



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:33 PM UTC

PDB ID : 3H1L / pdb_00003h1l
Title : Chicken cytochrome BC1 complex with ascochlorin bound at QO and QI sites
Authors : Berry, E.A.; Huang, L.S.; Minagawa, N.
Deposited on : 2009-04-12
Resolution : 3.21 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

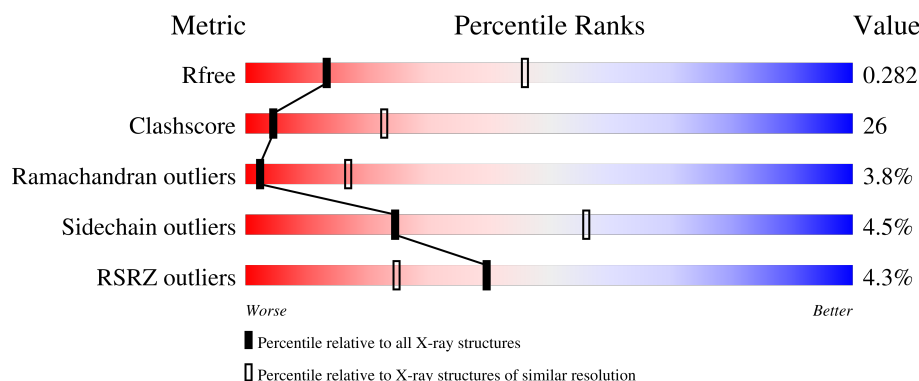
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	3% 52% 40% 7%
1	N	446	4% 52% 42% 5%
2	B	441	7% 45% 44% 6% 5%
2	O	441	4% 45% 44% 5%
3	C	380	0% 54% 42%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEE	P	3008	-	X	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32657 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	571	160	157	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	571	160	157	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			

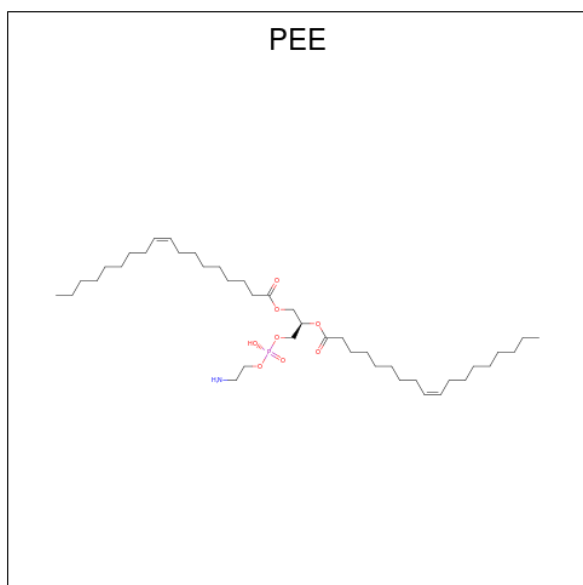
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



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

- Molecule 12 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

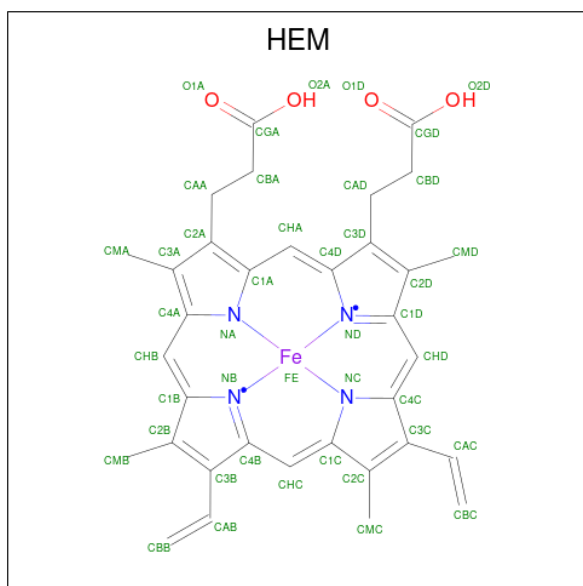
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total 1 O 1	0	0

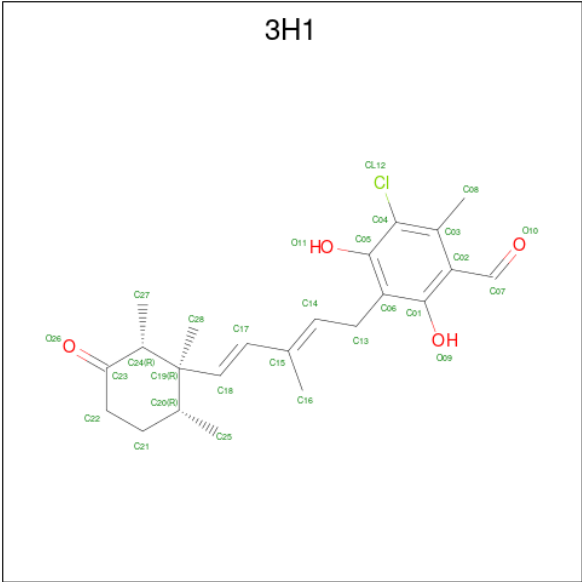
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	4	Total	O	0	0
			4	4		
12	E	1	Total	O	0	0
			1	1		
12	P	5	Total	O	0	0
			5	5		
12	R	1	Total	O	0	0
			1	1		

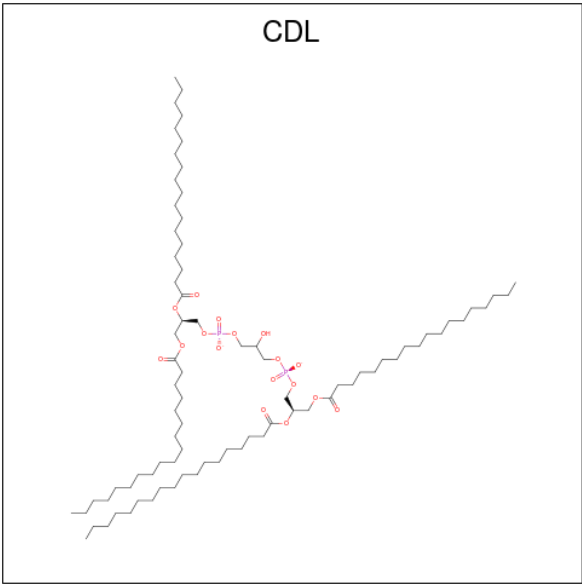
- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





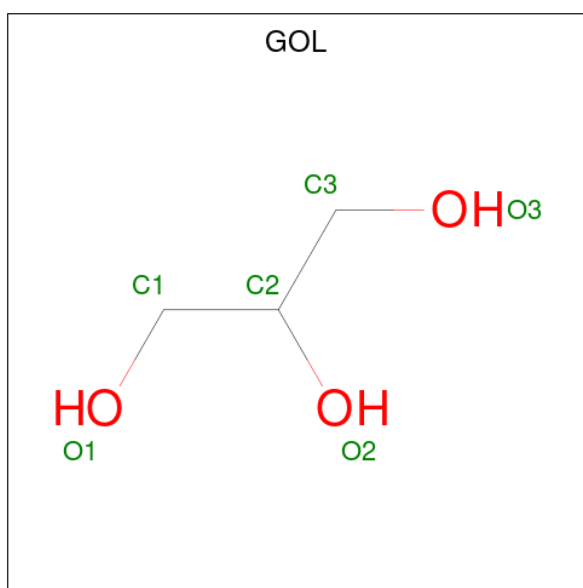
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Cl	O	0	0
			28	23	1	4		
14	C	1	Total	C	Cl	O	0	0
			28	23	1	4		
14	P	1	Total	C	Cl	O	0	0
			28	23	1	4		
14	P	1	Total	C	Cl	O	0	0
			28	23	1	4		

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



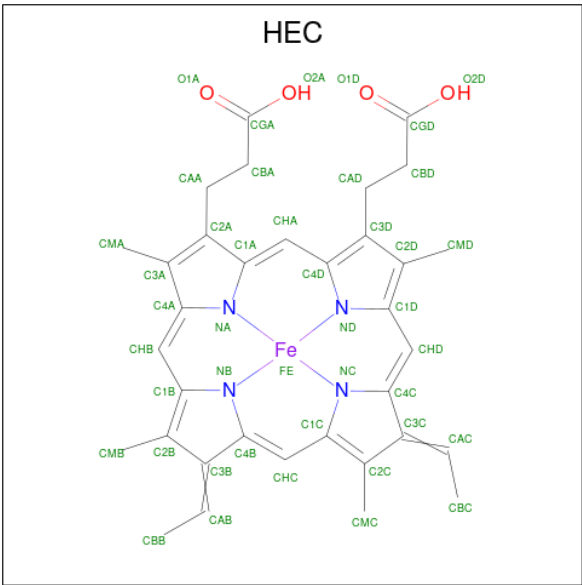
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			50	31	17	2		
15	G	1	Total	C	O	P	0	0
			40	21	17	2		
15	P	1	Total	C	O	P	0	0
			50	31	17	2		
15	T	1	Total	C	O	P	0	0
			40	21	17	2		

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



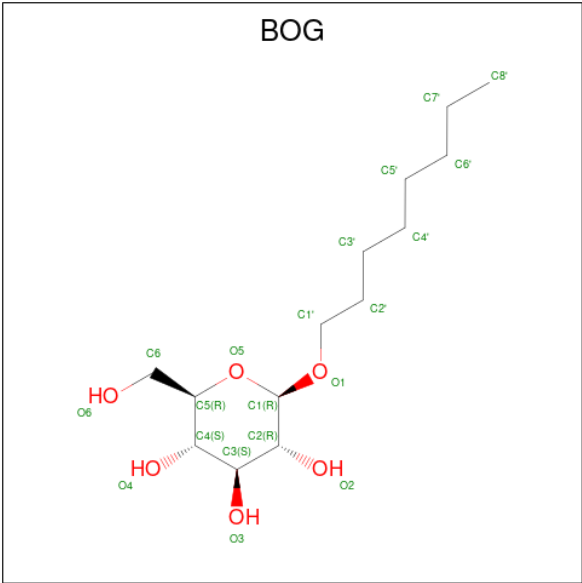
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

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



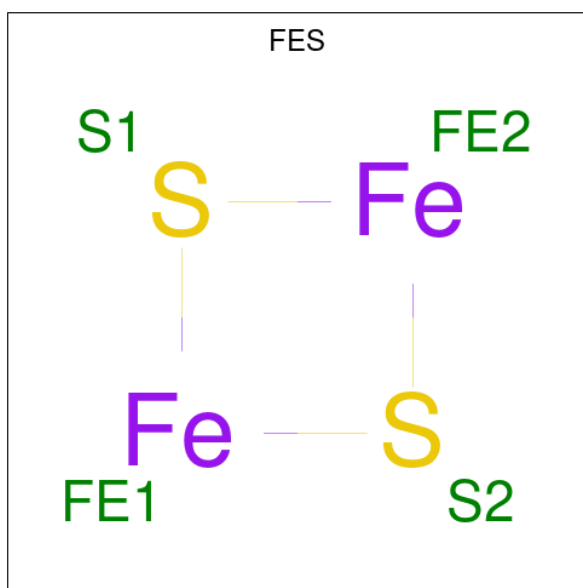
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
17	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 18 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	C	O	0	0
			20	14	6		
18	R	1	Total	C	O	0	0
			20	14	6		

- 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		

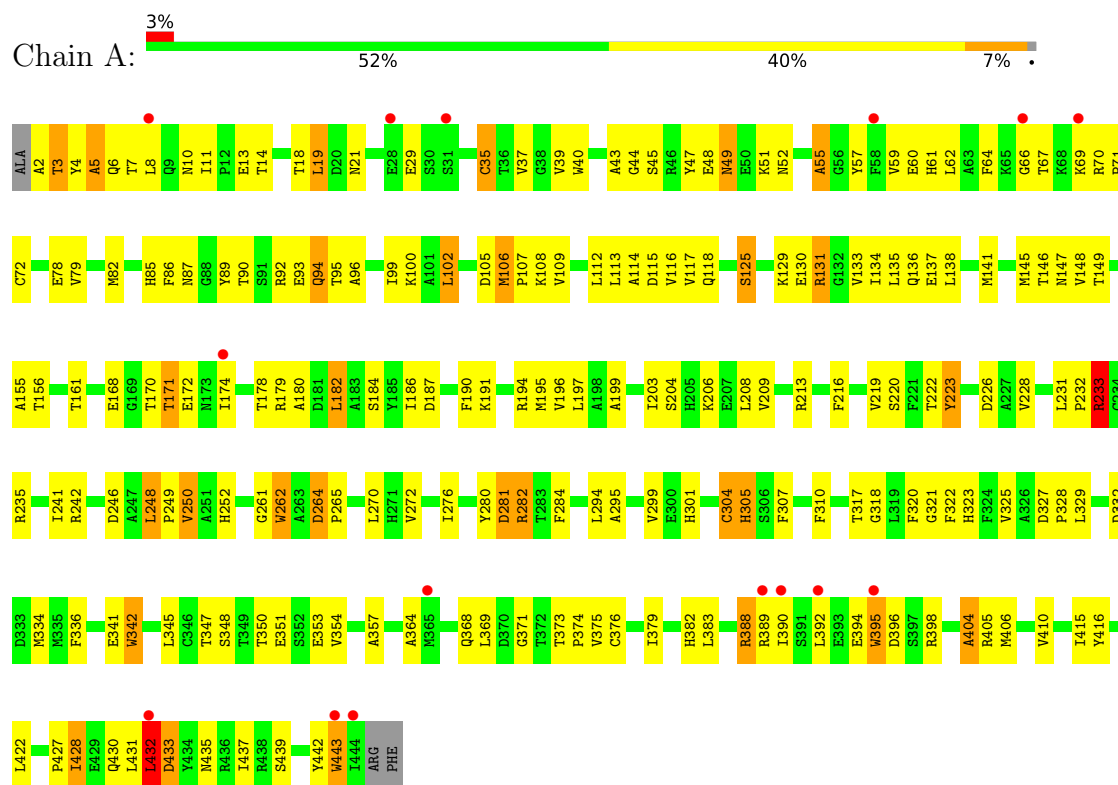
- Molecule 20 is water.

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

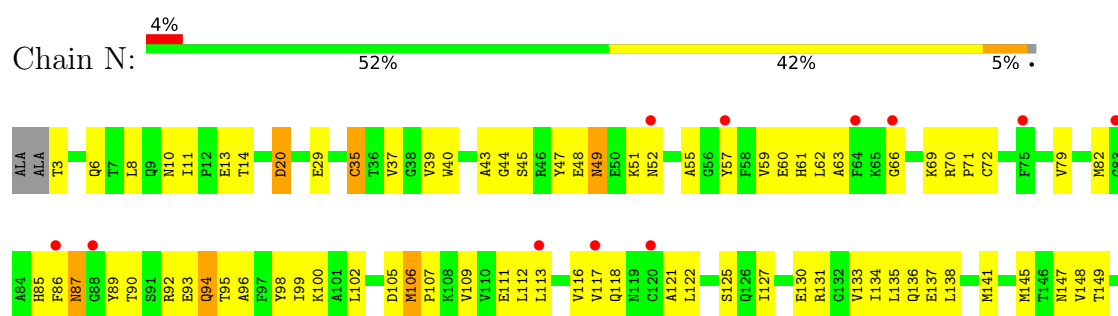
3 Residue-property plots [i](#)

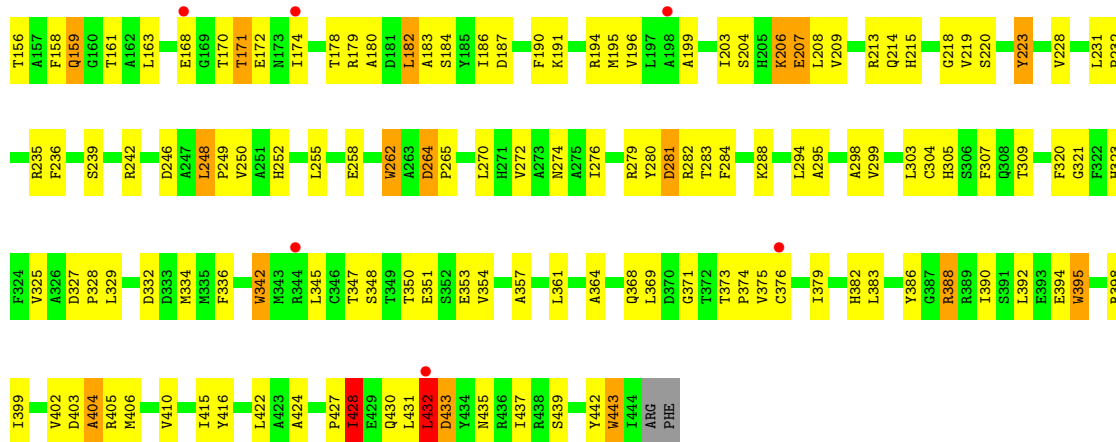
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

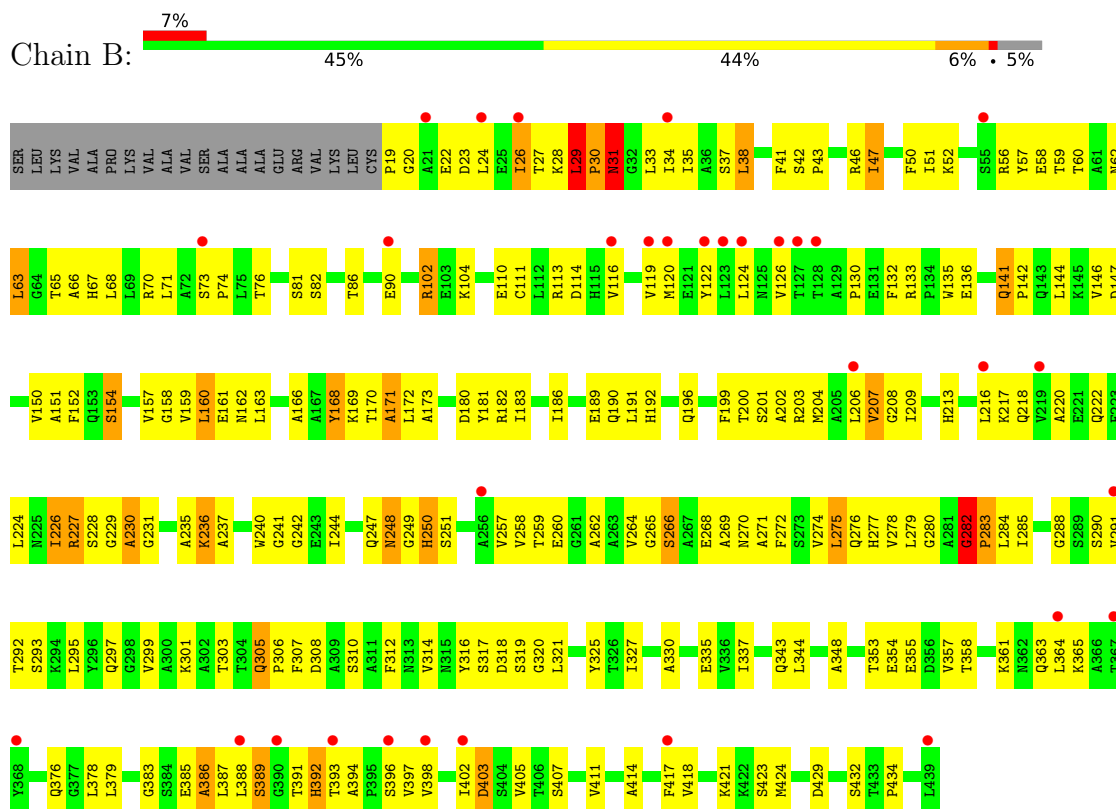


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

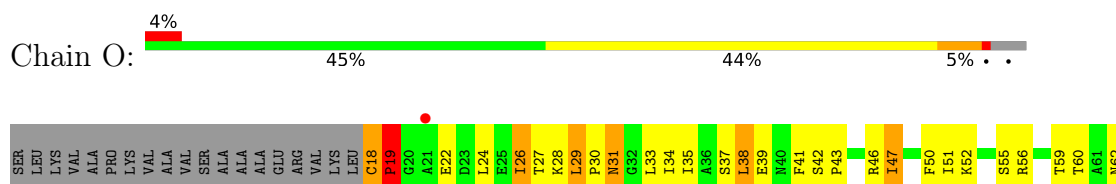


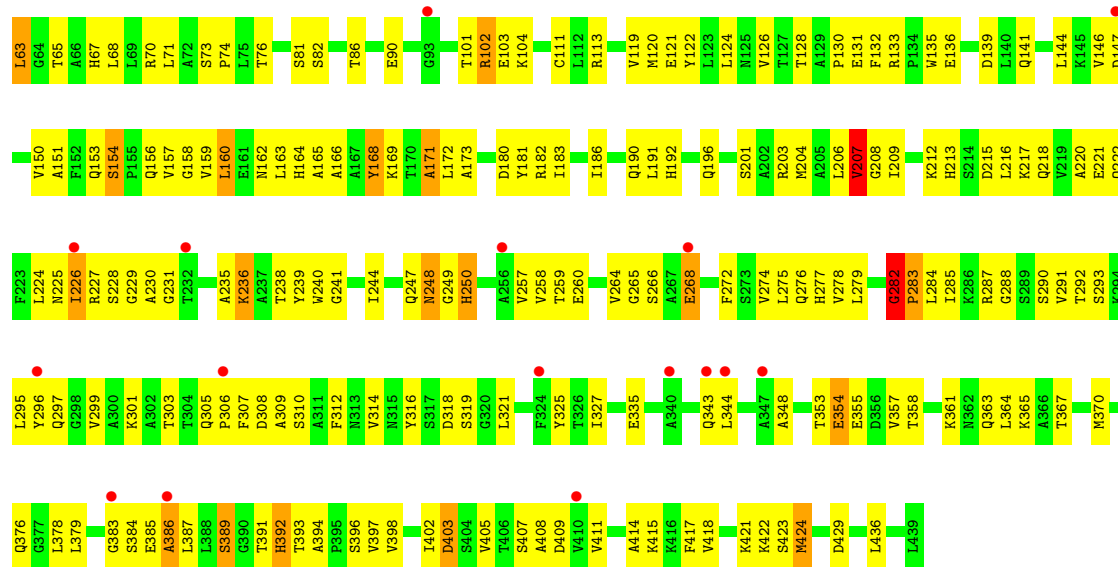


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

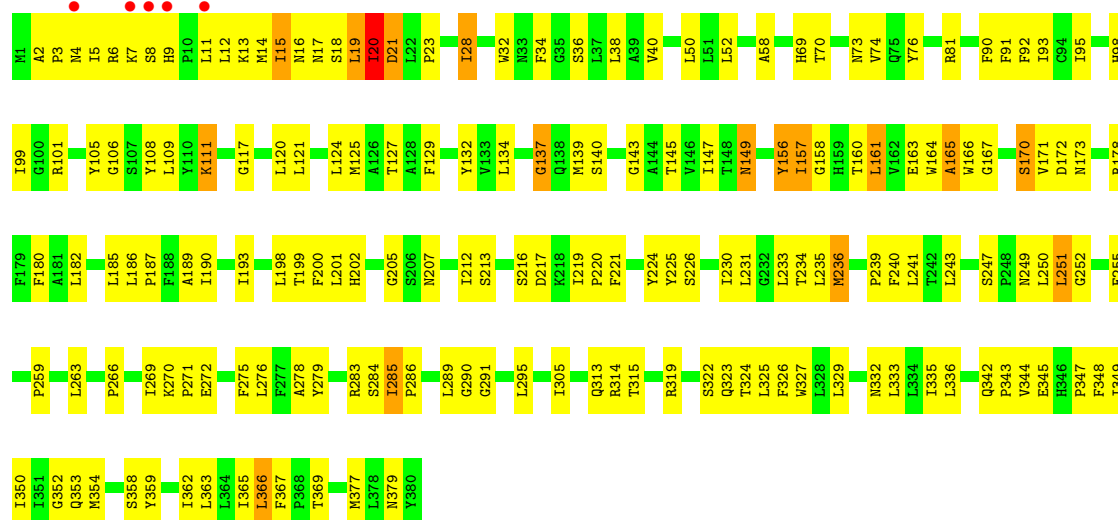


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

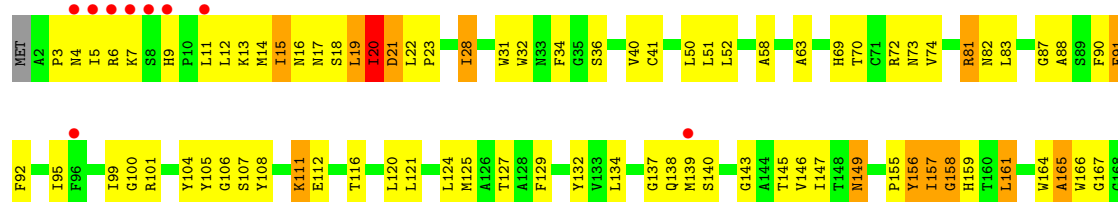


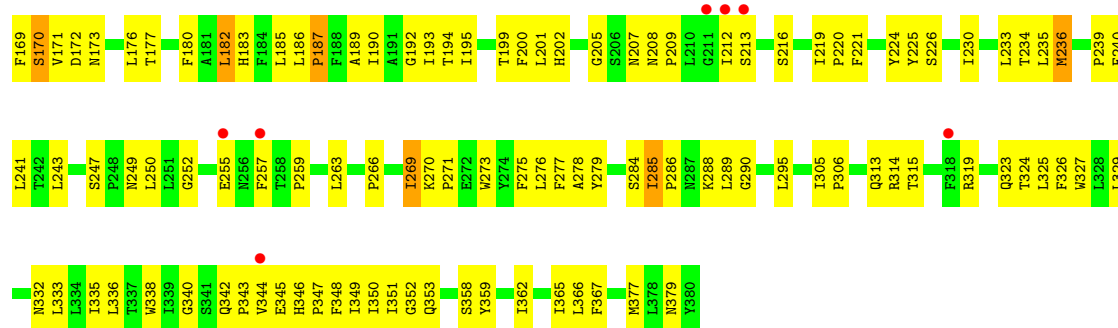


• Molecule 3: Cytochrome b

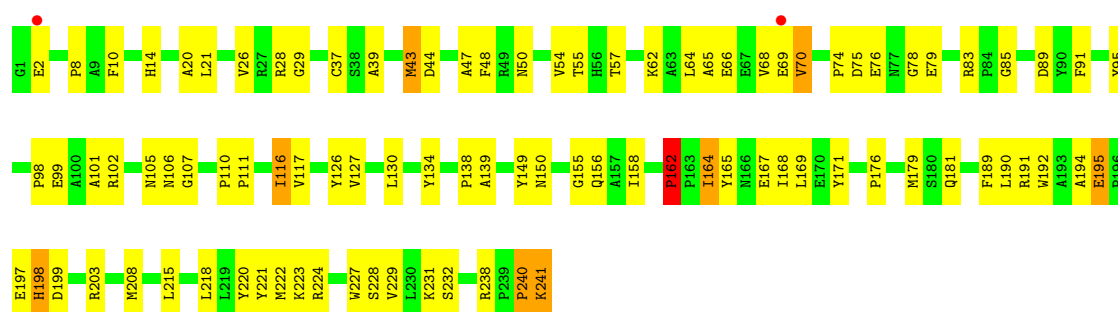


• Molecule 3: Cytochrome b

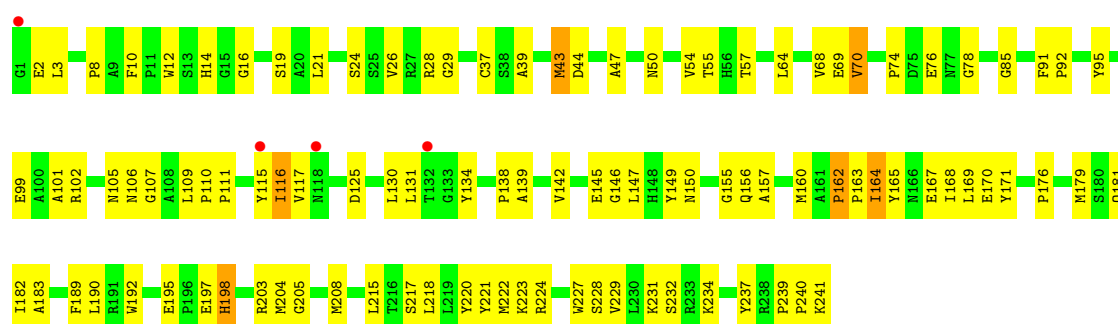




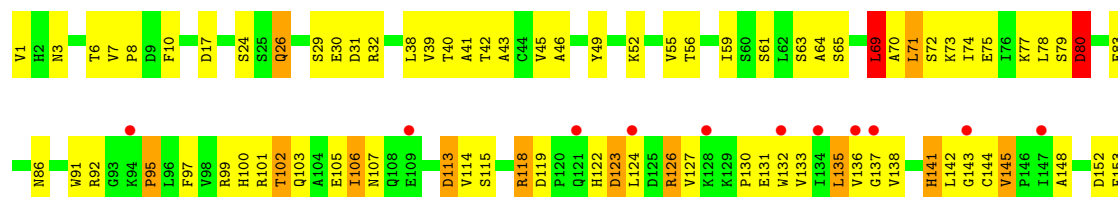
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

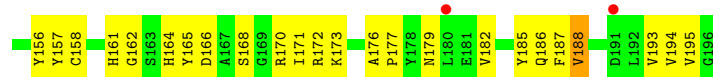


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

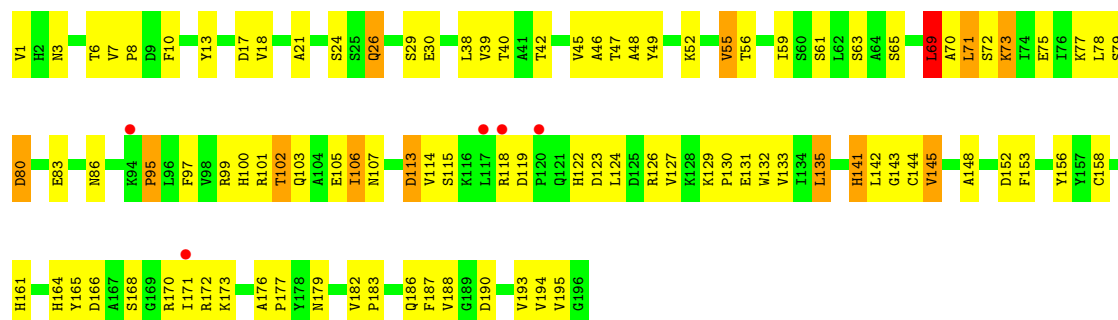


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

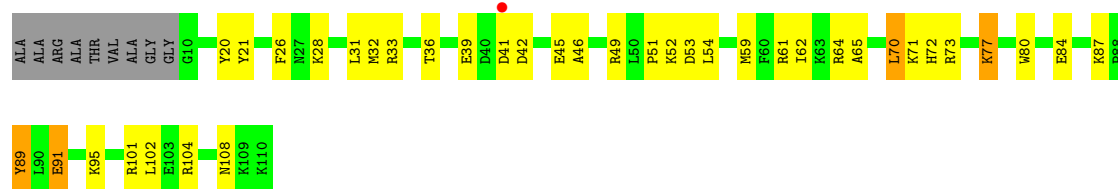




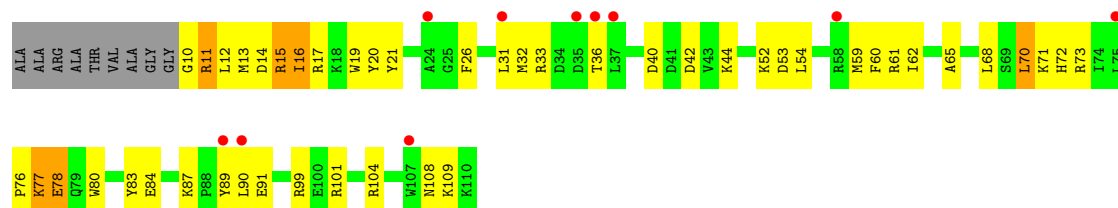
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



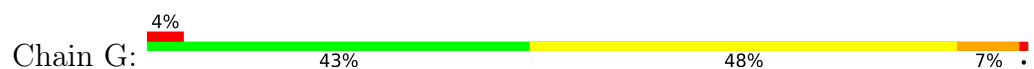
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



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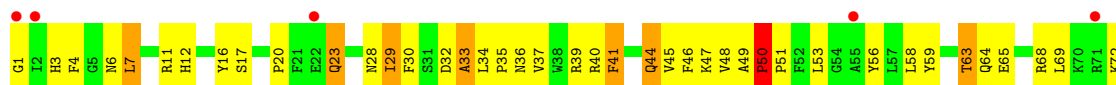


- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

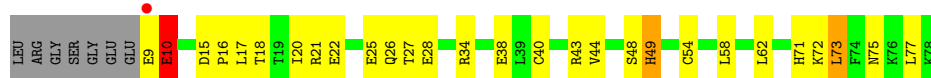




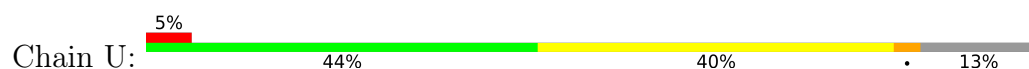
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



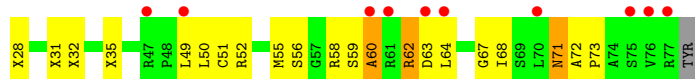
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



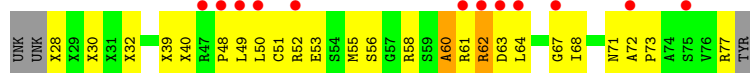
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



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



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



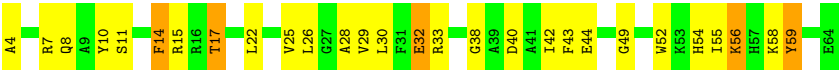
- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:

54%

38%

8%



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

Chain W:

2%

48%

41%

8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.14Å 182.36Å 241.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.21 29.99 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.99-3.21) 99.2 (29.99-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.295 0.250 , 0.282	Depositor DCC
R_{free} test set	2492 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32657	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: BOG, HEM, PEE, HEC, UNL, GOL, 3H1, CDL, FES

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	0.54	0/3511	1.05	25/4757 (0.5%)
1	N	0.53	0/3508	1.06	22/4753 (0.5%)
2	B	0.47	0/3196	1.00	17/4334 (0.4%)
2	O	0.54	0/3202	1.00	13/4343 (0.3%)
3	C	0.75	1/3122 (0.0%)	1.09	12/4273 (0.3%)
3	P	0.59	0/3114	1.04	14/4263 (0.3%)
4	D	0.64	0/1956	1.11	12/2658 (0.5%)
4	Q	0.50	0/1956	1.03	6/2658 (0.2%)
5	E	0.48	0/1547	1.05	10/2103 (0.5%)
5	R	0.51	0/1547	1.08	12/2103 (0.6%)
6	F	0.66	0/911	1.02	3/1218 (0.2%)
6	S	0.48	0/911	0.98	4/1218 (0.3%)
7	G	0.67	0/698	1.10	3/946 (0.3%)
7	T	0.50	0/680	1.05	4/923 (0.4%)
8	H	0.59	0/582	0.92	0/779
8	U	0.45	0/561	0.90	0/751
9	I	0.59	0/218	1.05	0/293
9	V	0.62	0/218	0.98	0/293
10	J	0.52	0/508	0.92	1/682 (0.1%)
10	W	0.49	0/489	0.93	1/658 (0.2%)
All	All	0.56	1/32435 (0.0%)	1.04	159/44006 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	354	MET	SD-CE	5.61	1.93	1.79

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	LEU	N-CA-C	10.31	123.09	110.41
5	E	71	LEU	N-CA-C	9.66	122.30	110.41
5	E	143	GLY	N-CA-C	9.19	129.05	114.90
1	N	272	VAL	N-CA-C	-9.02	102.05	110.53
5	R	143	GLY	N-CA-C	8.89	128.77	115.08
1	A	66	GLY	N-CA-C	8.47	121.78	112.29
1	A	248	LEU	CA-C-N	8.38	128.35	119.05
1	A	248	LEU	C-N-CA	8.38	128.35	119.05
4	D	116	ILE	N-CA-C	8.38	118.94	110.23
1	N	66	GLY	N-CA-C	8.26	121.54	112.29
7	G	37	VAL	N-CA-C	-8.05	102.41	110.62
1	A	432	LEU	N-CA-C	8.03	121.07	108.79
4	Q	116	ILE	N-CA-C	8.01	118.77	110.36
3	P	365	ILE	N-CA-C	7.94	118.39	111.56
10	W	14	PHE	N-CA-C	7.75	122.00	112.54
4	Q	195	GLU	CA-C-N	7.50	128.18	119.47
4	Q	195	GLU	C-N-CA	7.50	128.18	119.47
1	N	432	LEU	N-CA-C	7.47	119.51	108.60
10	J	14	PHE	N-CA-C	7.46	121.64	112.54
2	O	141	GLN	CA-C-N	-7.41	112.04	120.04
2	O	141	GLN	C-N-CA	-7.41	112.04	120.04
3	C	185	LEU	N-CA-C	7.40	119.25	111.03
1	A	415	ILE	N-CA-C	7.38	117.90	111.56
5	E	61	SER	N-CA-C	-7.33	104.31	113.18
1	N	415	ILE	N-CA-C	7.09	117.66	111.56
1	A	272	VAL	N-CA-C	-7.08	103.88	110.53
3	P	252	GLY	N-CA-C	7.05	123.52	111.04
1	N	348	SER	N-CA-C	6.99	118.82	110.44
1	N	304	CYS	N-CA-C	6.96	117.22	108.45
5	R	17	ASP	N-CA-C	6.90	120.96	112.54
4	D	164	ILE	N-CA-C	6.89	118.40	108.48
3	P	185	LEU	N-CA-C	6.88	118.67	111.03
6	F	39	GLU	N-CA-C	6.84	121.03	108.58
1	A	304	CYS	N-CA-C	6.80	117.02	108.45
1	N	264	ASP	N-CA-C	6.80	117.93	109.57
4	Q	44	ASP	N-CA-C	6.79	120.44	111.75
2	O	18	CYS	CA-C-N	6.75	128.28	119.84
2	O	18	CYS	C-N-CA	6.75	128.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	195	GLU	CA-C-N	6.75	127.30	119.47
4	D	195	GLU	C-N-CA	6.75	127.30	119.47
1	N	305	HIS	N-CA-C	-6.71	105.38	113.97
1	N	347	THR	N-CA-C	6.70	121.87	113.43
5	E	17	ASP	N-CA-C	6.70	120.71	112.54
5	R	118	ARG	N-CA-C	-6.68	103.92	111.07
1	A	264	ASP	N-CA-C	6.66	117.76	109.57
1	N	248	LEU	CA-C-N	6.66	125.89	118.97
1	N	248	LEU	C-N-CA	6.66	125.89	118.97
3	C	205	GLY	N-CA-C	-6.64	105.26	112.04
2	B	180	ASP	N-CA-C	6.63	118.20	110.97
3	C	365	ILE	N-CA-C	6.61	117.25	111.56
4	Q	164	ILE	N-CA-C	6.58	117.95	108.48
5	E	26	GLN	N-CA-C	6.57	119.26	111.71
5	E	118	ARG	N-CA-C	-6.56	104.05	111.07
1	N	415	ILE	CB-CA-C	-6.54	105.23	111.44
2	B	310	SER	N-CA-C	6.49	118.00	108.86
5	R	26	GLN	N-CA-C	6.45	119.13	111.71
6	S	15	ARG	N-CA-C	-6.42	105.75	113.97
1	A	348	SER	N-CA-C	6.41	118.13	110.44
4	D	44	ASP	N-CA-C	6.41	119.95	111.75
2	O	180	ASP	N-CA-C	6.35	117.89	110.97
7	T	47	LYS	N-CA-C	-6.33	105.68	113.41
7	T	37	VAL	N-CA-C	-6.29	104.21	110.62
1	N	125	SER	N-CA-C	-6.26	103.99	111.69
3	C	252	GLY	N-CA-C	6.24	122.09	111.04
1	A	347	THR	N-CA-C	6.23	121.28	113.43
3	C	21	ASP	N-CA-C	-6.13	103.89	113.02
5	R	190	ASP	N-CA-C	-6.06	104.01	111.40
5	R	73	LYS	CB-CA-C	-6.06	106.83	114.40
2	O	310	SER	N-CA-C	6.02	117.05	108.74
1	N	329	LEU	N-CA-C	6.00	120.29	113.15
5	R	145	VAL	N-CA-C	5.99	113.01	107.56
5	R	61	SER	N-CA-C	-5.97	105.96	113.18
1	A	415	ILE	CB-CA-C	-5.96	105.78	111.44
3	P	205	GLY	N-CA-C	-5.94	105.98	112.04
1	N	416	TYR	N-CA-C	5.93	118.80	109.96
6	S	109	LYS	N-CA-C	-5.93	104.40	111.69
1	N	218	GLY	N-CA-C	-5.91	100.86	111.19
1	N	428	ILE	N-CA-C	5.90	121.61	109.34
6	S	16	ILE	N-CA-C	-5.89	104.76	110.42
7	T	23	GLN	N-CA-C	5.85	118.11	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	LEU	N-CA-C	5.80	120.05	113.15
3	P	91	PHE	N-CA-C	-5.74	104.94	111.14
3	C	137	GLY	N-CA-C	-5.73	104.90	112.81
7	G	47	LYS	N-CA-C	-5.73	105.96	113.12
2	O	168	TYR	N-CA-C	5.72	116.93	108.86
1	A	428	ILE	N-CA-C	5.71	121.21	109.34
1	A	125	SER	N-CA-C	-5.68	104.70	111.69
2	B	23	ASP	N-CA-C	5.68	117.91	108.99
3	P	21	ASP	N-CA-C	-5.68	104.56	113.02
4	Q	155	GLY	N-CA-C	-5.67	107.23	114.37
1	A	305	HIS	N-CA-C	-5.59	106.81	113.97
2	O	213	HIS	N-CA-C	5.58	118.08	111.33
5	E	145	VAL	N-CA-C	5.57	112.63	107.56
6	F	41	ASP	N-CA-C	5.55	117.01	111.07
5	E	126	ARG	N-CA-C	-5.54	107.07	113.88
7	T	44	GLN	N-CA-C	5.50	120.12	113.41
2	B	237	ALA	N-CA-C	5.49	117.41	108.63
3	P	273	TRP	N-CA-C	5.48	117.96	111.33
2	B	29	LEU	N-CA-C	5.47	121.89	109.81
5	E	80	ASP	N-CA-C	-5.46	106.46	113.23
4	D	238	ARG	CA-C-N	5.44	123.63	119.66
4	D	238	ARG	C-N-CA	5.44	123.63	119.66
2	B	141	GLN	CA-C-N	-5.43	114.16	119.64
2	B	141	GLN	C-N-CA	-5.43	114.16	119.64
4	D	162	PRO	CA-C-N	5.43	124.94	119.19
4	D	162	PRO	C-N-CA	5.43	124.94	119.19
2	B	270	ASN	N-CA-C	-5.42	105.92	112.54
1	A	129	LYS	N-CA-C	-5.42	106.72	113.55
3	P	257	PHE	N-CA-C	-5.42	105.88	112.88
1	A	416	TYR	N-CA-C	5.41	118.41	110.30
1	N	214	GLN	N-CA-C	5.39	116.97	111.14
3	P	111	LYS	N-CA-C	5.39	122.29	110.80
7	G	44	GLN	N-CA-C	5.38	119.97	113.41
1	N	264	ASP	CA-C-N	5.36	125.18	119.28
1	N	264	ASP	C-N-CA	5.36	125.18	119.28
3	P	266	PRO	CA-C-N	5.36	124.87	119.19
3	P	266	PRO	C-N-CA	5.36	124.87	119.19
3	P	269	ILE	N-CA-C	5.36	115.35	107.15
3	C	111	LYS	N-CA-C	5.33	122.15	110.80
1	A	35	CYS	N-CA-C	5.29	115.34	107.88
1	A	131	ARG	N-CA-C	-5.28	105.44	111.14
3	C	93	ILE	N-CA-C	-5.26	105.20	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	91	PHE	CA-C-N	5.26	125.51	119.83
4	D	91	PHE	C-N-CA	5.26	125.51	119.83
3	C	266	PRO	CA-C-N	5.24	124.75	119.19
3	C	266	PRO	C-N-CA	5.24	124.75	119.19
3	P	107	SER	N-CA-C	-5.23	106.40	112.89
5	R	73	LYS	N-CA-C	5.23	116.67	109.29
2	O	354	GLU	N-CA-C	-5.23	106.73	113.01
2	B	41	PHE	N-CA-C	5.22	119.23	112.86
4	D	155	GLY	N-CA-C	-5.21	107.81	114.37
1	A	301	HIS	N-CA-C	5.20	119.61	113.16
2	O	139	ASP	N-CA-C	-5.19	106.79	113.23
1	A	55	ALA	N-CA-C	-5.18	104.59	112.04
2	B	168	TYR	N-CA-C	5.17	116.52	109.18
1	N	35	CYS	N-CA-C	5.16	115.15	107.88
1	N	309	THR	N-CA-C	-5.15	102.89	110.52
5	R	55	VAL	N-CA-C	-5.15	105.82	110.82
2	B	275	LEU	N-CA-C	-5.15	106.95	113.18
2	O	41	PHE	N-CA-C	5.13	118.83	112.47
5	R	102	THR	N-CA-C	-5.12	102.94	110.52
3	P	143	GLY	N-CA-C	-5.12	106.29	112.49
3	C	217	ASP	N-CA-C	5.12	118.47	108.18
2	B	251	SER	N-CA-C	5.11	118.29	111.75
2	O	282	GLY	CA-C-N	5.11	126.22	119.84
2	O	282	GLY	C-N-CA	5.11	126.22	119.84
5	E	102	THR	N-CA-C	-5.10	102.98	110.52
1	A	233	ARG	N-CA-C	5.09	116.86	110.24
2	B	282	GLY	CA-C-N	5.08	126.19	119.84
2	B	282	GLY	C-N-CA	5.08	126.19	119.84
1	A	264	ASP	CA-C-N	5.07	124.85	119.28
1	A	264	ASP	C-N-CA	5.07	124.85	119.28
2	B	305	GLN	CA-C-N	5.06	125.34	119.92
2	B	305	GLN	C-N-CA	5.06	125.34	119.92
3	C	251	LEU	N-CA-C	5.05	119.07	113.01
6	F	89	TYR	N-CA-C	5.05	117.52	111.71
6	S	68	LEU	N-CA-C	-5.04	105.44	111.03
1	A	282	ARG	N-CA-C	5.01	121.48	110.80
2	B	57	TYR	N-CA-C	-5.01	106.76	112.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	76	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	186	0
1	N	3437	0	3349	182	0
2	B	3141	0	3142	218	0
2	O	3147	0	3146	219	0
3	C	3020	0	3070	167	0
3	P	3012	0	3058	185	0
4	D	1898	0	1846	77	0
4	Q	1898	0	1846	95	0
5	E	1513	0	1478	84	0
5	R	1513	0	1478	82	0
6	F	891	0	900	39	0
6	S	891	0	900	39	0
7	G	676	0	659	51	0
7	T	658	0	647	57	0
8	H	574	0	548	24	0
8	U	553	0	535	38	0
9	I	285	0	239	31	0
9	V	275	0	238	34	0
10	J	497	0	490	22	0
10	W	478	0	478	30	0
11	A	21	0	13	0	0
11	C	49	0	72	0	0
11	E	50	0	77	0	0
11	P	54	0	72	3	0
11	R	50	0	77	3	0
12	A	1	0	0	0	0
12	C	4	0	0	1	0
12	E	1	0	0	0	0
12	P	5	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	11	0
13	P	86	0	60	7	0
14	C	56	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	56	0	58	7	0
15	C	50	0	44	2	0
15	G	40	0	24	1	0
15	P	50	0	44	1	0
15	T	40	0	24	1	0
16	C	6	0	8	0	0
16	P	6	0	8	0	0
17	D	43	0	30	2	0
17	Q	43	0	30	2	0
18	D	20	0	28	1	0
18	R	20	0	28	1	0
19	E	4	0	0	1	0
19	R	4	0	0	1	0
20	B	1	0	0	0	0
20	C	6	0	0	1	0
20	P	6	0	0	1	0
20	U	1	0	0	0	0
All	All	32657	0	32213	1693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (1693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.15	1.13
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.38	1.02
6:F:32:MET:HE2	6:F:87:LYS:HG2	1.41	1.01
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.40	0.99
3:C:139:MET:HE1	3:C:269:ILE:HA	1.43	0.99
3:P:139:MET:HE1	3:P:269:ILE:HA	1.41	0.99
6:F:52:LYS:HZ1	7:G:11:ARG:HH11	0.95	0.95
3:C:13:LYS:O	3:C:17:ASN:HB2	1.66	0.95
4:D:47:ALA:H	4:D:50:ASN:HD22	1.09	0.94
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.47	0.94
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.50	0.93
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.93
6:S:52:LYS:HZ1	7:T:11:ARG:NH1	1.67	0.93
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.69	0.93
2:O:76:THR:HG22	2:O:82:SER:H	1.31	0.92
2:O:353:THR:HG22	2:O:355:GLU:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG22	2:B:82:SER:H	1.32	0.91
6:S:52:LYS:NZ	7:T:11:ARG:HH11	1.69	0.91
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.51	0.91
3:P:13:LYS:O	3:P:17:ASN:HB2	1.69	0.90
3:P:19:LEU:O	3:P:20:ILE:HG13	1.71	0.90
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.06	0.90
6:F:32:MET:HE3	6:F:87:LYS:H	1.36	0.89
6:F:52:LYS:HZ1	7:G:11:ARG:NH1	1.71	0.89
3:C:19:LEU:O	3:C:20:ILE:HG13	1.73	0.88
3:P:157:ILE:HG13	3:P:158:GLY:H	1.39	0.88
2:B:227:ARG:HD3	2:B:228:SER:H	1.38	0.88
6:S:52:LYS:HZ1	7:T:11:ARG:HH11	0.89	0.88
2:O:128:THR:HA	2:O:226:ILE:HD11	1.54	0.88
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.56	0.87
6:F:32:MET:CE	6:F:87:LYS:HG2	2.04	0.87
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.56	0.86
2:B:353:THR:HG22	2:B:355:GLU:H	1.39	0.86
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.86
2:B:218:GLN:HG3	2:B:222:GLN:HE22	1.39	0.86
1:A:170:THR:HG22	1:A:171:THR:H	1.40	0.86
1:N:390:ILE:HG23	1:N:394:GLU:OE1	1.76	0.86
2:B:199:PHE:O	2:B:226:ILE:HG12	1.74	0.85
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.58	0.85
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.55	0.85
6:F:52:LYS:NZ	7:G:11:ARG:HH11	1.74	0.85
9:I:71:ASN:HD22	9:I:71:ASN:H	1.25	0.85
2:B:227:ARG:NE	2:B:227:ARG:HA	1.91	0.84
13:C:501:HEM:HBC2	13:C:501:HEM:HMC1	1.57	0.84
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.58	0.84
3:C:90:PHE:HB3	3:C:236:MET:HE3	1.57	0.84
2:B:207:VAL:HG12	2:B:208:GLY:H	1.43	0.84
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.59	0.84
2:O:27:THR:HG22	2:O:28:LYS:H	1.42	0.84
2:O:220:ALA:O	2:O:224:LEU:HB2	1.77	0.84
2:O:221:GLU:HG3	2:O:222:GLN:H	1.42	0.83
1:N:170:THR:HG22	1:N:171:THR:H	1.40	0.83
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	1.60	0.83
1:A:390:ILE:HG23	1:A:394:GLU:OE1	1.77	0.83
2:O:22:GLU:HG3	2:O:39:GLU:HB3	1.60	0.83
5:R:1:VAL:HG23	5:R:3:ASN:H	1.44	0.83
1:N:105:ASP:O	1:N:109:VAL:HG23	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:GLN:NE2	9:V:50:LEU:HB2	1.94	0.82
1:A:364:ALA:O	1:A:368:GLN:HG2	1.79	0.82
2:B:227:ARG:HA	2:B:227:ARG:HE	1.45	0.82
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.62	0.81
2:O:76:THR:CG2	2:O:82:SER:H	1.93	0.81
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.60	0.81
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.60	0.81
2:O:225:ASN:CG	2:O:226:ILE:H	1.88	0.81
1:N:49:ASN:ND2	1:N:52:ASN:H	1.79	0.81
3:P:15:ILE:HD12	3:P:15:ILE:H	1.45	0.81
3:C:6:ARG:HD3	3:C:16:ASN:OD1	1.81	0.81
3:C:15:ILE:H	3:C:15:ILE:HD12	1.45	0.81
1:A:170:THR:HG22	1:A:171:THR:N	1.96	0.81
3:P:17:ASN:HD21	7:T:1:GLY:HA2	1.46	0.81
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.63	0.81
6:S:32:MET:HE3	6:S:87:LYS:H	1.45	0.80
2:B:76:THR:CG2	2:B:82:SER:H	1.94	0.80
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.63	0.80
8:U:73:LEU:HD12	8:U:73:LEU:O	1.82	0.80
3:C:121:LEU:HG	3:C:125:MET:HE2	1.63	0.80
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.17	0.80
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.21	0.80
4:D:231:LYS:O	6:F:71:LYS:HE3	1.81	0.80
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.44	0.79
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.47	0.79
1:N:388:ARG:HH21	1:N:388:ARG:HG3	1.48	0.79
2:O:62:ASN:O	2:O:65:THR:HG22	1.83	0.79
2:O:27:THR:HG22	2:O:28:LYS:N	1.98	0.79
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.63	0.79
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.64	0.78
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.65	0.78
6:F:32:MET:CE	6:F:87:LYS:H	1.97	0.78
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.65	0.78
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.65	0.78
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.19	0.78
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.48	0.78
3:P:6:ARG:HD3	3:P:16:ASN:OD1	1.84	0.77
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.19	0.77
2:B:62:ASN:O	2:B:65:THR:HG22	1.84	0.77
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.66	0.77
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.07	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:ILE:HG22	2:O:227:ARG:N	1.99	0.77
1:N:364:ALA:O	1:N:368:GLN:HG2	1.84	0.77
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.66	0.77
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.19	0.77
3:P:157:ILE:HG13	3:P:158:GLY:N	1.99	0.77
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.19	0.77
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.10	0.76
1:N:170:THR:HG22	1:N:171:THR:N	1.98	0.76
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.66	0.76
1:A:373:THR:HB	1:A:374:PRO:HD3	1.67	0.76
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.66	0.76
2:O:207:VAL:HG12	2:O:208:GLY:H	1.50	0.76
13:P:501:HEM:HMC1	13:P:501:HEM:HBC2	1.67	0.76
4:Q:197:GLU:HG2	4:Q:198:HIS:N	1.99	0.76
5:E:73:LYS:HB3	5:E:195:VAL:O	1.86	0.76
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.51	0.76
3:P:101:ARG:HD2	3:P:101:ARG:C	2.11	0.76
2:B:201:SER:OG	2:B:228:SER:HB3	1.87	0.75
2:O:226:ILE:HG22	2:O:227:ARG:H	1.50	0.75
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.01	0.75
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.67	0.75
1:A:49:ASN:ND2	1:A:52:ASN:H	1.85	0.75
3:C:17:ASN:HD21	7:G:1:GLY:HA2	1.52	0.75
1:N:206:LYS:O	1:N:209:VAL:HG12	1.87	0.74
1:N:182:LEU:O	1:N:186:ILE:HG13	1.87	0.74
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.01	0.74
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.69	0.74
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.50	0.74
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.69	0.74
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.70	0.74
1:N:136:GLN:HE22	9:V:50:LEU:HD12	1.51	0.74
6:S:52:LYS:NZ	7:T:11:ARG:NH1	2.31	0.74
4:D:223:LYS:C	4:D:223:LYS:HD3	2.13	0.73
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.53	0.73
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.69	0.73
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.70	0.73
1:A:182:LEU:O	1:A:186:ILE:HG13	1.89	0.73
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.24	0.73
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.70	0.73
3:P:12:LEU:HA	3:P:15:ILE:HD13	1.71	0.73
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.70	0.73
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.24	0.73
3:P:70:THR:O	3:P:74:VAL:HB	1.89	0.72
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.53	0.72
2:O:225:ASN:CG	2:O:226:ILE:N	2.43	0.72
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.71	0.72
2:B:248:ASN:C	2:B:248:ASN:HD22	1.98	0.72
2:O:295:LEU:O	2:O:299:VAL:HG23	1.90	0.72
3:P:121:LEU:HG	3:P:125:MET:HE2	1.72	0.72
5:R:186:GLN:HE21	5:R:188:VAL:HG12	1.55	0.72
4:Q:76:GLU:H	4:Q:76:GLU:CD	1.98	0.72
7:T:29:ILE:H	7:T:29:ILE:HD12	1.55	0.72
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.20	0.72
6:F:52:LYS:NZ	7:G:11:ARG:NH1	2.36	0.72
2:O:398:VAL:O	2:O:402:ILE:HG13	1.90	0.72
4:Q:222:MET:HE3	5:R:40:THR:OG1	1.90	0.71
3:C:12:LEU:HA	3:C:15:ILE:HD13	1.72	0.71
17:D:501:HEC:HMB3	17:D:501:HEC:HBB3	1.72	0.71
2:O:248:ASN:C	2:O:248:ASN:HD22	1.96	0.71
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.24	0.71
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.25	0.71
1:N:49:ASN:HD21	1:N:52:ASN:H	1.39	0.71
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.71	0.71
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.71
5:E:1:VAL:HG23	5:E:3:ASN:H	1.56	0.71
9:I:71:ASN:HD22	9:I:71:ASN:N	1.87	0.71
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.88	0.71
2:B:295:LEU:O	2:B:299:VAL:HG23	1.90	0.70
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.53	0.70
2:O:393:THR:HG23	2:O:397:VAL:HB	1.74	0.70
3:P:90:PHE:HB3	3:P:236:MET:HE3	1.71	0.70
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.71	0.70
3:C:101:ARG:HD2	3:C:101:ARG:C	2.16	0.70
3:P:347:PRO:O	3:P:350:ILE:HG22	1.90	0.70
1:A:369:LEU:HD11	1:A:392:LEU:HD21	1.72	0.70
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.57	0.70
2:O:47:ILE:HD12	2:O:47:ILE:N	2.06	0.70
2:B:393:THR:HG23	2:B:397:VAL:HB	1.74	0.70
4:D:197:GLU:HG2	4:D:198:HIS:N	2.07	0.70
6:F:32:MET:HE3	6:F:87:LYS:N	2.05	0.70
8:U:52:GLU:HG2	8:U:53:GLN:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.74	0.70
2:B:393:THR:CG2	2:B:397:VAL:HB	2.21	0.70
1:N:373:THR:HB	1:N:374:PRO:HD3	1.71	0.70
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.07	0.69
1:N:49:ASN:ND2	1:N:49:ASN:C	2.48	0.69
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.22	0.69
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.27	0.69
1:A:49:ASN:ND2	1:A:49:ASN:C	2.48	0.69
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.74	0.69
7:G:78:GLU:C	7:G:79:ASN:HD22	2.00	0.69
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.74	0.69
1:A:233:ARG:HG2	1:A:233:ARG:HH11	1.58	0.69
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.27	0.69
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.73	0.69
3:P:285:ILE:N	3:P:285:ILE:HD12	2.08	0.69
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.28	0.69
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.57	0.69
3:C:285:ILE:HD12	3:C:285:ILE:N	2.07	0.69
2:O:376:GLN:HE22	9:V:77:ARG:HH22	1.40	0.69
3:P:235:LEU:O	3:P:239:PRO:HD2	1.93	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.58	0.68
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.29	0.68
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.12	0.68
2:O:357:VAL:O	2:O:361:LYS:HG3	1.93	0.68
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.26	0.68
2:B:47:ILE:HD12	2:B:47:ILE:N	2.09	0.68
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.59	0.68
2:B:357:VAL:O	2:B:361:LYS:HG3	1.94	0.68
3:C:139:MET:SD	3:C:269:ILE:HG13	2.34	0.68
2:O:227:ARG:NH1	2:O:228:SER:H	1.92	0.68
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.29	0.68
3:P:17:ASN:HD21	7:T:1:GLY:CA	2.07	0.68
2:B:398:VAL:O	2:B:402:ILE:HG13	1.94	0.67
3:C:15:ILE:HD12	3:C:15:ILE:N	2.08	0.67
1:N:342:TRP:O	1:N:345:LEU:HB2	1.93	0.67
2:O:34:ILE:HD13	2:O:386:ALA:O	1.94	0.67
2:O:393:THR:CG2	2:O:397:VAL:HB	2.24	0.67
3:C:2:ALA:CB	3:C:8:SER:HB3	2.24	0.67
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.29	0.67
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.75	0.67
8:U:34:ARG:O	8:U:38:GLU:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.76	0.67
5:E:52:LYS:C	5:E:52:LYS:HD3	2.20	0.67
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.30	0.67
8:H:73:LEU:HD12	8:H:73:LEU:O	1.95	0.67
2:B:24:LEU:HD12	2:B:37:SER:O	1.95	0.67
4:D:164:ILE:O	4:D:179:MET:HE2	1.93	0.67
1:A:49:ASN:C	1:A:49:ASN:HD22	2.01	0.67
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.77	0.67
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.24	0.67
1:N:49:ASN:C	1:N:49:ASN:HD22	2.01	0.67
2:O:59:THR:HG22	2:O:60:THR:N	2.08	0.67
1:N:369:LEU:HD11	1:N:392:LEU:HD21	1.77	0.66
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.28	0.66
3:P:17:ASN:ND2	7:T:1:GLY:HA2	2.10	0.66
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.77	0.66
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.77	0.66
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.60	0.66
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.75	0.66
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.30	0.66
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.95	0.66
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.10	0.66
3:C:90:PHE:CB	3:C:236:MET:HE3	2.26	0.66
2:B:227:ARG:CD	2:B:228:SER:H	2.08	0.66
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.31	0.66
3:P:236:MET:HA	15:P:3003:CDL:H162	1.78	0.66
1:A:170:THR:CG2	1:A:171:THR:H	2.09	0.66
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.77	0.66
4:D:47:ALA:N	4:D:50:ASN:HD22	1.90	0.66
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.95	0.66
1:A:137:GLU:O	1:A:141:MET:HG3	1.94	0.65
3:P:15:ILE:HD12	3:P:15:ILE:N	2.11	0.65
1:A:49:ASN:HD21	1:A:52:ASN:H	1.42	0.65
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.26	0.65
10:J:4:ALA:O	10:J:8:GLN:HG3	1.95	0.65
3:P:92:PHE:O	3:P:95:ILE:HG22	1.96	0.65
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.78	0.65
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.12	0.65
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.31	0.65
5:R:73:LYS:HB3	5:R:195:VAL:O	1.96	0.65
10:W:52:TRP:O	10:W:56:LYS:HB2	1.96	0.65
3:C:50:LEU:HD23	13:C:501:HEM:HBC1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:389:SER:O	2:O:391:THR:HG23	1.97	0.65
3:P:269:ILE:HG23	3:P:269:ILE:O	1.95	0.65
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.26	0.65
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.78	0.65
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.78	0.65
2:B:264:VAL:HG23	2:B:316:TYR:C	2.21	0.65
5:R:52:LYS:C	5:R:52:LYS:HD3	2.22	0.65
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.79	0.65
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.32	0.64
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.11	0.64
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.62	0.64
2:B:27:THR:HG22	2:B:28:LYS:N	2.12	0.64
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.79	0.64
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	1.79	0.64
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.16	0.64
2:B:218:GLN:HG3	2:B:222:GLN:NE2	2.10	0.64
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.80	0.64
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.79	0.64
1:N:44:GLY:H	1:N:47:TYR:HD1	1.44	0.64
7:T:3:HIS:O	7:T:7:LEU:HG	1.97	0.64
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.38	0.64
3:C:235:LEU:O	3:C:239:PRO:HD2	1.97	0.64
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.80	0.64
4:Q:76:GLU:CD	4:Q:76:GLU:N	2.56	0.64
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.26	0.64
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.28	0.64
2:B:389:SER:O	2:B:391:THR:HG23	1.97	0.64
2:B:162:ASN:O	2:B:244:ILE:HD12	1.98	0.64
2:O:226:ILE:CG2	2:O:227:ARG:H	2.11	0.64
1:N:161:THR:HG21	1:N:235:ARG:H	1.63	0.64
3:P:157:ILE:CG1	3:P:158:GLY:H	2.09	0.64
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.33	0.64
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.33	0.63
10:W:49:GLY:N	10:W:54:HIS:ND1	2.46	0.63
1:A:105:ASP:O	1:A:109:VAL:HG23	1.98	0.63
2:B:297:GLN:O	2:B:301:LYS:HG3	1.97	0.63
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.80	0.63
8:H:34:ARG:O	8:H:38:GLU:HG2	1.98	0.63
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.89	0.63
2:B:59:THR:HG22	2:B:60:THR:N	2.13	0.63
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.80	0.63
1:N:223:TYR:H	1:N:223:TYR:HD2	1.45	0.63
1:A:223:TYR:H	1:A:223:TYR:HD2	1.44	0.63
2:O:225:ASN:ND2	2:O:226:ILE:H	1.95	0.63
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.34	0.63
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.13	0.63
10:J:52:TRP:O	10:J:56:LYS:HB2	1.98	0.63
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.63
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.34	0.63
3:C:236:MET:HA	15:C:2003:CDL:H162	1.79	0.63
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.80	0.63
3:P:342:GLN:HA	3:P:342:GLN:NE2	2.14	0.63
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.81	0.63
4:D:116:ILE:HG23	4:D:117:VAL:N	2.13	0.62
1:N:178:THR:HG22	1:N:179:ARG:N	2.13	0.62
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.81	0.62
1:A:242:ARG:HH22	1:A:432:LEU:HA	1.63	0.62
2:B:28:LYS:O	2:B:29:LEU:O	2.17	0.62
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.81	0.62
2:O:274:VAL:O	2:O:278:VAL:HG23	1.99	0.62
3:C:347:PRO:O	3:C:350:ILE:HG22	1.99	0.62
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.64	0.62
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.65	0.62
1:N:284:PHE:CE2	9:V:71:ASN:O	2.52	0.62
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.63	0.62
2:B:71:LEU:O	2:B:74:PRO:HD2	2.00	0.62
7:G:3:HIS:O	7:G:7:LEU:HG	1.99	0.62
7:G:41:PHE:HD2	7:G:41:PHE:C	2.08	0.62
3:C:216:SER:HB3	6:F:59:MET:HE2	1.82	0.62
2:O:24:LEU:HD12	2:O:37:SER:O	1.98	0.62
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.35	0.62
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.08	0.62
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.82	0.62
10:W:56:LYS:O	10:W:60:GLU:HG2	1.99	0.62
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.35	0.62
2:O:227:ARG:HH11	2:O:228:SER:H	1.47	0.62
3:P:95:ILE:O	3:P:99:ILE:HG13	2.00	0.62
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.35	0.61
3:C:92:PHE:O	3:C:95:ILE:HG22	2.00	0.61
1:N:170:THR:CG2	1:N:171:THR:H	2.12	0.61
2:O:71:LEU:O	2:O:74:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.82	0.61
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.16	0.61
2:O:76:THR:HG22	2:O:82:SER:N	2.10	0.61
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.14	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.99	0.61
1:N:145:MET:HE2	1:N:145:MET:N	2.16	0.61
3:P:139:MET:SD	3:P:269:ILE:HG13	2.41	0.61
3:C:279:TYR:O	3:C:283:ARG:HG3	2.00	0.61
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.31	0.61
3:P:289:LEU:HD12	3:P:289:LEU:O	2.01	0.61
2:B:76:THR:HG22	2:B:82:SER:N	2.10	0.61
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.36	0.61
3:C:226:SER:O	3:C:230:ILE:HG12	2.01	0.61
3:C:269:ILE:HG23	3:C:269:ILE:O	2.01	0.61
1:N:45:SER:HA	1:N:48:GLU:HG3	1.82	0.61
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.35	0.61
3:C:15:ILE:H	3:C:15:ILE:CD1	2.14	0.61
3:C:17:ASN:HD21	7:G:1:GLY:CA	2.13	0.61
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.16	0.61
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.64	0.61
2:O:361:LYS:O	2:O:365:LYS:HG3	2.00	0.60
3:P:332:ASN:HD21	3:P:358:SER:CB	2.13	0.60
7:T:41:PHE:HD2	7:T:41:PHE:C	2.09	0.60
2:B:35:ILE:O	2:B:213:HIS:HE1	1.85	0.60
2:O:259:THR:HG22	2:O:260:GLU:N	2.16	0.60
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.01	0.60
4:D:47:ALA:H	4:D:50:ASN:ND2	1.92	0.60
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.70	0.60
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.17	0.60
3:P:332:ASN:ND2	3:P:358:SER:OG	2.35	0.60
9:V:64:LEU:HD12	9:V:77:ARG:O	2.02	0.60
6:S:11:ARG:HG2	6:S:11:ARG:O	2.01	0.60
6:S:70:LEU:C	6:S:70:LEU:HD12	2.26	0.60
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.42	0.60
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.37	0.60
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.32	0.60
10:W:4:ALA:O	10:W:8:GLN:HG3	2.01	0.60
1:A:161:THR:HG21	1:A:235:ARG:H	1.67	0.60
3:P:139:MET:HG2	3:P:255:GLU:HB3	1.84	0.60
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.02	0.60
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:40:ARG:HD2	15:T:3004:CDL:OA4	2.01	0.60
1:A:206:LYS:O	1:A:209:VAL:HG12	2.00	0.60
1:A:280:TYR:CG	1:A:281:ASP:N	2.70	0.60
3:P:155:PRO:O	3:P:156:TYR:HB2	2.02	0.60
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.66	0.60
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.37	0.60
1:A:106:MET:HE2	1:A:106:MET:O	2.01	0.59
1:A:170:THR:CG2	1:A:171:THR:N	2.65	0.59
3:C:36:SER:O	3:C:40:VAL:HG23	2.02	0.59
2:O:327:ILE:HG22	9:V:55:MET:HE3	1.84	0.59
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.32	0.59
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.30	0.59
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.83	0.59
3:C:156:TYR:C	3:C:158:GLY:H	2.10	0.59
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.84	0.59
1:N:137:GLU:O	1:N:141:MET:HG3	2.01	0.59
8:H:21:ARG:O	8:H:25:GLU:HG3	2.02	0.59
1:N:187:ASP:O	1:N:191:LYS:HE3	2.02	0.59
1:A:13:GLU:HG2	1:A:14:THR:N	2.17	0.59
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.31	0.59
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.59
3:P:189:ALA:O	3:P:193:ILE:HG13	2.03	0.59
7:T:41:PHE:C	7:T:41:PHE:CD2	2.81	0.59
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.37	0.59
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.33	0.59
2:B:31:ASN:HD22	2:B:31:ASN:N	2.01	0.59
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.83	0.59
2:O:407:SER:O	2:O:411:VAL:HG23	2.02	0.59
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.32	0.59
6:S:13:MET:HA	6:S:16:ILE:HB	1.85	0.59
7:G:41:PHE:C	7:G:41:PHE:CD2	2.79	0.59
2:O:226:ILE:CG2	2:O:227:ARG:N	2.66	0.59
3:P:247:SER:OG	3:P:250:LEU:HB2	2.02	0.59
9:V:55:MET:HA	9:V:58:ARG:HG3	1.84	0.59
1:A:43:ALA:HB2	1:A:194:ARG:HH21	1.68	0.59
8:U:32:LYS:O	8:U:36:ARG:HG3	2.03	0.59
1:A:45:SER:OG	1:A:92:ARG:HA	2.03	0.59
1:N:49:ASN:ND2	1:N:51:LYS:N	2.51	0.59
3:P:319:ARG:O	3:P:323:GLN:HG3	2.02	0.59
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.32	0.58
2:B:86:THR:O	2:B:90:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:UNK:N	9:I:72:ALA:HB2	2.18	0.58
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.58
7:T:29:ILE:HD12	7:T:29:ILE:N	2.17	0.58
2:B:312:PHE:HE1	9:I:62:ARG:O	1.85	0.58
3:C:132:TYR:OH	3:C:139:MET:HG3	2.03	0.58
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.17	0.58
1:A:44:GLY:H	1:A:47:TYR:HD1	1.52	0.58
1:A:95:THR:HG22	1:A:96:ALA:N	2.18	0.58
3:C:332:ASN:HD21	3:C:358:SER:CB	2.16	0.58
7:T:74:PRO:O	7:T:78:GLU:HG3	2.04	0.58
10:W:30:LEU:HD23	10:W:33:ARG:HH22	1.68	0.58
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.38	0.58
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.67	0.58
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.36	0.58
10:J:49:GLY:N	10:J:54:HIS:ND1	2.52	0.58
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.39	0.58
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.38	0.58
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.85	0.58
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.85	0.58
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.86	0.58
6:S:32:MET:CE	6:S:87:LYS:H	2.15	0.58
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.84	0.58
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.33	0.58
2:B:274:VAL:O	2:B:278:VAL:HG23	2.03	0.58
3:C:285:ILE:CD1	3:C:285:ILE:H	2.17	0.58
3:P:15:ILE:H	3:P:15:ILE:CD1	2.17	0.58
2:B:229:GLY:O	2:B:231:GLY:N	2.37	0.58
3:C:137:GLY:H	3:C:140:SER:HB2	1.68	0.58
3:C:207:ASN:ND2	3:C:314:ARG:NH1	2.52	0.58
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.85	0.58
1:N:45:SER:HA	1:N:48:GLU:CD	2.29	0.58
3:C:243:LEU:HD11	3:C:250:LEU:HD23	1.86	0.58
2:O:297:GLN:O	2:O:301:LYS:HG3	2.04	0.58
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.86	0.58
3:C:271:PRO:HD2	3:C:276:LEU:HD23	1.86	0.57
2:B:327:ILE:HD11	9:I:58:ARG:O	2.04	0.57
2:O:150:VAL:HG23	2:O:151:ALA:N	2.19	0.57
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.19	0.57
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.86	0.57
7:G:29:ILE:HD12	7:G:29:ILE:N	2.20	0.57
3:P:137:GLY:H	3:P:140:SER:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:O	2:B:292:THR:HG22	2.04	0.57
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.40	0.57
8:H:16:PRO:O	8:H:20:ILE:HG13	2.04	0.57
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.86	0.57
5:R:69:LEU:HD13	5:R:71:LEU:HD11	1.85	0.57
1:A:342:TRP:O	1:A:345:LEU:HB2	2.05	0.57
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.87	0.57
4:D:28:ARG:HD2	4:D:171:TYR:CE1	2.39	0.57
3:P:285:ILE:HD12	3:P:285:ILE:H	1.69	0.57
3:P:285:ILE:CD1	3:P:285:ILE:H	2.18	0.57
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.87	0.57
1:A:45:SER:HA	1:A:48:GLU:CD	2.30	0.57
1:A:130:GLU:O	1:A:134:ILE:HG13	2.05	0.57
3:C:121:LEU:HG	3:C:125:MET:CE	2.33	0.57
7:G:74:PRO:O	7:G:78:GLU:HG3	2.04	0.57
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.70	0.57
2:O:27:THR:CG2	2:O:28:LYS:N	2.68	0.57
5:R:122:HIS:CE1	5:R:124:LEU:HG	2.40	0.57
2:B:169:LYS:O	2:B:170:THR:HG23	2.04	0.57
3:C:17:ASN:ND2	7:G:1:GLY:HA2	2.20	0.57
3:C:319:ARG:O	3:C:323:GLN:HG3	2.04	0.57
2:O:162:ASN:O	2:O:244:ILE:HD12	2.05	0.57
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.15	0.57
5:R:161:HIS:HB2	19:R:501:FES:S1	2.44	0.57
3:C:285:ILE:N	3:C:285:ILE:CD1	2.68	0.57
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.86	0.57
3:P:139:MET:HE1	3:P:269:ILE:CA	2.27	0.57
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.87	0.57
2:O:59:THR:HG22	2:O:60:THR:H	1.68	0.57
2:O:292:THR:O	2:O:292:THR:HG22	2.05	0.57
3:P:332:ASN:HD21	3:P:358:SER:HB3	1.70	0.57
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.87	0.57
2:B:220:ALA:O	2:B:224:LEU:HB2	2.05	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.40	0.56
6:S:104:ARG:O	6:S:108:ASN:ND2	2.38	0.56
2:B:27:THR:HG22	2:B:28:LYS:H	1.71	0.56
2:B:62:ASN:HA	2:B:190:GLN:NE2	2.19	0.56
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.19	0.56
3:C:139:MET:HG2	3:C:255:GLU:HB3	1.87	0.56
6:F:104:ARG:O	6:F:108:ASN:ND2	2.38	0.56
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.40	0.56
2:B:157:VAL:HG22	2:B:157:VAL:O	2.06	0.56
2:B:268:GLU:O	2:B:271:ALA:HB3	2.05	0.56
3:C:132:TYR:CD2	12:C:2010:UNL:O1	2.58	0.56
3:C:332:ASN:HD21	3:C:358:SER:HB3	1.71	0.56
1:N:29:GLU:HG3	1:N:203:ILE:O	2.05	0.56
3:P:139:MET:HE1	3:P:270:LYS:H	1.70	0.56
8:U:52:GLU:HG2	8:U:53:GLN:H	1.69	0.56
1:A:170:THR:HG22	1:A:172:GLU:H	1.71	0.56
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.33	0.56
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.41	0.56
1:A:388:ARG:HG3	1:A:388:ARG:NH2	2.20	0.56
17:D:501:HEC:HHA	17:D:501:HEC:HBA1	1.86	0.56
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.05	0.56
2:B:248:ASN:C	2:B:248:ASN:ND2	2.63	0.56
4:D:203:ARG:NH1	10:J:43:PHE:HD2	2.04	0.56
9:I:71:ASN:H	9:I:71:ASN:ND2	1.99	0.56
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.71	0.56
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.40	0.56
1:A:29:GLU:HG3	1:A:203:ILE:O	2.06	0.56
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.68	0.56
9:I:59:SER:O	9:I:60:ALA:C	2.48	0.56
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.19	0.56
1:A:178:THR:HG22	1:A:179:ARG:N	2.21	0.56
5:E:95:PRO:HG3	3:P:263:LEU:CD2	2.36	0.56
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.87	0.56
3:P:95:ILE:HD13	3:P:121:LEU:HD12	1.87	0.56
4:D:37:CYS:C	4:D:39:ALA:H	2.12	0.56
2:O:403:ASP:C	2:O:405:VAL:H	2.14	0.56
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.41	0.56
2:B:227:ARG:NE	2:B:227:ARG:CA	2.68	0.56
3:C:366:LEU:O	3:C:369:THR:N	2.38	0.56
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.71	0.56
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.88	0.56
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.41	0.55
1:N:388:ARG:HG3	1:N:388:ARG:NH2	2.16	0.55
7:T:46:PHE:O	7:T:50:PRO:HG2	2.06	0.55
1:A:281:ASP:OD2	1:A:284:PHE:HE1	1.89	0.55
2:B:403:ASP:C	2:B:405:VAL:H	2.13	0.55
3:P:216:SER:HB3	6:S:59:MET:HE2	1.88	0.55
2:B:306:PRO:HA	9:I:52:ARG:CG	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.55
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.42	0.55
3:P:36:SER:O	3:P:40:VAL:HG23	2.06	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.42	0.55
4:Q:239:PRO:HB2	4:Q:240:PRO:HD2	1.88	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.06	0.55
4:D:197:GLU:HG2	4:D:198:HIS:H	1.72	0.55
1:N:49:ASN:HD21	1:N:52:ASN:N	2.04	0.55
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.72	0.55
1:A:133:VAL:O	1:A:137:GLU:HG3	2.06	0.55
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.40	0.55
2:O:192:HIS:O	2:O:196:GLN:HG3	2.06	0.55
3:P:345:GLU:O	3:P:348:PHE:HB2	2.07	0.55
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.17	0.55
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.89	0.55
8:U:12:GLU:O	8:U:12:GLU:HG2	2.07	0.55
3:C:129:PHE:CZ	3:C:147:ILE:HD12	2.41	0.55
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.41	0.55
1:N:62:LEU:CD2	1:N:130:GLU:HG3	2.36	0.55
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.06	0.55
1:A:106:MET:HE2	1:A:106:MET:C	2.32	0.55
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.88	0.55
2:B:59:THR:HG22	2:B:60:THR:H	1.72	0.55
7:G:29:ILE:HD12	7:G:29:ILE:H	1.70	0.55
2:B:189:GLU:O	2:B:192:HIS:N	2.39	0.55
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.89	0.55
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.36	0.55
1:A:406:MET:O	1:A:410:VAL:HG23	2.07	0.55
2:B:34:ILE:HD13	2:B:386:ALA:O	2.07	0.55
3:C:11:LEU:O	3:C:14:MET:HB2	2.06	0.55
3:C:329:LEU:O	3:C:332:ASN:HB3	2.06	0.55
2:B:154:SER:O	2:B:157:VAL:HG12	2.06	0.54
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.42	0.54
7:G:29:ILE:H	7:G:29:ILE:CD1	2.20	0.54
4:Q:139:ALA:CB	8:U:41:ASP:HA	2.38	0.54
6:S:10:GLY:C	6:S:12:LEU:H	2.15	0.54
3:C:137:GLY:N	3:C:140:SER:HB2	2.23	0.54
5:E:161:HIS:HB2	19:E:501:FES:S1	2.48	0.54
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.89	0.54
1:N:85:HIS:CE1	2:O:370:MET:HE1	2.42	0.54
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:275:PHE:HB3	14:P:3001:3H1:H16A	1.89	0.54
8:U:21:ARG:O	8:U:25:GLU:HG3	2.08	0.54
1:N:190:PHE:C	1:N:195:MET:HE2	2.33	0.54
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.72	0.54
3:P:243:LEU:HD11	3:P:250:LEU:HD23	1.90	0.54
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.88	0.54
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.43	0.54
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.40	0.54
10:W:14:PHE:N	10:W:14:PHE:CD2	2.73	0.54
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.43	0.54
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.89	0.54
1:N:133:VAL:O	1:N:137:GLU:HG3	2.08	0.54
10:W:40:ASP:O	10:W:44:GLU:HG3	2.06	0.54
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.88	0.54
1:N:136:GLN:HE22	9:V:50:LEU:CD1	2.21	0.54
3:P:329:LEU:O	3:P:332:ASN:HB3	2.08	0.54
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.55	0.54
1:N:112:LEU:O	1:N:116:VAL:HG23	2.07	0.54
2:O:229:GLY:O	2:O:231:GLY:N	2.40	0.54
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.73	0.54
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.73	0.54
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.07	0.54
1:N:281:ASP:OD2	1:N:284:PHE:HE1	1.90	0.54
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.73	0.54
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.31	0.54
2:B:262:ALA:HB3	2:B:269:ALA:HB2	1.90	0.54
1:N:106:MET:HE2	1:N:106:MET:C	2.33	0.54
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.54
3:P:285:ILE:N	3:P:285:ILE:CD1	2.71	0.54
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.43	0.54
1:A:49:ASN:HD21	1:A:52:ASN:N	2.06	0.53
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.53
2:B:344:LEU:HD23	2:B:417:PHE:CD2	2.44	0.53
5:E:69:LEU:HD13	5:E:71:LEU:HD11	1.90	0.53
1:N:106:MET:HE2	1:N:106:MET:O	2.08	0.53
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.73	0.53
3:C:95:ILE:O	3:C:99:ILE:HG13	2.09	0.53
6:F:31:LEU:HD21	6:F:65:ALA:CB	2.38	0.53
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.88	0.53
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.43	0.53
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:THR:O	5:E:106:ILE:HG13	2.09	0.53
6:S:17:ARG:HH11	6:S:17:ARG:HG3	1.73	0.53
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.21	0.53
2:O:217:LYS:O	2:O:221:GLU:HG2	2.08	0.53
3:P:145:THR:O	3:P:149:ASN:HB2	2.08	0.53
1:A:62:LEU:HD21	1:A:130:GLU:HG3	1.91	0.53
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.44	0.53
3:C:145:THR:O	3:C:149:ASN:HB2	2.09	0.53
1:N:178:THR:CG2	1:N:179:ARG:N	2.71	0.53
5:R:77:LYS:HE2	5:R:79:SER:CB	2.38	0.53
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.89	0.53
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.74	0.53
3:C:19:LEU:O	3:C:20:ILE:CG1	2.53	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG21	1.90	0.53
3:P:137:GLY:N	3:P:140:SER:HB2	2.24	0.53
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.44	0.53
1:A:209:VAL:O	1:A:213:ARG:HG3	2.09	0.53
2:B:361:LYS:O	2:B:365:LYS:HG3	2.08	0.53
4:D:150:ASN:O	4:D:156:GLN:HA	2.08	0.53
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.39	0.53
1:A:233:ARG:HG2	1:A:233:ARG:NH1	2.24	0.53
2:B:327:ILE:HG22	9:I:55:MET:HE3	1.91	0.53
1:N:62:LEU:HD21	1:N:130:GLU:HG3	1.90	0.53
1:N:178:THR:HG22	1:N:180:ALA:H	1.74	0.53
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.44	0.53
3:C:5:ILE:O	3:C:5:ILE:HG22	2.09	0.53
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.44	0.53
2:O:259:THR:O	2:O:260:GLU:C	2.51	0.53
3:C:157:ILE:O	3:C:161:LEU:HD12	2.09	0.52
3:C:180:PHE:HE1	3:P:180:PHE:HE1	1.56	0.52
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.44	0.52
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.90	0.52
2:O:264:VAL:HG23	2:O:316:TYR:C	2.34	0.52
8:U:36:ARG:HH11	8:U:36:ARG:HB2	1.73	0.52
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.09	0.52
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.52
9:V:32:UNK:C	9:V:73:PRO:HG2	2.39	0.52
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.44	0.52
3:C:366:LEU:O	3:C:367:PHE:C	2.52	0.52
1:N:242:ARG:HH22	1:N:432:LEU:HA	1.74	0.52
7:T:48:VAL:HG12	7:T:49:ALA:N	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLU:O	2:B:358:THR:HG23	2.09	0.52
3:C:285:ILE:HD12	3:C:285:ILE:H	1.72	0.52
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.24	0.52
1:A:49:ASN:ND2	1:A:51:LYS:N	2.58	0.52
1:A:62:LEU:CD2	1:A:130:GLU:HG3	2.40	0.52
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.92	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.44	0.52
2:B:307:PHE:CD1	2:B:308:ASP:N	2.78	0.52
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.91	0.52
2:O:128:THR:HG21	2:O:224:LEU:CD2	2.40	0.52
2:O:291:VAL:C	2:O:293:SER:H	2.16	0.52
3:P:90:PHE:CZ	3:P:240:PHE:HA	2.45	0.52
3:P:129:PHE:CZ	3:P:147:ILE:HD12	2.45	0.52
4:Q:37:CYS:C	4:Q:39:ALA:H	2.18	0.52
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.10	0.52
7:T:29:ILE:O	7:T:33:ALA:HB3	2.08	0.52
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.45	0.52
7:G:40:ARG:HD2	15:G:2004:CDL:OA4	2.09	0.52
2:O:31:ASN:HD22	2:O:31:ASN:N	2.07	0.52
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.90	0.52
1:A:422:LEU:HD22	1:A:437:ILE:HD13	1.92	0.52
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.91	0.52
3:C:105:TYR:HA	3:C:315:THR:HG22	1.92	0.52
3:C:139:MET:HE1	3:C:270:LYS:H	1.75	0.52
5:E:101:ARG:NH2	5:E:127:VAL:HG21	2.25	0.52
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.45	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.77	0.52
1:A:49:ASN:ND2	1:A:51:LYS:H	2.08	0.52
6:F:70:LEU:C	6:F:70:LEU:HD12	2.35	0.52
2:O:268:GLU:HG2	2:O:268:GLU:O	2.10	0.52
2:B:202:ALA:HB2	2:B:229:GLY:H	1.75	0.52
3:C:332:ASN:ND2	3:C:358:SER:OG	2.43	0.52
8:H:17:LEU:HD13	8:H:73:LEU:CD2	2.40	0.52
3:P:5:ILE:O	3:P:5:ILE:HG22	2.10	0.52
7:T:41:PHE:HD2	7:T:41:PHE:O	1.92	0.52
5:E:141:HIS:O	5:E:142:LEU:HD23	2.10	0.52
2:O:22:GLU:HG3	2:O:39:GLU:CB	2.37	0.52
2:O:50:PHE:HD2	2:O:104:LYS:HZ1	1.57	0.52
2:O:62:ASN:HA	2:O:190:GLN:NE2	2.25	0.52
6:S:32:MET:HE3	6:S:87:LYS:N	2.20	0.52
7:T:65:GLU:O	7:T:69:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:N	2:B:31:ASN:ND2	2.55	0.51
2:B:303:THR:HA	2:B:335:GLU:OE2	2.11	0.51
6:S:76:PRO:O	6:S:78:GLU:N	2.44	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.91	0.51
2:B:150:VAL:HG23	2:B:151:ALA:N	2.25	0.51
3:C:187:PRO:O	3:C:190:ILE:HB	2.10	0.51
1:A:305:HIS:ND1	9:I:35:UNK:CB	2.74	0.51
2:B:47:ILE:N	2:B:47:ILE:CD1	2.73	0.51
3:C:247:SER:OG	3:C:250:LEU:HB2	2.10	0.51
4:D:223:LYS:HD3	4:D:223:LYS:O	2.09	0.51
1:N:156:THR:HA	5:R:7:VAL:HG21	1.92	0.51
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.75	0.51
3:P:81:ARG:HH11	3:P:81:ARG:HG3	1.75	0.51
1:A:187:ASP:O	1:A:191:LYS:HE3	2.10	0.51
2:B:262:ALA:CB	2:B:269:ALA:HB2	2.39	0.51
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.45	0.51
1:N:433:ASP:OD2	1:N:435:ASN:N	2.43	0.51
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.92	0.51
3:P:271:PRO:HD2	3:P:276:LEU:HD23	1.91	0.51
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.26	0.51
5:R:102:THR:O	5:R:106:ILE:HG13	2.09	0.51
8:U:52:GLU:CG	8:U:53:GLN:N	2.74	0.51
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.23	0.51
3:C:167:GLY:HA3	3:C:178:ARG:NH2	2.25	0.51
8:H:9:GLU:C	8:H:10:GLU:HG3	2.34	0.51
1:N:45:SER:HA	1:N:48:GLU:CG	2.41	0.51
1:N:246:ASP:HA	1:N:427:PRO:HB3	1.91	0.51
3:P:11:LEU:O	3:P:14:MET:HB2	2.10	0.51
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.42	0.51
1:A:10:ASN:HD21	2:B:19:PRO:HD3	1.75	0.51
2:B:259:THR:HG22	2:B:260:GLU:N	2.24	0.51
5:E:52:LYS:C	5:E:52:LYS:CD	2.84	0.51
2:O:259:THR:CG2	2:O:260:GLU:N	2.73	0.51
6:S:40:ASP:O	6:S:44:LYS:HG3	2.11	0.51
8:U:72:LYS:HA	8:U:75:ASN:ND2	2.24	0.51
3:C:70:THR:O	3:C:74:VAL:HB	2.10	0.51
10:J:40:ASP:O	10:J:44:GLU:HG3	2.11	0.51
2:O:50:PHE:HD2	2:O:104:LYS:NZ	2.08	0.51
3:P:32:TRP:NE1	13:P:502:HEM:O2D	2.42	0.51
8:U:51:GLU:HG3	8:U:51:GLU:O	2.10	0.51
1:A:145:MET:HE2	1:A:145:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:LEU:C	4:D:208:MET:HE2	2.36	0.51
4:D:37:CYS:C	4:D:39:ALA:N	2.69	0.51
1:N:45:SER:OG	1:N:92:ARG:HA	2.11	0.51
1:N:136:GLN:HG2	9:V:51:CYS:HB3	1.92	0.51
2:O:248:ASN:C	2:O:248:ASN:ND2	2.63	0.51
2:O:376:GLN:HE22	9:V:77:ARG:NH2	2.06	0.51
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.51
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.46	0.51
8:U:36:ARG:HB2	8:U:36:ARG:NH1	2.26	0.51
1:A:93:GLU:O	1:A:94:GLN:HB2	2.09	0.51
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.93	0.51
2:B:394:ALA:C	2:B:396:SER:H	2.17	0.51
3:C:90:PHE:HB3	3:C:236:MET:CE	2.35	0.51
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.41	0.51
3:C:289:LEU:HD12	3:C:289:LEU:O	2.11	0.51
1:N:422:LEU:HD22	1:N:437:ILE:HD13	1.93	0.51
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.92	0.51
6:S:12:LEU:C	6:S:14:ASP:H	2.19	0.51
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.93	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.10	0.51
3:C:105:TYR:CA	3:C:315:THR:HG22	2.41	0.51
7:G:41:PHE:HD2	7:G:41:PHE:O	1.94	0.51
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.51
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.93	0.51
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.46	0.51
4:Q:203:ARG:HD2	18:R:3009:BOG:O6	2.11	0.51
4:Q:223:LYS:HD3	4:Q:223:LYS:O	2.10	0.51
3:C:172:ASP:OD1	3:C:173:ASN:N	2.35	0.50
3:C:272:GLU:OE1	3:C:272:GLU:HA	2.10	0.50
4:D:240:PRO:HD3	7:G:12:HIS:NE2	2.26	0.50
1:N:95:THR:HG22	1:N:96:ALA:N	2.25	0.50
3:P:31:TRP:O	3:P:101:ARG:HG3	2.11	0.50
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.26	0.50
7:G:81:GLN:OXT	8:H:49:HIS:HB3	2.11	0.50
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.10	0.50
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.45	0.50
6:F:91:GLU:O	6:F:95:LYS:HG3	2.11	0.50
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.46	0.50
3:P:139:MET:CE	3:P:270:LYS:H	2.23	0.50
3:P:183:HIS:O	3:P:187:PRO:HD2	2.12	0.50
2:B:50:PHE:HD2	2:B:104:LYS:HZ1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:GLU:HG2	1:N:14:THR:N	2.26	0.50
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.77	0.50
3:P:36:SER:HA	14:P:3002:3H1:H16B	1.92	0.50
3:P:241:LEU:C	4:Q:208:MET:HE2	2.36	0.50
4:Q:2:GLU:O	4:Q:2:GLU:HG2	2.11	0.50
8:U:13:LEU:HD23	8:U:13:LEU:H	1.77	0.50
1:A:95:THR:HG22	1:A:96:ALA:H	1.76	0.50
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.50
7:G:48:VAL:HG12	7:G:49:ALA:N	2.24	0.50
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.41	0.50
2:B:67:HIS:O	2:B:70:ARG:HB3	2.12	0.50
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.47	0.50
5:E:77:LYS:HE2	5:E:79:SER:CB	2.41	0.50
2:O:303:THR:HA	2:O:335:GLU:OE2	2.10	0.50
5:R:141:HIS:O	5:R:142:LEU:HD23	2.12	0.50
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.56	0.50
3:P:13:LYS:O	3:P:13:LYS:HG2	2.11	0.50
1:A:106:MET:HE3	1:A:208:LEU:HD13	1.93	0.50
1:A:241:ILE:HG23	1:A:241:ILE:O	2.10	0.50
10:J:30:LEU:HD23	10:J:33:ARG:HH22	1.77	0.50
1:N:79:VAL:O	1:N:82:MET:HG2	2.11	0.50
2:O:47:ILE:N	2:O:47:ILE:CD1	2.74	0.50
2:O:249:GLY:O	2:O:250:HIS:C	2.54	0.50
1:A:3:THR:O	1:A:4:TYR:C	2.55	0.50
1:A:307:PHE:CD1	1:A:307:PHE:C	2.89	0.50
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.93	0.50
2:B:249:GLY:O	2:B:250:HIS:C	2.54	0.50
5:E:38:LEU:HB2	10:J:14:PHE:HE1	1.76	0.50
2:O:156:GLN:HE22	9:V:77:ARG:C	2.20	0.50
4:Q:57:THR:CG2	10:W:59:TYR:HB2	2.42	0.50
8:U:73:LEU:HD12	8:U:73:LEU:C	2.35	0.50
2:O:62:ASN:O	2:O:65:THR:CG2	2.57	0.49
2:O:422:LYS:O	2:O:436:LEU:HD21	2.12	0.49
3:C:34:PHE:HB2	20:C:381:HOH:O	2.12	0.49
3:C:236:MET:HB2	15:C:2003:CDL:H161	1.94	0.49
5:E:122:HIS:CE1	5:E:124:LEU:HG	2.46	0.49
3:P:9:HIS:O	3:P:13:LYS:HB3	2.12	0.49
3:P:157:ILE:O	3:P:158:GLY:C	2.54	0.49
8:U:16:PRO:O	8:U:20:ILE:HG13	2.12	0.49
1:A:45:SER:HA	1:A:48:GLU:HG3	1.93	0.49
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:53:ASP:OD1	6:F:54:LEU:N	2.45	0.49
2:O:42:SER:OG	2:O:43:PRO:HD2	2.13	0.49
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.95	0.49
1:A:112:LEU:O	1:A:116:VAL:HG23	2.12	0.49
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.40	0.49
2:B:275:LEU:O	2:B:279:LEU:HD12	2.13	0.49
10:J:14:PHE:CD2	10:J:14:PHE:N	2.76	0.49
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.94	0.49
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.81	0.49
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.48	0.49
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.45	0.49
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.13	0.49
4:Q:223:LYS:C	4:Q:223:LYS:CD	2.84	0.49
6:S:21:TYR:C	6:S:21:TYR:CD2	2.91	0.49
1:A:295:ALA:O	1:A:299:VAL:HG23	2.12	0.49
2:B:76:THR:HG22	2:B:81:SER:HA	1.92	0.49
3:C:13:LYS:O	3:C:13:LYS:HG2	2.11	0.49
3:C:164:TRP:O	3:C:165:ALA:C	2.56	0.49
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.45	0.49
2:O:221:GLU:HG3	2:O:222:GLN:N	2.20	0.49
4:Q:70:VAL:HG21	4:Q:85:GLY:HA2	1.94	0.49
2:O:275:LEU:O	2:O:279:LEU:HD12	2.12	0.49
7:T:32:ASP:C	7:T:35:PRO:HD2	2.38	0.49
2:B:33:LEU:HD12	2:B:204:MET:O	2.12	0.49
2:B:306:PRO:HB3	9:I:52:ARG:N	2.27	0.49
2:O:154:SER:O	2:O:157:VAL:HG12	2.13	0.49
3:P:112:GLU:O	3:P:116:THR:HG23	2.13	0.49
2:B:265:GLY:O	2:B:266:SER:C	2.56	0.49
4:D:218:LEU:HD13	5:E:43:ALA:N	2.28	0.49
6:F:71:LYS:O	6:F:72:HIS:HB2	2.12	0.49
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.95	0.49
2:O:42:SER:O	2:O:113:ARG:HD2	2.13	0.49
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.28	0.49
9:V:67:GLY:O	9:V:68:ILE:HD13	2.13	0.49
1:A:228:VAL:HG13	1:A:228:VAL:O	2.12	0.49
1:N:93:GLU:O	1:N:94:GLN:HB2	2.12	0.49
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.48	0.49
7:T:41:PHE:CE2	7:T:45:VAL:HB	2.48	0.49
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.95	0.49
8:U:52:GLU:C	8:U:53:GLN:HG3	2.38	0.49
1:A:136:GLN:HE21	9:I:50:LEU:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:VAL:HG12	2:B:208:GLY:N	2.21	0.48
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.94	0.48
1:N:228:VAL:O	1:N:228:VAL:HG13	2.13	0.48
2:O:76:THR:HG23	2:O:82:SER:HB2	1.94	0.48
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.78	0.48
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.78	0.48
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.48	0.48
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.94	0.48
2:O:157:VAL:O	2:O:157:VAL:HG22	2.13	0.48
2:O:354:GLU:O	2:O:358:THR:HG23	2.13	0.48
3:P:90:PHE:CB	3:P:236:MET:HE3	2.41	0.48
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.95	0.48
3:C:156:TYR:C	3:C:158:GLY:N	2.71	0.48
5:E:186:GLN:NE2	5:E:188:VAL:CG1	2.76	0.48
1:N:295:ALA:O	1:N:298:ALA:HB3	2.12	0.48
3:P:121:LEU:HG	3:P:125:MET:CE	2.42	0.48
3:P:207:ASN:ND2	3:P:208:ASN:H	2.11	0.48
5:R:166:ASP:OD1	5:R:168:SER:HB3	2.13	0.48
10:W:26:LEU:HD13	10:W:26:LEU:O	2.13	0.48
3:C:137:GLY:H	3:C:140:SER:CB	2.26	0.48
7:G:32:ASP:C	7:G:35:PRO:HD2	2.39	0.48
9:I:55:MET:O	9:I:58:ARG:HG2	2.14	0.48
1:N:307:PHE:CD1	1:N:307:PHE:C	2.90	0.48
5:R:55:VAL:O	5:R:56:THR:C	2.55	0.48
2:B:318:ASP:O	2:B:319:SER:HB2	2.13	0.48
2:B:385:GLU:C	2:B:387:LEU:H	2.21	0.48
4:D:116:ILE:CG2	4:D:117:VAL:N	2.76	0.48
10:J:17:THR:O	10:J:17:THR:HG22	2.12	0.48
1:N:147:ASN:O	1:N:148:VAL:C	2.55	0.48
1:N:280:TYR:CG	1:N:281:ASP:N	2.81	0.48
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.38	0.48
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.95	0.48
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.95	0.48
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.96	0.48
5:R:77:LYS:CE	5:R:79:SER:HB2	2.44	0.48
5:R:95:PRO:HG2	5:R:145:VAL:HG21	1.94	0.48
1:A:178:THR:HG22	1:A:180:ALA:H	1.79	0.48
2:B:62:ASN:O	2:B:65:THR:CG2	2.58	0.48
9:I:31:UNK:C	9:I:73:PRO:HG2	2.43	0.48
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.27	0.48
7:G:2:ILE:HG13	7:G:2:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:GLU:O	7:G:69:LEU:HG	2.14	0.48
4:Q:203:ARG:NH1	10:W:43:PHE:HD2	2.12	0.48
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.94	0.48
3:C:137:GLY:O	3:C:140:SER:HB2	2.14	0.48
5:R:48:ALA:HB1	11:R:3005:PEE:H71	1.96	0.48
7:T:63:THR:HG22	7:T:64:GLN:N	2.29	0.48
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.49	0.48
2:B:50:PHE:HD2	2:B:104:LYS:NZ	2.12	0.48
3:C:143:GLY:HA2	14:C:2001:3H1:H08B	1.95	0.48
2:O:156:GLN:NE2	9:V:77:ARG:C	2.71	0.48
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.95	0.48
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.49	0.48
5:R:152:ASP:C	5:R:153:PHE:CD1	2.92	0.48
6:S:12:LEU:O	6:S:15:ARG:HG2	2.13	0.48
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.14	0.48
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.28	0.48
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.54	0.48
10:J:38:GLY:O	10:J:42:ILE:HG13	2.14	0.48
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.44	0.48
4:Q:138:PRO:HD3	8:U:58:LEU:HD23	1.95	0.48
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.77	0.48
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.29	0.48
2:B:189:GLU:O	2:B:190:GLN:C	2.57	0.47
2:B:306:PRO:CG	9:I:51:CYS:HA	2.44	0.47
4:D:57:THR:CG2	10:J:59:TYR:HB2	2.42	0.47
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.79	0.47
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.13	0.47
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.49	0.47
1:N:439:SER:HA	1:N:442:TYR:CE2	2.48	0.47
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.96	0.47
4:Q:227:TRP:O	4:Q:228:SER:C	2.56	0.47
2:B:26:ILE:HG12	2:B:26:ILE:O	2.12	0.47
3:C:90:PHE:CZ	3:C:240:PHE:HA	2.49	0.47
3:C:263:LEU:CD2	5:R:95:PRO:HG3	2.43	0.47
2:O:135:TRP:O	2:O:136:GLU:C	2.57	0.47
3:P:18:SER:O	3:P:19:LEU:HG	2.14	0.47
3:P:164:TRP:O	3:P:167:GLY:N	2.47	0.47
8:U:52:GLU:CG	8:U:53:GLN:H	2.28	0.47
4:D:102:ARG:HH11	4:D:102:ARG:HG2	1.78	0.47
4:D:223:LYS:C	4:D:223:LYS:CD	2.86	0.47
6:F:21:TYR:C	6:F:21:TYR:CD2	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:375:VAL:O	1:N:379:ILE:HD12	2.14	0.47
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.44	0.47
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.49	0.47
2:B:27:THR:CG2	2:B:28:LYS:N	2.77	0.47
2:B:280:GLY:HA3	2:B:293:SER:OG	2.14	0.47
2:B:385:GLU:CD	2:B:392:HIS:HA	2.40	0.47
5:E:152:ASP:C	5:E:153:PHE:CD1	2.92	0.47
2:O:394:ALA:C	2:O:396:SER:H	2.22	0.47
3:P:52:LEU:HD13	13:P:501:HEM:O2D	2.15	0.47
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.78	0.47
6:S:71:LYS:O	6:S:72:HIS:HB2	2.15	0.47
1:A:304:CYS:HB2	1:A:325:VAL:O	2.13	0.47
2:B:424:MET:HE1	2:B:434:PRO:O	2.15	0.47
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.49	0.47
4:D:197:GLU:O	4:D:198:HIS:C	2.57	0.47
7:G:78:GLU:C	7:G:79:ASN:ND2	2.71	0.47
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.29	0.47
2:O:158:GLY:O	2:O:162:ASN:ND2	2.47	0.47
2:O:318:ASP:O	2:O:319:SER:HB2	2.14	0.47
3:P:139:MET:HE1	3:P:270:LYS:N	2.28	0.47
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.15	0.47
4:Q:131:LEU:HD11	17:Q:501:HEC:HMB2	1.96	0.47
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.44	0.47
2:B:291:VAL:C	2:B:293:SER:H	2.23	0.47
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.49	0.47
4:D:227:TRP:O	4:D:228:SER:C	2.57	0.47
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.29	0.47
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.95	0.47
9:V:61:ARG:C	9:V:62:ARG:CG	2.88	0.47
1:A:248:LEU:HB3	1:A:249:PRO:HD2	1.97	0.47
2:B:146:VAL:HG12	2:B:147:ASP:N	2.30	0.47
3:C:9:HIS:O	3:C:13:LYS:HB3	2.14	0.47
3:C:189:ALA:O	3:C:193:ILE:HG13	2.15	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.49	0.47
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.96	0.47
1:N:130:GLU:O	1:N:134:ILE:HG13	2.15	0.47
3:P:41:CYS:HB3	3:P:91:PHE:CD2	2.49	0.47
3:P:187:PRO:O	3:P:190:ILE:HB	2.15	0.47
3:P:271:PRO:HB3	14:P:3001:3H1:CL12	2.52	0.47
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.45	0.47
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.15	0.47
8:U:17:LEU:O	8:U:21:ARG:HG3	2.14	0.47
1:A:4:TYR:O	1:A:5:ALA:C	2.58	0.47
3:C:18:SER:O	3:C:19:LEU:HG	2.13	0.47
5:E:103:GLN:O	5:E:107:ASN:ND2	2.48	0.47
3:P:193:ILE:O	3:P:194:THR:C	2.58	0.47
1:A:178:THR:CG2	1:A:179:ARG:N	2.78	0.47
3:C:160:THR:O	3:C:163:GLU:N	2.48	0.47
4:D:165:TYR:CE2	4:D:168:ILE:HG13	2.50	0.47
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.45	0.47
1:A:7:THR:HG21	2:B:113:ARG:CD	2.45	0.47
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.47
2:B:312:PHE:CE1	9:I:62:ARG:O	2.68	0.47
4:D:65:ALA:O	4:D:85:GLY:HA3	2.15	0.47
1:N:307:PHE:HA	1:N:323:HIS:O	2.15	0.47
5:R:113:ASP:C	5:R:115:SER:H	2.23	0.47
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.49	0.46
1:A:147:ASN:O	1:A:148:VAL:C	2.57	0.46
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.97	0.46
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.15	0.46
5:E:83:GLU:HA	5:E:100:HIS:CG	2.49	0.46
1:N:294:LEU:HD11	1:N:334:MET:CE	2.45	0.46
2:O:146:VAL:HG12	2:O:147:ASP:N	2.28	0.46
2:O:239:TYR:CD2	2:O:240:TRP:N	2.83	0.46
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.45	0.46
2:B:31:ASN:HB3	2:B:227:ARG:HH22	1.79	0.46
3:C:90:PHE:CD2	3:C:236:MET:HE3	2.51	0.46
7:G:63:THR:HG22	7:G:64:GLN:N	2.30	0.46
8:H:18:THR:O	8:H:22:GLU:HG3	2.15	0.46
1:N:236:PHE:CB	1:N:258:GLU:OE1	2.64	0.46
2:O:258:VAL:HG21	2:O:321:LEU:HD22	1.97	0.46
3:P:19:LEU:O	3:P:20:ILE:CG1	2.53	0.46
3:P:226:SER:O	3:P:230:ILE:HG12	2.16	0.46
3:P:342:GLN:HE21	3:P:342:GLN:CA	2.21	0.46
1:A:190:PHE:C	1:A:195:MET:HE2	2.40	0.46
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.30	0.46
1:N:106:MET:HE3	1:N:208:LEU:HD13	1.97	0.46
1:N:281:ASP:OD2	1:N:284:PHE:CE1	2.68	0.46
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.99	0.46
3:P:138:GLN:HB2	3:P:255:GLU:O	2.16	0.46
4:Q:234:LYS:HD2	5:R:10:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:18:VAL:HG23	5:R:18:VAL:O	2.14	0.46
13:C:501:HEM:HMC1	13:C:501:HEM:CBC	2.37	0.46
8:H:73:LEU:HD12	8:H:73:LEU:C	2.41	0.46
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.98	0.46
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.84	0.46
5:R:103:GLN:O	5:R:107:ASN:ND2	2.48	0.46
5:R:129:LYS:HG3	5:R:187:PHE:CE2	2.51	0.46
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.56	0.46
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.98	0.46
3:C:4:ASN:OD1	3:C:7:LYS:HD2	2.16	0.46
3:C:345:GLU:O	3:C:348:PHE:HB2	2.14	0.46
1:N:147:ASN:C	1:N:149:THR:N	2.71	0.46
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.29	0.46
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.16	0.46
3:C:275:PHE:HB3	14:C:2001:3H1:H16A	1.97	0.46
5:E:78:LEU:HB3	5:E:132:TRP:CH2	2.51	0.46
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.98	0.46
1:N:394:GLU:O	1:N:395:TRP:C	2.58	0.46
2:O:309:ALA:HA	2:O:325:TYR:O	2.16	0.46
3:C:362:ILE:HA	3:C:366:LEU:HB2	1.98	0.46
4:D:14:HIS:CB	4:D:21:LEU:HD23	2.46	0.46
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.98	0.46
1:N:371:GLY:C	1:N:374:PRO:HD2	2.41	0.46
2:O:67:HIS:O	2:O:70:ARG:HB3	2.15	0.46
2:O:385:GLU:C	2:O:387:LEU:H	2.23	0.46
2:O:417:PHE:C	2:O:417:PHE:CD2	2.94	0.46
3:P:200:PHE:O	3:P:201:LEU:C	2.58	0.46
1:A:156:THR:HA	5:E:7:VAL:HG21	1.98	0.46
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.96	0.46
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.97	0.46
2:O:76:THR:HG22	2:O:81:SER:HA	1.97	0.46
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.51	0.46
2:O:209:ILE:HG13	2:O:379:LEU:HD13	1.97	0.46
3:P:220:PRO:O	3:P:221:PHE:C	2.57	0.46
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.50	0.46
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.30	0.46
1:A:220:SER:HB2	1:A:226:ASP:OD1	2.16	0.46
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.46	0.46
2:B:394:ALA:C	2:B:396:SER:N	2.72	0.46
3:C:200:PHE:O	3:C:201:LEU:C	2.58	0.46
5:E:126:ARG:O	5:E:182:VAL:HG11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:ARG:HG3	1:N:131:ARG:NH1	2.27	0.46
1:N:191:LYS:N	1:N:195:MET:HE2	2.31	0.46
2:O:56:ARG:HE	2:O:171:ALA:HB1	1.81	0.46
4:Q:28:ARG:HD2	4:Q:171:TYR:CE1	2.51	0.46
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.15	0.46
5:R:77:LYS:HB3	5:R:80:ASP:OD2	2.16	0.46
1:A:106:MET:HE3	1:A:208:LEU:CD1	2.46	0.46
1:A:317:THR:OG1	1:A:318:GLY:N	2.49	0.46
1:A:327:ASP:HB3	1:A:328:PRO:HD2	1.98	0.46
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.98	0.46
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.51	0.46
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.51	0.46
3:P:132:TYR:OH	3:P:139:MET:HG3	2.16	0.46
3:P:137:GLY:H	3:P:140:SER:CB	2.28	0.46
4:D:62:LYS:O	4:D:66:GLU:HG3	2.16	0.45
1:N:49:ASN:HD21	1:N:51:LYS:N	2.13	0.45
1:N:406:MET:O	1:N:410:VAL:HG23	2.16	0.45
2:O:86:THR:O	2:O:90:GLU:HG3	2.15	0.45
2:O:327:ILE:CG2	9:V:55:MET:HE3	2.46	0.45
3:P:81:ARG:HG3	3:P:81:ARG:NH1	2.31	0.45
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.44	0.45
5:R:83:GLU:HA	5:R:100:HIS:CG	2.52	0.45
5:R:193:VAL:HG22	5:R:194:VAL:N	2.31	0.45
8:U:36:ARG:NH1	8:U:36:ARG:CB	2.80	0.45
1:A:203:ILE:HG22	1:A:204:SER:N	2.32	0.45
2:B:50:PHE:N	2:B:50:PHE:CD1	2.84	0.45
2:B:163:LEU:O	2:B:166:ALA:N	2.49	0.45
2:B:235:ALA:O	2:B:236:LYS:C	2.58	0.45
2:B:306:PRO:HG2	9:I:51:CYS:HA	1.98	0.45
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.28	0.45
5:E:77:LYS:CE	5:E:79:SER:HB2	2.46	0.45
7:G:46:PHE:O	7:G:50:PRO:HG2	2.15	0.45
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.32	0.45
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.98	0.45
10:J:59:TYR:N	10:J:59:TYR:CD1	2.85	0.45
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.97	0.45
3:P:105:TYR:CA	3:P:315:THR:HG22	2.46	0.45
3:P:270:LYS:HD2	3:P:340:GLY:O	2.16	0.45
4:Q:138:PRO:HB3	8:U:58:LEU:HD22	1.98	0.45
4:Q:197:GLU:O	4:Q:198:HIS:C	2.59	0.45
2:B:59:THR:CG2	2:B:60:THR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.46	0.45
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.51	0.45
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.45
5:E:186:GLN:HE21	5:E:188:VAL:HG12	1.80	0.45
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.63	0.45
7:G:74:PRO:C	7:G:76:ASP:H	2.25	0.45
9:I:71:ASN:N	9:I:71:ASN:ND2	2.51	0.45
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.99	0.45
2:O:38:LEU:HG	2:O:38:LEU:O	2.16	0.45
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.98	0.45
4:Q:234:LYS:HZ1	5:R:13:TYR:HE2	1.64	0.45
2:B:241:GLY:HA2	2:B:423:SER:OG	2.16	0.45
3:C:99:ILE:HG12	13:C:502:HEM:HBC2	1.97	0.45
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.45	0.45
4:D:139:ALA:HB3	8:H:54:CYS:SG	2.57	0.45
5:E:31:ASP:O	5:E:32:ARG:C	2.57	0.45
1:N:182:LEU:N	1:N:182:LEU:HD23	2.32	0.45
4:Q:165:TYR:CE2	4:Q:168:ILE:HG13	2.51	0.45
1:A:43:ALA:HA	1:A:47:TYR:CD1	2.50	0.45
3:C:90:PHE:CG	3:C:236:MET:HE3	2.52	0.45
4:D:138:PRO:HB3	8:H:58:LEU:HD22	1.98	0.45
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.16	0.45
7:G:53:LEU:O	7:G:57:LEU:HG	2.17	0.45
1:N:281:ASP:O	1:N:283:THR:N	2.50	0.45
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.98	0.45
2:O:163:LEU:O	2:O:166:ALA:N	2.49	0.45
2:O:215:ASP:O	2:O:216:LEU:C	2.59	0.45
5:R:186:GLN:HE21	5:R:188:VAL:CG1	2.26	0.45
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.45
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.44	0.45
2:B:135:TRP:O	2:B:136:GLU:C	2.60	0.45
4:D:203:ARG:HD2	18:D:2009:BOG:C6	2.47	0.45
2:O:130:PRO:HB2	2:O:132:PHE:CZ	2.51	0.45
2:O:150:VAL:CG2	2:O:151:ALA:N	2.80	0.45
2:O:235:ALA:O	2:O:236:LYS:C	2.60	0.45
2:O:268:GLU:HG2	2:O:272:PHE:CE1	2.52	0.45
3:P:333:LEU:HD11	11:P:3007:PEE:H38	1.98	0.45
4:Q:165:TYR:O	4:Q:168:ILE:HB	2.17	0.45
1:A:99:ILE:HG13	1:A:113:LEU:HD21	1.98	0.45
1:N:43:ALA:HB2	1:N:194:ARG:HH21	1.81	0.45
2:O:163:LEU:O	2:O:165:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:39:UNK:O	9:V:40:UNK:C	2.64	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.35	0.45
3:C:139:MET:O	3:C:140:SER:C	2.60	0.45
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.99	0.45
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.46	0.45
1:N:279:ARG:NH2	9:V:30:UNK:O	2.49	0.45
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.42	0.45
5:R:114:VAL:O	5:R:114:VAL:HG12	2.17	0.45
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.98	0.45
3:C:377:MET:HE2	6:F:20:TYR:CB	2.41	0.45
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.52	0.45
3:P:87:GLY:O	3:P:91:PHE:HB2	2.17	0.45
3:P:157:ILE:HD12	3:P:161:LEU:HD11	1.99	0.45
3:P:277:PHE:CD1	3:P:277:PHE:C	2.94	0.45
5:R:86:ASN:ND2	5:R:148:ALA:HB2	2.32	0.45
1:A:145:MET:HE2	1:A:145:MET:HA	1.99	0.45
5:E:55:VAL:O	5:E:56:THR:C	2.60	0.45
2:O:73:SER:N	2:O:74:PRO:CD	2.80	0.45
2:O:259:THR:HG23	2:O:421:LYS:O	2.17	0.45
2:O:385:GLU:CD	2:O:392:HIS:HA	2.42	0.45
3:P:164:TRP:O	3:P:166:TRP:N	2.50	0.45
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.31	0.45
1:A:6:GLN:C	1:A:8:LEU:N	2.72	0.44
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.82	0.44
2:B:414:ALA:O	2:B:418:VAL:HG23	2.17	0.44
3:C:285:ILE:HG21	3:C:290:GLY:HA3	1.97	0.44
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.52	0.44
3:C:352:GLY:O	3:C:353:GLN:C	2.59	0.44
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.81	0.44
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.52	0.44
1:N:43:ALA:HA	1:N:47:TYR:CD1	2.51	0.44
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.99	0.44
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.82	0.44
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.52	0.44
3:P:146:VAL:HG21	14:P:3001:3H1:C07	2.48	0.44
3:P:335:ILE:CD1	7:T:58:LEU:HD23	2.47	0.44
4:Q:130:LEU:HD12	4:Q:150:ASN:CG	2.42	0.44
1:A:250:VAL:HG21	1:A:325:VAL:CG1	2.47	0.44
3:C:139:MET:CE	3:C:270:LYS:H	2.29	0.44
7:G:74:PRO:O	7:G:76:ASP:N	2.51	0.44
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.35	0.44
6:S:99:ARG:HG2	6:S:99:ARG:HH11	1.82	0.44
2:B:227:ARG:NH1	2:B:228:SER:OG	2.50	0.44
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.44
1:N:145:MET:HE2	1:N:145:MET:CA	2.48	0.44
1:N:213:ARG:HG2	1:N:213:ARG:HH11	1.82	0.44
1:N:239:SER:HB2	7:T:17:SER:O	2.17	0.44
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.47	0.44
4:Q:139:ALA:HB2	8:U:41:ASP:HA	1.99	0.44
1:A:136:GLN:NE2	9:I:50:LEU:CB	2.81	0.44
3:C:164:TRP:O	3:C:167:GLY:N	2.51	0.44
3:C:220:PRO:O	3:C:221:PHE:C	2.60	0.44
3:C:284:SER:HB2	3:C:285:ILE:HD12	2.00	0.44
4:D:220:TYR:O	4:D:224:ARG:HG2	2.17	0.44
1:N:10:ASN:O	1:N:11:ILE:C	2.61	0.44
2:O:59:THR:CG2	2:O:60:THR:N	2.76	0.44
2:O:68:LEU:HD23	2:O:186:ILE:HG21	1.98	0.44
2:O:344:LEU:HD23	2:O:417:PHE:CD2	2.51	0.44
2:O:414:ALA:O	2:O:418:VAL:HG23	2.18	0.44
8:U:23:HIS:O	8:U:26:GLN:HB2	2.17	0.44
1:A:191:LYS:N	1:A:195:MET:HE2	2.32	0.44
2:B:27:THR:CG2	2:B:28:LYS:H	2.30	0.44
2:B:116:VAL:O	2:B:120:MET:HB2	2.17	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
1:N:6:GLN:C	1:N:8:LEU:N	2.74	0.44
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.32	0.44
4:D:76:GLU:CD	4:D:76:GLU:N	2.75	0.44
5:E:95:PRO:HG3	3:P:263:LEU:HA	2.00	0.44
6:F:45:GLU:O	6:F:46:ALA:C	2.59	0.44
2:O:218:GLN:O	2:O:221:GLU:HG3	2.18	0.44
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.16	0.44
3:P:338:TRP:NE1	7:T:59:TYR:HE1	2.16	0.44
1:A:375:VAL:O	1:A:379:ILE:HD12	2.18	0.44
5:E:29:SER:OG	5:E:30:GLU:N	2.50	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.79	0.44
4:D:68:VAL:HG12	4:D:69:GLU:N	2.32	0.44
2:O:26:ILE:HG23	2:O:26:ILE:O	2.17	0.44
2:O:62:ASN:O	2:O:63:LEU:C	2.61	0.44
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.99	0.44
4:Q:37:CYS:C	4:Q:39:ALA:N	2.75	0.44
7:T:30:PHE:O	7:T:35:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.44
1:A:246:ASP:HA	1:A:427:PRO:HB3	1.99	0.44
2:B:202:ALA:CB	2:B:229:GLY:H	2.30	0.44
3:C:91:PHE:CE1	3:C:124:LEU:HD22	2.52	0.44
5:E:41:ALA:O	5:E:45:VAL:HG23	2.18	0.44
5:E:91:TRP:O	5:E:92:ARG:C	2.61	0.44
1:N:276:ILE:HG12	1:N:357:ALA:HB2	2.00	0.44
3:P:19:LEU:HD13	14:P:3002:3H1:H25A	1.99	0.44
4:Q:54:VAL:HG11	4:Q:192:TRP:CE2	2.52	0.44
1:A:310:PHE:CE1	1:A:322:PHE:N	2.85	0.43
2:B:348:ALA:HA	2:B:414:ALA:HB3	2.00	0.43
3:C:117:GLY:O	3:C:120:LEU:HB2	2.18	0.43
4:D:167:GLU:C	4:D:169:LEU:N	2.76	0.43
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.52	0.43
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.31	0.43
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.18	0.43
1:N:106:MET:HE3	1:N:208:LEU:CD1	2.48	0.43
1:N:121:ALA:O	1:N:122:LEU:HB2	2.17	0.43
1:N:430:GLN:HG3	7:T:4:PHE:O	2.18	0.43
2:O:31:ASN:N	2:O:31:ASN:ND2	2.66	0.43
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.78	0.43
3:P:70:THR:HA	3:P:74:VAL:HG23	1.99	0.43
3:P:285:ILE:HG21	3:P:290:GLY:HA3	2.00	0.43
14:P:3002:3H1:H18	14:P:3002:3H1:H16	1.83	0.43
5:R:38:LEU:HD13	10:W:14:PHE:HZ	1.83	0.43
5:R:126:ARG:O	5:R:182:VAL:HG11	2.18	0.43
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.43
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.53	0.43
1:A:206:LYS:O	1:A:209:VAL:CG1	2.66	0.43
3:C:283:ARG:NH2	3:C:342:GLN:O	2.43	0.43
8:H:20:ILE:HD12	8:H:73:LEU:HA	2.00	0.43
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.47	0.43
2:O:73:SER:N	2:O:74:PRO:HD2	2.34	0.43
2:O:131:GLU:O	2:O:132:PHE:C	2.61	0.43
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.52	0.43
3:P:183:HIS:O	3:P:187:PRO:CD	2.66	0.43
5:R:38:LEU:HB2	10:W:14:PHE:CE1	2.51	0.43
1:A:55:ALA:C	1:A:57:TYR:N	2.76	0.43
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.30	0.43
4:D:197:GLU:O	4:D:199:ASP:N	2.51	0.43
5:E:123:ASP:O	5:E:127:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:PRO:O	6:F:52:LYS:C	2.61	0.43
3:P:22:LEU:HA	3:P:23:PRO:HD3	1.85	0.43
3:P:169:PHE:O	3:P:170:SER:HB3	2.19	0.43
4:Q:102:ARG:NH1	4:Q:109:LEU:HB2	2.34	0.43
1:A:7:THR:HG21	2:B:113:ARG:NE	2.34	0.43
1:A:10:ASN:O	1:A:11:ILE:C	2.61	0.43
1:A:85:HIS:HD2	2:B:284:LEU:HB3	1.82	0.43
2:B:71:LEU:HD11	2:B:144:LEU:HD23	2.00	0.43
3:C:285:ILE:HG21	3:C:290:GLY:C	2.43	0.43
4:D:20:ALA:HB1	4:D:199:ASP:OD2	2.18	0.43
4:D:48:PHE:CG	4:D:65:ALA:HB2	2.54	0.43
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.98	0.43
5:E:114:VAL:O	5:E:114:VAL:HG12	2.18	0.43
5:E:193:VAL:HG22	5:E:194:VAL:N	2.32	0.43
1:N:219:VAL:HG12	1:N:220:SER:N	2.33	0.43
1:N:371:GLY:O	1:N:375:VAL:HG23	2.19	0.43
3:P:134:LEU:HD12	13:P:501:HEM:C3D	2.54	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.52	0.43
5:R:113:ASP:C	5:R:115:SER:N	2.77	0.43
5:R:186:GLN:NE2	5:R:188:VAL:HG12	2.28	0.43
6:S:73:ARG:HD3	6:S:73:ARG:HA	1.65	0.43
8:U:67:HIS:C	8:U:67:HIS:ND1	2.76	0.43
1:A:45:SER:HA	1:A:48:GLU:CG	2.48	0.43
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.52	0.43
2:B:206:LEU:HG	2:B:206:LEU:O	2.19	0.43
3:C:212:ILE:HD12	6:F:62:ILE:HG12	2.01	0.43
3:C:243:LEU:HD21	3:C:251:LEU:HG	2.01	0.43
1:N:203:ILE:HG22	1:N:204:SER:N	2.34	0.43
1:N:206:LYS:O	1:N:208:LEU:N	2.52	0.43
2:O:81:SER:O	2:O:82:SER:C	2.61	0.43
10:W:38:GLY:O	10:W:42:ILE:HG13	2.17	0.43
4:D:241:LYS:HA	4:D:241:LYS:CE	2.39	0.43
5:E:105:GLU:C	5:E:107:ASN:N	2.77	0.43
7:G:41:PHE:CE2	7:G:45:VAL:HB	2.54	0.43
1:N:158:PHE:O	1:N:159:GLN:C	2.61	0.43
2:O:111:CYS:HB3	2:O:119:VAL:HG11	2.00	0.43
2:O:394:ALA:C	2:O:396:SER:N	2.77	0.43
3:P:4:ASN:OD1	3:P:7:LYS:HD2	2.19	0.43
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	3.07	0.43
5:R:105:GLU:C	5:R:107:ASN:N	2.77	0.43
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:HB	1:A:374:PRO:CD	2.44	0.43
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.48	0.43
2:B:272:PHE:O	2:B:276:GLN:N	2.52	0.43
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.83	0.43
3:C:263:LEU:HD23	5:R:95:PRO:HG3	2.01	0.43
3:C:326:PHE:HA	3:C:367:PHE:HZ	1.83	0.43
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.00	0.43
2:O:31:ASN:ND2	2:O:31:ASN:H	2.16	0.43
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.01	0.43
3:P:207:ASN:ND2	3:P:314:ARG:NH1	2.66	0.43
7:T:34:LEU:N	7:T:35:PRO:CD	2.81	0.43
1:A:223:TYR:CD2	1:A:223:TYR:N	2.87	0.43
2:B:24:LEU:HG	2:B:24:LEU:O	2.19	0.43
5:E:69:LEU:H	5:E:69:LEU:HG	1.59	0.43
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.19	0.43
8:H:15:ASP:O	8:H:17:LEU:N	2.51	0.43
1:N:20:ASP:OD2	1:N:20:ASP:N	2.50	0.43
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.46	0.43
2:O:408:ALA:O	2:O:411:VAL:N	2.51	0.43
3:P:58:ALA:O	3:P:177:THR:HG22	2.19	0.43
3:P:170:SER:O	3:P:171:VAL:C	2.60	0.43
3:P:186:LEU:HB2	3:P:187:PRO:HD3	2.01	0.43
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.54	0.43
1:A:281:ASP:OD2	1:A:284:PHE:CE1	2.71	0.43
1:A:294:LEU:HD11	1:A:334:MET:HE1	2.00	0.43
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.77	0.43
4:D:130:LEU:HD11	4:D:158:ILE:HD12	2.01	0.43
5:E:113:ASP:C	5:E:115:SER:H	2.27	0.43
5:E:153:PHE:CE2	5:E:172:ARG:HB3	2.54	0.43
3:P:172:ASP:OD1	3:P:173:ASN:N	2.42	0.43
4:Q:147:LEU:HD13	4:Q:157:ALA:HB1	2.01	0.43
8:U:50:THR:OG1	8:U:51:GLU:N	2.50	0.43
10:W:17:THR:O	10:W:17:THR:HG22	2.17	0.43
2:B:38:LEU:O	2:B:38:LEU:HG	2.18	0.43
3:C:263:LEU:HA	5:R:95:PRO:HG3	2.00	0.43
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.67	0.43
1:N:388:ARG:HD3	1:N:388:ARG:H	1.84	0.43
2:O:150:VAL:O	2:O:153:GLN:HB2	2.19	0.43
2:O:206:LEU:HG	2:O:206:LEU:O	2.18	0.43
2:O:241:GLY:HA2	2:O:423:SER:OG	2.19	0.43
2:O:285:ILE:O	2:O:288:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:164:TRP:O	3:P:165:ALA:C	2.61	0.43
3:P:326:PHE:O	3:P:329:LEU:HB3	2.19	0.43
8:U:27:THR:CG2	8:U:28:GLU:N	2.82	0.43
1:A:294:LEU:HB2	1:A:341:GLU:HG3	2.01	0.42
2:B:58:GLU:OE2	2:B:66:ALA:HB3	2.19	0.42
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.83	0.42
7:G:34:LEU:N	7:G:35:PRO:CD	2.81	0.42
7:G:68:ARG:HG2	7:G:68:ARG:HH11	1.83	0.42
8:H:40:CYS:O	8:H:44:VAL:HG23	2.18	0.42
1:N:274:ASN:HD22	1:N:274:ASN:HA	1.65	0.42
3:P:157:ILE:HD12	3:P:161:LEU:CD1	2.49	0.42
5:R:153:PHE:CE2	5:R:172:ARG:HB3	2.54	0.42
7:T:53:LEU:O	7:T:56:TYR:HB3	2.19	0.42
1:A:4:TYR:OH	1:A:396:ASP:OD2	2.33	0.42
1:A:39:VAL:O	1:A:39:VAL:HG13	2.19	0.42
1:A:147:ASN:C	1:A:149:THR:N	2.73	0.42
2:B:31:ASN:HB2	2:B:201:SER:OG	2.19	0.42
2:B:111:CYS:HB3	2:B:119:VAL:HG11	2.01	0.42
2:B:285:ILE:O	2:B:288:GLY:N	2.52	0.42
3:C:170:SER:O	3:C:171:VAL:C	2.61	0.42
4:D:126:TYR:O	4:D:127:VAL:C	2.61	0.42
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.54	0.42
2:O:24:LEU:O	2:O:24:LEU:HG	2.19	0.42
3:P:17:ASN:HD21	7:T:1:GLY:C	2.27	0.42
3:P:157:ILE:O	3:P:159:HIS:N	2.52	0.42
7:T:6:ASN:O	7:T:7:LEU:C	2.63	0.42
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.49	0.42
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.81	0.42
2:B:52:LYS:O	2:B:203:ARG:NH2	2.51	0.42
2:B:259:THR:HG23	2:B:421:LYS:O	2.19	0.42
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.78	0.42
2:B:295:LEU:HA	2:B:343:GLN:HG2	2.02	0.42
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.87	0.42
3:C:249:ASN:O	3:C:250:LEU:C	2.60	0.42
4:D:28:ARG:O	4:D:29:GLY:C	2.61	0.42
4:D:218:LEU:HD11	5:E:42:THR:HG22	2.01	0.42
5:E:78:LEU:HD22	5:E:132:TRP:CE3	2.53	0.42
1:N:39:VAL:HG13	1:N:39:VAL:O	2.19	0.42
3:P:70:THR:HA	3:P:74:VAL:CG2	2.49	0.42
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.84	0.42
7:T:28:ASN:HB2	7:T:32:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ILE:CD1	9:I:58:ARG:HB2	2.49	0.42
3:C:231:LEU:O	3:C:235:LEU:HG	2.19	0.42
3:C:344:VAL:HG12	3:C:349:ILE:HD11	2.01	0.42
5:E:118:ARG:HE	5:E:118:ARG:HB2	1.67	0.42
6:F:31:LEU:HD21	6:F:65:ALA:HB2	2.02	0.42
10:J:25:VAL:O	10:J:29:VAL:HG23	2.19	0.42
4:D:14:HIS:HB3	4:D:21:LEU:HA	2.01	0.42
5:E:136:VAL:HG12	5:E:138:VAL:HG23	2.01	0.42
6:F:28:LYS:HE3	6:F:80:TRP:CH2	2.55	0.42
1:N:109:VAL:HA	1:N:112:LEU:HD12	2.02	0.42
1:N:168:GLU:CD	1:N:168:GLU:H	2.27	0.42
1:N:262:TRP:O	1:N:386:TYR:HE1	2.02	0.42
2:O:264:VAL:C	2:O:266:SER:H	2.28	0.42
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.49	0.42
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.88	0.42
7:T:74:PRO:C	7:T:76:ASP:H	2.27	0.42
1:A:102:LEU:H	1:A:102:LEU:HG	1.62	0.42
1:A:102:LEU:HD12	1:A:105:ASP:OD2	2.19	0.42
1:A:350:THR:OG1	1:A:353:GLU:HG3	2.19	0.42
1:A:371:GLY:O	1:A:375:VAL:HG23	2.20	0.42
1:A:439:SER:HA	1:A:442:TYR:CE2	2.54	0.42
2:B:229:GLY:C	2:B:231:GLY:H	2.27	0.42
2:B:330:ALA:O	2:B:432:SER:HB2	2.19	0.42
3:C:121:LEU:CG	3:C:125:MET:HE2	2.43	0.42
3:C:333:LEU:HA	3:C:336:LEU:HD12	2.00	0.42
1:N:85:HIS:HD2	2:O:284:LEU:HB3	1.85	0.42
2:O:207:VAL:HG12	2:O:208:GLY:N	2.27	0.42
2:O:207:VAL:O	2:O:216:LEU:HD21	2.18	0.42
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.85	0.42
2:O:327:ILE:HG22	9:V:55:MET:CE	2.48	0.42
3:P:333:LEU:HA	3:P:336:LEU:HD12	2.02	0.42
5:R:40:THR:HG21	11:R:3005:PEE:O2P	2.19	0.42
7:T:29:ILE:H	7:T:29:ILE:CD1	2.12	0.42
2:B:147:ASP:O	2:B:150:VAL:HG22	2.19	0.42
3:C:14:MET:O	3:C:18:SER:OG	2.31	0.42
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.20	0.42
4:D:105:ASN:O	4:D:106:ASN:HB2	2.19	0.42
7:G:81:GLN:OXT	8:H:49:HIS:N	2.52	0.42
1:N:145:MET:HE2	1:N:145:MET:HA	2.02	0.42
2:O:101:THR:C	2:O:103:GLU:N	2.77	0.42
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:162:PRO:HA	4:Q:163:PRO:HD2	1.85	0.42
6:S:42:ASP:OD2	6:S:101:ARG:NH1	2.51	0.42
2:B:306:PRO:HB3	9:I:51:CYS:C	2.44	0.42
5:E:91:TRP:CH2	5:E:92:ARG:HD2	2.54	0.42
6:F:32:MET:O	6:F:33:ARG:C	2.62	0.42
7:G:49:ALA:O	7:G:50:PRO:C	2.62	0.42
1:N:332:ASP:HB2	1:N:430:GLN:HG2	2.00	0.42
2:O:43:PRO:C	2:O:113:ARG:HG3	2.45	0.42
2:O:59:THR:CG2	2:O:60:THR:H	2.32	0.42
3:P:350:ILE:HD12	3:P:350:ILE:HA	1.90	0.42
6:S:26:PHE:CE1	6:S:33:ARG:HA	2.55	0.42
2:B:229:GLY:C	2:B:231:GLY:N	2.78	0.42
6:F:52:LYS:NZ	7:G:11:ARG:HD3	2.35	0.42
6:F:89:TYR:CD1	6:F:89:TYR:C	2.97	0.42
10:J:32:GLU:O	10:J:33:ARG:C	2.63	0.42
1:N:106:MET:HB3	1:N:107:PRO:CD	2.50	0.42
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.19	0.42
2:O:52:LYS:O	2:O:203:ARG:NH2	2.53	0.42
2:O:306:PRO:HB3	9:V:52:ARG:N	2.35	0.42
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.55	0.42
4:Q:99:GLU:H	4:Q:99:GLU:CD	2.28	0.42
5:R:29:SER:OG	5:R:30:GLU:N	2.53	0.42
10:W:16:ARG:HB2	10:W:19:THR:OG1	2.19	0.42
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.03	0.42
2:B:56:ARG:HE	2:B:171:ALA:HB1	1.85	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.50	0.42
2:B:189:GLU:O	2:B:191:LEU:N	2.53	0.42
4:D:98:PRO:O	4:D:99:GLU:C	2.62	0.42
1:N:170:THR:HG22	1:N:172:GLU:H	1.83	0.42
1:N:180:ALA:O	1:N:183:ALA:HB3	2.20	0.42
1:N:255:LEU:O	1:N:321:GLY:HA3	2.20	0.42
1:N:398:ARG:NH1	1:N:398:ARG:HG2	2.35	0.42
3:P:155:PRO:O	3:P:156:TYR:CB	2.67	0.42
3:P:358:SER:O	3:P:362:ILE:HG13	2.20	0.42
4:Q:16:GLY:HA3	4:Q:19:SER:OG	2.20	0.42
4:Q:217:SER:O	4:Q:218:LEU:C	2.63	0.42
3:C:350:ILE:HD12	3:C:350:ILE:HA	1.90	0.41
5:E:64:ALA:HA	3:P:167:GLY:O	2.20	0.41
1:N:63:ALA:O	1:N:116:VAL:CG1	2.68	0.41
3:P:100:GLY:O	3:P:101:ARG:C	2.63	0.41
3:P:139:MET:O	3:P:140:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:346:HIS:CG	3:P:347:PRO:HA	2.55	0.41
3:P:352:GLY:O	3:P:353:GLN:C	2.63	0.41
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.37	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.91	0.41
5:R:78:LEU:HB3	5:R:132:TRP:CH2	2.55	0.41
10:W:42:ILE:O	10:W:46:LEU:HG	2.20	0.41
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.55	0.41
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.02	0.41
1:A:145:MET:HE2	1:A:145:MET:CA	2.50	0.41
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.55	0.41
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.56	0.41
6:F:102:LEU:HD23	6:F:102:LEU:HA	1.88	0.41
2:O:383:GLY:O	2:O:384:SER:C	2.62	0.41
3:P:88:ALA:O	3:P:92:PHE:HD1	2.03	0.41
3:P:182:LEU:HD13	3:P:182:LEU:HA	1.88	0.41
6:S:16:ILE:O	6:S:19:TRP:HB3	2.20	0.41
2:B:158:GLY:O	2:B:162:ASN:ND2	2.53	0.41
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.54	0.41
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.36	0.41
3:P:34:PHE:HB2	20:P:381:HOH:O	2.20	0.41
3:P:50:LEU:O	3:P:51:LEU:C	2.62	0.41
3:P:105:TYR:HA	3:P:315:THR:HG22	2.01	0.41
6:S:12:LEU:C	6:S:14:ASP:N	2.77	0.41
7:T:45:VAL:HG22	7:T:45:VAL:O	2.20	0.41
9:V:61:ARG:C	9:V:62:ARG:HG3	2.45	0.41
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.46	0.41
2:B:42:SER:O	2:B:113:ARG:HD2	2.20	0.41
3:C:70:THR:HA	3:C:74:VAL:HG23	2.02	0.41
3:C:319:ARG:NH1	3:C:322:SER:OG	2.53	0.41
5:E:164:HIS:HD2	5:E:173:LYS:HD3	1.84	0.41
1:N:351:GLU:O	1:N:354:VAL:HG22	2.21	0.41
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.02	0.41
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.56	0.41
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.72	0.41
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.51	0.41
5:R:49:TYR:CD1	10:W:32:GLU:HG3	2.55	0.41
8:U:13:LEU:HD23	8:U:13:LEU:N	2.34	0.41
8:U:58:LEU:HD12	8:U:58:LEU:O	2.21	0.41
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.03	0.41
3:C:212:ILE:HD12	6:F:62:ILE:HG23	2.01	0.41
4:D:165:TYR:O	4:D:168:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:187:PHE:CD1	5:E:193:VAL:HB	2.54	0.41
8:H:27:THR:CG2	8:H:28:GLU:N	2.82	0.41
9:I:67:GLY:O	9:I:68:ILE:HD13	2.21	0.41
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.02	0.41
2:O:376:GLN:NE2	9:V:77:ARG:HH22	2.12	0.41
7:T:29:ILE:N	7:T:29:ILE:CD1	2.80	0.41
1:A:78:GLU:OE1	1:A:108:LYS:HE3	2.21	0.41
2:B:76:THR:HG23	2:B:82:SER:HB2	2.01	0.41
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.41
2:B:169:LYS:C	2:B:170:THR:HG23	2.45	0.41
3:C:92:PHE:HA	3:C:95:ILE:HG22	2.02	0.41
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.55	0.41
3:P:201:LEU:HD23	14:P:3002:3H1:CL12	2.57	0.41
4:Q:102:ARG:HG2	4:Q:102:ARG:HH11	1.84	0.41
4:Q:134:TYR:OH	4:Q:160:MET:O	2.27	0.41
1:A:168:GLU:H	1:A:168:GLU:CD	2.28	0.41
1:A:307:PHE:HA	1:A:323:HIS:O	2.20	0.41
2:B:73:SER:N	2:B:74:PRO:HD2	2.35	0.41
2:B:161:GLU:OE1	2:B:161:GLU:HA	2.20	0.41
3:C:32:TRP:NE1	13:C:502:HEM:O2D	2.51	0.41
3:C:285:ILE:HB	3:C:291:GLY:HA2	2.02	0.41
4:D:191:ARG:O	4:D:192:TRP:C	2.63	0.41
4:D:194:ALA:O	4:D:195:GLU:HB3	2.21	0.41
5:E:105:GLU:O	5:E:107:ASN:N	2.54	0.41
1:N:156:THR:HA	1:N:159:GLN:HB3	2.02	0.41
1:N:320:PHE:CD2	1:N:320:PHE:C	2.99	0.41
2:O:154:SER:C	2:O:156:GLN:N	2.75	0.41
2:O:272:PHE:O	2:O:276:GLN:N	2.53	0.41
2:O:279:LEU:HD13	2:O:344:LEU:HD11	2.03	0.41
3:P:230:ILE:O	3:P:233:LEU:HB3	2.20	0.41
3:P:326:PHE:HA	3:P:367:PHE:HZ	1.85	0.41
5:R:105:GLU:O	5:R:107:ASN:N	2.53	0.41
9:V:49:LEU:O	9:V:50:LEU:HD23	2.20	0.41
1:A:4:TYR:O	1:A:6:GLN:N	2.54	0.41
1:A:106:MET:N	1:A:107:PRO:HD2	2.36	0.41
2:B:73:SER:N	2:B:74:PRO:CD	2.84	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.88	0.41
1:N:433:ASP:OD2	1:N:433:ASP:C	2.63	0.41
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.20	0.41
5:R:105:GLU:C	5:R:107:ASN:H	2.29	0.41
5:R:171:ILE:HD13	5:R:176:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:O	1:A:8:LEU:N	2.53	0.41
1:A:105:ASP:O	1:A:106:MET:C	2.64	0.41
1:A:182:LEU:N	1:A:182:LEU:HD23	2.35	0.41
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.56	0.41
2:B:259:THR:CG2	2:B:260:GLU:N	2.84	0.41
2:B:337:ILE:HD12	2:B:434:PRO:HD2	2.02	0.41
3:C:134:LEU:HD12	13:C:501:HEM:C3D	2.56	0.41
5:E:185:TYR:HB3	5:E:195:VAL:HA	2.03	0.41
7:G:6:ASN:O	7:G:7:LEU:C	2.63	0.41
7:G:30:PHE:O	7:G:35:PRO:HD3	2.20	0.41
8:H:17:LEU:CD1	8:H:73:LEU:HD22	2.51	0.41
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.02	0.41
1:N:163:LEU:HD23	1:N:163:LEU:HA	1.94	0.41
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.51	0.41
2:O:227:ARG:HG3	2:O:228:SER:N	2.36	0.41
2:O:279:LEU:CD2	2:O:344:LEU:HD12	2.51	0.41
2:O:291:VAL:C	2:O:293:SER:N	2.78	0.41
3:P:270:LYS:CD	3:P:279:TYR:HE2	2.34	0.41
3:P:350:ILE:HG23	3:P:351:ILE:N	2.36	0.41
5:R:47:THR:HG21	11:R:3005:PEE:H23	2.03	0.41
5:R:170:ARG:HA	5:R:179:ASN:HB3	2.03	0.41
7:T:72:LYS:NZ	8:U:52:GLU:OE1	2.46	0.41
1:A:2:ALA:HB3	2:B:113:ARG:HH21	1.87	0.41
1:A:294:LEU:HD11	1:A:334:MET:CE	2.50	0.41
1:A:369:LEU:HB3	1:A:375:VAL:HG22	2.03	0.41
2:B:42:SER:OG	2:B:43:PRO:HD2	2.21	0.41
2:B:43:PRO:C	2:B:113:ARG:HG3	2.46	0.41
2:B:169:LYS:O	2:B:170:THR:CG2	2.69	0.41
3:C:38:LEU:HB3	13:C:502:HEM:HMB1	2.03	0.41
3:C:40:VAL:HG11	3:C:233:LEU:HD11	2.02	0.41
3:C:52:LEU:HD13	13:C:501:HEM:O2D	2.21	0.41
3:C:284:SER:O	3:C:286:PRO:HD3	2.21	0.41
4:D:70:VAL:O	4:D:83:ARG:HG2	2.21	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.88	0.41
1:N:361:LEU:HD23	1:N:399:ILE:HD13	2.03	0.41
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.49	0.41
3:P:192:GLY:O	3:P:195:ILE:HB	2.21	0.41
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.03	0.41
3:P:366:LEU:O	3:P:367:PHE:C	2.64	0.41
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	2.03	0.41
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:89:TYR:CE1	6:S:90:LEU:HB2	2.56	0.41
8:U:20:ILE:HD12	8:U:73:LEU:HA	2.03	0.41
1:A:106:MET:HB3	1:A:107:PRO:HD3	2.03	0.40
1:A:261:GLY:O	1:A:262:TRP:C	2.65	0.40
1:A:388:ARG:HG2	1:A:389:ARG:N	2.36	0.40
2:B:146:VAL:O	2:B:147:ASP:C	2.64	0.40
3:C:164:TRP:O	3:C:166:TRP:N	2.54	0.40
4:D:222:MET:CE	5:E:40:THR:HG23	2.51	0.40
9:I:49:LEU:HB3	9:I:55:MET:HG3	2.02	0.40
2:O:293:SER:OG	2:O:296:TYR:HB2	2.21	0.40
3:P:104:TYR:CD2	11:P:3007:PEE:H14	2.56	0.40
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.20	0.40
1:A:233:ARG:NH1	1:A:233:ARG:CG	2.84	0.40
1:A:320:PHE:CD2	1:A:320:PHE:C	2.99	0.40
1:A:332:ASP:HB2	1:A:430:GLN:HG2	2.03	0.40
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.03	0.40
1:A:351:GLU:O	1:A:354:VAL:HG22	2.21	0.40
2:B:62:ASN:CB	2:B:190:GLN:HE21	2.34	0.40
2:B:141:GLN:N	2:B:142:PRO:CD	2.84	0.40
5:E:113:ASP:C	5:E:115:SER:N	2.79	0.40
1:N:89:TYR:O	1:N:95:THR:HG23	2.21	0.40
1:N:295:ALA:O	1:N:299:VAL:HG23	2.21	0.40
2:O:169:LYS:HD2	2:O:238:THR:HG21	2.03	0.40
3:P:249:ASN:O	3:P:250:LEU:C	2.64	0.40
3:P:284:SER:O	3:P:286:PRO:HD3	2.21	0.40
4:Q:145:GLU:HG2	4:Q:146:GLY:N	2.35	0.40
4:Q:204:MET:O	4:Q:205:GLY:C	2.65	0.40
5:R:24:SER:OG	5:R:26:GLN:HB2	2.22	0.40
6:S:53:ASP:OD1	6:S:54:LEU:N	2.55	0.40
6:S:70:LEU:HD12	6:S:70:LEU:O	2.20	0.40
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.22	0.40
7:T:73:ASN:HA	7:T:74:PRO:HD2	1.97	0.40
2:B:317:SER:OG	2:B:318:ASP:N	2.54	0.40
3:C:19:LEU:HD13	14:C:2002:3H1:H25A	2.04	0.40
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.76	0.40
3:C:219:ILE:HB	3:C:220:PRO:HD2	2.04	0.40
3:C:235:LEU:HD23	3:C:235:LEU:HA	1.88	0.40
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.57	0.40
10:J:10:TYR:HE2	10:J:15:ARG:HD2	1.79	0.40
1:N:351:GLU:OE2	1:N:404:ALA:CB	2.69	0.40
2:O:120:MET:O	2:O:121:GLU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:415:LYS:C	2:O:417:PHE:N	2.79	0.40
3:P:157:ILE:CG1	3:P:158:GLY:N	2.69	0.40
5:R:77:LYS:HE2	5:R:79:SER:OG	2.22	0.40
5:R:165:TYR:HA	5:R:170:ARG:O	2.22	0.40
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.20	0.40
1:A:19:LEU:HD23	1:A:19:LEU:N	2.36	0.40
1:A:191:LYS:CA	1:A:195:MET:HE2	2.51	0.40
1:A:404:ALA:O	1:A:405:ARG:C	2.64	0.40
2:B:209:ILE:HG13	2:B:379:LEU:HD13	2.02	0.40
2:B:353:THR:HG22	2:B:354:GLU:N	2.35	0.40
4:D:47:ALA:HB1	4:D:89:ASP:O	2.22	0.40
5:E:24:SER:OG	5:E:26:GLN:HB2	2.22	0.40
6:F:26:PHE:CE1	6:F:33:ARG:HA	2.56	0.40
1:N:402:VAL:HG12	1:N:403:ASP:N	2.37	0.40
2:O:33:LEU:HD12	2:O:204:MET:O	2.21	0.40
2:O:408:ALA:O	2:O:409:ASP:C	2.65	0.40
3:P:6:ARG:HD3	3:P:16:ASN:CG	2.43	0.40
4:Q:228:SER:O	4:Q:229:VAL:C	2.65	0.40
5:R:106:ILE:O	5:R:106:ILE:HG22	2.21	0.40
1:A:109:VAL:O	1:A:112:LEU:N	2.54	0.40
2:B:166:ALA:HB1	2:B:242:GLY:C	2.46	0.40
3:C:186:LEU:HD23	3:C:186:LEU:HA	1.75	0.40
3:C:216:SER:CB	6:F:59:MET:HE2	2.51	0.40
3:C:243:LEU:HD12	3:C:243:LEU:HA	1.90	0.40
7:G:48:VAL:O	7:G:51:PRO:HD2	2.22	0.40
8:H:15:ASP:O	8:H:16:PRO:C	2.63	0.40
8:H:27:THR:HG22	8:H:28:GLU:N	2.36	0.40
1:N:55:ALA:C	1:N:57:TYR:N	2.79	0.40
1:N:248:LEU:HB3	1:N:249:PRO:HD2	2.03	0.40
1:N:404:ALA:O	1:N:405:ARG:C	2.65	0.40
1:N:432:LEU:HG	1:N:433:ASP:H	1.85	0.40
2:O:24:LEU:HD21	2:O:392:HIS:CD2	2.56	0.40
2:O:101:THR:C	2:O:103:GLU:H	2.30	0.40
2:O:306:PRO:HA	9:V:52:ARG:HG3	2.03	0.40
3:P:82:ASN:O	3:P:83:LEU:C	2.64	0.40
4:Q:167:GLU:C	4:Q:169:LEU:N	2.79	0.40
7:T:68:ARG:HH11	7:T:68:ARG:HG2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	383 (87%)	47 (11%)	11 (2%)	4	25
1	N	440/446 (99%)	382 (87%)	45 (10%)	13 (3%)	3	22
2	B	419/441 (95%)	323 (77%)	73 (17%)	23 (6%)	1	11
2	O	420/441 (95%)	331 (79%)	67 (16%)	22 (5%)	1	11
3	C	378/380 (100%)	333 (88%)	33 (9%)	12 (3%)	3	20
3	P	377/380 (99%)	329 (87%)	36 (10%)	12 (3%)	3	20
4	D	239/241 (99%)	204 (85%)	32 (13%)	3 (1%)	9	39
4	Q	239/241 (99%)	201 (84%)	35 (15%)	3 (1%)	9	39
5	E	194/196 (99%)	153 (79%)	26 (13%)	15 (8%)	1	5
5	R	194/196 (99%)	153 (79%)	27 (14%)	14 (7%)	1	6
6	F	99/110 (90%)	90 (91%)	8 (8%)	1 (1%)	12	44
6	S	99/110 (90%)	88 (89%)	8 (8%)	3 (3%)	3	22
7	G	79/81 (98%)	64 (81%)	10 (13%)	5 (6%)	1	8
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	1	11
8	H	68/77 (88%)	59 (87%)	7 (10%)	2 (3%)	3	23
8	U	65/77 (84%)	53 (82%)	12 (18%)	0	100	100
9	I	29/47 (62%)	23 (79%)	4 (14%)	2 (7%)	1	6
9	V	29/47 (62%)	21 (72%)	5 (17%)	3 (10%)	0	2
10	J	59/61 (97%)	51 (86%)	5 (8%)	3 (5%)	1	12
10	W	57/61 (93%)	45 (79%)	10 (18%)	2 (4%)	3	19
All	All	4002/4160 (96%)	3349 (84%)	500 (12%)	153 (4%)	2	17

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	282	ARG
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	230	ALA
3	C	20	ILE
4	D	198	HIS
5	E	69	LEU
5	E	70	ALA
6	F	77	LYS
7	G	7	LEU
1	N	282	ARG
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	226	ILE
2	O	230	ALA
3	P	20	ILE
4	Q	198	HIS
5	R	69	LEU
5	R	70	ALA
6	S	77	LYS
7	T	7	LEU
10	W	60	GLU
1	A	5	ALA
1	A	72	CYS
1	A	433	ASP
2	B	22	GLU
2	B	38	LEU
2	B	63	LEU
2	B	207	VAL
2	B	282	GLY
2	B	389	SER
3	C	19	LEU
3	C	58	ALA
3	C	202	HIS
5	E	72	SER
5	E	123	ASP
5	E	188	VAL
7	G	75	ALA

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Mol	Chain	Res	Type
9	I	60	ALA
10	J	56	LYS
1	N	72	CYS
1	N	94	GLN
1	N	207	GLU
1	N	262	TRP
2	O	19	PRO
2	O	63	LEU
2	O	164	HIS
2	O	282	GLY
2	O	389	SER
3	P	19	LEU
3	P	111	LYS
3	P	158	GLY
3	P	165	ALA
3	P	170	SER
3	P	202	HIS
5	R	8	PRO
5	R	63	SER
5	R	72	SER
5	R	113	ASP
7	T	75	ALA
10	W	56	LYS
1	A	404	ALA
2	B	31	ASN
2	B	266	SER
2	B	283	PRO
2	B	386	ALA
3	C	156	TYR
3	C	165	ALA
5	E	63	SER
5	E	95	PRO
5	E	113	ASP
8	H	10	GLU
10	J	17	THR
1	N	159	GLN
2	O	38	LEU
2	O	207	VAL
2	O	283	PRO
3	P	156	TYR
3	P	379	ASN
5	R	21	ALA

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Mol	Chain	Res	Type
5	R	123	ASP
5	R	130	PRO
6	S	11	ARG
7	T	33	ALA
1	A	3	THR
1	A	71	PRO
1	A	155	ALA
1	A	262	TRP
2	B	30	PRO
2	B	152	PHE
2	B	250	HIS
2	B	290	SER
2	B	392	HIS
3	C	111	LYS
3	C	170	SER
5	E	8	PRO
5	E	130	PRO
5	E	141	HIS
8	H	49	HIS
1	N	206	LYS
1	N	288	LYS
1	N	404	ALA
1	N	428	ILE
2	O	201	SER
2	O	265	GLY
2	O	268	GLU
3	P	3	PRO
3	P	288	LYS
5	R	95	PRO
6	S	83	TYR
9	V	62	ARG
2	B	110	GLU
3	C	3	PRO
3	C	379	ASN
7	G	50	PRO
7	G	61	TRP
1	N	20	ASP
2	O	55	SER
2	O	236	LYS
2	O	250	HIS
2	O	290	SER
2	O	386	ALA

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Mol	Chain	Res	Type
2	O	392	HIS
3	P	157	ILE
5	R	106	ILE
5	R	141	HIS
5	R	183	PRO
7	T	50	PRO
1	A	428	ILE
2	B	236	LYS
3	C	366	LEU
4	D	176	PRO
5	E	106	ILE
5	E	177	PRO
7	G	33	ALA
9	I	62	ARG
10	J	32	GLU
1	N	71	PRO
4	Q	162	PRO
4	Q	176	PRO
9	V	60	ALA
5	E	137	GLY
5	R	177	PRO
3	C	157	ILE
4	D	162	PRO
9	V	48	PRO
2	O	29	LEU
5	E	74	ILE

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%)	341 (93%)	24 (7%)	15	45
1	N	365/368 (99%)	347 (95%)	18 (5%)	22	53
2	B	332/347 (96%)	323 (97%)	9 (3%)	39	66
2	O	333/347 (96%)	320 (96%)	13 (4%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	329/329 (100%)	315 (96%)	14 (4%)	26	57
3	P	328/329 (100%)	313 (95%)	15 (5%)	24	56
4	D	200/200 (100%)	194 (97%)	6 (3%)	36	64
4	Q	200/200 (100%)	195 (98%)	5 (2%)	42	67
5	E	166/166 (100%)	160 (96%)	6 (4%)	31	61
5	R	166/166 (100%)	160 (96%)	6 (4%)	31	61
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	57
6	S	93/96 (97%)	89 (96%)	4 (4%)	26	57
7	G	71/71 (100%)	65 (92%)	6 (8%)	10	35
7	T	69/71 (97%)	64 (93%)	5 (7%)	13	42
8	H	65/71 (92%)	60 (92%)	5 (8%)	12	40
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	54
9	I	23/26 (88%)	22 (96%)	1 (4%)	26	57
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	45 (92%)	4 (8%)	10	37
10	W	47/49 (96%)	43 (92%)	4 (8%)	10	35
All	All	3380/3446 (98%)	3228 (96%)	152 (4%)	24	56

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	19	LEU
1	A	49	ASN
1	A	59	VAL
1	A	87	ASN
1	A	102	LEU
1	A	106	MET
1	A	125	SER
1	A	135	LEU
1	A	171	THR
1	A	182	LEU
1	A	184	SER
1	A	219	VAL
1	A	222	THR
1	A	223	TYR

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Mol	Chain	Res	Type
1	A	233	ARG
1	A	250	VAL
1	A	281	ASP
1	A	342	TRP
1	A	388	ARG
1	A	395	TRP
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	47	ILE
2	B	102	ARG
2	B	124	LEU
2	B	154	SER
2	B	160	LEU
2	B	227	ARG
2	B	248	ASN
2	B	403	ASP
3	C	15	ILE
3	C	20	ILE
3	C	28	ILE
3	C	81	ARG
3	C	149	ASN
3	C	161	LEU
3	C	182	LEU
3	C	199	THR
3	C	213	SER
3	C	234	THR
3	C	236	MET
3	C	259	PRO
3	C	285	ILE
3	C	324	THR
4	D	2	GLU
4	D	43	MET
4	D	64	LEU
4	D	70	VAL
4	D	240	PRO
4	D	241	LYS
5	E	6	THR
5	E	59	ILE
5	E	65	SER
5	E	69	LEU

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Mol	Chain	Res	Type
5	E	80	ASP
5	E	135	LEU
6	F	64	ARG
6	F	70	LEU
6	F	84	GLU
6	F	91	GLU
7	G	15	THR
7	G	29	ILE
7	G	41	PHE
7	G	50	PRO
7	G	53	LEU
7	G	63	THR
8	H	10	GLU
8	H	26	GLN
8	H	48	SER
8	H	71	HIS
8	H	73	LEU
9	I	71	ASN
10	J	11	SER
10	J	22	LEU
10	J	26	LEU
10	J	59	TYR
1	N	3	THR
1	N	49	ASN
1	N	59	VAL
1	N	87	ASN
1	N	102	LEU
1	N	106	MET
1	N	135	LEU
1	N	171	THR
1	N	182	LEU
1	N	184	SER
1	N	223	TYR
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	31	ASN

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Mol	Chain	Res	Type
2	O	47	ILE
2	O	102	ARG
2	O	124	LEU
2	O	154	SER
2	O	160	LEU
2	O	207	VAL
2	O	212	LYS
2	O	248	ASN
2	O	367	THR
2	O	403	ASP
2	O	424	MET
3	P	15	ILE
3	P	20	ILE
3	P	28	ILE
3	P	81	ARG
3	P	149	ASN
3	P	161	LEU
3	P	182	LEU
3	P	187	PRO
3	P	199	THR
3	P	213	SER
3	P	234	THR
3	P	236	MET
3	P	259	PRO
3	P	285	ILE
3	P	324	THR
4	Q	3	LEU
4	Q	43	MET
4	Q	64	LEU
4	Q	70	VAL
4	Q	241	LYS
5	R	6	THR
5	R	59	ILE
5	R	65	SER
5	R	69	LEU
5	R	80	ASP
5	R	135	LEU
6	S	70	LEU
6	S	78	GLU
6	S	84	GLU
6	S	91	GLU
7	T	16	TYR

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Mol	Chain	Res	Type
7	T	29	ILE
7	T	41	PHE
7	T	50	PRO
7	T	63	THR
8	U	26	GLN
8	U	49	HIS
8	U	73	LEU
10	W	11	SER
10	W	22	LEU
10	W	26	LEU
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	ASN
1	A	49	ASN
1	A	53	ASN
1	A	85	HIS
1	A	87	ASN
1	A	118	GLN
1	A	136	GLN
1	A	159	GLN
1	A	274	ASN
1	A	301	HIS
1	A	308	GLN
1	A	359	ASN
1	A	435	ASN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	162	ASN
2	B	196	GLN
2	B	197	ASN
2	B	222	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	305	GLN
2	B	329	GLN
2	B	342	ASN

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Mol	Chain	Res	Type
2	B	343	GLN
2	B	363	GLN
2	B	376	GLN
2	B	400	GLN
3	C	17	ASN
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	71	GLN
4	D	105	ASN
5	E	57	GLN
5	E	86	ASN
5	E	103	GLN
5	E	107	ASN
5	E	164	HIS
5	E	186	GLN
6	F	22	ASN
6	F	79	GLN
7	G	12	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
7	G	81	GLN
9	I	71	ASN
1	N	9	GLN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	87	ASN
1	N	118	GLN
1	N	119	ASN
1	N	136	GLN
1	N	159	GLN
1	N	274	ASN
1	N	305	HIS
1	N	308	GLN

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Mol	Chain	Res	Type
2	O	31	ASN
2	O	115	HIS
2	O	153	GLN
2	O	156	GLN
2	O	162	ASN
2	O	196	GLN
2	O	222	GLN
2	O	225	ASN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	305	GLN
2	O	329	GLN
2	O	342	ASN
2	O	343	GLN
2	O	363	GLN
2	O	376	GLN
2	O	400	GLN
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	71	GLN
4	Q	105	ASN
5	R	57	GLN
5	R	86	ASN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
6	S	22	ASN
6	S	72	HIS
6	S	79	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 12 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	CDL	G	2004	-	39,39,99	1.35	5 (12%)	45,51,111	1.11	4 (8%)
13	HEM	C	502	3	50,50,50	1.62	11 (22%)	67,82,82	1.47	9 (13%)
17	HEC	D	501	4	46,50,50	1.90	12 (26%)	58,82,82	2.35	12 (20%)
16	GOL	C	2011	-	5,5,5	1.49	0	5,5,5	0.68	0
11	PEE	P	3008	-	4,4,50	3.74	4 (100%)	6,6,55	0.57	0
11	PEE	E	2005	-	49,49,50	1.49	10 (20%)	52,54,55	0.89	3 (5%)
14	3H1	C	2002	-	27,29,29	2.26	12 (44%)	33,43,43	1.60	8 (24%)
16	GOL	P	3011	-	5,5,5	1.34	0	5,5,5	0.63	0
18	BOG	D	2009	-	20,20,20	0.76	0	25,25,25	0.85	1 (4%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
11	PEE	R	3005	-	49,49,50	1.52	8 (16%)	52,54,55	0.88	3 (5%)
15	CDL	T	3004	-	39,39,99	1.28	5 (12%)	45,51,111	1.15	5 (11%)
13	HEM	P	502	3	50,50,50	1.46	6 (12%)	67,82,82	1.31	6 (8%)
11	PEE	C	2007	-	48,48,50	1.42	6 (12%)	51,53,55	0.79	2 (3%)
18	BOG	R	3009	-	20,20,20	1.08	2 (10%)	25,25,25	0.99	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PEE	P	3007	-	48,48,50	1.41	6 (12%)	51,53,55	0.77	2 (3%)
15	CDL	P	3003	-	49,49,99	1.19	5 (10%)	55,61,111	0.94	2 (3%)
11	PEE	A	2008	-	20,20,50	1.73	5 (25%)	23,25,55	0.66	0
14	3H1	P	3001	-	27,29,29	2.71	13 (48%)	33,43,43	1.58	8 (24%)
14	3H1	P	3002	-	27,29,29	2.27	12 (44%)	33,43,43	1.68	9 (27%)
13	HEM	P	501	3	50,50,50	1.59	8 (16%)	67,82,82	1.30	9 (13%)
14	3H1	C	2001	-	27,29,29	2.60	12 (44%)	33,43,43	1.68	7 (21%)
17	HEC	Q	501	4	46,50,50	1.83	7 (15%)	58,82,82	2.16	7 (12%)
13	HEM	C	501	3	50,50,50	1.75	12 (24%)	67,82,82	1.80	17 (25%)
15	CDL	C	2003	-	49,49,99	1.24	4 (8%)	55,61,111	0.90	1 (1%)
19	FES	E	501	5	0,4,4	-	-	-	-	-

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	CDL	G	2004	-	-	18/49/49/110	-
13	HEM	C	502	3	-	4/14/54/54	-
17	HEC	D	501	4	-	10/14/54/54	-
16	GOL	C	2011	-	-	0/4/4/4	-
11	PEE	E	2005	-	-	27/53/53/54	-
14	3H1	C	2002	-	-	3/13/34/34	0/2/2/2
16	GOL	P	3011	-	-	2/4/4/4	-
18	BOG	D	2009	-	-	7/11/31/31	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
11	PEE	R	3005	-	-	27/53/53/54	-
15	CDL	T	3004	-	-	18/49/49/110	-
13	HEM	P	502	3	-	4/14/54/54	-
11	PEE	C	2007	-	-	26/52/52/54	-
18	BOG	R	3009	-	-	7/11/31/31	0/1/1/1
11	PEE	P	3007	-	-	25/52/52/54	-
15	CDL	P	3003	-	-	14/59/59/110	-
11	PEE	A	2008	-	-	14/24/24/54	-
14	3H1	P	3001	-	-	2/13/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	3H1	P	3002	-	-	3/13/34/34	0/2/2/2
13	HEM	P	501	3	-	6/14/54/54	-
14	3H1	C	2001	-	-	2/13/34/34	0/2/2/2
17	HEC	Q	501	4	-	10/14/54/54	-
13	HEM	C	501	3	-	6/14/54/54	-
15	CDL	C	2003	-	-	16/59/59/110	-
19	FES	E	501	5	-	-	0/1/1/1

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	CAC-C3C	6.30	1.55	1.35
14	P	3001	3H1	C13-C06	6.26	1.58	1.51
17	Q	501	HEC	CAB-C3B	5.51	1.52	1.35
14	C	2001	3H1	C13-C06	5.34	1.57	1.51
17	D	501	HEC	CAB-C3B	5.09	1.51	1.35
11	P	3008	PEE	P-O1P	5.07	1.62	1.50
13	C	502	HEM	CBC-CAC	4.91	1.54	1.30
17	D	501	HEC	CAC-C3C	4.89	1.50	1.35
14	P	3002	3H1	C17-C15	-4.88	1.35	1.46
13	P	501	HEM	CBB-CAB	4.85	1.53	1.30
14	C	2001	3H1	C17-C15	-4.84	1.35	1.46
14	P	3002	3H1	C21-C20	4.78	1.60	1.53
14	P	3001	3H1	C24-C23	4.70	1.57	1.52
14	C	2002	3H1	C21-C20	4.69	1.60	1.53
13	P	502	HEM	CBC-CAC	4.67	1.52	1.30
13	C	501	HEM	CBC-CAC	4.64	1.52	1.30
14	C	2002	3H1	C17-C15	-4.57	1.36	1.46
14	P	3001	3H1	C17-C15	-4.45	1.36	1.46
11	C	2007	PEE	C39-C38	4.36	1.56	1.31
11	P	3007	PEE	C39-C38	4.27	1.55	1.31
11	E	2005	PEE	C39-C38	4.07	1.54	1.31
11	R	3005	PEE	C39-C38	4.06	1.54	1.31
13	P	502	HEM	CBB-CAB	3.99	1.49	1.30
14	C	2001	3H1	C04-CL12	3.95	1.81	1.72
13	C	501	HEM	CAB-C3B	-3.93	1.36	1.47
13	P	501	HEM	CBC-CAC	3.92	1.49	1.30
13	P	501	HEM	CAB-C3B	-3.87	1.37	1.47
13	C	501	HEM	CBB-CAB	3.84	1.48	1.30
14	C	2001	3H1	C21-C20	3.80	1.58	1.53
13	C	502	HEM	CAB-C3B	-3.78	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	502	HEM	CAB-C3B	-3.64	1.37	1.47
11	C	2007	PEE	O2-C10	3.56	1.44	1.34
11	A	2008	PEE	O2-C10	3.54	1.44	1.34
11	E	2005	PEE	O3-C30	3.47	1.43	1.33
11	P	3008	PEE	P-O4P	3.47	1.64	1.54
11	R	3005	PEE	P-O1P	3.47	1.62	1.50
11	R	3005	PEE	O2-C10	3.43	1.44	1.34
11	P	3008	PEE	P-O3P	3.43	1.64	1.54
14	P	3002	3H1	C02-C03	3.43	1.46	1.41
14	P	3001	3H1	C19-C24	3.40	1.61	1.56
14	P	3001	3H1	C21-C20	3.39	1.58	1.53
11	P	3007	PEE	C21-C22	-3.39	1.34	1.51
13	C	501	HEM	C3B-C4B	3.35	1.51	1.44
17	D	501	HEC	C1D-ND	-3.35	1.33	1.39
14	P	3001	3H1	C05-C06	3.35	1.44	1.40
14	C	2001	3H1	C19-C24	3.31	1.61	1.56
14	C	2002	3H1	C28-C19	3.31	1.59	1.54
11	R	3005	PEE	O3-C30	3.31	1.43	1.33
14	P	3001	3H1	C04-CL12	3.29	1.79	1.72
11	C	2007	PEE	O3-C30	3.28	1.42	1.33
11	P	3007	PEE	O3-C30	3.26	1.42	1.33
11	P	3007	PEE	O2-C10	3.24	1.43	1.34
14	C	2001	3H1	C05-C06	3.22	1.44	1.40
11	E	2005	PEE	C21-C22	-3.21	1.35	1.51
11	E	2005	PEE	O2-C10	3.19	1.43	1.34
14	P	3001	3H1	C28-C19	3.17	1.59	1.54
14	C	2002	3H1	C02-C03	3.16	1.45	1.41
11	C	2007	PEE	C21-C22	-3.16	1.36	1.51
11	R	3005	PEE	C21-C22	-3.16	1.36	1.51
14	C	2001	3H1	C04-C03	3.15	1.45	1.39
17	D	501	HEC	C1C-C2C	3.15	1.50	1.43
14	P	3002	3H1	C28-C19	3.15	1.58	1.54
14	C	2001	3H1	C24-C23	3.14	1.55	1.52
13	C	502	HEM	C2A-C3A	-3.11	1.30	1.38
14	C	2002	3H1	C04-C03	3.07	1.45	1.39
11	E	2005	PEE	P-O1P	3.07	1.61	1.50
17	D	501	HEC	C3B-C2B	-3.05	1.30	1.41
13	P	501	HEM	CAC-C3C	-3.05	1.39	1.47
18	R	3009	BOG	C4-C5	3.05	1.59	1.53
11	A	2008	PEE	P-O1P	3.03	1.61	1.50
13	C	502	HEM	CBB-CAB	3.01	1.44	1.30
17	Q	501	HEC	C3B-C2B	-2.93	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	2001	3H1	C01-C06	2.93	1.44	1.40
17	Q	501	HEC	C1D-ND	-2.91	1.34	1.39
14	P	3001	3H1	C22-C23	2.90	1.55	1.50
17	D	501	HEC	C3C-C2C	-2.88	1.31	1.41
14	P	3002	3H1	C22-C23	2.86	1.55	1.50
14	C	2002	3H1	C04-CL12	2.85	1.78	1.72
13	C	501	HEM	CAC-C3C	-2.85	1.39	1.47
14	C	2001	3H1	C02-C03	2.79	1.45	1.41
11	P	3007	PEE	P-O1P	2.76	1.60	1.50
13	C	502	HEM	CAC-C3C	-2.74	1.40	1.47
17	Q	501	HEC	C1B-NB	-2.71	1.34	1.39
13	C	501	HEM	FE-NB	-2.69	1.86	1.94
15	T	3004	CDL	CA3-CA4	2.65	1.59	1.50
14	P	3002	3H1	C02-C07	2.64	1.52	1.46
13	C	502	HEM	CHC-C1C	-2.64	1.33	1.38
15	G	2004	CDL	OA6-CA5	2.59	1.41	1.34
14	P	3001	3H1	C02-C03	2.57	1.44	1.41
14	C	2001	3H1	C28-C19	2.55	1.58	1.54
17	D	501	HEC	C4C-NC	-2.55	1.34	1.39
14	C	2002	3H1	C01-C06	2.54	1.43	1.40
11	P	3008	PEE	P-O2P	2.54	1.62	1.54
11	R	3005	PEE	C11-C10	2.54	1.58	1.50
13	P	502	HEM	CAC-C3C	-2.53	1.40	1.47
15	C	2003	CDL	OB8-CB7	2.51	1.40	1.33
11	C	2007	PEE	P-O1P	2.50	1.59	1.50
13	C	502	HEM	C1B-C2B	2.48	1.49	1.44
14	C	2001	3H1	C08-C03	2.44	1.56	1.51
17	D	501	HEC	CHA-C1A	-2.43	1.33	1.38
15	G	2004	CDL	O1-C1	2.43	1.50	1.43
17	D	501	HEC	C3D-C2D	-2.43	1.32	1.38
15	G	2004	CDL	CA3-CA4	2.42	1.58	1.50
11	A	2008	PEE	O3-C30	2.42	1.40	1.33
15	G	2004	CDL	OA8-CA6	-2.41	1.39	1.45
14	C	2002	3H1	C24-C23	2.40	1.55	1.52
14	C	2002	3H1	C27-C24	2.39	1.57	1.53
15	T	3004	CDL	OA8-CA6	-2.39	1.39	1.45
13	P	501	HEM	C1B-NB	-2.38	1.36	1.40
11	A	2008	PEE	C1-C2	2.38	1.58	1.50
14	P	3002	3H1	C19-C24	2.37	1.60	1.56
14	P	3001	3H1	C27-C24	2.37	1.57	1.53
11	R	3005	PEE	C31-C30	2.37	1.57	1.50
14	P	3002	3H1	C13-C06	2.37	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	501	HEM	C2A-C3A	-2.35	1.32	1.38
14	P	3002	3H1	C04-C03	2.34	1.44	1.39
15	T	3004	CDL	O1-C1	2.33	1.50	1.43
13	C	501	HEM	CHD-C4C	-2.32	1.33	1.38
14	P	3002	3H1	C04-CL12	2.32	1.77	1.72
11	E	2005	PEE	C31-C30	2.31	1.57	1.50
11	R	3005	PEE	C3-C2	2.30	1.58	1.50
14	C	2002	3H1	C08-C03	2.28	1.56	1.51
14	C	2002	3H1	C22-C23	2.28	1.54	1.50
17	Q	501	HEC	CHA-C4D	-2.27	1.34	1.39
13	C	501	HEM	C3C-C4C	-2.26	1.42	1.46
15	G	2004	CDL	OB8-CB7	2.26	1.39	1.33
13	C	501	HEM	C1D-C2D	2.25	1.49	1.44
13	P	502	HEM	CMB-C2B	2.25	1.55	1.50
13	C	501	HEM	CMA-C3A	2.24	1.55	1.50
13	C	502	HEM	C1C-C2C	-2.22	1.40	1.45
13	C	501	HEM	CHA-C1A	-2.21	1.34	1.39
13	P	501	HEM	C1C-C2C	2.20	1.49	1.45
14	C	2002	3H1	C16-C15	2.19	1.55	1.50
15	C	2003	CDL	OA2-CA2	-2.19	1.36	1.44
11	A	2008	PEE	C11-C10	2.19	1.57	1.50
15	T	3004	CDL	OB8-CB7	2.18	1.39	1.33
13	C	502	HEM	C3B-C4B	2.17	1.49	1.44
15	P	3003	CDL	CA3-CA4	2.17	1.57	1.50
11	E	2005	PEE	C3-C2	2.14	1.57	1.50
15	P	3003	CDL	OA2-CA2	-2.14	1.36	1.44
18	R	3009	BOG	C1-C2	2.14	1.58	1.52
13	P	502	HEM	C1C-NC	-2.14	1.35	1.39
14	P	3001	3H1	C08-C03	2.13	1.55	1.51
11	E	2005	PEE	C1-C2	2.13	1.57	1.50
17	D	501	HEC	CHD-C1D	-2.13	1.34	1.39
13	P	501	HEM	C3B-C2B	-2.12	1.32	1.37
15	P	3003	CDL	O1-C1	2.11	1.49	1.43
13	C	502	HEM	C3C-C2C	-2.10	1.32	1.37
11	E	2005	PEE	C11-C10	2.10	1.56	1.50
15	P	3003	CDL	OB2-CB2	-2.09	1.36	1.44
15	C	2003	CDL	O1-C1	2.09	1.49	1.43
14	P	3002	3H1	C24-C23	2.08	1.54	1.52
17	D	501	HEC	C4D-ND	-2.07	1.35	1.39
15	P	3003	CDL	OB5-CB3	-2.07	1.36	1.44
13	C	502	HEM	C4D-C3D	2.06	1.48	1.45
15	T	3004	CDL	OA6-CA5	2.05	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	3H1	C27-C24	2.04	1.57	1.53
17	Q	501	HEC	CHB-C1B	-2.04	1.34	1.39
14	P	3001	3H1	C01-C06	2.03	1.43	1.40
15	C	2003	CDL	OB2-CB2	-2.02	1.36	1.44
13	C	501	HEM	C1B-C2B	2.02	1.48	1.44
11	P	3007	PEE	C31-C30	2.01	1.56	1.50
11	E	2005	PEE	P-O4P	2.01	1.67	1.59
17	D	501	HEC	C4A-C3A	2.01	1.49	1.45
11	C	2007	PEE	C31-C30	2.00	1.56	1.50

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	501	HEC	CBC-CAC-C3C	-9.65	108.15	127.43
17	D	501	HEC	CBB-CAB-C3B	-9.00	109.45	127.43
17	D	501	HEC	CBC-CAC-C3C	-8.83	109.79	127.43
17	Q	501	HEC	CBB-CAB-C3B	-8.41	110.63	127.43
13	C	501	HEM	C3B-C2B-C1B	-5.57	102.23	106.41
13	C	502	HEM	C3B-C2B-C1B	-5.03	102.64	106.41
17	D	501	HEC	CAA-C2A-C3A	-5.02	118.47	127.87
17	D	501	HEC	CAA-C2A-C1A	4.78	134.58	124.85
14	P	3002	3H1	C28-C19-C18	-4.78	102.11	110.86
13	P	502	HEM	C3B-C2B-C1B	-4.76	102.84	106.41
13	C	501	HEM	C2B-C1B-NB	4.48	114.99	109.84
14	C	2002	3H1	C28-C19-C18	-4.30	102.99	110.86
17	Q	501	HEC	CAA-C2A-C1A	4.26	133.52	124.85
17	D	501	HEC	CMC-C2C-C1C	4.08	131.63	125.42
17	Q	501	HEC	CAA-C2A-C3A	-4.06	120.26	127.87
14	P	3001	3H1	C18-C17-C15	3.60	131.12	125.53
17	Q	501	HEC	CMC-C2C-C1C	3.57	130.86	125.42
13	C	502	HEM	C2B-C1B-NB	3.44	113.79	109.84
14	C	2001	3H1	C03-C04-CL12	3.43	124.18	118.74
18	R	3009	BOG	C1'-O1-C1	3.41	119.51	113.68
14	C	2001	3H1	C05-C04-C03	-3.40	119.02	122.65
13	P	502	HEM	CBD-CAD-C3D	-3.36	103.25	112.53
14	C	2001	3H1	C27-C24-C23	-3.30	106.30	111.36
17	D	501	HEC	CAD-C3D-C4D	3.26	131.31	124.94
14	C	2001	3H1	C18-C17-C15	3.26	130.59	125.53
13	C	501	HEM	CBA-CAA-C2A	-3.23	103.61	112.53
13	P	502	HEM	C3B-C4B-NB	3.14	111.72	109.47
17	D	501	HEC	CMA-C3A-C4A	3.10	130.19	124.73
13	C	501	HEM	C3D-C4D-ND	3.09	113.56	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	3004	CDL	CB4-OB6-CB5	-3.08	110.43	117.80
14	P	3001	3H1	C25-C20-C21	-3.03	105.92	110.33
13	C	501	HEM	C2D-C1D-ND	3.01	113.38	109.90
14	C	2001	3H1	C16-C15-C17	2.98	122.65	118.09
13	C	502	HEM	CAD-C3D-C4D	2.97	129.88	124.70
13	C	501	HEM	CBD-CAD-C3D	2.95	120.68	112.53
13	P	501	HEM	C4D-ND-C1D	-2.95	101.72	105.21
14	P	3001	3H1	C16-C15-C17	2.94	122.59	118.09
13	C	501	HEM	C4D-ND-C1D	-2.93	101.74	105.21
13	C	501	HEM	CHD-C4C-C3C	-2.93	120.28	125.21
13	C	501	HEM	C2A-C1A-NA	2.92	113.40	110.15
14	P	3002	3H1	C25-C20-C21	-2.90	106.11	110.33
15	C	2003	CDL	CB4-OB6-CB5	-2.88	110.89	117.80
11	E	2005	PEE	C22-C21-C20	2.88	127.70	113.86
11	R	3005	PEE	C22-C21-C20	2.84	127.52	113.86
18	D	2009	BOG	C1'-O1-C1	2.82	118.50	113.68
14	P	3001	3H1	C27-C24-C23	-2.80	107.06	111.36
14	C	2002	3H1	C22-C21-C20	2.79	117.34	112.52
17	D	501	HEC	CMD-C2D-C1D	2.79	129.66	125.42
13	C	502	HEM	C3B-C4B-NB	2.77	111.46	109.47
13	P	502	HEM	C2B-C1B-NB	2.77	113.02	109.84
13	C	502	HEM	CMB-C2B-C1B	2.76	129.35	125.03
13	P	501	HEM	C2B-C1B-NB	2.74	112.99	109.84
14	P	3002	3H1	C22-C21-C20	2.73	117.25	112.52
11	C	2007	PEE	C22-C21-C20	2.72	126.95	113.86
13	C	502	HEM	CBD-CAD-C3D	-2.72	105.00	112.53
14	P	3002	3H1	C27-C24-C23	-2.72	107.19	111.36
13	C	501	HEM	CBB-CAB-C3B	-2.68	114.13	127.53
13	P	501	HEM	C2D-C1D-ND	2.68	113.00	109.90
14	C	2002	3H1	C25-C20-C21	-2.68	106.43	110.33
11	P	3007	PEE	C22-C21-C20	2.67	126.71	113.86
15	P	3003	CDL	CB4-OB6-CB5	-2.64	111.47	117.80
14	C	2002	3H1	C03-C04-CL12	2.63	122.90	118.74
14	C	2002	3H1	C27-C24-C23	-2.61	107.35	111.36
13	C	501	HEM	CMD-C2D-C1D	2.61	129.11	125.03
15	G	2004	CDL	CB6-CB4-CB3	-2.60	105.73	111.78
11	R	3005	PEE	C21-C22-C23	2.58	127.42	114.37
13	C	501	HEM	C1D-C2D-C3D	-2.56	104.29	106.98
11	E	2005	PEE	C21-C22-C23	2.55	127.25	114.37
14	P	3002	3H1	C16-C15-C17	2.55	121.98	118.09
11	C	2007	PEE	C21-C22-C23	2.55	127.23	114.37
14	C	2002	3H1	C05-C04-C03	-2.53	119.94	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	3001	3H1	C05-C04-C03	-2.53	119.94	122.65
13	P	501	HEM	C4C-C3C-C2C	-2.50	104.64	106.81
13	C	501	HEM	CMC-C2C-C1C	2.47	129.07	124.73
14	P	3002	3H1	C16-C15-C14	-2.44	119.51	123.73
14	P	3002	3H1	C03-C04-CL12	2.44	122.60	118.74
13	P	501	HEM	CBA-CAA-C2A	-2.43	105.83	112.53
14	C	2002	3H1	C16-C15-C14	-2.42	119.54	123.73
13	C	501	HEM	C4A-NA-C1A	-2.42	101.88	105.82
11	P	3007	PEE	C21-C22-C23	2.41	126.53	114.37
17	D	501	HEC	CHA-C1A-NA	-2.38	121.86	124.45
15	T	3004	CDL	CA6-OA8-CA7	-2.37	111.25	117.08
11	E	2005	PEE	O3-C3-C2	2.36	115.20	108.40
13	C	501	HEM	CMB-C2B-C1B	2.34	128.68	125.03
14	C	2001	3H1	C25-C20-C21	-2.32	106.95	110.33
14	C	2002	3H1	C16-C15-C17	2.32	121.63	118.09
17	Q	501	HEC	CMA-C3A-C4A	2.32	128.81	124.73
15	G	2004	CDL	CA6-OA8-CA7	-2.31	111.39	117.08
13	P	501	HEM	C3D-C4D-ND	2.30	112.69	110.17
14	P	3002	3H1	C05-C04-C03	-2.29	120.21	122.65
17	D	501	HEC	C2A-C1A-NA	2.28	112.53	110.32
15	G	2004	CDL	CB4-OB6-CB5	-2.27	112.36	117.80
13	C	502	HEM	C4D-C3D-C2D	-2.24	103.63	106.89
14	P	3001	3H1	C03-C04-CL12	2.24	122.29	118.74
14	P	3001	3H1	C28-C19-C18	-2.23	106.77	110.86
13	C	501	HEM	CHB-C1B-C2B	-2.23	120.61	126.95
11	R	3005	PEE	O3-C3-C2	2.23	114.82	108.40
15	G	2004	CDL	CA6-CA4-CA3	-2.16	106.74	111.78
15	P	3003	CDL	CA6-CA4-CA3	-2.16	106.75	111.78
15	T	3004	CDL	CB6-CB4-CB3	-2.15	106.78	111.78
17	Q	501	HEC	C3D-C4D-ND	2.13	112.52	110.15
13	P	502	HEM	CAD-C3D-C4D	2.13	128.41	124.70
17	D	501	HEC	CHC-C4B-NB	-2.12	122.14	124.45
13	C	502	HEM	C2C-C1C-NC	2.09	113.51	109.64
13	P	501	HEM	CMA-C3A-C4A	2.08	128.59	125.42
17	D	501	HEC	C3D-C4D-ND	2.08	112.46	110.15
13	P	501	HEM	CBD-CAD-C3D	2.08	118.29	112.53
15	T	3004	CDL	CA6-CA4-CA3	-2.08	106.94	111.78
14	C	2001	3H1	C28-C19-C18	-2.06	107.08	110.86
14	P	3002	3H1	C06-C13-C14	2.05	115.56	112.06
13	P	501	HEM	C4A-NA-C1A	-2.03	102.50	105.82
13	P	502	HEM	C3C-C2C-C1C	-2.03	105.12	107.05
13	C	502	HEM	C4A-NA-C1A	-2.03	102.51	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	HEM	C4C-NC-C1C	-2.01	102.54	105.82
15	T	3004	CDL	OA6-CA4-CA3	2.01	115.55	108.34
14	P	3001	3H1	C02-C03-C04	2.01	119.55	117.44

There are no chirality outliers.

All (251) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C1-O3P-P-O2P
11	A	2008	PEE	C1-O3P-P-O4P
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C1-O3P-P-O1P
11	E	2005	PEE	C1-O3P-P-O4P
11	E	2005	PEE	C4-O4P-P-O3P
11	E	2005	PEE	C4-O4P-P-O2P
11	E	2005	PEE	O4P-C4-C5-N
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C1-O3P-P-O1P
11	R	3005	PEE	C1-O3P-P-O4P
11	R	3005	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C4-O4P-P-O2P
11	R	3005	PEE	O4P-C4-C5-N
13	P	501	HEM	C4B-C3B-CAB-CBB
14	C	2002	3H1	C17-C18-C19-C20
14	C	2002	3H1	C17-C18-C19-C28
14	P	3002	3H1	C17-C18-C19-C20
14	P	3002	3H1	C17-C18-C19-C28
15	C	2003	CDL	CB2-OB2-PB2-OB3
15	G	2004	CDL	CB3-OB5-PB2-OB2
15	G	2004	CDL	CB3-OB5-PB2-OB3
15	G	2004	CDL	CB3-OB5-PB2-OB4
15	P	3003	CDL	CB2-OB2-PB2-OB3
15	P	3003	CDL	CB2-OB2-PB2-OB5
15	T	3004	CDL	CB3-OB5-PB2-OB2
15	T	3004	CDL	CB3-OB5-PB2-OB3
15	T	3004	CDL	CB3-OB5-PB2-OB4
16	P	3011	GOL	C1-C2-C3-O3
17	D	501	HEC	C3A-C2A-CAA-CBA
17	D	501	HEC	C2B-C3B-CAB-CBB
17	D	501	HEC	C4B-C3B-CAB-CBB
17	D	501	HEC	C2C-C3C-CAC-CBC
17	D	501	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	Q	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C2B-C3B-CAB-CBB
17	Q	501	HEC	C4B-C3B-CAB-CBB
17	Q	501	HEC	C4C-C3C-CAC-CBC
11	E	2005	PEE	O5-C30-O3-C3
11	R	3005	PEE	O5-C30-O3-C3
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	O4-C10-O2-C2
11	E	2005	PEE	C31-C30-O3-C3
11	R	3005	PEE	C31-C30-O3-C3
11	A	2008	PEE	C31-C30-O3-C3
11	E	2005	PEE	C37-C38-C39-C40
11	R	3005	PEE	C37-C38-C39-C40
11	A	2008	PEE	O5-C30-O3-C3
17	D	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C1A-C2A-CAA-CBA
15	G	2004	CDL	O1-C1-CA2-OA2
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
15	G	2004	CDL	CB2-C1-CA2-OA2
15	T	3004	CDL	O1-C1-CA2-OA2
11	C	2007	PEE	O3P-C1-C2-O2
11	P	3007	PEE	O3P-C1-C2-O2
18	D	2009	BOG	O5-C5-C6-O6
18	D	2009	BOG	O1-C1'-C2'-C3'
18	R	3009	BOG	O1-C1'-C2'-C3'
11	R	3005	PEE	C30-C31-C32-C33
18	D	2009	BOG	C4-C5-C6-O6
11	E	2005	PEE	C30-C31-C32-C33
15	C	2003	CDL	CA5-C11-C12-C13
15	P	3003	CDL	CA5-C11-C12-C13
18	D	2009	BOG	O5-C1-O1-C1'
11	E	2005	PEE	C17-C18-C19-C20
11	R	3005	PEE	C17-C18-C19-C20
15	G	2004	CDL	C71-CB7-OB8-CB6
15	P	3003	CDL	C71-CB7-OB8-CB6
15	C	2003	CDL	C71-CB7-OB8-CB6
15	T	3004	CDL	C71-CB7-OB8-CB6
18	D	2009	BOG	C2-C1-O1-C1'
18	R	3009	BOG	C2-C1-O1-C1'
15	C	2003	CDL	OB9-CB7-OB8-CB6
15	C	2003	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
14	C	2001	3H1	C05-C06-C13-C14
14	P	3001	3H1	C05-C06-C13-C14
18	R	3009	BOG	O5-C1-O1-C1'
15	G	2004	CDL	C51-CB5-OB6-CB4
15	T	3004	CDL	C51-CB5-OB6-CB4
15	P	3003	CDL	OB9-CB7-OB8-CB6
11	C	2007	PEE	C12-C13-C14-C15
11	P	3007	PEE	C12-C13-C14-C15
15	G	2004	CDL	OB9-CB7-OB8-CB6
15	T	3004	CDL	OB7-CB5-OB6-CB4
16	P	3011	GOL	O2-C2-C3-O3
11	R	3005	PEE	C39-C40-C41-C42
15	P	3003	CDL	CB7-C71-C72-C73
15	G	2004	CDL	CB5-C51-C52-C53
15	T	3004	CDL	CB5-C51-C52-C53
15	T	3004	CDL	OB9-CB7-OB8-CB6
15	C	2003	CDL	C15-C16-C17-C18
15	G	2004	CDL	OB7-CB5-OB6-CB4
15	P	3003	CDL	C15-C16-C17-C18
18	R	3009	BOG	C4-C5-C6-O6
11	P	3007	PEE	C42-C43-C44-C45
11	C	2007	PEE	C15-C16-C17-C18
11	E	2005	PEE	C39-C40-C41-C42
11	C	2007	PEE	C34-C35-C36-C37
11	C	2007	PEE	C32-C33-C34-C35
11	C	2007	PEE	C42-C43-C44-C45
11	P	3007	PEE	C32-C33-C34-C35
11	P	3007	PEE	C34-C35-C36-C37
11	R	3005	PEE	C13-C14-C15-C16
11	E	2005	PEE	C13-C14-C15-C16
11	P	3007	PEE	C17-C18-C19-C20
13	C	501	HEM	C2B-C3B-CAB-CBB
13	C	501	HEM	C4B-C3B-CAB-CBB
11	R	3005	PEE	C23-C24-C25-C26
15	C	2003	CDL	C16-C17-C18-C19
15	T	3004	CDL	CB2-C1-CA2-OA2
14	C	2001	3H1	C01-C06-C13-C14
14	P	3001	3H1	C01-C06-C13-C14
18	R	3009	BOG	O5-C5-C6-O6
11	E	2005	PEE	C15-C16-C17-C18
11	A	2008	PEE	O3P-C1-C2-C3
11	C	2007	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O3P-C1-C2-C3
15	T	3004	CDL	CA3-CA4-CA6-OA8
11	P	3007	PEE	C15-C16-C17-C18
11	R	3005	PEE	C15-C16-C17-C18
11	E	2005	PEE	C23-C24-C25-C26
15	P	3003	CDL	C16-C17-C18-C19
11	P	3007	PEE	C21-C22-C23-C24
11	R	3005	PEE	C40-C41-C42-C43
11	E	2005	PEE	C31-C32-C33-C34
11	E	2005	PEE	C40-C41-C42-C43
11	C	2007	PEE	C17-C18-C19-C20
11	R	3005	PEE	C2-C3-O3-C30
15	C	2003	CDL	C71-C72-C73-C74
15	P	3003	CDL	C71-C72-C73-C74
11	A	2008	PEE	C10-C11-C12-C13
11	C	2007	PEE	C33-C34-C35-C36
11	R	3005	PEE	C32-C33-C34-C35
15	G	2004	CDL	CA3-CA4-CA6-OA8
15	T	3004	CDL	CB3-CB4-CB6-OB8
11	E	2005	PEE	C32-C33-C34-C35
11	P	3007	PEE	C33-C34-C35-C36
15	T	3004	CDL	C31-CA7-OA8-CA6
11	R	3005	PEE	C31-C32-C33-C34
15	C	2003	CDL	C14-C15-C16-C17
11	P	3007	PEE	C39-C40-C41-C42
11	C	2007	PEE	C21-C22-C23-C24
18	D	2009	BOG	C1'-C2'-C3'-C4'
11	P	3007	PEE	C13-C14-C15-C16
11	P	3007	PEE	C30-C31-C32-C33
11	E	2005	PEE	C2-C3-O3-C30
11	C	2007	PEE	C13-C14-C15-C16
15	P	3003	CDL	C13-C14-C15-C16
13	P	501	HEM	C2B-C3B-CAB-CBB
11	R	3005	PEE	C1-C2-O2-C10
18	R	3009	BOG	C2'-C3'-C4'-C5'
15	G	2004	CDL	CB3-CB4-CB6-OB8
11	A	2008	PEE	O2-C2-C3-O3
11	C	2007	PEE	C39-C40-C41-C42
15	T	3004	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C30-C31-C32-C33
15	C	2003	CDL	C13-C14-C15-C16
11	E	2005	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	C	2003	CDL	C1-CA2-OA2-PA1
15	G	2004	CDL	C1-CB2-OB2-PB2
15	P	3003	CDL	C1-CA2-OA2-PA1
15	T	3004	CDL	C1-CB2-OB2-PB2
11	A	2008	PEE	O3P-C1-C2-O2
15	G	2004	CDL	OA6-CA4-CA6-OA8
15	G	2004	CDL	OB6-CB4-CB6-OB8
15	T	3004	CDL	OB6-CB4-CB6-OB8
11	C	2007	PEE	C41-C42-C43-C44
11	R	3005	PEE	C21-C22-C23-C24
11	P	3007	PEE	C20-C21-C22-C23
11	A	2008	PEE	C1-O3P-P-O1P
11	C	2007	PEE	C1-O3P-P-O2P
11	C	2007	PEE	C1-O3P-P-O1P
11	C	2007	PEE	C1-O3P-P-O4P
11	P	3007	PEE	C1-O3P-P-O2P
11	P	3007	PEE	C1-O3P-P-O1P
11	P	3007	PEE	C1-O3P-P-O4P
15	C	2003	CDL	CB2-OB2-PB2-OB5
15	G	2004	CDL	CA3-OA5-PA1-OA4
15	T	3004	CDL	CA3-OA5-PA1-OA4
17	Q	501	HEC	C2C-C3C-CAC-CBC
11	A	2008	PEE	O3-C30-C31-C32
11	P	3007	PEE	C41-C42-C43-C44
11	E	2005	PEE	C1-C2-O2-C10
15	P	3003	CDL	C14-C15-C16-C17
11	A	2008	PEE	O4-C10-O2-C2
11	C	2007	PEE	C20-C21-C22-C23
11	E	2005	PEE	C20-C21-C22-C23
18	R	3009	BOG	C1'-C2'-C3'-C4'
11	E	2005	PEE	C41-C42-C43-C44
11	C	2007	PEE	C36-C37-C38-C39
11	P	3007	PEE	C36-C37-C38-C39
15	G	2004	CDL	C31-CA7-OA8-CA6
18	D	2009	BOG	C2'-C3'-C4'-C5'
11	A	2008	PEE	C11-C10-O2-C2
11	R	3005	PEE	C18-C19-C20-C21
13	P	502	HEM	CAA-CBA-CGA-O2A
13	C	502	HEM	CAD-CBD-CGD-O2D
11	E	2005	PEE	C18-C19-C20-C21
13	C	502	HEM	CAD-CBD-CGD-O1D
11	R	3005	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
15	T	3004	CDL	OA9-CA7-OA8-CA6
13	C	502	HEM	CAA-CBA-CGA-O2A
13	C	502	HEM	CAA-CBA-CGA-O1A
17	Q	501	HEC	CAD-CBD-CGD-O2D
11	A	2008	PEE	C1-C2-C3-O3
17	D	501	HEC	CAD-CBD-CGD-O2D
13	P	502	HEM	CAA-CBA-CGA-O1A
17	Q	501	HEC	CAA-CBA-CGA-O2A
13	P	501	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAD-CBD-CGD-O2D
17	D	501	HEC	CAA-CBA-CGA-O2A
11	P	3007	PEE	C31-C30-O3-C3
11	E	2005	PEE	C38-C39-C40-C41
11	R	3005	PEE	C38-C39-C40-C41
13	P	502	HEM	CAD-CBD-CGD-O1D
11	R	3005	PEE	C36-C37-C38-C39
13	P	501	HEM	CAD-CBD-CGD-O1D
17	Q	501	HEC	CAA-CBA-CGA-O1A
17	D	501	HEC	CAD-CBD-CGD-O1D
17	Q	501	HEC	CAD-CBD-CGD-O1D
13	C	501	HEM	CAD-CBD-CGD-O2D
13	P	501	HEM	CAA-CBA-CGA-O1A
13	C	501	HEM	CAD-CBD-CGD-O1D
13	C	501	HEM	CAA-CBA-CGA-O1A
13	P	501	HEM	CAA-CBA-CGA-O2A
17	D	501	HEC	CAA-CBA-CGA-O1A
11	P	3007	PEE	O5-C30-O3-C3
11	C	2007	PEE	C38-C39-C40-C41
11	E	2005	PEE	C36-C37-C38-C39
15	C	2003	CDL	C52-C51-CB5-OB6
13	C	501	HEM	CAA-CBA-CGA-O2A
14	C	2002	3H1	C01-C06-C13-C14
11	C	2007	PEE	O4-C10-O2-C2
15	P	3003	CDL	C52-C51-CB5-OB6
15	G	2004	CDL	OB5-CB3-CB4-OB6
11	C	2007	PEE	O2-C10-C11-C12
11	R	3005	PEE	C14-C15-C16-C17
11	P	3007	PEE	O2-C10-C11-C12
11	C	2007	PEE	C11-C10-O2-C2
14	P	3002	3H1	C01-C06-C13-C14
15	C	2003	CDL	C12-C11-CA5-OA6
11	C	2007	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O4-C10-C11-C12
11	A	2008	PEE	O5-C30-C31-C32
15	P	3003	CDL	C52-C51-CB5-OB7
11	P	3007	PEE	C38-C39-C40-C41
11	C	2007	PEE	O4-C10-C11-C12
15	C	2003	CDL	C52-C51-CB5-OB7
15	C	2003	CDL	C12-C11-CA5-OA7

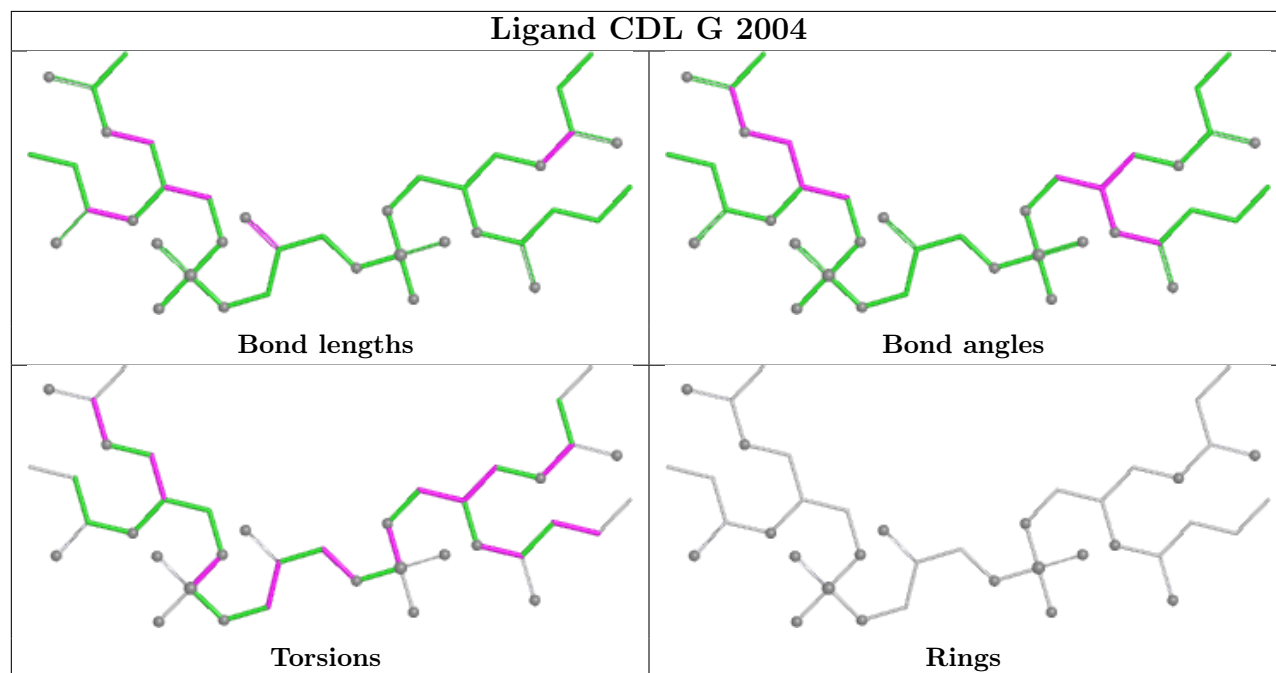
There are no ring outliers.

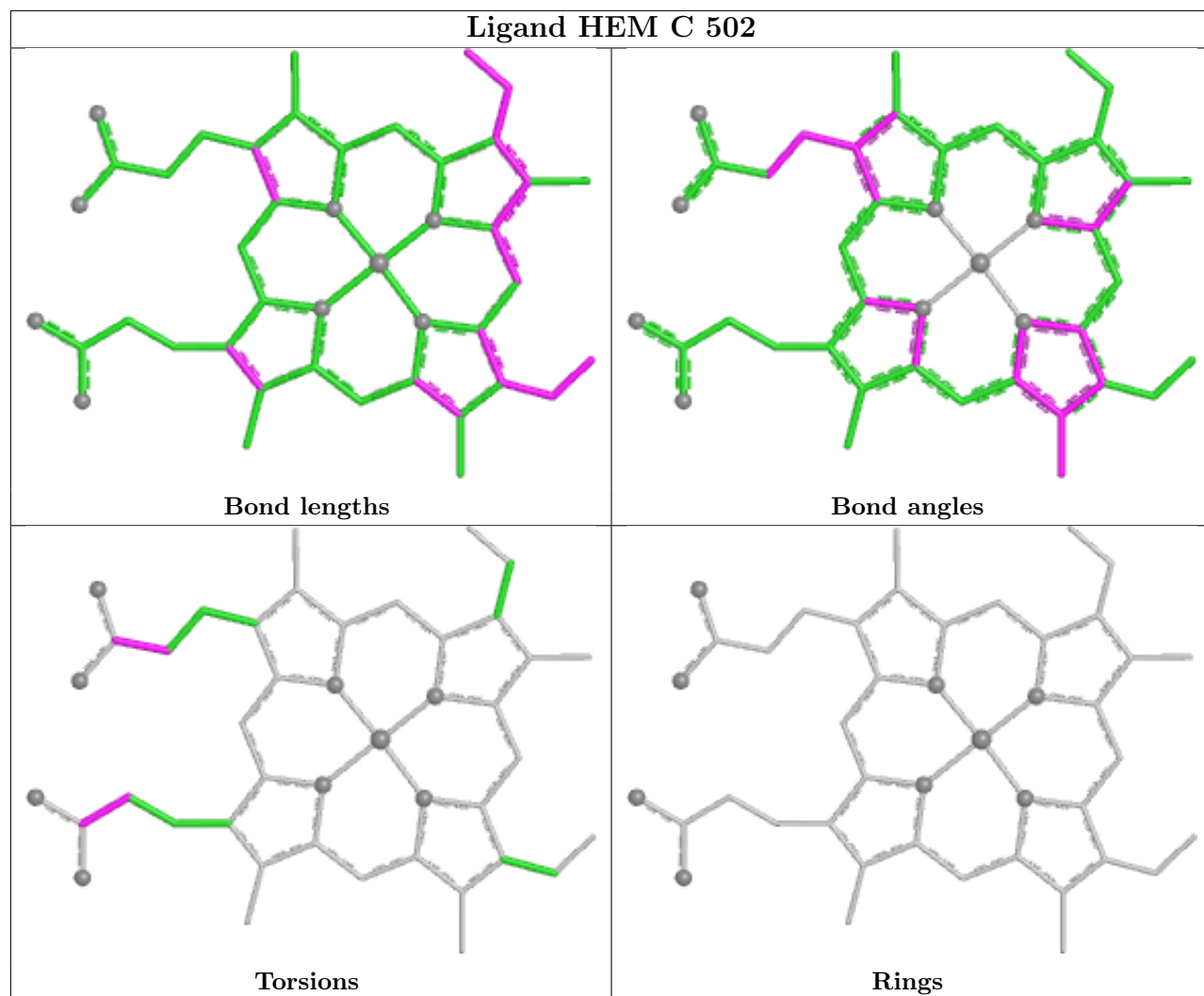
20 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	G	2004	CDL	1	0
13	C	502	HEM	5	0
17	D	501	HEC	2	0
14	C	2002	3H1	1	0
18	D	2009	BOG	1	0
19	R	501	FES	1	0
11	R	3005	PEE	3	0
15	T	3004	CDL	1	0
13	P	502	HEM	2	0
18	R	3009	BOG	1	0
11	P	3007	PEE	3	0
15	P	3003	CDL	1	0
14	P	3001	3H1	3	0
14	P	3002	3H1	4	0
13	P	501	HEM	5	0
14	C	2001	3H1	2	0
17	Q	501	HEC	2	0
13	C	501	HEM	6	0
15	C	2003	CDL	2	0
19	E	501	FES	1	0

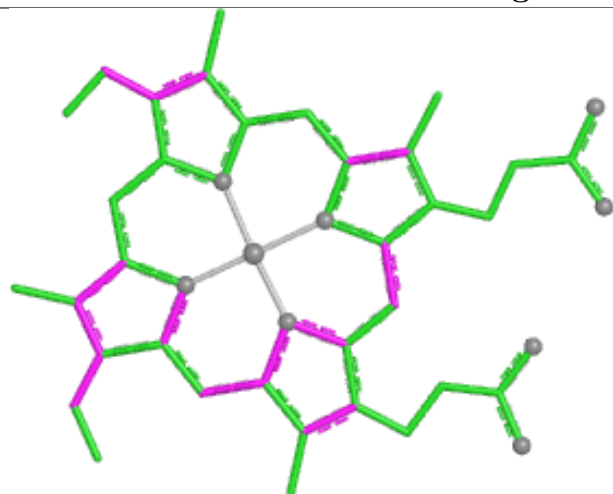
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

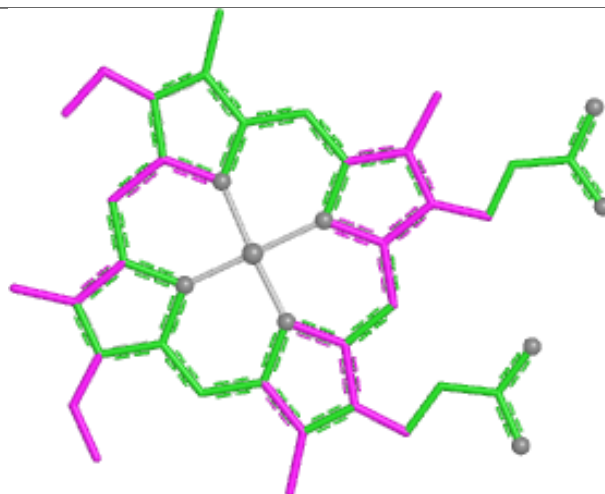




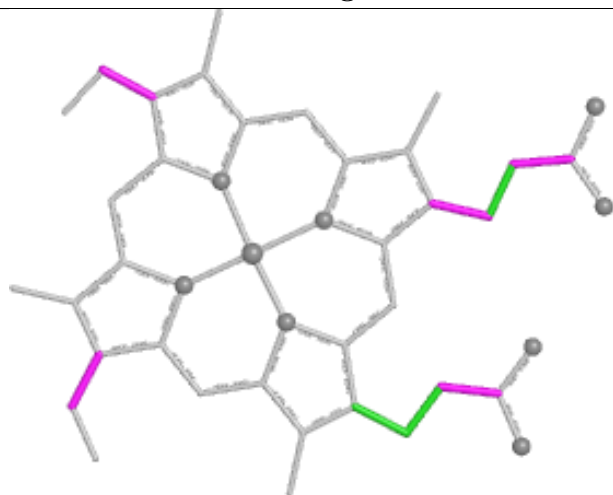
Ligand HEC D 501



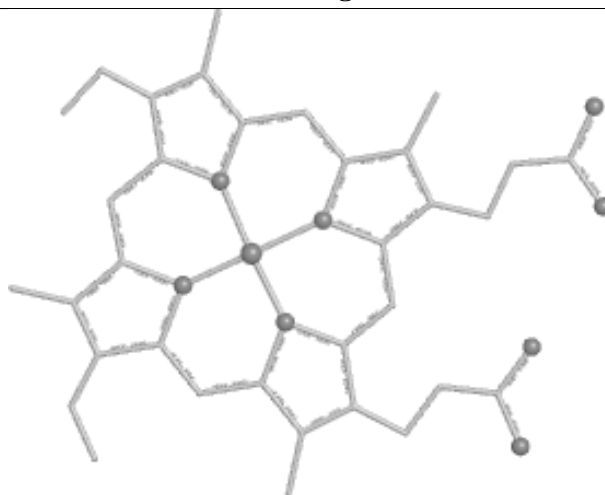
Bond lengths



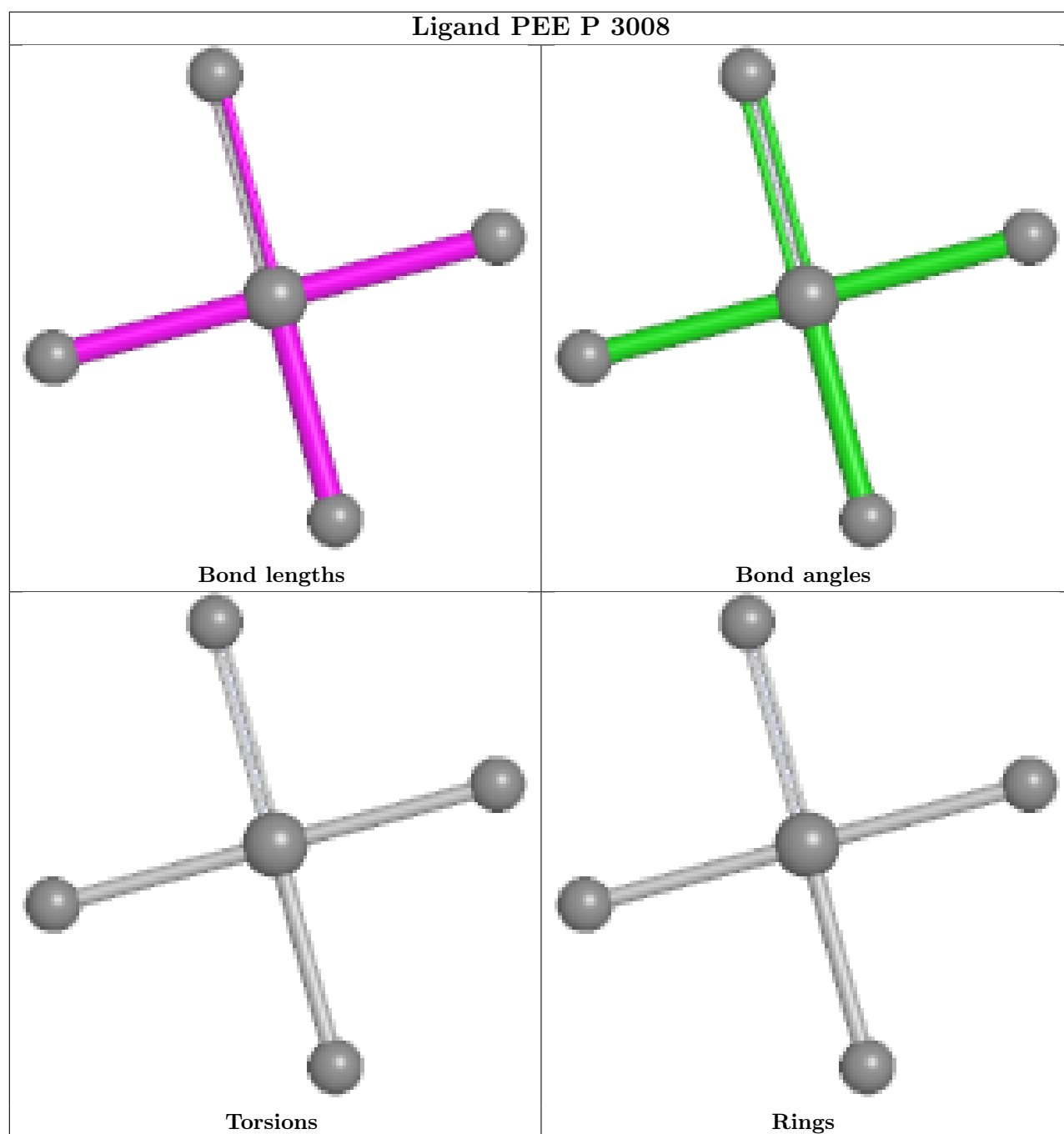
Bond angles

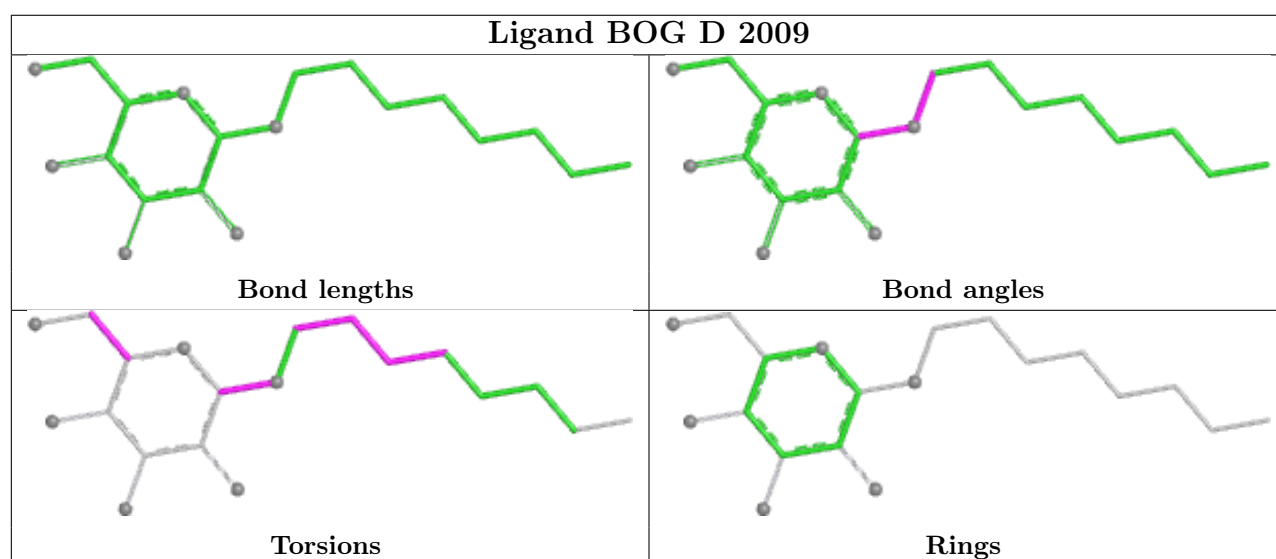
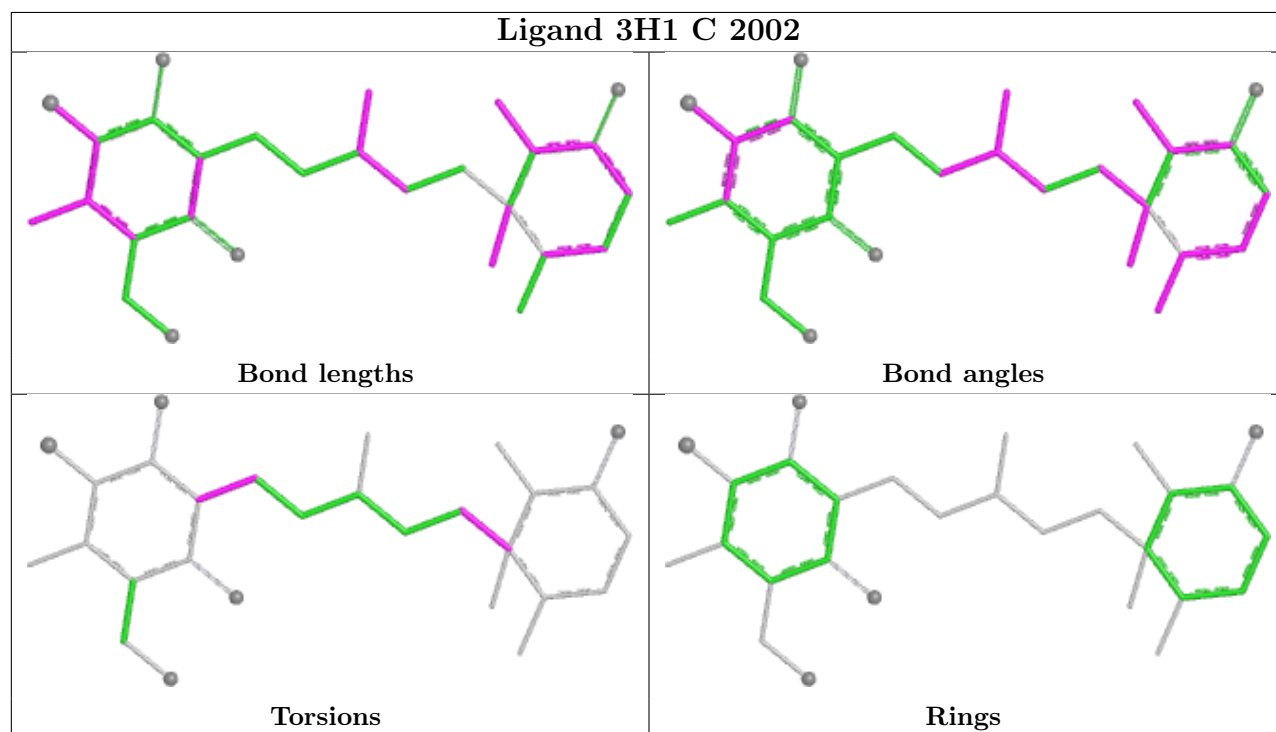
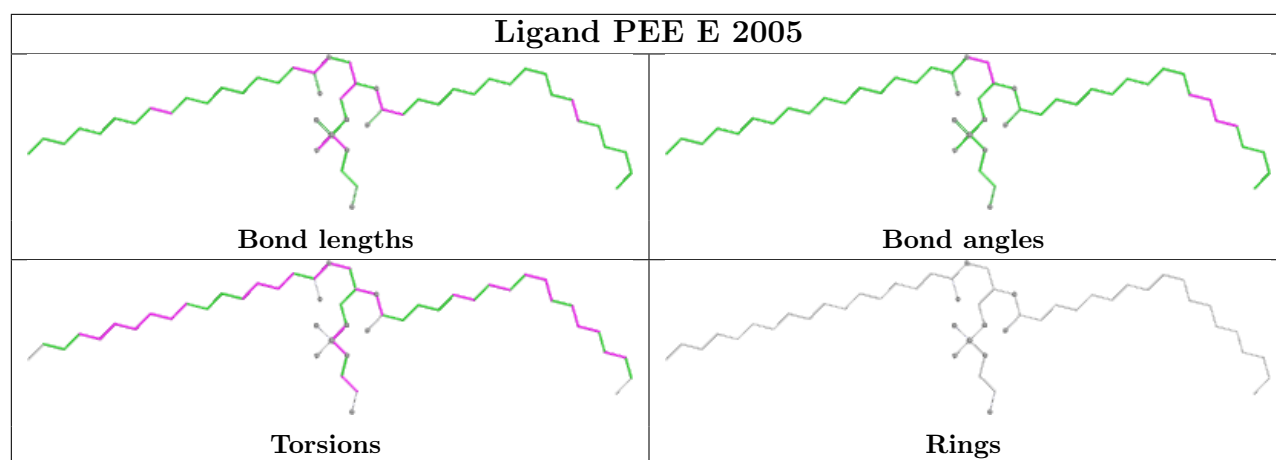


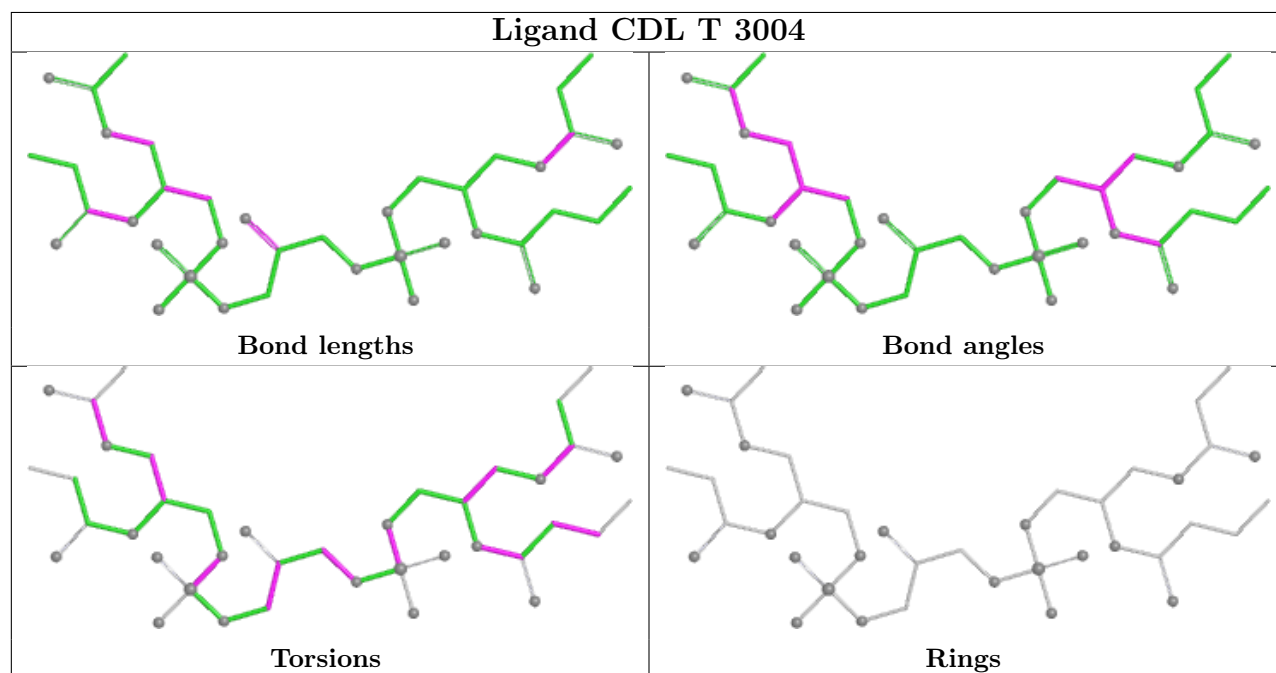
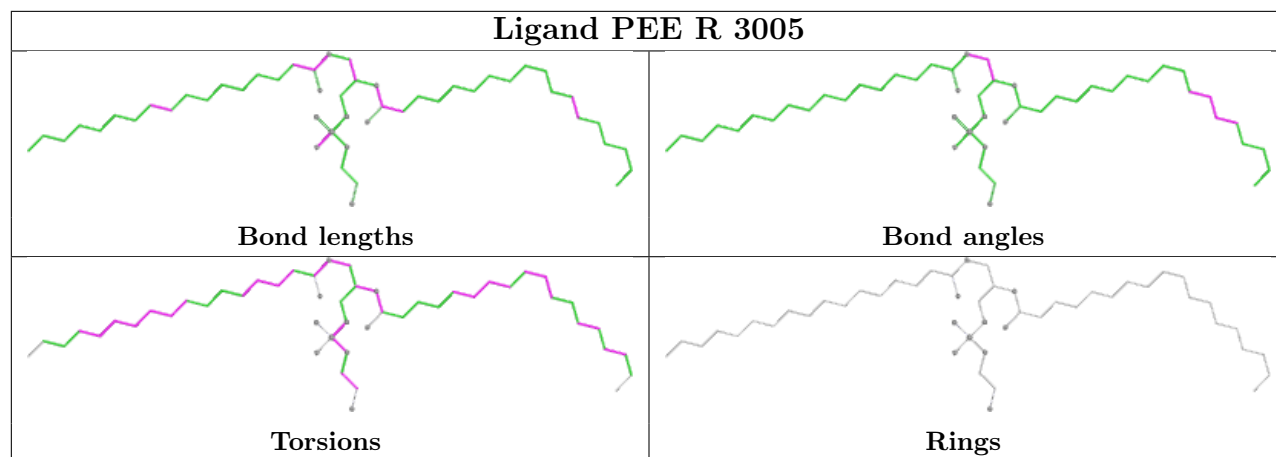
Torsions

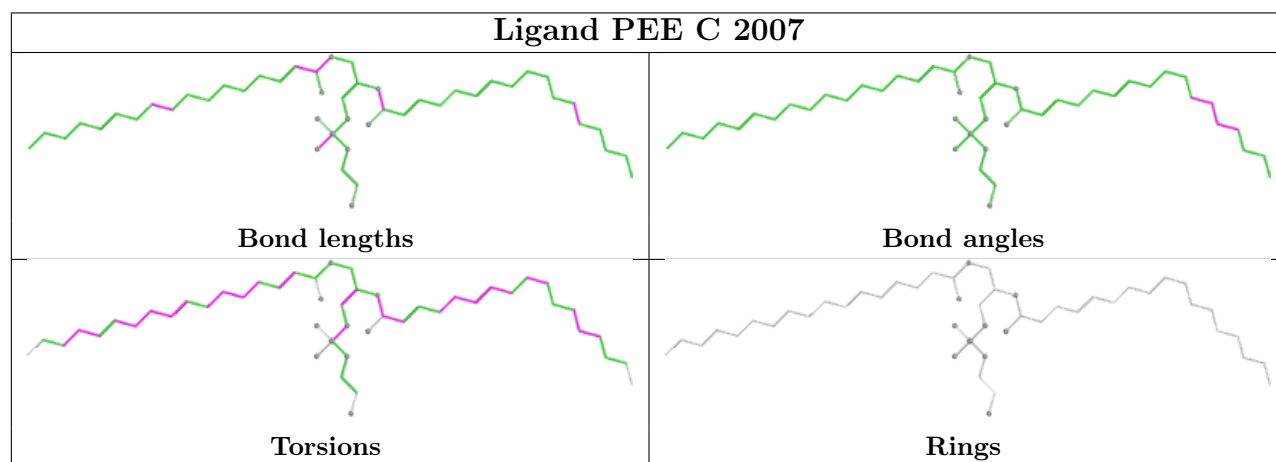
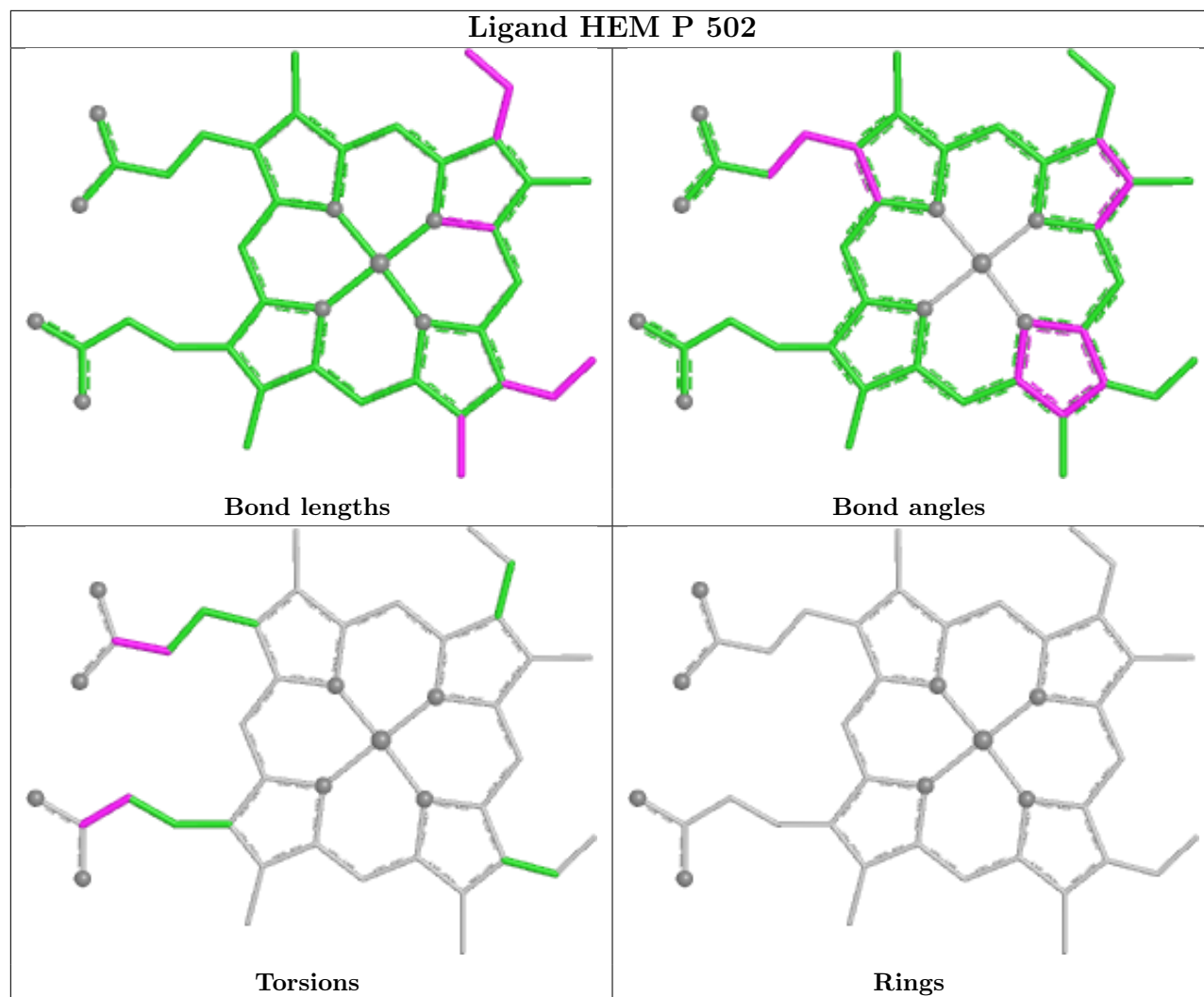


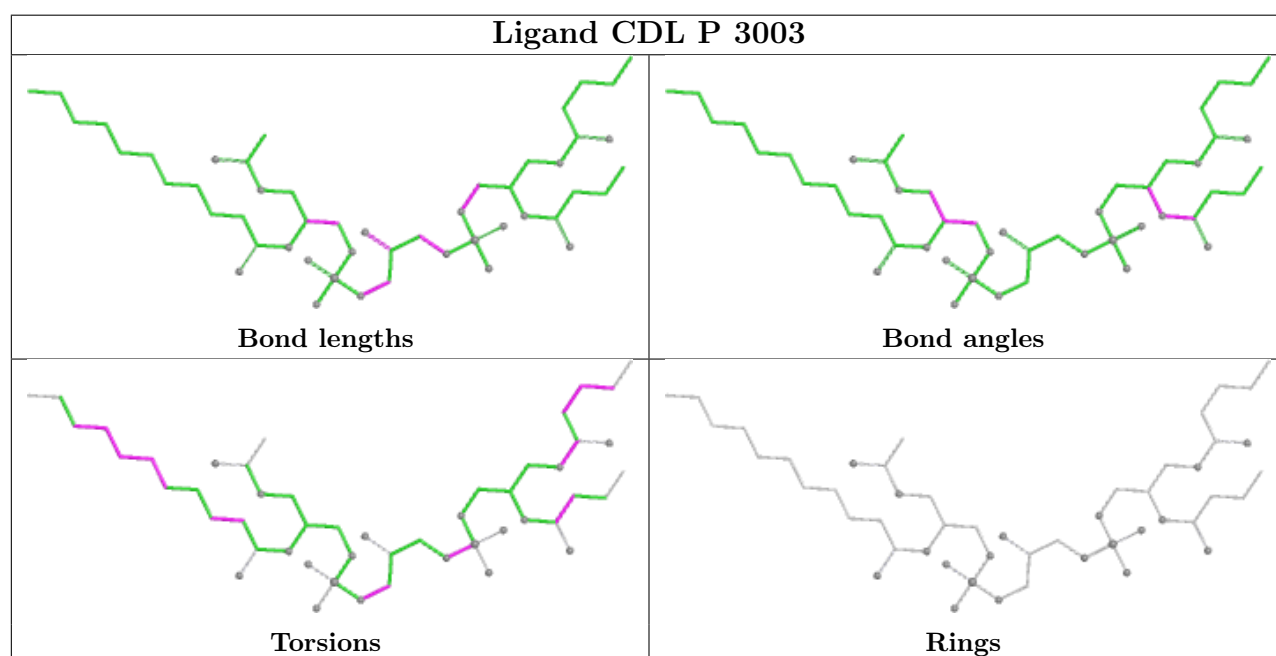
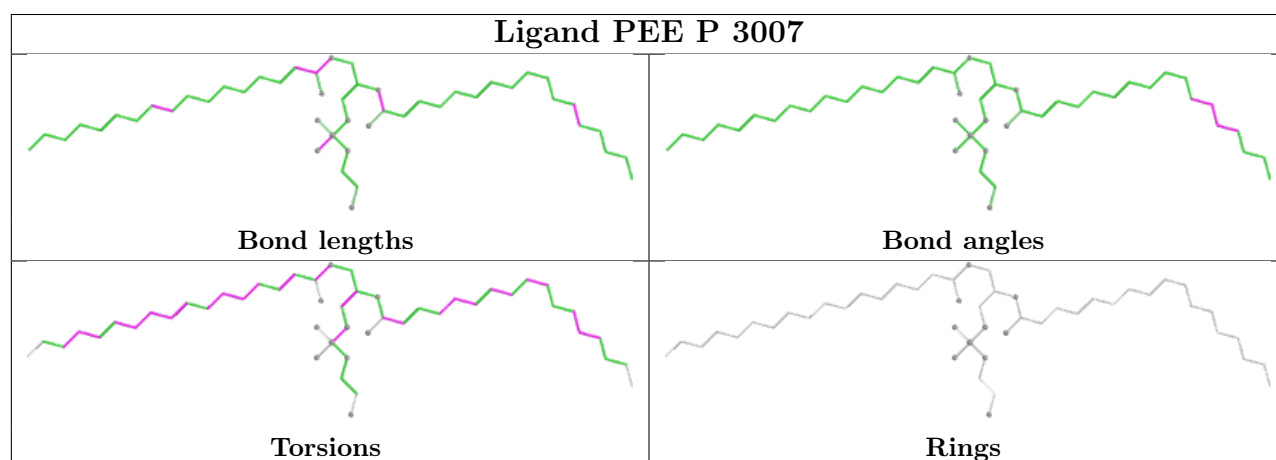
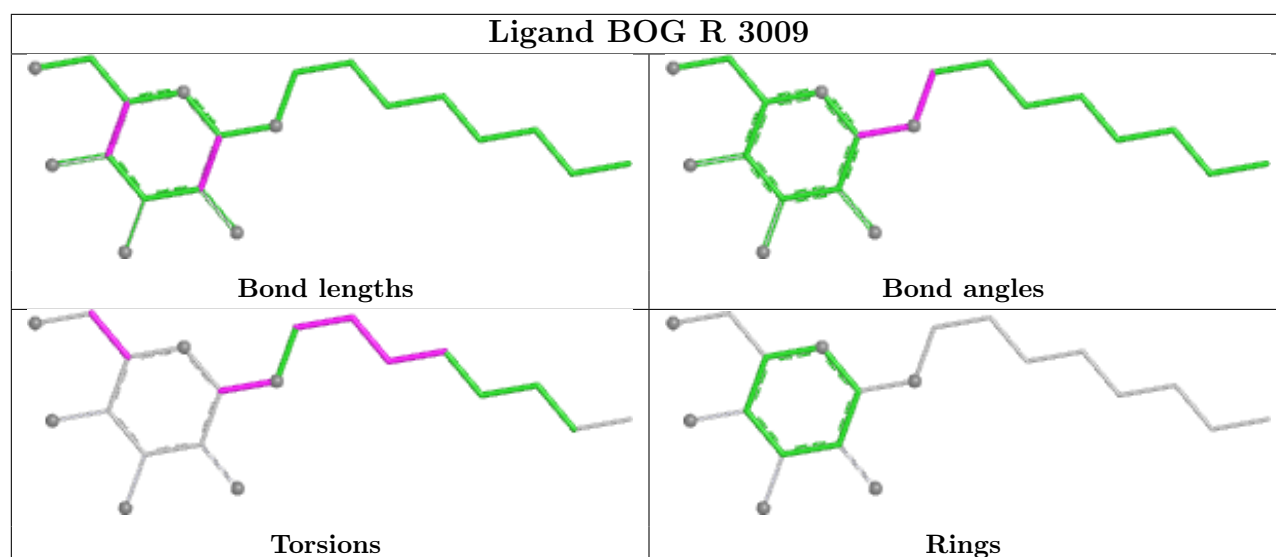
Rings

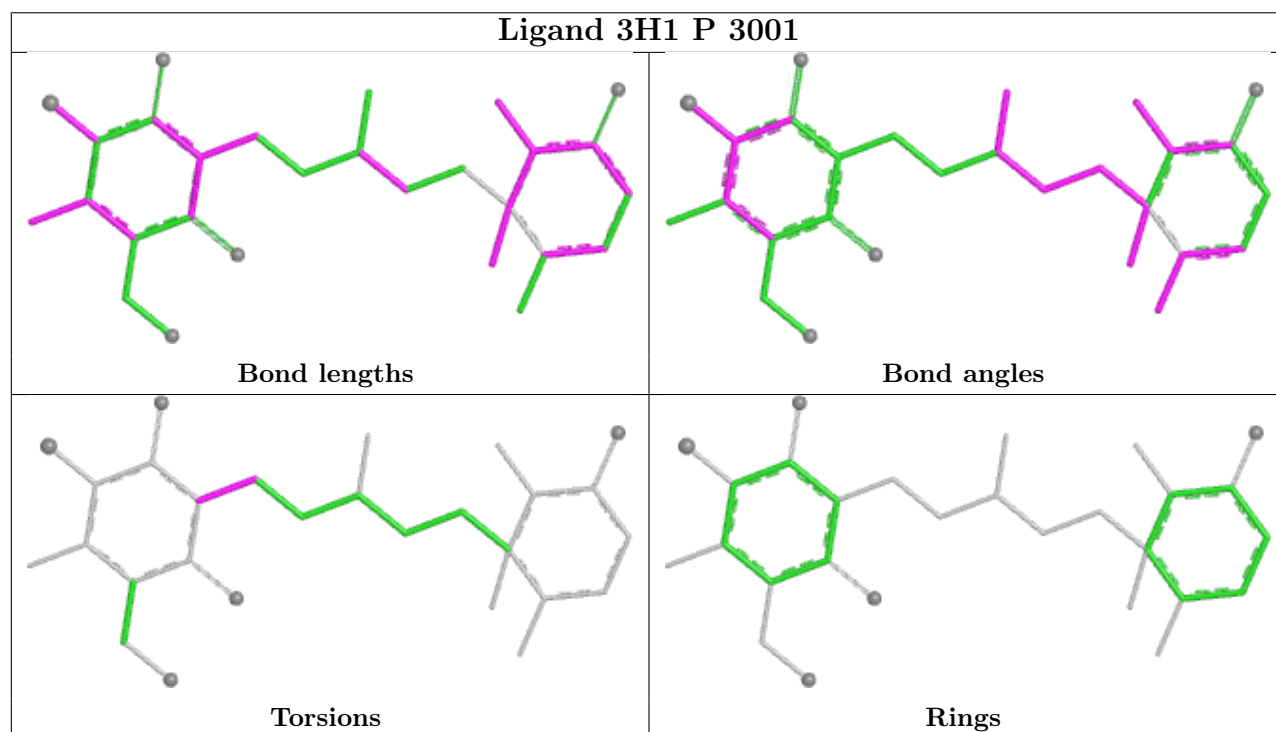
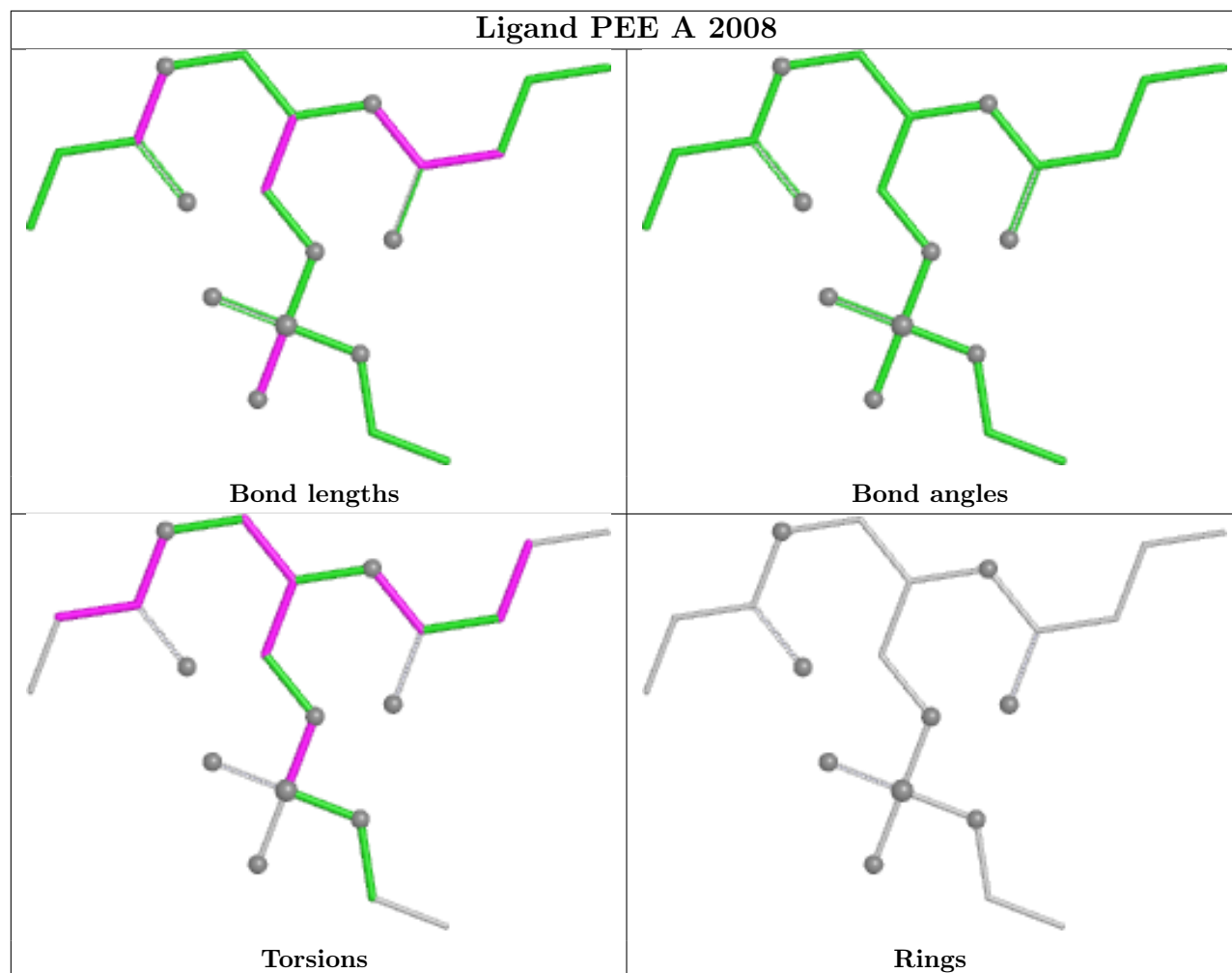


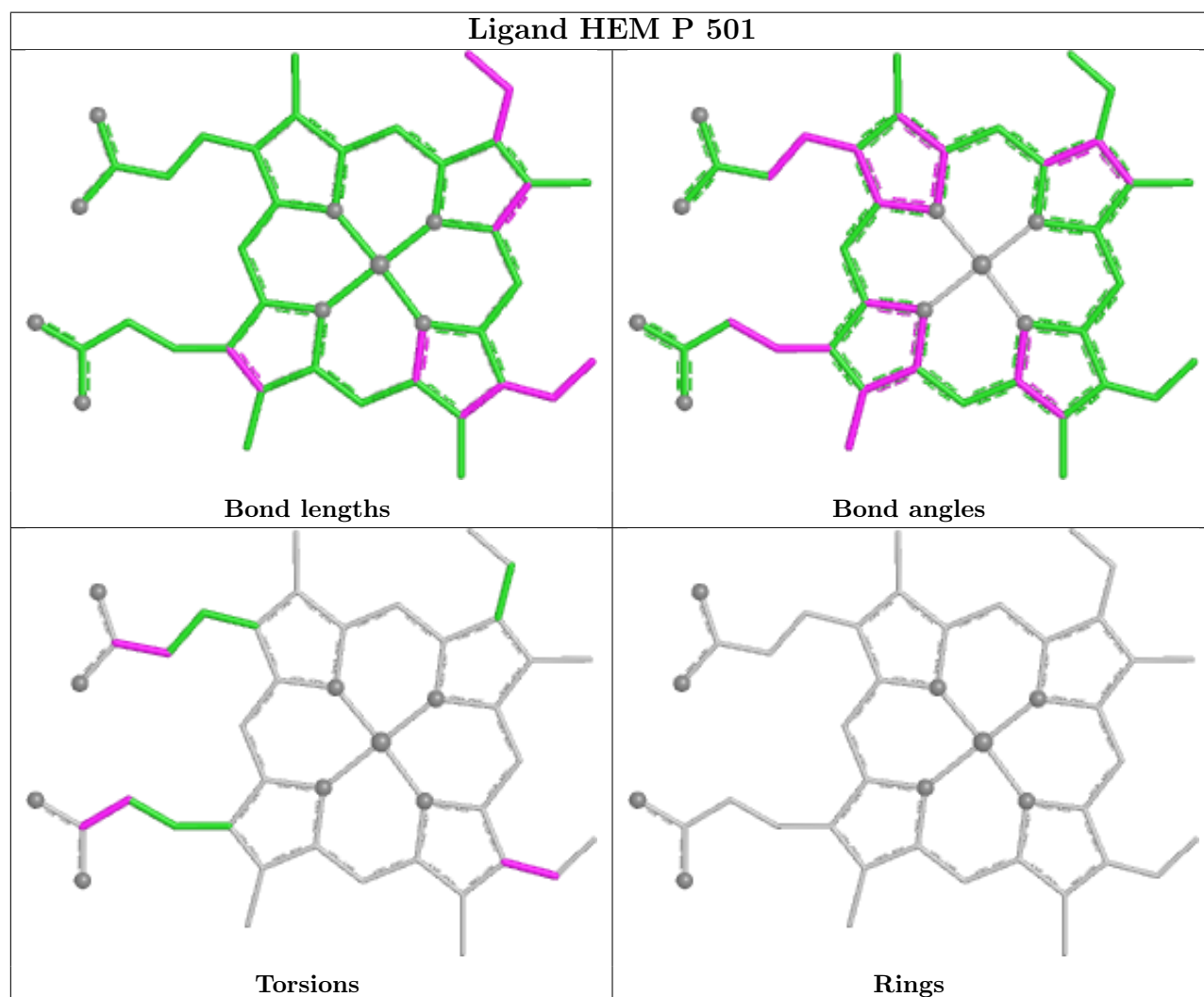
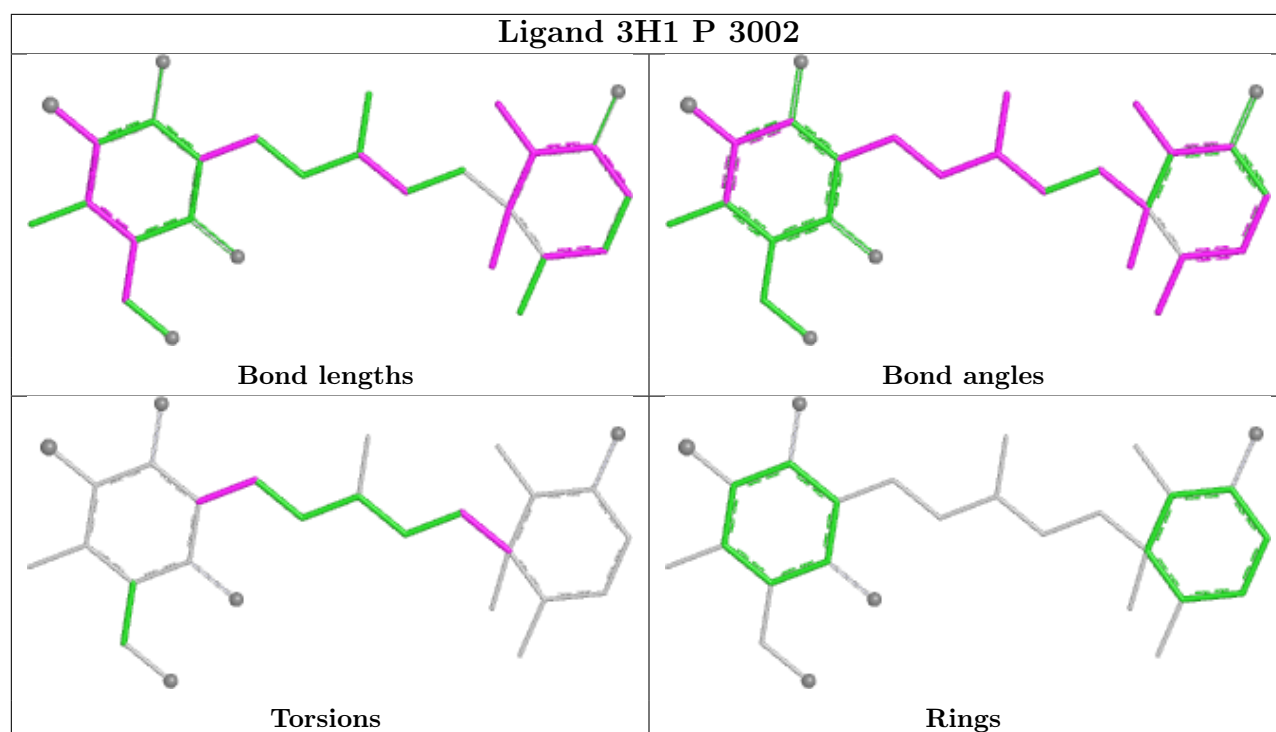


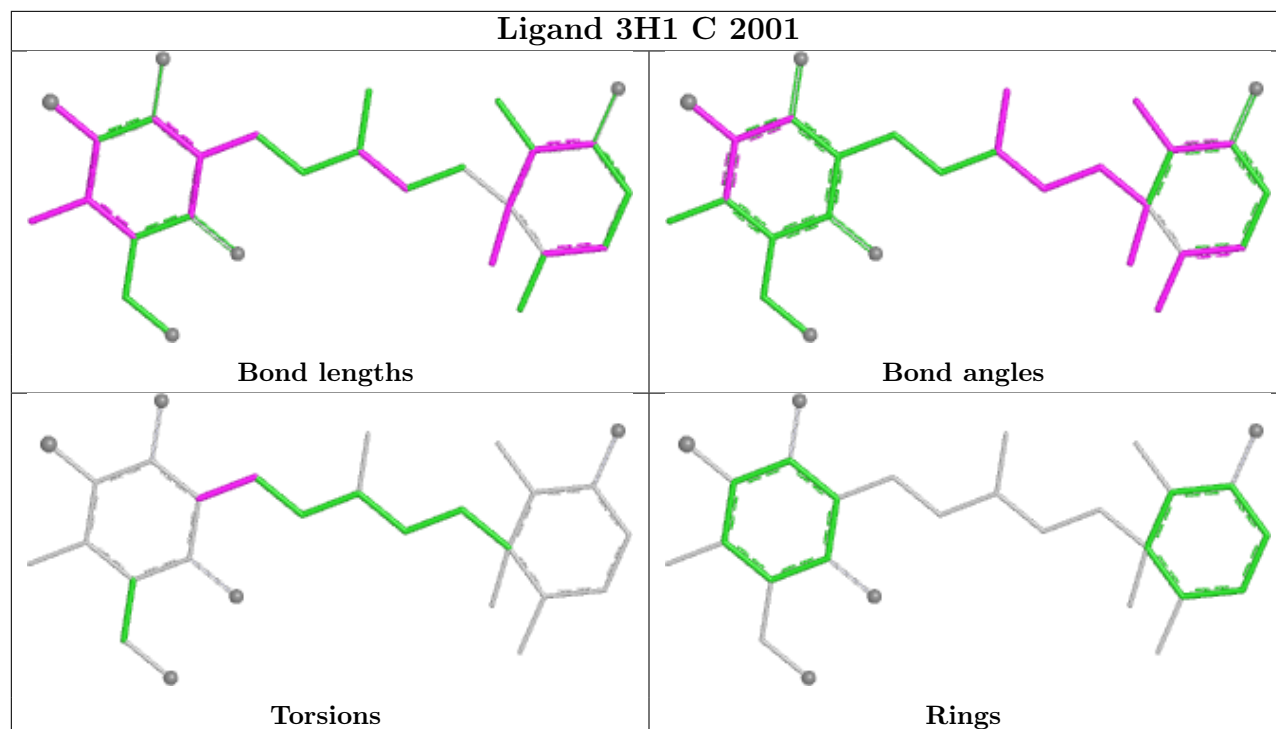




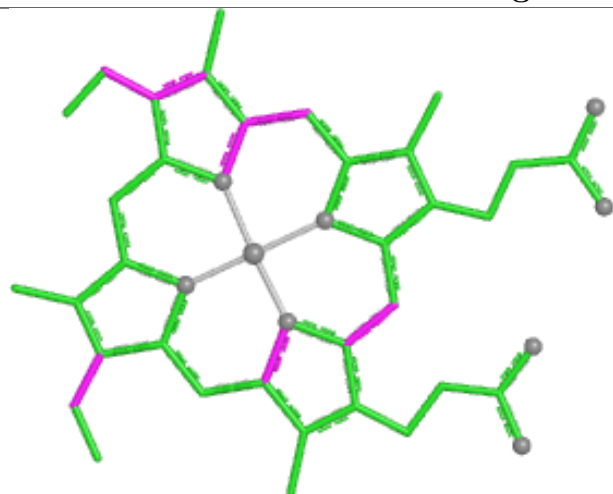




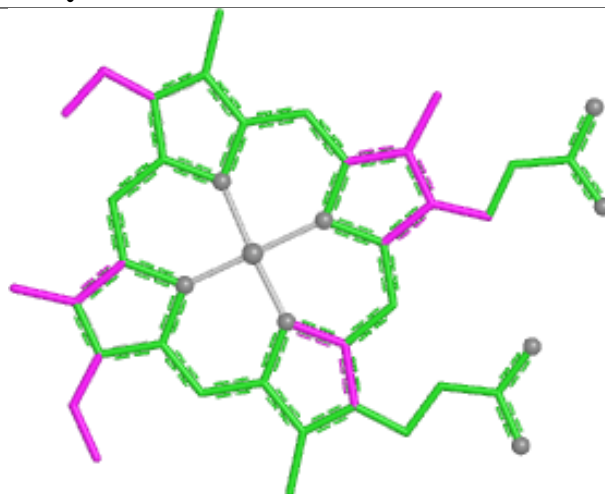




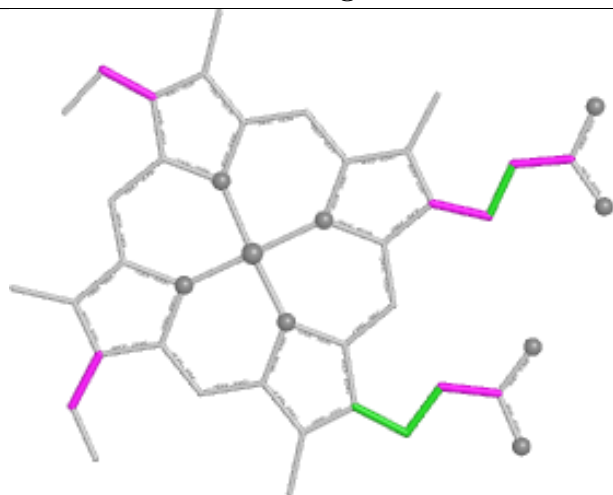
Ligand HEC Q 501



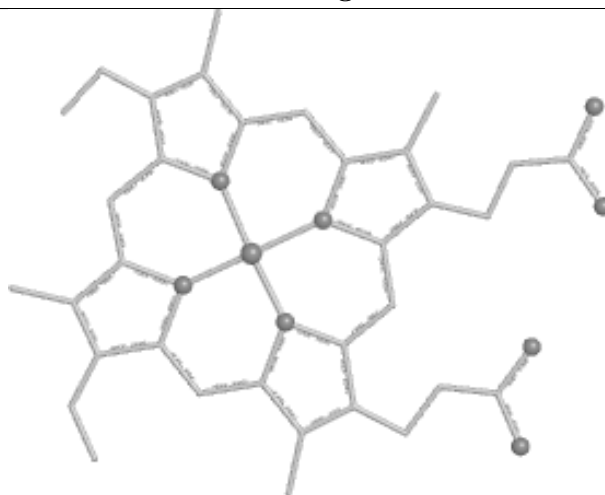
Bond lengths



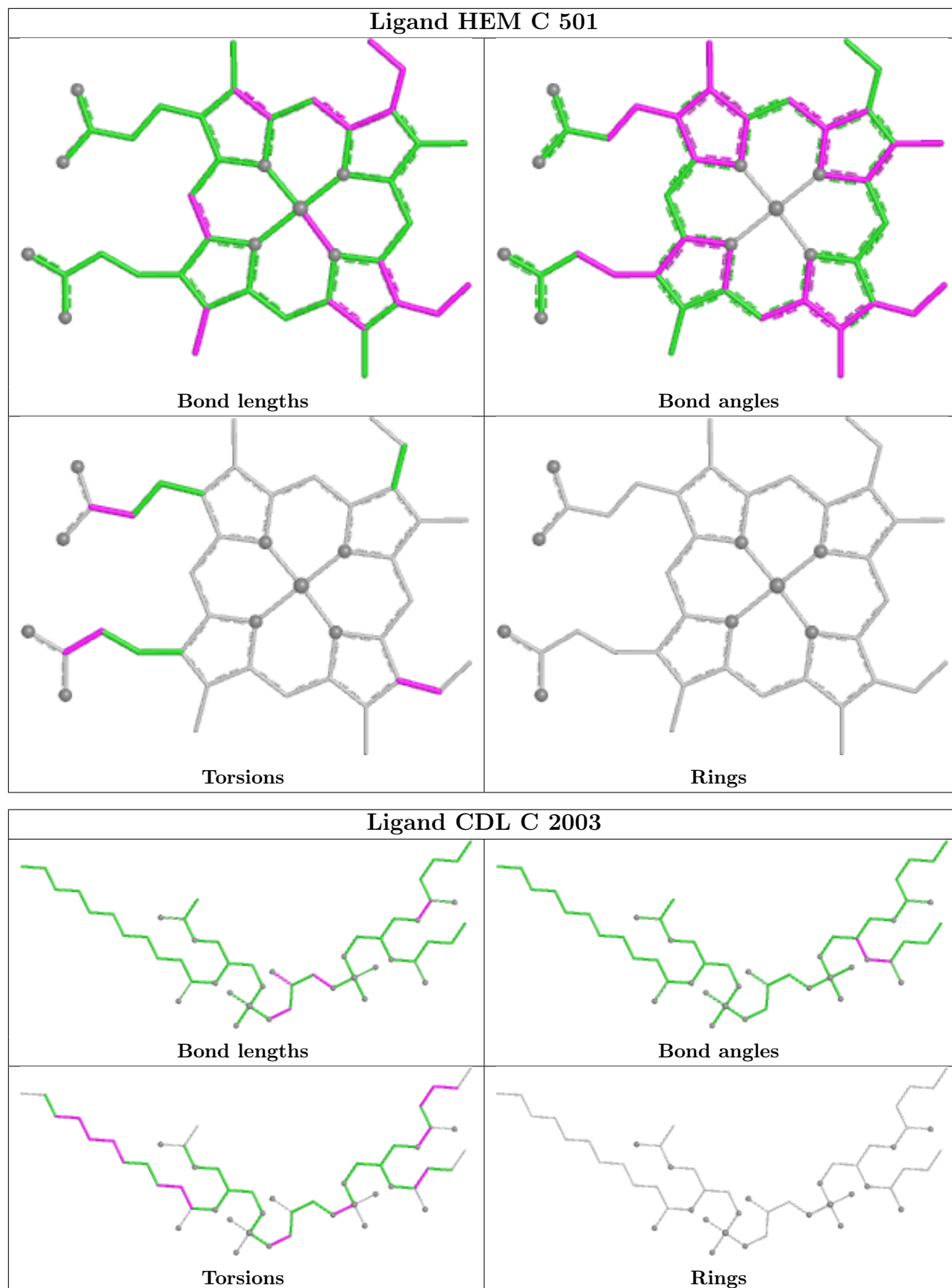
Bond angles



Torsions



Rings



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%)	0.29	15 (3%)	48	30	56, 105, 138, 156	0
1	N	442/446 (99%)	0.46	17 (3%)	44	28	66, 108, 138, 151	0
2	B	421/441 (95%)	0.63	32 (7%)	20	13	85, 124, 160, 177	0
2	O	422/441 (95%)	0.43	17 (4%)	42	26	68, 111, 142, 166	0
3	C	380/380 (100%)	-0.31	5 (1%)	75	55	39, 61, 113, 164	0
3	P	379/380 (99%)	0.36	16 (4%)	40	25	59, 104, 140, 164	0
4	D	241/241 (100%)	-0.33	2 (0%)	82	67	53, 68, 111, 136	0
4	Q	241/241 (100%)	0.37	4 (1%)	69	49	84, 117, 150, 163	0
5	E	196/196 (100%)	0.58	13 (6%)	24	15	63, 137, 182, 186	0
5	R	196/196 (100%)	0.32	5 (2%)	57	38	64, 107, 152, 165	0
6	F	101/110 (91%)	-0.31	1 (0%)	79	62	52, 68, 86, 121	0
6	S	101/110 (91%)	0.65	10 (9%)	13	9	96, 122, 162, 177	0
7	G	81/81 (100%)	-0.02	3 (3%)	45	28	53, 74, 134, 148	0
7	T	79/81 (97%)	0.72	5 (6%)	26	16	89, 132, 184, 194	0
8	H	70/77 (90%)	-0.03	1 (1%)	73	54	56, 95, 116, 154	0
8	U	67/77 (87%)	0.73	4 (5%)	27	17	143, 165, 185, 187	0
9	I	31/47 (65%)	1.59	10 (32%)	1	1	128, 157, 170, 174	0
9	V	31/47 (65%)	1.62	12 (38%)	1	1	109, 147, 196, 198	0
10	J	61/61 (100%)	-0.10	0	100	100	73, 93, 137, 168	0
10	W	59/61 (96%)	0.29	1 (1%)	69	49	91, 109, 133, 159	0
All	All	4042/4160 (97%)	0.30	173 (4%)	40	25	39, 106, 159, 198	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	120	MET	6.2
2	B	122	TYR	5.3
9	I	63	ASP	5.1
1	A	444	ILE	4.9
1	N	75	PHE	4.9
3	P	212	ILE	4.6
3	P	8	SER	4.5
2	B	206	LEU	4.3
5	R	118	ARG	4.2
1	N	64	PHE	4.1
2	B	402	ILE	4.1
6	F	41	ASP	4.1
7	T	1	GLY	4.1
2	B	216	LEU	4.0
1	A	392	LEU	3.9
5	E	137	GLY	3.8
9	I	61	ARG	3.8
2	B	116	VAL	3.8
9	V	63	ASP	3.7
6	S	35	ASP	3.7
1	A	8	LEU	3.6
1	N	86	PHE	3.6
1	A	395	TRP	3.6
9	I	64	LEU	3.6
2	B	119	VAL	3.5
4	Q	118	ASN	3.5
3	P	7	LYS	3.5
9	V	49	LEU	3.5
2	O	226	ILE	3.5
2	B	388	LEU	3.4
1	N	174	ILE	3.4
2	B	124	LEU	3.4
3	P	211	GLY	3.3
1	N	57	TYR	3.3
3	P	9	HIS	3.2
3	P	96	PHE	3.2
2	B	123	LEU	3.2
8	U	24	CYS	3.2
1	A	432	LEU	3.2
3	P	213	SER	3.2
1	N	66	GLY	3.2
2	B	219	VAL	3.1
9	I	76	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
9	V	75	SER	3.1
2	B	368	TYR	3.1
3	P	139	MET	3.1
3	P	4	ASN	3.0
2	O	410	VAL	3.0
7	G	2	ILE	3.0
7	T	22	GLU	3.0
1	N	376	CYS	3.0
3	P	344	VAL	3.0
10	W	60	GLU	3.0
9	V	48	PRO	2.9
3	P	6	ARG	2.9
5	E	143	GLY	2.9
2	B	90	GLU	2.9
8	U	30	CYS	2.9
1	A	174	ILE	2.9
2	O	256	ALA	2.9
3	C	9	HIS	2.8
5	E	109	GLU	2.8
7	T	55	ALA	2.8
9	V	61	ARG	2.8
7	G	4	PHE	2.8
2	B	21	ALA	2.8
8	H	9	GLU	2.8
9	V	50	LEU	2.8
6	S	36	THR	2.7
5	E	136	VAL	2.7
2	B	34	ILE	2.7
4	Q	115	TYR	2.7
2	O	232	THR	2.7
5	R	94	LYS	2.7
3	P	255	GLU	2.6
2	O	268	GLU	2.6
1	N	432	LEU	2.6
3	P	257	PHE	2.6
7	T	71	ARG	2.6
2	O	324	PHE	2.5
1	N	198	ALA	2.5
1	A	66	GLY	2.5
5	E	128	LYS	2.5
9	V	52	ARG	2.5
2	O	21	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	365	MET	2.5
3	P	318	PHE	2.5
1	N	117	VAL	2.5
2	B	398	VAL	2.5
1	A	443	TRP	2.5
9	V	47	ARG	2.5
2	O	343	GLN	2.5
8	U	54	CYS	2.5
1	N	344	ARG	2.5
3	P	11	LEU	2.5
9	V	62	ARG	2.5
2	B	367	THR	2.4
5	E	121	GLN	2.4
6	S	90	LEU	2.4
2	O	383	GLY	2.4
2	O	93	GLY	2.3
1	N	113	LEU	2.3
2	B	127	THR	2.3
2	B	390	GLY	2.3
2	O	347	ALA	2.3
2	O	386	ALA	2.3
2	B	439	LEU	2.3
1	N	88	GLY	2.3
2	O	344	LEU	2.3
2	O	147	ASP	2.3
5	R	117	LEU	2.3
6	S	89	TYR	2.3
1	A	58	PHE	2.3
7	T	2	ILE	2.3
2	B	55	SER	2.3
8	U	74	PHE	2.3
5	E	94	LYS	2.3
3	P	5	ILE	2.2
9	V	67	GLY	2.2
9	I	49	LEU	2.2
3	C	7	LYS	2.2
5	R	120	PRO	2.2
2	B	24	LEU	2.2
9	V	64	LEU	2.2
5	E	132	TRP	2.2
2	O	296	TYR	2.2
2	B	291	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	168	GLU	2.2
5	R	171	ILE	2.2
5	E	180	LEU	2.2
6	S	58	ARG	2.2
2	B	128	THR	2.1
1	N	83	GLY	2.1
5	E	147	ILE	2.1
1	A	69	LYS	2.1
2	O	340	ALA	2.1
9	I	60	ALA	2.1
1	A	31	SER	2.1
3	C	8	SER	2.1
1	N	52	ASN	2.1
2	B	417	PHE	2.1
1	A	390	ILE	2.1
2	B	393	THR	2.1
9	I	47	ARG	2.1
2	B	256	ALA	2.1
9	V	72	ALA	2.1
2	B	73	SER	2.1
2	B	396	SER	2.1
3	C	4	ASN	2.1
5	E	134	ILE	2.1
4	Q	132	THR	2.1
6	S	24	ALA	2.1
1	A	28	GLU	2.1
4	D	69	GLU	2.1
6	S	31	LEU	2.1
9	I	77	ARG	2.1
1	N	120	CYS	2.1
2	O	306	PRO	2.1
9	I	75	SER	2.0
2	B	364	LEU	2.0
4	D	2	GLU	2.0
7	G	67	GLU	2.0
5	E	124	LEU	2.0
2	B	26	ILE	2.0
6	S	107	TRP	2.0
5	E	191	ASP	2.0
4	Q	1	GLY	2.0
1	A	389	ARG	2.0
2	B	126	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	11	LEU	2.0
6	S	37	LEU	2.0
6	S	75	LEU	2.0
9	I	70	LEU	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($\text{\AA}^2$)	Q<0.9
12	UNL	P	3103	1/-	0.54	0.25	76,76,76,76	0
12	UNL	P	2106	1/-	0.67	0.07	63,63,63,63	0
12	UNL	A	3016	1/-	0.73	0.29	69,69,69,69	0
11	PEE	A	2008	21/51	0.75	0.20	149,161,164,166	0
12	UNL	P	3010	1/-	0.76	0.13	60,60,60,60	0
12	UNL	E	2105	1/-	0.79	0.17	82,82,82,82	0
11	PEE	P	3008	5/51	0.80	0.11	149,149,150,151	0
15	CDL	P	3003	50/100	0.80	0.28	150,158,162,162	0
12	UNL	P	3104	1/-	0.82	0.17	83,83,83,83	0
12	UNL	C	3015	1/-	0.82	0.33	53,53,53,53	0
12	UNL	C	2104	1/-	0.84	0.13	85,85,85,85	0
12	UNL	C	3106	1/-	0.84	0.08	44,44,44,44	0
12	UNL	P	2015	1/-	0.86	0.17	48,48,48,48	0
12	UNL	C	2010	1/-	0.86	0.44	30,30,30,30	0
15	CDL	T	3004	40/100	0.86	0.17	117,124,129,131	0
12	UNL	R	2103	1/-	0.87	0.18	53,53,53,53	0
11	PEE	E	2005	50/51	0.88	0.26	95,113,124,126	0
11	PEE	R	3005	50/51	0.88	0.26	102,123,129,130	0
14	3H1	P	3002	28/28	0.89	0.20	101,108,114,114	0

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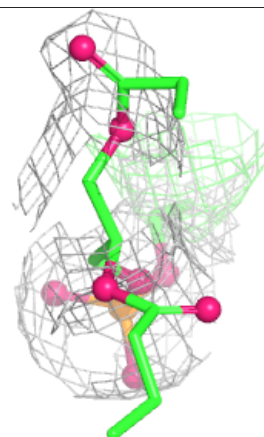
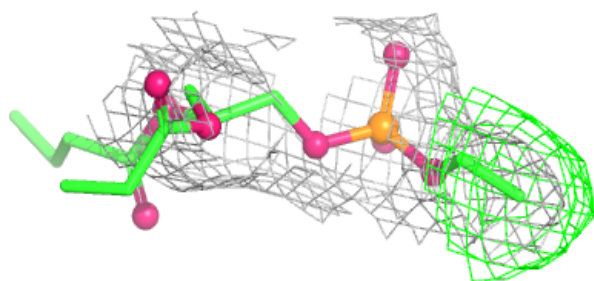
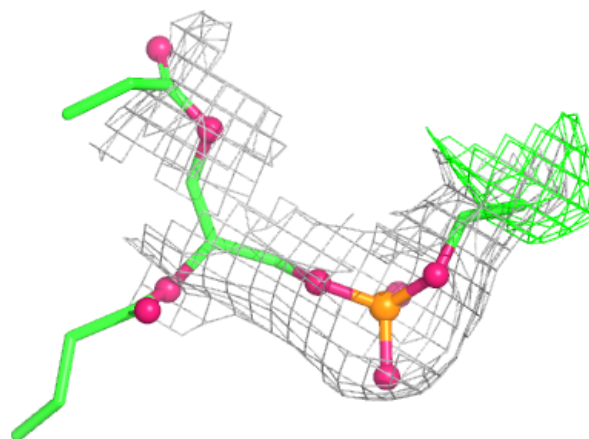
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CDL	C	2003	50/100	0.89	0.18	82,93,106,107	0
18	BOG	R	3009	20/20	0.89	0.21	101,121,124,124	0
14	3H1	C	2002	28/28	0.90	0.17	66,76,89,89	0
16	GOL	C	2011	6/6	0.91	0.21	84,87,88,88	0
14	3H1	P	3001	28/28	0.92	0.17	101,106,112,112	0
15	CDL	G	2004	40/100	0.92	0.13	65,79,101,103	0
14	3H1	C	2001	28/28	0.93	0.13	47,56,60,61	0
11	PEE	P	3007	49/51	0.93	0.23	107,121,139,140	0
18	BOG	D	2009	20/20	0.94	0.12	75,88,91,92	0
11	PEE	C	2007	49/51	0.96	0.14	55,72,95,97	0
17	HEC	Q	501	43/43	0.96	0.12	95,99,103,105	0
16	GOL	P	3011	6/6	0.97	0.22	108,110,111,113	0
19	FES	E	501	4/4	0.97	0.05	118,119,120,120	0
13	HEM	P	502	43/43	0.98	0.08	79,81,93,100	0
17	HEC	D	501	43/43	0.98	0.08	38,48,57,60	0
13	HEM	P	501	43/43	0.98	0.09	72,78,85,88	0
13	HEM	C	502	43/43	0.99	0.06	37,42,47,56	0
13	HEM	C	501	43/43	0.99	0.07	47,53,58,62	0
19	FES	R	501	4/4	0.99	0.03	69,69,69,69	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.

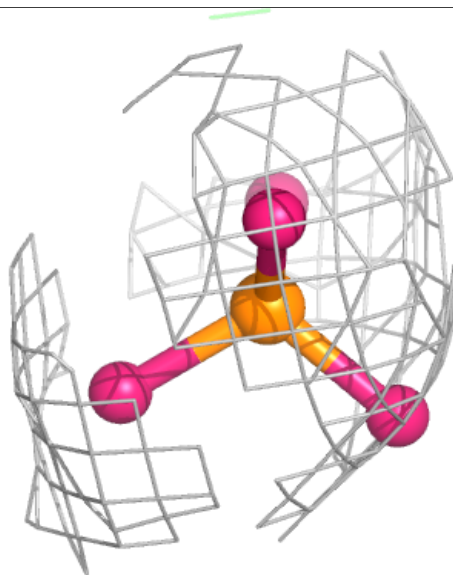
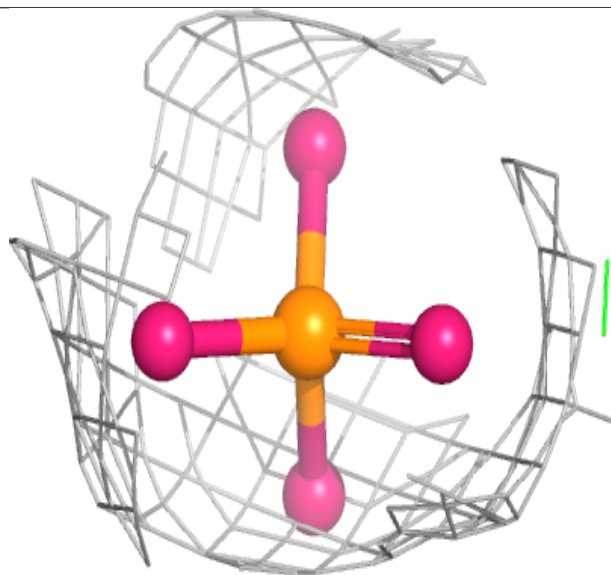
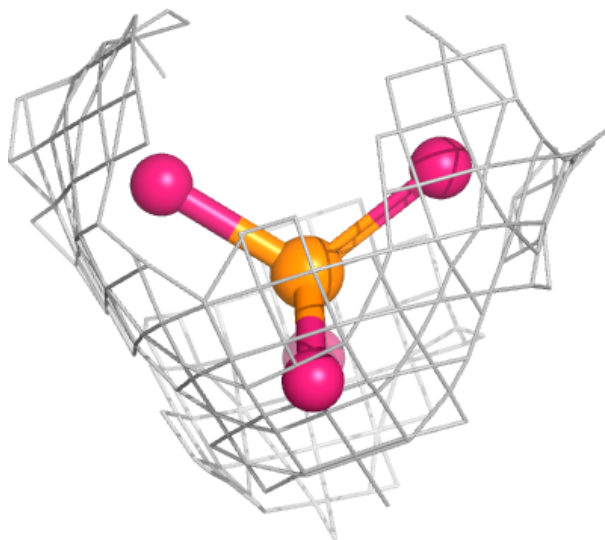
Electron density around PEE A 2008:

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



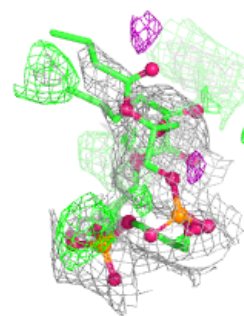
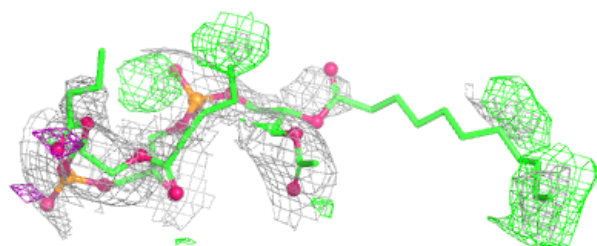
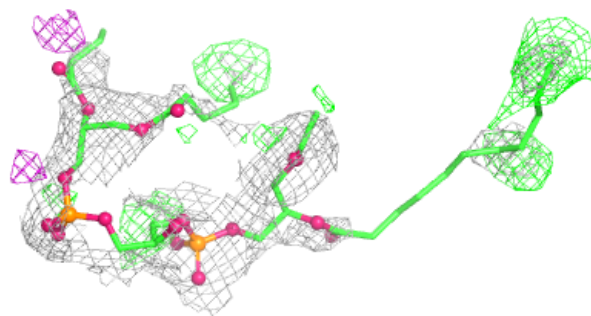
Electron density around PEE P 3008:

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



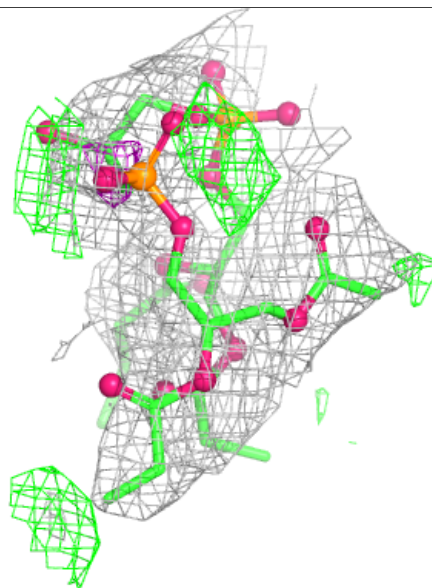
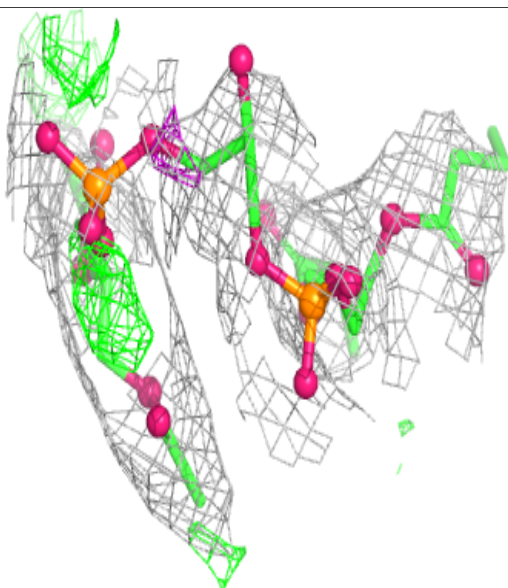
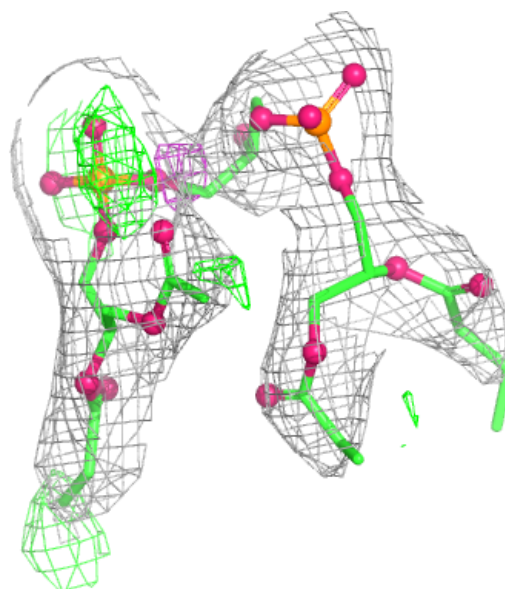
Electron density around CDL P 3003:

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



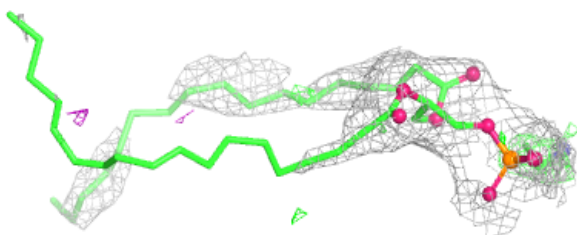
Electron density around CDL T 3004:

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



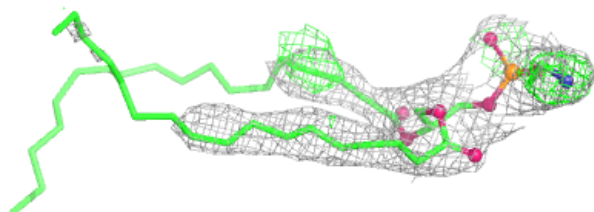
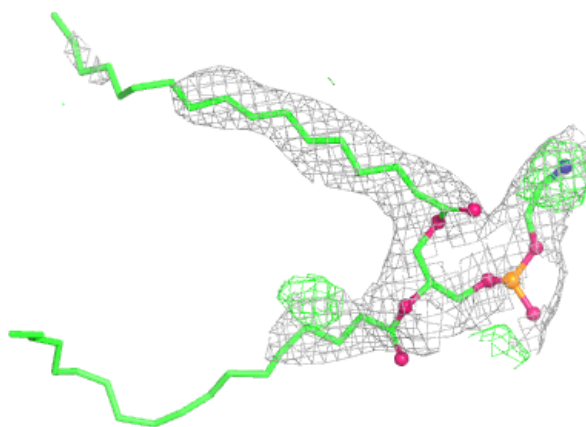
Electron density around PEE E 2005:

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

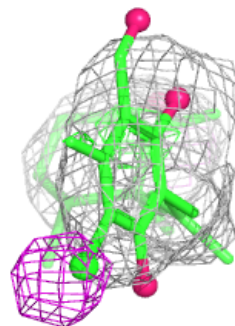
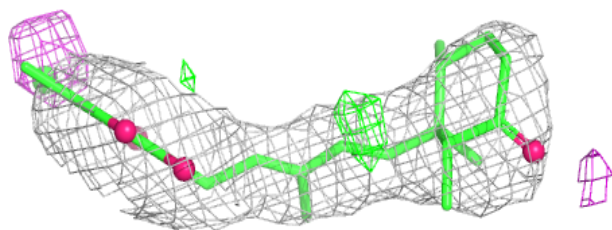
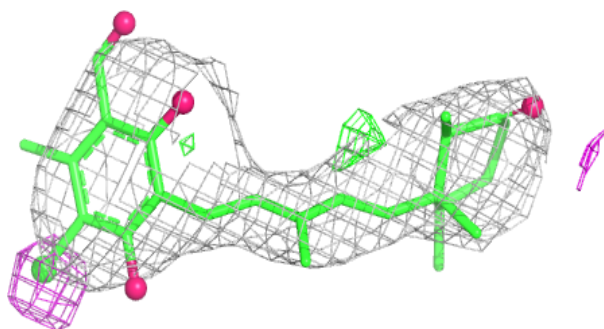


Electron density around PEE R 3005:

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

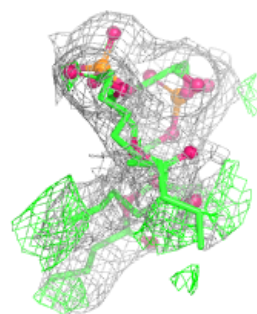
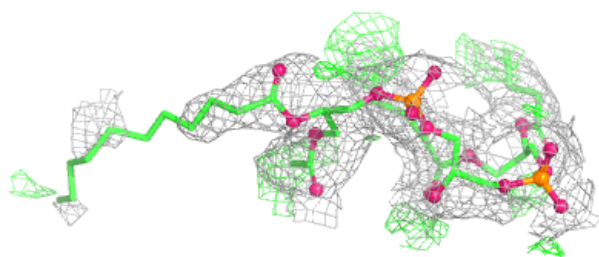
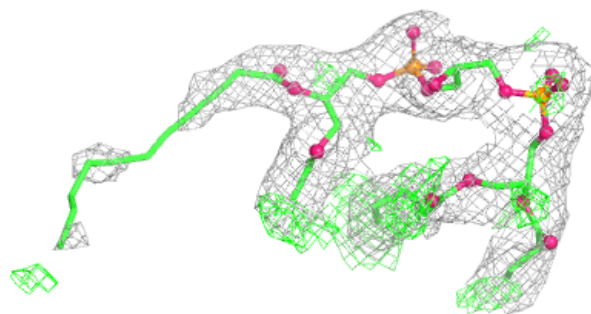
**Electron density around 3H1 P 3002:**

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and green (positive)

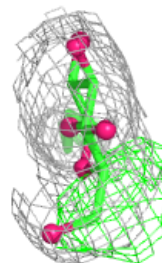
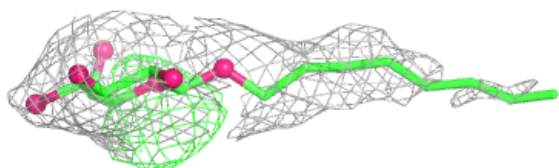
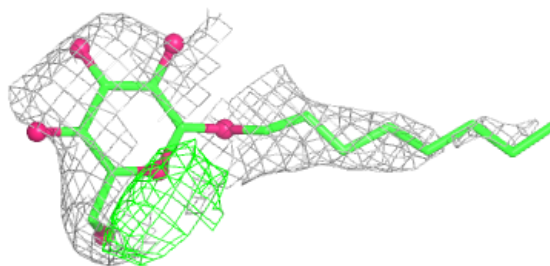


Electron density around CDL C 2003:

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

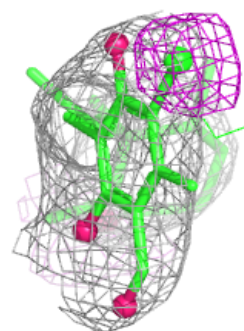
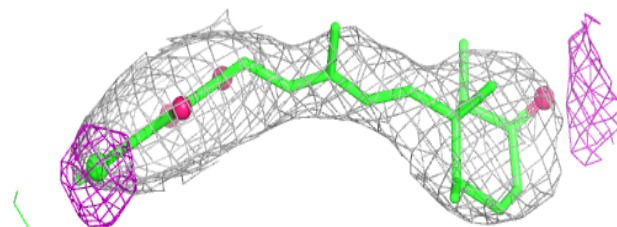
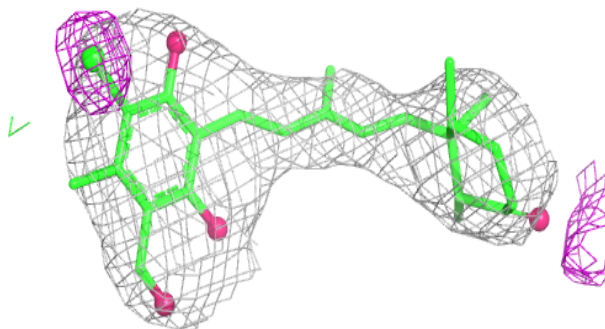
**Electron density around BOG R 3009:**

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

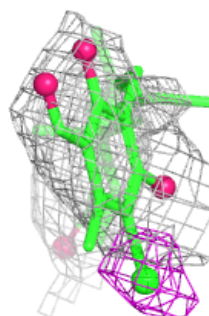
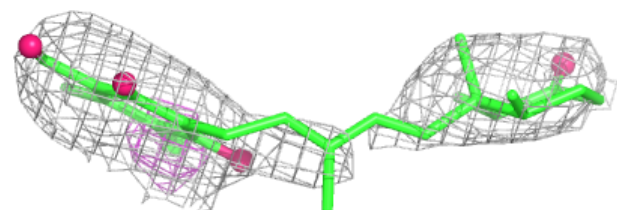
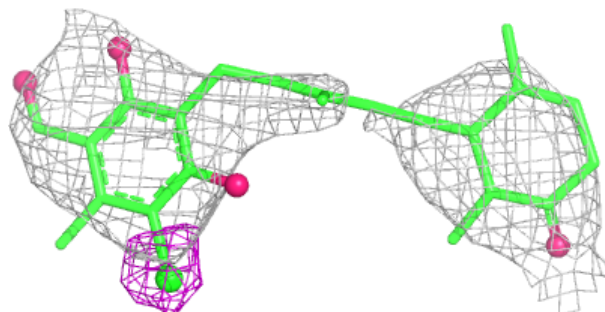


Electron density around 3H1 C 2002:

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

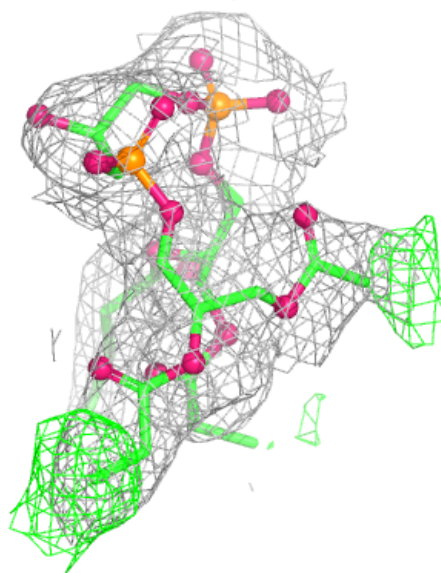
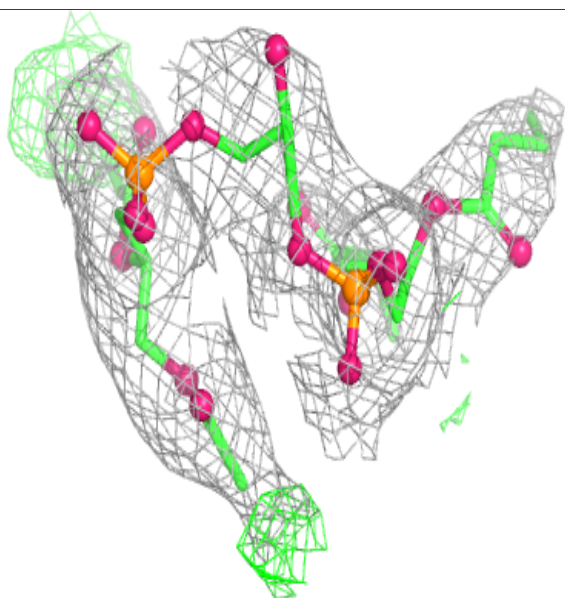
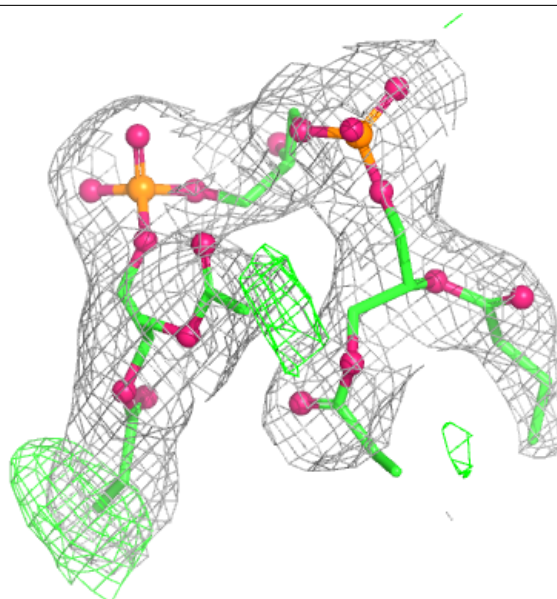
**Electron density around 3H1 P 3001:**

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



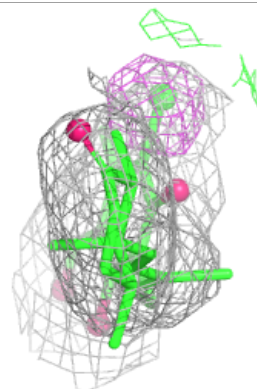
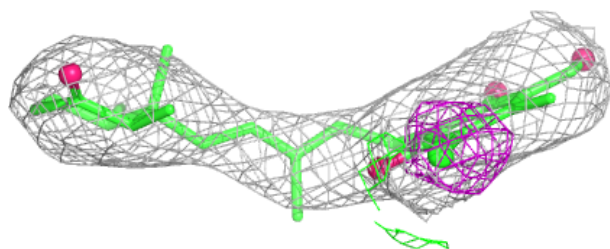
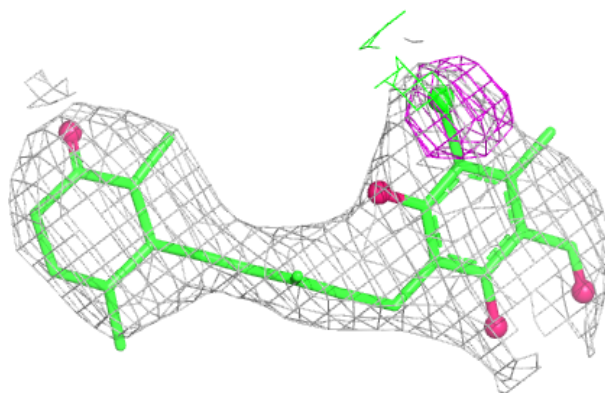
Electron density around CDL G 2004:

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and green (positive)

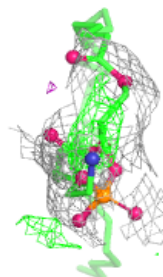
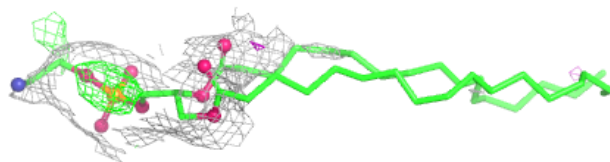
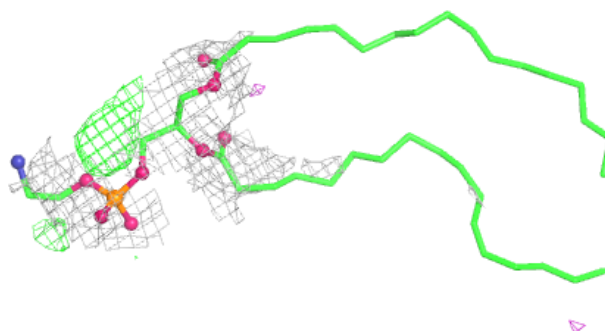


Electron density around 3H1 C 2001:

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and green (positive)

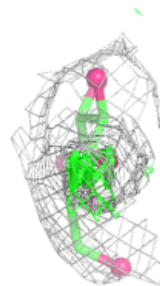
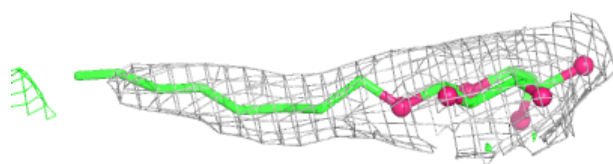
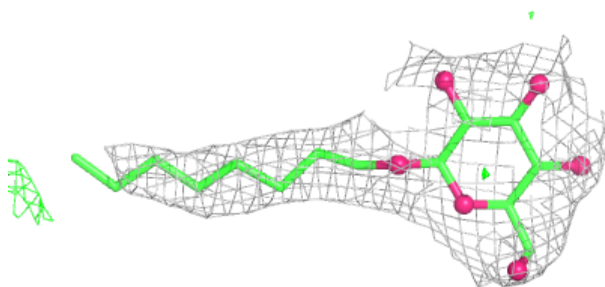
**Electron density around PEE P 3007:**

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and green (positive)

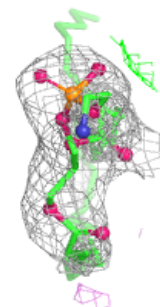
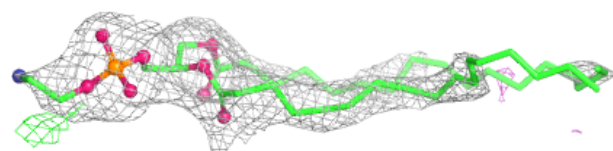
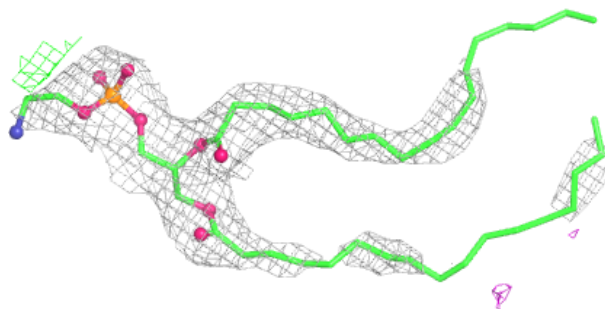


Electron density around BOG D 2009:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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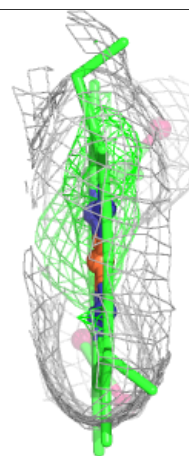
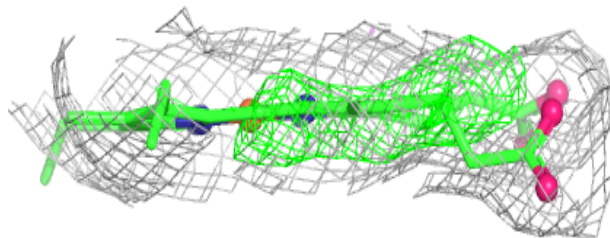
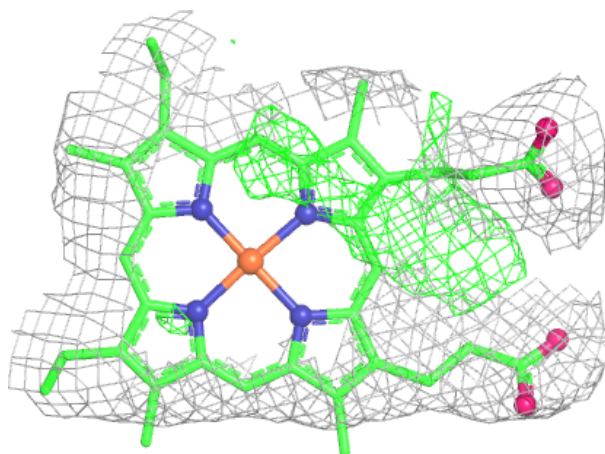
**Electron density around PEE C 2007:**

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and green (positive)



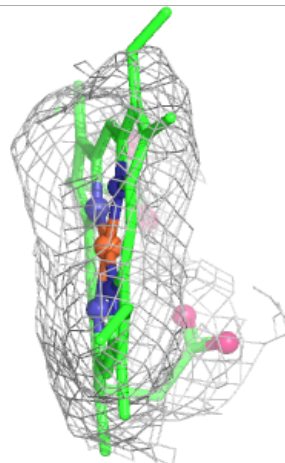
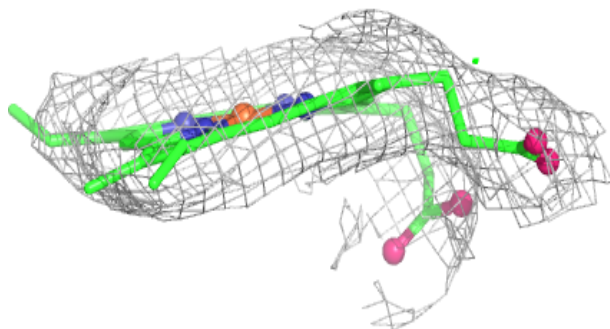
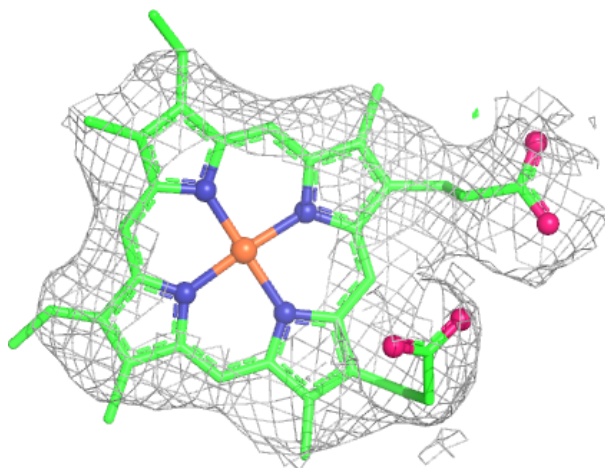
Electron density around HEC Q 501:

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



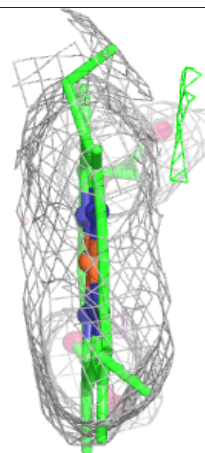
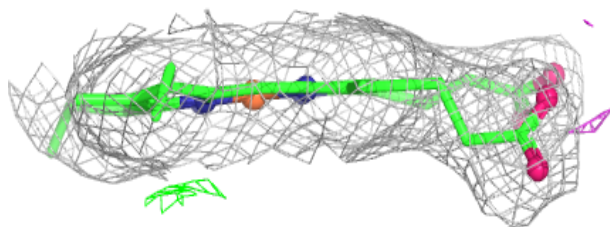
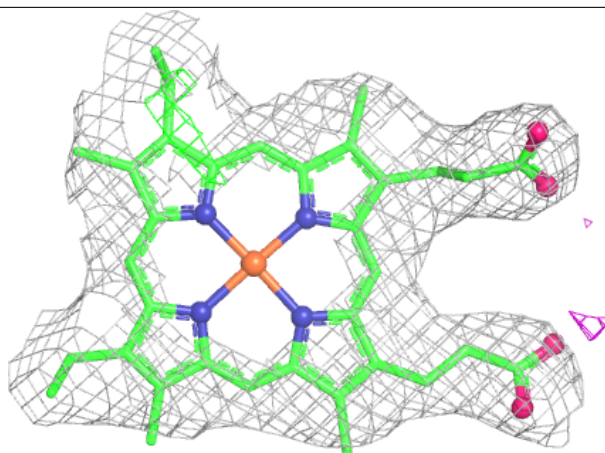
Electron density around HEM P 502:

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



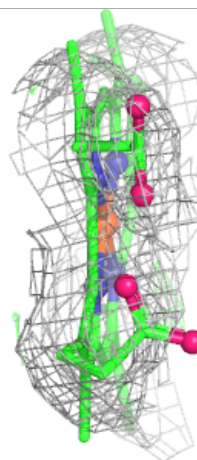
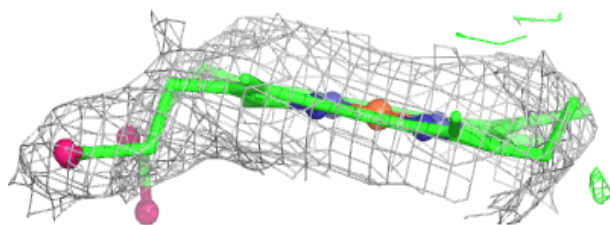
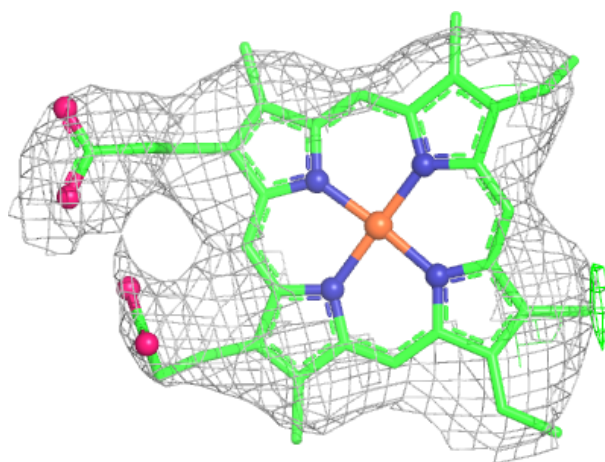
Electron density around HEC D 501:

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



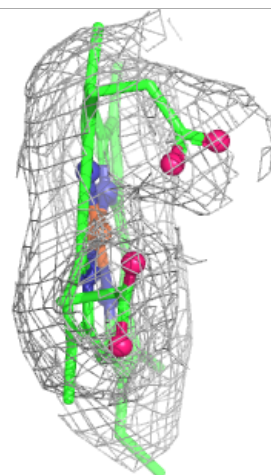
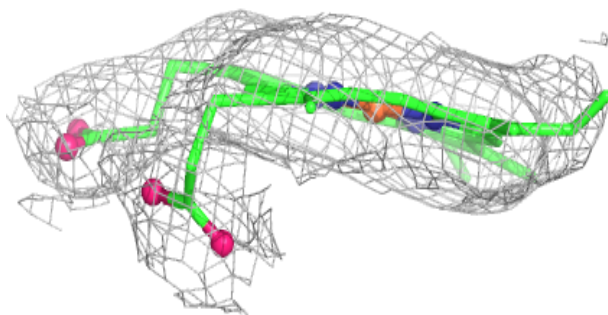
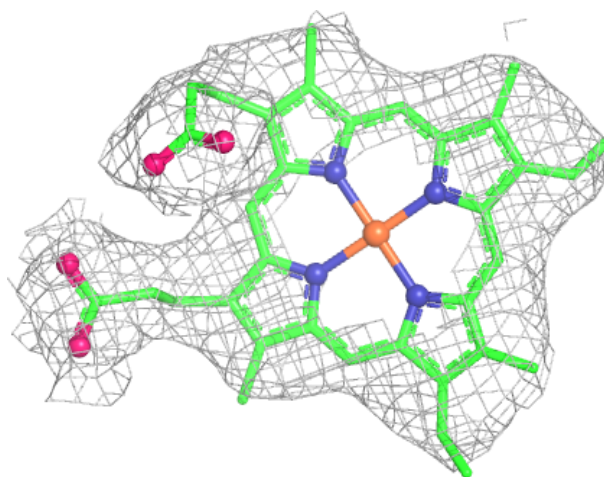
Electron density around HEM P 501:

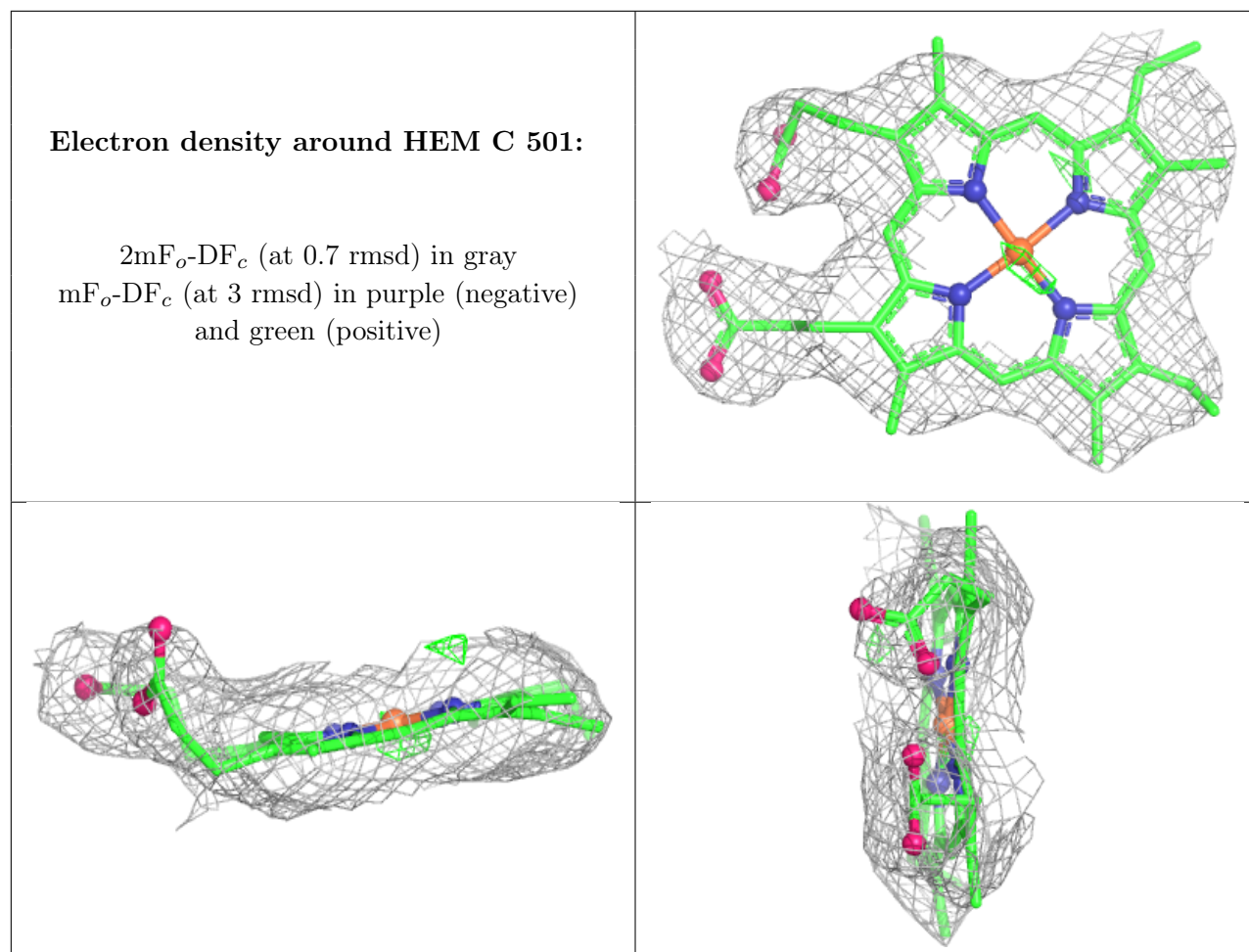
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.