



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 10:13 AM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

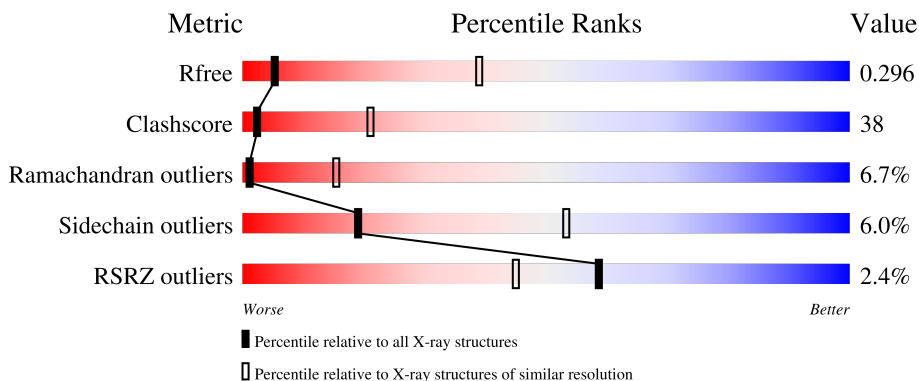
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	446	 41% 52% 7%
1	N	446	 39% 52% 7%
2	B	441	 36% 52% 7%
2	O	441	 38% 50% 7%
3	C	380	 39% 53% 7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEE	N	3008	-	X	-	-
11	PEE	P	3005	-	-	-	X
12	UNL	C	3015	-	-	-	X
12	UNL	P	3104	-	-	-	X
15	ANY	C	2002	X	-	-	-
15	ANY	P	3002	X	-	-	-
16	CDL	Q	3003	-	-	-	X
19	FES	E	501	-	-	X	-

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

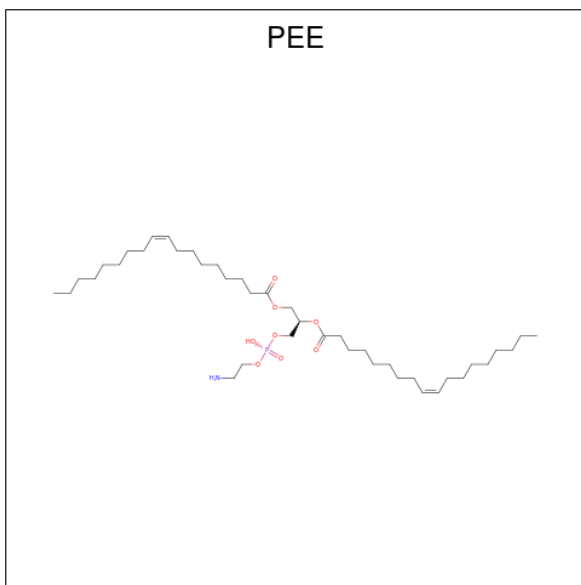
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

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

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

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P).



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

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

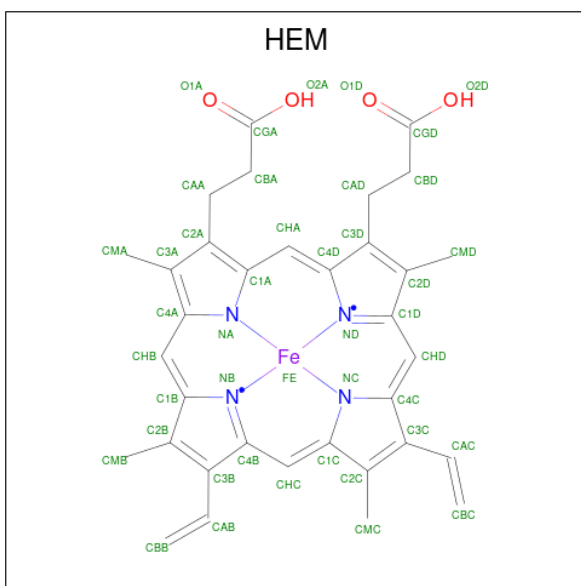
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total	0	0
			1	1	

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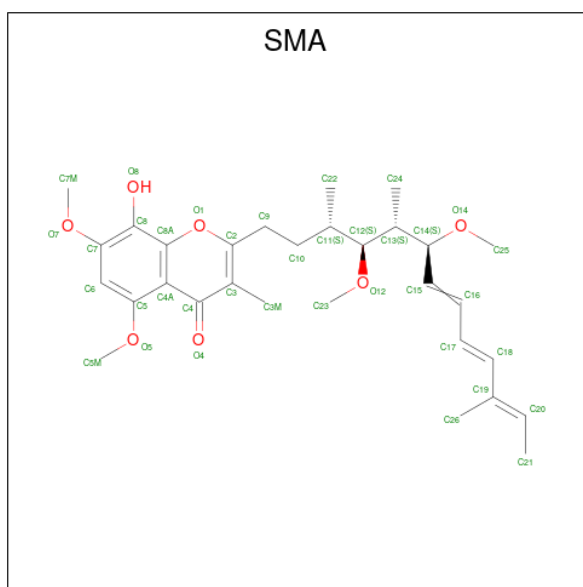
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	3	Total O 3 3	0	0
12	E	2	Total O 2 2	0	0
12	P	3	Total O 3 3	0	0
12	R	1	Total O 1 1	0	0

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



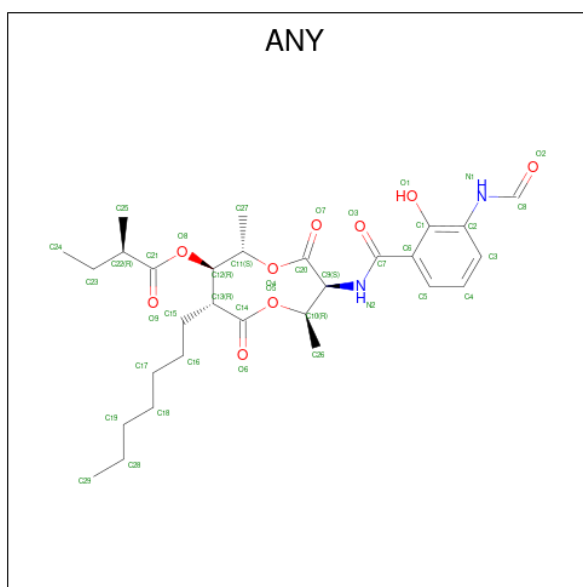
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

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



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

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



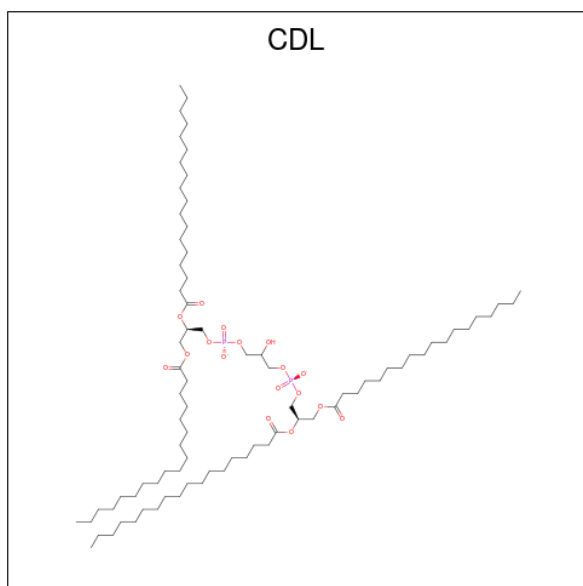
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	N	O	0	0
			37	26	2	9		

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

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



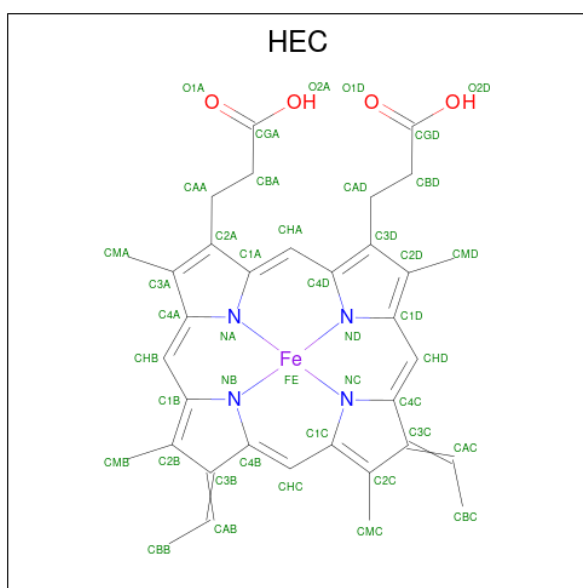
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
16	C	1	40	21	17	2	0	0
16	D	1	50	31	17	2	0	0
16	P	1	40	21	17	2	0	0
16	Q	1	50	31	17	2	0	0

- Molecule 17 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



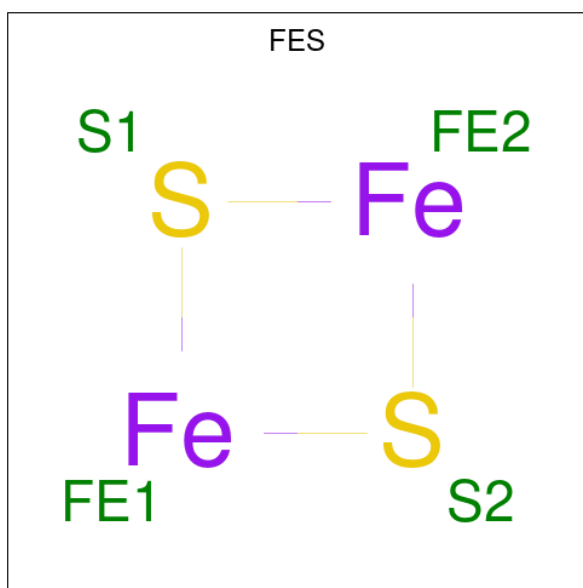
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			6	3	3		
17	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



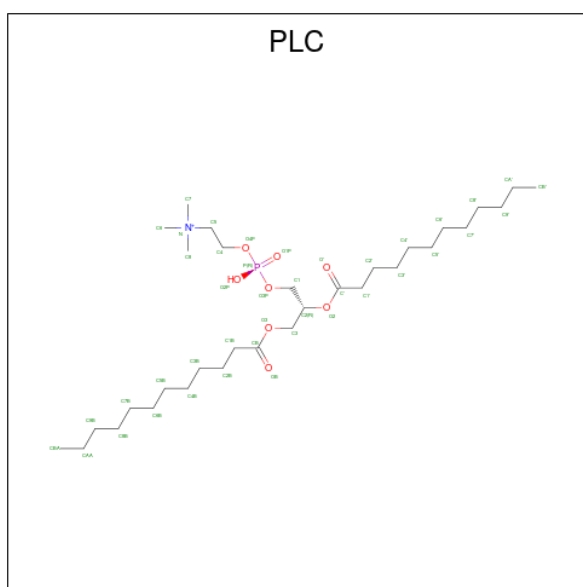
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
18	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
18	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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).

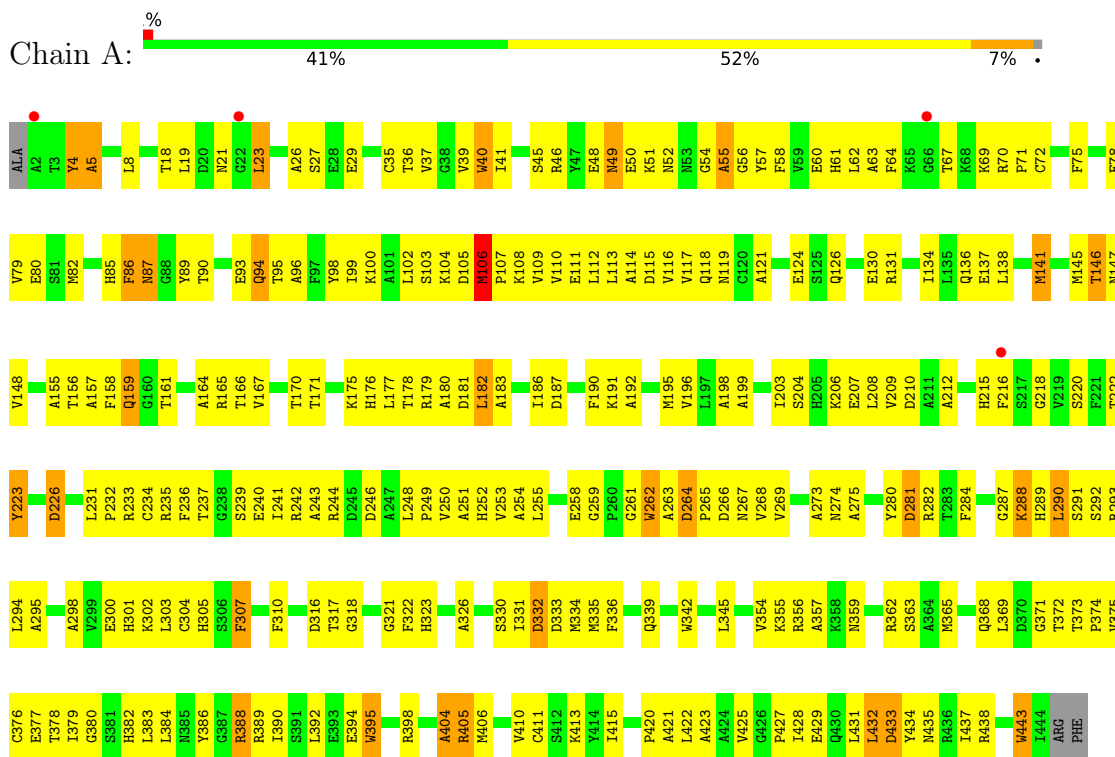


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

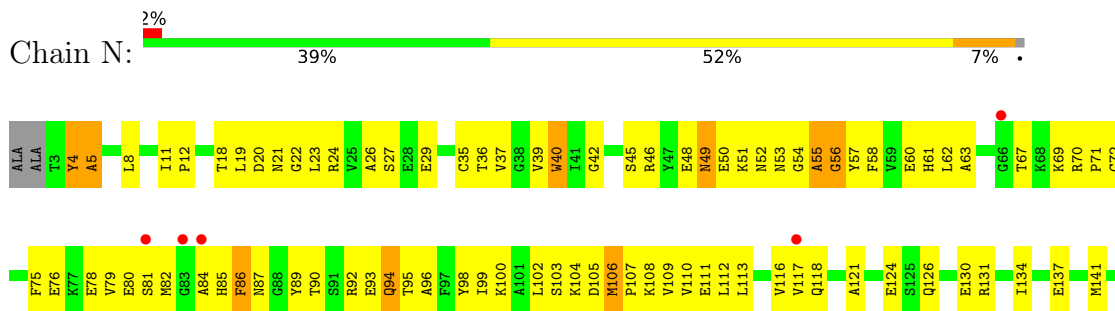
3 Residue-property plots

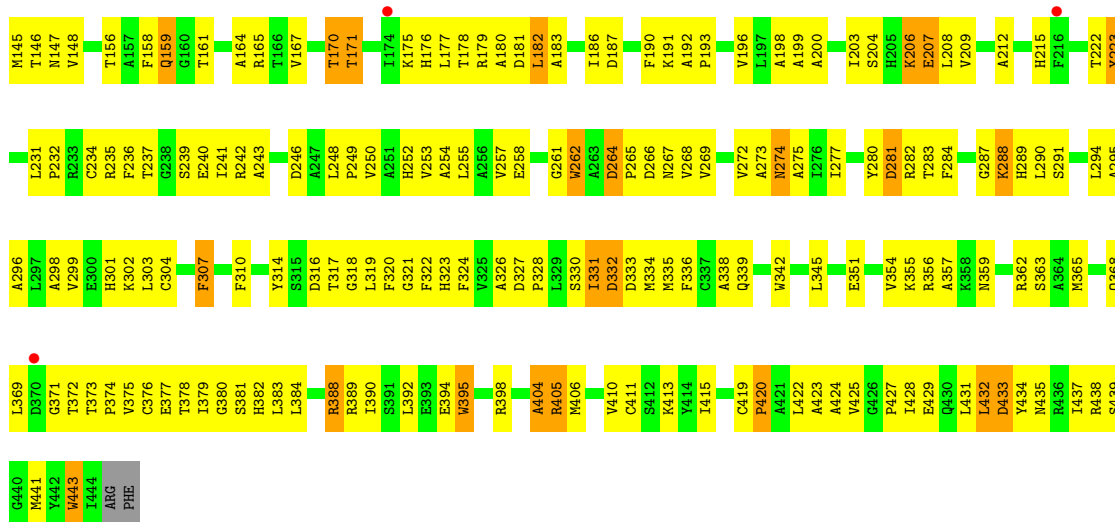
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

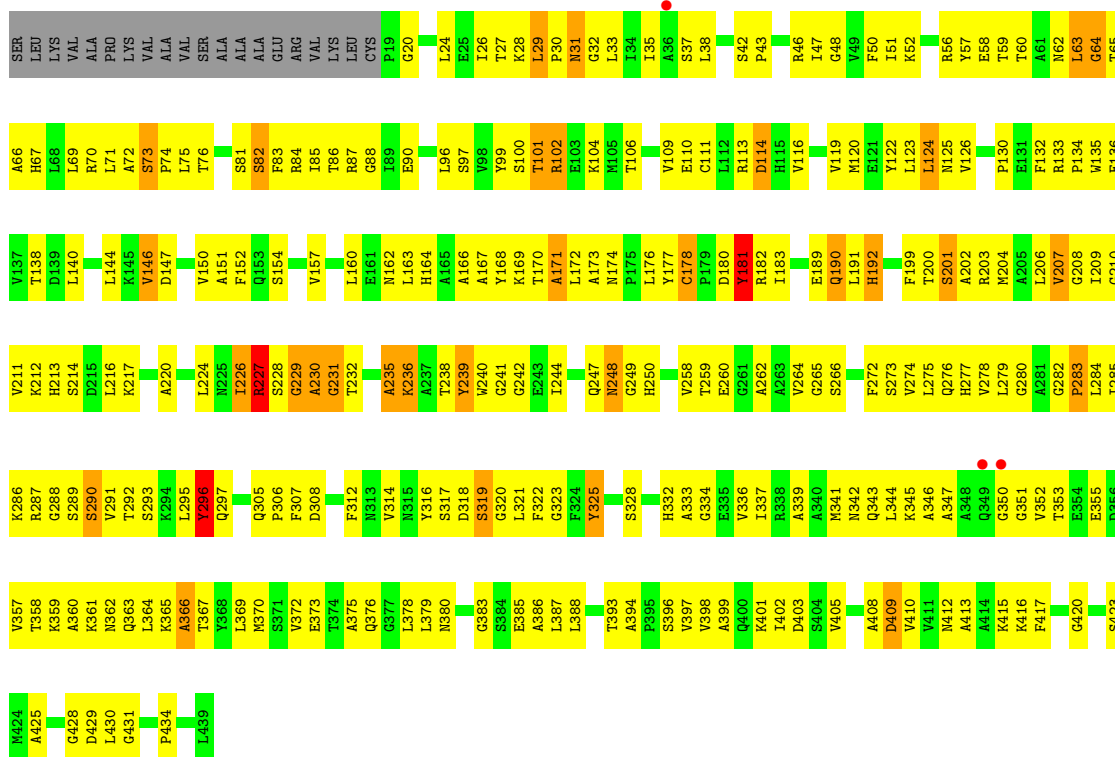


- Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL



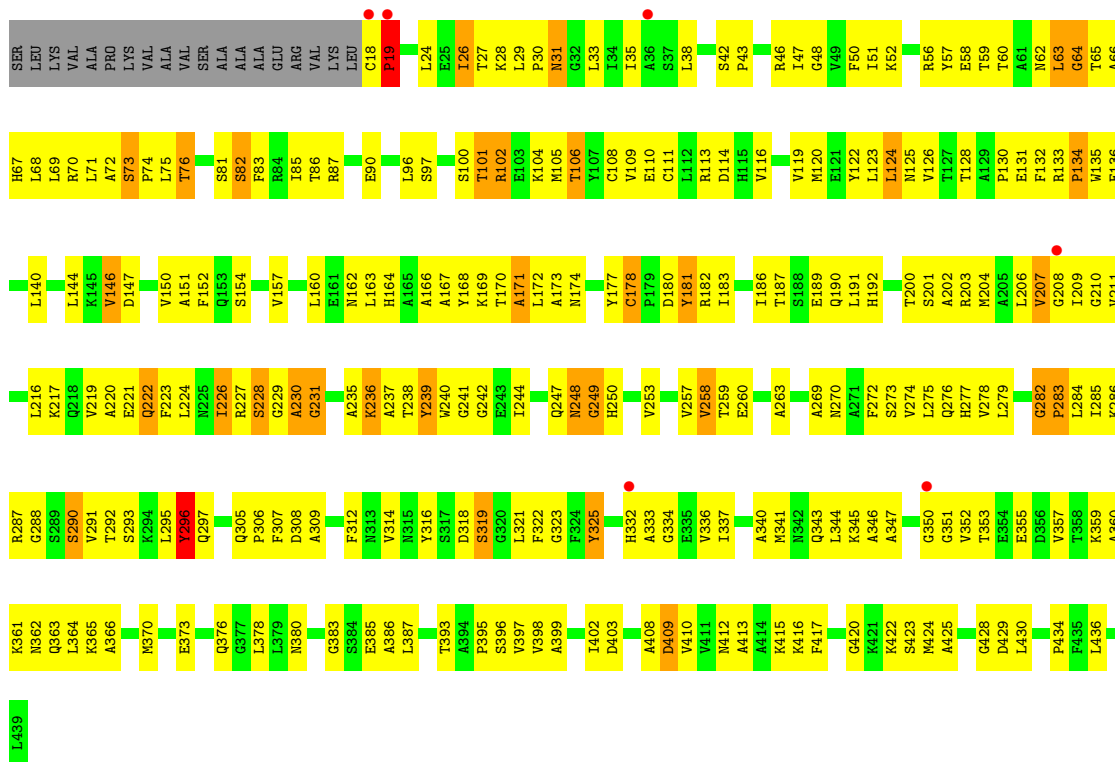


• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL

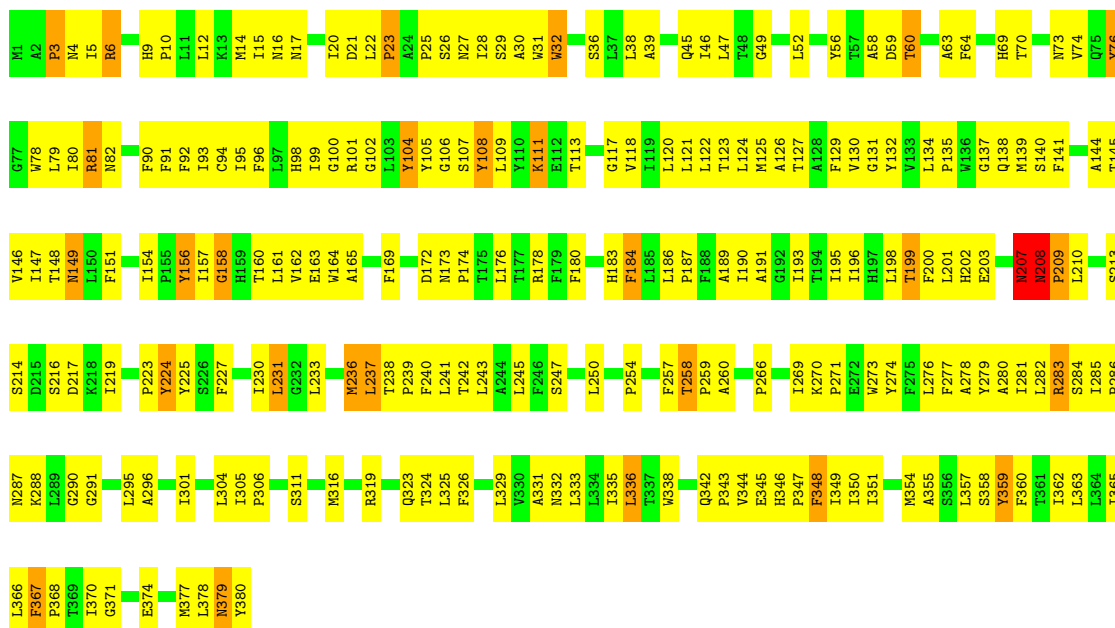
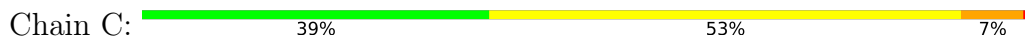


• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL



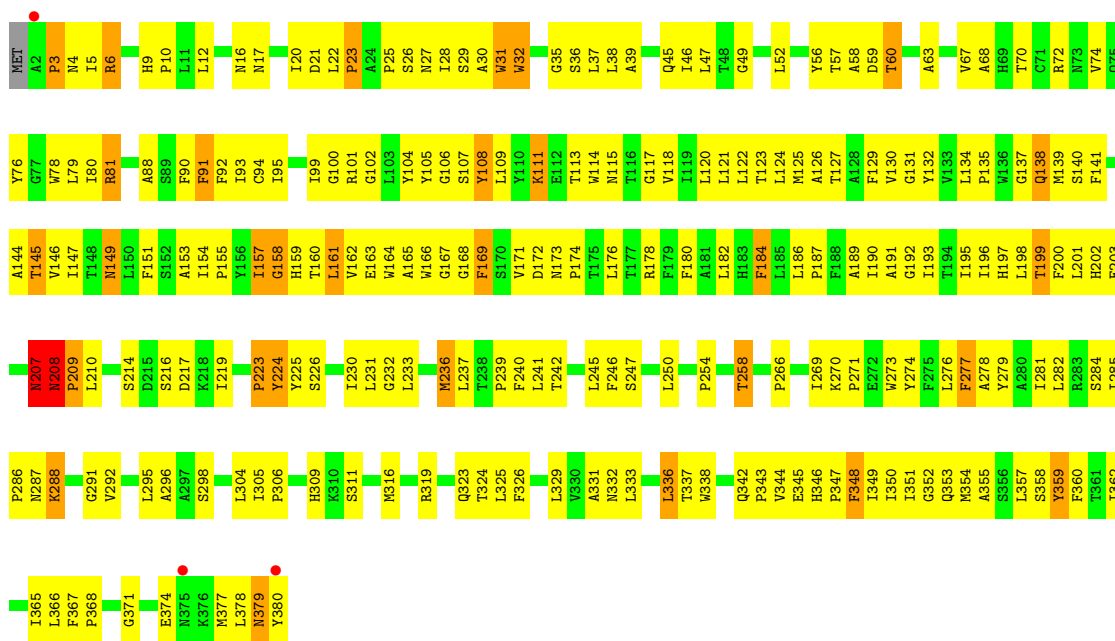


• Molecule 3: Cytochrome b

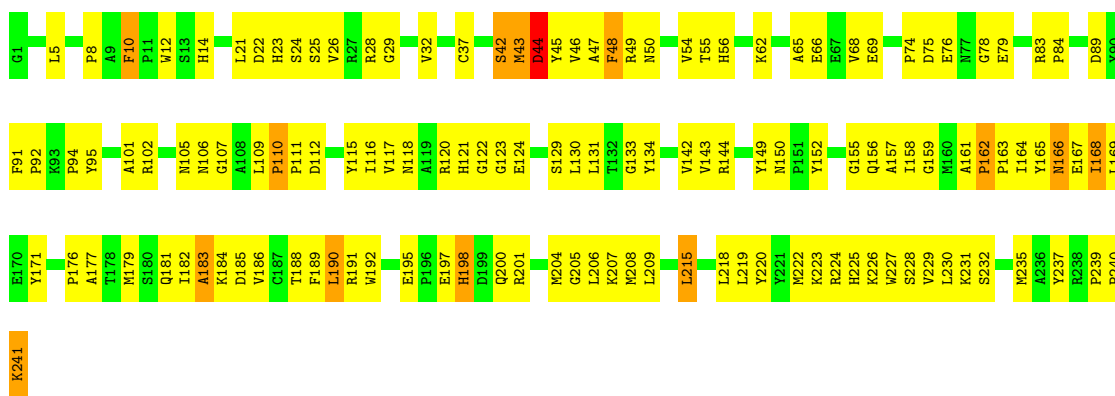


• Molecule 3: Cytochrome b

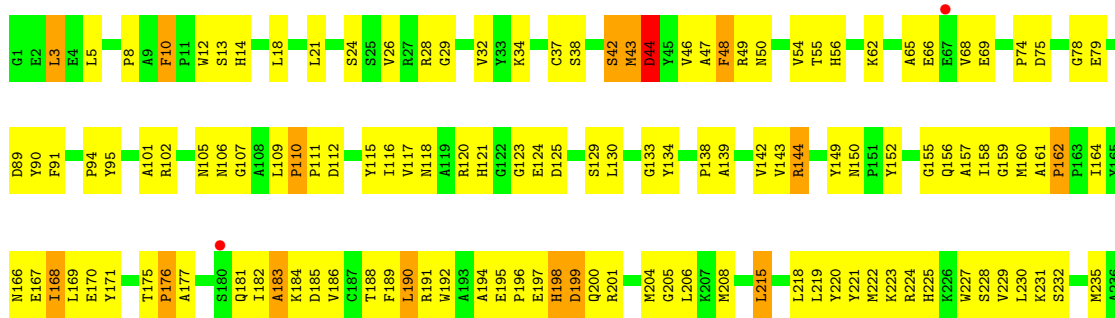




• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

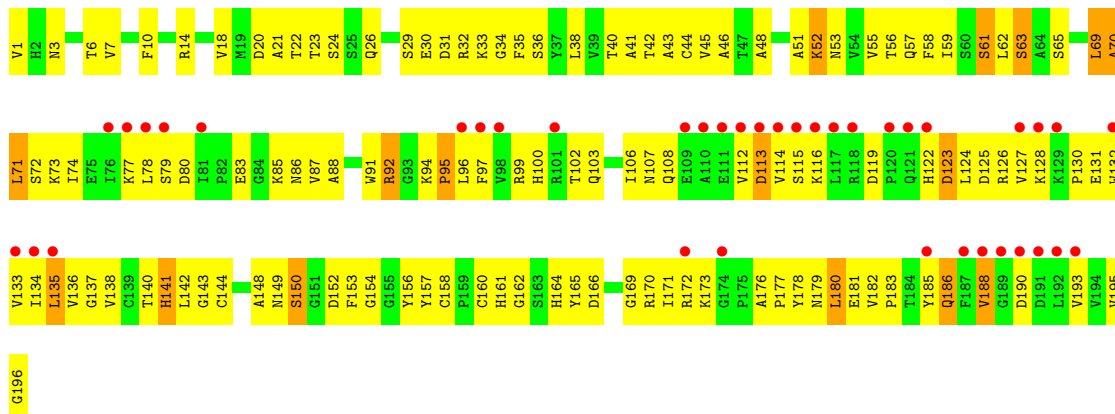


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

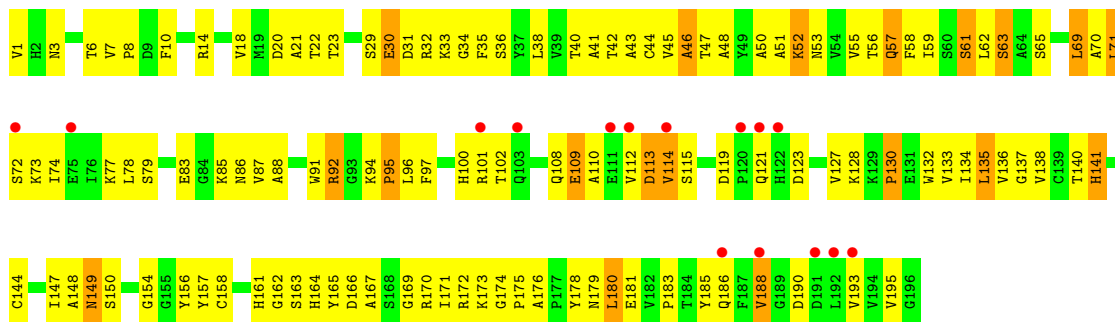




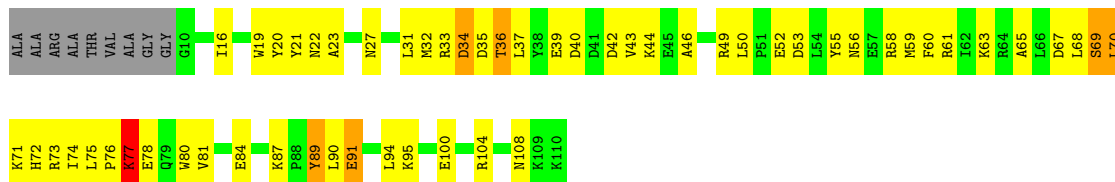
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



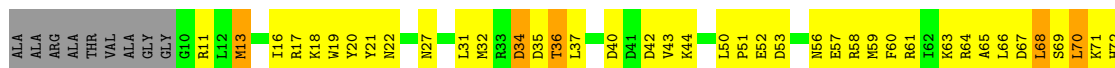
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

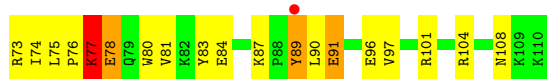


• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN



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

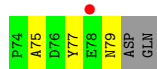
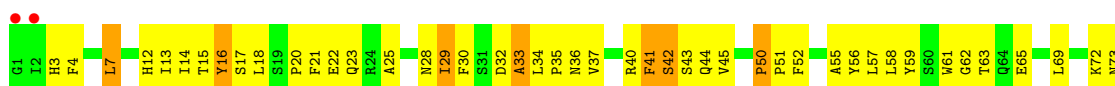




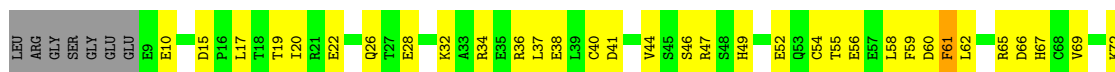
- Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



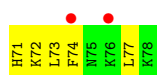
- Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



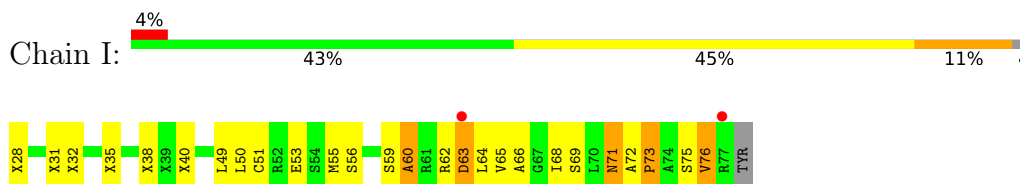
- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



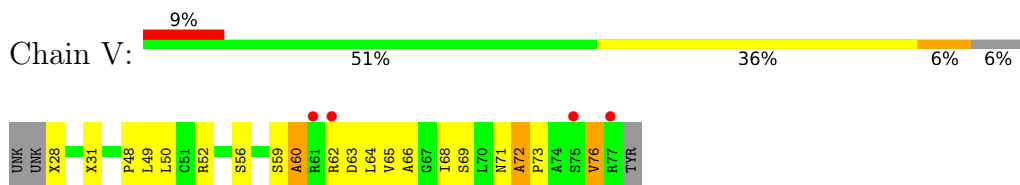
- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



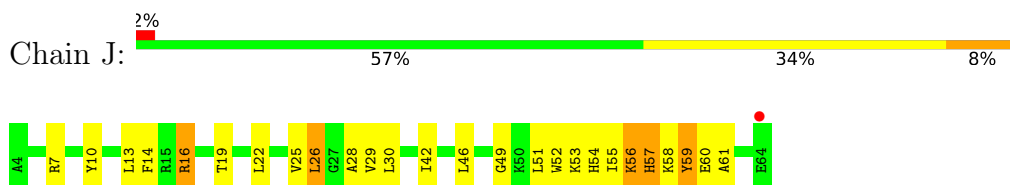
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



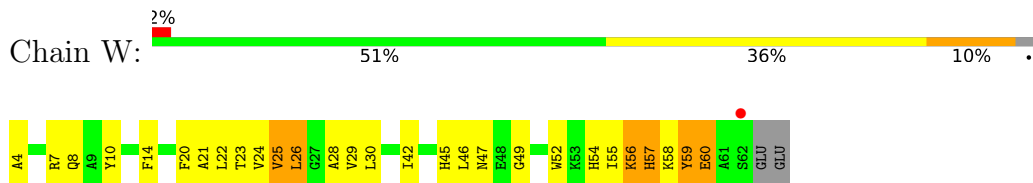
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.69Å 181.67Å 240.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.53 49.53 – 3.53	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.99-3.53) 90.6 (49.53-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.57Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.306 0.250 , 0.296	Depositor DCC
R_{free} test set	2560 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtrriage
Anisotropy	0.513	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.026 for k,h,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	32701	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/3511	0.69	0/4757
1	N	0.49	0/3508	0.69	0/4753
2	B	0.43	0/3196	0.67	0/4334
2	O	0.44	0/3202	0.67	0/4343
3	C	0.59	0/3122	0.76	0/4273
3	P	0.53	0/3114	0.72	0/4263
4	D	0.52	0/1956	0.69	0/2658
4	Q	0.43	0/1956	0.67	0/2658
5	E	0.43	0/1547	0.70	3/2103 (0.1%)
5	R	0.46	0/1547	0.71	1/2103 (0.0%)
6	F	0.55	0/911	0.70	0/1219
6	S	0.49	0/911	0.65	0/1219
7	G	0.56	0/698	0.68	0/946
7	T	0.49	0/680	0.64	0/923
8	H	0.48	0/582	0.61	0/779
8	U	0.39	0/561	0.58	0/751
9	I	0.45	0/218	0.69	0/293
9	V	0.44	0/218	0.66	0/293
10	J	0.48	0/508	0.62	0/682
10	W	0.46	0/489	0.63	0/658
All	All	0.49	0/32435	0.69	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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	LEU	N-CA-C	5.94	127.03	111.00
5	E	143	GLY	N-CA-C	5.88	127.80	113.10
5	E	71	LEU	N-CA-C	5.87	126.84	111.00
5	E	70	ALA	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	104	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	266	0
1	N	3437	0	3349	273	0
2	B	3141	0	3142	276	0
2	O	3147	0	3146	300	0
3	C	3020	0	3070	259	0
3	P	3012	0	3058	284	0
4	D	1898	0	1846	154	0
4	Q	1898	0	1846	161	0
5	E	1513	0	1478	136	0
5	R	1513	0	1478	120	0
6	F	891	0	893	65	0
6	S	891	0	893	73	0
7	G	676	0	659	58	0
7	T	658	0	647	63	0
8	H	574	0	548	27	0
8	U	553	0	535	38	0
9	I	285	0	239	30	0
9	V	275	0	238	30	0
10	J	497	0	490	25	0
10	W	478	0	478	33	0
11	A	21	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	49	0	72	2	0
11	E	50	0	77	1	0
11	N	5	0	0	0	0
11	P	99	0	149	6	0
12	A	1	0	0	0	0
12	C	3	0	0	0	0
12	E	2	0	0	0	0
12	P	3	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	20	0
13	P	86	0	60	22	0
14	C	37	0	42	3	0
14	P	37	0	42	4	0
15	C	37	0	28	3	0
15	P	37	0	29	1	0
16	C	40	0	24	2	0
16	D	50	0	44	1	0
16	P	40	0	24	2	0
16	Q	50	0	44	5	0
17	C	6	0	8	1	0
17	P	6	0	8	0	0
18	D	43	0	30	6	0
18	Q	43	0	30	4	0
19	E	4	0	0	2	0
19	R	4	0	0	1	0
20	E	32	0	38	2	0
20	R	32	0	38	3	0
All	All	32701	0	32246	2460	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 38.

All (2460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:157:ILE:HG13	3:P:158:GLY:H	1.04	1.15
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.19	1.12
5:E:119:ASP:HB3	5:E:179:ASN:ND2	1.67	1.07
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.36	1.04
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.38	1.03
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:ILE:H	7:T:29:ILE:HD12	1.25	1.01
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.43	1.00
3:P:271:PRO:HA	14:P:3001:SMA:H10	1.42	1.00
4:D:47:ALA:H	4:D:50:ASN:HD22	1.07	0.97
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.43	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.97
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.31	0.95
2:B:207:VAL:HG12	2:B:208:GLY:H	1.29	0.95
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.33	0.94
7:G:29:ILE:H	7:G:29:ILE:HD12	1.30	0.93
18:D:501:HEC:HMB1	18:D:501:HEC:HBB3	1.50	0.93
5:E:103:GLN:HA	5:E:106:ILE:HB	1.49	0.93
8:U:13:LEU:HD23	8:U:13:LEU:H	1.34	0.93
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.51	0.92
2:O:207:VAL:HG12	2:O:208:GLY:H	1.34	0.92
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.31	0.91
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.52	0.91
2:O:76:THR:HG22	2:O:82:SER:H	1.34	0.90
3:P:157:ILE:HG13	3:P:158:GLY:N	1.81	0.90
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.54	0.90
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.11	0.90
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.50	0.90
1:A:137:GLU:O	1:A:141:MET:HG3	1.73	0.89
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.08	0.89
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.53	0.89
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.53	0.88
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.53	0.88
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.55	0.88
4:D:32:VAL:HG11	4:D:186:VAL:HB	1.56	0.88
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.56	0.87
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.37	0.87
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.56	0.87
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.21	0.86
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.38	0.86
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.40	0.86
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.38	0.86
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.11	0.85
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.58	0.85
2:B:47:ILE:HG12	2:B:120:MET:HE3	1.58	0.85
1:N:137:GLU:O	1:N:141:MET:HG3	1.77	0.85
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.07	0.84
1:N:388:ARG:HH21	1:N:388:ARG:HG3	1.41	0.84
2:O:361:LYS:O	2:O:365:LYS:HG3	1.77	0.84
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.24	0.84
4:Q:215:LEU:HD22	5:R:46:ALA:HB1	1.60	0.84
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.58	0.84
5:R:128:LYS:O	5:R:130:PRO:HD3	1.78	0.83
4:D:235:MET:HB3	7:G:15:THR:HG22	1.61	0.83
2:B:76:THR:HG22	2:B:82:SER:H	1.43	0.83
3:C:46:ILE:HA	13:C:501:HEM:CMC	2.07	0.83
1:A:206:LYS:O	1:A:209:VAL:HG12	1.78	0.83
2:B:274:VAL:O	2:B:278:VAL:HG23	1.78	0.83
10:J:16:ARG:HB3	10:J:19:THR:HG23	1.60	0.83
2:O:398:VAL:O	2:O:402:ILE:HG13	1.79	0.83
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.77	0.83
2:O:274:VAL:O	2:O:278:VAL:HG23	1.78	0.83
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.13	0.82
4:D:47:ALA:N	4:D:50:ASN:HD22	1.75	0.82
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.61	0.82
1:A:130:GLU:O	1:A:134:ILE:HG13	1.80	0.82
2:B:47:ILE:HG12	2:B:120:MET:CE	2.08	0.82
3:C:101:ARG:HD2	3:C:102:GLY:N	1.94	0.81
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.80	0.81
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.62	0.81
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.44	0.81
3:C:247:SER:OG	3:C:250:LEU:HB2	1.81	0.81
18:Q:501:HEC:HMB1	18:Q:501:HEC:HBB3	1.63	0.81
3:P:101:ARG:HD2	3:P:102:GLY:N	1.96	0.81
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.45	0.80
4:Q:32:VAL:HG11	4:Q:186:VAL:HB	1.63	0.80
3:C:101:ARG:HD2	3:C:101:ARG:C	2.01	0.80
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.64	0.80
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.11	0.80
2:O:128:THR:HA	2:O:226:ILE:HD11	1.63	0.80
3:C:146:VAL:HG21	14:C:2001:SMA:H6	1.63	0.80
2:O:150:VAL:HG23	2:O:151:ALA:H	1.47	0.80
3:P:46:ILE:HA	13:P:501:HEM:CMC	2.11	0.80
5:E:73:LYS:HB3	5:E:195:VAL:O	1.80	0.80
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.62	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.47	0.79
2:O:150:VAL:HG23	2:O:151:ALA:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:101:ARG:HD2	3:P:101:ARG:C	2.02	0.79
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.62	0.79
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.17	0.79
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.65	0.79
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.64	0.78
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.65	0.78
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.84	0.78
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.17	0.78
2:B:150:VAL:HG23	2:B:151:ALA:N	1.98	0.78
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.18	0.78
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.47	0.78
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.49	0.78
4:Q:200:GLN:HE21	20:R:3009:PLC:H51	1.48	0.78
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.64	0.78
2:B:361:LYS:O	2:B:365:LYS:HG3	1.83	0.78
1:A:362:ARG:O	1:A:365:MET:HB3	1.84	0.78
1:N:390:ILE:HG23	1:N:394:GLU:OE1	1.84	0.78
3:C:132:TYR:O	3:C:135:PRO:HD2	1.84	0.78
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.48	0.77
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.13	0.77
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.64	0.77
1:A:4:TYR:HA	2:B:113:ARG:HD3	1.66	0.77
2:B:398:VAL:O	2:B:402:ILE:HG13	1.84	0.77
3:C:113:THR:HG21	3:C:201:LEU:HD13	1.67	0.77
7:T:29:ILE:O	7:T:33:ALA:HB3	1.84	0.77
2:B:43:PRO:O	2:B:113:ARG:HG3	1.85	0.77
1:N:90:THR:O	1:N:167:VAL:HG11	1.84	0.77
2:O:76:THR:CG2	2:O:82:SER:H	1.97	0.77
3:P:118:VAL:N	13:P:502:HEM:HBC2	1.99	0.77
2:B:46:ARG:NH2	2:B:376:GLN:HG3	1.99	0.77
2:B:227:ARG:HA	2:B:227:ARG:HE	1.49	0.77
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.66	0.77
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.65	0.76
1:N:49:ASN:ND2	1:N:52:ASN:H	1.83	0.76
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.49	0.76
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.15	0.76
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.68	0.76
2:O:56:ARG:HB2	2:O:171:ALA:HB1	1.67	0.76
8:H:34:ARG:O	8:H:38:GLU:HG2	1.84	0.76
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.68	0.75
3:C:355:ALA:O	3:C:358:SER:HB3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:MET:CE	6:F:87:LYS:H	1.98	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.66	0.75
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.69	0.75
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.01	0.75
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.01	0.75
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.22	0.75
1:N:429:GLU:OE1	7:T:7:LEU:HB2	1.87	0.74
4:Q:120:ARG:HG2	4:Q:120:ARG:HH11	1.51	0.74
6:F:89:TYR:HD1	6:F:90:LEU:N	1.84	0.74
1:N:362:ARG:O	1:N:365:MET:HB3	1.86	0.74
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.70	0.74
3:P:132:TYR:O	3:P:135:PRO:HD2	1.88	0.74
3:C:271:PRO:HA	14:C:2001:SMA:H10	1.69	0.74
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.23	0.74
2:O:325:TYR:HD1	9:V:60:ALA:HB2	1.50	0.74
5:R:58:PHE:O	5:R:61:SER:HB3	1.87	0.73
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.89	0.73
2:B:199:PHE:O	2:B:226:ILE:HG12	1.88	0.73
1:A:390:ILE:HG23	1:A:394:GLU:OE1	1.88	0.73
2:B:207:VAL:HG12	2:B:208:GLY:N	2.02	0.73
1:N:19:LEU:HB3	1:N:21:ASN:OD1	1.88	0.73
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.54	0.73
1:N:45:SER:HA	1:N:48:GLU:HG3	1.69	0.73
2:B:169:LYS:O	2:B:170:THR:HG23	1.88	0.73
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.04	0.73
5:E:102:THR:O	5:E:106:ILE:HG13	1.88	0.73
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.19	0.73
2:O:248:ASN:C	2:O:248:ASN:HD22	1.92	0.73
2:O:345:LYS:C	2:O:347:ALA:H	1.92	0.73
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.70	0.73
8:U:34:ARG:O	8:U:38:GLU:HG2	1.89	0.73
3:C:332:ASN:HD21	3:C:359:TYR:N	1.86	0.73
2:B:76:THR:CG2	2:B:82:SER:H	2.02	0.73
2:O:221:GLU:HG3	2:O:222:GLN:H	1.54	0.73
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.04	0.73
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.71	0.72
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.18	0.72
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.71	0.72
2:B:357:VAL:O	2:B:361:LYS:HG3	1.89	0.72
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.52	0.72
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.23	0.72
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.25	0.72
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.89	0.72
2:B:162:ASN:O	2:B:244:ILE:HD12	1.90	0.72
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.24	0.72
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.05	0.72
1:N:223:TYR:H	1:N:223:TYR:HD2	1.37	0.72
6:S:89:TYR:HD1	6:S:90:LEU:N	1.88	0.72
2:B:248:ASN:C	2:B:248:ASN:HD22	1.92	0.72
2:O:71:LEU:O	2:O:74:PRO:HD2	1.90	0.72
1:N:69:LYS:CE	1:N:70:ARG:HH21	2.02	0.72
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.20	0.72
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.24	0.72
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.53	0.72
5:R:53:ASN:O	5:R:57:GLN:HG3	1.90	0.72
1:A:90:THR:O	1:A:167:VAL:HG11	1.89	0.72
2:B:227:ARG:HA	2:B:227:ARG:NE	2.05	0.71
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.53	0.71
3:P:277:PHE:CD1	3:P:278:ALA:N	2.58	0.71
4:Q:223:LYS:O	4:Q:223:LYS:HD3	1.90	0.71
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.89	0.71
9:I:71:ASN:HD22	9:I:71:ASN:H	1.36	0.71
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.24	0.71
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.71	0.71
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.52	0.71
8:H:40:CYS:O	8:H:44:VAL:HG23	1.89	0.71
1:N:130:GLU:O	1:N:134:ILE:HG13	1.90	0.71
3:P:184:PHE:CD2	13:P:501:HEM:HBC1	2.26	0.71
2:B:111:CYS:HB3	2:B:119:VAL:HG11	1.72	0.71
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.39	0.71
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.72	0.71
1:A:294:LEU:HD11	1:A:334:MET:CE	2.20	0.71
5:E:141:HIS:O	5:E:142:LEU:HD23	1.91	0.71
1:A:45:SER:HA	1:A:48:GLU:HG3	1.71	0.70
3:C:189:ALA:O	3:C:193:ILE:HG13	1.90	0.70
4:D:46:VAL:HG12	4:D:47:ALA:N	2.06	0.70
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.71	0.70
1:A:49:ASN:ND2	1:A:52:ASN:H	1.89	0.70
1:A:269:VAL:HG11	1:A:410:VAL:HG21	1.73	0.70
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.27	0.70
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:53:ASN:O	5:E:57:GLN:HG3	1.91	0.70
1:N:294:LEU:HD11	1:N:334:MET:CE	2.21	0.70
1:N:373:THR:HB	1:N:374:PRO:HD3	1.71	0.70
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.31	0.70
1:A:373:THR:HB	1:A:374:PRO:HD3	1.73	0.70
4:D:222:MET:HE3	5:E:40:THR:HG23	1.74	0.70
4:D:231:LYS:O	6:F:71:LYS:HE3	1.91	0.70
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.74	0.70
7:G:29:ILE:O	7:G:33:ALA:HB3	1.92	0.70
2:O:219:VAL:O	2:O:223:PHE:HB2	1.92	0.70
4:Q:171:TYR:OH	4:Q:182:ILE:HA	1.91	0.70
4:Q:215:LEU:HD22	5:R:46:ALA:CB	2.21	0.70
1:A:294:LEU:HD11	1:A:334:MET:HE1	1.74	0.70
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.25	0.70
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.74	0.70
2:O:24:LEU:HD13	2:O:38:LEU:HB2	1.72	0.70
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.74	0.70
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.73	0.70
3:C:92:PHE:O	3:C:95:ILE:HG22	1.92	0.70
3:C:134:LEU:HB2	3:C:135:PRO:HD3	1.73	0.70
2:O:47:ILE:HG12	2:O:120:MET:HE3	1.72	0.70
3:P:189:ALA:O	3:P:193:ILE:HG13	1.91	0.70
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.73	0.70
8:U:73:LEU:HD12	8:U:73:LEU:O	1.92	0.70
1:A:223:TYR:H	1:A:223:TYR:HD2	1.38	0.69
5:E:58:PHE:O	5:E:61:SER:HB3	1.92	0.69
6:F:61:ARG:NH2	6:F:89:TYR:HE2	1.89	0.69
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.27	0.69
3:P:126:ALA:O	3:P:129:PHE:HB3	1.92	0.69
3:P:247:SER:OG	3:P:250:LEU:HB2	1.91	0.69
2:B:150:VAL:HG23	2:B:151:ALA:H	1.56	0.69
4:D:215:LEU:HD22	5:E:46:ALA:HB1	1.74	0.69
1:N:206:LYS:O	1:N:209:VAL:HG12	1.92	0.69
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.58	0.69
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.22	0.69
16:C:2004:CDL:OA4	7:G:40:ARG:HD2	1.92	0.69
4:D:47:ALA:N	4:D:50:ASN:ND2	2.41	0.69
2:O:150:VAL:CG2	2:O:151:ALA:H	2.06	0.69
2:O:154:SER:O	2:O:157:VAL:HG12	1.92	0.69
2:O:226:ILE:HG22	2:O:227:ARG:N	2.07	0.69
1:A:429:GLU:OE1	7:G:7:LEU:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:PHE:C	7:G:41:PHE:CD2	2.66	0.69
7:G:41:PHE:C	7:G:41:PHE:HD2	1.96	0.69
1:N:49:ASN:C	1:N:49:ASN:HD22	1.95	0.69
2:O:43:PRO:O	2:O:113:ARG:HG3	1.93	0.69
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.08	0.69
2:O:357:VAL:O	2:O:361:LYS:HG3	1.93	0.69
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.28	0.69
1:N:161:THR:HG21	1:N:235:ARG:H	1.57	0.69
3:P:92:PHE:O	3:P:95:ILE:HG22	1.93	0.69
3:P:146:VAL:HG21	14:P:3001:SMA:H6	1.74	0.69
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.22	0.69
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.27	0.68
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.74	0.68
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.56	0.68
2:O:47:ILE:HG12	2:O:120:MET:CE	2.22	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
3:C:282:LEU:O	3:C:282:LEU:HD23	1.94	0.68
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.28	0.68
2:O:207:VAL:HG12	2:O:208:GLY:N	2.07	0.68
2:B:312:PHE:N	2:B:323:GLY:O	2.22	0.68
4:D:223:LYS:O	4:D:223:LYS:HD3	1.94	0.68
8:H:73:LEU:HD12	8:H:73:LEU:O	1.93	0.68
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.76	0.68
3:P:113:THR:HG21	3:P:201:LEU:HD13	1.74	0.68
3:P:135:PRO:HG3	13:P:501:HEM:O1D	1.94	0.68
1:A:49:ASN:C	1:A:49:ASN:HD22	1.97	0.68
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.08	0.68
2:B:341:MET:O	2:B:344:LEU:N	2.26	0.68
1:A:209:VAL:O	1:A:212:ALA:HB3	1.94	0.68
3:C:319:ARG:HB3	3:C:374:GLU:OE1	1.93	0.68
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.75	0.68
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.75	0.68
1:N:246:ASP:HA	1:N:427:PRO:HB3	1.74	0.68
4:D:46:VAL:HG12	4:D:47:ALA:H	1.59	0.67
2:B:353:THR:HG22	2:B:355:GLU:H	1.58	0.67
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.58	0.67
3:P:104:TYR:HD2	3:P:105:TYR:CE1	2.11	0.67
1:A:136:GLN:HG2	9:I:51:CYS:HB3	1.77	0.67
3:C:269:ILE:HG23	3:C:269:ILE:O	1.93	0.67
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.75	0.67
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:94:PRO:HG2	4:Q:95:TYR:HD1	1.60	0.67
2:B:345:LYS:C	2:B:347:ALA:H	1.95	0.67
2:B:359:LYS:HA	2:B:362:ASN:ND2	2.10	0.67
3:C:118:VAL:N	13:C:502:HEM:HBC2	2.10	0.67
8:U:32:LYS:O	8:U:36:ARG:HG3	1.94	0.67
1:A:69:LYS:CE	1:A:70:ARG:HH21	2.03	0.67
2:O:75:LEU:CD2	2:O:136:GLU:HB3	2.24	0.67
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.60	0.67
5:R:77:LYS:HE2	5:R:79:SER:CB	2.24	0.67
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.75	0.67
2:B:62:ASN:O	2:B:65:THR:HG22	1.95	0.67
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.77	0.67
2:O:248:ASN:ND2	2:O:250:HIS:H	1.93	0.67
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.60	0.67
3:C:236:MET:O	3:C:239:PRO:HD2	1.93	0.67
5:E:40:THR:HG21	11:E:2005:PEE:O2P	1.96	0.67
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.76	0.67
4:D:94:PRO:HG2	4:D:95:TYR:CD1	2.30	0.66
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.77	0.66
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.30	0.66
1:A:136:GLN:NE2	9:I:50:LEU:HB2	2.09	0.66
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.31	0.66
4:D:47:ALA:H	4:D:50:ASN:ND2	1.86	0.66
5:R:113:ASP:C	5:R:115:SER:H	1.99	0.66
7:T:41:PHE:C	7:T:41:PHE:CD2	2.67	0.66
2:B:212:LYS:HD2	2:B:214:SER:OG	1.94	0.66
2:O:293:SER:OG	2:O:296:TYR:HB2	1.96	0.66
3:P:254:PRO:HB2	4:Q:118:ASN:O	1.96	0.66
3:P:332:ASN:HD21	3:P:359:TYR:N	1.94	0.66
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.20	0.66
6:F:33:ARG:O	6:F:36:THR:HG23	1.96	0.66
7:T:41:PHE:C	7:T:41:PHE:HD2	1.99	0.66
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.31	0.66
9:V:72:ALA:HB1	9:V:73:PRO:HD3	1.77	0.66
1:A:182:LEU:N	1:A:182:LEU:HD23	2.11	0.66
2:O:29:LEU:HD12	2:O:33:LEU:HD23	1.78	0.66
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.26	0.66
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.96	0.66
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.10	0.66
2:O:47:ILE:HD12	2:O:47:ILE:N	2.08	0.66
3:P:355:ALA:O	3:P:358:SER:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:111:CYS:HB3	2:O:119:VAL:HG11	1.78	0.65
4:Q:94:PRO:HG2	4:Q:95:TYR:CD1	2.30	0.65
4:Q:198:HIS:O	4:Q:201:ARG:HB3	1.95	0.65
4:D:198:HIS:O	4:D:201:ARG:HB3	1.96	0.65
3:C:316:MET:HG2	3:C:319:ARG:HH21	1.61	0.65
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.78	0.65
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.11	0.65
3:C:135:PRO:HG3	13:C:501:HEM:O1D	1.97	0.65
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.43	0.65
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.26	0.65
3:C:254:PRO:HB2	4:D:118:ASN:O	1.95	0.65
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.78	0.65
1:N:295:ALA:O	1:N:298:ALA:HB3	1.96	0.65
2:O:72:ALA:CB	2:O:75:LEU:HD12	2.25	0.65
4:Q:46:VAL:HG12	4:Q:47:ALA:N	2.12	0.65
1:A:161:THR:HG21	1:A:234:CYS:HA	1.77	0.65
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.77	0.65
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.88	0.65
1:A:246:ASP:HA	1:A:427:PRO:HB3	1.78	0.65
2:B:47:ILE:HD12	2:B:47:ILE:N	2.11	0.65
1:N:335:MET:HG3	1:N:339:GLN:HE21	1.60	0.65
6:S:50:LEU:HD21	6:S:90:LEU:HD12	1.79	0.65
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.79	0.65
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.43	0.65
8:U:13:LEU:HD23	8:U:13:LEU:N	2.08	0.65
1:A:5:ALA:O	1:A:8:LEU:HB2	1.97	0.65
3:C:277:PHE:CD1	3:C:278:ALA:N	2.64	0.65
3:P:157:ILE:HD12	3:P:161:LEU:HD12	1.79	0.65
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.64	0.65
1:A:388:ARG:HG3	1:A:388:ARG:NH2	2.12	0.64
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.27	0.64
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.17	0.64
18:D:501:HEC:HBC3	18:D:501:HEC:HMC1	1.79	0.64
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.63	0.64
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.79	0.64
2:O:29:LEU:CD2	2:O:30:PRO:HD2	2.27	0.64
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.31	0.64
5:R:91:TRP:CE3	5:R:96:LEU:HD22	2.33	0.64
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.62	0.64
3:P:6:ARG:HD3	3:P:16:ASN:OD1	1.97	0.64
5:R:166:ASP:HB3	5:R:172:ARG:HH11	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:13:MET:HA	6:S:16:ILE:HB	1.79	0.64
6:S:63:LYS:HD3	7:T:13:ILE:HG21	1.79	0.64
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.80	0.64
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.33	0.64
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.13	0.64
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.32	0.64
1:A:35:CYS:HA	1:A:372:THR:HG21	1.78	0.64
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.32	0.64
2:O:353:THR:HG22	2:O:355:GLU:H	1.62	0.64
2:O:359:LYS:HA	2:O:362:ASN:ND2	2.12	0.64
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.28	0.64
1:N:23:LEU:HA	1:N:192:ALA:O	1.98	0.64
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.33	0.64
4:Q:46:VAL:HG12	4:Q:47:ALA:H	1.63	0.64
1:N:379:ILE:HG12	1:N:389:ARG:HE	1.64	0.64
3:P:157:ILE:O	3:P:159:HIS:N	2.31	0.64
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.66	0.64
4:D:218:LEU:HD13	5:E:43:ALA:HA	1.80	0.63
1:N:432:LEU:HD23	1:N:433:ASP:H	1.62	0.63
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.25	0.63
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.80	0.63
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.34	0.63
6:S:13:MET:O	6:S:17:ARG:HG3	1.97	0.63
4:D:10:PHE:CD1	4:D:10:PHE:N	2.66	0.63
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.34	0.63
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.38	0.63
6:F:31:LEU:HD21	6:F:65:ALA:HB2	1.79	0.63
9:I:32:UNK:N	9:I:73:PRO:HG2	2.14	0.63
7:T:41:PHE:HD2	7:T:41:PHE:O	1.80	0.63
2:B:71:LEU:O	2:B:74:PRO:HD2	1.98	0.63
2:B:72:ALA:CB	2:B:75:LEU:HD12	2.29	0.63
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.80	0.63
4:D:171:TYR:OH	4:D:182:ILE:HA	1.99	0.63
4:D:235:MET:HE3	6:F:60:PHE:CE1	2.31	0.63
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.63	0.63
1:N:5:ALA:O	1:N:8:LEU:HB2	1.98	0.63
2:O:62:ASN:O	2:O:65:THR:HG22	1.98	0.63
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.79	0.63
1:N:35:CYS:HA	1:N:372:THR:HG21	1.81	0.63
1:N:49:ASN:ND2	1:N:51:LYS:H	1.96	0.63
1:N:253:VAL:HG11	1:N:335:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.62	0.63
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.63	0.63
5:R:73:LYS:HB3	5:R:195:VAL:O	1.98	0.63
5:R:165:TYR:CE2	5:R:180:LEU:HG	2.33	0.63
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.28	0.63
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.81	0.63
5:R:32:ARG:HH12	7:T:22:GLU:CD	2.01	0.63
7:G:58:LEU:HD12	7:G:58:LEU:O	1.99	0.63
2:O:341:MET:O	2:O:344:LEU:N	2.30	0.63
3:P:123:THR:HG21	3:P:190:ILE:HG13	1.79	0.63
3:C:30:ALA:O	3:C:32:TRP:N	2.31	0.62
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.12	0.62
2:O:147:ASP:OD1	9:V:68:ILE:HD11	1.98	0.62
2:B:24:LEU:HD13	2:B:38:LEU:HB2	1.79	0.62
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.14	0.62
3:C:207:ASN:O	3:C:208:ASN:HB3	1.98	0.62
4:D:164:ILE:HG21	4:D:182:ILE:HG21	1.81	0.62
6:S:68:LEU:O	6:S:71:LYS:N	2.26	0.62
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.82	0.62
1:A:182:LEU:O	1:A:186:ILE:HG13	1.98	0.62
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.34	0.62
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.14	0.62
3:C:36:SER:O	3:C:39:ALA:HB3	1.99	0.62
3:C:316:MET:HG2	3:C:319:ARG:NH2	2.14	0.62
1:N:105:ASP:O	1:N:109:VAL:HG23	1.99	0.62
3:P:70:THR:HA	3:P:74:VAL:CG2	2.29	0.62
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.34	0.62
2:B:220:ALA:O	2:B:224:LEU:HB2	1.98	0.62
9:I:65:VAL:HG12	9:I:66:ALA:N	2.15	0.62
1:A:406:MET:O	1:A:410:VAL:HG23	1.99	0.62
1:N:49:ASN:HD21	1:N:52:ASN:H	1.46	0.62
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.35	0.62
6:S:11:ARG:HG2	6:S:11:ARG:O	2.00	0.62
6:S:67:ASP:OD1	6:S:71:LYS:HD2	1.99	0.62
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.64	0.62
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.82	0.62
6:F:68:LEU:O	6:F:71:LYS:N	2.30	0.62
1:N:61:HIS:CE1	1:N:137:GLU:OE1	2.53	0.62
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.15	0.62
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.64	0.62
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:501:HEC:HMB1	18:D:501:HEC:CBB	2.28	0.62
2:O:226:ILE:HG22	2:O:227:ARG:H	1.63	0.62
5:R:109:GLU:O	5:R:123:ASP:HB2	1.99	0.62
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.35	0.62
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.34	0.62
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.35	0.62
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.15	0.61
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.15	0.61
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.81	0.61
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.34	0.61
4:D:116:ILE:HG23	4:D:117:VAL:N	2.14	0.61
8:H:58:LEU:HG	8:H:62:LEU:HD12	1.82	0.61
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.82	0.61
3:P:95:ILE:CD1	3:P:121:LEU:HD13	2.29	0.61
5:R:109:GLU:OE1	5:R:166:ASP:HB2	2.00	0.61
1:A:161:THR:HG21	1:A:235:ARG:H	1.65	0.61
1:A:240:GLU:OE1	1:A:434:TYR:HB2	1.99	0.61
2:B:58:GLU:OE1	2:B:64:GLY:N	2.33	0.61
2:B:109:VAL:CG1	2:B:123:LEU:HB2	2.30	0.61
3:C:63:ALA:HB2	3:C:176:LEU:HD21	1.80	0.61
4:D:8:PRO:HG2	4:D:10:PHE:HE1	1.63	0.61
1:N:406:MET:O	1:N:410:VAL:HG23	2.00	0.61
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.66	0.61
2:B:150:VAL:CG2	2:B:151:ALA:H	2.13	0.61
4:D:43:MET:HE3	4:D:91:PHE:HE2	1.65	0.61
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.30	0.61
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.35	0.61
3:C:345:GLU:O	3:C:349:ILE:HG13	2.01	0.61
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.16	0.61
3:P:282:LEU:HD23	3:P:282:LEU:C	2.20	0.61
2:B:150:VAL:CG2	2:B:151:ALA:N	2.63	0.61
1:N:49:ASN:ND2	1:N:49:ASN:C	2.51	0.61
2:O:150:VAL:CG2	2:O:151:ALA:N	2.62	0.61
4:D:94:PRO:HG2	4:D:95:TYR:HD1	1.66	0.61
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.66	0.61
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.30	0.61
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.81	0.61
4:D:167:GLU:O	4:D:169:LEU:N	2.34	0.61
4:D:223:LYS:HD3	4:D:223:LYS:C	2.20	0.61
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.82	0.61
2:O:312:PHE:N	2:O:323:GLY:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.15	0.61
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.36	0.61
1:A:156:THR:HA	5:E:7:VAL:HG21	1.83	0.61
1:A:335:MET:CG	1:A:339:GLN:HE21	2.13	0.61
3:C:70:THR:HA	3:C:74:VAL:HG23	1.82	0.61
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.31	0.61
1:N:281:ASP:O	1:N:284:PHE:HD1	1.84	0.61
1:N:307:PHE:CD1	1:N:307:PHE:C	2.74	0.61
5:R:34:GLY:HA2	10:W:10:TYR:HB2	1.83	0.61
3:C:30:ALA:C	3:C:32:TRP:H	2.04	0.60
3:C:282:LEU:HD23	3:C:282:LEU:C	2.21	0.60
4:D:155:GLY:C	4:D:157:ALA:H	2.04	0.60
3:P:242:THR:N	4:Q:208:MET:HE1	2.15	0.60
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.01	0.60
6:S:32:MET:CE	6:S:87:LYS:H	2.13	0.60
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.83	0.60
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.31	0.60
3:C:173:ASN:N	3:C:174:PRO:HD2	2.16	0.60
3:C:184:PHE:CD2	13:C:501:HEM:HBC1	2.35	0.60
1:N:240:GLU:OE1	1:N:434:TYR:HB2	2.02	0.60
1:A:27:SER:HB2	1:A:199:ALA:O	2.01	0.60
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.35	0.60
2:O:312:PHE:HE1	9:V:62:ARG:O	1.84	0.60
3:P:70:THR:HA	3:P:74:VAL:HG23	1.83	0.60
3:P:342:GLN:HA	3:P:342:GLN:NE2	2.15	0.60
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.83	0.60
1:N:388:ARG:HG3	1:N:388:ARG:NH2	2.15	0.60
1:A:89:TYR:O	1:A:95:THR:HG23	2.01	0.60
5:E:128:LYS:O	5:E:130:PRO:HD3	2.02	0.60
1:N:182:LEU:N	1:N:182:LEU:HD23	2.17	0.60
3:P:123:THR:HG22	3:P:190:ILE:HD11	1.83	0.60
1:N:182:LEU:O	1:N:186:ILE:HG13	2.00	0.60
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.37	0.60
3:P:134:LEU:HB2	3:P:135:PRO:HD3	1.82	0.60
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.65	0.60
2:B:396:SER:O	2:B:399:ALA:HB3	2.01	0.60
4:D:102:ARG:HH11	4:D:102:ARG:HG2	1.67	0.60
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.84	0.60
1:N:86:PHE:CD2	1:N:99:ILE:HD11	2.36	0.60
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.37	0.60
2:B:109:VAL:HG13	2:B:123:LEU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.83	0.60
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.02	0.60
2:O:219:VAL:HG13	2:O:223:PHE:CD1	2.37	0.60
2:B:230:ALA:O	2:B:232:THR:N	2.35	0.59
1:N:86:PHE:HB3	2:O:285:ILE:HG22	1.83	0.59
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.84	0.59
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.82	0.59
3:P:325:LEU:HD21	3:P:366:LEU:CB	2.32	0.59
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.36	0.59
2:B:140:LEU:HD12	2:B:140:LEU:O	2.02	0.59
2:B:332:HIS:O	2:B:336:VAL:HG23	2.02	0.59
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.84	0.59
1:N:255:LEU:HD13	1:N:422:LEU:CD1	2.31	0.59
2:O:332:HIS:O	2:O:336:VAL:HG23	2.02	0.59
2:B:248:ASN:ND2	2:B:250:HIS:H	2.00	0.59
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.84	0.59
2:O:76:THR:HG22	2:O:82:SER:N	2.13	0.59
3:P:27:ASN:ND2	3:P:209:PRO:HD2	2.16	0.59
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.36	0.59
10:J:25:VAL:O	10:J:29:VAL:HG23	2.01	0.59
1:N:161:THR:HG21	1:N:234:CYS:HA	1.83	0.59
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.84	0.59
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.03	0.59
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.37	0.59
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.37	0.59
2:O:73:SER:N	2:O:74:PRO:HD2	2.17	0.59
2:O:227:ARG:HG3	2:O:228:SER:N	2.17	0.59
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.84	0.59
3:C:21:ASP:O	3:C:23:PRO:HD3	2.03	0.59
3:P:21:ASP:O	3:P:23:PRO:HD3	2.01	0.59
4:Q:167:GLU:O	4:Q:169:LEU:N	2.36	0.59
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.32	0.59
1:A:310:PHE:HE1	1:A:322:PHE:N	2.00	0.59
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.66	0.59
9:V:65:VAL:HG12	9:V:66:ALA:N	2.17	0.59
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.38	0.59
2:B:295:LEU:HA	2:B:343:GLN:HG2	1.85	0.59
4:D:215:LEU:HD22	5:E:46:ALA:CB	2.31	0.59
5:E:171:ILE:HG12	5:E:176:ALA:O	2.02	0.59
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.84	0.59
2:O:220:ALA:O	2:O:224:LEU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.21	0.59
1:A:242:ARG:O	7:G:14:ILE:HA	2.03	0.59
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.83	0.59
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.84	0.59
16:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.03	0.59
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.36	0.59
3:C:104:TYR:HD2	3:C:105:TYR:CE1	2.21	0.58
3:P:154:ILE:HG23	3:P:155:PRO:HD2	1.84	0.58
3:P:173:ASN:N	3:P:174:PRO:HD2	2.17	0.58
5:R:134:ILE:HB	5:R:185:TYR:CE2	2.38	0.58
1:A:241:ILE:HG23	1:A:241:ILE:O	2.03	0.58
4:D:130:LEU:HD12	4:D:150:ASN:ND2	2.17	0.58
5:E:38:LEU:HA	10:J:14:PHE:CE1	2.38	0.58
7:G:41:PHE:HD2	7:G:41:PHE:O	1.85	0.58
1:N:45:SER:HA	1:N:48:GLU:CG	2.33	0.58
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.17	0.58
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.03	0.58
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.85	0.58
2:B:75:LEU:CD2	2:B:136:GLU:HB3	2.33	0.58
3:C:76:TYR:CE1	5:E:57:GLN:HG2	2.39	0.58
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.19	0.58
1:N:253:VAL:HG11	1:N:335:MET:CE	2.33	0.58
2:O:58:GLU:OE1	2:O:64:GLY:N	2.36	0.58
2:O:162:ASN:O	2:O:244:ILE:HD12	2.03	0.58
6:S:61:ARG:NH2	6:S:89:TYR:HE2	1.95	0.58
1:A:45:SER:HA	1:A:48:GLU:CG	2.34	0.58
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.38	0.58
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.85	0.58
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.38	0.58
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.86	0.58
2:O:206:LEU:HG	2:O:216:LEU:HD11	1.85	0.58
2:O:207:VAL:O	2:O:216:LEU:HD21	2.03	0.58
3:P:26:SER:HA	3:P:219:ILE:CD1	2.33	0.58
3:P:36:SER:O	3:P:39:ALA:HB3	2.03	0.58
6:S:32:MET:HE3	6:S:87:LYS:HB2	1.83	0.58
3:C:311:SER:HB2	3:C:319:ARG:HH11	1.68	0.58
4:D:43:MET:HE3	4:D:91:PHE:CE2	2.38	0.58
5:E:185:TYR:O	5:E:186:GLN:HB2	2.04	0.58
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.38	0.58
3:P:52:LEU:HD13	13:P:501:HEM:HBD1	1.85	0.58
3:P:365:ILE:HG22	3:P:366:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CE1	1:A:322:PHE:N	2.71	0.58
2:B:102:ARG:CZ	2:B:164:HIS:CD2	2.87	0.58
3:P:120:LEU:HD22	13:P:502:HEM:HBB1	1.84	0.58
9:V:65:VAL:O	9:V:76:VAL:HG23	2.04	0.58
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.68	0.58
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.33	0.58
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.38	0.58
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.58
1:A:379:ILE:HG12	1:A:389:ARG:HE	1.69	0.58
4:D:167:GLU:C	4:D:169:LEU:H	2.06	0.58
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.31	0.58
3:P:141:PHE:O	3:P:144:ALA:HB3	2.04	0.58
3:P:333:LEU:HD11	11:P:3007:PEE:H38	1.86	0.58
5:R:69:LEU:HD13	5:R:71:LEU:HD11	1.85	0.58
1:N:410:VAL:O	1:N:413:LYS:HB3	2.03	0.58
2:O:109:VAL:HG13	2:O:123:LEU:HB2	1.86	0.58
3:P:130:VAL:HG23	3:P:131:GLY:N	2.19	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.38	0.58
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.85	0.58
2:B:189:GLU:O	2:B:191:LEU:N	2.36	0.58
2:B:203:ARG:O	2:B:387:LEU:HD11	2.04	0.58
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.38	0.58
3:C:247:SER:HG	3:C:250:LEU:HB2	1.68	0.58
5:R:57:GLN:OE1	20:R:3009:PLC:H12	2.03	0.58
6:S:71:LYS:O	6:S:72:HIS:HB2	2.04	0.58
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.39	0.57
1:A:40:TRP:O	1:A:384:LEU:HD22	2.04	0.57
4:D:116:ILE:HG23	4:D:117:VAL:H	1.69	0.57
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.85	0.57
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.39	0.57
2:O:248:ASN:C	2:O:248:ASN:ND2	2.54	0.57
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.38	0.57
1:A:49:ASN:ND2	1:A:49:ASN:C	2.56	0.57
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.57
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.34	0.57
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.24	0.57
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.22	0.57
3:P:166:TRP:CD1	3:P:171:VAL:HG22	2.40	0.57
4:Q:224:ARG:HH12	16:Q:3003:CDL:HB21	1.69	0.57
1:A:61:HIS:CE1	1:A:137:GLU:OE1	2.57	0.57
2:B:67:HIS:O	2:B:70:ARG:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:GLU:O	2:B:192:HIS:N	2.37	0.57
2:B:293:SER:OG	2:B:296:TYR:HB2	2.05	0.57
6:F:32:MET:HE3	6:F:87:LYS:H	1.67	0.57
3:P:76:TYR:CE1	5:R:57:GLN:HG2	2.40	0.57
3:P:282:LEU:HD23	3:P:282:LEU:O	2.04	0.57
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.39	0.57
8:U:40:CYS:O	8:U:44:VAL:HG23	2.04	0.57
1:A:86:PHE:HB3	2:B:285:ILE:HG22	1.86	0.57
1:A:178:THR:HB	1:A:181:ASP:OD1	2.05	0.57
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.40	0.57
2:O:27:THR:HG22	2:O:28:LYS:N	2.17	0.57
7:T:42:SER:O	7:T:45:VAL:HG12	2.05	0.57
2:B:318:ASP:O	2:B:319:SER:HB2	2.04	0.57
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.40	0.57
1:N:254:ALA:HB3	1:N:423:ALA:HB3	1.87	0.57
3:P:137:GLY:N	3:P:140:SER:HB2	2.20	0.57
3:P:184:PHE:HA	13:P:501:HEM:CBC	2.34	0.57
6:S:21:TYR:C	6:S:21:TYR:CD2	2.78	0.57
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.87	0.57
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.03	0.57
2:B:258:VAL:HB	2:B:322:PHE:O	2.05	0.57
4:D:42:SER:HB2	4:D:112:ASP:OD2	2.04	0.57
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.40	0.57
1:N:239:SER:HB2	7:T:17:SER:O	2.04	0.57
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.19	0.57
3:P:5:ILE:HG22	3:P:12:LEU:HD12	1.86	0.57
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.25	0.57
2:O:146:VAL:HG12	2:O:147:ASP:N	2.19	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.87	0.57
3:P:207:ASN:O	3:P:208:ASN:HB3	2.03	0.57
3:P:269:ILE:HG23	3:P:269:ILE:O	2.05	0.57
4:D:10:PHE:H	4:D:10:PHE:HD1	1.52	0.57
4:D:227:TRP:O	4:D:228:SER:C	2.41	0.57
5:E:108:GLN:O	5:E:112:VAL:HG23	2.04	0.57
6:F:27:ASN:HB2	6:F:81:VAL:HB	1.86	0.57
2:O:42:SER:OG	2:O:43:PRO:HD2	2.05	0.57
2:O:209:ILE:HG22	2:O:210:GLY:N	2.19	0.57
3:P:30:ALA:C	3:P:32:TRP:H	2.09	0.57
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	1.87	0.57
10:W:56:LYS:HE2	10:W:60:GLU:CD	2.25	0.57
1:A:49:ASN:HD21	1:A:52:ASN:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:ILE:O	4:D:168:ILE:HG12	2.05	0.57
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.40	0.57
5:R:135:LEU:CD2	5:R:169:GLY:HA3	2.35	0.57
2:B:86:THR:O	2:B:90:GLU:HG3	2.05	0.56
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.87	0.56
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.35	0.56
3:C:126:ALA:O	3:C:129:PHE:HB3	2.04	0.56
4:D:232:SER:HB3	7:G:23:GLN:NE2	2.19	0.56
5:E:35:PHE:O	5:E:38:LEU:N	2.38	0.56
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.86	0.56
1:N:333:ASP:O	1:N:336:PHE:HB3	2.05	0.56
1:N:394:GLU:O	1:N:395:TRP:C	2.44	0.56
10:W:14:PHE:N	10:W:14:PHE:CD2	2.70	0.56
10:W:22:LEU:N	10:W:22:LEU:HD23	2.20	0.56
2:B:272:PHE:O	2:B:275:LEU:N	2.38	0.56
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.69	0.56
6:F:72:HIS:O	6:F:73:ARG:HD3	2.05	0.56
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.40	0.56
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.86	0.56
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.34	0.56
1:A:46:ARG:HD3	1:A:231:LEU:HD13	1.88	0.56
1:A:180:ALA:O	1:A:183:ALA:HB3	2.05	0.56
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.35	0.56
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.40	0.56
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.05	0.56
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.38	0.56
3:P:230:ILE:HG23	11:P:3005:PEE:H25	1.88	0.56
6:S:68:LEU:O	6:S:70:LEU:N	2.38	0.56
6:S:73:ARG:HH11	6:S:73:ARG:HG3	1.70	0.56
7:T:58:LEU:HD12	7:T:58:LEU:O	2.06	0.56
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.87	0.56
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.86	0.56
5:E:103:GLN:HA	5:E:106:ILE:CB	2.30	0.56
2:O:308:ASP:OD1	9:V:56:SER:HA	2.06	0.56
3:P:106:GLY:HA2	3:P:108:TYR:CD2	2.39	0.56
4:Q:155:GLY:C	4:Q:157:ALA:H	2.08	0.56
4:Q:218:LEU:HD13	5:R:43:ALA:HA	1.87	0.56
1:A:23:LEU:HA	1:A:192:ALA:O	2.06	0.56
3:C:22:LEU:HD12	3:C:23:PRO:N	2.20	0.56
3:C:134:LEU:HD21	3:C:180:PHE:HA	1.86	0.56
5:R:44:CYS:HB3	10:W:24:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASP:O	1:A:333:ASP:C	2.43	0.56
4:D:235:MET:HE3	6:F:60:PHE:HE1	1.69	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.56
5:R:62:LEU:O	5:R:63:SER:O	2.23	0.56
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.39	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.41	0.56
3:C:70:THR:HA	3:C:74:VAL:CG2	2.36	0.56
5:E:148:ALA:HA	5:E:156:TYR:CD2	2.41	0.56
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.06	0.56
2:B:333:ALA:O	2:B:337:ILE:HG13	2.05	0.56
6:F:32:MET:O	6:F:35:ASP:HB2	2.06	0.56
10:J:22:LEU:N	10:J:22:LEU:HD23	2.20	0.56
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.41	0.56
4:Q:47:ALA:HB1	4:Q:89:ASP:O	2.05	0.56
18:Q:501:HEC:HBC3	18:Q:501:HEC:HMC1	1.87	0.56
3:C:45:GLN:CB	13:C:501:HEM:HAB	2.36	0.56
3:C:285:ILE:HD12	3:C:285:ILE:N	2.21	0.56
7:G:42:SER:O	7:G:45:VAL:HG12	2.06	0.56
1:N:335:MET:CG	1:N:339:GLN:HE21	2.18	0.56
2:O:396:SER:O	2:O:399:ALA:HB3	2.06	0.56
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.86	0.56
2:B:239:TYR:HE1	2:B:260:GLU:N	2.04	0.56
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.71	0.56
5:E:29:SER:HA	5:E:32:ARG:HH21	1.71	0.56
1:N:209:VAL:O	1:N:212:ALA:HB3	2.05	0.56
2:O:47:ILE:N	2:O:47:ILE:CD1	2.68	0.56
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.42	0.56
2:O:345:LYS:C	2:O:347:ALA:N	2.59	0.56
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.06	0.56
6:S:27:ASN:HB2	6:S:81:VAL:HB	1.87	0.56
1:A:186:ILE:O	1:A:190:PHE:HB2	2.06	0.55
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.70	0.55
2:B:146:VAL:HG12	2:B:147:ASP:N	2.22	0.55
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.41	0.55
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.36	0.55
10:J:14:PHE:CD2	10:J:14:PHE:N	2.71	0.55
3:P:45:GLN:CB	13:P:501:HEM:HAB	2.36	0.55
3:P:231:LEU:HD11	4:Q:220:TYR:HA	1.88	0.55
5:R:1:VAL:HG23	5:R:3:ASN:H	1.70	0.55
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.32	0.55
1:A:49:ASN:ND2	1:A:51:LYS:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:O	1:A:110:VAL:HG23	2.06	0.55
3:C:9:HIS:ND1	3:C:10:PRO:HD2	2.21	0.55
1:N:318:GLY:O	1:N:319:LEU:HD23	2.07	0.55
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.15	0.55
3:P:27:ASN:ND2	3:P:208:ASN:OD1	2.35	0.55
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.88	0.55
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.87	0.55
1:A:342:TRP:O	1:A:345:LEU:HB2	2.06	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.88	0.55
5:E:171:ILE:N	5:E:179:ASN:OD1	2.37	0.55
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.22	0.55
3:P:276:LEU:O	3:P:279:TYR:HB3	2.06	0.55
7:T:29:ILE:O	7:T:34:LEU:HG	2.07	0.55
2:B:27:THR:HG22	2:B:28:LYS:H	1.71	0.55
3:C:365:ILE:HG22	3:C:366:LEU:HD23	1.86	0.55
5:E:136:VAL:O	5:E:138:VAL:N	2.37	0.55
5:E:157:TYR:HE1	5:E:162:GLY:HA2	1.69	0.55
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.06	0.55
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.41	0.55
2:O:273:SER:O	2:O:276:GLN:HB3	2.07	0.55
4:Q:167:GLU:C	4:Q:169:LEU:H	2.10	0.55
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.41	0.55
6:F:63:LYS:HD3	7:G:13:ILE:HG21	1.88	0.55
6:F:71:LYS:O	6:F:72:HIS:HB2	2.04	0.55
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.72	0.55
4:Q:235:MET:HE3	6:S:60:PHE:CE1	2.40	0.55
2:B:248:ASN:C	2:B:248:ASN:ND2	2.56	0.55
2:O:170:THR:O	2:O:172:LEU:N	2.40	0.55
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.41	0.55
3:P:117:GLY:C	13:P:502:HEM:HBC2	2.27	0.55
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.41	0.55
2:B:47:ILE:N	2:B:47:ILE:CD1	2.70	0.55
2:B:292:THR:O	2:B:292:THR:HG22	2.06	0.55
3:P:316:MET:HG2	3:P:319:ARG:HH21	1.70	0.55
1:A:75:PHE:O	1:A:79:VAL:HG23	2.07	0.55
2:B:229:GLY:O	2:B:231:GLY:N	2.39	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.55
3:C:79:LEU:O	3:C:79:LEU:HD12	2.06	0.55
1:N:19:LEU:O	1:N:21:ASN:N	2.40	0.55
1:N:86:PHE:O	2:O:285:ILE:HA	2.06	0.55
3:P:137:GLY:H	3:P:140:SER:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:32:MET:O	6:S:35:ASP:HB2	2.06	0.55
2:B:393:THR:CG2	2:B:397:VAL:HB	2.37	0.55
1:N:4:TYR:HA	2:O:113:ARG:HD3	1.89	0.55
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.42	0.55
1:N:281:ASP:HB3	1:N:284:PHE:HE1	1.71	0.55
2:O:122:TYR:O	2:O:126:VAL:HG23	2.07	0.55
4:Q:220:TYR:CE2	16:Q:3003:CDL:H722	2.42	0.55
5:R:188:VAL:HG23	5:R:188:VAL:O	2.06	0.55
6:S:13:MET:HB2	6:S:17:ARG:NH1	2.21	0.55
10:W:59:TYR:O	10:W:60:GLU:O	2.24	0.55
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.88	0.55
2:O:272:PHE:O	2:O:276:GLN:N	2.40	0.55
4:Q:120:ARG:HG2	4:Q:120:ARG:NH1	2.18	0.55
6:S:32:MET:HE1	6:S:87:LYS:HG2	1.88	0.55
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.42	0.54
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.42	0.54
2:B:170:THR:O	2:B:172:LEU:N	2.40	0.54
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.88	0.54
1:N:124:GLU:O	1:N:124:GLU:HG2	2.08	0.54
2:O:81:SER:O	2:O:83:PHE:N	2.40	0.54
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.07	0.54
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.07	0.54
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.42	0.54
1:A:410:VAL:O	1:A:413:LYS:HB3	2.08	0.54
3:C:156:TYR:CD2	3:C:156:TYR:N	2.74	0.54
5:E:136:VAL:HB	5:E:181:GLU:HB3	1.88	0.54
2:O:239:TYR:CD2	2:O:240:TRP:N	2.75	0.54
3:P:27:ASN:HD21	3:P:208:ASN:CG	2.10	0.54
3:P:231:LEU:CD1	4:Q:220:TYR:HA	2.37	0.54
5:R:83:GLU:CG	5:R:102:THR:HG22	2.28	0.54
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.43	0.54
2:B:272:PHE:O	2:B:276:GLN:N	2.37	0.54
3:C:286:PRO:HA	5:R:175:PRO:HB3	1.90	0.54
2:O:258:VAL:HB	2:O:322:PHE:O	2.06	0.54
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.42	0.54
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.07	0.54
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.88	0.54
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.42	0.54
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.16	0.54
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.88	0.54
2:O:169:LYS:O	2:O:170:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:37:LEU:HD21	3:P:232:GLY:O	2.07	0.54
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.54
1:A:339:GLN:HE22	1:A:437:ILE:HG23	1.71	0.54
3:C:162:VAL:O	3:C:163:GLU:C	2.45	0.54
3:C:278:ALA:HB1	3:C:295:LEU:HD13	1.87	0.54
3:C:347:PRO:O	3:C:350:ILE:HG22	2.08	0.54
3:C:380:TYR:OH	6:F:34:ASP:HA	2.08	0.54
1:N:206:LYS:O	1:N:208:LEU:N	2.40	0.54
8:U:13:LEU:H	8:U:13:LEU:CD2	2.15	0.54
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.69	0.54
1:A:269:VAL:HG11	1:A:410:VAL:CG2	2.38	0.54
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.07	0.54
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.88	0.54
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.43	0.54
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.89	0.54
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.89	0.54
4:D:191:ARG:O	4:D:192:TRP:C	2.45	0.54
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.88	0.54
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.88	0.54
3:P:101:ARG:HH22	13:P:502:HEM:CGA	2.21	0.54
3:P:273:TRP:CE3	3:P:274:TYR:HA	2.43	0.54
5:R:140:THR:HG21	5:R:178:TYR:HB2	1.89	0.54
1:A:295:ALA:O	1:A:298:ALA:HB3	2.08	0.54
2:B:31:ASN:HD22	2:B:32:GLY:H	1.56	0.54
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.90	0.54
2:B:273:SER:O	2:B:276:GLN:HB3	2.08	0.54
6:F:52:GLU:HG2	6:F:56:ASN:ND2	2.22	0.54
2:O:63:LEU:O	2:O:65:THR:N	2.38	0.54
2:O:350:GLY:O	2:O:352:VAL:N	2.32	0.54
3:P:95:ILE:HD13	3:P:121:LEU:HD12	1.90	0.54
3:P:236:MET:O	3:P:239:PRO:HD2	2.08	0.54
6:S:72:HIS:O	6:S:73:ARG:HD3	2.07	0.54
1:A:248:LEU:HB3	1:A:249:PRO:HD2	1.90	0.54
3:C:6:ARG:HD3	3:C:16:ASN:OD1	2.07	0.54
4:D:142:VAL:HG23	4:D:142:VAL:O	2.08	0.54
5:E:83:GLU:HA	5:E:100:HIS:CG	2.43	0.54
6:F:74:ILE:HG13	6:F:75:LEU:N	2.22	0.54
1:N:158:PHE:O	1:N:159:GLN:O	2.26	0.54
1:N:371:GLY:O	1:N:375:VAL:HG23	2.08	0.54
4:Q:54:VAL:HG11	4:Q:192:TRP:CE2	2.43	0.54
4:Q:191:ARG:O	4:Q:192:TRP:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.89	0.54
2:B:312:PHE:HE1	9:I:62:ARG:O	1.91	0.54
1:N:433:ASP:O	1:N:437:ILE:HG13	2.08	0.54
3:P:366:LEU:HD23	3:P:366:LEU:N	2.23	0.54
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.89	0.53
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.39	0.53
2:O:97:SER:HA	9:V:69:SER:HA	1.90	0.53
3:P:104:TYR:HD2	3:P:105:TYR:CD1	2.27	0.53
5:R:136:VAL:O	5:R:138:VAL:N	2.35	0.53
3:C:160:THR:O	3:C:163:GLU:HB3	2.09	0.53
5:E:177:PRO:O	5:E:178:TYR:HD1	1.91	0.53
2:O:318:ASP:O	2:O:319:SER:HB2	2.08	0.53
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.23	0.53
6:F:50:LEU:HD21	6:F:90:LEU:HD12	1.89	0.53
7:G:81:GLN:O	8:H:47:ARG:HA	2.08	0.53
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.71	0.53
3:P:113:THR:HG21	3:P:201:LEU:CD1	2.39	0.53
4:Q:164:ILE:HD11	4:Q:183:ALA:HB2	1.89	0.53
2:B:239:TYR:HE1	2:B:260:GLU:H	1.56	0.53
3:C:242:THR:N	4:D:208:MET:HE1	2.22	0.53
3:C:325:LEU:HD21	3:C:366:LEU:CB	2.38	0.53
4:D:167:GLU:C	4:D:169:LEU:N	2.62	0.53
6:F:67:ASP:OD1	6:F:71:LYS:HD2	2.08	0.53
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.49	0.53
1:N:304:CYS:HA	1:N:326:ALA:HB2	1.91	0.53
2:O:428:GLY:O	2:O:430:LEU:HG	2.08	0.53
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.89	0.53
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.08	0.53
4:Q:222:MET:HE3	5:R:40:THR:HA	1.90	0.53
1:A:307:PHE:CD1	1:A:307:PHE:C	2.82	0.53
5:E:62:LEU:O	5:E:63:SER:O	2.27	0.53
1:N:411:CYS:O	1:N:415:ILE:HG13	2.09	0.53
5:R:51:ALA:O	5:R:52:LYS:C	2.47	0.53
2:B:122:TYR:O	2:B:126:VAL:HG23	2.08	0.53
3:C:148:THR:O	3:C:151:PHE:HD1	1.92	0.53
4:D:44:ASP:OD1	4:D:44:ASP:N	2.42	0.53
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.74	0.53
2:O:109:VAL:CG1	2:O:123:LEU:HB2	2.38	0.53
2:O:207:VAL:CG1	2:O:208:GLY:H	2.16	0.53
3:P:273:TRP:CE3	3:P:274:TYR:N	2.77	0.53
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.90	0.53
3:C:113:THR:HG21	3:C:201:LEU:CD1	2.37	0.53
3:C:120:LEU:HB3	13:C:502:HEM:HAB	1.90	0.53
3:C:123:THR:HG21	3:C:190:ILE:HG13	1.89	0.53
9:I:71:ASN:HD22	9:I:71:ASN:N	1.97	0.53
1:N:330:SER:O	1:N:331:ILE:C	2.46	0.53
2:O:67:HIS:O	2:O:70:ARG:HB3	2.09	0.53
4:Q:44:ASP:N	4:Q:44:ASP:OD1	2.40	0.53
2:B:350:GLY:O	2:B:352:VAL:N	2.39	0.53
4:D:158:ILE:HG12	4:D:159:GLY:H	1.74	0.53
4:D:197:GLU:HG2	4:D:198:HIS:N	2.24	0.53
1:N:26:ALA:O	1:N:198:ALA:HA	2.09	0.53
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.89	0.53
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.44	0.53
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.43	0.53
8:U:13:LEU:N	8:U:13:LEU:CD2	2.71	0.53
8:U:58:LEU:HG	8:U:62:LEU:HD12	1.91	0.53
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.44	0.53
1:A:432:LEU:HD23	1:A:433:ASP:H	1.72	0.53
2:B:28:LYS:O	2:B:29:LEU:O	2.27	0.53
2:B:312:PHE:CD1	9:I:60:ALA:HB1	2.44	0.53
4:D:76:GLU:CD	4:D:76:GLU:H	2.12	0.53
10:J:59:TYR:N	10:J:59:TYR:CD1	2.77	0.53
2:O:147:ASP:O	2:O:150:VAL:HG22	2.08	0.53
2:O:239:TYR:HD2	2:O:240:TRP:N	2.07	0.53
3:P:78:TRP:CD2	3:P:79:LEU:N	2.77	0.53
1:A:255:LEU:HD12	1:A:421:ALA:O	2.08	0.53
2:B:200:THR:O	2:B:202:ALA:N	2.42	0.53
2:B:207:VAL:CG1	2:B:208:GLY:H	2.12	0.53
2:B:209:ILE:HG22	2:B:210:GLY:N	2.24	0.53
2:B:307:PHE:CD1	2:B:308:ASP:N	2.77	0.53
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.24	0.53
4:D:68:VAL:HG12	4:D:69:GLU:N	2.23	0.53
4:D:102:ARG:HG2	4:D:102:ARG:NH1	2.24	0.53
1:N:281:ASP:O	1:N:284:PHE:CD1	2.61	0.53
1:N:433:ASP:OD1	1:N:435:ASN:HB2	2.08	0.53
3:P:245:LEU:O	4:Q:201:ARG:CG	2.57	0.53
6:S:77:LYS:HA	6:S:80:TRP:NE1	2.23	0.53
3:C:344:VAL:HG12	3:C:349:ILE:HD11	1.90	0.52
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.39	0.52
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:22:GLY:O	1:N:193:PRO:HA	2.09	0.52
5:R:35:PHE:O	5:R:38:LEU:N	2.42	0.52
6:S:104:ARG:O	6:S:108:ASN:ND2	2.42	0.52
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.75	0.52
3:P:285:ILE:N	3:P:285:ILE:HD12	2.24	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.76	0.52
3:C:49:GLY:HA3	13:C:501:HEM:C2C	2.44	0.52
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.35	0.52
1:N:170:THR:HG22	1:N:171:THR:H	1.73	0.52
1:N:170:THR:HG22	1:N:171:THR:N	2.25	0.52
5:R:108:GLN:C	5:R:110:ALA:H	2.13	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.90	0.52
3:C:326:PHE:O	3:C:329:LEU:HB3	2.08	0.52
1:N:40:TRP:O	1:N:384:LEU:HD22	2.09	0.52
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.44	0.52
1:N:180:ALA:O	1:N:183:ALA:HB3	2.09	0.52
1:N:186:ILE:O	1:N:190:PHE:HB2	2.08	0.52
1:N:356:ARG:O	1:N:357:ALA:C	2.47	0.52
2:O:226:ILE:CG2	2:O:227:ARG:H	2.23	0.52
3:P:162:VAL:O	3:P:163:GLU:C	2.47	0.52
2:B:97:SER:HA	9:I:69:SER:HA	1.92	0.52
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.22	0.52
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.69	0.52
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.09	0.52
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.92	0.52
2:B:182:ARG:NH2	2:B:190:GLN:OE1	2.43	0.52
3:C:52:LEU:HD11	3:C:81:ARG:HA	1.92	0.52
8:H:19:THR:O	8:H:22:GLU:HB2	2.09	0.52
2:O:307:PHE:CD1	2:O:308:ASP:N	2.78	0.52
3:P:326:PHE:O	3:P:329:LEU:HB3	2.08	0.52
5:R:148:ALA:O	5:R:149:ASN:HB2	2.10	0.52
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.44	0.52
3:C:279:TYR:CZ	3:C:283:ARG:HD3	2.45	0.52
1:N:342:TRP:O	1:N:345:LEU:HB2	2.10	0.52
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.91	0.52
3:P:347:PRO:HG3	7:T:62:GLY:HA2	1.90	0.52
9:V:31:UNK:C	9:V:73:PRO:HG2	2.39	0.52
1:A:45:SER:HA	1:A:48:GLU:CD	2.30	0.52
1:A:239:SER:HB2	7:G:17:SER:O	2.09	0.52
1:A:287:GLY:O	1:A:289:HIS:N	2.43	0.52
1:A:294:LEU:HD11	1:A:334:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.74	0.52
3:C:245:LEU:HD13	4:D:205:GLY:HA2	1.92	0.52
3:C:276:LEU:O	3:C:279:TYR:HB3	2.10	0.52
4:D:186:VAL:O	4:D:190:LEU:HG	2.10	0.52
6:F:58:ARG:HA	6:F:61:ARG:NH2	2.25	0.52
3:P:107:SER:C	3:P:109:LEU:H	2.13	0.52
3:C:183:HIS:O	3:C:187:PRO:HD3	2.10	0.52
5:E:34:GLY:HA2	10:J:10:TYR:HB2	1.92	0.52
5:E:41:ALA:O	5:E:44:CYS:HB2	2.09	0.52
7:G:65:GLU:O	7:G:69:LEU:HG	2.10	0.52
3:P:186:LEU:O	3:P:187:PRO:C	2.46	0.52
4:Q:55:THR:HG1	4:Q:56:HIS:CE1	2.23	0.52
5:R:157:TYR:HE1	5:R:162:GLY:HA2	1.72	0.52
10:W:42:ILE:O	10:W:46:LEU:HG	2.10	0.52
2:B:28:LYS:O	2:B:28:LYS:HG2	2.10	0.52
2:B:31:ASN:HD22	2:B:31:ASN:N	2.08	0.52
2:B:345:LYS:C	2:B:347:ALA:N	2.63	0.52
3:C:3:PRO:HG2	3:C:4:ASN:H	1.75	0.52
6:F:32:MET:HE3	6:F:87:LYS:CG	2.32	0.52
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.52
11:P:3005:PEE:O2P	5:R:40:THR:HG21	2.10	0.52
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.33	0.51
1:A:404:ALA:O	1:A:405:ARG:C	2.48	0.51
2:B:428:GLY:O	2:B:430:LEU:N	2.43	0.51
3:C:101:ARG:CD	3:C:102:GLY:N	2.71	0.51
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.92	0.51
8:H:15:ASP:O	8:H:17:LEU:N	2.43	0.51
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.19	0.51
1:A:159:GLN:NE2	1:A:237:THR:HG21	2.25	0.51
2:B:428:GLY:O	2:B:430:LEU:HG	2.10	0.51
3:C:201:LEU:O	3:C:203:GLU:N	2.44	0.51
3:C:208:ASN:C	3:C:208:ASN:OD1	2.48	0.51
6:F:58:ARG:HA	6:F:61:ARG:CZ	2.41	0.51
2:O:135:TRP:O	2:O:136:GLU:C	2.46	0.51
2:O:272:PHE:O	2:O:275:LEU:N	2.42	0.51
3:P:201:LEU:O	3:P:203:GLU:N	2.43	0.51
6:F:32:MET:CE	6:F:87:LYS:HG2	2.32	0.51
2:O:29:LEU:CD1	2:O:33:LEU:HD23	2.41	0.51
3:P:9:HIS:ND1	3:P:10:PRO:HD2	2.25	0.51
3:P:284:SER:O	3:P:286:PRO:HD3	2.11	0.51
1:A:239:SER:HB2	7:G:18:LEU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PHE:N	2:B:50:PHE:CD1	2.78	0.51
2:B:63:LEU:O	2:B:65:THR:N	2.43	0.51
2:B:229:GLY:C	2:B:231:GLY:H	2.13	0.51
2:B:239:TYR:CD2	2:B:240:TRP:N	2.78	0.51
3:C:210:LEU:HD11	6:F:69:SER:HB2	1.91	0.51
3:C:332:ASN:O	3:C:336:LEU:HD12	2.11	0.51
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.46	0.51
6:F:68:LEU:O	6:F:70:LEU:N	2.44	0.51
6:F:104:ARG:O	6:F:108:ASN:ND2	2.44	0.51
1:N:49:ASN:ND2	1:N:51:LYS:N	2.58	0.51
1:N:89:TYR:O	1:N:95:THR:HG23	2.11	0.51
2:O:101:THR:OG1	2:O:104:LYS:HB3	2.11	0.51
3:P:26:SER:HA	3:P:219:ILE:HD11	1.92	0.51
5:R:38:LEU:CA	10:W:14:PHE:CE1	2.94	0.51
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.58	0.51
1:A:356:ARG:O	1:A:357:ALA:C	2.47	0.51
2:B:102:ARG:NH1	2:B:172:LEU:O	2.44	0.51
2:B:181:TYR:CE1	2:O:249:GLY:HA3	2.45	0.51
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.40	0.51
8:H:37:LEU:O	8:H:38:GLU:C	2.48	0.51
2:O:187:THR:OG1	2:O:189:GLU:HB2	2.10	0.51
2:O:226:ILE:CG2	2:O:227:ARG:N	2.73	0.51
2:O:385:GLU:C	2:O:387:LEU:H	2.13	0.51
3:P:139:MET:O	3:P:140:SER:C	2.49	0.51
3:P:237:LEU:O	3:P:241:LEU:HG	2.10	0.51
1:A:180:ALA:O	1:A:183:ALA:N	2.44	0.51
2:B:177:TYR:O	2:B:178:CYS:C	2.49	0.51
3:C:5:ILE:HG22	3:C:12:LEU:HD12	1.93	0.51
2:O:86:THR:O	2:O:90:GLU:HG3	2.11	0.51
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.75	0.51
4:Q:46:VAL:HB	4:Q:91:PHE:CE2	2.45	0.51
1:A:86:PHE:O	2:B:285:ILE:HA	2.10	0.51
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.92	0.51
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.45	0.51
1:A:394:GLU:O	1:A:395:TRP:C	2.49	0.51
1:N:61:HIS:ND1	1:N:134:ILE:HG12	2.25	0.51
1:N:171:THR:O	1:N:175:LYS:HG3	2.11	0.51
2:O:81:SER:C	2:O:83:PHE:N	2.64	0.51
4:Q:183:ALA:HA	4:Q:186:VAL:HG12	1.93	0.51
6:S:16:ILE:O	6:S:19:TRP:HB3	2.10	0.51
1:A:114:ALA:HA	1:A:216:PHE:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:231:LEU:CD1	4:D:220:TYR:HA	2.41	0.51
4:D:43:MET:HG2	4:D:91:PHE:HD2	1.76	0.51
5:E:186:GLN:HE21	5:E:188:VAL:HG12	1.75	0.51
6:F:87:LYS:O	6:F:89:TYR:N	2.44	0.51
7:G:29:ILE:H	7:G:29:ILE:CD1	2.01	0.51
7:G:29:ILE:O	7:G:34:LEU:HG	2.11	0.51
10:J:42:ILE:O	10:J:46:LEU:HG	2.11	0.51
1:N:388:ARG:HD3	1:N:388:ARG:H	1.76	0.51
2:O:221:GLU:O	2:O:223:PHE:N	2.43	0.51
2:O:308:ASP:OD2	9:V:59:SER:HB2	2.11	0.51
3:P:107:SER:HB2	13:P:502:HEM:HMD3	1.93	0.51
3:P:245:LEU:HD13	4:Q:205:GLY:HA2	1.91	0.51
3:P:345:GLU:O	3:P:349:ILE:HG13	2.11	0.51
4:Q:227:TRP:O	4:Q:228:SER:C	2.49	0.51
5:R:31:ASP:OD2	10:W:7:ARG:HG3	2.11	0.51
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.10	0.51
3:C:245:LEU:O	4:D:201:ARG:CG	2.58	0.51
3:C:304:LEU:O	3:C:305:ILE:C	2.50	0.51
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.92	0.51
5:R:41:ALA:O	5:R:44:CYS:HB2	2.11	0.51
5:R:108:GLN:O	5:R:110:ALA:N	2.44	0.51
2:B:385:GLU:C	2:B:387:LEU:H	2.14	0.51
4:D:54:VAL:HG11	4:D:192:TRP:CE2	2.45	0.51
6:F:40:ASP:O	6:F:44:LYS:HG3	2.11	0.51
7:G:55:ALA:O	7:G:56:TYR:C	2.48	0.51
1:N:107:PRO:HG2	1:N:108:LYS:H	1.75	0.51
1:N:332:ASP:O	1:N:333:ASP:C	2.50	0.51
3:P:230:ILE:O	3:P:233:LEU:HB3	2.11	0.51
7:T:55:ALA:O	7:T:58:LEU:N	2.44	0.51
2:B:370:MET:O	2:B:373:GLU:HG3	2.11	0.50
3:C:92:PHE:CA	3:C:95:ILE:HG22	2.38	0.50
3:C:230:ILE:O	3:C:233:LEU:HB3	2.11	0.50
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.26	0.50
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.41	0.50
2:O:272:PHE:HB3	2:O:322:PHE:CE1	2.46	0.50
4:Q:134:TYR:CD1	4:Q:162:PRO:HG3	2.46	0.50
7:T:56:TYR:O	7:T:59:TYR:HB3	2.11	0.50
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.76	0.50
2:B:100:SER:HA	2:B:104:LYS:O	2.11	0.50
2:B:275:LEU:O	2:B:279:LEU:HD12	2.12	0.50
4:D:232:SER:CB	7:G:23:GLN:HE22	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:SER:CB	5:E:32:ARG:HH21	2.25	0.50
7:G:34:LEU:O	7:G:37:VAL:N	2.45	0.50
1:N:27:SER:HB2	1:N:199:ALA:O	2.11	0.50
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.47	0.50
2:O:263:ALA:HA	2:O:319:SER:O	2.11	0.50
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.26	0.50
2:O:393:THR:CG2	2:O:397:VAL:HB	2.42	0.50
3:P:134:LEU:HD21	3:P:180:PHE:HA	1.92	0.50
3:P:332:ASN:ND2	3:P:359:TYR:HA	2.26	0.50
5:R:74:ILE:HG23	5:R:74:ILE:O	2.11	0.50
3:C:273:TRP:CE3	3:C:274:TYR:N	2.79	0.50
1:N:45:SER:HA	1:N:48:GLU:CD	2.31	0.50
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.93	0.50
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.46	0.50
5:R:35:PHE:O	5:R:36:SER:C	2.50	0.50
1:A:55:ALA:O	1:A:57:TYR:N	2.44	0.50
1:A:124:GLU:O	1:A:124:GLU:HG2	2.11	0.50
1:A:253:VAL:HG11	1:A:335:MET:CE	2.40	0.50
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.41	0.50
2:B:81:SER:O	2:B:83:PHE:N	2.45	0.50
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.92	0.50
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.92	0.50
3:C:104:TYR:HD2	3:C:105:TYR:CD1	2.29	0.50
4:D:102:ARG:NH1	4:D:107:GLY:O	2.44	0.50
2:O:227:ARG:HG3	2:O:228:SER:H	1.77	0.50
2:O:275:LEU:HD12	2:O:275:LEU:O	2.11	0.50
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.46	0.50
1:A:138:LEU:HD22	5:E:3:ASN:ND2	2.26	0.50
2:B:393:THR:HG23	2:B:397:VAL:HB	1.94	0.50
3:C:284:SER:O	3:C:286:PRO:HD3	2.12	0.50
4:D:26:VAL:HG13	4:D:189:PHE:HD1	1.76	0.50
4:D:47:ALA:HB1	4:D:89:ASP:O	2.12	0.50
6:F:32:MET:HE1	6:F:87:LYS:H	1.75	0.50
1:N:54:GLY:O	1:N:55:ALA:C	2.49	0.50
1:N:269:VAL:HG11	1:N:410:VAL:CG2	2.39	0.50
1:N:335:MET:O	1:N:338:ALA:HB3	2.11	0.50
3:P:198:LEU:HD11	15:P:3002:ANY:O4	2.12	0.50
3:P:354:MET:O	3:P:357:LEU:N	2.45	0.50
8:U:66:ASP:O	8:U:69:VAL:HB	2.11	0.50
1:A:206:LYS:O	1:A:209:VAL:CG1	2.56	0.50
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.92	0.50
3:C:273:TRP:HA	3:C:276:LEU:HG	1.93	0.50
5:E:45:VAL:O	5:E:48:ALA:HB3	2.11	0.50
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.93	0.50
4:Q:102:ARG:HG2	4:Q:102:ARG:HH11	1.77	0.50
4:Q:235:MET:HE1	6:S:63:LYS:C	2.32	0.50
10:W:22:LEU:HD23	10:W:22:LEU:H	1.75	0.50
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.47	0.50
3:C:139:MET:O	3:C:140:SER:C	2.50	0.50
3:C:273:TRP:CE3	3:C:274:TYR:HA	2.47	0.50
3:C:354:MET:O	3:C:357:LEU:N	2.45	0.50
5:E:29:SER:OG	5:E:30:GLU:N	2.44	0.50
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.94	0.50
6:F:21:TYR:C	6:F:21:TYR:CD2	2.84	0.50
6:F:73:ARG:HH11	6:F:73:ARG:HG3	1.75	0.50
1:N:55:ALA:O	1:N:57:TYR:N	2.45	0.50
1:N:180:ALA:O	1:N:183:ALA:N	2.45	0.50
6:S:89:TYR:CD1	6:S:90:LEU:N	2.75	0.50
1:A:333:ASP:O	1:A:336:PHE:HB3	2.12	0.50
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.50
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.39	0.50
4:Q:215:LEU:HD12	4:Q:215:LEU:O	2.12	0.50
5:R:78:LEU:HD21	5:R:193:VAL:HG11	1.92	0.50
1:A:161:THR:HB	1:A:234:CYS:SG	2.51	0.50
2:B:272:PHE:HB3	2:B:322:PHE:CE1	2.47	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.11	0.50
5:E:171:ILE:HG23	5:E:171:ILE:O	2.12	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.12	0.50
1:N:310:PHE:HE1	1:N:322:PHE:N	2.10	0.50
2:O:66:ALA:O	2:O:69:LEU:HB3	2.12	0.50
4:Q:167:GLU:HG3	8:U:13:LEU:HD11	1.94	0.50
7:T:41:PHE:CE2	7:T:45:VAL:HB	2.47	0.50
1:A:176:HIS:O	1:A:177:LEU:C	2.50	0.49
1:A:233:ARG:HG3	1:A:233:ARG:NH1	2.27	0.49
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.41	0.49
1:A:411:CYS:O	1:A:415:ILE:HG13	2.11	0.49
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.93	0.49
2:B:206:LEU:HG	2:B:206:LEU:O	2.11	0.49
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.47	0.49
8:H:32:LYS:O	8:H:36:ARG:HG3	2.12	0.49
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.94	0.49
3:P:242:THR:N	4:Q:208:MET:CE	2.75	0.49
4:Q:232:SER:CB	7:T:23:GLN:HE22	2.25	0.49
1:A:4:TYR:O	1:A:5:ALA:C	2.51	0.49
1:A:107:PRO:HG2	1:A:108:LYS:H	1.76	0.49
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.94	0.49
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.77	0.49
3:C:241:LEU:CB	4:D:208:MET:HE2	2.42	0.49
1:N:40:TRP:CD1	1:N:96:ALA:CB	2.95	0.49
2:O:345:LYS:O	2:O:347:ALA:N	2.46	0.49
8:U:37:LEU:O	8:U:38:GLU:C	2.51	0.49
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.42	0.49
1:A:21:ASN:HD22	1:A:192:ALA:CB	2.25	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
3:C:186:LEU:O	3:C:187:PRO:C	2.51	0.49
8:H:58:LEU:HG	8:H:62:LEU:CD1	2.43	0.49
8:H:66:ASP:O	8:H:69:VAL:HB	2.12	0.49
10:J:60:GLU:O	10:J:61:ALA:HB3	2.12	0.49
1:N:45:SER:CA	1:N:48:GLU:HG3	2.41	0.49
1:N:356:ARG:O	1:N:359:ASN:N	2.46	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB2	1.95	0.49
6:S:63:LYS:O	6:S:63:LYS:HG2	2.12	0.49
1:A:220:SER:HB2	1:A:226:ASP:OD1	2.12	0.49
2:B:272:PHE:HZ	2:B:416:LYS:HD3	1.78	0.49
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.48	0.49
5:E:152:ASP:C	5:E:153:PHE:CD1	2.85	0.49
6:F:16:ILE:O	6:F:19:TRP:HB3	2.13	0.49
1:N:104:LYS:O	1:N:107:PRO:HD2	2.13	0.49
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.94	0.49
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.95	0.49
5:E:113:ASP:C	5:E:115:SER:H	2.16	0.49
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.47	0.49
3:P:80:ILE:O	3:P:81:ARG:C	2.51	0.49
3:P:92:PHE:CA	3:P:95:ILE:HG22	2.42	0.49
3:P:192:GLY:O	3:P:195:ILE:HB	2.12	0.49
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.12	0.49
2:B:408:ALA:O	2:B:410:VAL:N	2.46	0.49
3:C:26:SER:HA	3:C:219:ILE:CD1	2.43	0.49
3:C:92:PHE:C	3:C:95:ILE:HG22	2.32	0.49
3:C:366:LEU:HD23	3:C:366:LEU:N	2.28	0.49
3:C:377:MET:HE1	6:F:20:TYR:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.94	0.49
5:E:51:ALA:O	5:E:52:LYS:C	2.50	0.49
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.13	0.49
2:O:239:TYR:HE1	2:O:260:GLU:N	2.11	0.49
3:P:79:LEU:HD12	3:P:79:LEU:O	2.12	0.49
4:Q:116:ILE:HG23	4:Q:117:VAL:H	1.76	0.49
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.95	0.49
3:C:78:TRP:CD2	3:C:79:LEU:N	2.80	0.49
4:D:55:THR:HG1	4:D:56:HIS:CE1	2.30	0.49
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.94	0.49
2:B:31:ASN:ND2	2:B:32:GLY:H	2.11	0.49
7:G:45:VAL:HG13	7:G:46:PHE:N	2.28	0.49
2:O:292:THR:O	2:O:292:THR:HG22	2.12	0.49
3:P:30:ALA:O	3:P:32:TRP:N	2.45	0.49
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.13	0.49
5:R:29:SER:OG	5:R:30:GLU:N	2.46	0.49
5:R:114:VAL:O	5:R:114:VAL:HG12	2.12	0.49
2:B:72:ALA:O	2:B:75:LEU:HB2	2.12	0.49
2:B:209:ILE:HD11	2:B:378:LEU:HG	1.94	0.49
4:D:24:SER:OG	10:J:55:ILE:HD11	2.13	0.49
5:E:29:SER:HA	5:E:32:ARG:HE	1.78	0.49
1:N:241:ILE:HG23	1:N:241:ILE:O	2.11	0.49
1:N:420:PRO:HD2	1:N:434:TYR:OH	2.13	0.49
3:P:172:ASP:C	3:P:174:PRO:HD2	2.33	0.49
3:C:172:ASP:C	3:C:174:PRO:HD2	2.33	0.49
4:D:109:LEU:O	4:D:111:PRO:HD3	2.12	0.49
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.48	0.49
1:N:255:LEU:O	1:N:321:GLY:HA3	2.13	0.49
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.14	0.49
3:P:292:VAL:O	3:P:295:LEU:HB3	2.12	0.49
4:Q:47:ALA:O	4:Q:49:ARG:N	2.46	0.49
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.48	0.48
4:D:215:LEU:HD12	4:D:215:LEU:O	2.13	0.48
5:E:113:ASP:HB3	5:E:116:LYS:HB2	1.95	0.48
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.26	0.48
1:N:310:PHE:CE1	1:N:322:PHE:N	2.81	0.48
2:O:81:SER:O	2:O:82:SER:C	2.52	0.48
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.28	0.48
3:P:287:ASN:O	3:P:288:LYS:C	2.50	0.48
5:R:165:TYR:HA	5:R:170:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:61:PHE:O	8:U:62:LEU:C	2.50	0.48
10:W:25:VAL:O	10:W:29:VAL:HG23	2.13	0.48
1:A:334:MET:O	1:A:335:MET:C	2.51	0.48
2:B:239:TYR:HD2	2:B:240:TRP:N	2.12	0.48
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.95	0.48
3:C:365:ILE:C	3:C:368:PRO:HD2	2.33	0.48
7:G:29:ILE:HD12	7:G:29:ILE:N	2.13	0.48
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.76	0.48
8:U:59:PHE:O	8:U:60:ASP:C	2.52	0.48
1:A:36:THR:OG1	1:A:100:LYS:HG2	2.13	0.48
2:B:325:TYR:C	2:B:325:TYR:CD2	2.87	0.48
3:C:287:ASN:O	3:C:288:LYS:C	2.52	0.48
1:N:63:ALA:O	1:N:116:VAL:HG11	2.13	0.48
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.94	0.48
1:N:334:MET:O	1:N:335:MET:C	2.52	0.48
1:N:404:ALA:O	1:N:405:ARG:C	2.52	0.48
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.13	0.48
18:Q:501:HEC:HMB1	18:Q:501:HEC:CBB	2.40	0.48
1:A:170:THR:HG22	1:A:171:THR:N	2.29	0.48
1:A:239:SER:CB	7:G:18:LEU:HA	2.43	0.48
2:B:135:TRP:O	2:B:136:GLU:C	2.51	0.48
3:C:106:GLY:HA2	3:C:108:TYR:CD2	2.49	0.48
2:O:307:PHE:H	9:V:52:ARG:HG2	1.78	0.48
3:P:157:ILE:O	3:P:158:GLY:C	2.52	0.48
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.13	0.48
2:B:31:ASN:N	2:B:31:ASN:ND2	2.61	0.48
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.96	0.48
5:E:69:LEU:HD13	5:E:71:LEU:HD11	1.96	0.48
1:N:4:TYR:O	1:N:5:ALA:C	2.52	0.48
3:P:184:PHE:CG	13:P:501:HEM:HBC1	2.49	0.48
3:P:311:SER:HB2	3:P:319:ARG:HH11	1.79	0.48
4:Q:167:GLU:C	4:Q:169:LEU:N	2.65	0.48
5:R:163:SER:HA	5:R:174:GLY:HA3	1.94	0.48
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.95	0.48
1:A:21:ASN:HB3	1:A:218:GLY:O	2.12	0.48
4:D:131:LEU:HD11	18:D:501:HEC:HMB2	1.96	0.48
5:E:142:LEU:HD22	3:P:149:ASN:HB3	1.96	0.48
1:N:46:ARG:HD3	1:N:231:LEU:HD13	1.95	0.48
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.44	0.48
2:O:75:LEU:HD21	2:O:136:GLU:HB3	1.95	0.48
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.94	0.48
2:B:167:ALA:C	2:B:168:TYR:CD1	2.87	0.48
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.96	0.48
3:C:245:LEU:O	4:D:201:ARG:HG2	2.14	0.48
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.95	0.48
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.14	0.48
2:O:272:PHE:HZ	2:O:416:LYS:HD3	1.79	0.48
3:P:127:THR:O	3:P:130:VAL:HG22	2.14	0.48
3:P:158:GLY:O	3:P:161:LEU:N	2.47	0.48
2:B:66:ALA:O	2:B:69:LEU:HB3	2.14	0.48
3:C:164:TRP:O	3:C:165:ALA:C	2.50	0.48
4:D:28:ARG:O	4:D:29:GLY:C	2.52	0.48
5:E:55:VAL:O	5:E:56:THR:C	2.52	0.48
1:N:85:HIS:CD2	2:O:284:LEU:HB3	2.48	0.48
2:O:177:TYR:O	2:O:178:CYS:C	2.51	0.48
2:O:253:VAL:HG13	2:O:430:LEU:CD2	2.44	0.48
3:P:273:TRP:CE3	3:P:274:TYR:CA	2.97	0.48
5:R:134:ILE:C	5:R:135:LEU:HG	2.33	0.48
1:A:191:LYS:O	1:A:195:MET:HG3	2.13	0.48
1:N:93:GLU:O	1:N:93:GLU:HG3	2.14	0.48
1:N:93:GLU:O	1:N:94:GLN:HB2	2.14	0.48
2:O:29:LEU:HD23	2:O:30:PRO:HD2	1.95	0.48
3:P:191:ALA:O	3:P:195:ILE:HG12	2.13	0.48
1:A:63:ALA:O	1:A:116:VAL:HG11	2.14	0.48
2:B:147:ASP:O	2:B:150:VAL:HG22	2.14	0.48
4:D:26:VAL:CG1	4:D:189:PHE:HD1	2.27	0.48
4:D:218:LEU:HD13	5:E:43:ALA:N	2.28	0.48
1:N:178:THR:HG22	1:N:180:ALA:H	1.79	0.48
2:O:163:LEU:HD13	2:O:425:ALA:CB	2.44	0.48
1:A:244:ARG:HH22	1:A:429:GLU:CD	2.17	0.47
3:C:196:ILE:O	3:C:199:THR:N	2.46	0.47
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.29	0.47
4:D:161:ALA:O	4:D:162:PRO:C	2.53	0.47
7:G:61:TRP:CE3	7:G:62:GLY:N	2.82	0.47
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.79	0.47
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.49	0.47
2:O:59:THR:HG22	2:O:60:THR:N	2.28	0.47
3:P:3:PRO:HG2	3:P:4:ASN:H	1.78	0.47
3:P:246:PHE:CZ	4:Q:205:GLY:C	2.87	0.47
3:P:304:LEU:O	3:P:305:ILE:C	2.52	0.47
1:A:171:THR:O	1:A:175:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.96	0.47
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.28	0.47
2:B:163:LEU:HD13	2:B:425:ALA:CB	2.43	0.47
2:B:166:ALA:O	2:B:242:GLY:N	2.37	0.47
2:B:402:ILE:O	2:B:405:VAL:HG23	2.14	0.47
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.44	0.47
5:E:52:LYS:HD3	5:E:56:THR:OG1	2.13	0.47
1:N:35:CYS:HB2	1:N:200:ALA:O	2.14	0.47
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.49	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.49	0.47
1:N:145:MET:O	1:N:146:THR:C	2.52	0.47
1:N:287:GLY:O	1:N:289:HIS:N	2.47	0.47
1:N:438:ARG:HH11	1:N:438:ARG:HG3	1.80	0.47
2:O:182:ARG:NH2	2:O:190:GLN:OE1	2.47	0.47
2:O:206:LEU:HG	2:O:206:LEU:O	2.14	0.47
3:P:107:SER:O	3:P:109:LEU:N	2.47	0.47
3:P:120:LEU:HB3	13:P:502:HEM:HAB	1.96	0.47
3:P:154:ILE:CG2	3:P:155:PRO:HD2	2.43	0.47
3:P:201:LEU:HD11	13:P:502:HEM:HAD2	1.95	0.47
7:T:4:PHE:CD2	7:T:7:LEU:HD11	2.49	0.47
9:V:49:LEU:O	9:V:50:LEU:HG	2.14	0.47
3:C:165:ALA:O	3:C:178:ARG:HD2	2.14	0.47
4:D:200:GLN:HE21	20:E:2009:PLC:H51	1.79	0.47
5:E:152:ASP:O	5:E:153:PHE:CD1	2.67	0.47
1:N:45:SER:OG	1:N:92:ARG:HA	2.13	0.47
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.50	0.47
4:Q:26:VAL:CG1	4:Q:189:PHE:HD1	2.27	0.47
4:Q:26:VAL:HG13	4:Q:189:PHE:HD1	1.79	0.47
6:S:58:ARG:HA	6:S:61:ARG:CZ	2.44	0.47
1:A:106:MET:HE3	1:A:208:LEU:CD1	2.45	0.47
3:C:123:THR:HG22	3:C:190:ILE:HD11	1.95	0.47
6:F:19:TRP:O	6:F:22:ASN:N	2.47	0.47
8:H:37:LEU:O	8:H:40:CYS:N	2.47	0.47
3:P:31:TRP:O	3:P:101:ARG:HG3	2.13	0.47
4:Q:12:TRP:CZ2	4:Q:124:GLU:HB2	2.49	0.47
7:T:16:TYR:N	7:T:16:TYR:CD1	2.82	0.47
1:A:69:LYS:HE3	1:A:70:ARG:NH2	2.14	0.47
2:B:81:SER:C	2:B:83:PHE:N	2.65	0.47
2:B:343:GLN:O	2:B:347:ALA:HB2	2.15	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.28	0.47
3:C:371:GLY:O	3:C:374:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:LYS:HG2	5:E:86:ASN:N	2.29	0.47
6:F:52:GLU:HG2	6:F:56:ASN:HD21	1.78	0.47
7:G:49:ALA:O	7:G:50:PRO:C	2.53	0.47
7:G:56:TYR:O	7:G:59:TYR:HB3	2.15	0.47
9:I:38:UNK:C	9:I:40:UNK:N	2.76	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.13	0.47
2:O:259:THR:O	2:O:260:GLU:C	2.51	0.47
3:P:117:GLY:HA3	13:P:502:HEM:HBC2	1.97	0.47
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.47	0.47
4:Q:130:LEU:HD12	4:Q:150:ASN:ND2	2.30	0.47
10:W:26:LEU:O	10:W:30:LEU:HG	2.14	0.47
1:A:29:GLU:HG3	1:A:203:ILE:O	2.15	0.47
2:B:239:TYR:HD1	2:B:260:GLU:HB2	1.76	0.47
3:C:78:TRP:CG	3:C:79:LEU:N	2.83	0.47
3:C:95:ILE:HD13	3:C:121:LEU:HD12	1.96	0.47
1:N:176:HIS:O	1:N:177:LEU:C	2.53	0.47
1:N:422:LEU:HD22	1:N:437:ILE:HD12	1.96	0.47
2:O:67:HIS:ND1	2:O:177:TYR:HA	2.30	0.47
3:P:347:PRO:O	3:P:350:ILE:HG22	2.14	0.47
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.29	0.47
6:S:90:LEU:O	6:S:91:GLU:C	2.53	0.47
7:T:34:LEU:O	7:T:37:VAL:N	2.47	0.47
8:U:15:ASP:O	8:U:17:LEU:N	2.48	0.47
1:A:27:SER:CB	1:A:199:ALA:O	2.62	0.47
1:A:45:SER:CA	1:A:48:GLU:HG3	2.42	0.47
3:C:92:PHE:HA	3:C:95:ILE:CG2	2.41	0.47
3:C:213:SER:HB2	6:F:39:GLU:OE2	2.15	0.47
3:C:241:LEU:HB3	4:D:208:MET:HE2	1.97	0.47
4:D:47:ALA:O	4:D:50:ASN:N	2.38	0.47
4:D:182:ILE:O	4:D:184:LYS:N	2.48	0.47
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.95	0.47
5:E:126:ARG:O	5:E:182:VAL:HG11	2.15	0.47
6:F:77:LYS:HA	6:F:80:TRP:NE1	2.30	0.47
8:H:44:VAL:HG22	8:H:52:GLU:HG2	1.97	0.47
9:I:65:VAL:HG12	9:I:66:ALA:H	1.79	0.47
1:N:103:SER:O	1:N:106:MET:HB2	2.15	0.47
1:N:253:VAL:CG1	1:N:335:MET:HE1	2.45	0.47
3:P:122:LEU:O	3:P:125:MET:HB2	2.13	0.47
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.96	0.47
3:P:277:PHE:CD1	3:P:277:PHE:C	2.88	0.47
4:Q:158:ILE:HG12	4:Q:159:GLY:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:THR:HA	1:N:121:ALA:H	1.78	0.47
2:O:29:LEU:HD22	2:O:30:PRO:HD2	1.96	0.47
2:O:200:THR:O	2:O:202:ALA:N	2.47	0.47
2:O:209:ILE:HD11	2:O:378:LEU:HG	1.97	0.47
2:O:275:LEU:O	2:O:279:LEU:HD12	2.15	0.47
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.50	0.47
6:S:76:PRO:O	6:S:78:GLU:N	2.48	0.47
1:A:281:ASP:HB3	1:A:284:PHE:CE1	2.50	0.47
2:B:412:ASN:O	2:B:415:LYS:N	2.47	0.47
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.62	0.47
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.33	0.47
1:N:42:GLY:HA2	1:N:384:LEU:HD21	1.97	0.47
1:N:388:ARG:NH2	1:N:388:ARG:CG	2.78	0.47
2:O:309:ALA:HA	2:O:325:TYR:O	2.15	0.47
3:P:130:VAL:HG23	3:P:131:GLY:H	1.80	0.47
3:P:380:TYR:OH	6:S:34:ASP:HA	2.15	0.47
4:Q:191:ARG:O	4:Q:194:ALA:N	2.46	0.47
4:Q:220:TYR:HE2	16:Q:3003:CDL:H722	1.79	0.47
4:Q:230:LEU:O	6:S:70:LEU:HD11	2.15	0.47
1:A:54:GLY:O	1:A:55:ALA:C	2.54	0.47
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.50	0.47
2:B:176:LEU:HD12	2:B:176:LEU:O	2.15	0.47
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.45	0.47
3:C:199:THR:HG22	3:C:200:PHE:N	2.30	0.47
4:D:46:VAL:CG1	4:D:47:ALA:N	2.76	0.47
8:H:61:PHE:O	8:H:62:LEU:C	2.53	0.47
1:N:105:ASP:O	1:N:106:MET:C	2.54	0.47
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.96	0.47
1:N:106:MET:O	1:N:110:VAL:HG23	2.14	0.47
1:N:178:THR:HG22	1:N:179:ARG:N	2.30	0.47
1:N:280:TYR:CG	1:N:281:ASP:N	2.83	0.47
2:O:100:SER:HB3	2:O:105:MET:HA	1.97	0.47
3:P:29:SER:O	3:P:32:TRP:HB2	2.15	0.47
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.50	0.47
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.55	0.47
1:A:235:ARG:NH2	5:E:14:ARG:NH2	2.63	0.46
1:A:305:HIS:ND1	9:I:35:UNK:CB	2.79	0.46
3:C:101:ARG:HD2	3:C:102:GLY:CA	2.45	0.46
4:D:62:LYS:O	4:D:66:GLU:HG3	2.15	0.46
2:O:393:THR:HG23	2:O:397:VAL:HB	1.96	0.46
2:O:428:GLY:O	2:O:430:LEU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.29	0.46
10:W:52:TRP:O	10:W:56:LYS:HB2	2.15	0.46
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.80	0.46
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.30	0.46
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.81	0.46
3:C:30:ALA:C	3:C:32:TRP:N	2.67	0.46
5:E:148:ALA:O	5:E:149:ASN:HB2	2.15	0.46
1:N:50:GLU:HB2	1:N:165:ARG:NH2	2.30	0.46
1:N:435:ASN:O	1:N:438:ARG:HB3	2.15	0.46
3:P:63:ALA:CB	3:P:176:LEU:HD21	2.44	0.46
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.30	0.46
5:R:47:THR:O	5:R:48:ALA:C	2.52	0.46
10:W:49:GLY:N	10:W:54:HIS:ND1	2.63	0.46
1:A:21:ASN:HD22	1:A:192:ALA:HB1	1.79	0.46
1:A:86:PHE:CD2	1:A:99:ILE:HD11	2.50	0.46
1:A:330:SER:O	1:A:331:ILE:C	2.53	0.46
3:C:4:ASN:O	3:C:4:ASN:OD1	2.33	0.46
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.78	0.46
1:N:19:LEU:C	1:N:21:ASN:H	2.18	0.46
1:N:307:PHE:HA	1:N:324:PHE:HA	1.97	0.46
2:O:314:VAL:HG11	2:O:316:TYR:CZ	2.50	0.46
5:R:136:VAL:HB	5:R:181:GLU:HB3	1.97	0.46
1:A:372:THR:O	1:A:373:THR:C	2.54	0.46
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.30	0.46
2:B:101:THR:OG1	2:B:104:LYS:HB3	2.16	0.46
2:B:280:GLY:HA3	2:B:293:SER:OG	2.16	0.46
3:C:122:LEU:O	3:C:125:MET:HB2	2.15	0.46
3:C:172:ASP:OD1	3:C:173:ASN:N	2.43	0.46
3:C:285:ILE:HG21	3:C:290:GLY:HA3	1.98	0.46
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.81	0.46
3:P:59:ASP:O	3:P:60:THR:C	2.54	0.46
3:P:104:TYR:CD2	3:P:105:TYR:CE1	2.97	0.46
3:P:281:ILE:O	3:P:285:ILE:HD13	2.16	0.46
3:P:365:ILE:C	3:P:368:PRO:HD2	2.36	0.46
5:R:38:LEU:CA	10:W:14:PHE:HE1	2.28	0.46
2:B:189:GLU:C	2:B:191:LEU:N	2.67	0.46
2:B:239:TYR:CD2	2:B:239:TYR:C	2.89	0.46
3:C:338:TRP:CE2	7:G:59:TYR:HD1	2.32	0.46
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.41	0.46
6:F:36:THR:O	6:F:37:LEU:C	2.54	0.46
6:F:89:TYR:CD1	6:F:90:LEU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:33:ALA:O	7:G:34:LEU:C	2.54	0.46
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.50	0.46
3:P:350:ILE:HG23	3:P:351:ILE:N	2.30	0.46
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.98	0.46
4:Q:182:ILE:O	4:Q:184:LYS:N	2.49	0.46
1:A:104:LYS:O	1:A:107:PRO:HD2	2.16	0.46
1:A:388:ARG:NH2	1:A:388:ARG:CG	2.77	0.46
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.50	0.46
3:C:270:LYS:HA	3:C:271:PRO:HD3	1.77	0.46
3:C:277:PHE:CD1	3:C:277:PHE:C	2.88	0.46
4:D:10:PHE:N	4:D:10:PHE:HD1	2.07	0.46
1:N:284:PHE:CE2	9:V:71:ASN:O	2.69	0.46
2:O:113:ARG:O	2:O:116:VAL:HG23	2.16	0.46
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.46	0.46
3:P:277:PHE:HD2	11:P:3007:PEE:H77	1.79	0.46
3:P:332:ASN:HD21	3:P:359:TYR:CA	2.29	0.46
5:R:171:ILE:O	5:R:171:ILE:HG23	2.16	0.46
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.98	0.46
3:C:219:ILE:HD11	3:C:225:TYR:CE1	2.51	0.46
3:C:258:THR:HG22	3:C:258:THR:O	2.15	0.46
3:C:335:ILE:O	3:C:336:LEU:C	2.53	0.46
3:C:357:LEU:HD12	3:C:357:LEU:HA	1.68	0.46
10:J:52:TRP:O	10:J:56:LYS:HB2	2.15	0.46
1:N:112:LEU:H	1:N:112:LEU:HG	1.48	0.46
2:O:168:TYR:CD2	2:O:237:ALA:HB1	2.51	0.46
2:O:307:PHE:HE2	9:V:52:ARG:HE	1.64	0.46
3:P:295:LEU:O	3:P:296:ALA:C	2.54	0.46
4:Q:121:HIS:C	4:Q:123:GLY:H	2.18	0.46
6:S:18:LYS:HA	6:S:83:TYR:CD1	2.50	0.46
10:W:14:PHE:N	10:W:14:PHE:HD2	2.13	0.46
2:B:67:HIS:ND1	2:B:177:TYR:HA	2.31	0.46
2:B:239:TYR:HE2	2:B:241:GLY:CA	2.29	0.46
3:C:344:VAL:CG1	3:C:349:ILE:HD11	2.46	0.46
8:H:40:CYS:O	8:H:41:ASP:C	2.54	0.46
8:H:65:ARG:O	8:H:69:VAL:HG23	2.15	0.46
2:O:128:THR:CA	2:O:226:ILE:HD11	2.41	0.46
2:O:241:GLY:HA2	2:O:423:SER:OG	2.16	0.46
3:P:25:PRO:HG2	3:P:207:ASN:O	2.16	0.46
3:P:56:TYR:OH	3:P:176:LEU:HD11	2.16	0.46
3:P:199:THR:HG22	3:P:200:PHE:N	2.31	0.46
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:29:GLY:HA3	4:Q:185:ASP:O	2.16	0.46
1:A:93:GLU:O	1:A:94:GLN:HB2	2.16	0.46
1:A:243:ALA:O	1:A:425:VAL:HA	2.16	0.46
2:B:72:ALA:CA	2:B:75:LEU:HD12	2.46	0.46
2:B:113:ARG:O	2:B:116:VAL:HG23	2.15	0.46
3:C:70:THR:O	3:C:70:THR:HG22	2.15	0.46
4:D:109:LEU:O	4:D:109:LEU:HG	2.15	0.46
5:E:29:SER:CA	5:E:32:ARG:HH21	2.29	0.46
5:E:122:HIS:O	5:E:124:LEU:N	2.49	0.46
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.97	0.46
3:P:166:TRP:NE1	3:P:171:VAL:HG22	2.31	0.46
3:P:198:LEU:HA	3:P:198:LEU:HD23	1.64	0.46
3:P:355:ALA:HA	3:P:358:SER:HB3	1.97	0.46
5:R:29:SER:HA	5:R:32:ARG:HE	1.81	0.46
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.81	0.46
8:U:46:SER:OG	8:U:47:ARG:N	2.48	0.46
1:A:103:SER:O	1:A:106:MET:HB2	2.15	0.46
3:C:104:TYR:CD2	3:C:105:TYR:CE1	3.04	0.46
3:C:117:GLY:HA3	13:C:502:HEM:HBC2	1.97	0.46
3:C:183:HIS:O	3:C:187:PRO:CD	2.64	0.46
3:C:378:LEU:O	3:C:379:ASN:CB	2.63	0.46
5:E:140:THR:HG21	5:E:178:TYR:HB2	1.97	0.46
7:G:81:GLN:OXT	8:H:49:HIS:HB3	2.16	0.46
2:O:63:LEU:C	2:O:65:THR:H	2.20	0.46
2:O:378:LEU:C	2:O:380:ASN:N	2.70	0.46
4:Q:5:LEU:HG	4:Q:152:TYR:HE1	1.81	0.46
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.96	0.46
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.46	0.46
6:S:58:ARG:HA	6:S:61:ARG:NH2	2.30	0.46
6:S:74:ILE:HG13	6:S:75:LEU:N	2.30	0.46
1:A:411:CYS:HB3	1:A:415:ILE:HD12	1.98	0.45
2:B:76:THR:HG22	2:B:82:SER:N	2.21	0.45
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.51	0.45
3:C:269:ILE:O	3:C:269:ILE:CG2	2.63	0.45
1:N:79:VAL:O	1:N:82:MET:HG2	2.16	0.45
1:N:159:GLN:NE2	1:N:237:THR:HG21	2.31	0.45
3:P:332:ASN:O	3:P:336:LEU:HD12	2.16	0.45
3:P:338:TRP:CE2	7:T:59:TYR:CD1	3.02	0.45
4:Q:5:LEU:HG	4:Q:152:TYR:CE1	2.51	0.45
5:R:18:VAL:HG23	5:R:18:VAL:O	2.15	0.45
5:R:150:SER:OG	5:R:157:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:O	1:A:148:VAL:C	2.55	0.45
2:B:57:TYR:CD1	2:B:57:TYR:N	2.84	0.45
3:C:141:PHE:O	3:C:144:ALA:HB3	2.16	0.45
3:C:295:LEU:O	3:C:296:ALA:C	2.51	0.45
8:H:59:PHE:O	8:H:60:ASP:C	2.54	0.45
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.46	0.45
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.50	0.45
1:N:235:ARG:NH2	5:R:14:ARG:NH2	2.65	0.45
1:N:242:ARG:O	7:T:14:ILE:HA	2.15	0.45
1:N:301:HIS:HB2	1:N:303:LEU:HD21	1.97	0.45
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.46	0.45
3:P:100:GLY:O	3:P:101:ARG:C	2.54	0.45
3:P:208:ASN:OD1	3:P:208:ASN:C	2.54	0.45
4:Q:42:SER:HB2	4:Q:112:ASP:OD2	2.16	0.45
7:T:41:PHE:HE2	7:T:45:VAL:HB	1.81	0.45
1:A:21:ASN:ND2	1:A:192:ALA:HB1	2.30	0.45
2:B:42:SER:OG	2:B:43:PRO:HD2	2.16	0.45
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.97	0.45
3:C:38:LEU:HB3	13:C:502:HEM:CMB	2.46	0.45
3:C:154:ILE:O	3:C:158:GLY:HA3	2.16	0.45
3:C:273:TRP:CE3	3:C:274:TYR:CA	3.00	0.45
5:E:35:PHE:O	5:E:38:LEU:HB3	2.17	0.45
1:N:22:GLY:C	1:N:193:PRO:HA	2.35	0.45
1:N:49:ASN:HD21	1:N:52:ASN:N	2.13	0.45
1:N:178:THR:HB	1:N:181:ASP:OD1	2.16	0.45
1:N:354:VAL:HG23	1:N:355:LYS:N	2.31	0.45
2:O:422:LYS:O	2:O:436:LEU:HD21	2.16	0.45
3:P:27:ASN:HD22	3:P:209:PRO:HD2	1.82	0.45
3:P:117:GLY:CA	13:P:502:HEM:HBC2	2.46	0.45
1:A:433:ASP:O	1:A:437:ILE:HG13	2.16	0.45
2:B:99:TYR:HA	9:I:66:ALA:O	2.16	0.45
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.16	0.45
3:C:52:LEU:HD13	13:C:501:HEM:HBD1	1.97	0.45
3:C:316:MET:HA	3:C:319:ARG:HE	1.81	0.45
4:D:46:VAL:HB	4:D:91:PHE:CD2	2.51	0.45
4:D:48:PHE:CE2	4:D:65:ALA:HA	2.51	0.45
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.77	0.45
1:N:206:LYS:O	1:N:207:GLU:C	2.55	0.45
2:O:209:ILE:CG2	2:O:210:GLY:N	2.80	0.45
2:O:408:ALA:O	2:O:410:VAL:N	2.48	0.45
3:P:164:TRP:O	3:P:165:ALA:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:28:ARG:O	4:Q:29:GLY:C	2.53	0.45
7:T:29:ILE:H	7:T:29:ILE:CD1	2.00	0.45
2:B:275:LEU:O	2:B:275:LEU:HD12	2.16	0.45
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.34	0.45
5:E:119:ASP:CB	5:E:179:ASN:ND2	2.59	0.45
6:F:32:MET:O	6:F:33:ARG:C	2.53	0.45
2:O:209:ILE:O	2:O:211:VAL:HG22	2.16	0.45
2:O:235:ALA:O	2:O:236:LYS:C	2.54	0.45
3:P:157:ILE:CG1	3:P:158:GLY:H	1.96	0.45
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.52	0.45
3:P:377:MET:HE1	6:S:20:TYR:HD1	1.82	0.45
5:R:55:VAL:O	5:R:56:THR:C	2.54	0.45
5:R:113:ASP:C	5:R:115:SER:N	2.65	0.45
5:R:135:LEU:HA	5:R:183:PRO:HD3	1.98	0.45
6:S:52:GLU:HG2	6:S:56:ASN:ND2	2.31	0.45
8:U:19:THR:O	8:U:22:GLU:HB2	2.16	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.51	0.45
1:A:87:ASN:ND2	1:A:98:TYR:OH	2.50	0.45
1:A:261:GLY:O	1:A:262:TRP:C	2.55	0.45
1:A:289:HIS:O	1:A:290:LEU:C	2.55	0.45
3:C:45:GLN:HB3	13:C:501:HEM:HAB	1.99	0.45
3:C:231:LEU:HD11	4:D:220:TYR:HA	1.98	0.45
3:C:285:ILE:N	3:C:285:ILE:CD1	2.79	0.45
3:C:325:LEU:HD22	3:C:370:ILE:HG13	1.97	0.45
1:N:187:ASP:O	1:N:191:LYS:HE3	2.16	0.45
3:P:92:PHE:C	3:P:95:ILE:HG22	2.37	0.45
3:P:95:ILE:O	3:P:99:ILE:HG13	2.16	0.45
3:P:182:LEU:HD23	14:P:3001:SMA:H26	1.98	0.45
10:W:20:PHE:O	10:W:23:THR:HB	2.17	0.45
2:B:73:SER:N	2:B:74:PRO:HD2	2.31	0.45
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.97	0.45
5:E:161:HIS:HB2	19:E:501:FES:S1	2.56	0.45
1:N:84:ALA:HB1	1:N:99:ILE:CG2	2.47	0.45
2:O:259:THR:HG22	2:O:260:GLU:N	2.31	0.45
3:P:295:LEU:O	3:P:298:SER:OG	2.29	0.45
6:S:40:ASP:O	6:S:44:LYS:HG3	2.15	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
2:B:412:ASN:O	2:B:413:ALA:C	2.56	0.45
3:C:331:ALA:HB2	7:G:52:PHE:CD2	2.52	0.45
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.95	0.45
3:P:271:PRO:CA	14:P:3001:SMA:H10	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:221:TYR:CE1	7:T:25:ALA:HB2	2.51	0.45
6:S:36:THR:O	6:S:37:LEU:C	2.54	0.45
6:S:77:LYS:HA	6:S:80:TRP:CD1	2.51	0.45
10:W:21:ALA:O	10:W:24:VAL:N	2.50	0.45
1:A:50:GLU:HB2	1:A:165:ARG:NH2	2.32	0.45
1:A:249:PRO:HG2	1:A:250:VAL:H	1.81	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.67	0.45
1:A:266:ASP:O	1:A:267:ASN:C	2.54	0.45
2:B:67:HIS:ND1	2:B:178:CYS:N	2.65	0.45
3:C:173:ASN:O	3:C:174:PRO:C	2.53	0.45
3:C:365:ILE:O	3:C:368:PRO:HD2	2.17	0.45
7:G:28:ASN:HB2	7:G:32:ASP:HB3	1.99	0.45
1:N:261:GLY:HA2	1:N:317:THR:O	2.17	0.45
1:N:288:LYS:HE3	1:N:289:HIS:NE2	2.31	0.45
3:P:35:GLY:O	3:P:38:LEU:HB2	2.16	0.45
3:P:129:PHE:CD1	3:P:129:PHE:C	2.89	0.45
6:S:19:TRP:O	6:S:22:ASN:N	2.50	0.45
6:S:65:ALA:O	6:S:68:LEU:HB2	2.17	0.45
6:S:96:GLU:O	6:S:97:VAL:C	2.55	0.45
1:A:61:HIS:ND1	1:A:134:ILE:HG12	2.32	0.45
2:B:84:ARG:O	2:B:88:GLY:N	2.47	0.45
5:E:165:TYR:HA	5:E:170:ARG:O	2.17	0.45
2:O:203:ARG:O	2:O:387:LEU:HD11	2.17	0.45
2:O:239:TYR:HE2	2:O:241:GLY:CA	2.30	0.45
2:O:279:LEU:O	2:O:295:LEU:HB3	2.17	0.45
3:P:186:LEU:HD23	3:P:186:LEU:HA	1.71	0.45
2:B:325:TYR:C	2:B:325:TYR:HD2	2.19	0.44
2:B:379:LEU:HG	2:B:379:LEU:O	2.15	0.44
3:C:49:GLY:HA3	13:C:501:HEM:C3C	2.52	0.44
3:C:63:ALA:CB	3:C:176:LEU:HD21	2.46	0.44
2:O:47:ILE:HG22	2:O:48:GLY:N	2.31	0.44
2:O:171:ALA:O	2:O:174:ASN:HB2	2.16	0.44
3:P:130:VAL:O	3:P:131:GLY:C	2.56	0.44
5:R:87:VAL:HG12	5:R:88:ALA:N	2.32	0.44
1:A:49:ASN:ND2	1:A:51:LYS:N	2.65	0.44
1:A:62:LEU:HD21	1:A:126:GLN:HG3	1.99	0.44
1:A:289:HIS:O	1:A:290:LEU:O	2.34	0.44
1:A:300:GLU:HG2	1:A:301:HIS:CE1	2.52	0.44
2:B:59:THR:HG22	2:B:60:THR:N	2.31	0.44
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.98	0.44
3:C:316:MET:CG	3:C:319:ARG:HH21	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.52	0.44
5:E:87:VAL:HG12	5:E:88:ALA:N	2.31	0.44
8:H:56:GLU:O	8:H:59:PHE:HB2	2.16	0.44
9:I:49:LEU:O	9:I:50:LEU:HG	2.17	0.44
9:I:49:LEU:HB3	9:I:55:MET:CG	2.48	0.44
1:N:368:GLN:O	1:N:374:PRO:HB3	2.18	0.44
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.82	0.44
3:P:38:LEU:HD21	3:P:95:ILE:N	2.32	0.44
3:P:151:PHE:C	3:P:153:ALA:N	2.70	0.44
3:P:323:GLN:O	3:P:326:PHE:HB3	2.17	0.44
7:T:28:ASN:HB2	7:T:32:ASP:HB3	1.99	0.44
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.30	0.44
10:W:4:ALA:N	10:W:8:GLN:HE21	2.16	0.44
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.48	0.44
2:B:259:THR:O	2:B:260:GLU:C	2.56	0.44
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.85	0.44
3:C:109:LEU:C	3:C:111:LYS:H	2.21	0.44
3:C:156:TYR:N	3:C:156:TYR:HD2	2.16	0.44
5:E:135:LEU:HA	5:E:183:PRO:HD3	1.99	0.44
5:E:141:HIS:HB3	19:E:501:FES:S2	2.57	0.44
7:G:30:PHE:O	7:G:35:PRO:CD	2.65	0.44
2:O:279:LEU:O	2:O:295:LEU:CB	2.66	0.44
4:Q:208:MET:SD	4:Q:208:MET:C	2.96	0.44
4:Q:224:ARG:O	4:Q:225:HIS:C	2.55	0.44
6:S:73:ARG:NH1	7:T:32:ASP:OD1	2.49	0.44
1:A:67:THR:HB	1:A:119:ASN:O	2.17	0.44
1:A:170:THR:HG22	1:A:171:THR:H	1.82	0.44
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.53	0.44
2:B:235:ALA:O	2:B:236:LYS:C	2.54	0.44
3:C:100:GLY:O	3:C:101:ARG:C	2.54	0.44
3:C:332:ASN:ND2	3:C:359:TYR:CA	2.81	0.44
4:D:22:ASP:O	4:D:25:SER:N	2.51	0.44
4:D:183:ALA:HA	4:D:186:VAL:HG12	2.00	0.44
1:N:294:LEU:O	1:N:298:ALA:HB2	2.17	0.44
2:O:277:HIS:HB2	2:O:360:ALA:HB1	1.98	0.44
2:O:286:LYS:O	2:O:287:ARG:HB2	2.17	0.44
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.98	0.44
5:R:85:LYS:HG2	5:R:86:ASN:N	2.32	0.44
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.50	0.44
3:C:29:SER:HB2	16:C:2004:CDL:HB21	2.00	0.44
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:57:GLN:OE1	20:E:2009:PLC:H12	2.18	0.44
5:E:122:HIS:C	5:E:124:LEU:N	2.71	0.44
5:E:160:CYS:HB3	5:E:161:HIS:CE1	2.53	0.44
1:N:36:THR:OG1	1:N:100:LYS:HG2	2.18	0.44
1:N:191:LYS:C	1:N:193:PRO:HD2	2.38	0.44
1:N:253:VAL:O	1:N:323:HIS:HA	2.17	0.44
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.97	0.44
4:Q:26:VAL:HG13	4:Q:189:PHE:HA	2.00	0.44
4:Q:43:MET:HE3	4:Q:91:PHE:HE2	1.82	0.44
1:A:105:ASP:O	1:A:106:MET:C	2.55	0.44
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.18	0.44
3:C:184:PHE:HA	13:C:501:HEM:CBC	2.48	0.44
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.98	0.44
5:E:29:SER:O	5:E:30:GLU:C	2.56	0.44
6:F:77:LYS:HA	6:F:80:TRP:CD1	2.53	0.44
7:G:73:ASN:O	7:G:75:ALA:N	2.50	0.44
1:N:86:PHE:CE2	1:N:99:ILE:HD11	2.53	0.44
1:N:248:LEU:HB3	1:N:249:PRO:HD2	1.99	0.44
1:N:419:CYS:SG	7:T:21:PHE:HB2	2.58	0.44
2:O:50:PHE:CD2	2:O:106:THR:HG23	2.53	0.44
2:O:333:ALA:O	2:O:337:ILE:HG13	2.17	0.44
3:P:108:TYR:HE1	3:P:309:HIS:HB2	1.81	0.44
3:P:145:THR:O	3:P:149:ASN:HB2	2.17	0.44
3:P:358:SER:O	3:P:362:ILE:HG13	2.18	0.44
4:Q:55:THR:OG1	4:Q:56:HIS:CE1	2.69	0.44
8:U:40:CYS:O	8:U:41:ASP:C	2.55	0.44
2:B:96:LEU:HD13	2:B:109:VAL:HG12	2.00	0.44
2:B:189:GLU:O	2:B:190:GLN:C	2.55	0.44
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.82	0.44
6:F:16:ILE:O	6:F:19:TRP:N	2.48	0.44
9:I:65:VAL:CG1	9:I:66:ALA:N	2.81	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.72	0.44
1:N:277:ILE:O	1:N:277:ILE:HG22	2.17	0.44
1:N:372:THR:O	1:N:373:THR:C	2.56	0.44
2:O:253:VAL:HG13	2:O:430:LEU:HD22	1.99	0.44
2:O:306:PRO:HB3	9:V:52:ARG:N	2.32	0.44
4:Q:102:ARG:HG2	4:Q:102:ARG:NH1	2.33	0.44
6:S:75:LEU:O	6:S:80:TRP:NE1	2.39	0.44
1:A:57:TYR:O	1:A:60:GLU:N	2.51	0.44
1:A:304:CYS:HA	1:A:326:ALA:HB2	2.00	0.44
2:B:56:ARG:NH1	2:B:172:LEU:HD21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:VAL:HG11	2:B:388:LEU:CD1	2.41	0.44
3:C:198:LEU:HD11	15:C:2002:ANY:O4	2.17	0.44
13:C:502:HEM:CMB	13:C:502:HEM:HBB2	2.48	0.44
2:O:229:GLY:O	2:O:231:GLY:N	2.49	0.44
2:O:269:ALA:O	2:O:270:ASN:C	2.56	0.44
3:P:146:VAL:O	3:P:147:ILE:C	2.56	0.44
3:P:151:PHE:N	3:P:151:PHE:CD1	2.85	0.44
4:Q:29:GLY:O	4:Q:32:VAL:HB	2.18	0.44
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.53	0.44
5:R:29:SER:HA	5:R:32:ARG:HH21	1.82	0.44
5:R:112:VAL:HG12	5:R:113:ASP:N	2.32	0.44
7:T:36:ASN:O	7:T:40:ARG:HG3	2.17	0.44
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.51	0.44
1:A:206:LYS:C	1:A:209:VAL:HG12	2.37	0.44
1:A:207:GLU:O	1:A:210:ASP:HB2	2.17	0.44
1:A:254:ALA:HB3	1:A:423:ALA:HB3	2.00	0.44
2:B:163:LEU:HD13	2:B:425:ALA:HB2	1.99	0.44
3:C:107:SER:HB2	13:C:502:HEM:HMD3	2.00	0.44
3:C:123:THR:O	3:C:124:LEU:C	2.56	0.44
3:C:129:PHE:CD1	3:C:129:PHE:C	2.88	0.44
5:E:1:VAL:HG23	5:E:3:ASN:H	1.83	0.44
1:N:19:LEU:C	1:N:21:ASN:N	2.72	0.44
1:N:55:ALA:C	1:N:57:TYR:N	2.71	0.44
1:N:81:SER:HB2	2:O:359:LYS:HE2	1.99	0.44
1:N:192:ALA:N	1:N:193:PRO:HD2	2.33	0.44
1:N:266:ASP:O	1:N:267:ASN:C	2.56	0.44
2:O:163:LEU:CD1	2:O:425:ALA:HB2	2.47	0.44
2:O:370:MET:O	2:O:373:GLU:HG3	2.18	0.44
3:P:95:ILE:CD1	3:P:121:LEU:CD1	2.89	0.44
3:P:354:MET:O	3:P:358:SER:N	2.41	0.44
4:Q:235:MET:CE	6:S:64:ARG:HA	2.48	0.44
1:A:291:SER:OG	2:B:87:ARG:HD3	2.18	0.43
2:B:169:LYS:HD2	2:B:238:THR:HG21	2.00	0.43
4:D:227:TRP:O	4:D:230:LEU:N	2.50	0.43
8:H:66:ASP:O	8:H:67:HIS:C	2.55	0.43
1:N:388:ARG:HD3	1:N:388:ARG:N	2.33	0.43
2:O:100:SER:HA	2:O:104:LYS:O	2.18	0.43
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.99	0.43
2:B:81:SER:O	2:B:82:SER:C	2.57	0.43
2:B:171:ALA:O	2:B:174:ASN:HB2	2.17	0.43
2:B:344:LEU:HD12	2:B:344:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:PHE:O	4:D:191:ARG:N	2.50	0.43
4:D:204:MET:O	4:D:205:GLY:C	2.56	0.43
7:G:34:LEU:O	7:G:35:PRO:C	2.56	0.43
7:G:48:VAL:O	7:G:51:PRO:HD2	2.18	0.43
2:O:166:ALA:O	2:O:242:GLY:N	2.35	0.43
2:O:296:TYR:O	2:O:297:GLN:C	2.57	0.43
2:O:408:ALA:O	2:O:409:ASP:C	2.56	0.43
3:P:60:THR:HG23	3:P:173:ASN:HA	2.00	0.43
3:P:111:LYS:O	3:P:114:TRP:HB3	2.18	0.43
3:P:245:LEU:HD12	4:Q:208:MET:HE2	2.00	0.43
4:Q:197:GLU:O	4:Q:199:ASP:N	2.51	0.43
4:Q:225:HIS:CE1	7:T:20:PRO:HB2	2.53	0.43
1:A:108:LYS:O	1:A:112:LEU:HG	2.19	0.43
1:A:301:HIS:HB2	1:A:303:LEU:HD21	1.99	0.43
3:C:92:PHE:O	3:C:96:PHE:CD2	2.71	0.43
3:C:242:THR:N	4:D:208:MET:CE	2.80	0.43
5:E:135:LEU:HD22	5:E:180:LEU:HD12	1.99	0.43
6:F:31:LEU:HD21	6:F:65:ALA:CB	2.48	0.43
7:G:57:LEU:C	7:G:59:TYR:N	2.70	0.43
1:N:94:GLN:NE2	1:N:381:SER:OG	2.44	0.43
2:O:124:LEU:HG	2:O:125:ASN:N	2.34	0.43
2:O:160:LEU:HD12	9:V:64:LEU:HB2	1.99	0.43
2:O:235:ALA:O	2:O:236:LYS:O	2.36	0.43
2:O:395:PRO:O	2:O:398:VAL:HG12	2.19	0.43
3:P:78:TRP:CG	3:P:79:LEU:N	2.86	0.43
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.84	0.43
4:Q:235:MET:HE1	6:S:64:ARG:N	2.34	0.43
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.82	0.43
6:S:67:ASP:HA	6:S:70:LEU:CD2	2.46	0.43
1:A:155:ALA:O	5:E:7:VAL:HG23	2.19	0.43
1:A:354:VAL:HG23	1:A:355:LYS:N	2.33	0.43
3:C:93:ILE:O	3:C:94:CYS:C	2.56	0.43
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.54	0.43
4:D:155:GLY:C	4:D:157:ALA:N	2.71	0.43
5:E:74:ILE:HG23	5:E:74:ILE:O	2.17	0.43
10:J:22:LEU:HD23	10:J:22:LEU:H	1.82	0.43
2:O:31:ASN:ND2	2:O:31:ASN:H	2.17	0.43
2:O:50:PHE:N	2:O:50:PHE:CD1	2.86	0.43
2:O:167:ALA:C	2:O:168:TYR:CD1	2.92	0.43
2:O:207:VAL:CG1	2:O:208:GLY:N	2.79	0.43
3:P:29:SER:HB2	16:P:3004:CDL:HB21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:184:PHE:CD2	3:P:184:PHE:C	2.92	0.43
3:P:371:GLY:O	3:P:374:GLU:HB2	2.18	0.43
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.43
4:Q:227:TRP:O	4:Q:230:LEU:N	2.50	0.43
5:R:32:ARG:HD2	7:T:21:PHE:O	2.18	0.43
7:T:33:ALA:O	7:T:34:LEU:C	2.57	0.43
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.32	0.43
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.18	0.43
1:A:85:HIS:CD2	2:B:284:LEU:HB3	2.54	0.43
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.53	0.43
1:A:292:SER:O	1:A:293:ARG:C	2.55	0.43
2:B:135:TRP:O	2:B:138:THR:N	2.51	0.43
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.53	0.43
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.31	0.43
4:D:206:LEU:O	4:D:207:LYS:C	2.57	0.43
6:F:42:ASP:O	6:F:43:VAL:C	2.55	0.43
10:J:26:LEU:O	10:J:30:LEU:HG	2.18	0.43
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.54	0.43
1:N:294:LEU:HD23	1:N:307:PHE:CE1	2.53	0.43
2:O:72:ALA:O	2:O:75:LEU:HB2	2.18	0.43
2:O:239:TYR:CD2	2:O:239:TYR:C	2.91	0.43
2:O:306:PRO:HA	9:V:52:ARG:HG3	2.00	0.43
3:P:22:LEU:HD12	3:P:23:PRO:CD	2.49	0.43
3:P:123:THR:O	3:P:124:LEU:C	2.57	0.43
4:Q:109:LEU:HA	4:Q:110:PRO:HD2	1.91	0.43
5:R:94:LYS:O	5:R:95:PRO:O	2.37	0.43
8:U:37:LEU:O	8:U:40:CYS:N	2.50	0.43
1:A:86:PHE:CG	1:A:99:ILE:HG12	2.54	0.43
3:C:28:ILE:HD12	15:C:2002:ANY:H3	2.00	0.43
3:C:101:ARG:C	3:C:101:ARG:CD	2.77	0.43
3:C:117:GLY:C	13:C:502:HEM:HBC2	2.39	0.43
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.25	0.43
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.49	0.43
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.83	0.43
1:N:317:THR:HG23	1:N:318:GLY:N	2.33	0.43
1:N:351:GLU:OE2	1:N:404:ALA:HB3	2.19	0.43
1:N:429:GLU:CD	7:T:7:LEU:HB2	2.37	0.43
2:O:96:LEU:HD13	2:O:109:VAL:HG12	2.00	0.43
3:P:101:ARG:HD2	3:P:102:GLY:CA	2.48	0.43
3:P:232:GLY:HA2	16:Q:3003:CDL:H121	2.00	0.43
4:Q:43:MET:HE3	4:Q:91:PHE:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:29:SER:O	5:R:30:GLU:C	2.56	0.43
5:R:52:LYS:C	5:R:52:LYS:HD3	2.39	0.43
5:R:141:HIS:HB3	19:R:501:FES:S2	2.58	0.43
1:A:259:GLY:HA3	1:A:318:GLY:HA3	1.99	0.43
1:A:287:GLY:C	1:A:289:HIS:H	2.22	0.43
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.48	0.43
2:B:163:LEU:O	2:B:167:ALA:N	2.52	0.43
3:C:95:ILE:CD1	3:C:121:LEU:HD13	2.49	0.43
3:C:104:TYR:HB2	3:C:326:PHE:CE1	2.53	0.43
3:C:149:ASN:HD22	3:C:149:ASN:HA	1.54	0.43
4:D:116:ILE:CG2	4:D:117:VAL:N	2.82	0.43
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.54	0.43
8:H:20:ILE:HG22	8:H:20:ILE:O	2.18	0.43
1:N:382:HIS:HE1	1:N:390:ILE:O	2.02	0.43
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.49	0.43
3:P:88:ALA:O	3:P:91:PHE:HB3	2.19	0.43
3:P:138:GLN:NE2	3:P:266:PRO:HD3	2.34	0.43
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.81	0.43
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.43
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.54	0.43
1:A:368:GLN:O	1:A:374:PRO:HB3	2.18	0.43
2:B:241:GLY:HA2	2:B:423:SER:OG	2.19	0.43
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.83	0.43
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.54	0.43
3:C:130:VAL:HG23	3:C:131:GLY:N	2.33	0.43
4:D:46:VAL:CG1	4:D:47:ALA:H	2.30	0.43
4:D:130:LEU:HD12	4:D:150:ASN:CG	2.39	0.43
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.47	0.43
5:E:114:VAL:O	5:E:114:VAL:HG12	2.19	0.43
6:F:67:ASP:HA	6:F:70:LEU:CD2	2.47	0.43
9:I:59:SER:O	9:I:60:ALA:C	2.56	0.43
1:N:261:GLY:HA2	1:N:314:TYR:O	2.19	0.43
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.75	0.43
2:O:344:LEU:HD12	2:O:344:LEU:HA	1.92	0.43
2:O:350:GLY:C	2:O:352:VAL:H	2.17	0.43
3:P:169:PHE:HD2	3:P:169:PHE:HA	1.77	0.43
4:Q:10:PHE:HB3	8:U:74:PHE:CE1	2.54	0.43
5:R:78:LEU:HG	5:R:193:VAL:HG12	2.00	0.43
9:V:65:VAL:HG12	9:V:66:ALA:H	1.82	0.43
3:C:81:ARG:HH22	17:C:2011:GOL:H2	1.83	0.43
3:C:241:LEU:O	3:C:245:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:165:TYR:O	4:D:166:ASN:C	2.57	0.43
4:D:209:LEU:HD23	4:D:209:LEU:HA	1.82	0.43
10:J:14:PHE:N	10:J:14:PHE:HD2	2.15	0.43
1:N:63:ALA:O	1:N:116:VAL:CG1	2.67	0.43
2:O:182:ARG:HH11	2:O:182:ARG:HG2	1.84	0.43
4:Q:47:ALA:O	4:Q:50:ASN:N	2.39	0.43
4:Q:189:PHE:O	4:Q:191:ARG:N	2.52	0.43
1:A:55:ALA:C	1:A:57:TYR:N	2.72	0.43
1:A:255:LEU:HA	1:A:421:ALA:O	2.19	0.43
2:B:47:ILE:HG22	2:B:48:GLY:N	2.32	0.43
3:C:22:LEU:HD12	3:C:23:PRO:HD2	2.01	0.43
3:C:56:TYR:OH	3:C:134:LEU:O	2.30	0.43
3:C:137:GLY:N	3:C:140:SER:HB2	2.33	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB1	1.84	0.43
5:E:113:ASP:C	5:E:115:SER:N	2.72	0.43
7:G:28:ASN:HB3	7:G:31:SER:OG	2.18	0.43
7:G:57:LEU:O	7:G:59:TYR:N	2.52	0.43
2:O:102:ARG:CZ	2:O:164:HIS:CD2	3.02	0.43
2:O:258:VAL:HG21	2:O:321:LEU:HD22	2.01	0.43
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.01	0.43
2:O:337:ILE:O	2:O:340:ALA:HB3	2.18	0.43
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.18	0.43
7:T:55:ALA:O	7:T:56:TYR:C	2.57	0.43
8:U:58:LEU:HG	8:U:62:LEU:CD1	2.49	0.43
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.49	0.42
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.02	0.42
1:A:422:LEU:HD22	1:A:437:ILE:HD12	2.00	0.42
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.42
3:C:25:PRO:HG2	3:C:207:ASN:O	2.18	0.42
3:C:29:SER:O	3:C:32:TRP:HB2	2.18	0.42
3:C:82:ASN:HD22	3:C:82:ASN:N	2.16	0.42
3:C:237:LEU:O	3:C:241:LEU:HG	2.19	0.42
4:D:134:TYR:CD1	4:D:162:PRO:HG3	2.54	0.42
4:D:143:VAL:O	4:D:144:ARG:C	2.57	0.42
7:G:55:ALA:O	7:G:58:LEU:N	2.52	0.42
1:N:261:GLY:O	1:N:262:TRP:C	2.57	0.42
1:N:273:ALA:O	1:N:275:ALA:N	2.52	0.42
1:N:277:ILE:CD1	1:N:345:LEU:HD11	2.49	0.42
1:N:319:LEU:HD23	1:N:319:LEU:HA	1.73	0.42
2:O:47:ILE:CG2	2:O:48:GLY:N	2.81	0.42
2:O:144:LEU:CB	2:O:183:ILE:CD1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:248:ASN:HD22	2:O:250:HIS:H	1.65	0.42
2:O:399:ALA:HA	2:O:402:ILE:HD12	2.00	0.42
4:Q:47:ALA:O	4:Q:48:PHE:C	2.56	0.42
5:R:97:PHE:O	5:R:134:ILE:HA	2.19	0.42
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.49	0.42
3:C:28:ILE:HG13	3:C:225:TYR:HE2	1.82	0.42
4:D:237:TYR:CD2	4:D:239:PRO:HD3	2.54	0.42
5:E:35:PHE:O	5:E:36:SER:C	2.56	0.42
6:F:20:TYR:O	6:F:23:ALA:HB3	2.19	0.42
1:N:54:GLY:O	1:N:56:GLY:N	2.52	0.42
1:N:284:PHE:HD1	1:N:284:PHE:H	1.66	0.42
2:O:230:ALA:O	2:O:231:GLY:C	2.57	0.42
2:O:412:ASN:O	2:O:413:ALA:C	2.56	0.42
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.20	0.42
2:B:169:LYS:HB2	2:B:238:THR:HB	2.00	0.42
2:B:358:THR:HA	2:B:361:LYS:HD2	2.02	0.42
3:C:141:PHE:HB2	3:C:260:ALA:HB1	2.02	0.42
3:C:154:ILE:HG21	3:C:157:ILE:HD11	2.01	0.42
3:C:378:LEU:O	3:C:379:ASN:HB3	2.19	0.42
4:D:22:ASP:O	4:D:24:SER:N	2.52	0.42
5:E:113:ASP:CB	5:E:116:LYS:HB2	2.49	0.42
5:E:177:PRO:C	5:E:178:TYR:HD1	2.22	0.42
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.49	0.42
1:N:90:THR:HB	1:N:95:THR:HG23	2.02	0.42
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.46	0.42
3:P:99:ILE:HD11	3:P:121:LEU:HD22	2.01	0.42
3:P:107:SER:C	3:P:109:LEU:N	2.72	0.42
3:P:151:PHE:C	3:P:153:ALA:H	2.21	0.42
1:A:78:GLU:OE1	1:A:108:LYS:CE	2.67	0.42
3:C:14:MET:O	3:C:15:ILE:C	2.57	0.42
2:O:239:TYR:HE1	2:O:260:GLU:H	1.65	0.42
3:P:196:ILE:O	3:P:197:HIS:C	2.57	0.42
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.80	0.42
5:R:186:GLN:HE21	5:R:188:VAL:HG12	1.84	0.42
1:A:261:GLY:HA2	1:A:317:THR:O	2.20	0.42
1:A:301:HIS:HB2	1:A:303:LEU:CD2	2.50	0.42
2:B:317:SER:OG	2:B:318:ASP:N	2.52	0.42
8:H:49:HIS:CG	8:H:49:HIS:O	2.71	0.42
10:J:13:LEU:O	10:J:19:THR:OG1	2.36	0.42
2:O:168:TYR:HD2	2:O:237:ALA:HB1	1.83	0.42
2:O:247:GLN:HE21	2:O:249:GLY:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:70:THR:HA	3:P:74:VAL:HG21	2.01	0.42
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.27	0.42
4:Q:46:VAL:CG1	4:Q:47:ALA:N	2.81	0.42
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.42
5:R:29:SER:O	5:R:31:ASP:N	2.52	0.42
6:S:16:ILE:O	6:S:19:TRP:N	2.52	0.42
2:B:209:ILE:O	2:B:211:VAL:HG22	2.19	0.42
3:C:193:ILE:HG13	3:C:193:ILE:H	1.67	0.42
3:C:243:LEU:HD12	3:C:243:LEU:HA	1.76	0.42
3:C:285:ILE:HB	3:C:291:GLY:HA2	2.01	0.42
3:C:380:TYR:HH	6:F:33:ARG:HE	1.68	0.42
4:D:121:HIS:C	4:D:123:GLY:H	2.22	0.42
5:E:185:TYR:HB2	5:E:186:GLN:H	1.63	0.42
8:H:15:ASP:C	8:H:17:LEU:N	2.72	0.42
1:N:439:SER:C	1:N:441:MET:H	2.23	0.42
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.50	0.42
2:O:57:TYR:N	2:O:57:TYR:CD1	2.87	0.42
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.54	0.42
6:S:50:LEU:HA	6:S:51:PRO:HD3	1.83	0.42
7:T:30:PHE:O	7:T:35:PRO:CD	2.67	0.42
1:A:284:PHE:H	1:A:284:PHE:HD1	1.66	0.42
2:B:258:VAL:HB	2:B:322:PHE:C	2.40	0.42
3:C:36:SER:HA	15:C:2002:ANY:O7	2.20	0.42
3:C:191:ALA:O	3:C:195:ILE:HG12	2.20	0.42
3:C:273:TRP:CD2	3:C:274:TYR:N	2.88	0.42
3:C:301:ILE:HD13	3:C:363:LEU:HD13	2.02	0.42
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.01	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.19	0.42
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.19	0.42
1:N:257:VAL:HG23	1:N:320:PHE:HB3	2.01	0.42
1:N:378:THR:O	1:N:382:HIS:N	2.50	0.42
2:O:76:THR:HG23	2:O:82:SER:HB2	2.02	0.42
3:P:49:GLY:HA3	13:P:501:HEM:C2C	2.55	0.42
5:R:83:GLU:HA	5:R:100:HIS:CG	2.54	0.42
7:T:73:ASN:O	7:T:75:ALA:N	2.53	0.42
8:U:50:THR:OG1	8:U:51:GLU:N	2.52	0.42
10:W:45:HIS:C	10:W:47:ASN:H	2.23	0.42
1:A:178:THR:O	1:A:179:ARG:C	2.57	0.42
1:A:187:ASP:O	1:A:191:LYS:HE3	2.20	0.42
1:A:236:PHE:HB2	1:A:258:GLU:OE1	2.19	0.42
2:B:163:LEU:CD1	2:B:425:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:VAL:O	3:C:165:ALA:N	2.52	0.42
5:E:94:LYS:O	5:E:95:PRO:O	2.37	0.42
6:F:49:ARG:HH22	6:F:100:GLU:CD	2.23	0.42
1:N:29:GLU:OE1	1:N:204:SER:HA	2.19	0.42
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.60	0.42
1:N:301:HIS:HB2	1:N:303:LEU:CD2	2.50	0.42
3:P:273:TRP:CD2	3:P:274:TYR:N	2.88	0.42
7:T:12:HIS:O	7:T:13:ILE:HG13	2.19	0.42
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.33	0.42
2:B:50:PHE:HD1	2:B:50:PHE:H	1.68	0.42
3:C:38:LEU:HD21	3:C:95:ILE:N	2.35	0.42
5:E:29:SER:O	5:E:31:ASP:N	2.53	0.42
5:E:103:GLN:O	5:E:107:ASN:ND2	2.53	0.42
5:E:127:VAL:HG11	5:E:133:VAL:HG23	2.02	0.42
5:E:149:ASN:O	5:E:150:SER:HB3	2.19	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HB	2.55	0.42
1:N:78:GLU:OE1	1:N:108:LYS:CE	2.67	0.42
2:O:47:ILE:O	2:O:108:CYS:HB2	2.20	0.42
3:P:223:PRO:HA	3:P:226:SER:OG	2.20	0.42
4:Q:18:LEU:HD22	4:Q:206:LEU:HD13	2.02	0.42
4:Q:44:ASP:O	4:Q:90:TYR:HD2	2.03	0.42
5:R:108:GLN:C	5:R:110:ALA:N	2.73	0.42
6:S:73:ARG:HG3	6:S:73:ARG:NH1	2.33	0.42
1:A:40:TRP:CD1	1:A:96:ALA:CB	3.03	0.42
1:A:89:TYR:O	1:A:95:THR:CG2	2.65	0.42
1:A:90:THR:HB	1:A:95:THR:HG23	2.01	0.42
1:A:138:LEU:HD22	5:E:3:ASN:HD21	1.84	0.42
1:A:182:LEU:HD23	1:A:182:LEU:H	1.85	0.42
1:A:251:ALA:HB1	1:A:428:ILE:HG22	2.02	0.42
2:B:62:ASN:HD22	2:B:65:THR:HG21	1.85	0.42
3:C:107:SER:C	3:C:109:LEU:H	2.23	0.42
4:D:186:VAL:HG21	18:D:501:HEC:HBB3	2.02	0.42
5:E:78:LEU:HD21	5:E:193:VAL:HG11	2.02	0.42
5:E:141:HIS:HB3	5:E:142:LEU:H	1.66	0.42
1:N:112:LEU:O	1:N:113:LEU:C	2.57	0.42
1:N:433:ASP:OD2	1:N:435:ASN:N	2.53	0.42
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.50	0.42
3:P:93:ILE:O	3:P:94:CYS:C	2.57	0.42
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.42
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.20	0.42
1:A:239:SER:O	1:A:421:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:O	1:A:359:ASN:N	2.53	0.41
2:B:35:ILE:O	2:B:213:HIS:HE1	2.03	0.41
2:B:209:ILE:CG2	2:B:210:GLY:N	2.82	0.41
3:C:59:ASP:O	3:C:60:THR:C	2.58	0.41
3:C:80:ILE:O	3:C:81:ARG:C	2.56	0.41
14:C:2001:SMA:H4	5:R:161:HIS:CE1	2.55	0.41
4:D:182:ILE:O	4:D:185:ASP:N	2.53	0.41
18:D:501:HEC:HBC3	18:D:501:HEC:CMC	2.44	0.41
5:E:78:LEU:HD22	5:E:132:TRP:CD2	2.54	0.41
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.55	0.41
9:I:49:LEU:HB3	9:I:55:MET:HG2	2.02	0.41
1:N:317:THR:OG1	1:N:318:GLY:N	2.51	0.41
2:O:163:LEU:O	2:O:166:ALA:N	2.52	0.41
4:Q:160:MET:HB2	18:Q:501:HEC:C1D	2.50	0.41
4:Q:215:LEU:HD12	4:Q:219:LEU:HG	2.02	0.41
1:A:158:PHE:O	1:A:159:GLN:O	2.37	0.41
2:B:408:ALA:O	2:B:409:ASP:C	2.58	0.41
3:C:145:THR:O	3:C:149:ASN:HB2	2.20	0.41
3:C:269:ILE:O	3:C:270:LYS:HD3	2.20	0.41
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.55	0.41
2:O:169:LYS:HB2	2:O:238:THR:HB	2.01	0.41
2:O:183:ILE:HD13	2:O:183:ILE:HA	1.88	0.41
2:O:189:GLU:O	2:O:191:LEU:N	2.53	0.41
3:P:6:ARG:CD	3:P:16:ASN:OD1	2.65	0.41
3:P:352:GLY:O	3:P:353:GLN:C	2.58	0.41
4:Q:3:LEU:HD23	4:Q:3:LEU:H	1.85	0.41
4:Q:218:LEU:HD13	5:R:43:ALA:CA	2.50	0.41
7:T:57:LEU:C	7:T:59:TYR:N	2.73	0.41
8:U:15:ASP:C	8:U:17:LEU:N	2.73	0.41
1:A:80:GLU:CD	2:B:290:SER:HA	2.41	0.41
1:A:178:THR:HG22	1:A:179:ARG:N	2.36	0.41
1:A:233:ARG:NH2	1:A:316:ASP:HB2	2.35	0.41
2:B:201:SER:N	2:B:227:ARG:O	2.53	0.41
2:B:378:LEU:C	2:B:380:ASN:N	2.72	0.41
2:B:431:GLY:HA3	2:O:60:THR:HG21	2.01	0.41
3:C:236:MET:O	3:C:238:THR:N	2.53	0.41
5:E:18:VAL:O	5:E:18:VAL:HG23	2.20	0.41
1:N:76:GLU:HG2	2:O:285:ILE:HD12	2.03	0.41
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.41
1:N:249:PRO:HG2	1:N:250:VAL:H	1.85	0.41
1:N:288:LYS:N	1:N:299:VAL:HG11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:26:ILE:HG23	2:O:26:ILE:O	2.20	0.41
3:P:30:ALA:C	3:P:32:TRP:N	2.72	0.41
5:R:20:ASP:C	5:R:22:THR:H	2.23	0.41
5:R:45:VAL:O	5:R:48:ALA:HB3	2.21	0.41
7:T:77:TYR:C	7:T:79:ASN:H	2.23	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.38	0.41
2:B:366:ALA:O	2:B:369:LEU:N	2.53	0.41
3:C:95:ILE:O	3:C:99:ILE:HG13	2.21	0.41
4:D:197:GLU:HG2	4:D:198:HIS:H	1.83	0.41
5:E:24:SER:OG	5:E:26:GLN:HB2	2.21	0.41
5:E:38:LEU:CA	10:J:14:PHE:CE1	3.01	0.41
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.36	0.41
2:O:417:PHE:CD2	2:O:417:PHE:C	2.94	0.41
3:P:57:THR:O	3:P:57:THR:HG22	2.20	0.41
3:P:160:THR:O	3:P:163:GLU:HB3	2.21	0.41
3:P:331:ALA:HB2	7:T:52:PHE:CD2	2.55	0.41
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.01	0.41
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.37	0.41
6:S:89:TYR:CD1	6:S:89:TYR:C	2.93	0.41
10:W:55:ILE:O	10:W:56:LYS:C	2.58	0.41
1:A:40:TRP:CD2	1:A:380:GLY:HA3	2.56	0.41
1:A:86:PHE:HD1	1:A:87:ASN:N	2.18	0.41
1:A:166:THR:HG21	5:E:3:ASN:OD1	2.20	0.41
2:B:111:CYS:SG	2:B:119:VAL:HG21	2.60	0.41
2:B:259:THR:HG22	2:B:260:GLU:N	2.34	0.41
4:D:195:GLU:HG3	4:D:195:GLU:O	2.20	0.41
5:E:20:ASP:C	5:E:22:THR:H	2.24	0.41
8:H:55:THR:O	8:H:58:LEU:N	2.54	0.41
10:J:55:ILE:O	10:J:56:LYS:C	2.59	0.41
1:N:69:LYS:HE3	1:N:70:ARG:NH2	2.15	0.41
1:N:291:SER:OG	2:O:87:ARG:HD3	2.20	0.41
2:O:144:LEU:HB3	2:O:183:ILE:CD1	2.51	0.41
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.85	0.41
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.56	0.41
8:U:20:ILE:O	8:U:20:ILE:HG22	2.20	0.41
1:A:281:ASP:O	1:A:284:PHE:HD1	2.03	0.41
4:D:42:SER:C	4:D:112:ASP:OD2	2.59	0.41
4:D:241:LYS:HA	4:D:241:LYS:CE	2.42	0.41
5:E:33:LYS:HG2	7:G:21:PHE:CD1	2.56	0.41
5:E:134:ILE:C	5:E:135:LEU:HG	2.40	0.41
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:75:SER:O	9:I:76:VAL:HB	2.20	0.41
1:N:147:ASN:O	1:N:148:VAL:C	2.59	0.41
2:O:283:PRO:CG	9:V:56:SER:HB2	2.47	0.41
2:O:362:ASN:HA	2:O:365:LYS:HD2	2.01	0.41
3:P:38:LEU:HB3	13:P:502:HEM:CMB	2.51	0.41
3:P:60:THR:N	3:P:176:LEU:HD23	2.36	0.41
4:Q:48:PHE:CE2	4:Q:65:ALA:HA	2.56	0.41
4:Q:195:GLU:N	4:Q:196:PRO:HD3	2.36	0.41
6:S:18:LYS:HA	6:S:83:TYR:CE1	2.55	0.41
6:S:53:ASP:O	6:S:57:GLU:HG3	2.21	0.41
9:V:65:VAL:CG1	9:V:66:ALA:N	2.83	0.41
1:A:29:GLU:OE1	1:A:204:SER:HA	2.21	0.41
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.56	0.41
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.83	0.41
1:A:206:LYS:CA	1:A:209:VAL:HG12	2.50	0.41
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.21	0.41
3:C:99:ILE:O	3:C:100:GLY:C	2.58	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41
6:F:63:LYS:HD3	7:G:13:ILE:HD13	2.01	0.41
6:F:90:LEU:O	6:F:91:GLU:C	2.59	0.41
1:N:80:GLU:CD	2:O:290:SER:HA	2.41	0.41
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.41
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.55	0.41
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.01	0.41
1:N:434:TYR:O	1:N:435:ASN:C	2.58	0.41
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.02	0.41
2:O:31:ASN:N	2:O:31:ASN:HD22	2.18	0.41
2:O:144:LEU:HB3	2:O:183:ILE:HD11	2.02	0.41
2:O:166:ALA:HB1	2:O:242:GLY:O	2.20	0.41
2:O:227:ARG:NH1	2:O:228:SER:H	2.17	0.41
2:O:248:ASN:HD21	2:O:250:HIS:CB	2.29	0.41
3:P:22:LEU:HD12	3:P:23:PRO:N	2.35	0.41
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.56	0.41
3:P:285:ILE:HB	3:P:291:GLY:HA2	2.03	0.41
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.36	0.41
3:P:332:ASN:ND2	3:P:359:TYR:CA	2.82	0.41
4:Q:171:TYR:HH	4:Q:182:ILE:HA	1.83	0.41
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.55	0.41
6:S:76:PRO:O	6:S:77:LYS:C	2.59	0.41
1:A:67:THR:HA	1:A:121:ALA:H	1.85	0.41
1:A:95:THR:HG22	1:A:96:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.55	0.41
2:B:235:ALA:O	2:B:236:LYS:O	2.38	0.41
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.55	0.41
3:C:186:LEU:HD23	3:C:186:LEU:HA	1.71	0.41
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.46	0.41
6:F:53:ASP:O	6:F:55:TYR:N	2.53	0.41
6:F:87:LYS:CG	6:F:87:LYS:O	2.69	0.41
1:N:272:VAL:O	1:N:275:ALA:HB3	2.21	0.41
2:O:75:LEU:HD11	2:O:140:LEU:HD23	2.03	0.41
3:P:92:PHE:HA	3:P:95:ILE:CG2	2.45	0.41
3:P:241:LEU:O	3:P:245:LEU:N	2.54	0.41
3:P:378:LEU:O	3:P:379:ASN:CB	2.68	0.41
4:Q:34:LYS:O	4:Q:38:SER:OG	2.34	0.41
4:Q:220:TYR:CE1	4:Q:224:ARG:HG3	2.56	0.41
6:S:52:GLU:HG2	6:S:56:ASN:HD21	1.86	0.41
1:A:210:ASP:C	1:A:212:ALA:N	2.73	0.41
1:A:235:ARG:CZ	5:E:14:ARG:NH2	2.84	0.41
1:A:287:GLY:C	1:A:289:HIS:N	2.74	0.41
1:A:288:LYS:HE3	1:A:289:HIS:NE2	2.36	0.41
2:B:47:ILE:CG2	2:B:48:GLY:N	2.83	0.41
2:B:124:LEU:HG	2:B:125:ASN:N	2.36	0.41
2:B:289:SER:O	2:B:290:SER:C	2.58	0.41
2:B:366:ALA:O	2:B:367:THR:C	2.59	0.41
3:C:227:PHE:CD2	4:D:226:LYS:HG3	2.56	0.41
3:C:358:SER:O	3:C:362:ILE:HG13	2.21	0.41
3:C:367:PHE:HD2	3:C:367:PHE:HA	1.73	0.41
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.02	0.41
4:D:208:MET:SD	4:D:208:MET:C	2.99	0.41
4:D:215:LEU:HD12	4:D:219:LEU:HG	2.03	0.41
4:D:224:ARG:HH12	16:D:2003:CDL:HB21	1.86	0.41
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.41
6:F:43:VAL:O	6:F:46:ALA:N	2.54	0.41
6:F:89:TYR:HD1	6:F:89:TYR:C	2.24	0.41
10:J:51:LEU:C	10:J:53:LYS:N	2.74	0.41
1:N:29:GLU:HG3	1:N:203:ILE:O	2.21	0.41
1:N:40:TRP:HZ3	1:N:376:CYS:SG	2.27	0.41
1:N:62:LEU:HD21	1:N:126:GLN:HG3	2.01	0.41
1:N:223:TYR:N	1:N:223:TYR:CD2	2.81	0.41
1:N:411:CYS:HB3	1:N:415:ILE:HD12	2.02	0.41
2:O:72:ALA:CA	2:O:75:LEU:HD12	2.50	0.41
2:O:130:PRO:CB	2:O:132:PHE:CE2	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.56	0.41
2:O:207:VAL:HG21	2:O:383:GLY:HA3	2.03	0.41
2:O:325:TYR:C	2:O:325:TYR:CD2	2.94	0.41
2:O:412:ASN:O	2:O:415:LYS:N	2.53	0.41
3:P:28:ILE:HG13	3:P:225:TYR:HE2	1.84	0.41
3:P:99:ILE:O	3:P:100:GLY:C	2.58	0.41
3:P:104:TYR:CD1	3:P:316:MET:SD	3.14	0.41
3:P:165:ALA:O	3:P:178:ARG:HD2	2.20	0.41
3:P:201:LEU:C	3:P:203:GLU:H	2.24	0.41
3:P:230:ILE:CG2	11:P:3005:PEE:H25	2.50	0.41
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.89	0.41
4:Q:43:MET:HG2	4:Q:91:PHE:HD2	1.85	0.41
4:Q:237:TYR:CD2	4:Q:239:PRO:HD3	2.56	0.41
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	2.03	0.41
5:R:50:ALA:HA	20:R:3009:PLC:OB	2.21	0.41
6:S:32:MET:HE1	6:S:87:LYS:H	1.85	0.41
6:S:42:ASP:O	6:S:43:VAL:C	2.59	0.41
7:T:40:ARG:O	7:T:41:PHE:C	2.59	0.41
1:A:46:ARG:NH1	1:A:316:ASP:OD1	2.36	0.41
1:A:157:ALA:HB1	1:A:236:PHE:HE1	1.86	0.41
1:A:373:THR:HB	1:A:374:PRO:CD	2.46	0.41
3:C:323:GLN:O	3:C:326:PHE:HB3	2.21	0.41
4:D:43:MET:O	4:D:45:TYR:N	2.54	0.41
4:D:47:ALA:O	4:D:49:ARG:N	2.54	0.41
1:N:177:LEU:HA	1:N:177:LEU:HD23	1.86	0.41
2:O:312:PHE:CE1	9:V:62:ARG:O	2.69	0.41
3:P:245:LEU:O	4:Q:201:ARG:HG2	2.20	0.41
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.97	0.41
3:P:365:ILE:O	3:P:368:PRO:HD2	2.21	0.41
5:R:46:ALA:O	5:R:47:THR:C	2.58	0.41
2:B:328:SER:OG	2:B:333:ALA:HA	2.21	0.40
2:B:339:ALA:HA	2:B:342:ASN:ND2	2.36	0.40
2:B:369:LEU:O	2:B:372:VAL:HG22	2.21	0.40
4:D:158:ILE:HG12	4:D:159:GLY:N	2.34	0.40
5:E:122:HIS:C	5:E:124:LEU:H	2.24	0.40
2:O:62:ASN:O	2:O:65:THR:CG2	2.67	0.40
2:O:221:GLU:C	2:O:223:PHE:H	2.25	0.40
2:O:295:LEU:O	2:O:296:TYR:C	2.60	0.40
3:P:78:TRP:CE3	3:P:79:LEU:N	2.89	0.40
3:P:164:TRP:O	3:P:167:GLY:N	2.54	0.40
5:R:29:SER:CB	5:R:32:ARG:HH21	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.36	0.40
2:B:130:PRO:HB2	2:B:132:PHE:CD2	2.56	0.40
3:C:29:SER:O	3:C:30:ALA:C	2.59	0.40
3:C:64:PHE:HD2	4:D:45:TYR:HH	1.67	0.40
1:N:11:ILE:HA	1:N:12:PRO:HD2	1.86	0.40
1:N:106:MET:HB3	1:N:107:PRO:CD	2.51	0.40
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.40
1:N:296:ALA:O	1:N:299:VAL:HB	2.22	0.40
2:O:131:GLU:O	2:O:132:PHE:C	2.59	0.40
3:P:38:LEU:HD23	3:P:38:LEU:HA	1.85	0.40
3:P:200:PHE:O	3:P:203:GLU:HB2	2.21	0.40
3:P:273:TRP:HA	3:P:276:LEU:HG	2.02	0.40
3:P:357:LEU:HD12	3:P:357:LEU:HA	1.69	0.40
3:P:378:LEU:O	3:P:379:ASN:HB3	2.22	0.40
3:P:378:LEU:HD23	3:P:378:LEU:HA	1.94	0.40
4:Q:143:VAL:O	4:Q:144:ARG:C	2.59	0.40
4:Q:204:MET:O	4:Q:205:GLY:C	2.59	0.40
5:R:113:ASP:O	5:R:115:SER:N	2.53	0.40
2:B:394:ALA:HB3	2:B:397:VAL:HG23	2.03	0.40
3:C:27:ASN:ND2	3:C:209:PRO:HD2	2.36	0.40
3:C:184:PHE:CD2	3:C:184:PHE:C	2.95	0.40
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.87	0.40
3:C:346:HIS:CG	3:C:347:PRO:HA	2.56	0.40
4:D:164:ILE:HD11	4:D:183:ALA:HB2	2.02	0.40
5:E:10:PHE:O	5:E:14:ARG:HG3	2.22	0.40
1:N:61:HIS:NE2	1:N:137:GLU:OE1	2.53	0.40
1:N:86:PHE:HD1	1:N:87:ASN:N	2.19	0.40
2:O:68:LEU:HD22	2:O:186:ILE:HD12	2.02	0.40
2:O:73:SER:N	2:O:74:PRO:CD	2.84	0.40
3:P:67:VAL:O	3:P:68:ALA:C	2.59	0.40
3:P:115:ASN:O	3:P:118:VAL:HG23	2.21	0.40
3:P:146:VAL:O	3:P:149:ASN:N	2.54	0.40
4:Q:175:THR:HA	4:Q:176:PRO:HD3	1.85	0.40
16:Q:3003:CDL:H732	16:Q:3003:CDL:HA61	2.04	0.40
1:A:112:LEU:HG	1:A:112:LEU:H	1.49	0.40
1:A:241:ILE:O	1:A:241:ILE:CG2	2.70	0.40
1:A:339:GLN:NE2	1:A:437:ILE:HG23	2.37	0.40
3:C:280:ALA:O	3:C:281:ILE:C	2.59	0.40
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.21	0.40
5:E:52:LYS:C	5:E:52:LYS:HD3	2.41	0.40
1:N:246:ASP:HA	1:N:427:PRO:CB	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:LEU:CD1	2:O:38:LEU:HB2	2.46	0.40
2:O:163:LEU:HD12	2:O:163:LEU:HA	1.83	0.40
3:P:285:ILE:N	3:P:285:ILE:CD1	2.85	0.40
3:P:338:TRP:CZ2	7:T:59:TYR:HD1	2.39	0.40
3:P:346:HIS:CG	3:P:347:PRO:HA	2.57	0.40
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.21	0.40
5:R:186:GLN:O	5:R:193:VAL:HG23	2.21	0.40
6:S:32:MET:HE3	6:S:87:LYS:CB	2.50	0.40
7:T:61:TRP:CE3	7:T:62:GLY:N	2.89	0.40
8:U:56:GLU:O	8:U:59:PHE:HB2	2.22	0.40
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.57	0.40
1:A:262:TRP:HE3	1:A:386:TYR:CZ	2.39	0.40
1:A:273:ALA:O	1:A:275:ALA:N	2.55	0.40
1:A:378:THR:O	1:A:382:HIS:N	2.52	0.40
2:B:345:LYS:O	2:B:347:ALA:N	2.54	0.40
3:C:56:TYR:OH	3:C:176:LEU:HD11	2.21	0.40
3:C:311:SER:OG	3:C:319:ARG:HD3	2.21	0.40
3:C:333:LEU:HD11	11:C:2007:PEE:H38	2.04	0.40
5:E:91:TRP:O	5:E:92:ARG:C	2.59	0.40
5:E:170:ARG:HA	5:E:179:ASN:CB	2.51	0.40
6:F:76:PRO:O	6:F:78:GLU:N	2.54	0.40
6:F:89:TYR:CD1	6:F:89:TYR:C	2.94	0.40
6:F:94:LEU:O	6:F:95:LYS:C	2.60	0.40
7:G:40:ARG:O	7:G:41:PHE:C	2.59	0.40
7:G:41:PHE:HE2	7:G:45:VAL:HB	1.87	0.40
1:N:51:LYS:HE3	1:N:51:LYS:HB2	1.94	0.40
1:N:110:VAL:HA	1:N:113:LEU:HD12	2.03	0.40
1:N:158:PHE:O	1:N:159:GLN:C	2.59	0.40
1:N:283:THR:O	1:N:284:PHE:C	2.59	0.40
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.37	0.40
3:P:166:TRP:C	3:P:168:GLY:H	2.24	0.40
3:P:184:PHE:CE2	13:P:501:HEM:HBC1	2.57	0.40
3:P:270:LYS:HA	3:P:271:PRO:HD3	1.94	0.40
4:Q:46:VAL:HB	4:Q:91:PHE:CD2	2.57	0.40
6:S:89:TYR:HD1	6:S:89:TYR:C	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	323 (73%)	94 (21%)	24 (5%)	2	19
1	N	440/446 (99%)	320 (73%)	95 (22%)	25 (6%)	1	18
2	B	419/441 (95%)	302 (72%)	77 (18%)	40 (10%)	0	8
2	O	420/441 (95%)	302 (72%)	85 (20%)	33 (8%)	1	11
3	C	378/380 (100%)	284 (75%)	72 (19%)	22 (6%)	1	18
3	P	377/380 (99%)	284 (75%)	73 (19%)	20 (5%)	2	19
4	D	239/241 (99%)	188 (79%)	37 (16%)	14 (6%)	1	17
4	Q	239/241 (99%)	186 (78%)	40 (17%)	13 (5%)	2	19
5	E	194/196 (99%)	136 (70%)	42 (22%)	16 (8%)	1	10
5	R	194/196 (99%)	136 (70%)	36 (19%)	22 (11%)	0	6
6	F	99/110 (90%)	73 (74%)	24 (24%)	2 (2%)	7	42
6	S	99/110 (90%)	73 (74%)	23 (23%)	3 (3%)	4	33
7	G	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	1	12
7	T	77/81 (95%)	52 (68%)	20 (26%)	5 (6%)	1	16
8	H	68/77 (88%)	46 (68%)	18 (26%)	4 (6%)	1	17
8	U	65/77 (84%)	41 (63%)	20 (31%)	4 (6%)	1	17
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0	4
9	V	29/47 (62%)	21 (72%)	4 (14%)	4 (14%)	0	4
10	J	59/61 (97%)	41 (70%)	16 (27%)	2 (3%)	3	31
10	W	57/61 (93%)	36 (63%)	17 (30%)	4 (7%)	1	14
All	All	4002/4160 (96%)	2919 (73%)	816 (20%)	267 (7%)	1	15

All (267) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA

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Mol	Chain	Res	Type
1	A	72	CYS
1	A	94	GLN
1	A	159	GLN
1	A	282	ARG
1	A	290	LEU
2	B	29	LEU
2	B	171	ALA
2	B	201	SER
2	B	226	ILE
2	B	230	ALA
2	B	236	LYS
2	B	283	PRO
3	C	31	TRP
3	C	58	ALA
3	C	111	LYS
3	C	224	TYR
3	C	348	PHE
4	D	44	ASP
4	D	198	HIS
5	E	63	SER
5	E	95	PRO
5	E	113	ASP
5	E	141	HIS
6	F	69	SER
7	G	7	LEU
7	G	33	ALA
9	I	63	ASP
10	J	56	LYS
1	N	4	TYR
1	N	55	ALA
1	N	72	CYS
1	N	159	GLN
1	N	206	LYS
1	N	282	ARG
1	N	433	ASP
2	O	171	ALA
2	O	201	SER
2	O	226	ILE
2	O	230	ALA
2	O	236	LYS
2	O	283	PRO
3	P	58	ALA

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Mol	Chain	Res	Type
3	P	111	LYS
3	P	224	TYR
4	Q	198	HIS
5	R	63	SER
5	R	95	PRO
5	R	141	HIS
6	S	69	SER
7	T	7	LEU
7	T	33	ALA
10	W	56	LYS
10	W	60	GLU
1	A	288	LYS
1	A	404	ALA
1	A	433	ASP
2	B	20	GLY
2	B	26	ILE
2	B	64	GLY
2	B	110	GLU
2	B	190	GLN
2	B	231	GLY
2	B	249	GLY
2	B	290	SER
2	B	319	SER
2	B	366	ALA
2	B	386	ALA
2	B	420	GLY
3	C	6	ARG
3	C	17	ASN
3	C	202	HIS
4	D	133	GLY
4	D	168	ILE
4	D	177	ALA
4	D	183	ALA
5	E	92	ARG
5	E	137	GLY
5	E	154	GLY
5	E	180	LEU
5	E	188	VAL
6	F	77	LYS
9	I	60	ALA
9	I	73	PRO
9	I	76	VAL

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Mol	Chain	Res	Type
10	J	57	HIS
1	N	20	ASP
1	N	94	GLN
1	N	207	GLU
1	N	288	LYS
1	N	290	LEU
1	N	404	ALA
2	O	19	PRO
2	O	26	ILE
2	O	64	GLY
2	O	222	GLN
2	O	231	GLY
2	O	290	SER
2	O	351	GLY
2	O	420	GLY
3	P	6	ARG
3	P	17	ASN
3	P	31	TRP
3	P	108	TYR
3	P	158	GLY
3	P	202	HIS
3	P	217	ASP
3	P	348	PHE
4	Q	44	ASP
4	Q	48	PHE
4	Q	133	GLY
4	Q	168	ILE
4	Q	177	ALA
4	Q	183	ALA
5	R	8	PRO
5	R	92	ARG
5	R	109	GLU
5	R	113	ASP
5	R	137	GLY
5	R	180	LEU
6	S	77	LYS
7	T	42	SER
8	U	46	SER
10	W	57	HIS
1	A	4	TYR
1	A	5	ALA
1	A	164	ALA

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Mol	Chain	Res	Type
1	A	222	THR
1	A	274	ASN
2	B	114	ASP
2	B	180	ASP
2	B	265	GLY
2	B	334	GLY
2	B	409	ASP
3	C	3	PRO
3	C	158	GLY
3	C	207	ASN
3	C	217	ASP
3	C	359	TYR
4	D	48	PHE
4	D	166	ASN
4	D	190	LEU
5	E	69	LEU
5	E	70	ALA
5	E	72	SER
5	E	123	ASP
5	E	150	SER
7	G	42	SER
8	H	28	GLU
1	N	222	THR
1	N	262	TRP
1	N	274	ASN
1	N	405	ARG
2	O	110	GLU
2	O	249	GLY
2	O	319	SER
2	O	334	GLY
2	O	346	ALA
2	O	366	ALA
2	O	386	ALA
2	O	409	ASP
3	P	207	ASN
4	Q	162	PRO
4	Q	190	LEU
5	R	21	ALA
5	R	70	ALA
5	R	72	SER
8	U	28	GLU
9	V	48	PRO

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	56	GLY
1	A	71	PRO
1	A	262	TRP
1	A	332	ASP
1	A	405	ARG
2	B	82	SER
2	B	227	ARG
2	B	346	ALA
2	B	351	GLY
3	C	60	THR
3	C	108	TYR
3	C	156	TYR
3	C	379	ASN
4	D	23	HIS
5	E	186	GLN
8	H	72	LYS
1	N	56	GLY
1	N	164	ALA
1	N	332	ASP
2	O	76	THR
2	O	82	SER
2	O	180	ASP
2	O	296	TYR
3	P	3	PRO
3	P	60	THR
3	P	288	LYS
3	P	359	TYR
3	P	379	ASN
4	Q	144	ARG
4	Q	166	ASN
5	R	114	VAL
5	R	121	GLN
8	U	61	PHE
8	U	72	LYS
9	V	72	ALA
9	V	76	VAL
1	A	141	MET
2	B	63	LEU
2	B	235	ALA
2	B	296	TYR
2	B	375	ALA

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Mol	Chain	Res	Type
2	B	401	LYS
3	C	208	ASN
3	C	209	PRO
3	C	237	LEU
4	D	162	PRO
4	D	176	PRO
5	E	21	ALA
7	G	50	PRO
7	G	61	TRP
8	H	46	SER
8	H	61	PHE
1	N	71	PRO
1	N	170	THR
2	O	114	ASP
3	P	157	ILE
3	P	209	PRO
5	R	30	GLU
5	R	46	ALA
5	R	57	GLN
5	R	69	LEU
5	R	130	PRO
5	R	154	GLY
5	R	188	VAL
6	S	68	LEU
7	T	43	SER
9	V	60	ALA
1	A	106	MET
1	A	263	ALA
1	A	268	VAL
2	B	181	TYR
2	B	207	VAL
2	B	229	GLY
2	B	266	SER
3	C	76	TYR
4	D	110	PRO
1	N	5	ALA
2	O	63	LEU
2	O	178	CYS
3	P	208	ASN
4	Q	176	PRO
5	R	149	ASN
7	T	50	PRO

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Mol	Chain	Res	Type
2	O	134	PRO
2	O	207	VAL
4	Q	110	PRO
3	C	259	PRO
7	G	74	PRO
1	N	268	VAL
1	N	331	ILE
10	W	25	VAL
2	O	85	ILE
2	B	85	ILE
2	B	178	CYS
2	B	282	GLY
2	O	282	GLY
4	D	122	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	342 (94%)	23 (6%)	18	52
1	N	365/368 (99%)	343 (94%)	22 (6%)	19	53
2	B	332/347 (96%)	316 (95%)	16 (5%)	25	60
2	O	333/347 (96%)	315 (95%)	18 (5%)	22	56
3	C	329/329 (100%)	306 (93%)	23 (7%)	15	47
3	P	328/329 (100%)	304 (93%)	24 (7%)	14	46
4	D	200/200 (100%)	192 (96%)	8 (4%)	31	65
4	Q	200/200 (100%)	190 (95%)	10 (5%)	24	59
5	E	166/166 (100%)	156 (94%)	10 (6%)	19	53
5	R	166/166 (100%)	157 (95%)	9 (5%)	22	56
6	F	93/96 (97%)	85 (91%)	8 (9%)	10	40
6	S	93/96 (97%)	83 (89%)	10 (11%)	6	31
7	G	71/71 (100%)	65 (92%)	6 (8%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	69/71 (97%)	65 (94%)	4 (6%)	20	54
8	H	65/71 (92%)	63 (97%)	2 (3%)	40	71
8	U	63/71 (89%)	59 (94%)	4 (6%)	18	52
9	I	23/26 (88%)	21 (91%)	2 (9%)	10	40
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	46 (94%)	3 (6%)	18	53
10	W	47/49 (96%)	45 (96%)	2 (4%)	29	63
All	All	3380/3446 (98%)	3176 (94%)	204 (6%)	19	53

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	40	TRP
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	87	ASN
1	A	102	LEU
1	A	106	MET
1	A	146	THR
1	A	182	LEU
1	A	223	TYR
1	A	226	ASP
1	A	264	ASP
1	A	281	ASP
1	A	302	LYS
1	A	307	PHE
1	A	363	SER
1	A	388	ARG
1	A	395	TRP
1	A	420	PRO
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	73	SER
2	B	101	THR
2	B	102	ARG
2	B	106	THR

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Mol	Chain	Res	Type
2	B	124	LEU
2	B	146	VAL
2	B	152	PHE
2	B	181	TYR
2	B	192	HIS
2	B	227	ARG
2	B	239	TYR
2	B	248	ASN
2	B	296	TYR
2	B	325	TYR
2	B	403	ASP
3	C	23	PRO
3	C	32	TRP
3	C	47	LEU
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	161	LEU
3	C	169	PHE
3	C	184	PHE
3	C	199	THR
3	C	207	ASN
3	C	208	ASN
3	C	214	SER
3	C	216	SER
3	C	223	PRO
3	C	231	LEU
3	C	236	MET
3	C	258	THR
3	C	266	PRO
3	C	283	ARG
3	C	324	THR
3	C	336	LEU
3	C	367	PHE
4	D	10	PHE
4	D	37	CYS
4	D	42	SER
4	D	43	MET
4	D	44	ASP
4	D	179	MET
4	D	215	LEU
4	D	241	LYS

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Mol	Chain	Res	Type
5	E	6	THR
5	E	23	THR
5	E	52	LYS
5	E	59	ILE
5	E	61	SER
5	E	65	SER
5	E	123	ASP
5	E	125	ASP
5	E	135	LEU
5	E	190	ASP
6	F	34	ASP
6	F	36	THR
6	F	59	MET
6	F	70	LEU
6	F	77	LYS
6	F	84	GLU
6	F	89	TYR
6	F	91	GLU
7	G	16	TYR
7	G	29	ILE
7	G	41	PHE
7	G	63	THR
7	G	80	ASP
7	G	81	GLN
8	H	10	GLU
8	H	26	GLN
9	I	63	ASP
9	I	71	ASN
10	J	16	ARG
10	J	26	LEU
10	J	59	TYR
1	N	40	TRP
1	N	49	ASN
1	N	53	ASN
1	N	58	PHE
1	N	86	PHE
1	N	102	LEU
1	N	106	MET
1	N	171	THR
1	N	182	LEU
1	N	223	TYR
1	N	264	ASP

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Mol	Chain	Res	Type
1	N	274	ASN
1	N	281	ASP
1	N	302	LYS
1	N	307	PHE
1	N	363	SER
1	N	388	ARG
1	N	395	TRP
1	N	420	PRO
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	73	SER
2	O	101	THR
2	O	102	ARG
2	O	106	THR
2	O	124	LEU
2	O	146	VAL
2	O	152	PHE
2	O	181	TYR
2	O	192	HIS
2	O	228	SER
2	O	239	TYR
2	O	248	ASN
2	O	258	VAL
2	O	296	TYR
2	O	325	TYR
2	O	403	ASP
3	P	23	PRO
3	P	32	TRP
3	P	47	LEU
3	P	81	ARG
3	P	91	PHE
3	P	138	GLN
3	P	145	THR
3	P	149	ASN
3	P	161	LEU
3	P	169	PHE
3	P	184	PHE
3	P	199	THR
3	P	207	ASN

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Mol	Chain	Res	Type
3	P	208	ASN
3	P	214	SER
3	P	216	SER
3	P	223	PRO
3	P	236	MET
3	P	258	THR
3	P	277	PHE
3	P	324	THR
3	P	336	LEU
3	P	337	THR
3	P	367	PHE
4	Q	3	LEU
4	Q	10	PHE
4	Q	13	SER
4	Q	37	CYS
4	Q	42	SER
4	Q	43	MET
4	Q	44	ASP
4	Q	199	ASP
4	Q	215	LEU
4	Q	241	LYS
5	R	6	THR
5	R	23	THR
5	R	52	LYS
5	R	59	ILE
5	R	61	SER
5	R	65	SER
5	R	135	LEU
5	R	147	ILE
5	R	190	ASP
6	S	13	MET
6	S	34	ASP
6	S	36	THR
6	S	59	MET
6	S	70	LEU
6	S	77	LYS
6	S	78	GLU
6	S	84	GLU
6	S	89	TYR
6	S	91	GLU
7	T	16	TYR
7	T	29	ILE

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Mol	Chain	Res	Type
7	T	41	PHE
7	T	63	THR
8	U	13	LEU
8	U	26	GLN
8	U	51	GLU
8	U	71	HIS
10	W	26	LEU
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	87	ASN
1	A	118	GLN
1	A	136	GLN
1	A	159	GLN
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	332	HIS
2	B	362	ASN
2	B	363	GLN
2	B	376	GLN
2	B	400	GLN
3	C	33	ASN
3	C	73	ASN
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN

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Mol	Chain	Res	Type
4	D	105	ASN
4	D	200	GLN
4	D	225	HIS
5	E	86	ASN
5	E	107	ASN
5	E	164	HIS
5	E	186	GLN
6	F	56	ASN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
7	G	81	GLN
8	H	26	GLN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	87	ASN
1	N	118	GLN
1	N	136	GLN
1	N	159	GLN
1	N	173	ASN
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	222	GLN
2	O	247	GLN
2	O	248	ASN
2	O	297	GLN
2	O	329	GLN
2	O	332	HIS
2	O	362	ASN
2	O	363	GLN
2	O	376	GLN
2	O	400	GLN
3	P	33	ASN
3	P	69	HIS
3	P	82	ASN

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Mol	Chain	Res	Type
3	P	149	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	105	ASN
4	Q	200	GLN
4	Q	225	HIS
5	R	164	HIS
5	R	186	GLN
6	S	56	ASN
6	S	79	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
16	CDL	C	2004	-	39,39,99	1.27	5 (12%)	45,51,111	1.13	2 (4%)
17	GOL	C	2011	-	5,5,5	1.25	0	5,5,5	0.61	0
20	PLC	E	2009	-	31,31,41	1.71	6 (19%)	37,39,49	0.71	0
18	HEC	D	501	4	32,50,50	2.19	2 (6%)	24,82,82	1.78	5 (20%)
11	PEE	P	3005	-	49,49,50	1.53	10 (20%)	52,54,55	0.87	3 (5%)
15	ANY	P	3002	-	38,38,41	1.83	9 (23%)	34,52,55	2.22	7 (20%)
20	PLC	R	3009	-	31,31,41	1.63	9 (29%)	37,39,49	0.59	0
16	CDL	P	3004	-	39,39,99	1.26	4 (10%)	45,51,111	1.13	2 (4%)
16	CDL	D	2003	-	49,49,99	1.18	4 (8%)	55,61,111	0.91	1 (1%)
13	HEM	P	502	3	41,50,50	1.78	8 (19%)	45,82,82	1.77	11 (24%)
16	CDL	Q	3003	-	49,49,99	1.15	3 (6%)	55,61,111	0.93	1 (1%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
14	SMA	C	2001	-	38,38,38	1.35	4 (10%)	48,52,52	0.85	3 (6%)
13	HEM	C	502	3	41,50,50	1.95	10 (24%)	45,82,82	2.27	12 (26%)
13	HEM	P	501	3	41,50,50	1.91	9 (21%)	45,82,82	1.85	13 (28%)
13	HEM	C	501	3	41,50,50	1.84	9 (21%)	45,82,82	2.13	11 (24%)
15	ANY	C	2002	-	38,38,41	1.56	4 (10%)	34,52,55	2.22	9 (26%)
11	PEE	E	2005	-	49,49,50	1.43	9 (18%)	52,54,55	0.87	3 (5%)
11	PEE	P	3007	-	48,48,50	1.42	6 (12%)	51,53,55	0.84	3 (5%)
11	PEE	A	2008	-	20,20,50	1.81	5 (25%)	23,25,55	0.71	1 (4%)
17	GOL	P	3011	-	5,5,5	1.21	0	5,5,5	0.59	0
19	FES	E	501	5	0,4,4	-	-	-	-	-
11	PEE	N	3008	-	4,4,50	3.60	4 (100%)	6,6,55	0.66	0
11	PEE	C	2007	-	48,48,50	1.44	8 (16%)	51,53,55	0.85	3 (5%)
18	HEC	Q	501	4	32,50,50	2.34	5 (15%)	24,82,82	1.76	5 (20%)
14	SMA	P	3001	-	38,38,38	1.54	7 (18%)	48,52,52	0.82	1 (2%)

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
16	CDL	C	2004	-	-	24/49/49/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GOL	C	2011	-	-	1/4/4/4	-
20	PLC	E	2009	-	-	14/35/35/45	-
18	HEC	D	501	4	-	4/10/54/54	-
11	PEE	P	3005	-	-	27/53/53/54	-
15	ANY	P	3002	-	1/1/10/13	1/37/52/56	0/1/2/2
20	PLC	R	3009	-	-	14/35/35/45	-
16	CDL	P	3004	-	-	22/49/49/110	-
16	CDL	D	2003	-	-	29/59/59/110	-
13	HEM	P	502	3	-	4/12/54/54	-
16	CDL	Q	3003	-	-	28/59/59/110	-
19	FES	R	501	5	-	-	0/1/1/1
14	SMA	C	2001	-	-	15/34/34/34	0/2/2/2
13	HEM	C	502	3	-	5/12/54/54	-
13	HEM	P	501	3	-	6/12/54/54	-
13	HEM	C	501	3	-	6/12/54/54	-
15	ANY	C	2002	-	1/1/10/13	1/37/52/56	0/1/2/2
11	PEE	E	2005	-	-	28/53/53/54	-
11	PEE	P	3007	-	-	28/52/52/54	-
11	PEE	A	2008	-	-	15/24/24/54	-
17	GOL	P	3011	-	-	2/4/4/4	-
19	FES	E	501	5	-	-	0/1/1/1
11	PEE	C	2007	-	-	29/52/52/54	-
18	HEC	Q	501	4	-	6/10/54/54	-
14	SMA	P	3001	-	-	15/34/34/34	0/2/2/2

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	501	HEC	C2B-C3B	-8.63	1.31	1.40
18	D	501	HEC	C2B-C3B	-8.01	1.32	1.40
18	Q	501	HEC	C3C-C2C	-7.38	1.33	1.40
18	D	501	HEC	C3C-C2C	-7.32	1.33	1.40
13	C	502	HEM	C3C-CAC	-5.89	1.35	1.47
15	P	3002	ANY	C8-N1	5.83	1.42	1.34
15	C	2002	ANY	C8-N1	5.59	1.41	1.34
14	C	2001	SMA	C7-C8	5.10	1.47	1.40
13	C	502	HEM	CBB-CAB	5.04	1.55	1.30
13	C	501	HEM	C3C-C2C	-5.00	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	501	HEM	CBB-CAB	4.66	1.53	1.30
13	P	502	HEM	C3C-CAC	-4.65	1.38	1.47
13	P	502	HEM	C3C-C2C	-4.58	1.34	1.40
13	P	501	HEM	C3C-C2C	-4.56	1.34	1.40
13	C	502	HEM	C3C-C2C	-4.50	1.34	1.40
13	P	501	HEM	C3C-CAC	-4.50	1.38	1.47
11	N	3008	PEE	P-O1P	4.50	1.61	1.50
20	E	2009	PLC	O2-C'	4.41	1.46	1.34
13	C	501	HEM	C3C-CAC	-4.23	1.39	1.47
14	P	3001	SMA	O1-C2	4.20	1.41	1.36
11	E	2005	PEE	C39-C38	4.17	1.55	1.31
11	P	3005	PEE	C39-C38	4.14	1.55	1.31
11	C	2007	PEE	C39-C38	4.12	1.55	1.31
11	P	3007	PEE	C39-C38	4.08	1.55	1.31
13	C	501	HEM	CBC-CAC	3.99	1.55	1.29
13	C	501	HEM	CAB-C3B	-3.91	1.36	1.47
13	P	502	HEM	CBB-CAB	3.89	1.49	1.30
15	P	3002	ANY	C2-C1	3.86	1.46	1.40
20	R	3009	PLC	O2-C'	3.81	1.45	1.34
13	P	502	HEM	CAB-C3B	-3.70	1.37	1.47
11	N	3008	PEE	P-O3P	3.67	1.65	1.54
14	P	3001	SMA	C20-C19	3.66	1.36	1.33
13	P	501	HEM	CBC-CAC	3.64	1.53	1.29
11	C	2007	PEE	O2-C10	3.62	1.44	1.34
13	C	501	HEM	CBB-CAB	3.58	1.48	1.30
11	N	3008	PEE	P-O4P	3.55	1.65	1.54
11	P	3007	PEE	O2-C10	3.52	1.44	1.34
11	P	3005	PEE	P-O1P	3.41	1.63	1.50
13	P	502	HEM	CBC-CAC	3.38	1.51	1.29
11	P	3005	PEE	O2-C10	3.34	1.43	1.34
20	E	2009	PLC	P-O1P	3.31	1.62	1.50
11	A	2008	PEE	O2-C10	3.29	1.43	1.34
11	P	3005	PEE	O3-C30	3.26	1.42	1.33
20	E	2009	PLC	O2-C2	3.24	1.54	1.46
14	P	3001	SMA	C7-C8	3.23	1.44	1.40
13	P	501	HEM	CAB-C3B	-3.18	1.38	1.47
15	P	3002	ANY	O8-C21	3.14	1.41	1.34
11	C	2007	PEE	P-O1P	3.11	1.61	1.50
11	E	2005	PEE	O3-C30	3.08	1.42	1.33
20	R	3009	PLC	P-O1P	3.07	1.61	1.50
11	A	2008	PEE	P-O1P	3.07	1.61	1.50
15	P	3002	ANY	C12-C11	3.06	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	E	2009	PLC	O3-CB	3.03	1.42	1.33
11	E	2005	PEE	P-O1P	3.03	1.61	1.50
15	C	2002	ANY	C12-C11	3.02	1.59	1.52
11	E	2005	PEE	O2-C10	3.01	1.42	1.34
11	A	2008	PEE	O3-C30	3.00	1.42	1.33
15	C	2002	ANY	C2-C1	3.00	1.44	1.40
11	P	3007	PEE	C21-C22	-2.99	1.34	1.51
20	R	3009	PLC	O3-CB	2.95	1.41	1.33
20	E	2009	PLC	C1-C2	2.94	1.59	1.50
11	P	3005	PEE	C31-C30	2.93	1.59	1.50
13	C	502	HEM	C1B-C2B	2.93	1.50	1.44
11	C	2007	PEE	C21-C22	-2.93	1.35	1.51
11	E	2005	PEE	C21-C22	-2.91	1.35	1.51
13	C	502	HEM	CBC-CAC	2.86	1.48	1.29
14	P	3001	SMA	C6-C5	2.85	1.44	1.38
11	P	3007	PEE	O3-C30	2.84	1.41	1.33
18	Q	501	HEC	CAD-C3D	2.84	1.56	1.52
11	P	3007	PEE	P-O1P	2.84	1.61	1.50
11	P	3005	PEE	C21-C22	-2.77	1.36	1.51
13	P	501	HEM	C3D-C2D	-2.77	1.30	1.36
11	A	2008	PEE	C1-C2	2.70	1.59	1.50
16	D	2003	CDL	CA6-CA4	2.69	1.58	1.50
18	Q	501	HEC	C1C-CHC	-2.69	1.33	1.41
15	P	3002	ANY	C13-C12	2.65	1.58	1.53
20	R	3009	PLC	C1-C2	2.62	1.58	1.50
11	C	2007	PEE	O3-C30	2.59	1.40	1.33
16	D	2003	CDL	O1-C1	2.59	1.51	1.43
14	P	3001	SMA	C3-C2	2.58	1.39	1.34
11	P	3005	PEE	C11-C10	2.58	1.58	1.50
13	C	502	HEM	C3D-C2D	-2.58	1.31	1.36
15	C	2002	ANY	O8-C21	2.57	1.40	1.34
14	C	2001	SMA	C6-C5	2.54	1.43	1.38
14	P	3001	SMA	C8-C8A	2.50	1.43	1.39
15	P	3002	ANY	C6-C1	2.50	1.45	1.41
16	P	3004	CDL	CA3-CA4	2.49	1.58	1.50
13	C	501	HEM	C3B-C2B	-2.48	1.32	1.37
13	C	502	HEM	CAB-C3B	-2.47	1.40	1.47
13	P	501	HEM	C1A-CHA	-2.42	1.34	1.41
13	P	502	HEM	CAA-C2A	2.40	1.55	1.52
11	E	2005	PEE	C31-C30	2.40	1.57	1.50
13	P	502	HEM	C4D-C3D	2.38	1.49	1.45
16	C	2004	CDL	CA3-CA4	2.38	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	2003	CDL	CA3-CA4	2.38	1.58	1.50
16	C	2004	CDL	OA6-CA5	2.37	1.41	1.34
11	N	3008	PEE	P-O2P	2.36	1.61	1.54
16	C	2004	CDL	CB3-CB4	2.36	1.57	1.50
13	C	502	HEM	C4D-ND	-2.35	1.36	1.40
13	P	501	HEM	C2C-C1C	2.34	1.47	1.42
15	P	3002	ANY	C3-C2	2.34	1.43	1.39
20	E	2009	PLC	C3-C2	2.32	1.57	1.50
20	R	3009	PLC	O2-C2	2.31	1.52	1.46
16	Q	3003	CDL	CA3-CA4	2.31	1.57	1.50
18	Q	501	HEC	C2A-C1A	2.29	1.47	1.42
16	P	3004	CDL	O1-C1	2.28	1.50	1.43
11	P	3007	PEE	C3-C2	2.27	1.57	1.50
14	C	2001	SMA	O1-C2	2.27	1.39	1.36
14	C	2001	SMA	C4A-C5	2.26	1.44	1.40
14	P	3001	SMA	C4A-C5	2.26	1.44	1.40
16	Q	3003	CDL	O1-C1	2.24	1.50	1.43
11	E	2005	PEE	C11-C10	2.24	1.57	1.50
20	R	3009	PLC	C1B-CB	2.22	1.57	1.50
16	C	2004	CDL	OB8-CB7	2.21	1.39	1.33
13	C	501	HEM	CMD-C2D	2.20	1.55	1.50
11	P	3005	PEE	C3-C2	2.20	1.57	1.50
16	D	2003	CDL	OB8-CB7	2.18	1.39	1.33
15	P	3002	ANY	O5-C14	2.17	1.39	1.34
11	C	2007	PEE	C3-C2	2.17	1.57	1.50
16	Q	3003	CDL	CA6-CA4	2.16	1.57	1.50
20	R	3009	PLC	C5-C4	2.16	1.58	1.51
13	C	502	HEM	C3B-C4B	2.15	1.49	1.44
13	C	502	HEM	C4A-NA	-2.15	1.31	1.36
11	A	2008	PEE	C3-C2	2.14	1.57	1.50
15	P	3002	ANY	C7-N2	2.14	1.38	1.34
13	P	501	HEM	C3B-C2B	-2.13	1.33	1.37
11	P	3005	PEE	P-O4P	2.12	1.67	1.59
13	C	501	HEM	C1A-CHA	-2.12	1.35	1.41
11	C	2007	PEE	C1-C2	2.11	1.57	1.50
20	R	3009	PLC	C1'-C'	2.10	1.56	1.50
11	P	3005	PEE	C1-C2	2.09	1.57	1.50
11	E	2005	PEE	P-O4P	2.09	1.67	1.59
16	C	2004	CDL	O1-C1	2.09	1.49	1.43
20	R	3009	PLC	C3-C2	2.08	1.57	1.50
16	P	3004	CDL	OB8-CB7	2.06	1.39	1.33
13	C	501	HEM	C1D-C2D	2.06	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	502	HEM	C1D-C2D	2.05	1.48	1.44
11	E	2005	PEE	C3-C2	2.04	1.56	1.50
16	P	3004	CDL	OA6-CA5	2.02	1.40	1.34
11	C	2007	PEE	P-O4P	2.01	1.67	1.59

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	3002	ANY	C25-C22-C21	8.03	135.38	111.02
15	C	2002	ANY	C25-C22-C21	7.83	134.77	111.02
13	C	502	HEM	C3B-C2B-C1B	-7.09	101.22	106.49
13	C	502	HEM	C4A-C3A-C2A	6.51	111.52	107.00
13	C	502	HEM	CMB-C2B-C1B	6.05	134.25	125.04
13	C	501	HEM	CAD-C3D-C4D	5.48	134.24	124.66
15	C	2002	ANY	O5-C14-O6	-5.44	117.22	124.08
13	C	501	HEM	C2C-C3C-C4C	-5.42	103.11	106.90
18	Q	501	HEC	CBA-CAA-C2A	5.38	121.67	112.60
15	P	3002	ANY	C25-C22-C23	-5.35	89.40	111.69
13	C	501	HEM	CBA-CAA-C2A	-5.28	103.62	112.62
18	D	501	HEC	CBA-CAA-C2A	5.20	121.37	112.60
15	C	2002	ANY	C25-C22-C23	-4.59	92.54	111.69
15	P	3002	ANY	O5-C14-O6	-4.43	118.50	124.08
13	P	501	HEM	C2C-C3C-C4C	-4.25	103.93	106.90
13	C	501	HEM	CMB-C2B-C1B	4.16	131.38	125.04
13	P	502	HEM	C4A-C3A-C2A	4.15	109.89	107.00
13	P	501	HEM	CAD-C3D-C4D	4.05	131.73	124.66
13	P	502	HEM	C3B-C2B-C1B	-3.98	103.53	106.49
13	C	502	HEM	CAD-C3D-C4D	3.93	131.53	124.66
13	P	501	HEM	CBA-CAA-C2A	-3.89	105.98	112.62
13	C	501	HEM	C3D-C4D-ND	3.89	114.50	110.17
16	P	3004	CDL	CB4-OB6-CB5	-3.75	108.55	117.79
13	P	502	HEM	CBD-CAD-C3D	-3.69	102.36	112.63
13	P	502	HEM	CAD-C3D-C4D	3.66	131.05	124.66
16	C	2004	CDL	CB4-OB6-CB5	-3.57	109.00	117.79
13	C	501	HEM	C4A-C3A-C2A	3.54	109.46	107.00
13	C	502	HEM	CHB-C1B-NB	-3.52	120.03	124.38
13	P	501	HEM	C4D-ND-C1D	-3.39	101.57	105.07
15	P	3002	ANY	O4-C20-O7	-3.28	119.95	124.08
11	P	3005	PEE	C22-C21-C20	3.18	127.64	113.79
15	C	2002	ANY	O4-C20-O7	-3.17	120.08	124.08
11	E	2005	PEE	C22-C21-C20	3.14	127.45	113.79
13	P	501	HEM	CMB-C2B-C1B	3.08	129.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	501	HEC	CMC-C2C-C3C	-3.06	122.22	125.82
11	P	3007	PEE	C22-C21-C20	3.03	126.98	113.79
18	D	501	HEC	CMB-C2B-C3B	-3.03	122.26	125.82
18	Q	501	HEC	CMC-C2C-C3C	-3.01	122.28	125.82
13	P	501	HEM	CMD-C2D-C1D	2.98	129.58	125.04
11	C	2007	PEE	C22-C21-C20	2.96	126.69	113.79
13	C	501	HEM	CAD-C3D-C2D	-2.96	122.37	127.88
13	P	502	HEM	C4C-CHD-C1D	2.92	126.41	122.56
13	C	502	HEM	CAD-C3D-C2D	-2.92	122.44	127.88
13	P	501	HEM	C1B-NB-C4B	-2.84	102.14	105.07
13	P	502	HEM	C1B-NB-C4B	-2.77	102.21	105.07
18	Q	501	HEC	CBD-CAD-C3D	2.77	117.34	112.62
14	C	2001	SMA	O7-C7-C8	2.75	117.31	114.54
15	P	3002	ANY	C12-O8-C21	2.72	122.45	117.78
13	P	501	HEM	CAD-C3D-C2D	-2.71	122.83	127.88
13	P	502	HEM	CMA-C3A-C4A	-2.63	124.42	128.46
13	C	502	HEM	C2B-C1B-NB	2.61	112.94	109.84
13	P	502	HEM	CAD-C3D-C2D	-2.60	123.04	127.88
15	C	2002	ANY	C23-C22-C21	2.58	118.85	111.02
16	D	2003	CDL	CB4-OB6-CB5	-2.57	111.47	117.79
11	P	3005	PEE	C21-C22-C23	2.56	127.43	114.42
13	P	501	HEM	C2D-C1D-ND	2.54	112.93	109.88
11	C	2007	PEE	C21-C22-C23	2.54	127.33	114.42
13	C	502	HEM	C4C-CHD-C1D	2.52	125.88	122.56
11	E	2005	PEE	C21-C22-C23	2.51	127.15	114.42
13	P	501	HEM	C3B-C2B-C1B	-2.50	104.63	106.49
13	P	501	HEM	C3D-C4D-ND	2.50	112.95	110.17
13	C	501	HEM	C4D-ND-C1D	-2.50	102.49	105.07
13	P	502	HEM	CMB-C2B-C1B	2.48	128.82	125.04
18	D	501	HEC	CAA-C2A-C3A	-2.48	120.12	127.25
14	P	3001	SMA	C4A-C4-C3	-2.45	115.18	118.79
13	C	502	HEM	CBD-CAD-C3D	-2.44	105.85	112.63
18	Q	501	HEC	CAA-C2A-C3A	-2.43	120.27	127.25
11	P	3007	PEE	C21-C22-C23	2.43	126.74	114.42
13	C	501	HEM	C4D-C3D-C2D	-2.41	103.38	106.90
15	C	2002	ANY	C12-O8-C21	2.36	121.83	117.78
13	C	501	HEM	C1B-NB-C4B	-2.35	102.65	105.07
16	Q	3003	CDL	CB4-OB6-CB5	-2.34	112.03	117.79
13	C	502	HEM	C1B-NB-C4B	-2.33	102.67	105.07
15	C	2002	ANY	O8-C21-O9	-2.30	119.65	123.94
14	C	2001	SMA	C4A-C4-C3	-2.30	115.41	118.79
14	C	2001	SMA	C9-C10-C11	-2.29	110.33	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	2005	PEE	O3-C3-C2	2.28	115.08	108.43
18	Q	501	HEC	CMB-C2B-C3B	-2.28	123.14	125.82
15	C	2002	ANY	O1-C1-C6	2.28	125.11	121.07
18	D	501	HEC	C1D-C2D-C3D	2.25	108.56	107.00
13	P	501	HEM	C4B-CHC-C1C	2.25	125.53	122.56
13	P	502	HEM	CMC-C2C-C3C	2.23	128.85	124.68
13	P	502	HEM	C4B-CHC-C1C	2.18	125.44	122.56
15	P	3002	ANY	C23-C22-C21	2.17	117.62	111.02
15	P	3002	ANY	O1-C1-C6	2.17	124.92	121.07
11	C	2007	PEE	O3-C3-C2	2.16	114.72	108.43
11	A	2008	PEE	O3-C3-C2	2.14	114.65	108.43
11	P	3007	PEE	O3-C3-C2	2.14	114.65	108.43
16	C	2004	CDL	OB6-CB4-CB3	2.13	116.12	108.40
11	P	3005	PEE	O3-C3-C2	2.12	114.62	108.43
13	C	501	HEM	CMB-C2B-C3B	-2.10	123.17	128.30
15	C	2002	ANY	O7-C20-C9	2.08	130.49	124.72
13	P	501	HEM	C2B-C1B-NB	2.08	112.30	109.84
16	P	3004	CDL	CA6-CA4-CA3	-2.07	106.89	111.79
13	C	502	HEM	CMC-C2C-C3C	2.06	128.53	124.68
13	C	502	HEM	CBA-CAA-C2A	-2.03	109.15	112.62

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	2002	ANY	C22
15	P	3002	ANY	C22

All (324) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	O3P-C1-C2-O2
11	C	2007	PEE	C1-O3P-P-O2P
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C1-O3P-P-O1P
11	E	2005	PEE	C4-O4P-P-O3P
11	E	2005	PEE	C4-O4P-P-O2P
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	O4P-C4-C5-N
11	P	3005	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
11	P	3005	PEE	C1-O3P-P-O1P
11	P	3005	PEE	C4-O4P-P-O3P
11	P	3005	PEE	C4-O4P-P-O2P
11	P	3005	PEE	C4-O4P-P-O1P
11	P	3005	PEE	O4P-C4-C5-N
11	P	3007	PEE	O3P-C1-C2-O2
11	P	3007	PEE	C1-O3P-P-O2P
11	P	3007	PEE	C4-O4P-P-O3P
11	P	3007	PEE	C4-O4P-P-O2P
11	P	3007	PEE	C4-O4P-P-O1P
13	C	501	HEM	C2B-C3B-CAB-CBB
13	P	501	HEM	C2B-C3B-CAB-CBB
14	C	2001	SMA	C3-C2-C9-C10
14	C	2001	SMA	O1-C2-C9-C10
14	C	2001	SMA	C24-C13-C14-O14
14	C	2001	SMA	C13-C14-O14-C25
14	C	2001	SMA	C15-C14-O14-C25
14	C	2001	SMA	C14-C15-C16-C17
14	P	3001	SMA	C3-C2-C9-C10
14	P	3001	SMA	O1-C2-C9-C10
14	P	3001	SMA	C13-C14-O14-C25
14	P	3001	SMA	C15-C14-O14-C25
14	P	3001	SMA	C14-C15-C16-C17
16	C	2004	CDL	O1-C1-CA2-OA2
16	C	2004	CDL	CA3-OA5-PA1-OA2
16	C	2004	CDL	CA3-OA5-PA1-OA3
16	C	2004	CDL	CA3-OA5-PA1-OA4
16	C	2004	CDL	OB5-CB3-CB4-OB6
16	D	2003	CDL	O1-C1-CB2-OB2
16	D	2003	CDL	CA2-OA2-PA1-OA5
16	D	2003	CDL	CB2-OB2-PB2-OB3
16	D	2003	CDL	CB2-OB2-PB2-OB4
16	D	2003	CDL	CB2-OB2-PB2-OB5
16	P	3004	CDL	O1-C1-CA2-OA2
16	P	3004	CDL	CA3-OA5-PA1-OA3
16	P	3004	CDL	CA3-OA5-PA1-OA4
16	P	3004	CDL	OB5-CB3-CB4-OB6
16	Q	3003	CDL	CA2-OA2-PA1-OA5
16	Q	3003	CDL	CB2-OB2-PB2-OB3
16	Q	3003	CDL	CB2-OB2-PB2-OB4
16	Q	3003	CDL	CB2-OB2-PB2-OB5
18	D	501	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	D	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
20	E	2009	PLC	C1-O3P-P-O4P
11	E	2005	PEE	O5-C30-O3-C3
11	P	3005	PEE	O5-C30-O3-C3
11	E	2005	PEE	O4-C10-O2-C2
11	P	3005	PEE	O4-C10-O2-C2
11	E	2005	PEE	C31-C30-O3-C3
11	P	3005	PEE	C31-C30-O3-C3
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
14	C	2001	SMA	C8-C7-O7-C7M
14	P	3001	SMA	C8-C7-O7-C7M
16	Q	3003	CDL	O1-C1-CB2-OB2
11	A	2008	PEE	C31-C30-O3-C3
16	Q	3003	CDL	C31-CA7-OA8-CA6
16	P	3004	CDL	C51-CB5-OB6-CB4
16	D	2003	CDL	C31-CA7-OA8-CA6
14	P	3001	SMA	C6-C7-O7-C7M
14	C	2001	SMA	C6-C7-O7-C7M
11	A	2008	PEE	O5-C30-O3-C3
16	C	2004	CDL	C51-CB5-OB6-CB4
20	E	2009	PLC	C1'-C'-O2-C2
16	Q	3003	CDL	CA2-C1-CB2-OB2
16	D	2003	CDL	C71-CB7-OB8-CB6
16	Q	3003	CDL	C71-CB7-OB8-CB6
16	P	3004	CDL	C31-CA7-OA8-CA6
14	C	2001	SMA	C17-C18-C19-C26
14	P	3001	SMA	C17-C18-C19-C26
14	C	2001	SMA	C17-C18-C19-C20
14	P	3001	SMA	C17-C18-C19-C20
20	E	2009	PLC	O'-C'-O2-C2
20	R	3009	PLC	C1'-C'-O2-C2
16	Q	3003	CDL	OA9-CA7-OA8-CA6
16	D	2003	CDL	CA5-C11-C12-C13
16	Q	3003	CDL	CA5-C11-C12-C13
11	E	2005	PEE	C37-C38-C39-C40
11	P	3005	PEE	C37-C38-C39-C40
16	D	2003	CDL	OA9-CA7-OA8-CA6
11	E	2005	PEE	C10-C11-C12-C13
11	P	3005	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	P	3004	CDL	OB7-CB5-OB6-CB4
16	Q	3003	CDL	OB9-CB7-OB8-CB6
16	D	2003	CDL	OB9-CB7-OB8-CB6
14	C	2001	SMA	C16-C17-C18-C19
14	P	3001	SMA	C16-C17-C18-C19
16	C	2004	CDL	OB7-CB5-OB6-CB4
20	R	3009	PLC	O'-C'-O2-C2
16	P	3004	CDL	C71-CB7-OB8-CB6
11	P	3007	PEE	C17-C18-C19-C20
11	C	2007	PEE	C1-O3P-P-O4P
11	E	2005	PEE	C1-O3P-P-O4P
11	P	3005	PEE	C1-O3P-P-O4P
11	P	3007	PEE	C1-O3P-P-O4P
16	P	3004	CDL	CA3-OA5-PA1-OA2
16	C	2004	CDL	C71-CB7-OB8-CB6
20	E	2009	PLC	C'-C1'-C2'-C3'
16	C	2004	CDL	CB2-C1-CA2-OA2
16	D	2003	CDL	CA2-C1-CB2-OB2
16	P	3004	CDL	CB2-C1-CA2-OA2
11	C	2007	PEE	C21-C22-C23-C24
11	E	2005	PEE	C40-C41-C42-C43
11	P	3005	PEE	C40-C41-C42-C43
11	P	3007	PEE	C21-C22-C23-C24
16	C	2004	CDL	C31-CA7-OA8-CA6
11	C	2007	PEE	C32-C33-C34-C35
11	P	3007	PEE	C34-C35-C36-C37
11	C	2007	PEE	C34-C35-C36-C37
20	R	3009	PLC	C'-C1'-C2'-C3'
11	P	3007	PEE	C32-C33-C34-C35
11	C	2007	PEE	C33-C34-C35-C36
16	Q	3003	CDL	CB7-C71-C72-C73
11	P	3007	PEE	C33-C34-C35-C36
17	P	3011	GOL	C1-C2-C3-O3
16	D	2003	CDL	C14-C15-C16-C17
16	D	2003	CDL	C12-C13-C14-C15
16	C	2004	CDL	OB9-CB7-OB8-CB6
16	Q	3003	CDL	C14-C15-C16-C17
16	P	3004	CDL	OB9-CB7-OB8-CB6
11	C	2007	PEE	C41-C42-C43-C44
11	P	3007	PEE	C41-C42-C43-C44
11	C	2007	PEE	C17-C18-C19-C20
16	Q	3003	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
16	C	2004	CDL	CB5-C51-C52-C53
16	P	3004	CDL	CB5-C51-C52-C53
11	P	3005	PEE	C39-C40-C41-C42
11	P	3007	PEE	C15-C16-C17-C18
16	P	3004	CDL	OA9-CA7-OA8-CA6
11	P	3005	PEE	C13-C14-C15-C16
11	P	3005	PEE	C33-C34-C35-C36
11	E	2005	PEE	C13-C14-C15-C16
11	E	2005	PEE	C39-C40-C41-C42
16	C	2004	CDL	OA7-CA5-OA6-CA4
16	D	2003	CDL	CB7-C71-C72-C73
20	E	2009	PLC	C1B-CB-O3-C3
20	R	3009	PLC	C1B-CB-O3-C3
11	E	2005	PEE	C33-C34-C35-C36
11	E	2005	PEE	C14-C15-C16-C17
11	P	3005	PEE	C23-C24-C25-C26
11	P	3005	PEE	C14-C15-C16-C17
16	C	2004	CDL	C11-CA5-OA6-CA4
16	P	3004	CDL	C11-CA5-OA6-CA4
13	C	501	HEM	C4B-C3B-CAB-CBB
13	P	501	HEM	C4B-C3B-CAB-CBB
14	P	3001	SMA	C24-C13-C14-C15
14	P	3001	SMA	C24-C13-C14-O14
14	C	2001	SMA	C12-C13-C14-C15
14	C	2001	SMA	C12-C13-C14-O14
14	P	3001	SMA	C12-C13-C14-C15
14	P	3001	SMA	C12-C13-C14-O14
16	P	3004	CDL	OA7-CA5-OA6-CA4
16	C	2004	CDL	OA9-CA7-OA8-CA6
11	A	2008	PEE	C1-O3P-P-O4P
16	C	2004	CDL	CA2-OA2-PA1-OA5
16	P	3004	CDL	CA2-OA2-PA1-OA5
20	R	3009	PLC	C1-O3P-P-O4P
11	C	2007	PEE	O3P-C1-C2-C3
11	P	3007	PEE	O3P-C1-C2-C3
16	C	2004	CDL	OB5-CB3-CB4-CB6
16	P	3004	CDL	OB5-CB3-CB4-CB6
11	E	2005	PEE	C30-C31-C32-C33
11	E	2005	PEE	C2-C3-O3-C30
11	E	2005	PEE	C23-C24-C25-C26
11	P	3007	PEE	C12-C13-C14-C15
15	P	3002	ANY	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	R	3009	PLC	C4'-C5'-C6'-C7'
17	P	3011	GOL	O2-C2-C3-O3
11	A	2008	PEE	C10-C11-C12-C13
11	C	2007	PEE	C15-C16-C17-C18
20	E	2009	PLC	OB-CB-O3-C3
20	R	3009	PLC	OB-CB-O3-C3
16	D	2003	CDL	C71-C72-C73-C74
16	Q	3003	CDL	C71-C72-C73-C74
15	C	2002	ANY	C16-C17-C18-C19
20	E	2009	PLC	C4'-C5'-C6'-C7'
11	P	3007	PEE	C40-C41-C42-C43
11	C	2007	PEE	C40-C41-C42-C43
11	C	2007	PEE	C12-C13-C14-C15
11	P	3005	PEE	C2-C3-O3-C30
11	P	3007	PEE	C43-C44-C45-C46
11	P	3005	PEE	C30-C31-C32-C33
11	C	2007	PEE	C43-C44-C45-C46
20	E	2009	PLC	C2'-C3'-C4'-C5'
11	C	2007	PEE	C10-C11-C12-C13
16	C	2004	CDL	OA6-CA4-CA6-OA8
16	D	2003	CDL	OA6-CA4-CA6-OA8
16	Q	3003	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C23-C24-C25-C26
11	P	3007	PEE	C23-C24-C25-C26
16	D	2003	CDL	C16-C17-C18-C19
20	R	3009	PLC	C2'-C3'-C4'-C5'
14	C	2001	SMA	C13-C14-C15-C16
16	Q	3003	CDL	C16-C17-C18-C19
16	P	3004	CDL	CA3-CA4-CA6-OA8
16	P	3004	CDL	CB3-CB4-CB6-OB8
16	Q	3003	CDL	CA3-CA4-CA6-OA8
20	E	2009	PLC	O3P-C1-C2-O2
13	C	502	HEM	C4D-C3D-CAD-CBD
14	C	2001	SMA	C24-C13-C14-C15
16	C	2004	CDL	OB6-CB4-CB6-OB8
16	P	3004	CDL	OB6-CB4-CB6-OB8
11	A	2008	PEE	O4-C10-O2-C2
20	E	2009	PLC	C1B-C2B-C3B-C4B
16	D	2003	CDL	C1-CA2-OA2-PA1
16	Q	3003	CDL	C1-CA2-OA2-PA1
11	A	2008	PEE	C1-O3P-P-O1P
11	C	2007	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C1-O3P-P-O1P
16	C	2004	CDL	CA2-OA2-PA1-OA4
16	D	2003	CDL	CA3-OA5-PA1-OA3
16	P	3004	CDL	CA2-OA2-PA1-OA4
16	Q	3003	CDL	CA3-OA5-PA1-OA3
11	A	2008	PEE	C11-C10-O2-C2
20	R	3009	PLC	O3P-C1-C2-O2
11	P	3007	PEE	C10-C11-C12-C13
16	C	2004	CDL	CA3-CA4-CA6-OA8
16	C	2004	CDL	CB3-CB4-CB6-OB8
20	E	2009	PLC	O4P-C4-C5-N
20	R	3009	PLC	O4P-C4-C5-N
11	A	2008	PEE	O2-C2-C3-O3
16	P	3004	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C31-C32-C33-C34
11	P	3007	PEE	C31-C32-C33-C34
11	E	2005	PEE	C1-C2-O2-C10
11	P	3005	PEE	C1-C2-O2-C10
11	E	2005	PEE	C12-C13-C14-C15
20	E	2009	PLC	C4-O4P-P-O3P
20	R	3009	PLC	C4-O4P-P-O3P
14	P	3001	SMA	C13-C14-C15-C16
11	P	3007	PEE	C11-C12-C13-C14
16	Q	3003	CDL	C15-C16-C17-C18
11	A	2008	PEE	O3P-C1-C2-C3
11	P	3007	PEE	C42-C43-C44-C45
13	C	502	HEM	CAA-CBA-CGA-O1A
16	D	2003	CDL	C15-C16-C17-C18
11	P	3005	PEE	C36-C37-C38-C39
16	D	2003	CDL	CA3-CA4-CA6-OA8
11	P	3005	PEE	C32-C33-C34-C35
13	P	502	HEM	CAA-CBA-CGA-O1A
11	P	3007	PEE	C13-C14-C15-C16
16	D	2003	CDL	CA3-OA5-PA1-OA2
20	R	3009	PLC	C1B-C2B-C3B-C4B
13	C	502	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C13-C14-C15-C16
11	E	2005	PEE	C36-C37-C38-C39
11	C	2007	PEE	C11-C12-C13-C14
13	P	501	HEM	CAA-CBA-CGA-O1A
13	P	501	HEM	CAA-CBA-CGA-O2A
13	C	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	C	502	HEM	CAD-CBD-CGD-O2D
16	Q	3003	CDL	C13-C14-C15-C16
13	P	502	HEM	CAA-CBA-CGA-O2A
13	P	502	HEM	CAD-CBD-CGD-O2D
11	E	2005	PEE	C32-C33-C34-C35
13	C	501	HEM	CAA-CBA-CGA-O2A
13	C	502	HEM	CAD-CBD-CGD-O1D
13	C	501	HEM	CAD-CBD-CGD-O2D
11	P	3005	PEE	C12-C13-C14-C15
16	D	2003	CDL	C13-C14-C15-C16
13	P	501	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAD-CBD-CGD-O1D
20	E	2009	PLC	O3P-C1-C2-C3
11	A	2008	PEE	O3-C30-C31-C32
16	C	2004	CDL	C1-CB2-OB2-PB2
11	P	3005	PEE	O2-C2-C3-O3
16	Q	3003	CDL	C72-C71-CB7-OB8
11	C	2007	PEE	C42-C43-C44-C45
11	A	2008	PEE	O5-C30-C31-C32
16	D	2003	CDL	C72-C71-CB7-OB8
18	Q	501	HEC	CAA-CBA-CGA-O2A
16	Q	3003	CDL	C12-C11-CA5-OA6
11	P	3005	PEE	C42-C43-C44-C45
16	D	2003	CDL	C12-C11-CA5-OA6
16	Q	3003	CDL	C52-C51-CB5-OB6
11	E	2005	PEE	C38-C39-C40-C41
11	A	2008	PEE	C1-C2-C3-O3
13	C	501	HEM	CAD-CBD-CGD-O1D
11	P	3005	PEE	C38-C39-C40-C41
16	D	2003	CDL	C52-C51-CB5-OB6
20	R	3009	PLC	O3P-C1-C2-C3
11	C	2007	PEE	O2-C2-C3-O3
11	E	2005	PEE	O2-C2-C3-O3
11	P	3007	PEE	O2-C2-C3-O3
20	E	2009	PLC	O2-C2-C3-O3
20	R	3009	PLC	O2-C2-C3-O3
13	P	501	HEM	CAD-CBD-CGD-O1D
18	Q	501	HEC	CAD-CBD-CGD-O2D
17	C	2011	GOL	O1-C1-C2-O2
11	A	2008	PEE	O2-C10-C11-C12
11	P	3007	PEE	O2-C10-C11-C12
11	C	2007	PEE	O2-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	D	2003	CDL	C72-C71-CB7-OB9
18	D	501	HEC	CAA-CBA-CGA-O2A
18	Q	501	HEC	CAA-CBA-CGA-O1A
16	Q	3003	CDL	C72-C71-CB7-OB9
16	D	2003	CDL	C52-C51-CB5-OB7
16	Q	3003	CDL	C52-C51-CB5-OB7
16	Q	3003	CDL	C12-C11-CA5-OA7
18	Q	501	HEC	CAD-CBD-CGD-O1D
11	E	2005	PEE	C42-C43-C44-C45
11	A	2008	PEE	C1-O3P-P-O2P
16	D	2003	CDL	C12-C11-CA5-OA7
11	E	2005	PEE	C22-C23-C24-C25
11	C	2007	PEE	C20-C21-C22-C23
11	P	3007	PEE	O4-C10-C11-C12
11	A	2008	PEE	O4-C10-C11-C12
11	C	2007	PEE	O4-C10-C11-C12
18	D	501	HEC	CAA-CBA-CGA-O1A
16	C	2004	CDL	C72-C71-CB7-OB8

There are no ring outliers.

23 monomers are involved in 91 short contacts:

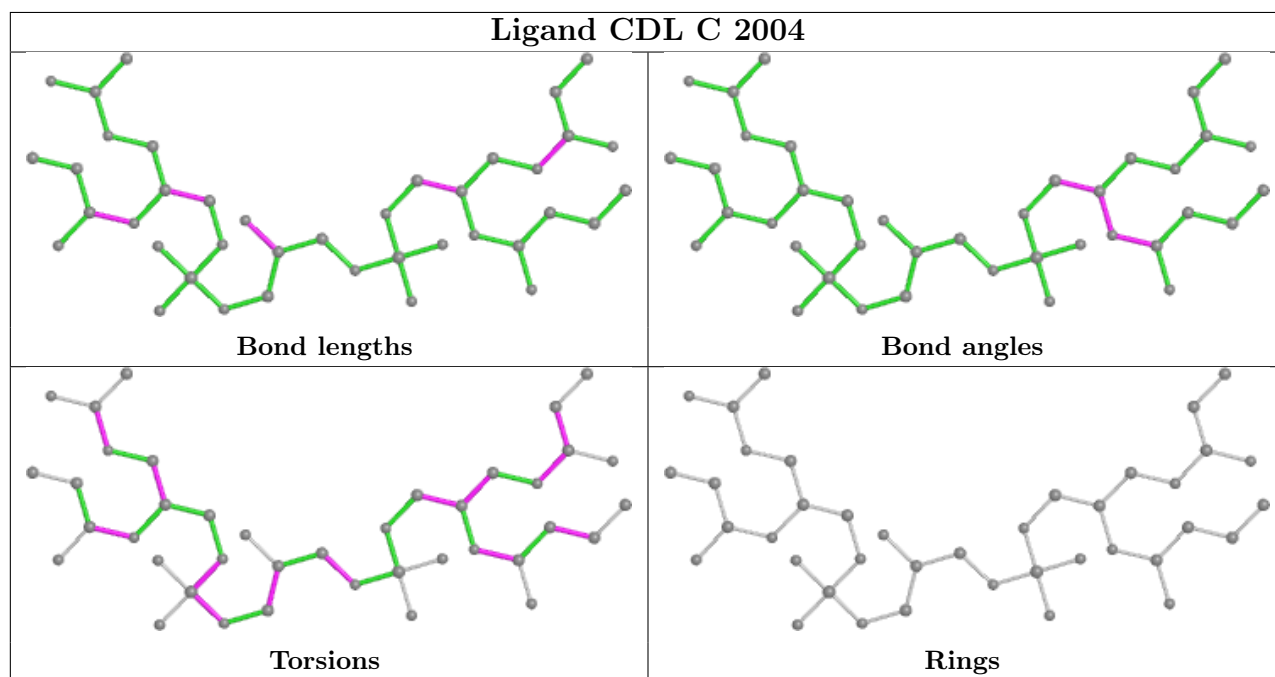
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	2004	CDL	2	0
17	C	2011	GOL	1	0
20	E	2009	PLC	2	0
18	D	501	HEC	6	0
11	P	3005	PEE	3	0
15	P	3002	ANY	1	0
20	R	3009	PLC	3	0
16	P	3004	CDL	2	0
16	D	2003	CDL	1	0
13	P	502	HEM	11	0
16	Q	3003	CDL	5	0
19	R	501	FES	1	0
14	C	2001	SMA	3	0
13	C	502	HEM	9	0
13	P	501	HEM	11	0
13	C	501	HEM	11	0
15	C	2002	ANY	3	0
11	E	2005	PEE	1	0
11	P	3007	PEE	3	0

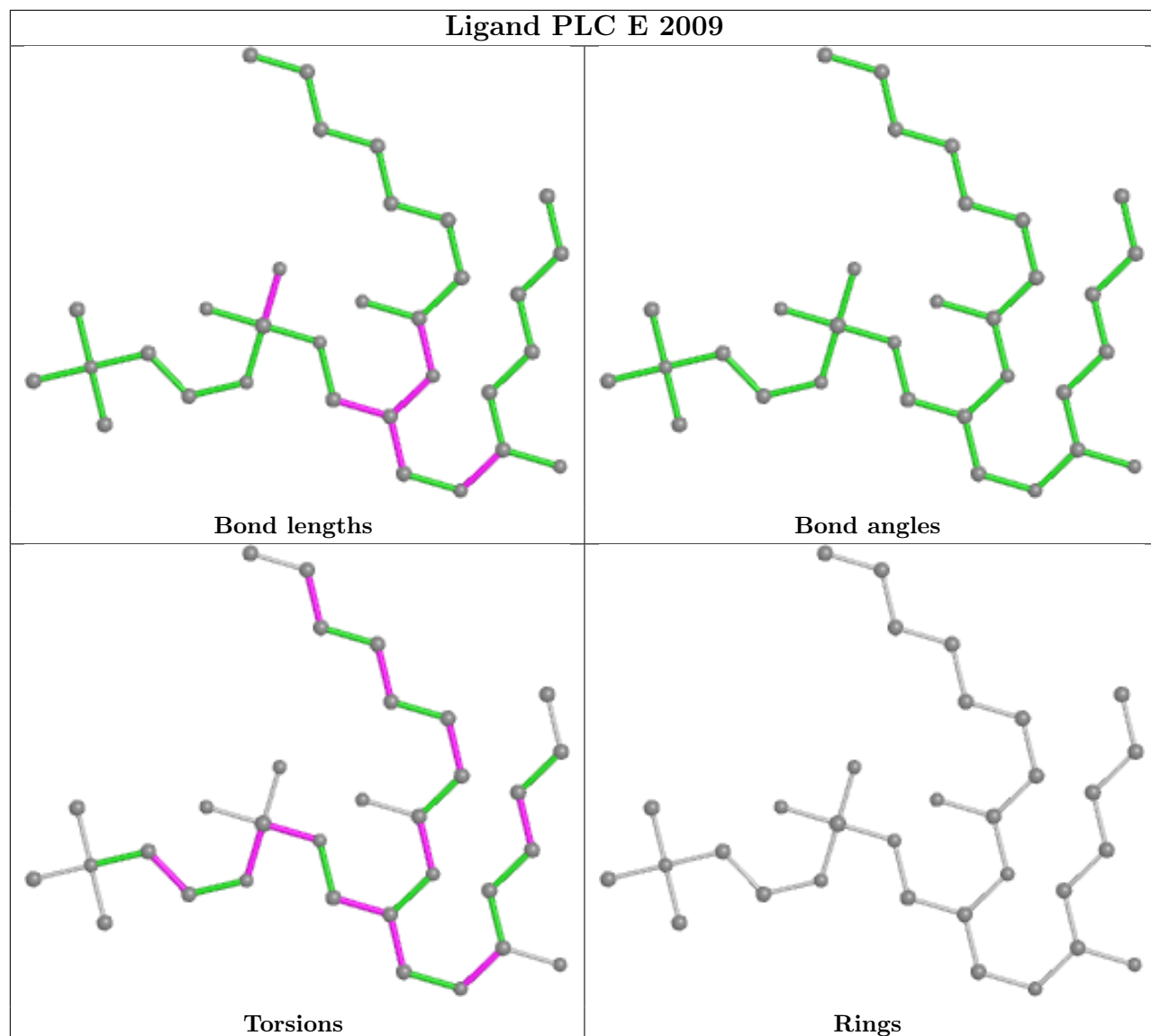
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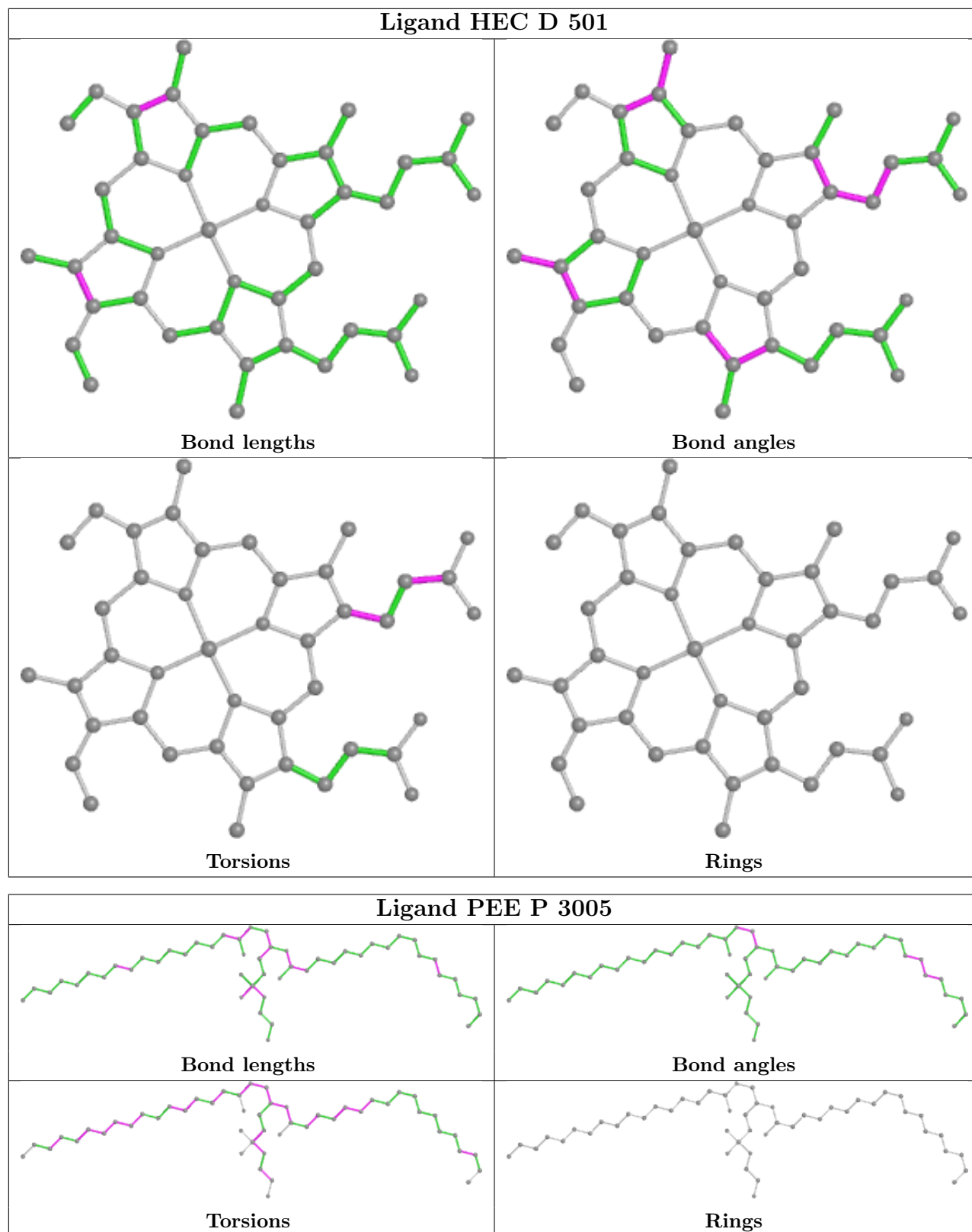
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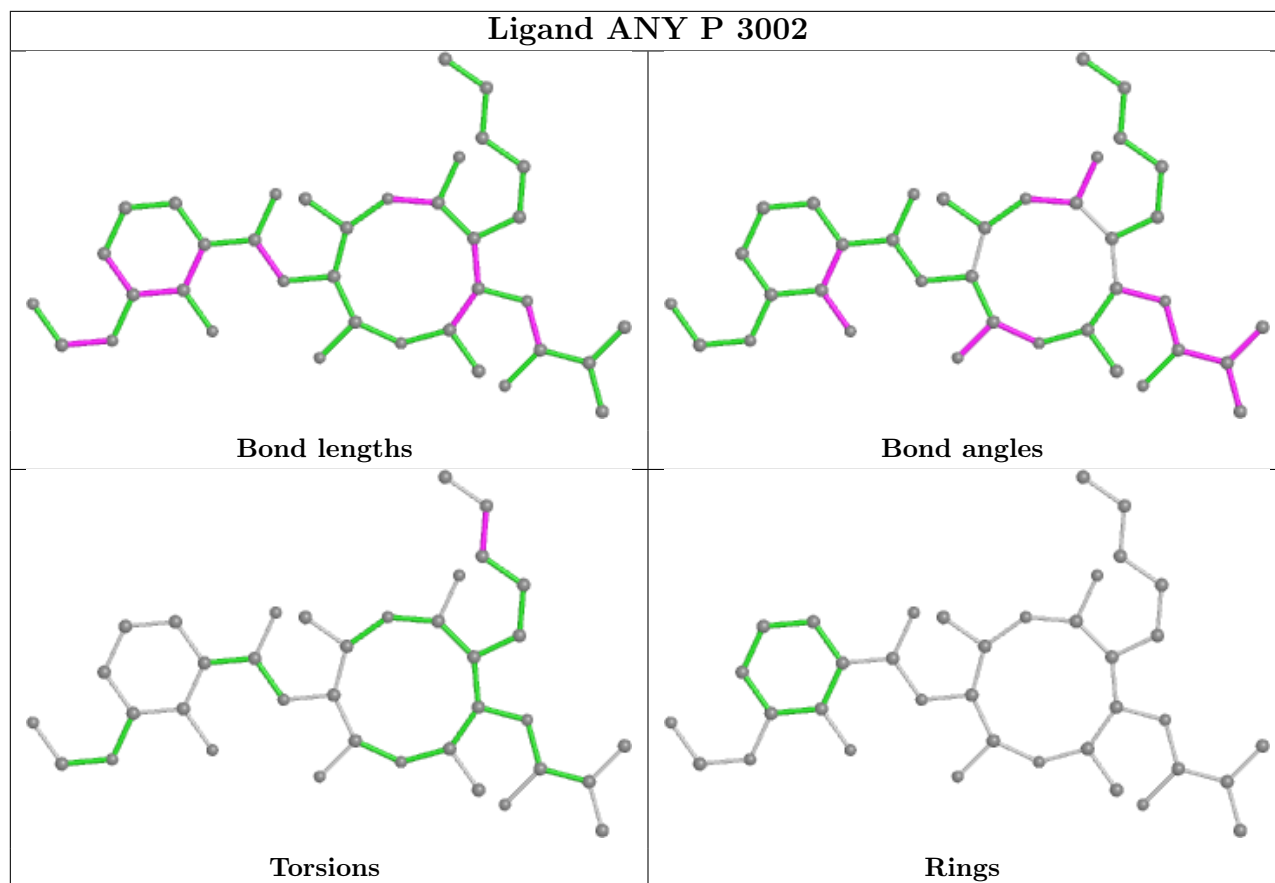
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	E	501	FES	2	0
11	C	2007	PEE	2	0
18	Q	501	HEC	4	0
14	P	3001	SMA	4	0

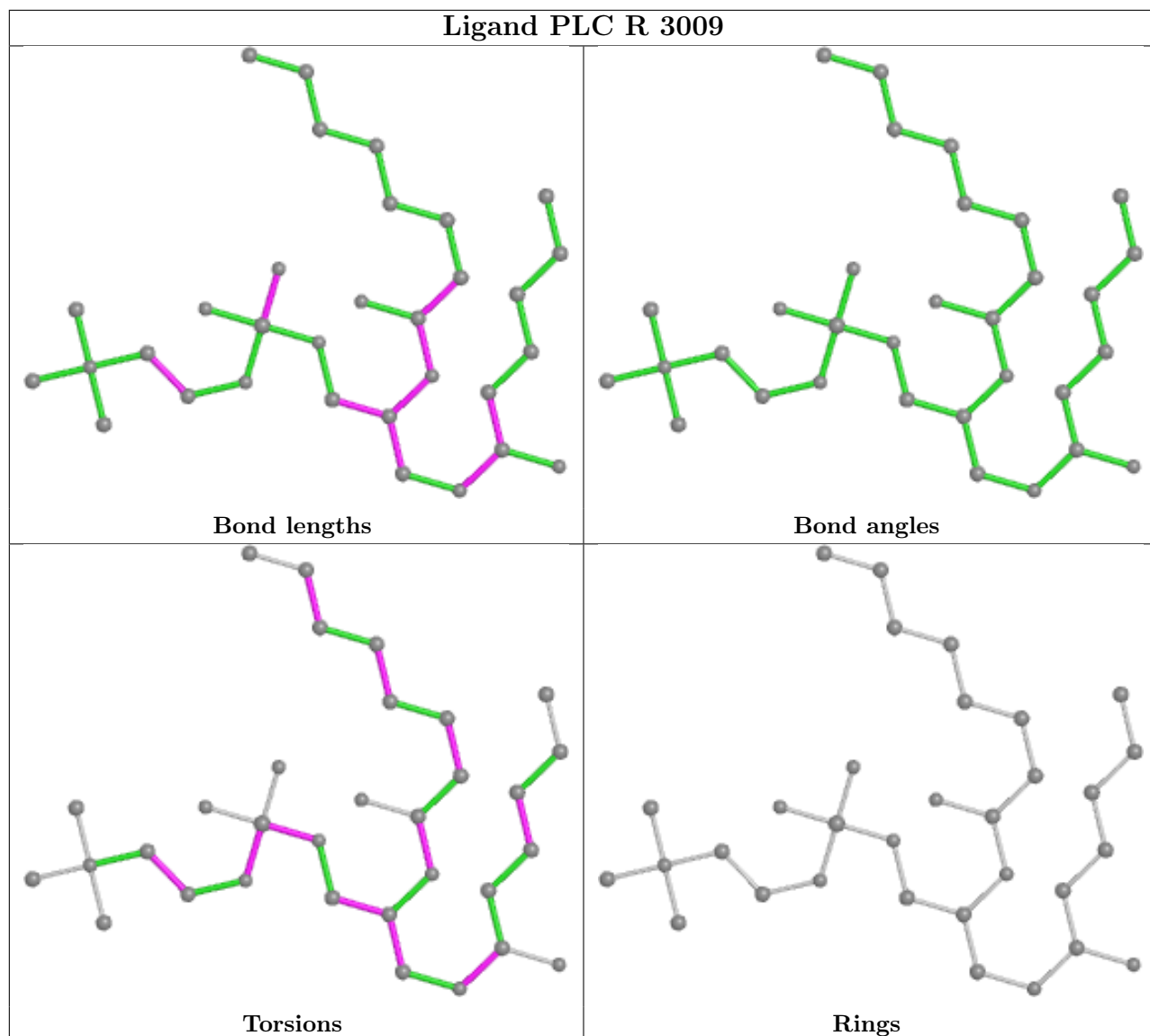
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

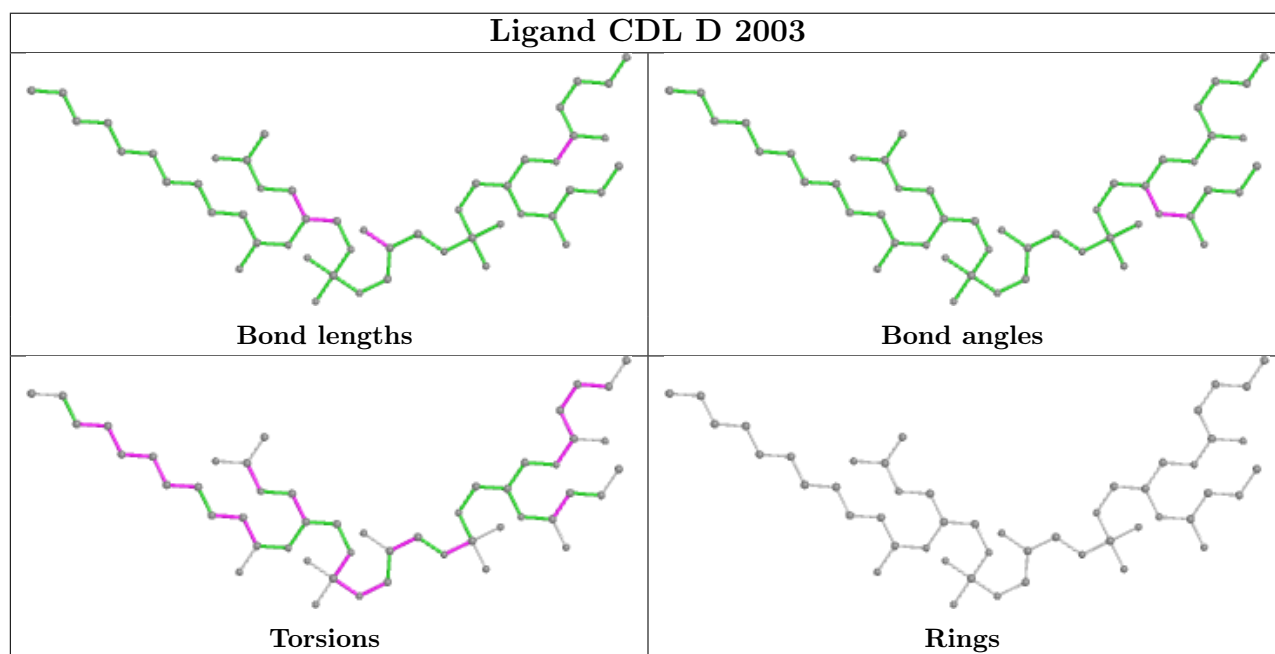
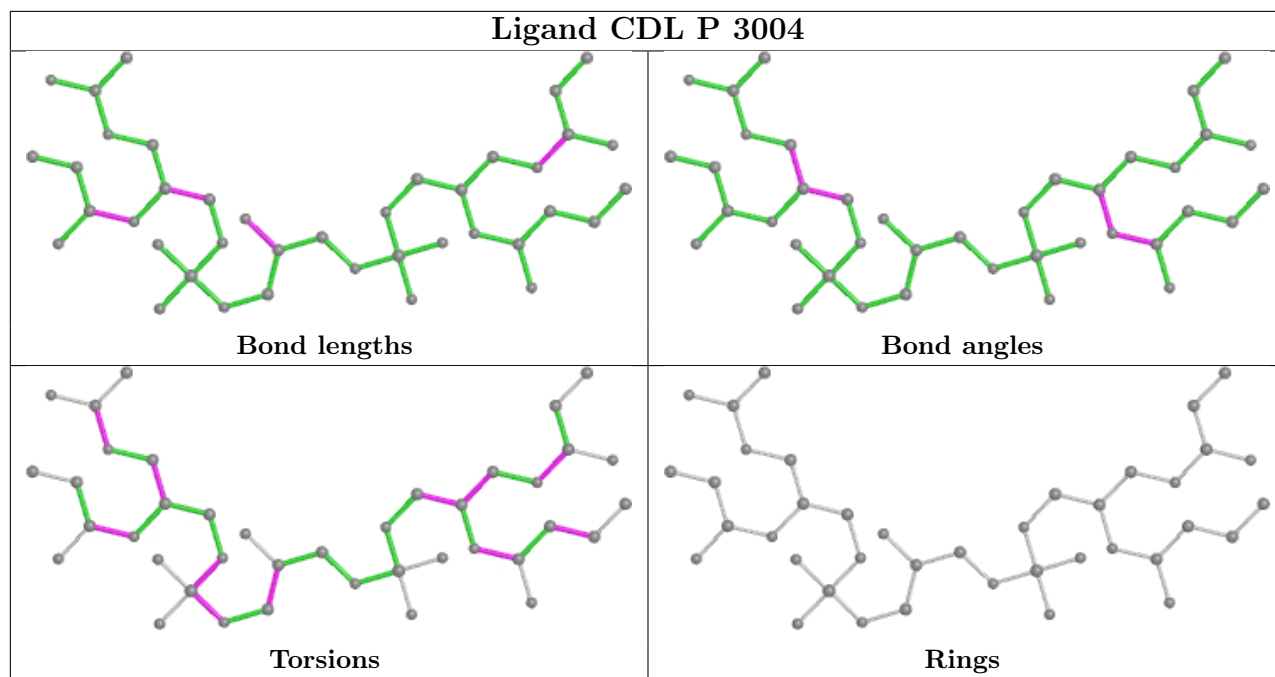


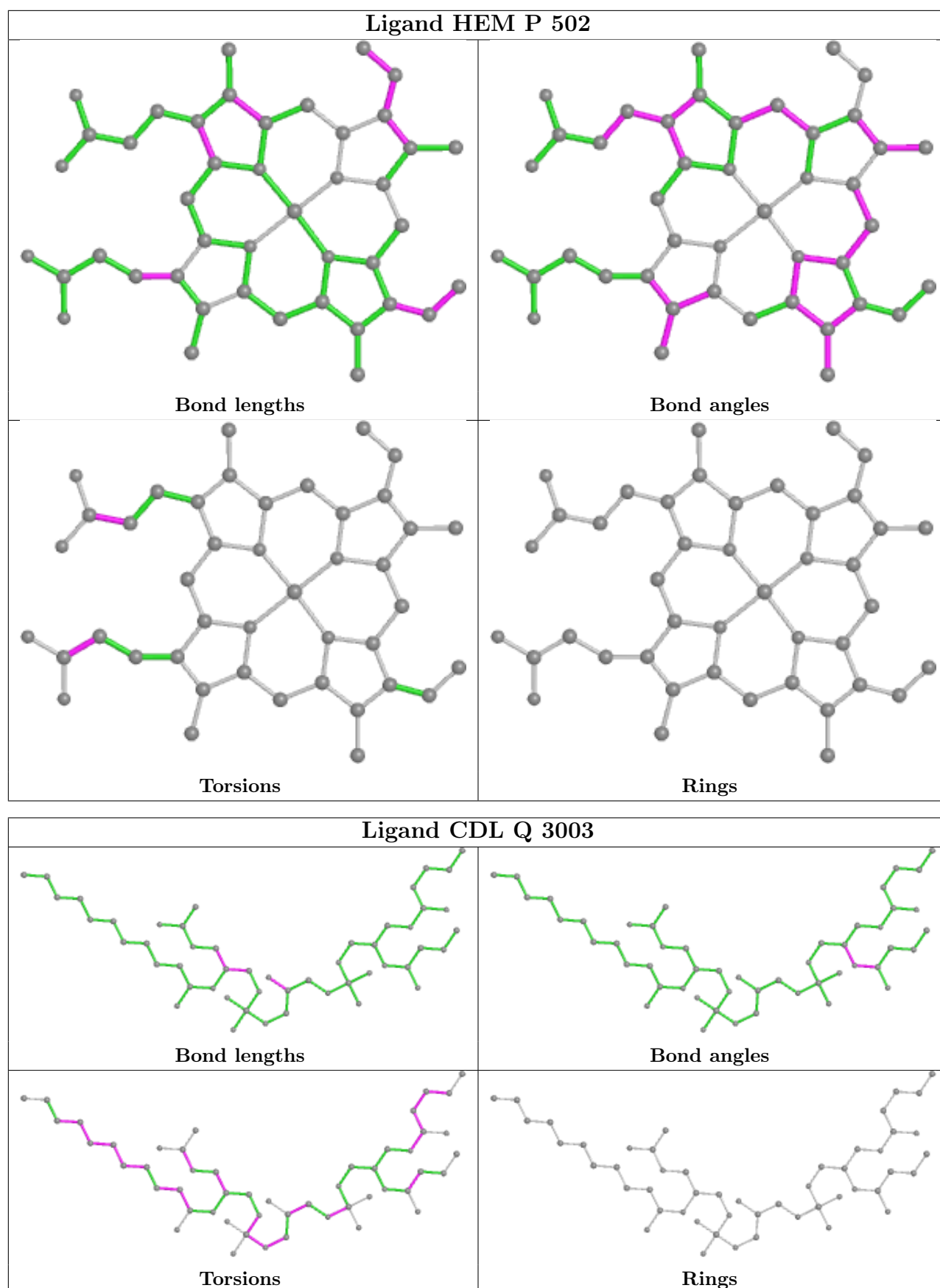


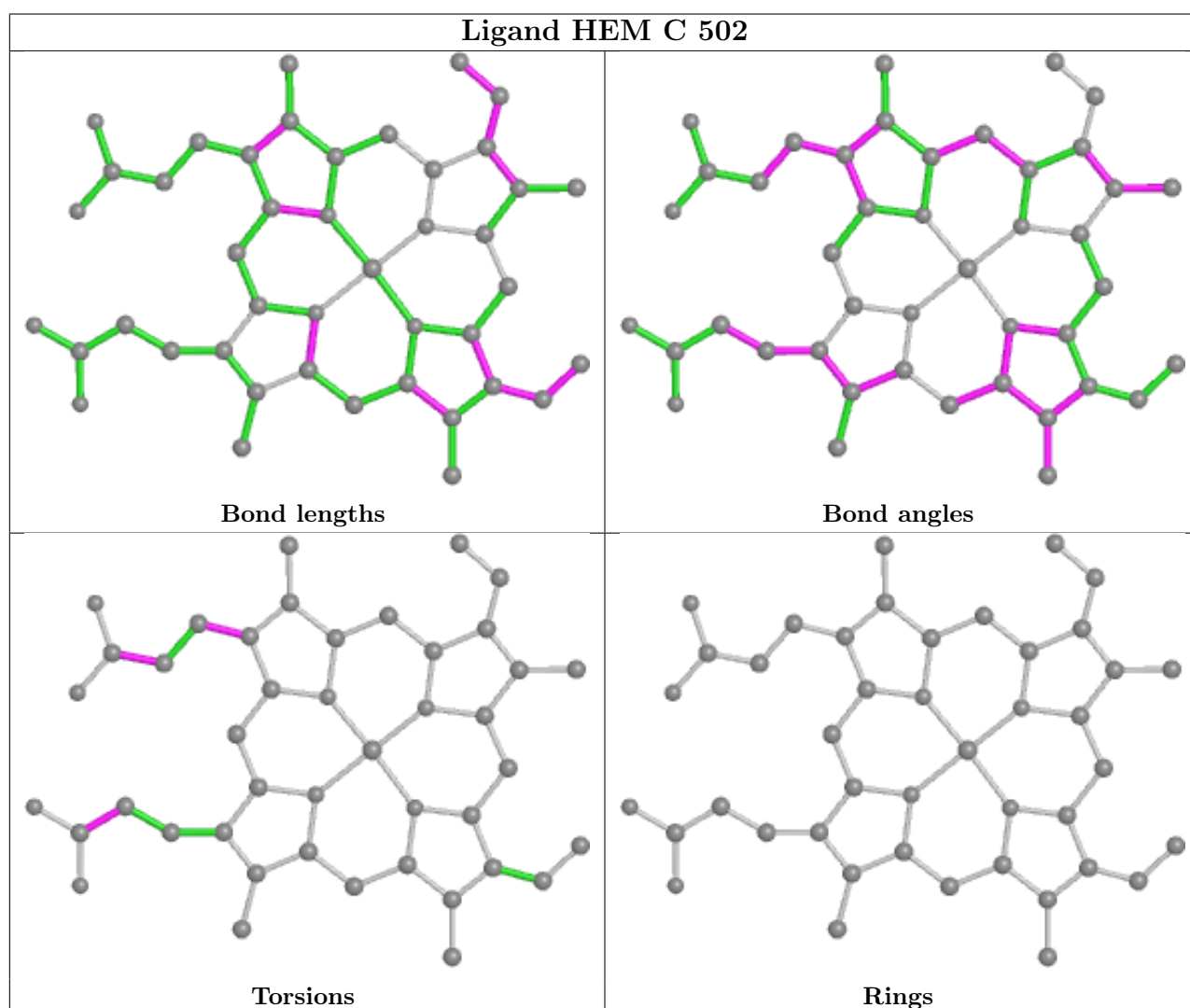
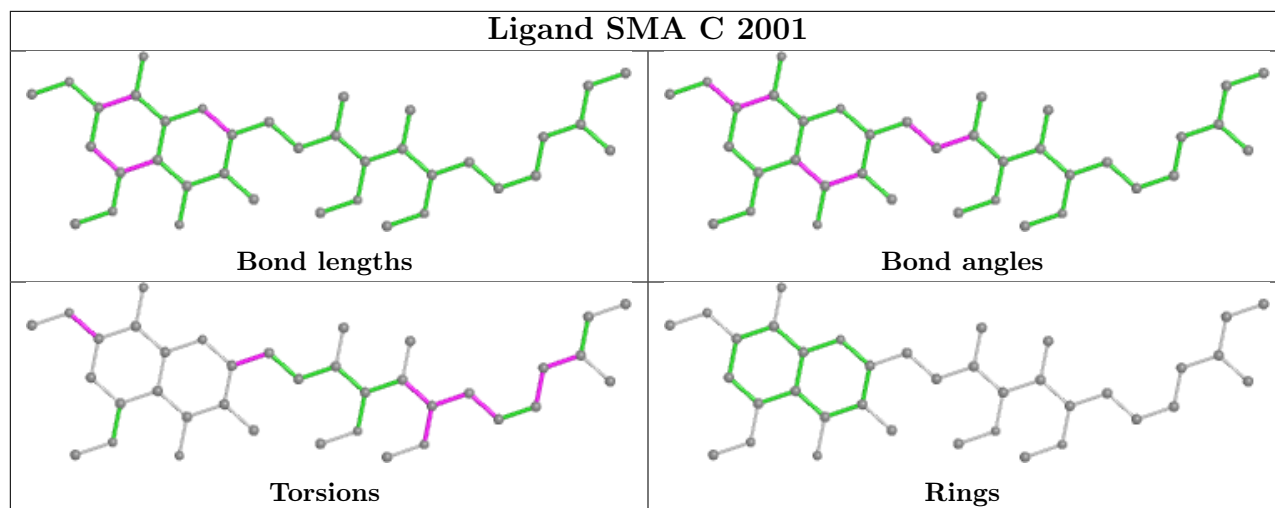


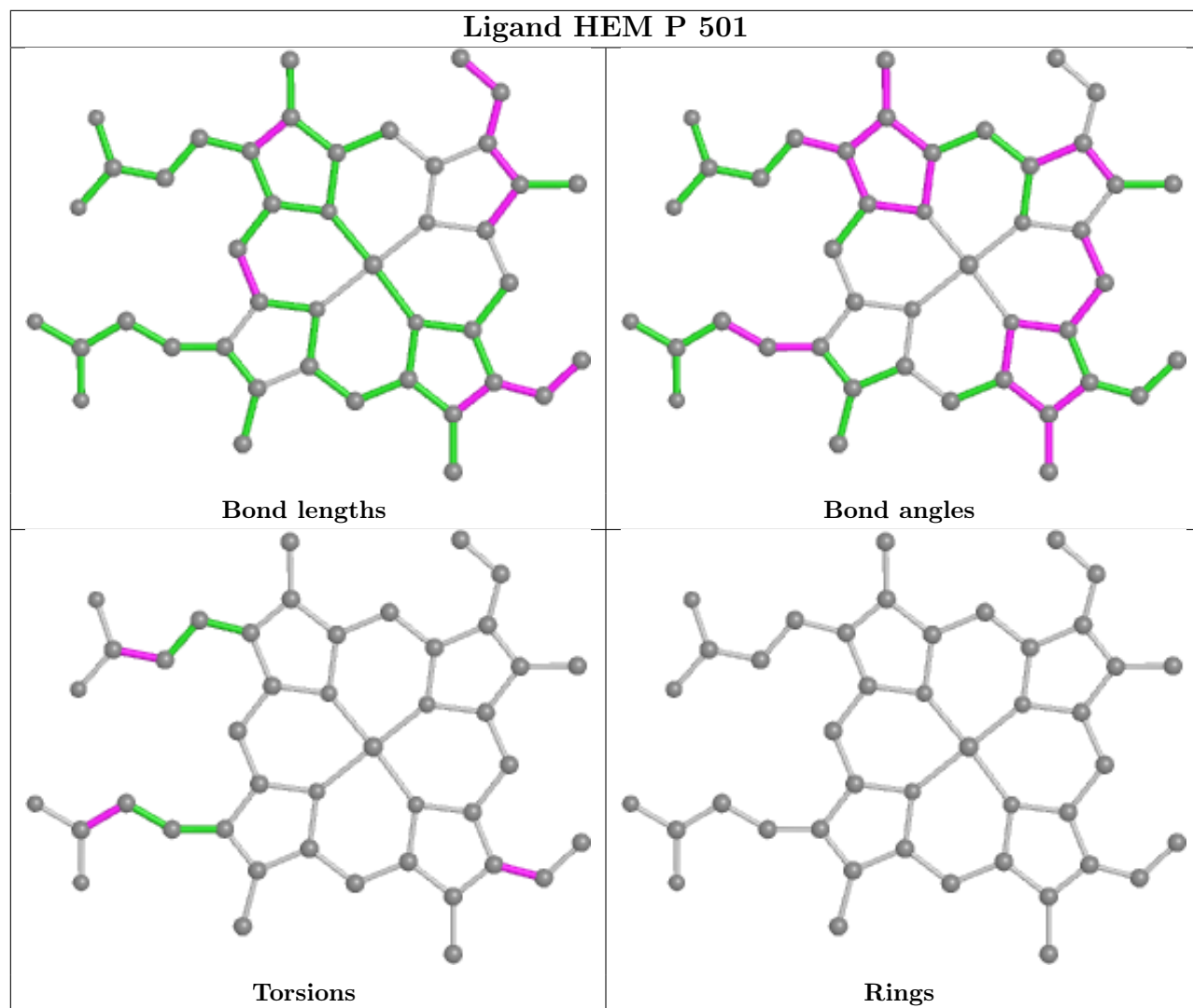


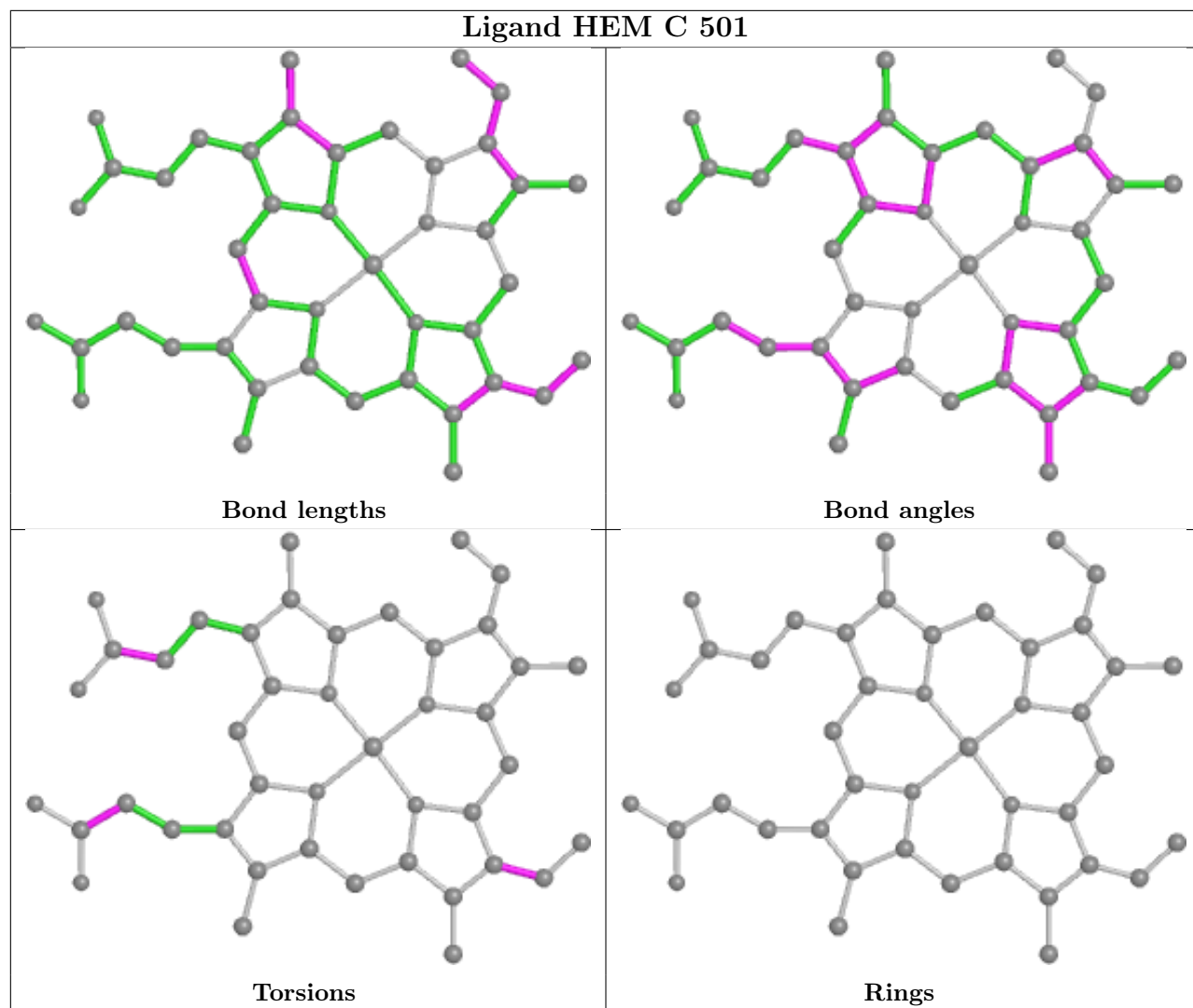


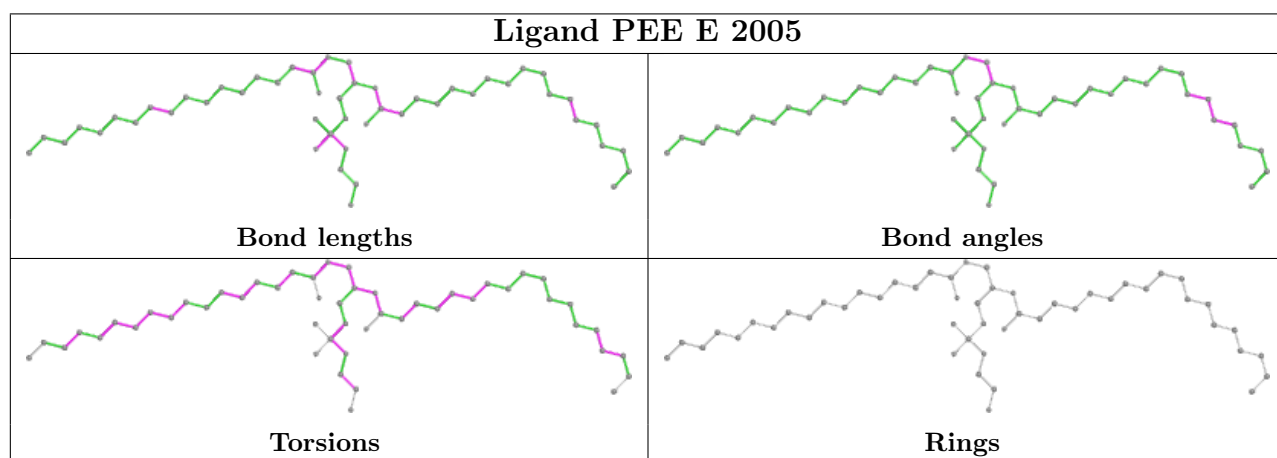
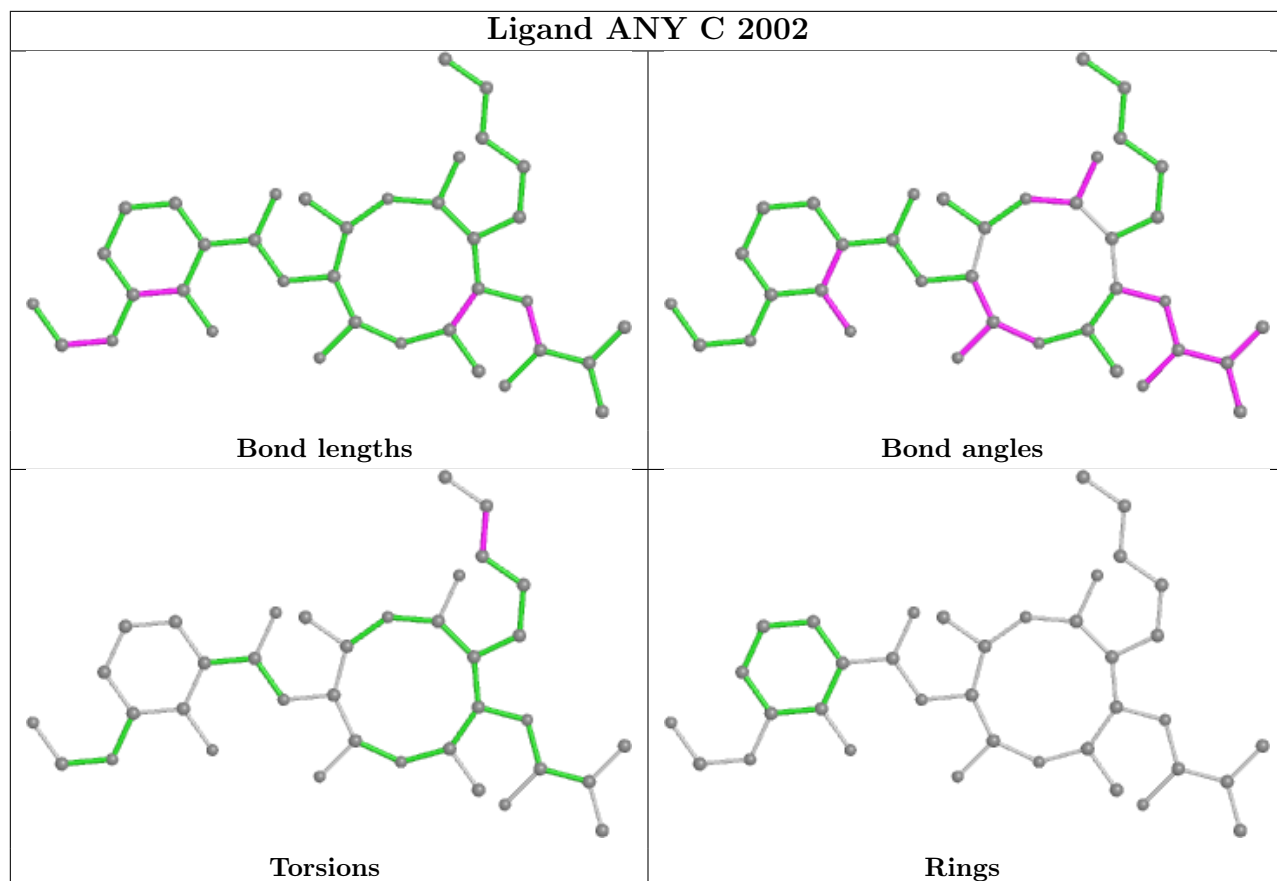


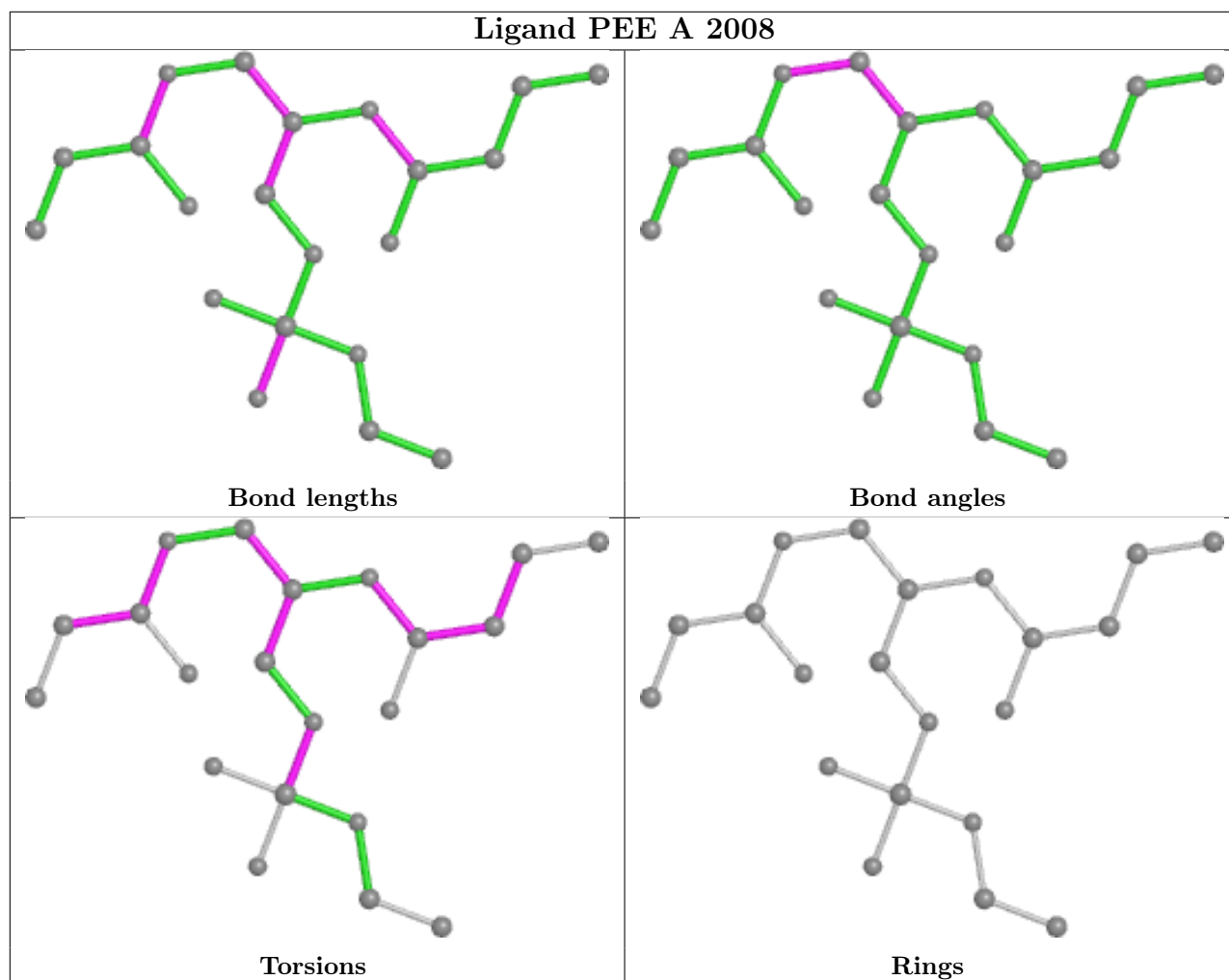
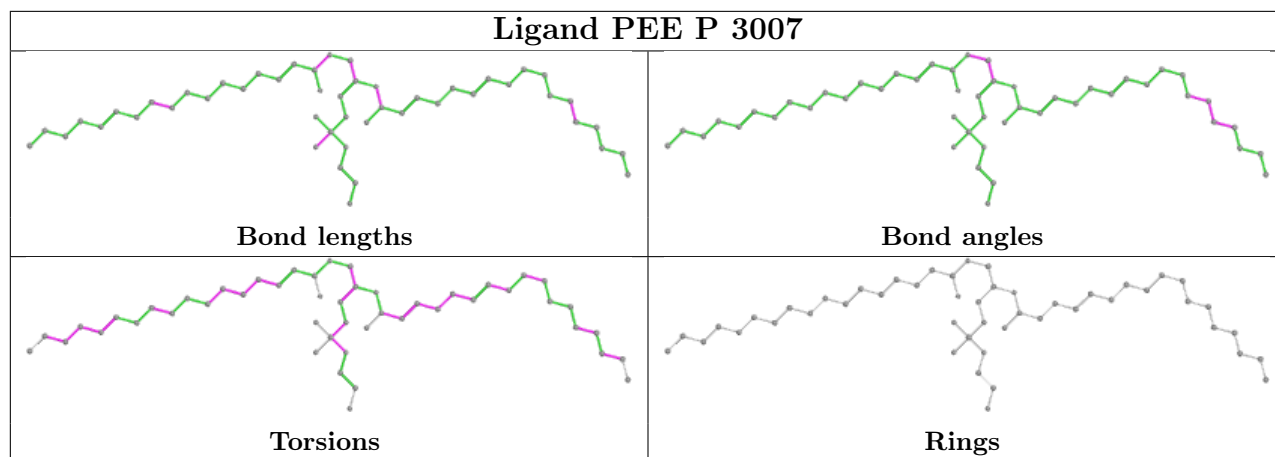


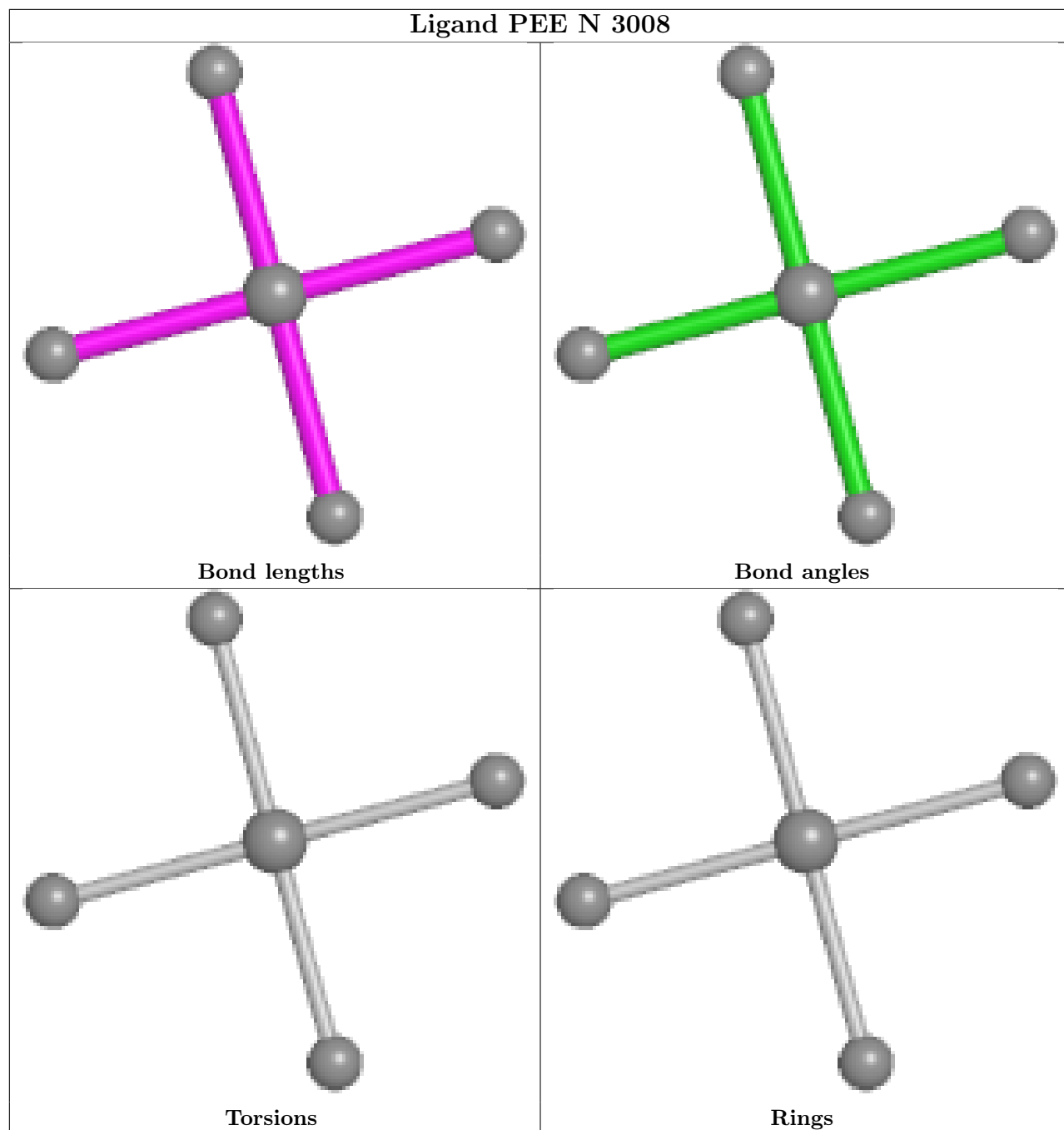


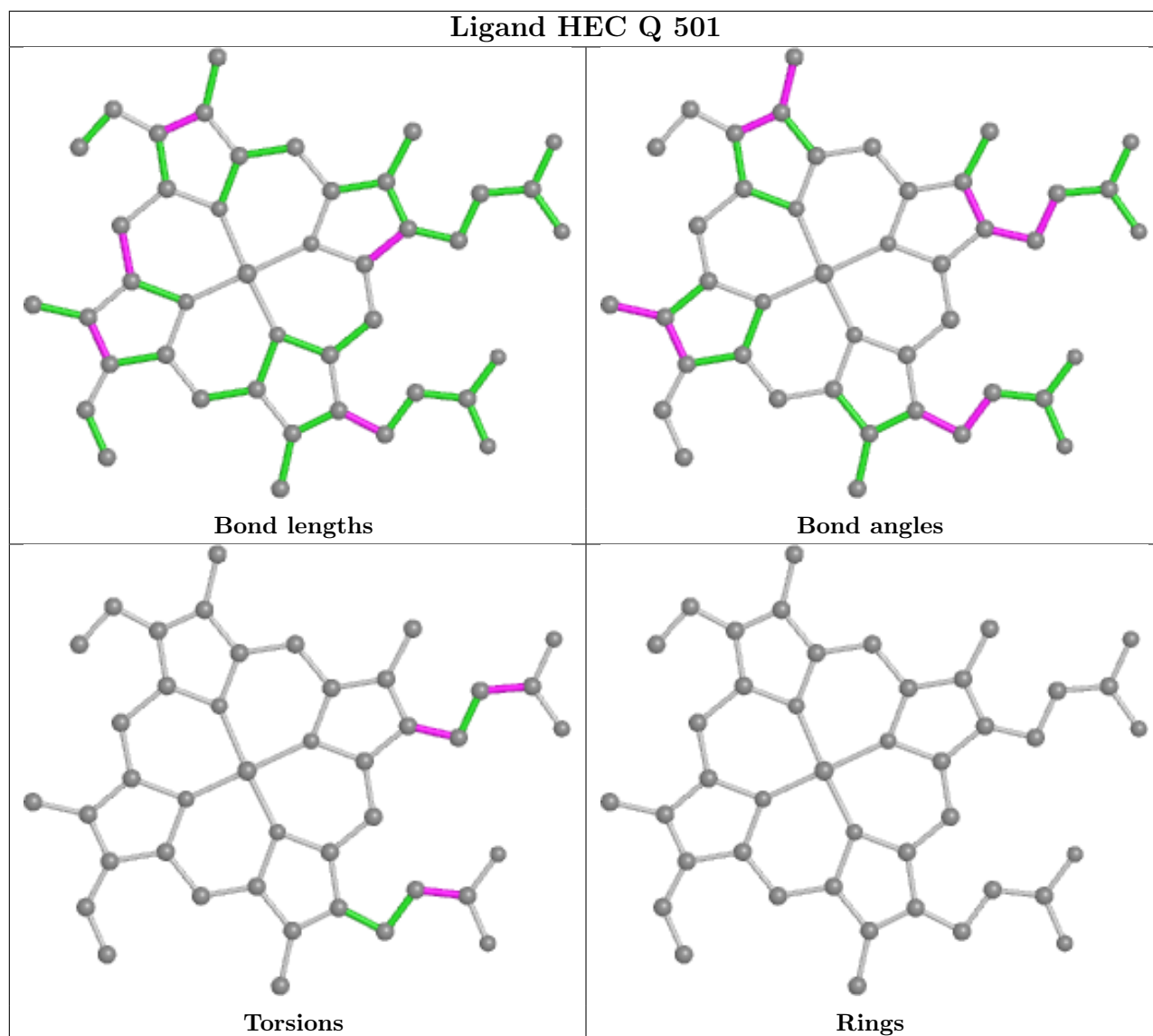
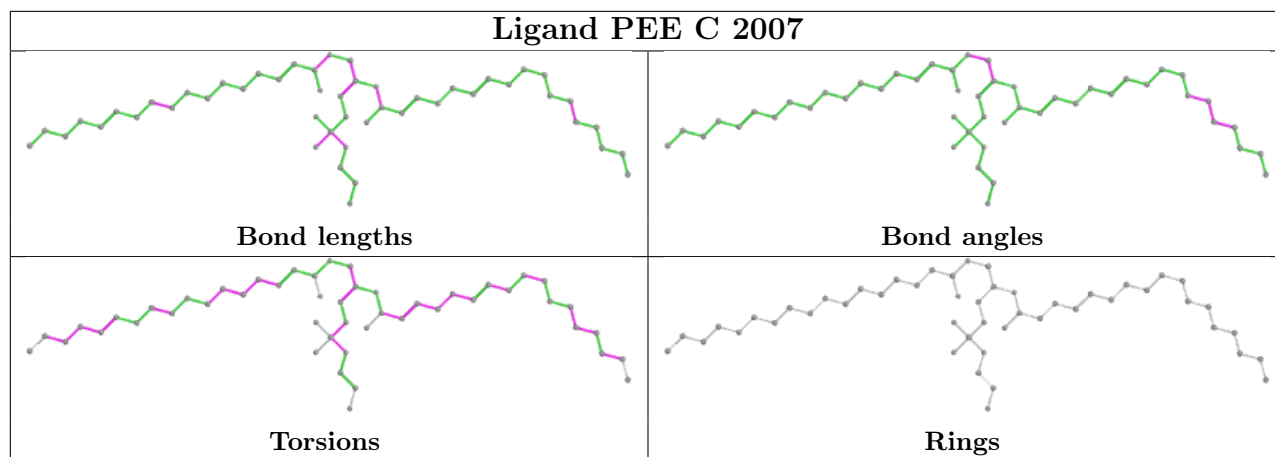


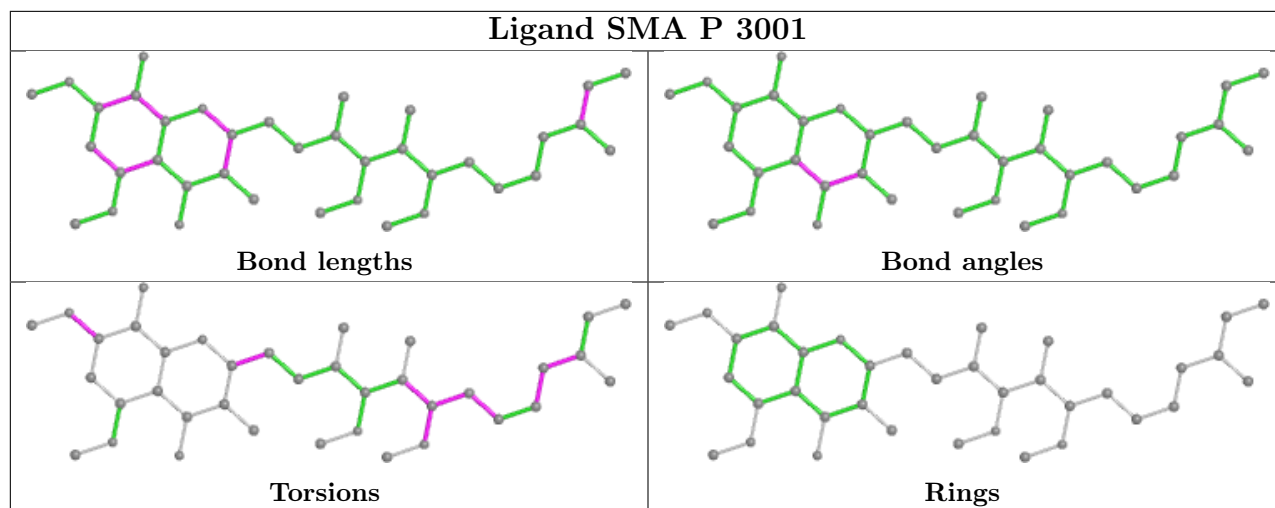












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	-0.23	4 (0%) 84 73	40, 85, 131, 143	0
1	N	442/446 (99%)	-0.17	8 (1%) 68 54	42, 91, 131, 143	0
2	B	421/441 (95%)	-0.12	3 (0%) 87 79	63, 107, 145, 173	0
2	O	422/441 (95%)	-0.20	6 (1%) 75 62	50, 97, 140, 150	0
3	C	380/380 (100%)	-0.75	0 100 100	17, 40, 73, 122	0
3	P	379/380 (99%)	-0.53	3 (0%) 86 75	20, 71, 106, 136	0
4	D	241/241 (100%)	-0.50	0 100 100	28, 55, 105, 118	0
4	Q	241/241 (100%)	-0.29	2 (0%) 86 75	51, 93, 136, 148	0
5	E	196/196 (100%)	0.50	39 (19%) 1 0	36, 123, 176, 180	0
5	R	196/196 (100%)	0.13	15 (7%) 13 10	50, 97, 152, 159	0
6	F	101/110 (91%)	-0.67	0 100 100	32, 57, 80, 112	0
6	S	101/110 (91%)	-0.24	1 (0%) 82 71	67, 103, 138, 161	0
7	G	81/81 (100%)	-0.43	0 100 100	38, 66, 112, 123	0
7	T	79/81 (97%)	-0.25	3 (3%) 40 29	62, 112, 176, 184	0
8	H	70/77 (90%)	-0.21	0 100 100	50, 90, 109, 132	0
8	U	67/77 (87%)	0.26	3 (4%) 33 24	129, 151, 171, 173	0
9	I	31/47 (65%)	0.64	2 (6%) 18 13	100, 143, 177, 178	0
9	V	31/47 (65%)	0.65	4 (12%) 3 3	107, 152, 194, 197	0
10	J	61/61 (100%)	-0.27	1 (1%) 72 59	57, 72, 124, 165	0
10	W	59/61 (96%)	0.04	1 (1%) 70 57	62, 89, 125, 148	0
All	All	4042/4160 (97%)	-0.24	95 (2%) 59 45	17, 87, 148, 197	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	132	TRP	5.4
5	E	134	ILE	4.5
9	I	77	ARG	4.3
5	E	121	GLN	3.9
5	E	133	VAL	3.9
5	E	77	LYS	3.9
5	R	188	VAL	3.9
5	E	111	GLU	3.8
10	J	64	GLU	3.8
5	E	117	LEU	3.8
5	E	122	HIS	3.8
5	E	127	VAL	3.8
5	E	128	LYS	3.7
5	E	78	LEU	3.7
5	R	122	HIS	3.6
9	V	77	ARG	3.6
5	E	192	LEU	3.5
5	E	114	VAL	3.3
5	E	112	VAL	3.3
8	U	76	LYS	3.3
5	E	110	ALA	3.3
5	E	76	ILE	3.2
2	B	350	GLY	3.1
5	E	187	PHE	3.1
2	O	36	ALA	3.1
1	A	216	PHE	3.1
5	E	98	VAL	3.0
5	R	114	VAL	3.0
1	N	83	GLY	2.9
5	E	174	GLY	2.9
7	T	2	ILE	2.9
2	O	208	GLY	2.9
10	W	62	SER	2.9
5	E	109	GLU	2.8
5	E	115	SER	2.8
5	R	111	GLU	2.8
3	P	380	TYR	2.8
5	E	96	LEU	2.8
5	E	188	VAL	2.8
5	R	192	LEU	2.8
5	E	120	PRO	2.8
1	N	66	GLY	2.8
5	E	172	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
5	R	75	GLU	2.7
5	E	135	LEU	2.7
5	R	121	GLN	2.7
5	E	185	TYR	2.7
8	U	74	PHE	2.7
5	R	103	GLN	2.6
1	A	2	ALA	2.6
2	O	18	CYS	2.6
1	N	370	ASP	2.6
5	R	112	VAL	2.5
3	P	375	ASN	2.5
3	P	2	ALA	2.5
5	E	193	VAL	2.4
1	N	81	SER	2.4
5	E	189	GLY	2.4
5	E	191	ASP	2.4
5	E	118	ARG	2.4
5	R	120	PRO	2.4
2	O	332	HIS	2.4
5	E	101	ARG	2.3
1	A	22	GLY	2.3
9	I	63	ASP	2.3
1	N	216	PHE	2.3
5	R	193	VAL	2.2
5	E	81	ILE	2.2
5	R	101	ARG	2.2
6	S	89	TYR	2.2
1	N	84	ALA	2.2
2	O	19	PRO	2.2
4	Q	180	SER	2.2
5	R	186	GLN	2.2
1	A	66	GLY	2.2
1	N	174	ILE	2.2
5	E	79	SER	2.2
9	V	61	ARG	2.1
8	U	29	LYS	2.1
2	B	36	ALA	2.1
5	E	97	PHE	2.1
2	O	350	GLY	2.1
5	R	72	SER	2.1
4	Q	67	GLU	2.1
5	E	190	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
9	V	75	SER	2.1
5	E	113	ASP	2.1
2	B	349	GLN	2.1
7	T	1	GLY	2.1
5	E	129	LYS	2.1
1	N	117	VAL	2.1
7	T	78	GLU	2.1
5	E	116	LYS	2.0
9	V	62	ARG	2.0
5	R	191	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	UNL	E	2105	1/-	0.60	0.34	35,35,35,35	0
12	UNL	C	3015	1/-	0.63	0.60	32,32,32,32	0
12	UNL	P	3104	1/-	0.69	0.63	42,42,42,42	0
16	CDL	Q	3003	50/100	0.75	0.40	116,149,158,158	0
11	PEE	P	3005	50/51	0.77	0.46	75,97,113,115	0
11	PEE	A	2008	21/51	0.79	0.35	121,125,130,130	0
12	UNL	C	2104	1/-	0.81	0.42	36,36,36,36	0
16	CDL	D	2003	50/100	0.83	0.34	63,103,110,111	0
20	PLC	R	3009	32/42	0.83	0.48	74,93,118,118	0
11	PEE	E	2005	50/51	0.85	0.46	66,86,100,101	0
20	PLC	E	2009	32/42	0.86	0.38	37,60,94,95	0
12	UNL	A	3016	1/-	0.86	0.36	10,10,10,10	0
16	CDL	P	3004	40/100	0.87	0.27	101,108,110,110	0

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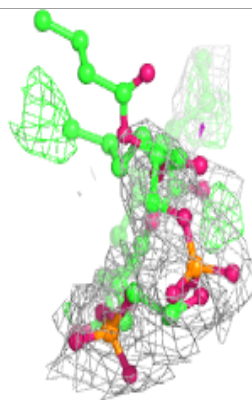
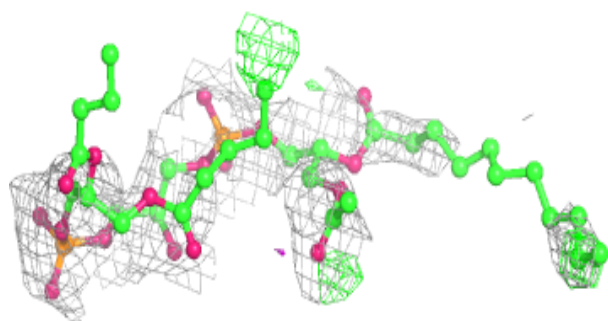
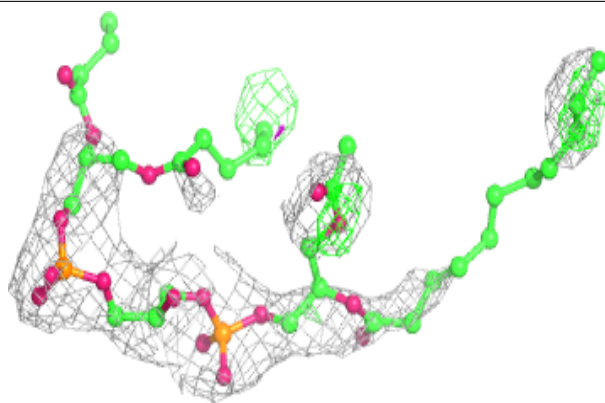
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PEE	P	3007	49/51	0.88	0.43	63,96,134,135	0
12	UNL	E	3103	1/-	0.90	0.52	32,32,32,32	0
17	GOL	C	2011	6/6	0.91	0.29	67,70,71,73	0
11	PEE	N	3008	5/51	0.91	0.36	105,105,106,106	0
11	PEE	C	2007	49/51	0.91	0.30	44,56,90,91	0
12	UNL	P	2015	1/-	0.92	0.54	25,25,25,25	0
12	UNL	C	2010	1/-	0.92	0.58	24,24,24,24	0
16	CDL	C	2004	40/100	0.92	0.24	50,72,90,92	0
12	UNL	R	2103	1/-	0.93	0.57	12,12,12,12	0
12	UNL	P	3010	1/-	0.93	0.35	24,24,24,24	0
14	SMA	P	3001	37/37	0.94	0.34	64,69,74,75	0
17	GOL	P	3011	6/6	0.94	0.43	46,48,50,50	0
15	ANY	P	3002	37/40	0.95	0.24	65,69,82,82	0
15	ANY	C	2002	37/40	0.96	0.21	27,36,48,50	0
13	HEM	P	502	43/43	0.96	0.22	49,52,70,77	0
14	SMA	C	2001	37/37	0.97	0.22	20,30,37,39	0
18	HEC	Q	501	43/43	0.97	0.20	64,68,72,76	0
18	HEC	D	501	43/43	0.98	0.16	34,39,48,55	0
13	HEM	P	501	43/43	0.98	0.21	44,49,55,56	0
13	HEM	C	501	43/43	0.98	0.20	24,32,36,39	0
13	HEM	C	502	43/43	0.98	0.20	21,28,43,49	0
19	FES	E	501	4/4	0.99	0.11	87,88,89,90	0
19	FES	R	501	4/4	0.99	0.12	55,56,58,58	0

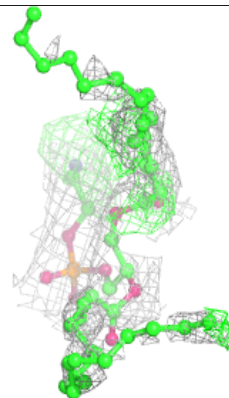
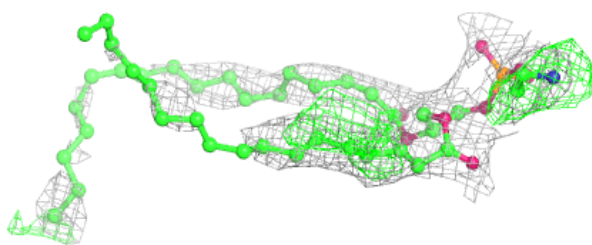
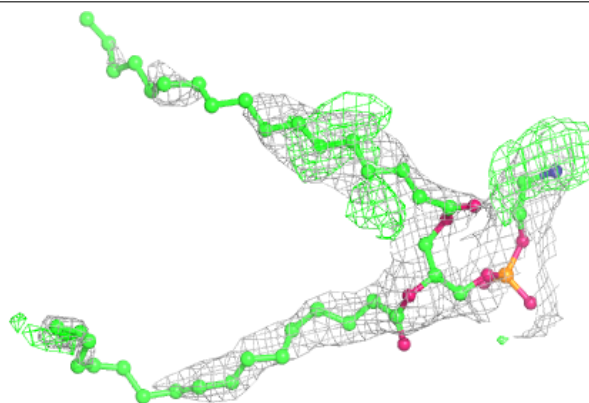
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL Q 3003:

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

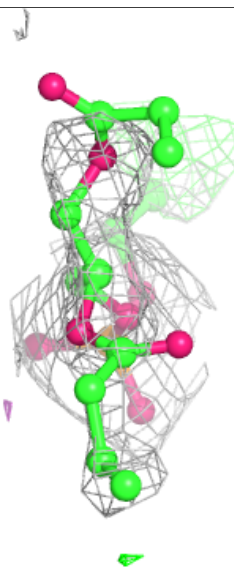
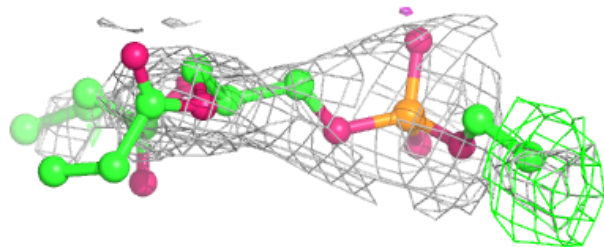
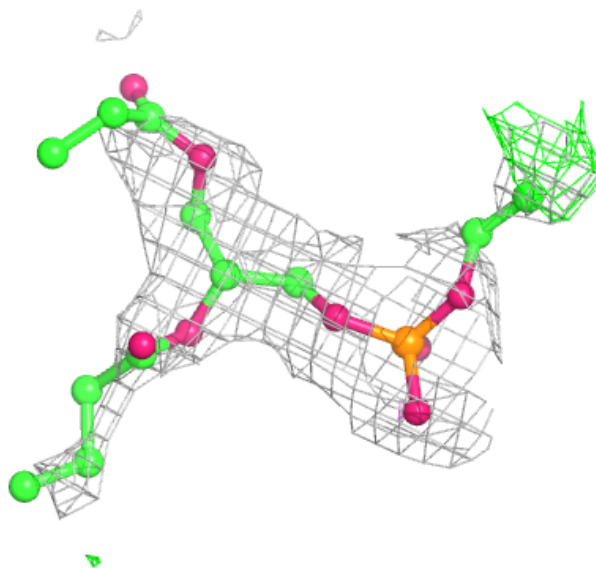
**Electron density around PEE P 3005:**

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



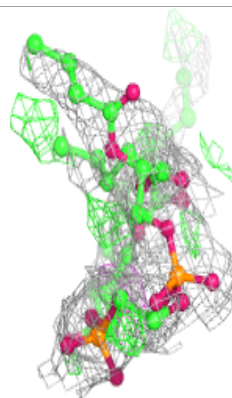
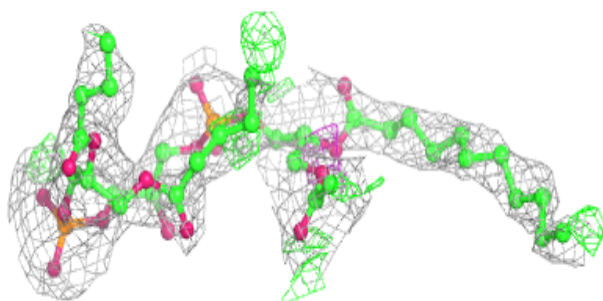
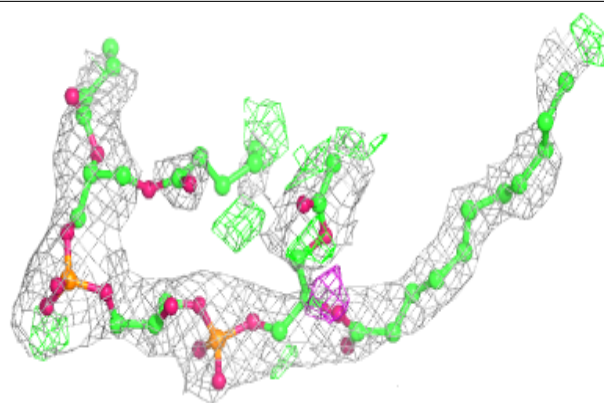
Electron density around PEE A 2008:

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

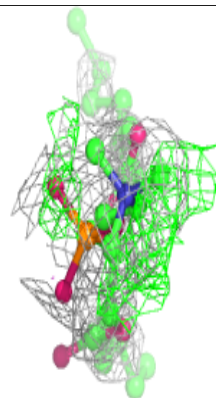
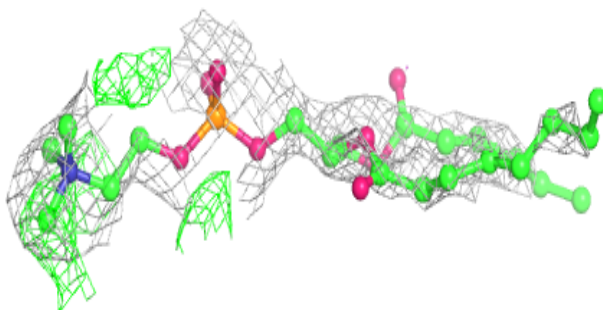
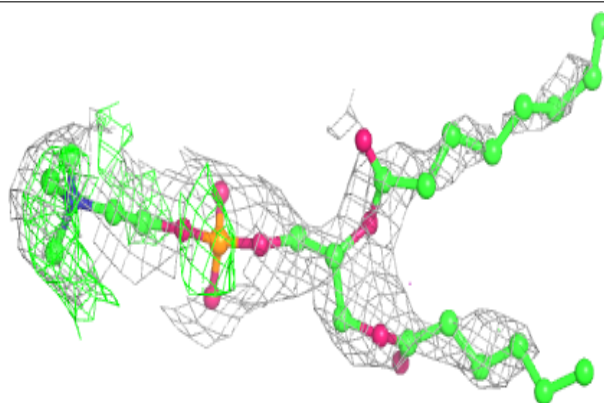


Electron density around CDL D 2003:

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

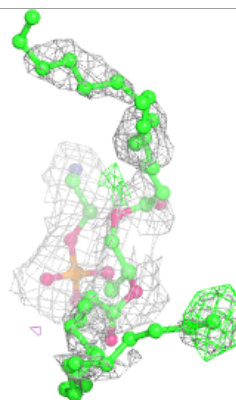
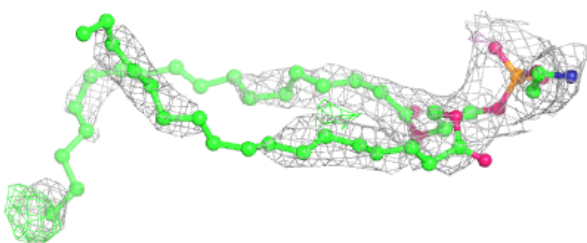
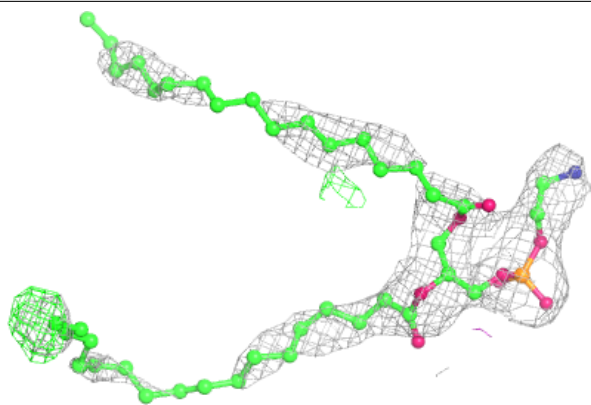
**Electron density around PLC R 3009:**

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

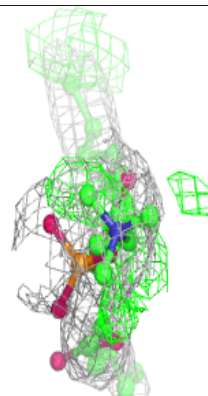
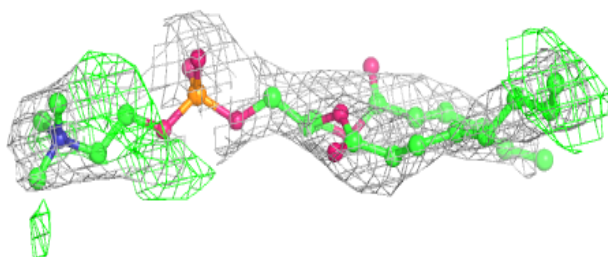
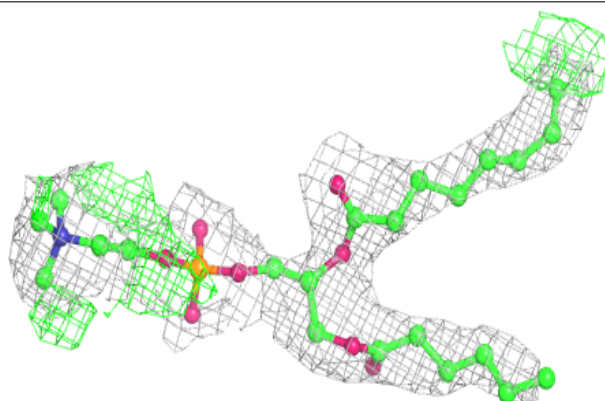


Electron density around PEE E 2005:

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

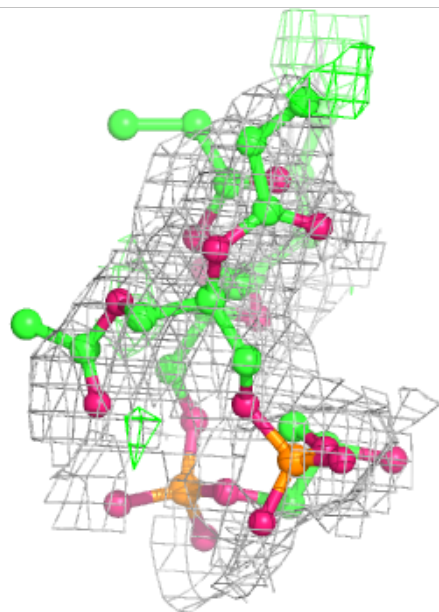
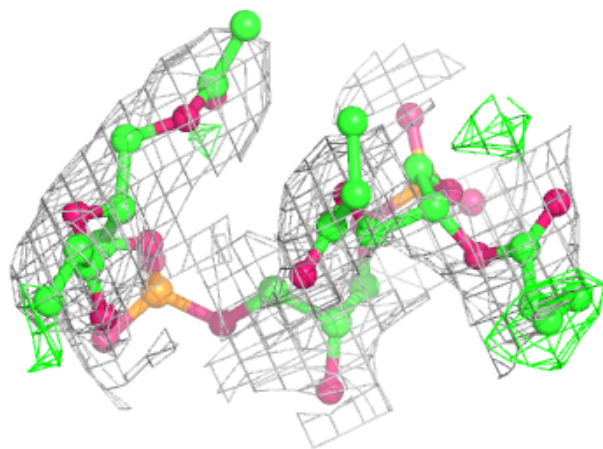
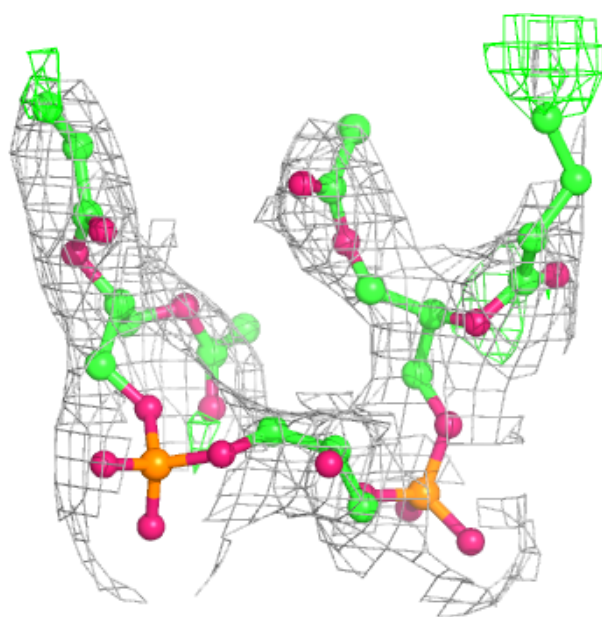
**Electron density around PLC E 2009:**

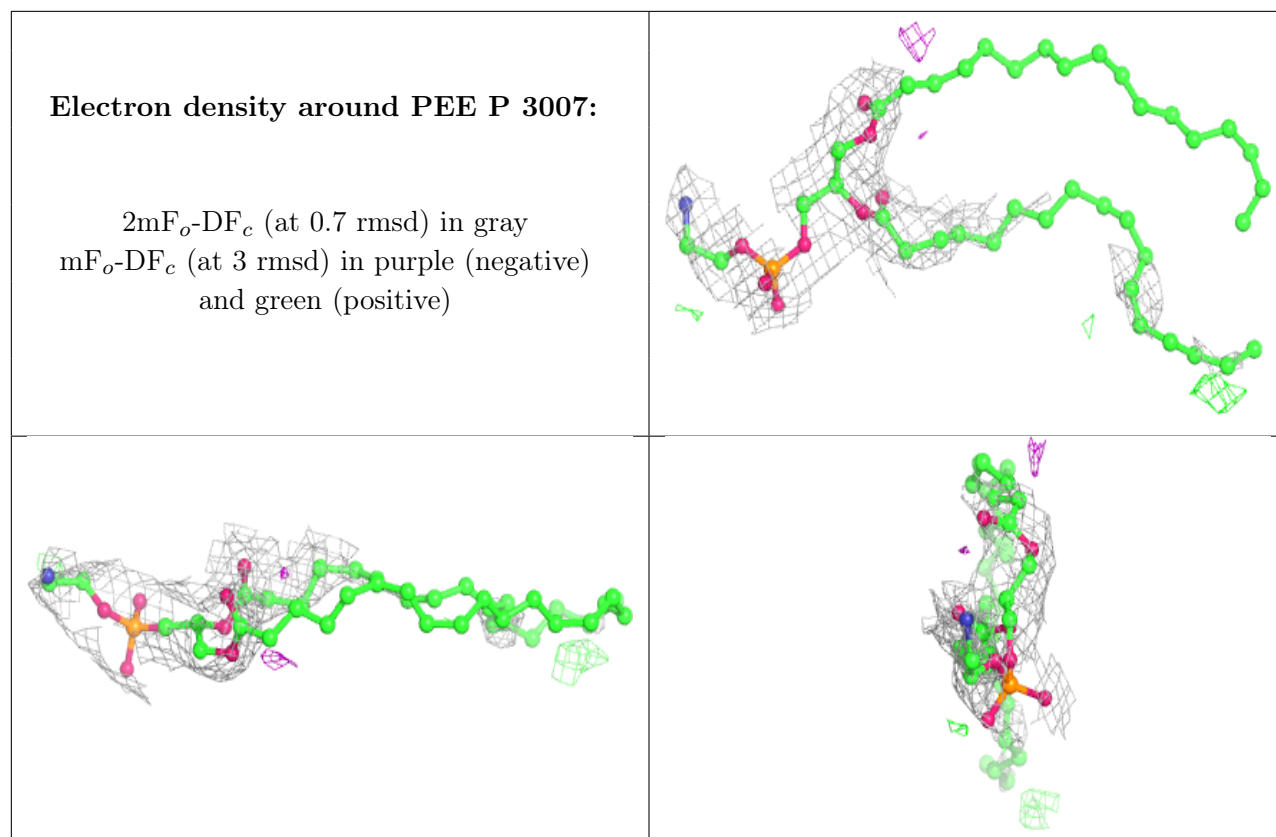
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CDL P 3004:

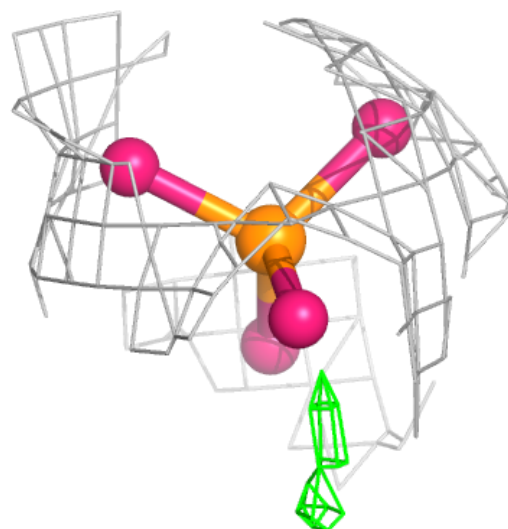
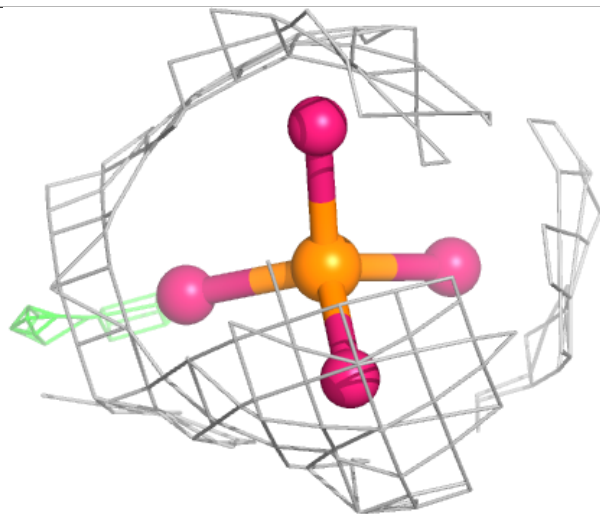
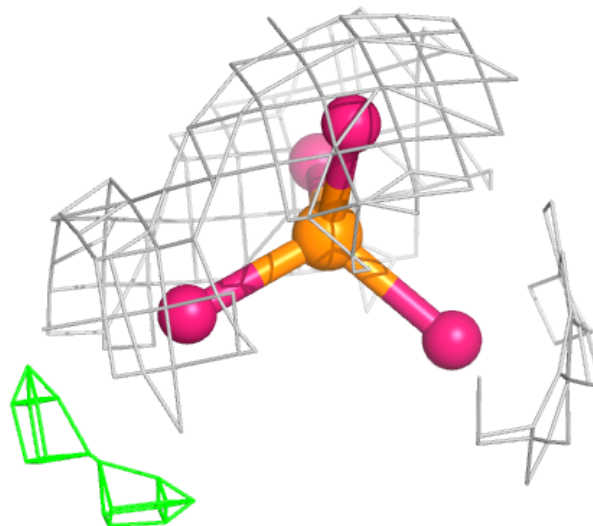
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

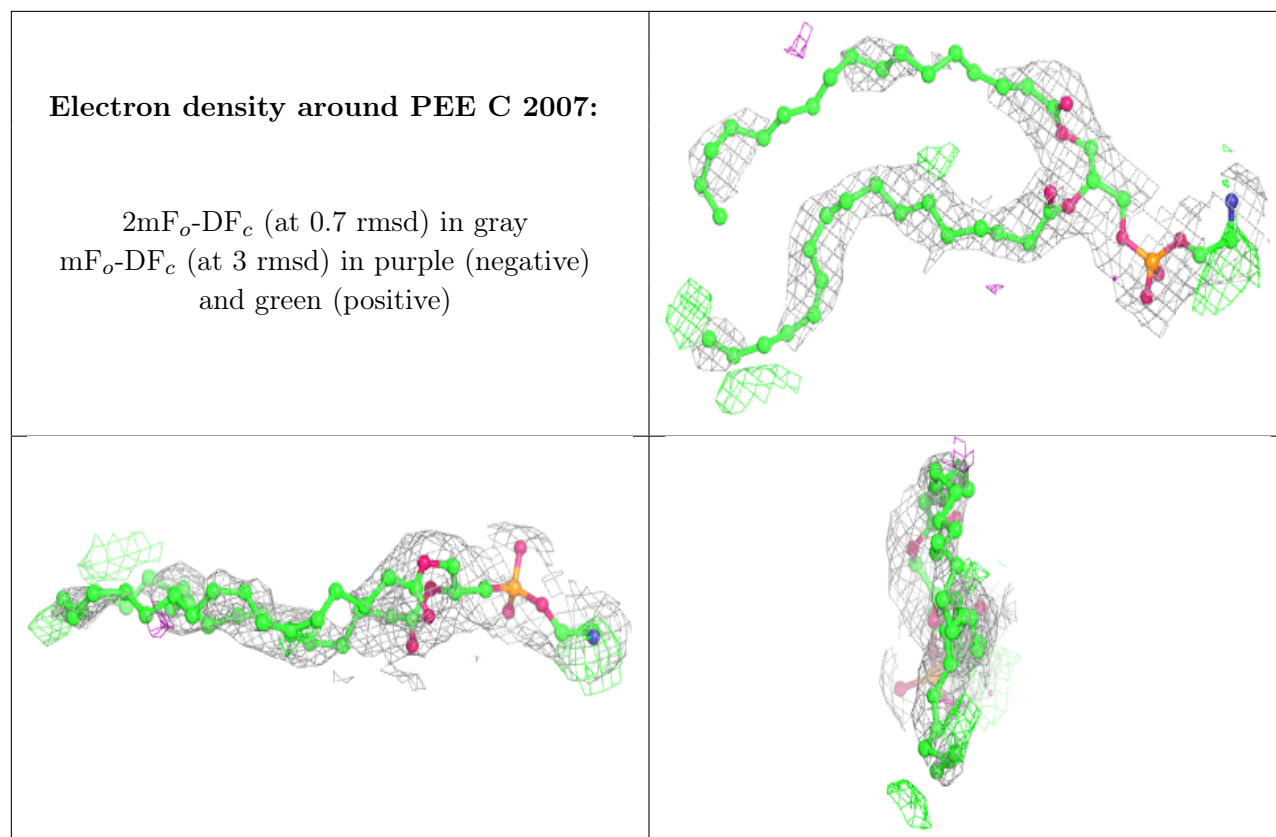




Electron density around PEE N 3008:

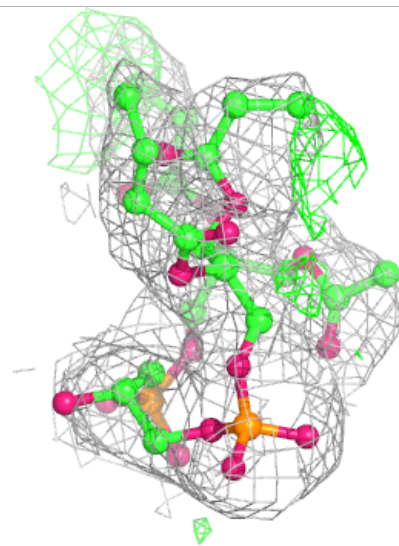
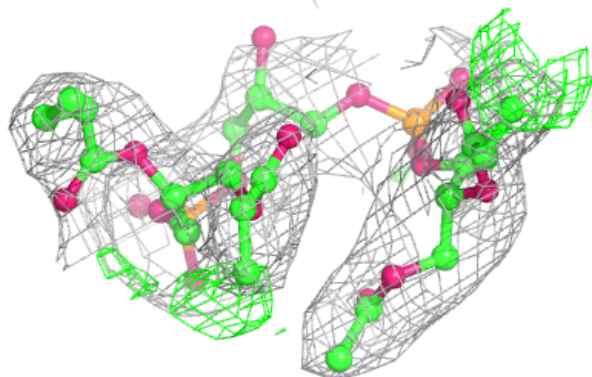
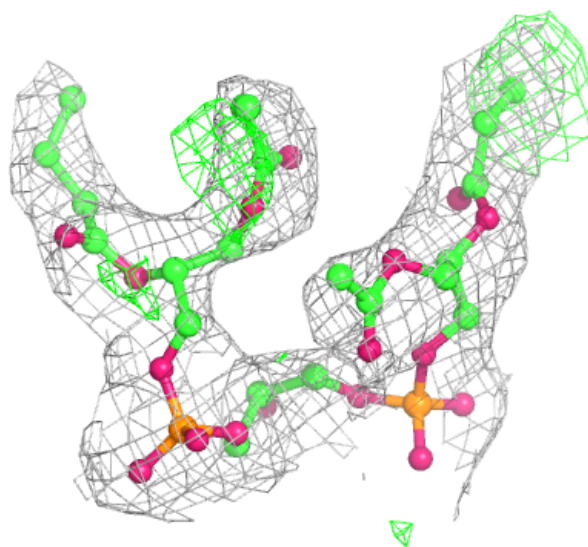
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





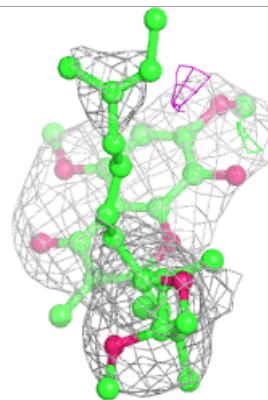
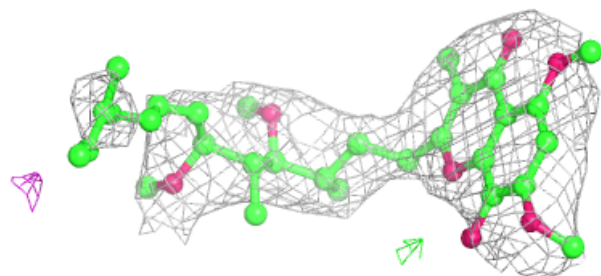
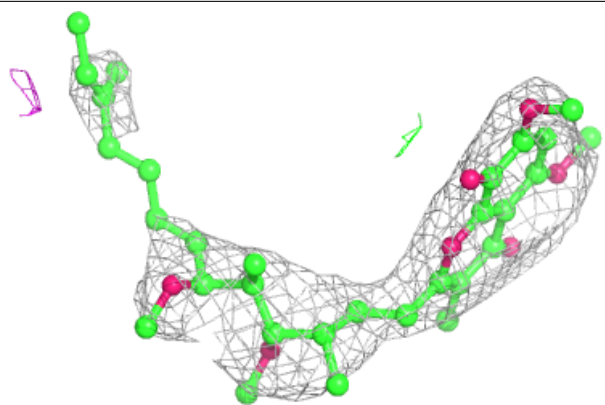
Electron density around CDL C 2004:

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

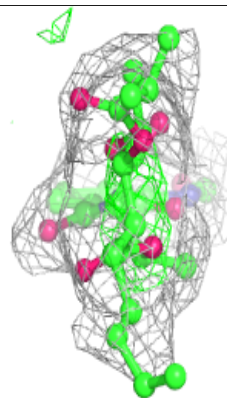
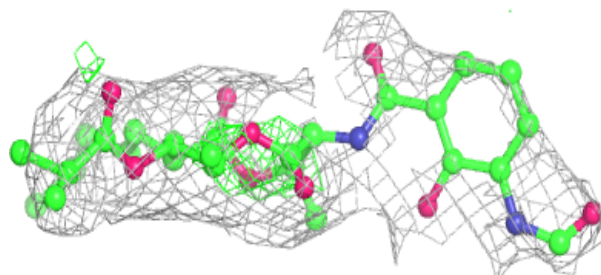
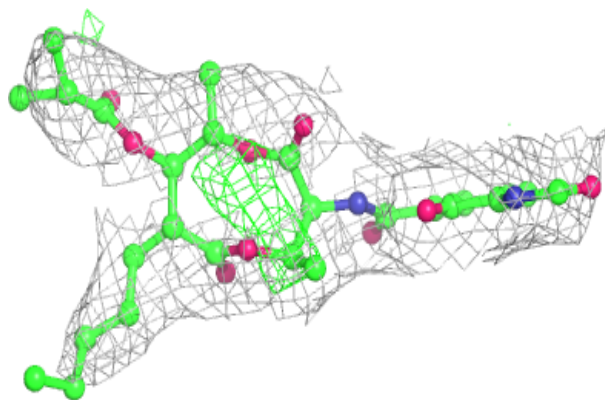


Electron density around SMA P 3001:

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

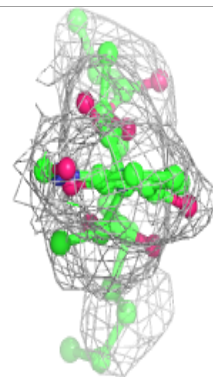
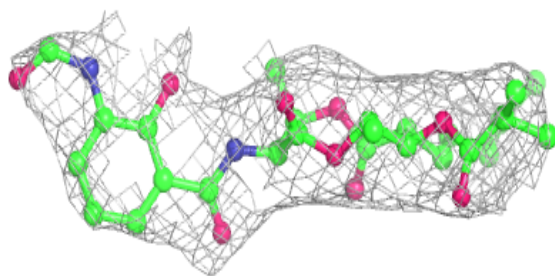
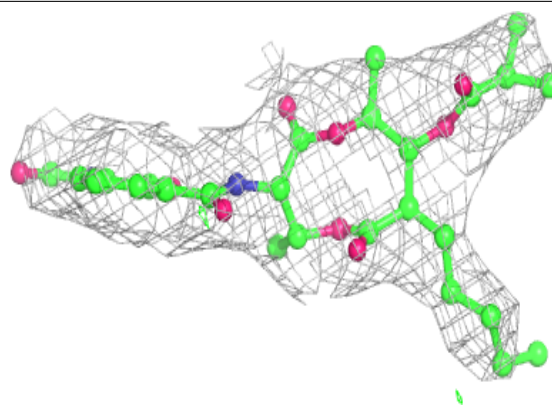
**Electron density around ANY P 3002:**

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



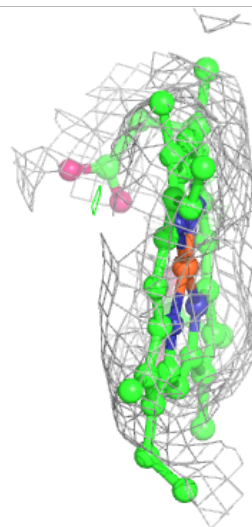
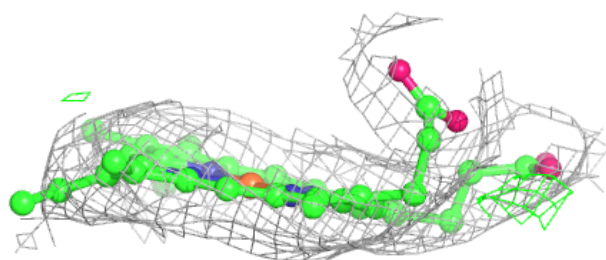
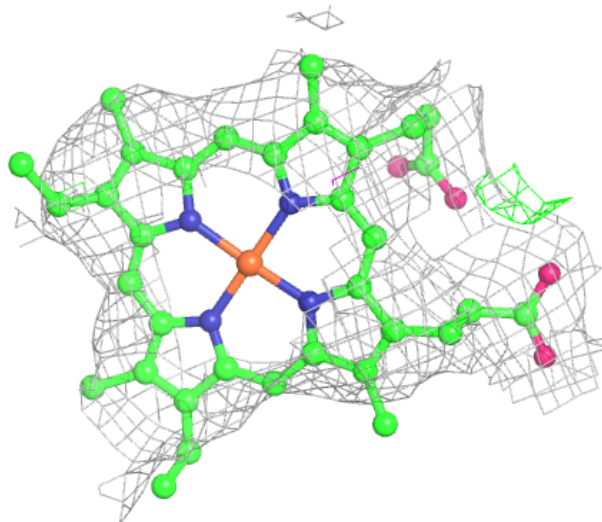
Electron density around ANY C 2002:

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



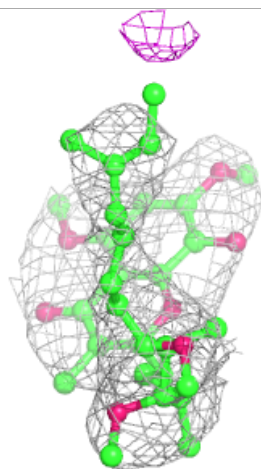
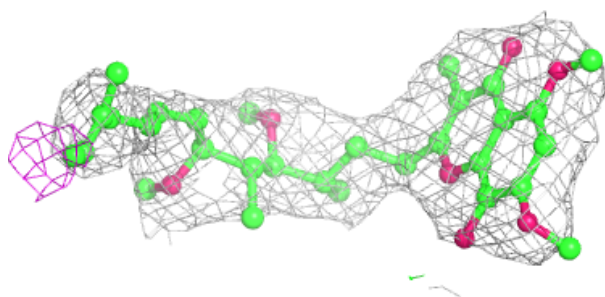
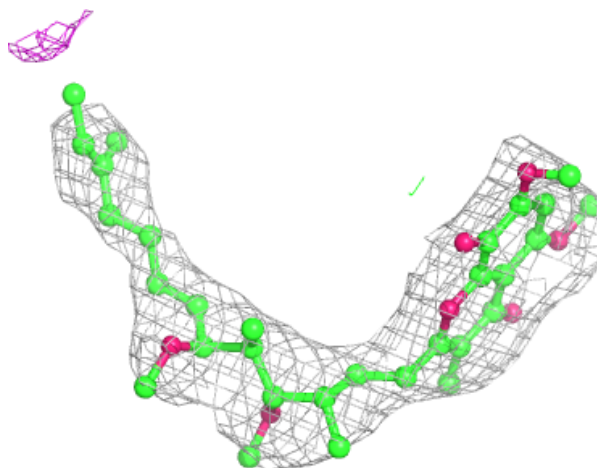
Electron density around HEM P 502:

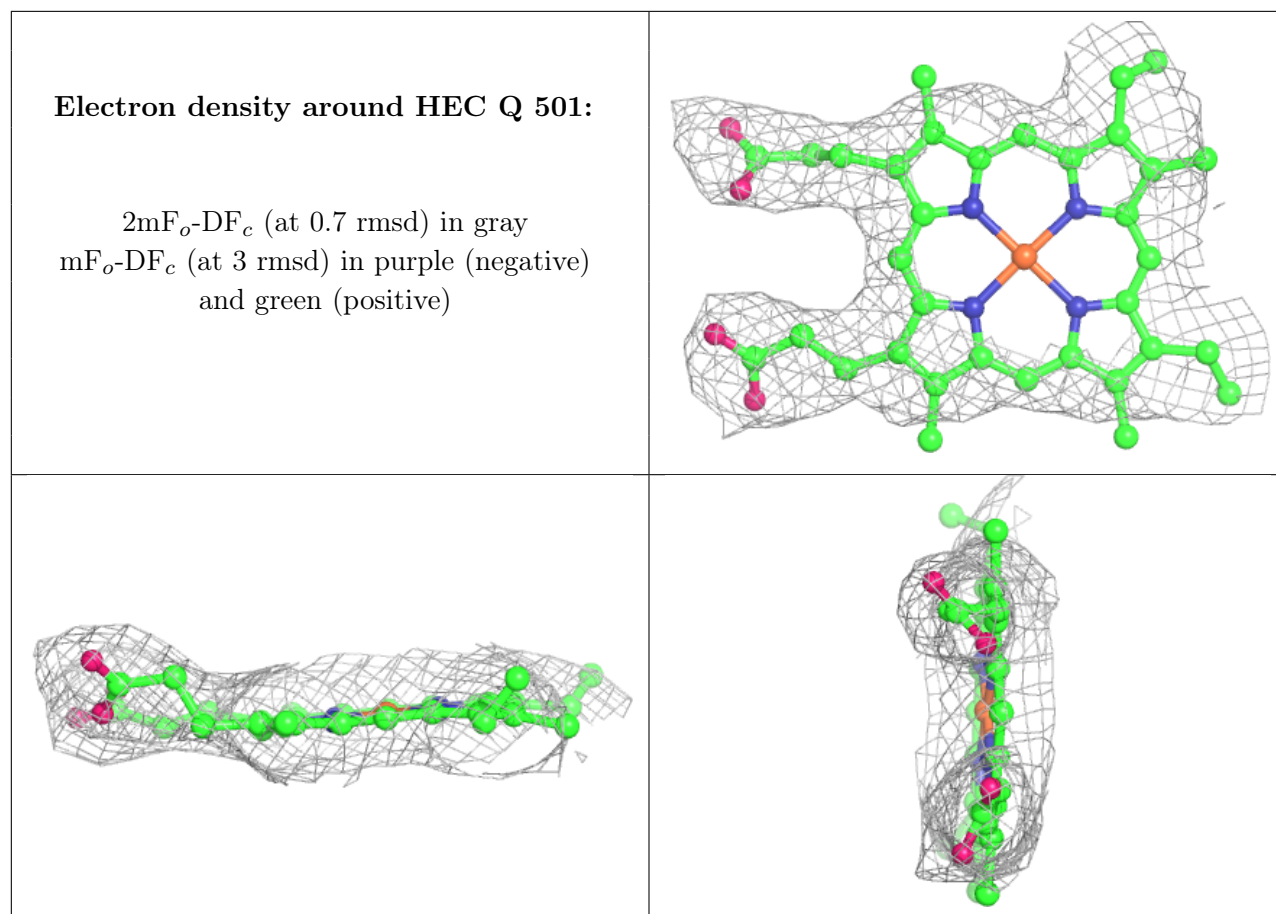
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

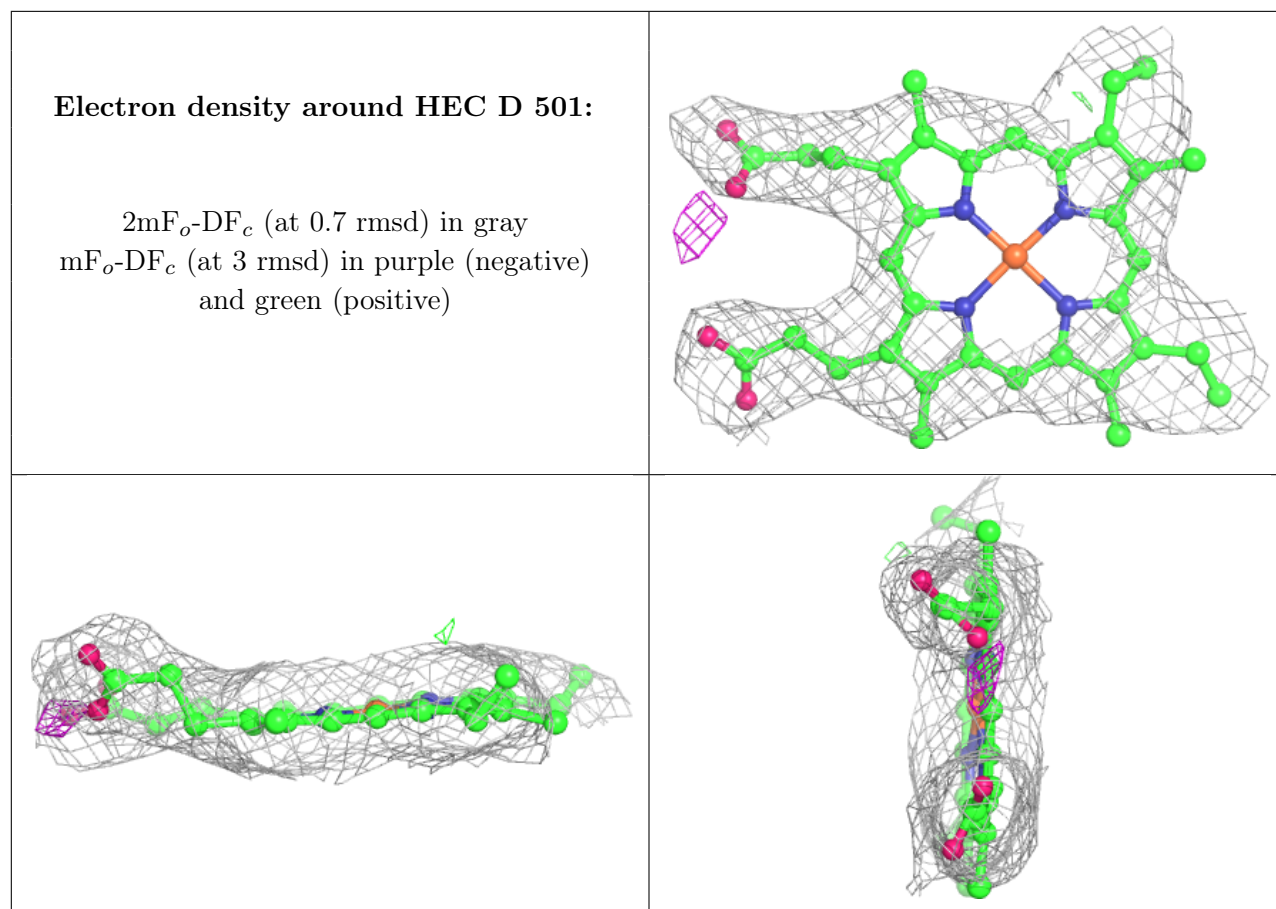


Electron density around SMA C 2001:

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

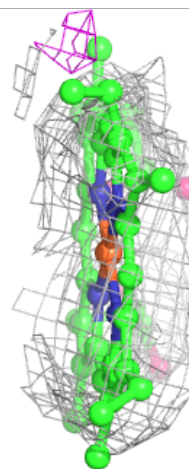
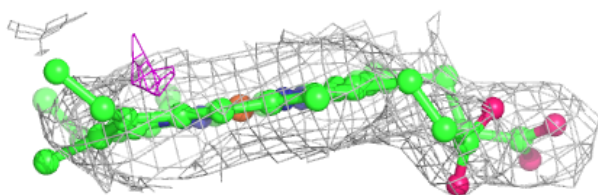
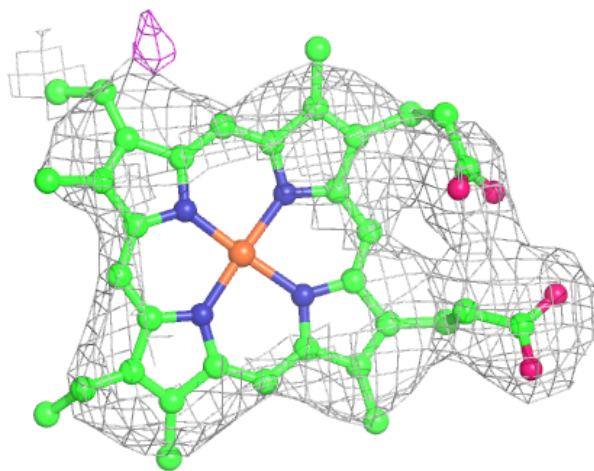






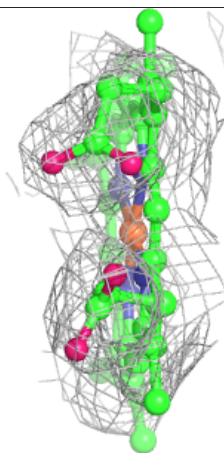
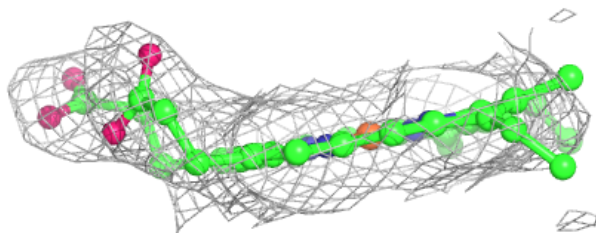
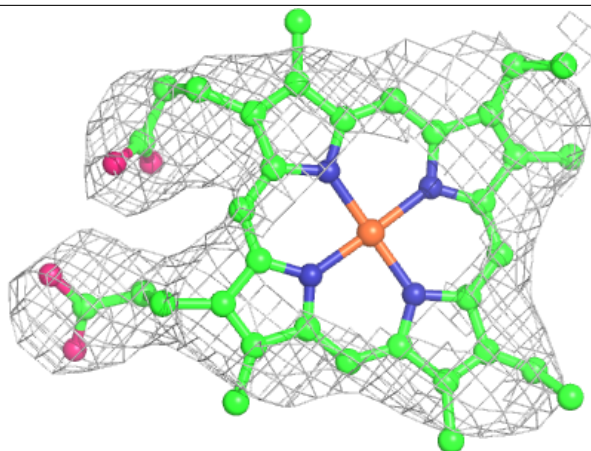
Electron density around HEM P 501:

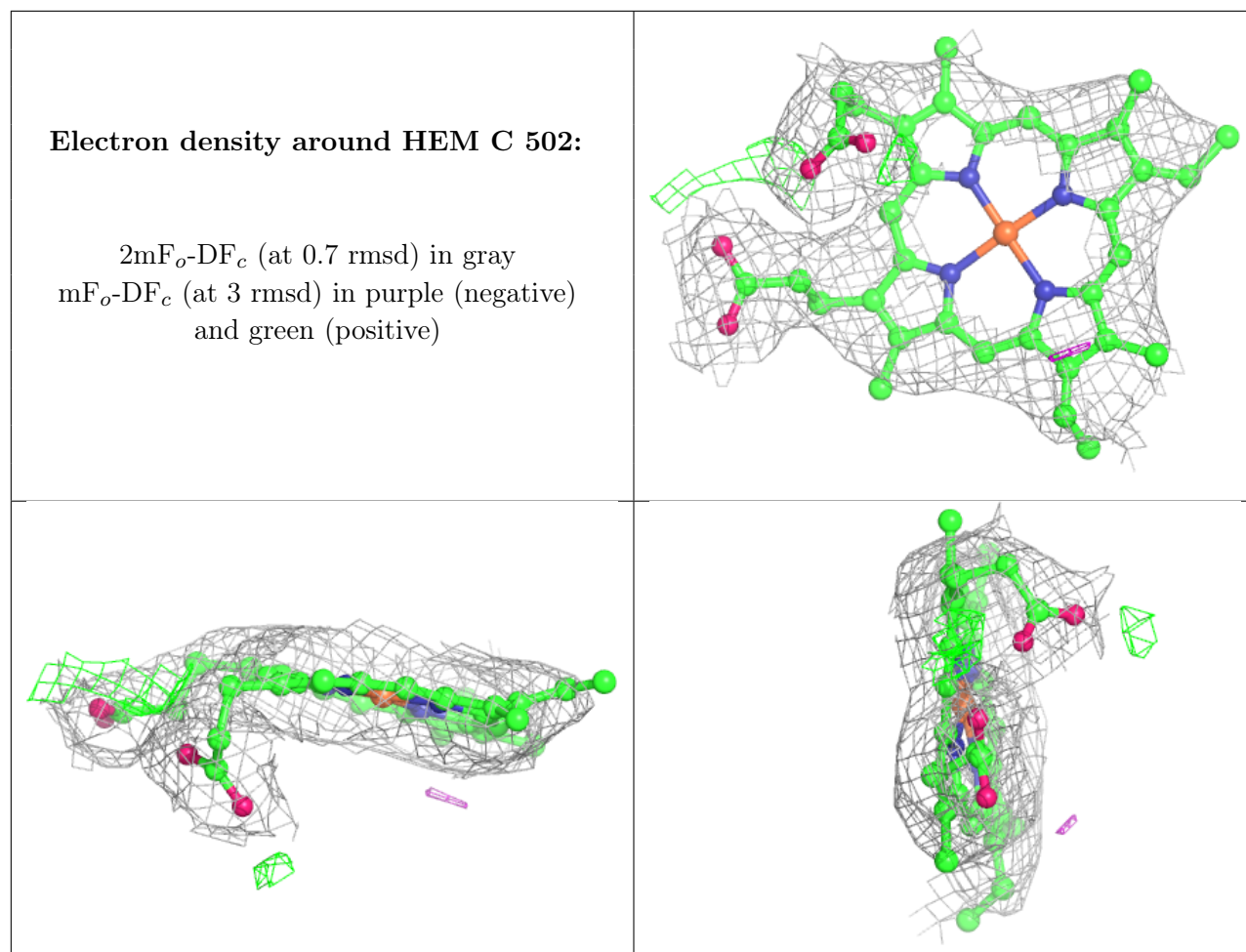
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.