



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:34 AM EDT

PDB ID : 3H1J / pdb_00003h1j
Title : Stigmatellin-bound cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.;
Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on : 2009-04-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

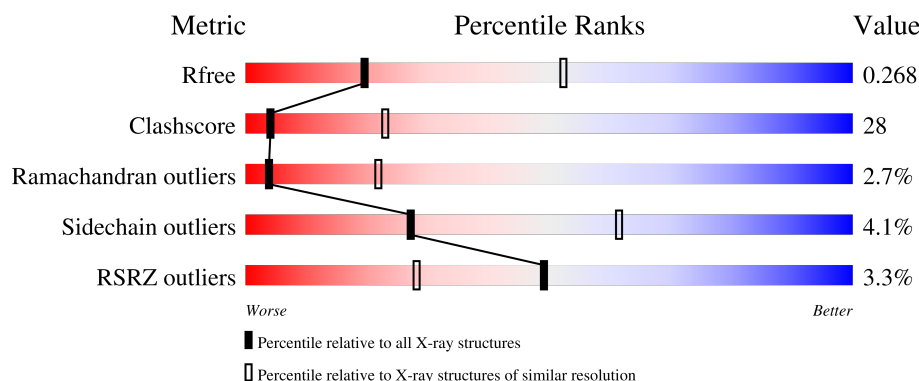
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

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

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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
15	PEE	N	3008	-	X	-	-
17	HEC	D	501	X	-	-	-
17	HEC	Q	501	X	-	-	-

2 Entry composition

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

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

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

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

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

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

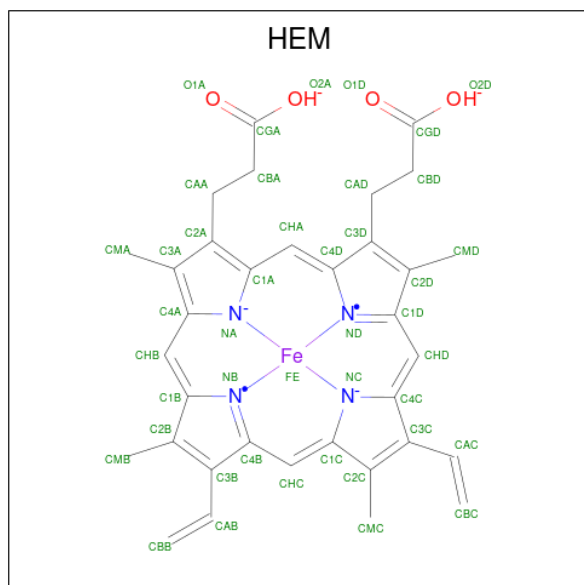
- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

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

- Molecule 11 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

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



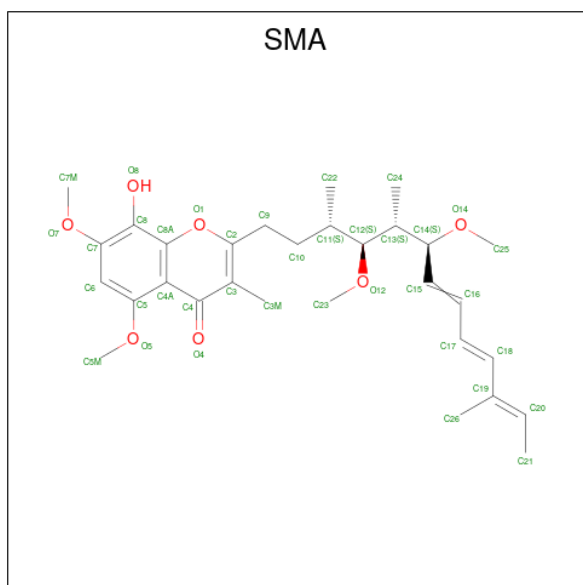
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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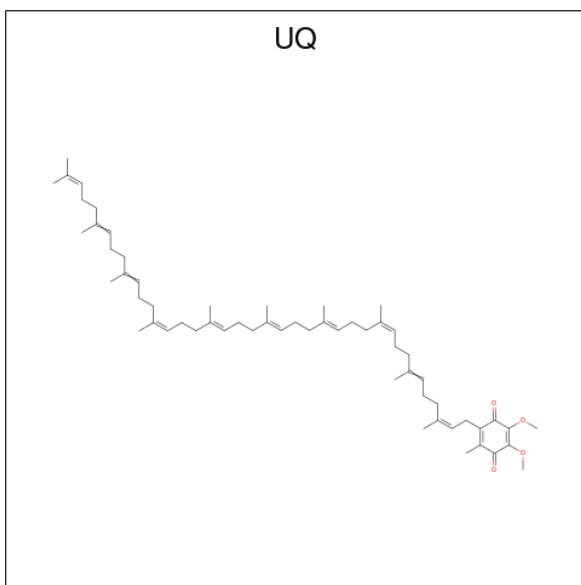
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



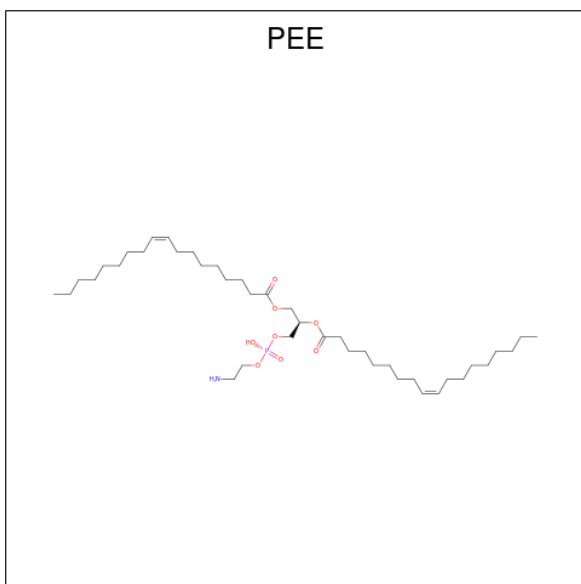
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			37	30	7		
13	P	1	Total	C	O	0	0
			37	30	7		

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



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

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



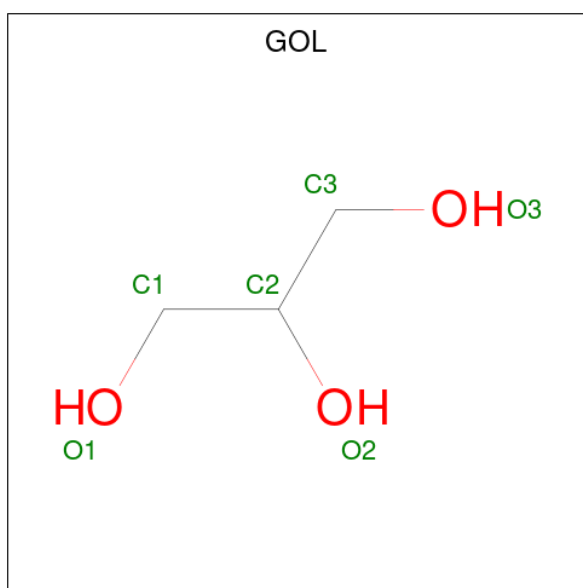
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

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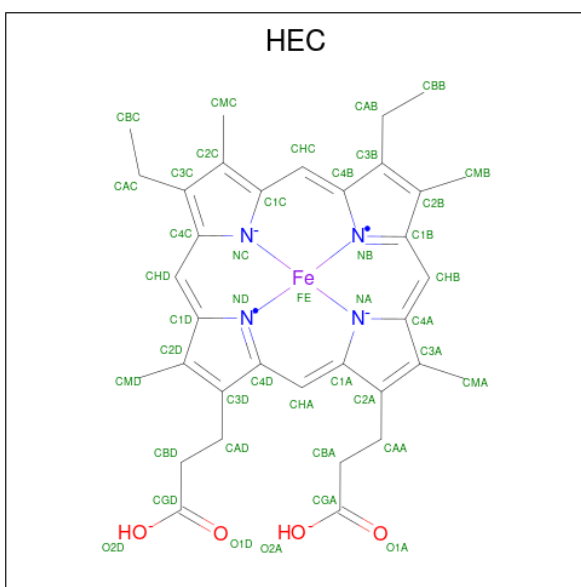
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	N	1	Total	O	P			0	0
			5	4	1				
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 16 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



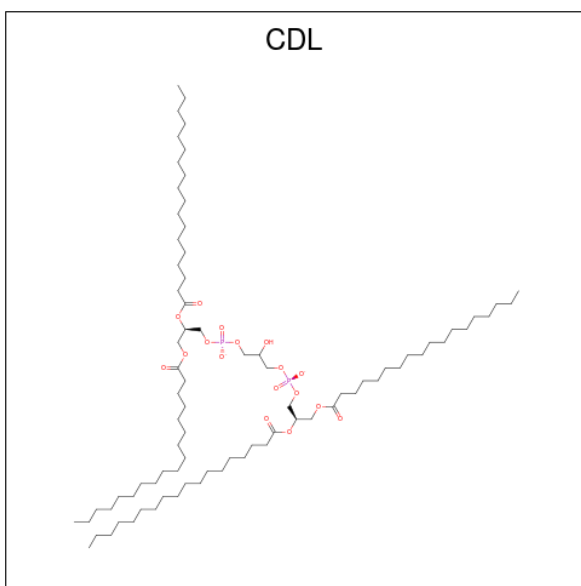
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



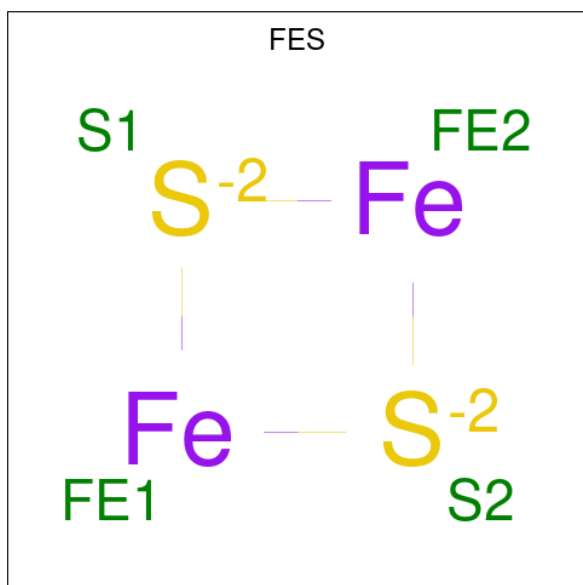
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total 50	C 31	O 17	P 2	0	0
18	G	1	Total 40	C 21	O 17	P 2	0	0

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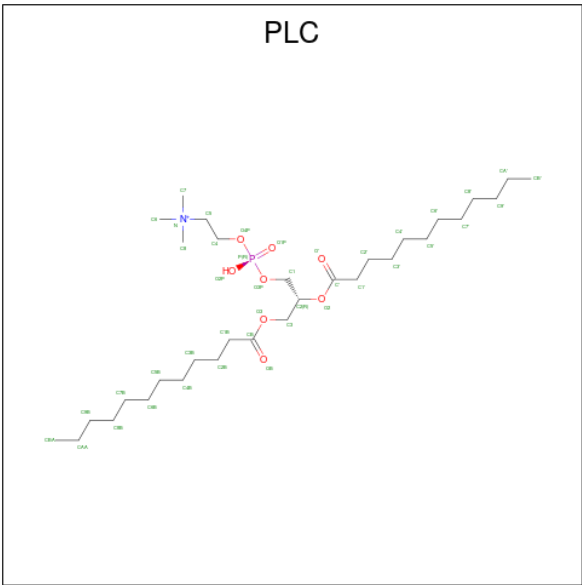
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			40	21	17	2		
18	S	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$).



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		

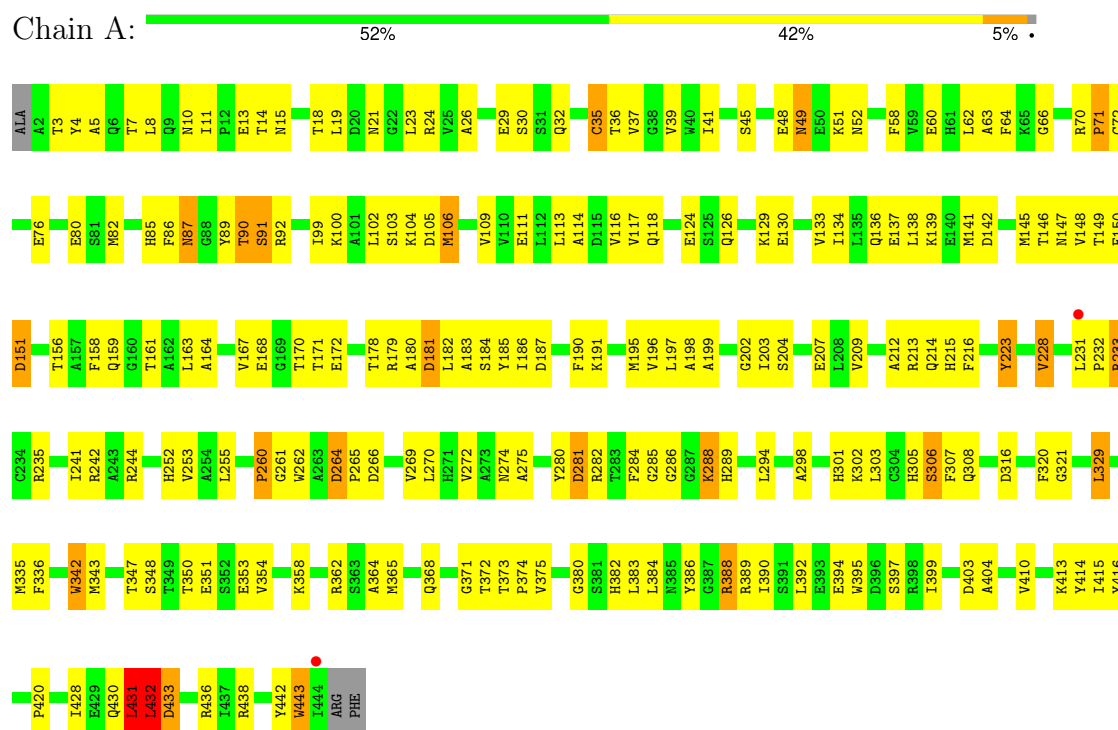
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	O	0	0
			1	1		
21	C	6	Total	O	0	0
			6	6		
21	P	6	Total	O	0	0
			6	6		
21	U	1	Total	O	0	0
			1	1		

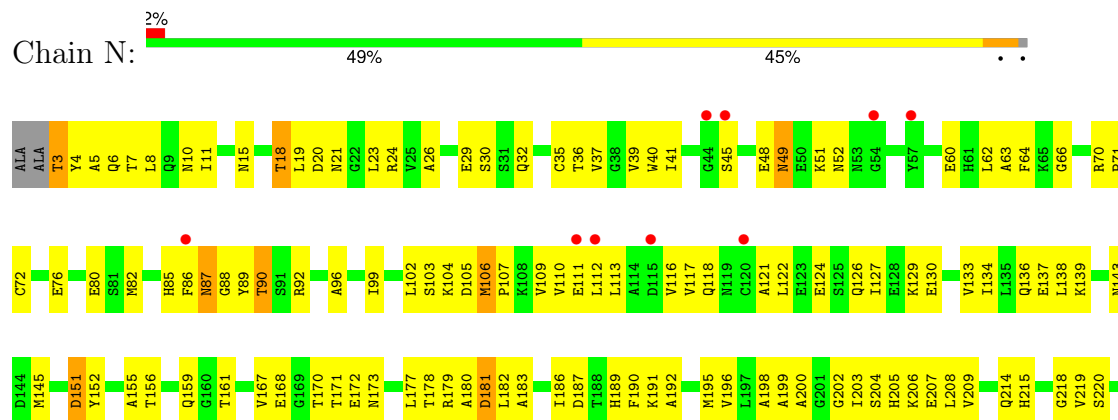
3 Residue-property plots

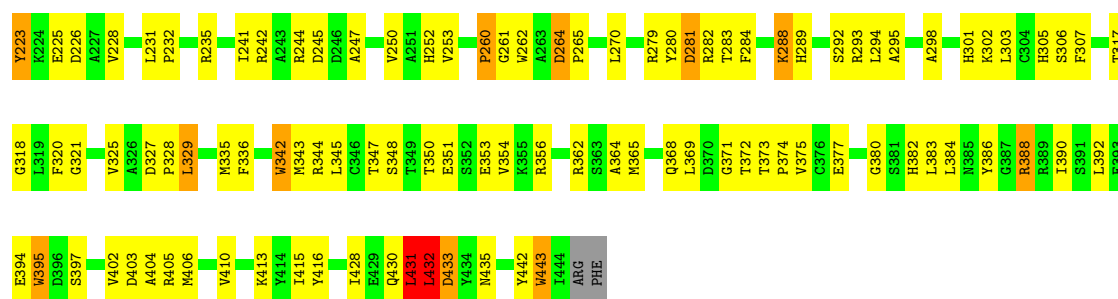
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

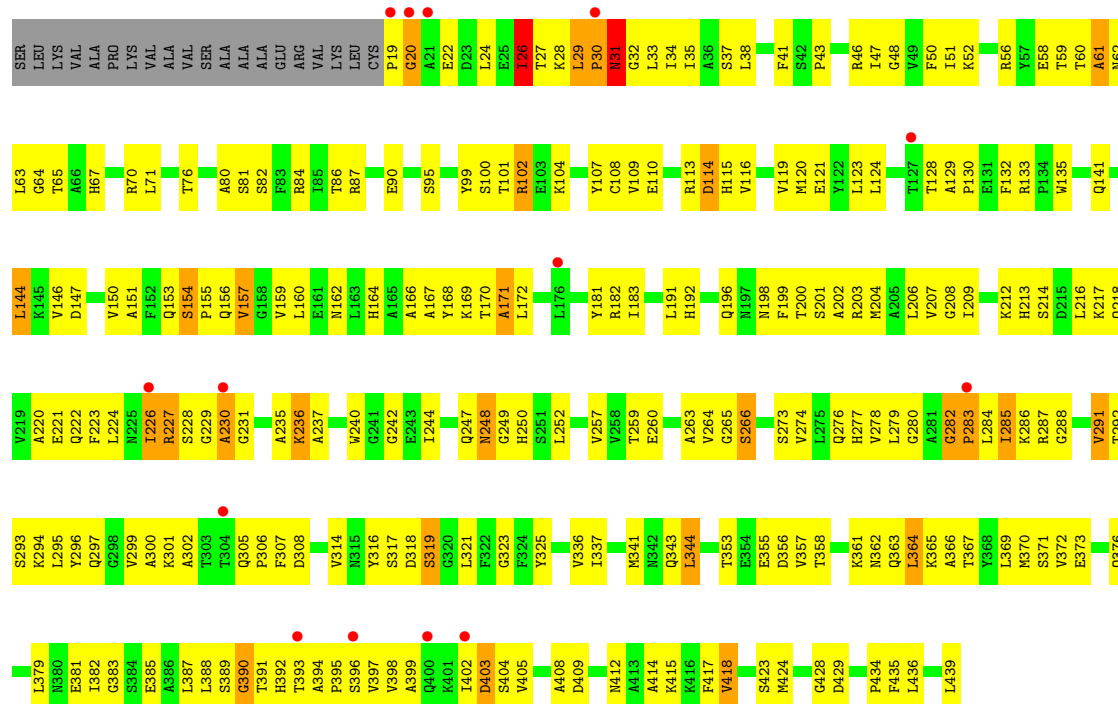


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

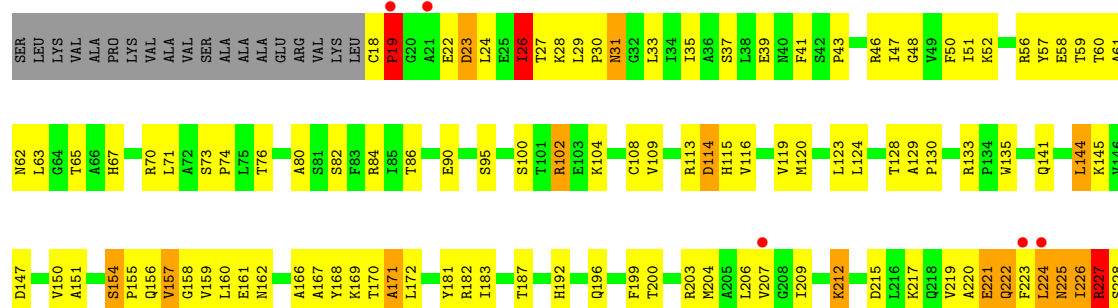
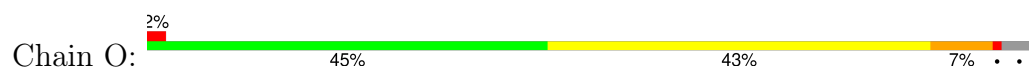




• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

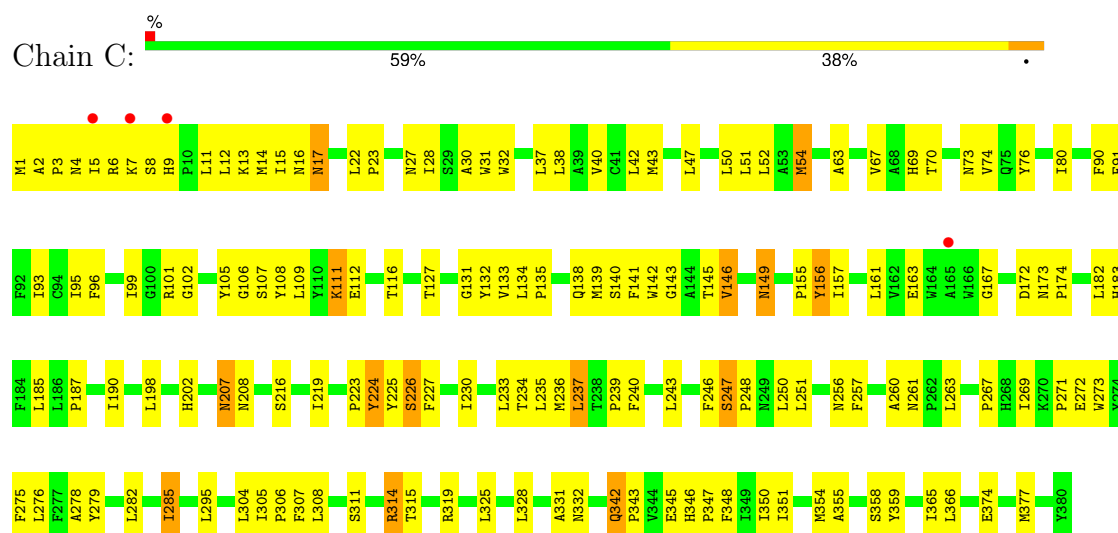


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

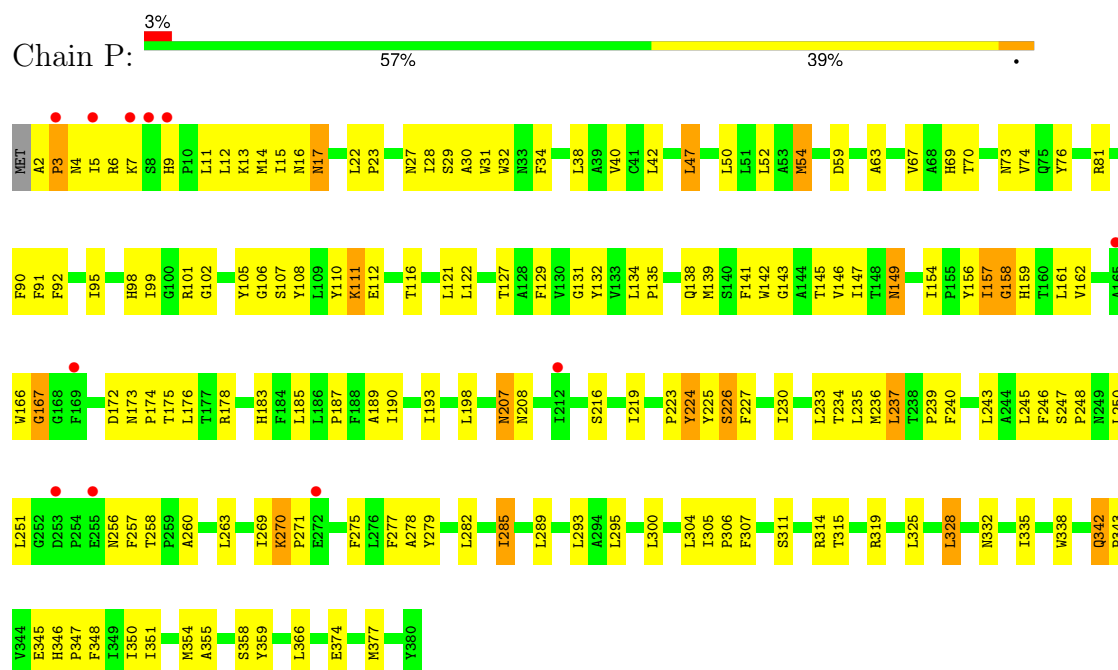




- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b



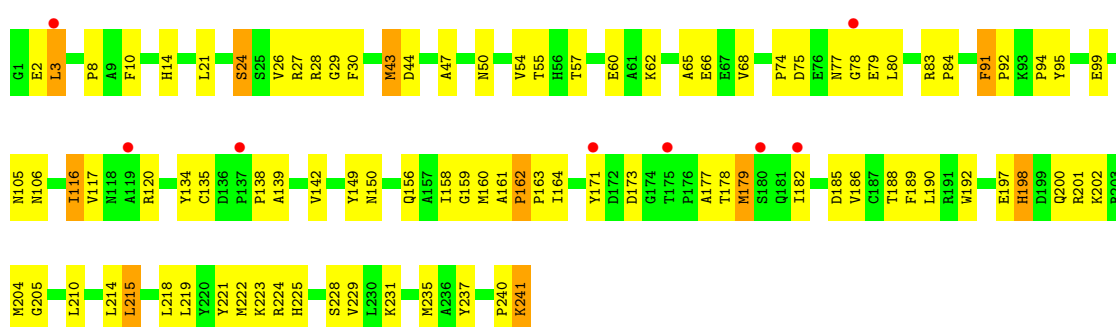
- Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:  64% 32% .



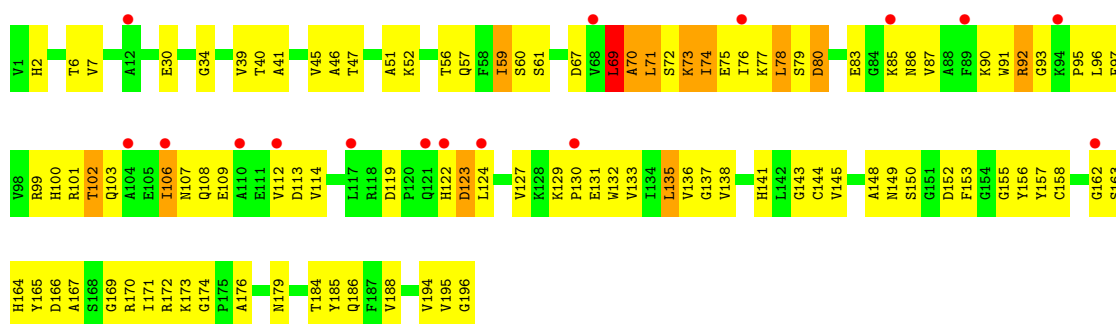
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:  3% 61% 34% .



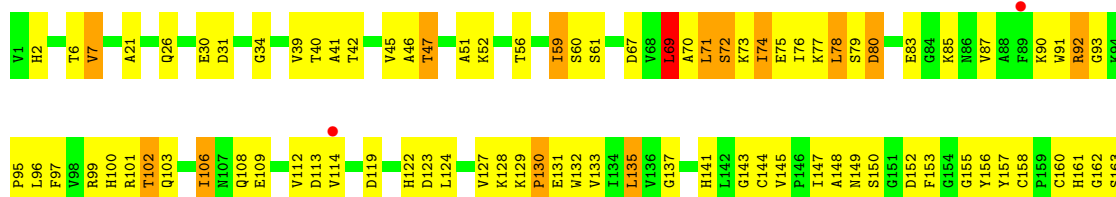
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

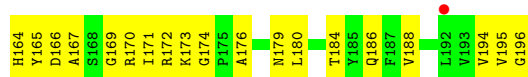
Chain E:  8% 48% 45% 6% .



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

Chain R:  2% 46% 46% 7% .





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



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



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



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



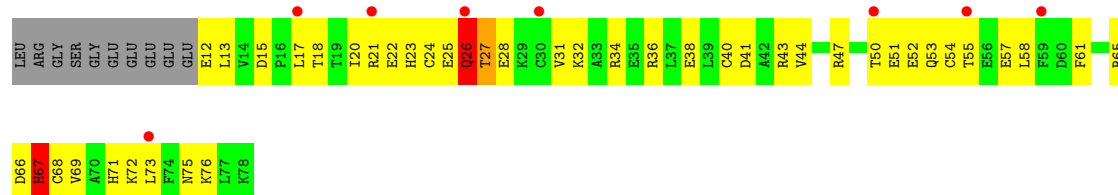
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H: 



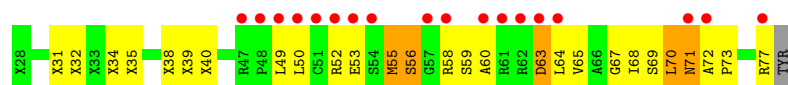
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U: 



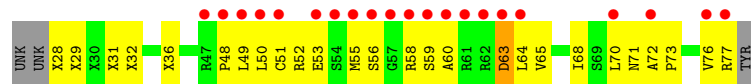
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 



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

Chain V: 



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

Chain J: 



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

Chain W:

51%

38%

8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.68-3.00) 92.5 (42.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.277 0.234 , 0.268	Depositor DCC
R_{free} test set	2796 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32679	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3511	1.01	17/4757 (0.4%)
1	N	0.51	0/3508	1.01	16/4753 (0.3%)
2	B	0.46	0/3196	0.98	8/4334 (0.2%)
2	O	0.51	0/3202	0.98	10/4343 (0.2%)
3	C	0.65	2/3122 (0.1%)	1.04	23/4273 (0.5%)
3	P	0.56	1/3114 (0.0%)	1.02	18/4263 (0.4%)
4	D	0.58	0/1956	1.04	10/2658 (0.4%)
4	Q	0.48	0/1956	1.01	6/2658 (0.2%)
5	E	0.46	0/1547	0.99	6/2103 (0.3%)
5	R	0.47	0/1547	1.05	10/2103 (0.5%)
6	F	0.61	0/911	1.00	4/1219 (0.3%)
6	S	0.50	0/911	0.96	6/1219 (0.5%)
7	G	0.62	0/698	1.03	3/946 (0.3%)
7	T	0.50	0/680	0.99	3/923 (0.3%)
8	H	0.52	0/582	0.88	1/779 (0.1%)
8	U	0.41	0/561	0.92	3/751 (0.4%)
9	I	0.58	0/218	0.99	0/293
9	V	0.63	0/218	1.00	0/293
10	J	0.54	0/508	0.94	1/682 (0.1%)
10	W	0.49	0/489	0.90	1/658 (0.2%)
All	All	0.53	3/32435 (0.0%)	1.00	146/44008 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	P	0	1
4	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	43	MET	SD-CE	6.73	1.96	1.79
3	C	54	MET	SD-CE	5.78	1.94	1.79
3	P	54	MET	SD-CE	5.44	1.93	1.79

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	143	GLY	N-CA-C	10.12	128.82	115.36
5	R	71	LEU	N-CA-C	10.12	125.02	110.14
5	R	143	GLY	N-CA-C	10.11	128.80	115.36
4	Q	116	ILE	N-CA-C	9.22	119.27	110.42
4	Q	91	PHE	CA-C-N	9.10	129.67	119.93
4	Q	91	PHE	C-N-CA	9.10	129.67	119.93
3	C	365	ILE	N-CA-C	8.88	118.63	111.62
4	D	91	PHE	CA-C-N	8.56	130.54	119.84
4	D	91	PHE	C-N-CA	8.56	130.54	119.84
1	N	415	ILE	CB-CA-C	-8.44	104.53	111.71
4	D	116	ILE	N-CA-C	8.36	118.45	110.42
3	P	226	SER	N-CA-C	-8.02	102.47	111.14
1	A	415	ILE	CB-CA-C	-7.84	105.04	111.71
1	A	264	ASP	CA-C-N	7.83	127.90	119.28
1	A	264	ASP	C-N-CA	7.83	127.90	119.28
1	A	348	SER	N-CA-C	7.70	120.24	110.61
1	N	415	ILE	N-CA-C	7.64	118.66	111.48
4	D	44	ASP	N-CA-C	7.59	121.46	111.75
5	R	129	LYS	CA-C-N	7.28	128.94	119.84
5	R	129	LYS	C-N-CA	7.28	128.94	119.84
1	A	214	GLN	N-CA-C	7.22	118.79	111.07
1	N	214	GLN	N-CA-C	7.04	118.61	111.07
3	C	226	SER	N-CA-C	-7.04	103.69	111.36
7	G	37	VAL	N-CA-C	-6.98	103.72	110.42
3	C	27	ASN	N-CA-C	6.92	121.80	112.88
5	E	102	THR	N-CA-C	-6.82	101.34	110.55
1	A	415	ILE	N-CA-C	6.73	117.81	111.48
5	R	7	VAL	N-CA-C	-6.72	102.85	108.63
5	E	71	LEU	N-CA-C	6.71	119.18	110.53
5	R	102	THR	N-CA-C	-6.65	101.57	110.55
1	N	432	LEU	N-CA-C	6.65	118.24	108.14
5	E	129	LYS	CA-C-N	6.50	127.97	119.84
5	E	129	LYS	C-N-CA	6.50	127.97	119.84
1	A	432	LEU	N-CA-C	6.48	117.98	108.14
1	N	348	SER	N-CA-C	6.46	120.48	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	264	ASP	CA-C-N	6.46	126.38	119.28
1	N	264	ASP	C-N-CA	6.46	126.38	119.28
3	P	185	LEU	N-CA-C	6.42	118.16	111.03
2	O	144	LEU	N-CA-C	-6.41	104.21	111.07
5	R	72	SER	N-CA-C	6.40	124.44	110.80
6	S	16	ILE	N-CA-C	-6.39	104.28	110.42
2	B	157	VAL	N-CA-C	6.38	117.16	110.72
3	C	111	LYS	N-CA-C	6.38	121.89	111.37
1	A	329	LEU	N-CA-C	6.32	120.60	113.02
3	P	270	LYS	CA-C-N	6.30	126.66	119.92
3	P	270	LYS	C-N-CA	6.30	126.66	119.92
4	Q	44	ASP	N-CA-C	6.26	119.77	111.75
2	B	61	ALA	N-CA-C	6.25	118.09	111.28
3	P	27	ASN	N-CA-C	6.24	120.92	112.88
3	P	91	PHE	N-CA-C	-6.19	104.46	111.14
3	C	134	LEU	CA-C-N	-6.16	113.47	119.87
3	C	134	LEU	C-N-CA	-6.16	113.47	119.87
6	S	15	ARG	N-CA-C	-6.15	105.91	113.41
3	C	207	ASN	N-CA-C	-6.12	100.87	110.36
3	C	247	SER	CA-C-N	6.10	125.58	119.24
3	C	247	SER	C-N-CA	6.10	125.58	119.24
4	Q	80	LEU	N-CA-C	-6.08	102.69	110.53
10	W	53	LYS	N-CA-C	-6.04	104.61	111.07
10	J	53	LYS	N-CA-C	-6.01	104.64	111.07
1	N	244	ARG	N-CA-C	6.00	119.03	109.24
1	N	329	LEU	N-CA-C	5.97	120.19	113.02
3	C	93	ILE	N-CA-C	-5.95	104.53	110.30
5	E	61	SER	N-CA-C	-5.94	105.99	113.18
2	O	61	ALA	N-CA-C	5.89	117.38	111.07
2	O	157	VAL	N-CA-C	5.88	117.41	111.00
4	D	80	LEU	N-CA-C	-5.86	102.97	110.53
5	R	61	SER	N-CA-C	-5.86	106.09	113.18
3	P	111	LYS	N-CA-C	5.84	120.95	111.37
1	N	218	GLY	N-CA-C	-5.84	100.11	111.03
2	O	141	GLN	CA-C-N	-5.83	113.81	119.87
2	O	141	GLN	C-N-CA	-5.83	113.81	119.87
2	B	144	LEU	N-CA-C	-5.82	104.85	111.07
3	P	110	TYR	N-CA-C	-5.82	101.51	109.71
3	P	257	PHE	N-CA-C	-5.81	105.77	112.92
4	D	95	TYR	CA-C-N	5.80	126.30	120.04
4	D	95	TYR	C-N-CA	5.80	126.30	120.04
3	C	146	VAL	N-CA-C	5.79	115.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	52	GLU	N-CA-C	5.77	117.24	111.07
3	C	224	TYR	N-CA-C	5.75	118.03	111.02
3	C	257	PHE	N-CA-C	-5.74	105.86	112.92
1	A	58	PHE	N-CA-C	-5.74	105.10	111.36
3	P	328	LEU	N-CA-C	-5.73	104.95	111.14
3	C	143	GLY	N-CA-C	-5.68	105.62	112.49
1	A	244	ARG	N-CA-C	5.67	118.48	109.24
8	H	67	HIS	N-CA-C	-5.63	105.04	111.07
6	F	39	GLU	N-CA-C	5.63	118.31	108.52
2	B	282	GLY	CA-C-N	5.62	126.86	119.84
2	B	282	GLY	C-N-CA	5.62	126.86	119.84
3	C	91	PHE	N-CA-C	-5.62	105.07	111.14
6	F	52	GLU	N-CA-C	5.61	117.08	111.07
1	N	431	LEU	N-CA-C	-5.61	102.10	110.23
2	O	282	GLY	CA-C-N	5.56	126.79	119.84
2	O	282	GLY	C-N-CA	5.56	126.79	119.84
3	C	261	ASN	CA-C-N	5.52	125.19	119.56
3	C	261	ASN	C-N-CA	5.52	125.19	119.56
8	U	67	HIS	N-CA-C	-5.52	105.17	111.07
3	C	342	GLN	CA-C-N	5.51	125.42	119.85
3	C	342	GLN	C-N-CA	5.51	125.42	119.85
2	O	356	ASP	N-CA-C	-5.50	105.19	111.07
3	P	134	LEU	CA-C-N	-5.49	114.01	119.56
3	P	134	LEU	C-N-CA	-5.49	114.01	119.56
4	D	107	GLY	N-CA-C	-5.48	108.08	115.21
1	N	66	GLY	N-CA-C	5.46	118.87	111.72
8	U	27	THR	N-CA-C	5.36	117.86	110.35
3	P	207	ASN	N-CA-C	-5.36	102.06	110.36
1	A	66	GLY	N-CA-C	5.35	118.73	111.72
4	D	19	SER	N-CA-C	5.35	117.03	108.41
1	A	35	CYS	N-CA-C	5.35	115.30	108.24
7	T	2	ILE	N-CA-C	5.35	115.90	108.84
6	S	39	GLU	N-CA-C	5.34	117.88	109.39
6	S	109	LYS	N-CA-C	-5.33	106.62	113.23
1	N	264	ASP	N-CA-C	5.31	118.87	109.58
1	N	442	TYR	N-CA-C	5.30	117.81	108.75
5	R	26	GLN	N-CA-C	5.28	117.72	111.33
3	C	185	LEU	N-CA-C	5.27	118.04	111.24
2	B	141	GLN	CA-C-N	-5.27	114.24	119.56
2	B	141	GLN	C-N-CA	-5.27	114.24	119.56
1	N	151	ASP	N-CA-C	-5.26	105.45	111.07
1	A	442	TYR	N-CA-C	5.24	117.22	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	LEU	N-CA-C	-5.24	102.63	110.23
5	R	70	ALA	N-CA-C	-5.22	98.51	107.23
3	C	365	ILE	CB-CA-C	-5.18	106.44	111.05
7	G	12	HIS	N-CA-C	5.17	118.85	111.92
3	P	143	GLY	N-CA-C	-5.16	106.25	112.49
3	P	342	GLN	CA-C-N	5.16	125.09	119.78
3	P	342	GLN	C-N-CA	5.16	125.09	119.78
3	P	167	GLY	N-CA-C	-5.15	106.97	114.90
7	G	23	GLN	N-CA-C	5.14	117.09	109.69
2	B	404	SER	N-CA-C	-5.14	106.96	113.18
6	F	34	ASP	N-CA-C	5.13	117.62	111.71
8	U	26	GLN	N-CA-C	-5.13	105.86	111.82
7	T	43	SER	N-CA-C	5.12	118.62	112.38
1	A	149	THR	N-CA-C	5.12	116.94	111.36
2	O	161	GLU	N-CA-C	-5.11	105.60	111.07
1	N	428	ILE	N-CA-C	5.10	119.94	109.34
3	P	314	ARG	N-CA-C	5.09	117.95	111.69
3	C	314	ARG	N-CA-C	5.07	117.92	111.69
7	T	12	HIS	N-CA-C	5.07	118.58	111.74
1	A	151	ASP	N-CA-C	-5.05	105.66	111.07
6	F	32	MET	N-CA-C	-5.05	102.59	110.42
4	D	215	LEU	N-CA-C	5.04	116.58	111.14
1	A	428	ILE	N-CA-C	5.04	119.81	109.34
6	S	32	MET	N-CA-C	-5.03	102.62	110.42
2	O	404	SER	N-CA-C	-5.02	107.10	113.18
3	C	37	LEU	N-CA-C	-5.01	105.70	111.07
4	Q	215	LEU	N-CA-C	5.01	116.83	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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	189	0
1	N	3437	0	3349	208	0
2	B	3141	0	3142	271	0
2	O	3147	0	3146	251	0
3	C	3020	0	3070	151	0
3	P	3012	0	3058	163	0
4	D	1898	0	1846	70	0
4	Q	1898	0	1846	89	0
5	E	1513	0	1478	95	0
5	R	1513	0	1478	96	0
6	F	891	0	893	41	0
6	S	891	0	893	47	0
7	G	676	0	659	48	0
7	T	658	0	647	48	0
8	H	574	0	548	35	0
8	U	553	0	535	48	0
9	I	285	0	237	53	0
9	V	275	0	238	43	0
10	J	497	0	490	20	0
10	W	478	0	478	31	0
11	A	1	0	0	0	0
11	C	3	0	0	0	0
11	E	2	0	0	0	0
11	P	3	0	0	0	0
11	R	1	0	0	0	0
12	C	86	0	60	11	0
12	P	86	0	60	12	0
13	C	37	0	42	4	0
13	P	37	0	42	4	0
14	C	19	0	17	4	0
14	P	19	0	17	2	0
15	C	70	0	85	1	0
15	E	50	0	77	4	0
15	N	5	0	0	0	0
15	P	49	0	72	1	0
15	R	50	0	77	4	0
16	C	6	0	8	0	0
16	P	6	0	8	1	0
17	D	43	0	30	0	0
17	Q	43	0	30	0	0
18	D	50	0	44	1	0
18	G	40	0	24	1	0
18	P	40	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	50	0	44	2	0
19	E	4	0	0	0	0
19	R	4	0	0	1	0
20	E	32	0	38	3	0
20	R	32	0	38	2	0
21	B	1	0	0	0	0
21	C	6	0	0	0	0
21	P	6	0	0	1	0
21	U	1	0	0	1	0
All	All	32679	0	32221	1792	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 28.

All (1792) 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)
6:F:32:MET:HE2	6:F:87:LYS:HG2	1.25	1.17
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.27	1.13
6:F:32:MET:HE3	6:F:87:LYS:H	1.11	1.12
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.23	1.10
2:B:353:THR:HG22	2:B:355:GLU:H	1.15	1.08
6:S:32:MET:HE3	6:S:87:LYS:H	1.16	1.07
3:C:17:ASN:HD21	7:G:1:GLY:HA2	0.98	1.07
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.35	1.06
2:O:353:THR:HG22	2:O:355:GLU:H	1.19	1.06
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.37	1.06
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.37	1.06
2:O:76:THR:HG22	2:O:82:SER:H	1.17	1.05
2:O:22:GLU:HG3	2:O:39:GLU:HB3	1.37	1.05
2:B:76:THR:HG22	2:B:82:SER:H	1.22	1.01
3:P:157:ILE:HG13	3:P:158:GLY:H	1.23	1.01
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.09	0.97
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.45	0.96
7:T:29:ILE:H	7:T:29:ILE:HD12	1.28	0.96
9:V:28:UNK:CB	9:V:72:ALA:HB2	1.95	0.95
6:S:13:MET:HA	6:S:16:ILE:HB	1.46	0.95
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.29	0.94
3:C:17:ASN:ND2	7:G:1:GLY:HA2	1.82	0.94
1:A:178:THR:HB	1:A:181:ASP:OD1	1.68	0.93
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.50	0.92
3:C:90:PHE:HB3	3:C:236:MET:HE3	1.50	0.92
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.52	0.91
7:G:29:ILE:H	7:G:29:ILE:HD12	1.35	0.90
1:N:49:ASN:C	1:N:49:ASN:HD22	1.79	0.90
6:F:32:MET:CE	6:F:87:LYS:H	1.84	0.90
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.89
3:P:101:ARG:HD2	3:P:101:ARG:C	1.97	0.89
1:N:136:GLN:HE22	9:V:50:LEU:HD12	1.38	0.89
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.54	0.89
3:P:207:ASN:ND2	3:P:208:ASN:H	1.70	0.88
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.56	0.88
3:C:13:LYS:O	3:C:17:ASN:HB2	1.74	0.88
3:P:90:PHE:HB3	3:P:236:MET:HE3	1.55	0.88
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.40	0.87
1:A:49:ASN:C	1:A:49:ASN:HD22	1.82	0.87
6:S:52:GLU:HG2	6:S:56:ASN:HD21	1.39	0.87
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.57	0.86
6:F:32:MET:CE	6:F:87:LYS:HG2	2.04	0.86
2:O:128:THR:HA	2:O:226:ILE:HD11	1.57	0.86
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.12	0.85
3:C:101:ARG:HD2	3:C:101:ARG:C	2.02	0.85
3:C:207:ASN:ND2	3:C:208:ASN:H	1.73	0.85
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.41	0.85
2:B:393:THR:HG23	2:B:397:VAL:HB	1.57	0.85
6:F:52:GLU:HG2	6:F:56:ASN:HD21	1.39	0.84
6:F:13:MET:HE2	6:F:13:MET:HA	1.60	0.84
2:B:31:ASN:HD22	2:B:32:GLY:N	1.74	0.84
9:V:65:VAL:HB	9:V:77:ARG:HD3	1.58	0.84
2:O:393:THR:HG23	2:O:397:VAL:HB	1.58	0.84
5:R:73:LYS:HB3	5:R:195:VAL:O	1.77	0.83
1:N:178:THR:HB	1:N:181:ASP:OD1	1.76	0.83
9:I:71:ASN:HD22	9:I:71:ASN:H	1.26	0.83
1:N:178:THR:HG22	1:N:180:ALA:H	1.41	0.83
6:S:52:GLU:HG2	6:S:56:ASN:ND2	1.94	0.83
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.42	0.83
3:P:13:LYS:O	3:P:17:ASN:HB2	1.77	0.83
1:A:178:THR:HG22	1:A:180:ALA:H	1.44	0.82
5:R:101:ARG:NH2	5:R:127:VAL:HG21	1.94	0.82
6:F:52:GLU:HG2	6:F:56:ASN:ND2	1.95	0.81
2:B:212:LYS:HD3	2:B:213:HIS:N	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ARG:HD3	2:B:228:SER:H	1.45	0.80
1:A:187:ASP:O	1:A:191:LYS:HE3	1.82	0.80
2:O:62:ASN:O	2:O:65:THR:HG22	1.81	0.80
3:P:139:MET:HE1	3:P:269:ILE:HA	1.63	0.80
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.63	0.80
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.64	0.80
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.64	0.80
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.64	0.80
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.22	0.79
6:F:32:MET:HE3	6:F:87:LYS:N	1.95	0.79
2:B:62:ASN:O	2:B:65:THR:HG22	1.82	0.79
5:E:101:ARG:NH2	5:E:127:VAL:HG21	1.97	0.79
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.63	0.79
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.18	0.79
2:O:76:THR:HG22	2:O:82:SER:N	1.95	0.79
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.78
1:N:187:ASP:O	1:N:191:LYS:HE3	1.84	0.78
1:N:99:ILE:HD12	1:N:109:VAL:HG13	1.65	0.78
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.18	0.78
1:A:106:MET:HE2	1:A:106:MET:O	1.84	0.78
2:B:76:THR:HG22	2:B:82:SER:N	1.97	0.78
2:B:248:ASN:C	2:B:248:ASN:HD22	1.90	0.77
1:A:99:ILE:HD12	1:A:109:VAL:HG13	1.67	0.77
2:B:227:ARG:HA	2:B:227:ARG:HE	1.48	0.76
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.67	0.76
2:B:76:THR:CG2	2:B:82:SER:H	1.97	0.76
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.20	0.76
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.66	0.76
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.50	0.76
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.50	0.76
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.15	0.76
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.68	0.76
2:B:154:SER:O	2:B:157:VAL:HG12	1.86	0.75
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.26	0.75
2:O:248:ASN:C	2:O:248:ASN:HD22	1.91	0.75
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.21	0.75
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.51	0.75
4:D:224:ARG:HE	7:G:26:ILE:HG12	1.52	0.75
9:I:32:UNK:N	9:I:73:PRO:HG2	2.01	0.75
2:B:201:SER:OG	2:B:228:SER:HB3	1.87	0.74
1:A:136:GLN:NE2	9:I:50:LEU:HB2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:ILE:HG22	2:O:227:ARG:N	2.01	0.74
3:C:139:MET:HE1	3:C:269:ILE:HA	1.69	0.74
7:T:29:ILE:HD12	7:T:29:ILE:N	2.01	0.74
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.69	0.74
2:B:385:GLU:OE1	2:B:392:HIS:HA	1.87	0.74
1:N:373:THR:HB	1:N:374:PRO:HD3	1.68	0.74
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.70	0.74
2:B:47:ILE:HG12	2:B:120:MET:CE	2.13	0.74
2:O:219:VAL:O	2:O:223:PHE:HB2	1.88	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.70	0.73
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.70	0.73
6:S:32:MET:CE	6:S:87:LYS:H	1.96	0.73
7:G:29:ILE:H	7:G:29:ILE:CD1	1.93	0.73
2:B:47:ILE:CG1	2:B:120:MET:HE1	2.12	0.73
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.70	0.73
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.23	0.73
2:O:154:SER:O	2:O:157:VAL:HG12	1.89	0.73
2:B:218:GLN:HG3	2:B:222:GLN:NE2	2.04	0.73
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.71	0.73
2:O:361:LYS:O	2:O:365:LYS:HG3	1.87	0.73
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.19	0.72
2:B:389:SER:O	2:B:391:THR:HG23	1.88	0.72
2:O:76:THR:CG2	2:O:82:SER:H	1.99	0.72
2:O:220:ALA:O	2:O:224:LEU:HB2	1.89	0.72
8:U:32:LYS:O	8:U:36:ARG:HG3	1.89	0.72
1:N:136:GLN:NE2	9:V:50:LEU:HB2	2.04	0.72
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.18	0.72
2:B:31:ASN:HB3	2:B:227:ARG:HH22	1.54	0.72
7:G:29:ILE:HD12	7:G:29:ILE:N	2.04	0.72
9:I:71:ASN:H	9:I:71:ASN:ND2	1.88	0.72
2:O:389:SER:O	2:O:391:THR:HG23	1.90	0.72
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.84	0.72
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.24	0.72
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.55	0.71
3:C:4:ASN:HD21	3:C:7:LYS:NZ	1.87	0.71
6:F:70:LEU:C	6:F:70:LEU:HD12	2.15	0.71
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.72	0.71
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.72	0.71
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.26	0.71
1:N:182:LEU:O	1:N:186:ILE:HG13	1.91	0.71
8:U:27:THR:O	8:U:31:VAL:HG23	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.30	0.71
1:N:106:MET:O	1:N:106:MET:HE2	1.90	0.71
2:O:22:GLU:HG3	2:O:39:GLU:CB	2.18	0.71
2:O:29:LEU:HD12	2:O:33:LEU:HD23	1.72	0.71
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.72	0.71
2:B:227:ARG:HA	2:B:227:ARG:NE	2.05	0.71
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.56	0.71
9:V:64:LEU:HD12	9:V:77:ARG:O	1.89	0.71
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.72	0.71
8:H:43:ARG:HD2	8:H:47:ARG:NH1	2.06	0.71
3:P:285:ILE:N	3:P:285:ILE:HD12	2.06	0.71
2:B:203:ARG:CD	2:B:230:ALA:HA	2.19	0.71
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.72	0.71
6:S:70:LEU:C	6:S:70:LEU:HD12	2.16	0.71
4:D:75:ASP:OD2	4:D:79:GLU:HB2	1.90	0.70
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.71	0.70
2:B:212:LYS:HD2	2:B:214:SER:OG	1.91	0.70
9:I:55:MET:O	9:I:58:ARG:HG2	1.92	0.70
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.72	0.70
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.27	0.70
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.06	0.70
7:T:29:ILE:H	7:T:29:ILE:CD1	1.90	0.70
1:N:90:THR:O	1:N:167:VAL:HG11	1.91	0.70
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.06	0.70
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.27	0.70
2:B:124:LEU:HD21	2:B:223:PHE:HB3	1.73	0.70
1:N:388:ARG:HH21	1:N:388:ARG:HG3	1.56	0.70
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.55	0.70
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.74	0.70
3:P:346:HIS:ND1	3:P:347:PRO:HA	2.06	0.70
2:B:353:THR:HG22	2:B:355:GLU:N	2.00	0.69
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.73	0.69
2:O:385:GLU:OE1	2:O:392:HIS:HA	1.92	0.69
3:P:187:PRO:HG2	12:P:501:HEM:HMC3	1.72	0.69
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.91	0.69
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.69
3:P:17:ASN:HD21	7:T:1:GLY:HA3	1.57	0.69
1:A:288:LYS:HE3	1:A:289:HIS:NE2	2.07	0.69
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.74	0.69
3:P:207:ASN:ND2	3:P:208:ASN:N	2.40	0.69
2:O:33:LEU:HD21	2:O:220:ALA:HB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.58	0.69
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.73	0.69
2:B:24:LEU:HD12	2:B:37:SER:O	1.92	0.69
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.73	0.69
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.75	0.68
1:A:10:ASN:HD21	2:B:19:PRO:HD3	1.56	0.68
2:B:31:ASN:HD22	2:B:32:GLY:H	1.39	0.68
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.08	0.68
1:A:45:SER:HA	1:A:48:GLU:HG3	1.74	0.68
1:A:281:ASP:HB3	1:A:284:PHE:CE1	2.29	0.68
9:I:31:UNK:C	9:I:73:PRO:HG2	2.23	0.68
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.28	0.68
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.75	0.68
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.75	0.68
5:R:91:TRP:CE3	5:R:96:LEU:HD22	2.28	0.68
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.20	0.68
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	1.94	0.68
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.23	0.68
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.29	0.68
1:A:373:THR:HB	1:A:374:PRO:HD3	1.75	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.58	0.68
1:A:350:THR:OG1	1:A:353:GLU:HG3	1.93	0.67
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.20	0.67
5:E:40:THR:HG21	15:E:2005:PEE:O2P	1.94	0.67
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.59	0.67
2:O:192:HIS:O	2:O:196:GLN:HG3	1.94	0.67
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.10	0.67
2:B:295:LEU:HA	2:B:343:GLN:HG2	1.76	0.67
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.60	0.67
3:P:226:SER:O	3:P:230:ILE:HG12	1.95	0.67
3:P:271:PRO:HA	13:P:3001:SMA:H10	1.75	0.67
2:O:47:ILE:CG1	2:O:120:MET:HE1	2.16	0.67
3:P:247:SER:OG	3:P:250:LEU:HB2	1.95	0.67
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.77	0.67
2:O:217:LYS:O	2:O:221:GLU:HG2	1.95	0.67
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.67
3:P:4:ASN:HD21	3:P:7:LYS:NZ	1.92	0.67
2:O:227:ARG:HH11	2:O:227:ARG:HA	1.59	0.67
6:S:11:ARG:HG2	6:S:11:ARG:O	1.95	0.67
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.76	0.66
2:O:274:VAL:O	2:O:278:VAL:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.78	0.66
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.28	0.66
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.59	0.66
1:N:30:SER:O	1:N:202:GLY:HA2	1.95	0.66
3:C:187:PRO:HG2	12:C:501:HEM:HMC3	1.78	0.66
8:H:34:ARG:O	8:H:38:GLU:HG2	1.96	0.66
1:N:432:LEU:HD23	1:N:433:ASP:N	2.11	0.66
8:H:27:THR:O	8:H:31:VAL:HG23	1.95	0.66
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.31	0.66
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.76	0.66
2:B:199:PHE:O	2:B:226:ILE:HG12	1.95	0.66
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.60	0.66
3:P:345:GLU:O	3:P:348:PHE:HB2	1.95	0.66
9:V:64:LEU:HA	9:V:77:ARG:O	1.96	0.66
2:B:43:PRO:O	2:B:113:ARG:HG3	1.96	0.65
3:C:202:HIS:NE2	14:C:2002:UQ:O4	2.29	0.65
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.78	0.65
3:P:157:ILE:HG13	3:P:158:GLY:N	2.01	0.65
3:P:216:SER:HB3	6:S:59:MET:HE2	1.77	0.65
15:P:3007:PEE:H7	7:T:44:GLN:HE21	1.60	0.65
8:H:32:LYS:O	8:H:36:ARG:HG3	1.96	0.65
2:O:95:SER:HB3	9:V:28:UNK:H2	1.61	0.65
1:N:136:GLN:NE2	9:V:50:LEU:HD12	2.10	0.65
2:O:95:SER:HB3	9:V:28:UNK:N	2.11	0.65
2:B:229:GLY:O	2:B:231:GLY:N	2.28	0.65
3:C:207:ASN:ND2	3:C:208:ASN:N	2.45	0.65
2:O:124:LEU:HD13	2:O:224:LEU:HD23	1.79	0.65
1:A:156:THR:O	1:A:159:GLN:HG2	1.97	0.65
2:B:361:LYS:O	2:B:365:LYS:HG3	1.96	0.65
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.61	0.65
2:O:250:HIS:HE1	2:O:252:LEU:HB2	1.61	0.65
3:P:347:PRO:O	3:P:351:ILE:HG13	1.97	0.65
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.79	0.64
3:C:285:ILE:HD12	3:C:285:ILE:N	2.10	0.64
4:D:200:GLN:HE21	20:E:2009:PLC:H51	1.62	0.64
2:O:357:VAL:O	2:O:361:LYS:HG3	1.97	0.64
2:B:307:PHE:H	9:I:52:ARG:HG2	1.61	0.64
5:E:83:GLU:HA	5:E:100:HIS:CG	2.32	0.64
4:Q:200:GLN:HE21	20:R:3009:PLC:H51	1.62	0.64
1:A:288:LYS:HE3	1:A:289:HIS:HE2	1.62	0.64
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:LEU:O	8:H:21:ARG:HG3	1.97	0.64
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.62	0.64
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.13	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.12	0.64
1:N:180:ALA:O	1:N:183:ALA:HB3	1.98	0.64
2:B:113:ARG:O	2:B:116:VAL:HG23	1.98	0.64
3:C:282:LEU:HD23	3:C:282:LEU:C	2.22	0.64
5:E:52:LYS:C	5:E:52:LYS:HD3	2.22	0.64
2:O:24:LEU:HD12	2:O:37:SER:O	1.97	0.64
1:N:45:SER:HA	1:N:48:GLU:HG3	1.79	0.64
1:N:288:LYS:HE3	1:N:289:HIS:NE2	2.13	0.64
1:N:351:GLU:O	1:N:354:VAL:HG22	1.98	0.64
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.78	0.64
2:B:409:ASP:HA	2:B:412:ASN:HD22	1.63	0.64
3:C:226:SER:O	3:C:230:ILE:HG12	1.98	0.64
6:S:32:MET:HE3	6:S:87:LYS:N	2.01	0.64
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.98	0.64
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.79	0.64
2:B:357:VAL:O	2:B:361:LYS:HG3	1.98	0.64
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.33	0.64
2:O:409:ASP:HA	2:O:412:ASN:HD22	1.63	0.64
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.32	0.64
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.13	0.64
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.64	0.63
2:B:124:LEU:CD2	2:B:223:PHE:HB3	2.27	0.63
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.13	0.63
2:O:222:GLN:O	2:O:223:PHE:HD2	1.79	0.63
3:P:146:VAL:HG21	13:P:3001:SMA:H6	1.79	0.63
3:P:355:ALA:O	3:P:358:SER:HB3	1.98	0.63
2:B:370:MET:O	2:B:373:GLU:HG3	1.97	0.63
1:N:87:ASN:OD1	2:O:286:LYS:HD2	1.99	0.63
1:A:182:LEU:O	1:A:186:ILE:HG13	1.97	0.63
3:C:243:LEU:HD21	3:C:251:LEU:HD11	1.79	0.63
3:C:247:SER:OG	3:C:250:LEU:HB2	1.97	0.63
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.62	0.63
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.28	0.63
1:A:4:TYR:HA	2:B:113:ARG:HD3	1.81	0.63
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.33	0.63
2:O:325:TYR:HD1	9:V:60:ALA:HB2	1.64	0.63
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.13	0.63
5:R:83:GLU:HA	5:R:100:HIS:CG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:3009:PLC:H1'1	20:R:3009:PLC:H1A1	1.79	0.63
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.79	0.63
3:C:90:PHE:HB3	3:C:236:MET:CE	2.26	0.63
3:C:346:HIS:ND1	3:C:347:PRO:HA	2.14	0.63
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.32	0.63
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.81	0.63
15:C:2007:PEE:H7	7:G:44:GLN:HE21	1.64	0.63
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.13	0.63
5:E:41:ALA:O	5:E:45:VAL:HG23	1.99	0.63
1:N:136:GLN:HG2	9:V:51:CYS:HB3	1.81	0.63
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.29	0.63
1:A:371:GLY:O	1:A:375:VAL:HG23	1.99	0.62
2:B:250:HIS:HE1	2:B:252:LEU:HB2	1.64	0.62
2:O:226:ILE:CG2	2:O:227:ARG:N	2.62	0.62
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.80	0.62
7:G:81:GLN:O	8:H:47:ARG:HA	2.00	0.62
1:N:126:GLN:NE2	1:N:129:LYS:HD3	2.15	0.62
1:N:49:ASN:C	1:N:49:ASN:ND2	2.50	0.62
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.63	0.62
2:B:229:GLY:C	2:B:231:GLY:H	2.07	0.62
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.35	0.62
1:N:103:SER:HB3	1:N:202:GLY:O	1.99	0.62
3:P:207:ASN:HD22	3:P:208:ASN:H	1.45	0.62
3:C:354:MET:HE2	3:C:354:MET:HA	1.81	0.62
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.34	0.62
6:F:53:ASP:OD1	6:F:54:LEU:N	2.31	0.62
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.82	0.62
2:B:26:ILE:HG12	2:B:26:ILE:O	1.98	0.62
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.81	0.62
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.83	0.62
7:G:40:ARG:HD2	18:G:2004:CDL:OA4	1.99	0.62
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.29	0.62
1:A:30:SER:O	1:A:202:GLY:HA2	2.00	0.62
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.35	0.62
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.81	0.62
2:O:26:ILE:O	2:O:26:ILE:HG12	1.99	0.62
2:B:150:VAL:HG23	2:B:151:ALA:N	2.15	0.62
2:B:274:VAL:O	2:B:278:VAL:HG23	2.00	0.62
3:C:173:ASN:N	3:C:174:PRO:HD2	2.15	0.62
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.82	0.62
6:S:52:GLU:CG	6:S:56:ASN:HD21	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:ILE:O	7:T:34:LEU:HG	2.00	0.62
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.00	0.62
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.81	0.61
1:A:103:SER:HB3	1:A:202:GLY:O	2.00	0.61
6:F:18:LYS:O	6:F:22:ASN:ND2	2.32	0.61
2:B:86:THR:O	2:B:90:GLU:HG3	2.00	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.97	0.61
1:N:82:MET:HE3	1:N:105:ASP:OD2	2.00	0.61
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.35	0.61
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.31	0.61
2:O:47:ILE:HG12	2:O:120:MET:CE	2.18	0.61
2:O:199:PHE:O	2:O:226:ILE:HG21	2.00	0.61
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.82	0.61
6:S:10:GLY:C	6:S:12:LEU:H	2.08	0.61
4:D:47:ALA:H	4:D:50:ASN:ND2	1.91	0.61
7:G:74:PRO:O	7:G:78:GLU:HG3	2.01	0.61
2:O:221:GLU:O	2:O:223:PHE:N	2.33	0.61
3:P:76:TYR:HE2	4:Q:204:MET:HE1	1.66	0.61
2:B:306:PRO:HA	9:I:52:ARG:CG	2.31	0.61
8:U:17:LEU:O	8:U:21:ARG:HG3	2.01	0.61
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.82	0.61
2:B:28:LYS:O	2:B:29:LEU:O	2.19	0.61
1:N:279:ARG:NH2	9:V:31:UNK:O	2.33	0.61
2:O:227:ARG:NH1	2:O:228:SER:H	1.98	0.61
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.82	0.60
2:O:259:THR:HG22	2:O:260:GLU:N	2.16	0.60
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.35	0.60
5:R:52:LYS:C	5:R:52:LYS:HD3	2.26	0.60
1:A:76:GLU:HG2	2:B:285:ILE:HD12	1.82	0.60
20:E:2009:PLC:H1A1	20:E:2009:PLC:H1'1	1.83	0.60
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.36	0.60
10:W:52:TRP:O	10:W:56:LYS:HB2	2.01	0.60
2:B:409:ASP:O	2:B:412:ASN:HB2	2.01	0.60
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.82	0.60
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.31	0.60
3:P:90:PHE:HB3	3:P:236:MET:CE	2.31	0.60
1:A:159:GLN:HE22	7:G:18:LEU:HD21	1.64	0.60
1:N:76:GLU:HG2	2:O:285:ILE:HD12	1.81	0.60
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.83	0.60
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.32	0.60
2:B:230:ALA:O	2:B:231:GLY:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.16	0.60
2:O:27:THR:HG22	2:O:28:LYS:N	2.17	0.60
5:R:102:THR:O	5:R:106:ILE:HG13	2.02	0.60
2:B:259:THR:HG22	2:B:260:GLU:N	2.17	0.60
9:I:65:VAL:HB	9:I:77:ARG:HD2	1.83	0.60
5:R:40:THR:HG21	15:R:3005:PEE:O2P	2.01	0.60
8:U:13:LEU:HD23	8:U:13:LEU:H	1.66	0.60
1:A:90:THR:O	1:A:167:VAL:HG11	2.02	0.60
4:Q:224:ARG:HE	7:T:26:ILE:HG12	1.67	0.60
8:U:34:ARG:O	8:U:38:GLU:HG2	2.01	0.60
2:O:409:ASP:O	2:O:412:ASN:HB2	2.02	0.60
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.84	0.60
8:U:52:GLU:HG2	8:U:53:GLN:N	2.14	0.60
2:B:227:ARG:CD	2:B:228:SER:H	2.15	0.60
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.20	0.60
3:C:347:PRO:O	3:C:351:ILE:HG13	2.02	0.60
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.31	0.60
7:T:41:PHE:C	7:T:41:PHE:CD2	2.80	0.60
2:O:287:ARG:HD3	9:V:53:GLU:CG	2.32	0.59
2:B:56:ARG:HA	2:B:171:ALA:O	2.02	0.59
3:C:377:MET:HE1	6:F:19:TRP:HZ3	1.67	0.59
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.66	0.59
1:A:272:VAL:O	1:A:275:ALA:HB3	2.02	0.59
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.84	0.59
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.84	0.59
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.17	0.59
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.85	0.59
1:N:105:ASP:O	1:N:109:VAL:HG23	2.02	0.59
3:P:285:ILE:HD12	3:P:285:ILE:H	1.66	0.59
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.85	0.59
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.31	0.59
5:E:108:GLN:O	5:E:112:VAL:HG23	2.02	0.59
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.36	0.59
7:T:29:ILE:O	7:T:33:ALA:HB3	2.02	0.59
9:I:71:ASN:ND2	9:I:71:ASN:N	2.45	0.59
1:N:432:LEU:HD23	1:N:433:ASP:H	1.67	0.59
7:T:73:ASN:HB3	7:T:76:ASP:OD2	2.02	0.59
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.18	0.59
2:O:150:VAL:HG23	2:O:151:ALA:N	2.18	0.58
9:I:71:ASN:HD22	9:I:71:ASN:N	1.90	0.58
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:13:MET:CA	6:S:16:ILE:HB	2.28	0.58
2:B:292:THR:O	2:B:292:THR:HG22	2.03	0.58
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.85	0.58
2:B:47:ILE:HD12	2:B:47:ILE:N	2.17	0.58
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.39	0.58
2:O:113:ARG:O	2:O:116:VAL:HG23	2.02	0.58
3:C:90:PHE:CB	3:C:236:MET:HE3	2.31	0.58
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.02	0.58
1:N:371:GLY:O	1:N:375:VAL:HG23	2.02	0.58
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.03	0.58
6:S:32:MET:CE	6:S:87:LYS:HG2	2.33	0.58
1:A:380:GLY:O	1:A:384:LEU:HB2	2.04	0.58
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.39	0.58
5:E:90:LYS:HD3	3:P:263:LEU:HD11	1.84	0.58
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.86	0.58
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.58
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.83	0.58
2:B:279:LEU:HD13	2:B:344:LEU:HD11	1.86	0.58
3:C:146:VAL:HG21	13:C:2001:SMA:H6	1.85	0.58
5:E:102:THR:O	5:E:106:ILE:HG13	2.03	0.58
5:E:103:GLN:HA	5:E:106:ILE:HD12	1.86	0.58
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.58
2:O:292:THR:O	2:O:292:THR:HG22	2.04	0.58
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.22	0.58
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.17	0.58
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.38	0.58
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.04	0.58
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.38	0.58
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.33	0.58
2:O:385:GLU:CD	2:O:392:HIS:HA	2.29	0.58
3:P:90:PHE:CB	3:P:236:MET:HE3	2.31	0.58
4:Q:28:ARG:HD2	4:Q:185:ASP:OD2	2.04	0.58
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.34	0.58
2:B:31:ASN:ND2	2:B:33:LEU:H	2.00	0.58
8:H:18:THR:O	8:H:22:GLU:HG3	2.04	0.58
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.84	0.58
4:D:88:SER:HB2	5:E:69:LEU:HD22	1.85	0.57
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.39	0.57
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.84	0.57
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.85	0.57
3:C:269:ILE:HG23	3:C:269:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.04	0.57
2:O:370:MET:O	2:O:373:GLU:HG3	2.04	0.57
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.18	0.57
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.69	0.57
5:E:109:GLU:CG	5:E:167:ALA:HB3	2.34	0.57
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.39	0.57
5:R:51:ALA:HA	15:R:3005:PEE:H42	1.86	0.57
1:A:156:THR:HA	5:E:7:VAL:HG21	1.86	0.57
2:O:95:SER:CB	9:V:28:UNK:H2	2.17	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.86	0.57
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.52	0.57
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.03	0.57
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.69	0.57
1:A:106:MET:HE2	1:A:106:MET:C	2.29	0.57
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.05	0.57
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.19	0.57
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.86	0.57
2:O:250:HIS:CE1	2:O:252:LEU:HB2	2.39	0.57
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.35	0.57
2:B:144:LEU:HB3	2:B:183:ILE:HD12	1.86	0.57
2:B:402:ILE:O	2:B:405:VAL:HG23	2.05	0.57
10:J:52:TRP:O	10:J:56:LYS:HB2	2.05	0.57
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.05	0.57
1:N:35:CYS:HA	1:N:372:THR:HG21	1.87	0.57
1:A:388:ARG:HG3	1:A:388:ARG:NH2	2.20	0.57
2:B:385:GLU:CD	2:B:392:HIS:HA	2.29	0.57
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.40	0.57
1:A:233:ARG:CG	1:A:233:ARG:HH11	2.17	0.57
2:B:144:LEU:HB2	2:B:183:ILE:HG23	1.87	0.57
1:N:156:THR:HA	5:R:7:VAL:HG21	1.86	0.57
3:P:243:LEU:HD21	3:P:251:LEU:HD11	1.86	0.57
3:P:76:TYR:CE2	4:Q:204:MET:HE1	2.41	0.56
6:S:46:ALA:HB1	6:S:90:LEU:HD11	1.86	0.56
2:O:86:THR:O	2:O:90:GLU:HG3	2.05	0.56
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.16	0.56
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.87	0.56
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.40	0.56
8:U:65:ARG:O	8:U:68:CYS:HB3	2.04	0.56
1:A:130:GLU:O	1:A:134:ILE:HG13	2.05	0.56
1:A:343:MET:O	1:A:347:THR:HG23	2.06	0.56
5:E:73:LYS:HB3	5:E:195:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:MET:HB2	3:P:256:ASN:OD1	2.05	0.56
2:B:264:VAL:HG11	2:B:388:LEU:CD1	2.36	0.56
8:H:11:GLU:O	8:H:12:GLU:HB2	2.05	0.56
8:H:40:CYS:O	8:H:44:VAL:HG23	2.05	0.56
1:N:219:VAL:HG12	1:N:220:SER:H	1.71	0.56
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.29	0.56
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.40	0.56
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.86	0.56
3:C:15:ILE:N	3:C:15:ILE:HD12	2.20	0.56
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.04	0.56
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.86	0.56
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.88	0.56
2:B:212:LYS:HD2	2:B:214:SER:H	1.69	0.56
3:C:101:ARG:C	3:C:101:ARG:CD	2.78	0.56
6:F:77:LYS:CE	6:F:78:GLU:HG3	2.36	0.56
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.87	0.56
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.04	0.56
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.41	0.56
1:A:180:ALA:O	1:A:183:ALA:HB3	2.06	0.56
3:C:216:SER:HB3	6:F:59:MET:HE2	1.87	0.56
2:O:248:ASN:C	2:O:248:ASN:ND2	2.62	0.56
1:A:29:GLU:HG3	1:A:203:ILE:O	2.05	0.56
1:A:432:LEU:HD23	1:A:433:ASP:N	2.21	0.56
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.87	0.56
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.88	0.56
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.46	0.56
15:E:2005:PEE:H67	10:J:25:VAL:HG22	1.87	0.56
1:N:106:MET:HE2	1:N:106:MET:C	2.31	0.56
7:G:60:SER:HB3	7:G:64:GLN:NE2	2.21	0.56
3:C:101:ARG:NH2	12:C:502:HEM:HBD2	2.22	0.55
5:E:112:VAL:HG11	5:E:172:ARG:NH2	2.21	0.55
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.88	0.55
5:R:153:PHE:HD2	5:R:172:ARG:NH1	2.04	0.55
7:T:53:LEU:O	7:T:56:TYR:HB3	2.06	0.55
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.41	0.55
7:G:41:PHE:C	7:G:41:PHE:CD2	2.83	0.55
1:N:431:LEU:HG	1:N:432:LEU:N	2.22	0.55
1:A:233:ARG:HG3	1:A:233:ARG:NH1	2.20	0.55
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.70	0.55
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.21	0.55
7:G:24:ARG:NH2	7:G:28:ASN:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:33:ARG:O	10:J:37:GLN:HG3	2.06	0.55
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.42	0.55
5:R:112:VAL:HG11	5:R:172:ARG:NH2	2.21	0.55
9:V:28:UNK:CB	9:V:71:ASN:ND2	2.70	0.55
10:W:38:GLY:O	10:W:42:ILE:HG13	2.06	0.55
1:A:170:THR:HG22	1:A:171:THR:N	2.22	0.55
1:A:351:GLU:O	1:A:354:VAL:HG22	2.07	0.55
4:Q:94:PRO:HG2	4:Q:95:TYR:CD1	2.42	0.55
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.88	0.55
7:T:41:PHE:C	7:T:41:PHE:HD2	2.13	0.55
7:G:53:LEU:O	7:G:56:TYR:HB3	2.07	0.55
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.21	0.55
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.88	0.55
3:C:38:LEU:HB3	12:C:502:HEM:CMB	2.37	0.55
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.37	0.55
3:P:90:PHE:CZ	3:P:240:PHE:HA	2.42	0.55
3:P:101:ARG:C	3:P:101:ARG:CD	2.74	0.55
5:R:78:LEU:HD22	5:R:132:TRP:CD2	2.42	0.55
5:R:108:GLN:O	5:R:112:VAL:HG23	2.06	0.55
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.22	0.55
3:C:5:ILE:O	3:C:5:ILE:HG22	2.07	0.55
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.42	0.55
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.06	0.55
1:A:305:HIS:O	1:A:306:SER:HB3	2.07	0.55
2:B:252:LEU:CD1	9:I:49:LEU:HB2	2.36	0.55
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.07	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.42	0.55
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.72	0.54
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.72	0.54
5:E:195:VAL:HG12	5:E:196:GLY:N	2.22	0.54
2:O:47:ILE:HD12	2:O:47:ILE:N	2.22	0.54
2:O:70:ARG:HD3	2:O:100:SER:OG	2.06	0.54
3:P:5:ILE:O	3:P:5:ILE:HG22	2.06	0.54
1:A:49:ASN:C	1:A:49:ASN:ND2	2.53	0.54
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.42	0.54
3:C:111:LYS:HE2	3:C:307:PHE:CE1	2.42	0.54
1:N:130:GLU:O	1:N:134:ILE:HG13	2.08	0.54
5:R:47:THR:HG21	15:R:3005:PEE:H23	1.89	0.54
6:S:105:GLU:O	6:S:109:LYS:HG3	2.07	0.54
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.07	0.54
9:I:55:MET:O	9:I:56:SER:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:ILE:CG2	2:O:227:ARG:H	2.20	0.54
3:P:332:ASN:ND2	3:P:358:SER:OG	2.40	0.54
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.89	0.54
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.89	0.54
1:N:301:HIS:HB2	1:N:303:LEU:HG	1.90	0.54
3:C:207:ASN:HD22	3:C:208:ASN:H	1.53	0.54
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.88	0.54
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.43	0.54
1:N:223:TYR:H	1:N:223:TYR:HD2	1.56	0.54
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.38	0.54
3:P:90:PHE:CD2	3:P:236:MET:HE3	2.42	0.54
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.89	0.54
7:T:67:GLU:O	7:T:70:LYS:HB2	2.08	0.54
9:V:32:UNK:C	9:V:73:PRO:HG2	2.38	0.54
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.43	0.54
2:B:300:ALA:C	2:B:302:ALA:H	2.14	0.54
3:P:17:ASN:HD21	7:T:1:GLY:CA	2.20	0.54
2:B:59:THR:HG22	2:B:60:THR:N	2.23	0.54
2:B:250:HIS:CE1	2:B:252:LEU:HB2	2.41	0.54
2:B:287:ARG:HB3	9:I:53:GLU:CG	2.38	0.54
3:C:2:ALA:CB	3:C:8:SER:HB3	2.38	0.54
7:G:41:PHE:C	7:G:41:PHE:HD2	2.16	0.54
2:O:47:ILE:O	2:O:108:CYS:HB2	2.07	0.54
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.41	0.54
1:A:82:MET:HE3	1:A:105:ASP:OD2	2.08	0.54
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.38	0.54
2:B:58:GLU:OE1	2:B:64:GLY:N	2.37	0.54
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.23	0.54
3:C:271:PRO:HG2	3:C:279:TYR:CG	2.42	0.54
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.43	0.54
5:E:155:GLY:HA3	5:E:166:ASP:C	2.33	0.54
1:N:15:ASN:O	1:N:26:ALA:HA	2.07	0.54
2:O:162:ASN:O	2:O:244:ILE:HD12	2.08	0.54
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.41	0.54
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.37	0.54
4:D:94:PRO:HG2	4:D:95:TYR:CD1	2.43	0.53
1:N:10:ASN:HD21	2:O:18:CYS:HB3	1.73	0.53
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.89	0.53
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.77	0.53
5:R:69:LEU:HD12	5:R:71:LEU:HG	1.90	0.53
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:THR:HG22	1:N:171:THR:N	2.23	0.53
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.89	0.53
6:S:18:LYS:O	6:S:22:ASN:ND2	2.42	0.53
2:B:47:ILE:HG22	2:B:48:GLY:N	2.23	0.53
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.53
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.53
7:T:77:TYR:C	7:T:79:ASN:H	2.16	0.53
2:B:47:ILE:O	2:B:108:CYS:HB2	2.08	0.53
4:D:150:ASN:O	4:D:156:GLN:HA	2.08	0.53
6:F:46:ALA:CB	6:F:90:LEU:HD11	2.39	0.53
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.73	0.53
1:A:223:TYR:H	1:A:223:TYR:HD2	1.57	0.53
3:C:285:ILE:HD12	3:C:285:ILE:H	1.71	0.53
2:O:47:ILE:HG22	2:O:48:GLY:N	2.24	0.53
3:P:4:ASN:HD21	3:P:7:LYS:CE	2.21	0.53
3:P:38:LEU:HB3	12:P:502:HEM:CMB	2.38	0.53
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.90	0.53
4:D:86:LYS:NZ	5:E:71:LEU:HD13	2.24	0.53
4:D:164:ILE:O	4:D:179:MET:HE2	2.09	0.53
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.91	0.53
1:N:260:PRO:HG2	1:N:261:GLY:H	1.73	0.53
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.91	0.53
1:A:364:ALA:O	1:A:368:GLN:HG2	2.09	0.53
2:B:102:ARG:NH1	2:B:164:HIS:CD2	2.76	0.53
2:B:167:ALA:HB1	2:B:321:LEU:HD21	1.91	0.53
2:B:280:GLY:HA3	2:B:293:SER:OG	2.08	0.53
5:E:100:HIS:HB2	5:E:132:TRP:CZ3	2.43	0.53
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.44	0.53
2:O:279:LEU:HD13	2:O:344:LEU:HD11	1.90	0.53
5:R:135:LEU:CD2	5:R:169:GLY:HA3	2.39	0.53
7:T:60:SER:HB3	7:T:64:GLN:NE2	2.24	0.53
3:C:90:PHE:CZ	3:C:240:PHE:HA	2.44	0.53
5:E:78:LEU:HD22	5:E:132:TRP:CD2	2.44	0.53
2:O:318:ASP:O	2:O:319:SER:HB2	2.08	0.53
3:P:354:MET:HE2	3:P:354:MET:HA	1.90	0.53
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.90	0.53
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.53
2:B:156:GLN:NE2	9:I:77:ARG:C	2.67	0.53
3:C:76:TYR:CE2	4:D:204:MET:HE1	2.44	0.53
3:C:345:GLU:O	3:C:348:PHE:HB2	2.09	0.53
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:80:GLU:OE2	2:O:291:VAL:HG23	2.09	0.53
1:N:219:VAL:HG12	1:N:220:SER:N	2.24	0.53
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.73	0.53
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.25	0.53
2:B:67:HIS:O	2:B:70:ARG:HB3	2.09	0.53
5:E:150:SER:OG	5:E:157:TYR:HB3	2.08	0.53
2:O:222:GLN:O	2:O:222:GLN:HG2	2.08	0.53
3:P:282:LEU:HD23	3:P:282:LEU:C	2.33	0.53
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.90	0.53
3:P:30:ALA:HB1	18:S:3003:CDL:H111	1.92	0.52
5:R:195:VAL:HG12	5:R:196:GLY:N	2.24	0.52
1:A:289:HIS:O	2:B:87:ARG:NE	2.35	0.52
3:C:4:ASN:HD21	3:C:7:LYS:CE	2.22	0.52
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.08	0.52
3:C:263:LEU:HD11	5:R:90:LYS:HD3	1.91	0.52
2:O:227:ARG:NH1	2:O:228:SER:N	2.57	0.52
3:P:271:PRO:HG2	3:P:279:TYR:CG	2.44	0.52
8:U:47:ARG:HG2	8:U:47:ARG:HH11	1.74	0.52
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.40	0.52
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.43	0.52
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.39	0.52
3:P:31:TRP:O	3:P:101:ARG:HG3	2.09	0.52
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.40	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.75	0.52
1:A:431:LEU:HG	1:A:432:LEU:N	2.23	0.52
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.89	0.52
1:N:49:ASN:ND2	1:N:51:LYS:N	2.57	0.52
1:N:181:ASP:OD1	1:N:181:ASP:N	2.43	0.52
2:O:168:TYR:CD2	2:O:237:ALA:HB1	2.44	0.52
2:O:217:LYS:HE2	2:O:221:GLU:OE1	2.10	0.52
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.25	0.52
3:P:101:ARG:HD2	3:P:101:ARG:O	2.08	0.52
9:V:77:ARG:HD2	9:V:77:ARG:N	2.24	0.52
10:J:38:GLY:O	10:J:42:ILE:HG13	2.09	0.52
2:O:56:ARG:HA	2:O:171:ALA:O	2.10	0.52
3:P:9:HIS:CE1	3:P:11:LEU:HB2	2.43	0.52
18:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.09	0.52
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.91	0.52
2:O:29:LEU:CD1	2:O:33:LEU:HD23	2.39	0.52
2:O:116:VAL:HG12	2:O:120:MET:HE2	1.92	0.52
5:R:100:HIS:HB2	5:R:132:TRP:CZ3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:ND2	1:A:52:ASN:OD1	2.42	0.52
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.45	0.52
1:A:301:HIS:HB2	1:A:303:LEU:HG	1.91	0.52
3:P:15:ILE:N	3:P:15:ILE:HD12	2.25	0.52
3:P:42:LEU:HD22	3:P:190:ILE:HG22	1.91	0.52
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.21	0.52
2:B:389:SER:O	2:B:391:THR:N	2.43	0.52
7:G:67:GLU:O	7:G:70:LYS:HB2	2.10	0.52
1:N:161:THR:HG21	1:N:235:ARG:H	1.74	0.52
2:O:300:ALA:C	2:O:302:ALA:H	2.18	0.52
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.74	0.52
1:A:394:GLU:O	1:A:397:SER:HB3	2.10	0.52
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.91	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.52
10:W:33:ARG:O	10:W:37:GLN:HG3	2.08	0.52
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.91	0.52
2:B:217:LYS:HE2	2:B:221:GLU:OE1	2.10	0.52
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.92	0.52
4:D:178:THR:HG23	8:H:13:LEU:HD11	1.92	0.52
1:N:380:GLY:O	1:N:384:LEU:HB2	2.09	0.52
3:P:187:PRO:HG2	12:P:501:HEM:CMC	2.39	0.52
5:R:114:VAL:O	5:R:114:VAL:HG12	2.10	0.52
6:S:53:ASP:OD1	6:S:54:LEU:N	2.39	0.52
1:A:190:PHE:C	1:A:195:MET:HE2	2.35	0.51
2:B:162:ASN:O	2:B:244:ILE:HD12	2.10	0.51
2:B:318:ASP:O	2:B:319:SER:HB2	2.10	0.51
6:F:46:ALA:HB1	6:F:90:LEU:HD11	1.91	0.51
1:N:136:GLN:HE22	9:V:50:LEU:CD1	2.19	0.51
8:U:20:ILE:HD11	8:U:76:LYS:CD	2.38	0.51
2:B:26:ILE:HA	2:B:35:ILE:O	2.11	0.51
3:C:76:TYR:HE2	4:D:204:MET:HE1	1.74	0.51
3:C:271:PRO:HA	13:C:2001:SMA:H10	1.93	0.51
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.92	0.51
4:D:158:ILE:HG12	4:D:160:MET:H	1.74	0.51
2:O:203:ARG:HD2	2:O:230:ALA:HA	1.92	0.51
2:O:219:VAL:HG13	2:O:223:PHE:CD1	2.45	0.51
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.92	0.51
5:R:45:VAL:HG13	10:W:28:ALA:N	2.24	0.51
3:C:198:LEU:HD13	14:C:2002:UQ:HM52	1.92	0.51
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.92	0.51
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:305:HIS:O	1:N:306:SER:HB3	2.10	0.51
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.09	0.51
2:O:59:THR:HG22	2:O:60:THR:N	2.25	0.51
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.41	0.51
2:O:306:PRO:HG2	9:V:51:CYS:HA	1.92	0.51
10:J:4:ALA:O	10:J:8:GLN:HG3	2.11	0.51
2:O:102:ARG:HH11	2:O:102:ARG:CG	2.15	0.51
2:O:297:GLN:O	2:O:301:LYS:HG3	2.09	0.51
2:O:226:ILE:HG22	2:O:227:ARG:H	1.74	0.51
2:O:306:PRO:HB3	9:V:52:ARG:N	2.25	0.51
3:P:131:GLY:HA3	3:P:183:HIS:CE1	2.45	0.51
3:P:154:ILE:HG21	3:P:157:ILE:HD11	1.93	0.51
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.11	0.51
10:W:42:ILE:O	10:W:46:LEU:HG	2.10	0.51
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.41	0.51
1:N:262:TRP:O	1:N:386:TYR:HE1	1.93	0.51
3:P:285:ILE:N	3:P:285:ILE:CD1	2.74	0.51
1:A:181:ASP:OD1	1:A:181:ASP:N	2.44	0.51
1:A:260:PRO:HG2	1:A:261:GLY:H	1.75	0.51
1:A:285:GLY:O	1:A:286:GLY:C	2.54	0.51
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.40	0.51
8:H:65:ARG:O	8:H:68:CYS:HB3	2.11	0.51
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.40	0.51
7:T:56:TYR:O	7:T:59:TYR:HB3	2.10	0.51
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.92	0.51
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.46	0.51
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.11	0.51
5:E:51:ALA:HA	15:E:2005:PEE:H42	1.93	0.51
3:P:173:ASN:N	3:P:174:PRO:HD2	2.25	0.51
5:R:155:GLY:HA3	5:R:166:ASP:C	2.36	0.51
7:T:74:PRO:O	7:T:78:GLU:HG3	2.11	0.51
1:A:10:ASN:ND2	2:B:19:PRO:HD3	2.23	0.51
1:A:86:PHE:HD1	1:A:87:ASN:H	1.58	0.51
1:A:178:THR:HG22	1:A:180:ALA:N	2.19	0.51
1:A:179:ARG:HG2	1:A:179:ARG:HH11	1.75	0.51
2:B:109:VAL:HG21	2:B:119:VAL:HG23	1.93	0.51
2:B:192:HIS:O	2:B:196:GLN:HG3	2.10	0.51
9:I:49:LEU:HB3	9:I:55:MET:HG2	1.93	0.51
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.92	0.51
1:N:159:GLN:HE22	7:T:18:LEU:HD21	1.76	0.51
3:P:223:PRO:O	3:P:227:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.93	0.51
1:A:410:VAL:O	1:A:413:LYS:HB3	2.11	0.50
2:B:306:PRO:HB3	9:I:52:ARG:N	2.26	0.50
2:B:308:ASP:OD1	9:I:56:SER:HA	2.11	0.50
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.93	0.50
5:R:41:ALA:O	5:R:45:VAL:HG23	2.10	0.50
5:R:103:GLN:HA	5:R:106:ILE:HB	1.92	0.50
1:A:432:LEU:HD23	1:A:433:ASP:H	1.76	0.50
1:N:63:ALA:HB1	1:N:116:VAL:CG1	2.41	0.50
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.94	0.50
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.46	0.50
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.90	0.50
5:R:90:LYS:O	5:R:91:TRP:HB2	2.11	0.50
1:A:8:LEU:HD22	1:A:392:LEU:HB2	1.92	0.50
2:B:325:TYR:HD1	9:I:60:ALA:CB	2.22	0.50
8:H:24:CYS:O	8:H:27:THR:HB	2.11	0.50
2:O:67:HIS:O	2:O:70:ARG:HB3	2.12	0.50
3:P:145:THR:O	3:P:149:ASN:HB2	2.12	0.50
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.11	0.50
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.40	0.50
3:C:246:PHE:C	3:C:248:PRO:HD3	2.36	0.50
1:N:179:ARG:HH11	1:N:179:ARG:HG2	1.75	0.50
1:A:45:SER:HA	1:A:48:GLU:CG	2.40	0.50
1:A:49:ASN:ND2	1:A:51:LYS:H	2.09	0.50
1:A:386:TYR:CD2	1:A:390:ILE:HD12	2.46	0.50
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.47	0.50
2:B:116:VAL:O	2:B:120:MET:HB2	2.11	0.50
2:B:394:ALA:C	2:B:396:SER:H	2.20	0.50
2:B:414:ALA:O	2:B:418:VAL:HG23	2.11	0.50
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.46	0.50
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.93	0.50
2:O:26:ILE:HA	2:O:35:ILE:O	2.10	0.50
1:A:308:GLN:O	1:A:308:GLN:HG3	2.11	0.50
3:C:38:LEU:HB3	12:C:502:HEM:HMB1	1.94	0.50
6:F:71:LYS:O	6:F:72:HIS:HB2	2.10	0.50
9:I:38:UNK:C	9:I:40:UNK:N	2.72	0.50
1:N:388:ARG:HG3	1:N:388:ARG:NH2	2.26	0.50
2:O:221:GLU:C	2:O:223:PHE:H	2.20	0.50
2:B:212:LYS:CD	2:B:214:SER:H	2.24	0.50
4:D:224:ARG:HH21	7:G:26:ILE:HG23	1.77	0.50
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:285:ILE:H	3:P:285:ILE:CD1	2.25	0.50
6:S:71:LYS:O	6:S:72:HIS:HB2	2.12	0.50
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.92	0.50
5:E:103:GLN:HA	5:E:106:ILE:HB	1.94	0.50
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.45	0.50
7:G:73:ASN:HB3	7:G:76:ASP:OD2	2.11	0.50
1:N:156:THR:O	1:N:159:GLN:HG2	2.12	0.50
2:O:227:ARG:HG3	2:O:228:SER:H	1.76	0.50
3:P:135:PRO:HG3	12:P:501:HEM:O1D	2.12	0.50
6:S:46:ALA:CB	6:S:90:LEU:HD11	2.41	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.50
8:U:24:CYS:O	8:U:27:THR:HB	2.12	0.50
2:B:153:GLN:HE22	9:I:34:UNK:CB	2.24	0.50
2:B:297:GLN:O	2:B:301:LYS:HG3	2.12	0.50
2:O:402:ILE:O	2:O:405:VAL:HG23	2.10	0.50
3:P:38:LEU:HB3	12:P:502:HEM:HMB1	1.94	0.50
3:P:101:ARG:NH2	12:P:502:HEM:HBD2	2.26	0.50
8:U:12:GLU:N	21:U:1233:HOH:O	2.45	0.50
8:U:52:GLU:CG	8:U:53:GLN:N	2.75	0.50
2:B:212:LYS:HD3	2:B:212:LYS:C	2.37	0.49
2:B:257:VAL:O	2:B:323:GLY:HA3	2.12	0.49
2:B:308:ASP:CG	9:I:56:SER:HA	2.37	0.49
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.11	0.49
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.20	0.49
10:J:42:ILE:O	10:J:46:LEU:HG	2.12	0.49
2:O:144:LEU:HB3	2:O:183:ILE:HD12	1.93	0.49
3:P:70:THR:HA	3:P:74:VAL:HG23	1.93	0.49
10:W:40:ASP:O	10:W:44:GLU:HG3	2.12	0.49
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.47	0.49
3:C:42:LEU:HD22	3:C:190:ILE:HG22	1.93	0.49
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.47	0.49
1:N:112:LEU:O	1:N:116:VAL:HG23	2.12	0.49
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.39	0.49
14:P:3002:UQ:HM51	14:P:3002:UQ:C8	2.41	0.49
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.94	0.49
2:B:248:ASN:C	2:B:248:ASN:ND2	2.60	0.49
1:N:152:TYR:HA	1:N:155:ALA:HB3	1.94	0.49
2:O:227:ARG:HG3	2:O:228:SER:N	2.27	0.49
2:O:341:MET:HG3	2:O:439:LEU:HB3	1.94	0.49
2:B:394:ALA:C	2:B:396:SER:N	2.70	0.49
2:O:381:GLU:OE1	2:O:381:GLU:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:158:GLY:O	3:P:161:LEU:N	2.41	0.49
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.26	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.52	0.49
2:B:116:VAL:HG12	2:B:120:MET:HE2	1.95	0.49
3:C:9:HIS:CE1	3:C:11:LEU:HB2	2.47	0.49
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.47	0.49
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.94	0.49
1:A:233:ARG:CG	1:A:233:ARG:NH1	2.74	0.49
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.93	0.49
1:N:178:THR:HG22	1:N:180:ALA:N	2.19	0.49
1:N:329:LEU:HA	1:N:430:GLN:NE2	2.27	0.49
2:O:159:VAL:HG23	2:O:160:LEU:N	2.27	0.49
3:P:2:ALA:HA	3:P:3:PRO:C	2.37	0.49
6:S:12:LEU:O	6:S:15:ARG:HG2	2.13	0.49
2:B:95:SER:HA	9:I:71:ASN:OD1	2.11	0.49
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.42	0.49
2:O:124:LEU:HD22	2:O:223:PHE:HB3	1.95	0.49
2:O:283:PRO:CG	9:V:56:SER:HB2	2.43	0.49
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.94	0.49
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.43	0.49
3:C:332:ASN:HD21	3:C:359:TYR:N	2.10	0.49
7:G:56:TYR:O	7:G:59:TYR:HB3	2.13	0.49
1:N:49:ASN:ND2	1:N:52:ASN:OD1	2.46	0.49
10:W:49:GLY:N	10:W:54:HIS:ND1	2.60	0.49
2:B:212:LYS:HD3	2:B:213:HIS:H	1.77	0.49
3:C:243:LEU:HD21	3:C:251:LEU:CD1	2.42	0.49
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.47	0.49
5:R:77:LYS:C	5:R:79:SER:H	2.21	0.49
8:U:25:GLU:HG2	8:U:61:PHE:HZ	1.78	0.49
8:U:40:CYS:O	8:U:44:VAL:HG23	2.12	0.49
4:D:14:HIS:O	4:D:202:LYS:NZ	2.46	0.49
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.48	0.49
2:O:166:ALA:HB1	2:O:242:GLY:C	2.38	0.49
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.94	0.48
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.27	0.48
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.94	0.48
2:O:389:SER:O	2:O:391:THR:N	2.46	0.48
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.48	0.48
5:R:77:LYS:HB3	5:R:80:ASP:OD2	2.13	0.48
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.27	0.48
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:TYR:CD2	2:B:237:ALA:HB1	2.48	0.48
2:B:248:ASN:HD22	2:B:249:GLY:N	2.11	0.48
2:B:291:VAL:C	2:B:293:SER:H	2.21	0.48
1:N:86:PHE:HD1	1:N:87:ASN:H	1.62	0.48
1:N:394:GLU:O	1:N:397:SER:HB3	2.13	0.48
2:O:230:ALA:O	2:O:231:GLY:C	2.55	0.48
2:O:394:ALA:C	2:O:396:SER:N	2.72	0.48
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.94	0.48
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.26	0.48
13:C:2001:SMA:H4	5:R:160:CYS:HB3	1.94	0.48
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.95	0.48
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.95	0.48
8:H:43:ARG:HD2	8:H:47:ARG:HH12	1.78	0.48
1:N:5:ALA:O	1:N:8:LEU:HB2	2.13	0.48
2:O:170:THR:O	2:O:172:LEU:N	2.46	0.48
2:O:291:VAL:C	2:O:293:SER:H	2.21	0.48
3:P:81:ARG:HH22	16:P:3011:GOL:H2	1.76	0.48
2:B:70:ARG:HD3	2:B:100:SER:OG	2.14	0.48
2:B:76:THR:HG22	2:B:81:SER:HA	1.96	0.48
2:B:167:ALA:HA	2:B:423:SER:OG	2.13	0.48
2:B:285:ILE:O	2:B:288:GLY:N	2.46	0.48
2:O:50:PHE:CE1	2:O:207:VAL:HB	2.48	0.48
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.48	0.48
3:P:30:ALA:C	3:P:32:TRP:H	2.21	0.48
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.39	0.48
1:A:305:HIS:HB3	9:I:35:UNK:CB	2.42	0.48
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.13	0.48
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.48	0.48
4:D:28:ARG:HG2	4:D:171:TYR:CD2	2.48	0.48
4:D:43:MET:HE1	4:D:189:PHE:HE2	1.68	0.48
1:N:19:LEU:HD12	1:N:23:LEU:HD23	1.94	0.48
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.78	0.48
2:O:353:THR:HG22	2:O:355:GLU:N	2.04	0.48
3:P:111:LYS:HE2	3:P:307:PHE:CE1	2.49	0.48
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.96	0.48
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.48	0.48
1:A:80:GLU:OE2	2:B:291:VAL:HG23	2.14	0.48
1:A:133:VAL:O	1:A:137:GLU:HG3	2.14	0.48
2:B:47:ILE:CG2	2:B:48:GLY:N	2.77	0.48
2:B:170:THR:O	2:B:172:LEU:N	2.47	0.48
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:LYS:O	1:N:209:VAL:HG12	2.13	0.48
2:O:235:ALA:O	2:O:236:LYS:C	2.55	0.48
2:O:370:MET:O	2:O:372:VAL:N	2.47	0.48
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.48	0.48
3:P:95:ILE:O	3:P:99:ILE:HG13	2.13	0.48
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.14	0.48
4:D:223:LYS:C	4:D:223:LYS:HD3	2.39	0.48
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.49	0.48
5:R:122:HIS:CE1	5:R:124:LEU:HG	2.48	0.48
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.96	0.48
1:A:233:ARG:NH2	1:A:316:ASP:O	2.43	0.48
2:B:229:GLY:C	2:B:231:GLY:N	2.71	0.48
5:E:127:VAL:HG11	5:E:133:VAL:HA	1.94	0.48
1:N:19:LEU:O	1:N:21:ASN:N	2.47	0.48
1:N:205:HIS:O	1:N:208:LEU:HB3	2.14	0.48
2:O:212:LYS:HB2	2:O:215:ASP:OD2	2.14	0.48
3:P:132:TYR:HA	12:P:501:HEM:HAA2	1.96	0.48
3:P:141:PHE:HB2	3:P:260:ALA:CB	2.43	0.48
4:Q:43:MET:HE1	4:Q:189:PHE:HE2	1.73	0.48
3:C:236:MET:HA	18:D:2003:CDL:H162	1.94	0.48
4:D:235:MET:HB3	7:G:15:THR:HG22	1.96	0.48
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.49	0.48
2:O:113:ARG:O	2:O:115:HIS:N	2.47	0.48
8:U:47:ARG:HG2	8:U:47:ARG:NH1	2.28	0.48
1:A:35:CYS:HA	1:A:372:THR:HG21	1.95	0.48
2:B:59:THR:HG22	2:B:60:THR:H	1.78	0.48
2:B:166:ALA:HB1	2:B:242:GLY:C	2.39	0.48
2:B:220:ALA:O	2:B:224:LEU:HB2	2.14	0.48
3:C:135:PRO:HG3	12:C:501:HEM:O1D	2.14	0.48
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.95	0.48
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.49	0.48
5:E:171:ILE:HG23	5:E:171:ILE:O	2.13	0.48
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.29	0.48
1:N:191:LYS:CA	1:N:195:MET:HE2	2.44	0.48
2:O:43:PRO:C	2:O:113:ARG:HG3	2.38	0.48
3:P:142:TRP:O	3:P:146:VAL:HG23	2.13	0.48
3:P:246:PHE:C	3:P:248:PRO:HD3	2.39	0.48
2:B:28:LYS:O	2:B:28:LYS:HG2	2.14	0.47
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.28	0.47
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.70	0.47
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASN:O	1:A:26:ALA:HA	2.13	0.47
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.49	0.47
2:B:398:VAL:O	2:B:402:ILE:HG13	2.14	0.47
3:C:285:ILE:H	3:C:285:ILE:CD1	2.27	0.47
3:P:245:LEU:O	4:Q:201:ARG:HG2	2.14	0.47
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.47
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.49	0.47
2:B:235:ALA:O	2:B:236:LYS:C	2.57	0.47
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.95	0.47
1:N:35:CYS:HB2	1:N:200:ALA:O	2.14	0.47
1:N:280:TYR:CG	1:N:281:ASP:N	2.82	0.47
3:P:112:GLU:O	3:P:116:THR:HG23	2.14	0.47
2:B:35:ILE:O	2:B:213:HIS:HE1	1.98	0.47
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.49	0.47
2:B:353:THR:HB	2:B:356:ASP:CG	2.39	0.47
3:C:1:MET:HA	3:C:1:MET:HE2	1.96	0.47
3:C:63:ALA:O	3:C:67:VAL:HG23	2.15	0.47
5:E:114:VAL:O	5:E:114:VAL:HG12	2.14	0.47
6:F:77:LYS:HE3	6:F:78:GLU:HG3	1.95	0.47
1:N:223:TYR:CD2	1:N:223:TYR:N	2.82	0.47
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.96	0.47
3:P:189:ALA:O	3:P:193:ILE:HG13	2.15	0.47
2:B:147:ASP:O	2:B:150:VAL:HG22	2.15	0.47
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.28	0.47
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.49	0.47
5:E:90:LYS:O	5:E:91:TRP:HB2	2.15	0.47
1:N:26:ALA:O	1:N:198:ALA:HA	2.14	0.47
1:N:179:ARG:HG2	1:N:179:ARG:NH1	2.29	0.47
3:P:271:PRO:HA	13:P:3001:SMA:C7M	2.41	0.47
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.96	0.47
3:C:12:LEU:C	3:C:14:MET:N	2.70	0.47
8:H:25:GLU:HG2	8:H:61:PHE:HZ	1.78	0.47
2:O:29:LEU:HB2	2:O:31:ASN:HD21	1.80	0.47
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.44	0.47
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.14	0.47
1:A:329:LEU:HA	1:A:430:GLN:NE2	2.29	0.47
3:C:347:PRO:O	3:C:350:ILE:HG22	2.15	0.47
4:D:135:CYS:O	4:D:149:TYR:HB3	2.15	0.47
4:D:171:TYR:OH	4:D:182:ILE:HA	2.14	0.47
5:E:57:GLN:OE1	20:E:2009:PLC:H12	2.14	0.47
5:E:77:LYS:C	5:E:79:SER:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:HIS:O	10:J:62:SER:HB2	2.14	0.47
1:N:62:LEU:C	1:N:64:PHE:H	2.22	0.47
1:N:410:VAL:O	1:N:413:LYS:HB3	2.14	0.47
1:N:433:ASP:OD2	1:N:433:ASP:C	2.58	0.47
2:O:27:THR:CG2	2:O:28:LYS:N	2.77	0.47
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.76	0.47
3:P:158:GLY:O	3:P:161:LEU:HB2	2.14	0.47
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.96	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.95	0.47
5:R:171:ILE:O	5:R:171:ILE:HG23	2.15	0.47
6:S:73:ARG:HA	6:S:73:ARG:HD3	1.74	0.47
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.15	0.47
9:V:64:LEU:HD12	9:V:77:ARG:C	2.39	0.47
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.15	0.47
3:C:101:ARG:HD2	3:C:102:GLY:N	2.30	0.47
3:C:157:ILE:O	3:C:161:LEU:HD12	2.14	0.47
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.96	0.47
3:P:158:GLY:O	3:P:159:HIS:C	2.58	0.47
5:R:164:HIS:HB2	5:R:173:LYS:HB3	1.96	0.47
15:R:3005:PEE:H54	10:W:21:ALA:HA	1.97	0.47
2:B:150:VAL:CG2	2:B:151:ALA:N	2.77	0.47
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.45	0.47
8:H:57:GLU:H	8:H:57:GLU:CD	2.23	0.47
2:B:50:PHE:CE1	2:B:207:VAL:HB	2.50	0.47
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.50	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.49	0.47
5:E:69:LEU:HB2	5:E:70:ALA:H	1.34	0.47
8:H:43:ARG:HD2	8:H:47:ARG:CZ	2.44	0.47
1:N:382:HIS:O	1:N:386:TYR:N	2.48	0.47
2:O:306:PRO:CG	9:V:51:CYS:HA	2.45	0.47
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.44	0.47
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.62	0.47
2:B:341:MET:HG3	2:B:439:LEU:HB3	1.96	0.46
4:D:214:LEU:HD11	4:D:218:LEU:HD11	1.97	0.46
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.44	0.46
1:N:85:HIS:CE1	2:O:370:MET:HE1	2.50	0.46
5:R:101:ARG:N	5:R:131:GLU:O	2.45	0.46
1:A:18:THR:HG23	1:A:24:ARG:HG2	1.97	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.15	0.46
6:F:84:GLU:CD	6:F:84:GLU:H	2.24	0.46
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:ILE:CG2	2:O:48:GLY:N	2.78	0.46
2:O:394:ALA:C	2:O:396:SER:H	2.22	0.46
3:P:332:ASN:HD21	3:P:359:TYR:N	2.13	0.46
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.97	0.46
5:R:109:GLU:CD	5:R:167:ALA:HB3	2.41	0.46
8:U:50:THR:OG1	8:U:51:GLU:N	2.48	0.46
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.31	0.46
2:B:209:ILE:HD12	2:B:379:LEU:HB2	1.97	0.46
2:B:265:GLY:O	2:B:266:SER:C	2.58	0.46
3:C:243:LEU:CD2	3:C:251:LEU:HD11	2.45	0.46
4:D:21:LEU:HD13	4:D:192:TRP:HB2	1.97	0.46
10:J:40:ASP:O	10:J:44:GLU:HG3	2.15	0.46
1:N:145:MET:HE2	1:N:145:MET:N	2.31	0.46
4:Q:62:LYS:O	4:Q:65:ALA:HB3	2.15	0.46
2:B:86:THR:OG1	9:I:70:LEU:HD11	2.16	0.46
2:B:113:ARG:O	2:B:115:HIS:N	2.47	0.46
5:E:148:ALA:HA	5:E:156:TYR:CD2	2.50	0.46
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.50	0.46
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.96	0.46
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.50	0.46
1:A:416:TYR:HE1	1:A:443:TRP:H	1.64	0.46
3:C:285:ILE:N	3:C:285:ILE:CD1	2.77	0.46
5:E:101:ARG:N	5:E:131:GLU:O	2.45	0.46
7:G:29:ILE:O	7:G:33:ALA:HB3	2.15	0.46
1:N:364:ALA:O	1:N:368:GLN:HG2	2.16	0.46
1:N:365:MET:HG2	1:N:392:LEU:HD22	1.98	0.46
8:U:18:THR:O	8:U:22:GLU:HG3	2.16	0.46
8:U:57:GLU:CD	8:U:57:GLU:H	2.24	0.46
1:A:63:ALA:HB1	1:A:116:VAL:CG1	2.45	0.46
2:B:102:ARG:NH1	2:B:102:ARG:CG	2.78	0.46
3:C:325:LEU:HD11	3:C:366:LEU:HD12	1.98	0.46
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.51	0.46
8:U:67:HIS:C	8:U:67:HIS:ND1	2.73	0.46
2:B:99:TYR:HA	9:I:67:GLY:HA2	1.98	0.46
2:B:109:VAL:CG1	2:B:123:LEU:HB2	2.46	0.46
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.96	0.46
2:B:394:ALA:O	2:B:396:SER:N	2.48	0.46
3:C:355:ALA:O	3:C:358:SER:HB3	2.16	0.46
3:C:374:GLU:HG2	6:F:20:TYR:CZ	2.51	0.46
4:D:27:ARG:NH1	4:D:55:THR:O	2.48	0.46
2:O:167:ALA:HB1	2:O:321:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:70:THR:HA	3:P:74:VAL:CG2	2.46	0.46
5:R:150:SER:OG	5:R:157:TYR:HB3	2.15	0.46
2:B:159:VAL:HG23	2:B:160:LEU:N	2.30	0.46
3:C:133:VAL:O	3:C:133:VAL:HG12	2.15	0.46
3:C:141:PHE:HB2	3:C:260:ALA:CB	2.46	0.46
1:N:329:LEU:C	1:N:430:GLN:HE22	2.23	0.46
1:A:5:ALA:O	1:A:8:LEU:HB2	2.16	0.46
1:A:223:TYR:CD2	1:A:223:TYR:N	2.84	0.46
1:A:389:ARG:HD2	1:A:390:ILE:H	1.81	0.46
3:C:350:ILE:HG23	3:C:351:ILE:N	2.31	0.46
6:F:109:LYS:O	6:F:110:LYS:C	2.59	0.46
2:O:102:ARG:NH1	2:O:102:ARG:CG	2.75	0.46
2:O:235:ALA:O	2:O:236:LYS:O	2.34	0.46
2:O:269:ALA:O	2:O:270:ASN:C	2.59	0.46
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.97	0.46
3:P:346:HIS:CG	3:P:347:PRO:HA	2.50	0.46
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.15	0.46
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.51	0.46
5:R:75:GLU:C	5:R:76:ILE:HG13	2.41	0.46
2:B:203:ARG:HD2	2:B:230:ALA:CA	2.26	0.46
2:B:385:GLU:C	2:B:387:LEU:N	2.73	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.51	0.46
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.81	0.46
2:O:116:VAL:O	2:O:120:MET:HB2	2.16	0.46
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.50	0.46
5:R:67:ASP:O	5:R:69:LEU:HD23	2.15	0.46
6:S:77:LYS:CE	6:S:78:GLU:HG3	2.46	0.46
7:T:34:LEU:HA	7:T:37:VAL:HG23	1.97	0.46
1:A:7:THR:HB	2:B:41:PHE:O	2.16	0.45
1:A:255:LEU:HD11	1:A:420:PRO:HB2	1.97	0.45
2:B:43:PRO:C	2:B:113:ARG:HG3	2.40	0.45
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.47	0.45
3:C:31:TRP:O	3:C:101:ARG:HG3	2.15	0.45
3:C:142:TRP:CH2	5:R:145:VAL:HG23	2.51	0.45
3:C:377:MET:HE1	6:F:19:TRP:CZ3	2.50	0.45
1:N:373:THR:HB	1:N:374:PRO:CD	2.43	0.45
2:O:394:ALA:O	2:O:396:SER:N	2.49	0.45
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.16	0.45
5:R:148:ALA:O	5:R:149:ASN:HB2	2.16	0.45
3:C:223:PRO:O	3:C:227:PHE:HB2	2.16	0.45
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:UNK:O	9:I:39:UNK:C	2.65	0.45
9:I:49:LEU:HB3	9:I:55:MET:CG	2.46	0.45
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.31	0.45
2:O:73:SER:OG	2:O:74:PRO:HD3	2.16	0.45
4:Q:2:GLU:O	4:Q:2:GLU:HG2	2.16	0.45
6:S:10:GLY:C	6:S:12:LEU:N	2.74	0.45
5:E:136:VAL:HG12	5:E:138:VAL:HG23	1.98	0.45
1:N:145:MET:CB	1:N:252:HIS:CD2	2.99	0.45
1:N:253:VAL:HG11	1:N:335:MET:HE2	1.99	0.45
2:O:109:VAL:CG1	2:O:123:LEU:HB2	2.45	0.45
2:O:209:ILE:HD12	2:O:379:LEU:HB2	1.97	0.45
3:P:377:MET:HE1	6:S:19:TRP:HZ3	1.81	0.45
5:R:91:TRP:O	5:R:93:GLY:N	2.50	0.45
1:A:62:LEU:C	1:A:64:PHE:H	2.25	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.15	0.45
1:A:403:ASP:O	1:A:404:ALA:C	2.58	0.45
2:B:60:THR:CG2	2:B:61:ALA:N	2.80	0.45
2:B:101:THR:HG22	9:I:65:VAL:HG22	1.99	0.45
2:B:102:ARG:HH11	2:B:102:ARG:CG	2.21	0.45
3:C:237:LEU:HD12	3:C:237:LEU:HA	1.68	0.45
5:E:122:HIS:CE1	5:E:124:LEU:HG	2.51	0.45
6:F:28:LYS:HB3	6:F:74:ILE:HD12	1.97	0.45
7:G:29:ILE:O	7:G:34:LEU:HG	2.17	0.45
1:N:102:LEU:C	1:N:104:LYS:N	2.74	0.45
1:N:121:ALA:O	1:N:122:LEU:HB2	2.15	0.45
1:N:126:GLN:HE22	1:N:129:LYS:HD3	1.79	0.45
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.45	0.45
2:O:150:VAL:CG2	2:O:151:ALA:N	2.80	0.45
2:O:366:ALA:O	2:O:367:THR:C	2.59	0.45
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.68	0.45
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.99	0.45
1:A:124:GLU:O	1:A:124:GLU:HG2	2.16	0.45
3:C:70:THR:HA	3:C:74:VAL:HG23	1.99	0.45
4:D:102:ARG:NH1	4:D:107:GLY:O	2.47	0.45
1:N:88:GLY:O	2:O:286:LYS:NZ	2.43	0.45
1:N:416:TYR:HE1	1:N:443:TRP:H	1.64	0.45
3:P:157:ILE:CG1	3:P:158:GLY:H	2.07	0.45
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	1.99	0.45
8:U:52:GLU:CG	8:U:53:GLN:H	2.30	0.45
1:A:212:ALA:O	1:A:216:PHE:HB2	2.16	0.45
2:B:198:ASN:HB3	2:B:203:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ALA:C	2:B:302:ALA:N	2.74	0.45
3:C:132:TYR:HA	12:C:501:HEM:HAA2	1.98	0.45
5:E:145:VAL:HG23	3:P:142:TRP:CH2	2.52	0.45
7:G:9:ARG:HG3	7:G:9:ARG:HH11	1.82	0.45
1:N:36:THR:HG21	1:N:373:THR:HA	1.99	0.45
1:N:145:MET:CB	1:N:252:HIS:NE2	2.80	0.45
1:N:190:PHE:C	1:N:195:MET:HE2	2.42	0.45
2:O:269:ALA:O	2:O:272:PHE:N	2.49	0.45
3:P:342:GLN:HE21	3:P:342:GLN:CA	2.25	0.45
6:S:13:MET:HA	6:S:16:ILE:CB	2.33	0.45
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.99	0.45
2:B:27:THR:H	2:B:213:HIS:CE1	2.34	0.45
2:B:128:THR:C	2:B:130:PRO:HD2	2.42	0.45
2:B:279:LEU:HA	2:B:294:LYS:HB2	1.99	0.45
2:B:408:ALA:O	2:B:409:ASP:C	2.60	0.45
3:C:23:PRO:HG2	7:G:3:HIS:CB	2.47	0.45
5:E:148:ALA:O	5:E:149:ASN:HB2	2.17	0.45
8:H:32:LYS:HA	8:H:32:LYS:HD3	1.82	0.45
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.45
5:R:91:TRP:C	5:R:93:GLY:N	2.75	0.45
10:W:59:TYR:CD1	10:W:59:TYR:N	2.84	0.45
1:A:4:TYR:O	1:A:5:ALA:C	2.59	0.45
1:A:161:THR:HG21	1:A:235:ARG:H	1.82	0.45
3:C:155:PRO:O	3:C:156:TYR:HB2	2.17	0.45
4:D:86:LYS:HZ2	5:E:71:LEU:HD13	1.81	0.45
5:E:59:ILE:HG22	5:E:60:SER:N	2.31	0.45
9:I:69:SER:CB	9:I:72:ALA:HB3	2.46	0.45
1:N:80:GLU:OE1	2:O:290:SER:HA	2.16	0.45
1:N:364:ALA:HB2	9:V:29:UNK:CB	2.47	0.45
2:O:31:ASN:HD22	2:O:31:ASN:N	2.14	0.45
2:O:367:THR:HG22	2:O:368:TYR:N	2.30	0.45
2:O:414:ALA:O	2:O:418:VAL:HG23	2.16	0.45
3:P:12:LEU:C	3:P:14:MET:N	2.73	0.45
3:P:325:LEU:HD11	3:P:366:LEU:HD12	1.99	0.45
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.99	0.45
8:U:52:GLU:HG2	8:U:53:GLN:H	1.80	0.45
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.32	0.45
5:E:85:LYS:HG2	5:E:86:ASN:N	2.31	0.45
7:G:71:ARG:NH2	8:H:56:GLU:OE1	2.50	0.45
10:J:49:GLY:N	10:J:54:HIS:ND1	2.65	0.45
1:N:29:GLU:HG3	1:N:203:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:294:LEU:HD23	1:N:307:PHE:CE1	2.52	0.45
1:N:386:TYR:CD2	1:N:390:ILE:HD12	2.52	0.45
2:O:398:VAL:O	2:O:402:ILE:HG13	2.17	0.45
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.98	0.45
5:R:153:PHE:CE2	5:R:172:ARG:HB3	2.52	0.45
2:B:385:GLU:C	2:B:387:LEU:H	2.25	0.45
3:C:4:ASN:HD21	3:C:7:LYS:HZ2	1.64	0.45
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.99	0.45
1:N:106:MET:HB3	1:N:107:PRO:CD	2.47	0.45
2:O:259:THR:CG2	2:O:260:GLU:N	2.80	0.45
3:P:269:ILE:HG23	3:P:269:ILE:O	2.16	0.45
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.52	0.45
5:R:122:HIS:ND1	5:R:124:LEU:HG	2.32	0.45
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.99	0.45
2:B:155:PRO:O	2:B:156:GLN:C	2.59	0.44
2:B:398:VAL:HG13	2:B:399:ALA:N	2.33	0.44
3:C:90:PHE:CD2	3:C:236:MET:HE3	2.53	0.44
5:E:69:LEU:HD13	5:E:71:LEU:HD21	1.99	0.44
6:F:31:LEU:HD21	6:F:65:ALA:HB2	1.99	0.44
6:F:52:GLU:CG	6:F:56:ASN:HD21	2.21	0.44
2:O:229:GLY:C	2:O:231:GLY:H	2.25	0.44
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.00	0.44
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.52	0.44
4:Q:120:ARG:HG2	4:Q:120:ARG:HH11	1.81	0.44
5:R:135:LEU:HD22	5:R:169:GLY:HA3	1.99	0.44
1:A:228:VAL:HG13	1:A:228:VAL:O	2.18	0.44
2:B:51:ILE:HG22	2:B:52:LYS:N	2.33	0.44
9:I:32:UNK:N	9:I:73:PRO:CG	2.75	0.44
2:O:144:LEU:HB2	2:O:183:ILE:HG23	1.97	0.44
3:P:107:SER:HB3	12:P:502:HEM:HAD1	1.99	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
2:B:249:GLY:O	2:B:250:HIS:C	2.60	0.44
6:F:105:GLU:O	6:F:109:LYS:HG3	2.17	0.44
7:G:71:ARG:CZ	8:H:56:GLU:OE1	2.65	0.44
8:H:20:ILE:HD12	8:H:73:LEU:HA	1.99	0.44
2:O:144:LEU:O	2:O:145:LYS:C	2.61	0.44
2:O:344:LEU:HD23	2:O:417:PHE:CD2	2.53	0.44
3:P:47:LEU:HD12	3:P:47:LEU:O	2.17	0.44
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	2.00	0.44
7:T:57:LEU:O	7:T:58:LEU:C	2.60	0.44
2:B:38:LEU:C	2:B:38:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:N	2:B:47:ILE:CD1	2.80	0.44
2:B:202:ALA:HB3	2:B:229:GLY:H	1.83	0.44
5:E:185:TYR:HB3	5:E:195:VAL:HG13	2.00	0.44
10:J:27:GLY:O	10:J:28:ALA:C	2.59	0.44
1:N:189:HIS:O	1:N:191:LYS:N	2.49	0.44
1:N:342:TRP:O	1:N:345:LEU:HB2	2.18	0.44
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.98	0.44
3:P:304:LEU:O	3:P:305:ILE:C	2.60	0.44
4:Q:214:LEU:HD11	4:Q:218:LEU:HD11	1.98	0.44
5:R:128:LYS:O	5:R:130:PRO:HD3	2.17	0.44
6:S:84:GLU:H	6:S:84:GLU:CD	2.25	0.44
1:A:191:LYS:CA	1:A:195:MET:HE2	2.47	0.44
2:B:107:TYR:O	2:B:108:CYS:HB3	2.17	0.44
2:B:129:ALA:N	2:B:130:PRO:CD	2.81	0.44
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.98	0.44
1:N:343:MET:O	1:N:347:THR:HG23	2.17	0.44
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.73	0.44
2:O:287:ARG:HD3	9:V:53:GLU:HG2	1.98	0.44
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.16	0.44
1:A:86:PHE:HD1	1:A:87:ASN:N	2.15	0.44
1:A:91:SER:OG	1:A:92:ARG:N	2.49	0.44
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.52	0.44
3:C:51:LEU:HD23	3:C:51:LEU:HA	1.88	0.44
1:N:138:LEU:O	1:N:139:LYS:C	2.60	0.44
1:N:242:ARG:NH1	1:N:432:LEU:HA	2.20	0.44
2:O:408:ALA:O	2:O:409:ASP:C	2.60	0.44
3:P:141:PHE:HB2	3:P:260:ALA:HB1	1.98	0.44
6:S:77:LYS:HE3	6:S:78:GLU:HG3	2.00	0.44
8:U:72:LYS:HA	8:U:75:ASN:HD22	1.83	0.44
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.47	0.44
1:A:329:LEU:C	1:A:430:GLN:HE22	2.25	0.44
2:B:209:ILE:HG13	2:B:379:LEU:HD13	1.98	0.44
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.18	0.44
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.53	0.44
3:P:289:LEU:HG	3:P:293:LEU:HD11	2.00	0.44
4:Q:55:THR:O	10:W:52:TRP:CZ3	2.71	0.44
4:Q:178:THR:HG21	8:U:15:ASP:HA	1.99	0.44
1:A:253:VAL:HG11	1:A:335:MET:HE2	1.99	0.44
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.99	0.44
5:E:165:TYR:HA	5:E:170:ARG:O	2.16	0.44
8:H:15:ASP:C	8:H:17:LEU:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:166:TRP:HA	3:P:175:THR:HG23	1.99	0.44
3:P:235:LEU:O	3:P:239:PRO:HD2	2.18	0.44
3:P:300:LEU:HD23	3:P:300:LEU:HA	1.84	0.44
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.47	0.44
5:R:171:ILE:N	5:R:179:ASN:OD1	2.49	0.44
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.82	0.44
1:A:87:ASN:OD1	2:B:286:LYS:HD2	2.17	0.44
3:C:132:TYR:O	3:C:135:PRO:HD2	2.18	0.44
3:C:187:PRO:HG2	12:C:501:HEM:CMC	2.46	0.44
4:D:27:ARG:O	4:D:30:PHE:HB3	2.17	0.44
1:N:18:THR:HG23	1:N:24:ARG:CG	2.40	0.44
1:N:45:SER:HA	1:N:48:GLU:CG	2.46	0.44
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.33	0.44
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.99	0.44
1:N:382:HIS:HB3	1:N:388:ARG:O	2.18	0.44
2:O:248:ASN:HD22	2:O:249:GLY:N	2.15	0.44
3:P:132:TYR:O	3:P:135:PRO:HD2	2.18	0.44
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	2.00	0.44
4:Q:241:LYS:HE3	4:Q:241:LYS:CA	2.43	0.44
1:A:45:SER:HA	1:A:48:GLU:CD	2.43	0.43
1:A:168:GLU:CD	1:A:168:GLU:H	2.26	0.43
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.74	0.43
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.32	0.43
1:N:170:THR:HG22	1:N:172:GLU:H	1.82	0.43
1:N:403:ASP:O	1:N:404:ALA:C	2.61	0.43
2:O:249:GLY:O	2:O:250:HIS:C	2.61	0.43
3:P:138:GLN:N	3:P:258:THR:O	2.48	0.43
4:Q:197:GLU:O	4:Q:198:HIS:C	2.60	0.43
6:S:40:ASP:O	6:S:44:LYS:HG3	2.17	0.43
1:A:105:ASP:O	1:A:109:VAL:HG23	2.18	0.43
2:B:395:PRO:C	2:B:398:VAL:HG12	2.43	0.43
4:D:3:LEU:HD23	4:D:3:LEU:HA	1.83	0.43
1:N:220:SER:HA	1:N:225:GLU:OE1	2.18	0.43
2:O:129:ALA:N	2:O:130:PRO:CD	2.82	0.43
5:R:99:ARG:HB3	5:R:133:VAL:HG12	1.99	0.43
8:U:73:LEU:HD12	8:U:73:LEU:O	2.18	0.43
1:A:261:GLY:O	1:A:262:TRP:C	2.60	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.61	0.43
2:O:222:GLN:C	2:O:223:PHE:HD2	2.27	0.43
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.48	0.43
3:P:159:HIS:O	3:P:162:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.43
7:T:56:TYR:HD2	7:T:57:LEU:HD23	1.82	0.43
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.48	0.43
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.52	0.43
2:B:393:THR:CG2	2:B:397:VAL:HB	2.39	0.43
4:D:75:ASP:CG	4:D:79:GLU:HB2	2.42	0.43
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.86	0.43
5:R:148:ALA:HA	5:R:156:TYR:CD2	2.53	0.43
6:S:28:LYS:HB3	6:S:74:ILE:HD12	2.01	0.43
8:U:23:HIS:O	8:U:26:GLN:HB2	2.19	0.43
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.81	0.43
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.53	0.43
1:A:362:ARG:O	1:A:365:MET:HB3	2.18	0.43
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.48	0.43
2:B:344:LEU:HD23	2:B:417:PHE:CD2	2.53	0.43
3:C:52:LEU:HD21	3:C:80:ILE:HG22	2.01	0.43
5:E:109:GLU:O	5:E:123:ASP:HB2	2.18	0.43
1:N:133:VAL:O	1:N:137:GLU:HG3	2.18	0.43
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.53	0.43
2:O:22:GLU:HB3	2:O:23:ASP:H	1.61	0.43
3:P:105:TYR:O	3:P:315:THR:HG22	2.18	0.43
1:A:358:LYS:HE3	1:A:399:ILE:O	2.19	0.43
3:C:101:ARG:CZ	12:C:502:HEM:HBD2	2.48	0.43
3:C:282:LEU:HD23	3:C:282:LEU:O	2.18	0.43
5:E:75:GLU:C	5:E:76:ILE:HG13	2.43	0.43
5:E:163:SER:HA	5:E:174:GLY:HA3	2.00	0.43
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.99	0.43
8:H:67:HIS:C	8:H:67:HIS:ND1	2.76	0.43
1:N:4:TYR:HA	2:O:113:ARG:HD3	2.01	0.43
2:O:257:VAL:O	2:O:323:GLY:HA3	2.18	0.43
2:O:325:TYR:C	2:O:325:TYR:CD2	2.97	0.43
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.18	0.43
3:P:76:TYR:HE2	4:Q:204:MET:CE	2.30	0.43
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.40	0.43
5:R:109:GLU:O	5:R:123:ASP:HB2	2.19	0.43
7:T:46:PHE:O	7:T:50:PRO:HG2	2.18	0.43
2:B:31:ASN:CB	2:B:227:ARG:HH22	2.29	0.43
3:C:112:GLU:O	3:C:116:THR:HG23	2.19	0.43
4:D:83:ARG:HB2	4:D:84:PRO:HD2	1.99	0.43
5:E:69:LEU:O	5:E:70:ALA:HB2	2.19	0.43
2:O:147:ASP:O	2:O:150:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:243:LEU:HD21	3:P:251:LEU:CD1	2.49	0.43
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.18	0.43
8:U:25:GLU:HG2	8:U:61:PHE:CZ	2.54	0.43
1:A:102:LEU:C	1:A:104:LYS:N	2.76	0.43
2:B:31:ASN:HD22	2:B:31:ASN:C	2.21	0.43
2:B:217:LYS:O	2:B:218:GLN:C	2.62	0.43
2:B:385:GLU:O	2:B:387:LEU:N	2.52	0.43
3:C:52:LEU:CD2	3:C:80:ILE:HG22	2.48	0.43
5:E:85:LYS:HE2	5:E:87:VAL:CG2	2.45	0.43
5:E:135:LEU:HD22	5:E:169:GLY:HA3	2.00	0.43
3:P:34:PHE:HB2	21:P:381:HOH:O	2.19	0.43
4:Q:60:GLU:OE1	10:W:59:TYR:HB3	2.18	0.43
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.83	0.43
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.54	0.43
5:R:179:ASN:O	5:R:180:LEU:C	2.62	0.43
3:C:131:GLY:HA3	3:C:183:HIS:CE1	2.54	0.43
4:D:142:VAL:HG23	4:D:142:VAL:O	2.18	0.43
6:F:13:MET:CE	6:F:16:ILE:HD12	2.49	0.43
1:N:293:ARG:HH21	1:N:344:ARG:NE	2.17	0.43
1:N:433:ASP:OD2	1:N:435:ASN:N	2.52	0.43
2:O:353:THR:HB	2:O:356:ASP:CG	2.44	0.43
5:R:165:TYR:HA	5:R:170:ARG:O	2.19	0.43
7:T:77:TYR:CD2	8:U:52:GLU:HB2	2.54	0.43
1:A:7:THR:HG21	2:B:113:ARG:CD	2.49	0.43
1:A:26:ALA:O	1:A:198:ALA:HA	2.19	0.43
3:C:107:SER:HB3	12:C:502:HEM:HAD1	2.01	0.43
4:D:62:LYS:HE2	4:D:66:GLU:OE2	2.19	0.43
5:E:152:ASP:C	5:E:153:PHE:CD1	2.97	0.43
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.84	0.43
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.54	0.43
1:N:161:THR:HG21	1:N:235:ARG:N	2.34	0.43
1:N:245:ASP:C	1:N:247:ALA:H	2.27	0.43
3:P:2:ALA:HA	3:P:3:PRO:O	2.19	0.43
3:P:275:PHE:CD2	13:P:3001:SMA:H11	2.54	0.43
5:R:186:GLN:NE2	5:R:188:VAL:HG12	2.34	0.43
2:B:84:ARG:HH22	2:B:121:GLU:CD	2.27	0.42
2:B:295:LEU:O	2:B:296:TYR:C	2.62	0.42
5:E:72:SER:HB2	5:E:73:LYS:H	1.62	0.42
6:F:103:GLU:O	6:F:104:ARG:C	2.60	0.42
1:N:86:PHE:HD1	1:N:87:ASN:N	2.17	0.42
1:N:220:SER:HB2	1:N:226:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.78	0.42
1:A:159:GLN:HE22	7:G:18:LEU:CD2	2.30	0.42
2:B:146:VAL:HG12	2:B:147:ASP:N	2.34	0.42
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.18	0.42
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.54	0.42
2:O:147:ASP:OD1	9:V:68:ILE:HD11	2.19	0.42
3:P:101:ARG:HD2	3:P:102:GLY:N	2.31	0.42
4:Q:14:HIS:O	4:Q:202:LYS:NZ	2.52	0.42
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.19	0.42
6:S:21:TYR:C	6:S:21:TYR:CD2	2.97	0.42
1:A:178:THR:O	1:A:179:ARG:C	2.62	0.42
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.83	0.42
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.83	0.42
5:E:47:THR:HG21	15:E:2005:PEE:H23	2.01	0.42
1:N:86:PHE:O	2:O:285:ILE:HA	2.19	0.42
1:N:178:THR:O	1:N:179:ARG:C	2.60	0.42
6:S:16:ILE:O	6:S:19:TRP:HB3	2.19	0.42
8:U:15:ASP:C	8:U:17:LEU:N	2.76	0.42
3:C:95:ILE:CG2	3:C:96:PHE:N	2.82	0.42
5:E:122:HIS:ND1	5:E:124:LEU:HG	2.35	0.42
7:G:34:LEU:HA	7:G:37:VAL:HG23	2.01	0.42
2:O:155:PRO:O	2:O:156:GLN:C	2.61	0.42
2:O:395:PRO:C	2:O:398:VAL:HG12	2.45	0.42
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.87	0.42
7:T:73:ASN:HA	7:T:74:PRO:HD2	1.90	0.42
3:C:95:ILE:O	3:C:99:ILE:HG13	2.20	0.42
3:C:235:LEU:O	3:C:239:PRO:HD2	2.19	0.42
2:O:415:LYS:C	2:O:417:PHE:N	2.77	0.42
4:Q:62:LYS:HE2	4:Q:66:GLU:OE2	2.19	0.42
4:Q:210:LEU:HD23	4:Q:210:LEU:HA	1.82	0.42
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.99	0.42
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.52	0.42
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.55	0.42
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.88	0.42
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.55	0.42
2:B:366:ALA:O	2:B:367:THR:C	2.62	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.64	0.42
5:E:52:LYS:C	5:E:52:LYS:CD	2.90	0.42
5:E:69:LEU:HD12	5:E:71:LEU:HG	2.01	0.42
7:G:68:ARG:C	7:G:70:LYS:H	2.27	0.42
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:73:LEU:HD12	8:H:73:LEU:O	2.20	0.42
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.54	0.42
1:N:62:LEU:C	1:N:64:PHE:N	2.78	0.42
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.02	0.42
1:A:76:GLU:O	1:A:80:GLU:HG3	2.19	0.42
1:A:191:LYS:N	1:A:195:MET:HE2	2.35	0.42
3:C:133:VAL:HA	3:C:140:SER:HB3	2.01	0.42
3:C:246:PHE:CZ	4:D:205:GLY:HA3	2.55	0.42
4:D:105:ASN:O	4:D:106:ASN:HB2	2.20	0.42
8:H:15:ASP:O	8:H:17:LEU:N	2.52	0.42
9:I:52:ARG:O	9:I:56:SER:HB3	2.19	0.42
2:O:225:ASN:O	2:O:226:ILE:O	2.36	0.42
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.32	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.65	0.42
1:A:365:MET:HG2	1:A:392:LEU:HD22	2.02	0.42
3:C:50:LEU:O	3:C:54:MET:HG3	2.20	0.42
3:C:141:PHE:HB2	3:C:260:ALA:HB1	2.02	0.42
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.55	0.42
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.50	0.42
1:N:10:ASN:O	1:N:11:ILE:C	2.63	0.42
1:N:39:VAL:HG11	1:N:117:VAL:CG1	2.49	0.42
2:O:59:THR:HG22	2:O:60:THR:H	1.85	0.42
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.20	0.42
3:P:335:ILE:HD13	7:T:58:LEU:HD23	2.01	0.42
10:W:27:GLY:O	10:W:28:ALA:C	2.63	0.42
1:A:26:ALA:CB	1:A:383:LEU:HD11	2.49	0.42
1:A:388:ARG:NH2	1:A:388:ARG:CG	2.83	0.42
2:B:305:GLN:HB3	2:B:306:PRO:HD2	2.01	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.19	0.42
7:G:81:GLN:OXT	8:H:49:HIS:N	2.53	0.42
1:N:178:THR:CG2	1:N:179:ARG:N	2.82	0.42
1:N:178:THR:H	1:N:181:ASP:CG	2.28	0.42
1:N:301:HIS:O	1:N:302:LYS:C	2.62	0.42
1:N:404:ALA:O	1:N:405:ARG:C	2.63	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.88	0.42
5:R:59:ILE:HG22	5:R:60:SER:N	2.35	0.42
2:B:169:LYS:C	2:B:170:THR:HG23	2.45	0.42
3:C:105:TYR:O	3:C:315:THR:HG22	2.20	0.42
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.83	0.42
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.32	0.42
3:P:187:PRO:O	3:P:190:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:198:LEU:HD21	12:P:502:HEM:CMA	2.47	0.42
3:P:270:LYS:HA	3:P:271:PRO:HD3	1.84	0.42
4:Q:74:PRO:HA	4:Q:79:GLU:O	2.20	0.42
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.49	0.42
7:T:41:PHE:HD2	7:T:41:PHE:O	2.02	0.42
1:A:13:GLU:HG2	1:A:14:THR:N	2.35	0.41
1:A:105:ASP:O	1:A:106:MET:C	2.63	0.41
2:B:100:SER:HA	2:B:104:LYS:O	2.20	0.41
2:B:109:VAL:HG21	2:B:119:VAL:CG2	2.50	0.41
3:C:76:TYR:HE2	4:D:204:MET:CE	2.33	0.41
4:D:28:ARG:NH1	4:D:173:ASP:OD2	2.53	0.41
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.50	0.41
7:G:68:ARG:C	7:G:70:LYS:N	2.78	0.41
1:N:37:VAL:HG12	1:N:199:ALA:HB2	2.00	0.41
1:N:63:ALA:O	1:N:116:VAL:HG13	2.20	0.41
3:P:237:LEU:HD12	3:P:237:LEU:HA	1.70	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.54	0.41
6:S:13:MET:O	6:S:17:ARG:HG3	2.21	0.41
9:V:55:MET:HA	9:V:58:ARG:HG3	2.01	0.41
1:A:147:ASN:O	1:A:148:VAL:C	2.63	0.41
1:A:158:PHE:O	1:A:164:ALA:HB2	2.19	0.41
2:B:113:ARG:C	2:B:115:HIS:H	2.29	0.41
3:C:30:ALA:C	3:C:32:TRP:H	2.28	0.41
4:D:62:LYS:O	4:D:65:ALA:HB3	2.20	0.41
6:F:91:GLU:N	6:F:92:PRO:HD2	2.35	0.41
7:G:9:ARG:HG3	7:G:9:ARG:NH1	2.35	0.41
8:H:40:CYS:O	8:H:41:ASP:C	2.63	0.41
2:O:113:ARG:C	2:O:115:HIS:H	2.28	0.41
4:Q:28:ARG:HH11	4:Q:28:ARG:HG3	1.85	0.41
5:R:31:ASP:OD1	10:W:7:ARG:HG3	2.20	0.41
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.50	0.41
1:A:126:GLN:NE2	1:A:129:LYS:HD3	2.35	0.41
2:B:128:THR:HG21	2:B:224:LEU:CD2	2.50	0.41
2:B:362:ASN:O	2:B:363:GLN:C	2.62	0.41
3:C:275:PHE:CD2	13:C:2001:SMA:H11	2.55	0.41
9:I:49:LEU:O	9:I:50:LEU:HD23	2.19	0.41
1:N:136:GLN:O	1:N:139:LYS:N	2.54	0.41
2:O:307:PHE:CD1	2:O:307:PHE:C	2.98	0.41
3:P:31:TRP:HE1	18:P:3004:CDL:H1	1.85	0.41
5:R:152:ASP:C	5:R:153:PHE:CD1	2.98	0.41
6:S:89:TYR:CD1	6:S:89:TYR:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:34:LEU:HA	7:T:37:VAL:CG2	2.50	0.41
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.49	0.41
1:A:242:ARG:NH1	1:A:432:LEU:HA	2.20	0.41
1:A:260:PRO:HD3	1:A:414:TYR:CE2	2.55	0.41
2:B:24:LEU:HD23	2:B:392:HIS:CE1	2.55	0.41
3:C:15:ILE:N	3:C:15:ILE:CD1	2.82	0.41
3:C:273:TRP:HA	3:C:276:LEU:HG	2.02	0.41
5:E:67:ASP:O	5:E:69:LEU:HD23	2.19	0.41
5:E:103:GLN:O	5:E:107:ASN:ND2	2.53	0.41
1:N:99:ILE:HD12	1:N:109:VAL:CG1	2.43	0.41
1:N:402:VAL:HA	1:N:406:MET:SD	2.61	0.41
2:O:47:ILE:N	2:O:47:ILE:CD1	2.84	0.41
2:O:59:THR:O	2:O:60:THR:C	2.62	0.41
2:O:385:GLU:C	2:O:387:LEU:N	2.77	0.41
3:P:59:ASP:HA	3:P:173:ASN:OD1	2.20	0.41
5:R:69:LEU:HD23	5:R:69:LEU:H	1.84	0.41
1:A:433:ASP:OD2	1:A:433:ASP:C	2.62	0.41
9:I:59:SER:O	9:I:60:ALA:C	2.64	0.41
9:I:64:LEU:HD12	9:I:77:ARG:O	2.20	0.41
1:N:21:ASN:O	1:N:192:ALA:HB3	2.20	0.41
1:N:252:HIS:CE1	1:N:325:VAL:HG22	2.55	0.41
1:N:356:ARG:HG3	2:O:90:GLU:O	2.21	0.41
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.20	0.41
2:O:50:PHE:HE1	2:O:207:VAL:HB	1.85	0.41
3:P:172:ASP:HB3	3:P:174:PRO:HD2	2.02	0.41
8:U:13:LEU:H	8:U:13:LEU:CD2	2.30	0.41
8:U:51:GLU:HA	8:U:51:GLU:OE1	2.20	0.41
8:U:58:LEU:HD12	8:U:58:LEU:O	2.21	0.41
10:W:14:PHE:HA	10:W:20:PHE:HD2	1.85	0.41
1:A:30:SER:OG	1:A:32:GLN:HB2	2.20	0.41
2:B:207:VAL:HG12	2:B:208:GLY:N	2.34	0.41
3:C:172:ASP:C	3:C:174:PRO:HD2	2.46	0.41
4:D:10:PHE:CD1	4:D:10:PHE:N	2.87	0.41
8:H:15:ASP:O	8:H:16:PRO:C	2.64	0.41
10:J:59:TYR:CD1	10:J:59:TYR:N	2.88	0.41
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.02	0.41
2:O:100:SER:HA	2:O:104:LYS:O	2.21	0.41
2:O:128:THR:C	2:O:130:PRO:HD2	2.46	0.41
2:O:389:SER:O	2:O:390:GLY:C	2.63	0.41
2:O:398:VAL:HG13	2:O:399:ALA:N	2.35	0.41
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.51	0.41
6:S:90:LEU:O	6:S:91:GLU:C	2.62	0.41
9:V:77:ARG:N	9:V:77:ARG:CD	2.83	0.41
1:A:49:ASN:ND2	1:A:51:LYS:N	2.68	0.41
1:A:99:ILE:HG22	1:A:100:LYS:N	2.35	0.41
1:A:184:SER:O	1:A:185:TYR:C	2.63	0.41
1:A:204:SER:HB3	1:A:207:GLU:HB2	2.02	0.41
3:C:40:VAL:HG11	3:C:233:LEU:HD11	2.03	0.41
9:I:49:LEU:HD22	9:I:55:MET:HA	2.03	0.41
10:J:7:ARG:HB3	10:J:7:ARG:CZ	2.50	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
1:N:261:GLY:O	1:N:262:TRP:C	2.62	0.41
3:P:122:LEU:HA	3:P:122:LEU:HD23	1.86	0.41
4:Q:158:ILE:HG12	4:Q:159:GLY:N	2.35	0.41
1:A:136:GLN:HE22	9:I:50:LEU:CD1	2.34	0.41
1:A:138:LEU:O	1:A:139:LYS:C	2.64	0.41
1:A:233:ARG:NH2	1:A:316:ASP:HB2	2.36	0.41
1:A:280:TYR:CD2	1:A:281:ASP:N	2.89	0.41
2:B:156:GLN:HE22	9:I:77:ARG:C	2.28	0.41
2:B:259:THR:HG22	2:B:260:GLU:H	1.84	0.41
2:B:325:TYR:C	2:B:325:TYR:CD2	2.99	0.41
3:C:308:LEU:HD23	3:C:308:LEU:HA	1.85	0.41
4:D:196:PRO:C	4:D:198:HIS:N	2.78	0.41
5:E:195:VAL:HG12	5:E:196:GLY:H	1.83	0.41
4:Q:27:ARG:NH2	10:W:59:TYR:CD2	2.88	0.41
4:Q:57:THR:HG23	10:W:59:TYR:HB2	2.03	0.41
6:S:77:LYS:HE2	6:S:77:LYS:HB3	1.88	0.41
9:V:49:LEU:HD22	9:V:55:MET:HG2	2.03	0.41
1:A:23:LEU:HD22	1:A:216:PHE:HB3	2.02	0.41
1:A:209:VAL:O	1:A:213:ARG:HG3	2.21	0.41
1:A:242:ARG:O	7:G:14:ILE:HA	2.20	0.41
1:A:266:ASP:O	1:A:269:VAL:N	2.54	0.41
2:B:26:ILE:HD11	2:B:390:GLY:O	2.21	0.41
2:B:33:LEU:HD21	2:B:220:ALA:HB1	2.02	0.41
2:B:263:ALA:HB1	2:B:317:SER:O	2.21	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.50	0.41
2:B:369:LEU:O	2:B:372:VAL:HG22	2.21	0.41
2:B:415:LYS:C	2:B:417:PHE:N	2.76	0.41
2:B:429:ASP:OD1	2:O:60:THR:HG21	2.20	0.41
3:C:272:GLU:H	3:C:272:GLU:CD	2.29	0.41
3:C:304:LEU:O	3:C:305:ILE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:331:ALA:HB2	7:G:52:PHE:CD2	2.56	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.55	0.41
5:E:133:VAL:O	5:E:133:VAL:HG13	2.21	0.41
6:F:82:LYS:O	6:F:83:TYR:C	2.64	0.41
6:F:89:TYR:CD1	6:F:89:TYR:C	2.99	0.41
6:F:104:ARG:O	6:F:108:ASN:ND2	2.53	0.41
9:I:64:LEU:HD12	9:I:77:ARG:C	2.46	0.41
10:J:32:GLU:O	10:J:33:ARG:C	2.64	0.41
1:N:317:THR:OG1	1:N:318:GLY:N	2.53	0.41
1:N:368:GLN:O	1:N:369:LEU:HD23	2.20	0.41
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.85	0.41
2:O:29:LEU:HB2	2:O:31:ASN:ND2	2.36	0.41
2:O:62:ASN:O	2:O:63:LEU:C	2.63	0.41
2:O:203:ARG:CD	2:O:230:ALA:HA	2.51	0.41
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.33	0.41
2:O:300:ALA:C	2:O:302:ALA:N	2.77	0.41
2:O:307:PHE:H	9:V:52:ARG:HG2	1.86	0.41
3:P:40:VAL:HG11	3:P:233:LEU:HD11	2.02	0.41
3:P:50:LEU:O	3:P:54:MET:HG3	2.21	0.41
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.55	0.41
5:R:166:ASP:HB3	5:R:172:ARG:HH11	1.85	0.41
7:T:56:TYR:CD2	7:T:56:TYR:C	2.97	0.41
1:A:10:ASN:ND2	2:B:19:PRO:CD	2.84	0.41
1:A:10:ASN:O	1:A:11:ILE:C	2.64	0.41
1:A:146:THR:O	1:A:150:PHE:HD1	2.03	0.41
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.50	0.41
3:C:145:THR:O	3:C:149:ASN:HB2	2.21	0.41
6:F:90:LEU:C	6:F:92:PRO:HD2	2.46	0.41
1:N:45:SER:OG	1:N:92:ARG:HA	2.20	0.41
1:N:168:GLU:CD	1:N:168:GLU:H	2.29	0.41
2:O:56:ARG:HG3	2:O:57:TYR:CD1	2.56	0.41
2:O:124:LEU:CD2	2:O:223:PHE:HB3	2.51	0.41
3:P:42:LEU:CD2	3:P:190:ILE:HG22	2.51	0.41
3:P:167:GLY:HA3	3:P:178:ARG:NH2	2.36	0.41
3:P:207:ASN:HD22	3:P:208:ASN:N	2.10	0.41
3:P:243:LEU:CD2	3:P:251:LEU:HD11	2.50	0.41
3:P:347:PRO:O	3:P:350:ILE:HG22	2.21	0.41
4:Q:228:SER:O	4:Q:229:VAL:C	2.64	0.41
6:S:70:LEU:C	6:S:70:LEU:CD1	2.87	0.41
1:A:39:VAL:HG13	1:A:39:VAL:O	2.21	0.40
3:C:163:GLU:O	3:C:167:GLY:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:PHE:CE1	4:D:222:MET:HE2	2.54	0.40
4:D:171:TYR:C	4:D:173:ASP:H	2.29	0.40
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.85	0.40
6:F:67:ASP:O	6:F:70:LEU:HG	2.21	0.40
1:N:30:SER:OG	1:N:32:GLN:HB2	2.22	0.40
1:N:292:SER:O	1:N:295:ALA:HB3	2.22	0.40
1:N:362:ARG:O	1:N:365:MET:HB3	2.21	0.40
2:O:157:VAL:HG13	2:O:158:GLY:N	2.34	0.40
2:O:209:ILE:HG13	2:O:379:LEU:HD13	2.01	0.40
2:O:367:THR:O	2:O:368:TYR:C	2.64	0.40
3:P:29:SER:HB2	18:P:3004:CDL:HB21	2.03	0.40
3:P:47:LEU:HD12	3:P:47:LEU:C	2.45	0.40
3:P:63:ALA:O	3:P:67:VAL:HG23	2.21	0.40
3:P:236:MET:HA	18:S:3003:CDL:H162	2.02	0.40
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.04	0.40
4:Q:138:PRO:HD3	8:U:58:LEU:HD23	2.02	0.40
4:Q:235:MET:CB	7:T:15:THR:HG22	2.51	0.40
5:R:69:LEU:CD1	5:R:71:LEU:HD11	2.51	0.40
6:S:77:LYS:HE2	6:S:78:GLU:OE2	2.21	0.40
6:S:91:GLU:N	6:S:92:PRO:HD2	2.36	0.40
2:B:19:PRO:O	2:B:20:GLY:O	2.39	0.40
2:B:259:THR:CG2	2:B:260:GLU:N	2.83	0.40
3:C:11:LEU:O	3:C:14:MET:HB2	2.21	0.40
3:C:216:SER:O	6:F:63:LYS:NZ	2.53	0.40
3:C:267:PRO:HA	5:R:147:ILE:HD11	2.03	0.40
4:D:228:SER:O	4:D:229:VAL:C	2.64	0.40
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.03	0.40
1:N:223:TYR:HD2	1:N:223:TYR:N	2.17	0.40
2:O:51:ILE:HG22	2:O:52:LYS:N	2.36	0.40
2:O:307:PHE:CD1	2:O:308:ASP:N	2.89	0.40
3:P:11:LEU:O	3:P:14:MET:HB2	2.21	0.40
4:Q:161:ALA:O	4:Q:163:PRO:HD3	2.22	0.40
4:Q:171:TYR:C	4:Q:173:ASP:H	2.29	0.40
1:A:62:LEU:C	1:A:64:PHE:N	2.78	0.40
1:A:178:THR:H	1:A:181:ASP:CG	2.29	0.40
1:A:438:ARG:HG3	1:A:438:ARG:HH11	1.86	0.40
3:C:70:THR:HA	3:C:74:VAL:CG2	2.51	0.40
3:C:109:LEU:HB2	3:C:314:ARG:HH21	1.86	0.40
5:E:91:TRP:C	5:E:93:GLY:N	2.79	0.40
5:E:103:GLN:CA	5:E:106:ILE:HD12	2.50	0.40
1:N:37:VAL:HG23	1:N:113:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.04	0.40
1:N:173:ASN:O	1:N:177:LEU:HG	2.21	0.40
1:N:281:ASP:O	1:N:283:THR:N	2.54	0.40
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	3.04	0.40
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.50	0.40
4:Q:139:ALA:HB2	8:U:41:ASP:HA	2.02	0.40
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.55	0.40
5:R:127:VAL:HG11	5:R:133:VAL:HG23	2.03	0.40
10:W:51:LEU:C	10:W:53:LYS:N	2.77	0.40
1:A:301:HIS:O	1:A:302:LYS:C	2.64	0.40
2:B:56:ARG:HB2	2:B:171:ALA:HB1	2.02	0.40
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.57	0.40
4:D:105:ASN:O	4:D:108:ALA:HB3	2.21	0.40
5:E:91:TRP:O	5:E:92:ARG:C	2.64	0.40
5:E:103:GLN:HA	5:E:106:ILE:CG1	2.52	0.40
2:O:19:PRO:HB3	2:O:41:PHE:CG	2.57	0.40
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.56	0.40
3:P:338:TRP:CZ2	3:P:348:PHE:HE2	2.38	0.40
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.37	0.40
5:R:122:HIS:O	5:R:123:ASP:C	2.64	0.40
7:T:65:GLU:HA	7:T:65:GLU:OE1	2.22	0.40
8:U:40:CYS:O	8:U:41:ASP:C	2.64	0.40
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.62	0.40
9:V:59:SER:O	9:V:60:ALA:C	2.65	0.40
1:A:36:THR:HG21	1:A:373:THR:HA	2.04	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.84	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.76	0.40
2:B:34:ILE:HD13	2:B:390:GLY:HA2	2.04	0.40
3:C:6:ARG:HD3	3:C:16:ASN:OD1	2.22	0.40
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.51	0.40
4:D:47:ALA:HB1	4:D:89:ASP:O	2.21	0.40
4:D:139:ALA:HB3	8:H:54:CYS:SG	2.62	0.40
5:E:52:LYS:HD3	5:E:52:LYS:O	2.21	0.40
8:H:20:ILE:HD11	8:H:76:LYS:CD	2.44	0.40
1:N:15:ASN:HB3	1:N:205:HIS:CD2	2.57	0.40
2:O:109:VAL:HG21	2:O:119:VAL:HG23	2.02	0.40
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.04	0.40
2:O:325:TYR:C	2:O:325:TYR:HD2	2.30	0.40
2:O:422:LYS:O	2:O:436:LEU:HD21	2.21	0.40
3:P:30:ALA:C	3:P:32:TRP:N	2.80	0.40
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	2.04	0.40
4:Q:224:ARG:O	4:Q:225:HIS:C	2.65	0.40
5:R:34:GLY:HA2	10:W:10:TYR:HB2	2.04	0.40
5:R:103:GLN:HA	5:R:106:ILE:CG1	2.51	0.40
10:W:7:ARG:HB3	10:W:7:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	393 (89%)	40 (9%)	8 (2%)	6	31
1	N	440/446 (99%)	397 (90%)	36 (8%)	7 (2%)	7	34
2	B	419/441 (95%)	339 (81%)	63 (15%)	17 (4%)	2	13
2	O	420/441 (95%)	336 (80%)	66 (16%)	18 (4%)	2	12
3	C	378/380 (100%)	358 (95%)	18 (5%)	2 (0%)	24	60
3	P	377/380 (99%)	349 (93%)	24 (6%)	4 (1%)	11	43
4	D	239/241 (99%)	217 (91%)	20 (8%)	2 (1%)	16	50
4	Q	239/241 (99%)	214 (90%)	22 (9%)	3 (1%)	9	38
5	E	194/196 (99%)	157 (81%)	24 (12%)	13 (7%)	1	5
5	R	194/196 (99%)	161 (83%)	21 (11%)	12 (6%)	1	6
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	12	45
7	G	79/81 (98%)	66 (84%)	9 (11%)	4 (5%)	1	10
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	1	9
8	H	68/77 (88%)	57 (84%)	8 (12%)	3 (4%)	2	12
8	U	65/77 (84%)	48 (74%)	16 (25%)	1 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	29/47 (62%)	19 (66%)	7 (24%)	3 (10%)	0	2
9	V	29/47 (62%)	20 (69%)	7 (24%)	2 (7%)	1	5
10	J	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	7	32
10	W	57/61 (93%)	45 (79%)	8 (14%)	4 (7%)	1	4
All	All	4002/4160 (96%)	3475 (87%)	418 (10%)	109 (3%)	4	22

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	114	ASP
2	B	171	ALA
2	B	230	ALA
2	B	236	LYS
5	E	69	LEU
5	E	70	ALA
5	E	95	PRO
7	G	7	LEU
8	H	12	GLU
10	J	56	LYS
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	114	ASP
2	O	171	ALA
2	O	222	GLN
2	O	225	ASN
2	O	226	ILE
2	O	236	LYS
3	P	157	ILE
5	R	69	LEU
5	R	72	SER
5	R	95	PRO
7	T	7	LEU
10	W	56	LYS
1	A	71	PRO
1	A	72	CYS
1	A	282	ARG
1	A	433	ASP

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Mol	Chain	Res	Type
2	B	31	ASN
2	B	226	ILE
2	B	283	PRO
2	B	371	SER
2	B	390	GLY
5	E	74	ILE
5	E	113	ASP
5	E	137	GLY
7	G	33	ALA
8	H	49	HIS
9	I	56	SER
1	N	20	ASP
1	N	72	CYS
1	N	282	ARG
2	O	221	GLU
2	O	230	ALA
2	O	283	PRO
2	O	371	SER
2	O	390	GLY
3	P	158	GLY
4	Q	177	ALA
5	R	113	ASP
7	T	33	ALA
2	B	30	PRO
3	C	3	PRO
5	E	73	LYS
5	E	78	LEU
5	E	141	HIS
8	H	72	LYS
9	I	55	MET
1	N	71	PRO
1	N	288	LYS
2	O	224	LEU
3	P	3	PRO
3	P	156	TYR
5	R	92	ARG
6	S	11	ARG
10	W	60	GLU
1	A	3	THR
1	A	306	SER
3	C	156	TYR
5	E	92	ARG

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Mol	Chain	Res	Type
5	E	130	PRO
9	I	63	ASP
2	O	227	ARG
4	Q	198	HIS
5	R	78	LEU
5	R	141	HIS
10	W	57	HIS
10	W	61	ALA
1	A	288	LYS
2	B	22	GLU
2	B	266	SER
2	B	382	ILE
4	D	177	ALA
5	E	123	ASP
4	Q	162	PRO
5	R	21	ALA
5	R	74	ILE
5	R	130	PRO
5	R	137	GLY
9	V	63	ASP
2	B	319	SER
1	N	260	PRO
2	O	319	SER
5	R	106	ILE
7	T	27	PRO
8	U	28	GLU
1	A	260	PRO
5	E	106	ILE
7	G	27	PRO
2	O	382	ILE
7	G	50	PRO
7	T	50	PRO
9	V	76	VAL
2	O	288	GLY
4	D	162	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	349 (96%)	16 (4%)	25	60
1	N	365/368 (99%)	346 (95%)	19 (5%)	21	55
2	B	332/347 (96%)	319 (96%)	13 (4%)	28	62
2	O	333/347 (96%)	315 (95%)	18 (5%)	20	53
3	C	329/329 (100%)	323 (98%)	6 (2%)	51	77
3	P	328/329 (100%)	323 (98%)	5 (2%)	57	80
4	D	200/200 (100%)	194 (97%)	6 (3%)	36	69
4	Q	200/200 (100%)	194 (97%)	6 (3%)	36	69
5	E	166/166 (100%)	158 (95%)	8 (5%)	23	57
5	R	166/166 (100%)	157 (95%)	9 (5%)	20	53
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	60
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	53
7	G	71/71 (100%)	68 (96%)	3 (4%)	26	61
7	T	69/71 (97%)	66 (96%)	3 (4%)	26	60
8	H	65/71 (92%)	62 (95%)	3 (5%)	24	58
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	57
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	35
9	V	23/26 (88%)	22 (96%)	1 (4%)	26	60
10	J	49/49 (100%)	45 (92%)	4 (8%)	10	37
10	W	47/49 (96%)	44 (94%)	3 (6%)	16	48
All	All	3380/3446 (98%)	3243 (96%)	137 (4%)	27	61

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	87	ASN
1	A	90	THR
1	A	91	SER
1	A	106	MET
1	A	181	ASP
1	A	223	TYR
1	A	228	VAL
1	A	233	ARG

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Mol	Chain	Res	Type
1	A	241	ILE
1	A	281	ASP
1	A	342	TRP
1	A	388	ARG
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	26	ILE
2	B	31	ASN
2	B	102	ARG
2	B	154	SER
2	B	227	ARG
2	B	248	ASN
2	B	285	ILE
2	B	291	VAL
2	B	344	LEU
2	B	358	THR
2	B	364	LEU
2	B	403	ASP
2	B	418	VAL
3	C	17	ASN
3	C	47	LEU
3	C	149	ASN
3	C	182	LEU
3	C	237	LEU
3	C	285	ILE
4	D	24	SER
4	D	43	MET
4	D	77	ASN
4	D	179	MET
4	D	240	PRO
4	D	241	LYS
5	E	6	THR
5	E	56	THR
5	E	59	ILE
5	E	69	LEU
5	E	74	ILE
5	E	80	ASP
5	E	135	LEU
5	E	184	THR
6	F	70	LEU
6	F	77	LYS

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Mol	Chain	Res	Type
6	F	84	GLU
6	F	91	GLU
7	G	27	PRO
7	G	29	ILE
7	G	41	PHE
8	H	10	GLU
8	H	26	GLN
8	H	67	HIS
9	I	70	LEU
9	I	71	ASN
10	J	16	ARG
10	J	22	LEU
10	J	26	LEU
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	70	ARG
1	N	87	ASN
1	N	90	THR
1	N	106	MET
1	N	124	GLU
1	N	181	ASP
1	N	223	TYR
1	N	228	VAL
1	N	241	ILE
1	N	281	ASP
1	N	342	TRP
1	N	388	ARG
1	N	395	TRP
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	23	ASP
2	O	26	ILE
2	O	31	ASN
2	O	102	ARG
2	O	154	SER
2	O	187	THR
2	O	212	LYS
2	O	227	ARG

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Mol	Chain	Res	Type
2	O	248	ASN
2	O	285	ILE
2	O	291	VAL
2	O	325	TYR
2	O	344	LEU
2	O	358	THR
2	O	364	LEU
2	O	403	ASP
2	O	418	VAL
3	P	17	ASN
3	P	47	LEU
3	P	149	ASN
3	P	237	LEU
3	P	285	ILE
4	Q	3	LEU
4	Q	24	SER
4	Q	43	MET
4	Q	77	ASN
4	Q	179	MET
4	Q	241	LYS
5	R	6	THR
5	R	47	THR
5	R	56	THR
5	R	59	ILE
5	R	69	LEU
5	R	74	ILE
5	R	80	ASP
5	R	135	LEU
5	R	184	THR
6	S	13	MET
6	S	70	LEU
6	S	84	GLU
6	S	91	GLU
6	S	110	LYS
7	T	27	PRO
7	T	29	ILE
7	T	41	PHE
8	U	26	GLN
8	U	67	HIS
8	U	71	HIS
9	V	70	LEU
10	W	22	LEU

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	ASN
1	A	49	ASN
1	A	85	HIS
1	A	94	GLN
1	A	118	GLN
1	A	126	GLN
1	A	136	GLN
1	A	147	ASN
1	A	159	GLN
1	A	176	HIS
1	A	274	ASN
1	A	308	GLN
1	A	360	HIS
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	192	HIS
2	B	222	GLN
2	B	248	ASN
2	B	276	GLN
2	B	313	ASN
2	B	315	ASN
2	B	362	ASN
2	B	363	GLN
2	B	380	ASN
2	B	400	GLN
2	B	412	ASN
3	C	4	ASN
3	C	17	ASN
3	C	55	HIS
3	C	69	HIS
3	C	82	ASN
3	C	86	ASN
3	C	149	ASN
3	C	207	ASN

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Mol	Chain	Res	Type
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
3	C	379	ASN
4	D	50	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	72	HIS
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	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	94	GLN
1	N	118	GLN
1	N	126	GLN
1	N	136	GLN
1	N	143	ASN
1	N	147	ASN
1	N	159	GLN
1	N	176	HIS
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
1	N	360	HIS
1	N	385	ASN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	192	HIS
2	O	222	GLN

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Mol	Chain	Res	Type
2	O	225	ASN
2	O	248	ASN
2	O	270	ASN
2	O	276	GLN
2	O	313	ASN
2	O	362	ASN
2	O	363	GLN
2	O	380	ASN
2	O	400	GLN
2	O	412	ASN
3	P	4	ASN
3	P	17	ASN
3	P	55	HIS
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	149	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	50	ASN
4	Q	200	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
6	S	56	ASN
6	S	72	HIS
6	S	79	GLN
7	T	23	GLN
7	T	28	ASN
7	T	44	GLN
7	T	64	GLN
7	T	73	ASN
8	U	71	HIS
8	U	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
15	PEE	E	2005	-	49,49,50	1.51	10 (20%)	52,54,55	0.86	3 (5%)
19	FES	R	501	5	0,4,4	-	-	-		
18	CDL	P	3004	-	39,39,99	1.25	3 (7%)	45,51,111	1.17	4 (8%)
15	PEE	C	2007	-	48,48,50	1.49	8 (16%)	51,53,55	0.86	3 (5%)
12	HEM	C	502	3	50,50,50	1.51	6 (12%)	67,82,82	1.41	9 (13%)
13	SMA	P	3001	-	38,38,38	1.71	10 (26%)	47,52,52	0.91	2 (4%)
17	HEC	Q	501	4	50,50,50	1.09	4 (8%)	68,82,82	1.58	11 (16%)
14	UQ	P	3002	-	19,19,63	2.62	9 (47%)	24,26,79	1.09	2 (8%)
12	HEM	C	501	3	50,50,50	1.53	8 (16%)	67,82,82	1.41	9 (13%)
13	SMA	C	2001	-	38,38,38	1.68	10 (26%)	47,52,52	0.96	3 (6%)
18	CDL	S	3003	-	49,49,99	1.14	2 (4%)	55,61,111	1.03	2 (3%)
15	PEE	R	3005	-	49,49,50	1.53	9 (18%)	52,54,55	0.85	3 (5%)
15	PEE	C	2008	-	20,20,50	1.75	5 (25%)	23,25,55	0.64	0
20	PLC	E	2009	-	31,31,41	1.70	6 (19%)	37,39,49	0.66	0
12	HEM	P	502	3	50,50,50	1.44	6 (12%)	67,82,82	1.26	6 (8%)
14	UQ	C	2002	-	19,19,63	2.66	9 (47%)	24,26,79	1.08	2 (8%)
17	HEC	D	501	4	50,50,50	0.93	0	68,82,82	1.55	10 (14%)
19	FES	E	501	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	HEM	P	501	3	50,50,50	1.44	6 (12%)	67,82,82	1.36	9 (13%)
15	PEE	P	3007	-	48,48,50	1.44	7 (14%)	51,53,55	0.81	2 (3%)
16	GOL	P	3011	-	5,5,5	1.51	1 (20%)	5,5,5	0.70	0
18	CDL	G	2004	-	39,39,99	1.33	5 (12%)	45,51,111	1.16	4 (8%)
20	PLC	R	3009	-	31,31,41	1.63	7 (22%)	37,39,49	0.63	1 (2%)
15	PEE	N	3008	-	4,4,50	3.63	4 (100%)	6,6,55	0.65	0
16	GOL	C	2011	-	5,5,5	1.32	0	5,5,5	0.57	0
18	CDL	D	2003	-	49,49,99	1.16	2 (4%)	55,61,111	1.03	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEE	E	2005	-	-	27/53/53/54	-
19	FES	R	501	5	-	-	0/1/1/1
18	CDL	P	3004	-	-	22/49/49/110	-
15	PEE	C	2007	-	-	21/52/52/54	-
12	HEM	C	502	3	-	8/14/54/54	-
13	SMA	P	3001	-	-	5/34/34/34	0/2/2/2
17	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
14	UQ	P	3002	-	-	3/11/35/87	0/1/1/1
12	HEM	C	501	3	-	6/14/54/54	-
13	SMA	C	2001	-	-	5/34/34/34	0/2/2/2
18	CDL	S	3003	-	-	24/59/59/110	-
15	PEE	R	3005	-	-	27/53/53/54	-
15	PEE	C	2008	-	-	9/24/24/54	-
20	PLC	E	2009	-	-	13/35/35/45	-
12	HEM	P	502	3	-	8/14/54/54	-
14	UQ	C	2002	-	-	3/11/35/87	0/1/1/1
17	HEC	D	501	4	1/1/3/7	8/14/54/54	-
19	FES	E	501	5	-	-	0/1/1/1
12	HEM	P	501	3	-	6/14/54/54	-
15	PEE	P	3007	-	-	23/52/52/54	-
16	GOL	P	3011	-	-	0/4/4/4	-
18	CDL	G	2004	-	-	21/49/49/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PLC	R	3009	-	-	12/35/35/45	-
16	GOL	C	2011	-	-	2/4/4/4	-
18	CDL	D	2003	-	-	24/59/59/110	-

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	C6-C5	5.27	1.44	1.35
14	C	2002	UQ	C6-C5	4.95	1.44	1.35
13	C	2001	SMA	C7-C8	4.88	1.47	1.40
14	P	3002	UQ	C7-C6	4.82	1.60	1.51
15	N	3008	PEE	P-O1P	4.77	1.61	1.50
12	P	502	HEM	CBC-CAC	4.76	1.53	1.30
12	C	502	HEM	CBB-CAB	4.71	1.53	1.30
12	C	501	HEM	CBC-CAC	4.66	1.52	1.30
13	P	3001	SMA	O1-C2	4.65	1.42	1.36
12	P	501	HEM	CBC-CAC	4.60	1.52	1.30
14	C	2002	UQ	C7-C6	4.48	1.59	1.51
12	P	502	HEM	CBB-CAB	4.39	1.51	1.30
15	C	2007	PEE	C39-C38	4.35	1.56	1.31
15	E	2005	PEE	C39-C38	4.31	1.56	1.31
15	R	3005	PEE	C39-C38	4.18	1.55	1.31
15	P	3007	PEE	C39-C38	4.16	1.55	1.31
20	E	2009	PLC	O2-C'	4.13	1.46	1.34
13	P	3001	SMA	C7-C8	4.05	1.46	1.40
12	P	501	HEM	CBB-CAB	4.04	1.49	1.30
12	C	502	HEM	CBC-CAC	3.99	1.49	1.30
14	C	2002	UQ	C6-C1	3.99	1.57	1.46
14	C	2002	UQ	O3-C3	3.94	1.46	1.36
13	C	2001	SMA	C20-C19	3.81	1.36	1.33
14	P	3002	UQ	C6-C1	3.81	1.57	1.46
13	C	2001	SMA	O1-C2	3.77	1.41	1.36
20	R	3009	PLC	O2-C'	3.76	1.44	1.34
12	C	501	HEM	CBB-CAB	3.73	1.48	1.30
12	C	502	HEM	C4D-C3D	3.68	1.51	1.45
20	E	2009	PLC	P-O1P	3.54	1.63	1.50
20	R	3009	PLC	P-O1P	3.52	1.63	1.50
15	R	3005	PEE	P-O1P	3.49	1.62	1.50
15	E	2005	PEE	P-O1P	3.46	1.62	1.50
15	N	3008	PEE	P-O4P	3.44	1.64	1.54
13	P	3001	SMA	C6-C5	3.44	1.44	1.38
15	N	3008	PEE	P-O3P	3.44	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	2005	PEE	O3-C30	3.44	1.43	1.33
15	R	3005	PEE	O3-C30	3.42	1.43	1.33
12	C	501	HEM	CAB-C3B	-3.42	1.38	1.47
14	C	2002	UQ	O2-C2	3.35	1.44	1.36
14	P	3002	UQ	O3-C3	3.31	1.44	1.36
15	C	2008	PEE	P-O1P	3.25	1.62	1.50
15	R	3005	PEE	O2-C10	3.25	1.43	1.34
12	P	501	HEM	CAB-C3B	-3.23	1.38	1.47
15	R	3005	PEE	C21-C22	-3.22	1.35	1.51
15	E	2005	PEE	C21-C22	-3.21	1.35	1.51
12	C	502	HEM	C3B-C4B	3.18	1.51	1.44
15	P	3007	PEE	O2-C10	3.16	1.43	1.34
12	P	501	HEM	CAC-C3C	-3.15	1.39	1.47
15	C	2008	PEE	O2-C10	3.12	1.43	1.34
20	E	2009	PLC	O2-C2	3.10	1.53	1.46
15	P	3007	PEE	C21-C22	-3.09	1.36	1.51
15	C	2007	PEE	O2-C10	3.02	1.42	1.34
15	C	2007	PEE	C21-C22	-3.01	1.36	1.51
15	P	3007	PEE	P-O1P	3.00	1.61	1.50
12	P	502	HEM	C4D-C3D	3.00	1.50	1.45
20	R	3009	PLC	O3-CB	2.99	1.42	1.33
14	P	3002	UQ	O2-C2	2.95	1.43	1.36
14	C	2002	UQ	C2-C1	2.93	1.57	1.48
20	E	2009	PLC	O3-CB	2.93	1.41	1.33
13	C	2001	SMA	C6-C5	2.92	1.43	1.38
14	P	3002	UQ	CM5-C5	2.90	1.56	1.50
14	C	2002	UQ	CM5-C5	2.88	1.56	1.50
15	C	2007	PEE	O3-C30	2.85	1.41	1.33
14	P	3002	UQ	C2-C1	2.83	1.57	1.48
15	P	3007	PEE	O3-C30	2.83	1.41	1.33
13	P	3001	SMA	C4A-C5	2.79	1.45	1.40
15	C	2008	PEE	O3-C30	2.79	1.41	1.33
15	C	2007	PEE	P-O1P	2.78	1.60	1.50
14	C	2002	UQ	C5-C4	2.73	1.56	1.47
14	P	3002	UQ	C3-C4	2.71	1.56	1.48
15	E	2005	PEE	O2-C10	2.70	1.41	1.34
12	C	501	HEM	CHD-C1D	-2.68	1.33	1.39
14	C	2002	UQ	C3-C4	2.67	1.56	1.48
18	D	2003	CDL	O1-C1	2.67	1.51	1.43
18	G	2004	CDL	OA6-CA5	2.65	1.41	1.34
20	R	3009	PLC	O2-C2	2.62	1.52	1.46
20	E	2009	PLC	C1-C2	2.61	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	C5-C4	2.60	1.56	1.47
12	P	502	HEM	CAB-C3B	-2.60	1.40	1.47
18	S	3003	CDL	O1-C1	2.60	1.50	1.43
12	C	501	HEM	CHA-C1A	-2.59	1.33	1.39
12	P	502	HEM	CAC-C3C	-2.58	1.40	1.47
18	G	2004	CDL	O1-C1	2.58	1.50	1.43
12	C	502	HEM	CAC-C3C	-2.55	1.40	1.47
15	N	3008	PEE	P-O2P	2.53	1.62	1.54
15	E	2005	PEE	C31-C30	2.53	1.58	1.50
13	P	3001	SMA	C6-C7	2.52	1.43	1.38
15	R	3005	PEE	C31-C30	2.50	1.58	1.50
18	P	3004	CDL	O1-C1	2.49	1.50	1.43
12	C	501	HEM	CAC-C3C	-2.48	1.40	1.47
13	P	3001	SMA	O7-C7	2.44	1.41	1.37
13	P	3001	SMA	C8-C8A	2.43	1.43	1.39
12	C	502	HEM	CAB-C3B	-2.42	1.40	1.47
13	P	3001	SMA	O5-C5	2.40	1.41	1.37
18	G	2004	CDL	CA3-CA4	2.40	1.58	1.50
13	P	3001	SMA	C20-C19	2.40	1.35	1.33
15	E	2005	PEE	C1-C2	2.39	1.58	1.50
17	Q	501	HEC	CMC-C2C	2.37	1.55	1.50
13	C	2001	SMA	O7-C7	2.36	1.41	1.37
13	C	2001	SMA	C11-C12	2.32	1.57	1.53
13	C	2001	SMA	C4A-C5	2.32	1.44	1.40
20	R	3009	PLC	C1-C2	2.30	1.58	1.50
16	P	3011	GOL	O2-C2	2.26	1.49	1.43
17	Q	501	HEC	C4B-NB	-2.26	1.36	1.40
13	C	2001	SMA	C6-C7	2.26	1.42	1.38
15	R	3005	PEE	C11-C10	2.25	1.57	1.50
15	C	2007	PEE	C3-C2	2.23	1.57	1.50
13	P	3001	SMA	C3-C2	2.22	1.39	1.34
12	P	501	HEM	CHA-C4D	-2.21	1.34	1.38
20	E	2009	PLC	C3-C2	2.20	1.57	1.50
12	P	502	HEM	C3B-C4B	2.18	1.49	1.44
15	R	3005	PEE	C1-C2	2.17	1.57	1.50
15	C	2008	PEE	C1-C2	2.16	1.57	1.50
12	P	501	HEM	C2A-C3A	-2.16	1.33	1.38
20	R	3009	PLC	C3-C2	2.16	1.57	1.50
15	E	2005	PEE	C3-C2	2.15	1.57	1.50
15	P	3007	PEE	C11-C10	2.15	1.56	1.50
13	C	2001	SMA	C8-C8A	2.14	1.43	1.39
15	C	2008	PEE	C11-C10	2.13	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	2005	PEE	P-O4P	2.13	1.67	1.59
15	C	2007	PEE	C11-C10	2.13	1.56	1.50
20	R	3009	PLC	C1B-CB	2.11	1.56	1.50
15	R	3005	PEE	C3-C2	2.11	1.57	1.50
18	S	3003	CDL	OA6-CA5	2.09	1.40	1.34
17	Q	501	HEC	FE-NC	-2.08	1.88	1.95
17	Q	501	HEC	FE-NA	2.07	2.02	1.95
18	G	2004	CDL	OA8-CA6	-2.06	1.40	1.45
18	P	3004	CDL	OA8-CA6	-2.06	1.40	1.45
15	C	2007	PEE	P-O4P	2.05	1.67	1.59
12	C	501	HEM	C3B-C4B	2.05	1.48	1.44
15	P	3007	PEE	C3-C2	2.05	1.57	1.50
18	G	2004	CDL	CB3-CB4	2.04	1.57	1.50
18	D	2003	CDL	OA6-CA5	2.03	1.40	1.34
13	C	2001	SMA	C3-C2	2.03	1.38	1.34
15	E	2005	PEE	C11-C10	2.02	1.56	1.50
12	C	501	HEM	CMA-C3A	2.02	1.54	1.50
18	P	3004	CDL	OA6-CA5	2.01	1.40	1.34

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CAA-C2A-C3A	-4.58	119.29	127.87
17	D	501	HEC	CAC-C3C-C4C	-4.52	118.69	124.91
17	Q	501	HEC	CAC-C3C-C4C	-4.39	118.88	124.91
17	Q	501	HEC	CAA-C2A-C3A	-4.31	119.80	127.87
12	P	502	HEM	CAD-C3D-C4D	4.20	132.01	124.70
17	D	501	HEC	CBA-CAA-C2A	3.91	123.33	112.53
12	C	501	HEM	C3B-C4B-NB	3.78	112.18	109.47
12	C	502	HEM	CAD-C3D-C4D	3.70	131.14	124.70
12	C	502	HEM	C2B-C1B-NB	3.68	114.07	109.84
17	D	501	HEC	CAC-C3C-C2C	3.64	132.64	126.89
17	Q	501	HEC	CAA-C2A-C1A	3.58	132.14	124.85
13	C	2001	SMA	O7-C7-C8	3.56	118.25	114.53
18	P	3004	CDL	CB4-OB6-CB5	-3.56	109.27	117.80
17	Q	501	HEC	CAC-C3C-C2C	3.49	132.42	126.89
17	Q	501	HEC	CBA-CAA-C2A	3.49	122.19	112.53
18	G	2004	CDL	CB4-OB6-CB5	-3.47	109.48	117.80
12	P	501	HEM	C3B-C4B-NB	3.41	111.92	109.47
12	P	502	HEM	C3B-C4B-NB	3.32	111.85	109.47
12	P	501	HEM	C3D-C4D-ND	3.32	113.81	110.17
17	D	501	HEC	CAA-C2A-C1A	3.30	131.57	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	3002	UQ	C8-C7-C6	3.29	120.18	112.08
14	C	2002	UQ	C8-C7-C6	3.28	120.15	112.08
12	C	501	HEM	CBA-CAA-C2A	-3.13	103.89	112.53
12	P	501	HEM	C2B-C1B-NB	3.06	113.36	109.84
12	C	501	HEM	C3B-C2B-C1B	-2.99	104.17	106.41
12	C	502	HEM	C3B-C4B-NB	2.94	111.58	109.47
12	P	501	HEM	C3B-C2B-C1B	-2.92	104.22	106.41
13	P	3001	SMA	C9-C10-C11	-2.91	109.03	114.46
17	D	501	HEC	CMA-C3A-C4A	2.86	129.77	124.73
15	E	2005	PEE	C22-C21-C20	2.85	127.58	113.86
12	C	501	HEM	CHC-C4B-NB	-2.85	121.35	124.42
15	C	2007	PEE	C22-C21-C20	2.82	127.40	113.86
13	C	2001	SMA	C9-C10-C11	-2.78	109.26	114.46
14	P	3002	UQ	C7-C6-C1	-2.78	115.28	118.52
15	R	3005	PEE	C22-C21-C20	2.78	127.20	113.86
15	P	3007	PEE	C22-C21-C20	2.77	127.19	113.86
18	D	2003	CDL	CA6-CA4-CA3	-2.77	105.33	111.78
17	Q	501	HEC	CAD-C3D-C4D	2.76	129.51	124.70
17	Q	501	HEC	CHC-C4B-NB	-2.73	120.99	124.37
12	C	501	HEM	CMD-C2D-C1D	2.72	129.28	125.03
17	Q	501	HEC	C3D-C4D-ND	2.70	112.96	110.35
12	C	501	HEM	C2B-C1B-NB	2.66	112.90	109.84
18	S	3003	CDL	CA6-CA4-CA3	-2.65	105.61	111.78
15	C	2007	PEE	C21-C22-C23	2.64	127.71	114.37
12	C	502	HEM	C4D-C3D-C2D	-2.62	103.08	106.89
17	D	501	HEC	C3D-C4D-ND	2.62	112.88	110.35
14	C	2002	UQ	C7-C6-C1	-2.61	115.49	118.52
15	P	3007	PEE	C21-C22-C23	2.59	127.48	114.37
15	R	3005	PEE	C21-C22-C23	2.58	127.42	114.37
12	C	502	HEM	C1D-C2D-C3D	2.58	109.69	106.98
12	C	502	HEM	C4D-ND-C1D	-2.57	102.16	105.21
18	D	2003	CDL	CB4-OB6-CB5	-2.57	111.66	117.80
15	E	2005	PEE	C21-C22-C23	2.56	127.29	114.37
12	C	501	HEM	CMB-C2B-C1B	2.54	129.00	125.03
12	P	501	HEM	CMD-C2D-C1D	2.54	129.00	125.03
17	D	501	HEC	CMD-C2D-C1D	2.52	128.97	125.03
13	P	3001	SMA	O7-C7-C8	2.51	117.15	114.53
12	P	502	HEM	C4C-C3C-C2C	-2.50	104.64	106.81
12	P	502	HEM	C2B-C1B-NB	2.47	112.68	109.84
12	C	502	HEM	CHA-C4D-ND	-2.45	121.33	124.37
18	G	2004	CDL	OB6-CB4-CB3	2.44	117.10	108.34
12	C	502	HEM	C3D-C4D-ND	2.44	112.85	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	501	HEM	CMB-C2B-C1B	2.39	128.77	125.03
18	P	3004	CDL	OB6-CB4-CB3	2.39	116.92	108.34
12	P	501	HEM	C2A-C1A-NA	2.39	112.80	110.15
18	G	2004	CDL	CB6-CB4-CB3	-2.36	106.29	111.78
17	Q	501	HEC	CAB-C3B-C2B	2.35	131.87	127.56
12	P	501	HEM	C4D-ND-C1D	-2.34	102.43	105.21
15	E	2005	PEE	O3-C3-C2	2.33	115.10	108.40
15	C	2007	PEE	O3-C3-C2	2.32	115.07	108.40
18	P	3004	CDL	CB6-CB4-CB3	-2.31	106.39	111.78
17	D	501	HEC	CHC-C4B-NB	-2.31	121.51	124.37
13	C	2001	SMA	C4A-C4-C3	-2.31	115.38	118.78
18	S	3003	CDL	CB4-OB6-CB5	-2.31	112.27	117.80
12	P	501	HEM	CBA-CAA-C2A	-2.30	106.16	112.53
15	R	3005	PEE	O3-C3-C2	2.27	114.95	108.40
18	P	3004	CDL	CA6-CA4-CA3	-2.26	106.51	111.78
12	P	502	HEM	CAD-C3D-C2D	-2.26	123.64	127.87
17	Q	501	HEC	CMD-C2D-C1D	2.21	128.49	125.03
12	P	502	HEM	C4D-C3D-C2D	-2.20	103.69	106.89
12	C	502	HEM	C4C-C3C-C2C	-2.16	104.94	106.81
17	D	501	HEC	CAD-C3D-C4D	2.16	128.47	124.70
12	C	501	HEM	C1B-NB-C4B	-2.15	102.67	105.21
12	C	501	HEM	C2A-C1A-NA	2.14	112.53	110.15
18	G	2004	CDL	CA6-CA4-CA3	-2.14	106.81	111.78
17	Q	501	HEC	CMA-C3A-C4A	2.12	128.47	124.73
20	R	3009	PLC	O3-C3-C2	2.01	114.20	108.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	D	501	HEC	NA
17	Q	501	HEC	NA

All (285) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	2001	SMA	C3-C2-C9-C10
13	C	2001	SMA	O1-C2-C9-C10
13	P	3001	SMA	C3-C2-C9-C10
13	P	3001	SMA	O1-C2-C9-C10
14	C	2002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	C	2007	PEE	C1-O3P-P-O2P
15	C	2008	PEE	C1-O3P-P-O2P
15	C	2008	PEE	C1-O3P-P-O1P
15	C	2008	PEE	C1-O3P-P-O4P
15	E	2005	PEE	C11-C10-O2-C2
15	E	2005	PEE	C1-O3P-P-O1P
15	E	2005	PEE	O4P-C4-C5-N
15	P	3007	PEE	C1-O3P-P-O2P
15	P	3007	PEE	C1-O3P-P-O4P
15	R	3005	PEE	C11-C10-O2-C2
15	R	3005	PEE	C1-O3P-P-O1P
15	R	3005	PEE	O4P-C4-C5-N
16	C	2011	GOL	C1-C2-C3-O3
18	D	2003	CDL	O1-C1-CB2-OB2
18	D	2003	CDL	OA6-CA4-CA6-OA8
18	D	2003	CDL	CB2-OB2-PB2-OB4
18	D	2003	CDL	CB2-OB2-PB2-OB5
18	G	2004	CDL	CA3-OA5-PA1-OA2
18	G	2004	CDL	CA3-OA5-PA1-OA3
18	G	2004	CDL	OB5-CB3-CB4-OB6
18	G	2004	CDL	C51-CB5-OB6-CB4
18	P	3004	CDL	CA3-OA5-PA1-OA2
18	P	3004	CDL	CA3-OA5-PA1-OA3
18	P	3004	CDL	OB5-CB3-CB4-OB6
18	P	3004	CDL	C51-CB5-OB6-CB4
18	S	3003	CDL	O1-C1-CB2-OB2
18	S	3003	CDL	OA6-CA4-CA6-OA8
18	S	3003	CDL	CB2-OB2-PB2-OB4
18	S	3003	CDL	CB2-OB2-PB2-OB5
20	E	2009	PLC	O4P-C4-C5-N
20	E	2009	PLC	C1'-C'-O2-C2
20	R	3009	PLC	O4P-C4-C5-N
20	R	3009	PLC	C1'-C'-O2-C2
15	E	2005	PEE	O5-C30-O3-C3
15	R	3005	PEE	O5-C30-O3-C3
15	E	2005	PEE	C31-C30-O3-C3
15	R	3005	PEE	C31-C30-O3-C3
18	S	3003	CDL	C31-CA7-OA8-CA6
15	E	2005	PEE	O4-C10-O2-C2
15	R	3005	PEE	O4-C10-O2-C2
18	G	2004	CDL	OB7-CB5-OB6-CB4
18	P	3004	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	E	2009	PLC	O'-C'-O2-C2
20	R	3009	PLC	O'-C'-O2-C2
18	D	2003	CDL	C31-CA7-OA8-CA6
17	D	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
15	C	2008	PEE	C31-C30-O3-C3
18	P	3004	CDL	C71-CB7-OB8-CB6
18	G	2004	CDL	O1-C1-CA2-OA2
18	P	3004	CDL	O1-C1-CA2-OA2
18	G	2004	CDL	C71-CB7-OB8-CB6
15	C	2008	PEE	O5-C30-O3-C3
18	P	3004	CDL	OB9-CB7-OB8-CB6
18	S	3003	CDL	OA9-CA7-OA8-CA6
18	G	2004	CDL	OB9-CB7-OB8-CB6
18	P	3004	CDL	C31-CA7-OA8-CA6
18	G	2004	CDL	CB2-C1-CA2-OA2
18	P	3004	CDL	CB2-C1-CA2-OA2
18	D	2003	CDL	OA9-CA7-OA8-CA6
18	G	2004	CDL	C31-CA7-OA8-CA6
17	Q	501	HEC	C2B-C3B-CAB-CBB
15	E	2005	PEE	C17-C18-C19-C20
18	P	3004	CDL	OA9-CA7-OA8-CA6
12	C	502	HEM	C4D-C3D-CAD-CBD
15	E	2005	PEE	C30-C31-C32-C33
15	R	3005	PEE	C30-C31-C32-C33
18	D	2003	CDL	CA5-C11-C12-C13
18	S	3003	CDL	CA5-C11-C12-C13
13	P	3001	SMA	C6-C7-O7-C7M
18	G	2004	CDL	OA9-CA7-OA8-CA6
15	R	3005	PEE	C17-C18-C19-C20
13	C	2001	SMA	C6-C7-O7-C7M
12	P	502	HEM	C4D-C3D-CAD-CBD
18	D	2003	CDL	CA2-C1-CB2-OB2
18	S	3003	CDL	CA2-C1-CB2-OB2
20	R	3009	PLC	C'-C1'-C2'-C3'
17	D	501	HEC	C4B-C3B-CAB-CBB
15	C	2007	PEE	C17-C18-C19-C20
15	C	2007	PEE	C37-C38-C39-C40
15	P	3007	PEE	C17-C18-C19-C20
15	P	3007	PEE	C37-C38-C39-C40
15	E	2005	PEE	C10-C11-C12-C13
15	R	3005	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	P	3004	CDL	C11-CA5-OA6-CA4
18	S	3003	CDL	C71-CB7-OB8-CB6
17	D	501	HEC	C4C-C3C-CAC-CBC
15	C	2007	PEE	C32-C33-C34-C35
20	R	3009	PLC	C1B-CB-O3-C3
15	E	2005	PEE	C40-C41-C42-C43
15	P	3007	PEE	C34-C35-C36-C37
15	C	2007	PEE	C34-C35-C36-C37
15	C	2007	PEE	C12-C13-C14-C15
15	R	3005	PEE	C40-C41-C42-C43
18	G	2004	CDL	C11-CA5-OA6-CA4
20	E	2009	PLC	C'-C1'-C2'-C3'
20	E	2009	PLC	C1B-CB-O3-C3
18	D	2003	CDL	C15-C16-C17-C18
18	S	3003	CDL	C15-C16-C17-C18
18	P	3004	CDL	OA7-CA5-OA6-CA4
15	P	3007	PEE	C12-C13-C14-C15
15	P	3007	PEE	C32-C33-C34-C35
18	S	3003	CDL	OB9-CB7-OB8-CB6
18	D	2003	CDL	C71-CB7-OB8-CB6
20	E	2009	PLC	OB-CB-O3-C3
20	R	3009	PLC	OB-CB-O3-C3
15	E	2005	PEE	C23-C24-C25-C26
18	G	2004	CDL	OA7-CA5-OA6-CA4
15	R	3005	PEE	C13-C14-C15-C16
15	E	2005	PEE	C13-C14-C15-C16
15	R	3005	PEE	C23-C24-C25-C26
13	P	3001	SMA	C8-C7-O7-C7M
15	C	2008	PEE	C11-C10-O2-C2
18	S	3003	CDL	CB7-C71-C72-C73
17	Q	501	HEC	C1A-C2A-CAA-CBA
15	P	3007	PEE	C39-C40-C41-C42
14	C	2002	UQ	C5-C6-C7-C8
12	C	501	HEM	C2B-C3B-CAB-CBB
17	D	501	HEC	C2B-C3B-CAB-CBB
15	P	3007	PEE	O3P-C1-C2-O2
12	P	501	HEM	C4B-C3B-CAB-CBB
15	C	2007	PEE	C39-C40-C41-C42
17	Q	501	HEC	C4B-C3B-CAB-CBB
13	C	2001	SMA	C8-C7-O7-C7M
18	D	2003	CDL	OB9-CB7-OB8-CB6
18	D	2003	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
18	S	3003	CDL	OA5-CA3-CA4-CA6
15	C	2008	PEE	O4-C10-O2-C2
17	D	501	HEC	C1A-C2A-CAA-CBA
18	D	2003	CDL	CA3-CA4-CA6-OA8
18	S	3003	CDL	CA3-CA4-CA6-OA8
15	C	2007	PEE	C15-C16-C17-C18
18	D	2003	CDL	C13-C14-C15-C16
18	D	2003	CDL	CB7-C71-C72-C73
18	D	2003	CDL	C16-C17-C18-C19
20	E	2009	PLC	C2'-C3'-C4'-C5'
15	E	2005	PEE	C39-C40-C41-C42
15	R	3005	PEE	C39-C40-C41-C42
17	Q	501	HEC	C4C-C3C-CAC-CBC
15	C	2007	PEE	O3P-C1-C2-O2
18	S	3003	CDL	C13-C14-C15-C16
18	S	3003	CDL	C16-C17-C18-C19
15	P	3007	PEE	C42-C43-C44-C45
20	R	3009	PLC	C2'-C3'-C4'-C5'
18	S	3003	CDL	C71-C72-C73-C74
20	R	3009	PLC	C4'-C5'-C6'-C7'
15	P	3007	PEE	C15-C16-C17-C18
18	D	2003	CDL	C71-C72-C73-C74
20	E	2009	PLC	C4'-C5'-C6'-C7'
15	C	2008	PEE	O3P-C1-C2-C3
20	E	2009	PLC	O3P-C1-C2-C3
20	R	3009	PLC	O3P-C1-C2-C3
15	C	2007	PEE	C42-C43-C44-C45
18	G	2004	CDL	CB3-CB4-CB6-OB8
18	P	3004	CDL	CA3-CA4-CA6-OA8
18	P	3004	CDL	CB3-CB4-CB6-OB8
15	E	2005	PEE	C42-C43-C44-C45
15	C	2007	PEE	C33-C34-C35-C36
15	R	3005	PEE	C42-C43-C44-C45
15	C	2007	PEE	C30-C31-C32-C33
15	E	2005	PEE	C15-C16-C17-C18
15	P	3007	PEE	C33-C34-C35-C36
18	G	2004	CDL	OB6-CB4-CB6-OB8
18	P	3004	CDL	OB6-CB4-CB6-OB8
15	P	3007	PEE	C43-C44-C45-C46
15	E	2005	PEE	C12-C13-C14-C15
18	P	3004	CDL	OB5-CB3-CB4-CB6
15	R	3005	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
15	R	3005	PEE	C12-C13-C14-C15
15	C	2007	PEE	C43-C44-C45-C46
12	P	501	HEM	C2B-C3B-CAB-CBB
13	P	3001	SMA	C15-C14-O14-C25
15	R	3005	PEE	C15-C16-C17-C18
20	E	2009	PLC	O3P-C1-C2-O2
20	R	3009	PLC	O3P-C1-C2-O2
18	G	2004	CDL	CA3-CA4-CA6-OA8
12	C	501	HEM	C4B-C3B-CAB-CBB
18	P	3004	CDL	OA6-CA4-CA6-OA8
15	C	2007	PEE	C20-C21-C22-C23
15	E	2005	PEE	C31-C32-C33-C34
15	E	2005	PEE	C2-C3-O3-C30
18	G	2004	CDL	CA2-C1-CB2-OB2
15	P	3007	PEE	O3P-C1-C2-C3
18	G	2004	CDL	OB5-CB3-CB4-CB6
18	D	2003	CDL	OA5-CA3-CA4-OA6
18	S	3003	CDL	OA5-CA3-CA4-OA6
15	C	2007	PEE	C13-C14-C15-C16
18	G	2004	CDL	OA6-CA4-CA6-OA8
17	D	501	HEC	C2C-C3C-CAC-CBC
15	P	3007	PEE	C20-C21-C22-C23
15	C	2007	PEE	C1-O3P-P-O4P
15	E	2005	PEE	C1-O3P-P-O4P
18	D	2003	CDL	CB2-OB2-PB2-OB3
18	G	2004	CDL	CA3-OA5-PA1-OA4
18	P	3004	CDL	CA3-OA5-PA1-OA4
18	S	3003	CDL	CB2-OB2-PB2-OB3
15	E	2005	PEE	C18-C19-C20-C21
15	E	2005	PEE	C1-C2-O2-C10
15	R	3005	PEE	C1-C2-O2-C10
15	P	3007	PEE	C13-C14-C15-C16
15	R	3005	PEE	C2-C3-O3-C30
15	R	3005	PEE	C31-C32-C33-C34
18	P	3004	CDL	CA2-C1-CB2-OB2
18	D	2003	CDL	C1-CA2-OA2-PA1
18	S	3003	CDL	C1-CA2-OA2-PA1
12	P	502	HEM	C4C-C3C-CAC-CBC
15	E	2005	PEE	C37-C38-C39-C40
15	R	3005	PEE	C2-C1-O3P-P
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
15	R	3005	PEE	C33-C34-C35-C36
12	P	502	HEM	C2D-C3D-CAD-CBD
12	C	502	HEM	CAA-CBA-CGA-O2A
13	C	2001	SMA	C15-C14-O14-C25
12	C	501	HEM	CAA-CBA-CGA-O1A
12	P	501	HEM	CAA-CBA-CGA-O1A
16	C	2011	GOL	O2-C2-C3-O3
12	P	502	HEM	CAA-CBA-CGA-O2A
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAD-CBD-CGD-O2D
18	G	2004	CDL	O1-C1-CB2-OB2
12	P	502	HEM	CAD-CBD-CGD-O1D
15	C	2007	PEE	C36-C37-C38-C39
15	P	3007	PEE	C16-C17-C18-C19
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAA-CBA-CGA-O1A
15	C	2007	PEE	O3P-C1-C2-C3
12	C	501	HEM	CAA-CBA-CGA-O2A
12	P	501	HEM	CAA-CBA-CGA-O2A
15	R	3005	PEE	C36-C37-C38-C39
12	C	502	HEM	CAD-CBD-CGD-O2D
15	C	2007	PEE	C16-C17-C18-C19
15	E	2005	PEE	C2-C1-O3P-P
15	R	3005	PEE	C35-C36-C37-C38
15	E	2005	PEE	C36-C37-C38-C39
12	P	501	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	C2D-C3D-CAD-CBD
12	C	501	HEM	CAD-CBD-CGD-O2D
15	E	2005	PEE	C16-C17-C18-C19
12	C	502	HEM	C2C-C3C-CAC-CBC
12	P	502	HEM	C2C-C3C-CAC-CBC
15	P	3007	PEE	C36-C37-C38-C39
17	Q	501	HEC	CAD-CBD-CGD-O2D
12	P	501	HEM	CAD-CBD-CGD-O1D
15	R	3005	PEE	C37-C38-C39-C40
15	P	3007	PEE	C31-C30-O3-C3
15	P	3007	PEE	O5-C30-O3-C3
12	C	501	HEM	CAD-CBD-CGD-O1D
17	D	501	HEC	CAD-CBD-CGD-O2D
12	C	502	HEM	C4C-C3C-CAC-CBC
15	R	3005	PEE	C16-C17-C18-C19
17	Q	501	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	R	3005	PEE	C38-C39-C40-C41
20	E	2009	PLC	C2B-C1B-CB-O3
15	C	2008	PEE	O3-C30-C31-C32
20	R	3009	PLC	C2B-C1B-CB-O3
15	E	2005	PEE	C38-C39-C40-C41
18	D	2003	CDL	C12-C11-CA5-OA6
18	S	3003	CDL	C12-C11-CA5-OA6
17	D	501	HEC	CAD-CBD-CGD-O1D
20	E	2009	PLC	C3'-C4'-C5'-C6'
18	S	3003	CDL	C72-C71-CB7-OB8
15	P	3007	PEE	C30-C31-C32-C33
20	E	2009	PLC	C2B-C1B-CB-OB
17	Q	501	HEC	CAA-CBA-CGA-O2A
15	E	2005	PEE	C22-C23-C24-C25
15	C	2007	PEE	O3-C30-C31-C32
15	P	3007	PEE	O3-C30-C31-C32
15	P	3007	PEE	O2-C10-C11-C12
20	R	3009	PLC	C2B-C1B-CB-OB
18	D	2003	CDL	C72-C71-CB7-OB8
18	P	3004	CDL	C1-CB2-OB2-PB2
18	D	2003	CDL	C12-C11-CA5-OA7
18	S	3003	CDL	C12-C11-CA5-OA7
18	S	3003	CDL	C72-C71-CB7-OB9
18	P	3004	CDL	O1-C1-CB2-OB2
15	C	2007	PEE	O2-C10-C11-C12
18	D	2003	CDL	C72-C71-CB7-OB9

There are no ring outliers.

20 monomers are involved in 61 short contacts:

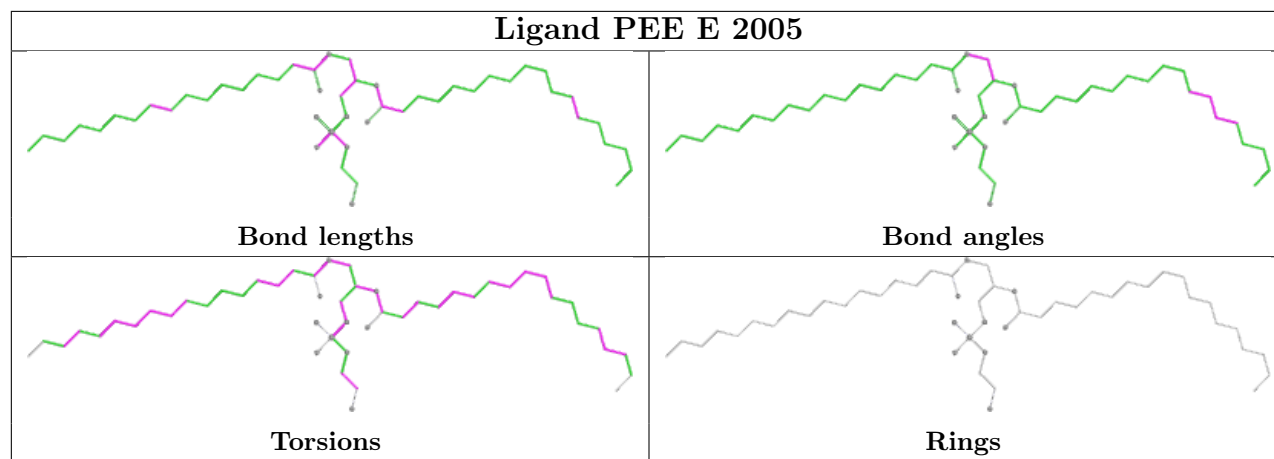
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	2005	PEE	4	0
19	R	501	FES	1	0
18	P	3004	CDL	3	0
15	C	2007	PEE	1	0
12	C	502	HEM	6	0
13	P	3001	SMA	4	0
14	P	3002	UQ	2	0
12	C	501	HEM	5	0
13	C	2001	SMA	4	0
18	S	3003	CDL	2	0
15	R	3005	PEE	4	0

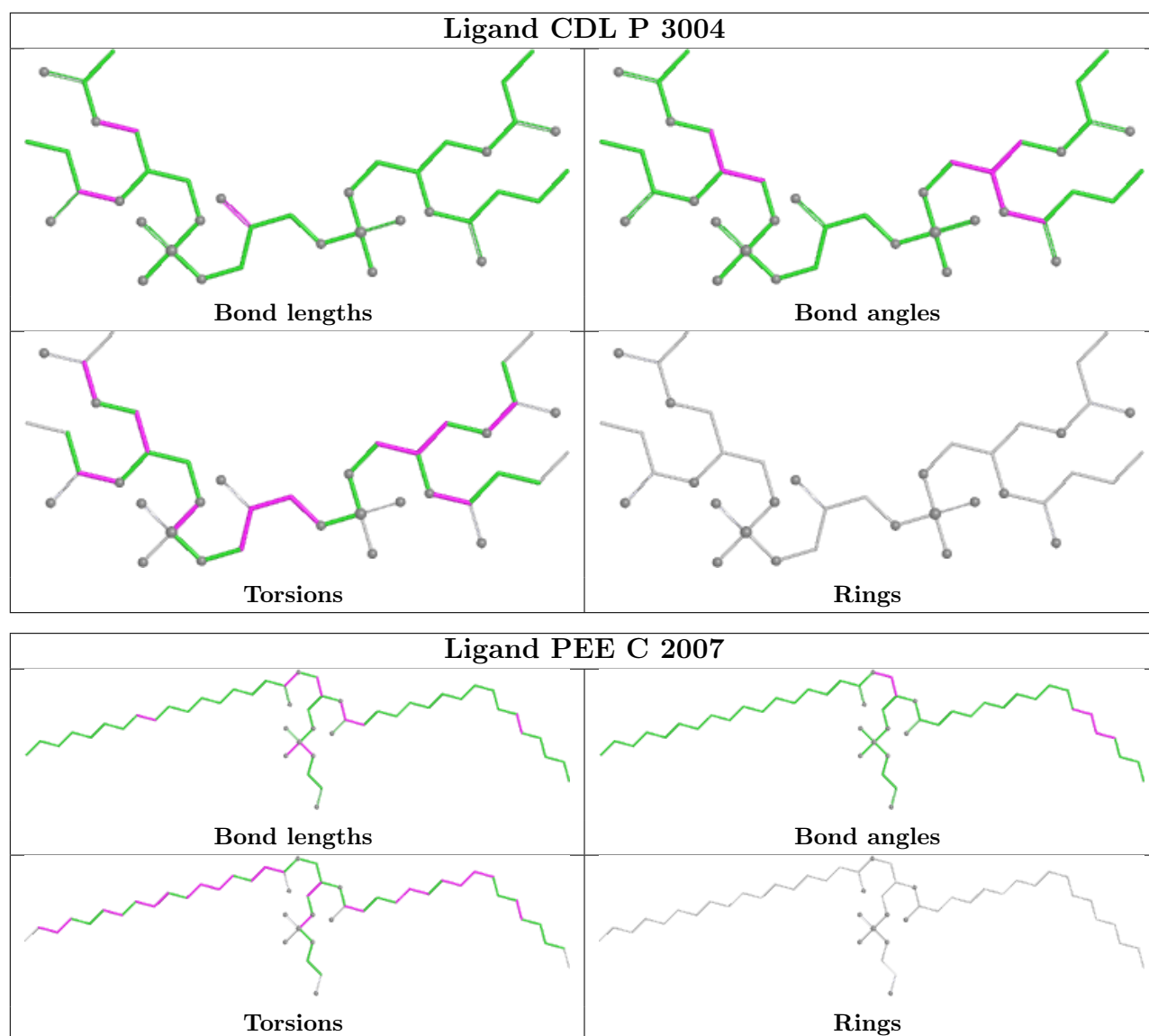
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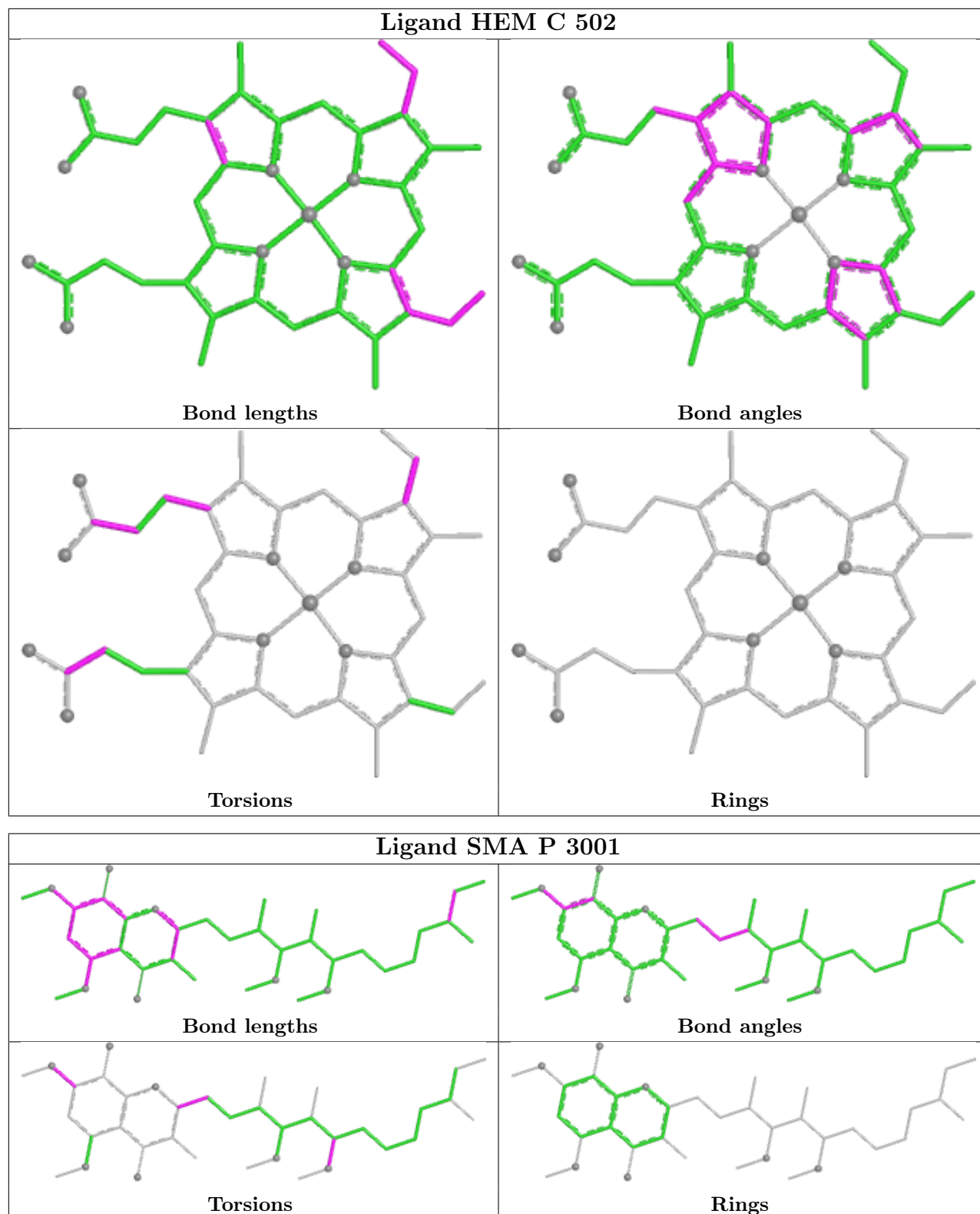
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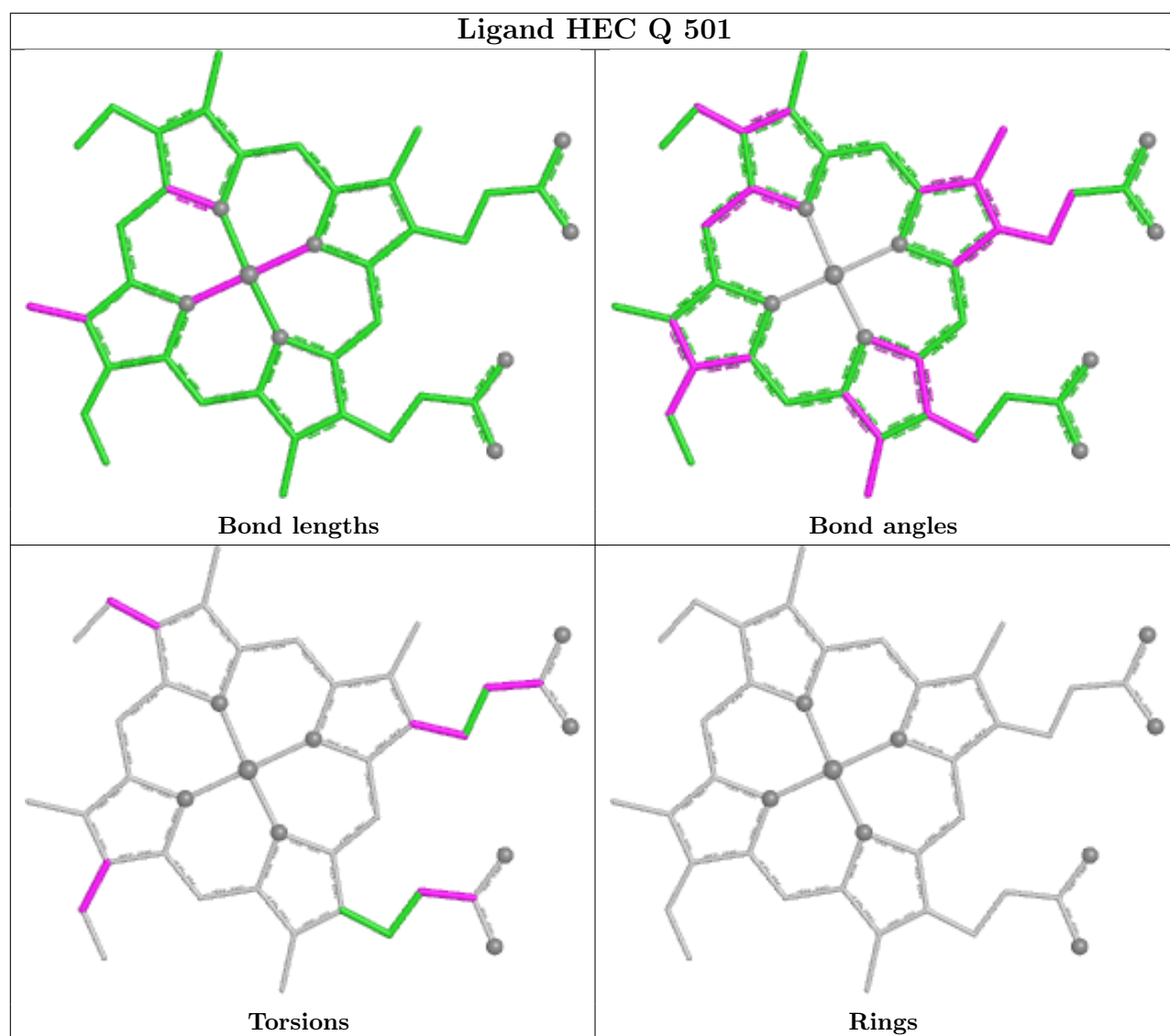
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	E	2009	PLC	3	0
12	P	502	HEM	7	0
14	C	2002	UQ	4	0
12	P	501	HEM	5	0
15	P	3007	PEE	1	0
16	P	3011	GOL	1	0
18	G	2004	CDL	1	0
20	R	3009	PLC	2	0
18	D	2003	CDL	1	0

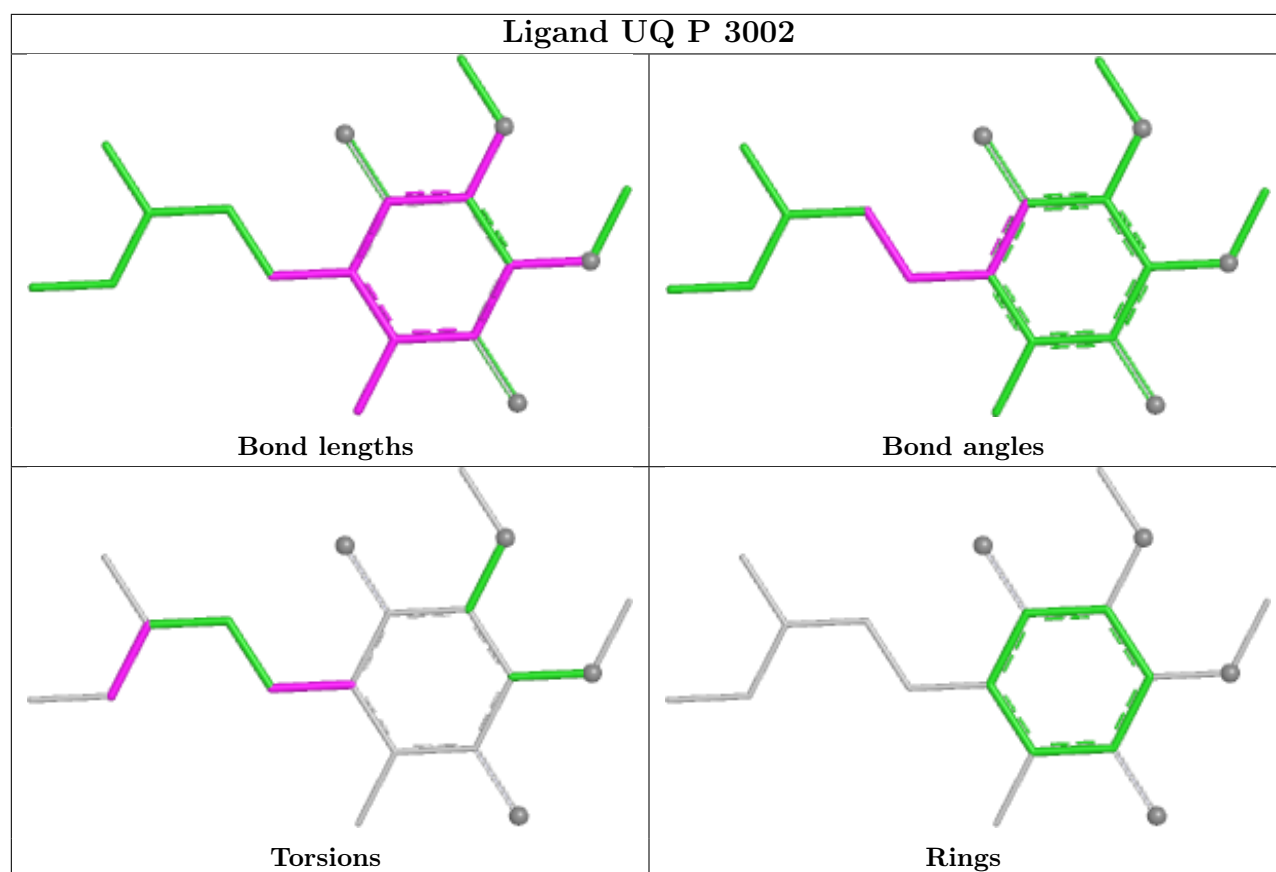
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

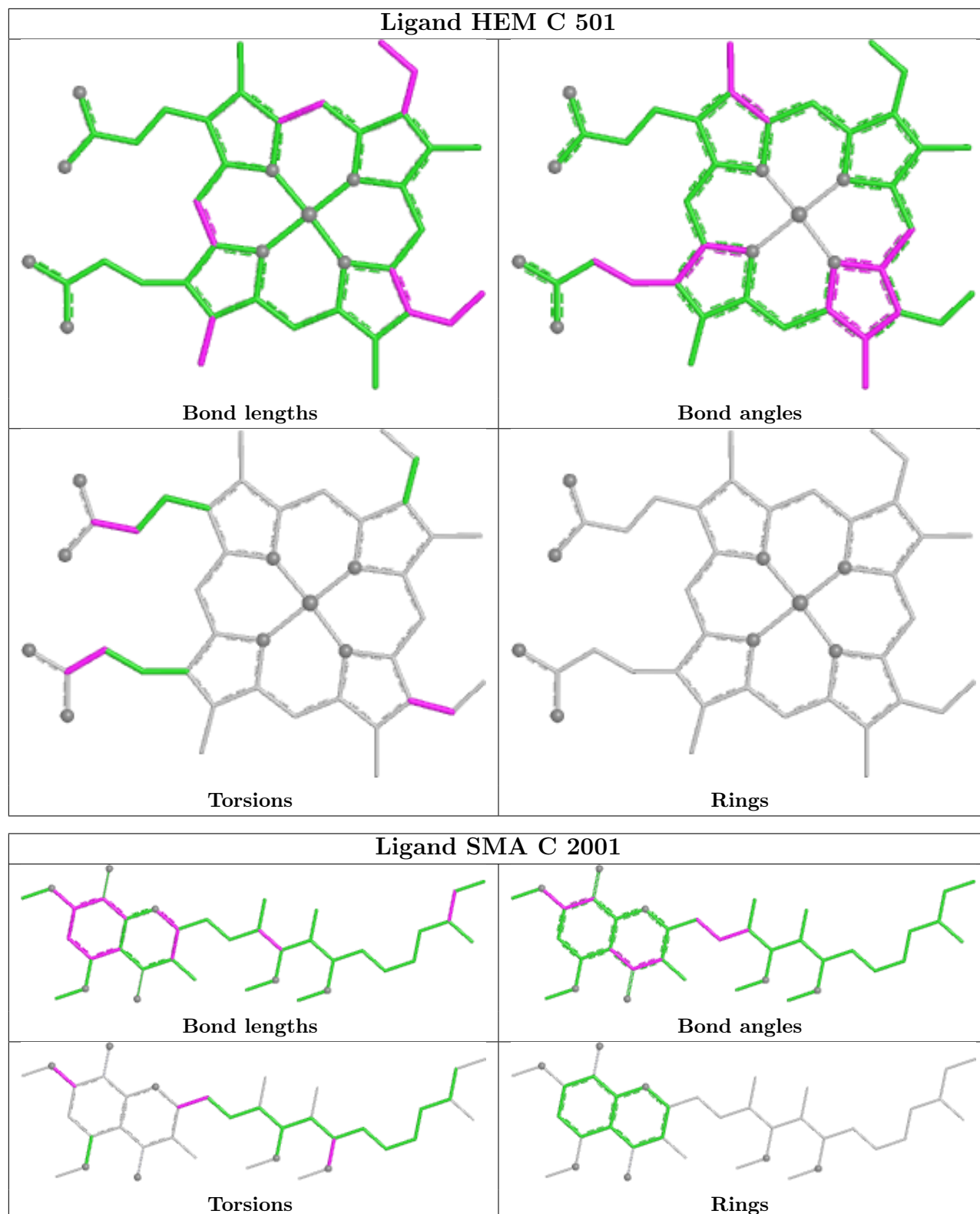


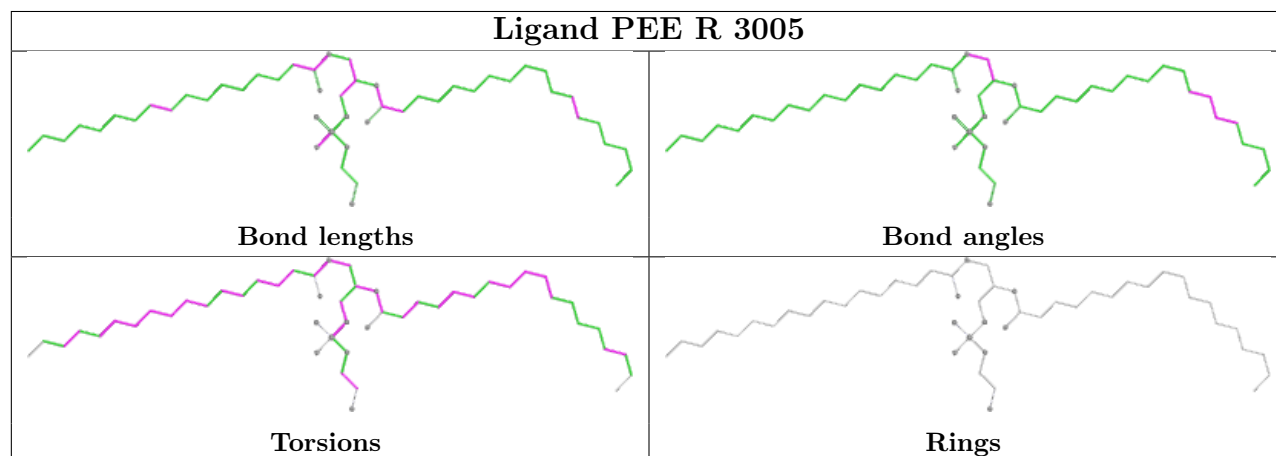
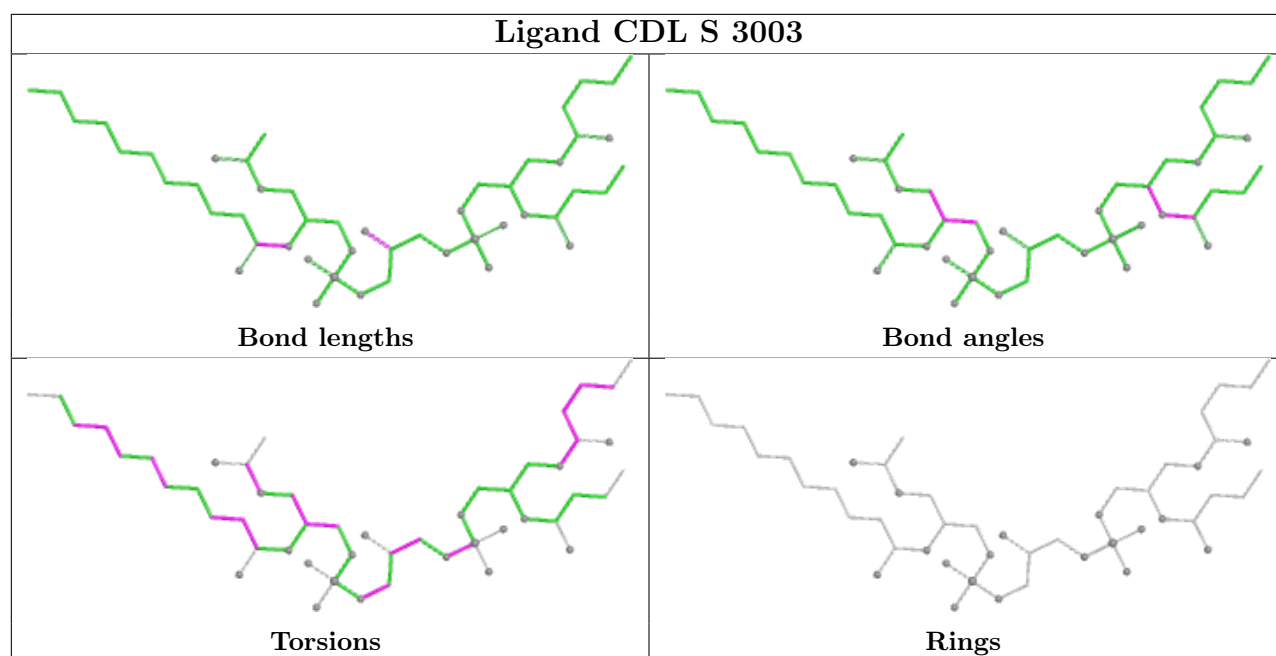


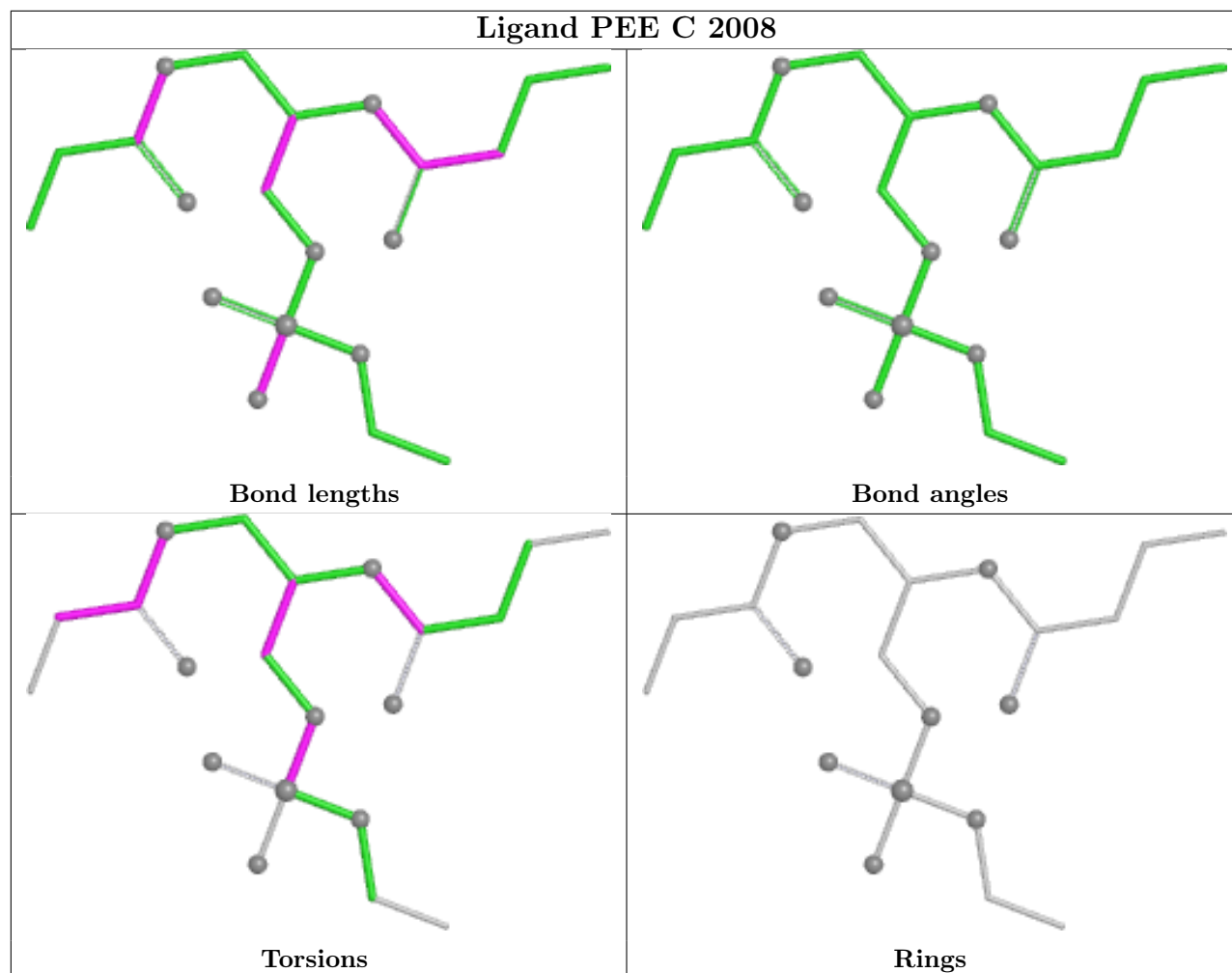


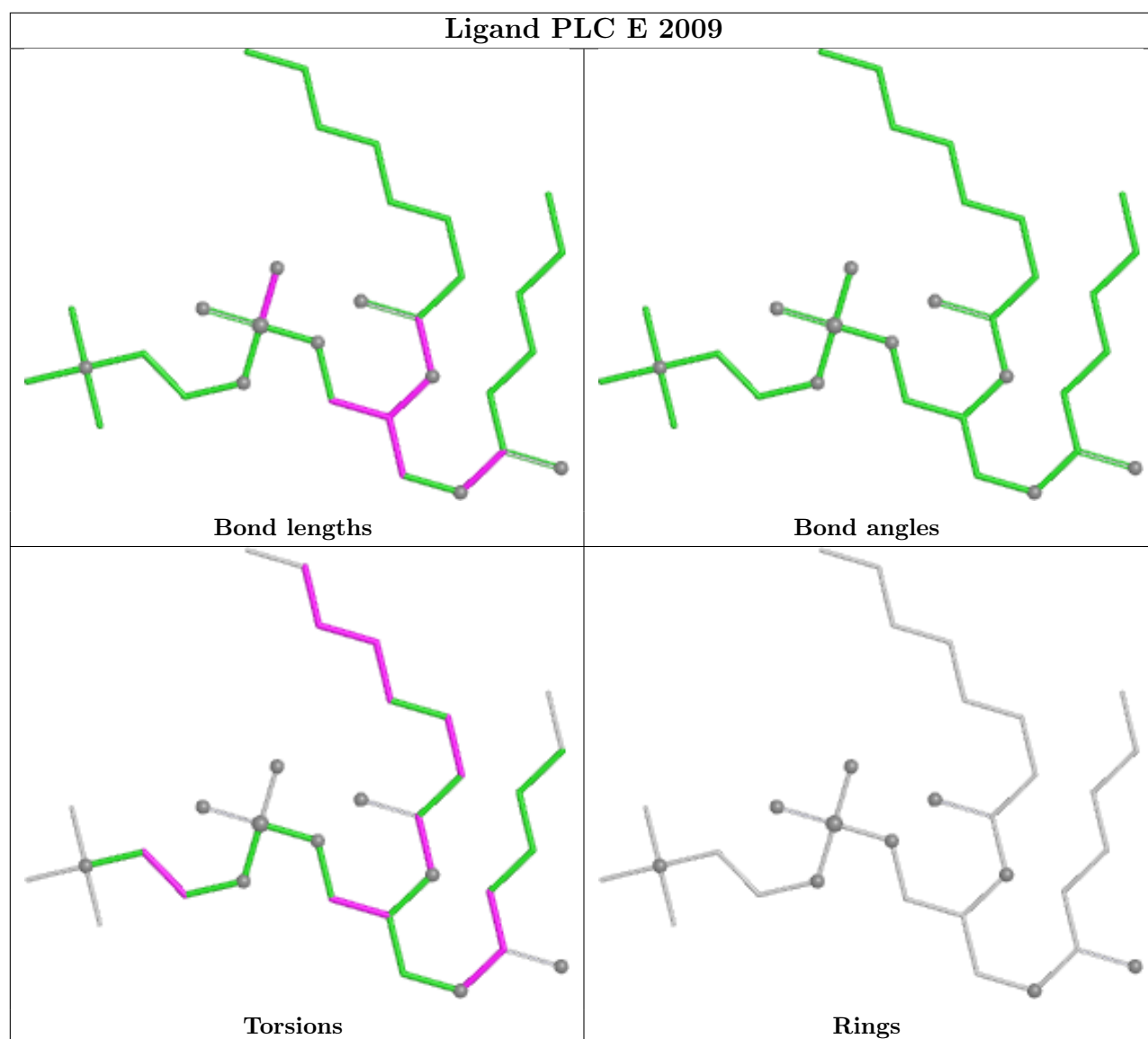


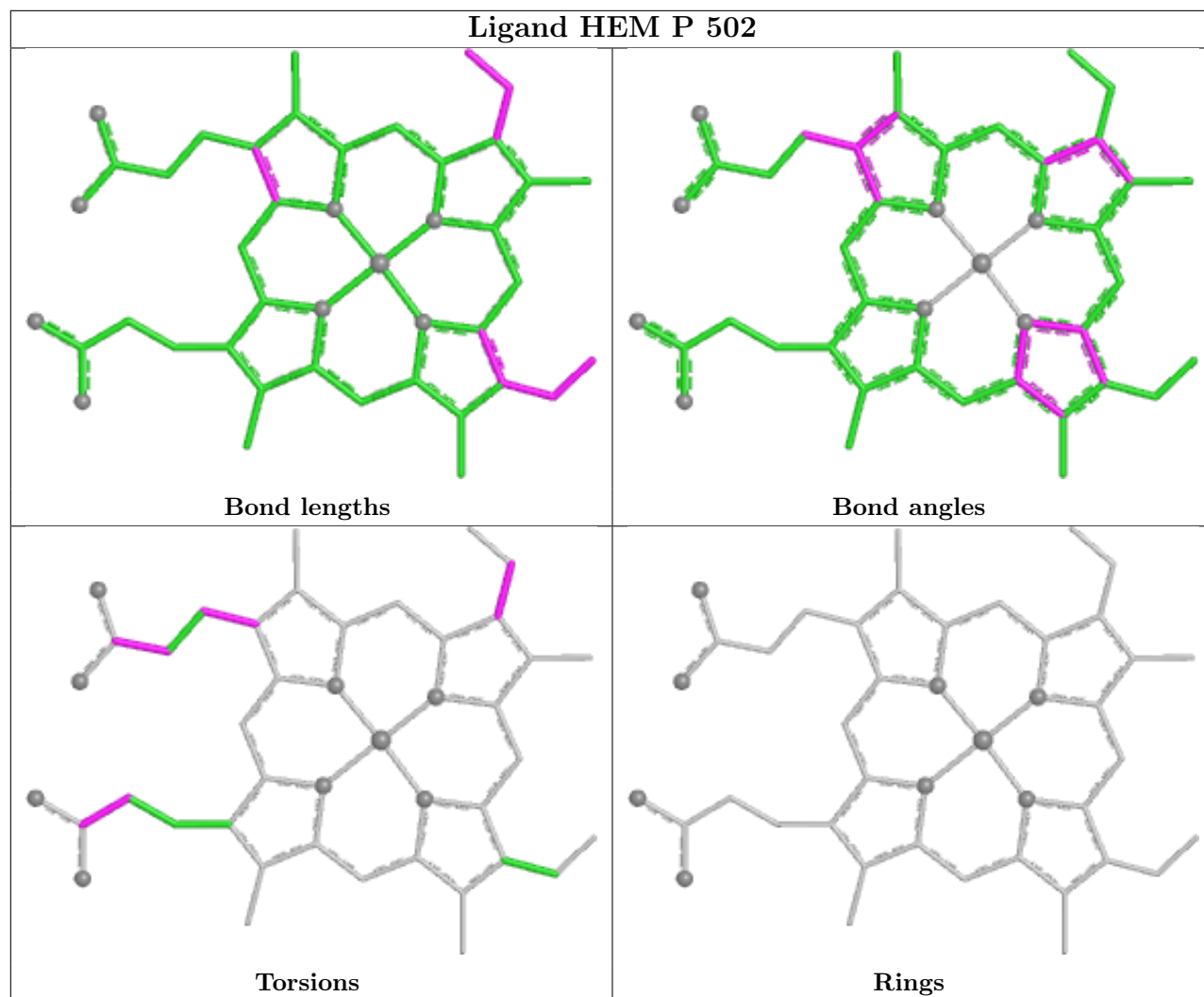


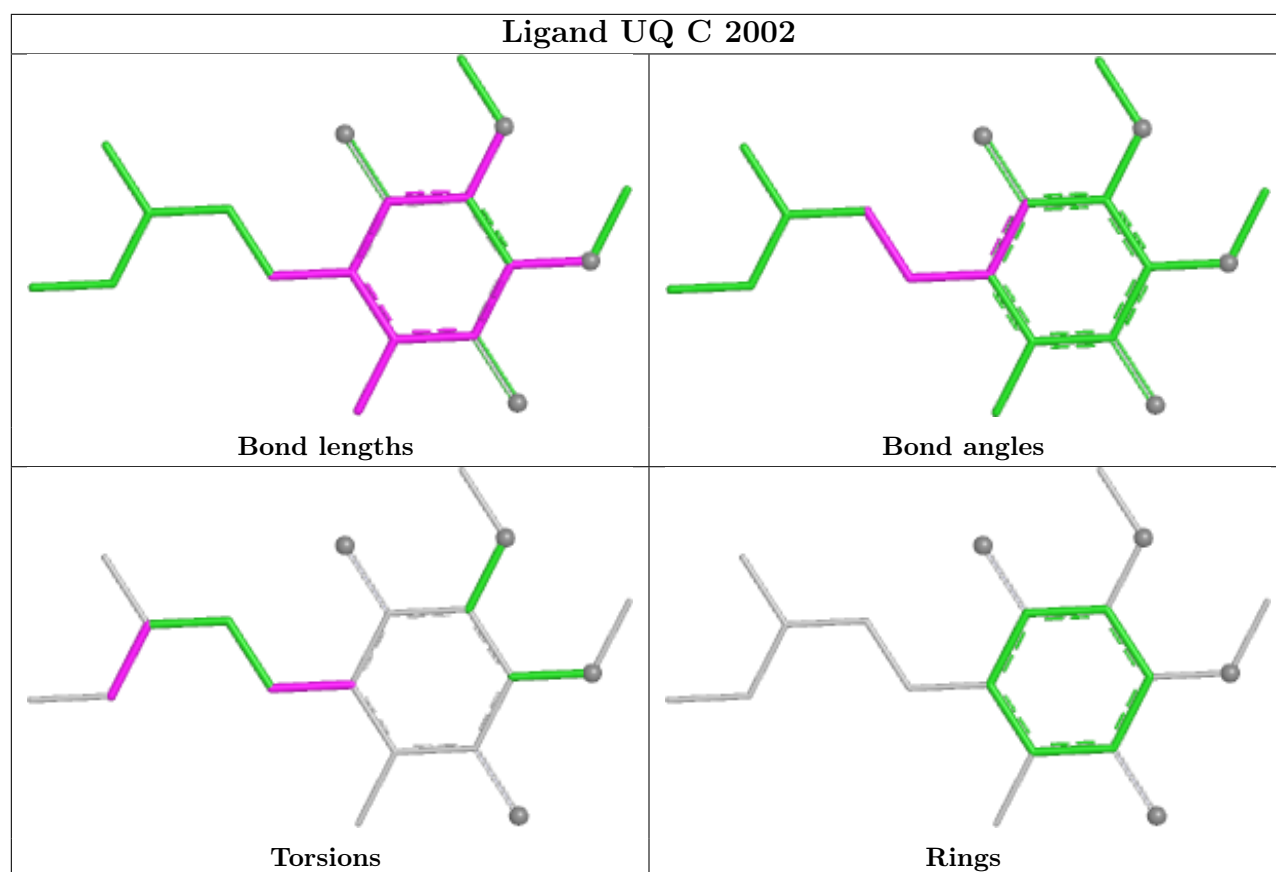


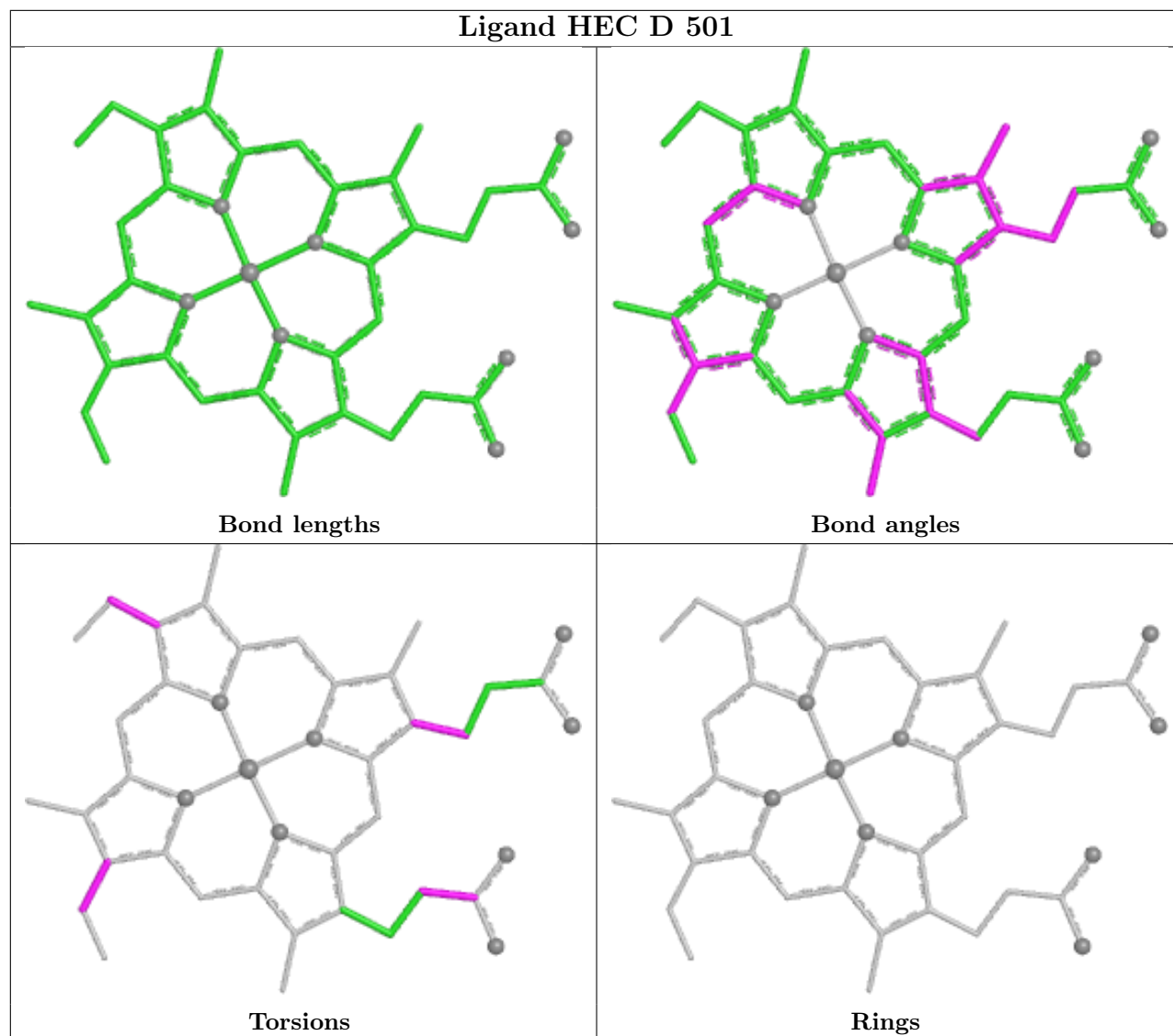


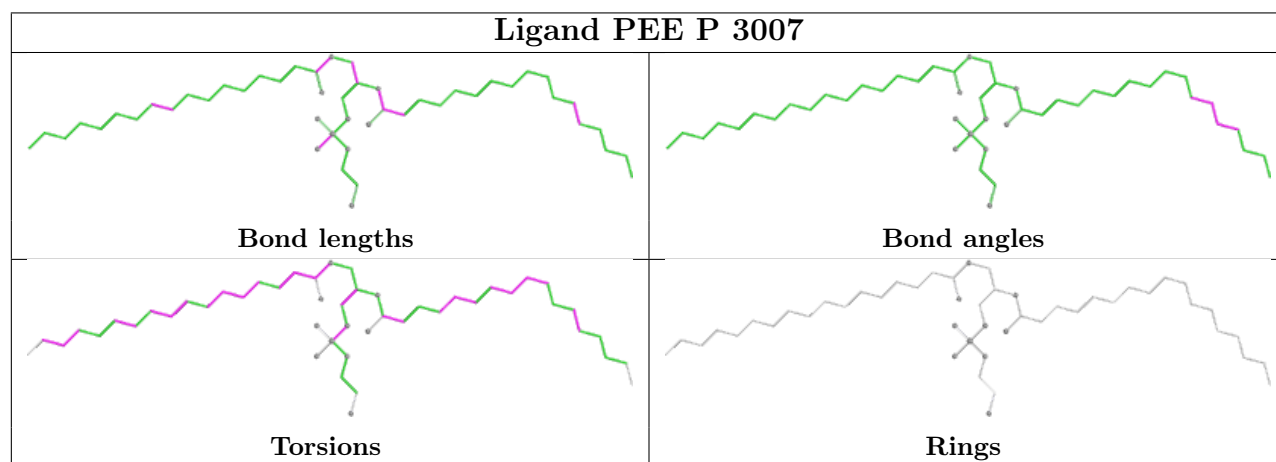
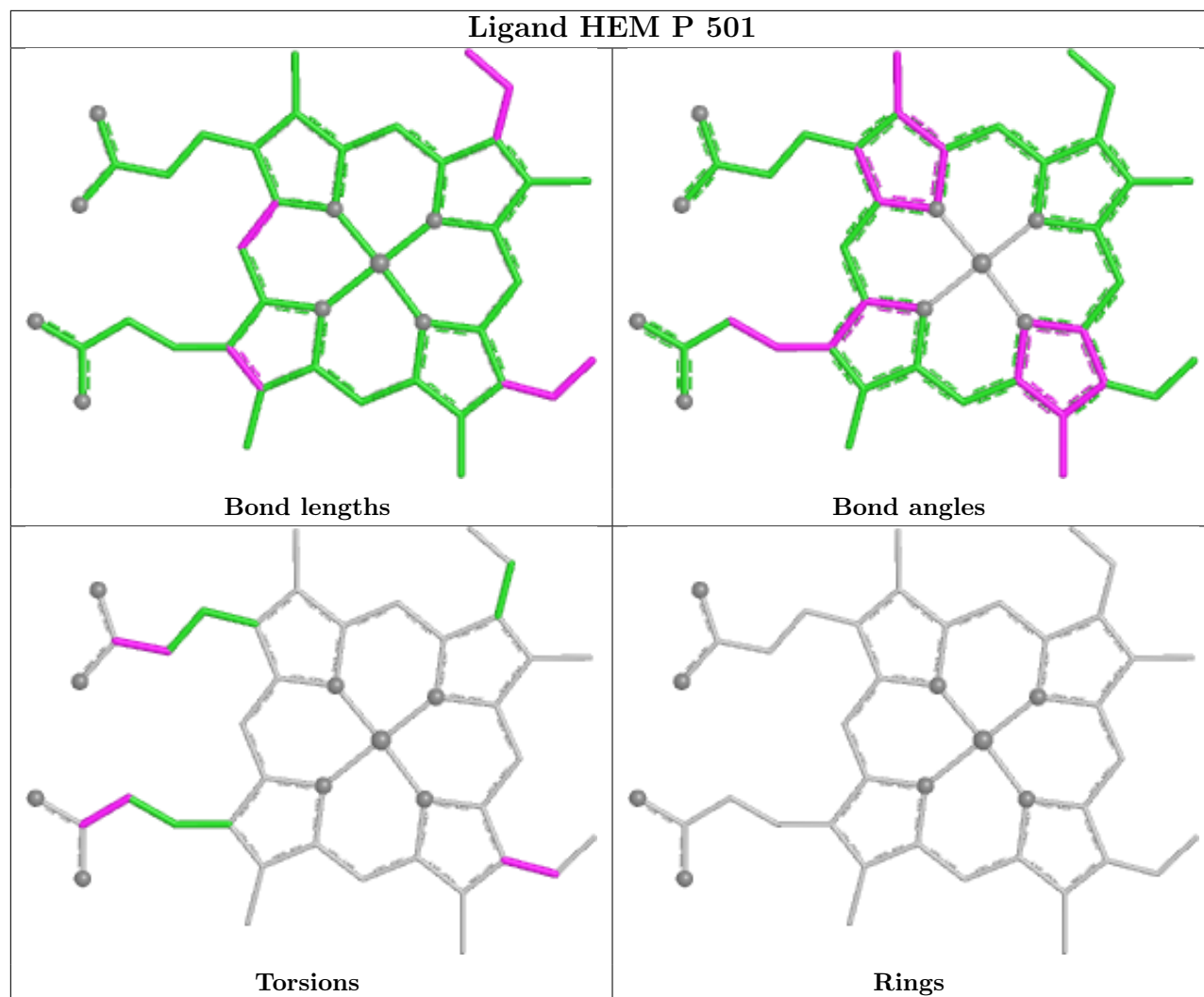


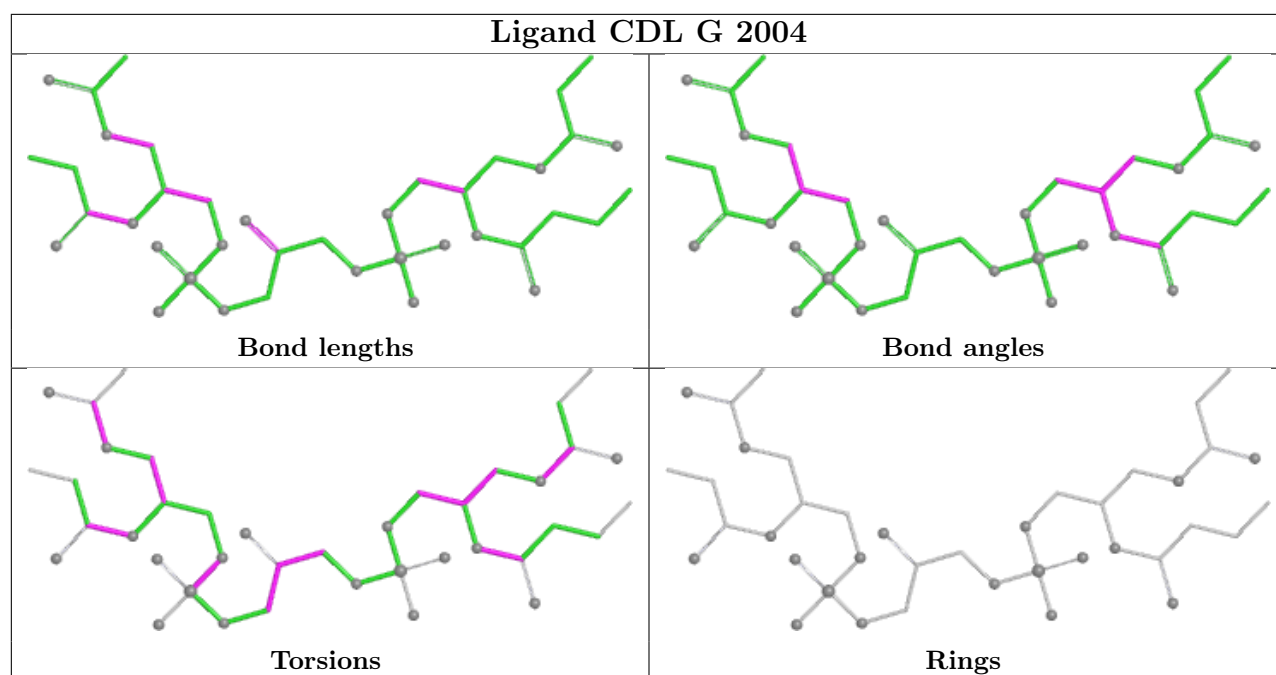


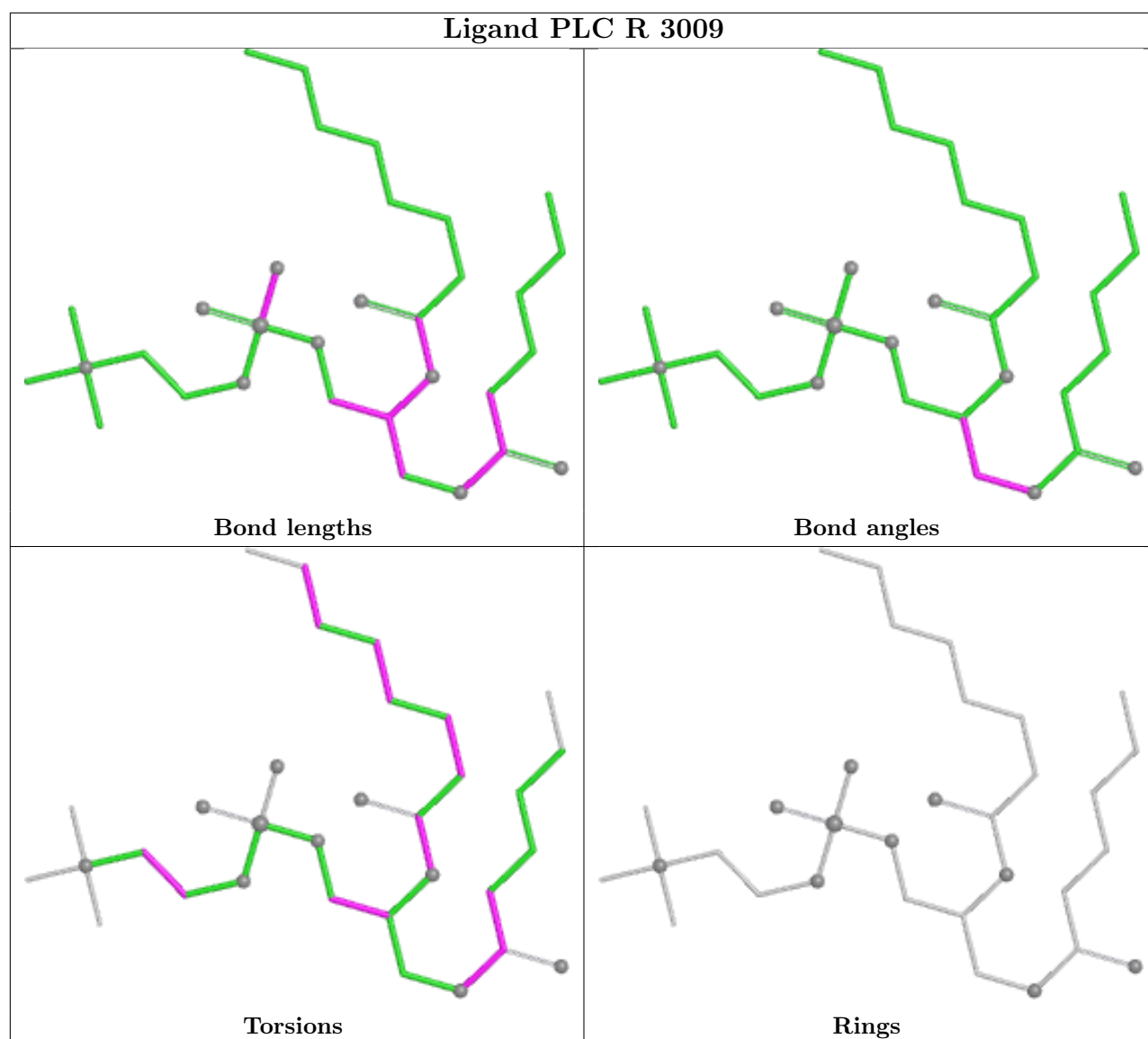


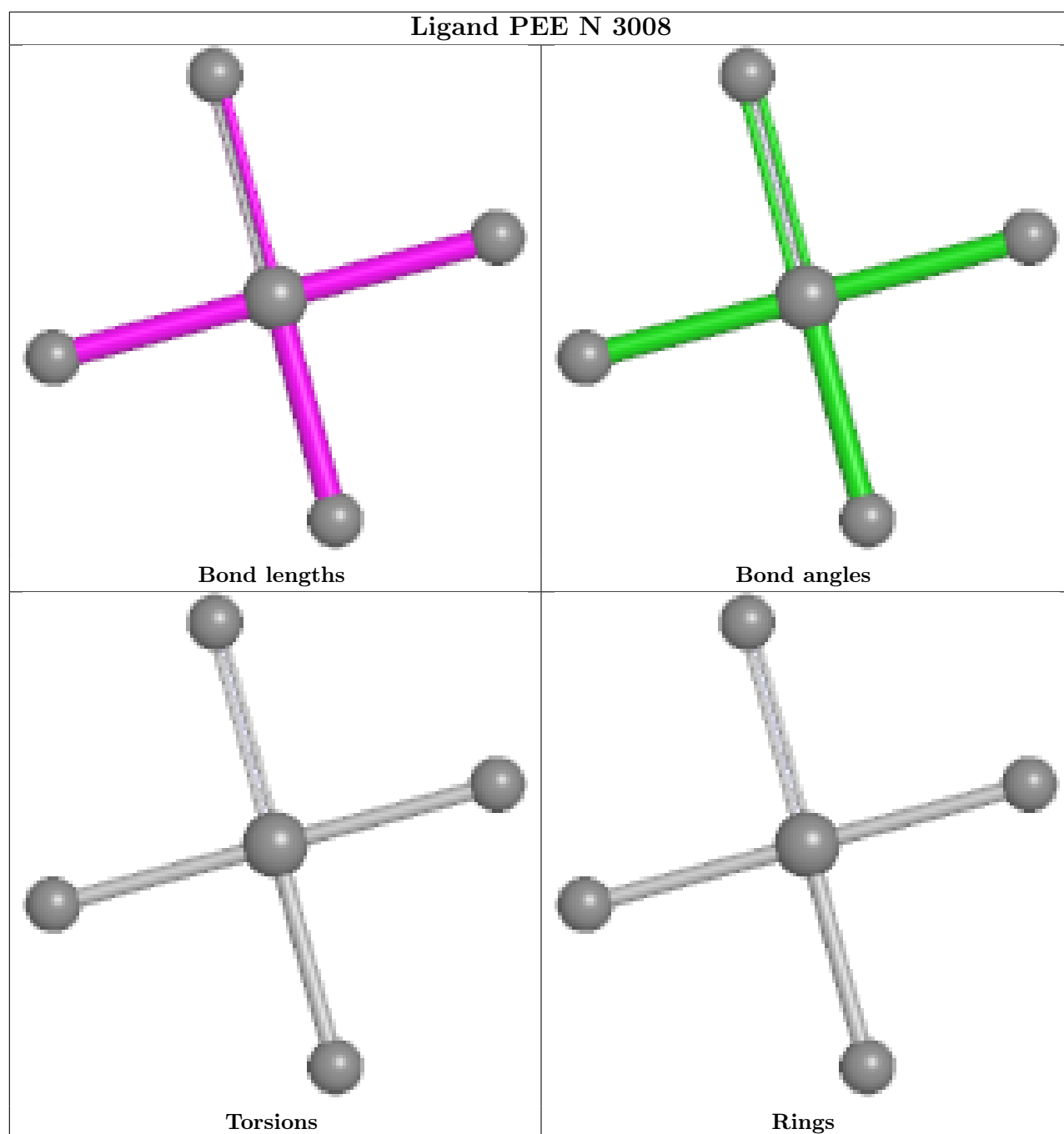


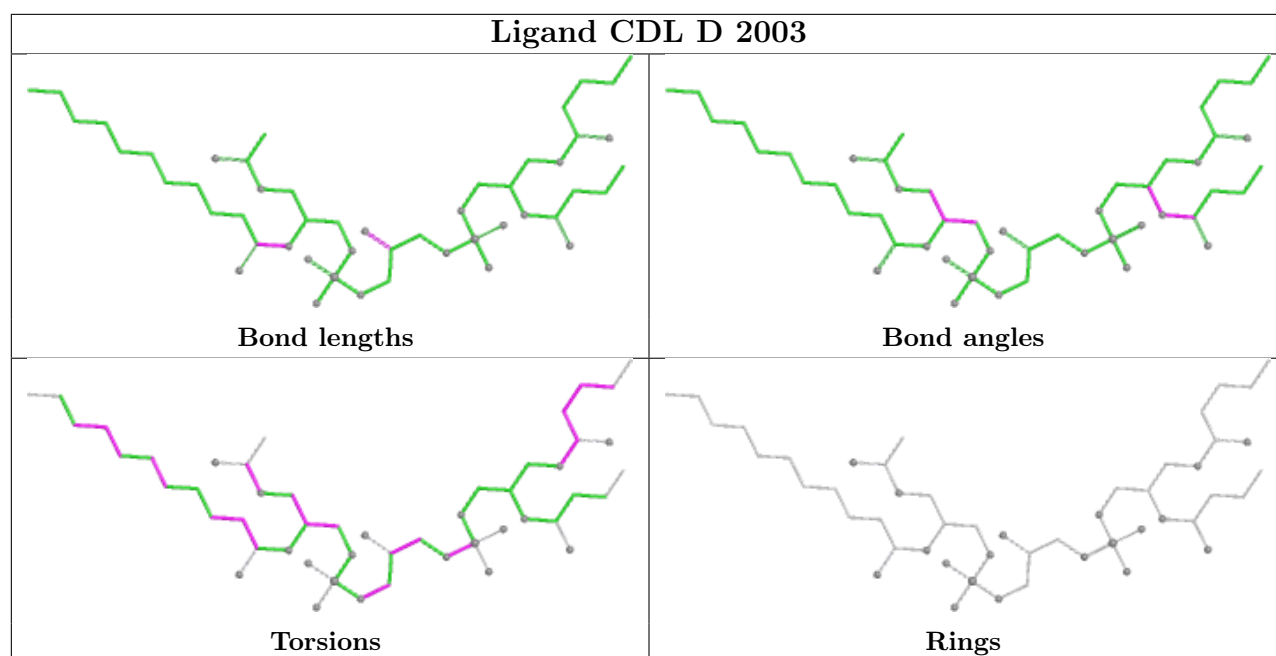












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.01	2 (0%) 87 72	44, 77, 105, 114	0
1	N	442/446 (99%)	0.23	9 (2%) 65 41	54, 80, 102, 110	0
2	B	421/441 (95%)	0.43	14 (3%) 49 28	66, 93, 122, 140	0
2	O	422/441 (95%)	0.21	9 (2%) 63 40	52, 85, 111, 124	0
3	C	380/380 (100%)	-0.44	4 (1%) 78 57	33, 49, 84, 140	0
3	P	379/380 (99%)	0.06	11 (2%) 53 31	44, 75, 99, 119	0
4	D	241/241 (100%)	-0.44	0 100 100	42, 55, 86, 114	0
4	Q	241/241 (100%)	0.36	8 (3%) 49 28	59, 86, 112, 127	0
5	E	196/196 (100%)	0.62	16 (8%) 17 9	48, 113, 165, 172	0
5	R	196/196 (100%)	0.38	3 (1%) 72 49	54, 85, 134, 151	0
6	F	101/110 (91%)	-0.50	0 100 100	37, 53, 67, 99	0
6	S	101/110 (91%)	0.11	0 100 100	64, 84, 112, 141	0
7	G	81/81 (100%)	0.09	2 (2%) 58 35	48, 62, 94, 113	0
7	T	79/81 (97%)	0.70	7 (8%) 15 8	69, 95, 147, 164	0
8	H	70/77 (90%)	0.05	1 (1%) 73 51	48, 73, 90, 133	0
8	U	67/77 (87%)	1.03	8 (11%) 9 5	102, 125, 148, 154	0
9	I	31/47 (65%)	2.41	18 (58%) 0 0	94, 127, 172, 178	0
9	V	31/47 (65%)	2.61	21 (67%) 0 0	93, 125, 184, 184	0
10	J	61/61 (100%)	-0.12	1 (1%) 70 47	57, 71, 109, 151	0
10	W	59/61 (96%)	0.14	0 100 100	69, 85, 101, 117	0
All	All	4042/4160 (97%)	0.16	134 (3%) 49 28	33, 79, 125, 184	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	49	LEU	6.5
1	A	444	ILE	5.9
9	V	61	ARG	5.8
9	I	63	ASP	5.5
9	V	50	LEU	5.4
9	I	49	LEU	5.4
7	G	2	ILE	5.0
2	B	21	ALA	4.8
9	I	61	ARG	4.3
9	I	50	LEU	4.1
2	B	19	PRO	4.0
8	H	9	GLU	4.0
7	T	78	GLU	3.9
9	I	47	ARG	3.9
9	V	63	ASP	3.9
9	V	62	ARG	3.8
2	O	19	PRO	3.7
7	T	2	ILE	3.6
2	O	387	LEU	3.5
5	E	162	GLY	3.5
9	I	57	GLY	3.5
9	V	47	ARG	3.4
2	B	226	ILE	3.4
9	I	54	SER	3.4
1	N	86	PHE	3.4
5	E	94	LYS	3.3
2	B	393	THR	3.3
9	V	76	VAL	3.3
9	V	51	CYS	3.3
9	V	77	ARG	3.3
9	I	53	GLU	3.2
4	Q	171	TYR	3.2
4	Q	180	SER	3.2
9	V	60	ALA	3.2
5	E	106	ILE	3.1
1	N	57	TYR	3.1
2	O	21	ALA	3.0
9	V	72	ALA	3.0
8	U	50	THR	2.9
2	O	383	GLY	2.9
3	P	7	LYS	2.8
9	V	59	SER	2.8
3	P	255	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	P	165	ALA	2.8
9	I	62	ARG	2.8
5	E	130	PRO	2.8
9	I	58	ARG	2.7
5	E	76	ILE	2.7
9	V	55	MET	2.7
1	N	44	GLY	2.7
3	P	5	ILE	2.7
9	I	52	ARG	2.7
3	P	253	ASP	2.7
2	B	304	THR	2.6
2	B	20	GLY	2.6
8	U	59	PHE	2.6
1	N	115	ASP	2.6
2	B	402	ILE	2.6
7	G	29	ILE	2.5
9	I	77	ARG	2.5
3	P	9	HIS	2.5
4	Q	137	PRO	2.5
4	Q	3	LEU	2.5
7	T	20	PRO	2.5
1	N	112	LEU	2.5
8	U	26	GLN	2.5
5	E	12	ALA	2.5
2	B	283	PRO	2.5
9	V	48	PRO	2.5
9	V	58	ARG	2.4
5	E	124	LEU	2.4
4	Q	119	ALA	2.4
2	B	127	THR	2.4
5	E	68	VAL	2.4
5	R	114	VAL	2.4
8	U	21	ARG	2.4
9	V	56	SER	2.4
9	I	51	CYS	2.4
9	V	57	GLY	2.4
3	C	5	ILE	2.4
3	C	165	ALA	2.4
3	P	3	PRO	2.4
5	E	121	GLN	2.4
5	E	89	PHE	2.4
2	B	396	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	8	SER	2.4
4	Q	175	THR	2.3
2	O	223	PHE	2.3
9	I	48	PRO	2.3
9	I	60	ALA	2.3
10	J	61	ALA	2.3
5	E	112	VAL	2.3
3	C	7	LYS	2.3
5	E	85	LYS	2.3
2	O	386	ALA	2.3
5	R	89	PHE	2.3
2	B	400	GLN	2.3
5	E	110	ALA	2.2
9	V	64	LEU	2.2
7	T	74	PRO	2.2
2	O	224	LEU	2.2
4	Q	78	GLY	2.2
7	T	1	GLY	2.2
9	I	71	ASN	2.2
8	U	30	CYS	2.2
3	P	212	ILE	2.2
2	B	30	PRO	2.2
2	O	207	VAL	2.1
4	Q	182	ILE	2.1
2	B	176	LEU	2.1
2	O	283	PRO	2.1
5	R	192	LEU	2.1
3	C	9	HIS	2.1
8	U	73	LEU	2.1
1	N	111	GLU	2.1
3	P	272	GLU	2.1
7	T	79	ASN	2.1
1	A	231	LEU	2.1
1	N	120	CYS	2.1
5	E	122	HIS	2.1
8	U	17	LEU	2.1
9	V	70	LEU	2.1
2	B	230	ALA	2.1
9	I	72	ALA	2.1
5	E	117	LEU	2.1
9	I	64	LEU	2.1
3	P	169	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
8	U	55	THR	2.0
1	N	45	SER	2.0
9	V	54	SER	2.0
5	E	104	ALA	2.0
7	T	77	TYR	2.0
1	N	54	GLY	2.0
9	V	53	GLU	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 oligosaccharides 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
15	PEE	N	3008	5/51	0.72	0.13	135,135,136,136	0
15	PEE	C	2008	21/51	0.77	0.23	139,142,144,144	0
18	CDL	P	3004	40/100	0.81	0.22	106,114,120,121	0
18	CDL	S	3003	50/100	0.81	0.30	126,140,153,153	0
20	PLC	E	2009	32/42	0.81	0.24	67,83,97,98	0
11	UNL	E	3103	1/-	0.83	0.14	45,45,45,45	0
18	CDL	D	2003	50/100	0.84	0.25	79,112,130,131	0
18	CDL	G	2004	40/100	0.85	0.17	81,90,97,98	0
11	UNL	A	3016	1/-	0.86	0.23	55,55,55,55	0
20	PLC	R	3009	32/42	0.86	0.26	91,99,116,116	0
14	UQ	P	3002	19/63	0.89	0.28	116,121,122,122	0
15	PEE	E	2005	50/51	0.90	0.19	76,90,95,95	0
14	UQ	C	2002	19/63	0.90	0.26	85,88,90,91	0
15	PEE	R	3005	50/51	0.90	0.20	95,108,116,119	0
15	PEE	P	3007	49/51	0.91	0.20	73,98,107,108	0
11	UNL	C	3015	1/-	0.91	0.12	47,47,47,47	0

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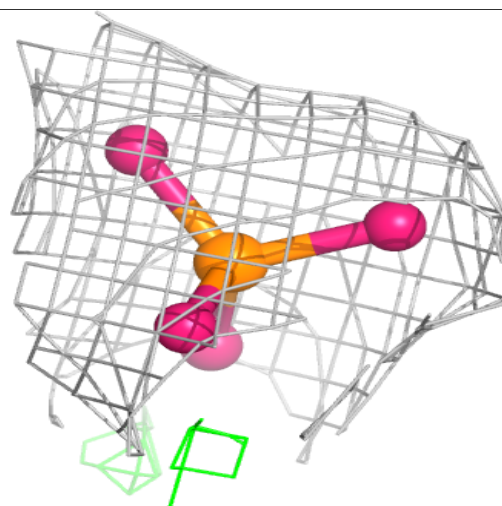
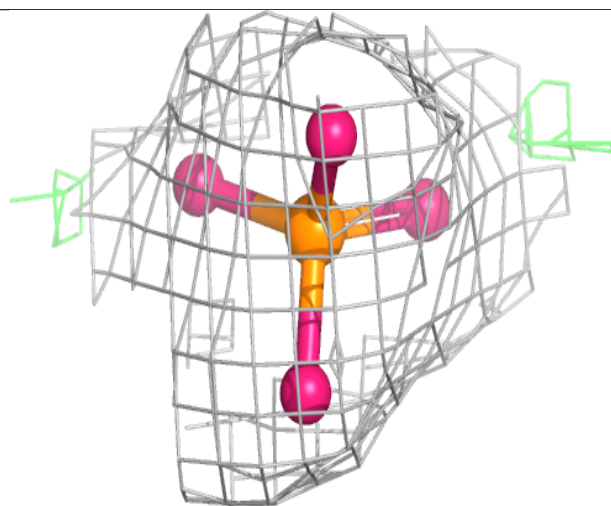
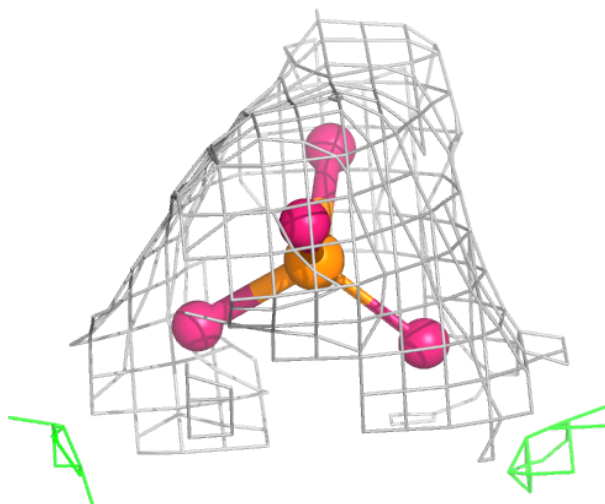
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	PEE	C	2007	49/51	0.92	0.17	52,68,87,89	0
11	UNL	P	2015	1/-	0.92	0.10	33,33,33,33	0
11	UNL	P	3104	1/-	0.93	0.08	59,59,59,59	0
16	GOL	C	2011	6/6	0.94	0.18	79,81,82,83	0
16	GOL	P	3011	6/6	0.94	0.18	69,71,72,72	0
11	UNL	E	2105	1/-	0.95	0.07	62,62,62,62	0
11	UNL	R	2103	1/-	0.95	0.12	45,45,45,45	0
11	UNL	C	2104	1/-	0.96	0.11	71,71,71,71	0
13	SMA	P	3001	37/37	0.96	0.12	67,73,75,78	0
11	UNL	C	2010	1/-	0.97	0.22	53,53,53,53	0
11	UNL	P	3010	1/-	0.97	0.22	67,67,67,67	0
12	HEM	P	501	43/43	0.97	0.10	56,61,69,75	0
17	HEC	Q	501	43/43	0.97	0.10	67,71,76,78	0
13	SMA	C	2001	37/37	0.97	0.09	41,44,46,52	0
19	FES	E	501	4/4	0.98	0.05	92,93,95,95	0
17	HEC	D	501	43/43	0.98	0.07	44,46,50,53	0
12	HEM	C	501	43/43	0.98	0.08	44,48,50,53	0
12	HEM	P	502	43/43	0.99	0.06	59,63,71,77	0
12	HEM	C	502	43/43	0.99	0.06	34,40,50,54	0
19	FES	R	501	4/4	1.00	0.02	52,54,56,57	0

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

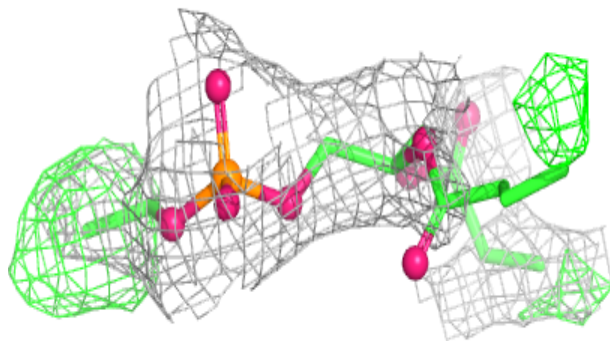
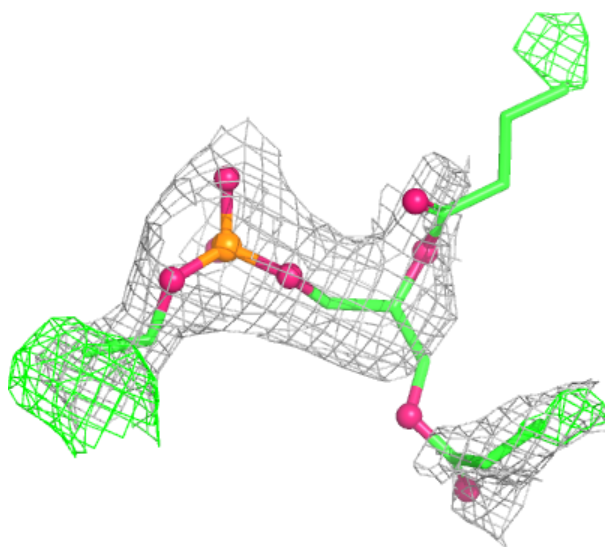
Electron density around PEE N 3008:

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



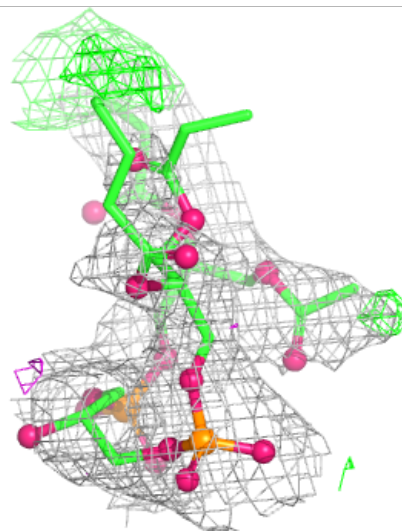
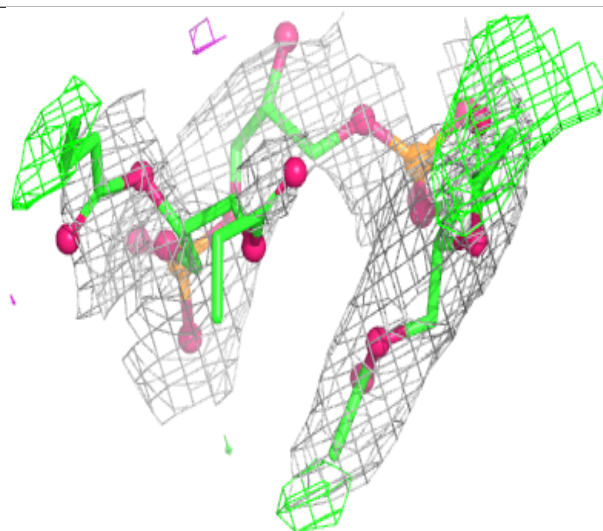
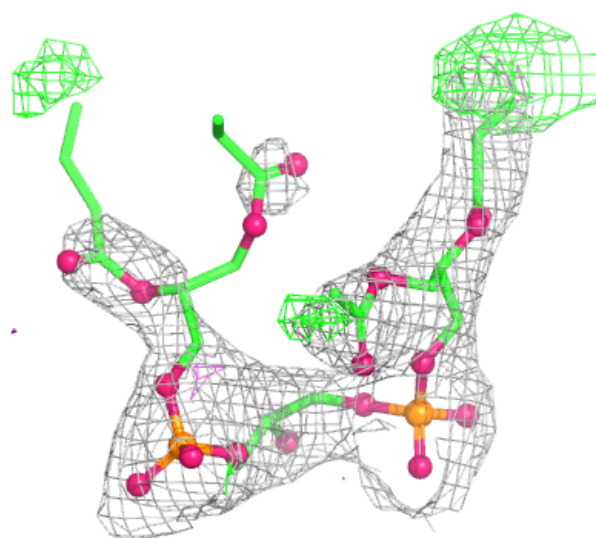
Electron density around PEE C 2008:

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



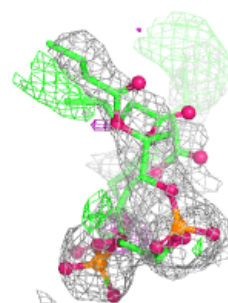
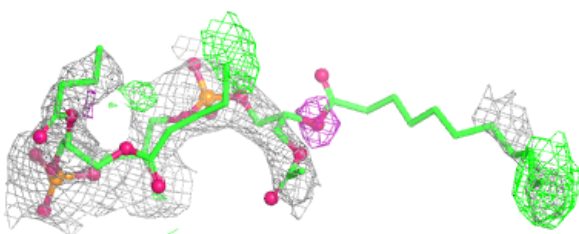
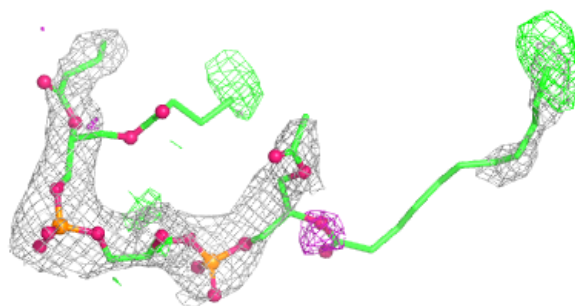
Electron density around CDL P 3004:

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

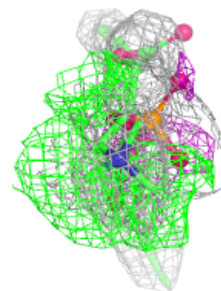
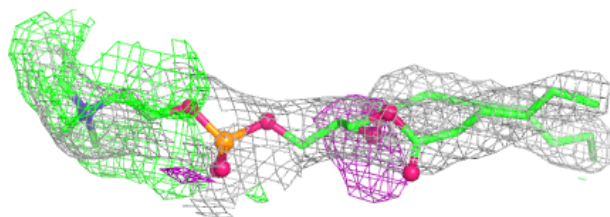
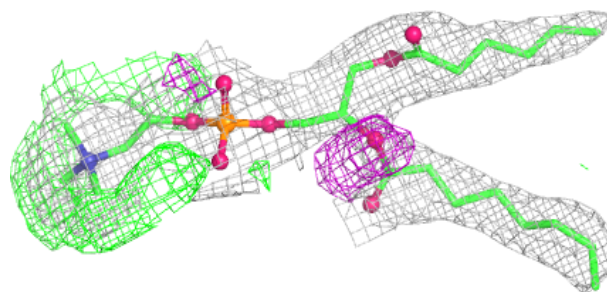


Electron density around CDL S 3003:

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

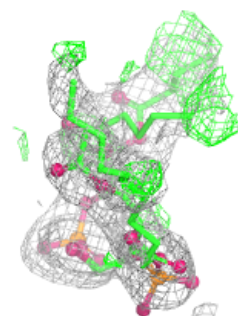
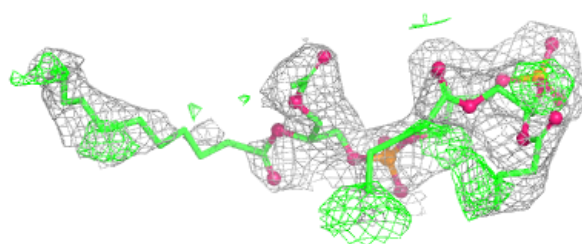
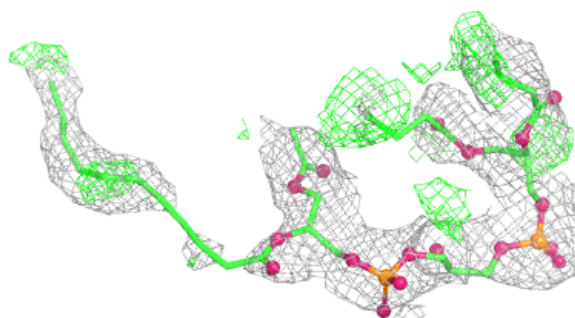
**Electron density around PLC E 2009:**

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



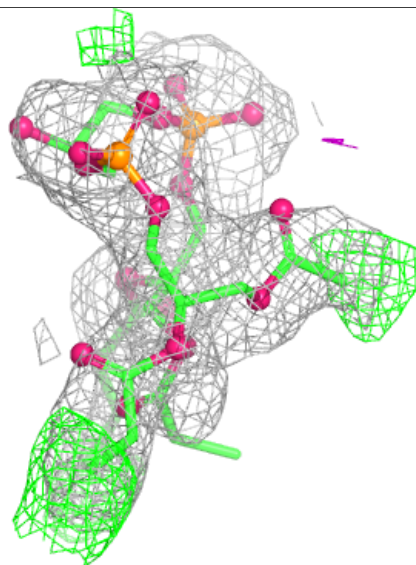
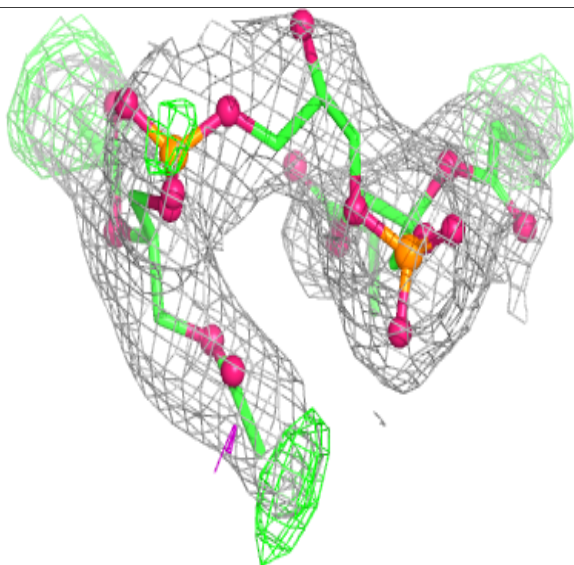
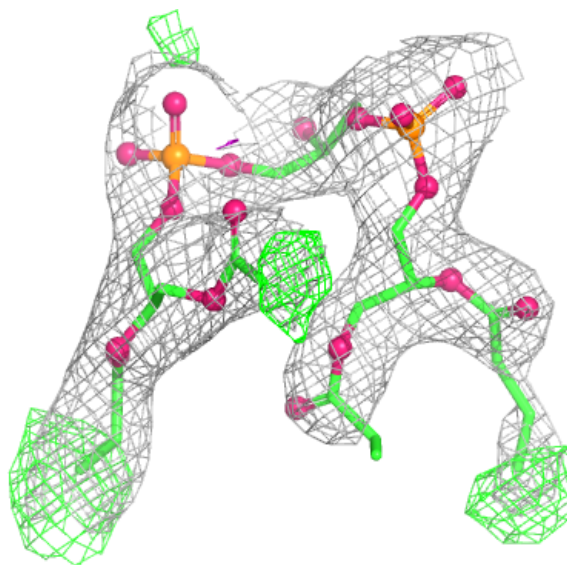
Electron density around CDL D 2003:

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



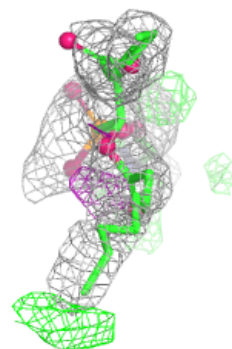
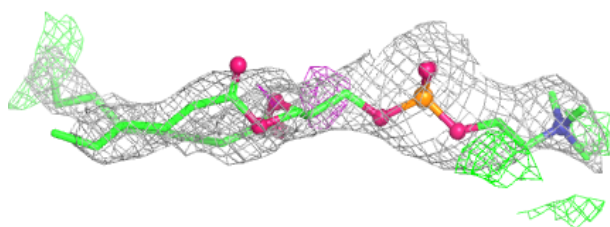
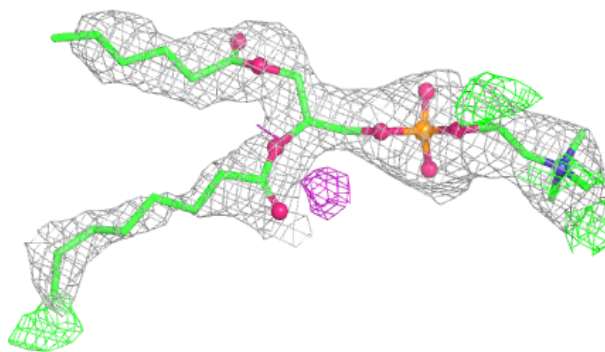
Electron density around CDL G 2004:

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

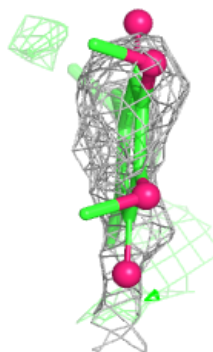
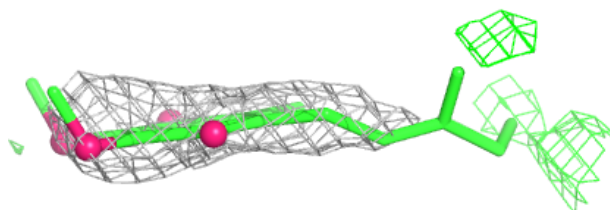
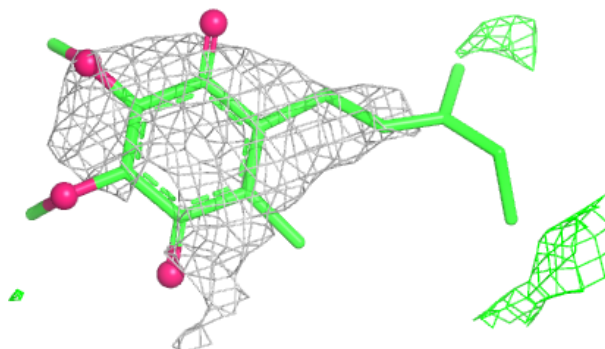


Electron density around PLC R 3009:

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

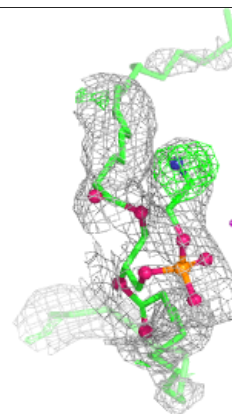
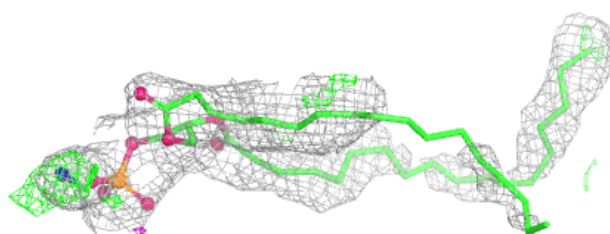
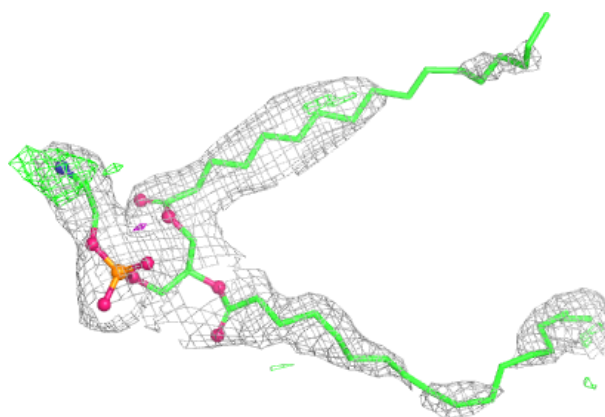
**Electron density around UQ P 3002:**

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

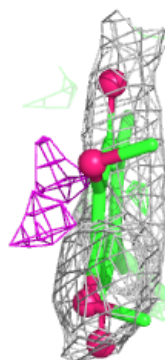
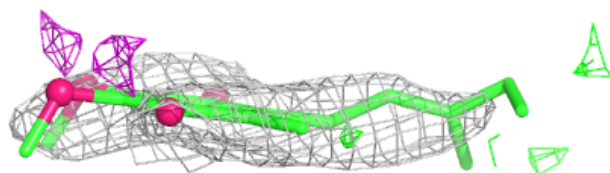


Electron density around PEE E 2005:

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

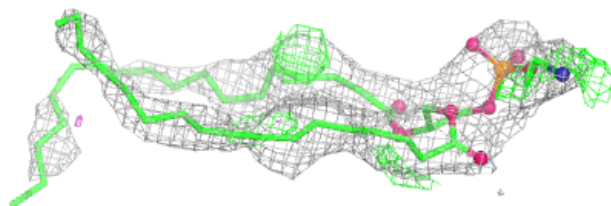
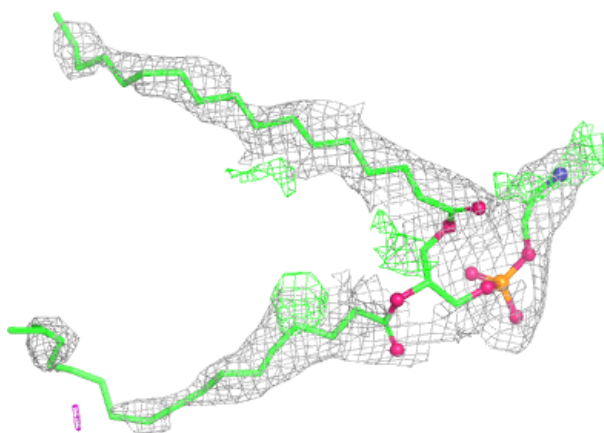
**Electron density around UQ C 2002:**

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

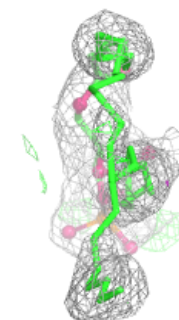
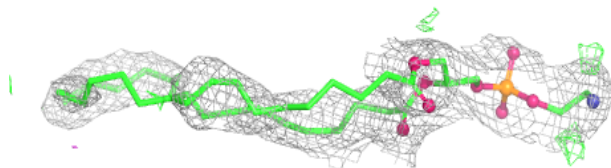
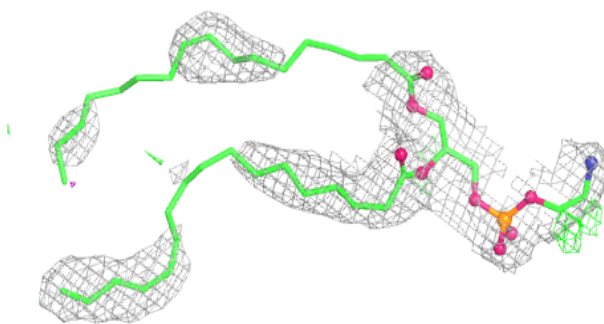


Electron density around PEE R 3005:

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

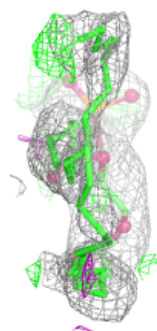
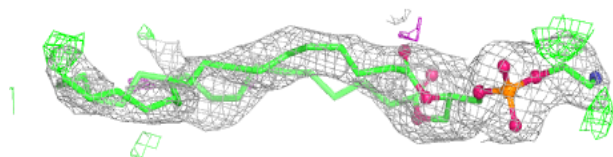
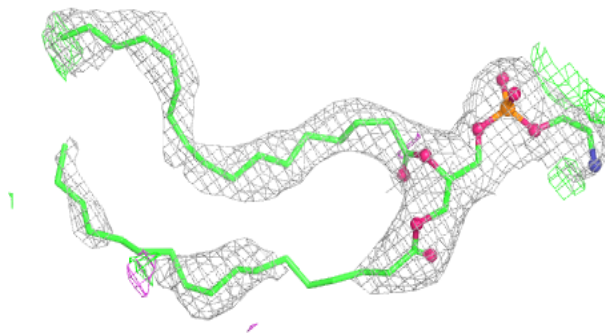
**Electron density around PEE P 3007:**

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

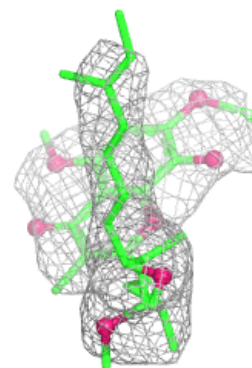
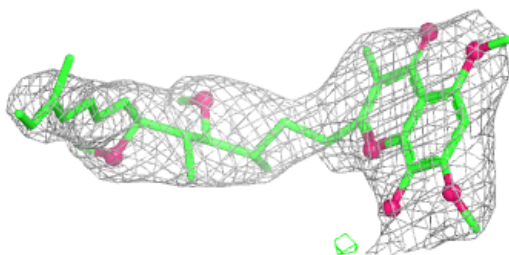
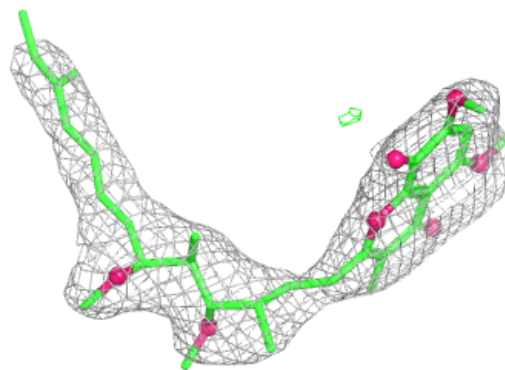


Electron density around PEE C 2007:

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

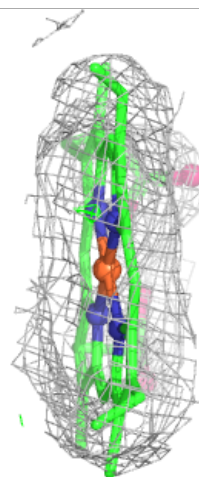
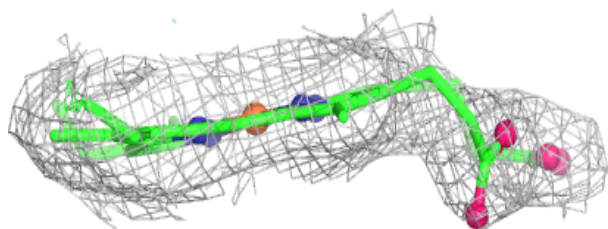
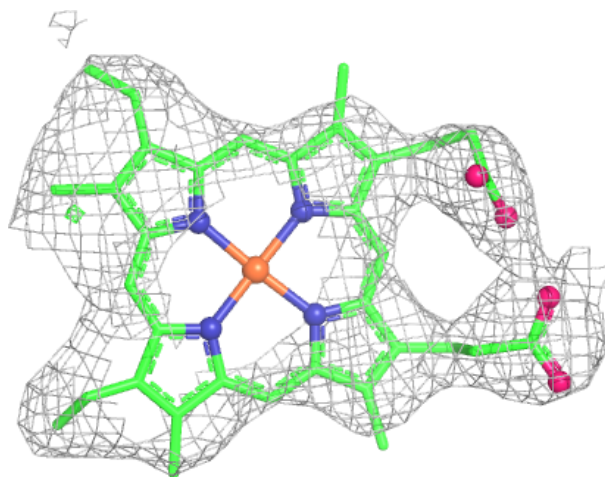
**Electron density around SMA P 3001:**

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



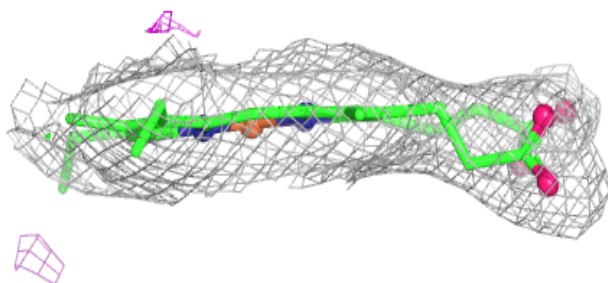
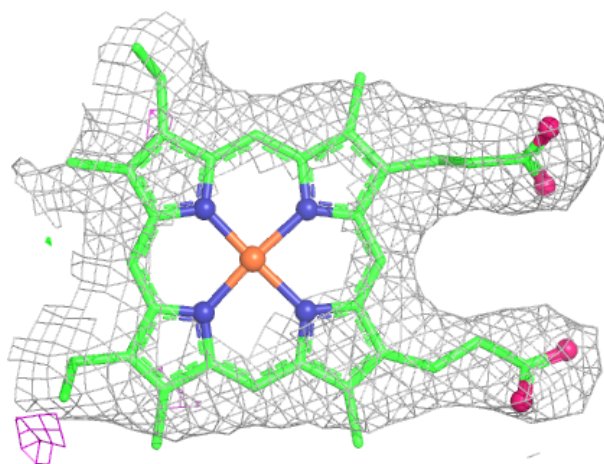
Electron density around HEM P 501:

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



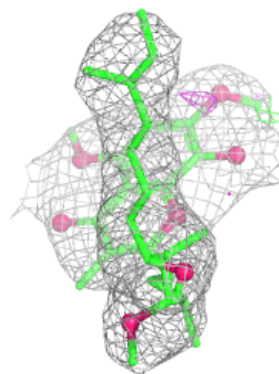
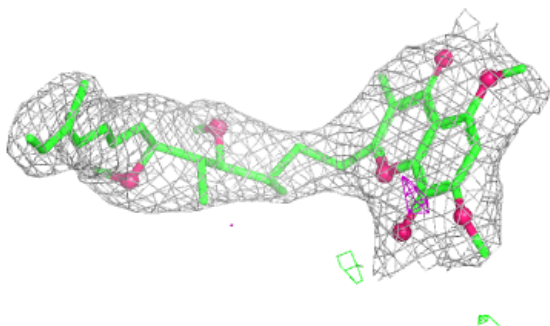
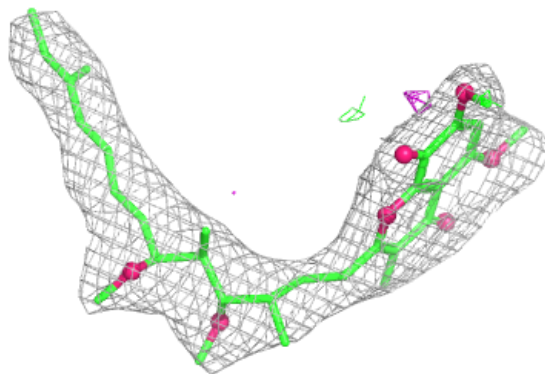
Electron density around HEC Q 501:

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



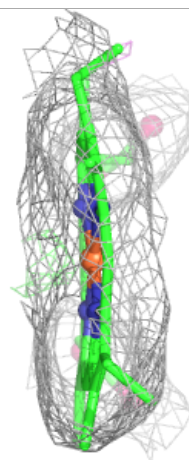
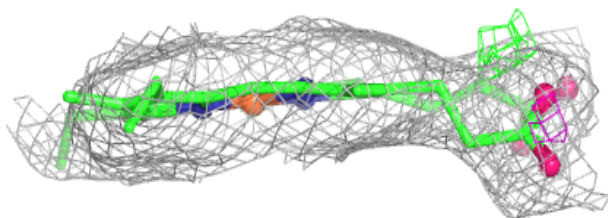
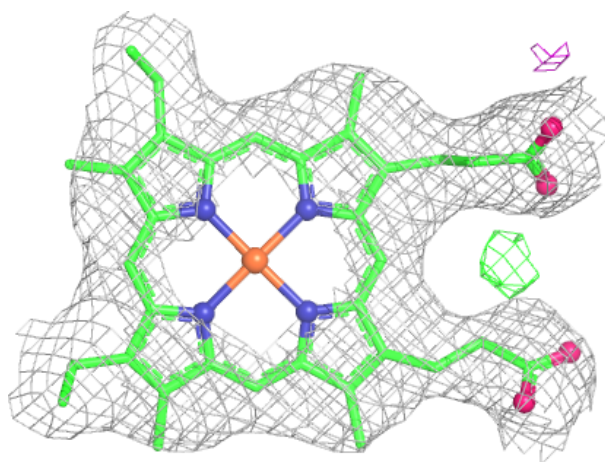
Electron density around SMA C 2001:

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



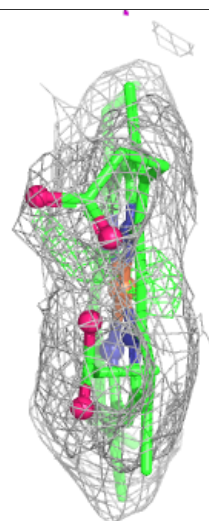
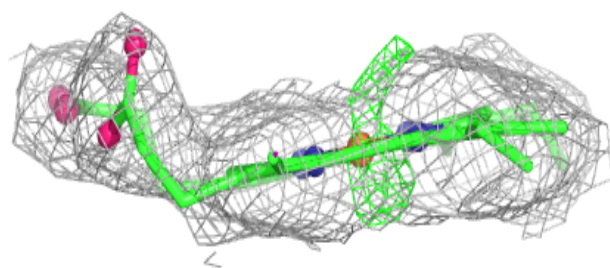
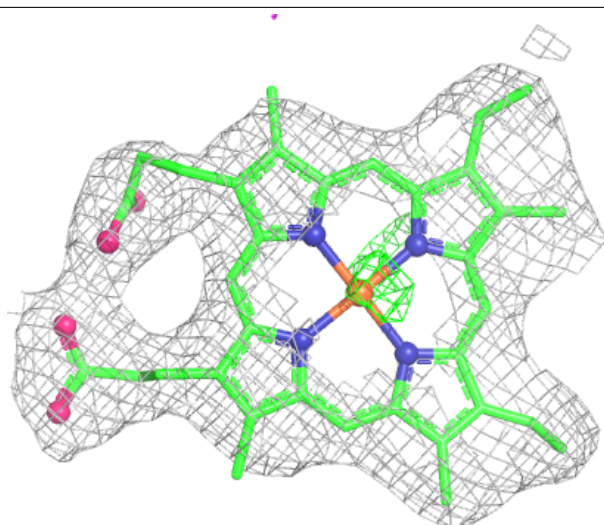
Electron density around HEC D 501:

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



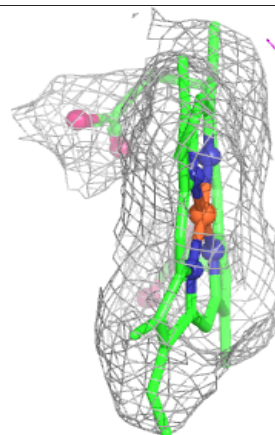
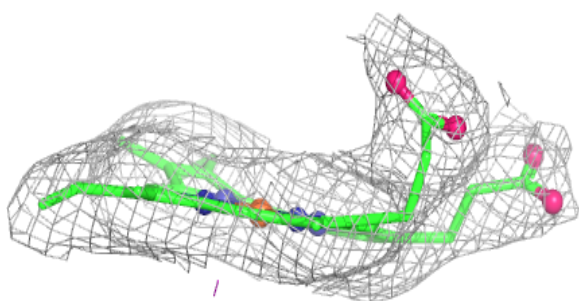
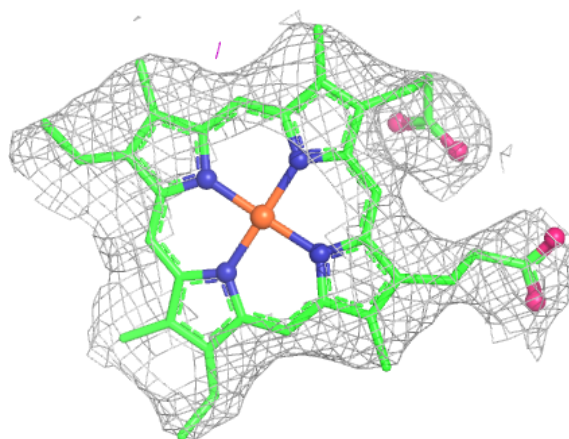
Electron density around HEM C 501:

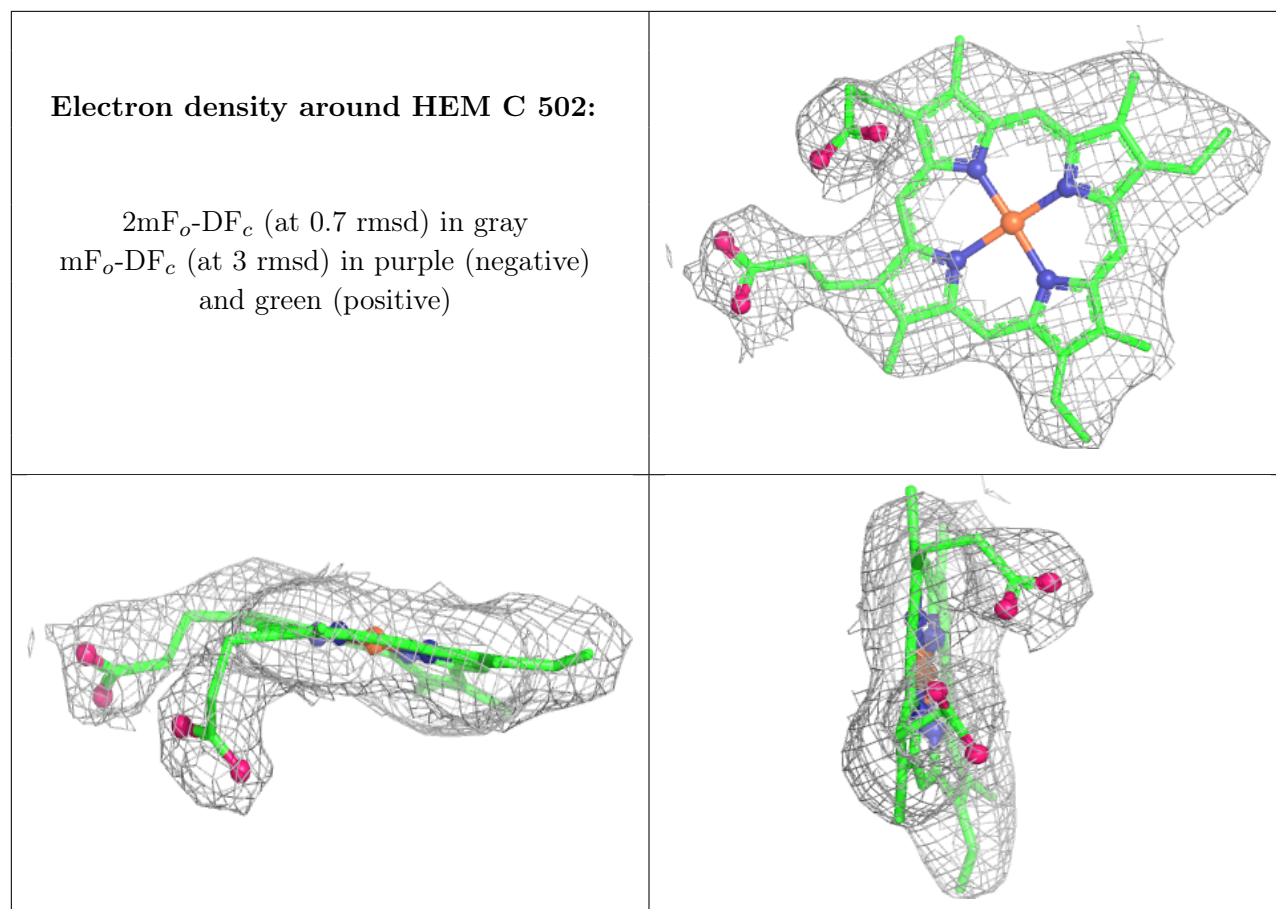
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.