4.73	132.24	125.04
11	P	501	HEM	CBA-CAA-C2A	-4.62	104.73	112.62
13	C	2002	UQ	C8-C7-C6	4.38	123.86	112.05
17	Q	501	HEC	CBA-CAA-C2A	4.35	119.93	112.60
13	P	3002	UQ	C8-C7-C6	4.25	123.50	112.05
11	C	502	HEM	C4A-C3A-C2A	-4.19	104.08	107.00
17	D	501	HEC	CMC-C2C-C3C	-4.18	120.90	125.82
11	P	501	HEM	C3B-C2B-C1B	-4.03	103.50	106.49
18	Q	3009	BOG	C1'-O1-C1	3.96	120.41	113.84
11	C	502	HEM	C2B-C1B-NB	3.86	114.41	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	502	HEM	CMB-C2B-C1B	3.79	130.81	125.04
18	D	2091	BOG	C1'-O1-C1	3.62	118.86	113.27
18	D	2009	BOG	C1'-O1-C1	3.56	119.74	113.84
13	P	3002	UQ	C7-C6-C1	-3.48	114.29	118.48
18	Q	3091	BOG	C1'-O1-C1	3.48	118.64	113.27
13	C	2002	UQ	C7-C6-C1	-3.38	114.41	118.48
17	D	501	HEC	CBA-CAA-C2A	3.33	118.22	112.60
11	C	501	HEM	CAD-C3D-C4D	3.28	130.39	124.66
12	P	3001	IKR	C40-C2-C3	-3.23	113.52	119.49
11	P	502	HEM	C4A-C3A-C2A	-3.21	104.76	107.00
15	E	2005	PEE	C22-C21-C20	3.21	127.77	113.79
11	P	502	HEM	C2B-C1B-NB	3.21	113.64	109.84
15	R	3005	PEE	C22-C21-C20	3.15	127.52	113.79
11	P	502	HEM	CBA-CAA-C2A	3.15	117.99	112.62
11	C	502	HEM	C4B-CHC-C1C	3.09	126.64	122.56
14	P	3004	CDL	CB4-OB6-CB5	-3.06	110.25	117.79
11	P	501	HEM	CAD-C3D-C4D	3.04	129.97	124.66
15	C	2007	PEE	C22-C21-C20	3.04	127.04	113.79
11	C	502	HEM	C4C-CHD-C1D	3.03	126.56	122.56
14	C	2004	CDL	CB4-OB6-CB5	-3.00	110.40	117.79
12	C	2001	IKR	C40-C2-C3	-2.96	114.02	119.49
17	Q	501	HEC	CMC-C2C-C3C	-2.90	122.41	125.82
11	C	501	HEM	C4B-CHC-C1C	2.90	126.38	122.56
11	P	502	HEM	C2C-C3C-C4C	-2.88	104.89	106.90
17	D	501	HEC	CMC-C2C-C1C	2.84	132.82	128.46
11	P	501	HEM	C4C-CHD-C1D	2.82	126.28	122.56
12	P	3001	IKR	C3-C2-C1	2.82	119.48	117.21
11	P	501	HEM	C2B-C1B-NB	2.81	113.17	109.84
11	P	502	HEM	CAD-C3D-C2D	-2.80	122.66	127.88
15	P	3007	PEE	C22-C21-C20	2.79	125.97	113.79
14	D	2003	CDL	CB4-OB6-CB5	-2.67	111.21	117.79
11	C	502	HEM	CAD-C3D-C2D	-2.67	122.91	127.88
11	C	501	HEM	CAD-C3D-C2D	-2.66	122.92	127.88
14	P	3004	CDL	CA6-CA4-CA3	-2.66	105.50	111.79
18	D	2091	BOG	O1-C1-C2	2.65	111.26	108.15
11	C	501	HEM	C3B-C2B-C1B	-2.65	104.52	106.49
12	P	3001	IKR	O31-C30-O36	2.64	128.62	123.53
15	C	2007	PEE	C21-C22-C23	2.61	127.69	114.42
11	P	501	HEM	C2D-C1D-ND	2.61	113.01	109.88
14	C	2004	CDL	CA4-OA6-CA5	-2.60	111.38	117.79
11	P	502	HEM	CAD-C3D-C4D	2.60	129.21	124.66
11	C	502	HEM	CAD-C3D-C4D	2.57	129.14	124.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	501	HEM	CAD-C3D-C2D	-2.56	123.11	127.88
15	E	2005	PEE	C21-C22-C23	2.49	127.09	114.42
12	C	2001	IKR	O31-C30-O36	2.48	128.31	123.53
15	P	3007	PEE	C21-C22-C23	2.47	126.98	114.42
12	C	2001	IKR	C3-C2-C1	2.47	119.20	117.21
15	R	3005	PEE	C21-C22-C23	2.47	126.94	114.42
18	Q	3091	BOG	O1-C1-C2	2.46	111.03	108.15
17	D	501	HEC	CAA-C2A-C3A	-2.45	120.22	127.25
12	P	3001	IKR	O15-C4-C5	2.44	119.73	115.10
11	P	502	HEM	C4C-CHD-C1D	2.41	125.75	122.56
14	Q	3003	CDL	CB4-OB6-CB5	-2.41	111.85	117.79
12	C	2001	IKR	O15-C4-C5	2.41	119.67	115.10
14	C	2004	CDL	CA6-CA4-CA3	-2.40	106.11	111.79
14	D	2003	CDL	CA6-CA4-CA3	-2.40	106.12	111.79
11	C	501	HEM	C3D-C4D-ND	2.31	112.74	110.17
14	Q	3003	CDL	CA6-CA4-CA3	-2.30	106.34	111.79
11	C	501	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
12	P	3001	IKR	O31-C30-C29	-2.30	109.19	111.83
12	C	2001	IKR	O31-C30-C29	-2.29	109.20	111.83
11	C	501	HEM	C4D-ND-C1D	-2.29	102.71	105.07
14	P	3004	CDL	OB6-CB4-CB3	2.26	116.58	108.40
14	P	3004	CDL	CA4-OA6-CA5	-2.24	112.26	117.79
17	Q	501	HEC	CBD-CAD-C3D	2.23	116.43	112.62
14	C	2004	CDL	OB6-CB4-CB3	2.22	116.45	108.40
11	C	502	HEM	C1B-NB-C4B	-2.20	102.80	105.07
13	P	3002	UQ	C10-C9-C8	-2.20	118.05	123.68
11	P	501	HEM	C4B-CHC-C1C	2.19	125.45	122.56
13	C	2002	UQ	C10-C9-C8	-2.17	118.11	123.68
11	C	501	HEM	C2B-C1B-NB	2.15	112.39	109.84
13	C	2002	UQ	C11-C9-C8	2.15	125.82	120.50
17	D	501	HEC	CMB-C2B-C3B	-2.15	123.30	125.82
11	P	502	HEM	C4B-CHC-C1C	2.15	125.39	122.56
15	R	3005	PEE	O3-C3-C2	2.14	114.66	108.43
17	D	501	HEC	CBD-CAD-C3D	2.13	116.26	112.62
11	C	502	HEM	C4D-ND-C1D	-2.11	102.89	105.07
11	P	501	HEM	C1D-C2D-C3D	-2.09	104.75	106.96
17	Q	501	HEC	CAA-C2A-C3A	-2.09	121.24	127.25
13	P	3002	UQ	C11-C9-C8	2.05	125.58	120.50
11	C	502	HEM	C2D-C1D-ND	2.05	112.34	109.88
15	E	2005	PEE	O3-C3-C2	2.03	114.36	108.43
11	C	501	HEM	C2D-C1D-ND	2.02	112.30	109.88

There are no chirality outliers.

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	2002	UQ	C1-C6-C7-C8
13	C	2002	UQ	C5-C6-C7-C8
13	C	2002	UQ	C12-C11-C9-C8
13	C	2002	UQ	C12-C11-C9-C10
13	P	3002	UQ	C1-C6-C7-C8
13	P	3002	UQ	C5-C6-C7-C8
13	P	3002	UQ	C12-C11-C9-C8
13	P	3002	UQ	C12-C11-C9-C10
14	C	2004	CDL	CB2-C1-CA2-OA2
14	C	2004	CDL	CB3-OB5-PB2-OB3
14	C	2004	CDL	C51-CB5-OB6-CB4
14	P	3004	CDL	CB2-C1-CA2-OA2
14	P	3004	CDL	CA2-C1-CB2-OB2
14	P	3004	CDL	CB3-OB5-PB2-OB3
14	P	3004	CDL	C51-CB5-OB6-CB4
15	C	2007	PEE	C1-O3P-P-O2P
15	C	2007	PEE	C1-O3P-P-O1P
15	C	2007	PEE	C4-O4P-P-O2P
15	C	2007	PEE	C4-O4P-P-O1P
15	C	2007	PEE	O4P-C4-C5-N
15	C	2008	PEE	C4-O4P-P-O3P
15	C	2008	PEE	C4-O4P-P-O2P
15	C	2008	PEE	C4-O4P-P-O1P
15	E	2005	PEE	C11-C10-O2-C2
15	E	2005	PEE	C1-O3P-P-O2P
15	E	2005	PEE	C1-O3P-P-O1P
15	E	2005	PEE	O4P-C4-C5-N
15	P	3007	PEE	C1-O3P-P-O2P
15	P	3007	PEE	C1-O3P-P-O1P
15	P	3007	PEE	C4-O4P-P-O2P
15	P	3007	PEE	C4-O4P-P-O1P
15	P	3007	PEE	O4P-C4-C5-N
15	R	3005	PEE	C11-C10-O2-C2
15	R	3005	PEE	C1-O3P-P-O2P
15	R	3005	PEE	C1-O3P-P-O1P
15	R	3005	PEE	O4P-C4-C5-N
16	C	2011	GOL	O1-C1-C2-C3
16	P	3011	GOL	O1-C1-C2-C3
17	D	501	HEC	C1A-C2A-CAA-CBA
17	D	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	D	2009	BOG	C2-C1-O1-C1'
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	C2-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
14	D	2003	CDL	C31-CA7-OA8-CA6
14	Q	3003	CDL	C31-CA7-OA8-CA6
15	C	2008	PEE	O5-C30-O3-C3
14	C	2004	CDL	OB9-CB7-OB8-CB6
14	P	3004	CDL	OB9-CB7-OB8-CB6
15	E	2005	PEE	O5-C30-O3-C3
15	R	3005	PEE	O5-C30-O3-C3
14	D	2003	CDL	OA9-CA7-OA8-CA6
15	E	2005	PEE	O4-C10-O2-C2
15	R	3005	PEE	O4-C10-O2-C2
15	C	2008	PEE	C31-C30-O3-C3
15	E	2005	PEE	C31-C30-O3-C3
15	R	3005	PEE	C31-C30-O3-C3
14	Q	3003	CDL	OA9-CA7-OA8-CA6
14	C	2004	CDL	C31-CA7-OA8-CA6
14	P	3004	CDL	C31-CA7-OA8-CA6
14	C	2004	CDL	C71-CB7-OB8-CB6
14	P	3004	CDL	C71-CB7-OB8-CB6
14	C	2004	CDL	OB7-CB5-OB6-CB4
14	P	3004	CDL	OB7-CB5-OB6-CB4
14	C	2004	CDL	O1-C1-CA2-OA2
14	P	3004	CDL	O1-C1-CA2-OA2
14	C	2004	CDL	OA9-CA7-OA8-CA6
18	Q	3091	BOG	O5-C5-C6-O6
14	D	2003	CDL	C71-CB7-OB8-CB6
14	Q	3003	CDL	C71-CB7-OB8-CB6
18	D	2091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	C4-C5-C6-O6
18	D	2091	BOG	O5-C1-O1-C1'
14	P	3004	CDL	OA9-CA7-OA8-CA6
14	D	2003	CDL	OB9-CB7-OB8-CB6
15	R	3005	PEE	C30-C31-C32-C33
18	Q	3009	BOG	O1-C1'-C2'-C3'
18	D	2009	BOG	O1-C1'-C2'-C3'
15	E	2005	PEE	C30-C31-C32-C33
14	Q	3003	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	2007	PEE	C17-C18-C19-C20
15	P	3007	PEE	C17-C18-C19-C20
14	D	2003	CDL	CA2-OA2-PA1-OA5
14	Q	3003	CDL	CA2-OA2-PA1-OA5
15	C	2007	PEE	C1-O3P-P-O4P
15	C	2007	PEE	C4-O4P-P-O3P
15	E	2005	PEE	C1-O3P-P-O4P
15	P	3007	PEE	C1-O3P-P-O4P
15	P	3007	PEE	C4-O4P-P-O3P
15	R	3005	PEE	C1-O3P-P-O4P
14	C	2004	CDL	C11-CA5-OA6-CA4
14	C	2004	CDL	OA7-CA5-OA6-CA4
15	C	2007	PEE	C10-C11-C12-C13
15	R	3005	PEE	C22-C23-C24-C25
14	P	3004	CDL	OA7-CA5-OA6-CA4
14	P	3004	CDL	C11-CA5-OA6-CA4
15	C	2007	PEE	C15-C16-C17-C18
15	E	2005	PEE	C35-C36-C37-C38
15	P	3007	PEE	C15-C16-C17-C18
15	R	3005	PEE	C35-C36-C37-C38
15	P	3007	PEE	C10-C11-C12-C13
15	E	2005	PEE	C22-C23-C24-C25
15	E	2005	PEE	C20-C21-C22-C23
15	R	3005	PEE	C34-C35-C36-C37
15	C	2007	PEE	C33-C34-C35-C36
15	E	2005	PEE	C34-C35-C36-C37
15	P	3007	PEE	C33-C34-C35-C36
15	R	3005	PEE	C20-C21-C22-C23
15	C	2008	PEE	C10-C11-C12-C13
15	C	2007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C20-C21-C22-C23
14	C	2004	CDL	CA2-C1-CB2-OB2
15	C	2007	PEE	C20-C21-C22-C23
14	Q	3003	CDL	CB7-C71-C72-C73
15	P	3007	PEE	C40-C41-C42-C43
14	D	2003	CDL	CB7-C71-C72-C73
15	R	3005	PEE	C11-C12-C13-C14
15	C	2007	PEE	O3P-C1-C2-O2
15	P	3007	PEE	O3P-C1-C2-O2
18	Q	3009	BOG	C2'-C3'-C4'-C5'
15	P	3007	PEE	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	E	2005	PEE	C11-C12-C13-C14
11	C	502	HEM	C4D-C3D-CAD-CBD
15	C	2007	PEE	C40-C41-C42-C43
14	P	3004	CDL	CB3-OB5-PB2-OB2
14	C	2004	CDL	CA3-CA4-CA6-OA8
14	P	3004	CDL	CA3-CA4-CA6-OA8
15	C	2007	PEE	C11-C12-C13-C14
18	D	2009	BOG	C2'-C3'-C4'-C5'
16	C	2011	GOL	O1-C1-C2-O2
16	P	3011	GOL	O1-C1-C2-O2
15	E	2005	PEE	O3P-C1-C2-O2
15	C	2007	PEE	C39-C40-C41-C42
14	D	2003	CDL	OA6-CA4-CA6-OA8
14	Q	3003	CDL	OA6-CA4-CA6-OA8
15	R	3005	PEE	C42-C43-C44-C45
15	C	2007	PEE	C43-C44-C45-C46
15	E	2005	PEE	C43-C44-C45-C46
15	R	3005	PEE	C43-C44-C45-C46
15	P	3007	PEE	C11-C12-C13-C14
15	P	3007	PEE	C43-C44-C45-C46
14	P	3004	CDL	O1-C1-CB2-OB2
11	C	501	HEM	C3D-CAD-CBD-CGD
14	Q	3003	CDL	C71-C72-C73-C74
14	D	2003	CDL	CA3-CA4-CA6-OA8
14	Q	3003	CDL	CA3-CA4-CA6-OA8
14	D	2003	CDL	C71-C72-C73-C74
14	Q	3003	CDL	CA3-OA5-PA1-OA2
14	C	2004	CDL	OB5-CB3-CB4-OB6
14	P	3004	CDL	OB5-CB3-CB4-OB6
15	C	2007	PEE	O3P-C1-C2-C3
15	C	2008	PEE	O3P-C1-C2-C3
15	P	3007	PEE	O3P-C1-C2-C3
15	E	2005	PEE	C42-C43-C44-C45
11	C	501	HEM	C2B-C3B-CAB-CBB
11	C	502	HEM	C2B-C3B-CAB-CBB
11	P	502	HEM	C2B-C3B-CAB-CBB
15	R	3005	PEE	O3P-C1-C2-O2
11	P	502	HEM	C4D-C3D-CAD-CBD
15	C	2008	PEE	O2-C2-C3-O3
16	C	2011	GOL	O2-C2-C3-O3
16	P	3011	GOL	O2-C2-C3-O3
15	R	3005	PEE	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	C	2004	CDL	CA3-OA5-PA1-OA2
14	C	2004	CDL	CB3-OB5-PB2-OB2
14	Q	3003	CDL	CB2-OB2-PB2-OB5
14	C	2004	CDL	CA3-OA5-PA1-OA3
14	C	2004	CDL	CB3-OB5-PB2-OB4
14	D	2003	CDL	CA2-OA2-PA1-OA4
14	P	3004	CDL	CA3-OA5-PA1-OA3
14	P	3004	CDL	CB3-OB5-PB2-OB4
14	Q	3003	CDL	CA2-OA2-PA1-OA4
15	E	2005	PEE	C4-O4P-P-O2P
14	C	2004	CDL	OB5-CB3-CB4-CB6
15	E	2005	PEE	C39-C40-C41-C42
11	P	501	HEM	C3D-CAD-CBD-CGD
14	P	3004	CDL	OB5-CB3-CB4-CB6
15	P	3007	PEE	C21-C22-C23-C24
14	Q	3003	CDL	OA5-CA3-CA4-OA6
14	C	2004	CDL	OA6-CA4-CA6-OA8
14	P	3004	CDL	OA6-CA4-CA6-OA8
14	D	2003	CDL	CA3-OA5-PA1-OA2
14	D	2003	CDL	CB2-OB2-PB2-OB5
14	D	2003	CDL	CB3-OB5-PB2-OB2
14	Q	3003	CDL	CB3-OB5-PB2-OB2
15	C	2008	PEE	C1-C2-C3-O3
15	C	2007	PEE	C21-C22-C23-C24
15	C	2007	PEE	C41-C42-C43-C44
15	C	2007	PEE	C34-C35-C36-C37
11	P	502	HEM	CAA-CBA-CGA-O1A
15	E	2005	PEE	C1-C2-O2-C10
15	R	3005	PEE	C1-C2-O2-C10
11	P	502	HEM	CAA-CBA-CGA-O2A
14	D	2003	CDL	C12-C11-CA5-OA6
11	C	502	HEM	CAA-CBA-CGA-O1A
11	C	502	HEM	CAA-CBA-CGA-O2A
14	C	2004	CDL	O1-C1-CB2-OB2
11	P	501	HEM	CAA-CBA-CGA-O2A
15	E	2005	PEE	C14-C15-C16-C17
15	R	3005	PEE	C14-C15-C16-C17
15	R	3005	PEE	C41-C42-C43-C44
17	D	501	HEC	CAA-CBA-CGA-O2A
15	E	2005	PEE	C40-C41-C42-C43
15	P	3007	PEE	C41-C42-C43-C44
18	D	2009	BOG	C1'-C2'-C3'-C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	P	3011	GOL	C1-C2-C3-O3
15	E	2005	PEE	C36-C37-C38-C39
14	D	2003	CDL	OA5-CA3-CA4-OA6
11	P	501	HEM	CAA-CBA-CGA-O1A
14	Q	3003	CDL	OA5-CA3-CA4-CA6
14	Q	3003	CDL	C12-C11-CA5-OA6
11	P	502	HEM	CAD-CBD-CGD-O1D
11	P	501	HEM	CAD-CBD-CGD-O2D
17	D	501	HEC	CAA-CBA-CGA-O1A
11	P	502	HEM	CAD-CBD-CGD-O2D
15	R	3005	PEE	C36-C37-C38-C39
11	C	501	HEM	CAD-CBD-CGD-O2D
11	P	501	HEM	C2B-C3B-CAB-CBB
15	E	2005	PEE	C41-C42-C43-C44
11	C	501	HEM	CAA-CBA-CGA-O2A
11	C	501	HEM	CAA-CBA-CGA-O1A
11	C	501	HEM	CAD-CBD-CGD-O1D
11	C	502	HEM	CAD-CBD-CGD-O2D
11	P	501	HEM	CAD-CBD-CGD-O1D
11	C	501	HEM	C4B-C3B-CAB-CBB
11	C	502	HEM	C4B-C3B-CAB-CBB
11	P	501	HEM	C4B-C3B-CAB-CBB
11	P	502	HEM	C4B-C3B-CAB-CBB
15	P	3007	PEE	O3-C30-C31-C32
17	D	501	HEC	CAD-CBD-CGD-O2D
17	Q	501	HEC	CAD-CBD-CGD-O2D
14	D	2003	CDL	OA5-CA3-CA4-CA6
14	D	2003	CDL	OB5-CB3-CB4-CB6
14	Q	3003	CDL	OB5-CB3-CB4-CB6
15	E	2005	PEE	O3P-C1-C2-C3
17	Q	501	HEC	CAA-CBA-CGA-O2A
15	C	2007	PEE	O2-C10-C11-C12
11	C	502	HEM	CAD-CBD-CGD-O1D
14	C	2004	CDL	CB5-C51-C52-C53
15	P	3007	PEE	O2-C10-C11-C12
15	E	2005	PEE	C23-C24-C25-C26
15	P	3007	PEE	C34-C35-C36-C37
15	C	2007	PEE	O3-C30-C31-C32
18	Q	3009	BOG	C1'-C2'-C3'-C4'
17	D	501	HEC	CAD-CBD-CGD-O1D
18	D	2091	BOG	C4-C5-C6-O6
17	Q	501	HEC	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	P	3004	CDL	CA3-OA5-PA1-OA2
14	Q	3003	CDL	CA3-OA5-PA1-OA4
15	C	2007	PEE	O5-C30-C31-C32
17	Q	501	HEC	CAA-CBA-CGA-O1A
15	C	2007	PEE	O4-C10-C11-C12
15	P	3007	PEE	O5-C30-C31-C32
14	D	2003	CDL	C72-C71-CB7-OB8
15	P	3007	PEE	O4-C10-C11-C12
15	E	2005	PEE	C31-C32-C33-C34
14	Q	3003	CDL	OB5-CB3-CB4-OB6
14	Q	3003	CDL	C72-C71-CB7-OB8

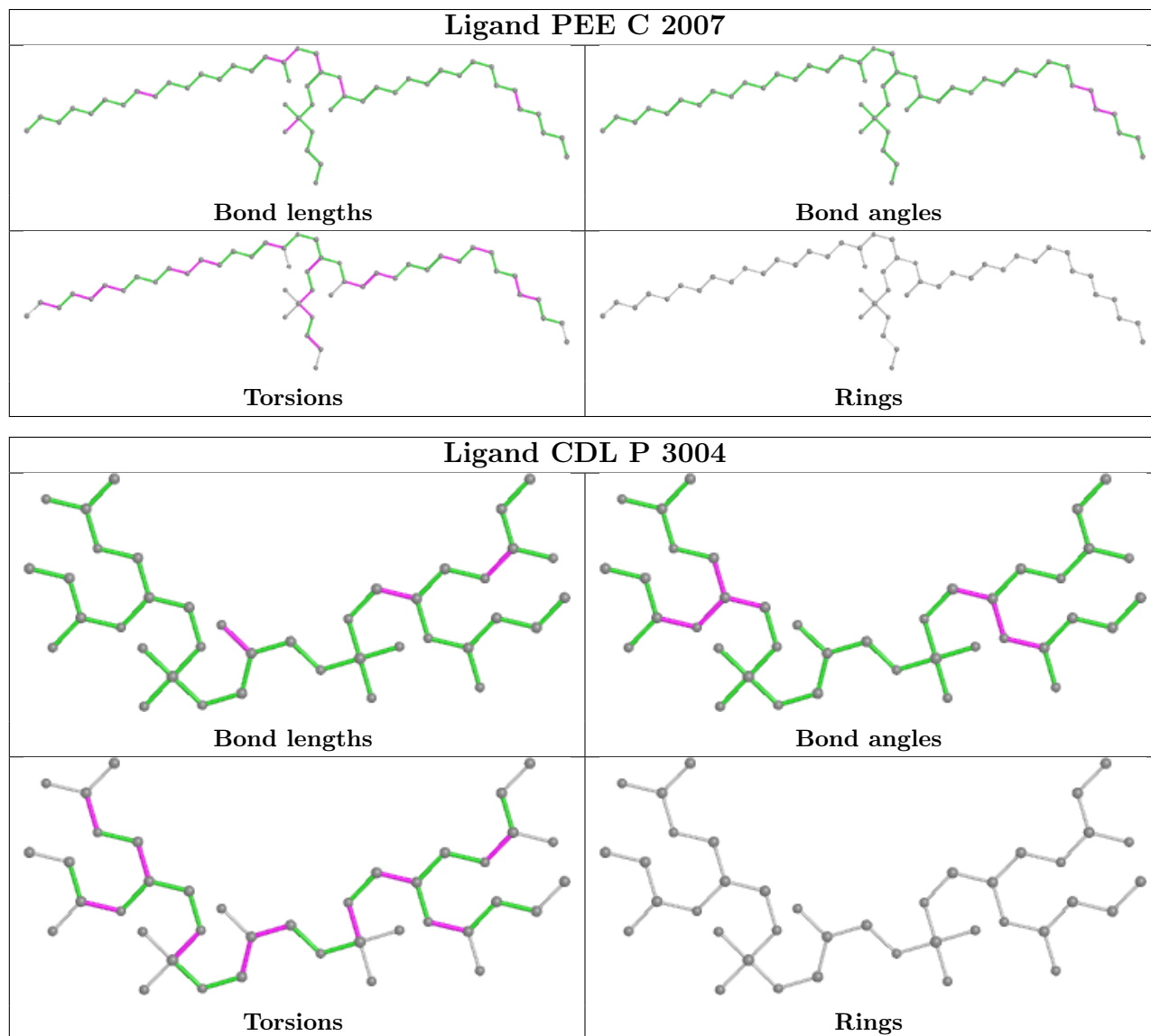
There are no ring outliers.

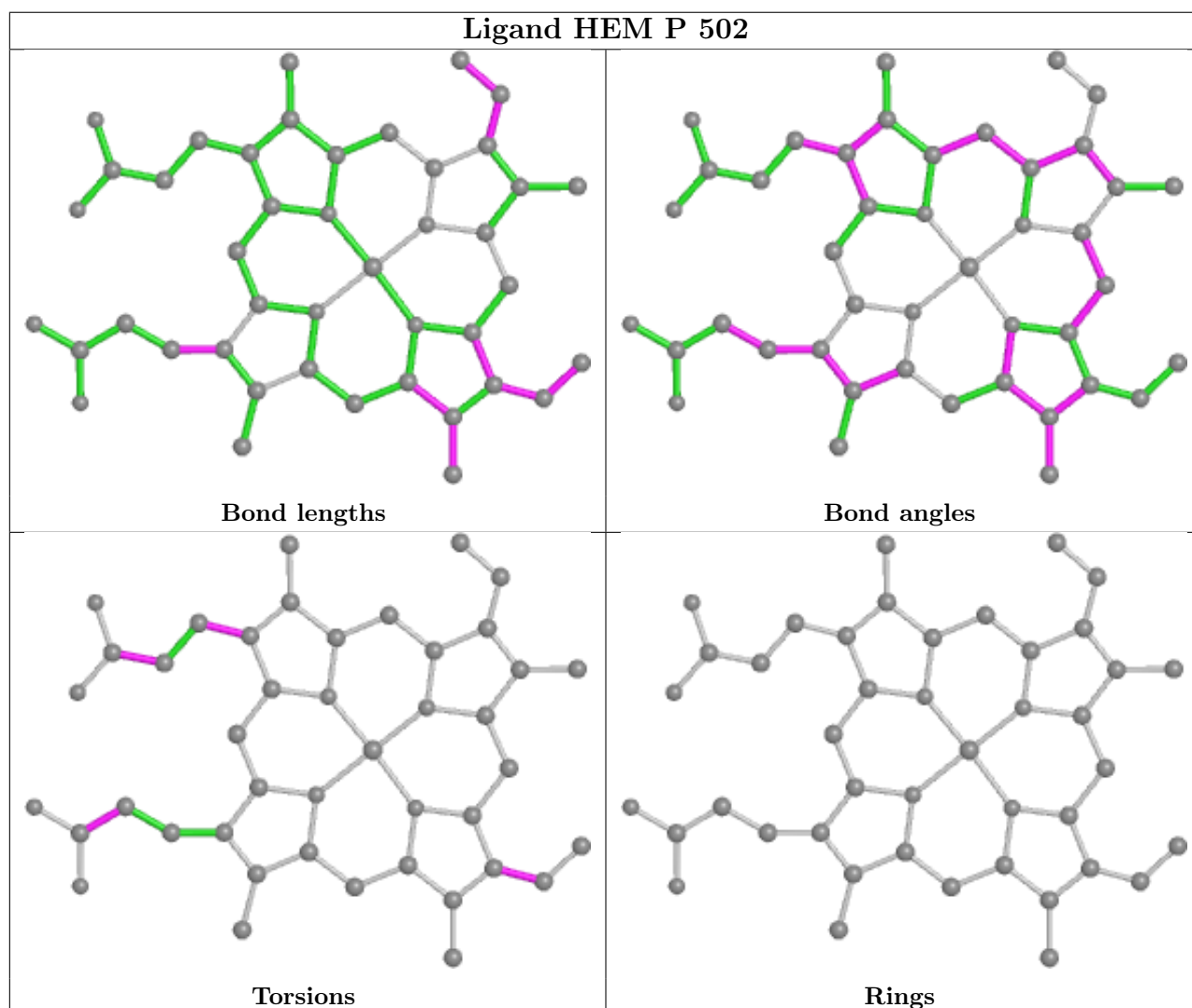
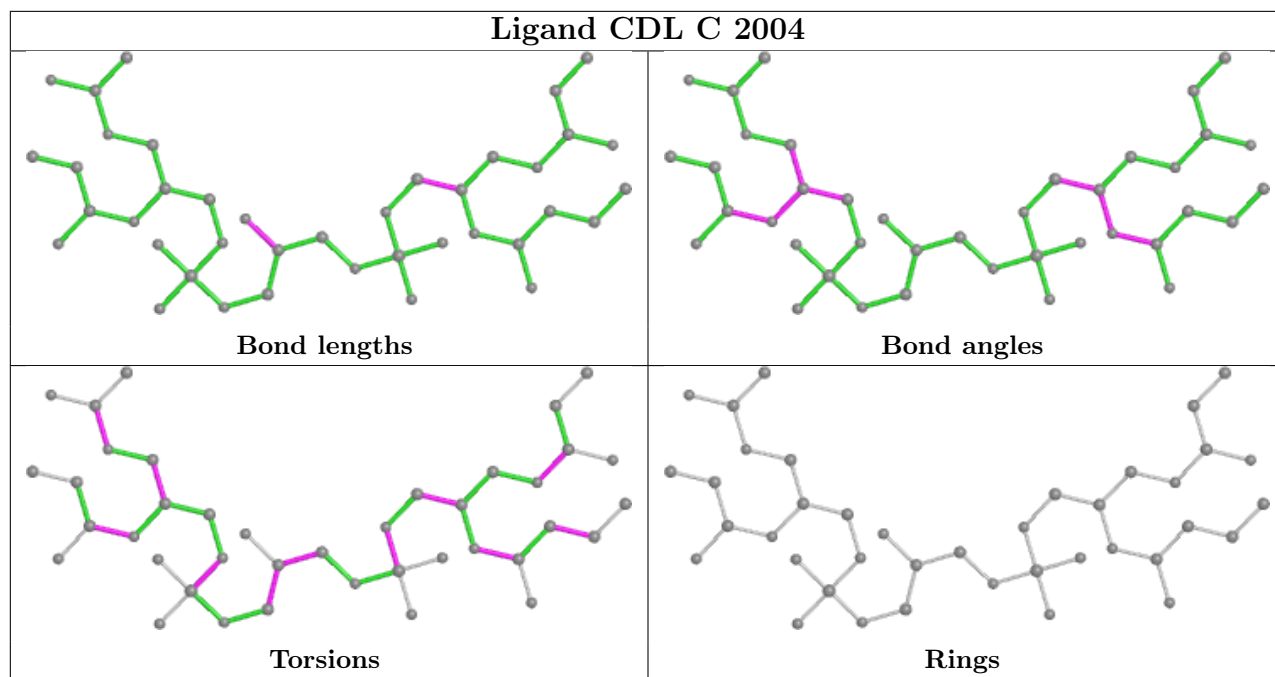
22 monomers are involved in 52 short contacts:

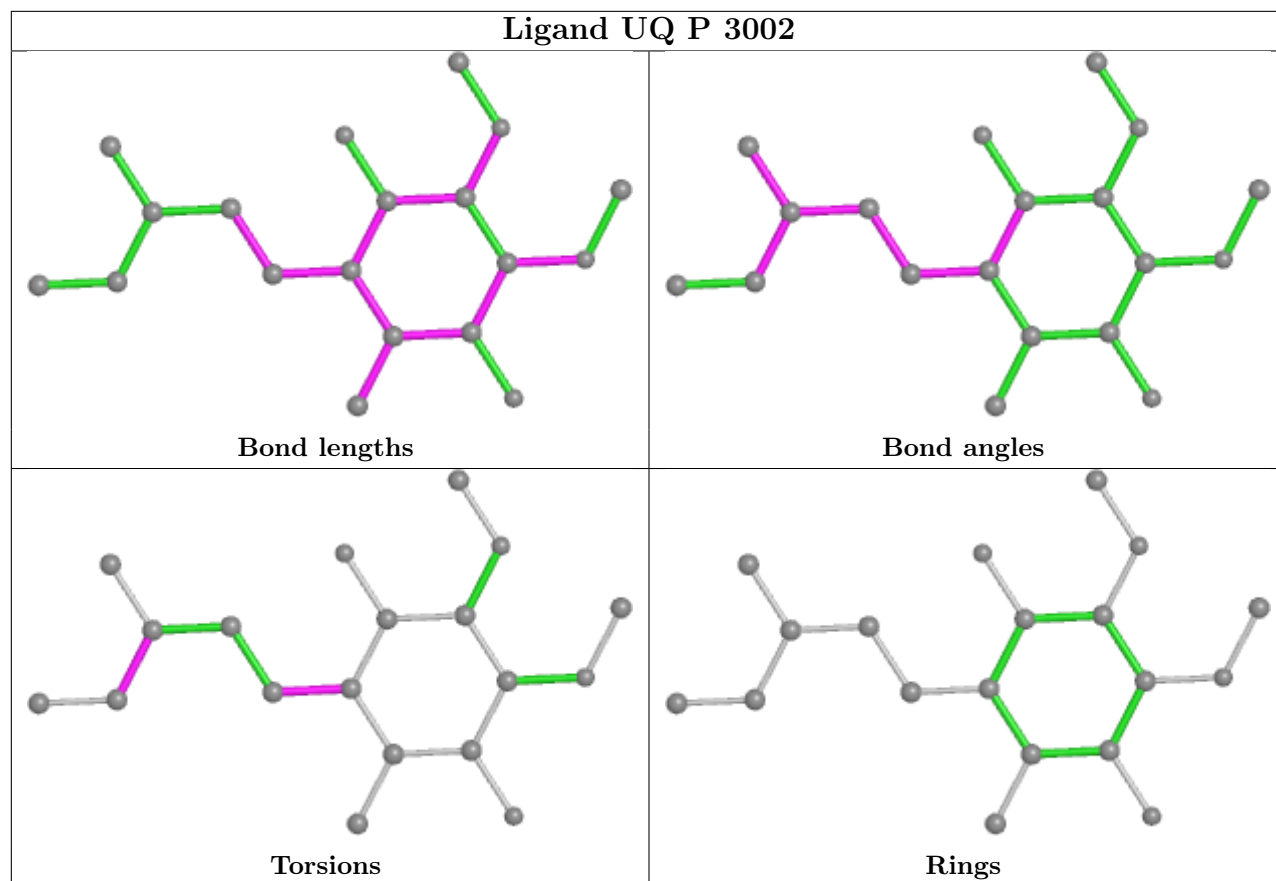
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	2007	PEE	1	0
14	P	3004	CDL	2	0
19	E	501	FES	2	0
14	C	2004	CDL	1	0
11	P	502	HEM	3	0
13	P	3002	UQ	5	0
17	Q	501	HEC	2	0
16	P	3011	GOL	2	0
17	D	501	HEC	2	0
19	R	501	FES	2	0
15	P	3007	PEE	2	0
18	D	2009	BOG	1	0
11	C	501	HEM	3	0
13	C	2002	UQ	6	0
18	Q	3009	BOG	1	0
11	P	501	HEM	2	0
18	P	2010	BOG	1	0
11	C	502	HEM	4	0
14	Q	3003	CDL	2	0
12	C	2001	IKR	4	0
12	P	3001	IKR	3	0
15	R	3005	PEE	1	0

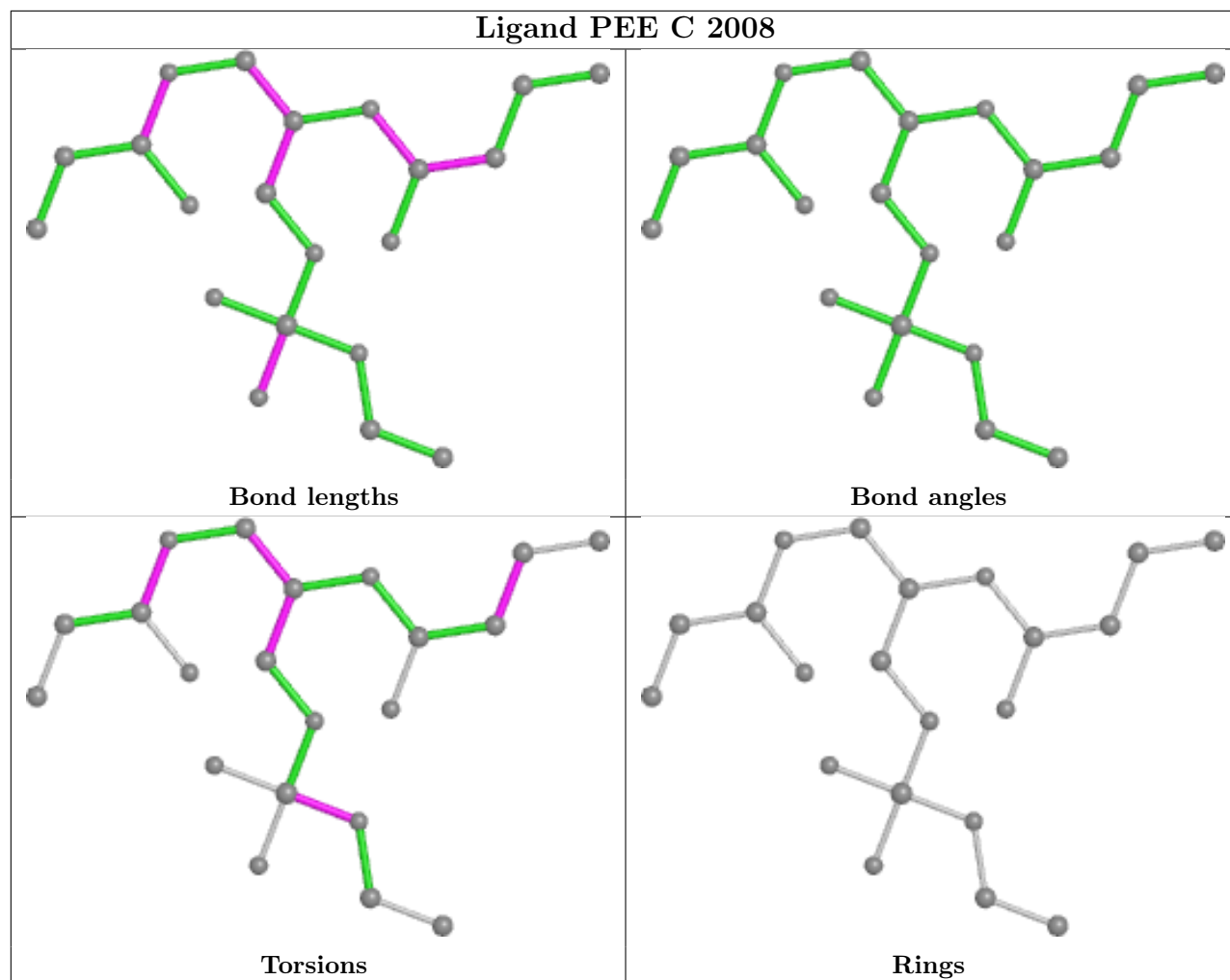
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

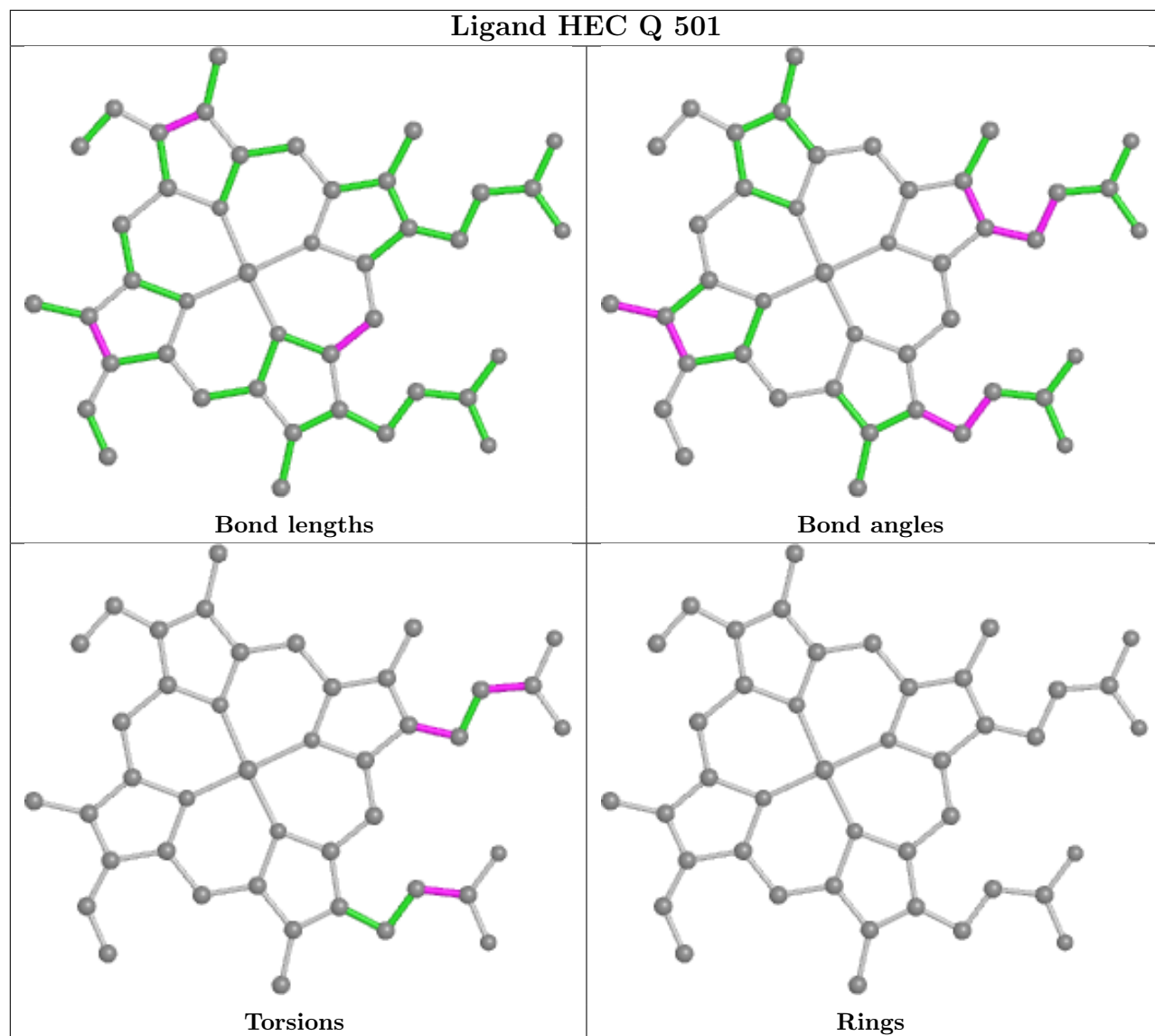
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

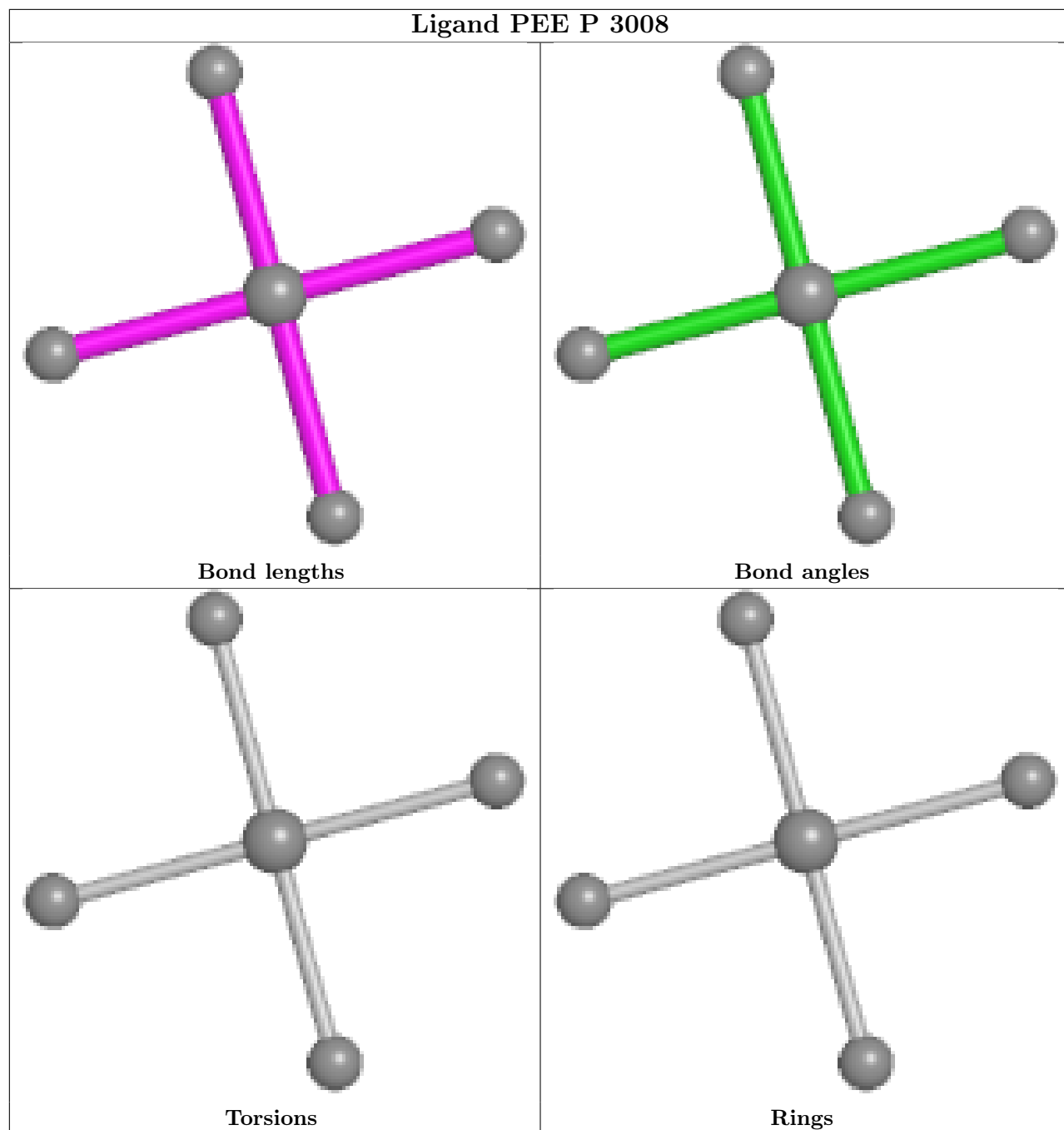


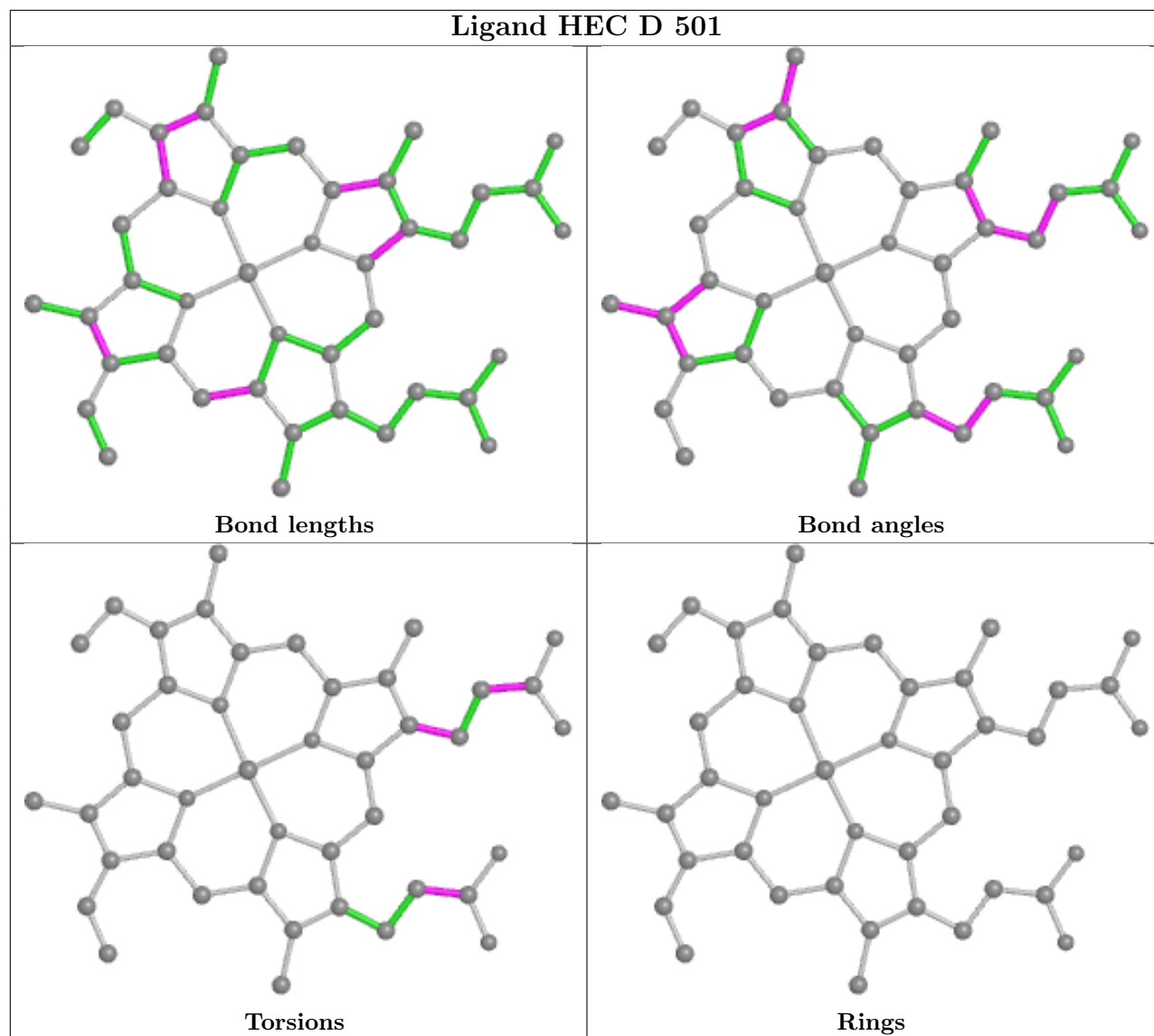


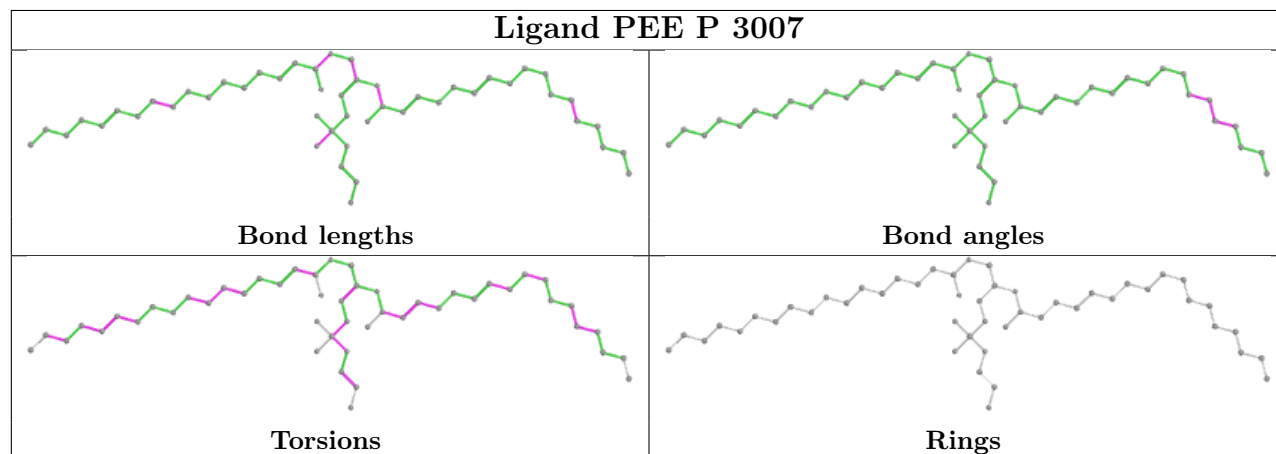
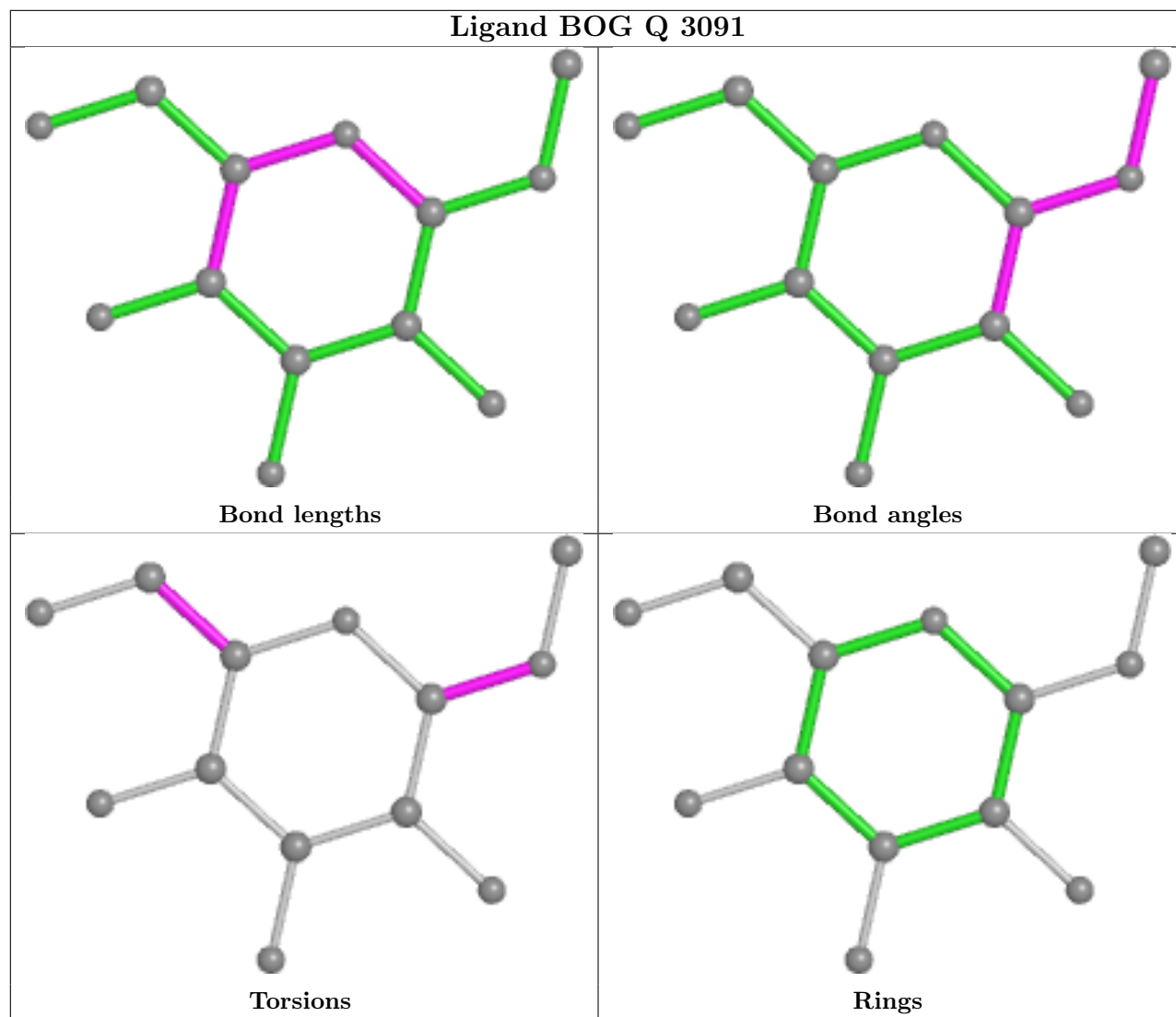


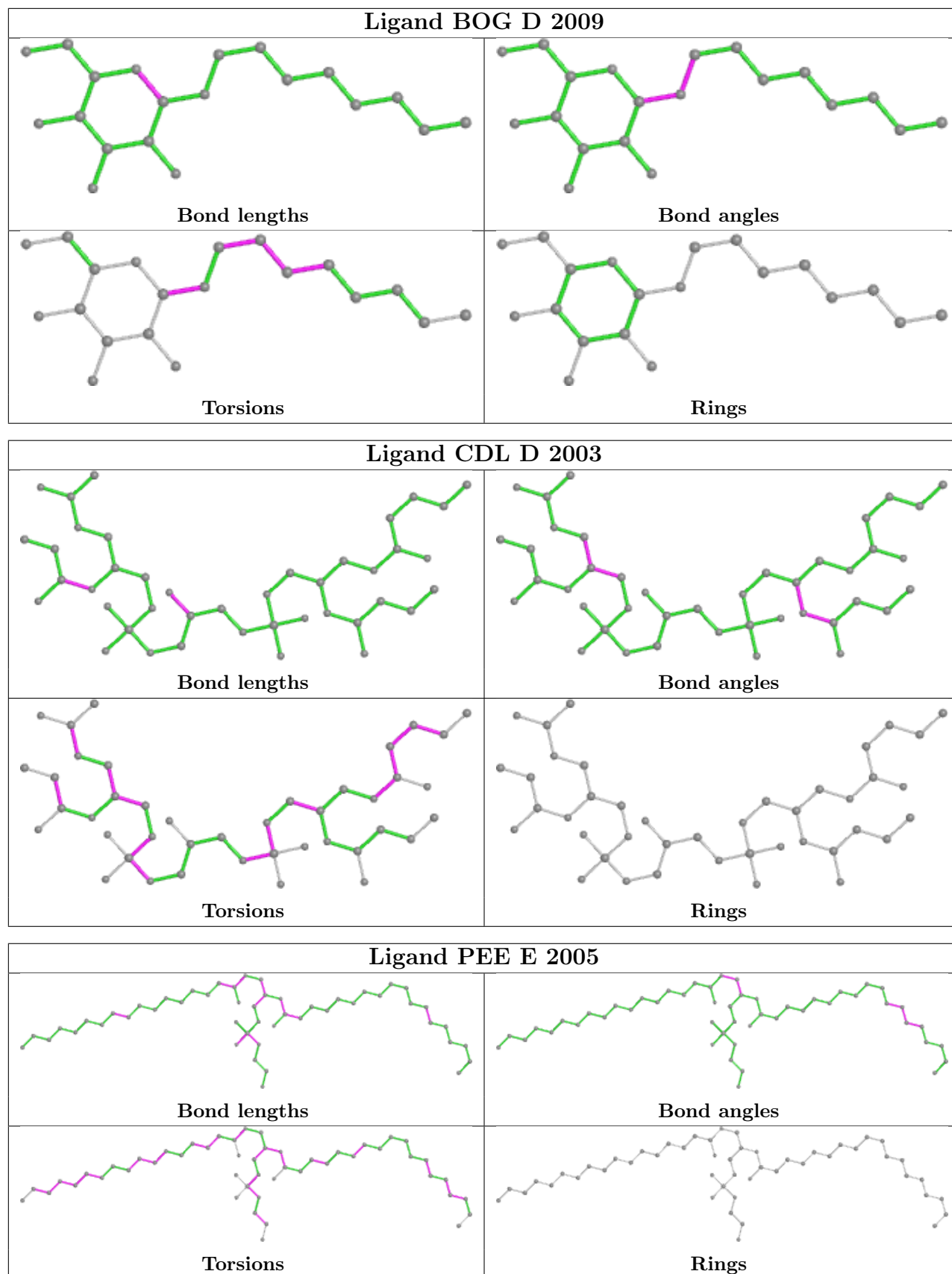


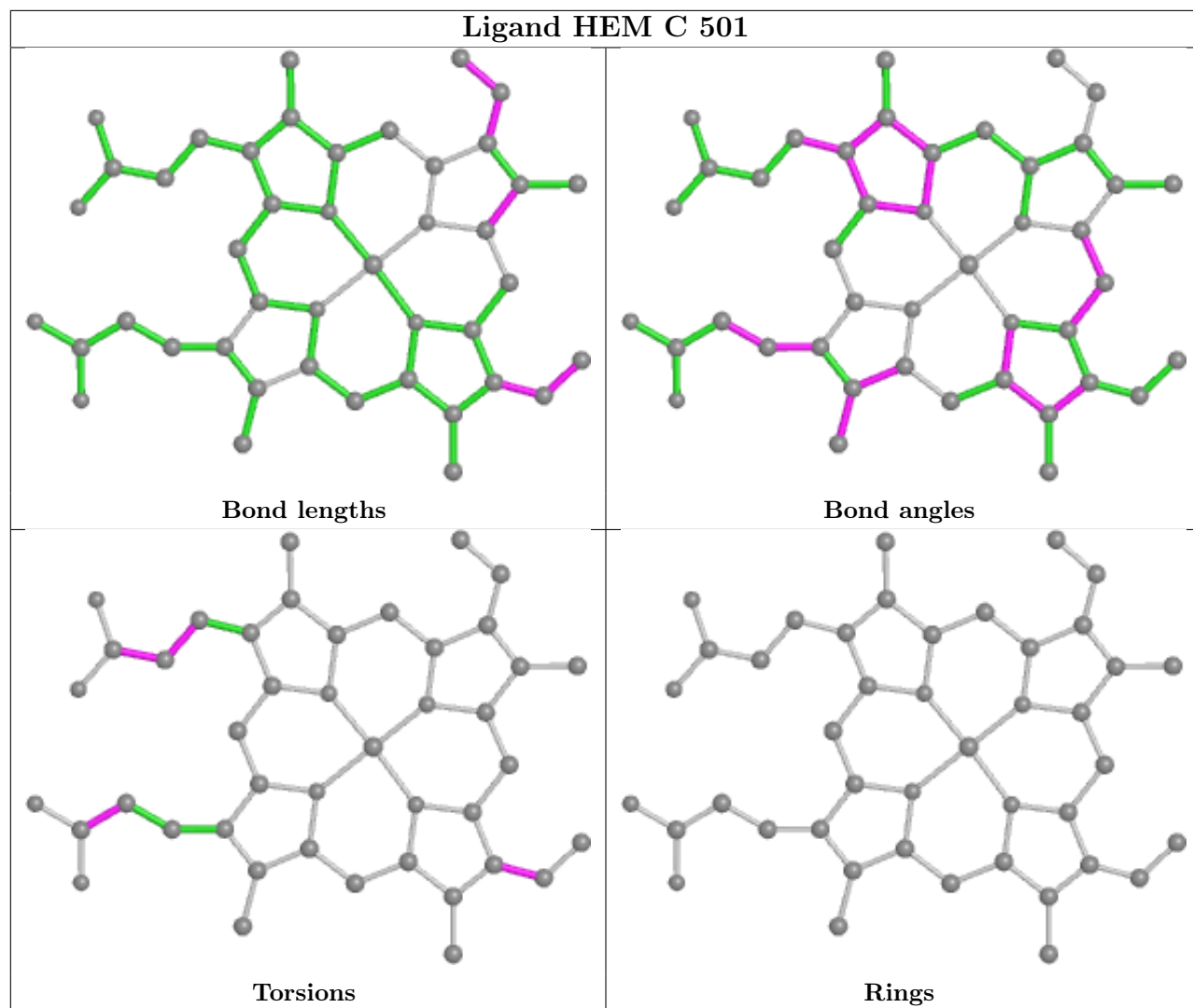


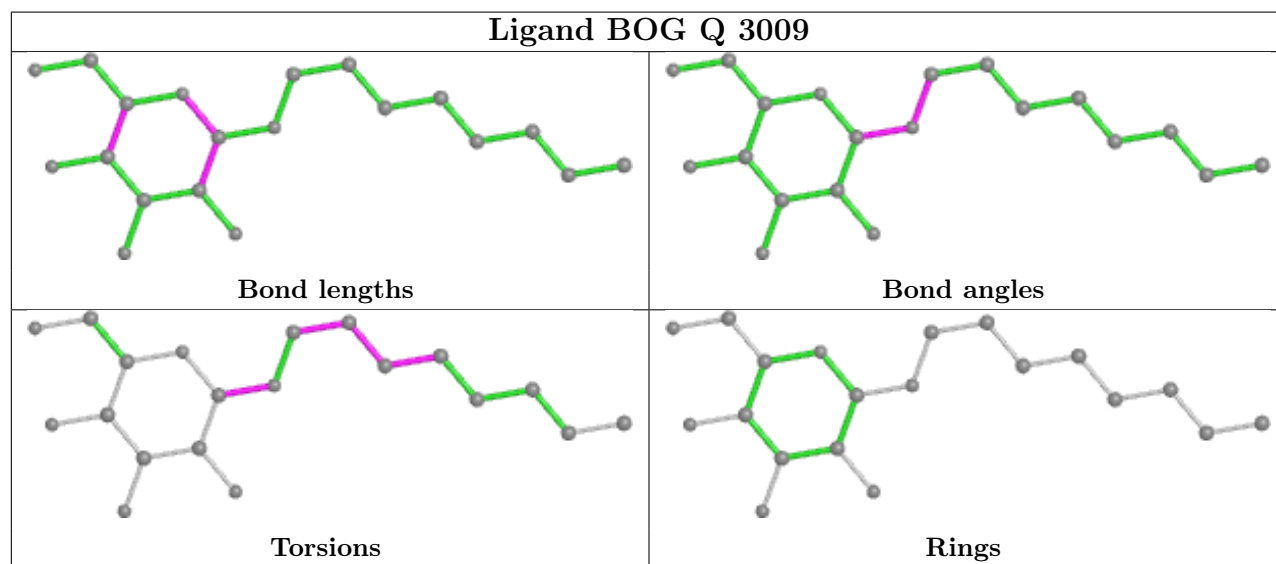
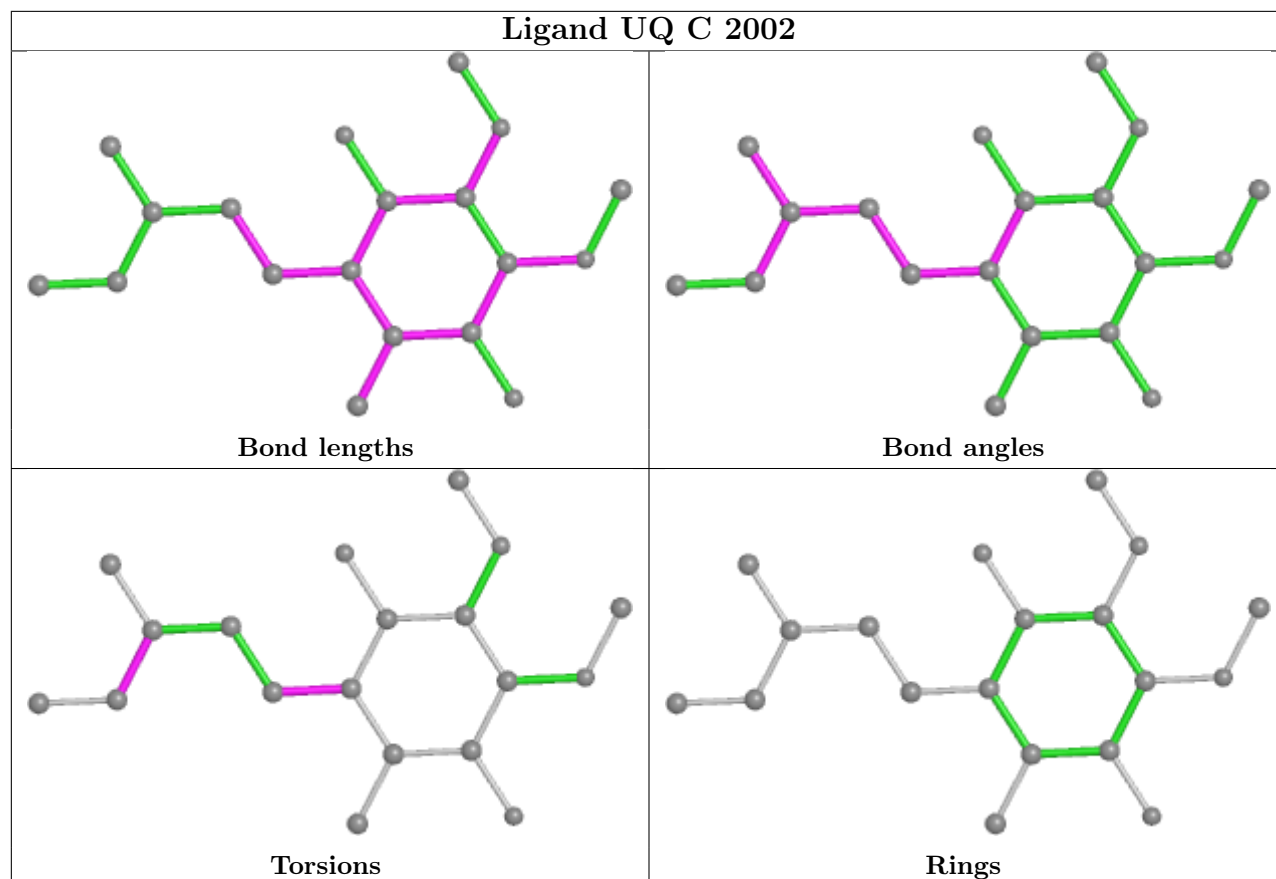


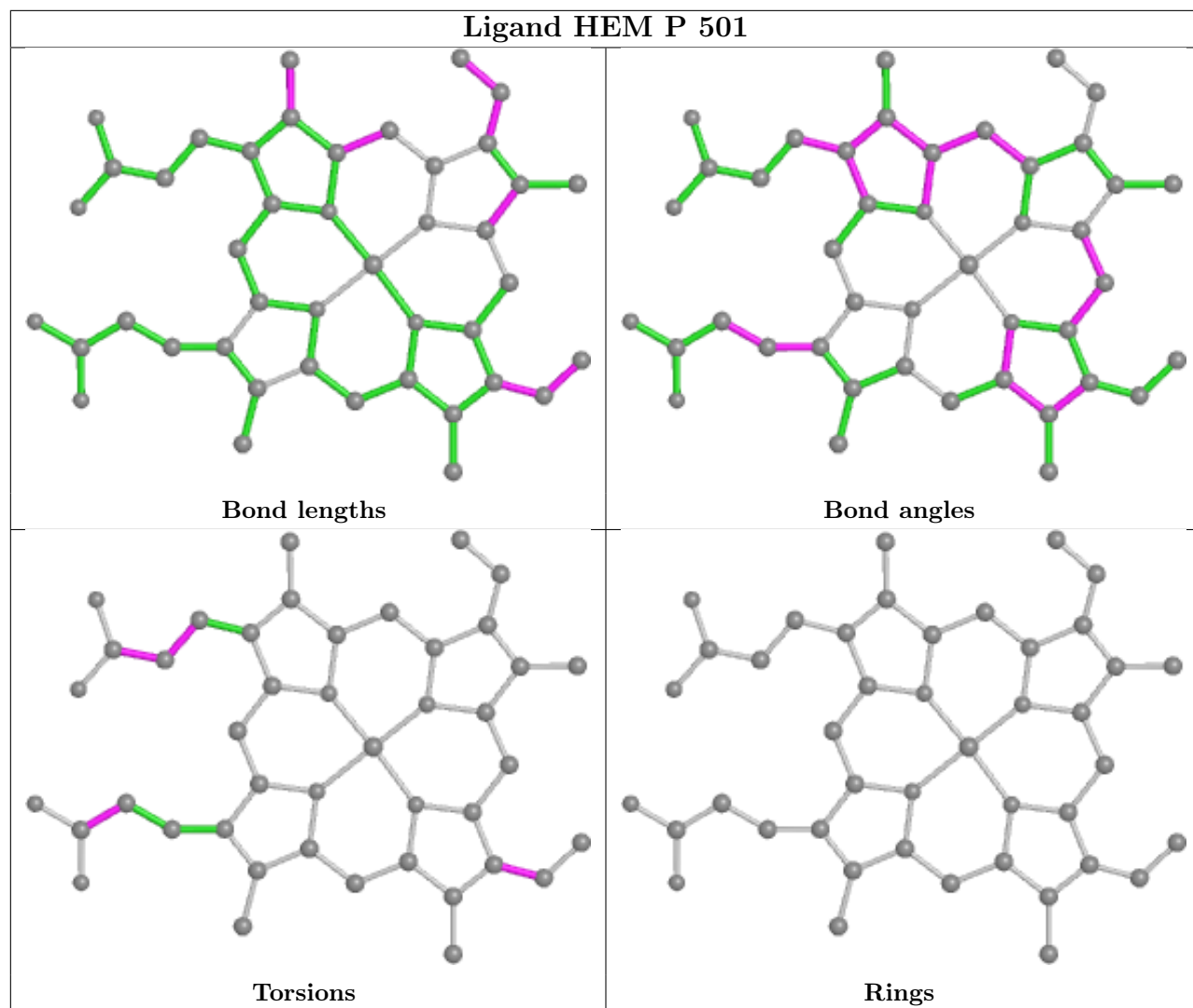


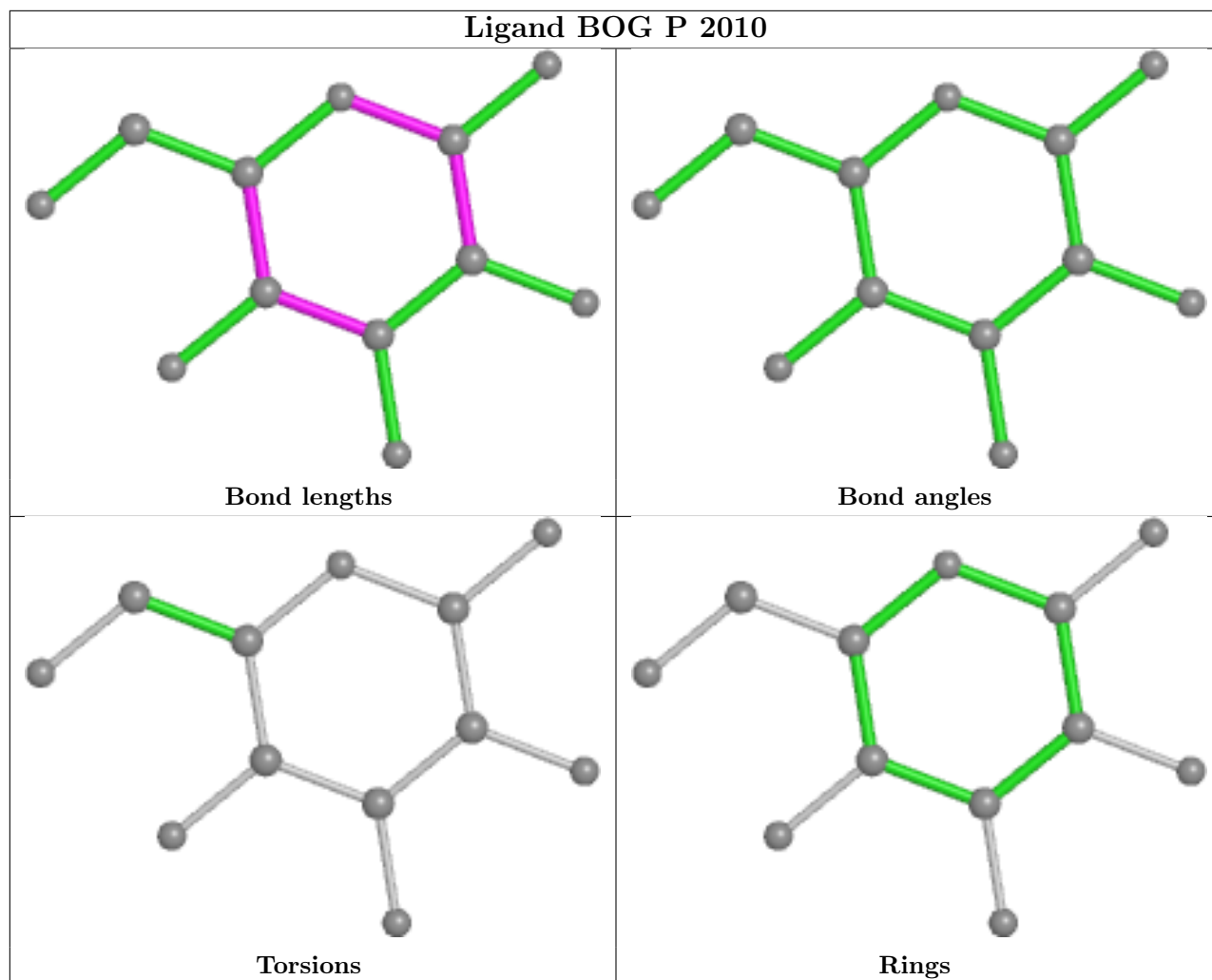


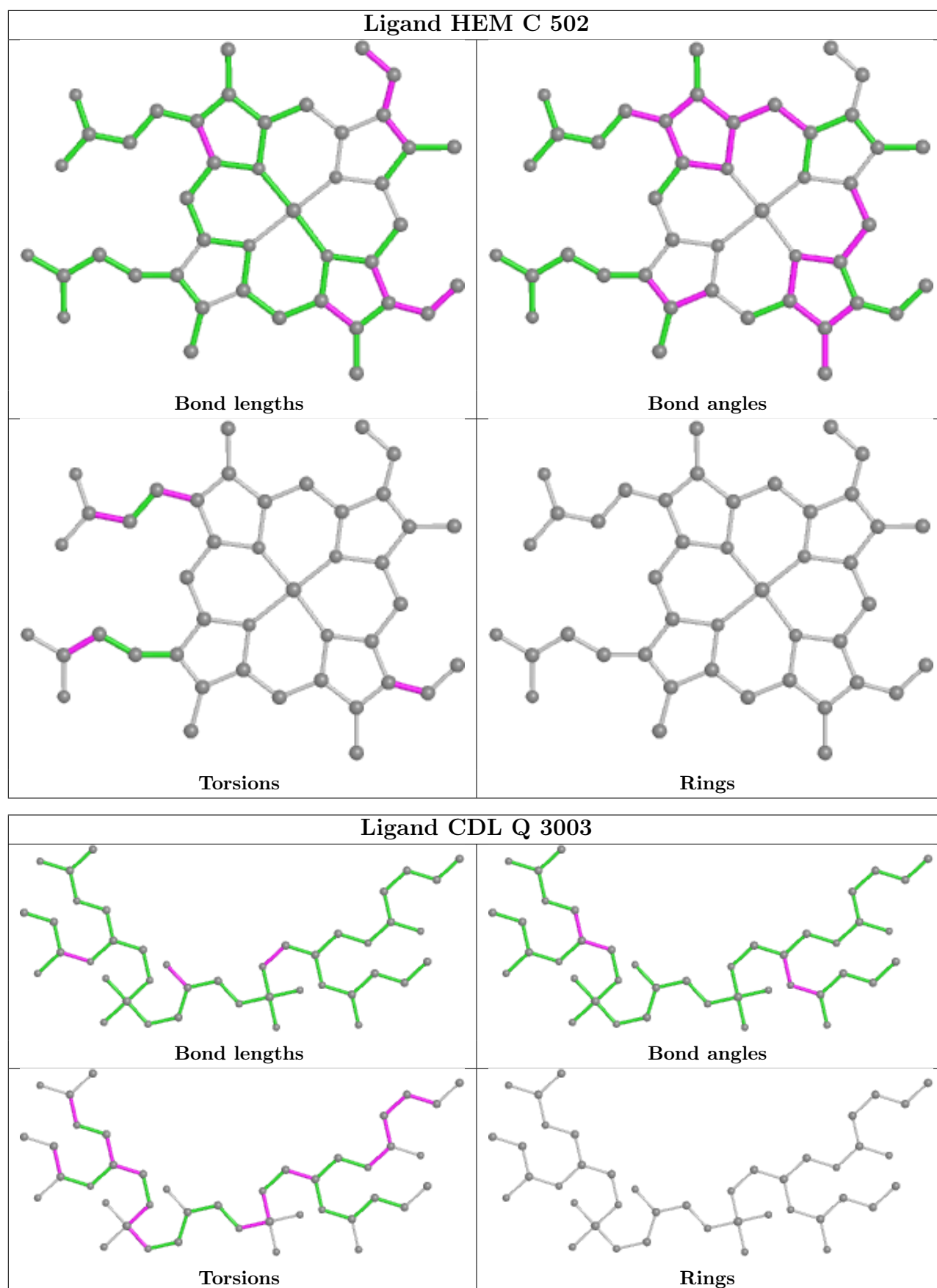


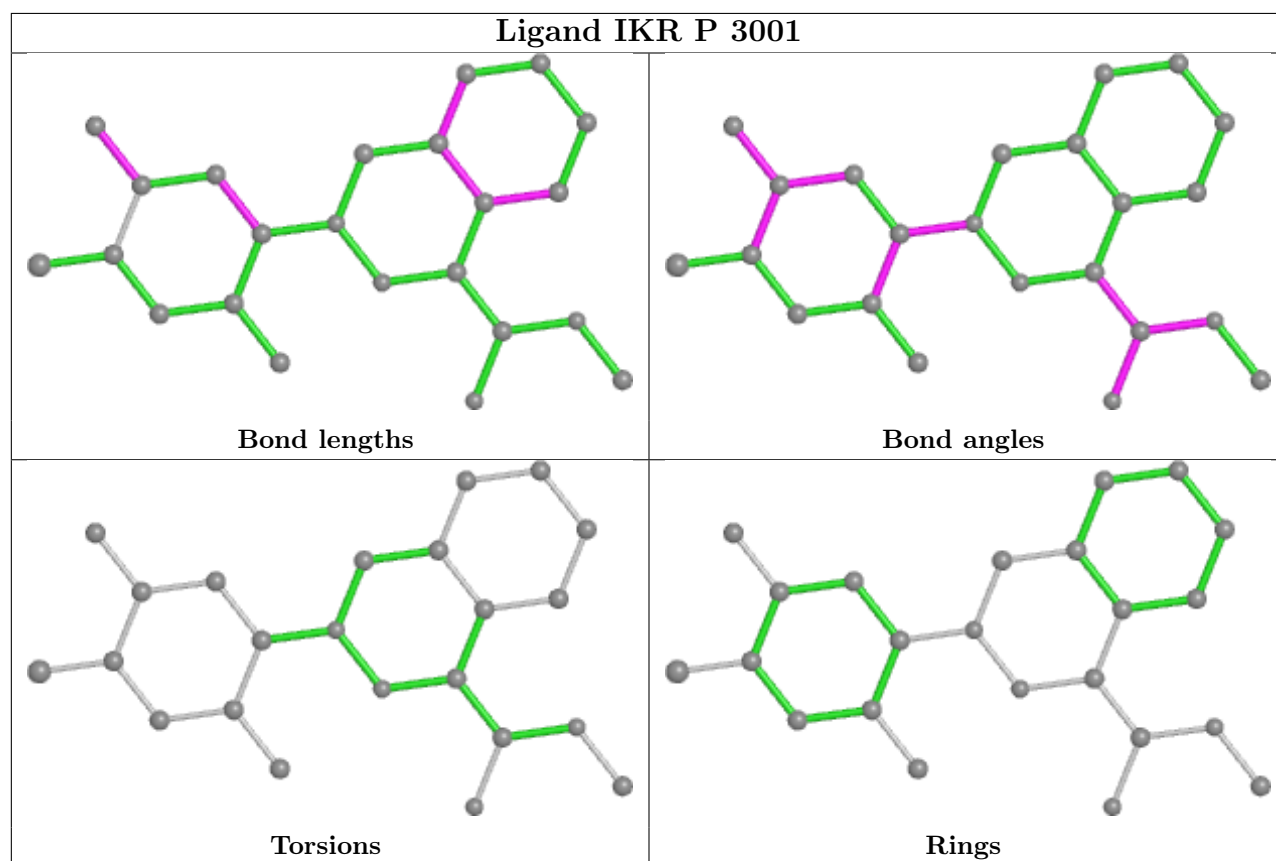
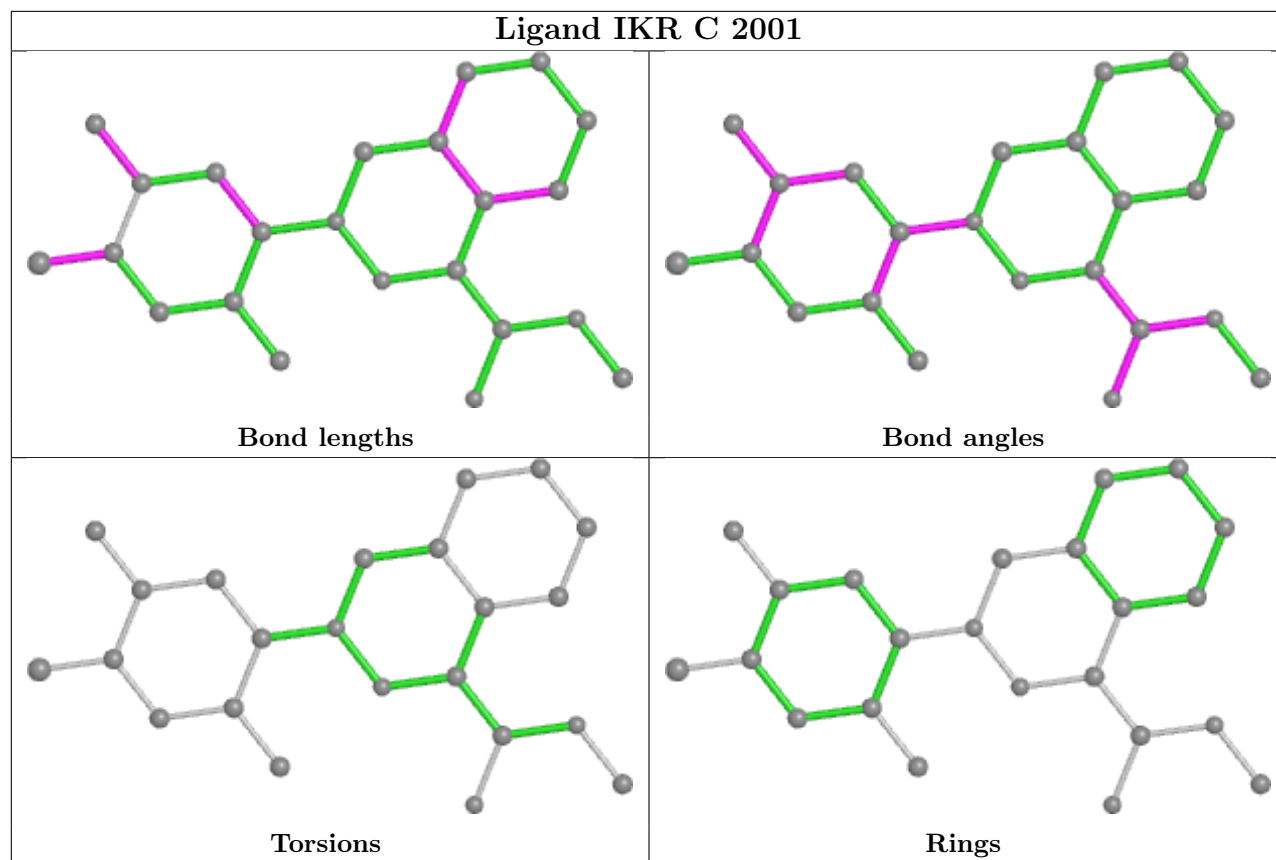


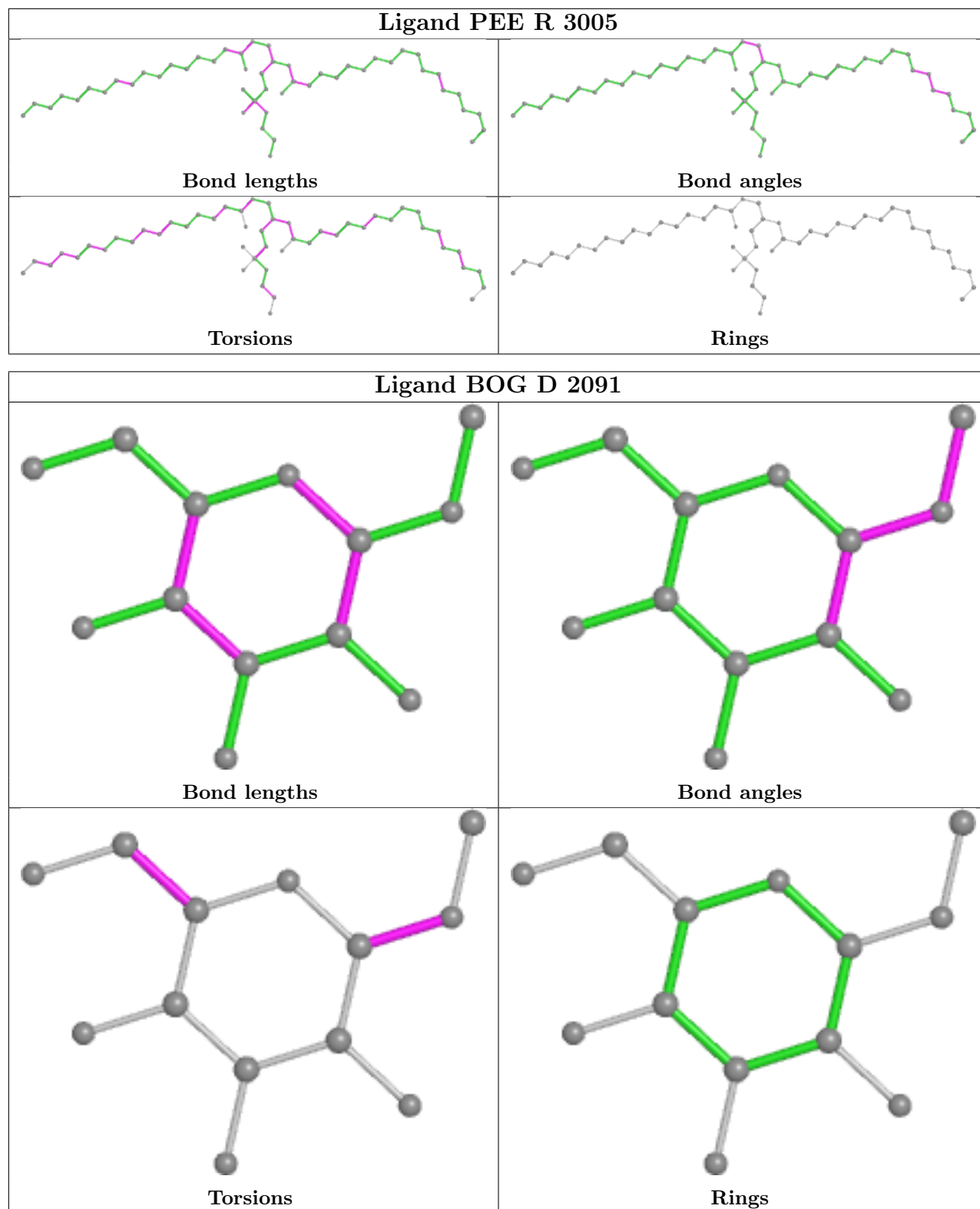












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/446 (99%)	-0.22	3 (0%) 87 72	39, 74, 106, 125	0
1	N	442/446 (99%)	-0.13	3 (0%) 87 72	43, 79, 111, 119	0
2	B	421/441 (95%)	-0.07	6 (1%) 75 53	63, 90, 121, 156	0
2	O	422/441 (95%)	-0.13	7 (1%) 70 46	50, 85, 115, 134	0
3	C	380/380 (100%)	-0.38	3 (0%) 86 70	23, 45, 98, 135	0
3	P	379/380 (99%)	-0.24	5 (1%) 77 56	32, 68, 104, 128	0
4	D	241/241 (100%)	-0.40	0 100 100	37, 51, 89, 114	0
4	Q	241/241 (100%)	-0.13	1 (0%) 92 82	55, 85, 118, 130	0
5	E	196/196 (100%)	1.26	63 (32%) 0 0	39, 140, 179, 186	125 (63%)
5	R	196/196 (100%)	0.68	38 (19%) 1 0	51, 99, 146, 165	0
6	F	101/110 (91%)	-0.55	0 100 100	38, 52, 70, 90	0
6	S	101/110 (91%)	-0.19	1 (0%) 82 63	62, 84, 126, 151	0
7	G	80/81 (98%)	-0.27	0 100 100	39, 61, 118, 127	0
7	T	79/81 (97%)	0.08	6 (7%) 13 5	55, 91, 154, 161	0
8	H	70/77 (90%)	-0.38	1 (1%) 75 53	52, 74, 95, 133	0
8	U	67/77 (87%)	0.49	6 (8%) 9 3	103, 131, 152, 157	0
9	I	31/47 (65%)	1.63	11 (35%) 0 0	92, 128, 164, 167	0
9	V	31/47 (65%)	1.54	10 (32%) 0 0	87, 119, 167, 170	0
10	J	61/61 (100%)	-0.26	1 (1%) 72 49	46, 63, 107, 143	0
10	W	60/61 (98%)	0.15	1 (1%) 70 46	65, 83, 120, 129	0
All	All	4043/4160 (97%)	-0.05	166 (4%) 37 18	23, 77, 138, 186	125 (3%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	11.2
5	E	107	ASN	8.4
9	I	51	CYS	7.8
5	E	167	ALA	6.6
5	E	98	VAL	6.3
5	E	168	SER	6.1
5	E	112	VAL	6.1
5	E	174	GLY	6.1
5	R	114	VAL	6.0
9	V	56	SER	5.7
5	E	86	ASN	5.6
5	E	84	GLY	5.4
5	E	102	THR	5.4
5	E	180	LEU	5.3
5	E	101	ARG	5.3
5	E	126	ARG	5.1
5	R	112	VAL	5.0
5	R	111	GLU	5.0
5	E	87	VAL	5.0
5	E	105	GLU	4.8
5	E	106	ILE	4.7
5	E	135	LEU	4.7
9	V	57	GLY	4.5
5	E	169	GLY	4.5
5	E	115	SER	4.4
9	I	50	LEU	4.3
5	R	122	HIS	4.3
5	E	148	ALA	4.3
5	E	114	VAL	4.3
5	E	99	ARG	4.2
5	R	98	VAL	4.2
5	E	104	ALA	4.1
5	E	109	GLU	4.1
8	U	13	LEU	4.0
5	R	86	ASN	4.0
5	E	120	PRO	3.8
5	E	187	PHE	3.8
2	O	222	GLN	3.8
2	B	350	GLY	3.8
5	E	173	LYS	3.8
2	B	225	ASN	3.7
9	V	63	ASP	3.7
7	T	74	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	R	113	ASP	3.7
3	C	4	ASN	3.7
5	E	103	GLN	3.6
5	E	134	ILE	3.6
5	E	157	TYR	3.6
5	E	108	GLN	3.5
5	R	120	PRO	3.5
5	E	81	ILE	3.5
5	E	116	LYS	3.5
5	E	149	ASN	3.5
7	T	73	ASN	3.4
5	E	171	ILE	3.4
5	E	133	VAL	3.3
5	R	121	GLN	3.3
5	R	186	GLN	3.3
5	E	111	GLU	3.3
5	R	124	LEU	3.3
5	R	130	PRO	3.3
9	I	53	GLU	3.3
2	O	350	GLY	3.3
5	E	117	LEU	3.2
2	B	227	ARG	3.2
10	J	63	GLU	3.2
5	R	172	ARG	3.2
1	A	69	LYS	3.1
5	E	100	HIS	3.1
9	I	63	ASP	3.1
2	B	228	SER	3.1
5	E	110	ALA	3.1
5	R	127	VAL	3.1
5	R	87	VAL	3.0
2	O	347	ALA	3.0
2	O	19	PRO	3.0
5	E	188	VAL	3.0
5	R	156	TYR	3.0
5	R	109	GLU	3.0
5	R	133	VAL	2.9
5	R	184	THR	2.9
5	E	78	LEU	2.9
5	R	89	PHE	2.9
1	N	217	SER	2.9
9	I	47	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	190	ASP	2.8
2	B	402	ILE	2.8
5	E	165	TYR	2.8
9	I	52	ARG	2.8
9	V	77	ARG	2.8
5	E	97	PHE	2.8
1	N	66	GLY	2.8
7	T	78	GLU	2.7
3	C	7	LYS	2.7
5	E	125	ASP	2.7
5	R	88	ALA	2.7
7	T	2	ILE	2.7
5	E	183	PRO	2.7
5	E	124	LEU	2.7
5	R	134	ILE	2.7
9	V	53	GLU	2.7
5	R	154	GLY	2.7
9	I	61	ARG	2.6
2	O	352	VAL	2.6
5	E	156	TYR	2.6
9	V	59	SER	2.6
9	I	77	ARG	2.6
5	R	115	SER	2.6
10	W	45	HIS	2.6
3	C	8	SER	2.6
5	R	76	ILE	2.6
9	V	61	ARG	2.5
7	T	80	ASP	2.5
8	U	44	VAL	2.4
3	P	156	TYR	2.4
9	I	62	ARG	2.4
5	E	146	PRO	2.4
5	R	96	LEU	2.4
5	E	85	LYS	2.4
5	E	122	HIS	2.4
5	R	97	PHE	2.4
5	E	150	SER	2.4
5	E	163	SER	2.4
2	O	410	VAL	2.4
8	U	50	THR	2.4
3	P	6	ARG	2.4
5	R	85	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	55	MET	2.4
3	P	4	ASN	2.4
5	R	108	GLN	2.4
3	P	7	LYS	2.4
5	E	147	ILE	2.4
5	E	121	GLN	2.4
5	E	175	PRO	2.4
8	U	12	GLU	2.4
5	R	125	ASP	2.3
6	S	11	ARG	2.3
5	R	128	LYS	2.3
9	V	55	MET	2.3
5	E	79	SER	2.3
5	R	135	LEU	2.3
9	I	56	SER	2.3
5	R	81	ILE	2.3
5	E	83	GLU	2.3
4	Q	139	ALA	2.2
5	R	110	ALA	2.2
8	U	39	LEU	2.2
5	E	159	PRO	2.2
1	A	219	VAL	2.2
3	P	157	ILE	2.2
5	R	165	TYR	2.2
5	E	89	PHE	2.2
5	E	145	VAL	2.1
7	T	77	TYR	2.1
8	U	14	VAL	2.1
2	B	33	LEU	2.1
5	R	171	ILE	2.1
2	O	23	ASP	2.1
1	A	217	SER	2.1
9	V	58	ARG	2.1
8	H	71	HIS	2.1
1	N	177	LEU	2.1
5	R	117	LEU	2.1
9	V	62	ARG	2.0
5	E	158	CYS	2.0
5	R	116	LYS	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.

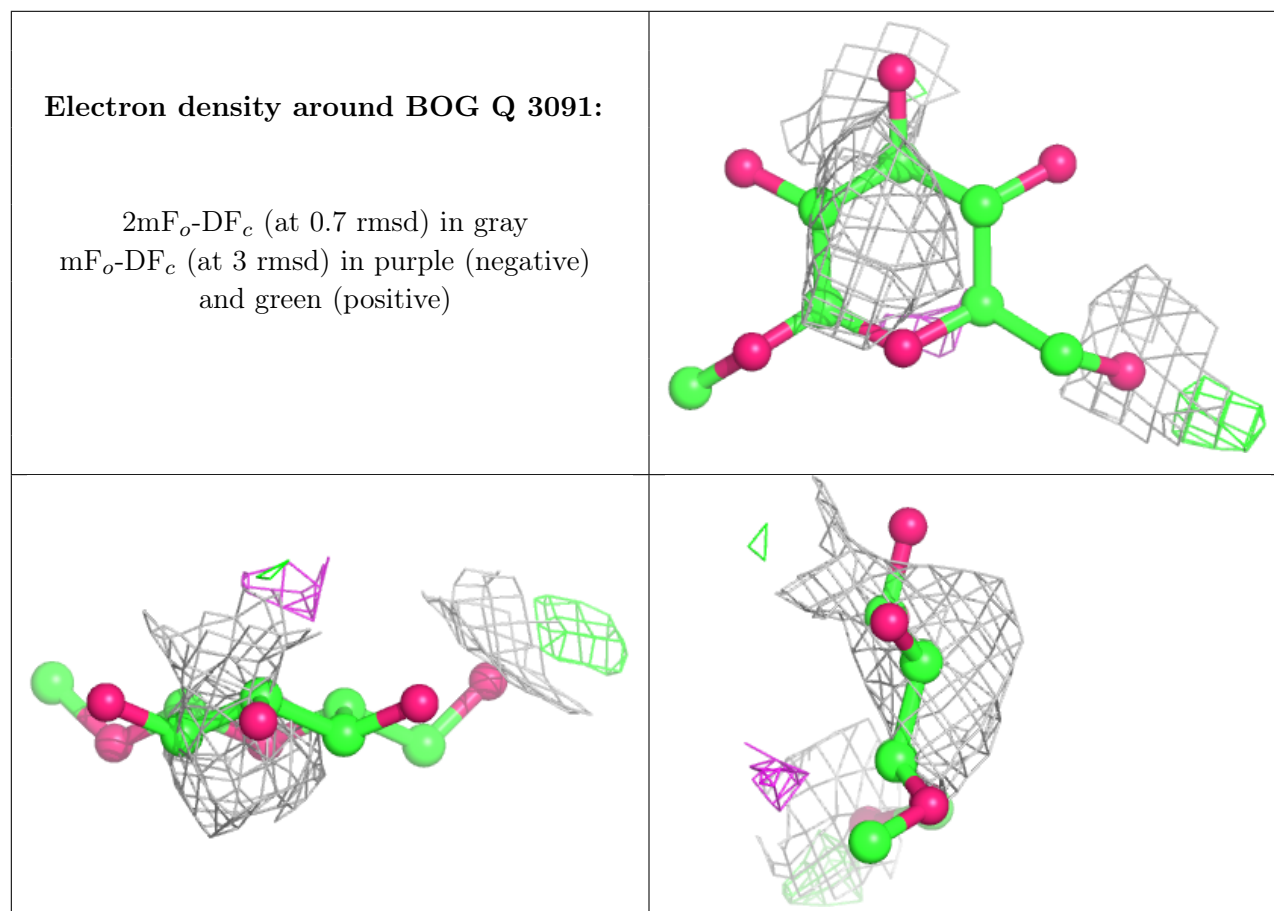
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	BOG	Q	3091	13/20	0.31	0.77	194,197,197,198	0
18	BOG	D	2091	13/20	0.50	0.63	167,171,171,171	0
18	BOG	P	2010	12/20	0.57	0.42	162,165,167,167	0
15	PEE	C	2008	21/51	0.67	0.39	132,138,141,142	0
14	CDL	Q	3003	42/100	0.76	0.34	120,141,152,153	0
15	PEE	R	3005	50/51	0.79	0.35	80,99,106,107	0
14	CDL	D	2003	42/100	0.80	0.29	112,121,125,126	0
15	PEE	P	3008	5/51	0.80	0.26	140,140,140,140	0
15	PEE	E	2005	50/51	0.82	0.42	79,91,105,106	0
14	CDL	P	3004	40/100	0.83	0.34	111,116,122,123	0
13	UQ	P	3002	19/63	0.85	0.29	97,111,114,115	0
13	UQ	C	2002	19/63	0.88	0.28	85,89,90,90	0
14	CDL	C	2004	40/100	0.89	0.25	72,82,99,101	0
15	PEE	P	3007	49/51	0.89	0.37	68,91,107,109	0
16	GOL	P	3011	6/6	0.89	0.32	79,79,79,80	0
18	BOG	Q	3009	20/20	0.90	0.31	71,99,102,102	0
16	GOL	C	2011	6/6	0.90	0.27	54,56,58,60	0
15	PEE	C	2007	49/51	0.92	0.29	49,59,88,90	0
18	BOG	D	2009	20/20	0.93	0.29	51,76,80,81	0
19	FES	E	501	4/4	0.95	0.11	151,151,152,152	4
17	HEC	Q	501	43/43	0.96	0.23	68,71,76,78	0
11	HEM	P	502	43/43	0.97	0.21	40,47,59,62	0
11	HEM	C	502	43/43	0.98	0.19	24,31,37,44	0
11	HEM	P	501	43/43	0.98	0.21	46,50,57,60	0
17	HEC	D	501	43/43	0.98	0.18	38,42,46,48	0
11	HEM	C	501	43/43	0.98	0.21	30,37,43,45	0
12	IKR	P	3001	25/25	0.98	0.19	66,67,76,78	0

Continued on next page...

Continued from previous page...

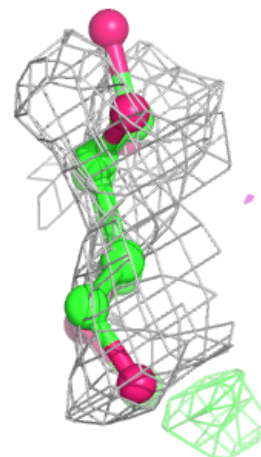
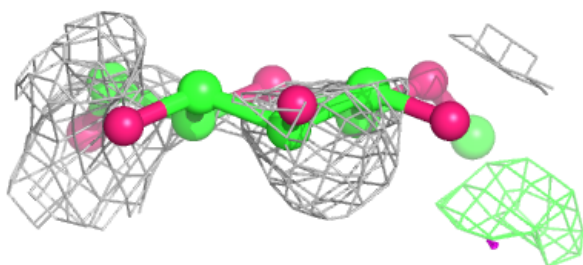
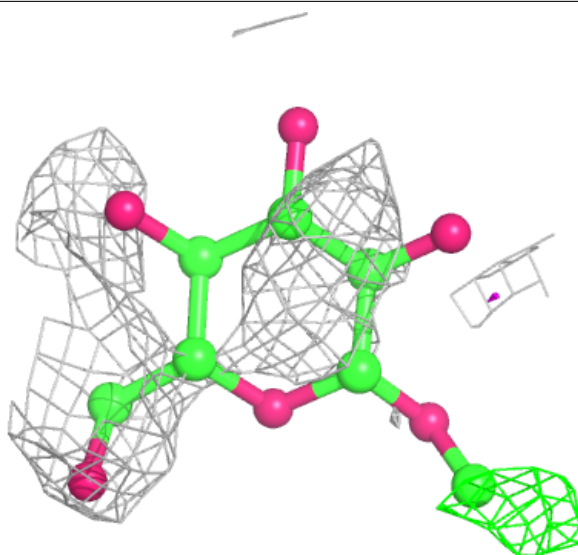
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	FES	R	501	4/4	0.98	0.09	88,90,91,91	0
12	IKR	C	2001	25/25	0.99	0.17	38,40,44,54	0

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.



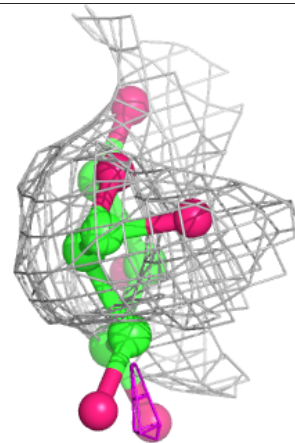
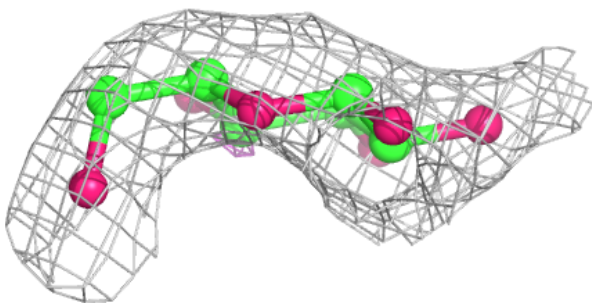
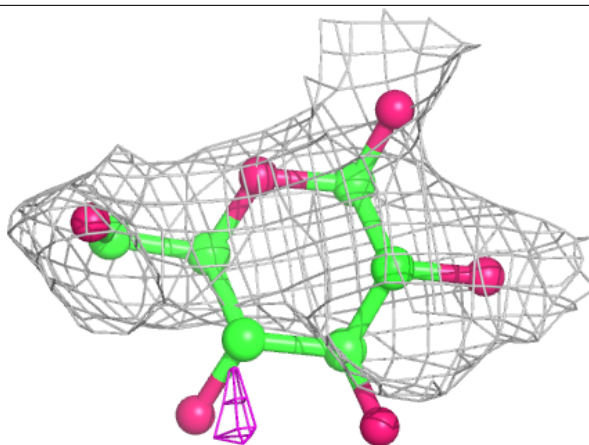
Electron density around BOG D 2091:

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



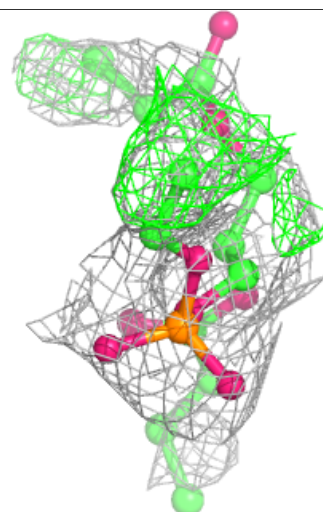
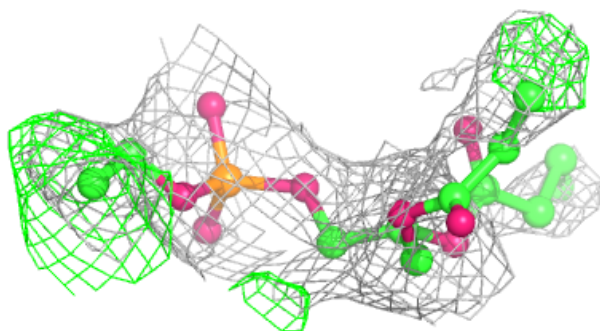
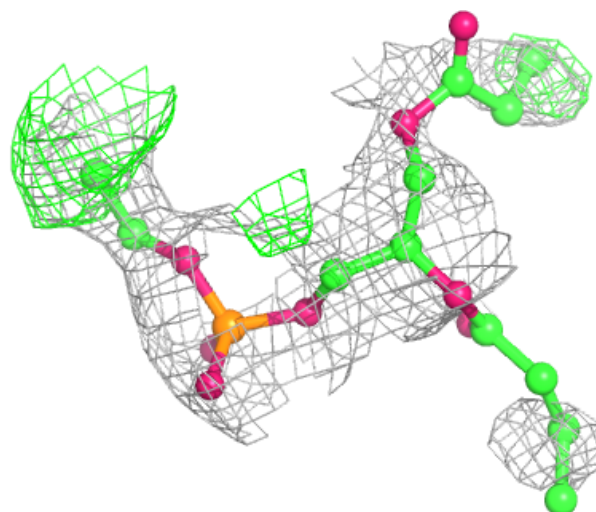
Electron density around BOG P 2010:

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



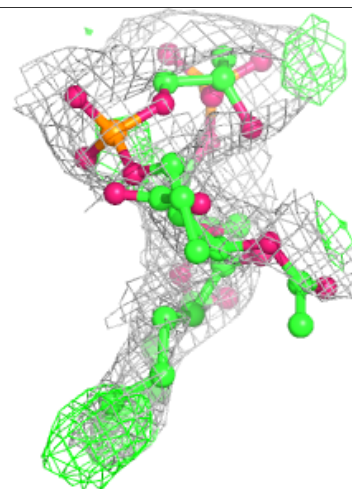
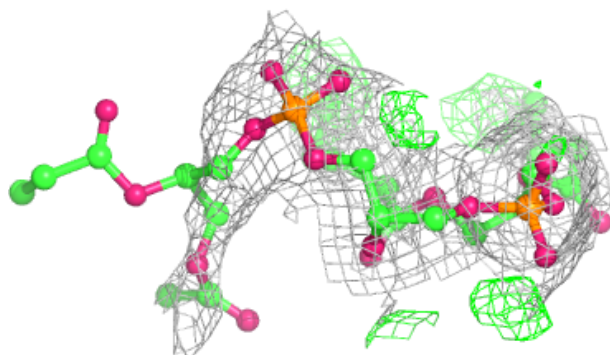
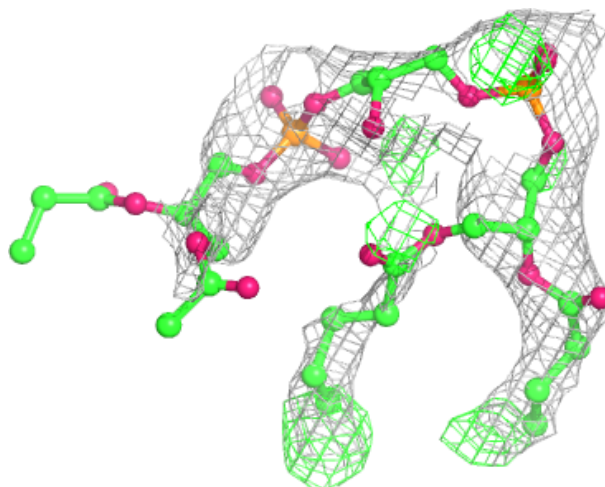
Electron density around PEE C 2008:

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



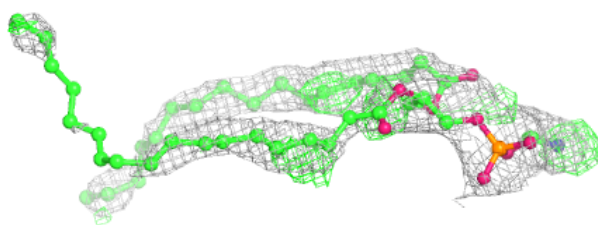
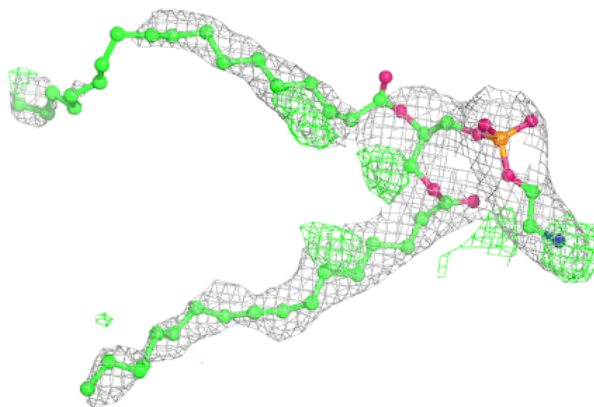
Electron density around CDL Q 3003:

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



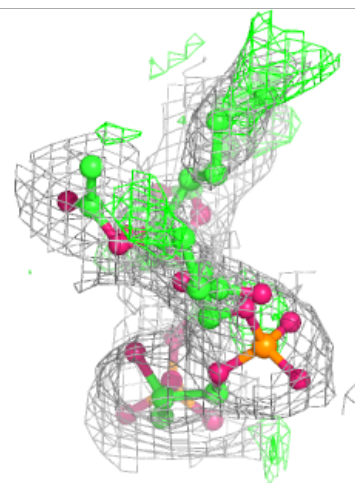
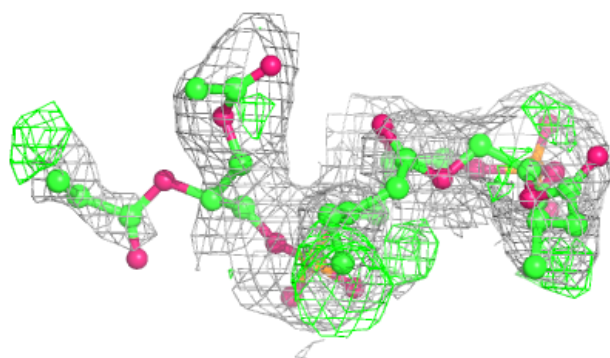
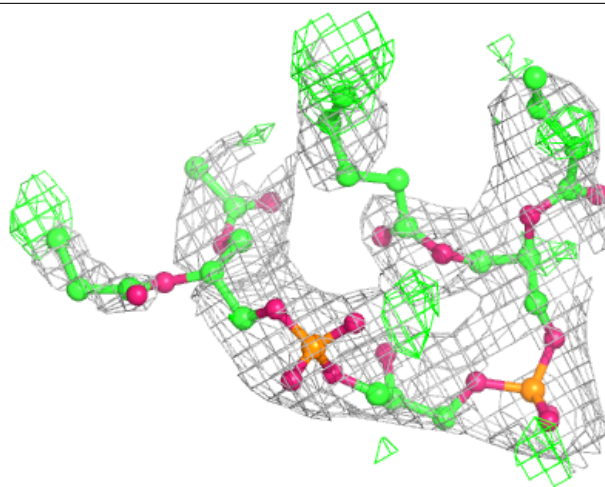
Electron density around PEE R 3005:

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



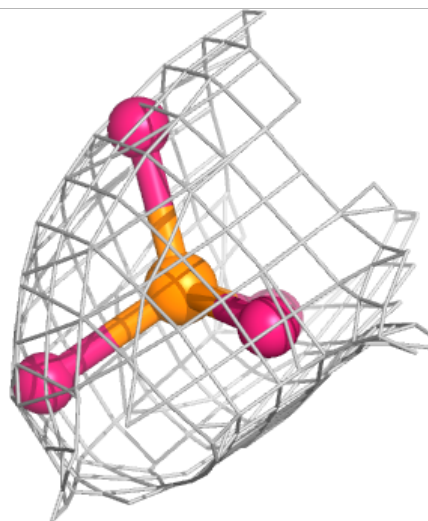
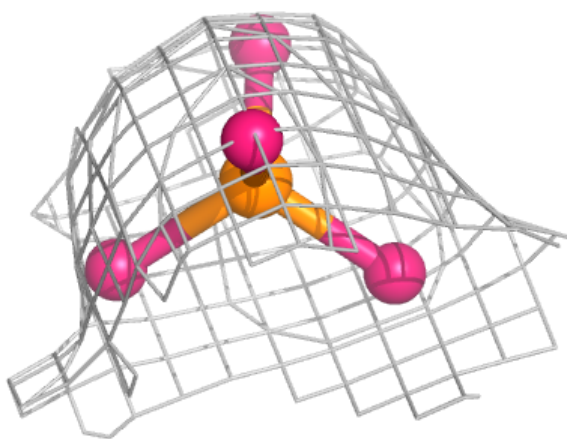
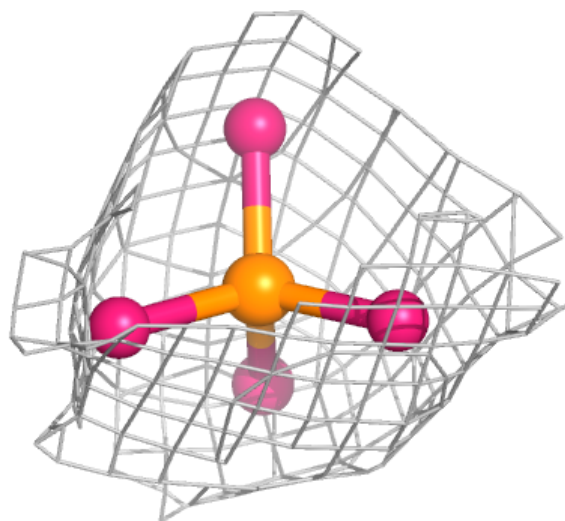
Electron density around CDL D 2003:

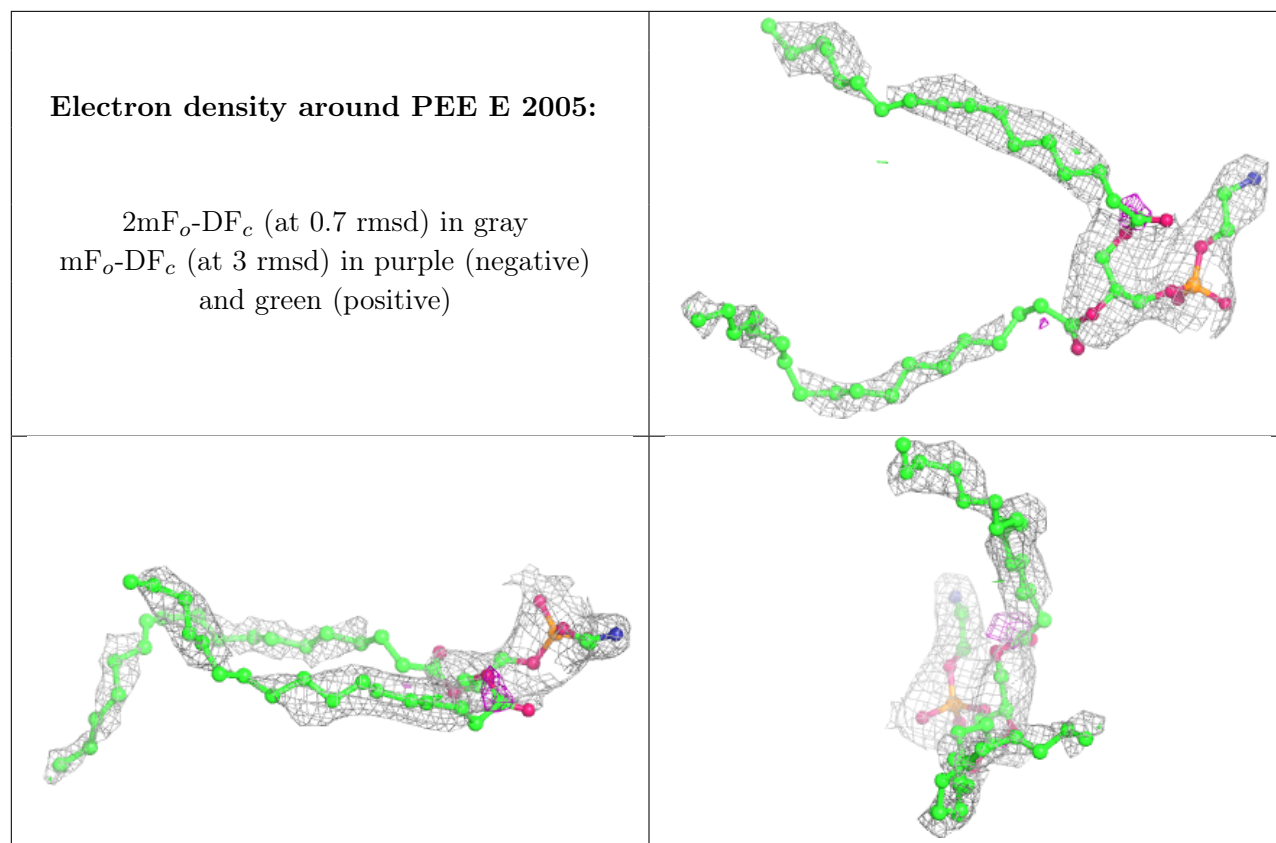
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEE P 3008:

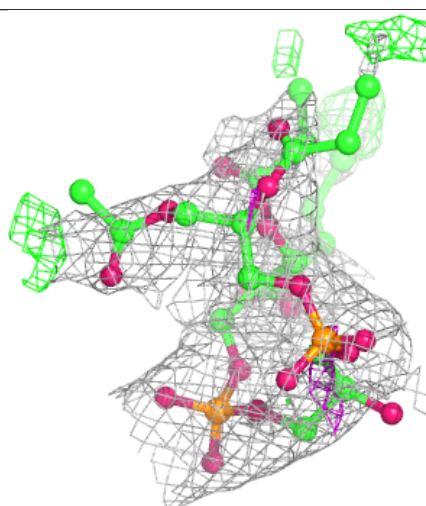
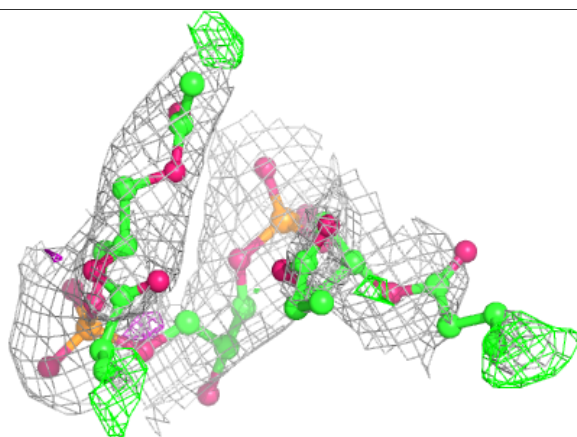
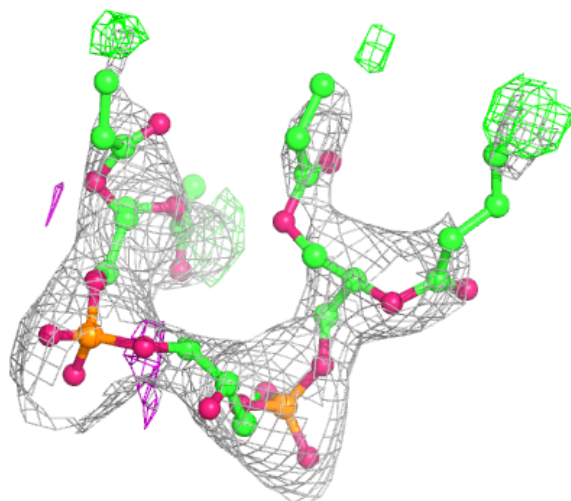
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





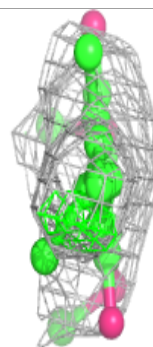
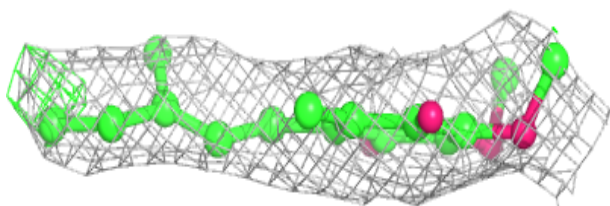
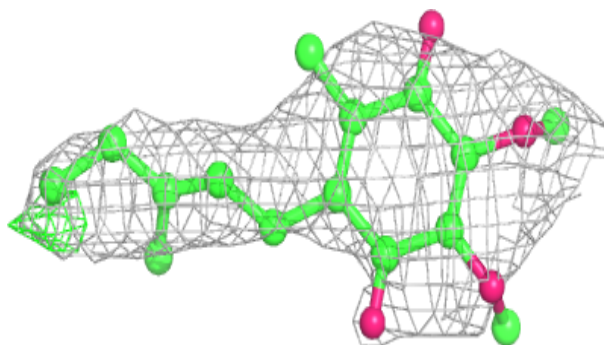
Electron density around CDL P 3004:

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

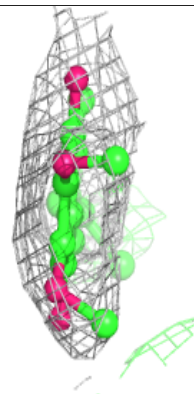
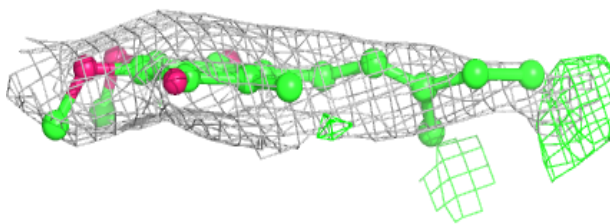
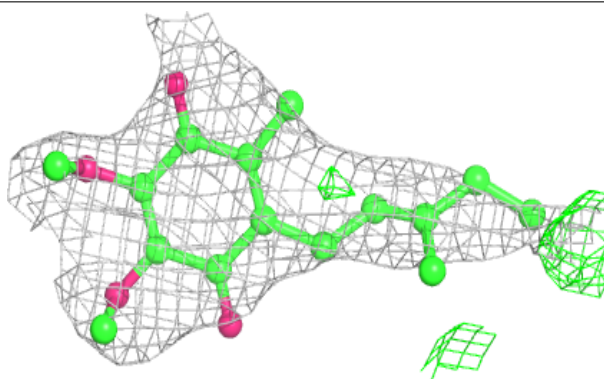


Electron density around UQ P 3002:

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

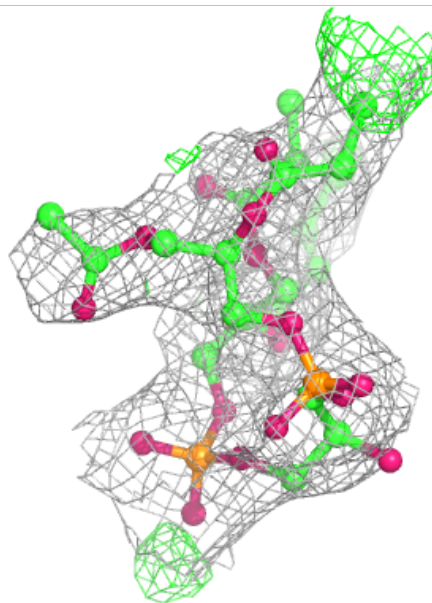
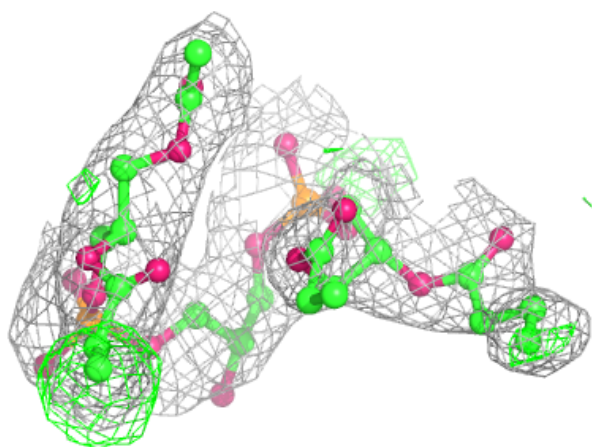
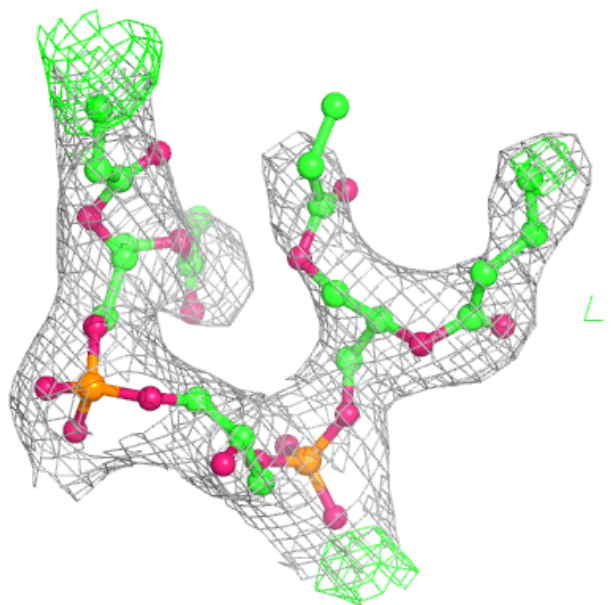
**Electron density around UQ C 2002:**

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



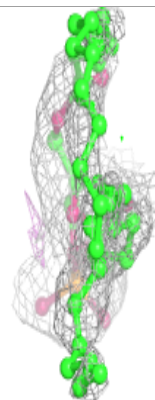
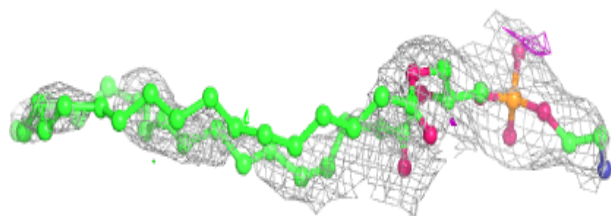
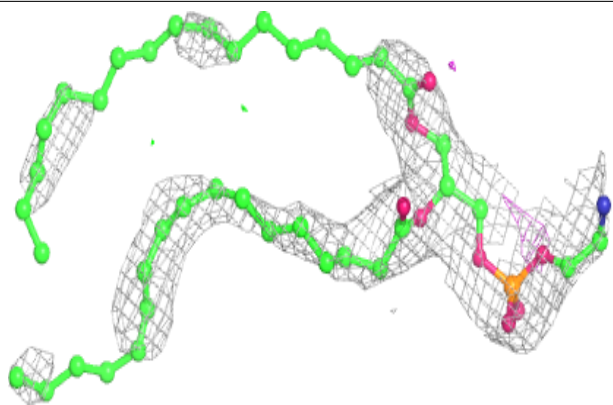
Electron density around CDL C 2004:

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

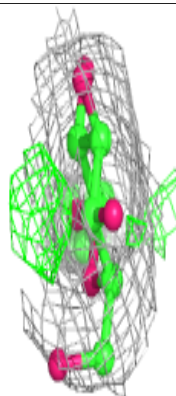
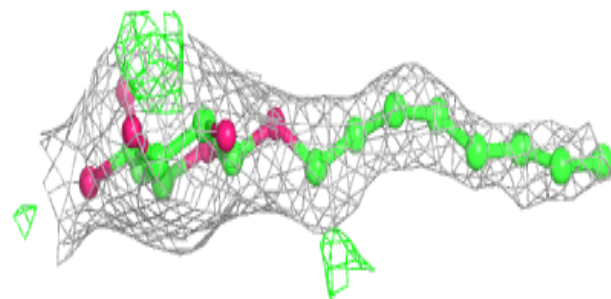
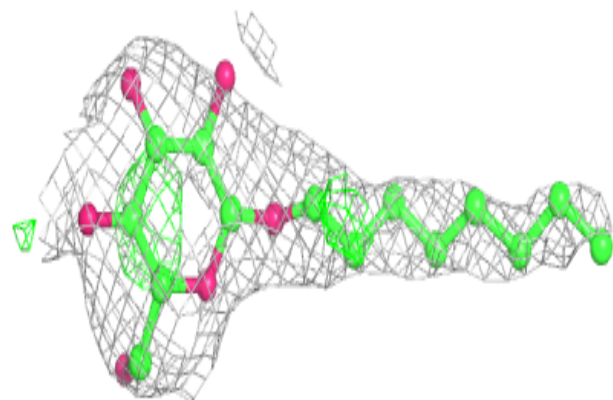


Electron density around PEE P 3007:

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

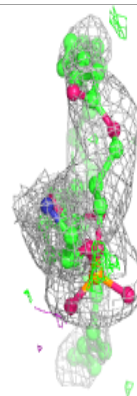
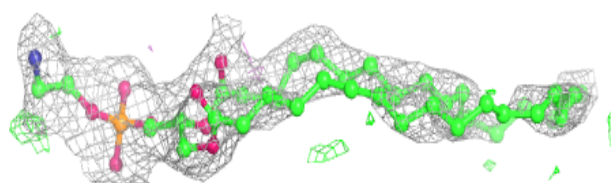
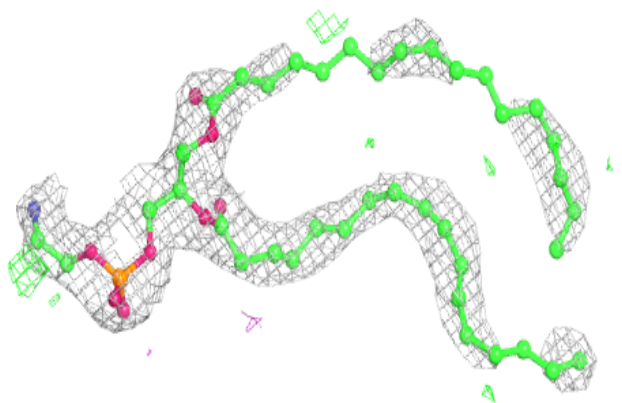
**Electron density around BOG Q 3009:**

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

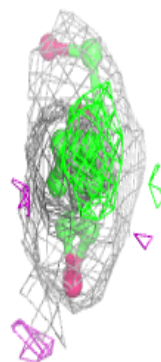
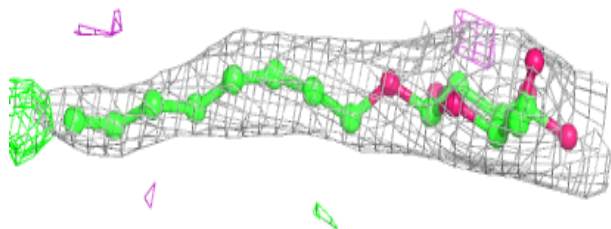
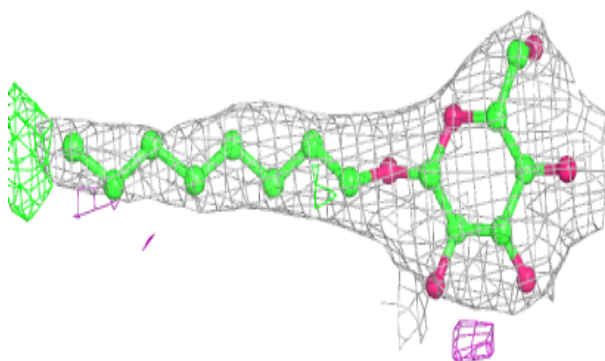


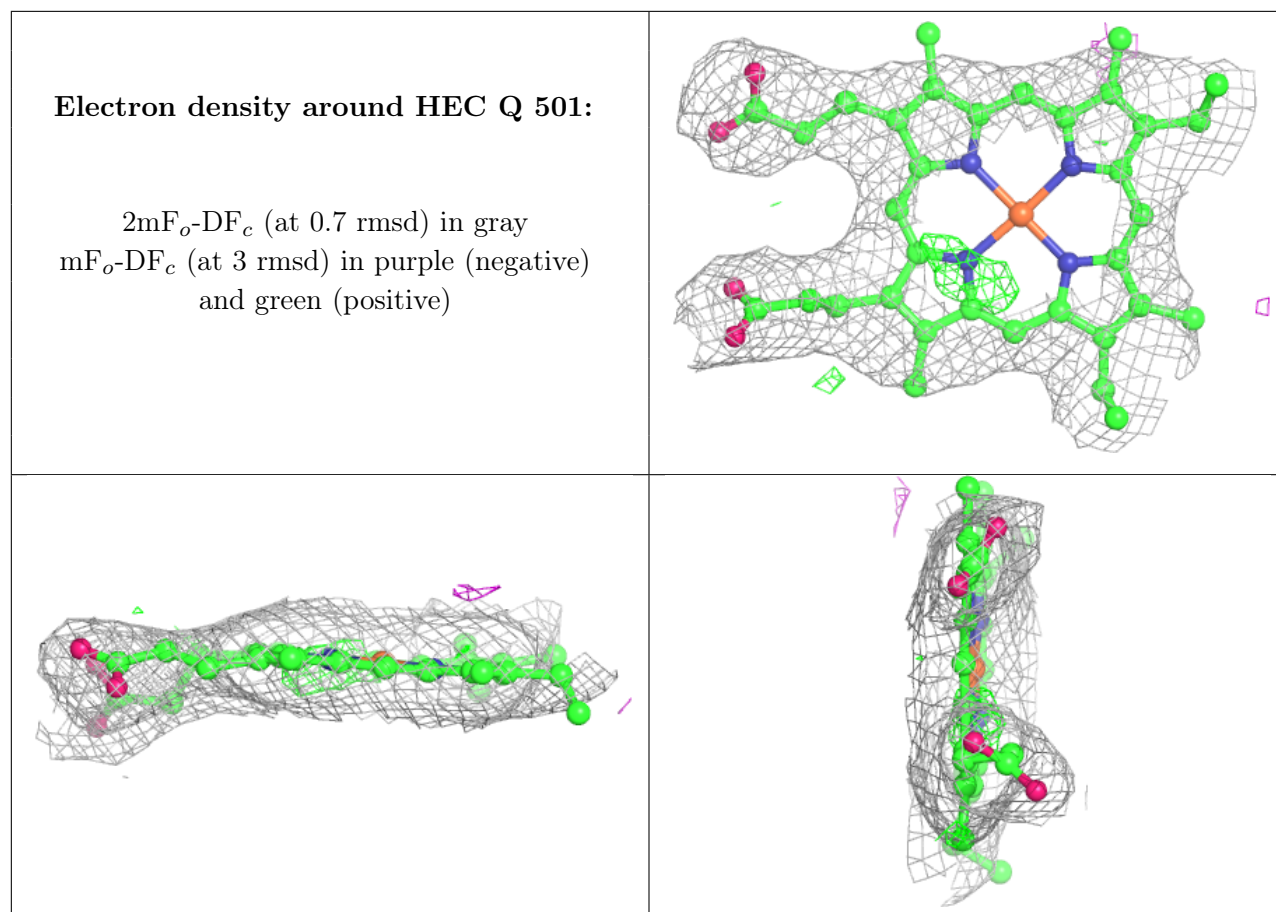
Electron density around PEE C 2007:

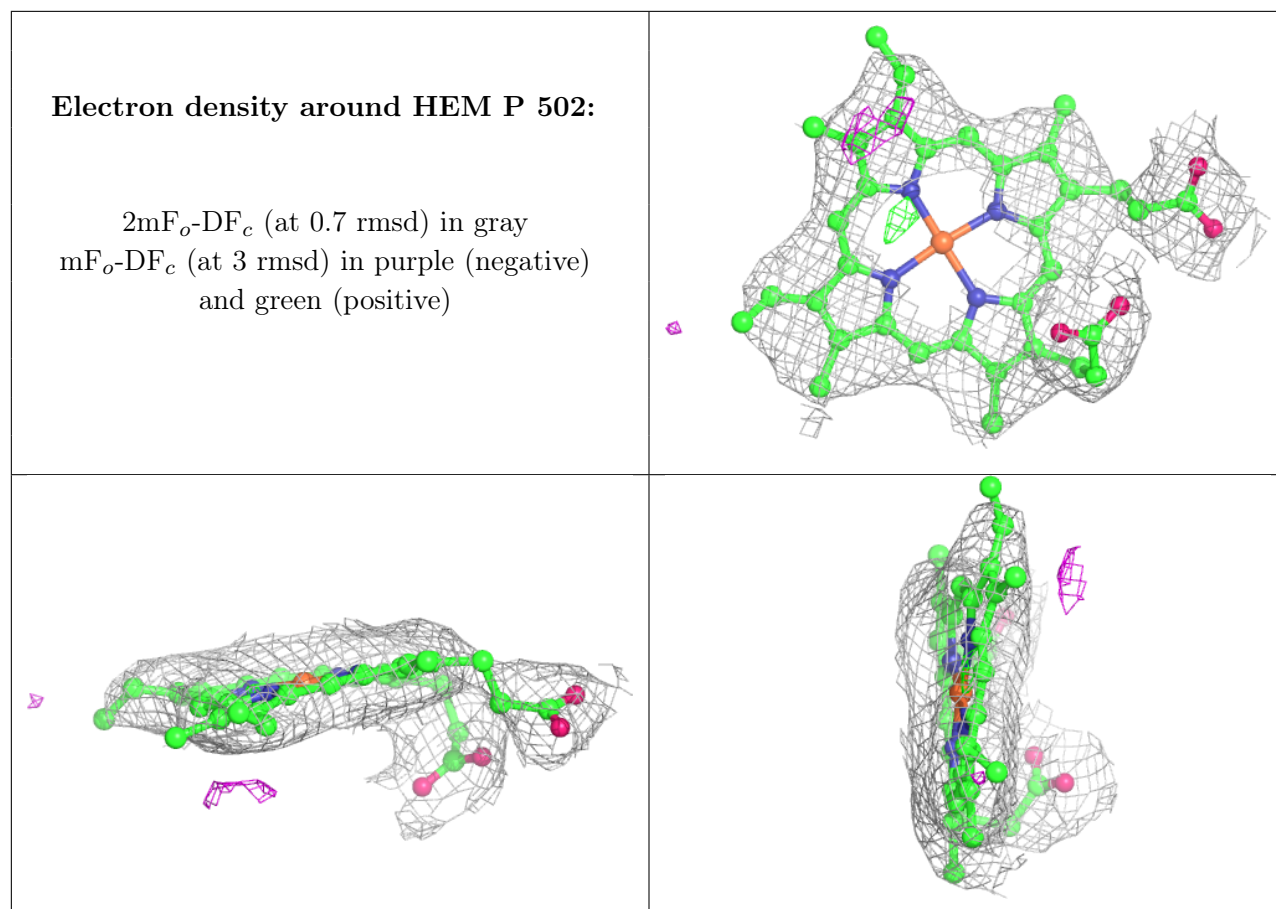
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BOG D 2009:**

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

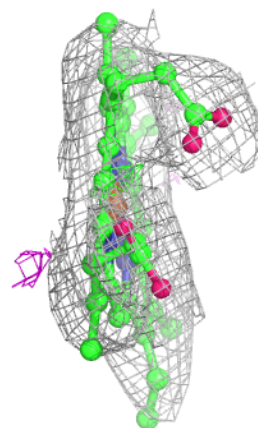
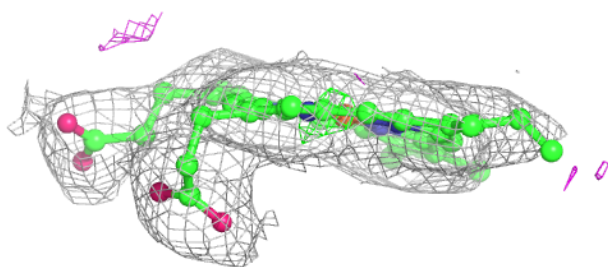
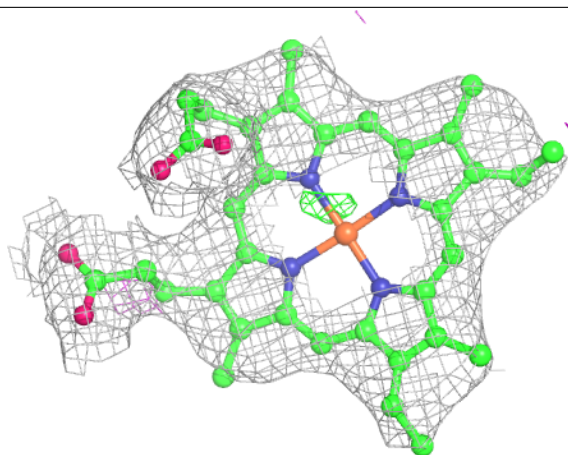






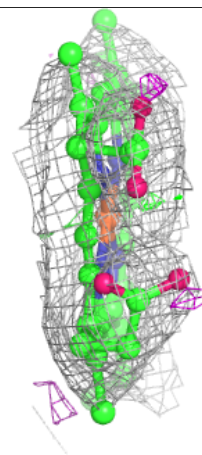
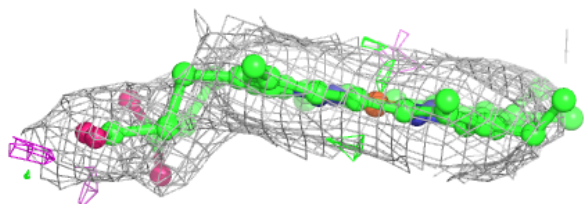
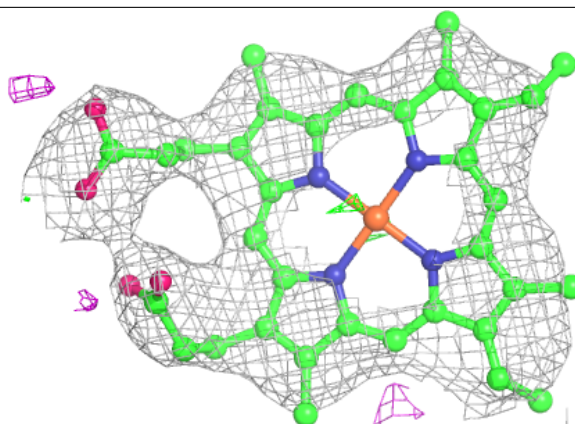
Electron density around HEM C 502:

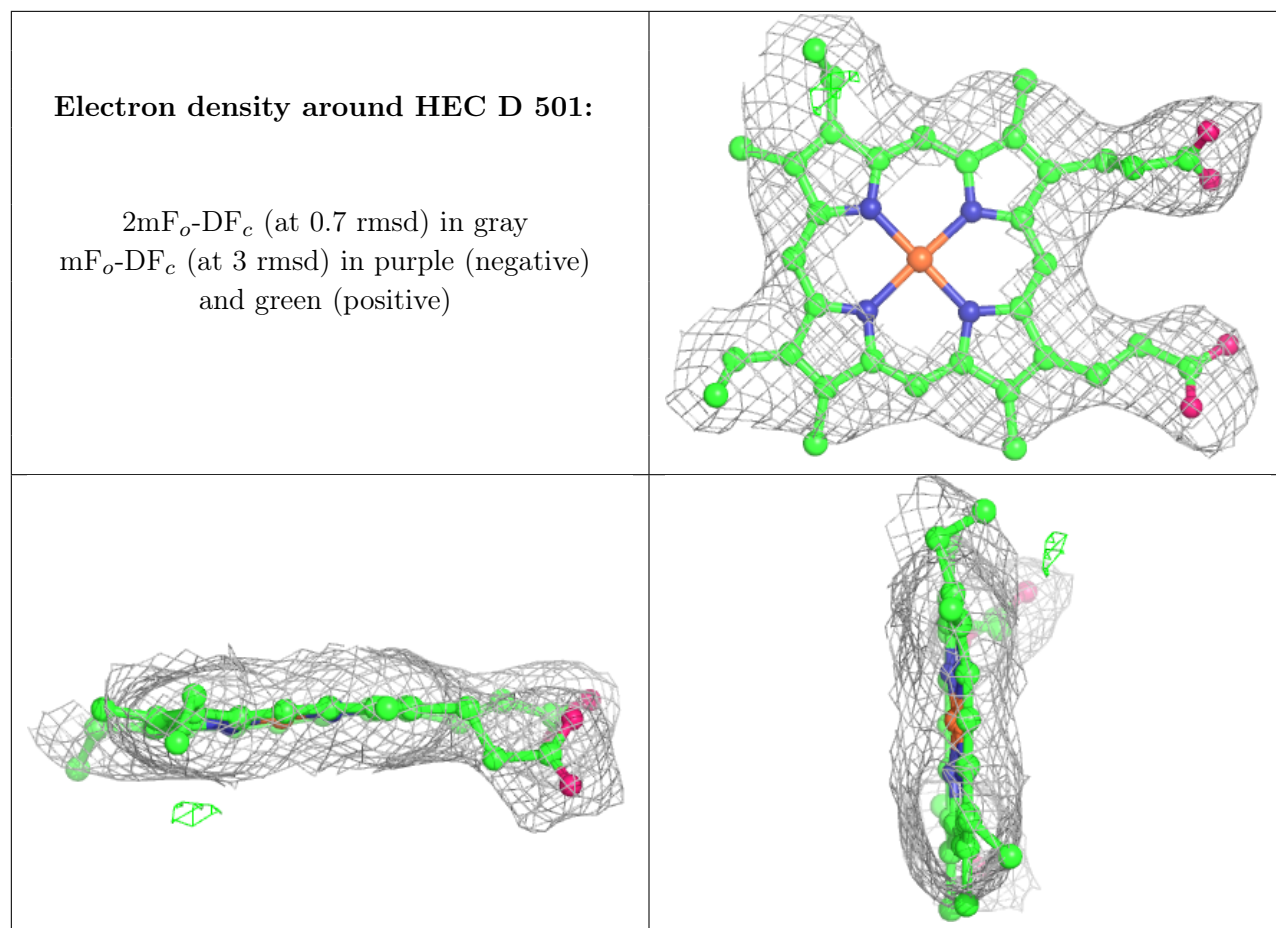
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM P 501:

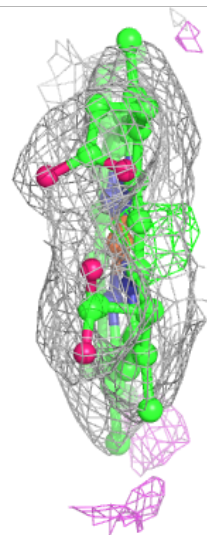
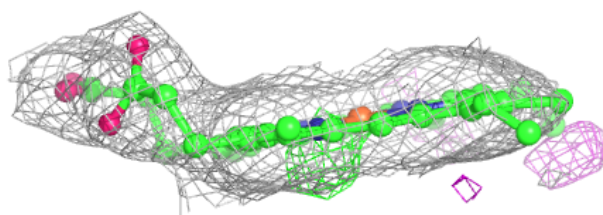
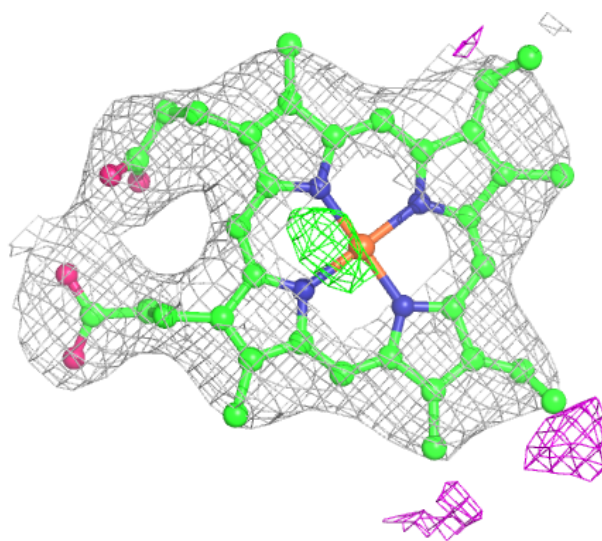
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





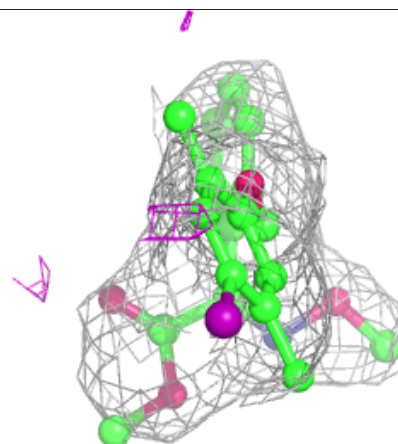
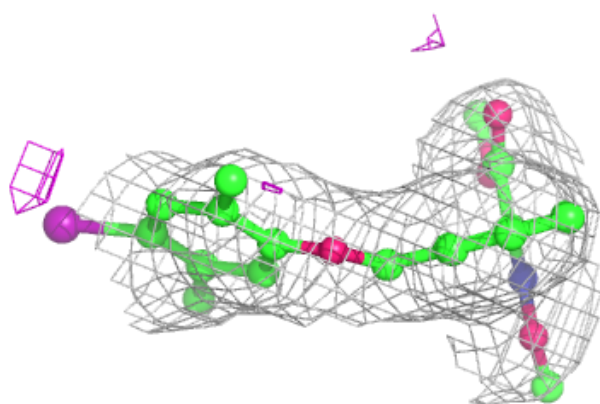
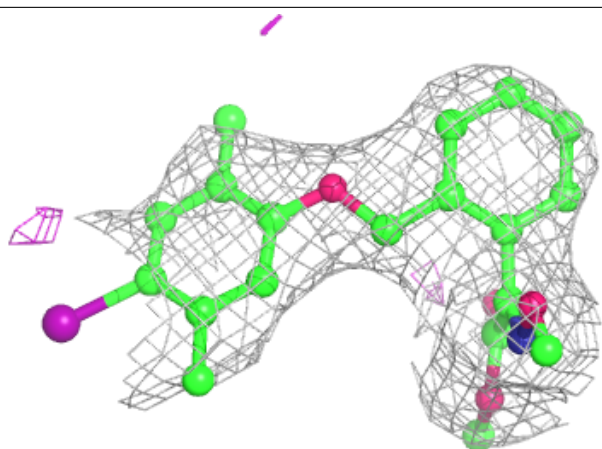
Electron density around HEM C 501:

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

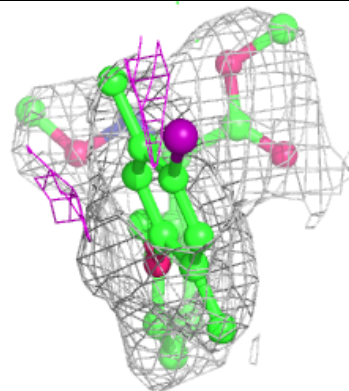
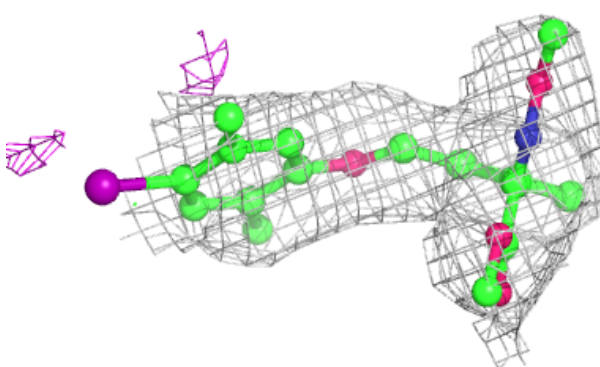
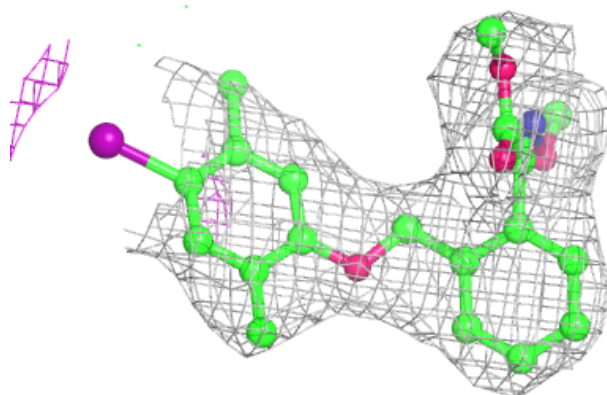


Electron density around IKR P 3001:

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

**Electron density around IKR C 2001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.