



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:44 pm BST

PDB ID : 3H1J
Title : Stigmatellin-bound cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.; Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on : 2009-04-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

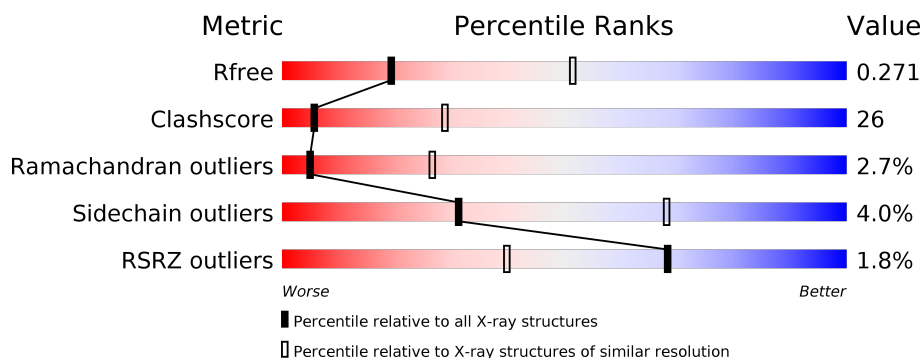
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>56%</div> <div>38%</div> <div>5%</div> </div>
1	N	446	<div> <div>53%</div> <div>41%</div> <div></div> </div>
2	B	441	<div> <div>43%</div> <div>47%</div> <div>5%</div> <div>5%</div> </div>
2	O	441	<div> <div>48%</div> <div>42%</div> <div>5%</div> </div>
3	C	380	<div> <div>63%</div> <div>36%</div> </div>
3	P	380	<div> <div>%</div> <div>59%</div> <div>38%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	UNL	C	2010	-	-	-	X
11	UNL	C	2104	-	-	-	X
11	UNL	C	3015	-	-	-	X
11	UNL	E	3103	-	-	-	X
11	UNL	P	3010	-	-	-	X
11	UNL	P	3104	-	-	-	X
11	UNL	R	2103	-	-	-	X
15	PEE	N	3008	-	X	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

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

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

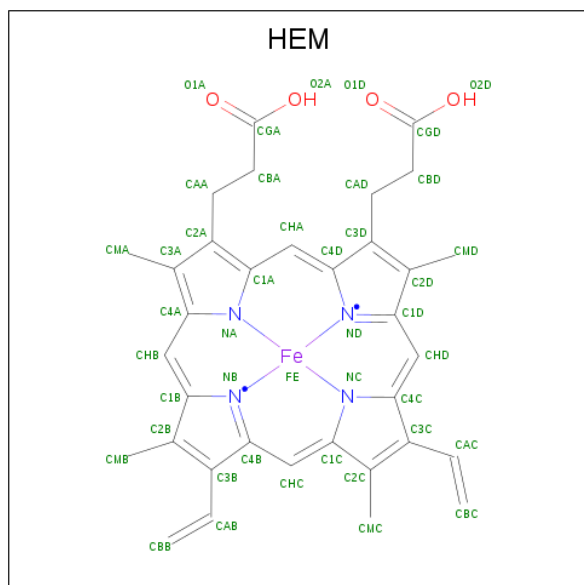
- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

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

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



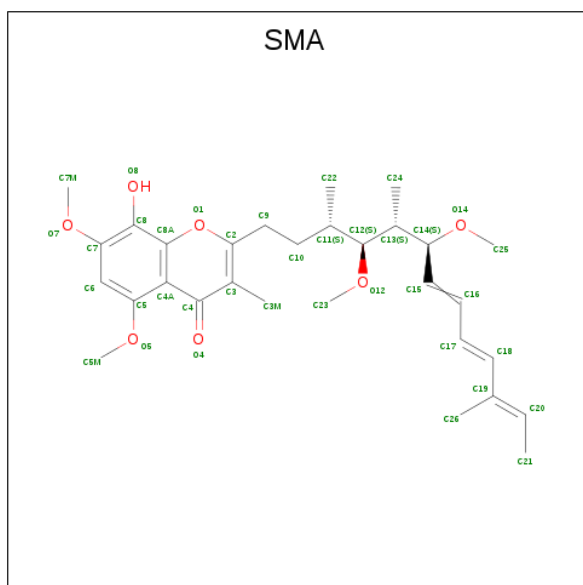
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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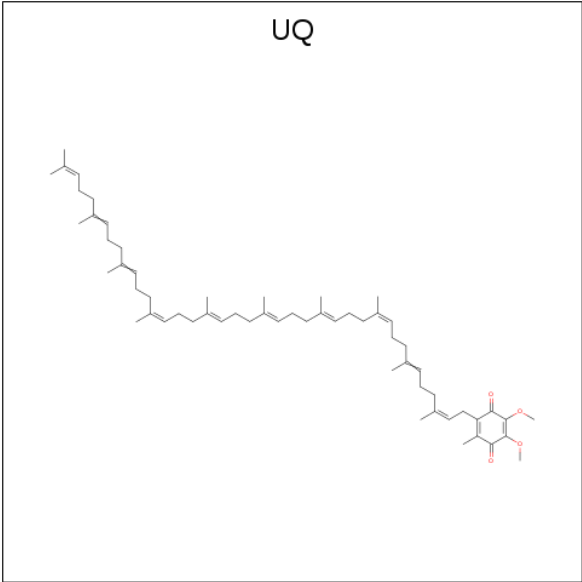
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 13 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



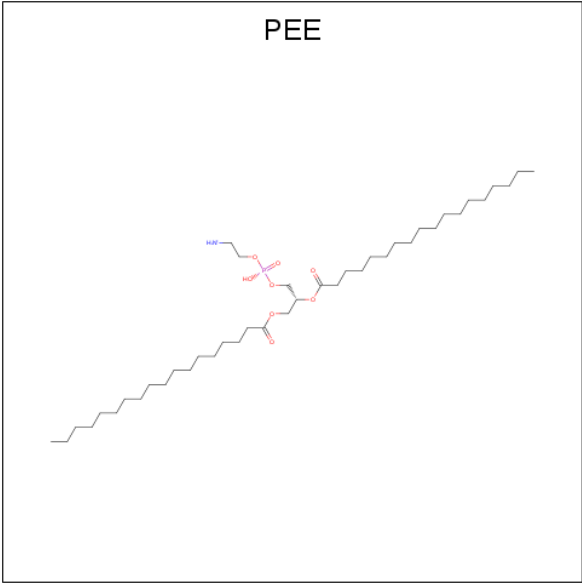
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O		
			37	30	7	0	0
13	P	1	Total	C	O		
			37	30	7	0	0

- Molecule 14 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



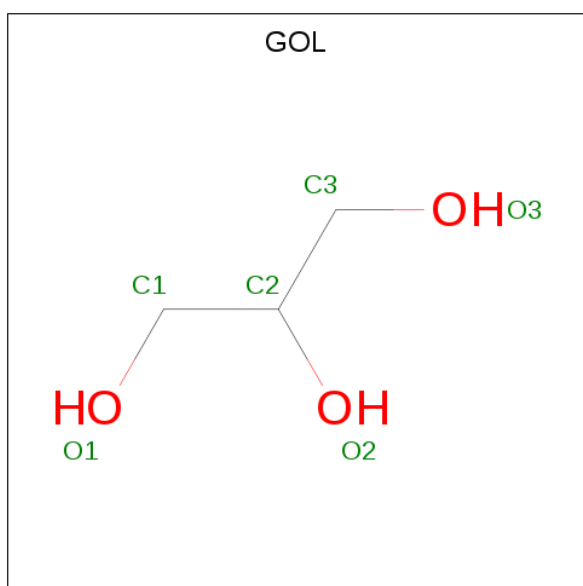
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

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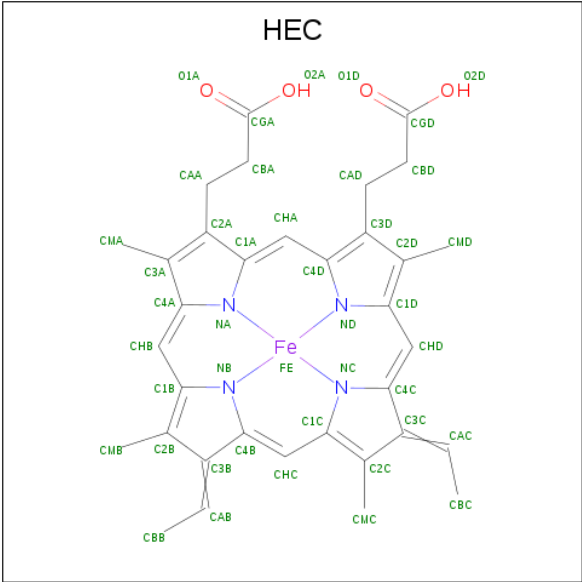
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	N	1	Total	O	P			0	0
			5	4	1				
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



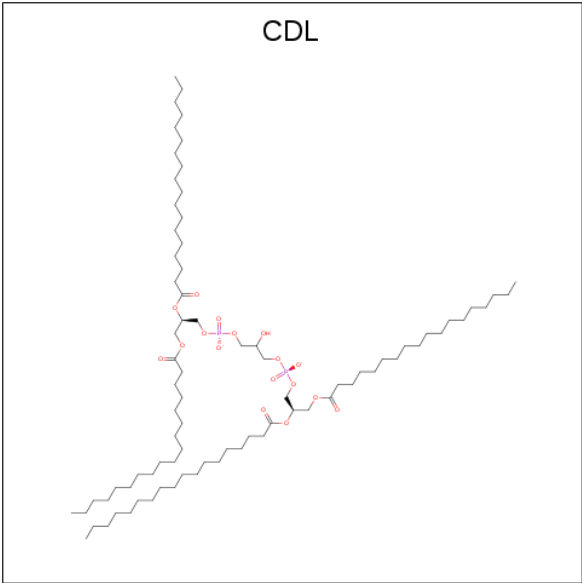
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



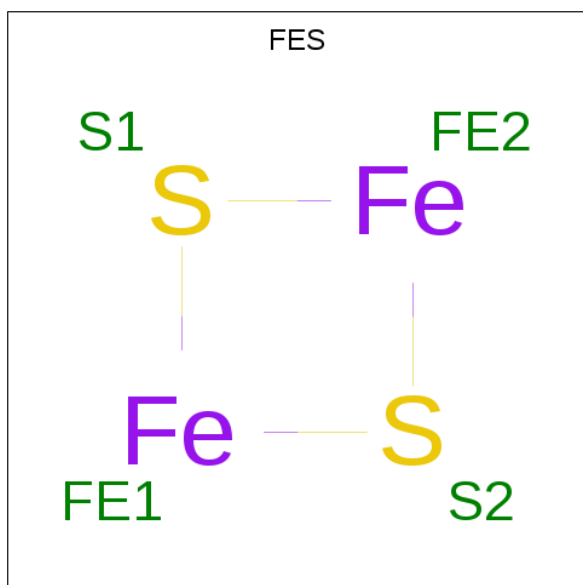
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			50	31	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		

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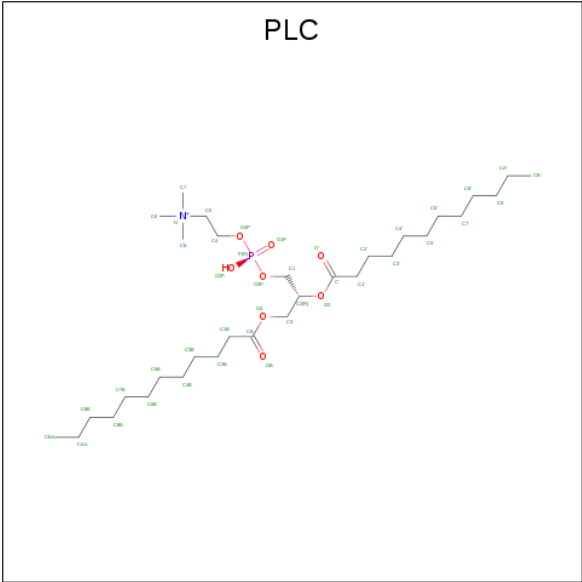
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			40	21	17	2		
18	S	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

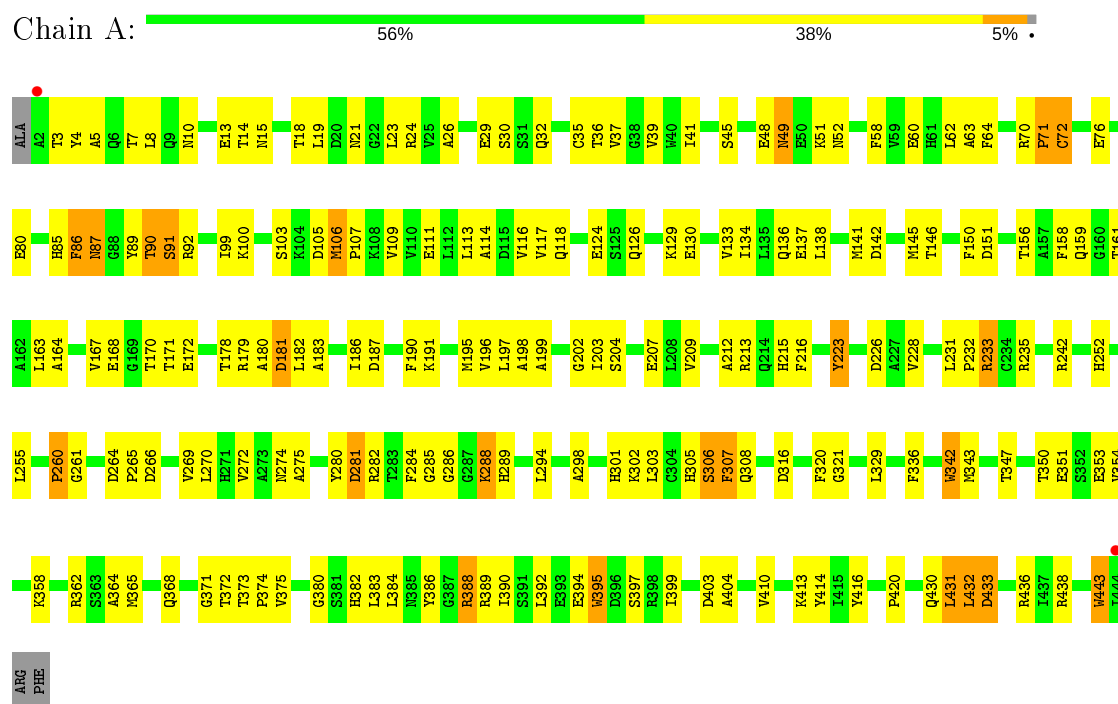
- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C₃₂H₆₅NO₈P).



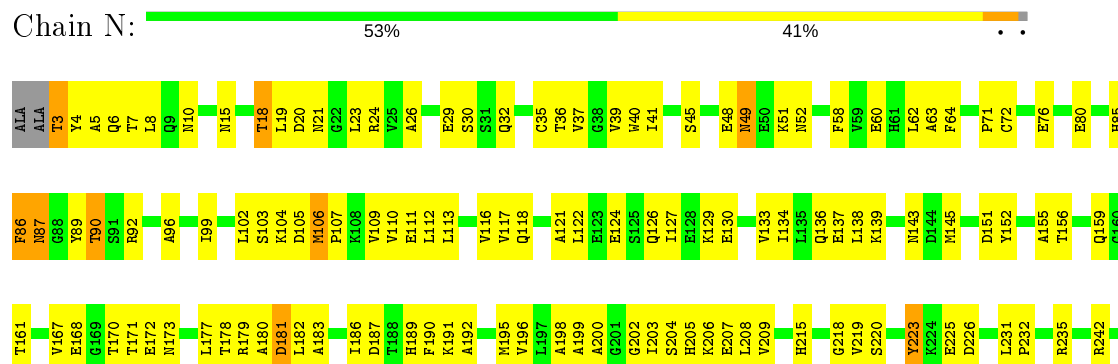
3 Residue-property plots

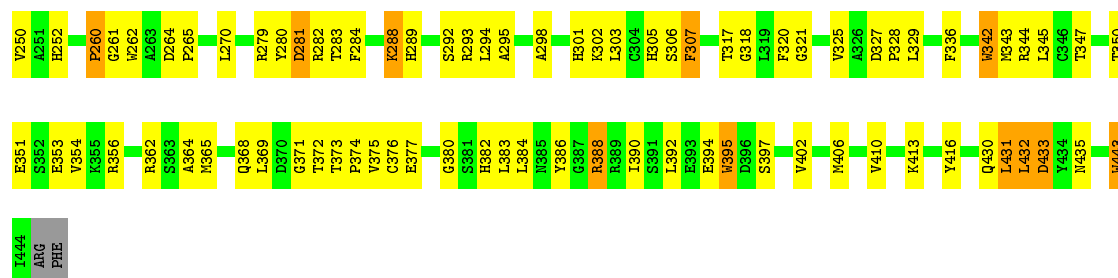
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



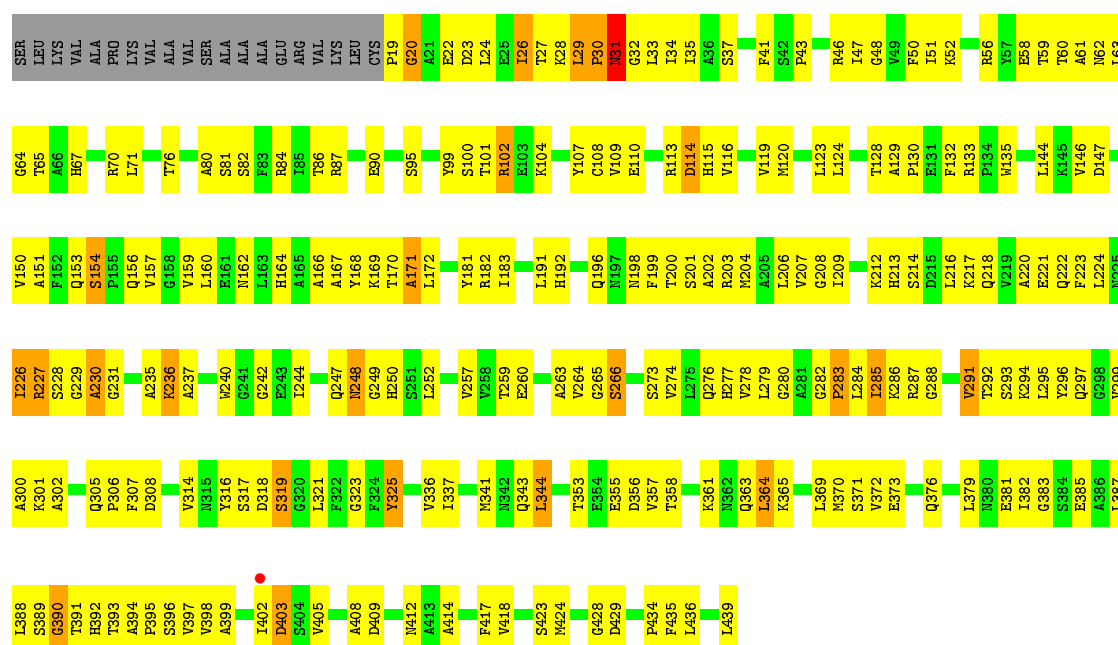
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I





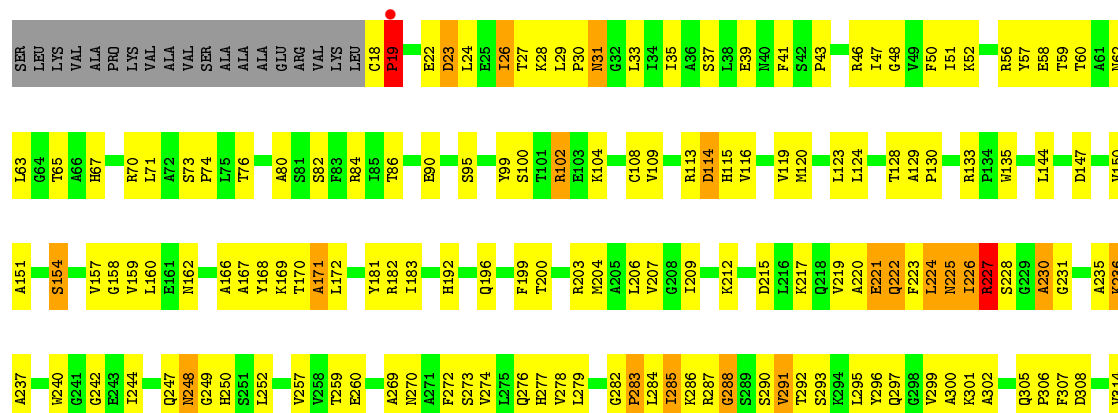
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

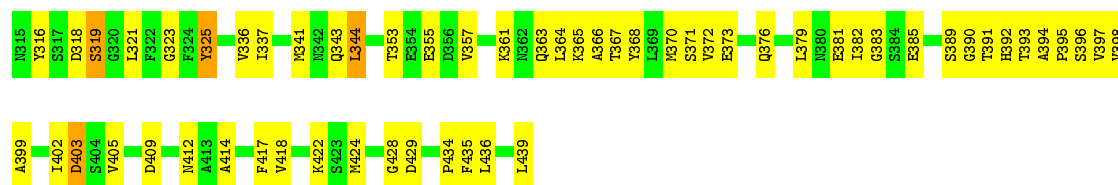
Chain B: 43% 47% 5% 5%



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

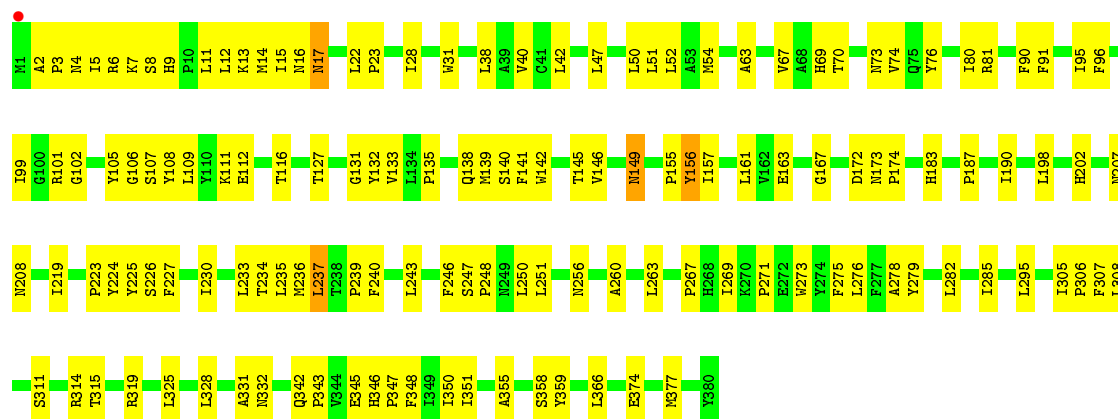
Chain O: 48% 42% 5%





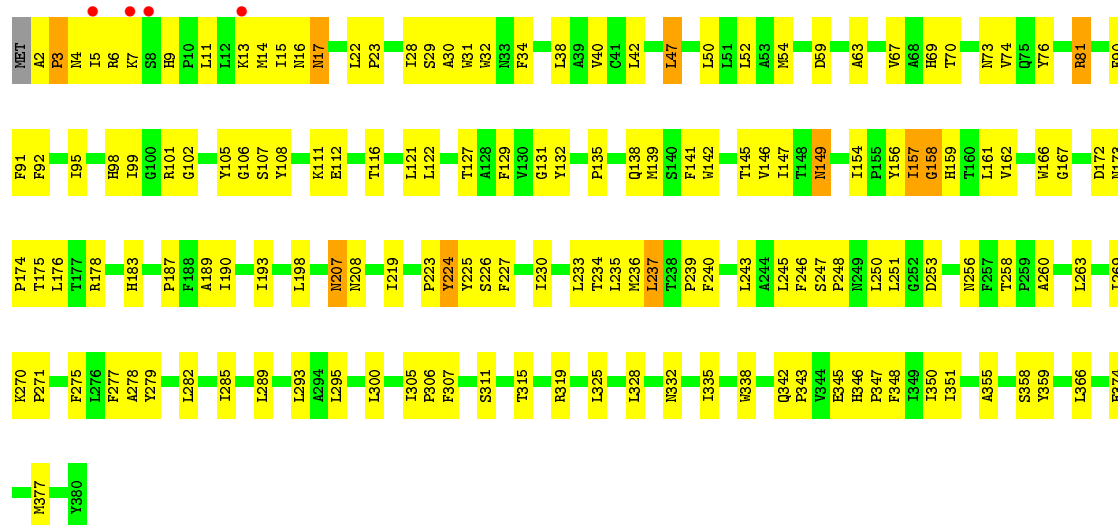
• Molecule 3: Cytochrome b

Chain C: 63% 36%



• Molecule 3: Cytochrome b

Chain P: 59% 38%



• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

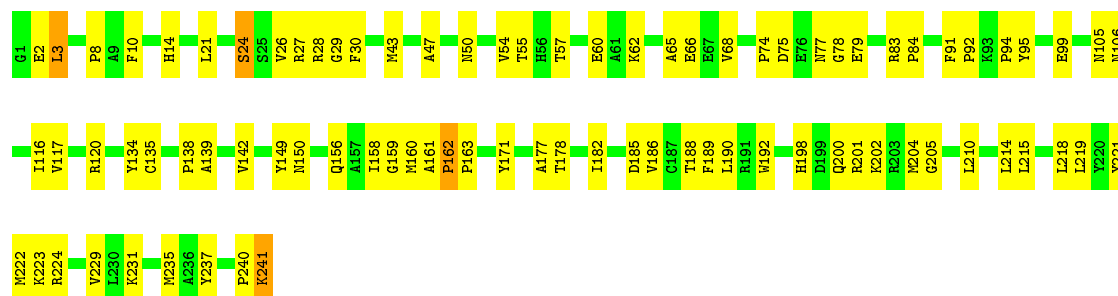
Chain D: 68% 31%





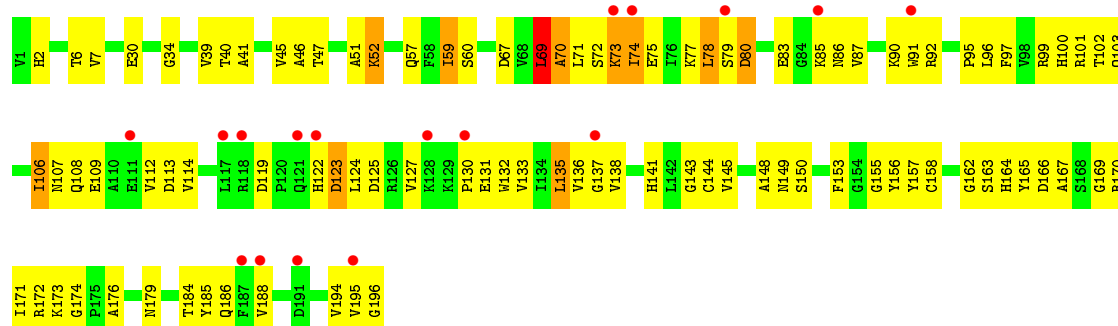
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q: 65% 34% .



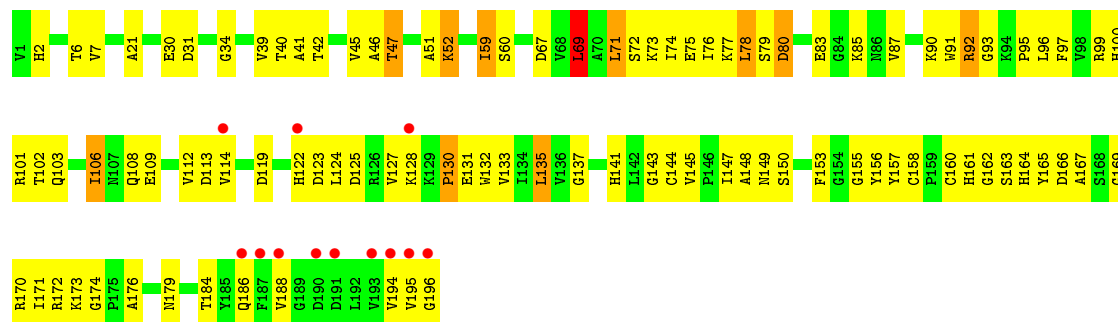
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 9% 51% 44% 5% .



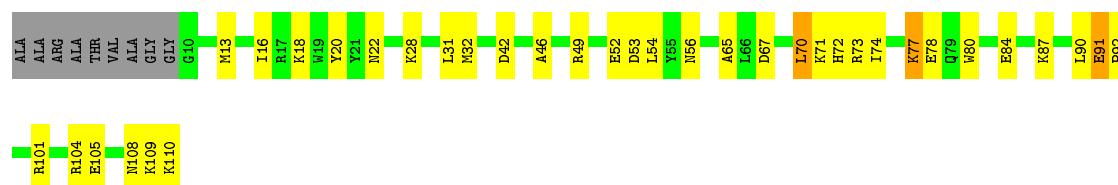
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R: 6% 49% 45% 5% .



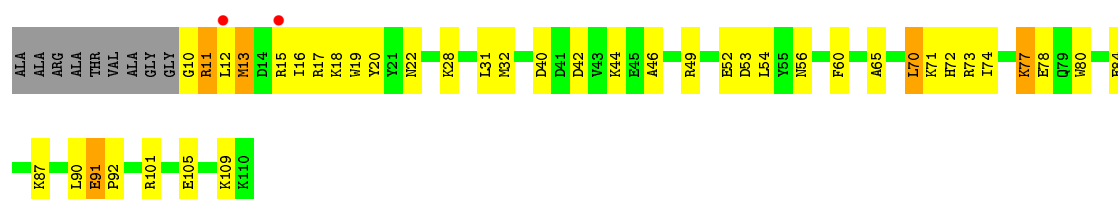
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain F: 



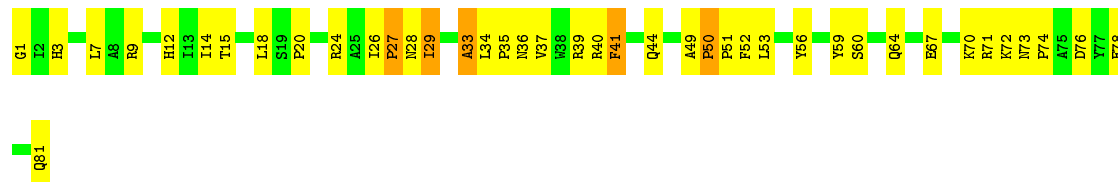
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S: 



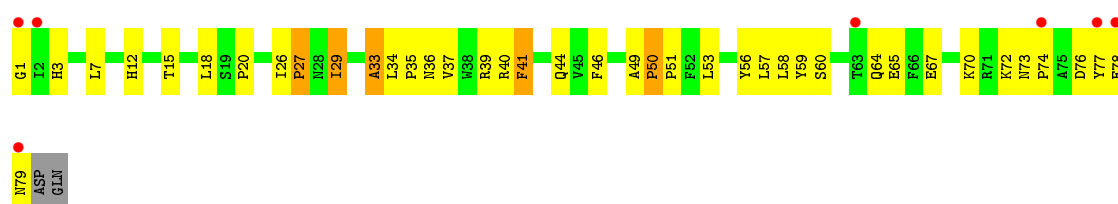
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



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

Chain T: 



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

Chain H: 



L77
K78

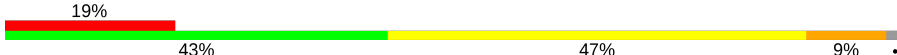
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U: 

LEU ARG GLY SER GLY GLU GLU GLU E12 L13 L14 D15 P16 L17 T18 T19 I20 R21 R22 R23 R24 C24 E25 Q26 T27 E28 V31 V32 A33 R34 R35 R36 L37 E38 L39 C40 D41 A42 R43 V44 R47 S48 R49 T50 E51 E52 Q53 C54 T55 E56 E57 L58 F61 R65 D66

H67 C68 V69 A70 K71 K72 L73 F74 N75 K76 L77 K78

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

Chain I: 

X28 X31 X32 X33 X34 X35 X38 X39 X40 R47 P48 L49 L50 R51 R52 E53 S54 M55 S56 S57 G57 S58 A60 R61 R62 D63 L64 V65 A66 G67 I68 S69 S69 N71 A72 P73 R77 TYR

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

Chain V: 

UNK UNK X28 X29 X30 X31 X32 X36 P48 L49 L50 C51 R52 E53 S54 M55 S56 S57 G57 S58 A60 R61 R62 D63 L64 V65 I68 S69 L70 N71 A72 P73 V76 R77 TYR

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

Chain J: 

A4 R7 Q8 A9 Y10 R16 L22 V25 L26 R33 Q37 Q38 A39 D40 A41 T42 F43 E44 H45 L46 G49 N52 K53 H54 I55 K56 H57 K58 Y59 S62 E63 E64

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

Chain W: 

A4 R7 Y10 F14 F20 A21 L22 L26 G27 A28 R33 Q37 Q38 A39 D40 A41 I42 F43 E44 H45 L46 G49 H52 K53 H54 I55 K56 H57 K58 Y59 E60 A61 S62 GLU GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.68-3.00) 92.5 (42.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.277 0.234 , 0.271	Depositor DCC
R_{free} test set	2796 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32679	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/3511	0.65	0/4757
1	N	0.43	0/3508	0.65	1/4753 (0.0%)
2	B	0.38	0/3196	0.63	0/4334
2	O	0.40	0/3202	0.63	0/4343
3	C	0.52	0/3122	0.67	0/4273
3	P	0.46	0/3114	0.65	0/4263
4	D	0.45	0/1956	0.64	0/2658
4	Q	0.40	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.64	1/2103 (0.0%)
5	R	0.39	0/1547	0.68	2/2103 (0.1%)
6	F	0.52	0/911	0.71	0/1219
6	S	0.43	0/911	0.63	0/1219
7	G	0.50	0/698	0.68	0/946
7	T	0.44	0/680	0.65	0/923
8	H	0.47	0/582	0.59	0/779
8	U	0.34	0/561	0.57	0/751
9	I	0.40	0/218	0.65	0/293
9	V	0.41	0/218	0.66	0/293
10	J	0.44	0/508	0.63	0/682
10	W	0.41	0/489	0.61	0/658
All	All	0.43	0/32435	0.65	4/44008 (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
3	P	0	1
4	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	143	GLY	N-CA-C	6.29	128.82	113.10
5	R	143	GLY	N-CA-C	6.28	128.80	113.10
1	N	218	GLY	N-CA-C	-5.19	100.11	113.10
5	R	71	LEU	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	33	TYR	Sidechain
3	P	224	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	169	0
1	N	3437	0	3349	192	0
2	B	3141	0	3142	255	0
2	O	3147	0	3146	228	0
3	C	3020	0	3070	136	0
3	P	3012	0	3058	152	0
4	D	1898	0	1846	63	0
4	Q	1898	0	1846	83	0
5	E	1513	0	1478	91	0
5	R	1513	0	1478	93	0
6	F	891	0	893	36	0
6	S	891	0	893	40	0
7	G	676	0	659	46	0
7	T	658	0	647	46	0
8	H	574	0	548	31	0
8	U	553	0	535	46	0
9	I	285	0	237	50	0
9	V	275	0	238	42	0
10	J	497	0	490	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	478	0	478	29	0
11	A	1	0	0	0	0
11	C	3	0	0	0	0
11	E	2	0	0	0	0
11	P	3	0	0	0	0
11	R	1	0	0	0	0
12	C	86	0	60	11	0
12	P	86	0	60	11	0
13	C	37	0	42	4	0
13	P	37	0	42	4	0
14	C	19	0	17	5	0
14	P	19	0	17	1	0
15	C	70	0	85	1	0
15	E	50	0	77	4	0
15	N	5	0	0	0	0
15	P	49	0	72	1	0
15	R	50	0	77	4	0
16	C	6	0	8	0	0
16	P	6	0	8	1	0
17	D	43	0	30	1	0
17	Q	43	0	30	1	0
18	D	50	0	44	1	0
18	G	40	0	24	1	0
18	P	40	0	24	3	0
18	S	50	0	44	2	0
19	E	4	0	0	0	0
19	R	4	0	0	1	0
20	E	32	0	38	3	0
20	R	32	0	38	2	0
21	B	1	0	0	0	0
21	C	6	0	0	0	0
21	P	6	0	0	1	0
21	U	1	0	0	1	0
All	All	32679	0	32221	1656	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 26.

All (1656) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:THR:HG22	2:B:355:GLU:H	1.15	1.08
3:C:17:ASN:HD21	7:G:1:GLY:HA2	0.98	1.07
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.35	1.06
2:O:353:THR:HG22	2:O:355:GLU:H	1.19	1.06
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.37	1.06
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.37	1.06
2:O:76:THR:HG22	2:O:82:SER:H	1.17	1.05
2:O:22:GLU:HG3	2:O:39:GLU:HB3	1.37	1.05
2:B:76:THR:HG22	2:B:82:SER:H	1.22	1.01
3:P:90:PHE:HB3	3:P:236:MET:HE3	1.41	1.01
3:P:157:ILE:HG13	3:P:158:GLY:H	1.23	1.01
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.09	0.97
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.45	0.96
3:C:90:PHE:HB3	3:C:236:MET:HE3	1.45	0.96
7:T:29:ILE:HD12	7:T:29:ILE:H	1.28	0.96
9:V:28:UNK:CB	9:V:72:ALA:HB2	1.95	0.95
6:S:13:MET:HA	6:S:16:ILE:HB	1.46	0.95
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.29	0.94
3:C:17:ASN:ND2	7:G:1:GLY:HA2	1.82	0.94
1:A:178:THR:HB	1:A:181:ASP:OD1	1.68	0.93
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.34	0.92
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.50	0.92
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.52	0.91
6:S:32:MET:HE3	6:S:87:LYS:H	1.37	0.90
7:G:29:ILE:HD12	7:G:29:ILE:H	1.35	0.90
6:F:32:MET:CE	6:F:87:LYS:H	1.84	0.90
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.89
1:N:136:GLN:HE22	9:V:50:LEU:HD12	1.38	0.89
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.54	0.89
3:P:207:ASN:ND2	3:P:208:ASN:H	1.70	0.88
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.56	0.88
3:C:13:LYS:O	3:C:17:ASN:HB2	1.74	0.88
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.40	0.87
6:S:52:GLU:HG2	6:S:56:ASN:HD21	1.39	0.87
6:F:32:MET:CE	6:F:87:LYS:HG2	2.04	0.87
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.57	0.86
2:O:128:THR:HA	2:O:226:ILE:HD11	1.57	0.86
1:N:49:ASN:C	1:N:49:ASN:HD22	1.79	0.85
3:C:207:ASN:ND2	3:C:208:ASN:H	1.73	0.85
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.41	0.85
2:B:393:THR:HG23	2:B:397:VAL:HB	1.57	0.85
6:F:52:GLU:HG2	6:F:56:ASN:HD21	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:HD22	2:B:32:GLY:N	1.74	0.84
9:V:65:VAL:HB	9:V:77:ARG:HD3	1.58	0.84
2:O:393:THR:HG23	2:O:397:VAL:HB	1.58	0.84
3:P:101:ARG:C	3:P:101:ARG:HD2	1.97	0.84
5:R:73:LYS:HB3	5:R:195:VAL:O	1.77	0.83
6:F:32:MET:HE3	6:F:87:LYS:H	1.42	0.83
1:N:178:THR:HB	1:N:181:ASP:OD1	1.76	0.83
9:I:71:ASN:HD22	9:I:71:ASN:H	1.26	0.83
1:N:178:THR:HG22	1:N:180:ALA:H	1.41	0.83
6:S:52:GLU:HG2	6:S:56:ASN:ND2	1.94	0.83
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.42	0.83
3:P:13:LYS:O	3:P:17:ASN:HB2	1.77	0.83
1:A:178:THR:HG22	1:A:180:ALA:H	1.44	0.82
1:A:49:ASN:C	1:A:49:ASN:HD22	1.82	0.82
5:R:101:ARG:NH2	5:R:127:VAL:HG21	1.94	0.82
6:F:52:GLU:HG2	6:F:56:ASN:ND2	1.95	0.81
2:B:212:LYS:HD3	2:B:213:HIS:N	1.96	0.81
2:B:227:ARG:HD3	2:B:228:SER:H	1.45	0.80
1:A:187:ASP:O	1:A:191:LYS:HE3	1.82	0.80
3:C:101:ARG:C	3:C:101:ARG:HD2	2.02	0.80
2:O:62:ASN:O	2:O:65:THR:HG22	1.81	0.80
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.63	0.80
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.64	0.80
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.64	0.80
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.64	0.80
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.22	0.79
2:B:62:ASN:O	2:B:65:THR:HG22	1.82	0.79
6:S:32:MET:CE	6:S:87:LYS:H	1.96	0.79
5:E:101:ARG:NH2	5:E:127:VAL:HG21	1.97	0.79
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.63	0.79
2:B:47:ILE:HG12	2:B:120:MET:CE	2.13	0.79
2:O:76:THR:HG22	2:O:82:SER:N	1.95	0.79
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.78
1:N:187:ASP:O	1:N:191:LYS:HE3	1.84	0.78
1:N:99:ILE:HD12	1:N:109:VAL:HG13	1.65	0.78
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.18	0.78
2:B:76:THR:HG22	2:B:82:SER:N	1.97	0.78
1:A:99:ILE:HD12	1:A:109:VAL:HG13	1.67	0.77
2:B:227:ARG:HE	2:B:227:ARG:HA	1.48	0.76
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.67	0.76
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:CG2	2:B:82:SER:H	1.97	0.76
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.66	0.76
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.50	0.76
2:B:102:ARG:HH11	2:B:102:ARG:HG2	1.50	0.76
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.15	0.76
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.68	0.76
2:O:226:ILE:HG22	2:O:227:ARG:N	2.01	0.75
2:B:154:SER:O	2:B:157:VAL:HG12	1.86	0.75
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.26	0.75
6:F:32:MET:HE2	6:F:87:LYS:HG2	1.66	0.75
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.21	0.75
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.51	0.75
4:D:224:ARG:HE	7:G:26:ILE:HG12	1.52	0.75
9:I:32:UNK:N	9:I:73:PRO:HG2	2.01	0.75
2:O:47:ILE:HG12	2:O:120:MET:HE3	1.69	0.75
2:B:201:SER:OG	2:B:228:SER:HB3	1.87	0.74
1:A:136:GLN:NE2	9:I:50:LEU:HB2	2.02	0.74
2:B:47:ILE:HG12	2:B:120:MET:HE3	1.69	0.74
7:T:29:ILE:HD12	7:T:29:ILE:N	2.01	0.74
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.69	0.74
2:B:385:GLU:OE1	2:B:392:HIS:HA	1.87	0.74
1:N:373:THR:HB	1:N:374:PRO:HD3	1.68	0.74
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.70	0.74
3:P:157:ILE:HG13	3:P:158:GLY:N	2.01	0.74
2:O:219:VAL:O	2:O:223:PHE:HB2	1.88	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.70	0.73
2:O:47:ILE:HG12	2:O:120:MET:CE	2.18	0.73
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.70	0.73
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.69	0.73
2:B:248:ASN:HD22	2:B:248:ASN:C	1.90	0.73
7:G:29:ILE:CD1	7:G:29:ILE:H	1.93	0.73
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.70	0.73
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.23	0.73
2:O:154:SER:O	2:O:157:VAL:HG12	1.89	0.73
2:B:218:GLN:HG3	2:B:222:GLN:NE2	2.04	0.73
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.71	0.73
2:O:361:LYS:O	2:O:365:LYS:HG3	1.87	0.73
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.19	0.72
2:B:389:SER:O	2:B:391:THR:HG23	1.88	0.72
2:O:220:ALA:O	2:O:224:LEU:HB2	1.89	0.72
2:O:76:THR:CG2	2:O:82:SER:H	1.99	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:32:LYS:O	8:U:36:ARG:HG3	1.89	0.72
1:N:136:GLN:NE2	9:V:50:LEU:HB2	2.04	0.72
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.18	0.72
3:C:139:MET:HE1	3:C:269:ILE:HA	1.70	0.72
2:B:31:ASN:HB3	2:B:227:ARG:HH22	1.54	0.72
7:G:29:ILE:HD12	7:G:29:ILE:N	2.04	0.72
9:I:71:ASN:H	9:I:71:ASN:ND2	1.88	0.72
2:O:389:SER:O	2:O:391:THR:HG23	1.90	0.72
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.84	0.72
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.24	0.72
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.55	0.71
3:C:4:ASN:HD21	3:C:7:LYS:NZ	1.87	0.71
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.72	0.71
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.26	0.71
1:N:182:LEU:O	1:N:186:ILE:HG13	1.91	0.71
8:U:27:THR:O	8:U:31:VAL:HG23	1.89	0.71
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.30	0.71
2:O:22:GLU:HG3	2:O:39:GLU:CB	2.18	0.71
2:O:29:LEU:HD12	2:O:33:LEU:HD23	1.72	0.71
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.72	0.71
2:O:248:ASN:HD22	2:O:248:ASN:C	1.91	0.71
2:B:227:ARG:NE	2:B:227:ARG:HA	2.05	0.71
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.56	0.71
9:V:64:LEU:HD12	9:V:77:ARG:O	1.89	0.71
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.72	0.71
8:H:43:ARG:HD2	8:H:47:ARG:NH1	2.06	0.71
3:P:285:ILE:N	3:P:285:ILE:HD12	2.06	0.71
2:B:203:ARG:CD	2:B:230:ALA:HA	2.19	0.71
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.72	0.71
4:D:75:ASP:OD2	4:D:79:GLU:HB2	1.90	0.70
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.71	0.70
2:B:212:LYS:HD2	2:B:214:SER:OG	1.91	0.70
9:I:55:MET:O	9:I:58:ARG:HG2	1.92	0.70
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.27	0.70
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.06	0.70
7:T:29:ILE:CD1	7:T:29:ILE:H	1.90	0.70
1:N:90:THR:O	1:N:167:VAL:HG11	1.91	0.70
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.06	0.70
2:B:124:LEU:HD21	2:B:223:PHE:HB3	1.73	0.70
1:N:388:ARG:HG3	1:N:388:ARG:HH21	1.56	0.70
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.74	0.70
3:P:346:HIS:ND1	3:P:347:PRO:HA	2.06	0.70
2:B:353:THR:HG22	2:B:355:GLU:N	2.00	0.69
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.73	0.69
2:O:385:GLU:OE1	2:O:392:HIS:HA	1.92	0.69
3:P:187:PRO:HG2	12:P:501:HEM:HMC3	1.72	0.69
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.91	0.69
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.69
3:P:17:ASN:HD21	7:T:1:GLY:HA3	1.57	0.69
1:A:288:LYS:HE3	1:A:289:HIS:NE2	2.07	0.69
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.74	0.69
3:P:207:ASN:ND2	3:P:208:ASN:N	2.40	0.69
2:O:33:LEU:HD21	2:O:220:ALA:HB1	1.74	0.69
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.58	0.69
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.73	0.69
2:B:24:LEU:HD12	2:B:37:SER:O	1.92	0.69
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.73	0.69
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.75	0.68
1:A:10:ASN:HD21	2:B:19:PRO:HD3	1.56	0.68
2:B:31:ASN:HD22	2:B:32:GLY:H	1.39	0.68
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.08	0.68
1:A:281:ASP:HB3	1:A:284:PHE:CE1	2.29	0.68
1:A:45:SER:HA	1:A:48:GLU:HG3	1.74	0.68
9:I:31:UNK:C	9:I:73:PRO:HG2	2.23	0.68
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.28	0.68
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.75	0.68
5:R:91:TRP:CE3	5:R:96:LEU:HD22	2.28	0.68
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.75	0.68
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	1.94	0.68
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.20	0.68
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.23	0.68
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.29	0.68
1:A:373:THR:HB	1:A:374:PRO:HD3	1.75	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.58	0.68
1:A:350:THR:OG1	1:A:353:GLU:HG3	1.93	0.67
5:E:40:THR:HG21	15:E:2005:PEE:O2P	1.94	0.67
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.20	0.67
2:O:192:HIS:O	2:O:196:GLN:HG3	1.94	0.67
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.59	0.67
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.10	0.67
2:B:295:LEU:HA	2:B:343:GLN:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.60	0.67
3:P:226:SER:O	3:P:230:ILE:HG12	1.95	0.67
3:P:271:PRO:HA	13:P:3001:SMA:H10	1.75	0.67
3:P:247:SER:OG	3:P:250:LEU:HB2	1.95	0.67
2:O:217:LYS:O	2:O:221:GLU:HG2	1.95	0.67
6:F:70:LEU:HD12	6:F:70:LEU:C	2.15	0.67
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.67
3:P:4:ASN:HD21	3:P:7:LYS:NZ	1.92	0.67
2:O:227:ARG:HA	2:O:227:ARG:HH11	1.59	0.67
6:S:11:ARG:O	6:S:11:ARG:HG2	1.95	0.67
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.76	0.66
2:O:274:VAL:O	2:O:278:VAL:HG23	1.96	0.66
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.78	0.66
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.28	0.66
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.59	0.66
1:N:30:SER:O	1:N:202:GLY:HA2	1.95	0.66
3:C:187:PRO:HG2	12:C:501:HEM:HMC3	1.78	0.66
8:H:34:ARG:O	8:H:38:GLU:HG2	1.96	0.66
1:N:432:LEU:HD23	1:N:433:ASP:N	2.11	0.66
8:H:27:THR:O	8:H:31:VAL:HG23	1.95	0.66
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.76	0.66
2:B:199:PHE:O	2:B:226:ILE:HG12	1.95	0.66
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.60	0.66
3:P:345:GLU:O	3:P:348:PHE:HB2	1.95	0.66
6:S:70:LEU:HD12	6:S:70:LEU:C	2.16	0.66
9:V:64:LEU:HA	9:V:77:ARG:O	1.96	0.66
2:B:43:PRO:O	2:B:113:ARG:HG3	1.96	0.65
3:C:202:HIS:NE2	14:C:2002:UQ:O4	2.29	0.65
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.78	0.65
15:P:3007:PEE:H7	7:T:44:GLN:HE21	1.60	0.65
8:H:32:LYS:O	8:H:36:ARG:HG3	1.96	0.65
2:O:95:SER:HB3	9:V:28:UNK:H2	1.61	0.65
1:N:136:GLN:NE2	9:V:50:LEU:HD12	2.10	0.65
1:N:49:ASN:C	1:N:49:ASN:ND2	2.50	0.65
2:O:95:SER:HB3	9:V:28:UNK:N	2.11	0.65
2:B:229:GLY:O	2:B:231:GLY:N	2.28	0.65
3:C:207:ASN:ND2	3:C:208:ASN:N	2.45	0.65
2:O:124:LEU:HD13	2:O:224:LEU:HD23	1.79	0.65
1:A:156:THR:O	1:A:159:GLN:HG2	1.97	0.65
2:B:361:LYS:O	2:B:365:LYS:HG3	1.96	0.65
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:MET:HE1	6:F:87:LYS:H	1.62	0.65
2:O:250:HIS:HE1	2:O:252:LEU:HB2	1.61	0.65
3:P:347:PRO:O	3:P:351:ILE:HG13	1.97	0.65
3:C:285:ILE:N	3:C:285:ILE:HD12	2.10	0.64
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.79	0.64
4:D:200:GLN:HE21	20:E:2009:PLC:H51	1.62	0.64
2:O:357:VAL:O	2:O:361:LYS:HG3	1.97	0.64
5:E:83:GLU:HA	5:E:100:HIS:CG	2.32	0.64
2:B:307:PHE:H	9:I:52:ARG:HG2	1.61	0.64
4:Q:200:GLN:HE21	20:R:3009:PLC:H51	1.62	0.64
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.79	0.64
8:H:17:LEU:O	8:H:21:ARG:HG3	1.97	0.64
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.62	0.64
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.13	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.12	0.64
1:N:180:ALA:O	1:N:183:ALA:HB3	1.98	0.64
2:B:113:ARG:O	2:B:116:VAL:HG23	1.98	0.64
2:O:24:LEU:HD12	2:O:37:SER:O	1.97	0.64
1:N:288:LYS:HE3	1:N:289:HIS:NE2	2.13	0.64
1:N:351:GLU:O	1:N:354:VAL:HG22	1.98	0.64
1:N:45:SER:HA	1:N:48:GLU:HG3	1.79	0.64
2:B:409:ASP:HA	2:B:412:ASN:HD22	1.63	0.64
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.78	0.64
3:C:226:SER:O	3:C:230:ILE:HG12	1.98	0.64
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.98	0.64
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.79	0.64
2:B:357:VAL:O	2:B:361:LYS:HG3	1.98	0.64
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.33	0.64
2:O:409:ASP:HA	2:O:412:ASN:HD22	1.63	0.64
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.32	0.64
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.13	0.64
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.64	0.63
2:B:124:LEU:CD2	2:B:223:PHE:HB3	2.27	0.63
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.13	0.63
2:O:222:GLN:O	2:O:223:PHE:HD2	1.79	0.63
3:P:146:VAL:HG21	13:P:3001:SMA:H6	1.79	0.63
3:P:355:ALA:O	3:P:358:SER:HB3	1.98	0.63
2:B:370:MET:O	2:B:373:GLU:HG3	1.97	0.63
1:N:87:ASN:OD1	2:O:286:LYS:HD2	1.99	0.63
1:A:182:LEU:O	1:A:186:ILE:HG13	1.97	0.63
3:C:243:LEU:HD21	3:C:251:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:SER:OG	3:C:250:LEU:HB2	1.97	0.63
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.62	0.63
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.28	0.63
1:A:4:TYR:HA	2:B:113:ARG:HD3	1.81	0.63
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.33	0.63
2:O:325:TYR:HD1	9:V:60:ALA:HB2	1.64	0.63
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.13	0.63
20:R:3009:PLC:H1A1	20:R:3009:PLC:H1'1	1.79	0.63
5:R:83:GLU:HA	5:R:100:HIS:CG	2.33	0.63
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.79	0.63
3:C:346:HIS:ND1	3:C:347:PRO:HA	2.14	0.63
3:C:90:PHE:HB3	3:C:236:MET:CE	2.26	0.63
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.32	0.63
15:C:2007:PEE:H7	7:G:44:GLN:HE21	1.64	0.63
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.81	0.63
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.13	0.63
5:E:41:ALA:O	5:E:45:VAL:HG23	1.99	0.63
1:N:136:GLN:HG2	9:V:51:CYS:HB3	1.81	0.63
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.29	0.63
1:A:371:GLY:O	1:A:375:VAL:HG23	1.99	0.62
2:B:250:HIS:HE1	2:B:252:LEU:HB2	1.64	0.62
2:O:226:ILE:CG2	2:O:227:ARG:N	2.62	0.62
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.80	0.62
7:G:81:GLN:O	8:H:47:ARG:HA	2.00	0.62
1:N:126:GLN:NE2	1:N:129:LYS:HD3	2.15	0.62
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.63	0.62
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.35	0.62
1:N:103:SER:HB3	1:N:202:GLY:O	1.99	0.62
3:P:207:ASN:HD22	3:P:208:ASN:H	1.45	0.62
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.34	0.62
6:F:53:ASP:OD1	6:F:54:LEU:N	2.31	0.62
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.82	0.62
2:B:26:ILE:O	2:B:26:ILE:HG12	1.98	0.62
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.83	0.62
7:G:40:ARG:HD2	18:G:2004:CDL:OA4	1.99	0.62
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.81	0.62
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.29	0.62
1:A:30:SER:O	1:A:202:GLY:HA2	2.00	0.62
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.81	0.62
2:O:26:ILE:O	2:O:26:ILE:HG12	1.99	0.62
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG23	2:B:151:ALA:N	2.15	0.62
2:B:274:VAL:O	2:B:278:VAL:HG23	2.00	0.62
3:C:173:ASN:N	3:C:174:PRO:HD2	2.15	0.62
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.82	0.62
6:S:52:GLU:CG	6:S:56:ASN:HD21	2.11	0.62
7:T:29:ILE:O	7:T:34:LEU:HG	2.00	0.62
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.00	0.62
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.81	0.61
1:A:103:SER:HB3	1:A:202:GLY:O	2.00	0.61
1:A:49:ASN:ND2	1:A:49:ASN:C	2.53	0.61
6:F:18:LYS:O	6:F:22:ASN:ND2	2.32	0.61
8:U:52:GLU:HG2	8:U:53:GLN:N	2.14	0.61
2:B:86:THR:O	2:B:90:GLU:HG3	2.00	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.97	0.61
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.35	0.61
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.31	0.61
2:O:199:PHE:O	2:O:226:ILE:HG21	2.00	0.61
2:O:259:THR:HG22	2:O:260:GLU:N	2.16	0.61
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.82	0.61
4:D:47:ALA:H	4:D:50:ASN:ND2	1.91	0.61
7:G:74:PRO:O	7:G:78:GLU:HG3	2.01	0.61
2:O:221:GLU:O	2:O:223:PHE:N	2.33	0.61
2:B:306:PRO:HA	9:I:52:ARG:CG	2.31	0.61
8:U:17:LEU:O	8:U:21:ARG:HG3	2.01	0.61
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.82	0.61
2:B:28:LYS:O	2:B:29:LEU:O	2.19	0.61
1:N:279:ARG:NH2	9:V:31:UNK:O	2.33	0.61
2:O:227:ARG:NH1	2:O:228:SER:H	1.98	0.61
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.82	0.60
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.35	0.60
1:A:76:GLU:HG2	2:B:285:ILE:HD12	1.82	0.60
20:E:2009:PLC:H1'1	20:E:2009:PLC:H1A1	1.83	0.60
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.36	0.60
10:W:52:TRP:O	10:W:56:LYS:HB2	2.01	0.60
2:B:409:ASP:O	2:B:412:ASN:HB2	2.01	0.60
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.82	0.60
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.31	0.60
4:D:43:MET:HE3	4:D:189:PHE:CZ	2.35	0.60
1:A:159:GLN:HE22	7:G:18:LEU:HD21	1.64	0.60
1:N:76:GLU:HG2	2:O:285:ILE:HD12	1.81	0.60
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.32	0.60
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.16	0.60
2:O:27:THR:HG22	2:O:28:LYS:N	2.17	0.60
5:R:102:THR:O	5:R:106:ILE:HG13	2.02	0.60
2:B:259:THR:HG22	2:B:260:GLU:N	2.17	0.60
9:I:65:VAL:HB	9:I:77:ARG:HD2	1.83	0.60
5:R:40:THR:HG21	15:R:3005:PEE:O2P	2.01	0.60
8:U:13:LEU:HD23	8:U:13:LEU:H	1.66	0.60
1:A:90:THR:O	1:A:167:VAL:HG11	2.02	0.60
4:Q:224:ARG:HE	7:T:26:ILE:HG12	1.67	0.60
8:U:34:ARG:O	8:U:38:GLU:HG2	2.01	0.60
2:O:409:ASP:O	2:O:412:ASN:HB2	2.02	0.60
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.84	0.60
2:B:227:ARG:CD	2:B:228:SER:H	2.15	0.60
3:C:347:PRO:O	3:C:351:ILE:HG13	2.02	0.60
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.20	0.60
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.31	0.60
2:O:287:ARG:HD3	9:V:53:GLU:CG	2.32	0.59
2:B:56:ARG:HA	2:B:171:ALA:O	2.02	0.59
5:E:52:LYS:C	5:E:52:LYS:HD3	2.22	0.59
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.66	0.59
1:A:272:VAL:O	1:A:275:ALA:HB3	2.02	0.59
3:C:282:LEU:HD23	3:C:282:LEU:C	2.22	0.59
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.84	0.59
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.84	0.59
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.17	0.59
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.85	0.59
1:N:105:ASP:O	1:N:109:VAL:HG23	2.02	0.59
3:P:285:ILE:H	3:P:285:ILE:HD12	1.66	0.59
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.85	0.59
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.31	0.59
5:E:108:GLN:O	5:E:112:VAL:HG23	2.02	0.59
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.36	0.59
7:T:29:ILE:O	7:T:33:ALA:HB3	2.02	0.59
9:I:71:ASN:N	9:I:71:ASN:ND2	2.45	0.59
1:N:432:LEU:HD23	1:N:433:ASP:H	1.67	0.59
7:T:73:ASN:HB3	7:T:76:ASP:OD2	2.02	0.59
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.84	0.59
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.18	0.59
2:O:150:VAL:HG23	2:O:151:ALA:N	2.18	0.58
9:I:71:ASN:N	9:I:71:ASN:HD22	1.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.03	0.58
6:S:13:MET:CA	6:S:16:ILE:HB	2.28	0.58
2:B:292:THR:O	2:B:292:THR:HG22	2.03	0.58
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.85	0.58
2:B:47:ILE:HD12	2:B:47:ILE:N	2.17	0.58
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.39	0.58
2:O:113:ARG:O	2:O:116:VAL:HG23	2.02	0.58
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.02	0.58
1:N:371:GLY:O	1:N:375:VAL:HG23	2.02	0.58
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.03	0.58
6:S:32:MET:CE	6:S:87:LYS:HG2	2.33	0.58
1:A:380:GLY:O	1:A:384:LEU:HB2	2.04	0.58
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.86	0.58
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.39	0.58
5:E:90:LYS:HD3	3:P:263:LEU:HD11	1.84	0.58
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.58
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.83	0.58
2:B:279:LEU:HD13	2:B:344:LEU:HD11	1.86	0.58
3:C:146:VAL:HG21	13:C:2001:SMA:H6	1.85	0.58
5:E:103:GLN:HA	5:E:106:ILE:HD12	1.86	0.58
5:E:102:THR:O	5:E:106:ILE:HG13	2.03	0.58
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.04	0.58
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.22	0.58
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.17	0.58
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.38	0.58
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.04	0.58
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.38	0.58
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.33	0.58
4:Q:28:ARG:HD2	4:Q:185:ASP:OD2	2.04	0.58
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.34	0.58
2:B:31:ASN:ND2	2:B:33:LEU:H	2.00	0.58
8:H:18:THR:O	8:H:22:GLU:HG3	2.04	0.58
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.84	0.58
4:D:88:SER:HB2	5:E:69:LEU:HD22	1.85	0.57
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.39	0.57
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.85	0.57
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.84	0.57
2:B:229:GLY:C	2:B:231:GLY:H	2.07	0.57
3:C:269:ILE:HG23	3:C:269:ILE:O	2.04	0.57
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:370:MET:O	2:O:373:GLU:HG3	2.04	0.57
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.18	0.57
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.69	0.57
5:E:109:GLU:CG	5:E:167:ALA:HB3	2.34	0.57
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.39	0.57
5:R:51:ALA:HA	15:R:3005:PEE:H42	1.86	0.57
1:A:156:THR:HA	5:E:7:VAL:HG21	1.86	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.86	0.57
2:O:95:SER:CB	9:V:28:UNK:H2	2.17	0.57
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.52	0.57
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.03	0.57
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.05	0.57
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.86	0.57
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.19	0.57
2:O:250:HIS:CE1	2:O:252:LEU:HB2	2.39	0.57
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.35	0.57
2:B:144:LEU:HB3	2:B:183:ILE:HD12	1.86	0.57
2:B:402:ILE:O	2:B:405:VAL:HG23	2.05	0.57
10:J:52:TRP:O	10:J:56:LYS:HB2	2.05	0.57
1:N:35:CYS:HA	1:N:372:THR:HG21	1.87	0.57
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.05	0.57
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.39	0.57
1:A:388:ARG:NH2	1:A:388:ARG:HG3	2.20	0.57
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.17	0.57
2:B:144:LEU:HB2	2:B:183:ILE:HG23	1.87	0.57
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.40	0.57
1:N:156:THR:HA	5:R:7:VAL:HG21	1.86	0.57
3:P:243:LEU:HD21	3:P:251:LEU:HD11	1.86	0.57
1:A:106:MET:HE2	1:A:107:PRO:HA	1.87	0.56
6:S:46:ALA:HB1	6:S:90:LEU:HD11	1.86	0.56
2:O:86:THR:O	2:O:90:GLU:HG3	2.05	0.56
8:U:65:ARG:O	8:U:68:CYS:HB3	2.04	0.56
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.16	0.56
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.40	0.56
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.87	0.56
1:A:130:GLU:O	1:A:134:ILE:HG13	2.05	0.56
1:A:343:MET:O	1:A:347:THR:HG23	2.06	0.56
5:E:73:LYS:HB3	5:E:195:VAL:O	2.04	0.56
3:P:139:MET:HB2	3:P:256:ASN:OD1	2.05	0.56
2:B:264:VAL:HG11	2:B:388:LEU:CD1	2.36	0.56
8:H:11:GLU:O	8:H:12:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:CYS:O	8:H:44:VAL:HG23	2.05	0.56
1:N:219:VAL:HG12	1:N:220:SER:H	1.71	0.56
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.29	0.56
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.40	0.56
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.86	0.56
3:C:15:ILE:HD12	3:C:15:ILE:N	2.20	0.56
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.04	0.56
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.86	0.56
6:S:10:GLY:C	6:S:12:LEU:H	2.08	0.56
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.88	0.56
2:B:212:LYS:HD2	2:B:214:SER:H	1.69	0.56
6:F:77:LYS:CE	6:F:78:GLU:HG3	2.36	0.56
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.87	0.56
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.04	0.56
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.41	0.56
1:A:180:ALA:O	1:A:183:ALA:HB3	2.06	0.56
1:A:29:GLU:HG3	1:A:203:ILE:O	2.05	0.56
1:A:432:LEU:HD23	1:A:433:ASP:N	2.21	0.56
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.88	0.56
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.46	0.56
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.87	0.56
15:E:2005:PEE:H67	10:J:25:VAL:HG22	1.87	0.56
7:G:60:SER:HB3	7:G:64:GLN:NE2	2.21	0.56
3:C:101:ARG:NH2	12:C:502:HEM:HBD2	2.22	0.55
5:E:112:VAL:HG11	5:E:172:ARG:NH2	2.21	0.55
2:B:230:ALA:O	2:B:231:GLY:C	2.45	0.55
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.41	0.55
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.88	0.55
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.41	0.55
5:R:153:PHE:HD2	5:R:172:ARG:NH1	2.04	0.55
7:T:53:LEU:O	7:T:56:TYR:HB3	2.06	0.55
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.41	0.55
1:N:431:LEU:HG	1:N:432:LEU:N	2.22	0.55
1:A:233:ARG:NH1	1:A:233:ARG:HG3	2.20	0.55
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.21	0.55
7:G:24:ARG:NH2	7:G:28:ASN:H	2.05	0.55
10:J:33:ARG:O	10:J:37:GLN:HG3	2.06	0.55
5:R:112:VAL:HG11	5:R:172:ARG:NH2	2.21	0.55
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.42	0.55
9:V:28:UNK:CB	9:V:71:ASN:ND2	2.70	0.55
10:W:38:GLY:O	10:W:42:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:HG22	1:A:171:THR:N	2.22	0.55
1:A:351:GLU:O	1:A:354:VAL:HG22	2.07	0.55
4:Q:94:PRO:HG2	4:Q:95:TYR:CD1	2.42	0.55
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.88	0.55
7:G:53:LEU:O	7:G:56:TYR:HB3	2.07	0.55
1:A:305:HIS:O	1:A:306:SER:HB3	2.07	0.55
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.88	0.55
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.21	0.55
3:C:38:LEU:HB3	12:C:502:HEM:CMB	2.37	0.55
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.37	0.55
3:P:90:PHE:CZ	3:P:240:PHE:HA	2.42	0.55
5:R:108:GLN:O	5:R:112:VAL:HG23	2.06	0.55
5:R:78:LEU:HD22	5:R:132:TRP:CD2	2.42	0.55
7:T:41:PHE:CD2	7:T:41:PHE:C	2.80	0.55
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.22	0.55
3:C:5:ILE:O	3:C:5:ILE:HG22	2.07	0.55
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.42	0.55
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.06	0.55
5:R:52:LYS:HD3	5:R:52:LYS:C	2.26	0.55
2:B:252:LEU:CD1	9:I:49:LEU:HB2	2.36	0.55
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.07	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.42	0.55
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.72	0.54
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.72	0.54
5:E:195:VAL:HG12	5:E:196:GLY:N	2.22	0.54
2:O:47:ILE:HD12	2:O:47:ILE:N	2.22	0.54
2:O:70:ARG:HD3	2:O:100:SER:OG	2.06	0.54
3:P:5:ILE:O	3:P:5:ILE:HG22	2.06	0.54
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.42	0.54
3:C:111:LYS:HE2	3:C:307:PHE:CE1	2.42	0.54
1:N:130:GLU:O	1:N:134:ILE:HG13	2.08	0.54
5:R:47:THR:HG21	15:R:3005:PEE:H23	1.89	0.54
6:S:105:GLU:O	6:S:109:LYS:HG3	2.07	0.54
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.07	0.54
2:O:226:ILE:CG2	2:O:227:ARG:H	2.20	0.54
3:P:332:ASN:ND2	3:P:358:SER:OG	2.40	0.54
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.89	0.54
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.89	0.54
2:B:248:ASN:ND2	2:B:248:ASN:C	2.60	0.54
1:N:301:HIS:HB2	1:N:303:LEU:HG	1.90	0.54
3:C:207:ASN:HD22	3:C:208:ASN:H	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.88	0.54
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.43	0.54
1:N:223:TYR:HD2	1:N:223:TYR:H	1.56	0.54
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.38	0.54
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.89	0.54
7:T:67:GLU:O	7:T:70:LYS:HB2	2.08	0.54
9:V:32:UNK:C	9:V:73:PRO:HG2	2.38	0.54
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.43	0.54
3:P:17:ASN:HD21	7:T:1:GLY:CA	2.20	0.54
2:B:250:HIS:CE1	2:B:252:LEU:HB2	2.41	0.54
2:B:287:ARG:HB3	9:I:53:GLU:CG	2.38	0.54
2:B:59:THR:HG22	2:B:60:THR:N	2.23	0.54
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.37	0.54
3:C:2:ALA:CB	3:C:8:SER:HB3	2.38	0.54
2:O:47:ILE:O	2:O:108:CYS:HB2	2.07	0.54
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.41	0.54
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.23	0.54
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.38	0.54
2:B:58:GLU:OE1	2:B:64:GLY:N	2.37	0.54
3:C:271:PRO:HG2	3:C:279:TYR:CG	2.42	0.54
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.43	0.54
1:N:15:ASN:O	1:N:26:ALA:HA	2.07	0.54
2:O:162:ASN:O	2:O:244:ILE:HD12	2.08	0.54
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.41	0.54
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.37	0.54
4:D:94:PRO:HG2	4:D:95:TYR:CD1	2.43	0.53
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.89	0.53
1:N:10:ASN:HD21	2:O:18:CYS:HB3	1.73	0.53
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.77	0.53
5:R:69:LEU:HD12	5:R:71:LEU:HG	1.90	0.53
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.08	0.53
1:N:170:THR:HG22	1:N:171:THR:N	2.23	0.53
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.89	0.53
6:S:18:LYS:O	6:S:22:ASN:ND2	2.42	0.53
2:B:47:ILE:HG22	2:B:48:GLY:N	2.23	0.53
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.53
2:B:47:ILE:O	2:B:108:CYS:HB2	2.08	0.53
4:D:150:ASN:O	4:D:156:GLN:HA	2.08	0.53
6:F:46:ALA:CB	6:F:90:LEU:HD11	2.39	0.53
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.73	0.53
1:A:223:TYR:HD2	1:A:223:TYR:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:ILE:H	3:C:285:ILE:HD12	1.71	0.53
2:O:385:GLU:CD	2:O:392:HIS:HA	2.29	0.53
2:O:47:ILE:HG22	2:O:48:GLY:N	2.24	0.53
3:P:38:LEU:HB3	12:P:502:HEM:CMB	2.38	0.53
3:P:4:ASN:HD21	3:P:7:LYS:CE	2.21	0.53
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.90	0.53
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.91	0.53
4:D:86:LYS:NZ	5:E:71:LEU:HD13	2.24	0.53
1:N:260:PRO:HG2	1:N:261:GLY:H	1.73	0.53
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.91	0.53
1:A:364:ALA:O	1:A:368:GLN:HG2	2.09	0.53
2:B:102:ARG:NH1	2:B:164:HIS:CD2	2.76	0.53
2:B:280:GLY:HA3	2:B:293:SER:OG	2.08	0.53
2:B:167:ALA:HB1	2:B:321:LEU:HD21	1.91	0.53
5:E:100:HIS:HB2	5:E:132:TRP:CZ3	2.43	0.53
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.44	0.53
2:O:279:LEU:HD13	2:O:344:LEU:HD11	1.90	0.53
5:R:135:LEU:CD2	5:R:169:GLY:HA3	2.39	0.53
7:T:60:SER:HB3	7:T:64:GLN:NE2	2.24	0.53
3:C:90:PHE:CZ	3:C:240:PHE:HA	2.44	0.53
5:E:78:LEU:HD22	5:E:132:TRP:CD2	2.44	0.53
2:O:318:ASP:O	2:O:319:SER:HB2	2.08	0.53
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.90	0.53
3:C:345:GLU:O	3:C:348:PHE:HB2	2.09	0.53
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.24	0.53
1:N:219:VAL:HG12	1:N:220:SER:N	2.24	0.53
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.73	0.53
1:N:80:GLU:OE2	2:O:291:VAL:HG23	2.09	0.53
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.25	0.53
2:B:67:HIS:O	2:B:70:ARG:HB3	2.09	0.53
5:E:150:SER:OG	5:E:157:TYR:HB3	2.08	0.53
2:O:222:GLN:HG2	2:O:222:GLN:O	2.08	0.53
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.90	0.53
3:P:30:ALA:HB1	18:S:3003:CDL:H111	1.92	0.52
5:R:195:VAL:HG12	5:R:196:GLY:N	2.24	0.52
1:A:289:HIS:O	2:B:87:ARG:NE	2.35	0.52
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.08	0.52
3:C:263:LEU:HD11	5:R:90:LYS:HD3	1.91	0.52
3:C:4:ASN:HD21	3:C:7:LYS:CE	2.22	0.52
2:O:227:ARG:NH1	2:O:228:SER:N	2.57	0.52
3:P:271:PRO:HG2	3:P:279:TYR:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:47:ARG:HG2	8:U:47:ARG:HH11	1.74	0.52
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.40	0.52
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.39	0.52
3:P:31:TRP:O	3:P:101:ARG:HG3	2.09	0.52
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.43	0.52
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.40	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.75	0.52
1:A:431:LEU:HG	1:A:432:LEU:N	2.23	0.52
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.89	0.52
1:N:181:ASP:N	1:N:181:ASP:OD1	2.43	0.52
1:N:49:ASN:ND2	1:N:51:LYS:N	2.57	0.52
2:O:217:LYS:HE2	2:O:221:GLU:OE1	2.10	0.52
2:O:168:TYR:CD2	2:O:237:ALA:HB1	2.44	0.52
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.25	0.52
3:P:101:ARG:O	3:P:101:ARG:HD2	2.08	0.52
9:V:77:ARG:HD2	9:V:77:ARG:N	2.24	0.52
2:B:385:GLU:CD	2:B:392:HIS:HA	2.29	0.52
10:J:38:GLY:O	10:J:42:ILE:HG13	2.09	0.52
2:O:56:ARG:HA	2:O:171:ALA:O	2.10	0.52
18:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.09	0.52
3:P:9:HIS:CE1	3:P:11:LEU:HB2	2.43	0.52
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.91	0.52
2:O:29:LEU:CD1	2:O:33:LEU:HD23	2.39	0.52
5:R:100:HIS:HB2	5:R:132:TRP:CZ3	2.44	0.52
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.45	0.52
1:A:301:HIS:HB2	1:A:303:LEU:HG	1.91	0.52
1:A:49:ASN:ND2	1:A:52:ASN:OD1	2.42	0.52
3:P:15:ILE:N	3:P:15:ILE:HD12	2.25	0.52
3:P:42:LEU:HD22	3:P:190:ILE:HG22	1.91	0.52
7:T:41:PHE:HD2	7:T:41:PHE:C	2.13	0.52
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.21	0.52
2:B:389:SER:O	2:B:391:THR:N	2.43	0.52
7:G:67:GLU:O	7:G:70:LYS:HB2	2.10	0.52
1:N:161:THR:HG21	1:N:235:ARG:H	1.74	0.52
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.74	0.52
1:A:394:GLU:O	1:A:397:SER:HB3	2.10	0.52
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.91	0.52
1:N:106:MET:HE2	1:N:107:PRO:HA	1.92	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.52
10:W:33:ARG:O	10:W:37:GLN:HG3	2.08	0.52
2:B:217:LYS:HE2	2:B:221:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.92	0.52
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.91	0.52
4:D:178:THR:HG23	8:H:13:LEU:HD11	1.92	0.52
1:N:380:GLY:O	1:N:384:LEU:HB2	2.09	0.52
3:P:187:PRO:HG2	12:P:501:HEM:CMC	2.39	0.52
5:R:114:VAL:HG12	5:R:114:VAL:O	2.10	0.52
6:S:53:ASP:OD1	6:S:54:LEU:N	2.39	0.52
2:B:162:ASN:O	2:B:244:ILE:HD12	2.10	0.51
2:B:318:ASP:O	2:B:319:SER:HB2	2.10	0.51
6:F:46:ALA:HB1	6:F:90:LEU:HD11	1.91	0.51
1:N:136:GLN:HE22	9:V:50:LEU:CD1	2.19	0.51
8:U:20:ILE:HD11	8:U:76:LYS:CD	2.38	0.51
2:B:26:ILE:HA	2:B:35:ILE:O	2.11	0.51
3:C:271:PRO:HA	13:C:2001:SMA:H10	1.93	0.51
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.92	0.51
4:D:158:ILE:HG12	4:D:160:MET:H	1.74	0.51
6:F:13:MET:HA	6:F:13:MET:CE	2.40	0.51
2:O:203:ARG:HD2	2:O:230:ALA:HA	1.92	0.51
2:O:219:VAL:HG13	2:O:223:PHE:CD1	2.45	0.51
2:O:248:ASN:C	2:O:248:ASN:ND2	2.62	0.51
5:R:45:VAL:HG13	10:W:28:ALA:N	2.24	0.51
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.92	0.51
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.92	0.51
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.46	0.51
1:N:305:HIS:O	1:N:306:SER:HB3	2.10	0.51
2:O:306:PRO:HG2	9:V:51:CYS:HA	1.92	0.51
2:O:59:THR:HG22	2:O:60:THR:N	2.25	0.51
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.09	0.51
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.41	0.51
14:P:3002:UQ:C8	14:P:3002:UQ:HM51	2.40	0.51
10:J:4:ALA:O	10:J:8:GLN:HG3	2.11	0.51
2:O:102:ARG:CG	2:O:102:ARG:HH11	2.15	0.51
2:O:297:GLN:O	2:O:301:LYS:HG3	2.09	0.51
2:O:226:ILE:HG22	2:O:227:ARG:H	1.74	0.51
2:O:306:PRO:HB3	9:V:52:ARG:N	2.25	0.51
3:P:154:ILE:HG21	3:P:157:ILE:HD11	1.93	0.51
3:P:131:GLY:HA3	3:P:183:HIS:CE1	2.45	0.51
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.11	0.51
10:W:42:ILE:O	10:W:46:LEU:HG	2.10	0.51
1:A:191:LYS:C	1:A:195:MET:HE2	2.31	0.51
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:262:TRP:O	1:N:386:TYR:HE1	1.93	0.51
3:P:285:ILE:N	3:P:285:ILE:CD1	2.74	0.51
1:A:181:ASP:N	1:A:181:ASP:OD1	2.44	0.51
1:A:260:PRO:HG2	1:A:261:GLY:H	1.75	0.51
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.40	0.51
8:H:65:ARG:O	8:H:68:CYS:HB3	2.11	0.51
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.40	0.51
7:T:56:TYR:O	7:T:59:TYR:HB3	2.10	0.51
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.92	0.51
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.46	0.51
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.11	0.51
4:D:43:MET:HE3	4:D:189:PHE:CE2	2.46	0.51
5:E:51:ALA:HA	15:E:2005:PEE:H42	1.93	0.51
3:P:173:ASN:N	3:P:174:PRO:HD2	2.25	0.51
7:T:74:PRO:O	7:T:78:GLU:HG3	2.11	0.51
1:A:178:THR:HG22	1:A:180:ALA:N	2.19	0.51
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.75	0.51
1:A:86:PHE:HD1	1:A:87:ASN:H	1.58	0.51
2:B:109:VAL:HG21	2:B:119:VAL:HG23	1.93	0.51
2:B:192:HIS:O	2:B:196:GLN:HG3	2.10	0.51
1:A:10:ASN:ND2	2:B:19:PRO:HD3	2.23	0.51
9:I:49:LEU:HB3	9:I:55:MET:HG2	1.93	0.51
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.92	0.51
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	1.91	0.51
7:G:41:PHE:CD2	7:G:41:PHE:C	2.83	0.51
3:P:223:PRO:O	3:P:227:PHE:HB2	2.10	0.51
1:N:159:GLN:HE22	7:T:18:LEU:HD21	1.76	0.51
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.93	0.51
1:A:410:VAL:O	1:A:413:LYS:HB3	2.11	0.50
2:B:308:ASP:OD1	9:I:56:SER:HA	2.11	0.50
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.93	0.50
2:B:306:PRO:HB3	9:I:52:ARG:N	2.26	0.50
5:R:103:GLN:HA	5:R:106:ILE:HB	1.92	0.50
5:R:41:ALA:O	5:R:45:VAL:HG23	2.10	0.50
1:A:432:LEU:HD23	1:A:433:ASP:H	1.76	0.50
1:N:63:ALA:HB1	1:N:116:VAL:CG1	2.41	0.50
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.46	0.50
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.90	0.50
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.94	0.50
5:R:90:LYS:O	5:R:91:TRP:HB2	2.11	0.50
1:A:8:LEU:HD22	1:A:392:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:TYR:HD1	9:I:60:ALA:CB	2.22	0.50
8:H:24:CYS:O	8:H:27:THR:HB	2.11	0.50
2:O:67:HIS:O	2:O:70:ARG:HB3	2.12	0.50
3:P:145:THR:O	3:P:149:ASN:HB2	2.12	0.50
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.11	0.50
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.40	0.50
1:N:179:ARG:HG2	1:N:179:ARG:HH11	1.75	0.50
1:A:386:TYR:CD2	1:A:390:ILE:HD12	2.46	0.50
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.47	0.50
1:A:45:SER:HA	1:A:48:GLU:CG	2.40	0.50
1:A:49:ASN:ND2	1:A:51:LYS:H	2.09	0.50
2:B:116:VAL:O	2:B:120:MET:HB2	2.11	0.50
2:B:414:ALA:O	2:B:418:VAL:HG23	2.11	0.50
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.46	0.50
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.93	0.50
2:O:26:ILE:HA	2:O:35:ILE:O	2.10	0.50
1:A:308:GLN:HG3	1:A:308:GLN:O	2.11	0.50
3:C:38:LEU:HB3	12:C:502:HEM:HMB1	1.94	0.50
6:F:71:LYS:O	6:F:72:HIS:HB2	2.10	0.50
9:I:38:UNK:C	9:I:40:UNK:N	2.72	0.50
1:N:388:ARG:NH2	1:N:388:ARG:HG3	2.26	0.50
2:B:212:LYS:CD	2:B:214:SER:H	2.24	0.50
4:D:224:ARG:HH21	7:G:26:ILE:HG23	1.77	0.50
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.12	0.50
3:P:285:ILE:H	3:P:285:ILE:CD1	2.25	0.50
6:S:71:LYS:O	6:S:72:HIS:HB2	2.12	0.50
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.92	0.50
5:E:103:GLN:HA	5:E:106:ILE:HB	1.94	0.50
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.45	0.50
7:G:73:ASN:HB3	7:G:76:ASP:OD2	2.11	0.50
1:N:156:THR:O	1:N:159:GLN:HG2	2.12	0.50
2:O:227:ARG:HG3	2:O:228:SER:H	1.76	0.50
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.93	0.50
3:P:135:PRO:HG3	12:P:501:HEM:O1D	2.12	0.50
6:S:46:ALA:CB	6:S:90:LEU:HD11	2.41	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.50
8:U:24:CYS:O	8:U:27:THR:HB	2.12	0.50
2:B:153:GLN:HE22	9:I:34:UNK:CB	2.24	0.50
2:B:297:GLN:O	2:B:301:LYS:HG3	2.12	0.50
2:O:402:ILE:O	2:O:405:VAL:HG23	2.10	0.50
3:P:101:ARG:NH2	12:P:502:HEM:HBD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:38:LEU:HB3	12:P:502:HEM:HMB1	1.94	0.50
8:U:12:GLU:N	21:U:1233:HOH:O	2.45	0.50
8:U:52:GLU:CG	8:U:53:GLN:N	2.75	0.50
2:B:257:VAL:O	2:B:323:GLY:HA3	2.12	0.49
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.11	0.49
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.20	0.49
10:J:42:ILE:O	10:J:46:LEU:HG	2.12	0.49
2:O:144:LEU:HB3	2:O:183:ILE:HD12	1.93	0.49
3:P:70:THR:HA	3:P:74:VAL:HG23	1.93	0.49
10:W:40:ASP:O	10:W:44:GLU:HG3	2.12	0.49
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.47	0.49
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.47	0.49
3:C:42:LEU:HD22	3:C:190:ILE:HG22	1.93	0.49
5:E:171:ILE:HG23	5:E:171:ILE:O	2.13	0.49
1:N:112:LEU:O	1:N:116:VAL:HG23	2.12	0.49
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.39	0.49
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.94	0.49
9:I:55:MET:O	9:I:56:SER:C	2.50	0.49
1:N:152:TYR:HA	1:N:155:ALA:HB3	1.94	0.49
2:O:227:ARG:HG3	2:O:228:SER:N	2.27	0.49
2:O:341:MET:HG3	2:O:439:LEU:HB3	1.94	0.49
2:O:381:GLU:OE1	2:O:381:GLU:HA	2.11	0.49
3:P:158:GLY:O	3:P:161:LEU:N	2.41	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.52	0.49
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.26	0.49
2:B:300:ALA:C	2:B:302:ALA:H	2.14	0.49
3:C:9:HIS:CE1	3:C:11:LEU:HB2	2.47	0.49
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.47	0.49
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.94	0.49
1:A:233:ARG:NH1	1:A:233:ARG:CG	2.74	0.49
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.93	0.49
1:N:178:THR:HG22	1:N:180:ALA:N	2.19	0.49
1:N:329:LEU:HA	1:N:430:GLN:NE2	2.27	0.49
2:O:159:VAL:HG23	2:O:160:LEU:N	2.27	0.49
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.77	0.49
6:S:12:LEU:O	6:S:15:ARG:HG2	2.13	0.49
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.42	0.49
2:B:95:SER:HA	9:I:71:ASN:OD1	2.11	0.49
2:O:124:LEU:HD22	2:O:223:PHE:HB3	1.95	0.49
2:O:283:PRO:CG	9:V:56:SER:HB2	2.43	0.49
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:ASN:HD21	3:C:359:TYR:N	2.10	0.49
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.43	0.49
5:E:155:GLY:HA3	5:E:166:ASP:C	2.33	0.49
7:G:56:TYR:O	7:G:59:TYR:HB3	2.13	0.49
1:N:49:ASN:ND2	1:N:52:ASN:OD1	2.46	0.49
10:W:49:GLY:N	10:W:54:HIS:ND1	2.60	0.49
2:B:212:LYS:HD3	2:B:213:HIS:H	1.77	0.49
3:C:243:LEU:HD21	3:C:251:LEU:CD1	2.42	0.49
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.47	0.49
8:U:40:CYS:O	8:U:44:VAL:HG23	2.12	0.49
8:U:25:GLU:HG2	8:U:61:PHE:HZ	1.78	0.49
4:D:14:HIS:O	4:D:202:LYS:NZ	2.46	0.49
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.48	0.49
7:T:77:TYR:C	7:T:79:ASN:H	2.16	0.49
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.94	0.48
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.27	0.48
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.48
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.94	0.48
2:O:389:SER:O	2:O:391:THR:N	2.46	0.48
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.48	0.48
4:Q:43:MET:HE3	4:Q:189:PHE:CZ	2.48	0.48
5:R:77:LYS:HB3	5:R:80:ASP:OD2	2.13	0.48
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.27	0.48
2:B:168:TYR:CD2	2:B:237:ALA:HB1	2.48	0.48
2:B:248:ASN:HD22	2:B:249:GLY:N	2.11	0.48
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.12	0.48
1:N:394:GLU:O	1:N:397:SER:HB3	2.13	0.48
1:N:86:PHE:HD1	1:N:87:ASN:H	1.62	0.48
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.94	0.48
13:C:2001:SMA:H4	5:R:160:CYS:HB3	1.94	0.48
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.26	0.48
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.95	0.48
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.95	0.48
8:H:43:ARG:HD2	8:H:47:ARG:HH12	1.78	0.48
1:N:5:ALA:O	1:N:8:LEU:HB2	2.13	0.48
2:O:170:THR:O	2:O:172:LEU:N	2.46	0.48
3:P:81:ARG:HH22	16:P:3011:GOL:H2	1.76	0.48
2:B:70:ARG:HD3	2:B:100:SER:OG	2.14	0.48
2:B:285:ILE:O	2:B:288:GLY:N	2.46	0.48
2:B:167:ALA:HA	2:B:423:SER:OG	2.13	0.48
2:B:76:THR:HG22	2:B:81:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:LYS:C	1:N:195:MET:HE2	2.33	0.48
2:O:50:PHE:CE1	2:O:207:VAL:HB	2.48	0.48
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.48	0.48
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.13	0.48
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.48	0.48
4:D:28:ARG:HG2	4:D:171:TYR:CD2	2.48	0.48
7:G:41:PHE:HD2	7:G:41:PHE:C	2.16	0.48
1:A:305:HIS:HB3	9:I:35:UNK:CB	2.42	0.48
1:N:19:LEU:HD12	1:N:23:LEU:HD23	1.94	0.48
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.78	0.48
2:O:353:THR:HG22	2:O:355:GLU:N	2.04	0.48
3:P:111:LYS:HE2	3:P:307:PHE:CE1	2.49	0.48
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.96	0.48
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.48	0.48
1:A:133:VAL:O	1:A:137:GLU:HG3	2.14	0.48
1:A:80:GLU:OE2	2:B:291:VAL:HG23	2.14	0.48
2:B:170:THR:O	2:B:172:LEU:N	2.47	0.48
2:B:47:ILE:CG2	2:B:48:GLY:N	2.77	0.48
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.14	0.48
1:N:191:LYS:CA	1:N:195:MET:HE2	2.44	0.48
1:N:206:LYS:O	1:N:209:VAL:HG12	2.13	0.48
2:O:370:MET:O	2:O:372:VAL:N	2.47	0.48
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.48	0.48
3:P:95:ILE:O	3:P:99:ILE:HG13	2.13	0.48
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.48
2:B:156:GLN:NE2	9:I:77:ARG:C	2.67	0.48
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.14	0.48
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.49	0.48
5:R:122:HIS:CE1	5:R:124:LEU:HG	2.48	0.48
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.96	0.48
1:A:233:ARG:NH2	1:A:316:ASP:O	2.43	0.48
5:E:127:VAL:HG11	5:E:133:VAL:HA	1.94	0.48
1:N:205:HIS:O	1:N:208:LEU:HB3	2.14	0.48
1:N:19:LEU:O	1:N:21:ASN:N	2.47	0.48
2:O:212:LYS:HB2	2:O:215:ASP:OD2	2.14	0.48
3:P:132:TYR:HA	12:P:501:HEM:HAA2	1.96	0.48
3:P:141:PHE:HB2	3:P:260:ALA:CB	2.43	0.48
3:P:282:LEU:HD23	3:P:282:LEU:C	2.33	0.48
3:C:236:MET:HA	18:D:2003:CDL:H162	1.94	0.48
4:D:235:MET:HB3	7:G:15:THR:HG22	1.96	0.48
5:E:114:VAL:O	5:E:114:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.49	0.48
2:O:113:ARG:O	2:O:115:HIS:N	2.47	0.48
8:U:47:ARG:NH1	8:U:47:ARG:HG2	2.28	0.48
1:A:35:CYS:HA	1:A:372:THR:HG21	1.95	0.48
2:B:220:ALA:O	2:B:224:LEU:HB2	2.14	0.48
2:B:59:THR:HG22	2:B:60:THR:H	1.78	0.48
3:C:135:PRO:HG3	12:C:501:HEM:O1D	2.14	0.48
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.95	0.48
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.49	0.48
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.29	0.48
3:P:142:TRP:O	3:P:146:VAL:HG23	2.13	0.48
2:B:28:LYS:HG2	2:B:28:LYS:O	2.14	0.47
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.28	0.47
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.70	0.47
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.96	0.47
1:A:15:ASN:O	1:A:26:ALA:HA	2.13	0.47
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.49	0.47
2:B:398:VAL:O	2:B:402:ILE:HG13	2.14	0.47
3:C:285:ILE:H	3:C:285:ILE:CD1	2.27	0.47
3:P:245:LEU:O	4:Q:201:ARG:HG2	2.14	0.47
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.47
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.49	0.47
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.95	0.47
1:N:280:TYR:CG	1:N:281:ASP:N	2.82	0.47
1:N:35:CYS:HB2	1:N:200:ALA:O	2.14	0.47
3:P:112:GLU:O	3:P:116:THR:HG23	2.14	0.47
2:B:35:ILE:O	2:B:213:HIS:HE1	1.98	0.47
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.49	0.47
3:C:63:ALA:O	3:C:67:VAL:HG23	2.15	0.47
6:F:77:LYS:HE3	6:F:78:GLU:HG3	1.95	0.47
1:N:223:TYR:CD2	1:N:223:TYR:N	2.82	0.47
3:P:189:ALA:O	3:P:193:ILE:HG13	2.15	0.47
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.96	0.47
2:B:147:ASP:O	2:B:150:VAL:HG22	2.15	0.47
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.28	0.47
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.49	0.47
5:E:90:LYS:O	5:E:91:TRP:HB2	2.15	0.47
1:N:179:ARG:HG2	1:N:179:ARG:NH1	2.29	0.47
1:N:26:ALA:O	1:N:198:ALA:HA	2.14	0.47
3:P:271:PRO:HA	13:P:3001:SMA:C7M	2.41	0.47
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:GLU:HG2	8:H:61:PHE:HZ	1.78	0.47
2:O:29:LEU:HB2	2:O:31:ASN:HD21	1.80	0.47
2:O:300:ALA:C	2:O:302:ALA:H	2.18	0.47
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.44	0.47
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.14	0.47
1:A:329:LEU:HA	1:A:430:GLN:NE2	2.29	0.47
3:C:347:PRO:O	3:C:350:ILE:HG22	2.15	0.47
4:D:135:CYS:O	4:D:149:TYR:HB3	2.15	0.47
10:J:57:HIS:O	10:J:62:SER:HB2	2.14	0.47
1:N:410:VAL:O	1:N:413:LYS:HB3	2.14	0.47
2:O:27:THR:CG2	2:O:28:LYS:N	2.77	0.47
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.76	0.47
3:P:158:GLY:O	3:P:161:LEU:HB2	2.14	0.47
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.97	0.47
4:D:171:TYR:OH	4:D:182:ILE:HA	2.14	0.47
5:E:57:GLN:OE1	20:E:2009:PLC:H12	2.14	0.47
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.96	0.47
5:R:171:ILE:HG23	5:R:171:ILE:O	2.15	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.95	0.47
6:S:73:ARG:HA	6:S:73:ARG:HD3	1.74	0.47
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.15	0.47
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.15	0.47
3:C:101:ARG:HD2	3:C:102:GLY:N	2.30	0.47
3:C:157:ILE:O	3:C:161:LEU:HD12	2.14	0.47
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.96	0.47
5:R:164:HIS:HB2	5:R:173:LYS:HB3	1.96	0.47
15:R:3005:PEE:H54	10:W:21:ALA:HA	1.97	0.47
2:B:150:VAL:CG2	2:B:151:ALA:N	2.77	0.47
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.45	0.47
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.50	0.47
2:B:50:PHE:CE1	2:B:207:VAL:HB	2.50	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.49	0.47
5:E:69:LEU:HB2	5:E:70:ALA:H	1.34	0.47
8:H:43:ARG:HD2	8:H:47:ARG:CZ	2.44	0.47
1:N:382:HIS:O	1:N:386:TYR:N	2.48	0.47
2:O:306:PRO:CG	9:V:51:CYS:HA	2.45	0.47
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.62	0.47
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.44	0.47
2:B:341:MET:HG3	2:B:439:LEU:HB3	1.96	0.46
4:D:214:LEU:HD11	4:D:218:LEU:HD11	1.97	0.46
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.97	0.46
5:R:101:ARG:N	5:R:131:GLU:O	2.45	0.46
1:A:18:THR:HG23	1:A:24:ARG:HG2	1.97	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.15	0.46
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.15	0.46
2:O:47:ILE:CG2	2:O:48:GLY:N	2.78	0.46
3:P:332:ASN:HD21	3:P:359:TYR:N	2.13	0.46
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.97	0.46
8:U:50:THR:OG1	8:U:51:GLU:N	2.48	0.46
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.31	0.46
1:A:191:LYS:CA	1:A:195:MET:HE2	2.45	0.46
2:B:209:ILE:HD12	2:B:379:LEU:HB2	1.97	0.46
3:C:243:LEU:CD2	3:C:251:LEU:HD11	2.45	0.46
4:D:21:LEU:HD13	4:D:192:TRP:HB2	1.97	0.46
10:J:40:ASP:O	10:J:44:GLU:HG3	2.15	0.46
4:Q:62:LYS:O	4:Q:65:ALA:HB3	2.15	0.46
1:A:285:GLY:O	1:A:286:GLY:C	2.54	0.46
2:B:113:ARG:O	2:B:115:HIS:N	2.47	0.46
2:B:86:THR:OG1	9:I:70:LEU:HD11	2.16	0.46
5:E:148:ALA:HA	5:E:156:TYR:CD2	2.50	0.46
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.50	0.46
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.96	0.46
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.50	0.46
1:A:416:TYR:HE1	1:A:443:TRP:H	1.64	0.46
3:C:285:ILE:N	3:C:285:ILE:CD1	2.77	0.46
5:E:101:ARG:N	5:E:131:GLU:O	2.45	0.46
7:G:29:ILE:O	7:G:33:ALA:HB3	2.15	0.46
1:N:364:ALA:O	1:N:368:GLN:HG2	2.16	0.46
1:N:365:MET:HG2	1:N:392:LEU:HD22	1.98	0.46
5:R:155:GLY:HA3	5:R:166:ASP:C	2.36	0.46
8:U:18:THR:O	8:U:22:GLU:HG3	2.16	0.46
1:A:124:GLU:O	1:A:124:GLU:HG2	2.16	0.46
1:A:63:ALA:HB1	1:A:116:VAL:CG1	2.45	0.46
2:B:102:ARG:CG	2:B:102:ARG:NH1	2.78	0.46
3:C:325:LEU:HD11	3:C:366:LEU:HD12	1.98	0.46
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.51	0.46
3:P:101:ARG:CD	3:P:101:ARG:C	2.74	0.46
2:B:109:VAL:CG1	2:B:123:LEU:HB2	2.46	0.46
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.96	0.46
2:B:394:ALA:O	2:B:396:SER:N	2.48	0.46
3:C:355:ALA:O	3:C:358:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:GLU:HG2	6:F:20:TYR:CZ	2.51	0.46
4:D:27:ARG:NH1	4:D:55:THR:O	2.48	0.46
2:B:99:TYR:HA	9:I:67:GLY:HA2	1.98	0.46
2:O:167:ALA:HB1	2:O:321:LEU:HD21	1.98	0.46
3:P:70:THR:HA	3:P:74:VAL:CG2	2.46	0.46
5:R:150:SER:OG	5:R:157:TYR:HB3	2.15	0.46
2:B:159:VAL:HG23	2:B:160:LEU:N	2.30	0.46
3:C:133:VAL:O	3:C:133:VAL:HG12	2.15	0.46
3:C:141:PHE:HB2	3:C:260:ALA:CB	2.46	0.46
1:A:223:TYR:CD2	1:A:223:TYR:N	2.84	0.46
1:A:389:ARG:HD2	1:A:390:ILE:H	1.81	0.46
1:A:5:ALA:O	1:A:8:LEU:HB2	2.16	0.46
3:C:246:PHE:C	3:C:248:PRO:HD3	2.36	0.46
3:C:350:ILE:HG23	3:C:351:ILE:N	2.31	0.46
2:O:102:ARG:CG	2:O:102:ARG:NH1	2.75	0.46
2:O:235:ALA:O	2:O:236:LYS:O	2.34	0.46
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.97	0.46
3:P:346:HIS:CG	3:P:347:PRO:HA	2.50	0.46
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.15	0.46
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.51	0.46
2:B:203:ARG:HD2	2:B:230:ALA:CA	2.26	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.51	0.46
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.81	0.46
2:O:116:VAL:O	2:O:120:MET:HB2	2.16	0.46
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.50	0.46
5:R:67:ASP:O	5:R:69:LEU:HD23	2.15	0.46
6:S:77:LYS:CE	6:S:78:GLU:HG3	2.46	0.46
7:T:34:LEU:HA	7:T:37:VAL:HG23	1.97	0.46
1:A:255:LEU:HD11	1:A:420:PRO:HB2	1.97	0.45
1:A:7:THR:HB	2:B:41:PHE:O	2.16	0.45
3:C:31:TRP:O	3:C:101:ARG:HG3	2.15	0.45
3:C:142:TRP:CH2	5:R:145:VAL:HG23	2.51	0.45
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.47	0.45
1:N:373:THR:HB	1:N:374:PRO:CD	2.43	0.45
2:O:394:ALA:O	2:O:396:SER:N	2.49	0.45
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.16	0.45
5:R:148:ALA:O	5:R:149:ASN:HB2	2.16	0.45
2:B:394:ALA:C	2:B:396:SER:H	2.20	0.45
3:C:223:PRO:O	3:C:227:PHE:HB2	2.16	0.45
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.46	0.45
9:I:38:UNK:O	9:I:39:UNK:C	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:LEU:HB3	9:I:55:MET:CG	2.46	0.45
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.31	0.45
2:O:73:SER:OG	2:O:74:PRO:HD3	2.16	0.45
4:Q:2:GLU:HG2	4:Q:2:GLU:O	2.16	0.45
5:E:136:VAL:HG12	5:E:138:VAL:HG23	1.98	0.45
1:N:145:MET:CB	1:N:252:HIS:CD2	2.99	0.45
2:O:109:VAL:CG1	2:O:123:LEU:HB2	2.45	0.45
2:O:209:ILE:HD12	2:O:379:LEU:HB2	1.97	0.45
5:R:91:TRP:O	5:R:93:GLY:N	2.50	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.15	0.45
2:B:101:THR:HG22	9:I:65:VAL:HG22	1.99	0.45
2:B:102:ARG:HH11	2:B:102:ARG:CG	2.21	0.45
2:B:60:THR:CG2	2:B:61:ALA:N	2.80	0.45
3:C:237:LEU:HD12	3:C:237:LEU:HA	1.68	0.45
5:E:122:HIS:CE1	5:E:124:LEU:HG	2.51	0.45
6:F:28:LYS:HB3	6:F:74:ILE:HD12	1.97	0.45
7:G:29:ILE:O	7:G:34:LEU:HG	2.17	0.45
1:N:121:ALA:O	1:N:122:LEU:HB2	2.15	0.45
1:N:126:GLN:HE22	1:N:129:LYS:HD3	1.79	0.45
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.45	0.45
2:O:150:VAL:CG2	2:O:151:ALA:N	2.80	0.45
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.68	0.45
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.99	0.45
3:C:70:THR:HA	3:C:74:VAL:HG23	1.99	0.45
4:D:102:ARG:NH1	4:D:107:GLY:O	2.47	0.45
5:E:59:ILE:HG22	5:E:60:SER:N	2.31	0.45
1:N:416:TYR:HE1	1:N:443:TRP:H	1.64	0.45
3:P:157:ILE:CG1	3:P:158:GLY:H	2.07	0.45
3:P:269:ILE:HG23	3:P:269:ILE:O	2.16	0.45
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	1.99	0.45
8:U:52:GLU:CG	8:U:53:GLN:H	2.30	0.45
1:A:212:ALA:O	1:A:216:PHE:HB2	2.16	0.45
2:B:198:ASN:HB3	2:B:203:ARG:HH21	1.81	0.45
3:C:132:TYR:HA	12:C:501:HEM:HAA2	1.98	0.45
5:E:145:VAL:HG23	3:P:142:TRP:CH2	2.52	0.45
7:G:9:ARG:HH11	7:G:9:ARG:HG3	1.82	0.45
1:N:145:MET:CB	1:N:252:HIS:NE2	2.80	0.45
1:N:36:THR:HG21	1:N:373:THR:HA	1.99	0.45
2:O:269:ALA:O	2:O:272:PHE:N	2.49	0.45
3:P:342:GLN:HE21	3:P:342:GLN:CA	2.25	0.45
6:S:13:MET:HA	6:S:16:ILE:CB	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.99	0.45
2:B:212:LYS:C	2:B:212:LYS:HD3	2.37	0.45
2:B:27:THR:H	2:B:213:HIS:CE1	2.34	0.45
2:B:279:LEU:HA	2:B:294:LYS:HB2	1.99	0.45
3:C:23:PRO:HG2	7:G:3:HIS:CB	2.47	0.45
5:E:148:ALA:O	5:E:149:ASN:HB2	2.17	0.45
8:H:32:LYS:HD3	8:H:32:LYS:HA	1.82	0.45
10:W:59:TYR:CD1	10:W:59:TYR:N	2.84	0.45
1:A:161:THR:HG21	1:A:235:ARG:H	1.82	0.45
3:C:155:PRO:O	3:C:156:TYR:HB2	2.17	0.45
5:E:85:LYS:HG2	5:E:86:ASN:N	2.31	0.45
2:B:308:ASP:CG	9:I:56:SER:HA	2.37	0.45
9:I:69:SER:CB	9:I:72:ALA:HB3	2.46	0.45
1:N:80:GLU:OE1	2:O:290:SER:HA	2.16	0.45
2:O:31:ASN:N	2:O:31:ASN:HD22	2.14	0.45
2:O:367:THR:HG22	2:O:368:TYR:N	2.30	0.45
2:O:414:ALA:O	2:O:418:VAL:HG23	2.16	0.45
3:P:325:LEU:HD11	3:P:366:LEU:HD12	1.99	0.45
3:P:76:TYR:HE2	4:Q:204:MET:CE	2.30	0.45
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.99	0.45
8:U:52:GLU:HG2	8:U:53:GLN:H	1.80	0.45
1:N:364:ALA:HB2	9:V:29:UNK:CB	2.47	0.45
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.32	0.45
2:B:107:TYR:O	2:B:108:CYS:HB3	2.17	0.45
7:G:71:ARG:NH2	8:H:56:GLU:OE1	2.50	0.45
10:J:49:GLY:N	10:J:54:HIS:ND1	2.65	0.45
1:N:29:GLU:HG3	1:N:203:ILE:O	2.17	0.45
1:N:294:LEU:HD23	1:N:307:PHE:CE1	2.52	0.45
1:N:386:TYR:CD2	1:N:390:ILE:HD12	2.52	0.45
2:O:398:VAL:O	2:O:402:ILE:HG13	2.17	0.45
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.98	0.45
5:R:153:PHE:CE2	5:R:172:ARG:HB3	2.52	0.45
2:B:394:ALA:C	2:B:396:SER:N	2.70	0.45
3:C:12:LEU:C	3:C:14:MET:N	2.70	0.45
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.99	0.45
1:N:106:MET:HB3	1:N:107:PRO:CD	2.47	0.45
2:O:221:GLU:C	2:O:223:PHE:H	2.20	0.45
2:O:259:THR:CG2	2:O:260:GLU:N	2.80	0.45
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.52	0.45
5:R:122:HIS:ND1	5:R:124:LEU:HG	2.32	0.45
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:VAL:HG13	2:B:399:ALA:N	2.33	0.44
5:E:69:LEU:HD13	5:E:71:LEU:HD21	1.99	0.44
6:F:31:LEU:HD21	6:F:65:ALA:HB2	1.99	0.44
6:F:52:GLU:CG	6:F:56:ASN:HD21	2.21	0.44
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.00	0.44
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.52	0.44
4:Q:120:ARG:HH11	4:Q:120:ARG:HG2	1.81	0.44
5:R:135:LEU:HD22	5:R:169:GLY:HA3	1.99	0.44
1:A:228:VAL:O	1:A:228:VAL:HG13	2.18	0.44
2:B:51:ILE:HG22	2:B:52:LYS:N	2.33	0.44
9:I:32:UNK:N	9:I:73:PRO:CG	2.75	0.44
2:O:144:LEU:HB2	2:O:183:ILE:HG23	1.97	0.44
3:P:107:SER:HB3	12:P:502:HEM:HAD1	1.99	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
6:F:105:GLU:O	6:F:109:LYS:HG3	2.17	0.44
7:G:71:ARG:CZ	8:H:56:GLU:OE1	2.65	0.44
8:H:20:ILE:HD12	8:H:73:LEU:HA	1.99	0.44
2:O:230:ALA:O	2:O:231:GLY:C	2.55	0.44
2:O:344:LEU:HD23	2:O:417:PHE:CD2	2.53	0.44
3:P:47:LEU:O	3:P:47:LEU:HD12	2.17	0.44
2:B:202:ALA:HB3	2:B:229:GLY:H	1.83	0.44
2:B:47:ILE:CD1	2:B:47:ILE:N	2.80	0.44
5:E:185:TYR:HB3	5:E:195:VAL:HG13	2.00	0.44
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.51	0.44
1:N:189:HIS:O	1:N:191:LYS:N	2.49	0.44
1:N:342:TRP:O	1:N:345:LEU:HB2	2.18	0.44
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.98	0.44
4:Q:214:LEU:HD11	4:Q:218:LEU:HD11	1.98	0.44
5:R:128:LYS:O	5:R:130:PRO:HD3	2.17	0.44
2:B:129:ALA:N	2:B:130:PRO:CD	2.81	0.44
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.98	0.44
1:N:343:MET:O	1:N:347:THR:HG23	2.17	0.44
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.73	0.44
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.16	0.44
5:R:77:LYS:C	5:R:79:SER:H	2.21	0.44
2:O:287:ARG:HD3	9:V:53:GLU:HG2	1.98	0.44
1:A:86:PHE:HD1	1:A:87:ASN:N	2.15	0.44
1:A:91:SER:OG	1:A:92:ARG:N	2.49	0.44
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.52	0.44
3:C:51:LEU:HD23	3:C:51:LEU:HA	1.88	0.44
1:N:242:ARG:NH1	1:N:432:LEU:HA	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:166:ALA:HB1	2:O:242:GLY:C	2.38	0.44
3:P:141:PHE:HB2	3:P:260:ALA:HB1	1.98	0.44
6:S:77:LYS:HE3	6:S:78:GLU:HG3	2.00	0.44
8:U:72:LYS:HA	8:U:75:ASN:HD22	1.83	0.44
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.47	0.44
2:B:209:ILE:HG13	2:B:379:LEU:HD13	1.98	0.44
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.18	0.44
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.53	0.44
3:P:198:LEU:HD21	12:P:502:HEM:CMA	2.47	0.44
3:P:289:LEU:HG	3:P:293:LEU:HD11	2.00	0.44
4:Q:178:THR:HG21	8:U:15:ASP:HA	1.99	0.44
4:Q:55:THR:O	10:W:52:TRP:CZ3	2.71	0.44
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.99	0.44
2:B:291:VAL:C	2:B:293:SER:H	2.21	0.44
5:E:165:TYR:HA	5:E:170:ARG:O	2.16	0.44
2:O:291:VAL:C	2:O:293:SER:H	2.21	0.44
2:O:394:ALA:C	2:O:396:SER:N	2.72	0.44
3:P:166:TRP:HA	3:P:175:THR:HG23	1.99	0.44
3:P:235:LEU:O	3:P:239:PRO:HD2	2.18	0.44
3:P:300:LEU:HA	3:P:300:LEU:HD23	1.84	0.44
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.47	0.44
5:R:171:ILE:N	5:R:179:ASN:OD1	2.49	0.44
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.82	0.44
1:A:87:ASN:OD1	2:B:286:LYS:HD2	2.17	0.44
3:C:132:TYR:O	3:C:135:PRO:HD2	2.18	0.44
3:C:187:PRO:HG2	12:C:501:HEM:CMC	2.46	0.44
4:D:27:ARG:O	4:D:30:PHE:HB3	2.17	0.44
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.33	0.44
1:N:18:THR:HG23	1:N:24:ARG:CG	2.40	0.44
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.99	0.44
1:N:382:HIS:HB3	1:N:388:ARG:O	2.18	0.44
1:N:45:SER:HA	1:N:48:GLU:CG	2.46	0.44
2:O:248:ASN:HD22	2:O:249:GLY:N	2.15	0.44
3:P:132:TYR:O	3:P:135:PRO:HD2	2.18	0.44
4:Q:241:LYS:CA	4:Q:241:LYS:HE3	2.43	0.44
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	2.00	0.44
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.74	0.43
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.32	0.43
1:N:170:THR:HG22	1:N:172:GLU:H	1.82	0.43
3:P:138:GLN:N	3:P:258:THR:O	2.48	0.43
6:S:40:ASP:O	6:S:44:LYS:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:O	1:A:109:VAL:HG23	2.18	0.43
3:C:198:LEU:HD13	14:C:2002:UQ:HM53	2.00	0.43
4:D:3:LEU:HA	4:D:3:LEU:HD23	1.83	0.43
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.53	0.43
1:N:220:SER:HA	1:N:225:GLU:OE1	2.18	0.43
2:O:129:ALA:N	2:O:130:PRO:CD	2.82	0.43
3:P:30:ALA:C	3:P:32:TRP:H	2.21	0.43
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.39	0.43
5:R:99:ARG:HB3	5:R:133:VAL:HG12	1.99	0.43
8:U:73:LEU:HD12	8:U:73:LEU:O	2.18	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.39	0.43
2:O:235:ALA:O	2:O:236:LYS:C	2.55	0.43
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.48	0.43
3:P:159:HIS:O	3:P:162:VAL:N	2.52	0.43
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.43
7:T:56:TYR:HD2	7:T:57:LEU:HD23	1.82	0.43
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.48	0.43
2:B:229:GLY:C	2:B:231:GLY:N	2.71	0.43
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.52	0.43
2:B:393:THR:CG2	2:B:397:VAL:HB	2.39	0.43
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.86	0.43
5:R:148:ALA:HA	5:R:156:TYR:CD2	2.53	0.43
6:S:28:LYS:HB3	6:S:74:ILE:HD12	2.01	0.43
8:U:23:HIS:O	8:U:26:GLN:HB2	2.19	0.43
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.81	0.43
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.53	0.43
1:A:362:ARG:O	1:A:365:MET:HB3	2.18	0.43
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.48	0.43
2:B:344:LEU:HD23	2:B:417:PHE:CD2	2.53	0.43
3:C:52:LEU:HD21	3:C:80:ILE:HG22	2.01	0.43
5:E:109:GLU:O	5:E:123:ASP:HB2	2.18	0.43
1:N:133:VAL:O	1:N:137:GLU:HG3	2.18	0.43
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.53	0.43
1:N:62:LEU:C	1:N:64:PHE:H	2.22	0.43
2:O:22:GLU:HB3	2:O:23:ASP:H	1.61	0.43
3:P:105:TYR:O	3:P:315:THR:HG22	2.18	0.43
1:A:358:LYS:HE3	1:A:399:ILE:O	2.19	0.43
3:C:282:LEU:HD23	3:C:282:LEU:O	2.18	0.43
3:C:101:ARG:CZ	12:C:502:HEM:HBD2	2.48	0.43
5:E:163:SER:HA	5:E:174:GLY:HA3	2.00	0.43
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:TYR:HA	2:O:113:ARG:HD3	2.01	0.43
2:O:257:VAL:O	2:O:323:GLY:HA3	2.18	0.43
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.40	0.43
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.18	0.43
5:R:109:GLU:O	5:R:123:ASP:HB2	2.19	0.43
7:T:46:PHE:O	7:T:50:PRO:HG2	2.18	0.43
2:B:166:ALA:HB1	2:B:242:GLY:C	2.39	0.43
2:B:31:ASN:CB	2:B:227:ARG:HH22	2.29	0.43
3:C:112:GLU:O	3:C:116:THR:HG23	2.19	0.43
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.82	0.43
4:D:83:ARG:HB2	4:D:84:PRO:HD2	1.99	0.43
5:E:59:ILE:CG2	5:E:60:SER:N	2.81	0.43
5:E:69:LEU:O	5:E:70:ALA:HB2	2.19	0.43
2:O:147:ASP:O	2:O:150:VAL:HG22	2.18	0.43
3:P:243:LEU:HD21	3:P:251:LEU:CD1	2.49	0.43
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.18	0.43
8:U:25:GLU:HG2	8:U:61:PHE:CZ	2.54	0.43
2:B:385:GLU:O	2:B:387:LEU:N	2.52	0.43
3:C:52:LEU:CD2	3:C:80:ILE:HG22	2.48	0.43
5:E:135:LEU:HD22	5:E:169:GLY:HA3	2.00	0.43
5:E:85:LYS:HE2	5:E:87:VAL:CG2	2.45	0.43
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.00	0.43
3:P:246:PHE:C	3:P:248:PRO:HD3	2.39	0.43
3:P:34:PHE:HB2	21:P:381:HOH:O	2.19	0.43
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.83	0.43
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.54	0.43
4:Q:60:GLU:OE1	10:W:59:TYR:HB3	2.18	0.43
3:C:131:GLY:HA3	3:C:183:HIS:CE1	2.54	0.43
4:D:142:VAL:O	4:D:142:VAL:HG23	2.18	0.43
6:F:13:MET:CE	6:F:16:ILE:HD12	2.49	0.43
1:N:293:ARG:HH21	1:N:344:ARG:NE	2.17	0.43
1:N:433:ASP:OD2	1:N:435:ASN:N	2.52	0.43
5:R:165:TYR:HA	5:R:170:ARG:O	2.19	0.43
7:T:77:TYR:CD2	8:U:52:GLU:HB2	2.54	0.43
1:A:26:ALA:O	1:A:198:ALA:HA	2.19	0.43
1:A:7:THR:HG21	2:B:113:ARG:CD	2.49	0.43
2:B:235:ALA:O	2:B:236:LYS:C	2.57	0.43
3:C:107:SER:HB3	12:C:502:HEM:HAD1	2.01	0.43
4:D:62:LYS:HE2	4:D:66:GLU:OE2	2.19	0.43
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.84	0.43
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:THR:HG21	1:N:235:ARG:N	2.34	0.43
3:P:139:MET:HE3	3:P:270:LYS:H	1.84	0.43
3:P:275:PHE:CD2	13:P:3001:SMA:H11	2.54	0.43
3:P:2:ALA:HA	3:P:3:PRO:O	2.19	0.43
5:R:186:GLN:NE2	5:R:188:VAL:HG12	2.34	0.43
2:B:353:THR:HB	2:B:356:ASP:CG	2.39	0.42
5:E:72:SER:HB2	5:E:73:LYS:H	1.62	0.42
1:N:220:SER:HB2	1:N:226:ASP:OD1	2.19	0.42
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.78	0.42
1:N:86:PHE:HD1	1:N:87:ASN:N	2.17	0.42
1:A:159:GLN:HE22	7:G:18:LEU:CD2	2.30	0.42
2:B:146:VAL:HG12	2:B:147:ASP:N	2.34	0.42
3:C:101:ARG:O	3:C:101:ARG:HD2	2.18	0.42
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.18	0.42
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.54	0.42
2:O:147:ASP:OD1	9:V:68:ILE:HD11	2.19	0.42
3:P:101:ARG:HD2	3:P:102:GLY:N	2.31	0.42
3:P:139:MET:HE2	3:P:253:ASP:OD2	2.18	0.42
4:Q:14:HIS:O	4:Q:202:LYS:NZ	2.52	0.42
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.83	0.42
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.83	0.42
5:E:47:THR:HG21	15:E:2005:PEE:H23	2.01	0.42
1:N:86:PHE:O	2:O:285:ILE:HA	2.19	0.42
3:P:2:ALA:HA	3:P:3:PRO:C	2.37	0.42
6:S:16:ILE:O	6:S:19:TRP:HB3	2.19	0.42
2:B:385:GLU:C	2:B:387:LEU:N	2.73	0.42
3:C:95:ILE:CG2	3:C:96:PHE:N	2.82	0.42
5:E:122:HIS:ND1	5:E:124:LEU:HG	2.35	0.42
7:G:34:LEU:HA	7:G:37:VAL:HG23	2.01	0.42
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.87	0.42
7:T:73:ASN:HA	7:T:74:PRO:HD2	1.90	0.42
3:C:235:LEU:O	3:C:239:PRO:HD2	2.19	0.42
3:C:95:ILE:O	3:C:99:ILE:HG13	2.20	0.42
4:Q:210:LEU:HD23	4:Q:210:LEU:HA	1.82	0.42
4:Q:62:LYS:HE2	4:Q:66:GLU:OE2	2.19	0.42
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.99	0.42
9:V:64:LEU:HD12	9:V:77:ARG:C	2.39	0.42
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.52	0.42
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.55	0.42
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.88	0.42
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ARG:CD	3:C:101:ARG:C	2.78	0.42
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.84	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.64	0.42
5:E:69:LEU:HD12	5:E:71:LEU:HG	2.01	0.42
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.59	0.42
8:H:73:LEU:O	8:H:73:LEU:HD12	2.20	0.42
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.54	0.42
1:N:433:ASP:C	1:N:433:ASP:OD2	2.58	0.42
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.02	0.42
3:P:158:GLY:O	3:P:159:HIS:C	2.58	0.42
1:A:76:GLU:O	1:A:80:GLU:HG3	2.19	0.42
2:B:116:VAL:HG12	2:B:120:MET:HE2	2.02	0.42
3:C:133:VAL:HA	3:C:140:SER:HB3	2.01	0.42
4:D:105:ASN:O	4:D:106:ASN:HB2	2.20	0.42
3:C:246:PHE:CZ	4:D:205:GLY:HA3	2.55	0.42
8:H:15:ASP:O	8:H:17:LEU:N	2.52	0.42
8:H:57:GLU:CD	8:H:57:GLU:H	2.23	0.42
9:I:52:ARG:O	9:I:56:SER:HB3	2.19	0.42
2:O:157:VAL:HG13	2:O:158:GLY:N	2.34	0.42
2:O:225:ASN:O	2:O:226:ILE:O	2.36	0.42
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.32	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.65	0.42
1:A:365:MET:HG2	1:A:392:LEU:HD22	2.02	0.42
3:C:141:PHE:HB2	3:C:260:ALA:HB1	2.02	0.42
3:C:50:LEU:O	3:C:54:MET:HG3	2.20	0.42
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.55	0.42
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.50	0.42
1:N:39:VAL:HG11	1:N:117:VAL:CG1	2.49	0.42
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.20	0.42
2:O:59:THR:HG22	2:O:60:THR:H	1.85	0.42
3:P:335:ILE:HD13	7:T:58:LEU:HD23	2.01	0.42
1:A:26:ALA:CB	1:A:383:LEU:HD11	2.49	0.42
1:A:388:ARG:NH2	1:A:388:ARG:CG	2.83	0.42
1:A:403:ASP:O	1:A:404:ALA:C	2.58	0.42
2:B:305:GLN:HB3	2:B:306:PRO:HD2	2.01	0.42
4:D:222:MET:HE1	5:E:40:THR:HG23	2.00	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.19	0.42
7:G:81:GLN:OXT	8:H:49:HIS:N	2.53	0.42
1:N:178:THR:CG2	1:N:179:ARG:N	2.82	0.42
2:O:394:ALA:C	2:O:396:SER:H	2.22	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:59:ILE:HG22	5:R:60:SER:N	2.35	0.42
3:C:105:TYR:O	3:C:315:THR:HG22	2.20	0.42
6:F:84:GLU:CD	6:F:84:GLU:H	2.24	0.42
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.83	0.42
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.32	0.42
3:P:187:PRO:O	3:P:190:ILE:HB	2.20	0.42
3:P:270:LYS:HA	3:P:271:PRO:HD3	1.84	0.42
4:Q:74:PRO:HA	4:Q:79:GLU:O	2.20	0.42
5:R:109:GLU:CD	5:R:167:ALA:HB3	2.41	0.42
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.49	0.42
7:T:41:PHE:HD2	7:T:41:PHE:O	2.02	0.42
1:A:13:GLU:HG2	1:A:14:THR:N	2.35	0.41
2:B:100:SER:HA	2:B:104:LYS:O	2.20	0.41
2:B:109:VAL:HG21	2:B:119:VAL:CG2	2.50	0.41
2:B:265:GLY:O	2:B:266:SER:C	2.58	0.41
3:C:76:TYR:HE2	4:D:204:MET:CE	2.33	0.41
4:D:28:ARG:NH1	4:D:173:ASP:OD2	2.53	0.41
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.50	0.41
1:N:37:VAL:HG12	1:N:199:ALA:HB2	2.00	0.41
1:N:63:ALA:O	1:N:116:VAL:HG13	2.20	0.41
3:P:237:LEU:HD12	3:P:237:LEU:HA	1.70	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.54	0.41
6:S:13:MET:O	6:S:17:ARG:HG3	2.21	0.41
9:V:55:MET:HA	9:V:58:ARG:HG3	2.01	0.41
1:A:158:PHE:O	1:A:164:ALA:HB2	2.19	0.41
4:D:62:LYS:O	4:D:65:ALA:HB3	2.20	0.41
6:F:91:GLU:N	6:F:92:PRO:HD2	2.35	0.41
7:G:9:ARG:NH1	7:G:9:ARG:HG3	2.35	0.41
4:Q:28:ARG:HG3	4:Q:28:ARG:HH11	1.85	0.41
5:R:31:ASP:OD1	10:W:7:ARG:HG3	2.20	0.41
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.50	0.41
1:A:126:GLN:NE2	1:A:129:LYS:HD3	2.35	0.41
2:B:128:THR:HG21	2:B:224:LEU:CD2	2.50	0.41
3:C:275:PHE:CD2	13:C:2001:SMA:H11	2.55	0.41
9:I:49:LEU:O	9:I:50:LEU:HD23	2.19	0.41
1:N:136:GLN:O	1:N:139:LYS:N	2.54	0.41
2:O:43:PRO:C	2:O:113:ARG:HG3	2.38	0.41
3:P:31:TRP:HE1	18:P:3004:CDL:H1	1.85	0.41
7:T:34:LEU:HA	7:T:37:VAL:CG2	2.50	0.41
8:U:57:GLU:CD	8:U:57:GLU:H	2.24	0.41
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PRO:HD3	1:A:414:TYR:CE2	2.55	0.41
1:A:242:ARG:NH1	1:A:432:LEU:HA	2.20	0.41
2:B:24:LEU:HD23	2:B:392:HIS:CE1	2.55	0.41
3:C:15:ILE:CD1	3:C:15:ILE:N	2.82	0.41
3:C:273:TRP:HA	3:C:276:LEU:HG	2.02	0.41
5:E:103:GLN:O	5:E:107:ASN:ND2	2.53	0.41
5:E:67:ASP:O	5:E:69:LEU:HD23	2.19	0.41
1:N:402:VAL:HA	1:N:406:MET:SD	2.61	0.41
1:N:99:ILE:HD12	1:N:109:VAL:CG1	2.43	0.41
2:O:47:ILE:CD1	2:O:47:ILE:N	2.84	0.41
3:P:59:ASP:HA	3:P:173:ASN:OD1	2.20	0.41
5:R:69:LEU:H	5:R:69:LEU:HD23	1.84	0.41
8:U:67:HIS:ND1	8:U:67:HIS:C	2.73	0.41
5:E:77:LYS:C	5:E:79:SER:H	2.23	0.41
9:I:64:LEU:HD12	9:I:77:ARG:O	2.20	0.41
1:N:21:ASN:O	1:N:192:ALA:HB3	2.20	0.41
1:N:252:HIS:CE1	1:N:325:VAL:HG22	2.55	0.41
1:N:356:ARG:HG3	2:O:90:GLU:O	2.21	0.41
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.20	0.41
2:O:50:PHE:HE1	2:O:207:VAL:HB	1.85	0.41
3:P:172:ASP:HB3	3:P:174:PRO:HD2	2.02	0.41
8:U:13:LEU:CD2	8:U:13:LEU:H	2.30	0.41
8:U:51:GLU:HA	8:U:51:GLU:OE1	2.20	0.41
8:U:58:LEU:HD12	8:U:58:LEU:O	2.21	0.41
10:W:14:PHE:HA	10:W:20:PHE:HD2	1.85	0.41
1:A:30:SER:OG	1:A:32:GLN:HB2	2.20	0.41
2:B:207:VAL:HG12	2:B:208:GLY:N	2.34	0.41
4:D:10:PHE:N	4:D:10:PHE:CD1	2.87	0.41
10:J:59:TYR:CD1	10:J:59:TYR:N	2.88	0.41
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.02	0.41
2:O:100:SER:HA	2:O:104:LYS:O	2.21	0.41
2:O:398:VAL:HG13	2:O:399:ALA:N	2.35	0.41
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.51	0.41
9:V:77:ARG:N	9:V:77:ARG:CD	2.83	0.41
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.20	0.41
1:A:204:SER:HB3	1:A:207:GLU:HB2	2.02	0.41
1:A:49:ASN:ND2	1:A:51:LYS:N	2.68	0.41
1:A:99:ILE:HG22	1:A:100:LYS:N	2.35	0.41
3:C:40:VAL:HG11	3:C:233:LEU:HD11	2.03	0.41
6:F:109:LYS:O	6:F:110:LYS:C	2.59	0.41
9:I:49:LEU:HD22	9:I:55:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:ARG:HB3	10:J:7:ARG:CZ	2.50	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
1:N:329:LEU:C	1:N:430:GLN:HE22	2.23	0.41
2:O:269:ALA:O	2:O:270:ASN:C	2.59	0.41
3:P:122:LEU:HD23	3:P:122:LEU:HA	1.86	0.41
4:Q:158:ILE:HG12	4:Q:159:GLY:N	2.35	0.41
5:R:75:GLU:C	5:R:76:ILE:HG13	2.41	0.41
1:A:233:ARG:NH2	1:A:316:ASP:HB2	2.36	0.41
1:A:280:TYR:CD2	1:A:281:ASP:N	2.89	0.41
2:B:259:THR:HG22	2:B:260:GLU:H	1.84	0.41
3:C:308:LEU:HD23	3:C:308:LEU:HA	1.85	0.41
5:E:195:VAL:HG12	5:E:196:GLY:H	1.83	0.41
1:A:136:GLN:HE22	9:I:50:LEU:CD1	2.34	0.41
4:Q:27:ARG:NH2	10:W:59:TYR:CD2	2.88	0.41
4:Q:57:THR:HG23	10:W:59:TYR:HB2	2.03	0.41
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.88	0.41
9:V:49:LEU:HD22	9:V:55:MET:HG2	2.03	0.41
1:A:209:VAL:O	1:A:213:ARG:HG3	2.21	0.41
2:B:263:ALA:HB1	2:B:317:SER:O	2.21	0.41
2:B:33:LEU:HD21	2:B:220:ALA:HB1	2.02	0.41
2:B:369:LEU:O	2:B:372:VAL:HG22	2.21	0.41
2:B:26:ILE:HD11	2:B:390:GLY:O	2.21	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.55	0.41
5:E:133:VAL:HG13	5:E:133:VAL:O	2.21	0.41
6:F:32:MET:HE3	6:F:87:LYS:N	2.22	0.41
1:A:242:ARG:O	7:G:14:ILE:HA	2.20	0.41
1:N:368:GLN:O	1:N:369:LEU:HD23	2.20	0.41
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.85	0.41
2:O:29:LEU:HB2	2:O:31:ASN:ND2	2.36	0.41
2:B:429:ASP:OD1	2:O:60:THR:HG21	2.20	0.41
3:P:40:VAL:HG11	3:P:233:LEU:HD11	2.02	0.41
3:P:50:LEU:O	3:P:54:MET:HG3	2.21	0.41
5:R:166:ASP:HB3	5:R:172:ARG:HH11	1.85	0.41
1:A:23:LEU:HD22	1:A:216:PHE:HB3	2.02	0.41
1:A:266:ASP:O	1:A:269:VAL:N	2.54	0.41
2:B:43:PRO:C	2:B:113:ARG:HG3	2.40	0.41
6:F:104:ARG:O	6:F:108:ASN:ND2	2.53	0.41
3:C:331:ALA:HB2	7:G:52:PHE:CD2	2.56	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.50	0.41
1:N:106:MET:HE2	1:N:106:MET:O	2.21	0.41
1:N:317:THR:OG1	1:N:318:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:203:ARG:CD	2:O:230:ALA:HA	2.51	0.41
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.33	0.41
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.55	0.41
6:S:10:GLY:C	6:S:12:LEU:N	2.74	0.41
2:O:307:PHE:H	9:V:52:ARG:HG2	1.86	0.41
1:A:10:ASN:ND2	2:B:19:PRO:CD	2.84	0.41
1:A:146:THR:O	1:A:150:PHE:HD1	2.03	0.41
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.50	0.41
3:C:145:THR:O	3:C:149:ASN:HB2	2.21	0.41
1:N:102:LEU:C	1:N:104:LYS:N	2.74	0.41
1:N:45:SER:OG	1:N:92:ARG:HA	2.20	0.41
2:O:124:LEU:CD2	2:O:223:PHE:HB3	2.51	0.41
2:O:56:ARG:HG3	2:O:57:TYR:CD1	2.56	0.41
3:P:167:GLY:HA3	3:P:178:ARG:NH2	2.36	0.41
3:P:42:LEU:CD2	3:P:190:ILE:HG22	2.51	0.41
3:P:207:ASN:HD22	3:P:208:ASN:N	2.10	0.41
3:P:243:LEU:CD2	3:P:251:LEU:HD11	2.50	0.41
3:P:347:PRO:O	3:P:350:ILE:HG22	2.21	0.41
1:A:39:VAL:O	1:A:39:VAL:HG13	2.21	0.40
3:C:163:GLU:O	3:C:167:GLY:N	2.52	0.40
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.85	0.40
6:F:67:ASP:O	6:F:70:LEU:HG	2.21	0.40
1:N:292:SER:O	1:N:295:ALA:HB3	2.22	0.40
1:N:30:SER:OG	1:N:32:GLN:HB2	2.22	0.40
1:N:362:ARG:O	1:N:365:MET:HB3	2.21	0.40
2:O:209:ILE:HG13	2:O:379:LEU:HD13	2.01	0.40
3:P:29:SER:HB2	18:P:3004:CDL:HB21	2.03	0.40
3:P:63:ALA:O	3:P:67:VAL:HG23	2.21	0.40
5:R:69:LEU:CD1	5:R:71:LEU:HD11	2.51	0.40
3:P:236:MET:HA	18:S:3003:CDL:H162	2.02	0.40
6:S:77:LYS:HE2	6:S:78:GLU:OE2	2.21	0.40
6:S:91:GLU:N	6:S:92:PRO:HD2	2.36	0.40
4:Q:235:MET:CB	7:T:15:THR:HG22	2.51	0.40
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.04	0.40
4:Q:138:PRO:HD3	8:U:58:LEU:HD23	2.02	0.40
1:A:62:LEU:C	1:A:64:PHE:H	2.25	0.40
2:B:19:PRO:O	2:B:20:GLY:O	2.39	0.40
2:B:259:THR:CG2	2:B:260:GLU:N	2.83	0.40
2:B:300:ALA:C	2:B:302:ALA:N	2.74	0.40
2:B:408:ALA:O	2:B:409:ASP:C	2.60	0.40
3:C:11:LEU:O	3:C:14:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:267:PRO:HA	5:R:147:ILE:HD11	2.03	0.40
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.03	0.40
1:N:223:TYR:HD2	1:N:223:TYR:N	2.17	0.40
2:O:307:PHE:CD1	2:O:308:ASP:N	2.89	0.40
2:O:366:ALA:O	2:O:367:THR:C	2.59	0.40
2:O:51:ILE:HG22	2:O:52:LYS:N	2.36	0.40
3:P:11:LEU:O	3:P:14:MET:HB2	2.21	0.40
4:Q:161:ALA:O	4:Q:163:PRO:HD3	2.22	0.40
6:S:84:GLU:H	6:S:84:GLU:CD	2.25	0.40
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.86	0.40
3:C:109:LEU:HB2	3:C:314:ARG:HH21	1.86	0.40
3:C:70:THR:HA	3:C:74:VAL:CG2	2.51	0.40
5:E:103:GLN:CA	5:E:106:ILE:HD12	2.50	0.40
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.04	0.40
1:N:37:VAL:HG23	1:N:113:LEU:HD11	2.03	0.40
1:N:173:ASN:O	1:N:177:LEU:HG	2.21	0.40
1:N:281:ASP:O	1:N:283:THR:N	2.54	0.40
4:Q:139:ALA:HB2	8:U:41:ASP:HA	2.02	0.40
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.55	0.40
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.50	0.40
5:R:127:VAL:HG11	5:R:133:VAL:HG23	2.03	0.40
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	3.04	0.40
2:B:128:THR:C	2:B:130:PRO:HD2	2.42	0.40
2:B:56:ARG:HB2	2:B:171:ALA:HB1	2.02	0.40
4:D:105:ASN:O	4:D:108:ALA:HB3	2.21	0.40
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.57	0.40
5:E:103:GLN:HA	5:E:106:ILE:CG1	2.52	0.40
2:O:19:PRO:HB3	2:O:41:PHE:CG	2.57	0.40
3:P:338:TRP:CZ2	3:P:348:PHE:HE2	2.38	0.40
3:P:76:TYR:HE2	4:Q:204:MET:HE3	1.86	0.40
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.37	0.40
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.56	0.40
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.40
5:R:91:TRP:C	5:R:93:GLY:N	2.75	0.40
7:T:65:GLU:OE1	7:T:65:GLU:HA	2.22	0.40
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.62	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.84	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.76	0.40
1:A:36:THR:HG21	1:A:373:THR:HA	2.04	0.40
1:A:4:TYR:O	1:A:5:ALA:C	2.59	0.40
2:B:34:ILE:HD13	2:B:390:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ARG:HD3	3:C:16:ASN:OD1	2.22	0.40
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.51	0.40
4:D:139:ALA:HB3	8:H:54:CYS:SG	2.62	0.40
4:D:47:ALA:HB1	4:D:89:ASP:O	2.21	0.40
5:E:52:LYS:O	5:E:52:LYS:HD3	2.21	0.40
8:H:20:ILE:HD11	8:H:76:LYS:CD	2.44	0.40
1:N:15:ASN:HB3	1:N:205:HIS:CD2	2.57	0.40
2:O:109:VAL:HG21	2:O:119:VAL:HG23	2.02	0.40
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.04	0.40
2:O:422:LYS:O	2:O:436:LEU:HD21	2.21	0.40
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.51	0.40
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	2.04	0.40
5:R:103:GLN:HA	5:R:106:ILE:CG1	2.51	0.40
5:R:34:GLY:HA2	10:W:10:TYR:HB2	2.04	0.40
10:W:7:ARG:HB3	10:W:7:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	393 (89%)	40 (9%)	8 (2%)	8	37
1	N	440/446 (99%)	397 (90%)	36 (8%)	7 (2%)	9	40
2	B	419/441 (95%)	339 (81%)	63 (15%)	17 (4%)	3	16
2	O	420/441 (95%)	336 (80%)	66 (16%)	18 (4%)	2	15
3	C	378/380 (100%)	358 (95%)	18 (5%)	2 (0%)	29	68
3	P	377/380 (99%)	349 (93%)	24 (6%)	4 (1%)	14	50
4	D	239/241 (99%)	217 (91%)	20 (8%)	2 (1%)	19	57
4	Q	239/241 (99%)	214 (90%)	22 (9%)	3 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	194/196 (99%)	157 (81%)	24 (12%)	13 (7%)	1	6
5	R	194/196 (99%)	161 (83%)	21 (11%)	12 (6%)	1	8
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	15	53
7	G	79/81 (98%)	66 (84%)	9 (11%)	4 (5%)	2	12
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	2	12
8	H	68/77 (88%)	57 (84%)	8 (12%)	3 (4%)	2	15
8	U	65/77 (84%)	48 (74%)	16 (25%)	1 (2%)	10	42
9	I	29/47 (62%)	19 (66%)	7 (24%)	3 (10%)	0	2
9	V	29/47 (62%)	20 (69%)	7 (24%)	2 (7%)	1	6
10	J	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	9	39
10	W	57/61 (93%)	45 (79%)	8 (14%)	4 (7%)	1	6
All	All	4002/4160 (96%)	3475 (87%)	418 (10%)	109 (3%)	5	26

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	114	ASP
2	B	171	ALA
2	B	230	ALA
2	B	236	LYS
5	E	69	LEU
5	E	70	ALA
5	E	95	PRO
7	G	7	LEU
8	H	12	GLU
10	J	56	LYS
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	114	ASP
2	O	171	ALA
2	O	222	GLN
2	O	225	ASN
2	O	226	ILE

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Mol	Chain	Res	Type
2	O	236	LYS
3	P	157	ILE
5	R	69	LEU
5	R	72	SER
5	R	95	PRO
7	T	7	LEU
10	W	56	LYS
1	A	71	PRO
1	A	72	CYS
1	A	282	ARG
1	A	433	ASP
2	B	31	ASN
2	B	226	ILE
2	B	283	PRO
2	B	371	SER
2	B	390	GLY
5	E	74	ILE
5	E	113	ASP
5	E	137	GLY
7	G	33	ALA
8	H	49	HIS
9	I	56	SER
1	N	20	ASP
1	N	72	CYS
1	N	282	ARG
2	O	221	GLU
2	O	230	ALA
2	O	283	PRO
2	O	371	SER
2	O	390	GLY
3	P	158	GLY
4	Q	177	ALA
5	R	113	ASP
7	T	33	ALA
2	B	30	PRO
3	C	3	PRO
5	E	73	LYS
5	E	78	LEU
5	E	141	HIS
8	H	72	LYS
9	I	55	MET
1	N	71	PRO

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Mol	Chain	Res	Type
1	N	288	LYS
2	O	224	LEU
3	P	3	PRO
3	P	156	TYR
5	R	92	ARG
6	S	11	ARG
10	W	60	GLU
1	A	3	THR
1	A	306	SER
3	C	156	TYR
5	E	92	ARG
5	E	130	PRO
9	I	63	ASP
2	O	227	ARG
4	Q	198	HIS
5	R	78	LEU
5	R	141	HIS
10	W	57	HIS
10	W	61	ALA
1	A	288	LYS
2	B	22	GLU
2	B	266	SER
2	B	382	ILE
4	D	177	ALA
5	E	123	ASP
4	Q	162	PRO
5	R	21	ALA
5	R	74	ILE
5	R	130	PRO
5	R	137	GLY
9	V	63	ASP
2	B	319	SER
1	N	260	PRO
2	O	319	SER
5	R	106	ILE
7	T	27	PRO
8	U	28	GLU
1	A	260	PRO
5	E	106	ILE
7	G	27	PRO
2	O	382	ILE
7	G	50	PRO

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Mol	Chain	Res	Type
7	T	50	PRO
9	V	76	VAL
2	O	288	GLY
4	D	162	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	344 (94%)	21 (6%)	20	55
1	N	365/368 (99%)	344 (94%)	21 (6%)	20	55
2	B	332/347 (96%)	318 (96%)	14 (4%)	30	66
2	O	333/347 (96%)	319 (96%)	14 (4%)	30	66
3	C	329/329 (100%)	323 (98%)	6 (2%)	59	85
3	P	328/329 (100%)	321 (98%)	7 (2%)	53	82
4	D	200/200 (100%)	196 (98%)	4 (2%)	55	83
4	Q	200/200 (100%)	196 (98%)	4 (2%)	55	83
5	E	166/166 (100%)	157 (95%)	9 (5%)	22	57
5	R	166/166 (100%)	157 (95%)	9 (5%)	22	57
6	F	93/96 (97%)	90 (97%)	3 (3%)	39	74
6	S	93/96 (97%)	89 (96%)	4 (4%)	29	66
7	G	71/71 (100%)	68 (96%)	3 (4%)	30	66
7	T	69/71 (97%)	66 (96%)	3 (4%)	29	66
8	H	65/71 (92%)	63 (97%)	2 (3%)	40	75
8	U	63/71 (89%)	61 (97%)	2 (3%)	39	74
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	66
9	V	23/26 (88%)	22 (96%)	1 (4%)	29	66
10	J	49/49 (100%)	45 (92%)	4 (8%)	11	39
10	W	47/49 (96%)	44 (94%)	3 (6%)	17	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3380/3446 (98%)	3245 (96%)	135 (4%)	31 68

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	72	CYS
1	A	86	PHE
1	A	87	ASN
1	A	90	THR
1	A	91	SER
1	A	106	MET
1	A	181	ASP
1	A	223	TYR
1	A	226	ASP
1	A	233	ARG
1	A	281	ASP
1	A	302	LYS
1	A	307	PHE
1	A	342	TRP
1	A	388	ARG
1	A	395	TRP
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	102	ARG
2	B	154	SER
2	B	227	ARG
2	B	248	ASN
2	B	285	ILE
2	B	291	VAL
2	B	296	TYR
2	B	325	TYR
2	B	344	LEU
2	B	358	THR
2	B	364	LEU
2	B	403	ASP
3	C	17	ASN
3	C	47	LEU

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Mol	Chain	Res	Type
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	237	LEU
4	D	24	SER
4	D	77	ASN
4	D	240	PRO
4	D	241	LYS
5	E	6	THR
5	E	52	LYS
5	E	59	ILE
5	E	69	LEU
5	E	74	ILE
5	E	80	ASP
5	E	125	ASP
5	E	135	LEU
5	E	184	THR
6	F	70	LEU
6	F	77	LYS
6	F	91	GLU
7	G	27	PRO
7	G	29	ILE
7	G	41	PHE
8	H	10	GLU
8	H	26	GLN
9	I	71	ASN
10	J	16	ARG
10	J	22	LEU
10	J	26	LEU
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	87	ASN
1	N	90	THR
1	N	106	MET
1	N	124	GLU
1	N	181	ASP
1	N	223	TYR
1	N	281	ASP

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Mol	Chain	Res	Type
1	N	302	LYS
1	N	307	PHE
1	N	342	TRP
1	N	376	CYS
1	N	388	ARG
1	N	395	TRP
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	23	ASP
2	O	31	ASN
2	O	99	TYR
2	O	102	ARG
2	O	154	SER
2	O	227	ARG
2	O	248	ASN
2	O	285	ILE
2	O	291	VAL
2	O	296	TYR
2	O	325	TYR
2	O	344	LEU
2	O	403	ASP
3	P	17	ASN
3	P	47	LEU
3	P	81	ARG
3	P	91	PHE
3	P	149	ASN
3	P	207	ASN
3	P	237	LEU
4	Q	3	LEU
4	Q	24	SER
4	Q	77	ASN
4	Q	241	LYS
5	R	6	THR
5	R	47	THR
5	R	52	LYS
5	R	59	ILE
5	R	69	LEU
5	R	80	ASP
5	R	125	ASP
5	R	135	LEU

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Mol	Chain	Res	Type
5	R	184	THR
6	S	13	MET
6	S	70	LEU
6	S	77	LYS
6	S	91	GLU
7	T	27	PRO
7	T	29	ILE
7	T	41	PHE
8	U	26	GLN
8	U	71	HIS
9	V	70	LEU
10	W	22	LEU
10	W	26	LEU
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	126	GLN
1	A	136	GLN
1	A	147	ASN
1	A	159	GLN
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
1	A	360	HIS
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	222	GLN
2	B	248	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	362	ASN
2	B	363	GLN
2	B	400	GLN
2	B	412	ASN

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Mol	Chain	Res	Type
3	C	4	ASN
3	C	17	ASN
3	C	69	HIS
3	C	82	ASN
3	C	149	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	200	GLN
5	E	86	ASN
5	E	107	ASN
5	E	164	HIS
5	E	186	GLN
6	F	56	ASN
6	F	72	HIS
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	64	GLN
7	G	79	ASN
7	G	81	GLN
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	126	GLN
1	N	136	GLN
1	N	143	ASN
1	N	147	ASN
1	N	159	GLN
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
1	N	360	HIS
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN

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Mol	Chain	Res	Type
2	O	192	HIS
2	O	222	GLN
2	O	225	ASN
2	O	248	ASN
2	O	270	ASN
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	329	GLN
2	O	362	ASN
2	O	363	GLN
2	O	400	GLN
2	O	412	ASN
3	P	4	ASN
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	200	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
6	S	56	ASN
6	S	72	HIS
6	S	79	GLN
7	T	23	GLN
7	T	44	GLN
7	T	64	GLN
8	U	71	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 10 are unknown - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEE	N	3008	-	4,4,50	3.52	4 (100%)	6,6,55	0.61	0
20	PLC	E	2009	-	31,31,41	1.67	6 (19%)	37,39,49	0.65	0
15	PEE	R	3005	-	49,49,50	1.43	9 (18%)	52,54,55	0.94	5 (9%)
17	HEC	Q	501	4	26,50,50	2.01	3 (11%)	18,82,82	1.63	3 (16%)
20	PLC	R	3009	-	31,31,41	1.61	7 (22%)	37,39,49	0.62	0
12	HEM	P	502	3	27,50,50	1.84	6 (22%)	17,82,82	1.69	6 (35%)
12	HEM	C	502	3	27,50,50	1.86	8 (29%)	17,82,82	1.90	7 (41%)
15	PEE	P	3007	-	48,48,50	1.32	7 (14%)	51,53,55	0.92	4 (7%)
12	HEM	P	501	3	27,50,50	1.87	5 (18%)	17,82,82	1.49	4 (23%)
17	HEC	D	501	4	26,50,50	2.00	5 (19%)	18,82,82	1.84	3 (16%)
16	GOL	P	3011	-	5,5,5	1.46	1 (20%)	5,5,5	0.68	0
15	PEE	C	2007	-	48,48,50	1.34	8 (16%)	51,53,55	0.97	5 (9%)
18	CDL	D	2003	-	49,49,99	1.14	2 (4%)	55,61,111	1.00	2 (3%)
14	UQ	C	2002	-	19,19,63	2.67	9 (47%)	23,26,79	1.11	2 (8%)
15	PEE	C	2008	-	20,20,50	1.73	6 (30%)	23,25,55	0.62	0
18	CDL	S	3003	-	49,49,99	1.13	2 (4%)	55,61,111	1.00	2 (3%)
18	CDL	P	3004	-	39,39,99	1.24	3 (7%)	45,51,111	1.14	4 (8%)
16	GOL	C	2011	-	5,5,5	1.28	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SMA	P	3001	-	35,38,38	1.69	9 (25%)	46,52,52	1.81	7 (15%)
14	UQ	P	3002	-	19,19,63	2.64	10 (52%)	23,26,79	1.11	2 (8%)
12	HEM	C	501	3	27,50,50	1.96	9 (33%)	17,82,82	1.80	4 (23%)
13	SMA	C	2001	-	35,38,38	1.73	9 (25%)	46,52,52	1.87	8 (17%)
15	PEE	E	2005	-	49,49,50	1.41	10 (20%)	52,54,55	0.95	5 (9%)
19	FES	E	501	5	0,4,4	0.00	-	-	-	-
18	CDL	G	2004	-	39,39,99	1.33	5 (12%)	45,51,111	1.13	4 (8%)
19	FES	R	501	5	0,4,4	0.00	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PLC	E	2009	-	-	15/35/35/45	-
15	PEE	R	3005	-	-	24/53/53/54	-
17	HEC	Q	501	4	-	2/6/54/54	-
20	PLC	R	3009	-	-	14/35/35/45	-
12	HEM	P	502	3	-	2/6/54/54	-
12	HEM	C	502	3	-	2/6/54/54	-
15	PEE	P	3007	-	-	28/52/52/54	-
12	HEM	P	501	3	-	0/6/54/54	-
17	HEC	D	501	4	-	2/6/54/54	-
16	GOL	P	3011	-	-	0/4/4/4	-
15	PEE	C	2007	-	-	24/52/52/54	-
18	CDL	D	2003	-	-	25/59/59/110	-
14	UQ	C	2002	-	-	3/11/35/87	0/1/1/1
15	PEE	C	2008	-	-	9/24/24/54	-
18	CDL	S	3003	-	-	25/59/59/110	-
18	CDL	P	3004	-	-	21/49/49/110	-
16	GOL	C	2011	-	-	2/4/4/4	-
13	SMA	P	3001	-	-	4/33/34/34	0/2/2/2
14	UQ	P	3002	-	-	3/11/35/87	0/1/1/1
12	HEM	C	501	3	-	0/6/54/54	-
13	SMA	C	2001	-	-	3/33/34/34	0/2/2/2
15	PEE	E	2005	-	-	24/53/53/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FES	E	501	5	-	-	0/1/1/1
18	CDL	G	2004	-	-	21/49/49/110	-
19	FES	R	501	5	-	-	0/1/1/1

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3B-C2B	-7.62	1.32	1.40
17	D	501	HEC	C3B-C2B	-6.34	1.34	1.40
14	P	3002	UQ	C7-C6	5.44	1.60	1.51
14	P	3002	UQ	C6-C5	5.17	1.44	1.35
13	C	2001	SMA	C7-C8	5.13	1.47	1.40
17	D	501	HEC	C3C-C2C	-5.10	1.35	1.40
14	C	2002	UQ	C7-C6	5.05	1.59	1.51
14	C	2002	UQ	C6-C5	4.86	1.44	1.35
13	P	3001	SMA	O1-C2	4.78	1.42	1.35
12	C	501	HEM	C3B-CAB	-4.75	1.38	1.47
15	N	3008	PEE	P-O1P	4.60	1.61	1.50
12	P	501	HEM	C3B-CAB	-4.50	1.38	1.47
12	P	501	HEM	C3C-CAC	-4.30	1.39	1.47
13	P	3001	SMA	C7-C8	4.27	1.46	1.40
20	E	2009	PLC	O2-C'	4.13	1.46	1.34
13	C	2001	SMA	O1-C2	4.08	1.41	1.35
17	Q	501	HEC	C3C-C2C	-3.96	1.36	1.40
14	C	2002	UQ	C6-C1	3.95	1.57	1.46
12	C	502	HEM	C4D-C3D	3.85	1.51	1.42
14	C	2002	UQ	O3-C3	3.85	1.46	1.36
14	P	3002	UQ	C6-C1	3.77	1.57	1.46
20	R	3009	PLC	O2-C'	3.75	1.44	1.34
12	P	502	HEM	C3B-CAB	-3.67	1.40	1.47
12	P	502	HEM	CBC-CAC	3.61	1.53	1.29
12	C	502	HEM	CBB-CAB	3.57	1.53	1.29
12	P	502	HEM	C3C-CAC	-3.57	1.40	1.47
13	C	2001	SMA	C4-C3	3.57	1.51	1.41
12	C	501	HEM	CBC-CAC	3.54	1.52	1.29
12	C	502	HEM	C3C-CAC	-3.53	1.40	1.47
12	P	501	HEM	CBC-CAC	3.50	1.52	1.29
12	C	502	HEM	C3B-CAB	-3.44	1.40	1.47
12	C	501	HEM	C3C-CAC	-3.44	1.40	1.47
13	P	3001	SMA	C4-C3	3.44	1.51	1.41
20	E	2009	PLC	P-O1P	3.43	1.63	1.50
15	E	2005	PEE	O3-C30	3.43	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	3005	PEE	O3-C30	3.42	1.43	1.33
20	R	3009	PLC	P-O1P	3.41	1.63	1.50
15	R	3005	PEE	P-O1P	3.39	1.62	1.50
15	E	2005	PEE	P-O1P	3.36	1.62	1.50
13	C	2001	SMA	C20-C19	3.36	1.36	1.33
15	N	3008	PEE	P-O4P	3.35	1.64	1.54
12	P	502	HEM	CBB-CAB	3.35	1.51	1.29
15	N	3008	PEE	P-O3P	3.34	1.64	1.54
12	P	502	HEM	C4D-C3D	3.34	1.50	1.42
14	C	2002	UQ	O2-C2	3.26	1.44	1.36
15	R	3005	PEE	O2-C10	3.24	1.43	1.34
14	P	3002	UQ	O3-C3	3.22	1.44	1.36
12	P	501	HEM	C3B-C2B	-3.20	1.35	1.40
15	C	2008	PEE	P-O1P	3.15	1.62	1.50
15	P	3007	PEE	O2-C10	3.15	1.43	1.34
15	C	2008	PEE	O2-C10	3.11	1.43	1.34
12	P	501	HEM	CBB-CAB	3.09	1.49	1.29
12	C	502	HEM	CBC-CAC	3.06	1.49	1.29
15	C	2007	PEE	O2-C10	3.01	1.42	1.34
20	R	3009	PLC	O3-CB	2.99	1.42	1.33
15	E	2005	PEE	C19-C18	-2.97	1.34	1.51
15	R	3005	PEE	C19-C18	-2.96	1.35	1.51
20	E	2009	PLC	O3-CB	2.93	1.41	1.33
14	C	2002	UQ	C2-C1	2.92	1.57	1.48
20	E	2009	PLC	O2-C2	2.91	1.53	1.46
15	P	3007	PEE	P-O1P	2.91	1.61	1.50
14	P	3002	UQ	O2-C2	2.87	1.43	1.36
12	C	501	HEM	CBB-CAB	2.87	1.48	1.29
15	C	2007	PEE	O3-C30	2.85	1.41	1.33
12	C	501	HEM	C1D-CHD	-2.84	1.33	1.41
15	P	3007	PEE	O3-C30	2.83	1.41	1.33
14	P	3002	UQ	C2-C1	2.82	1.57	1.48
15	R	3005	PEE	C22-C21	-2.82	1.35	1.51
15	E	2005	PEE	C22-C21	-2.81	1.35	1.51
12	P	502	HEM	C3C-C2C	-2.80	1.36	1.40
14	P	3002	UQ	CM5-C5	2.80	1.56	1.50
15	C	2008	PEE	O3-C30	2.79	1.41	1.33
14	C	2002	UQ	CM5-C5	2.77	1.56	1.50
20	E	2009	PLC	C1-C2	2.70	1.59	1.50
15	P	3007	PEE	C22-C21	-2.70	1.36	1.51
14	P	3002	UQ	C3-C4	2.70	1.56	1.48
15	E	2005	PEE	O2-C10	2.70	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2007	PEE	P-O1P	2.69	1.60	1.50
15	P	3007	PEE	C19-C18	-2.68	1.36	1.51
14	C	2002	UQ	C3-C4	2.66	1.56	1.48
12	C	501	HEM	C1A-CHA	-2.66	1.33	1.41
18	G	2004	CDL	OA6-CA5	2.64	1.41	1.34
15	C	2007	PEE	C22-C21	-2.63	1.36	1.51
14	C	2002	UQ	C5-C4	2.63	1.56	1.47
12	C	502	HEM	C3C-C2C	-2.59	1.36	1.40
18	D	2003	CDL	O1-C1	2.59	1.51	1.43
15	C	2007	PEE	C19-C18	-2.53	1.37	1.51
18	S	3003	CDL	O1-C1	2.52	1.50	1.43
13	P	3001	SMA	O1-C8A	2.52	1.40	1.36
15	E	2005	PEE	C31-C30	2.51	1.58	1.50
14	P	3002	UQ	C5-C4	2.51	1.56	1.47
18	G	2004	CDL	O1-C1	2.50	1.50	1.43
12	C	501	HEM	C1B-C2B	2.50	1.48	1.42
13	P	3001	SMA	O7-C7	2.50	1.41	1.37
18	G	2004	CDL	CA3-CA4	2.48	1.58	1.50
15	R	3005	PEE	C31-C30	2.48	1.58	1.50
15	E	2005	PEE	C1-C2	2.47	1.58	1.50
15	N	3008	PEE	P-O2P	2.47	1.62	1.54
20	R	3009	PLC	O2-C2	2.46	1.52	1.46
13	P	3001	SMA	O5-C5	2.46	1.41	1.36
18	P	3004	CDL	O1-C1	2.42	1.50	1.43
13	C	2001	SMA	O7-C7	2.41	1.41	1.37
17	D	501	HEC	C3C-C4C	2.39	1.47	1.43
20	R	3009	PLC	C1-C2	2.39	1.58	1.50
13	P	3001	SMA	C6-C7	2.38	1.43	1.38
12	C	501	HEM	C3C-C2C	-2.35	1.37	1.40
13	P	3001	SMA	C6-C5	2.32	1.44	1.37
15	C	2007	PEE	C3-C2	2.31	1.57	1.50
13	C	2001	SMA	C11-C12	2.29	1.57	1.53
20	E	2009	PLC	C3-C2	2.28	1.57	1.50
12	C	501	HEM	C3B-C2B	-2.27	1.37	1.40
15	R	3005	PEE	C1-C2	2.25	1.57	1.50
15	C	2008	PEE	C1-C2	2.24	1.57	1.50
20	R	3009	PLC	C3-C2	2.24	1.57	1.50
15	R	3005	PEE	C11-C10	2.23	1.57	1.50
15	E	2005	PEE	C3-C2	2.23	1.57	1.50
17	Q	501	HEC	C4D-CHA	-2.21	1.34	1.41
13	C	2001	SMA	O1-C8A	2.19	1.40	1.36
12	C	502	HEM	C1B-C2B	2.19	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	3011	GOL	O2-C2	2.19	1.49	1.43
15	R	3005	PEE	C3-C2	2.19	1.57	1.50
13	C	2001	SMA	C6-C7	2.14	1.42	1.38
15	P	3007	PEE	C11-C10	2.13	1.56	1.50
15	P	3007	PEE	C3-C2	2.12	1.57	1.50
18	G	2004	CDL	CB3-CB4	2.12	1.57	1.50
15	C	2008	PEE	C11-C10	2.12	1.56	1.50
15	C	2007	PEE	C11-C10	2.11	1.56	1.50
13	P	3001	SMA	C20-C19	2.11	1.35	1.33
20	R	3009	PLC	C1B-CB	2.09	1.56	1.50
18	S	3003	CDL	OA6-CA5	2.08	1.40	1.34
15	E	2005	PEE	P-O4P	2.08	1.67	1.59
17	D	501	HEC	C1C-NC	2.07	1.40	1.36
14	P	3002	UQ	C7-C8	2.07	1.53	1.50
13	C	2001	SMA	C6-C5	2.02	1.43	1.37
18	D	2003	CDL	OA6-CA5	2.02	1.40	1.34
15	C	2008	PEE	C3-C2	2.02	1.56	1.50
18	G	2004	CDL	OA8-CA6	-2.02	1.40	1.45
17	D	501	HEC	C4D-CHA	-2.01	1.35	1.41
18	P	3004	CDL	OA8-CA6	-2.01	1.40	1.45
12	C	502	HEM	C4B-NB	2.01	1.40	1.36
15	C	2007	PEE	P-O4P	2.01	1.67	1.59
15	E	2005	PEE	C11-C10	2.01	1.56	1.50
18	P	3004	CDL	OA6-CA5	2.00	1.40	1.34

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	3001	SMA	C9-C2-C3	6.58	129.72	120.39
13	C	2001	SMA	C9-C2-C3	6.55	129.68	120.39
17	D	501	HEC	CBA-CAA-C2A	5.89	123.33	112.48
17	Q	501	HEC	CBA-CAA-C2A	5.27	122.19	112.48
13	C	2001	SMA	C3-C4-C4A	-5.17	115.38	120.58
13	P	3001	SMA	C3-C4-C4A	-4.69	115.86	120.58
12	C	501	HEM	CBA-CAA-C2A	-4.66	103.89	112.49
13	P	3001	SMA	C9-C10-C11	-4.23	109.03	114.72
13	C	2001	SMA	C9-C10-C11	-4.05	109.26	114.72
12	C	502	HEM	C1D-C2D-C3D	3.88	109.69	107.00
13	C	2001	SMA	O7-C7-C8	3.68	118.25	114.54
13	C	2001	SMA	C4-C3-C2	3.60	120.58	116.63
18	P	3004	CDL	CB4-OB6-CB5	-3.46	109.27	117.79
12	P	501	HEM	CBA-CAA-C2A	-3.43	106.16	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	3001	SMA	C4-C3-C2	3.38	120.33	116.63
18	G	2004	CDL	CB4-OB6-CB5	-3.37	109.48	117.79
13	P	3001	SMA	O1-C2-C9	-3.30	108.00	111.91
13	C	2001	SMA	O1-C2-C9	-3.26	108.05	111.91
12	P	502	HEM	C4C-C3C-C2C	-3.23	104.64	106.90
14	P	3002	UQ	C8-C7-C6	3.02	120.18	112.05
14	C	2002	UQ	C8-C7-C6	3.01	120.15	112.05
12	C	501	HEM	CBD-CAD-C3D	2.99	117.99	112.48
15	C	2007	PEE	C20-C19-C18	2.93	129.31	114.42
15	E	2005	PEE	C20-C19-C18	2.89	129.12	114.42
15	P	3007	PEE	C19-C18-C17	2.86	128.97	114.42
15	R	3005	PEE	C20-C19-C18	2.85	128.92	114.42
15	C	2007	PEE	C19-C18-C17	2.85	128.87	114.42
12	C	502	HEM	CBA-CAA-C2A	2.83	117.71	112.49
12	C	502	HEM	C4C-C3C-C2C	-2.81	104.94	106.90
15	P	3007	PEE	C20-C19-C18	2.80	128.62	114.42
13	C	2001	SMA	C10-C9-C2	2.78	119.57	113.59
17	D	501	HEC	CAA-C2A-C3A	-2.77	119.29	127.25
12	P	502	HEM	CMB-C2B-C3B	2.76	129.85	124.68
18	D	2003	CDL	CA6-CA4-CA3	-2.73	105.33	111.79
13	P	3001	SMA	C10-C9-C2	2.71	119.41	113.59
14	P	3002	UQ	C7-C6-C1	-2.66	115.28	118.48
12	P	502	HEM	C1D-C2D-C3D	2.64	108.83	107.00
15	C	2007	PEE	C23-C22-C21	2.62	127.71	114.42
18	S	3003	CDL	CA6-CA4-CA3	-2.61	105.61	111.79
12	C	502	HEM	C4A-C3A-C2A	-2.60	105.19	107.00
17	Q	501	HEC	CAA-C2A-C3A	-2.59	119.80	127.25
15	E	2005	PEE	C22-C21-C20	2.59	127.58	114.42
13	P	3001	SMA	O7-C7-C8	2.59	117.15	114.54
15	P	3007	PEE	C23-C22-C21	2.57	127.48	114.42
15	R	3005	PEE	C19-C18-C17	2.56	127.44	114.42
15	R	3005	PEE	C23-C22-C21	2.56	127.42	114.42
15	C	2007	PEE	C22-C21-C20	2.56	127.40	114.42
12	P	502	HEM	CBA-CAA-C2A	2.55	117.18	112.49
15	E	2005	PEE	C23-C22-C21	2.53	127.29	114.42
12	P	502	HEM	CMD-C2D-C1D	-2.53	124.57	128.46
12	P	501	HEM	CBD-CAD-C3D	2.52	117.12	112.48
15	R	3005	PEE	C22-C21-C20	2.52	127.20	114.42
15	P	3007	PEE	C22-C21-C20	2.51	127.19	114.42
18	D	2003	CDL	CB4-OB6-CB5	-2.49	111.66	117.79
14	C	2002	UQ	C7-C6-C1	-2.49	115.49	118.48
15	E	2005	PEE	C19-C18-C17	2.47	126.98	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	501	HEM	CMC-C2C-C3C	2.47	129.29	124.68
17	D	501	HEC	CBD-CAD-C3D	2.41	116.94	112.49
18	G	2004	CDL	OB6-CB4-CB3	2.40	117.10	108.40
18	P	3004	CDL	OB6-CB4-CB3	2.35	116.92	108.40
12	C	502	HEM	CMB-C2B-C3B	2.34	129.06	124.68
18	G	2004	CDL	CB6-CB4-CB3	-2.33	106.29	111.79
13	C	2001	SMA	C7-C8-C8A	-2.31	118.15	120.18
12	C	501	HEM	C3B-C4B-NB	2.30	112.18	109.21
15	E	2005	PEE	O3-C3-C2	2.29	115.10	108.43
15	C	2007	PEE	O3-C3-C2	2.28	115.07	108.43
18	P	3004	CDL	CB6-CB4-CB3	-2.28	106.39	111.79
12	C	501	HEM	CMC-C2C-C3C	2.26	128.91	124.68
18	S	3003	CDL	CB4-OB6-CB5	-2.24	112.27	117.79
15	R	3005	PEE	O3-C3-C2	2.24	114.95	108.43
18	P	3004	CDL	CA6-CA4-CA3	-2.23	106.51	111.79
12	C	502	HEM	CMA-C3A-C2A	2.13	128.96	124.94
18	G	2004	CDL	CA6-CA4-CA3	-2.11	106.81	111.79
12	P	501	HEM	C3B-C4B-NB	2.09	111.92	109.21
17	Q	501	HEC	CBD-CAD-C3D	2.09	116.33	112.49
12	C	502	HEM	CMD-C2D-C1D	-2.08	125.26	128.46
12	P	502	HEM	C3B-C4B-NB	2.04	111.85	109.21

There are no chirality outliers.

All (253) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	E	2009	PLC	O4P-C4-C5-N
20	E	2009	PLC	C1'-C'-O2-C2
17	Q	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
20	R	3009	PLC	O4P-C4-C5-N
20	R	3009	PLC	C1'-C'-O2-C2
12	P	502	HEM	C4D-C3D-CAD-CBD
12	C	502	HEM	C4D-C3D-CAD-CBD
15	R	3005	PEE	O4P-C4-C5-N
15	R	3005	PEE	C11-C10-O2-C2
15	R	3005	PEE	C1-O3P-P-O1P
18	D	2003	CDL	O1-C1-CB2-OB2
18	D	2003	CDL	OA6-CA4-CA6-OA8
18	D	2003	CDL	CB2-OB2-PB2-OB4
18	D	2003	CDL	CB2-OB2-PB2-OB5
14	C	2002	UQ	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	C	2002	UQ	C5-C6-C7-C8
15	C	2008	PEE	C1-O3P-P-O1P
15	C	2008	PEE	C1-O3P-P-O2P
18	S	3003	CDL	O1-C1-CB2-OB2
18	S	3003	CDL	OA6-CA4-CA6-OA8
18	S	3003	CDL	CB2-OB2-PB2-OB4
18	S	3003	CDL	CB2-OB2-PB2-OB5
18	P	3004	CDL	CA3-OA5-PA1-OA3
18	P	3004	CDL	OB5-CB3-CB4-OB6
18	P	3004	CDL	C51-CB5-OB6-CB4
16	C	2011	GOL	C1-C2-C3-O3
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8
15	E	2005	PEE	O4P-C4-C5-N
15	E	2005	PEE	C11-C10-O2-C2
15	E	2005	PEE	C1-O3P-P-O1P
15	E	2005	PEE	C1-O3P-P-O4P
17	D	501	HEC	C1A-C2A-CAA-CBA
17	D	501	HEC	C3A-C2A-CAA-CBA
18	G	2004	CDL	CA3-OA5-PA1-OA3
18	G	2004	CDL	OB5-CB3-CB4-OB6
18	G	2004	CDL	C51-CB5-OB6-CB4
15	R	3005	PEE	O5-C30-O3-C3
15	E	2005	PEE	O5-C30-O3-C3
15	R	3005	PEE	C31-C30-O3-C3
15	E	2005	PEE	C31-C30-O3-C3
18	S	3003	CDL	C31-CA7-OA8-CA6
20	E	2009	PLC	O'-C'-O2-C2
20	R	3009	PLC	O'-C'-O2-C2
15	R	3005	PEE	O4-C10-O2-C2
18	P	3004	CDL	OB7-CB5-OB6-CB4
15	E	2005	PEE	O4-C10-O2-C2
18	G	2004	CDL	OB7-CB5-OB6-CB4
18	D	2003	CDL	C31-CA7-OA8-CA6
15	C	2008	PEE	C31-C30-O3-C3
18	P	3004	CDL	C71-CB7-OB8-CB6
18	P	3004	CDL	O1-C1-CA2-OA2
18	G	2004	CDL	O1-C1-CA2-OA2
18	G	2004	CDL	C71-CB7-OB8-CB6
15	C	2008	PEE	O5-C30-O3-C3
18	S	3003	CDL	OA9-CA7-OA8-CA6
18	P	3004	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
18	G	2004	CDL	OB9-CB7-OB8-CB6
18	P	3004	CDL	C31-CA7-OA8-CA6
18	D	2003	CDL	OA9-CA7-OA8-CA6
18	G	2004	CDL	C31-CA7-OA8-CA6
18	P	3004	CDL	CB2-C1-CA2-OA2
18	G	2004	CDL	CB2-C1-CA2-OA2
18	P	3004	CDL	OA9-CA7-OA8-CA6
15	R	3005	PEE	C30-C31-C32-C33
15	E	2005	PEE	C30-C31-C32-C33
18	D	2003	CDL	CA5-C11-C12-C13
18	S	3003	CDL	CA5-C11-C12-C13
18	G	2004	CDL	OA9-CA7-OA8-CA6
13	P	3001	SMA	C6-C7-O7-C7M
20	R	3009	PLC	C'-C1'-C2'-C3'
13	C	2001	SMA	C6-C7-O7-C7M
15	P	3007	PEE	C1-O3P-P-O4P
15	C	2008	PEE	C1-O3P-P-O4P
18	P	3004	CDL	CA3-OA5-PA1-OA2
18	G	2004	CDL	CA3-OA5-PA1-OA2
15	E	2005	PEE	C10-C11-C12-C13
15	R	3005	PEE	C10-C11-C12-C13
18	D	2003	CDL	CA2-C1-CB2-OB2
18	S	3003	CDL	CA2-C1-CB2-OB2
15	C	2007	PEE	C12-C13-C14-C15
15	P	3007	PEE	C34-C35-C36-C37
15	C	2007	PEE	C32-C33-C34-C35
18	D	2003	CDL	C15-C16-C17-C18
15	E	2005	PEE	C40-C41-C42-C43
15	P	3007	PEE	C12-C13-C14-C15
15	C	2007	PEE	C34-C35-C36-C37
18	S	3003	CDL	C15-C16-C17-C18
20	E	2009	PLC	C'-C1'-C2'-C3'
15	R	3005	PEE	C40-C41-C42-C43
15	E	2005	PEE	C39-C40-C41-C42
15	P	3007	PEE	C18-C19-C20-C21
15	C	2007	PEE	C39-C40-C41-C42
15	E	2005	PEE	C23-C24-C25-C26
15	C	2007	PEE	C18-C19-C20-C21
18	P	3004	CDL	C11-CA5-OA6-CA4
15	R	3005	PEE	C13-C14-C15-C16
15	E	2005	PEE	C13-C14-C15-C16
15	E	2005	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	C32-C33-C34-C35
15	P	3007	PEE	C39-C40-C41-C42
15	R	3005	PEE	C23-C24-C25-C26
15	R	3005	PEE	C39-C40-C41-C42
15	R	3005	PEE	C17-C18-C19-C20
18	S	3003	CDL	C71-CB7-OB8-CB6
18	P	3004	CDL	OA7-CA5-OA6-CA4
20	R	3009	PLC	C1B-CB-O3-C3
18	G	2004	CDL	C11-CA5-OA6-CA4
20	E	2009	PLC	C1B-CB-O3-C3
18	G	2004	CDL	OA7-CA5-OA6-CA4
18	S	3003	CDL	OB9-CB7-OB8-CB6
18	S	3003	CDL	CB7-C71-C72-C73
20	E	2009	PLC	OB-CB-O3-C3
20	R	3009	PLC	OB-CB-O3-C3
13	P	3001	SMA	C8-C7-O7-C7M
18	D	2003	CDL	C71-CB7-OB8-CB6
15	C	2008	PEE	C11-C10-O2-C2
15	P	3007	PEE	O3P-C1-C2-O2
18	D	2003	CDL	C13-C14-C15-C16
18	D	2003	CDL	C16-C17-C18-C19
20	E	2009	PLC	C2'-C3'-C4'-C5'
13	C	2001	SMA	C8-C7-O7-C7M
15	C	2008	PEE	O4-C10-O2-C2
15	R	3005	PEE	C1-O3P-P-O4P
18	D	2003	CDL	OA5-CA3-CA4-CA6
18	S	3003	CDL	OA5-CA3-CA4-CA6
18	S	3003	CDL	C13-C14-C15-C16
15	P	3007	PEE	C42-C43-C44-C45
18	D	2003	CDL	OB9-CB7-OB8-CB6
20	R	3009	PLC	C2'-C3'-C4'-C5'
18	S	3003	CDL	C16-C17-C18-C19
18	D	2003	CDL	CA3-CA4-CA6-OA8
18	S	3003	CDL	CA3-CA4-CA6-OA8
18	D	2003	CDL	CB7-C71-C72-C73
18	D	2003	CDL	C71-C72-C73-C74
20	R	3009	PLC	C4'-C5'-C6'-C7'
18	S	3003	CDL	C71-C72-C73-C74
15	C	2007	PEE	O3P-C1-C2-O2
15	C	2007	PEE	C15-C16-C17-C18
20	E	2009	PLC	C4'-C5'-C6'-C7'
15	C	2007	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	C17-C18-C19-C20
15	C	2007	PEE	C30-C31-C32-C33
15	C	2007	PEE	C17-C18-C19-C20
20	E	2009	PLC	O3P-C1-C2-C3
20	R	3009	PLC	O3P-C1-C2-C3
15	C	2008	PEE	O3P-C1-C2-C3
15	E	2005	PEE	C42-C43-C44-C45
15	C	2007	PEE	C33-C34-C35-C36
15	R	3005	PEE	C42-C43-C44-C45
15	P	3007	PEE	C15-C16-C17-C18
15	P	3007	PEE	C33-C34-C35-C36
18	P	3004	CDL	CA3-CA4-CA6-OA8
18	P	3004	CDL	CB3-CB4-CB6-OB8
18	G	2004	CDL	CB3-CB4-CB6-OB8
15	E	2005	PEE	C15-C16-C17-C18
15	C	2007	PEE	C1-O3P-P-O4P
15	P	3007	PEE	C43-C44-C45-C46
18	P	3004	CDL	OB6-CB4-CB6-OB8
18	G	2004	CDL	OB6-CB4-CB6-OB8
15	E	2005	PEE	C12-C13-C14-C15
15	C	2007	PEE	C43-C44-C45-C46
15	C	2007	PEE	C38-C39-C40-C41
15	R	3005	PEE	C12-C13-C14-C15
15	R	3005	PEE	C15-C16-C17-C18
15	P	3007	PEE	O3P-C1-C2-C3
18	P	3004	CDL	OB5-CB3-CB4-CB6
15	P	3007	PEE	C38-C39-C40-C41
15	C	2007	PEE	C20-C21-C22-C23
18	G	2004	CDL	CA3-CA4-CA6-OA8
20	E	2009	PLC	O3P-C1-C2-O2
20	R	3009	PLC	O3P-C1-C2-O2
15	E	2005	PEE	C31-C32-C33-C34
18	G	2004	CDL	CA2-C1-CB2-OB2
18	P	3004	CDL	OA6-CA4-CA6-OA8
15	E	2005	PEE	C2-C3-O3-C30
15	P	3007	PEE	C4-O4P-P-O3P
15	C	2007	PEE	C4-O4P-P-O3P
18	D	2003	CDL	C1-CA2-OA2-PA1
18	S	3003	CDL	C1-CA2-OA2-PA1
15	P	3007	PEE	C1-O3P-P-O2P
15	C	2007	PEE	C1-O3P-P-O2P
18	D	2003	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
18	S	3003	CDL	CB2-OB2-PB2-OB3
18	P	3004	CDL	CA3-OA5-PA1-OA4
18	G	2004	CDL	CA3-OA5-PA1-OA4
18	G	2004	CDL	OB5-CB3-CB4-CB6
15	C	2007	PEE	C13-C14-C15-C16
18	D	2003	CDL	OA5-CA3-CA4-OA6
18	S	3003	CDL	OA5-CA3-CA4-OA6
13	P	3001	SMA	C15-C14-O14-C25
15	P	3007	PEE	C20-C21-C22-C23
12	P	502	HEM	C2D-C3D-CAD-CBD
12	C	502	HEM	C2D-C3D-CAD-CBD
18	G	2004	CDL	OA6-CA4-CA6-OA8
15	P	3007	PEE	C13-C14-C15-C16
15	R	3005	PEE	C31-C32-C33-C34
15	R	3005	PEE	C1-C2-O2-C10
15	E	2005	PEE	C1-C2-O2-C10
15	R	3005	PEE	C2-C1-O3P-P
15	R	3005	PEE	C2-C3-O3-C30
20	E	2009	PLC	C1-O3P-P-O4P
20	E	2009	PLC	C4-O4P-P-O3P
20	R	3009	PLC	C1-O3P-P-O4P
20	R	3009	PLC	C4-O4P-P-O3P
18	D	2003	CDL	CA2-OA2-PA1-OA5
18	S	3003	CDL	CA2-OA2-PA1-OA5
15	R	3005	PEE	C35-C36-C37-C38
15	E	2005	PEE	C2-C1-O3P-P
18	P	3004	CDL	CA2-C1-CB2-OB2
15	R	3005	PEE	C33-C34-C35-C36
15	C	2007	PEE	O3P-C1-C2-C3
15	E	2005	PEE	C37-C38-C39-C40
18	G	2004	CDL	O1-C1-CB2-OB2
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10
15	E	2005	PEE	C35-C36-C37-C38
16	C	2011	GOL	O2-C2-C3-O3
15	P	3007	PEE	C31-C30-O3-C3
15	P	3007	PEE	O5-C30-O3-C3
20	E	2009	PLC	C2B-C1B-CB-O3
20	R	3009	PLC	C2B-C1B-CB-O3
13	C	2001	SMA	C15-C14-O14-C25
18	D	2003	CDL	C12-C11-CA5-OA6
18	S	3003	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C30-C31-C32-C33
20	E	2009	PLC	C2B-C1B-CB-OB
18	S	3003	CDL	C72-C71-CB7-OB8
15	C	2008	PEE	O3-C30-C31-C32
20	R	3009	PLC	C2B-C1B-CB-OB
20	E	2009	PLC	C3'-C4'-C5'-C6'
15	P	3007	PEE	O3-C30-C31-C32
15	C	2007	PEE	O3-C30-C31-C32
13	P	3001	SMA	C3-C2-C9-C10
15	P	3007	PEE	O2-C10-C11-C12
15	E	2005	PEE	C22-C23-C24-C25
15	P	3007	PEE	C1-O3P-P-O1P
15	R	3005	PEE	C37-C38-C39-C40
18	D	2003	CDL	C72-C71-CB7-OB8
18	S	3003	CDL	C72-C71-CB7-OB9
15	P	3007	PEE	C5-C4-O4P-P
15	C	2007	PEE	C5-C4-O4P-P
18	D	2003	CDL	C12-C11-CA5-OA7
18	S	3003	CDL	C12-C11-CA5-OA7
15	C	2007	PEE	O2-C10-C11-C12
18	P	3004	CDL	C1-CB2-OB2-PB2
15	P	3007	PEE	O4-C10-C11-C12
15	P	3007	PEE	O5-C30-C31-C32
15	C	2007	PEE	O5-C30-C31-C32
18	D	2003	CDL	C72-C71-CB7-OB9
15	C	2007	PEE	O4-C10-C11-C12

There are no ring outliers.

22 monomers are involved in 62 short contacts:

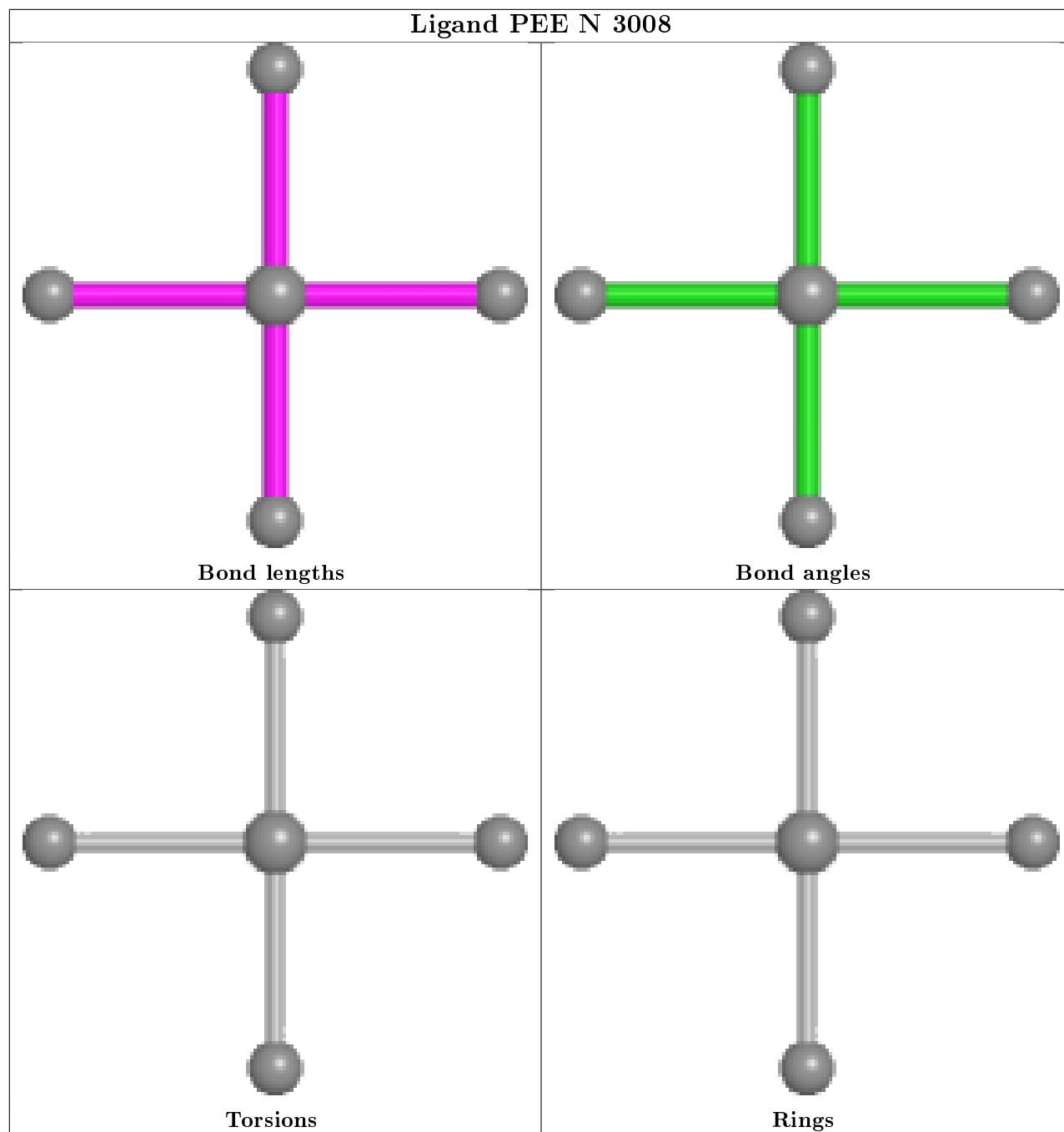
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	E	2009	PLC	3	0
15	R	3005	PEE	4	0
17	Q	501	HEC	1	0
20	R	3009	PLC	2	0
12	P	502	HEM	6	0
12	C	502	HEM	6	0
15	P	3007	PEE	1	0
12	P	501	HEM	5	0
17	D	501	HEC	1	0
16	P	3011	GOL	1	0

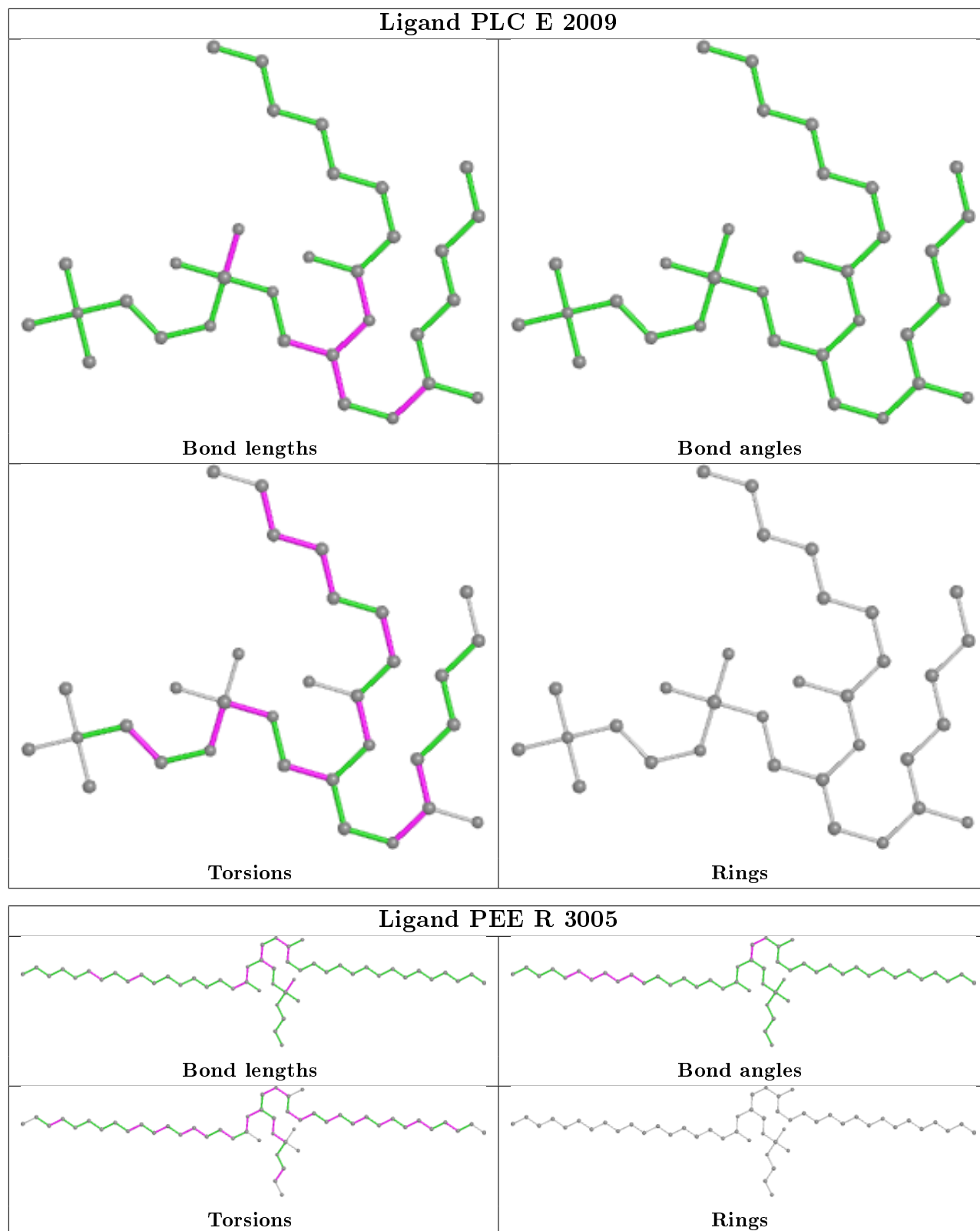
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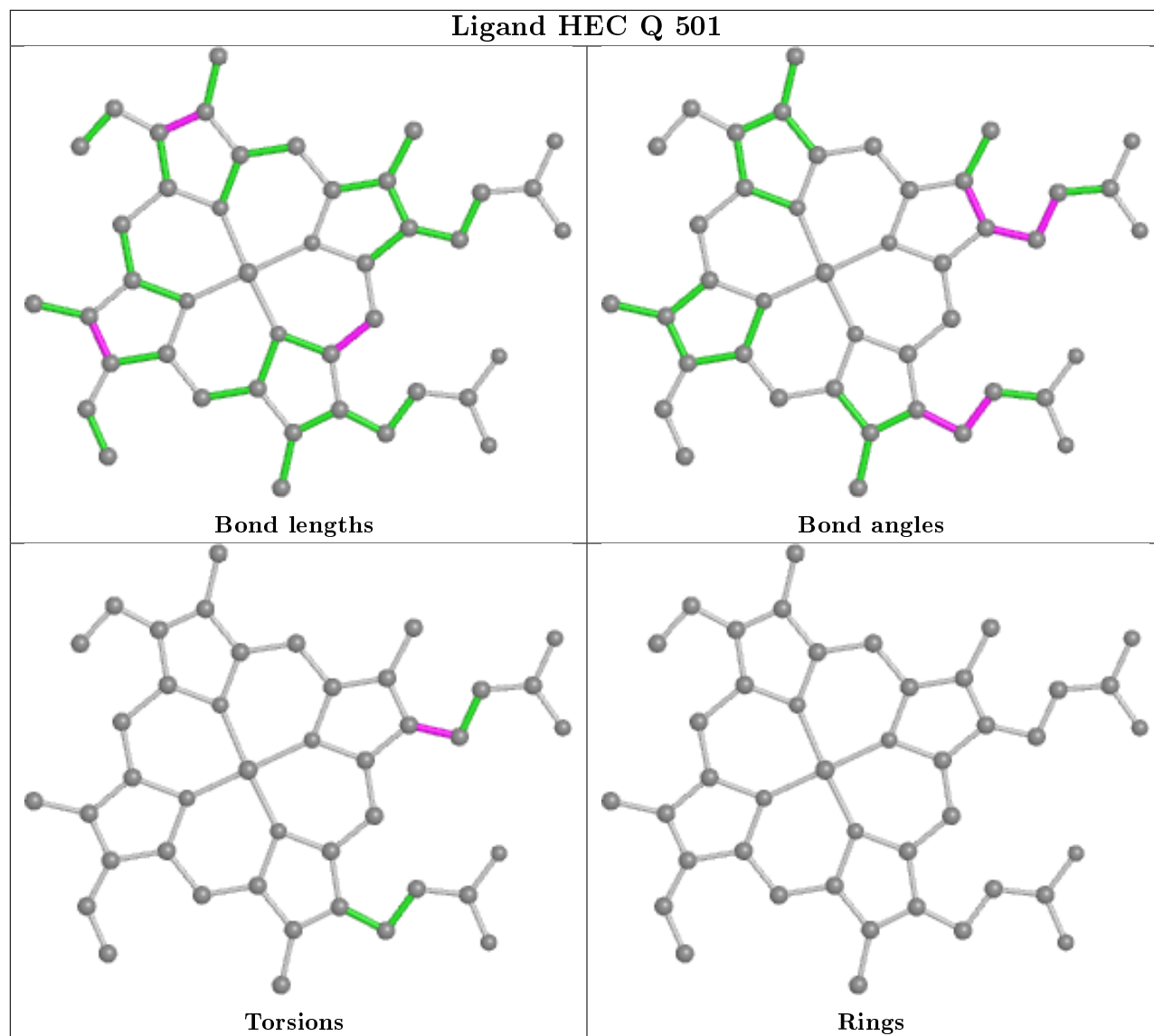
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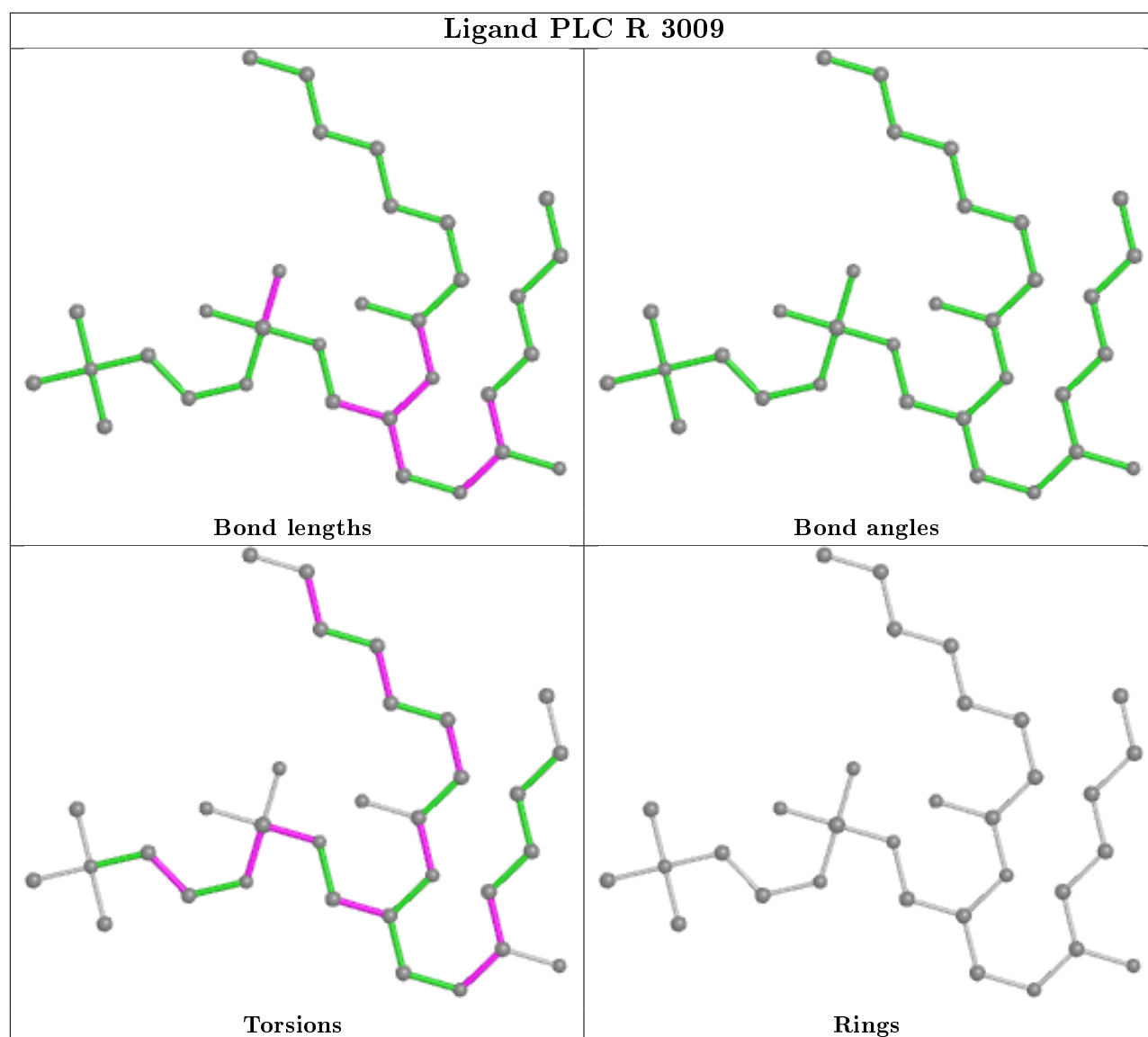
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	2007	PEE	1	0
18	D	2003	CDL	1	0
14	C	2002	UQ	5	0
18	S	3003	CDL	2	0
18	P	3004	CDL	3	0
13	P	3001	SMA	4	0
14	P	3002	UQ	1	0
12	C	501	HEM	5	0
13	C	2001	SMA	4	0
15	E	2005	PEE	4	0
18	G	2004	CDL	1	0
19	R	501	FES	1	0

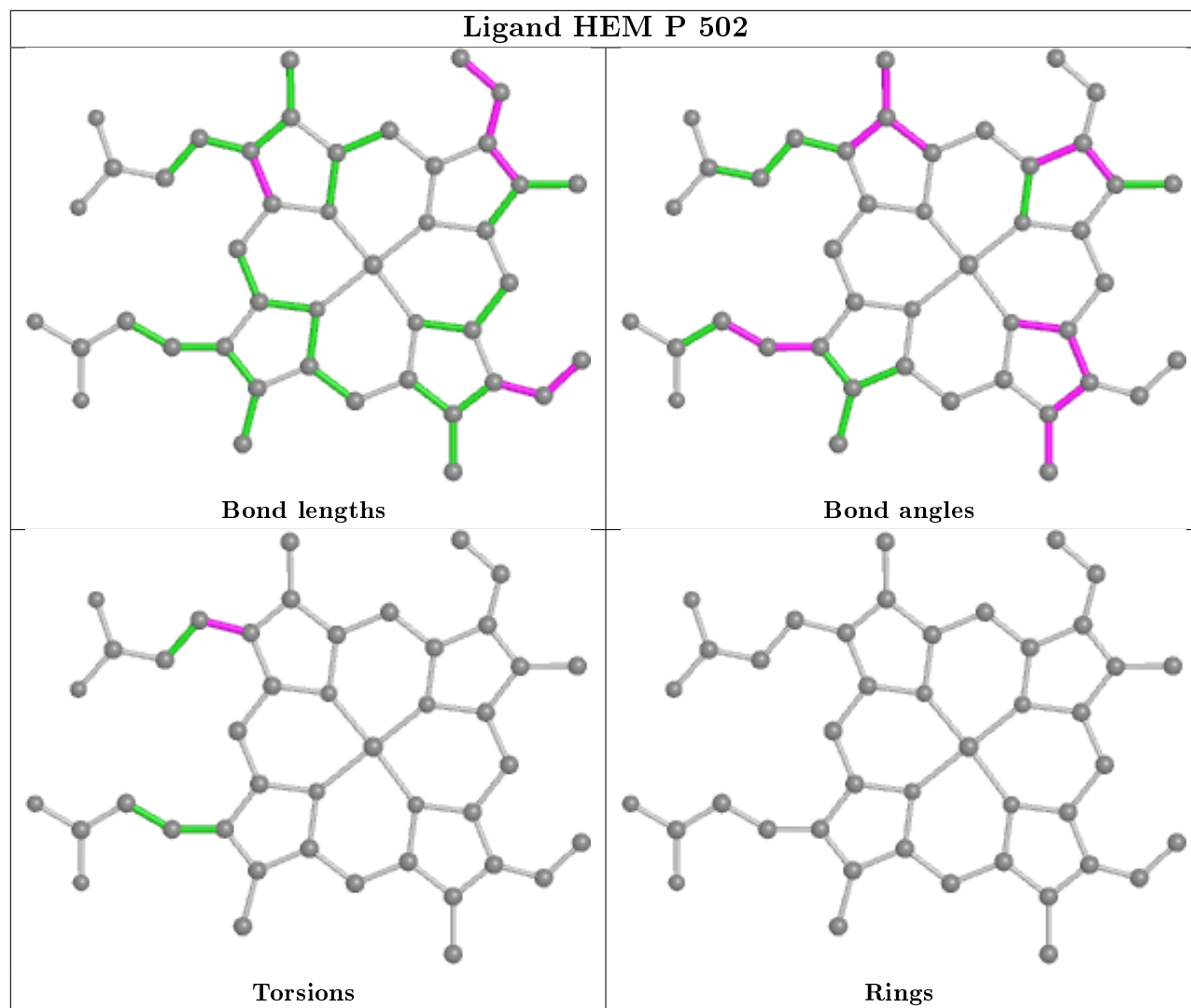
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



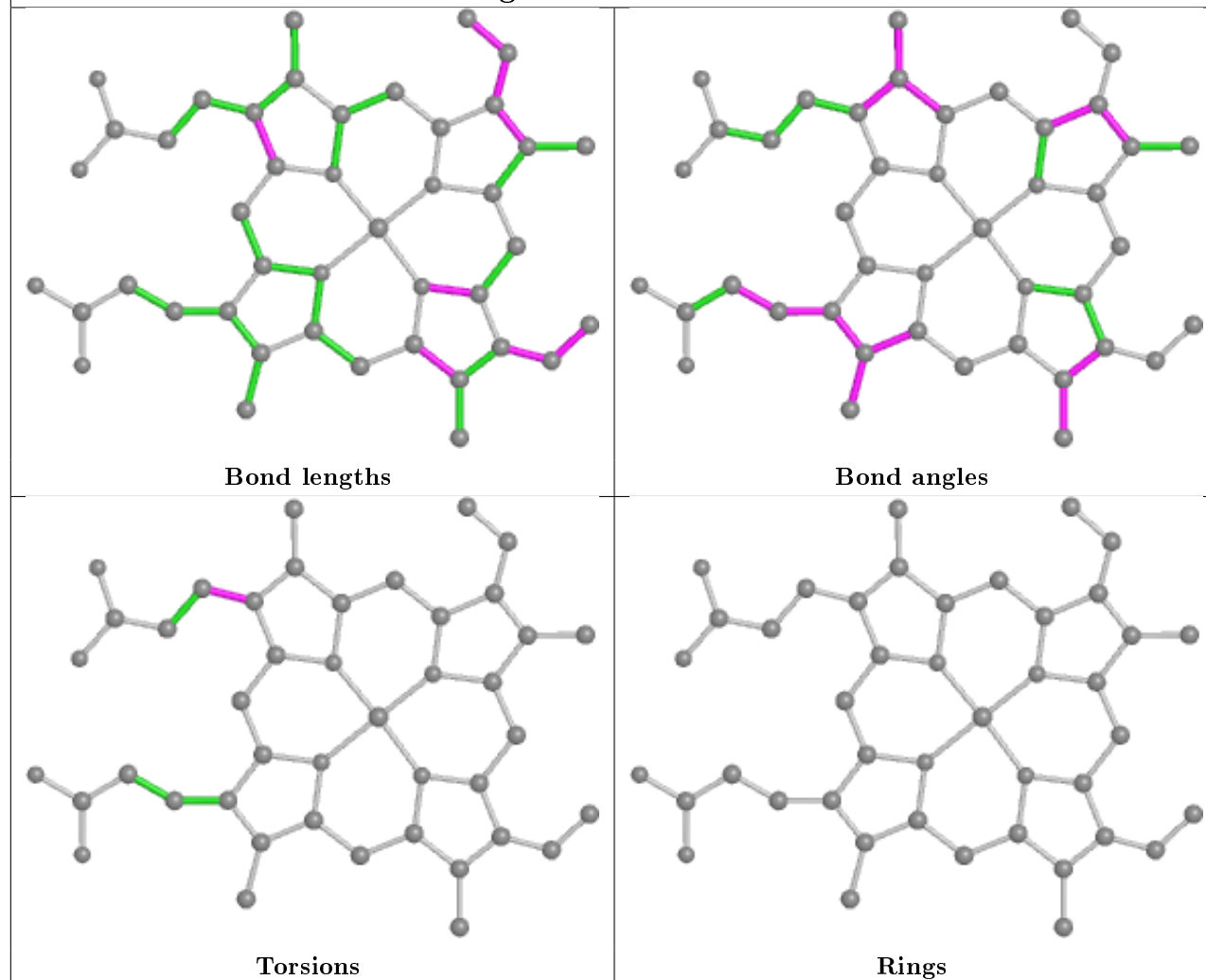




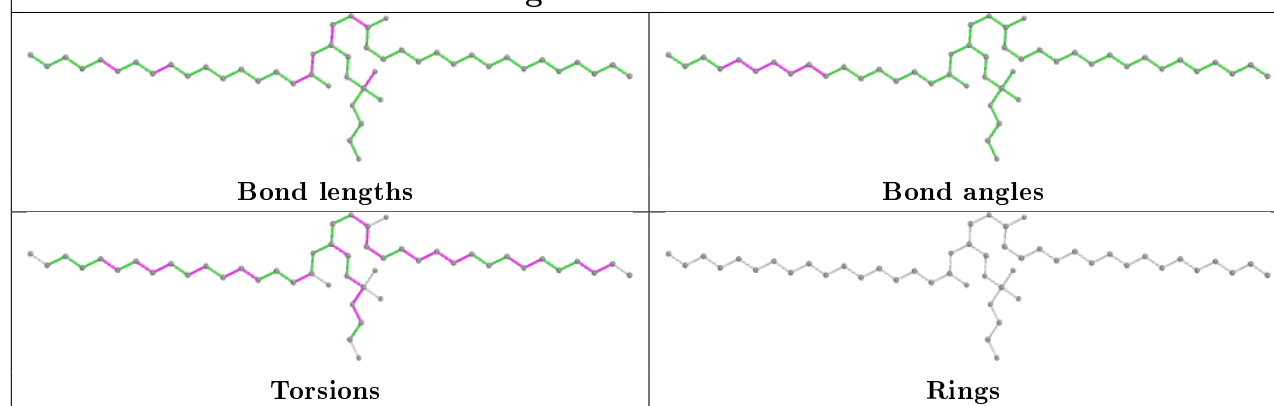


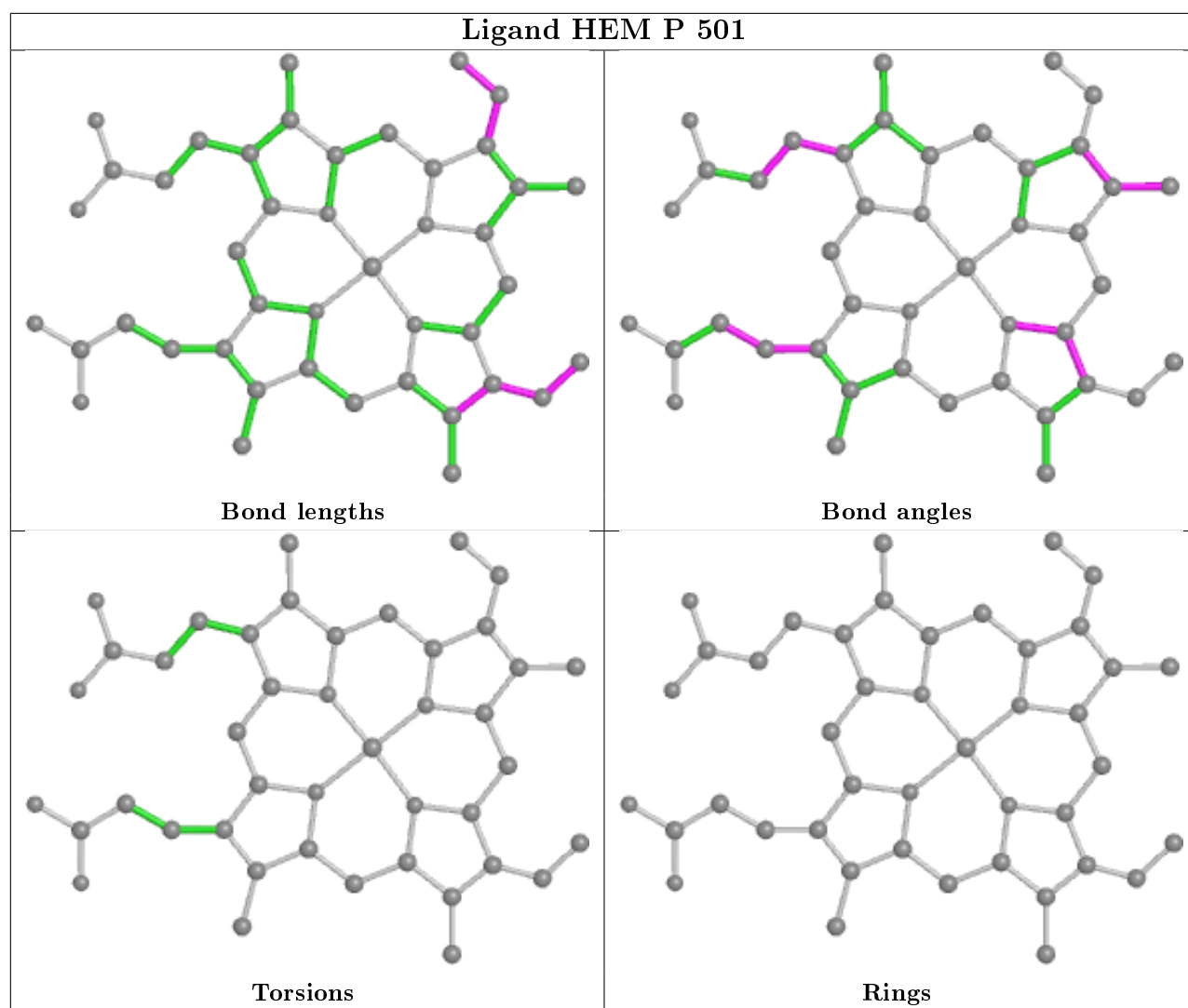


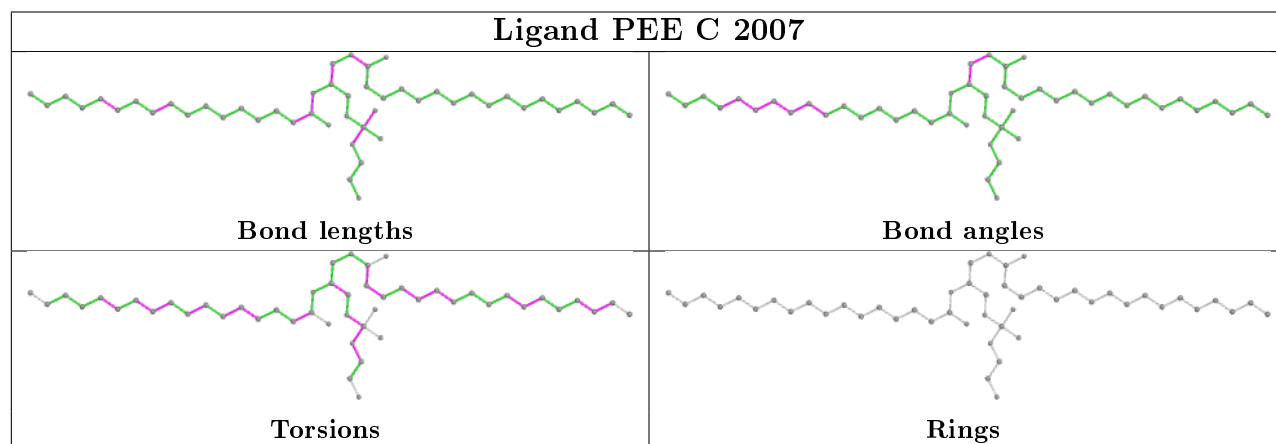
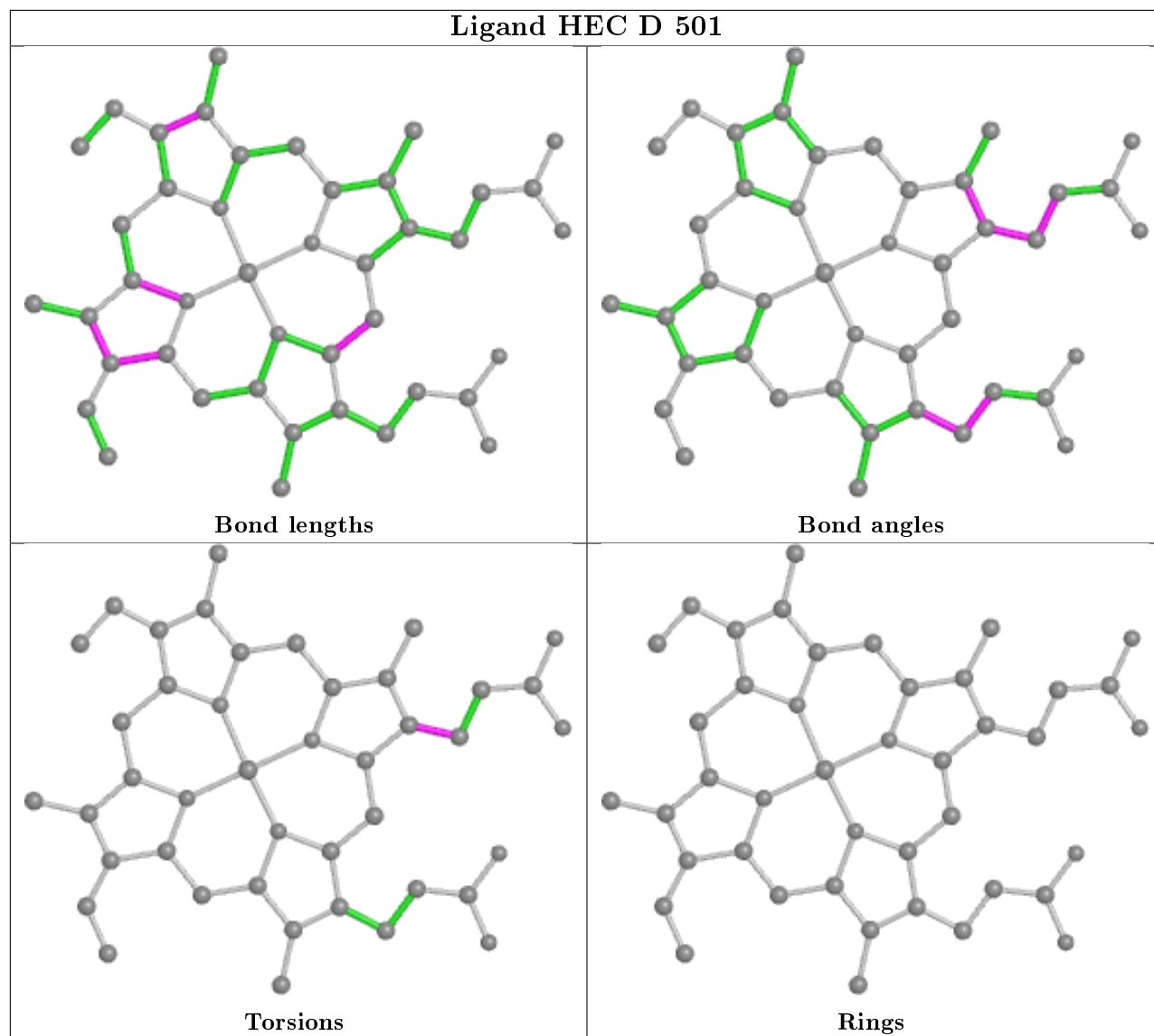
Ligand HEM C 502



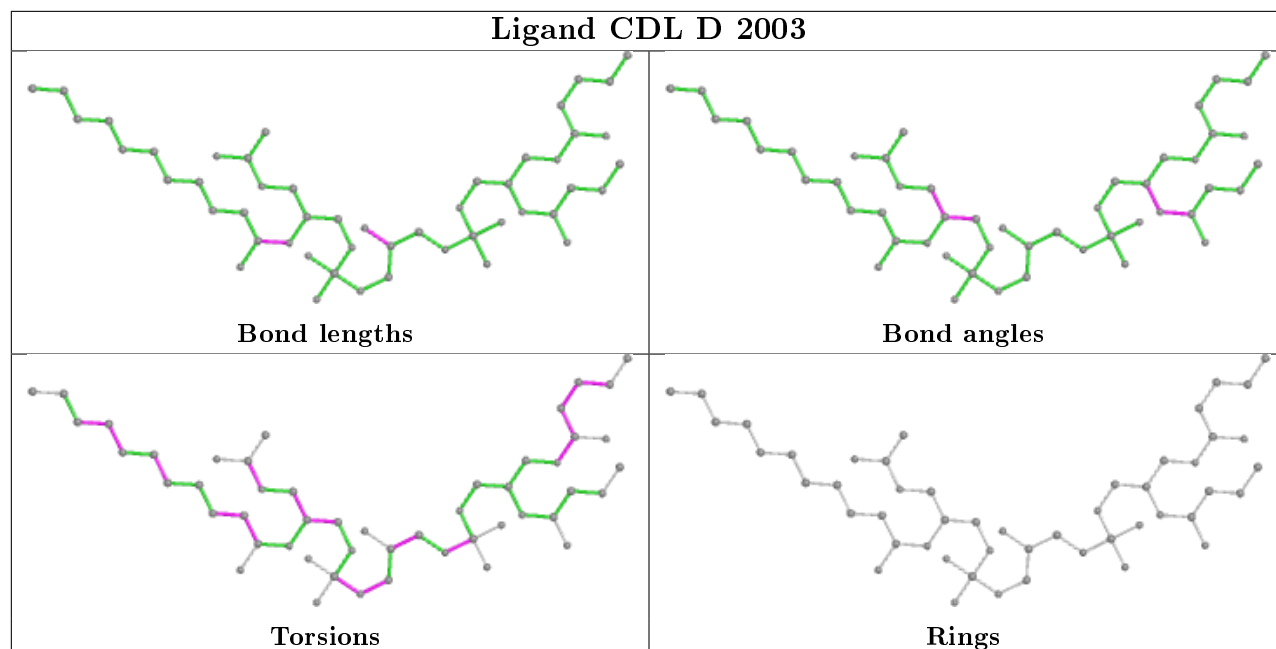
Ligand PEE P 3007



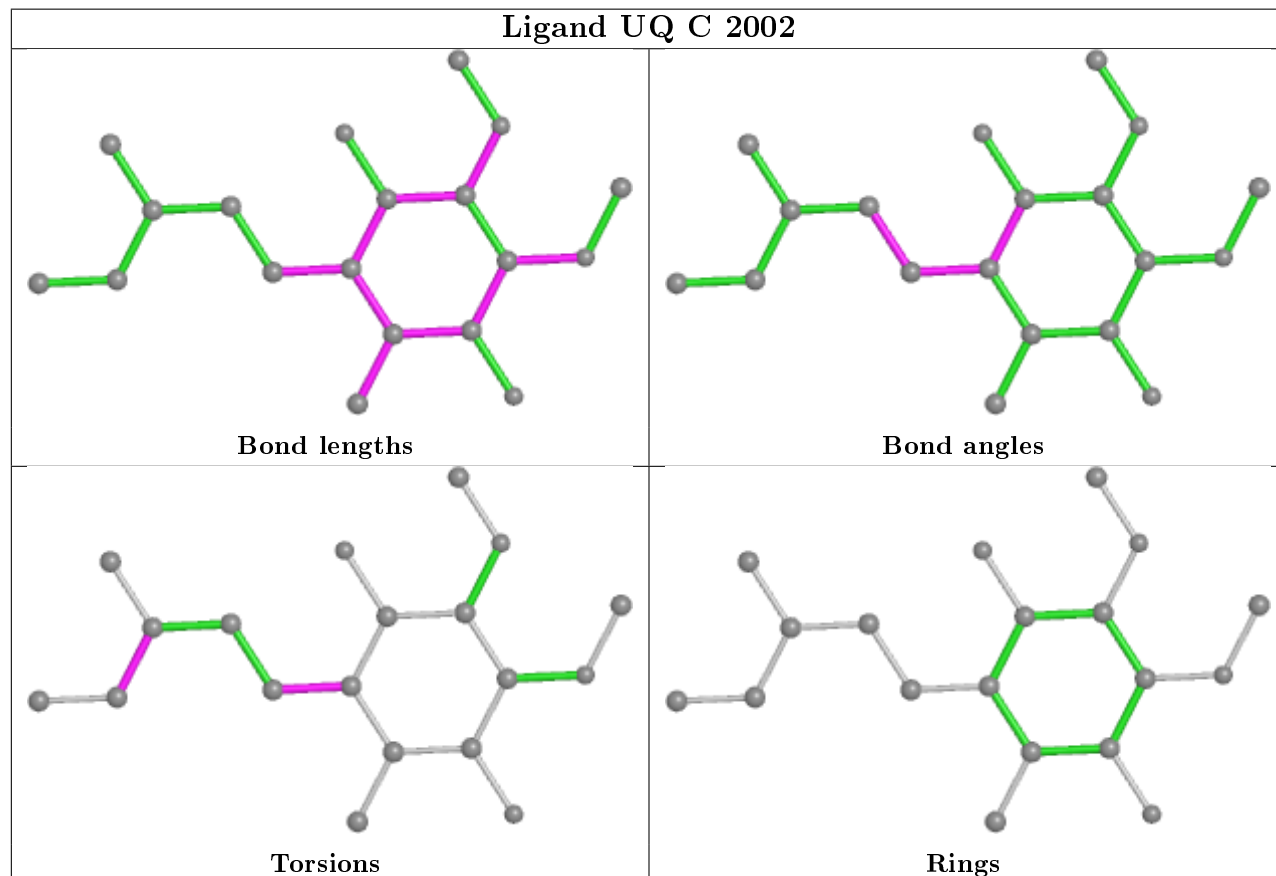


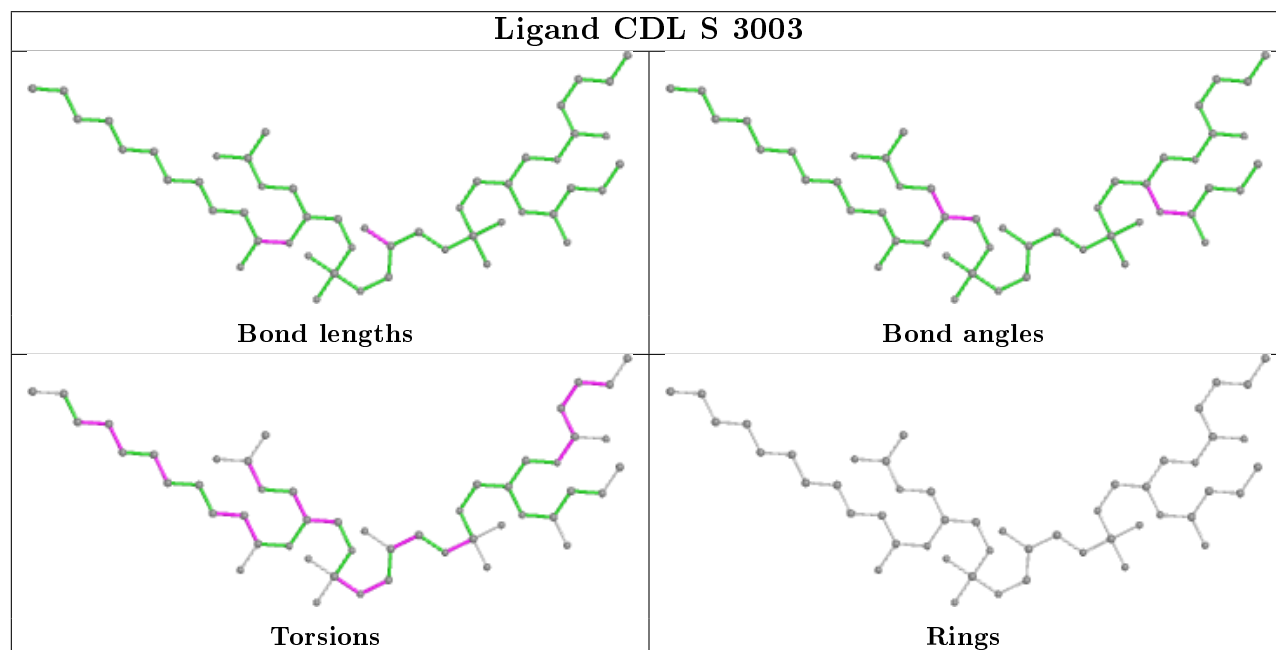
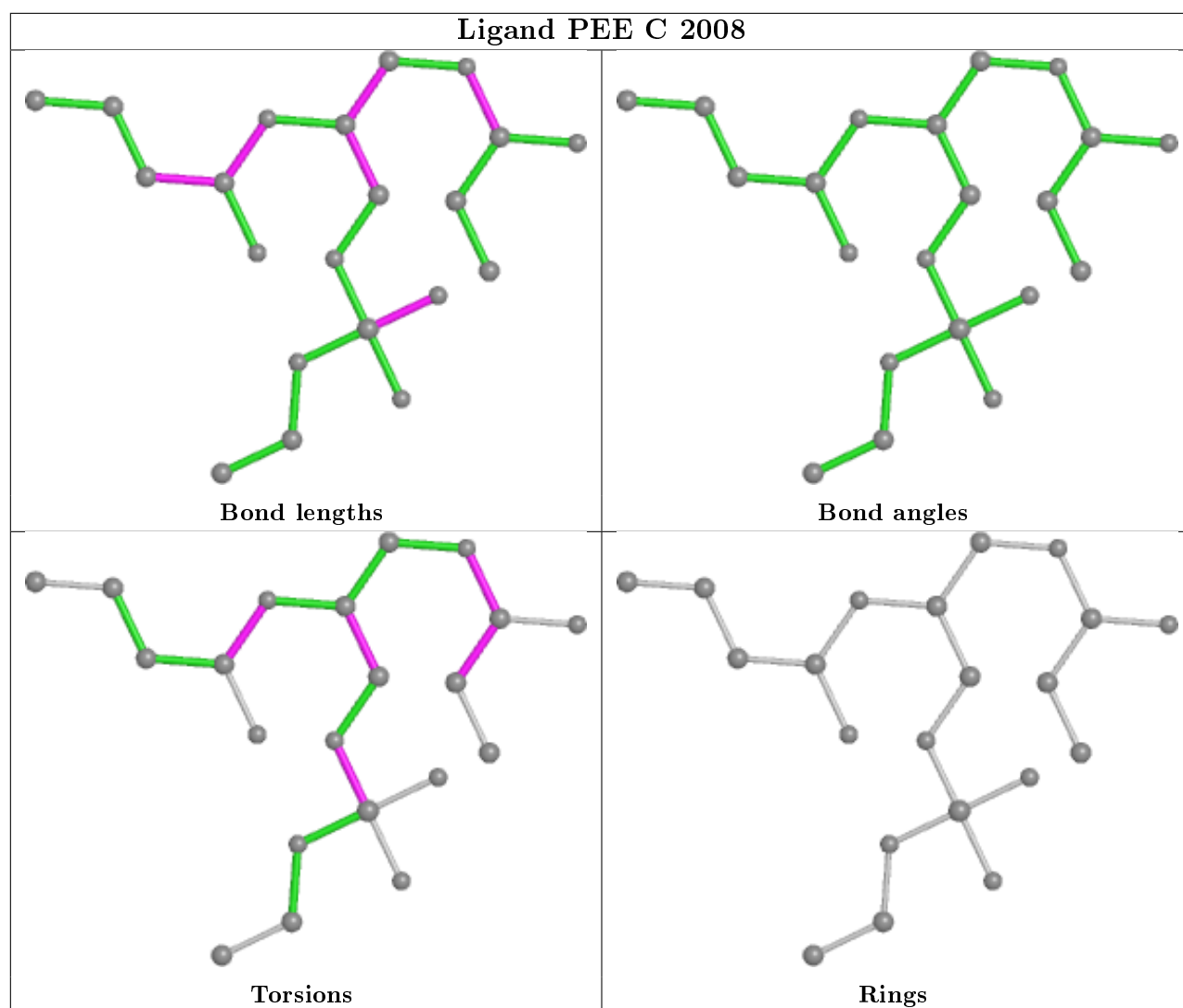


Ligand CDL D 2003

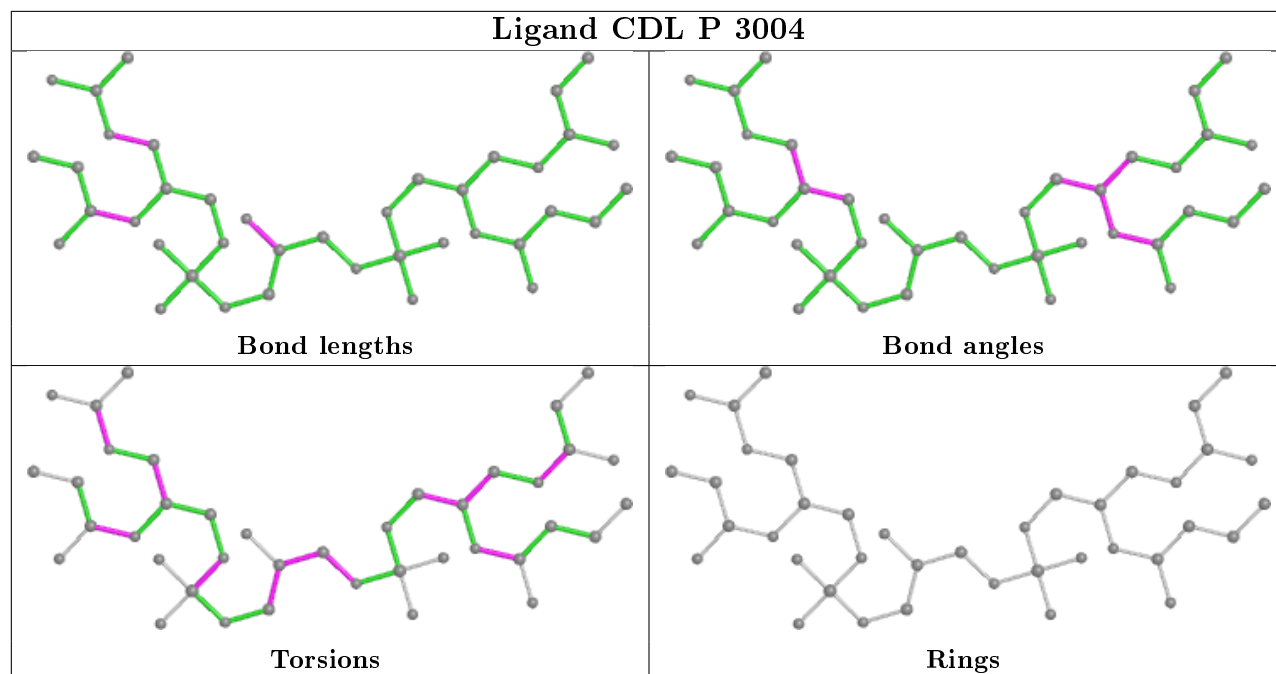


Ligand UQ C 2002

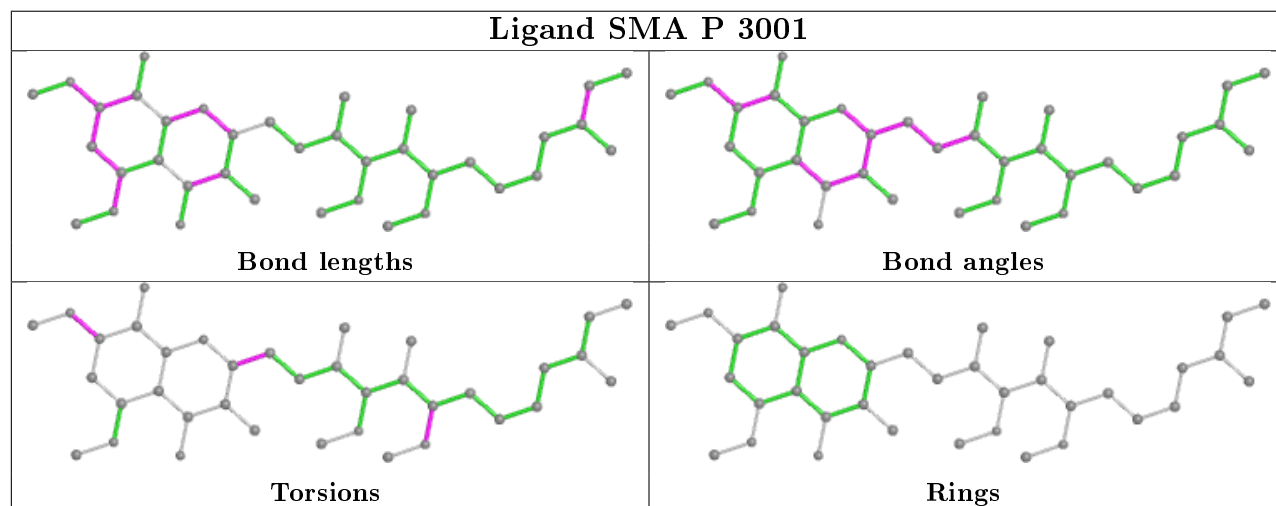


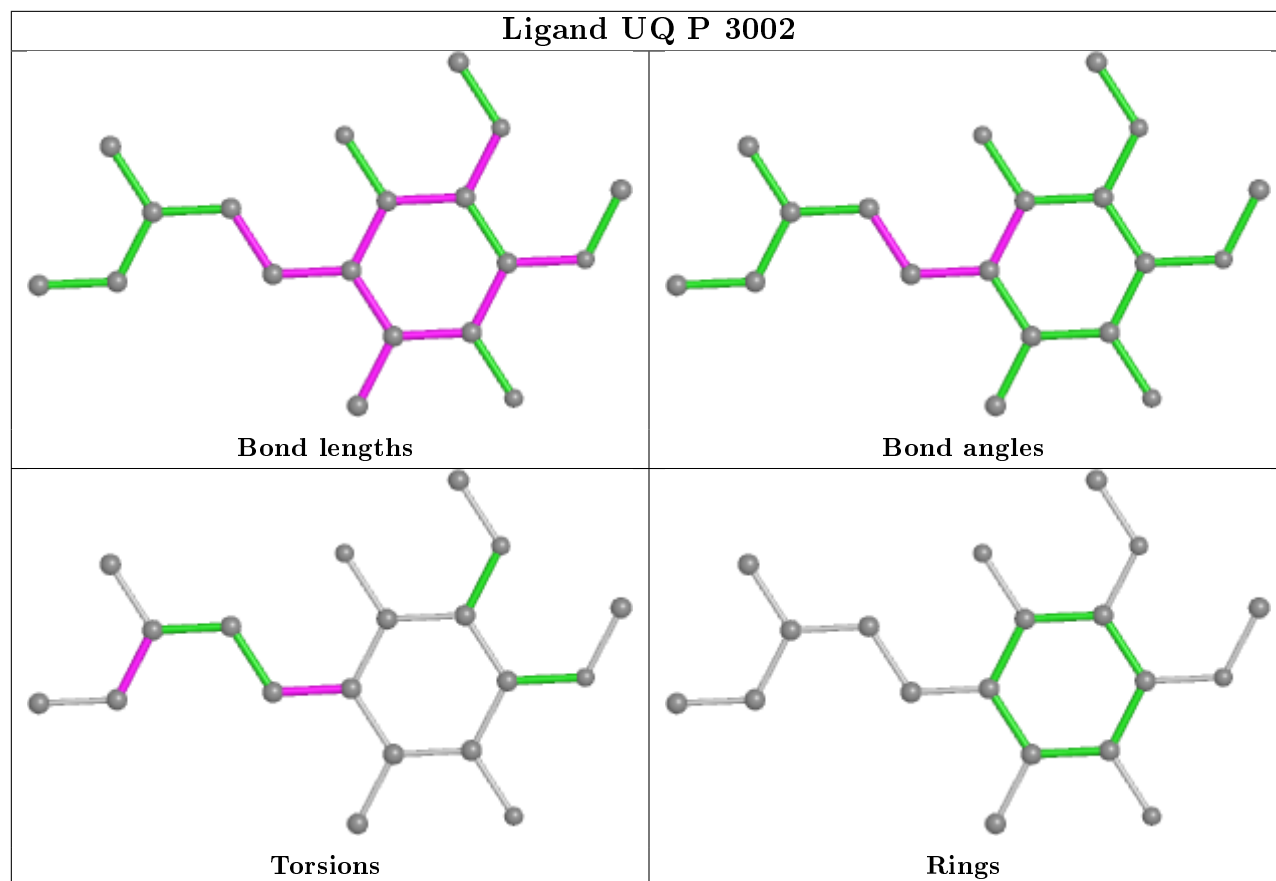


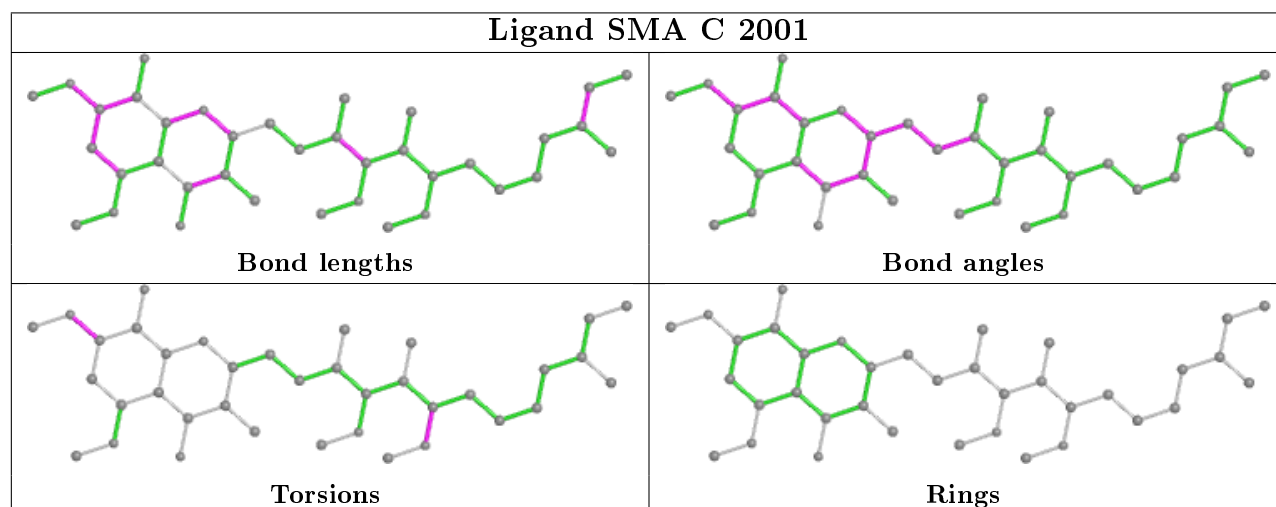
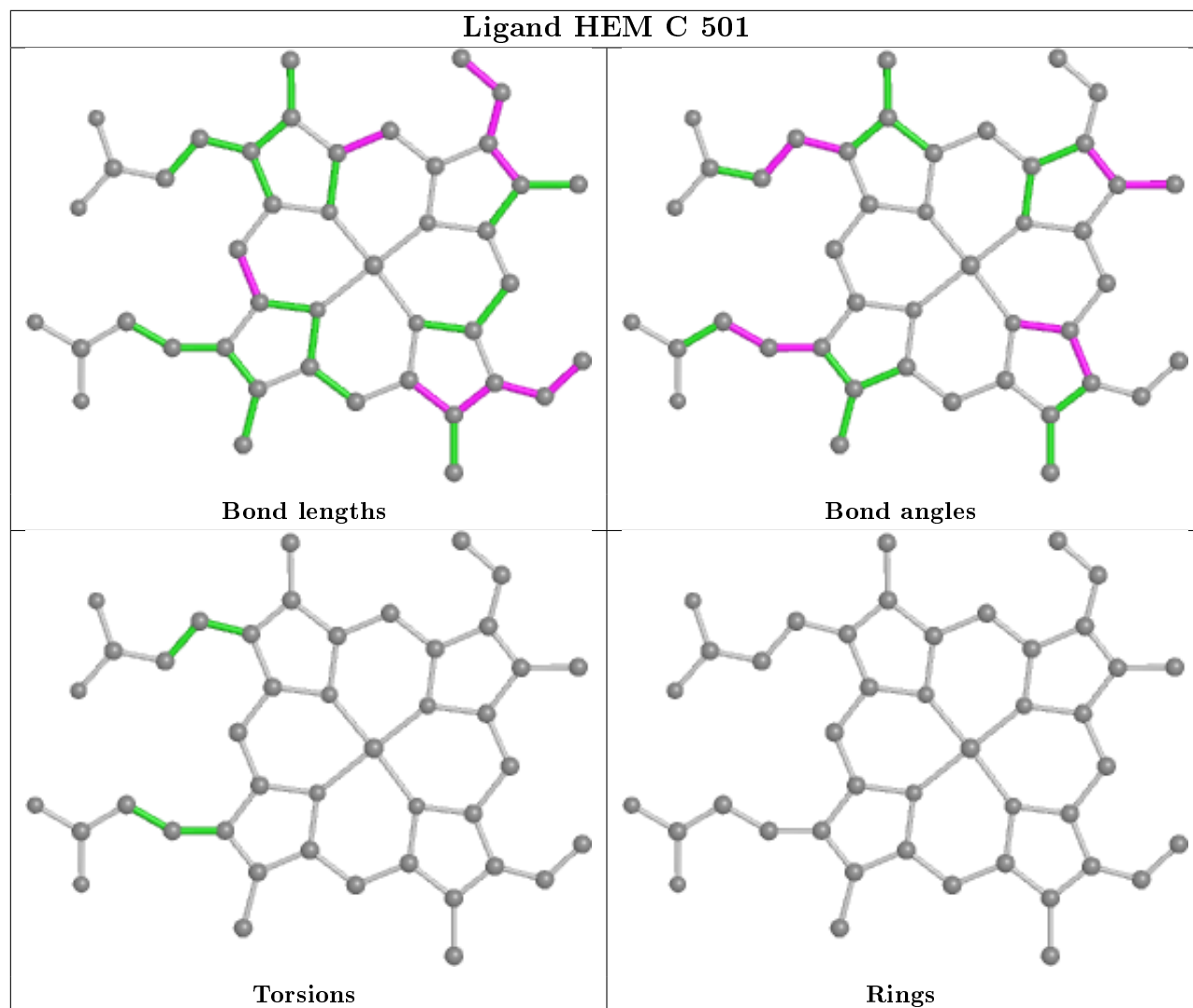
Ligand CDL P 3004

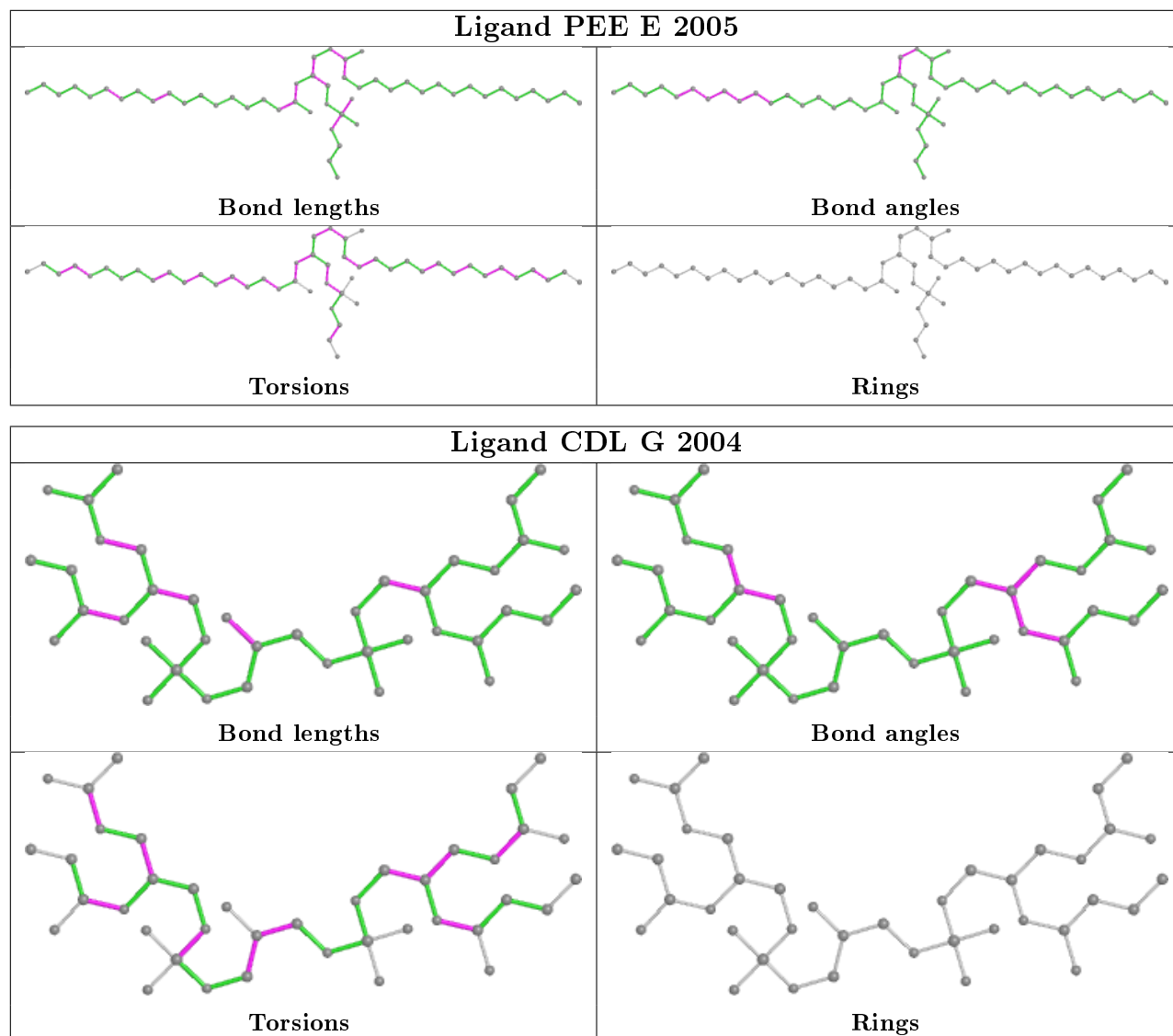


Ligand SMA P 3001









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	-0.34	2 (0%) 91 75	44, 77, 105, 114	0
1	N	442/446 (99%)	-0.31	0 100 100	54, 80, 102, 110	0
2	B	421/441 (95%)	-0.26	1 (0%) 95 87	66, 93, 122, 140	0
2	O	422/441 (95%)	-0.29	1 (0%) 95 87	52, 85, 111, 124	0
3	C	380/380 (100%)	-0.49	1 (0%) 94 84	33, 49, 84, 140	0
3	P	379/380 (99%)	-0.31	4 (1%) 80 56	44, 75, 99, 119	0
4	D	241/241 (100%)	-0.51	0 100 100	42, 55, 86, 114	0
4	Q	241/241 (100%)	-0.25	0 100 100	59, 86, 112, 127	0
5	E	196/196 (100%)	0.28	17 (8%) 10 3	48, 114, 165, 172	0
5	R	196/196 (100%)	0.05	12 (6%) 21 7	54, 85, 134, 151	0
6	F	101/110 (91%)	-0.64	0 100 100	37, 53, 67, 99	0
6	S	101/110 (91%)	-0.24	2 (1%) 65 36	64, 84, 112, 141	0
7	G	81/81 (100%)	-0.27	0 100 100	48, 62, 94, 113	0
7	T	79/81 (97%)	0.18	7 (8%) 9 3	69, 95, 147, 164	0
8	H	70/77 (90%)	-0.44	0 100 100	48, 73, 90, 133	0
8	U	67/77 (87%)	0.18	3 (4%) 33 12	102, 125, 148, 154	0
9	I	31/47 (65%)	1.32	9 (29%) 0 0	94, 127, 172, 178	0
9	V	31/47 (65%)	1.59	11 (35%) 0 0	93, 125, 184, 184	0
10	J	61/61 (100%)	-0.43	1 (1%) 72 44	57, 71, 109, 151	0
10	W	59/61 (96%)	-0.01	1 (1%) 70 41	69, 85, 101, 117	0
All	All	4042/4160 (97%)	-0.25	72 (1%) 68 40	33, 79, 125, 184	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	GLY	5.7
8	U	50	THR	5.3
9	V	51	CYS	5.3
7	T	78	GLU	4.8
7	T	2	ILE	4.1
5	E	187	PHE	4.0
3	P	8	SER	3.9
5	R	187	PHE	3.9
3	C	1	MET	3.7
9	I	48	PRO	3.7
10	W	62	SER	3.7
5	R	114	VAL	3.4
5	E	191	ASP	3.3
1	A	2	ALA	3.2
9	V	56	SER	3.2
9	V	53	GLU	3.2
7	T	79	ASN	3.2
5	R	194	VAL	3.1
9	V	57	GLY	3.1
5	R	190	ASP	3.0
5	R	191	ASP	3.0
9	V	59	SER	3.0
9	V	62	ARG	2.9
9	I	53	GLU	2.9
9	V	50	LEU	2.9
7	T	74	PRO	2.9
6	S	12	LEU	2.9
9	V	61	ARG	2.8
2	O	19	PRO	2.8
5	R	195	VAL	2.8
3	P	7	LYS	2.8
9	I	58	ARG	2.7
5	R	196	GLY	2.7
9	I	63	ASP	2.7
9	I	57	GLY	2.7
5	R	186	GLN	2.6
9	I	62	ARG	2.6
9	I	77	ARG	2.6
5	E	195	VAL	2.6
5	E	130	PRO	2.6
5	R	122	HIS	2.6
5	E	121	GLN	2.6
5	R	193	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	444	ILE	2.5
5	E	85	LYS	2.5
9	V	49	LEU	2.3
5	E	122	HIS	2.3
5	E	128	LYS	2.3
8	U	49	HIS	2.3
5	E	188	VAL	2.3
5	E	79	SER	2.3
8	U	28	GLU	2.3
5	R	128	LYS	2.3
2	B	402	ILE	2.2
5	E	74	ILE	2.2
5	E	73	LYS	2.2
7	T	77	TYR	2.2
10	J	64	GLU	2.2
3	P	5	ILE	2.2
9	I	47	ARG	2.1
9	I	51	CYS	2.1
9	V	77	ARG	2.1
5	R	188	VAL	2.1
9	V	63	ASP	2.1
5	E	111	GLU	2.1
3	P	13	LYS	2.1
5	E	118	ARG	2.1
5	E	117	LEU	2.1
5	E	137	GLY	2.0
6	S	15	ARG	2.0
7	T	63	THR	2.0
5	E	91	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

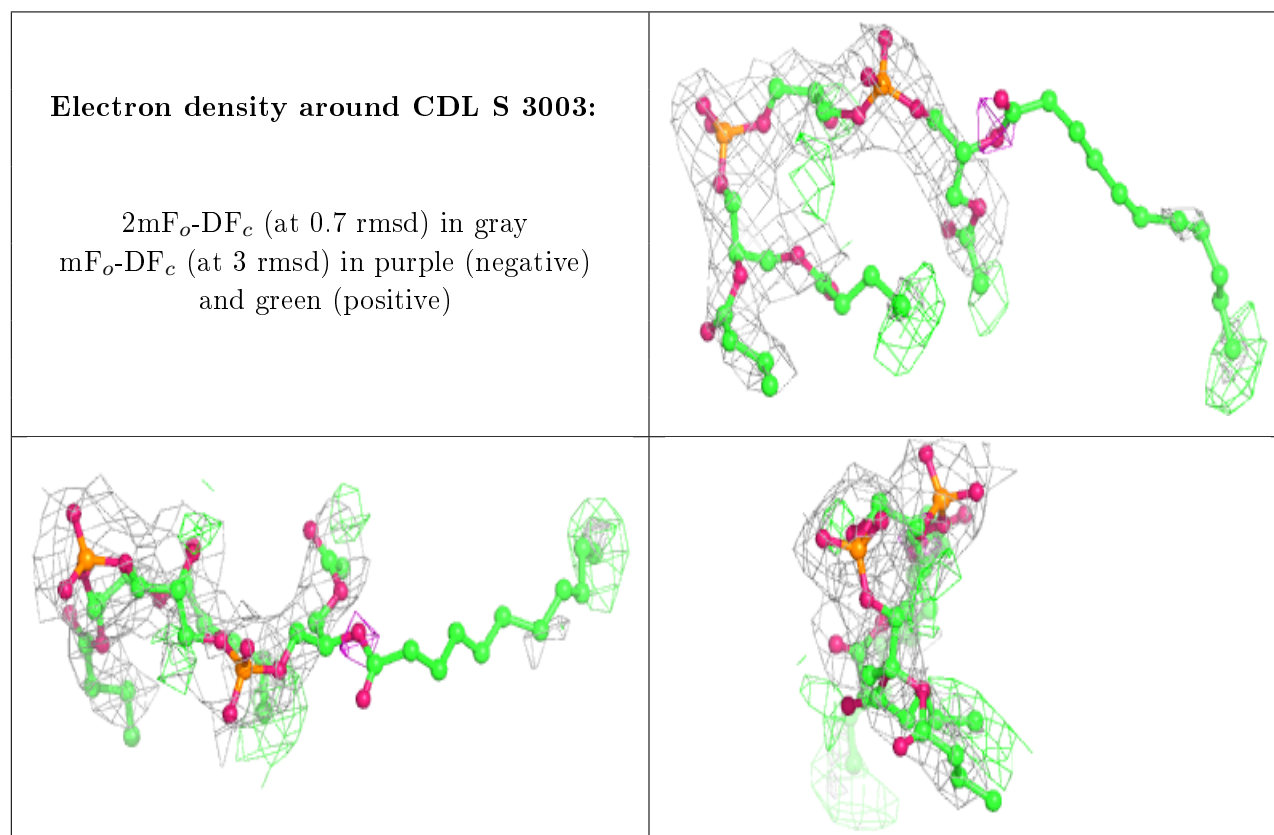
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

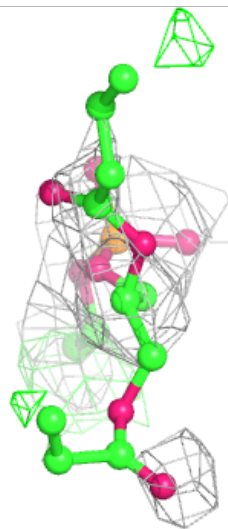
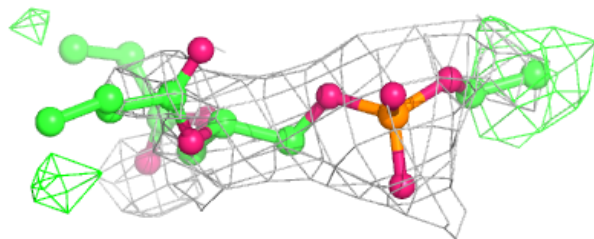
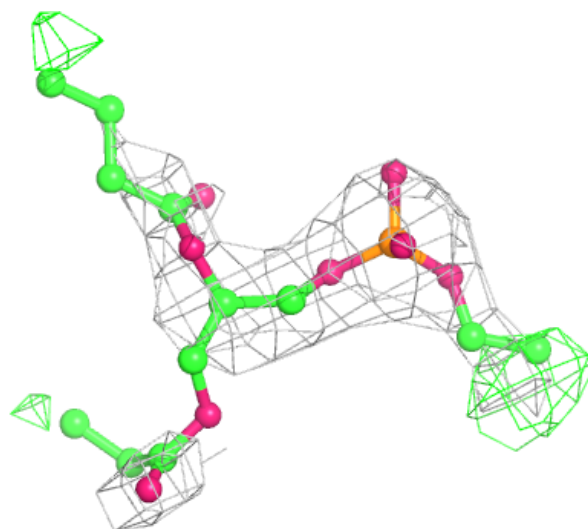
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	UNL	E	2105	1/-	0.51	0.38	62,62,62,62	0
11	UNL	C	2010	1/-	0.59	1.52	53,53,53,53	0
11	UNL	E	3103	1/-	0.65	0.43	45,45,45,45	0
11	UNL	P	3010	1/-	0.65	0.89	67,67,67,67	0
11	UNL	C	2104	1/-	0.67	0.62	71,71,71,71	0
11	UNL	P	2015	1/-	0.71	0.39	33,33,33,33	0
11	UNL	C	3015	1/-	0.73	0.48	47,47,47,47	0
11	UNL	A	3016	1/-	0.75	0.40	55,55,55,55	0
18	CDL	S	3003	50/100	0.76	0.38	126,140,153,153	0
11	UNL	P	3104	1/-	0.76	0.54	59,59,59,59	0
15	PEE	C	2008	21/51	0.76	0.33	139,142,144,144	0
15	PEE	R	3005	50/51	0.78	0.38	95,108,116,119	0
15	PEE	E	2005	50/51	0.79	0.34	76,90,95,95	0
11	UNL	R	2103	1/-	0.80	0.61	45,45,45,45	0
20	PLC	E	2009	32/42	0.82	0.32	67,83,97,98	0
20	PLC	R	3009	32/42	0.82	0.35	91,99,116,116	0
15	PEE	N	3008	5/51	0.82	0.34	135,135,136,136	0
16	GOL	C	2011	6/6	0.84	0.35	79,81,82,83	0
14	UQ	C	2002	19/63	0.84	0.28	85,88,90,91	0
18	CDL	P	3004	40/100	0.85	0.27	106,114,120,121	0
18	CDL	D	2003	50/100	0.85	0.27	79,112,130,131	0
14	UQ	P	3002	19/63	0.85	0.30	116,121,122,122	0
15	PEE	P	3007	49/51	0.87	0.34	73,98,107,108	0
18	CDL	G	2004	40/100	0.90	0.26	81,90,97,98	0
16	GOL	P	3011	6/6	0.92	0.27	69,71,72,72	0
15	PEE	C	2007	49/51	0.92	0.28	52,68,87,89	0
13	SMA	P	3001	37/37	0.94	0.23	67,73,75,78	0
17	HEC	Q	501	43/43	0.96	0.19	67,71,76,78	0
13	SMA	C	2001	37/37	0.97	0.20	41,44,46,52	0
12	HEM	C	501	43/43	0.98	0.20	44,48,50,53	0
17	HEC	D	501	43/43	0.98	0.17	44,46,50,53	0
19	FES	E	501	4/4	0.98	0.15	92,93,95,95	0
12	HEM	P	501	43/43	0.98	0.21	56,61,69,75	0
12	HEM	C	502	43/43	0.99	0.19	34,40,50,54	0
12	HEM	P	502	43/43	0.99	0.20	59,63,71,77	0
19	FES	R	501	4/4	1.00	0.16	52,54,56,57	0

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



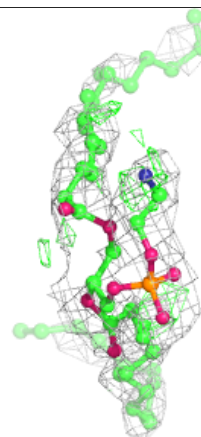
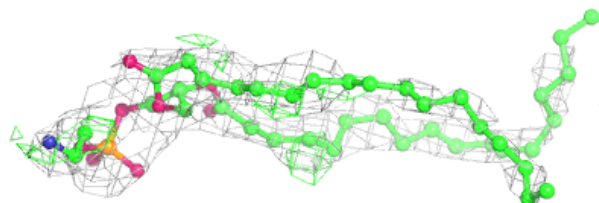
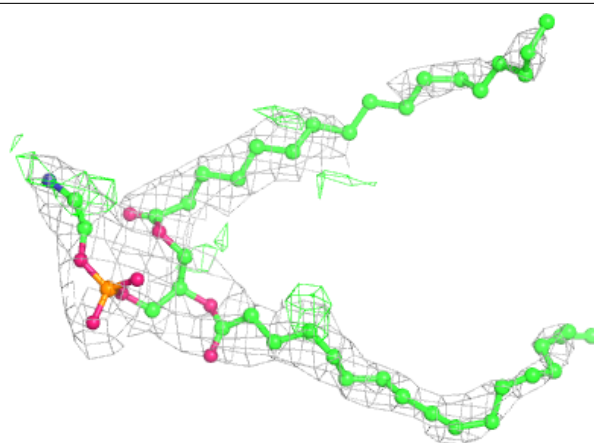
Electron density around PEE C 2008:

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



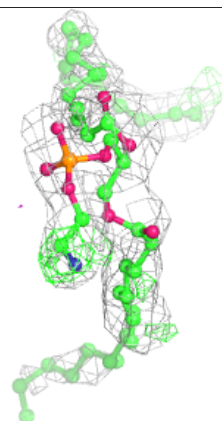
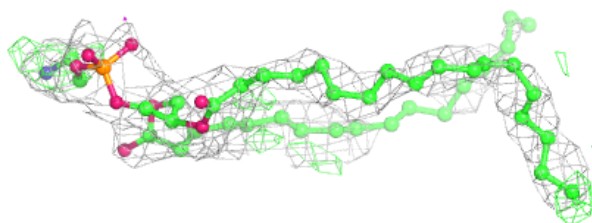
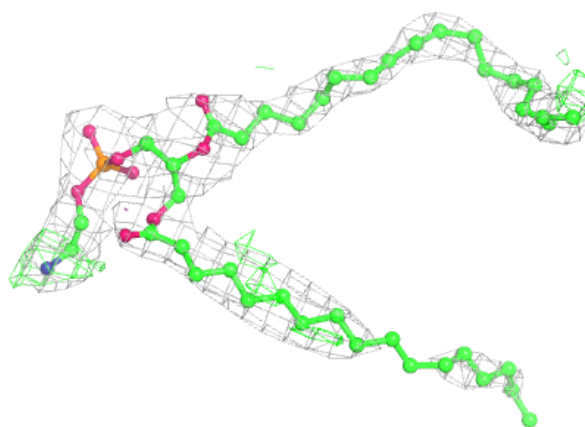
Electron density around PEE R 3005:

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

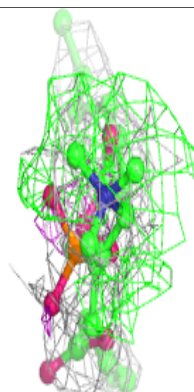
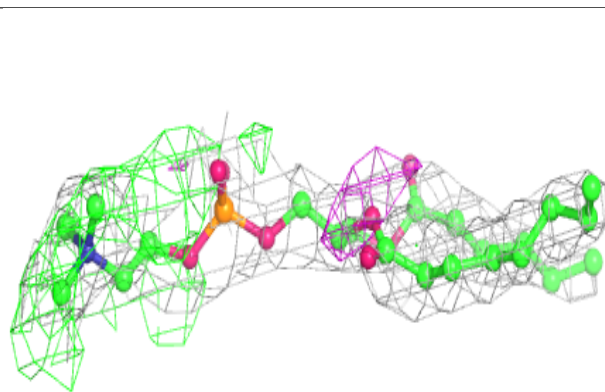
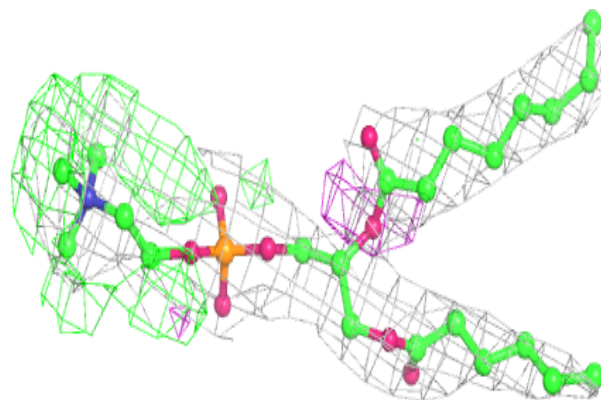


Electron density around PEE E 2005:

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

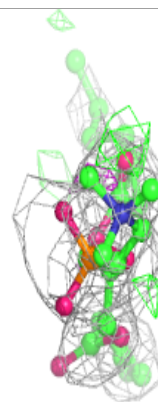
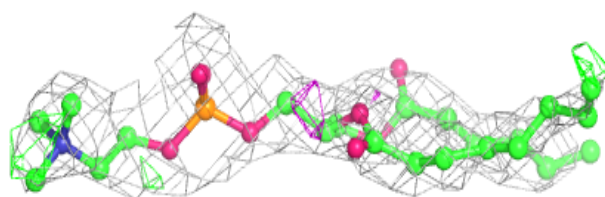
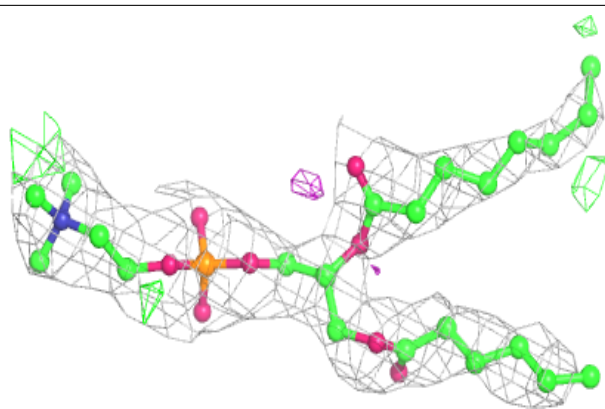
**Electron density around PLC E 2009:**

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



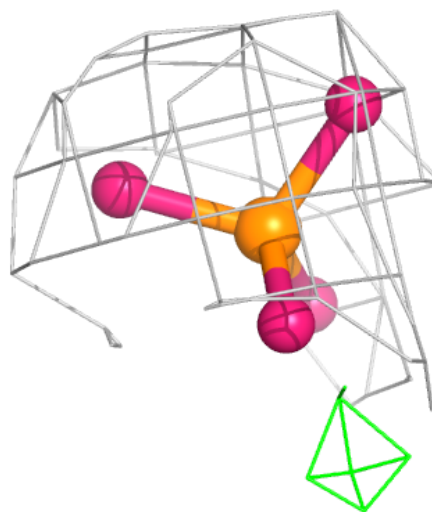
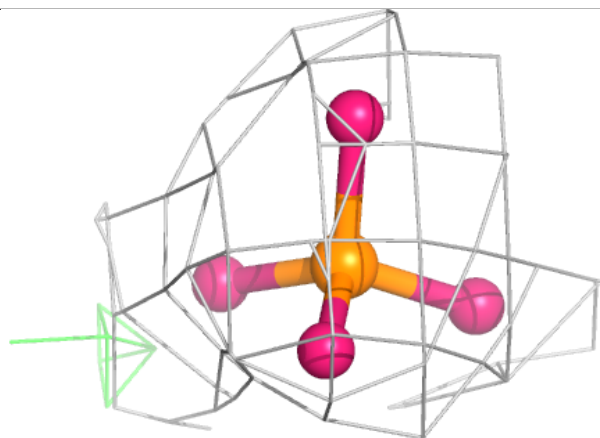
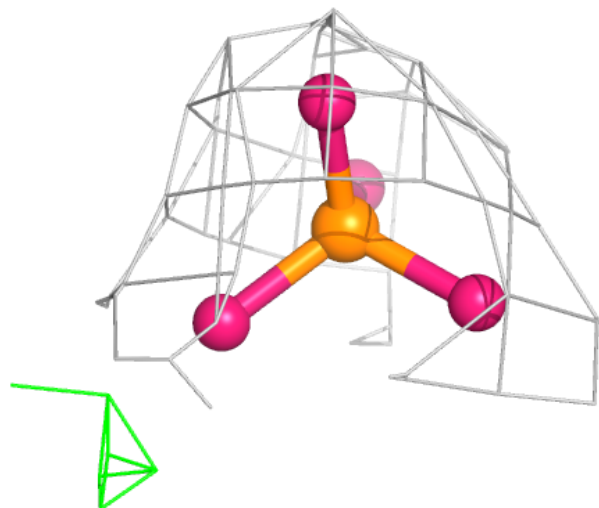
Electron density around PLC R 3009:

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



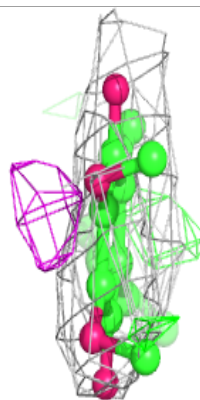
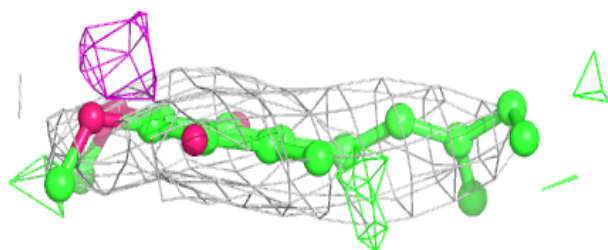
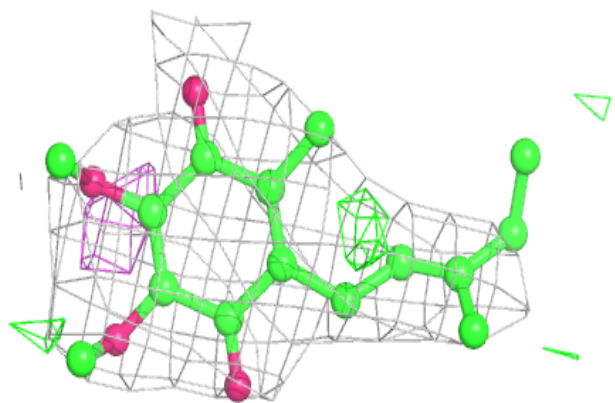
Electron density around PEE N 3008:

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



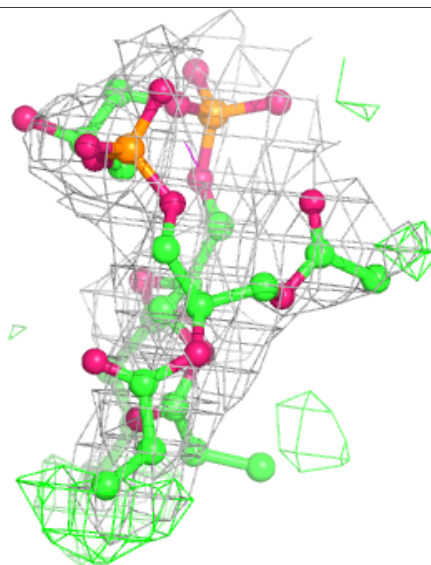
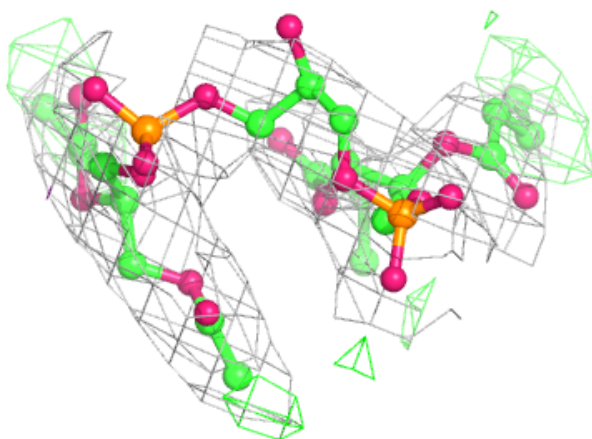
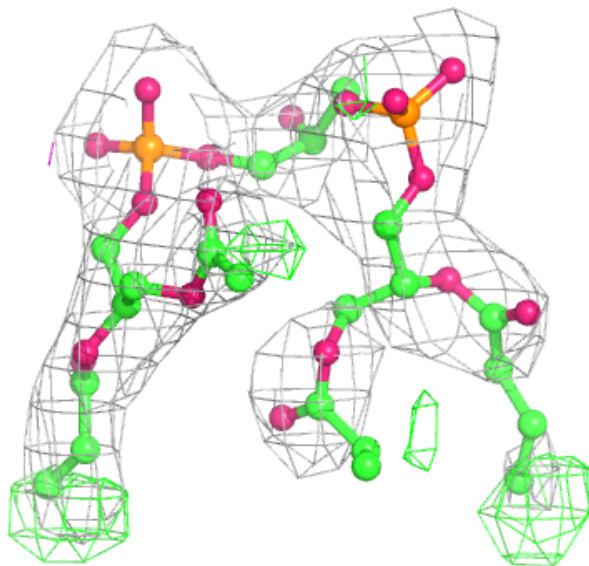
Electron density around UQ C 2002:

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



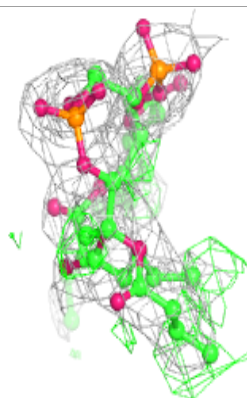
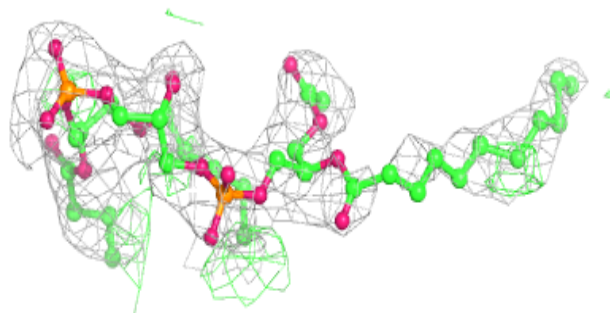
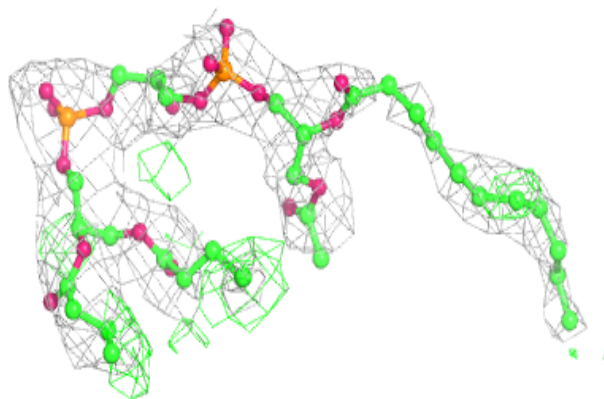
Electron density around CDL P 3004:

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

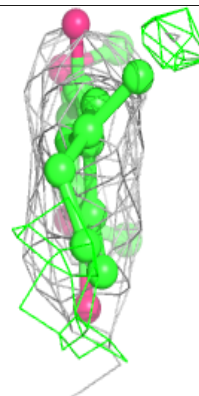
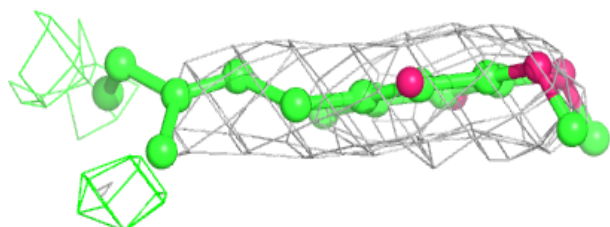
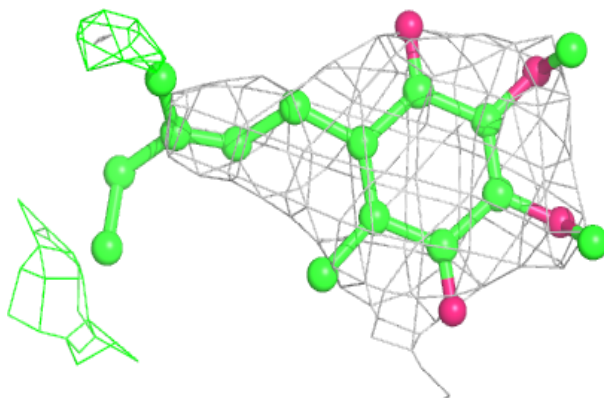


Electron density around CDL D 2003:

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

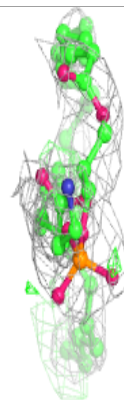
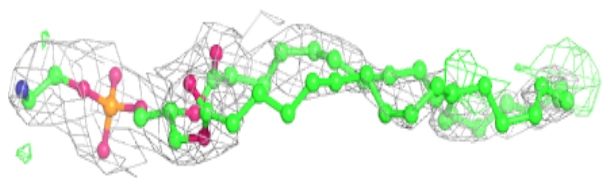
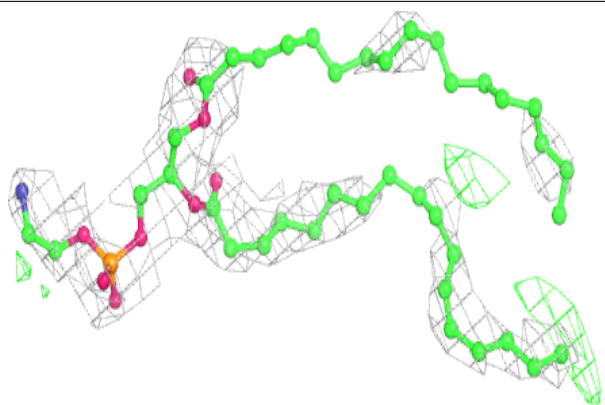
**Electron density around UQ P 3002:**

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



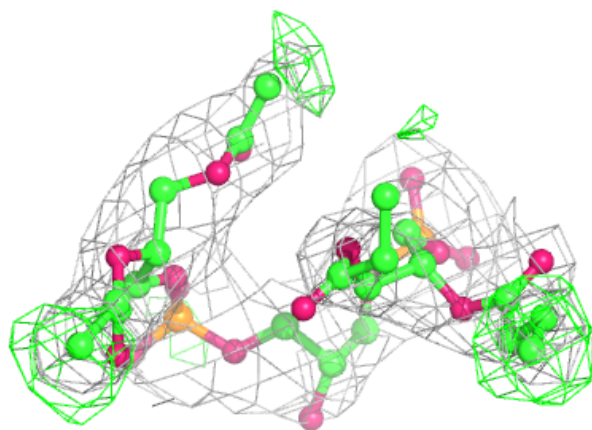
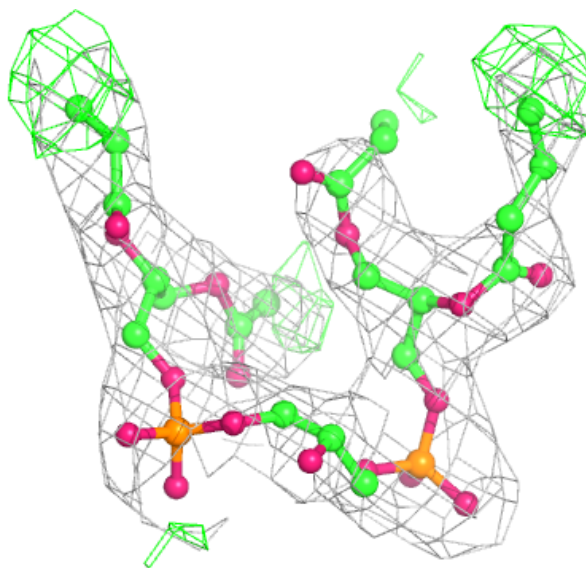
Electron density around PEE P 3007:

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



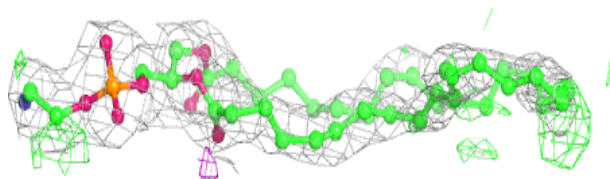
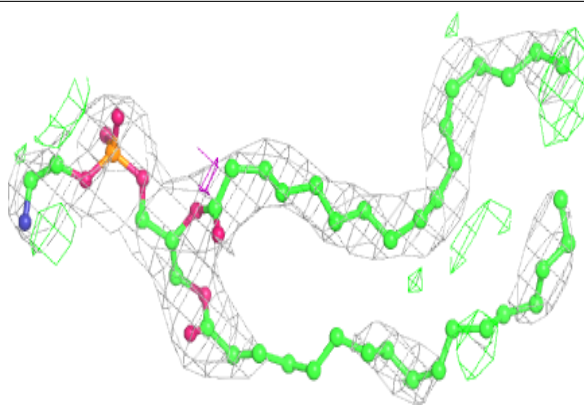
Electron density around CDL G 2004:

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

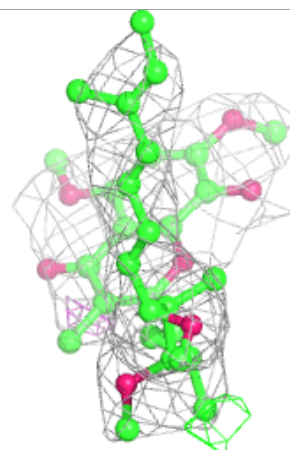
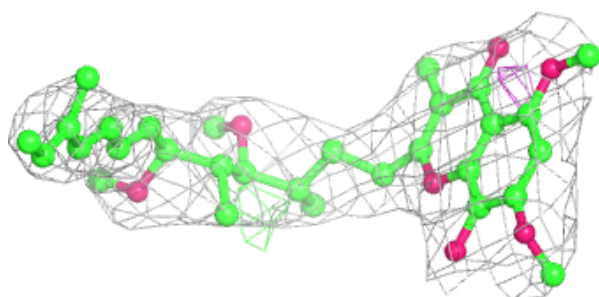
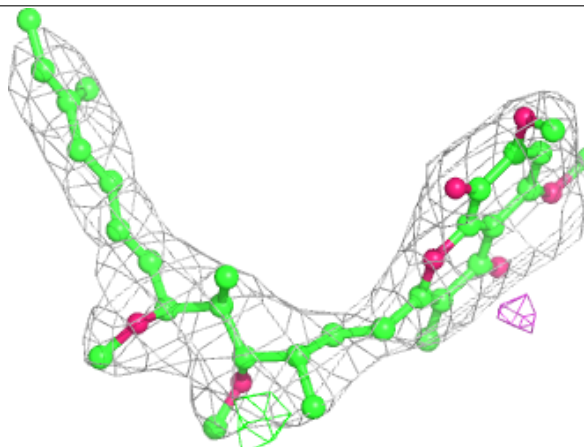


Electron density around PEE C 2007:

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

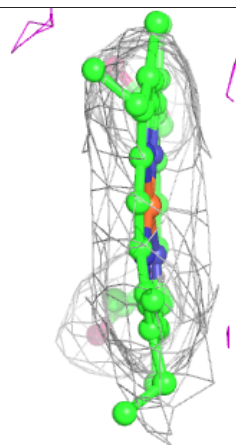
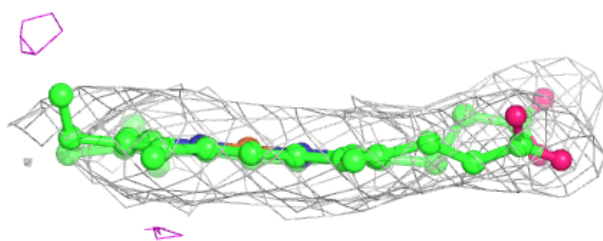
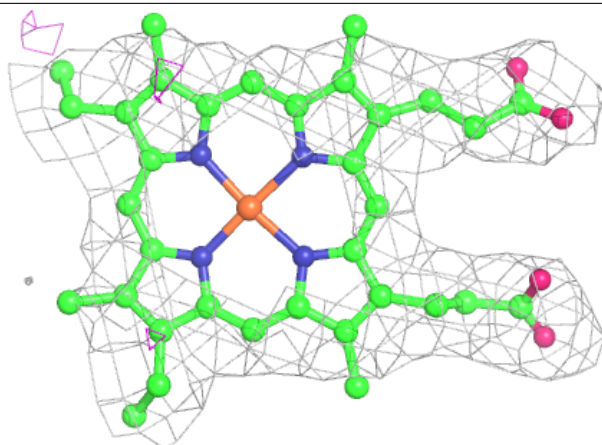
**Electron density around SMA P 3001:**

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

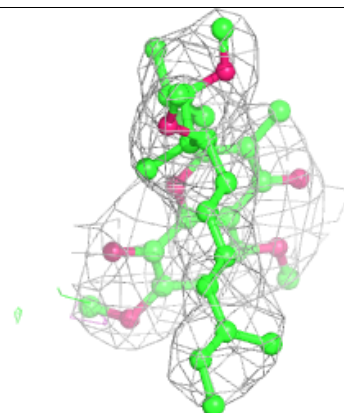
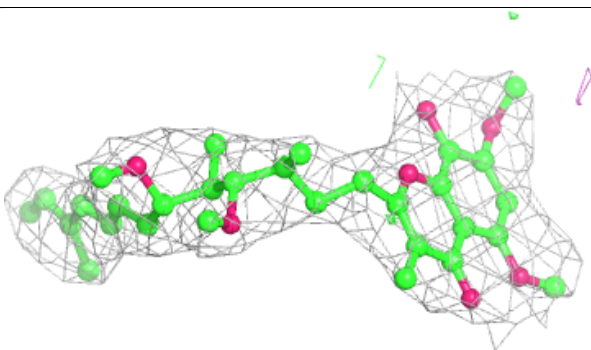
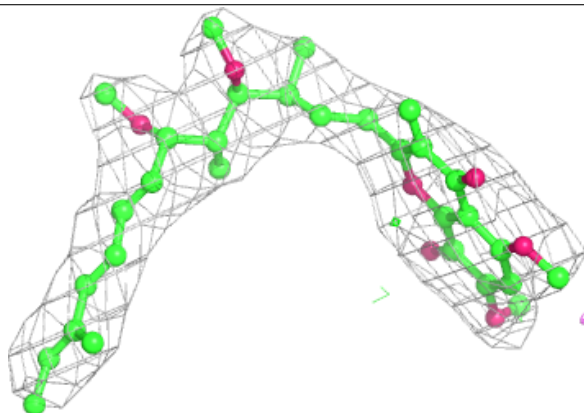


Electron density around HEC Q 501:

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

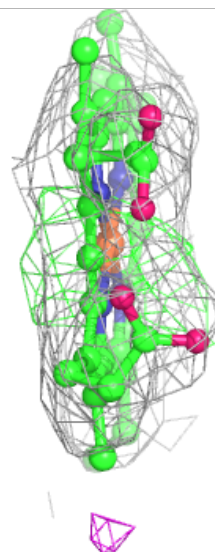
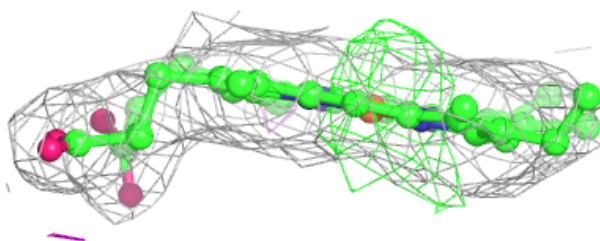
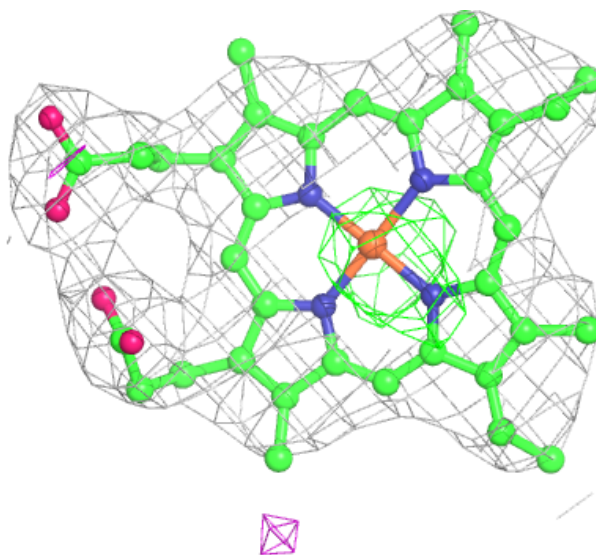
**Electron density around SMA C 2001:**

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



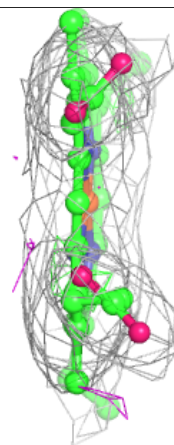
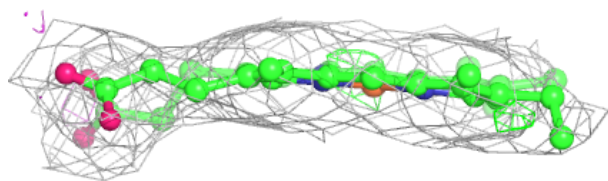
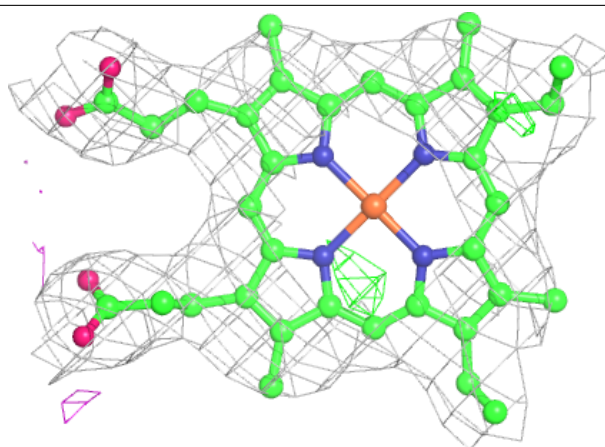
Electron density around HEM C 501:

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



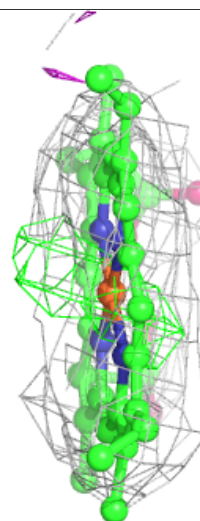
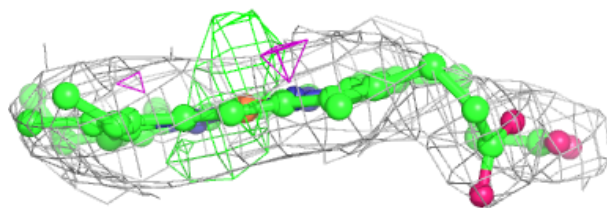
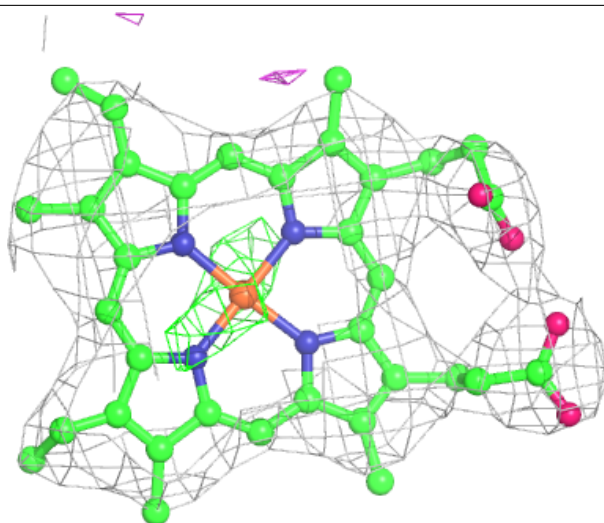
Electron density around HEC D 501:

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



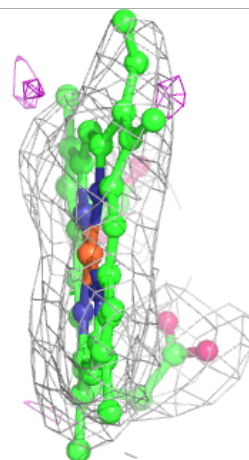
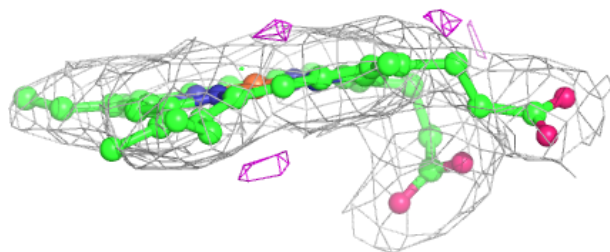
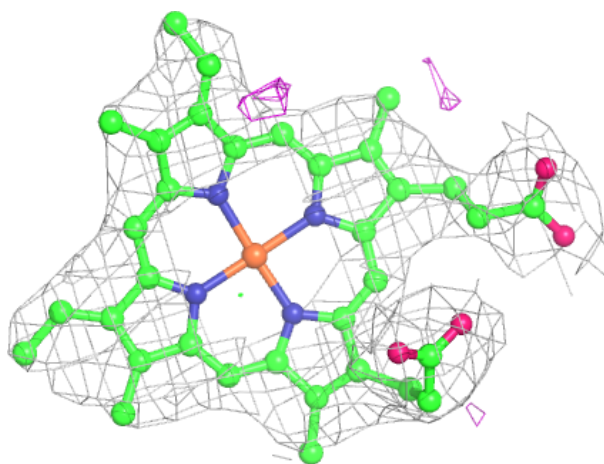
Electron density around HEM P 501:

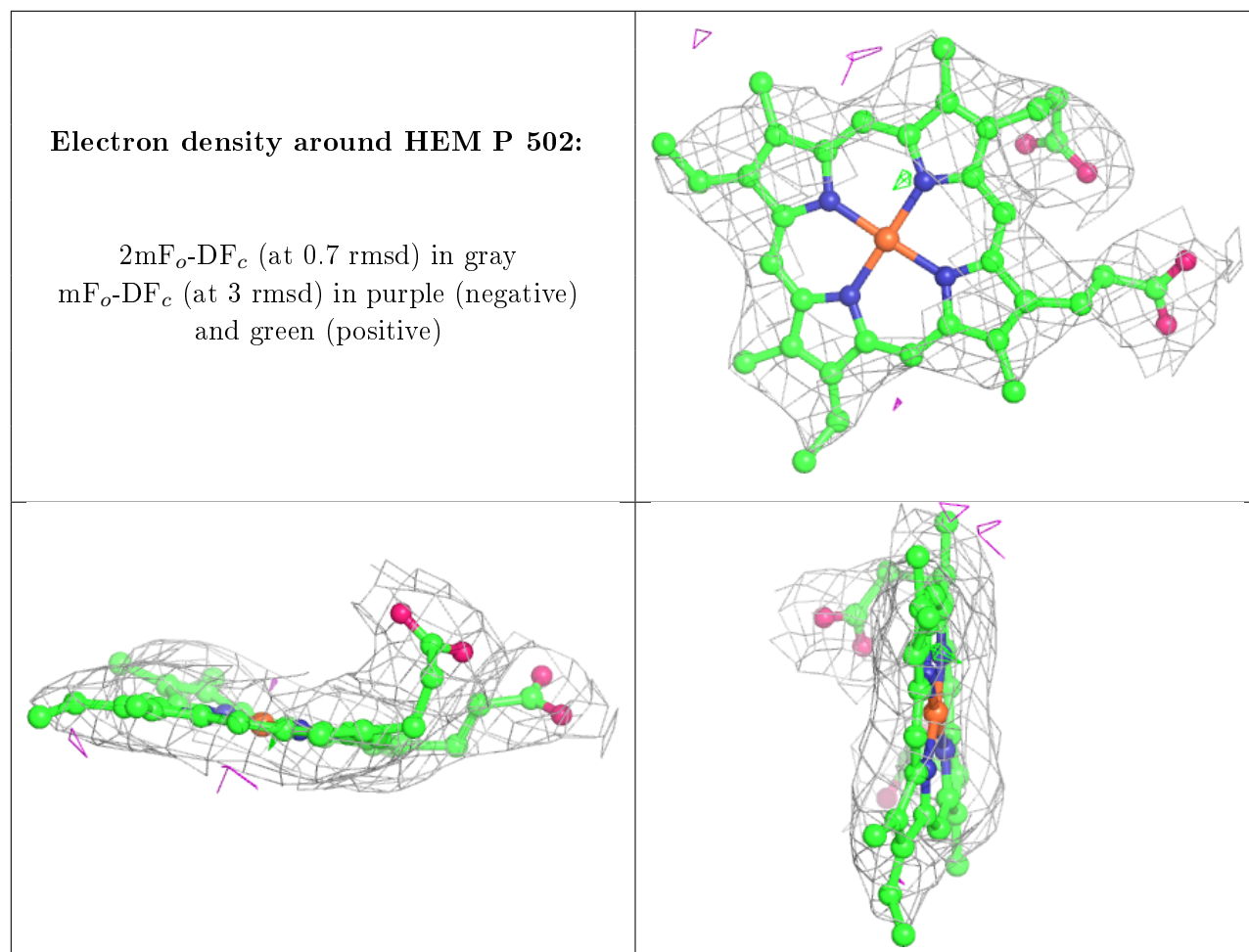
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.