



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:10 AM UTC

PDB ID : 3H1H / pdb_00003h1h
Title : Cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.;
Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on : 2009-04-12
Resolution : 3.16 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:

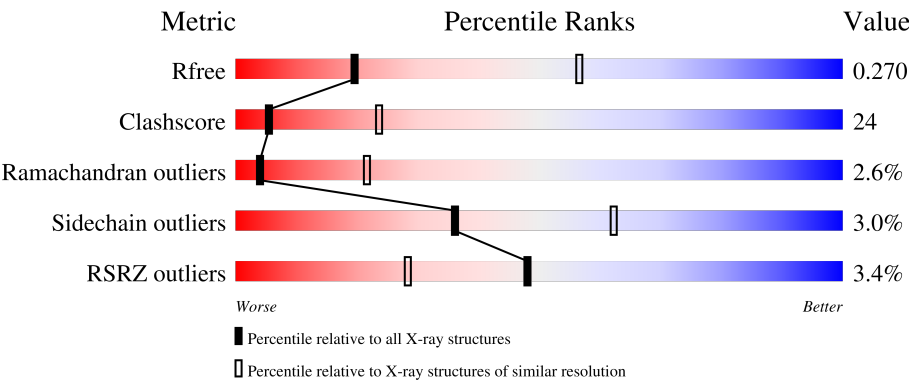
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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.



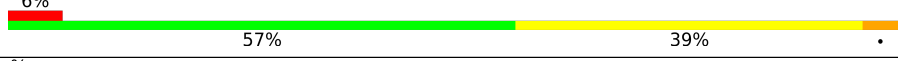
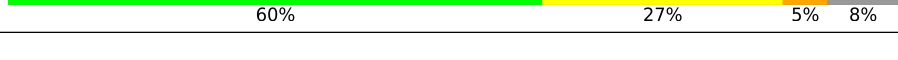
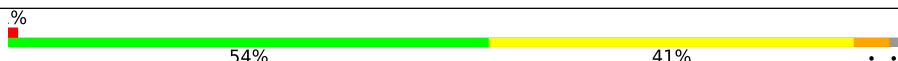
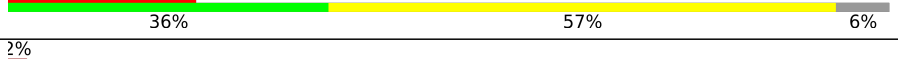
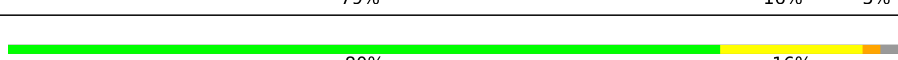
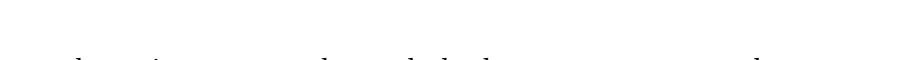
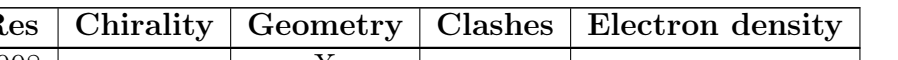
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PEE	N	3008	-	X	-	-
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1509	950	263	290	6			

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

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

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

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

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

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

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

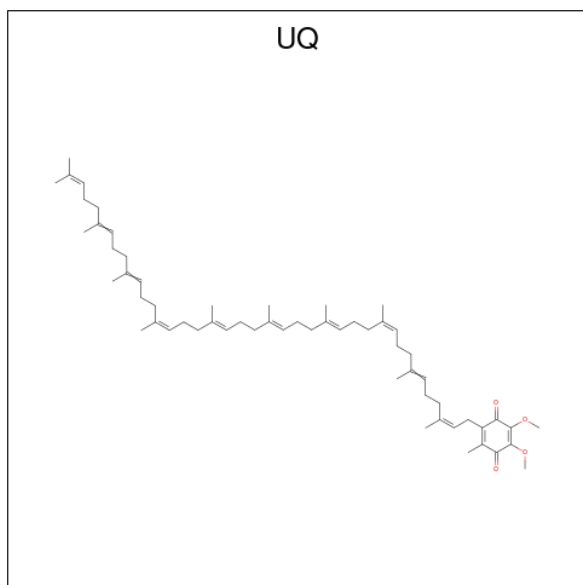
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

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

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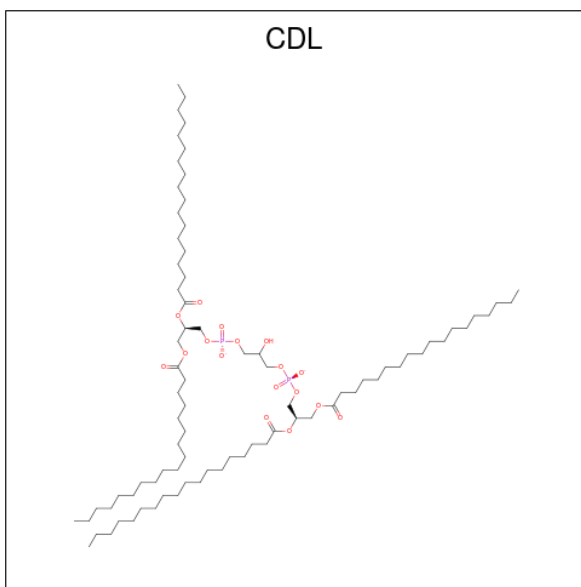
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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



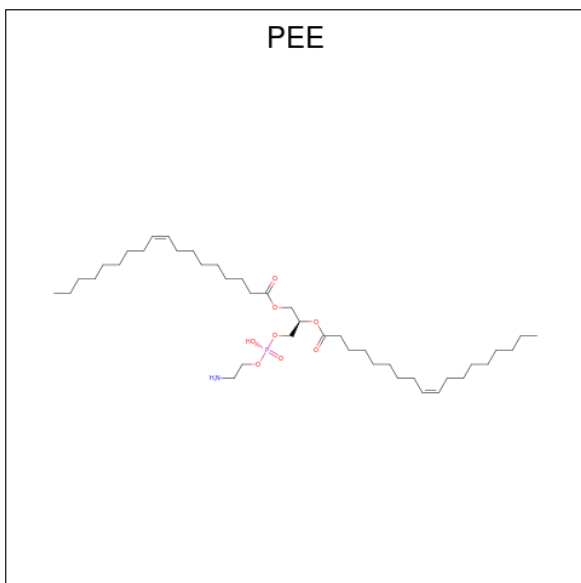
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O		
			19	15	4	0	0
13	P	1	Total	C	O		
			19	15	4	0	0

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



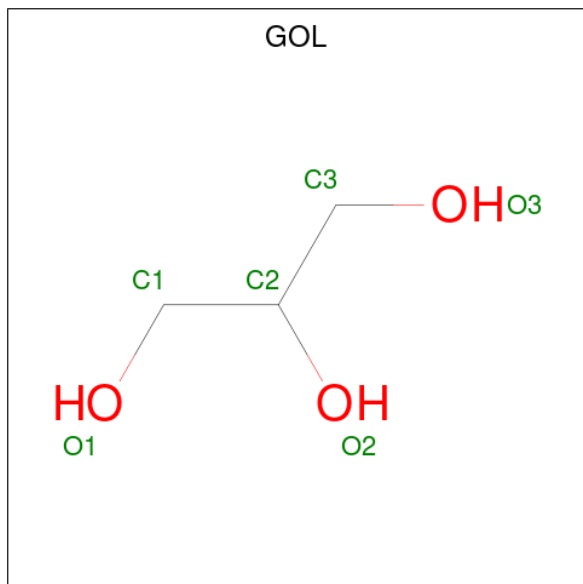
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			40	21	17	2		
14	D	1	Total	C	O	P	0	0
			42	23	17	2		
14	P	1	Total	C	O	P	0	0
			40	21	17	2		
14	Q	1	Total	C	O	P	0	0
			42	23	17	2		

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



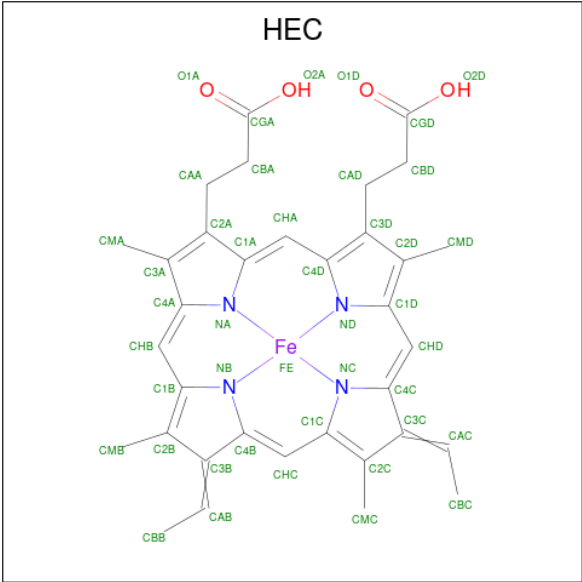
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	N	1	Total	O	P			0	0
			5	4	1				
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

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



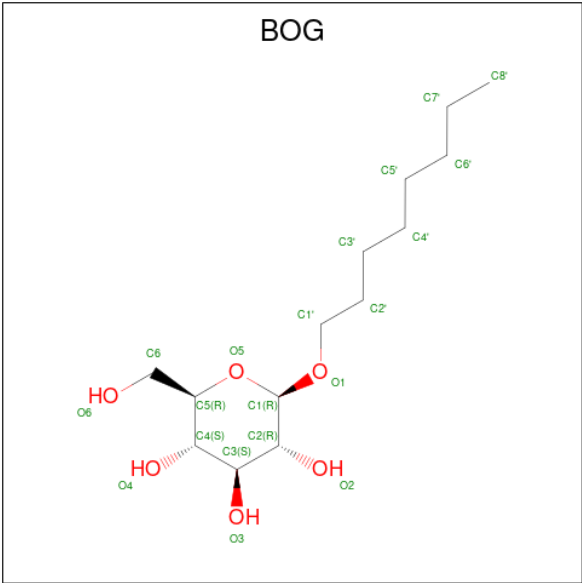
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

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



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).



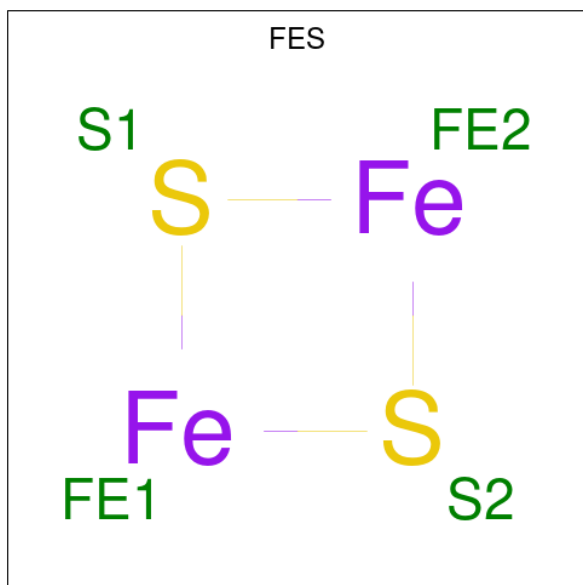
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	C	O	0	0
			20	14	6		
18	D	1	Total	C	O	0	0
			13	7	6		

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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (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		

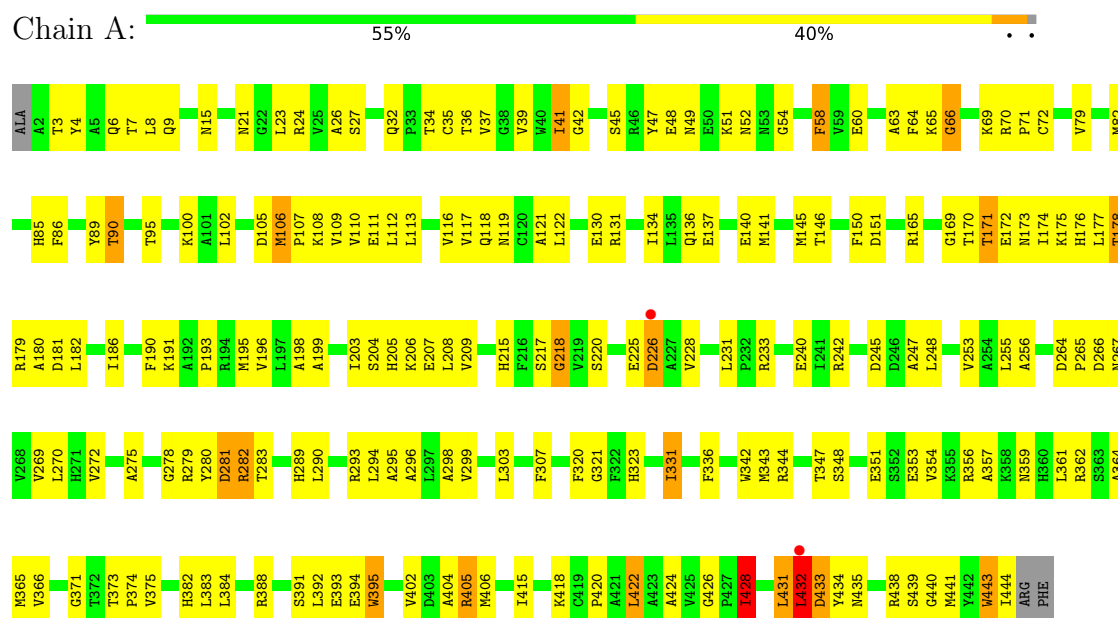
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	8	Total	O	0	0
			8	8		
20	E	1	Total	O	0	0
			1	1		
20	P	9	Total	O	0	0
			9	9		
20	R	1	Total	O	0	0
			1	1		

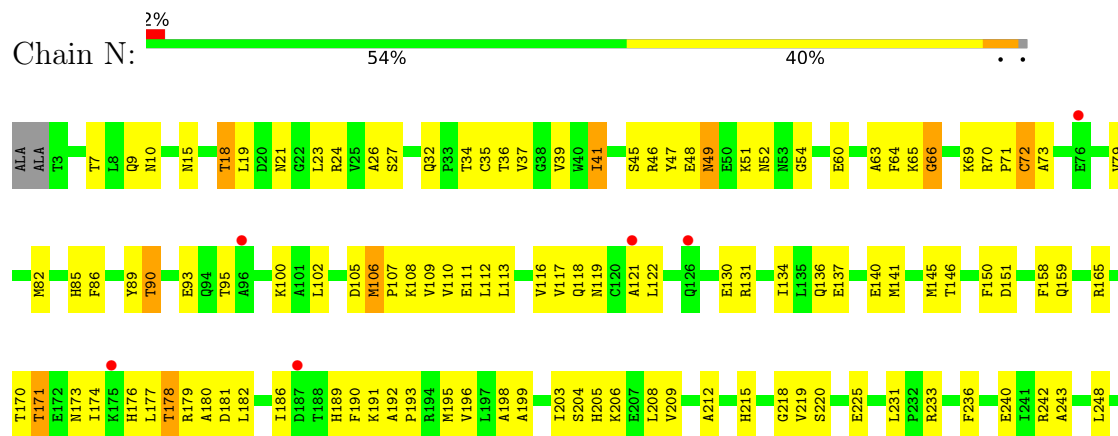
3 Residue-property plots [i](#)

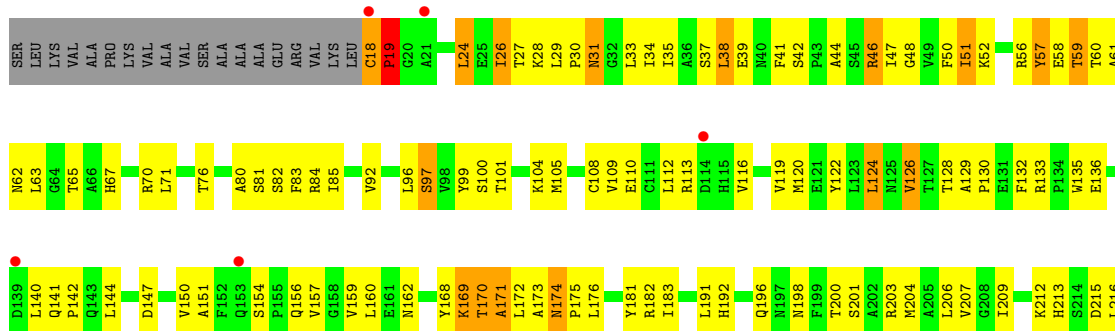
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

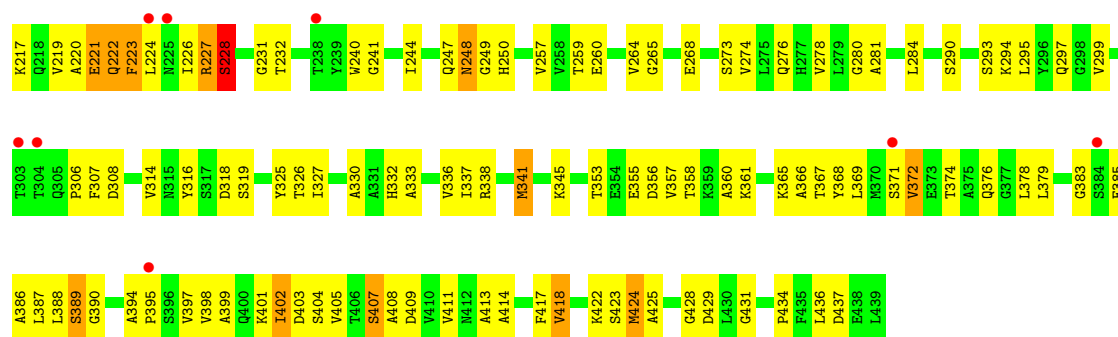
- Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL



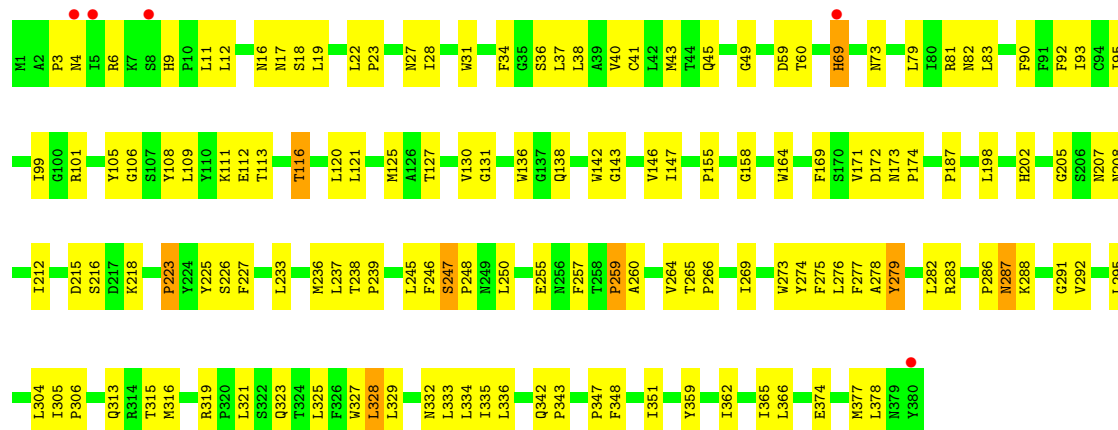
- Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL



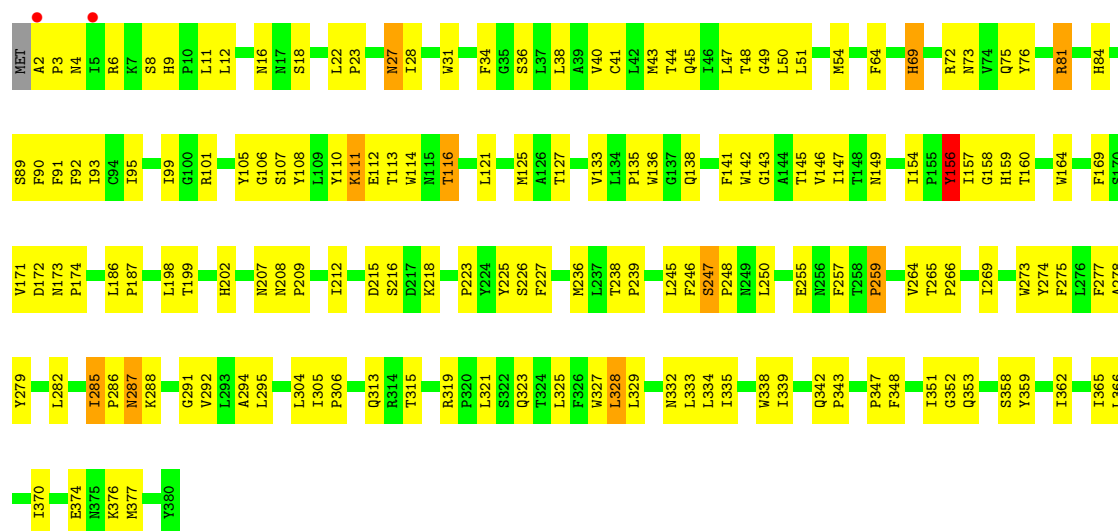




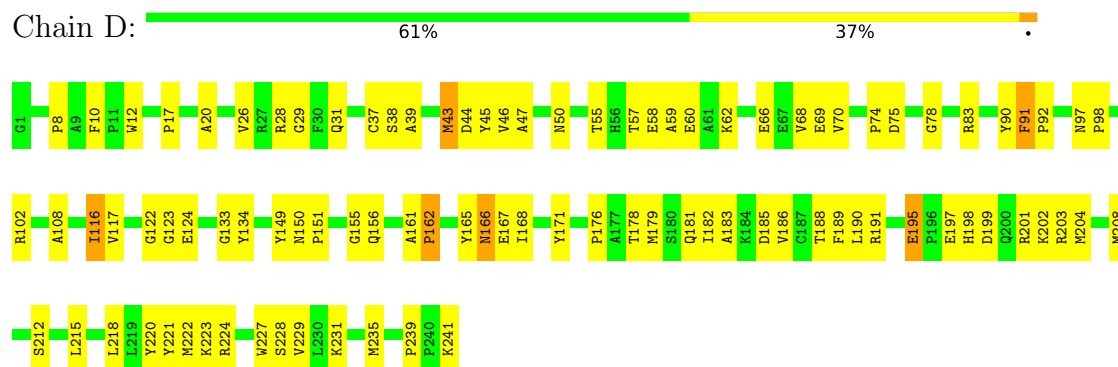
• Molecule 3: Cytochrome b



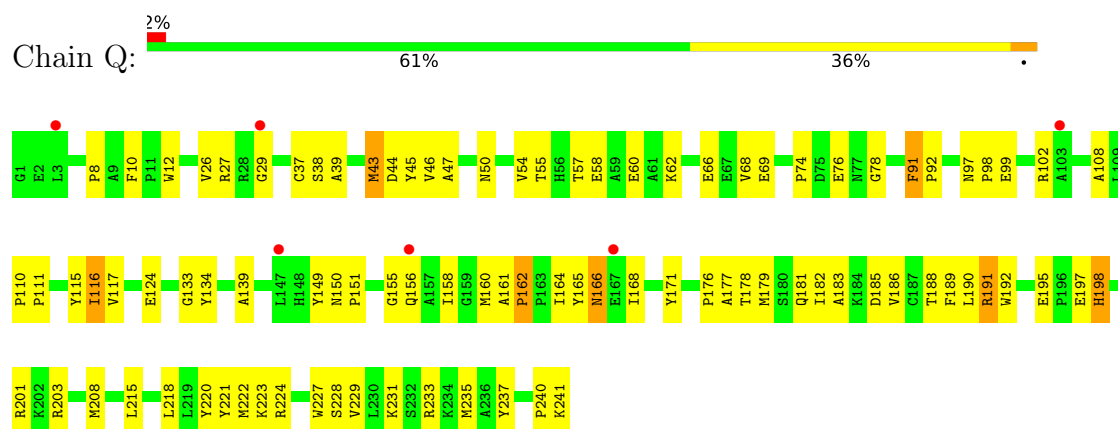
• Molecule 3: Cytochrome b



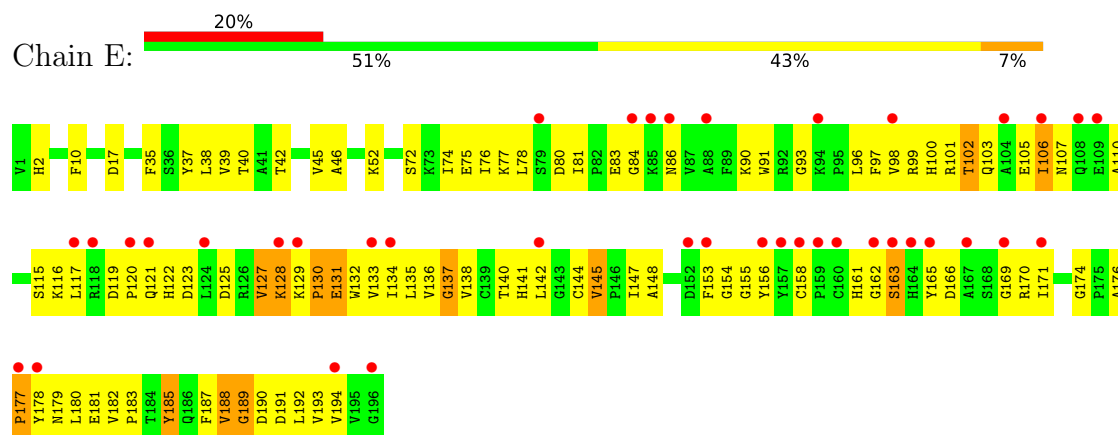
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



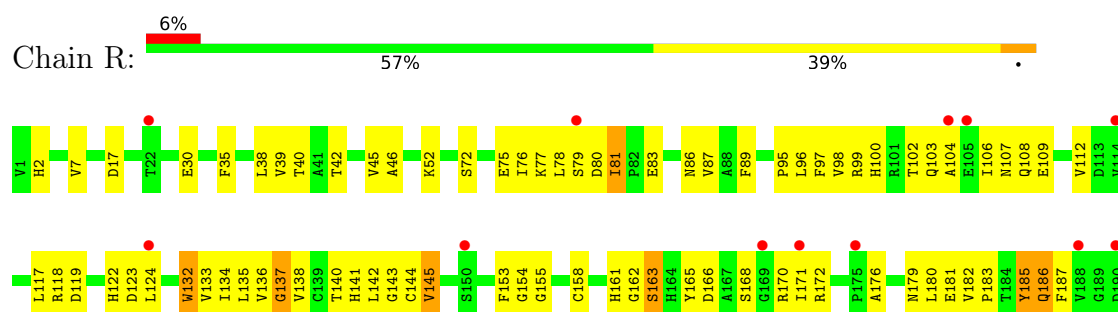
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



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

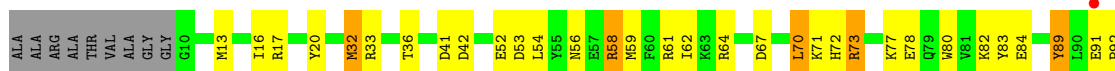


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial





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



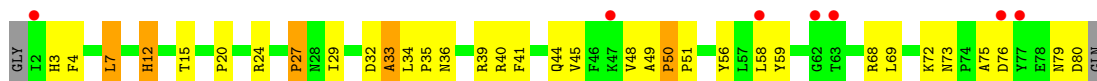
- Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN



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



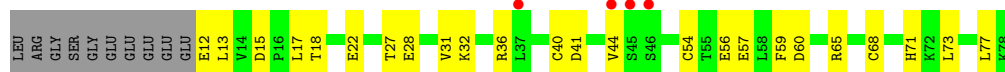
- Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



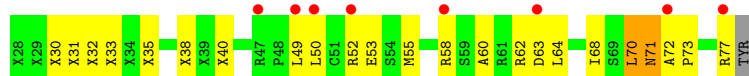
- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



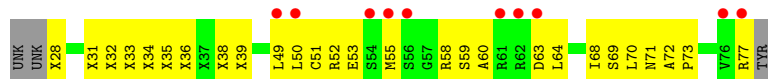
- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



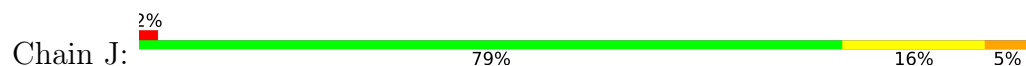
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



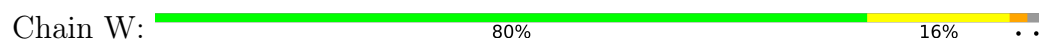
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.59Å 182.52Å 240.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.16 20.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-3.16) 96.7 (20.00-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.291 0.235 , 0.270	Depositor DCC
R_{free} test set	2453 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32608	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.59	0/3513	1.06	26/4760 (0.5%)
1	N	0.55	0/3508	1.04	25/4753 (0.5%)
2	B	0.50	0/3196	0.99	8/4334 (0.2%)
2	O	0.53	0/3202	1.02	13/4343 (0.3%)
3	C	0.69	1/3119 (0.0%)	1.06	17/4270 (0.4%)
3	P	0.61	1/3114 (0.0%)	1.03	14/4263 (0.3%)
4	D	0.61	0/1956	1.05	9/2658 (0.3%)
4	Q	0.48	0/1956	0.99	11/2658 (0.4%)
5	E	0.49	0/1547	0.95	4/2103 (0.2%)
5	R	0.47	0/1543	0.97	5/2098 (0.2%)
6	F	0.62	0/911	0.93	3/1219 (0.2%)
6	S	0.49	0/911	0.94	3/1219 (0.2%)
7	G	0.60	0/694	1.05	6/941 (0.6%)
7	T	0.49	0/684	1.02	3/929 (0.3%)
8	H	0.58	0/582	0.97	2/779 (0.3%)
8	U	0.44	0/561	0.89	0/751
9	I	0.67	0/218	1.14	2/293 (0.7%)
9	V	0.62	0/218	1.01	0/293
10	J	0.57	0/508	0.93	1/682 (0.1%)
10	W	0.51	0/490	0.89	1/660 (0.2%)
All	All	0.56	2/32431 (0.0%)	1.01	153/44006 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	43	MET	SD-CE	7.93	1.99	1.79
3	C	43	MET	SD-CE	5.17	1.92	1.79

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	227	ARG	N-CA-C	11.20	123.52	108.07
4	D	195	GLU	CA-C-N	9.33	129.54	119.28
4	D	195	GLU	C-N-CA	9.33	129.54	119.28
1	A	32	GLN	CA-C-N	8.82	128.55	119.56
1	A	32	GLN	C-N-CA	8.82	128.55	119.56
1	N	32	GLN	CA-C-N	8.72	128.46	119.56
1	N	32	GLN	C-N-CA	8.72	128.46	119.56
2	O	226	ILE	N-CA-C	-8.60	97.49	108.84
3	P	247	SER	CA-C-N	8.54	128.13	119.24
3	P	247	SER	C-N-CA	8.54	128.13	119.24
3	C	247	SER	CA-C-N	8.49	128.07	119.24
3	C	247	SER	C-N-CA	8.49	128.07	119.24
3	P	226	SER	N-CA-C	-7.59	102.95	111.07
1	A	248	LEU	CA-C-N	7.49	127.12	119.19
1	A	248	LEU	C-N-CA	7.49	127.12	119.19
3	P	365	ILE	N-CA-C	7.44	117.50	111.62
4	D	44	ASP	N-CA-C	7.42	121.25	111.75
4	Q	195	GLU	CA-C-N	7.29	128.95	119.84
4	Q	195	GLU	C-N-CA	7.29	128.95	119.84
2	B	174	ASN	CA-C-N	7.17	127.21	119.90
2	B	174	ASN	C-N-CA	7.17	127.21	119.90
3	P	328	LEU	N-CA-C	-7.16	103.09	111.03
6	F	89	TYR	N-CA-C	7.09	119.87	111.71
3	C	226	SER	N-CA-C	-7.08	103.50	111.07
1	N	426	GLY	CA-C-N	7.07	128.79	121.65
1	N	426	GLY	C-N-CA	7.07	128.79	121.65
2	B	326	THR	N-CA-C	6.95	119.73	108.34
4	Q	44	ASP	N-CA-C	6.91	120.60	111.75
2	O	174	ASN	CA-C-N	6.88	126.91	119.89
2	O	174	ASN	C-N-CA	6.88	126.91	119.89
1	A	426	GLY	CA-C-N	6.81	128.53	121.65
1	A	426	GLY	C-N-CA	6.81	128.53	121.65
1	A	119	ASN	N-CA-C	6.77	119.55	110.88
1	A	169	GLY	N-CA-C	6.76	118.94	112.04
1	A	440	GLY	N-CA-C	-6.72	104.70	115.66
3	P	257	PHE	N-CA-C	-6.57	104.84	112.92
1	A	32	GLN	N-CA-C	6.54	117.89	109.72
1	A	41	ILE	N-CA-C	6.52	118.43	108.71
2	O	326	THR	N-CA-C	6.51	119.08	108.26
3	C	365	ILE	N-CA-C	6.47	116.73	111.62
1	N	415	ILE	N-CA-C	6.46	117.12	111.56
3	C	328	LEU	N-CA-C	-6.44	103.95	110.97
3	C	279	TYR	N-CA-C	-6.44	104.26	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	415	ILE	CB-CA-C	-6.42	105.34	111.44
4	Q	116	ILE	N-CA-C	6.42	117.17	110.62
3	P	164	TRP	N-CA-C	-6.38	103.94	111.03
7	G	7	LEU	N-CA-C	6.37	118.10	111.03
1	A	233	ARG	N-CA-C	6.37	119.01	110.35
6	S	15	ARG	N-CA-C	-6.34	104.25	112.68
2	O	18	CYS	CA-C-N	6.30	127.72	119.84
2	O	18	CYS	C-N-CA	6.30	127.72	119.84
3	P	154	ILE	N-CA-C	-6.21	102.12	108.96
2	B	169	LYS	N-CA-C	-6.17	105.55	114.12
1	N	41	ILE	N-CA-C	6.10	118.16	108.89
3	C	27	ASN	N-CA-C	6.08	119.45	112.57
5	R	108	GLN	N-CA-C	-6.05	105.00	112.38
6	S	89	TYR	N-CA-C	6.05	118.67	111.71
2	B	230	ALA	N-CA-C	-6.04	106.88	114.56
1	A	415	ILE	N-CA-C	6.01	116.73	111.56
7	T	12	HIS	N-CA-C	6.00	119.96	111.92
1	N	32	GLN	N-CA-C	6.00	117.22	109.72
4	D	133	GLY	N-CA-C	5.99	127.39	113.18
3	C	265	THR	CA-C-N	-5.98	114.22	120.38
3	C	265	THR	C-N-CA	-5.98	114.22	120.38
3	P	116	THR	N-CA-C	-5.96	104.79	111.28
5	E	145	VAL	N-CA-C	5.93	114.41	107.77
5	R	17	ASP	N-CA-C	5.93	118.53	111.71
1	N	347	THR	N-CA-C	5.92	121.54	113.97
9	I	72	ALA	CA-C-N	5.91	126.83	119.98
9	I	72	ALA	C-N-CA	5.91	126.83	119.98
3	P	265	THR	CA-C-N	-5.90	114.30	120.38
3	P	265	THR	C-N-CA	-5.90	114.30	120.38
4	D	155	GLY	N-CA-C	-5.90	108.06	115.08
4	D	116	ILE	N-CA-C	5.89	116.63	110.62
1	N	248	LEU	CA-C-N	5.88	125.74	119.28
1	N	248	LEU	C-N-CA	5.88	125.74	119.28
1	A	428	ILE	N-CA-C	5.83	121.47	109.34
1	N	66	GLY	N-CA-C	5.82	119.52	112.48
3	C	116	THR	N-CA-C	-5.81	104.95	111.28
1	N	233	ARG	N-CA-C	5.79	118.17	110.53
1	A	66	GLY	N-CA-C	5.79	119.48	112.48
1	N	440	GLY	N-CA-C	-5.78	106.23	115.66
1	N	331	ILE	CB-CA-C	-5.76	104.59	111.97
4	D	91	PHE	CA-C-N	5.75	125.77	119.90
4	D	91	PHE	C-N-CA	5.75	125.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	76	ASP	N-CA-C	-5.74	106.62	113.97
1	A	348	SER	N-CA-C	5.72	118.70	109.83
4	Q	133	GLY	N-CA-C	5.70	126.69	113.18
2	O	126	VAL	N-CA-C	5.68	115.87	110.42
5	R	81	ILE	N-CA-C	5.66	113.66	107.60
3	P	27	ASN	N-CA-C	5.65	119.16	112.72
3	C	316	MET	N-CA-C	-5.61	105.64	112.88
1	N	348	SER	N-CA-C	5.57	118.46	109.83
3	C	90	PHE	N-CA-C	-5.56	105.22	111.28
6	S	14	ASP	N-CA-C	-5.53	106.48	113.18
1	N	431	LEU	CA-C-N	-5.52	112.82	121.87
1	N	431	LEU	C-N-CA	-5.52	112.82	121.87
1	A	178	THR	N-CA-C	5.51	118.54	109.72
4	Q	155	GLY	N-CA-C	-5.50	108.54	115.08
3	C	155	PRO	N-CA-C	5.47	119.67	111.14
1	A	431	LEU	CA-C-N	-5.46	112.91	121.87
1	A	431	LEU	C-N-CA	-5.46	112.91	121.87
5	E	17	ASP	N-CA-C	5.46	117.99	111.71
2	O	169	LYS	N-CA-C	-5.45	106.54	114.12
5	R	132	TRP	N-CA-C	5.44	117.28	108.41
8	H	52	GLU	N-CA-C	5.44	117.31	110.24
1	A	331	ILE	CB-CA-C	-5.44	105.01	111.97
7	T	7	LEU	N-CA-C	5.43	118.25	111.24
7	G	12	HIS	N-CA-C	5.43	119.20	111.92
4	Q	164	ILE	N-CA-C	5.43	116.30	108.48
4	Q	91	PHE	CA-C-N	5.40	125.41	119.90
4	Q	91	PHE	C-N-CA	5.40	125.41	119.90
1	A	58	PHE	N-CA-C	-5.37	105.43	111.28
2	O	228	SER	N-CA-C	5.36	122.21	110.80
5	R	143	GLY	N-CA-C	5.36	125.88	113.18
3	P	113	THR	N-CA-C	-5.35	105.35	111.07
1	N	178	THR	N-CA-C	5.35	117.95	109.50
3	C	164	TRP	N-CA-C	-5.34	105.11	111.03
6	F	41	ASP	N-CA-C	5.31	117.48	111.11
7	T	76	ASP	N-CA-C	-5.31	107.17	113.97
1	A	226	ASP	N-CA-C	5.30	119.31	112.41
1	N	301	HIS	N-CA-C	5.29	119.42	112.92
7	G	44	GLN	N-CA-C	5.28	120.20	113.55
3	P	285	ILE	N-CA-C	5.28	112.36	107.56
7	G	37	VAL	N-CA-C	-5.26	105.37	110.42
2	O	413	ALA	N-CA-C	-5.25	104.81	111.11
1	A	256	ALA	N-CA-C	5.24	117.03	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	53	LEU	N-CA-C	-5.21	105.51	111.14
1	N	119	ASN	N-CA-C	5.20	118.73	111.30
1	N	189	HIS	N-CA-C	5.18	119.60	113.12
10	W	14	PHE	N-CA-C	5.18	119.65	113.23
2	O	51	ILE	N-CA-C	5.17	117.19	108.81
4	Q	191	ARG	N-CA-C	-5.17	105.54	111.07
2	B	345	LYS	N-CA-C	-5.17	105.56	111.14
4	D	45	TYR	N-CA-C	5.16	119.56	113.16
3	C	257	PHE	N-CA-C	-5.16	106.30	112.59
5	E	106	ILE	N-CA-C	-5.14	106.55	112.98
3	C	205	GLY	N-CA-C	-5.13	105.22	112.81
6	F	99	ARG	N-CA-C	-5.12	105.59	111.07
2	O	407	SER	N-CA-C	-5.11	105.71	111.28
4	Q	45	TYR	N-CA-C	5.10	119.48	113.16
10	J	11	SER	N-CA-C	5.08	116.51	110.97
5	E	185	TYR	N-CA-C	5.08	114.94	108.24
1	N	416	TYR	N-CA-C	5.06	117.89	110.30
8	H	13	LEU	N-CA-C	5.06	116.94	107.99
1	A	278	GLY	N-CA-C	5.05	120.41	111.02
1	N	263	ALA	N-CA-C	5.04	117.43	111.33
1	N	256	ALA	N-CA-C	5.02	116.47	108.79
1	A	347	THR	N-CA-C	5.02	120.39	113.97
1	A	432	LEU	N-CA-C	5.02	116.44	108.96
2	B	51	ILE	N-CA-C	5.01	115.59	108.42
3	C	113	THR	N-CA-C	-5.01	105.71	111.07
2	B	61	ALA	N-CA-C	5.01	119.39	113.28

There are no chirality outliers.

There are no planarity outliers.

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	3442	0	3354	175	0
1	N	3437	0	3349	174	0
2	B	3141	0	3142	231	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	3147	0	3146	229	0
3	C	3017	0	3063	119	0
3	P	3012	0	3058	135	0
4	D	1898	0	1846	78	0
4	Q	1898	0	1846	84	0
5	E	1513	0	1478	98	0
5	R	1509	0	1474	94	0
6	F	891	0	893	28	0
6	S	891	0	893	36	0
7	G	672	0	653	31	0
7	T	662	0	645	34	0
8	H	574	0	548	20	0
8	U	553	0	535	26	0
9	I	287	0	250	41	0
9	V	278	0	253	39	0
10	J	497	0	490	10	0
10	W	479	0	478	9	0
11	A	3	0	0	0	0
11	C	2	0	0	0	0
11	N	3	0	0	0	0
11	P	1	0	0	0	0
12	C	86	0	60	6	0
12	P	86	0	60	8	0
13	C	19	0	17	5	0
13	P	19	0	17	2	0
14	C	40	0	24	2	0
14	D	42	0	28	2	0
14	P	40	0	24	2	0
14	Q	42	0	28	3	0
15	C	70	0	85	2	0
15	E	50	0	77	1	0
15	N	5	0	0	0	0
15	P	49	0	72	2	0
15	R	50	0	77	0	0
16	C	6	0	8	0	0
16	P	6	0	8	0	0
17	D	43	0	30	1	0
17	Q	43	0	30	0	0
18	D	33	0	39	0	0
18	P	12	0	11	1	0
18	Q	33	0	39	0	0
19	E	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	2	0
20	R	1	0	0	0	0
All	All	32608	0	32128	1537	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 24.

All (1537) 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	1.40	1.04
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.07	1.02
1:N:10:ASN:HD21	2:O:18:CYS:HB3	1.23	1.01
9:I:32:UNK:N	9:I:73:PRO:HG2	1.75	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.27	0.99
2:B:353:THR:HG22	2:B:355:GLU:H	1.27	0.98
2:O:353:THR:HG22	2:O:355:GLU:H	1.26	0.97
1:N:178:THR:HG22	1:N:180:ALA:H	1.26	0.97
9:I:33:UNK:HG2	9:I:73:PRO:CB	1.95	0.96
3:P:216:SER:HB3	6:S:59:MET:HE2	1.47	0.96
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.46	0.96
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.48	0.95
3:P:238:THR:HB	3:P:239:PRO:HD3	1.48	0.95
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.50	0.94
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.93
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.32	0.92
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.36	0.91
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.69	0.91
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.89
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.53	0.89
2:O:219:VAL:O	2:O:223:PHE:HB2	1.73	0.89
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.53	0.88
3:C:238:THR:HB	3:C:239:PRO:HD3	1.55	0.88
2:B:76:THR:HG22	2:B:82:SER:H	1.39	0.88
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.39	0.88
5:E:127:VAL:HG12	5:E:128:LYS:H	1.38	0.87
2:O:27:THR:HG22	2:O:28:LYS:H	1.37	0.86
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.57	0.86
2:O:76:THR:HG22	2:O:82:SER:H	1.39	0.86
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.55	0.85
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.55	0.85
2:B:24:LEU:HD12	2:B:37:SER:O	1.76	0.85
2:B:47:ILE:HD13	2:B:120:MET:CE	2.07	0.85
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.02	0.84
1:A:402:VAL:HA	1:A:406:MET:HE2	1.59	0.84
2:O:248:ASN:HD22	2:O:249:GLY:N	1.75	0.83
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.59	0.83
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.60	0.83
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.42	0.83
2:O:46:ARG:NH2	2:O:376:GLN:HG3	1.94	0.83
2:O:221:GLU:HG3	2:O:222:GLN:H	1.42	0.83
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.60	0.83
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.60	0.83
2:B:23:ASP:O	2:B:24:LEU:HB3	1.76	0.82
9:I:38:UNK:C	9:I:40:UNK:H	1.89	0.82
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.43	0.82
2:B:248:ASN:HD22	2:B:249:GLY:N	1.76	0.82
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.60	0.82
4:D:231:LYS:O	6:F:71:LYS:HE3	1.79	0.82
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.59	0.82
3:C:216:SER:HB3	6:F:59:MET:HE2	1.62	0.81
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.62	0.81
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.63	0.81
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.81	0.81
2:O:154:SER:O	2:O:157:VAL:HG12	1.81	0.80
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.64	0.80
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.64	0.79
1:N:402:VAL:HA	1:N:406:MET:HE2	1.64	0.79
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.61	0.79
2:O:27:THR:HG22	2:O:28:LYS:N	1.97	0.79
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.97	0.79
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.64	0.79
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.81	0.79
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.79
2:O:24:LEU:HD12	2:O:37:SER:O	1.83	0.78
2:O:47:ILE:HD13	2:O:120:MET:CE	2.13	0.78
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.66	0.78
5:E:101:ARG:HA	5:E:105:GLU:OE1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ASP:O	1:N:109:VAL:HG23	1.85	0.78
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.66	0.77
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.66	0.77
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.67	0.77
2:B:76:THR:CG2	2:B:82:SER:H	1.97	0.77
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.84	0.77
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.66	0.76
1:N:49:ASN:ND2	1:N:51:LYS:H	1.83	0.76
2:B:274:VAL:O	2:B:278:VAL:HG23	1.86	0.76
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.67	0.76
9:I:70:LEU:HD23	9:I:71:ASN:H	1.50	0.76
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.16	0.76
2:O:76:THR:CG2	2:O:82:SER:H	2.00	0.75
2:O:248:ASN:HD22	2:O:248:ASN:C	1.94	0.75
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.66	0.75
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.68	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.68	0.74
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.54	0.74
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.67	0.74
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.17	0.74
2:B:27:THR:HG22	2:B:28:LYS:N	2.02	0.74
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.50	0.74
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.54	0.74
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.69	0.74
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.74
2:B:27:THR:HG22	2:B:28:LYS:H	1.52	0.74
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.52	0.73
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.23	0.73
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.02	0.73
1:A:49:ASN:ND2	1:A:51:LYS:H	1.85	0.73
2:O:422:LYS:O	2:O:436:LEU:HD21	1.88	0.73
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.71	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.69	0.73
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.24	0.73
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.71	0.73
1:A:23:LEU:HD23	1:A:24:ARG:N	2.03	0.73
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.18	0.73
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.54	0.72
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.69	0.72
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:274:VAL:O	2:O:278:VAL:HG23	1.89	0.72
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.72	0.72
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.29	0.72
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.71	0.72
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.18	0.72
2:B:248:ASN:HD22	2:B:248:ASN:C	1.94	0.72
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.55	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.90	0.71
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.20	0.71
3:C:9:HIS:HD2	3:C:12:LEU:H	1.38	0.71
3:P:22:LEU:HD21	13:P:3002:UQ:HM32	1.70	0.71
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.70	0.71
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.23	0.71
7:G:29:ILE:O	7:G:33:ALA:HB3	1.91	0.71
1:A:140:GLU:OE2	9:I:50:LEU:N	2.19	0.71
3:C:236:MET:O	3:C:239:PRO:HD2	1.91	0.70
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.21	0.70
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.73	0.70
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.73	0.70
9:V:31:UNK:C	9:V:73:PRO:HG2	2.21	0.70
3:C:169:PHE:HE1	5:R:72:SER:HA	1.57	0.70
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.07	0.70
1:N:281:ASP:O	1:N:283:THR:N	2.24	0.70
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.71	0.70
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.26	0.70
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.26	0.70
1:A:130:GLU:O	1:A:134:ILE:HG13	1.91	0.70
2:B:341:MET:CE	2:B:417:PHE:HE2	2.05	0.69
3:P:9:HIS:HD2	3:P:12:LEU:H	1.40	0.69
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.74	0.69
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.74	0.69
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.73	0.69
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.22	0.69
1:A:281:ASP:O	1:A:283:THR:N	2.26	0.69
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.75	0.69
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.56	0.69
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.87	0.69
4:Q:222:MET:HE3	5:R:40:THR:OG1	1.93	0.69
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.56	0.69
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.75	0.69
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.56	0.68
2:B:399:ALA:O	2:B:402:ILE:HG22	1.94	0.68
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.29	0.68
1:N:112:LEU:O	1:N:116:VAL:HG23	1.94	0.68
7:T:29:ILE:O	7:T:33:ALA:HB3	1.93	0.68
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.19	0.68
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.75	0.68
2:B:31:ASN:HD22	2:B:31:ASN:N	1.90	0.67
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.76	0.67
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.74	0.67
1:A:178:THR:HB	1:A:181:ASP:OD1	1.94	0.67
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.26	0.67
1:N:130:GLU:O	1:N:134:ILE:HG13	1.94	0.67
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.74	0.67
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.56	0.67
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.76	0.67
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.57	0.67
8:U:18:THR:O	8:U:22:GLU:HG3	1.94	0.67
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.28	0.67
2:B:422:LYS:O	2:B:436:LEU:HD21	1.95	0.67
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.76	0.67
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.30	0.67
5:E:78:LEU:HD12	5:E:190:ASP:O	1.95	0.67
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.30	0.67
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.77	0.66
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.25	0.66
3:P:199:THR:HA	18:P:2010:BOG:O1	1.95	0.66
7:T:41:PHE:O	7:T:45:VAL:HG23	1.94	0.66
2:B:76:THR:HG22	2:B:81:SER:HA	1.78	0.66
3:C:286:PRO:O	3:C:287:ASN:HB2	1.94	0.66
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.29	0.66
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.26	0.66
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.11	0.66
5:R:102:THR:O	5:R:106:ILE:HG13	1.95	0.66
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.77	0.66
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.77	0.66
3:P:121:LEU:O	3:P:125:MET:HG3	1.96	0.66
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.76	0.65
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.76	0.65
6:F:13:MET:HA	6:F:13:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:27:THR:CG2	2:O:28:LYS:H	2.08	0.65
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.31	0.65
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.32	0.65
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.03	0.65
10:W:49:GLY:N	10:W:54:HIS:ND1	2.45	0.65
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.11	0.65
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.96	0.65
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.31	0.65
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.24	0.65
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.78	0.65
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.26	0.65
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.31	0.65
1:N:23:LEU:HD23	1:N:24:ARG:N	2.11	0.65
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.61	0.65
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.79	0.64
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.79	0.64
1:N:382:HIS:HB3	1:N:388:ARG:O	1.97	0.64
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.62	0.64
3:P:216:SER:CB	6:S:59:MET:HE2	2.27	0.64
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.32	0.64
5:R:136:VAL:HG21	5:R:181:GLU:OE1	1.97	0.64
5:E:101:ARG:HG2	5:E:105:GLU:OE2	1.98	0.64
2:O:273:SER:O	2:O:276:GLN:HB3	1.98	0.64
2:O:402:ILE:C	2:O:402:ILE:HD13	2.23	0.64
1:N:402:VAL:HG22	1:N:406:MET:CE	2.28	0.64
3:P:207:ASN:ND2	3:P:208:ASN:H	1.96	0.64
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.63	0.64
10:J:49:GLY:N	10:J:54:HIS:ND1	2.46	0.64
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.33	0.64
5:R:186:GLN:O	5:R:193:VAL:HG23	1.98	0.64
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.16	0.63
1:A:105:ASP:O	1:A:109:VAL:HG23	1.97	0.63
2:B:264:VAL:HG23	2:B:316:TYR:C	2.23	0.63
3:C:278:ALA:HB1	3:C:295:LEU:HD12	1.78	0.63
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.80	0.63
4:D:57:THR:HB	4:D:60:GLU:HG3	1.81	0.63
2:O:399:ALA:O	2:O:402:ILE:HG22	1.97	0.63
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.63	0.63
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.24	0.63
3:P:105:TYR:HA	3:P:315:THR:HG22	1.80	0.63
1:A:36:THR:HG21	1:A:373:THR:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.81	0.63
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.81	0.63
3:P:138:GLN:HA	3:P:138:GLN:OE1	1.99	0.63
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.35	0.62
2:O:76:THR:HG22	2:O:81:SER:HA	1.82	0.62
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.82	0.62
5:R:118:ARG:NH1	5:R:118:ARG:HB2	2.15	0.62
7:G:41:PHE:O	7:G:45:VAL:HG23	1.98	0.62
2:B:122:TYR:O	2:B:126:VAL:HG23	2.00	0.62
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.62
3:C:105:TYR:HA	3:C:315:THR:HG22	1.80	0.62
5:E:190:ASP:C	5:E:192:LEU:H	2.07	0.62
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.27	0.62
1:A:240:GLU:OE1	1:A:434:TYR:HB2	1.99	0.62
2:B:76:THR:HG22	2:B:82:SER:N	2.12	0.62
2:B:402:ILE:HD13	2:B:402:ILE:C	2.24	0.62
1:N:165:ARG:HH11	1:N:165:ARG:HG3	1.65	0.62
1:A:112:LEU:O	1:A:116:VAL:HG23	2.00	0.62
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.35	0.62
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.82	0.62
8:H:18:THR:O	8:H:22:GLU:HG3	1.99	0.61
2:O:361:LYS:O	2:O:365:LYS:HG3	1.99	0.61
1:A:371:GLY:O	1:A:375:VAL:HG23	2.00	0.61
2:B:38:LEU:C	2:B:38:LEU:HD12	2.24	0.61
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.30	0.61
4:D:62:LYS:O	4:D:66:GLU:HG3	2.00	0.61
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.82	0.61
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.35	0.61
2:O:341:MET:CE	2:O:417:PHE:HE2	2.11	0.61
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.81	0.61
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.80	0.61
8:H:12:GLU:HG2	8:H:13:LEU:N	2.15	0.61
1:N:371:GLY:O	1:N:375:VAL:HG23	2.00	0.61
5:E:72:SER:HA	3:P:169:PHE:HE1	1.64	0.61
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.81	0.61
2:O:353:THR:HB	2:O:356:ASP:OD1	2.00	0.61
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.83	0.61
5:E:137:GLY:O	5:E:145:VAL:HG13	2.00	0.61
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.82	0.61
1:N:359:ASN:HD22	2:O:92:VAL:HA	1.65	0.61
6:S:13:MET:O	6:S:17:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:HIS:O	2:B:336:VAL:HG23	2.01	0.61
9:I:31:UNK:C	9:I:73:PRO:HG2	2.30	0.61
3:P:236:MET:O	3:P:239:PRO:HD2	2.01	0.61
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.01	0.61
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.36	0.60
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.01	0.60
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.60
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.65	0.60
8:U:12:GLU:HG2	8:U:13:LEU:H	1.66	0.60
1:A:281:ASP:OD1	9:I:33:UNK:HB2	2.02	0.60
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.30	0.60
3:C:125:MET:HE2	3:C:275:PHE:CE2	2.36	0.60
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.83	0.60
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.83	0.60
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.01	0.60
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.34	0.60
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.83	0.60
2:O:46:ARG:HH22	2:O:376:GLN:HG3	1.67	0.60
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.84	0.60
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.37	0.60
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.66	0.60
2:B:333:ALA:O	2:B:337:ILE:HG13	2.01	0.60
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.33	0.60
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.36	0.60
1:A:178:THR:HG22	1:A:180:ALA:N	2.09	0.60
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.36	0.60
4:D:171:TYR:OH	4:D:182:ILE:HA	2.01	0.60
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.60
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.60
1:N:63:ALA:O	1:N:116:VAL:HG13	2.02	0.60
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.20	0.60
2:B:31:ASN:H	2:B:31:ASN:ND2	2.00	0.60
1:A:106:MET:HE2	1:A:106:MET:C	2.26	0.60
1:A:402:VAL:HG22	1:A:406:MET:CE	2.31	0.59
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.37	0.59
1:N:131:ARG:NH2	1:N:177:LEU:O	2.35	0.59
1:A:280:TYR:CG	1:A:281:ASP:N	2.70	0.59
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.84	0.59
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.00	0.59
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.32	0.59
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:286:PRO:O	3:P:287:ASN:HB2	2.02	0.59
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.82	0.59
2:B:223:PHE:O	2:B:225:ASN:HB2	2.03	0.59
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.32	0.59
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.85	0.59
2:O:76:THR:HG22	2:O:82:SER:N	2.12	0.59
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.59
2:B:294:LYS:HE3	2:B:356:ASP:OD2	2.03	0.59
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.83	0.59
1:N:15:ASN:O	1:N:26:ALA:HA	2.02	0.59
2:O:372:VAL:HG12	2:O:372:VAL:O	2.01	0.59
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.02	0.59
4:Q:161:ALA:O	4:Q:162:PRO:C	2.45	0.59
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.83	0.59
1:N:255:LEU:HD12	1:N:422:LEU:HB2	1.84	0.59
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.33	0.59
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.84	0.59
3:C:143:GLY:O	3:C:147:ILE:HG12	2.02	0.59
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.67	0.59
1:N:106:MET:C	1:N:106:MET:HE2	2.27	0.59
1:A:191:LYS:CA	1:A:195:MET:HE2	2.33	0.59
2:O:294:LYS:HE3	2:O:356:ASP:OD2	2.02	0.59
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.16	0.59
1:N:170:THR:HG22	1:N:171:THR:N	2.18	0.58
2:O:333:ALA:O	2:O:337:ILE:HG13	2.03	0.58
2:O:345:LYS:HG2	2:O:418:VAL:HG13	1.85	0.58
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.02	0.58
2:B:100:SER:HB2	2:B:105:MET:HG2	1.85	0.58
3:C:9:HIS:CD2	3:C:12:LEU:H	2.20	0.58
3:C:279:TYR:CE2	3:C:283:ARG:HD3	2.39	0.58
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.16	0.58
3:P:101:ARG:C	3:P:101:ARG:HD2	2.28	0.58
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.68	0.58
2:B:361:LYS:O	2:B:365:LYS:HG3	2.02	0.58
1:N:136:GLN:OE1	9:V:50:LEU:HD13	2.03	0.58
2:B:96:LEU:HD12	2:B:97:SER:N	2.19	0.58
5:E:136:VAL:O	5:E:138:VAL:N	2.31	0.58
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.85	0.58
5:E:141:HIS:O	5:E:142:LEU:HD23	2.04	0.58
1:N:36:THR:HG21	1:N:373:THR:HA	1.85	0.58
1:N:269:VAL:CG2	1:N:406:MET:HE3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:HIS:HB3	1:A:388:ARG:O	2.03	0.58
2:B:372:VAL:HG12	2:B:372:VAL:O	2.03	0.58
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.86	0.58
1:A:269:VAL:CG2	1:A:406:MET:HE3	2.34	0.58
3:C:45:GLN:CB	12:C:501:HEM:HAB	2.34	0.58
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.86	0.58
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.37	0.58
9:V:33:UNK:HA	9:V:73:PRO:HG3	1.86	0.58
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.86	0.58
2:O:99:TYR:HE1	2:O:108:CYS:SG	2.27	0.58
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.85	0.58
2:O:248:ASN:ND2	2:O:250:HIS:H	2.01	0.58
5:E:127:VAL:HG12	5:E:128:LYS:N	2.15	0.58
4:Q:139:ALA:HB2	8:U:41:ASP:HA	1.86	0.58
3:C:34:PHE:HB2	20:C:381:HOH:O	2.04	0.58
2:O:27:THR:CG2	2:O:28:LYS:N	2.67	0.58
2:O:52:LYS:O	2:O:203:ARG:NH2	2.37	0.58
5:E:84:GLY:N	5:E:102:THR:HG23	2.19	0.57
3:P:9:HIS:CD2	3:P:12:LEU:H	2.22	0.57
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.86	0.57
1:N:106:MET:O	1:N:110:VAL:HG23	2.04	0.57
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.39	0.57
2:O:100:SER:CB	2:O:105:MET:HG2	2.34	0.57
2:O:332:HIS:O	2:O:336:VAL:HG23	2.03	0.57
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.39	0.57
1:A:137:GLU:O	1:A:141:MET:HG3	2.04	0.57
2:B:31:ASN:HD22	2:B:31:ASN:H	1.52	0.57
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.85	0.57
2:B:290:SER:O	2:B:297:GLN:HG2	2.04	0.57
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.86	0.57
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.18	0.57
2:O:338:ARG:HG3	2:O:338:ARG:NH1	2.19	0.57
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.86	0.57
2:O:140:LEU:C	2:O:142:PRO:HD2	2.28	0.57
1:A:402:VAL:HA	1:A:406:MET:CE	2.32	0.57
2:B:353:THR:HB	2:B:356:ASP:OD1	2.04	0.57
1:N:90:THR:HB	1:N:95:THR:HG23	1.86	0.57
2:O:147:ASP:OD1	9:V:68:ILE:HD11	2.05	0.57
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.39	0.57
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.53	0.57
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.04	0.57
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.86	0.57
2:O:47:ILE:HG22	2:O:48:GLY:N	2.19	0.57
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.87	0.57
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.87	0.57
3:P:49:GLY:C	12:P:501:HEM:HAC	2.30	0.57
2:B:27:THR:CG2	2:B:28:LYS:H	2.18	0.57
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.87	0.57
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.35	0.57
5:E:147:ILE:O	5:E:156:TYR:HA	2.05	0.57
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.20	0.57
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.87	0.57
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.69	0.57
4:D:161:ALA:O	4:D:162:PRO:C	2.48	0.56
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.34	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.05	0.56
2:B:46:ARG:HG3	2:B:379:LEU:HD22	1.87	0.56
2:B:140:LEU:C	2:B:142:PRO:HD2	2.30	0.56
3:P:215:ASP:HA	3:P:218:LYS:HE2	1.87	0.56
12:P:502:HEM:HBD1	20:P:386:HOH:O	2.04	0.56
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.21	0.56
2:B:35:ILE:O	2:B:213:HIS:HE1	1.87	0.56
3:C:101:ARG:HD2	3:C:101:ARG:C	2.30	0.56
6:F:32:MET:O	6:F:33:ARG:C	2.49	0.56
1:N:182:LEU:O	1:N:186:ILE:HG13	2.05	0.56
2:O:306:PRO:HB3	9:V:52:ARG:N	2.21	0.56
3:P:238:THR:HB	3:P:239:PRO:CD	2.30	0.56
2:B:248:ASN:ND2	2:B:250:HIS:H	2.03	0.56
1:A:307:PHE:CD1	1:A:307:PHE:C	2.83	0.56
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.05	0.56
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.34	0.56
1:N:240:GLU:OE1	1:N:434:TYR:HB2	2.04	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.56
5:R:122:HIS:CD2	5:R:123:ASP:H	2.24	0.56
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.86	0.56
4:Q:139:ALA:CB	8:U:41:ASP:HA	2.35	0.56
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.86	0.56
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.40	0.56
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.88	0.56
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.36	0.56
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.88	0.56
3:C:37:LEU:O	3:C:41:CYS:HB2	2.05	0.56
3:C:245:LEU:O	4:D:201:ARG:HD3	2.06	0.56
3:P:142:TRP:O	3:P:146:VAL:HG23	2.05	0.56
1:A:106:MET:HE2	1:A:107:PRO:HA	1.86	0.56
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.87	0.56
2:B:385:GLU:O	2:B:387:LEU:N	2.39	0.56
5:E:52:LYS:C	5:E:52:LYS:HD3	2.30	0.56
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.88	0.56
2:O:38:LEU:HD12	2:O:38:LEU:C	2.31	0.56
2:O:156:GLN:HE22	9:V:77:ARG:C	2.14	0.56
2:O:338:ARG:O	2:O:341:MET:HB2	2.06	0.56
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.36	0.56
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.41	0.56
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.06	0.56
2:B:100:SER:CB	2:B:105:MET:HG2	2.36	0.56
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.88	0.56
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.28	0.56
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.53	0.56
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.20	0.55
13:C:2002:UQ:HM51	13:C:2002:UQ:H8	1.88	0.55
2:O:192:HIS:O	2:O:196:GLN:HG3	2.06	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.41	0.55
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.41	0.55
1:A:15:ASN:O	1:A:26:ALA:HA	2.04	0.55
3:C:286:PRO:O	3:C:287:ASN:CB	2.55	0.55
2:O:403:ASP:O	2:O:405:VAL:N	2.38	0.55
8:U:65:ARG:O	8:U:68:CYS:HB3	2.06	0.55
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.87	0.55
3:C:9:HIS:CD2	3:C:11:LEU:H	2.24	0.55
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.24	0.55
3:C:246:PHE:C	3:C:248:PRO:HD3	2.31	0.55
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.55
3:C:377:MET:HE2	6:F:20:TYR:CG	2.41	0.55
2:B:27:THR:CG2	2:B:28:LYS:N	2.70	0.55
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.87	0.55
1:N:362:ARG:O	1:N:365:MET:HG2	2.07	0.55
2:B:345:LYS:HG2	2:B:418:VAL:CG1	2.36	0.55
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.32	0.55
1:N:140:GLU:OE2	9:V:50:LEU:N	2.37	0.55
1:A:90:THR:HB	1:A:95:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.89	0.55
5:R:162:GLY:O	5:R:163:SER:C	2.50	0.55
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.21	0.55
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.37	0.55
5:E:76:ILE:O	5:E:193:VAL:HG12	2.07	0.55
5:E:130:PRO:C	5:E:132:TRP:H	2.14	0.55
3:P:138:GLN:HB2	3:P:255:GLU:O	2.06	0.55
3:P:245:LEU:O	4:Q:201:ARG:CD	2.55	0.55
9:V:34:UNK:N	9:V:35:UNK:N	2.54	0.55
2:B:52:LYS:O	2:B:203:ARG:NH2	2.40	0.55
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.88	0.55
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.35	0.55
3:P:34:PHE:HB2	20:P:381:HOH:O	2.06	0.55
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.71	0.55
4:Q:218:LEU:HD11	5:R:42:THR:CG2	2.37	0.55
1:N:373:THR:N	1:N:374:PRO:HD2	2.22	0.54
2:O:57:TYR:CD1	2:O:57:TYR:N	2.74	0.54
2:O:290:SER:O	2:O:297:GLN:HG2	2.07	0.54
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.35	0.54
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.88	0.54
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.89	0.54
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.89	0.54
4:Q:220:TYR:CZ	4:Q:224:ARG:HD3	2.42	0.54
9:V:69:SER:HB2	9:V:72:ALA:HB3	1.89	0.54
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.43	0.54
2:B:47:ILE:HG22	2:B:48:GLY:N	2.23	0.54
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.72	0.54
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.72	0.54
1:A:170:THR:HG22	1:A:171:THR:N	2.23	0.54
3:P:9:HIS:CD2	3:P:11:LEU:H	2.25	0.54
3:P:112:GLU:O	3:P:116:THR:HG23	2.08	0.54
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.07	0.54
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.42	0.54
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.34	0.54
3:C:22:LEU:HD21	13:C:2002:UQ:HM32	1.89	0.54
3:C:169:PHE:CE1	5:R:72:SER:HA	2.39	0.54
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.89	0.54
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.90	0.54
3:C:245:LEU:O	4:D:201:ARG:CD	2.55	0.54
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.48	0.54
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:100:SER:HB2	2:O:105:MET:HG2	1.90	0.54
2:O:385:GLU:O	2:O:387:LEU:N	2.41	0.54
3:P:173:ASN:N	3:P:174:PRO:HD2	2.22	0.54
5:R:52:LYS:HD3	5:R:52:LYS:C	2.33	0.54
3:C:207:ASN:ND2	3:C:208:ASN:H	2.05	0.54
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.42	0.54
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.42	0.54
1:N:106:MET:HE2	1:N:107:PRO:HA	1.90	0.54
1:N:295:ALA:O	1:N:298:ALA:HB3	2.07	0.54
2:O:407:SER:O	2:O:411:VAL:HG23	2.08	0.54
3:C:142:TRP:O	3:C:146:VAL:HG23	2.07	0.54
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.54
4:Q:227:TRP:O	4:Q:228:SER:C	2.51	0.54
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.54
1:A:131:ARG:NH2	1:A:177:LEU:O	2.41	0.54
1:A:255:LEU:HD12	1:A:422:LEU:HB2	1.90	0.54
1:N:402:VAL:HA	1:N:406:MET:CE	2.35	0.54
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.26	0.54
3:P:329:LEU:O	3:P:332:ASN:HB3	2.08	0.54
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.91	0.54
8:U:73:LEU:HD12	8:U:73:LEU:O	2.08	0.54
2:B:57:TYR:HE2	2:B:203:ARG:HH22	1.45	0.54
2:B:402:ILE:HG23	2:B:403:ASP:N	2.23	0.54
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.43	0.54
1:N:209:VAL:O	1:N:212:ALA:HB3	2.08	0.54
5:R:76:ILE:O	5:R:193:VAL:HG12	2.08	0.54
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.91	0.54
1:A:23:LEU:HD23	1:A:23:LEU:C	2.33	0.53
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.43	0.53
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.38	0.53
2:B:248:ASN:C	2:B:248:ASN:ND2	2.64	0.53
2:B:318:ASP:O	2:B:319:SER:HB2	2.08	0.53
6:F:13:MET:HE2	6:F:16:ILE:HD12	1.89	0.53
1:N:178:THR:HG22	1:N:180:ALA:N	2.09	0.53
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.90	0.53
6:S:91:GLU:HB3	6:S:92:PRO:HD3	1.91	0.53
3:C:49:GLY:C	12:C:501:HEM:HAC	2.33	0.53
4:D:47:ALA:H	4:D:50:ASN:ND2	1.96	0.53
5:E:116:LYS:HD2	5:E:116:LYS:N	2.23	0.53
2:O:46:ARG:HG3	2:O:379:LEU:HD22	1.90	0.53
2:O:57:TYR:HE2	2:O:203:ARG:HH22	1.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:O	1:A:186:ILE:HG13	2.07	0.53
1:A:191:LYS:N	1:A:195:MET:HE2	2.22	0.53
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.43	0.53
1:N:307:PHE:CD1	1:N:307:PHE:C	2.85	0.53
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.23	0.53
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.90	0.53
2:B:96:LEU:H	9:I:70:LEU:HD22	1.74	0.53
2:B:345:LYS:HG2	2:B:418:VAL:HG13	1.91	0.53
4:D:37:CYS:C	4:D:39:ALA:H	2.16	0.53
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.34	0.53
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.43	0.53
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.44	0.53
9:V:69:SER:CB	9:V:72:ALA:HB3	2.39	0.53
1:A:136:GLN:OE1	9:I:50:LEU:HD12	2.08	0.53
2:B:28:LYS:O	2:B:29:LEU:O	2.27	0.53
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.22	0.53
5:E:117:LEU:HD23	5:E:121:GLN:H	1.73	0.53
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.53
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.24	0.53
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.39	0.53
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.74	0.53
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.91	0.53
3:P:246:PHE:C	3:P:248:PRO:HD3	2.33	0.53
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.90	0.53
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.16	0.53
2:B:99:TYR:HE1	2:B:108:CYS:SG	2.32	0.53
2:B:268:GLU:O	2:B:271:ALA:HB3	2.09	0.53
3:C:92:PHE:O	3:C:95:ILE:HG22	2.08	0.53
1:N:191:LYS:C	1:N:193:PRO:HD2	2.34	0.53
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.24	0.53
3:P:143:GLY:O	3:P:147:ILE:HG12	2.09	0.53
3:P:156:TYR:CD2	3:P:156:TYR:N	2.75	0.53
5:E:102:THR:C	5:E:103:GLN:HG3	2.34	0.53
6:F:94:LEU:HD12	6:F:94:LEU:O	2.08	0.53
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.74	0.52
2:B:357:VAL:O	2:B:361:LYS:HG3	2.09	0.52
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.10	0.52
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.52
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.44	0.52
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.39	0.52
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:LEU:O	3:C:125:MET:HG3	2.08	0.52
5:R:136:VAL:O	5:R:138:VAL:N	2.38	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.76	0.52
5:E:117:LEU:HD23	5:E:119:ASP:O	2.10	0.52
2:O:248:ASN:C	2:O:248:ASN:ND2	2.64	0.52
3:P:92:PHE:O	3:P:95:ILE:HG22	2.08	0.52
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.91	0.52
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.28	0.52
2:B:385:GLU:C	2:B:387:LEU:H	2.17	0.52
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.92	0.52
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.92	0.52
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.39	0.52
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.74	0.52
3:P:347:PRO:O	3:P:351:ILE:HG13	2.09	0.52
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.92	0.52
3:C:99:ILE:HD11	3:C:121:LEU:HD22	1.91	0.52
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.44	0.52
2:O:67:HIS:O	2:O:70:ARG:HB3	2.10	0.52
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.45	0.52
3:P:278:ALA:HB1	3:P:295:LEU:HD12	1.91	0.52
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.43	0.52
1:A:359:ASN:HD22	2:B:92:VAL:HA	1.74	0.52
3:C:215:ASP:HA	3:C:218:LYS:HE2	1.90	0.52
4:D:68:VAL:HG12	4:D:69:GLU:N	2.24	0.52
1:N:23:LEU:HD23	1:N:23:LEU:C	2.35	0.52
1:N:39:VAL:HA	1:N:196:VAL:O	2.10	0.52
2:B:170:THR:O	2:B:172:LEU:N	2.43	0.52
7:G:36:ASN:O	7:G:40:ARG:HG3	2.10	0.52
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.45	0.52
3:P:202:HIS:NE2	13:P:3002:UQ:O4	2.38	0.52
1:A:362:ARG:O	1:A:365:MET:HG2	2.09	0.52
2:B:31:ASN:N	2:B:31:ASN:ND2	2.53	0.52
2:B:57:TYR:N	2:B:57:TYR:CD1	2.77	0.52
4:D:122:GLY:O	4:D:123:GLY:C	2.53	0.52
1:N:137:GLU:O	1:N:141:MET:HG3	2.09	0.52
4:Q:12:TRP:CZ2	4:Q:124:GLU:HB2	2.44	0.52
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.92	0.52
3:C:92:PHE:O	3:C:93:ILE:C	2.50	0.52
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.92	0.52
4:D:37:CYS:C	4:D:39:ALA:N	2.67	0.52
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:92:PHE:O	3:P:93:ILE:C	2.52	0.52
4:Q:43:MET:HE2	4:Q:91:PHE:HE2	1.75	0.52
2:B:338:ARG:O	2:B:341:MET:HB2	2.10	0.51
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.10	0.51
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.92	0.51
2:O:341:MET:CE	2:O:341:MET:HA	2.40	0.51
1:A:404:ALA:O	1:A:406:MET:N	2.43	0.51
3:P:282:LEU:HD12	3:P:291:GLY:O	2.10	0.51
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.91	0.51
8:U:40:CYS:O	8:U:44:VAL:HG23	2.10	0.51
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.39	0.51
1:A:269:VAL:HG22	1:A:406:MET:HE3	1.90	0.51
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.51
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.51
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.93	0.51
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.25	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
4:D:227:TRP:O	4:D:228:SER:C	2.51	0.51
2:B:22:GLU:HG3	2:B:23:ASP:H	1.74	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.43	0.51
2:O:414:ALA:O	2:O:418:VAL:HG23	2.11	0.51
3:P:377:MET:HE2	6:S:20:TYR:CG	2.46	0.51
4:D:102:ARG:HA	4:D:108:ALA:O	2.10	0.51
4:D:167:GLU:HG3	8:H:13:LEU:HD23	1.91	0.51
5:E:162:GLY:O	5:E:163:SER:C	2.53	0.51
8:H:65:ARG:O	8:H:68:CYS:HB3	2.10	0.51
2:O:170:THR:O	2:O:172:LEU:N	2.43	0.51
2:O:318:ASP:O	2:O:319:SER:HB2	2.11	0.51
2:B:38:LEU:HD12	2:B:39:GLU:N	2.26	0.51
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.75	0.51
2:B:307:PHE:CD1	2:B:308:ASP:N	2.79	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.11	0.51
3:C:173:ASN:N	3:C:174:PRO:HD2	2.26	0.51
1:N:10:ASN:ND2	2:O:19:PRO:HD2	2.26	0.51
1:N:178:THR:CG2	1:N:179:ARG:N	2.73	0.51
2:O:46:ARG:HG3	2:O:46:ARG:O	2.10	0.51
2:O:424:MET:HG2	2:O:425:ALA:N	2.24	0.51
5:R:179:ASN:O	5:R:180:LEU:C	2.54	0.51
1:A:106:MET:HE2	1:A:107:PRO:CA	2.39	0.51
8:H:40:CYS:O	8:H:44:VAL:HG23	2.10	0.51
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.93	0.51
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.40	0.51
1:N:295:ALA:O	1:N:299:VAL:HG23	2.10	0.51
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.42	0.51
3:P:31:TRP:CZ3	15:P:3007:PEE:H20	2.46	0.51
14:P:3004:CDL:HA32	7:T:40:ARG:HB3	1.92	0.51
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	1.92	0.51
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.92	0.51
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.93	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.93	0.51
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.45	0.51
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.26	0.51
2:O:385:GLU:C	2:O:387:LEU:H	2.19	0.51
3:P:332:ASN:ND2	3:P:358:SER:OG	2.42	0.51
1:A:64:PHE:C	1:A:66:GLY:H	2.20	0.50
1:A:121:ALA:O	1:A:122:LEU:HB2	2.11	0.50
5:E:131:GLU:CD	5:E:131:GLU:H	2.18	0.50
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.30	0.50
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.93	0.50
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.75	0.50
4:Q:47:ALA:O	4:Q:50:ASN:HB2	2.11	0.50
2:B:273:SER:O	2:B:276:GLN:HB3	2.11	0.50
3:C:138:GLN:HB2	3:C:255:GLU:O	2.11	0.50
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.50
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.46	0.50
1:N:26:ALA:O	1:N:198:ALA:HA	2.12	0.50
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.46	0.50
2:B:135:TRP:O	2:B:136:GLU:C	2.53	0.50
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.46	0.50
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.50
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.93	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.26	0.50
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.94	0.50
1:A:217:SER:O	1:A:218:GLY:C	2.54	0.50
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.76	0.50
2:O:422:LYS:C	2:O:436:LEU:HD21	2.36	0.50
4:Q:181:GLN:HE21	4:Q:185:ASP:CG	2.19	0.50
2:B:141:GLN:N	2:B:142:PRO:HD2	2.27	0.50
6:F:53:ASP:OD1	6:F:54:LEU:N	2.44	0.50
1:N:255:LEU:CD1	1:N:422:LEU:HB2	2.40	0.50
3:P:105:TYR:CA	3:P:315:THR:HG22	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:ILE:HD13	5:R:98:VAL:O	2.11	0.50
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.94	0.50
1:A:52:ASN:C	1:A:52:ASN:OD1	2.55	0.50
2:B:414:ALA:O	2:B:418:VAL:HG23	2.12	0.50
3:C:105:TYR:CA	3:C:315:THR:HG22	2.41	0.50
4:D:208:MET:SD	4:D:208:MET:C	2.95	0.50
1:N:64:PHE:C	1:N:66:GLY:H	2.20	0.50
1:N:255:LEU:O	1:N:321:GLY:HA3	2.12	0.50
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.12	0.50
9:V:64:LEU:HD12	9:V:77:ARG:O	2.12	0.50
1:A:190:PHE:C	1:A:195:MET:HE2	2.37	0.50
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.93	0.50
1:A:343:MET:HB3	1:A:444:ILE:HA	1.94	0.50
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.75	0.50
2:O:141:GLN:N	2:O:142:PRO:HD2	2.26	0.50
3:P:48:THR:HG1	3:P:84:HIS:HD1	1.57	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.91	0.50
2:B:341:MET:CE	2:B:341:MET:HA	2.42	0.50
3:C:31:TRP:NE1	15:C:2007:PEE:O4	2.45	0.50
3:C:347:PRO:O	3:C:351:ILE:HG13	2.12	0.50
5:E:72:SER:HA	3:P:169:PHE:CE1	2.46	0.50
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.42	0.50
10:J:59:TYR:CD1	10:J:59:TYR:N	2.79	0.50
1:N:48:GLU:CD	1:N:54:GLY:H	2.20	0.50
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.47	0.50
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.12	0.50
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.12	0.50
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.93	0.50
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.41	0.50
1:A:106:MET:O	1:A:110:VAL:HG23	2.11	0.49
1:A:255:LEU:O	1:A:321:GLY:HA3	2.11	0.49
3:C:28:ILE:HD11	3:C:225:TYR:CZ	2.47	0.49
4:D:183:ALA:O	4:D:186:VAL:HG12	2.11	0.49
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.94	0.49
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.77	0.49
2:B:46:ARG:HG3	2:B:46:ARG:O	2.11	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.49
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.45	0.49
1:N:178:THR:HB	1:N:181:ASP:OD1	2.12	0.49
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.47	0.49
3:P:125:MET:HE2	3:P:275:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.94	0.49
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.12	0.49
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.46	0.49
2:B:290:SER:C	2:B:297:GLN:HE21	2.20	0.49
3:C:287:ASN:O	3:C:288:LYS:C	2.55	0.49
5:E:84:GLY:N	5:E:100:HIS:O	2.43	0.49
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.46	0.49
2:O:206:LEU:O	2:O:206:LEU:HG	2.12	0.49
1:A:63:ALA:O	1:A:116:VAL:HG13	2.12	0.49
2:B:353:THR:HG22	2:B:355:GLU:N	2.10	0.49
5:E:84:GLY:CA	5:E:102:THR:HG23	2.42	0.49
9:I:70:LEU:HG	9:I:71:ASN:N	2.26	0.49
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.27	0.49
2:O:290:SER:C	2:O:297:GLN:HE21	2.20	0.49
4:Q:37:CYS:C	4:Q:39:ALA:H	2.20	0.49
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.95	0.49
1:A:48:GLU:CD	1:A:54:GLY:H	2.21	0.49
2:B:280:GLY:HA3	2:B:293:SER:OG	2.12	0.49
3:C:31:TRP:CZ3	15:C:2007:PEE:H20	2.48	0.49
4:D:222:MET:HE3	5:E:40:THR:OG1	2.13	0.49
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.43	0.49
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.27	0.49
3:P:45:GLN:CB	12:P:501:HEM:HAB	2.43	0.49
3:P:247:SER:OG	3:P:250:LEU:HB2	2.13	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
1:A:49:ASN:HD21	1:A:51:LYS:H	1.59	0.49
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.95	0.49
3:C:238:THR:HB	3:C:239:PRO:CD	2.36	0.49
4:D:239:PRO:C	4:D:241:LYS:H	2.20	0.49
5:E:127:VAL:O	5:E:128:LYS:HB2	2.13	0.49
1:N:165:ARG:HG3	1:N:165:ARG:NH1	2.26	0.49
1:N:317:THR:HG23	1:N:318:GLY:N	2.27	0.49
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.12	0.49
2:O:56:ARG:NH1	2:O:171:ALA:HB1	2.27	0.49
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.48	0.49
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.48	0.49
6:S:71:LYS:O	6:S:72:HIS:HB2	2.13	0.49
2:B:50:PHE:C	2:B:51:ILE:HG13	2.37	0.49
2:B:156:GLN:HE22	9:I:77:ARG:C	2.21	0.49
1:N:173:ASN:O	1:N:177:LEU:HG	2.13	0.49
3:P:319:ARG:O	3:P:323:GLN:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.13	0.49
5:R:153:PHE:C	5:R:155:GLY:H	2.20	0.49
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.42	0.49
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.24	0.49
3:C:112:GLU:O	3:C:116:THR:HG23	2.12	0.49
4:D:223:LYS:HD3	4:D:223:LYS:C	2.38	0.49
14:D:2003:CDL:H721	14:D:2003:CDL:HA62	1.93	0.49
5:E:101:ARG:HG2	5:E:105:GLU:CD	2.38	0.49
2:O:221:GLU:C	2:O:223:PHE:H	2.20	0.49
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.48	0.49
5:R:137:GLY:O	5:R:145:VAL:HG13	2.12	0.49
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.76	0.49
2:B:200:THR:OG1	2:B:203:ARG:HG3	2.13	0.49
4:D:37:CYS:O	4:D:39:ALA:N	2.44	0.49
1:N:121:ALA:O	1:N:122:LEU:HB2	2.12	0.49
1:N:191:LYS:CA	1:N:195:MET:HE2	2.43	0.49
2:O:129:ALA:N	2:O:130:PRO:CD	2.76	0.49
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.45	0.49
9:V:32:UNK:O	9:V:33:UNK:C	2.61	0.49
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.48	0.49
1:N:354:VAL:HG23	1:N:355:LYS:N	2.28	0.49
2:O:96:LEU:HD12	2:O:97:SER:N	2.28	0.49
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.48	0.49
3:P:292:VAL:O	3:P:295:LEU:HB3	2.13	0.49
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.94	0.48
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.43	0.48
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.48	0.48
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.46	0.48
14:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.27	0.48
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.77	0.48
9:V:51:CYS:HB2	9:V:53:GLU:OE1	2.13	0.48
1:A:279:ARG:HH22	9:I:30:UNK:C	2.26	0.48
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.95	0.48
14:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.28	0.48
7:G:3:HIS:O	7:G:7:LEU:HG	2.12	0.48
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.94	0.48
1:A:106:MET:HE2	1:A:107:PRO:N	2.29	0.48
2:B:366:ALA:O	2:B:367:THR:C	2.55	0.48
13:C:2002:UQ:HM51	13:C:2002:UQ:C8	2.42	0.48
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.48
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:282:LEU:HD12	3:P:291:GLY:C	2.38	0.48
3:P:286:PRO:O	3:P:287:ASN:CB	2.61	0.48
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.13	0.48
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.47	0.48
1:N:361:LEU:O	1:N:364:ALA:HB3	2.14	0.48
3:P:287:ASN:O	3:P:288:LYS:C	2.55	0.48
3:P:342:GLN:HB3	3:P:343:PRO:HD2	1.95	0.48
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.78	0.48
9:V:70:LEU:HD23	9:V:71:ASN:H	1.78	0.48
1:A:289:HIS:O	1:A:290:LEU:C	2.57	0.48
2:B:129:ALA:N	2:B:130:PRO:CD	2.77	0.48
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.78	0.48
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.48
1:A:178:THR:CG2	1:A:179:ARG:N	2.76	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.14	0.48
2:B:312:PHE:HE1	9:I:62:ARG:O	1.96	0.48
3:C:319:ARG:O	3:C:323:GLN:HG3	2.13	0.48
5:E:163:SER:HA	5:E:174:GLY:HA3	1.95	0.48
2:O:366:ALA:O	2:O:367:THR:C	2.57	0.48
3:P:28:ILE:HD11	3:P:225:TYR:CZ	2.48	0.48
4:Q:178:THR:CG2	8:U:15:ASP:HA	2.43	0.48
6:S:40:ASP:OD1	6:S:40:ASP:C	2.57	0.48
1:A:39:VAL:HA	1:A:196:VAL:O	2.13	0.48
1:A:295:ALA:O	1:A:299:VAL:HG23	2.14	0.48
2:O:374:THR:HG22	2:O:376:GLN:H	1.79	0.48
4:Q:116:ILE:CG2	4:Q:190:LEU:HD13	2.43	0.48
3:C:233:LEU:O	3:C:237:LEU:HB2	2.12	0.48
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.48	0.48
1:N:280:TYR:CG	1:N:281:ASP:N	2.81	0.48
2:O:221:GLU:HG3	2:O:222:GLN:N	2.21	0.48
3:P:319:ARG:HD2	3:P:374:GLU:OE2	2.14	0.48
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.44	0.48
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.96	0.48
4:D:150:ASN:O	4:D:156:GLN:HA	2.13	0.48
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.44	0.48
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.95	0.48
10:W:57:HIS:ND1	10:W:58:LYS:N	2.62	0.48
5:E:190:ASP:C	5:E:192:LEU:N	2.72	0.48
1:N:170:THR:HG22	1:N:171:THR:H	1.78	0.48
2:O:385:GLU:C	2:O:387:LEU:N	2.72	0.48
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:55:MET:O	9:I:58:ARG:HG2	2.13	0.47
2:O:124:LEU:HD23	2:O:124:LEU:C	2.39	0.47
2:O:135:TRP:O	2:O:136:GLU:C	2.57	0.47
2:O:353:THR:HG22	2:O:355:GLU:N	2.09	0.47
4:Q:208:MET:SD	4:Q:208:MET:C	2.97	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.96	0.47
2:B:259:THR:HG22	2:B:260:GLU:N	2.30	0.47
2:B:403:ASP:O	2:B:405:VAL:N	2.44	0.47
14:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.14	0.47
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.78	0.47
5:E:35:PHE:O	5:E:38:LEU:HB3	2.15	0.47
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.96	0.47
3:P:146:VAL:HG21	3:P:269:ILE:HG21	1.95	0.47
1:A:240:GLU:HA	1:A:422:LEU:O	2.14	0.47
2:B:385:GLU:C	2:B:387:LEU:N	2.72	0.47
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.49	0.47
4:D:165:TYR:O	4:D:166:ASN:C	2.57	0.47
5:E:119:ASP:O	5:E:121:GLN:N	2.47	0.47
9:I:49:LEU:O	9:I:50:LEU:HD23	2.15	0.47
3:P:172:ASP:C	3:P:174:PRO:HD2	2.39	0.47
7:T:3:HIS:O	7:T:7:LEU:HG	2.13	0.47
7:T:68:ARG:NH2	7:T:69:LEU:HD21	2.29	0.47
1:A:178:THR:O	1:A:179:ARG:C	2.58	0.47
2:B:306:PRO:HA	9:I:52:ARG:CG	2.45	0.47
2:B:374:THR:HG22	2:B:376:GLN:H	1.79	0.47
3:C:304:LEU:O	3:C:305:ILE:C	2.57	0.47
5:E:165:TYR:HA	5:E:170:ARG:O	2.15	0.47
2:O:38:LEU:HD12	2:O:39:GLU:N	2.29	0.47
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.39	0.47
1:A:170:THR:HB	1:A:173:ASN:HB2	1.96	0.47
3:C:36:SER:O	3:C:40:VAL:HG23	2.14	0.47
3:C:125:MET:HE2	3:C:275:PHE:HE2	1.76	0.47
3:C:216:SER:CB	6:F:59:MET:HE2	2.39	0.47
5:E:188:VAL:HG12	5:E:188:VAL:O	2.14	0.47
9:I:70:LEU:CD2	9:I:71:ASN:N	2.78	0.47
1:N:79:VAL:O	1:N:82:MET:HG2	2.14	0.47
1:N:438:ARG:HG3	1:N:438:ARG:HH11	1.80	0.47
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.95	0.47
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.54	0.47
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.45	0.47
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.39	0.47
4:D:116:ILE:CG2	4:D:190:LEU:HD13	2.43	0.47
9:V:70:LEU:HD23	9:V:71:ASN:N	2.30	0.47
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.82	0.47
7:G:68:ARG:NH2	7:G:69:LEU:HD21	2.29	0.47
8:H:59:PHE:O	8:H:60:ASP:C	2.55	0.47
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.47
1:N:289:HIS:O	1:N:290:LEU:C	2.58	0.47
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.32	0.47
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.50	0.47
5:R:96:LEU:HD12	5:R:135:LEU:O	2.14	0.47
5:R:153:PHE:O	5:R:155:GLY:N	2.48	0.47
7:T:36:ASN:O	7:T:40:ARG:HG3	2.14	0.47
2:B:206:LEU:O	2:B:216:LEU:HD21	2.14	0.47
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.50	0.47
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.47	0.47
10:W:20:PHE:O	10:W:24:VAL:HG23	2.15	0.47
1:N:219:VAL:HG12	1:N:220:SER:N	2.30	0.47
3:P:44:THR:O	3:P:48:THR:HG23	2.15	0.47
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.50	0.47
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.96	0.47
5:R:79:SER:OG	5:R:191:ASP:HB2	2.15	0.47
3:C:22:LEU:HD12	3:C:23:PRO:N	2.29	0.47
4:D:47:ALA:O	4:D:50:ASN:HB2	2.14	0.47
1:N:47:TYR:CE2	1:N:231:LEU:HD11	2.49	0.47
1:N:49:ASN:HD21	1:N:51:LYS:H	1.57	0.47
1:N:253:VAL:O	1:N:323:HIS:HA	2.14	0.47
1:N:394:GLU:O	1:N:395:TRP:C	2.58	0.47
2:O:31:ASN:N	2:O:31:ASN:HD22	2.13	0.47
3:P:18:SER:HA	3:P:22:LEU:HD22	1.96	0.47
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.50	0.47
2:B:28:LYS:O	2:B:28:LYS:HG2	2.14	0.46
3:C:292:VAL:O	3:C:295:LEU:HB3	2.15	0.46
4:D:17:PRO:O	4:D:202:LYS:HD3	2.14	0.46
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.46
4:D:220:TYR:O	4:D:224:ARG:HG2	2.15	0.46
5:E:140:THR:O	5:E:177:PRO:HD2	2.15	0.46
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.79	0.46
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.97	0.46
2:O:345:LYS:HG2	2:O:418:VAL:HG11	1.97	0.46
3:P:141:PHE:HE1	3:P:171:VAL:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:186:LEU:O	3:P:187:PRO:C	2.58	0.46
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.96	0.46
1:N:205:HIS:O	1:N:208:LEU:HB3	2.14	0.46
2:O:259:THR:O	2:O:260:GLU:C	2.56	0.46
2:O:408:ALA:O	2:O:409:ASP:C	2.57	0.46
4:Q:165:TYR:O	4:Q:166:ASN:C	2.58	0.46
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.46
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.84	0.46
8:U:15:ASP:O	8:U:17:LEU:N	2.49	0.46
1:A:45:SER:HA	1:A:48:GLU:CD	2.39	0.46
3:C:146:VAL:HG21	3:C:269:ILE:HG21	1.96	0.46
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.79	0.46
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.75	0.46
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.15	0.46
4:D:57:THR:HG22	4:D:58:GLU:N	2.30	0.46
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.41	0.46
2:O:33:LEU:HD12	2:O:204:MET:O	2.15	0.46
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.97	0.46
1:A:255:LEU:CD1	1:A:422:LEU:HB2	2.46	0.46
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.97	0.46
2:B:424:MET:HG2	2:B:425:ALA:N	2.30	0.46
3:C:202:HIS:NE2	13:C:2002:UQ:O4	2.46	0.46
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.96	0.46
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.16	0.46
5:R:163:SER:OG	5:R:176:ALA:HB2	2.16	0.46
6:S:32:MET:O	6:S:33:ARG:C	2.58	0.46
1:A:27:SER:HA	1:A:199:ALA:O	2.15	0.46
2:B:206:LEU:HG	2:B:206:LEU:O	2.15	0.46
2:B:370:MET:O	2:B:373:GLU:HG3	2.15	0.46
4:D:239:PRO:HG2	4:D:241:LYS:HB2	1.97	0.46
8:H:15:ASP:O	8:H:17:LEU:N	2.48	0.46
8:U:15:ASP:C	8:U:17:LEU:N	2.74	0.46
1:A:289:HIS:CD2	2:B:83:PHE:HD1	2.32	0.46
2:B:366:ALA:O	2:B:369:LEU:N	2.49	0.46
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.51	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
9:I:38:UNK:O	9:I:40:UNK:N	2.47	0.46
1:N:106:MET:HE2	1:N:107:PRO:CA	2.45	0.46
5:R:165:TYR:HA	5:R:170:ARG:O	2.15	0.46
1:A:89:TYR:CD1	1:A:89:TYR:C	2.94	0.46
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.97	0.46
5:E:133:VAL:O	5:E:133:VAL:HG13	2.15	0.46
5:E:153:PHE:C	5:E:155:GLY:H	2.24	0.46
8:H:15:ASP:C	8:H:17:LEU:N	2.74	0.46
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.98	0.46
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.56	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.50	0.46
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.37	0.46
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.46	0.46
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.46
2:O:307:PHE:HD1	2:O:308:ASP:N	2.14	0.46
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.57	0.45
1:A:404:ALA:O	1:A:405:ARG:C	2.59	0.45
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.42	0.45
5:E:96:LEU:HD12	5:E:135:LEU:O	2.16	0.45
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.56	0.45
2:O:57:TYR:N	2:O:57:TYR:HD1	2.14	0.45
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.46	0.45
2:O:355:GLU:O	2:O:358:THR:N	2.49	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.15	0.45
5:R:185:TYR:N	5:R:185:TYR:CD2	2.85	0.45
7:T:79:ASN:O	7:T:80:ASP:HB2	2.16	0.45
1:A:48:GLU:HB3	1:A:52:ASN:OD1	2.16	0.45
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.51	0.45
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.98	0.45
5:E:52:LYS:NZ	10:J:32:GLU:OE1	2.42	0.45
1:N:34:THR:HA	1:N:102:LEU:HA	1.97	0.45
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.41	0.45
1:N:436:ARG:HD2	1:N:436:ARG:HA	1.77	0.45
2:O:198:ASN:O	2:O:203:ARG:HD3	2.16	0.45
2:O:327:ILE:HD11	9:V:58:ARG:O	2.16	0.45
5:R:181:GLU:HG2	5:R:182:VAL:N	2.30	0.45
5:R:185:TYR:O	5:R:186:GLN:HB3	2.16	0.45
1:A:245:ASP:OD1	1:A:247:ALA:HB3	2.16	0.45
2:B:26:ILE:HG23	2:B:26:ILE:O	2.16	0.45
2:B:57:TYR:HE2	2:B:203:ARG:NH2	2.09	0.45
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.99	0.45
3:C:273:TRP:CG	3:C:274:TYR:N	2.84	0.45
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.96	0.45
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.98	0.45
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:GLU:O	8:H:32:LYS:HG3	2.16	0.45
1:N:281:ASP:C	1:N:283:THR:H	2.24	0.45
10:W:10:TYR:C	10:W:10:TYR:CD2	2.94	0.45
1:A:146:THR:O	1:A:150:PHE:HD1	1.98	0.45
2:B:292:THR:HG22	2:B:292:THR:O	2.15	0.45
4:D:57:THR:HG22	4:D:59:ALA:H	1.81	0.45
1:N:48:GLU:HB3	1:N:52:ASN:OD1	2.16	0.45
6:S:82:LYS:O	6:S:83:TYR:C	2.58	0.45
2:B:306:PRO:HB3	9:I:52:ARG:N	2.31	0.45
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.84	0.45
1:N:439:SER:C	1:N:441:MET:H	2.24	0.45
2:O:56:ARG:NH2	2:O:318:ASP:OD2	2.50	0.45
9:V:38:UNK:O	9:V:39:UNK:CB	2.63	0.45
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.84	0.45
8:H:10:GLU:O	8:H:11:GLU:HG3	2.17	0.45
1:N:45:SER:HA	1:N:48:GLU:CD	2.41	0.45
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.52	0.45
5:R:106:ILE:O	5:R:109:GLU:HB3	2.17	0.45
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.98	0.45
6:S:70:LEU:HD12	6:S:70:LEU:C	2.41	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.78	0.45
5:E:52:LYS:C	5:E:52:LYS:CD	2.89	0.45
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.16	0.45
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.17	0.45
3:P:238:THR:CB	3:P:239:PRO:HD3	2.34	0.45
3:P:376:LYS:O	6:S:17:ARG:NH1	2.50	0.45
6:S:94:LEU:O	6:S:94:LEU:HD12	2.17	0.45
7:T:56:TYR:O	7:T:59:TYR:HB3	2.16	0.45
2:B:47:ILE:HD13	2:B:120:MET:SD	2.56	0.45
3:C:28:ILE:CD1	13:C:2002:UQ:HM21	2.47	0.45
3:C:172:ASP:C	3:C:174:PRO:HD2	2.42	0.45
5:E:130:PRO:C	5:E:132:TRP:N	2.75	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.15	0.45
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.51	0.45
3:P:99:ILE:HD11	3:P:121:LEU:HD22	1.98	0.45
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.32	0.45
2:B:110:GLU:O	2:B:111:CYS:HB3	2.17	0.45
3:C:82:ASN:O	3:C:83:LEU:C	2.58	0.45
5:E:179:ASN:O	5:E:180:LEU:C	2.59	0.45
8:H:73:LEU:HD12	8:H:73:LEU:O	2.17	0.45
3:P:72:ARG:HH11	3:P:72:ARG:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:89:SER:O	3:P:90:PHE:C	2.58	0.45
5:R:133:VAL:O	5:R:133:VAL:HG13	2.16	0.45
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.31	0.45
1:A:281:ASP:C	1:A:283:THR:H	2.24	0.45
4:D:195:GLU:HG3	4:D:195:GLU:O	2.17	0.45
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.99	0.45
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.99	0.45
9:I:70:LEU:CG	9:I:71:ASN:N	2.78	0.45
10:J:10:TYR:C	10:J:10:TYR:CD2	2.95	0.45
1:N:10:ASN:ND2	2:O:18:CYS:HB3	2.08	0.45
1:N:106:MET:N	1:N:107:PRO:HD2	2.32	0.45
1:N:191:LYS:N	1:N:195:MET:HE2	2.32	0.45
1:N:269:VAL:HG22	1:N:406:MET:HE3	1.98	0.45
2:O:57:TYR:HE2	2:O:203:ARG:NH2	2.11	0.45
3:P:107:SER:OG	12:P:502:HEM:O1D	2.32	0.45
2:B:162:ASN:O	2:B:244:ILE:HD12	2.17	0.44
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.82	0.44
4:Q:178:THR:HG21	8:U:15:ASP:HA	1.99	0.44
1:A:404:ALA:C	1:A:406:MET:N	2.75	0.44
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.47	0.44
2:B:112:LEU:O	2:B:113:ARG:C	2.59	0.44
5:E:181:GLU:HG2	5:E:182:VAL:N	2.31	0.44
7:G:29:ILE:HA	7:G:33:ALA:HB3	1.99	0.44
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.99	0.44
2:O:96:LEU:HD13	2:O:109:VAL:CG1	2.38	0.44
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.52	0.44
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.98	0.44
8:U:59:PHE:O	8:U:60:ASP:C	2.58	0.44
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.17	0.44
2:B:360:ALA:O	2:B:361:LYS:C	2.60	0.44
3:C:187:PRO:HG2	12:C:501:HEM:HMC3	2.00	0.44
5:E:106:ILE:O	5:E:106:ILE:HG22	2.17	0.44
6:F:71:LYS:O	6:F:72:HIS:HB2	2.16	0.44
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.44
2:O:360:ALA:O	2:O:361:LYS:C	2.61	0.44
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.99	0.44
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.30	0.44
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.97	0.44
1:N:18:THR:HG23	1:N:24:ARG:CG	2.48	0.44
1:N:270:LEU:HD23	1:N:270:LEU:HA	1.81	0.44
3:P:223:PRO:O	3:P:227:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:37:CYS:C	4:Q:39:ALA:N	2.74	0.44
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	2.00	0.44
5:R:141:HIS:HB3	19:R:501:FES:S2	2.58	0.44
2:B:56:ARG:NH1	2:B:171:ALA:HB1	2.32	0.44
5:R:136:VAL:HG12	5:R:138:VAL:HG23	1.99	0.44
7:T:44:GLN:O	7:T:45:VAL:C	2.61	0.44
1:A:253:VAL:O	1:A:323:HIS:HA	2.17	0.44
2:B:42:SER:C	2:B:44:ALA:H	2.25	0.44
4:D:224:ARG:HH21	7:G:26:ILE:HA	1.81	0.44
2:O:200:THR:OG1	2:O:203:ARG:HG3	2.17	0.44
2:O:209:ILE:HD11	2:O:378:LEU:HG	2.00	0.44
3:P:81:ARG:O	3:P:81:ARG:HD3	2.18	0.44
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	3.00	0.44
2:B:22:GLU:HG3	2:B:23:ASP:N	2.32	0.44
5:E:102:THR:O	5:E:103:GLN:HG3	2.17	0.44
5:E:161:HIS:HB2	19:E:501:FES:S1	2.58	0.44
1:N:23:LEU:HA	1:N:192:ALA:O	2.17	0.44
2:O:19:PRO:HG3	2:O:41:PHE:CD2	2.52	0.44
1:A:373:THR:N	1:A:374:PRO:HD2	2.31	0.44
2:B:368:TYR:O	2:B:372:VAL:HG23	2.18	0.44
9:V:71:ASN:CG	9:V:71:ASN:O	2.59	0.44
1:A:7:THR:HG21	2:B:113:ARG:CD	2.44	0.44
1:A:79:VAL:O	1:A:82:MET:HG2	2.17	0.44
1:A:204:SER:O	1:A:205:HIS:C	2.60	0.44
1:A:394:GLU:O	1:A:395:TRP:C	2.60	0.44
2:B:63:LEU:O	2:B:182:ARG:NE	2.43	0.44
2:B:76:THR:HG22	2:B:81:SER:CA	2.45	0.44
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.98	0.44
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.18	0.44
4:D:116:ILE:HG21	4:D:190:LEU:HD13	2.00	0.44
8:H:17:LEU:HD13	8:H:73:LEU:CD2	2.47	0.44
1:N:158:PHE:O	1:N:159:GLN:C	2.60	0.44
2:O:33:LEU:HD21	2:O:224:LEU:HD12	2.00	0.44
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.18	0.44
2:O:101:THR:HG23	2:O:104:LYS:HE3	2.00	0.44
2:O:276:GLN:HG2	2:O:281:ALA:HB2	2.00	0.44
5:R:185:TYR:N	5:R:185:TYR:HD2	2.16	0.44
1:A:418:LYS:O	1:A:420:PRO:HD3	2.18	0.43
2:B:408:ALA:O	2:B:409:ASP:C	2.61	0.43
3:C:378:LEU:HD22	6:F:33:ARG:HG3	2.01	0.43
7:G:56:TYR:O	7:G:59:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.47	0.43
3:P:45:GLN:HB3	12:P:501:HEM:HAB	2.00	0.43
4:Q:197:GLU:O	4:Q:198:HIS:C	2.60	0.43
1:A:356:ARG:O	1:A:357:ALA:C	2.62	0.43
2:B:67:HIS:O	2:B:70:ARG:HB3	2.18	0.43
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.99	0.43
5:E:105:GLU:C	5:E:107:ASN:H	2.26	0.43
5:E:189:GLY:O	5:E:192:LEU:O	2.35	0.43
2:O:417:PHE:CD2	2:O:417:PHE:C	2.96	0.43
1:A:47:TYR:CE2	1:A:231:LEU:HD11	2.54	0.43
1:A:109:VAL:O	1:A:110:VAL:C	2.62	0.43
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.50	0.43
2:B:341:MET:HA	2:B:341:MET:HE2	2.00	0.43
2:B:379:LEU:O	2:B:379:LEU:HG	2.18	0.43
4:D:208:MET:O	4:D:212:SER:HB2	2.18	0.43
2:O:31:ASN:N	2:O:31:ASN:ND2	2.63	0.43
2:O:174:ASN:HA	2:O:175:PRO:HD2	1.85	0.43
2:O:280:GLY:HA3	2:O:293:SER:OG	2.18	0.43
3:P:36:SER:O	3:P:40:VAL:HG23	2.19	0.43
9:V:32:UNK:N	9:V:73:PRO:HG2	2.32	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.73	0.43
17:D:501:HEC:HBC3	17:D:501:HEC:HMC3	2.00	0.43
2:O:151:ALA:O	2:O:157:VAL:HG11	2.19	0.43
14:Q:3003:CDL:H721	14:Q:3003:CDL:HA62	1.99	0.43
5:R:102:THR:C	5:R:104:ALA:N	2.76	0.43
1:A:295:ALA:O	1:A:298:ALA:HB3	2.18	0.43
2:B:124:LEU:C	2:B:124:LEU:HD23	2.43	0.43
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.47	0.43
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.99	0.43
2:B:422:LYS:C	2:B:436:LEU:HD21	2.42	0.43
3:C:362:ILE:HA	3:C:366:LEU:HB2	2.01	0.43
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.82	0.43
2:O:341:MET:HA	2:O:341:MET:HE2	2.00	0.43
3:P:31:TRP:NE1	15:P:3007:PEE:O4	2.50	0.43
3:P:50:LEU:O	3:P:54:MET:HG3	2.17	0.43
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.32	0.43
5:R:155:GLY:HA3	5:R:165:TYR:O	2.18	0.43
1:A:272:VAL:O	1:A:275:ALA:HB3	2.18	0.43
1:A:402:VAL:CA	1:A:406:MET:HE2	2.40	0.43
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.43
3:C:377:MET:HE2	6:F:20:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.19	0.43
3:P:142:TRP:CD1	3:P:266:PRO:HD3	2.53	0.43
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.18	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.90	0.43
1:A:361:LEU:O	1:A:364:ALA:HB3	2.17	0.43
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.40	0.43
3:C:276:LEU:O	3:C:277:PHE:C	2.61	0.43
1:N:52:ASN:OD1	1:N:52:ASN:C	2.61	0.43
1:N:240:GLU:HA	1:N:422:LEU:O	2.18	0.43
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.83	0.43
1:N:404:ALA:O	1:N:405:ARG:C	2.62	0.43
2:O:295:LEU:O	2:O:299:VAL:HG23	2.19	0.43
3:P:2:ALA:HB3	3:P:8:SER:HB3	2.00	0.43
3:P:304:LEU:O	3:P:305:ILE:C	2.61	0.43
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.53	0.43
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.32	0.43
4:Q:220:TYR:CE2	14:Q:3003:CDL:H722	2.54	0.43
1:A:41:ILE:HG22	1:A:42:GLY:N	2.34	0.43
1:A:140:GLU:HG2	9:I:50:LEU:HG	1.99	0.43
2:B:57:TYR:N	2:B:57:TYR:HD1	2.16	0.43
2:B:207:VAL:HG21	2:B:383:GLY:HA2	2.01	0.43
3:C:313:GLN:HE21	6:F:36:THR:CB	2.31	0.43
6:F:52:GLU:HG3	6:F:56:ASN:ND2	2.34	0.43
1:N:178:THR:C	1:N:180:ALA:N	2.75	0.43
2:O:207:VAL:HG21	2:O:383:GLY:HA2	2.00	0.43
3:P:38:LEU:HD23	3:P:38:LEU:HA	1.86	0.43
3:P:285:ILE:HD12	3:P:294:ALA:HB2	2.00	0.43
3:C:273:TRP:CD2	3:C:274:TYR:N	2.87	0.43
9:I:49:LEU:C	9:I:50:LEU:HD23	2.44	0.43
1:N:18:THR:HG23	1:N:24:ARG:HG3	2.00	0.43
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.83	0.43
1:N:89:TYR:CD1	1:N:89:TYR:C	2.97	0.43
1:N:433:ASP:OD1	1:N:435:ASN:HB2	2.18	0.43
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.52	0.43
3:P:313:GLN:HE21	6:S:36:THR:CB	2.32	0.43
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.46	0.43
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.34	0.43
4:Q:240:PRO:O	4:Q:241:LYS:C	2.61	0.43
5:R:77:LYS:HA	5:R:192:LEU:HD23	2.01	0.43
5:R:109:GLU:CD	5:R:168:SER:HB2	2.43	0.43
5:R:135:LEU:CD2	5:R:182:VAL:HG22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:THR:C	2:B:61:ALA:N	2.75	0.43
3:C:247:SER:OG	3:C:250:LEU:HB2	2.19	0.43
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.54	0.43
4:D:182:ILE:O	4:D:183:ALA:C	2.61	0.43
8:H:15:ASP:O	8:H:16:PRO:C	2.62	0.43
10:J:57:HIS:ND1	10:J:58:LYS:N	2.67	0.43
2:O:402:ILE:C	2:O:402:ILE:CD1	2.92	0.43
3:P:22:LEU:HD12	3:P:23:PRO:N	2.34	0.43
3:P:41:CYS:SG	3:P:91:PHE:HA	2.58	0.43
3:P:273:TRP:C	3:P:275:PHE:H	2.26	0.43
3:P:279:TYR:O	3:P:282:LEU:HB3	2.18	0.43
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.19	0.43
7:T:50:PRO:HB2	7:T:51:PRO:HD2	1.99	0.43
2:B:209:ILE:HD11	2:B:378:LEU:HG	2.01	0.42
3:C:79:LEU:HD22	4:D:204:MET:HE1	2.01	0.42
5:E:130:PRO:O	5:E:132:TRP:N	2.52	0.42
1:N:27:SER:HA	1:N:199:ALA:O	2.19	0.42
2:O:62:ASN:O	2:O:63:LEU:C	2.61	0.42
2:O:355:GLU:O	2:O:356:ASP:C	2.62	0.42
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.54	0.42
5:R:134:ILE:HB	5:R:185:TYR:CE1	2.54	0.42
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.19	0.42
2:B:341:MET:O	2:B:342:ASN:C	2.62	0.42
3:C:329:LEU:O	3:C:332:ASN:HB3	2.20	0.42
1:N:356:ARG:O	1:N:357:ALA:C	2.62	0.42
3:P:325:LEU:HD12	3:P:325:LEU:HA	1.77	0.42
7:T:29:ILE:HA	7:T:33:ALA:HB3	2.00	0.42
8:U:27:THR:O	8:U:31:VAL:HG23	2.19	0.42
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.35	0.42
1:A:439:SER:C	1:A:441:MET:H	2.26	0.42
3:C:336:LEU:HD23	3:C:336:LEU:HA	1.86	0.42
4:D:178:THR:HG21	8:H:15:ASP:HA	2.00	0.42
10:J:52:TRP:O	10:J:53:LYS:C	2.62	0.42
1:N:404:ALA:O	1:N:406:MET:N	2.53	0.42
3:P:145:THR:O	3:P:149:ASN:HB2	2.20	0.42
6:S:70:LEU:HD12	6:S:70:LEU:O	2.19	0.42
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.54	0.42
2:O:96:LEU:HB3	9:V:70:LEU:HD22	2.01	0.42
2:O:162:ASN:O	2:O:244:ILE:HD12	2.19	0.42
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.54	0.42
2:O:357:VAL:O	2:O:361:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:362:ILE:HA	3:P:366:LEU:HB2	2.00	0.42
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.01	0.42
2:B:163:LEU:O	2:B:166:ALA:N	2.49	0.42
2:B:307:PHE:CD1	2:B:307:PHE:C	2.96	0.42
1:N:206:LYS:C	1:N:208:LEU:N	2.77	0.42
2:O:206:LEU:HG	2:O:216:LEU:HD11	2.01	0.42
2:O:264:VAL:HG12	2:O:265:GLY:N	2.34	0.42
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.02	0.42
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.42
8:U:28:GLU:O	8:U:32:LYS:HG3	2.19	0.42
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.42	0.42
2:B:355:GLU:O	2:B:358:THR:N	2.52	0.42
3:C:377:MET:CE	6:F:20:TYR:HB2	2.50	0.42
5:E:106:ILE:C	5:E:110:ALA:HB3	2.44	0.42
1:N:106:MET:HE2	1:N:107:PRO:N	2.34	0.42
1:A:176:HIS:O	1:A:177:LEU:C	2.63	0.42
1:A:365:MET:HG3	1:A:366:VAL:N	2.35	0.42
2:B:341:MET:CE	2:B:417:PHE:CE2	2.93	0.42
2:O:26:ILE:HG23	2:O:26:ILE:O	2.19	0.42
2:O:257:VAL:HG22	2:O:424:MET:HG3	2.02	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.88	0.42
3:P:377:MET:CE	6:S:20:TYR:HB2	2.50	0.42
5:R:99:ARG:HB3	5:R:133:VAL:HG12	2.02	0.42
7:T:34:LEU:HB2	7:T:35:PRO:HD3	2.02	0.42
1:A:191:LYS:C	1:A:193:PRO:HD2	2.44	0.42
1:A:281:ASP:OD2	9:I:33:UNK:HB2	2.18	0.42
2:B:437:ASP:OD1	2:B:437:ASP:C	2.62	0.42
3:C:245:LEU:O	4:D:201:ARG:HD2	2.19	0.42
3:C:282:LEU:HD12	3:C:291:GLY:C	2.45	0.42
8:H:55:THR:O	8:H:56:GLU:C	2.63	0.42
1:N:72:CYS:O	1:N:73:ALA:C	2.63	0.42
1:N:204:SER:O	1:N:205:HIS:C	2.62	0.42
2:O:59:THR:C	2:O:61:ALA:N	2.75	0.42
2:O:231:GLY:O	2:O:232:THR:C	2.62	0.42
5:R:141:HIS:O	5:R:142:LEU:HD23	2.19	0.42
6:S:52:GLU:HG3	6:S:56:ASN:ND2	2.35	0.42
1:A:228:VAL:O	1:A:228:VAL:HG13	2.20	0.42
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.46	0.42
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.55	0.42
2:B:266:SER:HB3	2:B:269:ALA:HB2	2.01	0.42
6:F:82:LYS:O	6:F:83:TYR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:ILE:HA	7:G:33:ALA:CB	2.50	0.42
2:O:221:GLU:O	2:O:223:PHE:N	2.51	0.42
2:O:306:PRO:HB3	9:V:52:ARG:H	1.85	0.42
2:O:307:PHE:CD1	2:O:307:PHE:C	2.98	0.42
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.50	0.42
5:R:107:ASN:C	5:R:109:GLU:N	2.78	0.42
1:A:3:THR:O	1:A:4:TYR:C	2.62	0.42
3:C:279:TYR:O	3:C:282:LEU:HB3	2.19	0.42
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.02	0.42
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.55	0.42
2:O:268:GLU:O	2:O:268:GLU:HG2	2.20	0.42
2:O:314:VAL:HG22	9:V:63:ASP:N	2.34	0.42
2:O:366:ALA:O	2:O:369:LEU:N	2.52	0.42
3:P:187:PRO:HG2	12:P:501:HEM:HMC3	2.00	0.42
3:P:338:TRP:O	3:P:339:ILE:C	2.63	0.42
1:A:205:HIS:O	1:A:208:LEU:HB3	2.20	0.41
2:B:192:HIS:O	2:B:196:GLN:HG3	2.19	0.41
2:B:264:VAL:HG23	2:B:316:TYR:O	2.20	0.41
5:E:37:TYR:CE2	15:E:2005:PEE:H10	2.56	0.41
5:E:177:PRO:HG2	5:E:178:TYR:H	1.85	0.41
1:N:146:THR:O	1:N:150:PHE:HD1	2.03	0.41
1:N:219:VAL:CG1	1:N:220:SER:N	2.83	0.41
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.47	0.41
1:N:365:MET:HG3	1:N:366:VAL:N	2.35	0.41
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.46	0.41
2:O:176:LEU:HD12	2:O:176:LEU:O	2.20	0.41
5:R:35:PHE:O	5:R:38:LEU:HB3	2.19	0.41
5:R:76:ILE:HD13	5:R:89:PHE:CD1	2.54	0.41
1:A:21:ASN:OD1	1:A:21:ASN:N	2.54	0.41
2:B:29:LEU:HB3	2:B:30:PRO:HD2	2.02	0.41
2:B:371:SER:C	2:B:372:VAL:HG23	2.46	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.41
14:C:2004:CDL:HA32	7:G:40:ARG:HB3	2.02	0.41
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.20	0.41
2:O:35:ILE:O	2:O:213:HIS:HE1	2.03	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.45	0.41
2:O:437:ASP:OD1	2:O:437:ASP:C	2.61	0.41
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.02	0.41
3:C:223:PRO:O	3:C:227:PHE:HB2	2.20	0.41
4:D:20:ALA:HB1	4:D:199:ASP:CG	2.45	0.41
4:D:181:GLN:HE21	4:D:185:ASP:CG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.30	0.41
1:N:190:PHE:C	1:N:195:MET:HE2	2.45	0.41
2:O:112:LEU:O	2:O:113:ARG:C	2.62	0.41
2:O:371:SER:C	2:O:372:VAL:HG23	2.45	0.41
3:P:159:HIS:O	3:P:160:THR:C	2.62	0.41
3:P:245:LEU:HD23	3:P:245:LEU:HA	1.90	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.75	0.41
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.50	0.41
5:R:97:PHE:O	5:R:134:ILE:HA	2.20	0.41
6:S:67:ASP:HA	6:S:70:LEU:HD23	2.02	0.41
1:A:191:LYS:O	1:A:195:MET:HG3	2.21	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.44	0.41
2:B:345:LYS:HG2	2:B:418:VAL:HG11	2.02	0.41
2:B:402:ILE:C	2:B:402:ILE:CD1	2.93	0.41
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.21	0.41
1:N:176:HIS:O	1:N:177:LEU:C	2.64	0.41
2:O:42:SER:C	2:O:44:ALA:H	2.28	0.41
2:O:85:ILE:HA	2:O:122:TYR:CD2	2.56	0.41
5:R:153:PHE:C	5:R:155:GLY:N	2.78	0.41
1:A:58:PHE:HZ	1:A:131:ARG:HB2	1.86	0.41
1:A:220:SER:HB2	1:A:225:GLU:HB2	2.03	0.41
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.84	0.41
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.55	0.41
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.51	0.41
3:P:64:PHE:CD2	3:P:259:PRO:HG3	2.56	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.55	0.41
1:A:172:GLU:O	1:A:175:LYS:N	2.51	0.41
1:A:281:ASP:C	1:A:283:THR:N	2.79	0.41
2:B:59:THR:O	2:B:60:THR:C	2.63	0.41
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.55	0.41
2:B:222:GLN:O	2:B:222:GLN:CG	2.68	0.41
3:C:59:ASP:O	3:C:60:THR:C	2.64	0.41
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.21	0.41
4:D:102:ARG:HG2	4:D:102:ARG:NH1	2.36	0.41
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.56	0.41
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.21	0.41
2:O:181:TYR:CD1	2:O:181:TYR:C	2.98	0.41
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.56	0.41
4:Q:37:CYS:O	4:Q:39:ALA:N	2.54	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.93	0.41
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.45	0.41
4:Q:233:ARG:O	6:S:71:LYS:NZ	2.53	0.41
9:V:70:LEU:HD21	9:V:71:ASN:OD1	2.20	0.41
1:A:34:THR:HA	1:A:102:LEU:HA	2.02	0.41
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.85	0.41
2:B:51:ILE:CG2	2:B:52:LYS:N	2.82	0.41
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.55	0.41
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.88	0.41
5:E:77:LYS:HA	5:E:192:LEU:HD23	2.01	0.41
1:N:404:ALA:C	1:N:406:MET:N	2.78	0.41
8:U:15:ASP:C	8:U:17:LEU:H	2.29	0.41
9:V:33:UNK:N	9:V:73:PRO:CG	2.83	0.41
1:A:266:ASP:O	1:A:267:ASN:C	2.64	0.41
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.35	0.41
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.55	0.41
2:B:307:PHE:HD1	2:B:308:ASP:N	2.19	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41
1:N:206:LYS:H	1:N:206:LYS:HD2	1.86	0.41
1:N:402:VAL:CA	1:N:406:MET:HE2	2.44	0.41
2:O:47:ILE:CG2	2:O:48:GLY:N	2.84	0.41
2:O:56:ARG:HA	2:O:171:ALA:O	2.20	0.41
2:O:169:LYS:HG3	2:O:240:TRP:HB2	2.01	0.41
1:A:178:THR:C	1:A:180:ALA:N	2.75	0.41
1:A:280:TYR:CD2	1:A:281:ASP:N	2.88	0.41
2:B:56:ARG:HA	2:B:171:ALA:O	2.21	0.41
2:B:59:THR:O	2:B:61:ALA:N	2.53	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.91	0.41
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.56	0.41
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.85	0.41
4:D:28:ARG:O	4:D:31:GLN:N	2.54	0.41
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.56	0.41
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.51	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.49	0.41
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.41
1:N:351:GLU:O	1:N:354:VAL:HG22	2.21	0.41
2:O:399:ALA:C	2:O:401:LYS:N	2.78	0.41
3:P:47:LEU:HD12	3:P:47:LEU:HA	1.93	0.41
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	2.03	0.41
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.35	0.41
5:R:122:HIS:HA	5:R:170:ARG:NH1	2.36	0.41
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:17:LEU:HD13	8:U:73:LEU:CD2	2.48	0.41
1:A:47:TYR:CZ	1:A:231:LEU:HD11	2.56	0.41
1:A:351:GLU:O	1:A:354:VAL:HG22	2.21	0.41
1:A:391:SER:O	1:A:392:LEU:C	2.63	0.41
2:B:219:VAL:O	2:B:220:ALA:C	2.64	0.41
3:C:101:ARG:C	3:C:101:ARG:CD	2.93	0.41
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.56	0.41
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.38	0.41
4:D:215:LEU:HD13	5:E:46:ALA:HB3	2.03	0.41
5:E:141:HIS:HB2	5:E:176:ALA:HB2	2.03	0.41
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.84	0.41
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.51	0.41
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.39	0.41
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.21	0.40
2:B:141:GLN:C	2:B:143:GLN:N	2.77	0.40
3:C:246:PHE:O	3:C:248:PRO:HD3	2.21	0.40
3:C:259:PRO:O	3:C:260:ALA:C	2.64	0.40
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.52	0.40
1:N:7:THR:HG21	2:O:113:ARG:CD	2.47	0.40
5:R:122:HIS:C	5:R:124:LEU:N	2.78	0.40
9:V:33:UNK:N	9:V:73:PRO:HG2	2.36	0.40
1:A:106:MET:N	1:A:107:PRO:HD2	2.36	0.40
9:I:38:UNK:C	9:I:40:UNK:N	2.64	0.40
1:N:159:GLN:NE2	5:R:7:VAL:HG11	2.37	0.40
1:N:439:SER:HA	1:N:442:TYR:CE2	2.56	0.40
1:N:443:TRP:O	1:N:444:ILE:C	2.64	0.40
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.55	0.40
3:P:23:PRO:HG2	7:T:3:HIS:HB3	2.03	0.40
3:P:92:PHE:CA	3:P:95:ILE:HG22	2.49	0.40
6:S:21:TYR:CD2	6:S:21:TYR:C	2.99	0.40
6:S:57:GLU:O	6:S:61:ARG:HG3	2.21	0.40
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.51	0.40
1:A:23:LEU:HD23	1:A:24:ARG:C	2.46	0.40
1:A:204:SER:HB3	1:A:207:GLU:HB2	2.03	0.40
1:A:293:ARG:CD	1:A:344:ARG:CZ	3.00	0.40
2:B:198:ASN:HA	2:B:203:ARG:NH1	2.37	0.40
2:B:209:ILE:HD12	2:B:379:LEU:HB2	2.03	0.40
2:B:231:GLY:O	2:B:232:THR:C	2.64	0.40
3:C:22:LEU:HD12	3:C:23:PRO:HD2	2.03	0.40
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.50	0.40
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.45	0.40
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.61	0.40
1:N:134:ILE:HG21	1:N:174:ILE:CD1	2.50	0.40
1:N:220:SER:HB2	1:N:225:GLU:HB2	2.03	0.40
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.21	0.40
3:P:75:GLN:O	3:P:76:TYR:HB2	2.21	0.40
3:P:133:VAL:C	3:P:135:PRO:HD2	2.46	0.40
5:R:52:LYS:C	5:R:52:LYS:CD	2.94	0.40
5:R:83:GLU:HA	5:R:100:HIS:CB	2.49	0.40
1:A:6:GLN:C	1:A:8:LEU:N	2.79	0.40
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.88	0.40
1:A:296:ALA:O	1:A:299:VAL:N	2.55	0.40
2:B:51:ILE:HG22	2:B:52:LYS:N	2.37	0.40
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.55	0.40
2:B:181:TYR:CD1	2:B:181:TYR:C	2.98	0.40
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.78	0.40
3:C:130:VAL:HG23	3:C:131:GLY:N	2.37	0.40
4:D:26:VAL:HG12	4:D:55:THR:HG21	2.03	0.40
5:E:101:ARG:HD2	5:E:105:GLU:HB3	2.03	0.40
2:O:368:TYR:O	2:O:372:VAL:HG23	2.21	0.40
2:O:388:LEU:O	2:O:389:SER:HB2	2.21	0.40
5:R:30:GLU:HB2	10:W:7:ARG:HG3	2.03	0.40
5:R:102:THR:C	5:R:104:ALA:H	2.28	0.40
2:B:62:ASN:O	2:B:65:THR:CG2	2.64	0.40
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.51	0.40
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.03	0.40
2:O:59:THR:O	2:O:60:THR:C	2.63	0.40
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.85	0.40
2:O:227:ARG:HB3	2:O:228:SER:H	1.42	0.40
3:P:51:LEU:HA	3:P:51:LEU:HD23	1.88	0.40
3:P:110:TYR:O	3:P:111:LYS:C	2.64	0.40
3:P:352:GLY:O	3:P:353:GLN:C	2.65	0.40
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.57	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%)	384 (87%)	48 (11%)	9 (2%)	6	27
1	N	440/446 (99%)	385 (88%)	45 (10%)	10 (2%)	5	24
2	B	419/441 (95%)	350 (84%)	51 (12%)	18 (4%)	2	13
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	2	16
3	C	378/380 (100%)	346 (92%)	25 (7%)	7 (2%)	6	28
3	P	377/380 (99%)	336 (89%)	33 (9%)	8 (2%)	5	26
4	D	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	7	30
4	Q	239/241 (99%)	216 (90%)	17 (7%)	6 (2%)	4	22
5	E	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	0	3
5	R	194/196 (99%)	162 (84%)	27 (14%)	5 (3%)	4	21
6	F	99/110 (90%)	93 (94%)	6 (6%)	0	100	100
6	S	99/110 (90%)	89 (90%)	10 (10%)	0	100	100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	4	21
7	T	77/81 (95%)	65 (84%)	10 (13%)	2 (3%)	4	21
8	H	68/77 (88%)	59 (87%)	9 (13%)	0	100	100
8	U	65/77 (84%)	53 (82%)	12 (18%)	0	100	100
9	I	29/47 (62%)	26 (90%)	3 (10%)	0	100	100
9	V	29/47 (62%)	23 (79%)	6 (21%)	0	100	100
10	J	59/61 (97%)	53 (90%)	5 (8%)	1 (2%)	7	30
10	W	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
All	All	4002/4160 (96%)	3481 (87%)	418 (10%)	103 (3%)	4	21

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG

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Mol	Chain	Res	Type
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	224	LEU
2	B	227	ARG
3	C	287	ASN
5	E	115	SER
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
5	E	191	ASP
1	N	282	ARG
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
1	A	71	PRO
1	A	218	GLY
1	A	405	ARG
1	A	433	ASP
2	B	21	ALA
2	B	201	SER
2	B	221	GLU
2	B	372	VAL
2	B	386	ALA
2	B	389	SER
5	E	102	THR
5	E	127	VAL
5	E	131	GLU
5	E	137	GLY
2	O	24	LEU
2	O	201	SER
2	O	221	GLU
2	O	222	GLN
2	O	372	VAL
2	O	386	ALA
2	O	389	SER
3	P	274	TYR
5	R	137	GLY
5	R	154	GLY

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Mol	Chain	Res	Type
5	R	163	SER
7	T	33	ALA
2	B	24	LEU
2	B	46	ARG
3	C	3	PRO
4	D	166	ASN
5	E	80	ASP
5	E	120	PRO
5	E	177	PRO
7	G	33	ALA
1	N	72	CYS
2	O	46	ARG
2	O	330	ALA
3	P	111	LYS
4	Q	166	ASN
4	Q	177	ALA
5	R	186	GLN
5	R	191	ASP
7	T	50	PRO
1	A	65	LYS
1	A	72	CYS
1	A	145	MET
2	B	189	GLU
3	C	111	LYS
5	E	123	ASP
5	E	154	GLY
1	N	65	LYS
1	N	71	PRO
1	N	145	MET
1	N	262	TRP
1	N	405	ARG
3	P	156	TYR
3	P	264	VAL
2	B	319	SER
3	C	17	ASN
4	D	38	SER
4	D	176	PRO
7	G	50	PRO
10	J	61	ALA
2	O	404	SER
3	P	158	GLY
4	Q	38	SER

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Mol	Chain	Res	Type
4	Q	176	PRO
4	Q	198	HIS
2	B	431	GLY
3	C	19	LEU
5	E	189	GLY
3	P	3	PRO
2	B	20	GLY
5	E	188	VAL
1	N	428	ILE
2	B	129	ALA
4	Q	162	PRO
3	C	158	GLY
3	C	264	VAL
1	N	218	GLY
3	P	157	ILE
1	A	428	ILE
4	D	162	PRO
2	O	431	GLY

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%)	354 (97%)	11 (3%)	36	62
1	N	365/368 (99%)	352 (96%)	13 (4%)	31	59
2	B	332/347 (96%)	317 (96%)	15 (4%)	24	53
2	O	333/347 (96%)	318 (96%)	15 (4%)	24	53
3	C	328/329 (100%)	323 (98%)	5 (2%)	57	72
3	P	328/329 (100%)	323 (98%)	5 (2%)	57	72
4	D	200/200 (100%)	196 (98%)	4 (2%)	48	68
4	Q	200/200 (100%)	197 (98%)	3 (2%)	57	72
5	E	166/166 (100%)	165 (99%)	1 (1%)	78	81
5	R	165/166 (99%)	162 (98%)	3 (2%)	51	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	93/96 (97%)	86 (92%)	7 (8%)	12	38
6	S	93/96 (97%)	85 (91%)	8 (9%)	10	32
7	G	71/71 (100%)	69 (97%)	2 (3%)	38	63
7	T	70/71 (99%)	68 (97%)	2 (3%)	37	63
8	H	65/71 (92%)	64 (98%)	1 (2%)	57	72
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	71
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	32
9	V	23/26 (88%)	22 (96%)	1 (4%)	26	54
10	J	49/49 (100%)	47 (96%)	2 (4%)	27	56
10	W	47/49 (96%)	46 (98%)	1 (2%)	47	67
All	All	3379/3446 (98%)	3277 (97%)	102 (3%)	36	62

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	106	MET
1	A	108	LYS
1	A	171	THR
1	A	226	ASP
1	A	281	ASP
1	A	384	LEU
1	A	395	TRP
1	A	422	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	38	LEU
2	B	57	TYR
2	B	59	THR
2	B	97	SER
2	B	150	VAL
2	B	170	THR
2	B	228	SER
2	B	248	ASN
2	B	264	VAL
2	B	304	THR
2	B	341	MET

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Mol	Chain	Res	Type
2	B	402	ILE
2	B	418	VAL
2	B	424	MET
3	C	69	HIS
3	C	81	ARG
3	C	223	PRO
3	C	259	PRO
3	C	334	LEU
4	D	43	MET
4	D	179	MET
4	D	203	ARG
4	D	235	MET
5	E	185	TYR
6	F	32	MET
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
6	F	78	GLU
6	F	84	GLU
7	G	4	PHE
7	G	17	SER
8	H	71	HIS
9	I	70	LEU
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	18	THR
1	N	49	ASN
1	N	90	THR
1	N	106	MET
1	N	108	LYS
1	N	171	THR
1	N	281	ASP
1	N	395	TRP
1	N	420	PRO
1	N	422	LEU
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	38	LEU
2	O	57	TYR
2	O	59	THR
2	O	97	SER
2	O	124	LEU
2	O	150	VAL
2	O	170	THR
2	O	223	PHE
2	O	248	ASN
2	O	341	MET
2	O	402	ILE
2	O	418	VAL
2	O	424	MET
3	P	69	HIS
3	P	81	ARG
3	P	156	TYR
3	P	259	PRO
3	P	334	LEU
4	Q	43	MET
4	Q	179	MET
4	Q	203	ARG
5	R	80	ASP
5	R	145	VAL
5	R	185	TYR
6	S	13	MET
6	S	32	MET
6	S	58	ARG
6	S	64	ARG
6	S	70	LEU
6	S	73	ARG
6	S	78	GLU
6	S	84	GLU
7	T	4	PHE
7	T	27	PRO
8	U	71	HIS
9	V	59	SER
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

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Mol	Chain	Res	Type
1	A	49	ASN
1	A	87	ASN
1	A	173	ASN
1	A	215	HIS
1	A	274	ASN
1	A	289	HIS
1	A	301	HIS
1	A	308	GLN
2	B	31	ASN
2	B	125	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
3	C	9	HIS
3	C	17	ASN
3	C	73	ASN
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	6	HIS
4	D	35	GLN
4	D	50	ASN
4	D	225	HIS
5	E	3	ASN
5	E	57	GLN
5	E	103	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	28	ASN
7	G	73	ASN
8	H	26	GLN
9	I	71	ASN
1	N	10	ASN
1	N	32	GLN

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Mol	Chain	Res	Type
1	N	49	ASN
1	N	87	ASN
1	N	118	GLN
1	N	176	HIS
1	N	274	ASN
1	N	301	HIS
1	N	435	ASN
2	O	31	ASN
2	O	125	ASN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	329	GLN
2	O	343	GLN
3	P	9	HIS
3	P	17	ASN
3	P	73	ASN
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	6	HIS
4	Q	14	HIS
4	Q	50	ASN
4	Q	200	GLN
5	R	57	GLN
5	R	122	HIS
5	R	164	HIS
6	S	72	HIS
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 9 are unknown - leaving 27 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
17	HEC	Q	501	4	46,50,50	1.78	10 (21%)	58,82,82	2.17	12 (20%)
14	CDL	Q	3003	-	41,41,99	1.16	1 (2%)	47,53,111	1.08	4 (8%)
14	CDL	C	2004	-	39,39,99	1.24	2 (5%)	45,51,111	1.16	3 (6%)
15	PEE	R	3005	-	49,49,50	1.56	10 (20%)	52,54,55	0.88	3 (5%)
16	GOL	P	3011	-	5,5,5	1.32	1 (20%)	5,5,5	0.55	0
19	FES	E	501	5	0,4,4	-	-	-	-	-
15	PEE	C	2008	-	20,20,50	1.87	6 (30%)	23,25,55	0.68	0
15	PEE	N	3008	-	4,4,50	3.83	4 (100%)	6,6,55	0.66	0
18	BOG	P	2010	-	12,12,20	1.40	3 (25%)	17,17,25	0.62	0
14	CDL	P	3004	-	39,39,99	1.21	3 (7%)	45,51,111	1.19	4 (8%)
12	HEM	C	502	3	50,50,50	1.81	14 (28%)	67,82,82	1.96	19 (28%)
12	HEM	C	501	3	50,50,50	1.62	6 (12%)	67,82,82	1.64	15 (22%)
12	HEM	P	502	3	50,50,50	1.47	5 (10%)	67,82,82	1.52	10 (14%)
12	HEM	P	501	3	50,50,50	1.55	8 (16%)	67,82,82	1.26	8 (11%)
18	BOG	Q	3009	-	20,20,20	0.95	1 (5%)	25,25,25	0.96	1 (4%)
15	PEE	E	2005	-	49,49,50	1.61	11 (22%)	52,54,55	0.89	3 (5%)
14	CDL	D	2003	-	41,41,99	1.18	2 (4%)	47,53,111	1.09	4 (8%)
15	PEE	P	3007	-	48,48,50	1.40	5 (10%)	51,53,55	0.77	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	UQ	P	3002	-	19,19,63	2.63	10 (52%)	24,26,79	1.33	3 (12%)
17	HEC	D	501	4	46,50,50	2.01	12 (26%)	58,82,82	2.38	18 (31%)
16	GOL	C	2011	-	5,5,5	1.22	0	5,5,5	0.48	0
18	BOG	D	2091	-	13,13,20	1.40	3 (23%)	18,18,25	1.20	2 (11%)
15	PEE	C	2007	-	48,48,50	1.47	6 (12%)	51,53,55	0.82	3 (5%)
13	UQ	C	2002	-	19,19,63	2.73	11 (57%)	24,26,79	1.29	3 (12%)
18	BOG	Q	3091	-	13,13,20	1.42	3 (23%)	18,18,25	1.12	2 (11%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
18	BOG	D	2009	-	20,20,20	1.00	1 (5%)	25,25,25	0.94	1 (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
17	HEC	Q	501	4	-	8/14/54/54	-
14	CDL	Q	3003	-	-	28/51/51/110	-
14	CDL	C	2004	-	-	23/49/49/110	-
15	PEE	R	3005	-	-	28/53/53/54	-
16	GOL	P	3011	-	-	3/4/4/4	-
19	FES	E	501	5	-	-	0/1/1/1
15	PEE	C	2008	-	-	8/24/24/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
14	CDL	P	3004	-	-	21/49/49/110	-
12	HEM	C	502	3	-	7/14/54/54	-
12	HEM	C	501	3	-	7/14/54/54	-
12	HEM	P	502	3	-	6/14/54/54	-
12	HEM	P	501	3	-	7/14/54/54	-
18	BOG	Q	3009	-	-	8/11/31/31	0/1/1/1
15	PEE	E	2005	-	-	28/53/53/54	-
14	CDL	D	2003	-	-	27/51/51/110	-
15	PEE	P	3007	-	-	28/52/52/54	-
13	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
17	HEC	D	501	4	-	8/14/54/54	-
16	GOL	C	2011	-	-	4/4/4/4	-
18	BOG	D	2091	-	-	0/4/24/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEE	C	2007	-	-	29/52/52/54	-
13	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
18	BOG	D	2009	-	-	8/11/31/31	0/1/1/1

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	501	HEM	CBC-CAC	5.52	1.56	1.30
12	C	501	HEM	CBC-CAC	5.42	1.56	1.30
17	Q	501	HEC	CAB-C3B	5.28	1.52	1.35
15	N	3008	PEE	P-O1P	5.23	1.62	1.50
17	Q	501	HEC	CAC-C3C	5.21	1.51	1.35
13	P	3002	UQ	C7-C6	5.04	1.60	1.51
13	C	2002	UQ	C7-C6	5.01	1.60	1.51
13	C	2002	UQ	C6-C5	4.95	1.44	1.35
17	D	501	HEC	CAB-C3B	4.88	1.50	1.35
17	D	501	HEC	CAC-C3C	4.71	1.50	1.35
13	P	3002	UQ	C6-C5	4.68	1.43	1.35
12	P	502	HEM	CBC-CAC	4.49	1.51	1.30
12	P	502	HEM	CBB-CAB	4.38	1.51	1.30
15	C	2007	PEE	C39-C38	4.29	1.56	1.31
13	C	2002	UQ	C6-C1	4.26	1.58	1.46
15	P	3007	PEE	C39-C38	4.21	1.55	1.31
15	R	3005	PEE	C39-C38	4.17	1.55	1.31
15	E	2005	PEE	C39-C38	4.13	1.55	1.31
12	C	502	HEM	CBB-CAB	4.08	1.50	1.30
13	P	3002	UQ	C6-C1	3.83	1.57	1.46
17	D	501	HEC	C3C-C2C	-3.77	1.28	1.41
17	D	501	HEC	C4C-NC	-3.77	1.32	1.39
12	C	502	HEM	CBC-CAC	3.75	1.48	1.30
15	N	3008	PEE	P-O4P	3.69	1.65	1.54
15	E	2005	PEE	O3-C30	3.65	1.44	1.33
13	C	2002	UQ	O3-C3	3.63	1.45	1.36
15	R	3005	PEE	O2-C10	3.63	1.44	1.34
12	C	501	HEM	CBB-CAB	3.61	1.47	1.30
12	P	501	HEM	CBB-CAB	3.59	1.47	1.30
15	E	2005	PEE	O2-C10	3.56	1.44	1.34
17	D	501	HEC	C3B-C2B	-3.49	1.29	1.41
12	P	501	HEM	CAB-C3B	-3.48	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2008	PEE	O3-C30	3.46	1.43	1.33
15	N	3008	PEE	P-O3P	3.38	1.64	1.54
15	R	3005	PEE	O3-C30	3.37	1.43	1.33
15	C	2007	PEE	O3-C30	3.35	1.43	1.33
13	P	3002	UQ	O3-C3	3.34	1.44	1.36
15	R	3005	PEE	P-O1P	3.33	1.62	1.50
15	C	2008	PEE	O2-C10	3.32	1.43	1.34
12	C	502	HEM	C4C-NC	-3.28	1.33	1.39
15	P	3007	PEE	O3-C30	3.28	1.42	1.33
15	C	2008	PEE	P-O1P	3.27	1.62	1.50
12	C	502	HEM	C4D-C3D	3.26	1.50	1.45
15	P	3007	PEE	C21-C22	-3.23	1.35	1.51
15	E	2005	PEE	P-O1P	3.23	1.62	1.50
15	R	3005	PEE	C21-C22	-3.21	1.35	1.51
12	P	502	HEM	CAC-C3C	-3.18	1.38	1.47
15	E	2005	PEE	C21-C22	-3.17	1.36	1.51
15	C	2007	PEE	P-O1P	3.15	1.61	1.50
12	C	501	HEM	CAB-C3B	-3.12	1.39	1.47
17	D	501	HEC	C1A-C2A	3.06	1.50	1.45
12	P	502	HEM	CAB-C3B	-3.05	1.39	1.47
15	C	2007	PEE	C21-C22	-2.98	1.37	1.51
13	C	2002	UQ	O2-C2	2.97	1.43	1.36
15	P	3007	PEE	O2-C10	2.94	1.42	1.34
17	D	501	HEC	C1D-ND	-2.93	1.34	1.39
15	C	2007	PEE	O2-C10	2.91	1.42	1.34
15	E	2005	PEE	C31-C30	2.89	1.59	1.50
15	P	3007	PEE	P-O1P	2.86	1.60	1.50
13	C	2002	UQ	C3-C4	2.86	1.57	1.48
13	C	2002	UQ	C2-C1	2.85	1.57	1.48
12	C	502	HEM	C3B-C4B	2.84	1.50	1.44
13	P	3002	UQ	O2-C2	2.80	1.43	1.36
13	P	3002	UQ	C2-C1	2.80	1.56	1.48
13	P	3002	UQ	C7-C8	2.80	1.55	1.50
12	C	502	HEM	CAC-C3C	-2.79	1.39	1.47
17	D	501	HEC	C1B-NB	-2.77	1.34	1.39
12	C	502	HEM	CAB-C3B	-2.76	1.40	1.47
13	C	2002	UQ	CM5-C5	2.75	1.56	1.50
13	C	2002	UQ	C7-C8	2.73	1.54	1.50
17	Q	501	HEC	C1D-ND	-2.73	1.34	1.39
13	P	3002	UQ	C5-C4	2.70	1.56	1.47
12	C	501	HEM	CHD-C4C	-2.69	1.33	1.38
12	C	502	HEM	C3C-C2C	-2.68	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C1A-NA	-2.66	1.34	1.39
13	P	3002	UQ	CM5-C5	2.66	1.56	1.50
17	D	501	HEC	C4D-C3D	2.61	1.49	1.44
18	D	2091	BOG	C4-C5	2.59	1.58	1.53
12	C	502	HEM	CHA-C1A	-2.59	1.33	1.39
12	C	502	HEM	C1B-C2B	2.58	1.49	1.44
17	Q	501	HEC	C3B-C2B	-2.58	1.32	1.41
18	Q	3091	BOG	C4-C5	2.56	1.58	1.53
13	P	3002	UQ	C3-C4	2.55	1.56	1.48
17	D	501	HEC	C3D-C2D	-2.55	1.32	1.38
15	R	3005	PEE	C31-C30	2.54	1.58	1.50
13	C	2002	UQ	C5-C4	2.54	1.55	1.47
12	P	501	HEM	CAC-C3C	-2.53	1.40	1.47
15	N	3008	PEE	P-O2P	2.50	1.61	1.54
15	R	3005	PEE	C11-C10	2.50	1.58	1.50
18	P	2010	BOG	C4-C5	2.49	1.58	1.53
18	Q	3091	BOG	O5-C1	2.48	1.48	1.41
12	P	501	HEM	C1A-NA	-2.46	1.35	1.39
18	D	2091	BOG	O5-C1	2.46	1.48	1.41
17	Q	501	HEC	CHA-C4D	-2.41	1.34	1.39
17	Q	501	HEC	C3C-C2C	-2.40	1.33	1.41
15	E	2005	PEE	C3-C2	2.39	1.58	1.50
18	P	2010	BOG	C1-C2	2.38	1.57	1.52
15	E	2005	PEE	C11-C10	2.36	1.57	1.50
18	D	2009	BOG	O5-C1	2.35	1.47	1.41
14	D	2003	CDL	O1-C1	2.34	1.50	1.43
12	C	502	HEM	C3D-C2D	-2.33	1.31	1.36
12	P	501	HEM	CHD-C4C	-2.32	1.33	1.38
14	P	3004	CDL	O1-C1	2.32	1.50	1.43
17	Q	501	HEC	C4C-NC	-2.30	1.35	1.39
15	E	2005	PEE	C1-C2	2.28	1.57	1.50
15	C	2008	PEE	C1-C2	2.28	1.57	1.50
12	P	502	HEM	C3B-C4B	2.27	1.49	1.44
15	C	2008	PEE	C11-C10	2.26	1.57	1.50
18	Q	3009	BOG	O5-C1	2.25	1.47	1.41
15	R	3005	PEE	C3-C2	2.25	1.57	1.50
12	C	502	HEM	C1C-C2C	2.24	1.49	1.45
14	Q	3003	CDL	O1-C1	2.23	1.49	1.43
14	C	2004	CDL	O1-C1	2.23	1.49	1.43
15	C	2008	PEE	C3-C2	2.21	1.57	1.50
15	E	2005	PEE	P-O4P	2.21	1.68	1.59
12	C	501	HEM	C1A-NA	-2.19	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	501	HEM	CAC-C3C	-2.17	1.41	1.47
17	Q	501	HEC	C3B-C4B	-2.16	1.42	1.46
15	R	3005	PEE	O2-C2	2.15	1.51	1.46
15	E	2005	PEE	O2-C2	2.14	1.51	1.46
12	P	501	HEM	C1C-NC	-2.13	1.35	1.39
17	Q	501	HEC	C1B-NB	-2.13	1.35	1.39
17	D	501	HEC	CHD-C1D	-2.11	1.34	1.39
14	P	3004	CDL	OB2-CB2	-2.11	1.36	1.44
13	C	2002	UQ	C8-C9	2.10	1.37	1.33
12	P	501	HEM	CHD-C1D	-2.10	1.34	1.39
15	R	3005	PEE	C1-C2	2.10	1.57	1.50
17	D	501	HEC	CHA-C1A	-2.09	1.34	1.38
18	P	2010	BOG	O5-C1	2.09	1.48	1.42
14	D	2003	CDL	OA6-CA5	2.08	1.40	1.34
17	Q	501	HEC	CHC-C4B	-2.07	1.34	1.38
18	Q	3091	BOG	C1-C2	2.07	1.58	1.52
14	P	3004	CDL	OB8-CB7	2.03	1.39	1.33
16	P	3011	GOL	O2-C2	2.02	1.49	1.43
12	C	502	HEM	C2A-C3A	-2.01	1.33	1.38
14	C	2004	CDL	OA6-CA4	-2.01	1.41	1.46
18	D	2091	BOG	C1-C2	2.00	1.58	1.52
15	C	2007	PEE	C3-C2	2.00	1.57	1.50

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CBB-CAB-C3B	-9.73	107.99	127.43
17	Q	501	HEC	CBC-CAC-C3C	-8.30	110.84	127.43
17	Q	501	HEC	CBB-CAB-C3B	-8.21	111.03	127.43
17	D	501	HEC	CBC-CAC-C3C	-6.85	113.75	127.43
12	C	502	HEM	C3B-C2B-C1B	-6.48	101.54	106.41
12	P	502	HEM	CAD-C3D-C4D	4.75	132.97	124.70
12	C	502	HEM	CAD-C3D-C4D	4.74	132.97	124.70
17	Q	501	HEC	CAA-C2A-C1A	4.70	134.40	124.85
12	C	502	HEM	C2B-C1B-NB	4.49	115.00	109.84
17	D	501	HEC	CAA-C2A-C1A	4.43	133.87	124.85
13	C	2002	UQ	C8-C7-C6	4.38	122.88	112.08
12	C	501	HEM	C3B-C2B-C1B	-4.34	103.15	106.41
13	P	3002	UQ	C8-C7-C6	4.34	122.76	112.08
18	D	2091	BOG	C1'-O1-C1	4.15	119.56	113.26
18	Q	3009	BOG	C1'-O1-C1	3.83	120.22	113.68
18	D	2009	BOG	C1'-O1-C1	3.78	120.13	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	HEM	CMB-C2B-C1B	3.72	130.85	125.03
12	C	502	HEM	CMC-C2C-C1C	3.68	131.22	124.73
14	P	3004	CDL	CB4-OB6-CB5	-3.65	109.06	117.80
12	C	501	HEM	CAD-C3D-C4D	3.61	130.98	124.70
17	D	501	HEC	CAA-C2A-C3A	-3.59	121.14	127.87
12	C	501	HEM	CAD-C3D-C2D	-3.54	121.23	127.87
12	C	502	HEM	CHD-C1D-ND	-3.49	120.67	124.42
14	C	2004	CDL	CA4-OA6-CA5	-3.48	109.47	117.80
18	Q	3091	BOG	C1'-O1-C1	3.45	118.50	113.26
14	C	2004	CDL	CB4-OB6-CB5	-3.43	109.58	117.80
17	Q	501	HEC	CAD-C3D-C4D	3.43	131.63	124.94
12	C	502	HEM	CAD-C3D-C2D	-3.38	121.54	127.87
12	P	502	HEM	C2B-C1B-NB	3.35	113.69	109.84
12	P	502	HEM	C3B-C2B-C1B	-3.35	103.89	106.41
17	D	501	HEC	CMA-C3A-C4A	3.35	130.63	124.73
17	Q	501	HEC	CAA-C2A-C3A	-3.31	121.67	127.87
12	C	501	HEM	C3B-C4B-NB	3.28	111.83	109.47
12	P	502	HEM	CAD-C3D-C2D	-3.27	121.75	127.87
17	D	501	HEC	C2A-C1A-NA	3.23	113.44	110.32
12	P	502	HEM	CMB-C2B-C1B	3.21	130.06	125.03
14	P	3004	CDL	CA4-OA6-CA5	-3.21	110.12	117.80
17	D	501	HEC	CAD-C3D-C4D	3.18	131.16	124.94
17	D	501	HEC	CMB-C2B-C1B	3.17	130.25	125.42
17	D	501	HEC	CMC-C2C-C1C	3.07	130.10	125.42
12	C	502	HEM	C2D-C1D-ND	3.06	113.44	109.90
17	Q	501	HEC	CMB-C2B-C1B	3.05	130.07	125.42
13	P	3002	UQ	C7-C6-C1	-3.00	115.03	118.52
17	D	501	HEC	C3D-C4D-ND	2.94	113.41	110.15
15	C	2007	PEE	C22-C21-C20	2.91	127.86	113.86
17	D	501	HEC	CMD-C2D-C1D	2.90	129.83	125.42
15	E	2005	PEE	C22-C21-C20	2.87	127.66	113.86
12	P	502	HEM	C3B-C4B-NB	2.86	111.53	109.47
17	Q	501	HEC	CBA-CAA-C2A	2.85	120.41	112.53
12	C	502	HEM	C3B-C4B-NB	2.83	111.50	109.47
15	R	3005	PEE	C22-C21-C20	2.82	127.43	113.86
12	C	502	HEM	C3C-C2C-C1C	-2.81	104.39	107.05
17	D	501	HEC	C4D-C3D-C2D	-2.80	102.53	106.87
12	C	502	HEM	CMB-C2B-C1B	2.80	129.41	125.03
12	P	501	HEM	CAD-C3D-C4D	2.79	129.57	124.70
12	C	502	HEM	CMD-C2D-C1D	2.78	129.38	125.03
13	C	2002	UQ	C7-C6-C1	-2.78	115.28	118.52
15	P	3007	PEE	C22-C21-C20	2.76	127.13	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	501	HEC	C1A-C2A-C3A	-2.76	103.48	107.11
17	D	501	HEC	C1A-C2A-C3A	-2.74	103.50	107.11
12	P	501	HEM	CMB-C2B-C1B	2.71	129.28	125.03
15	C	2007	PEE	C21-C22-C23	2.68	127.93	114.37
17	Q	501	HEC	C3D-C4D-ND	2.65	113.09	110.15
12	C	501	HEM	C2B-C1B-NB	2.64	112.88	109.84
12	P	501	HEM	C4C-C3C-C2C	-2.63	104.54	106.81
12	P	501	HEM	CAD-C3D-C2D	-2.60	122.99	127.87
15	P	3007	PEE	C21-C22-C23	2.59	127.48	114.37
12	C	502	HEM	C4D-ND-C1D	-2.59	102.14	105.21
12	C	501	HEM	C4C-CHD-C1D	-2.58	120.53	126.02
18	Q	3091	BOG	O1-C1-C2	2.58	111.12	108.14
14	D	2003	CDL	CB4-OB6-CB5	-2.57	111.65	117.80
15	E	2005	PEE	C21-C22-C23	2.54	127.19	114.37
14	Q	3003	CDL	CB4-OB6-CB5	-2.53	111.75	117.80
12	P	502	HEM	CHC-C1C-NC	-2.45	121.79	124.45
17	D	501	HEC	C4B-NB-C1B	-2.40	101.90	105.82
17	D	501	HEC	CHC-C4B-NB	-2.38	121.86	124.45
15	R	3005	PEE	C21-C22-C23	2.38	126.39	114.37
17	Q	501	HEC	C4D-C3D-C2D	-2.35	103.23	106.87
14	P	3004	CDL	OB6-CB4-CB3	2.35	116.77	108.34
18	D	2091	BOG	O1-C1-C2	2.34	110.84	108.14
14	D	2003	CDL	CA6-CA4-CA3	-2.34	106.33	111.78
15	R	3005	PEE	O3-C3-C2	2.29	115.01	108.40
12	C	501	HEM	C4C-NC-C1C	-2.27	102.11	105.82
12	P	501	HEM	C2B-C1B-NB	2.27	112.45	109.84
12	C	501	HEM	CMA-C3A-C2A	2.27	130.43	125.62
17	Q	501	HEC	CMC-C2C-C1C	2.27	128.87	125.42
13	P	3002	UQ	C10-C9-C8	-2.26	117.82	123.63
14	Q	3003	CDL	CA6-CA4-CA3	-2.24	106.56	111.78
12	C	502	HEM	CHA-C4D-ND	-2.24	121.60	124.37
12	C	502	HEM	CHD-C4C-NC	-2.22	122.03	124.45
14	Q	3003	CDL	CA4-OA6-CA5	-2.20	112.52	117.80
12	C	501	HEM	CBB-CAB-C3B	-2.20	116.54	127.53
12	P	502	HEM	C2D-C1D-ND	2.20	112.44	109.90
12	C	502	HEM	CHC-C1C-NC	-2.20	122.06	124.45
17	D	501	HEC	CHA-C1A-NA	-2.19	122.07	124.45
17	D	501	HEC	C4A-NA-C1A	-2.19	102.26	105.82
15	E	2005	PEE	O3-C3-C2	2.19	114.70	108.40
12	P	501	HEM	CBB-CAB-C3B	-2.17	116.66	127.53
12	C	502	HEM	C2A-C1A-NA	2.17	112.56	110.15
14	P	3004	CDL	CA6-CA4-CA3	-2.15	106.78	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	HEM	C2C-C1C-NC	2.14	113.60	109.64
14	D	2003	CDL	CA6-OA8-CA7	-2.13	111.81	117.08
12	C	502	HEM	CAA-C2A-C1A	2.13	129.11	124.94
17	D	501	HEC	CBA-CAA-C2A	2.13	118.42	112.53
17	Q	501	HEC	CHA-C1A-NA	-2.12	122.14	124.45
12	C	502	HEM	C3D-C4D-ND	2.12	112.49	110.17
14	Q	3003	CDL	CA6-OA8-CA7	-2.10	111.89	117.08
12	P	502	HEM	CHB-C4A-C3A	-2.10	121.33	127.43
13	C	2002	UQ	C10-C9-C8	-2.10	118.24	123.63
12	P	502	HEM	C3C-C2C-C1C	-2.09	105.07	107.05
12	C	502	HEM	C4A-NA-C1A	-2.07	102.45	105.82
12	C	501	HEM	CBD-CAD-C3D	2.06	118.23	112.53
15	C	2007	PEE	O3-C3-C2	2.06	114.32	108.40
12	P	501	HEM	C3B-C4B-NB	2.05	110.94	109.47
14	C	2004	CDL	OB6-CB4-CB3	2.04	115.65	108.34
12	C	501	HEM	CHD-C4C-C3C	-2.03	121.78	125.21
12	C	501	HEM	CHD-C1D-C2D	-2.03	121.82	125.03
14	D	2003	CDL	CA4-OA6-CA5	-2.03	112.95	117.80
12	C	501	HEM	CHB-C4A-C3A	-2.01	121.61	127.43
12	P	501	HEM	C3B-C2B-C1B	-2.00	104.91	106.41

There are no chirality outliers.

All (298) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	501	HEM	C2B-C3B-CAB-CBB
12	C	501	HEM	C4B-C3B-CAB-CBB
12	P	501	HEM	C2B-C3B-CAB-CBB
12	P	501	HEM	C4B-C3B-CAB-CBB
13	C	2002	UQ	C1-C6-C7-C8
13	C	2002	UQ	C5-C6-C7-C8
13	C	2002	UQ	C12-C11-C9-C8
13	P	3002	UQ	C1-C6-C7-C8
13	P	3002	UQ	C5-C6-C7-C8
13	P	3002	UQ	C12-C11-C9-C8
14	C	2004	CDL	O1-C1-CA2-OA2
14	C	2004	CDL	CA3-OA5-PA1-OA2
14	C	2004	CDL	CA3-OA5-PA1-OA3
14	C	2004	CDL	CA3-OA5-PA1-OA4
14	C	2004	CDL	C51-CB5-OB6-CB4
14	D	2003	CDL	CB2-OB2-PB2-OB4
14	D	2003	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
14	D	2003	CDL	CB3-OB5-PB2-OB4
14	P	3004	CDL	O1-C1-CA2-OA2
14	P	3004	CDL	CA3-OA5-PA1-OA2
14	P	3004	CDL	CA3-OA5-PA1-OA3
14	P	3004	CDL	CA3-OA5-PA1-OA4
14	P	3004	CDL	C51-CB5-OB6-CB4
14	Q	3003	CDL	CB2-OB2-PB2-OB4
14	Q	3003	CDL	CB2-OB2-PB2-OB5
14	Q	3003	CDL	CB3-OB5-PB2-OB4
15	C	2007	PEE	C1-O3P-P-O2P
15	C	2007	PEE	C1-O3P-P-O4P
15	C	2007	PEE	C4-O4P-P-O3P
15	C	2007	PEE	C4-O4P-P-O2P
15	C	2007	PEE	C4-O4P-P-O1P
15	C	2007	PEE	O4P-C4-C5-N
15	C	2008	PEE	C4-O4P-P-O3P
15	C	2008	PEE	C4-O4P-P-O2P
15	C	2008	PEE	C4-O4P-P-O1P
15	E	2005	PEE	C11-C10-O2-C2
15	E	2005	PEE	C4-O4P-P-O3P
15	E	2005	PEE	C4-O4P-P-O2P
15	P	3007	PEE	C1-O3P-P-O2P
15	P	3007	PEE	C1-O3P-P-O4P
15	P	3007	PEE	C4-O4P-P-O3P
15	P	3007	PEE	C4-O4P-P-O2P
15	P	3007	PEE	C4-O4P-P-O1P
15	P	3007	PEE	O4P-C4-C5-N
15	R	3005	PEE	C11-C10-O2-C2
15	R	3005	PEE	C4-O4P-P-O3P
15	R	3005	PEE	C4-O4P-P-O2P
16	C	2011	GOL	O1-C1-C2-C3
16	C	2011	GOL	C1-C2-C3-O3
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
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	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	Q	501	HEC	C4C-C3C-CAC-CBC
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
14	P	3004	CDL	C31-CA7-OA8-CA6
14	C	2004	CDL	OB9-CB7-OB8-CB6
14	P	3004	CDL	OB9-CB7-OB8-CB6
15	E	2005	PEE	O5-C30-O3-C3
15	R	3005	PEE	O5-C30-O3-C3
14	C	2004	CDL	C31-CA7-OA8-CA6
14	D	2003	CDL	C31-CA7-OA8-CA6
14	Q	3003	CDL	C31-CA7-OA8-CA6
14	C	2004	CDL	OB7-CB5-OB6-CB4
14	P	3004	CDL	OB7-CB5-OB6-CB4
15	E	2005	PEE	O4-C10-O2-C2
15	R	3005	PEE	O4-C10-O2-C2
15	R	3005	PEE	C31-C30-O3-C3
14	C	2004	CDL	OA9-CA7-OA8-CA6
14	P	3004	CDL	OA9-CA7-OA8-CA6
14	C	2004	CDL	C71-CB7-OB8-CB6
14	P	3004	CDL	C71-CB7-OB8-CB6
15	E	2005	PEE	C31-C30-O3-C3
17	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	3091	BOG	C4-C5-C6-O6
14	D	2003	CDL	OA9-CA7-OA8-CA6
14	Q	3003	CDL	OA9-CA7-OA8-CA6
18	Q	3091	BOG	O5-C5-C6-O6
14	D	2003	CDL	C71-CB7-OB8-CB6
14	Q	3003	CDL	C71-CB7-OB8-CB6
15	C	2007	PEE	C17-C18-C19-C20
18	D	2009	BOG	C4-C5-C6-O6
14	D	2003	CDL	OB9-CB7-OB8-CB6
14	Q	3003	CDL	OB9-CB7-OB8-CB6
14	D	2003	CDL	CB7-C71-C72-C73
14	Q	3003	CDL	CB7-C71-C72-C73
14	Q	3003	CDL	O1-C1-CA2-OA2
18	D	2009	BOG	O1-C1'-C2'-C3'
15	P	3007	PEE	C17-C18-C19-C20
18	Q	3009	BOG	O1-C1'-C2'-C3'
14	C	2004	CDL	CB2-C1-CA2-OA2
14	P	3004	CDL	CB2-C1-CA2-OA2
14	C	2004	CDL	C11-CA5-OA6-CA4
14	P	3004	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
14	C	2004	CDL	OA7-CA5-OA6-CA4
18	D	2009	BOG	C2-C1-O1-C1'
18	Q	3009	BOG	C2-C1-O1-C1'
14	D	2003	CDL	O1-C1-CA2-OA2
18	D	2009	BOG	O5-C5-C6-O6
17	D	501	HEC	C1A-C2A-CAA-CBA
14	P	3004	CDL	OA7-CA5-OA6-CA4
16	C	2011	GOL	O1-C1-C2-O2
16	C	2011	GOL	O2-C2-C3-O3
16	P	3011	GOL	O2-C2-C3-O3
15	C	2007	PEE	C41-C42-C43-C44
15	P	3007	PEE	C41-C42-C43-C44
15	R	3005	PEE	C34-C35-C36-C37
15	E	2005	PEE	C34-C35-C36-C37
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
18	D	2009	BOG	C1'-C2'-C3'-C4'
18	Q	3009	BOG	C1'-C2'-C3'-C4'
14	D	2003	CDL	C51-CB5-OB6-CB4
14	Q	3003	CDL	C51-CB5-OB6-CB4
12	C	502	HEM	C4D-C3D-CAD-CBD
14	Q	3003	CDL	OB7-CB5-OB6-CB4
15	C	2007	PEE	C15-C16-C17-C18
15	C	2007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C15-C16-C17-C18
15	P	3007	PEE	C35-C36-C37-C38
15	C	2007	PEE	C10-C11-C12-C13
15	P	3007	PEE	C31-C32-C33-C34
15	C	2007	PEE	C31-C32-C33-C34
15	R	3005	PEE	C20-C21-C22-C23
15	E	2005	PEE	C35-C36-C37-C38
15	R	3005	PEE	C35-C36-C37-C38
15	R	3005	PEE	C42-C43-C44-C45
14	D	2003	CDL	OB7-CB5-OB6-CB4
15	E	2005	PEE	C42-C43-C44-C45
15	E	2005	PEE	C39-C40-C41-C42
15	R	3005	PEE	C39-C40-C41-C42
15	R	3005	PEE	O3P-C1-C2-C3
15	E	2005	PEE	C20-C21-C22-C23
15	C	2008	PEE	C11-C10-O2-C2
15	R	3005	PEE	C23-C24-C25-C26
12	P	502	HEM	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
15	C	2007	PEE	C42-C43-C44-C45
15	P	3007	PEE	C42-C43-C44-C45
15	E	2005	PEE	C23-C24-C25-C26
15	P	3007	PEE	C10-C11-C12-C13
18	Q	3009	BOG	C4-C5-C6-O6
14	D	2003	CDL	OB5-CB3-CB4-OB6
14	Q	3003	CDL	OB5-CB3-CB4-OB6
15	E	2005	PEE	O3P-C1-C2-O2
15	C	2007	PEE	C43-C44-C45-C46
15	P	3007	PEE	C43-C44-C45-C46
15	E	2005	PEE	C40-C41-C42-C43
15	C	2007	PEE	C11-C12-C13-C14
14	Q	3003	CDL	C71-C72-C73-C74
15	P	3007	PEE	C11-C12-C13-C14
14	D	2003	CDL	OA5-CA3-CA4-CA6
14	Q	3003	CDL	OA5-CA3-CA4-CA6
15	E	2005	PEE	O3P-C1-C2-C3
14	D	2003	CDL	C71-C72-C73-C74
15	P	3007	PEE	C40-C41-C42-C43
13	C	2002	UQ	C12-C11-C9-C10
13	P	3002	UQ	C12-C11-C9-C10
14	C	2004	CDL	CA3-CA4-CA6-OA8
14	P	3004	CDL	CA3-CA4-CA6-OA8
15	R	3005	PEE	C40-C41-C42-C43
18	D	2009	BOG	C4'-C5'-C6'-C7'
15	P	3007	PEE	C14-C15-C16-C17
15	R	3005	PEE	C21-C22-C23-C24
14	C	2004	CDL	OB5-CB3-CB4-OB6
14	P	3004	CDL	OB5-CB3-CB4-OB6
14	Q	3003	CDL	OA5-CA3-CA4-OA6
15	C	2007	PEE	O3P-C1-C2-O2
15	P	3007	PEE	O3P-C1-C2-O2
15	R	3005	PEE	O3P-C1-C2-O2
14	C	2004	CDL	OA6-CA4-CA6-OA8
14	P	3004	CDL	OA6-CA4-CA6-OA8
15	E	2005	PEE	C10-C11-C12-C13
15	R	3005	PEE	C10-C11-C12-C13
15	E	2005	PEE	C21-C22-C23-C24
15	C	2007	PEE	C40-C41-C42-C43
16	P	3011	GOL	O1-C1-C2-O2
18	Q	3009	BOG	O5-C5-C6-O6
15	E	2005	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
15	C	2008	PEE	O3P-C1-C2-C3
18	D	2009	BOG	C2'-C3'-C4'-C5'
15	C	2007	PEE	C12-C13-C14-C15
15	E	2005	PEE	C33-C34-C35-C36
15	R	3005	PEE	C31-C32-C33-C34
15	R	3005	PEE	C33-C34-C35-C36
15	R	3005	PEE	C30-C31-C32-C33
15	C	2008	PEE	O4-C10-O2-C2
12	C	501	HEM	C2C-C3C-CAC-CBC
12	P	501	HEM	C2C-C3C-CAC-CBC
14	D	2003	CDL	OA5-CA3-CA4-OA6
15	C	2008	PEE	O3P-C1-C2-O2
15	P	3007	PEE	C12-C13-C14-C15
15	C	2007	PEE	C14-C15-C16-C17
14	P	3004	CDL	OB5-CB3-CB4-CB6
15	E	2005	PEE	C41-C42-C43-C44
18	Q	3009	BOG	C4'-C5'-C6'-C7'
15	R	3005	PEE	C22-C23-C24-C25
15	E	2005	PEE	C14-C15-C16-C17
14	C	2004	CDL	CB3-OB5-PB2-OB2
14	C	2004	CDL	CB3-OB5-PB2-OB4
14	D	2003	CDL	CA3-OA5-PA1-OA2
14	D	2003	CDL	CA3-OA5-PA1-OA3
14	D	2003	CDL	CA3-OA5-PA1-OA4
14	D	2003	CDL	CB3-OB5-PB2-OB2
14	D	2003	CDL	CB3-OB5-PB2-OB3
14	P	3004	CDL	CB3-OB5-PB2-OB2
14	P	3004	CDL	CB3-OB5-PB2-OB4
14	Q	3003	CDL	CA3-OA5-PA1-OA2
14	Q	3003	CDL	CA3-OA5-PA1-OA3
14	Q	3003	CDL	CA3-OA5-PA1-OA4
14	Q	3003	CDL	CB3-OB5-PB2-OB2
14	Q	3003	CDL	CB3-OB5-PB2-OB3
15	C	2008	PEE	C1-O3P-P-O1P
15	E	2005	PEE	C30-C31-C32-C33
15	E	2005	PEE	C19-C20-C21-C22
18	Q	3009	BOG	C2'-C3'-C4'-C5'
15	R	3005	PEE	C14-C15-C16-C17
15	E	2005	PEE	C43-C44-C45-C46
14	D	2003	CDL	OB5-CB3-CB4-CB6
14	Q	3003	CDL	OB5-CB3-CB4-CB6
15	R	3005	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	O4-C10-O2-C2
15	C	2007	PEE	O2-C2-C3-O3
15	P	3007	PEE	C20-C21-C22-C23
15	P	3007	PEE	C11-C10-O2-C2
15	P	3007	PEE	C19-C20-C21-C22
15	C	2007	PEE	C20-C21-C22-C23
15	R	3005	PEE	C43-C44-C45-C46
15	E	2005	PEE	C22-C23-C24-C25
12	C	502	HEM	C2C-C3C-CAC-CBC
14	C	2004	CDL	OB5-CB3-CB4-CB6
12	C	501	HEM	C4C-C3C-CAC-CBC
14	D	2003	CDL	OA6-CA4-CA6-OA8
14	Q	3003	CDL	OA6-CA4-CA6-OA8
15	P	3007	PEE	O2-C2-C3-O3
14	C	2004	CDL	CB5-C51-C52-C53
14	P	3004	CDL	C1-CB2-OB2-PB2
15	C	2007	PEE	C19-C20-C21-C22
15	R	3005	PEE	C19-C20-C21-C22
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAD-CBD-CGD-O1D
15	E	2005	PEE	C1-C2-O2-C10
15	R	3005	PEE	C1-C2-O2-C10
15	E	2005	PEE	C11-C12-C13-C14
12	C	502	HEM	CAA-CBA-CGA-O2A
12	P	502	HEM	CAA-CBA-CGA-O2A
14	D	2003	CDL	C1-CA2-OA2-PA1
14	Q	3003	CDL	C1-CA2-OA2-PA1
12	P	502	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAA-CBA-CGA-O1A
17	Q	501	HEC	CAA-CBA-CGA-O2A
14	C	2004	CDL	C1-CB2-OB2-PB2
15	C	2007	PEE	O4-C10-O2-C2
15	C	2007	PEE	C38-C39-C40-C41
12	C	501	HEM	CAA-CBA-CGA-O2A
15	R	3005	PEE	C11-C12-C13-C14
17	Q	501	HEC	CAA-CBA-CGA-O1A
15	P	3007	PEE	C38-C39-C40-C41
15	R	3005	PEE	C38-C39-C40-C41
12	P	501	HEM	CAA-CBA-CGA-O2A
14	Q	3003	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
12	C	501	HEM	CAA-CBA-CGA-O1A
15	P	3007	PEE	C16-C17-C18-C19
12	P	501	HEM	C4C-C3C-CAC-CBC
17	D	501	HEC	CAA-CBA-CGA-O2A
14	P	3004	CDL	OB6-CB4-CB6-OB8
12	P	501	HEM	CAA-CBA-CGA-O1A
15	E	2005	PEE	C38-C39-C40-C41
14	C	2004	CDL	C12-C11-CA5-OA6
14	Q	3003	CDL	CB4-CB3-OB5-PB2
15	C	2007	PEE	C16-C17-C18-C19
15	C	2007	PEE	C11-C10-O2-C2
15	P	3007	PEE	O2-C10-C11-C12
15	C	2007	PEE	C33-C34-C35-C36
15	C	2007	PEE	O2-C10-C11-C12
14	D	2003	CDL	CB4-CB3-OB5-PB2
14	D	2003	CDL	CA3-CA4-CA6-OA8
14	Q	3003	CDL	CA3-CA4-CA6-OA8
14	D	2003	CDL	C72-C71-CB7-OB8
14	Q	3003	CDL	C72-C71-CB7-OB8
17	D	501	HEC	CAA-CBA-CGA-O1A
15	P	3007	PEE	O4-C10-C11-C12
15	C	2007	PEE	O4-C10-C11-C12
12	C	501	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAD-CBD-CGD-O2D
14	Q	3003	CDL	C72-C71-CB7-OB9
14	C	2004	CDL	OB6-CB4-CB6-OB8
12	C	502	HEM	C2B-C3B-CAB-CBB
12	P	502	HEM	C2B-C3B-CAB-CBB
14	D	2003	CDL	C72-C71-CB7-OB9

There are no ring outliers.

17 monomers are involved in 41 short contacts:

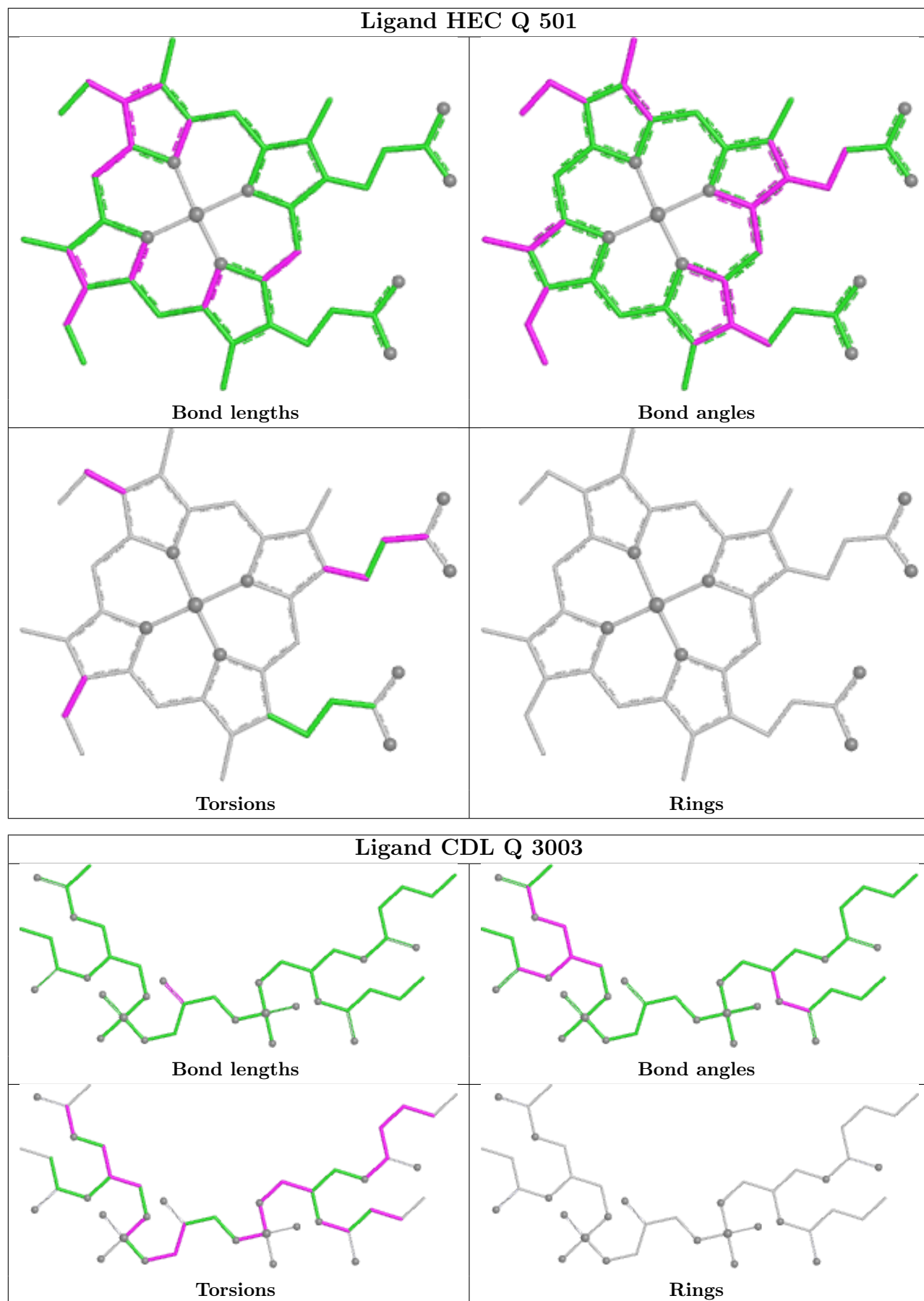
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Q	3003	CDL	3	0
14	C	2004	CDL	2	0
19	E	501	FES	2	0
18	P	2010	BOG	1	0
14	P	3004	CDL	2	0
12	C	502	HEM	1	0
12	C	501	HEM	5	0
12	P	502	HEM	3	0

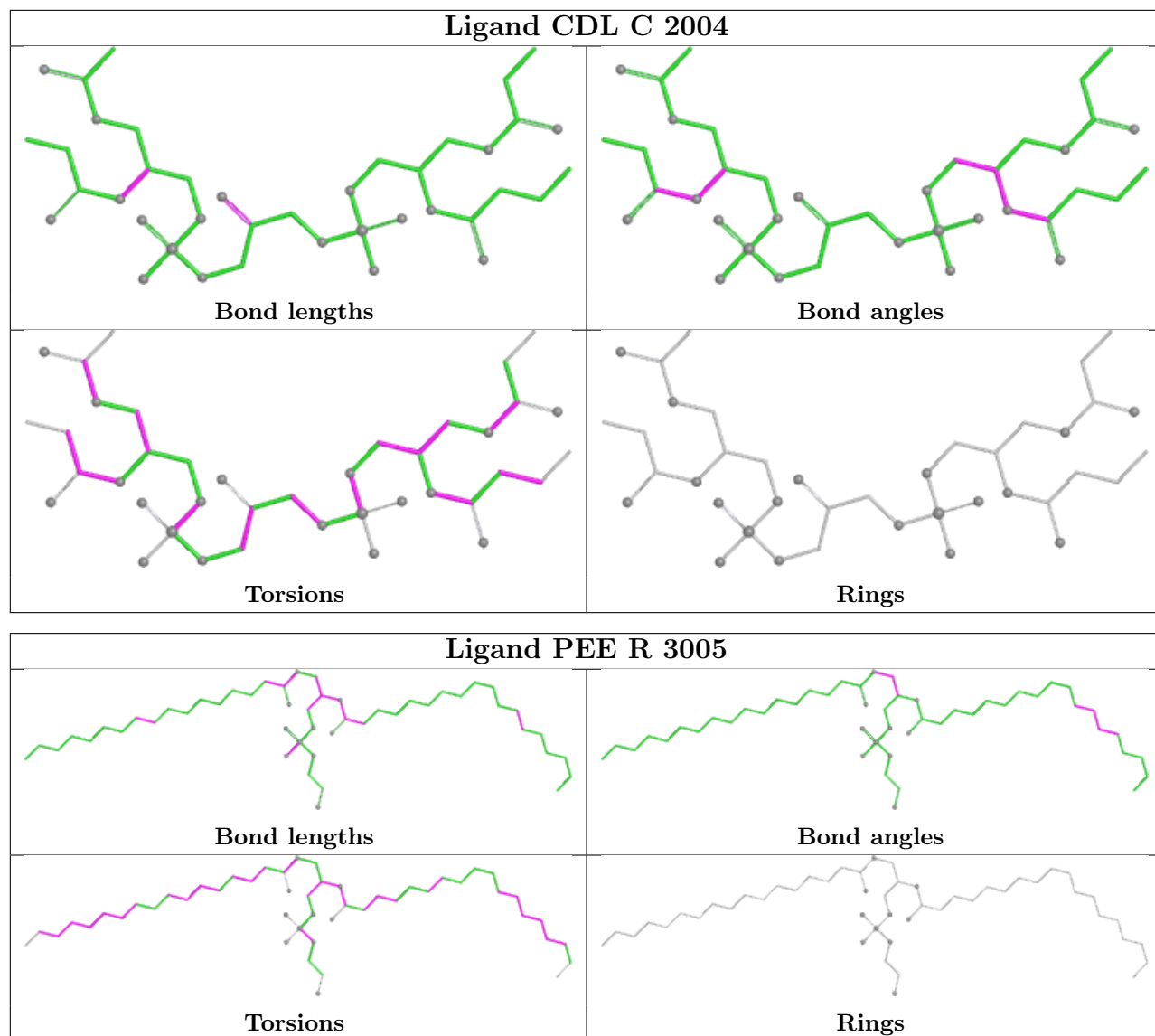
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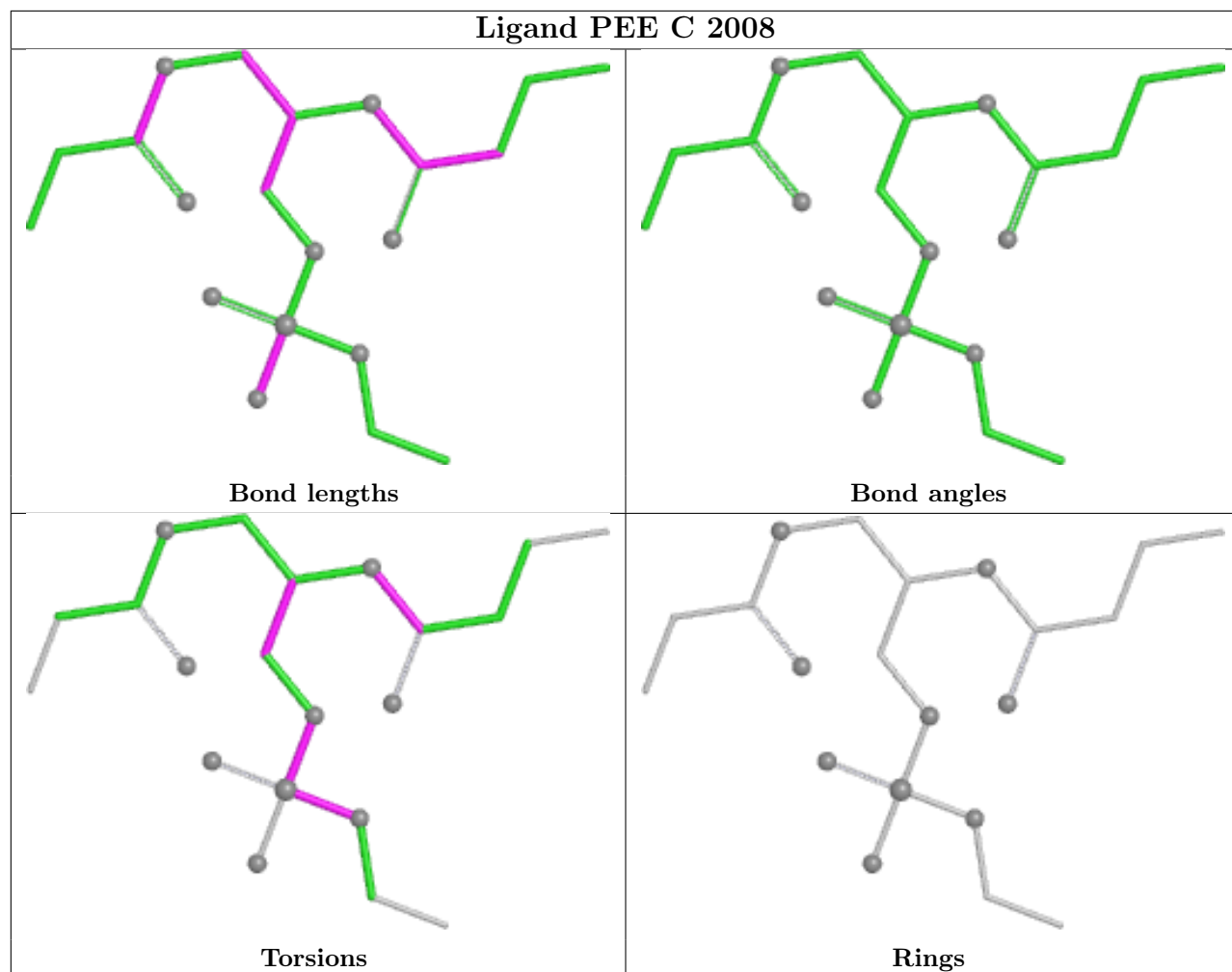
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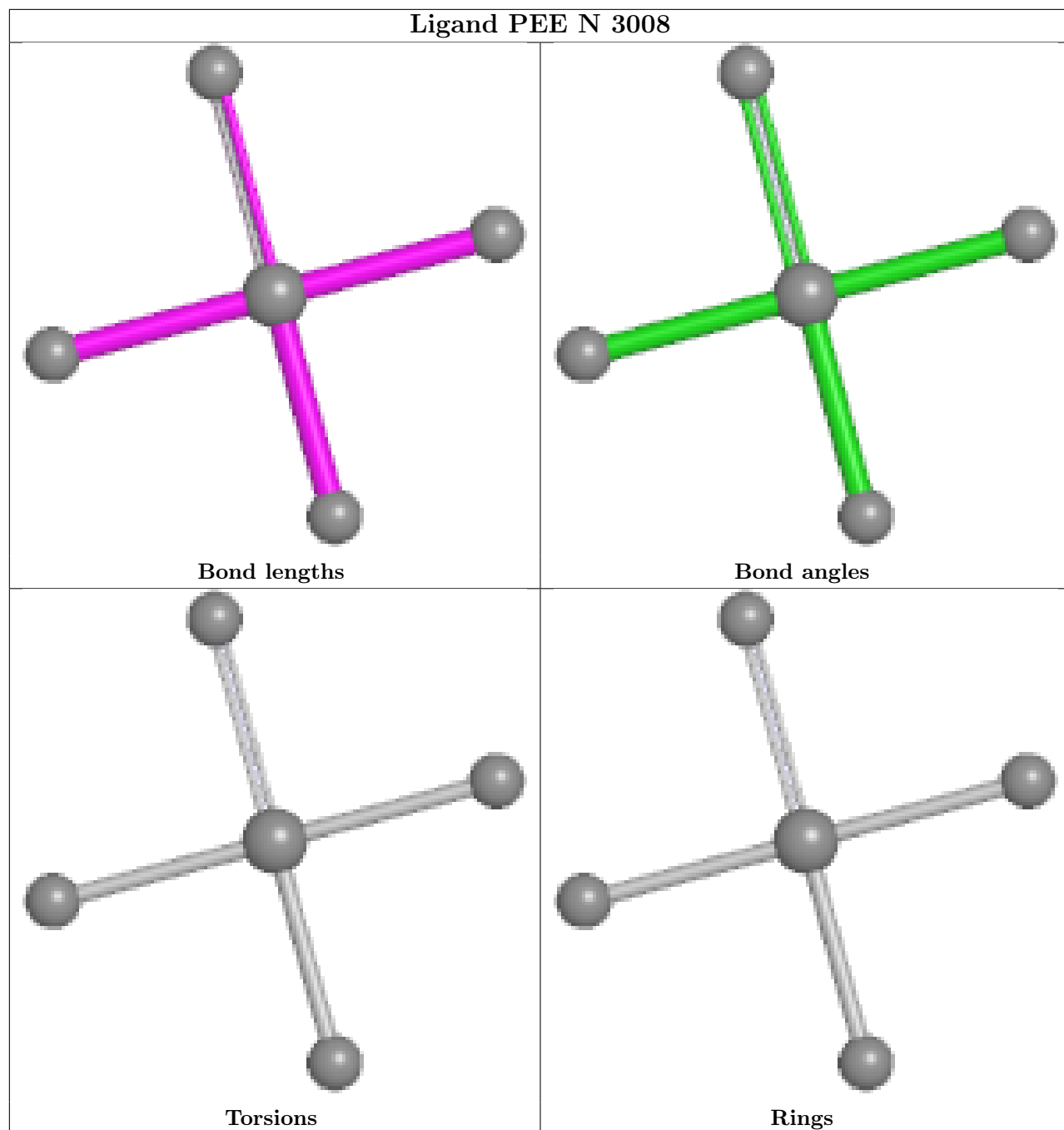
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	501	HEM	5	0
15	E	2005	PEE	1	0
14	D	2003	CDL	2	0
15	P	3007	PEE	2	0
13	P	3002	UQ	2	0
17	D	501	HEC	1	0
15	C	2007	PEE	2	0
13	C	2002	UQ	5	0
19	R	501	FES	2	0

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.

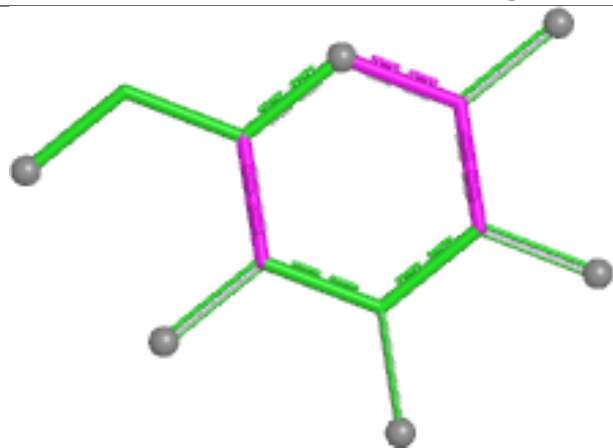




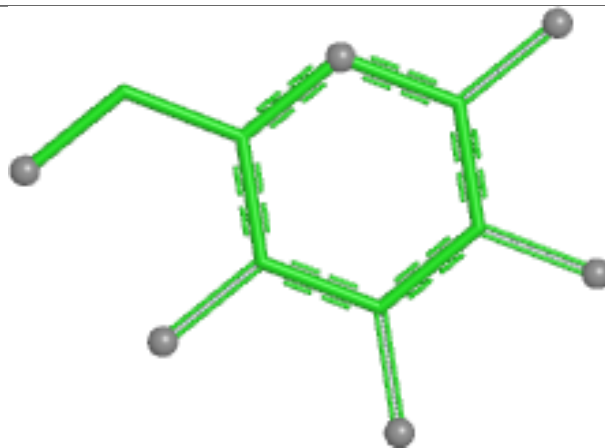




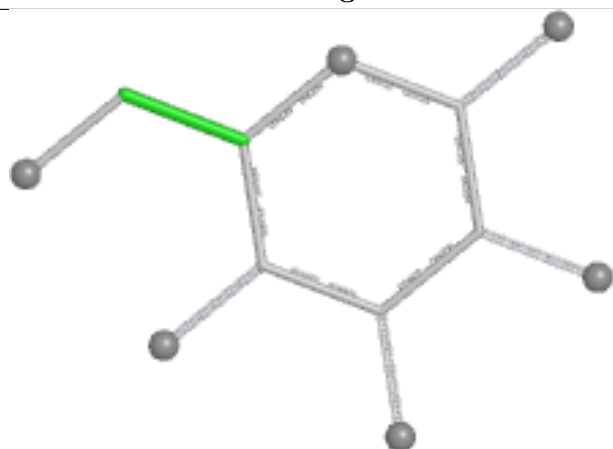
Ligand BOG P 2010



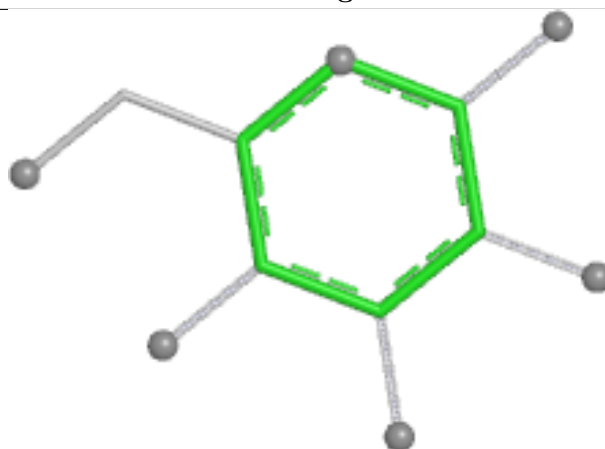
Bond lengths



Bond angles

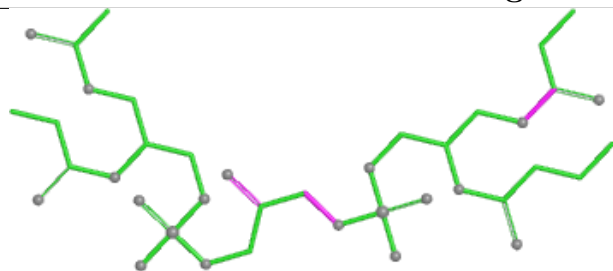


Torsions

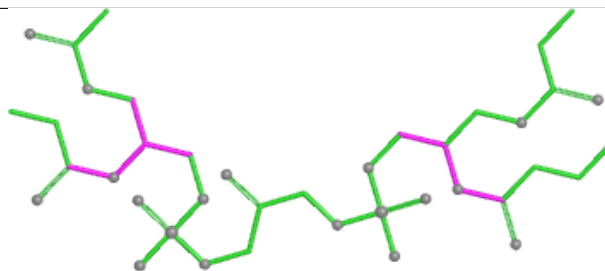


Rings

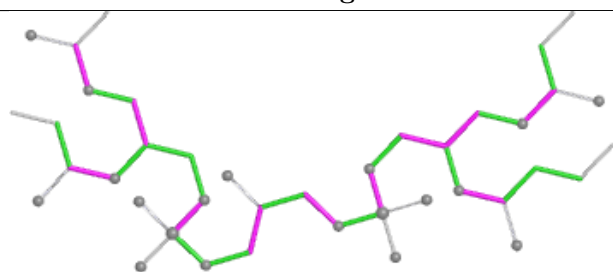
Ligand CDL P 3004



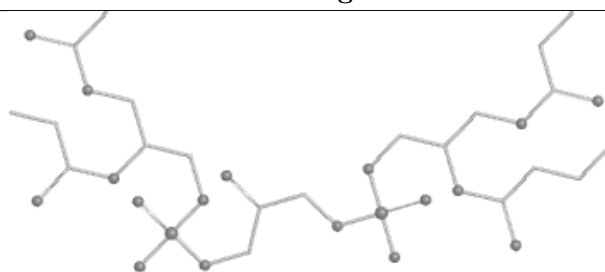
Bond lengths



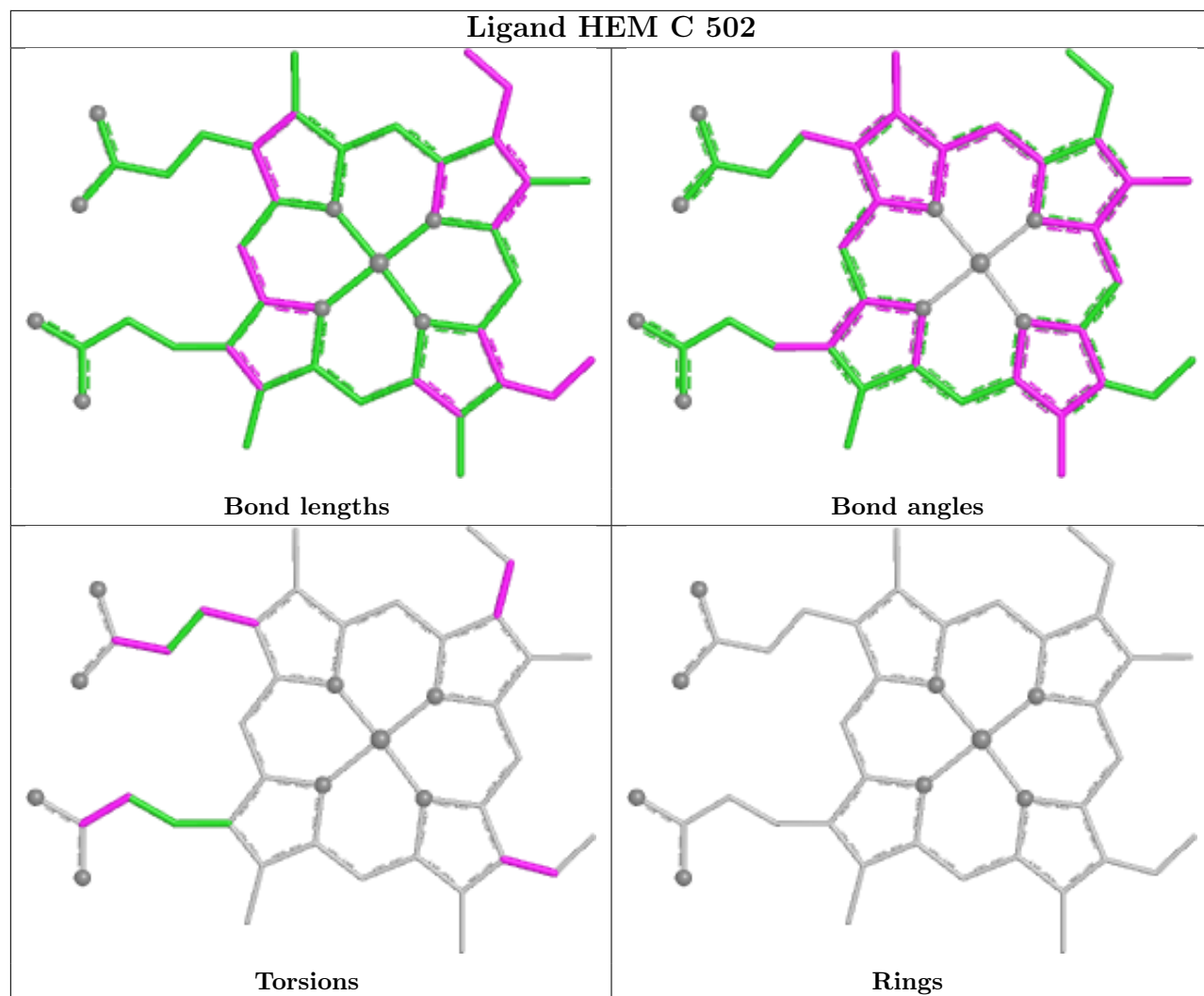
Bond angles

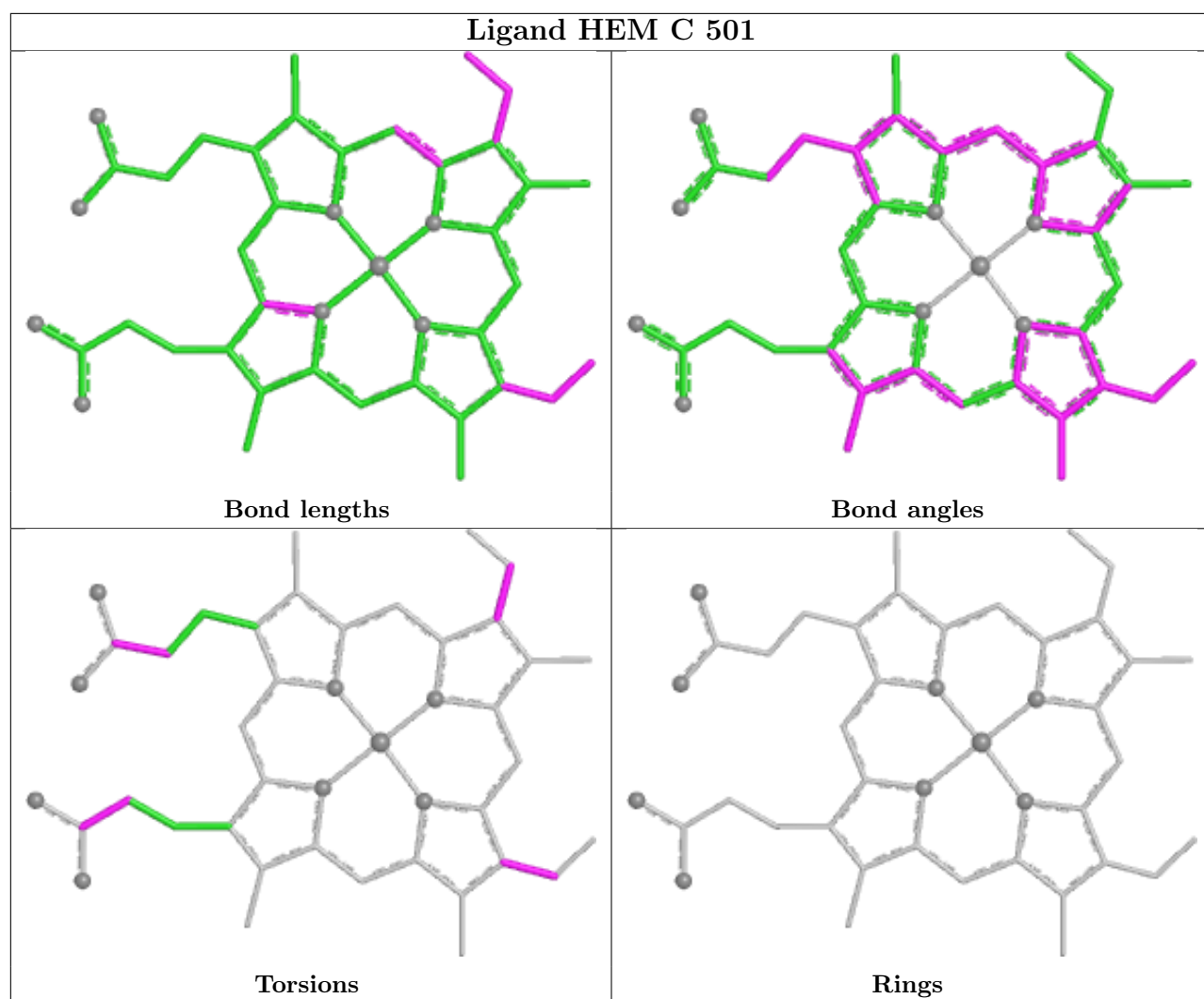


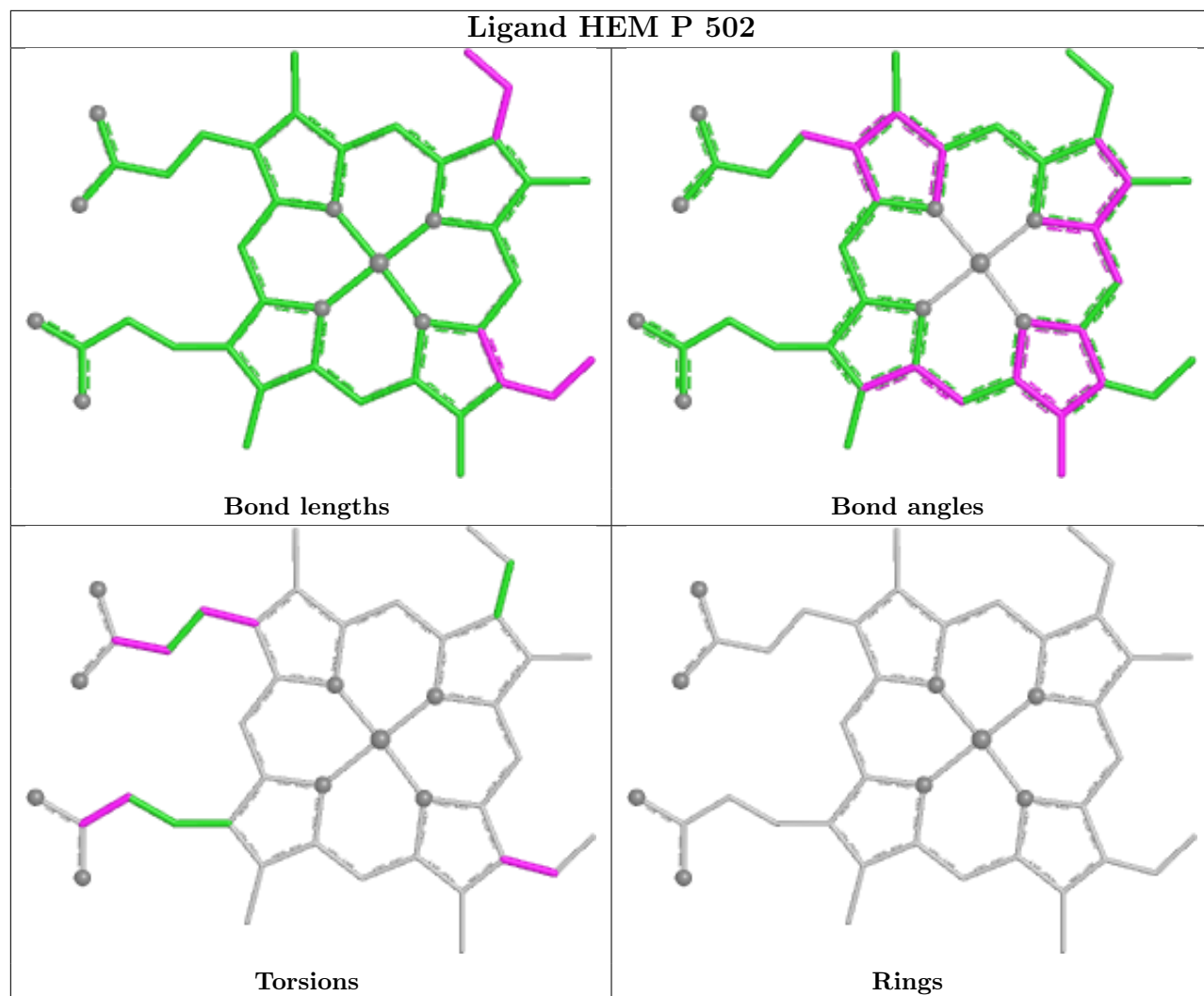
Torsions

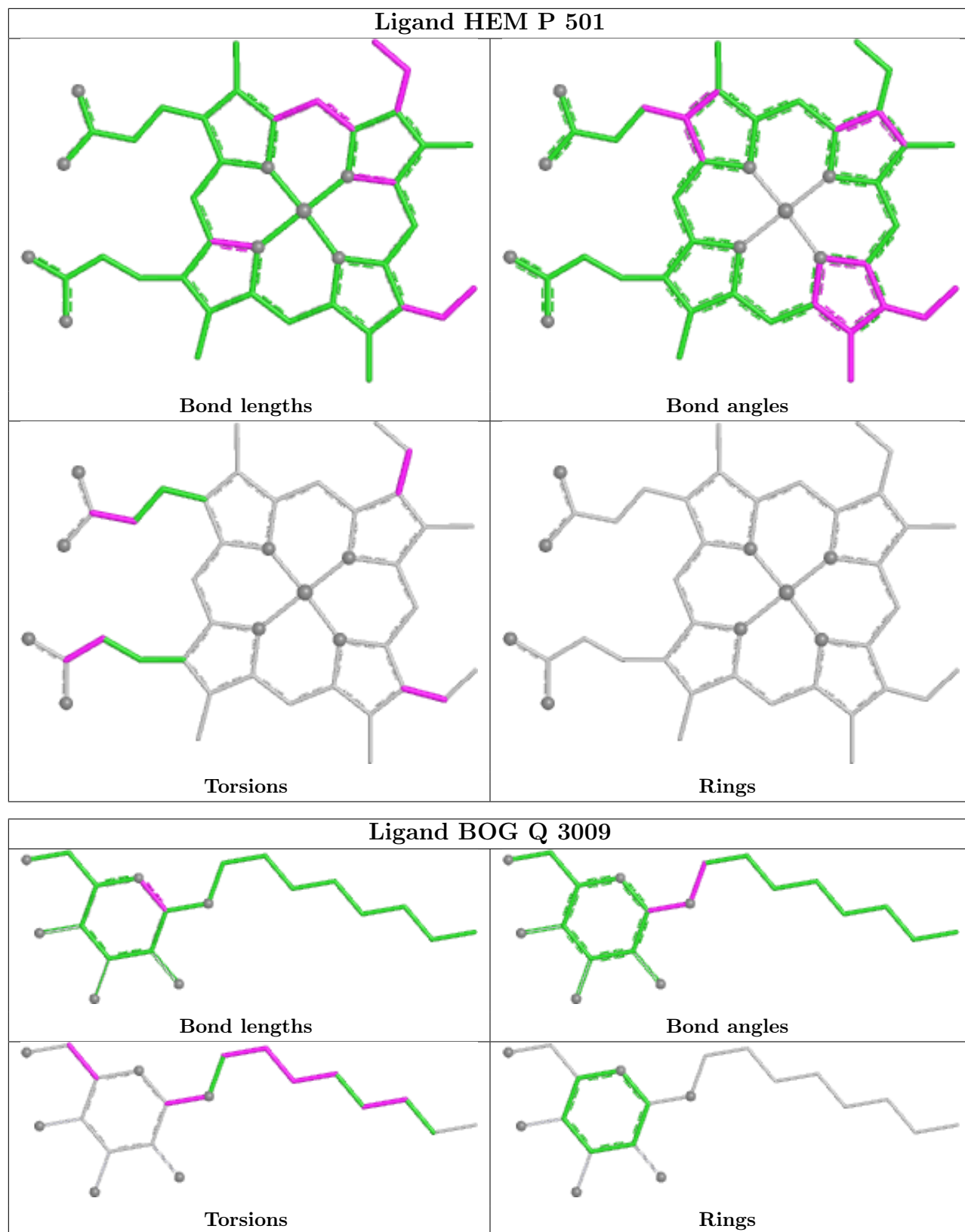


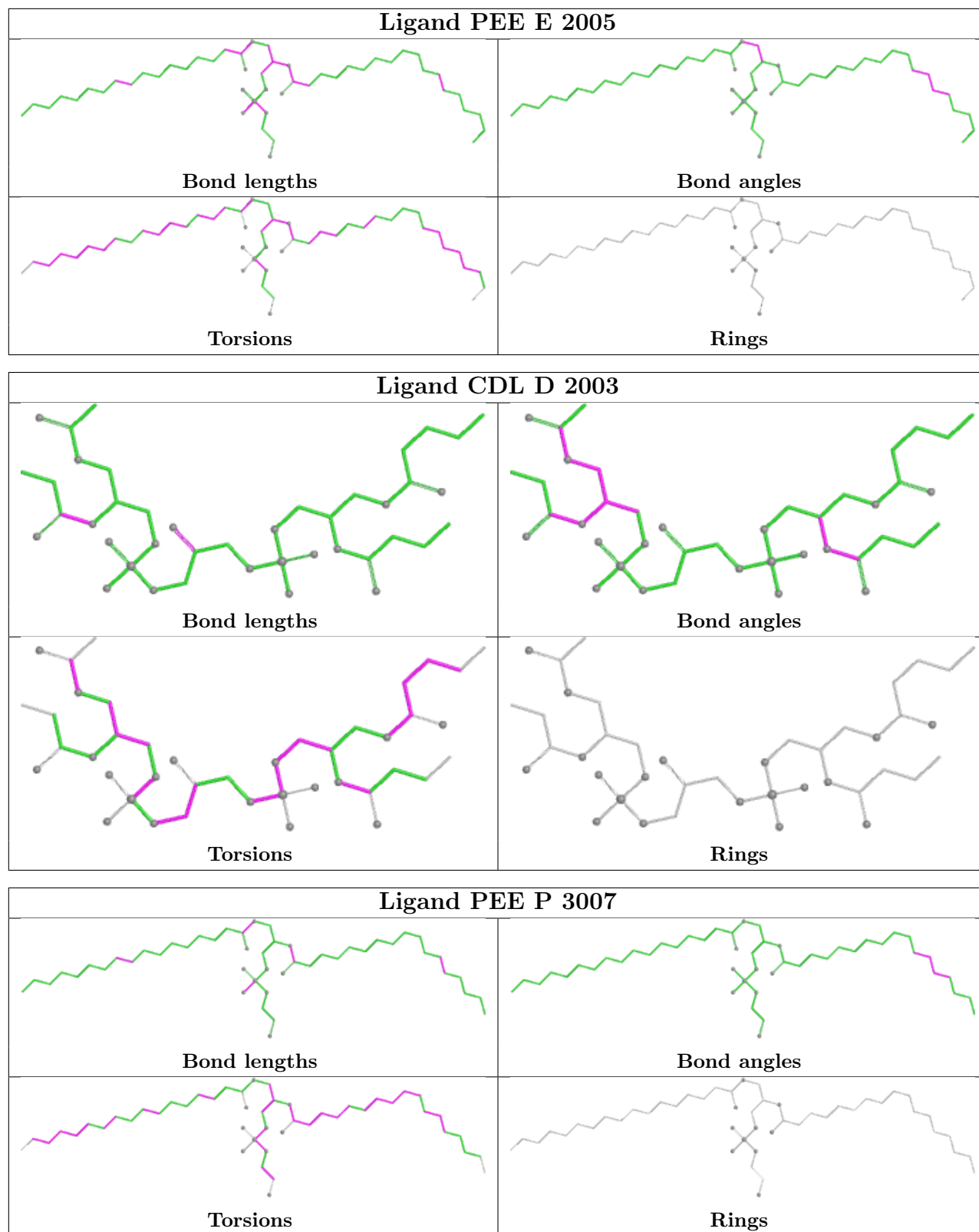
Rings

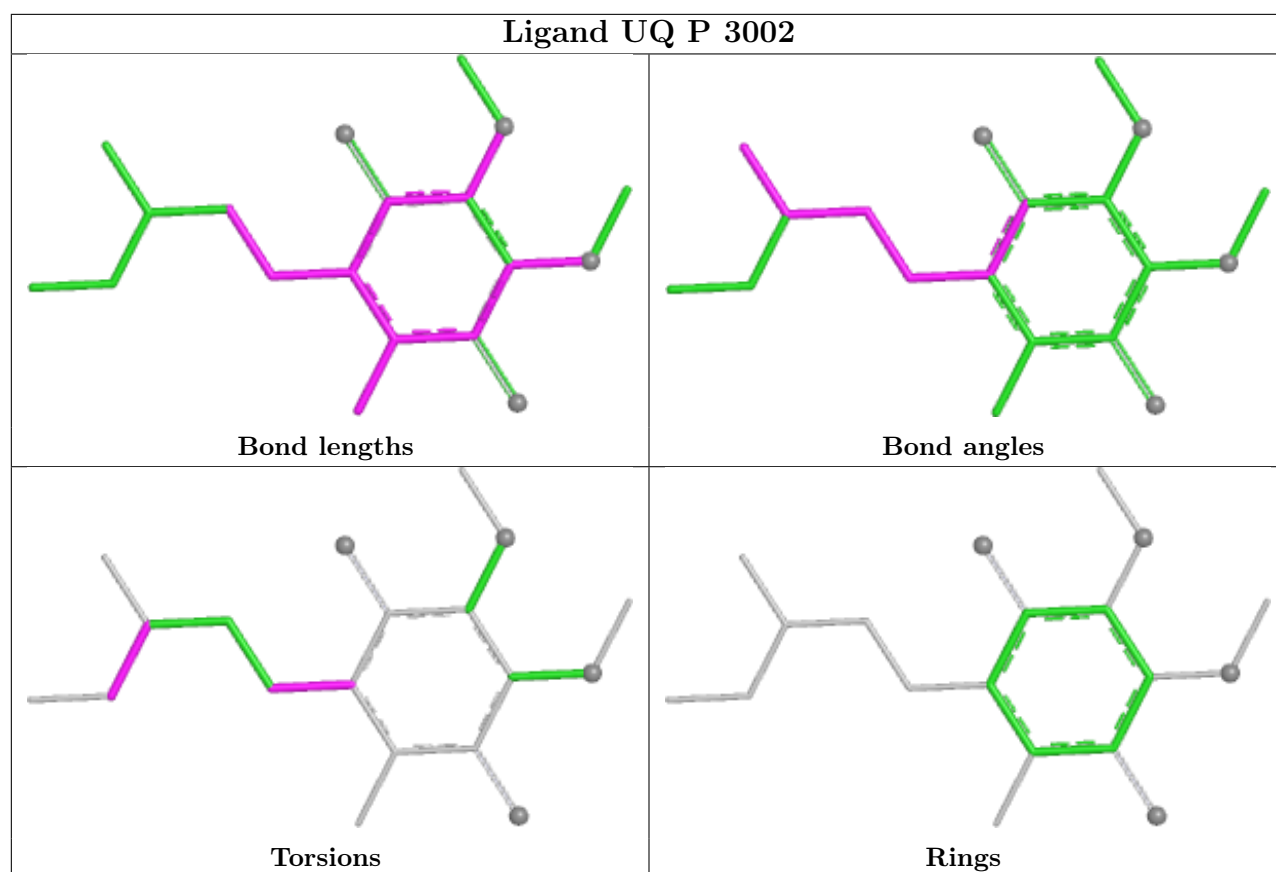




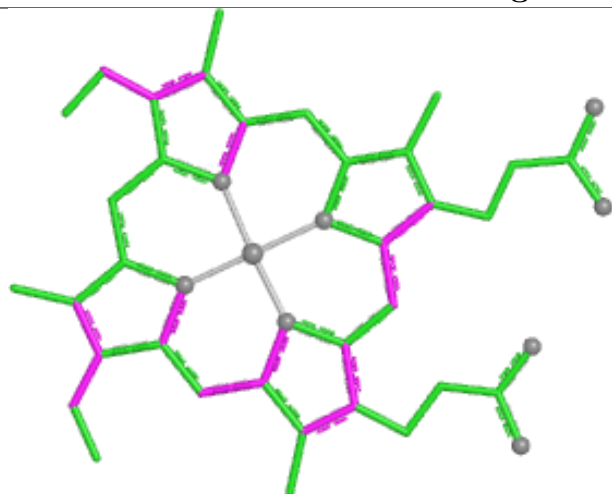




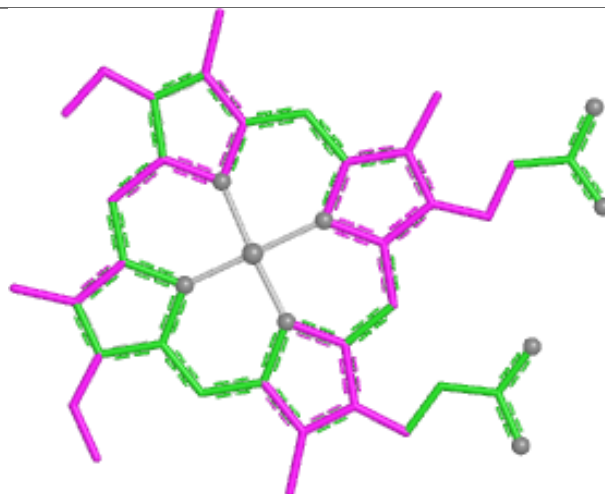




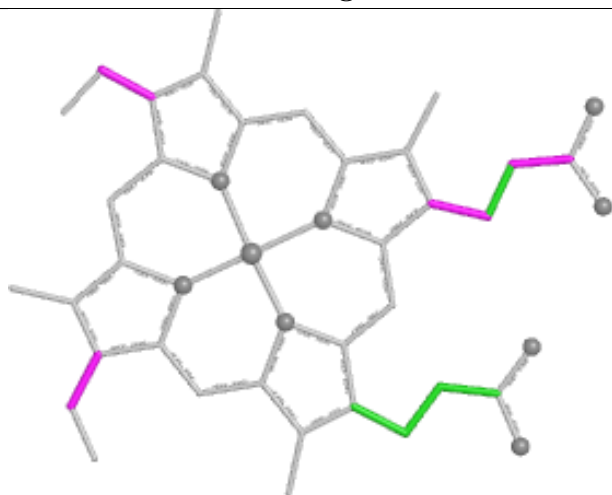
Ligand HEC D 501



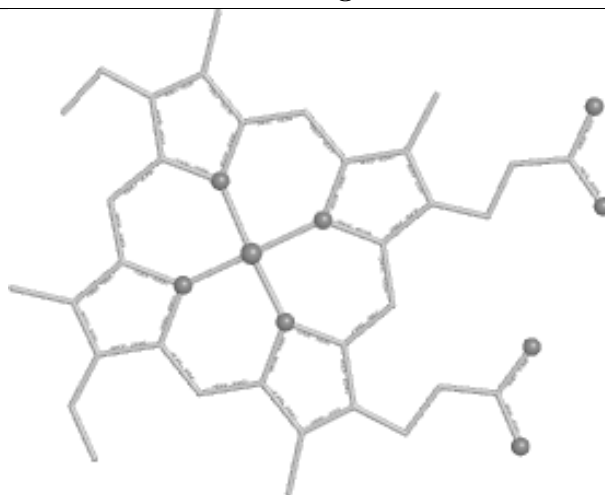
Bond lengths



Bond angles

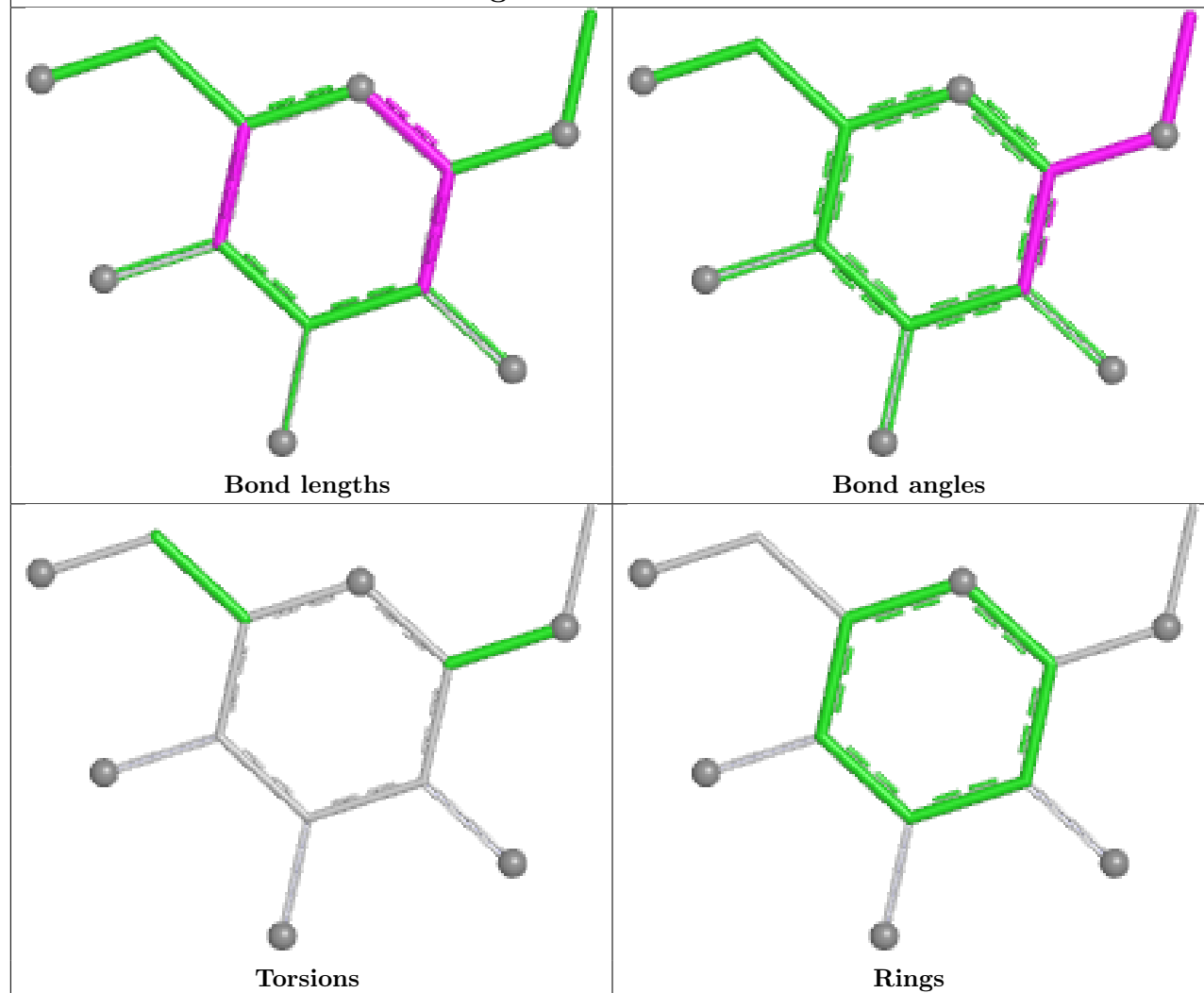


Torsions

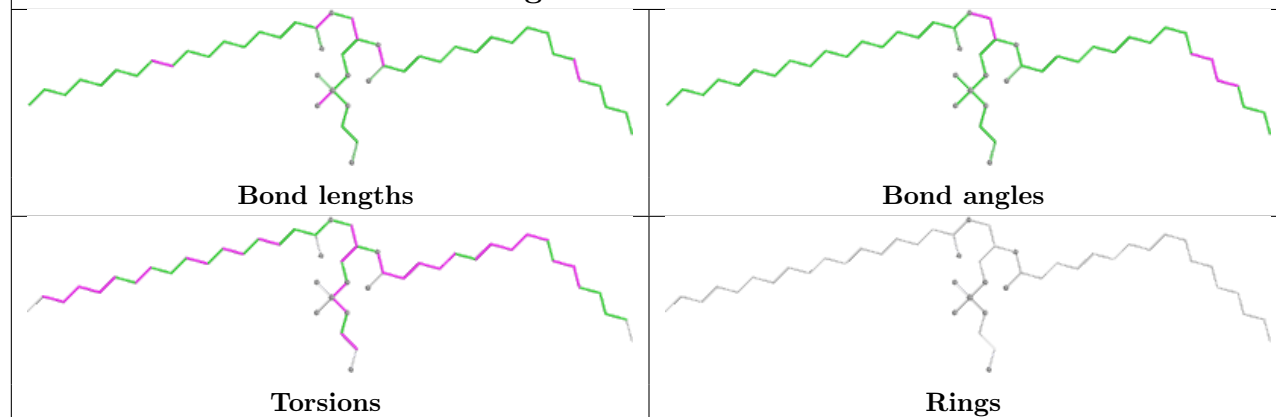


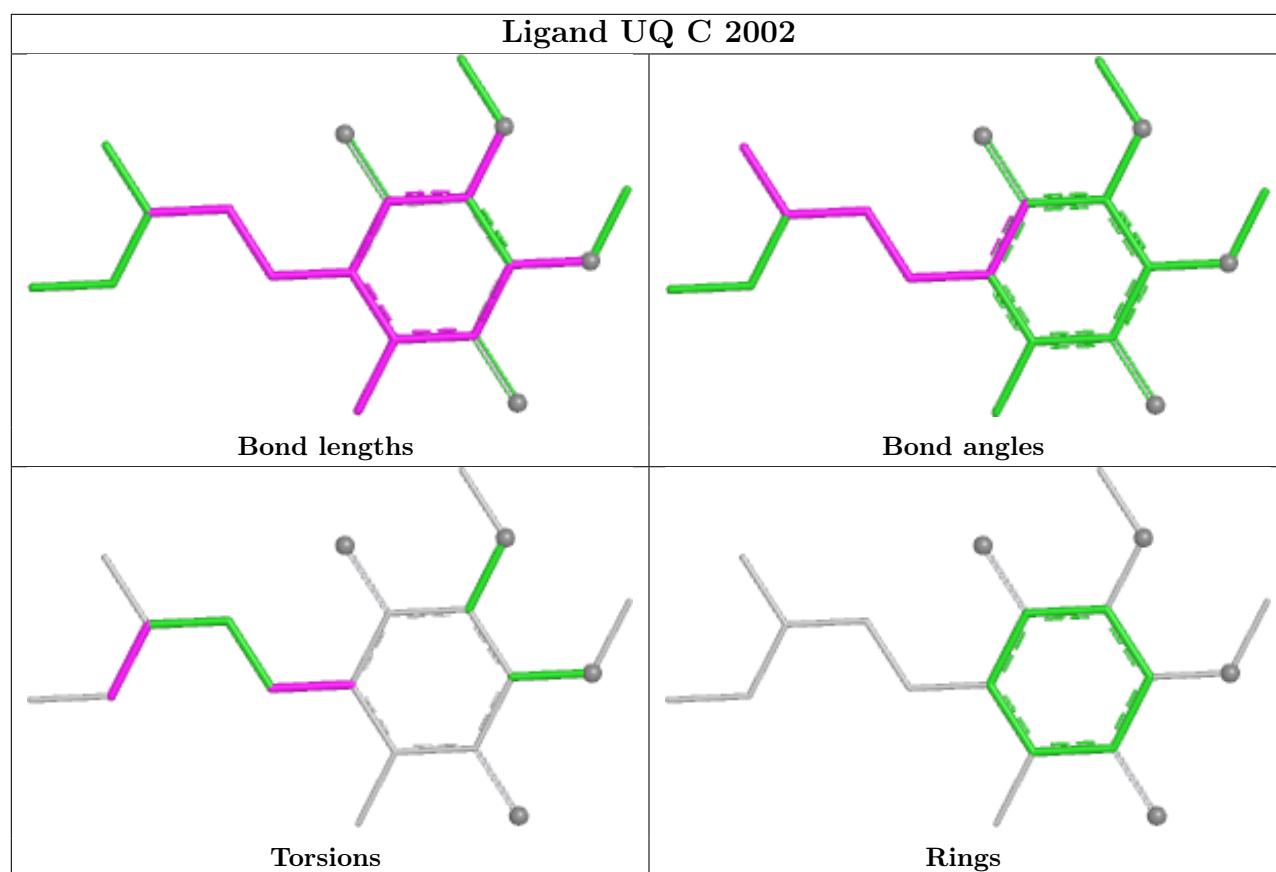
Rings

Ligand BOG D 2091

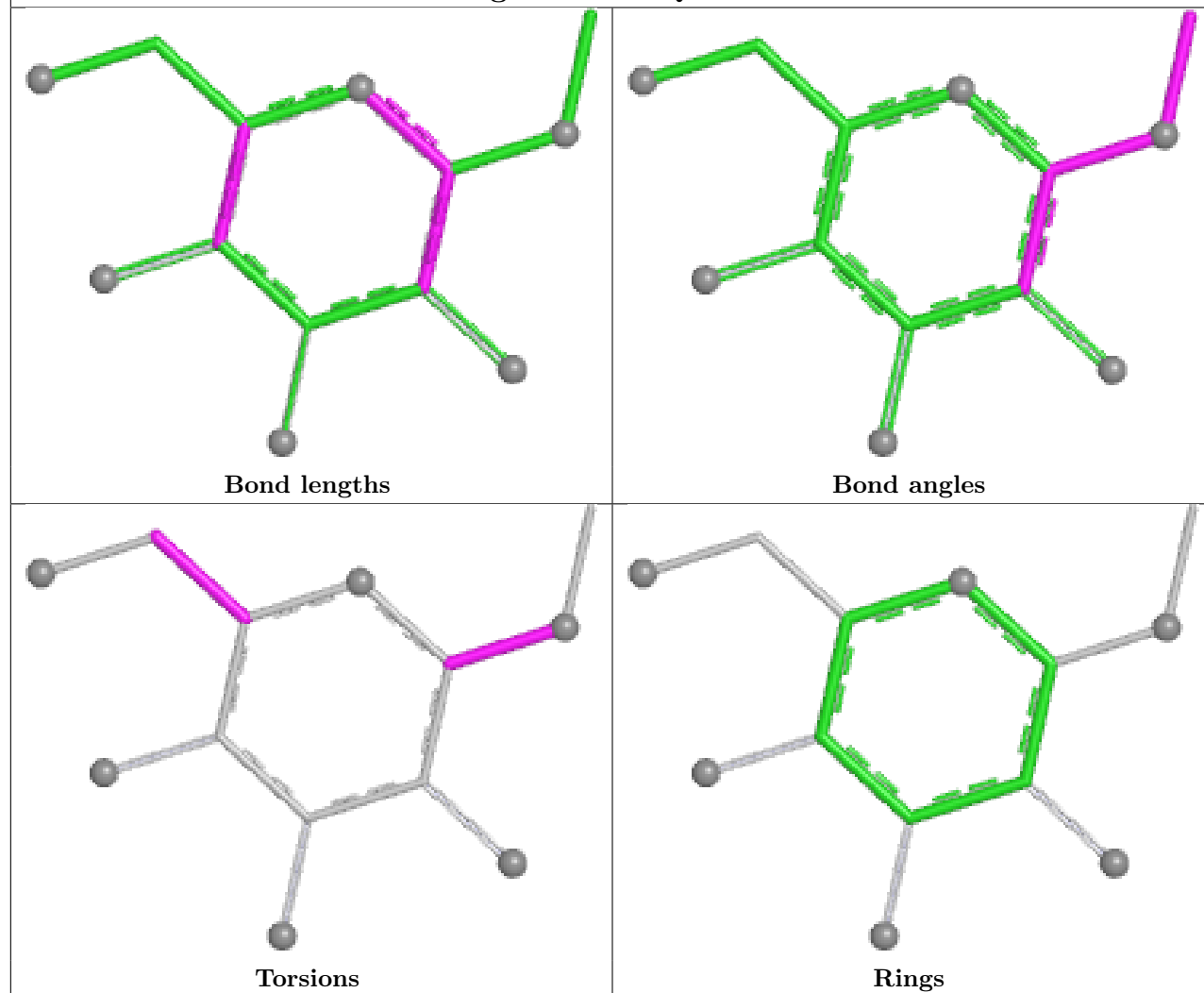


Ligand PEE C 2007

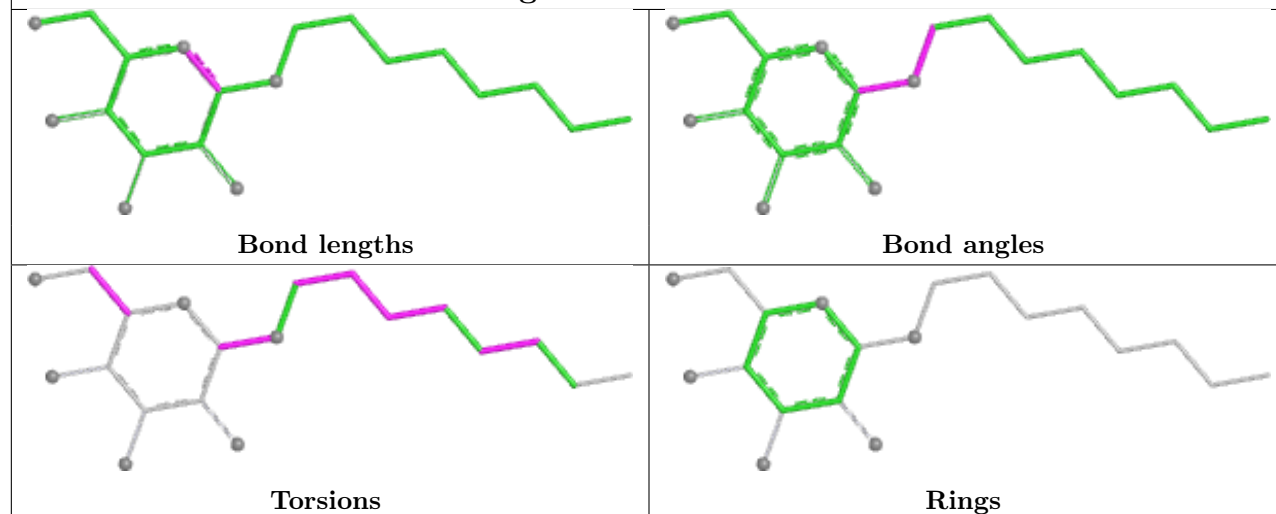




Ligand BOG Q 3091



Ligand BOG D 2009



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%)	-0.03	2 (0%) 87 75	38, 72, 106, 123	0
1	N	442/446 (99%)	0.13	7 (1%) 70 50	41, 79, 111, 121	0
2	B	421/441 (95%)	0.36	17 (4%) 42 24	59, 90, 133, 158	0
2	O	422/441 (95%)	0.25	13 (3%) 51 31	49, 86, 120, 149	0
3	C	380/380 (100%)	-0.44	5 (1%) 75 55	25, 46, 88, 131	0
3	P	379/380 (99%)	-0.13	2 (0%) 87 75	34, 70, 102, 127	0
4	D	241/241 (100%)	-0.38	0 100 100	38, 51, 105, 124	0
4	Q	241/241 (100%)	0.24	6 (2%) 58 37	55, 88, 124, 142	0
5	E	196/196 (100%)	0.94	39 (19%) 3 2	42, 120, 141, 149	125 (63%)
5	R	196/196 (100%)	0.58	12 (6%) 27 15	51, 90, 126, 137	127 (64%)
6	F	101/110 (91%)	-0.45	1 (0%) 79 62	32, 53, 74, 109	0
6	S	101/110 (91%)	0.13	0 100 100	56, 79, 121, 145	0
7	G	80/81 (98%)	-0.16	1 (1%) 75 55	37, 63, 111, 120	0
7	T	79/81 (97%)	0.56	7 (8%) 15 9	54, 99, 162, 174	0
8	H	70/77 (90%)	0.07	1 (1%) 73 53	44, 73, 98, 145	0
8	U	67/77 (87%)	0.87	4 (5%) 27 16	110, 132, 150, 155	0
9	I	31/47 (65%)	1.60	8 (25%) 1 1	80, 125, 161, 162	0
9	V	31/47 (65%)	1.96	10 (32%) 1 1	81, 114, 162, 165	0
10	J	61/61 (100%)	-0.05	1 (1%) 70 50	51, 66, 113, 156	0
10	W	60/61 (98%)	0.23	0 100 100	66, 86, 130, 135	0
All	All	4042/4160 (97%)	0.13	136 (3%) 48 28	25, 77, 131, 174	252 (6%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	9.6
9	I	63	ASP	6.5
2	B	19	PRO	6.1
5	E	134	ILE	5.9
5	E	158	CYS	5.4
5	E	120	PRO	5.4
5	E	85	LYS	4.9
5	E	177	PRO	4.5
9	V	50	LEU	4.5
9	V	49	LEU	4.4
3	C	380	TYR	4.3
5	E	109	GLU	4.1
5	E	165	TYR	4.1
5	E	104	ALA	4.0
5	E	121	GLN	3.5
1	N	175	LYS	3.5
5	E	106	ILE	3.5
9	V	62	ARG	3.5
5	E	117	LEU	3.4
2	B	114	ASP	3.4
8	U	37	LEU	3.4
2	O	371	SER	3.3
9	V	61	ARG	3.3
5	E	159	PRO	3.3
7	G	2	ILE	3.3
1	A	226	ASP	3.3
5	E	129	LYS	3.2
6	F	91	GLU	3.2
5	E	79	SER	3.2
9	V	77	ARG	3.2
2	B	412	ASN	3.2
5	R	114	VAL	3.1
2	B	389	SER	3.1
2	O	153	GLN	3.1
3	P	2	ALA	3.0
9	V	55	MET	3.0
4	Q	167	GLU	2.9
5	E	84	GLY	2.9
5	E	163	SER	2.9
5	R	150	SER	2.9
9	I	77	ARG	2.9
5	E	142	LEU	2.8
5	E	152	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	24	LEU	2.8
5	R	190	ASP	2.8
5	R	169	GLY	2.8
5	E	157	TYR	2.8
5	E	167	ALA	2.8
5	R	79	SER	2.8
2	B	20	GLY	2.7
5	E	178	TYR	2.7
3	C	5	ILE	2.7
5	E	156	TYR	2.7
2	B	232	THR	2.7
7	T	63	THR	2.7
2	O	139	ASP	2.7
2	B	396	SER	2.7
5	E	88	ALA	2.6
5	E	86	ASN	2.6
7	T	2	ILE	2.6
5	E	108	GLN	2.6
9	I	49	LEU	2.6
4	Q	103	ALA	2.6
3	C	8	SER	2.6
5	R	124	LEU	2.6
9	V	56	SER	2.5
9	I	50	LEU	2.5
5	E	194	VAL	2.5
2	B	375	ALA	2.5
9	I	47	ARG	2.5
1	N	187	ASP	2.5
5	E	160	CYS	2.5
2	O	21	ALA	2.5
9	I	72	ALA	2.5
3	C	69	HIS	2.5
1	N	444	ILE	2.4
2	O	238	THR	2.4
8	U	45	SER	2.4
1	N	126	GLN	2.4
9	I	52	ARG	2.4
5	R	22	THR	2.4
5	E	133	VAL	2.4
1	A	432	LEU	2.4
2	O	384	SER	2.4
2	O	304	THR	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	169	GLY	2.3
1	N	96	ALA	2.3
9	I	58	ARG	2.3
5	R	105	GLU	2.3
8	H	9	GLU	2.3
9	V	54	SER	2.3
10	J	61	ALA	2.3
7	T	58	LEU	2.3
5	E	171	ILE	2.3
2	B	224	LEU	2.3
2	O	224	LEU	2.3
5	E	124	LEU	2.3
2	B	403	ASP	2.3
7	T	47	LYS	2.3
4	Q	147	LEU	2.3
5	R	175	PRO	2.2
7	T	77	TYR	2.2
5	R	104	ALA	2.2
5	E	128	LYS	2.2
8	U	46	SER	2.2
1	N	121	ALA	2.2
5	E	162	GLY	2.2
5	E	94	LYS	2.2
5	R	188	VAL	2.2
9	V	76	VAL	2.2
2	O	18	CYS	2.2
7	T	62	GLY	2.2
5	E	118	ARG	2.2
2	O	225	ASN	2.2
5	E	196	GLY	2.2
2	B	111	CYS	2.2
1	N	76	GLU	2.1
2	B	229	GLY	2.1
2	B	23	ASP	2.1
2	O	114	ASP	2.1
2	B	238	THR	2.1
2	B	280	GLY	2.1
5	E	153	PHE	2.1
7	T	76	ASP	2.1
4	Q	29	GLY	2.1
4	Q	156	GLN	2.1
4	Q	3	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	171	ALA	2.0
2	O	303	THR	2.0
5	E	98	VAL	2.0
8	U	44	VAL	2.0
3	P	5	ILE	2.0
3	C	4	ASN	2.0
5	E	164	HIS	2.0
2	O	395	PRO	2.0
5	R	171	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	PEE	C	2008	21/51	0.46	0.29	150,154,158,159	0
15	PEE	N	3008	5/51	0.63	0.19	117,118,119,119	0
18	BOG	Q	3091	13/20	0.65	0.21	195,196,196,196	0
14	CDL	Q	3003	42/100	0.69	0.21	134,150,157,158	0
18	BOG	D	2091	13/20	0.72	0.26	185,187,187,187	0
14	CDL	D	2003	42/100	0.76	0.19	97,106,116,117	0
11	UNL	N	3291	1/-	0.76	0.17	37,37,37,37	0
18	BOG	P	2010	12/20	0.78	0.19	155,156,157,158	0
14	CDL	P	3004	40/100	0.78	0.16	107,115,122,124	0
15	PEE	R	3005	50/51	0.79	0.19	87,109,125,125	0
13	UQ	P	3002	19/63	0.81	0.23	121,130,133,133	0
15	PEE	E	2005	50/51	0.83	0.18	72,96,104,105	0
15	PEE	P	3007	49/51	0.83	0.15	65,94,110,112	0
11	UNL	P	3286	1/-	0.84	0.08	55,55,55,55	0

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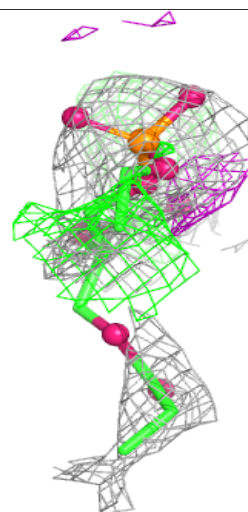
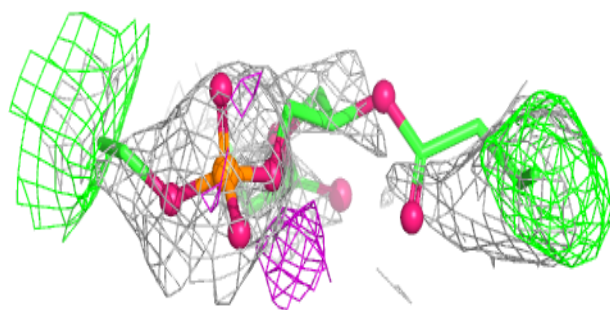
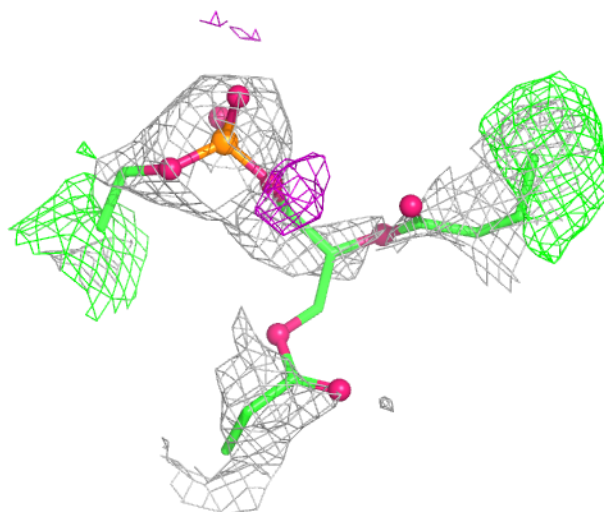
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	FES	E	501	4/4	0.84	0.15	161,162,162,162	4
11	UNL	C	3288	1/-	0.85	0.26	84,84,84,84	0
13	UQ	C	2002	19/63	0.86	0.16	82,84,86,86	0
11	UNL	A	3289	1/-	0.86	0.11	38,38,38,38	0
14	CDL	C	2004	40/100	0.87	0.13	69,86,100,102	0
15	PEE	C	2007	49/51	0.88	0.13	42,65,85,87	0
11	UNL	C	3287	1/-	0.88	0.18	88,88,88,88	0
11	UNL	A	3284	1/-	0.90	0.09	28,28,28,28	0
18	BOG	D	2009	20/20	0.90	0.10	52,70,74,76	0
11	UNL	N	4231	1/-	0.90	0.11	67,67,67,67	0
16	GOL	P	3011	6/6	0.91	0.16	86,87,88,89	0
18	BOG	Q	3009	20/20	0.91	0.12	82,93,95,95	0
16	GOL	C	2011	6/6	0.92	0.13	70,71,72,75	0
11	UNL	A	3231	1/-	0.92	0.18	91,91,91,91	0
11	UNL	N	3290	1/-	0.93	0.14	53,53,53,53	0
17	HEC	Q	501	43/43	0.95	0.10	70,75,81,84	0
19	FES	R	501	4/4	0.97	0.12	92,94,94,95	4
12	HEM	C	502	43/43	0.98	0.07	23,30,38,44	0
17	HEC	D	501	43/43	0.98	0.06	35,40,48,52	0
12	HEM	P	501	43/43	0.98	0.07	48,52,61,66	0
12	HEM	P	502	43/43	0.98	0.07	43,50,60,65	0
12	HEM	C	501	43/43	0.98	0.07	30,36,47,53	0

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

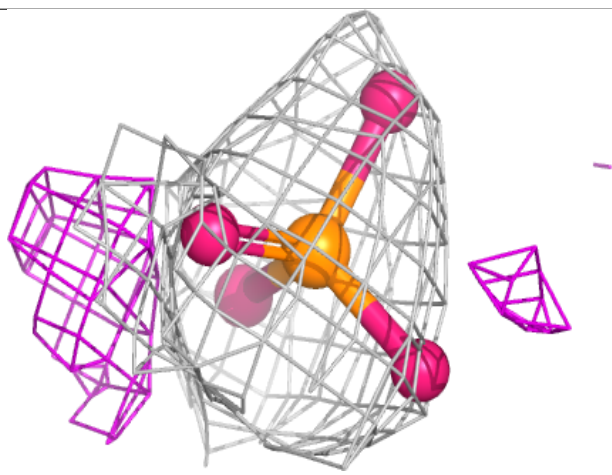
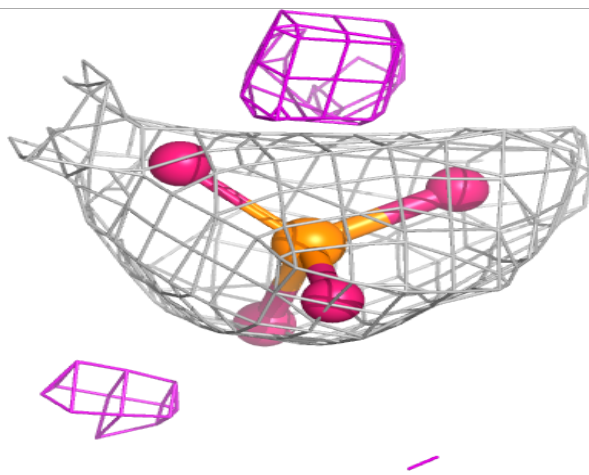
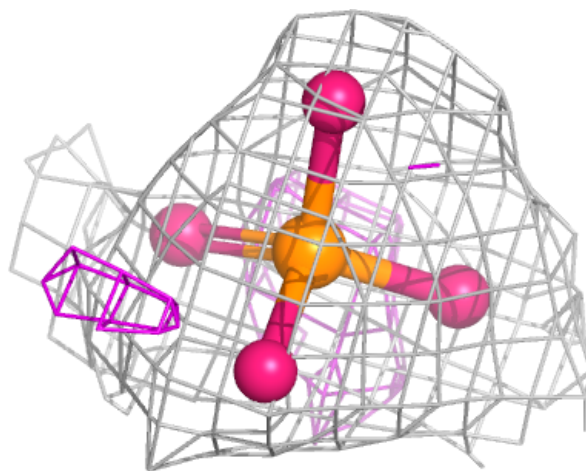
Electron density around PEE C 2008:

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



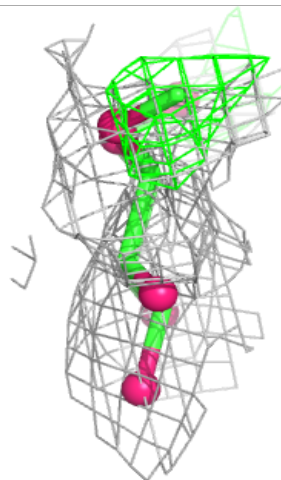
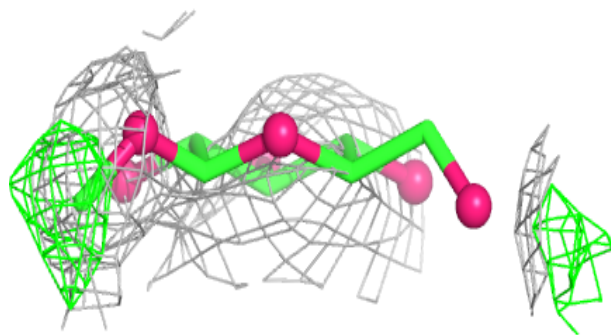
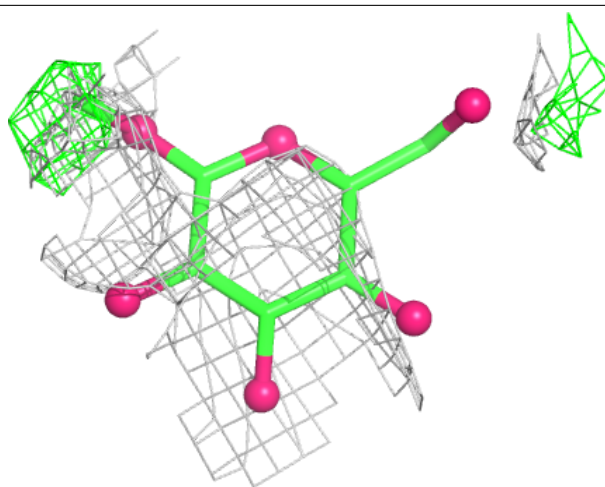
Electron density around PEE N 3008:

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



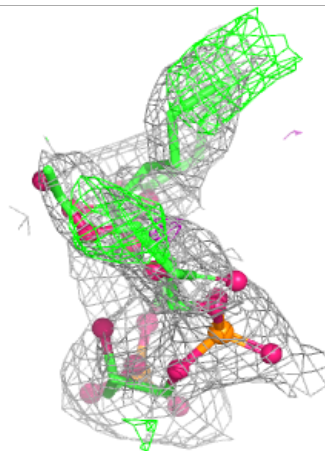
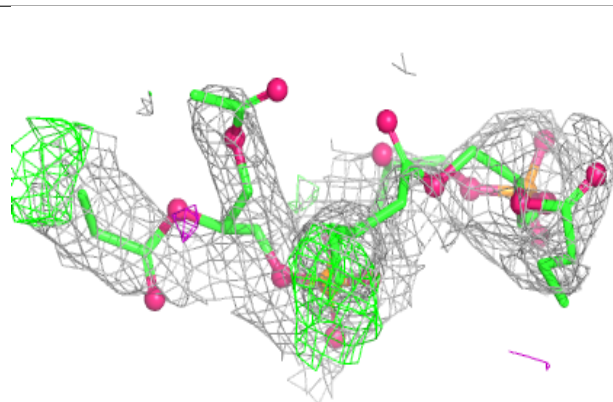
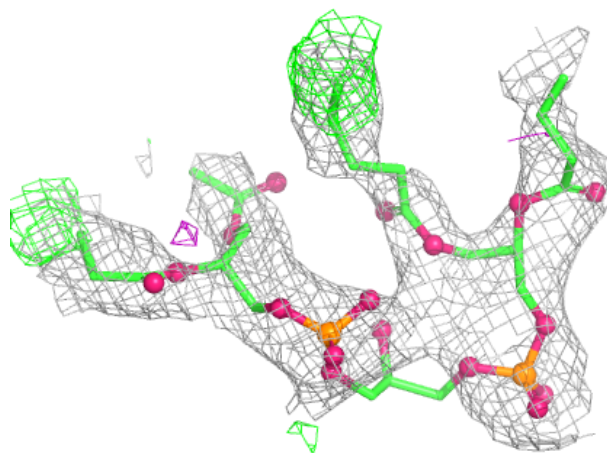
Electron density around BOG Q 3091:

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



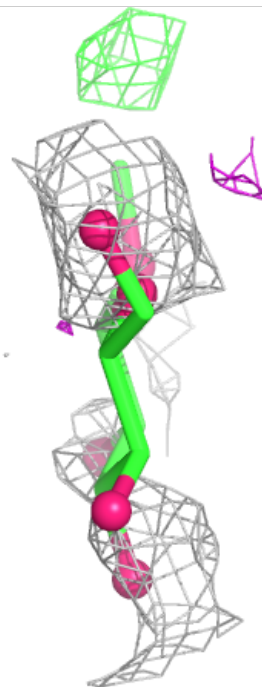
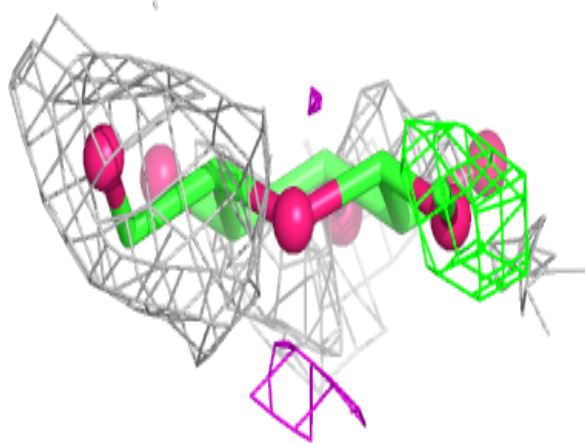
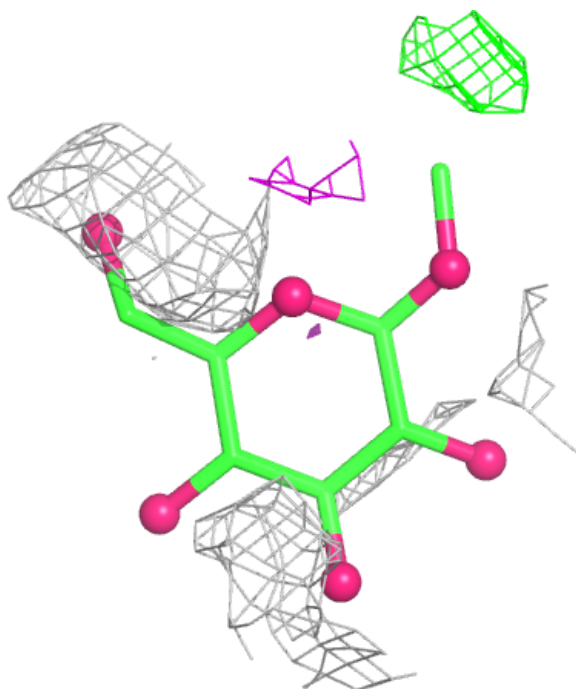
Electron density around CDL Q 3003:

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



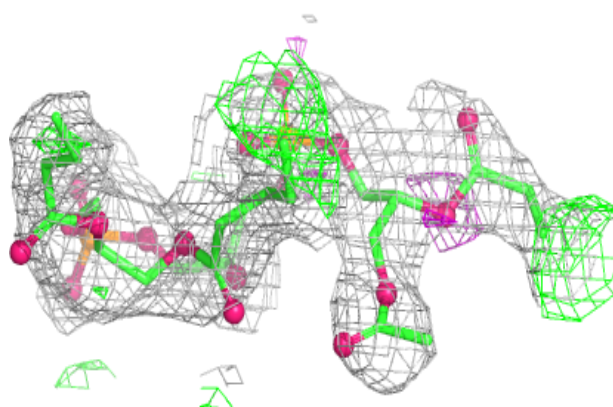
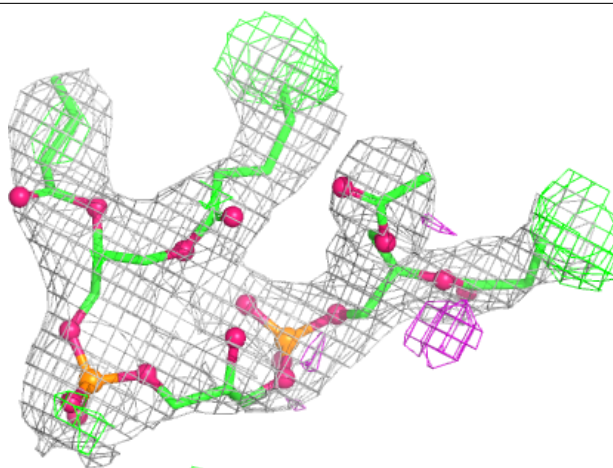
Electron density around BOG D 2091:

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



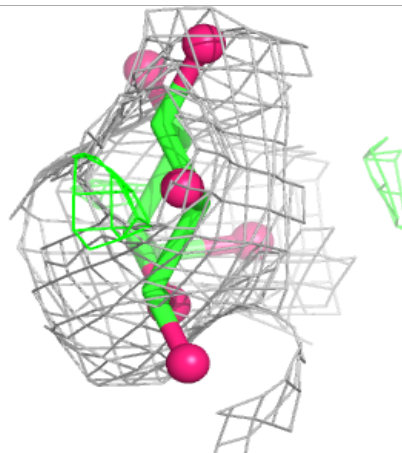
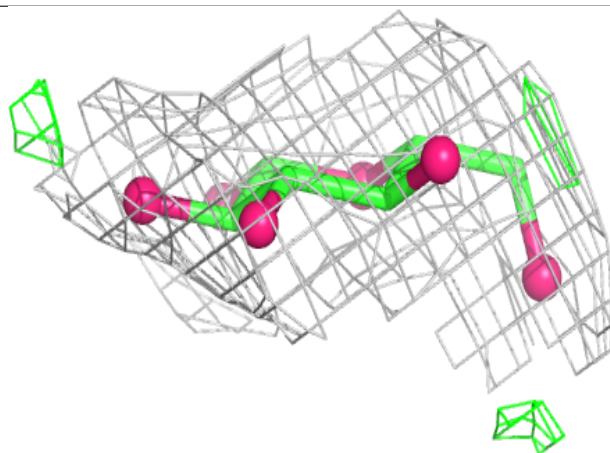
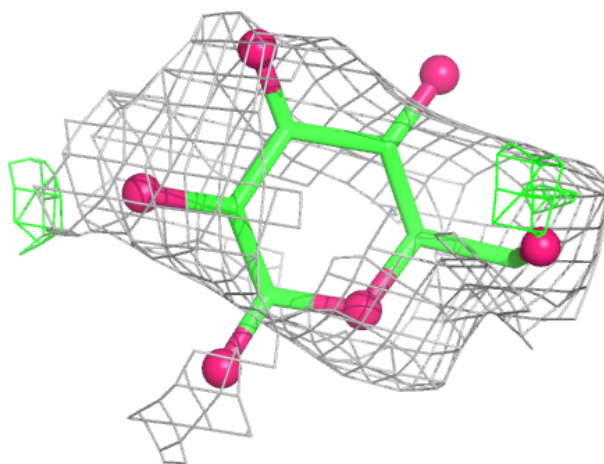
Electron density around CDL D 2003:

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



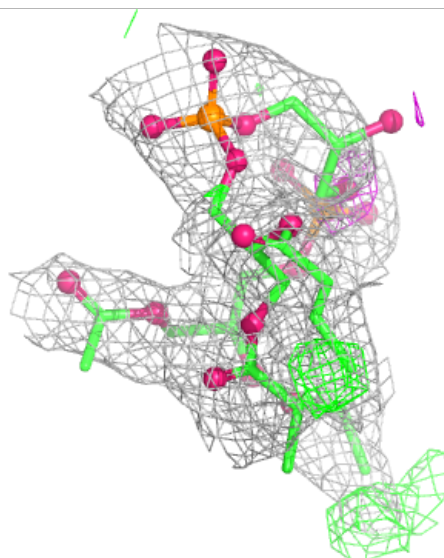
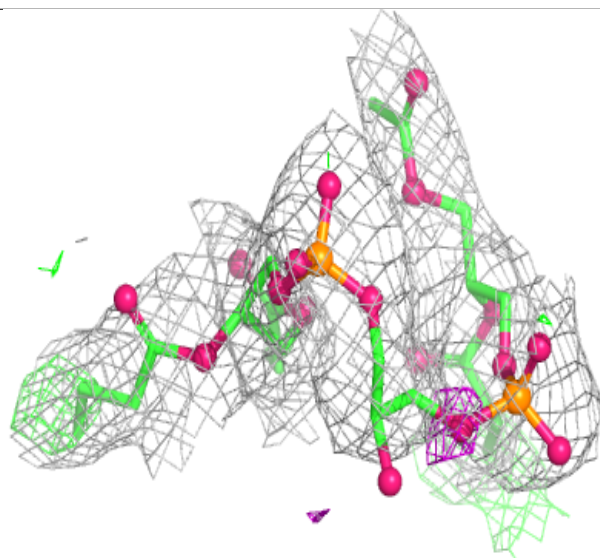
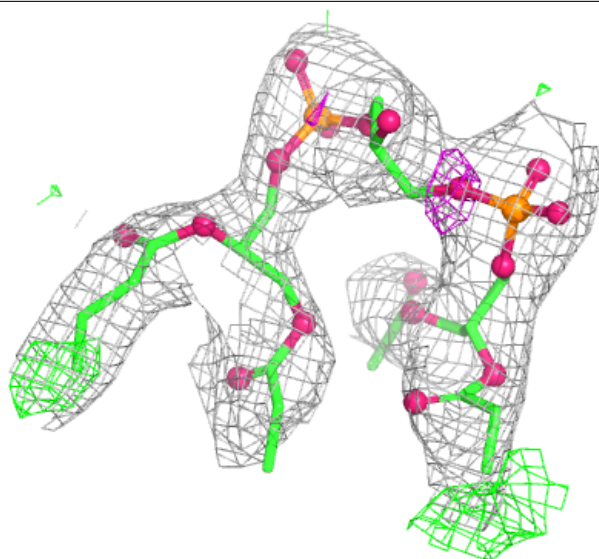
Electron density around BOG P 2010:

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



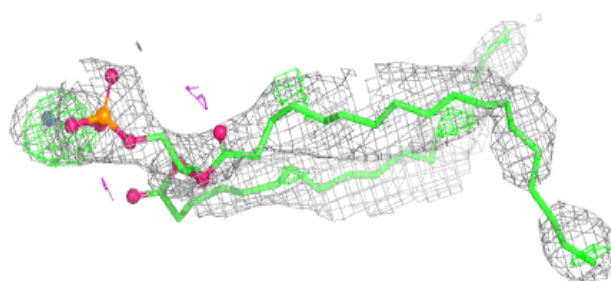
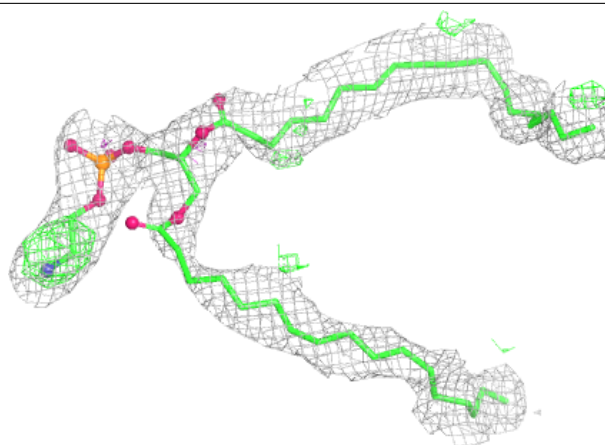
Electron density around CDL P 3004:

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

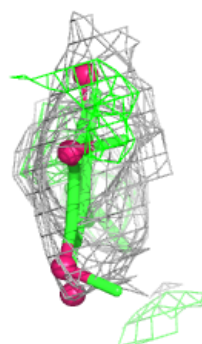
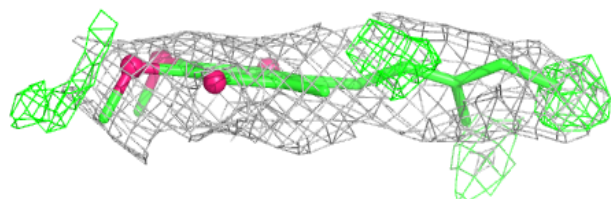
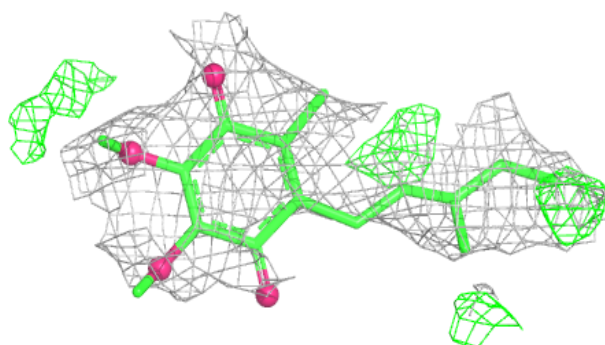


Electron density around PEE R 3005:

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

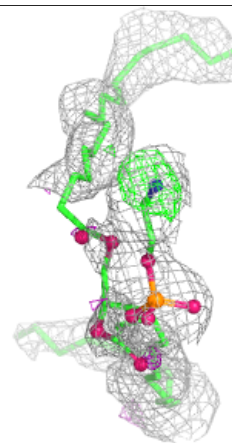
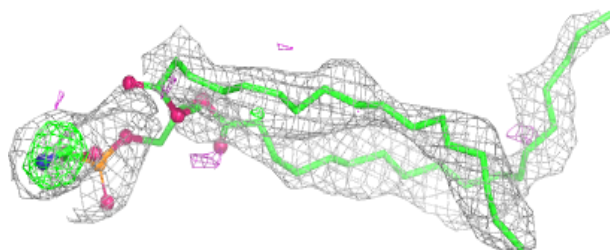
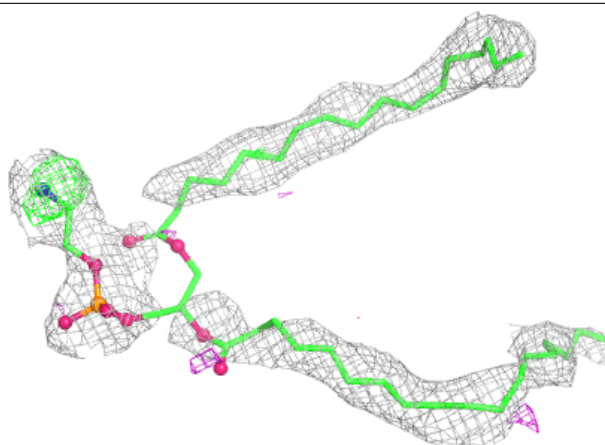
**Electron density around UQ P 3002:**

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

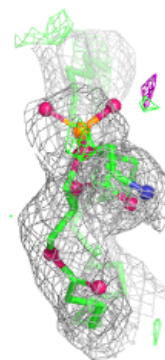
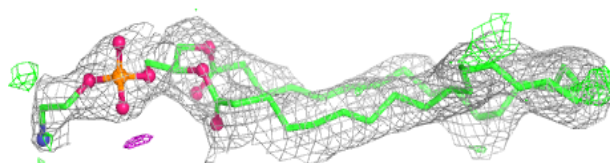
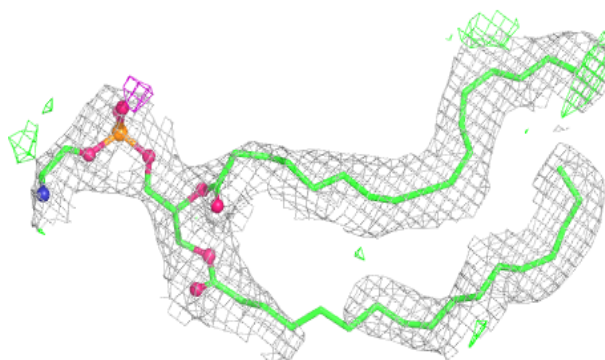


Electron density around PEE E 2005:

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

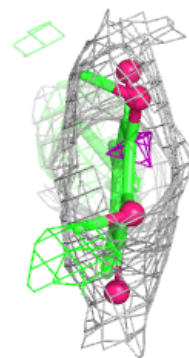
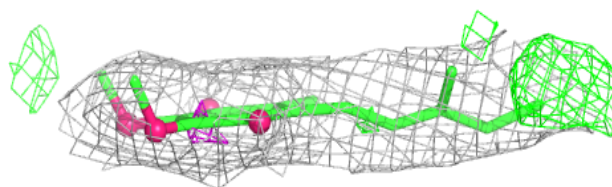
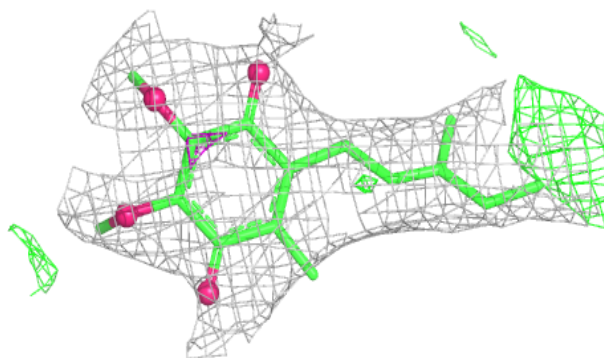
**Electron density around PEE P 3007:**

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and green (positive)



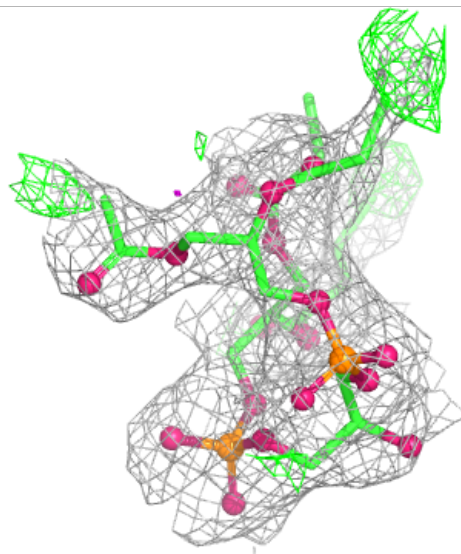
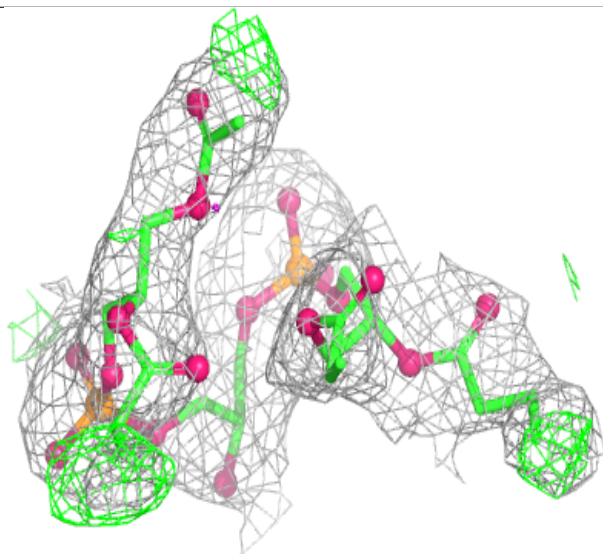
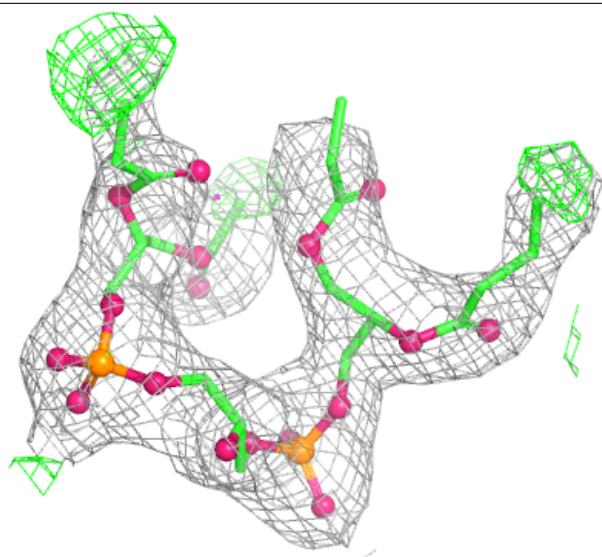
Electron density around UQ C 2002:

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



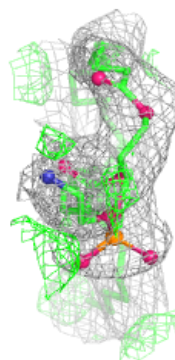
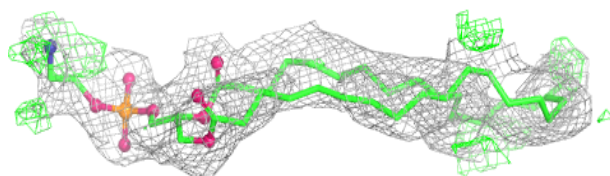
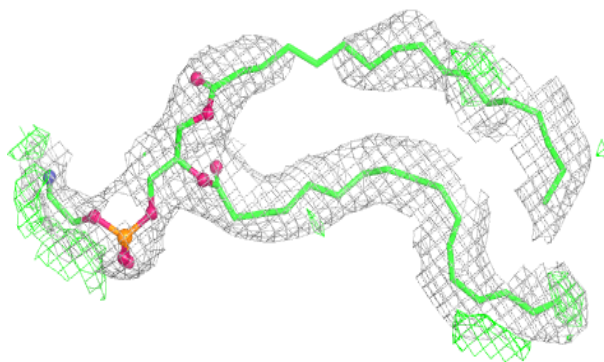
Electron density around CDL C 2004:

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

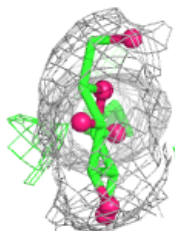
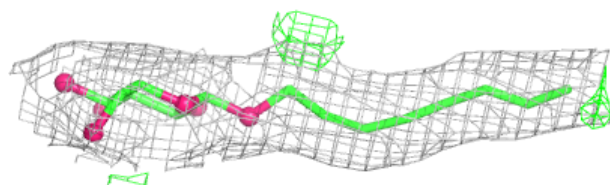
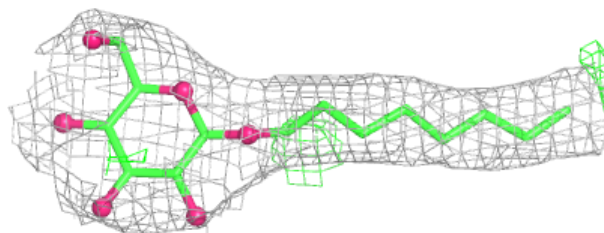


Electron density around PEE C 2007:

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

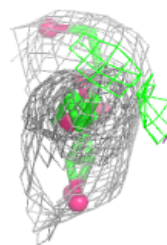
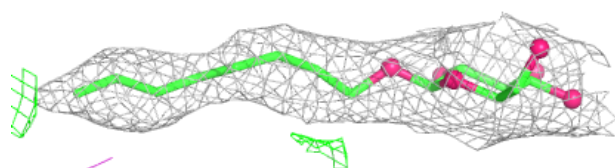
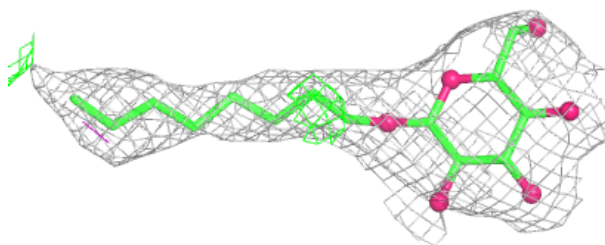
**Electron density around BOG D 2009:**

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

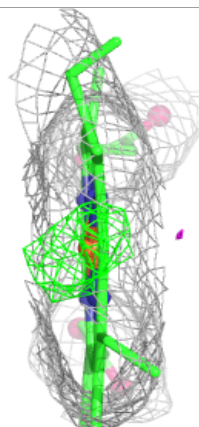
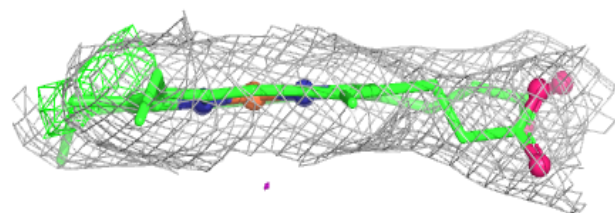
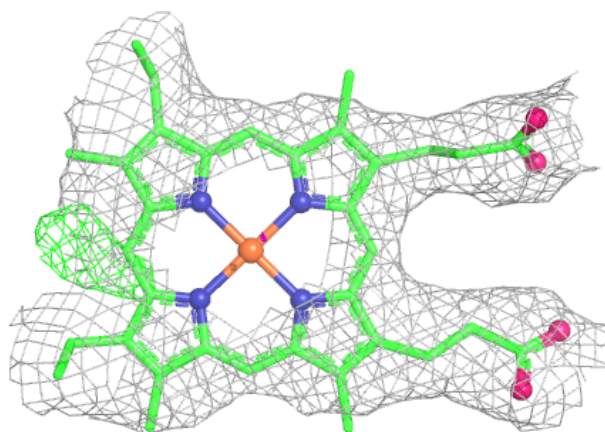


Electron density around BOG Q 3009:

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

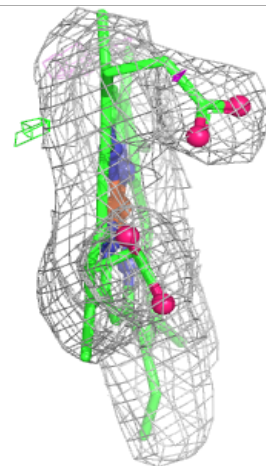
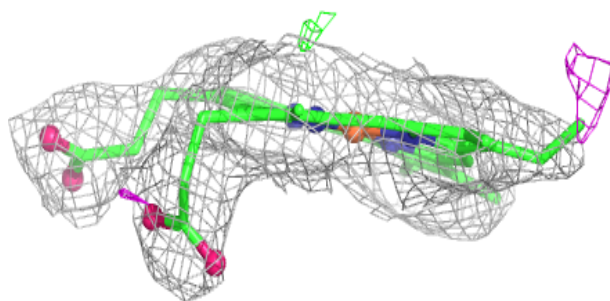
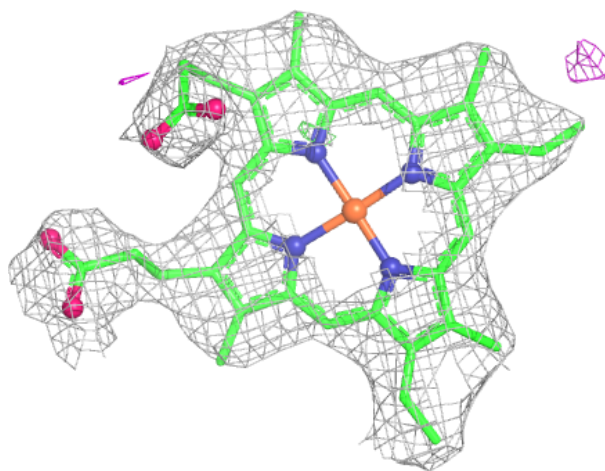
**Electron density around HEC Q 501:**

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



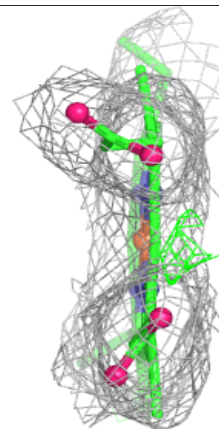
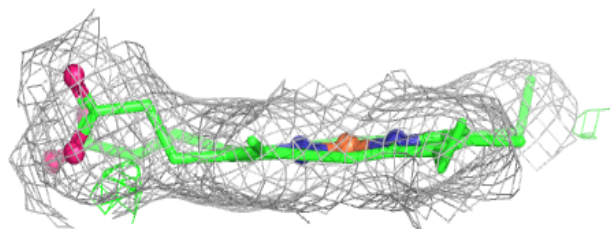
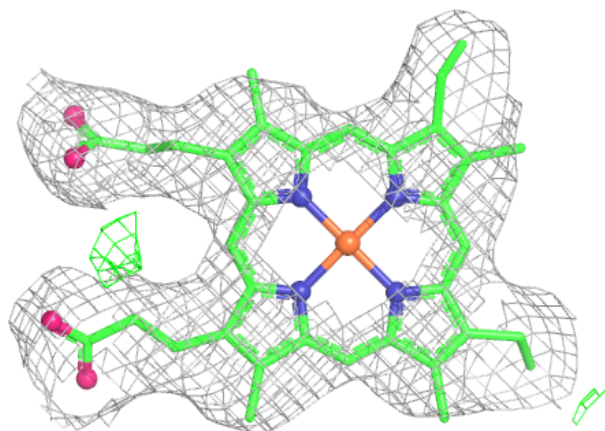
Electron density around HEM C 502:

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



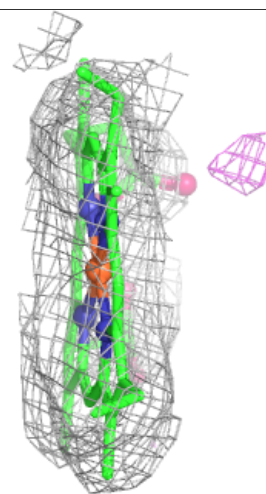
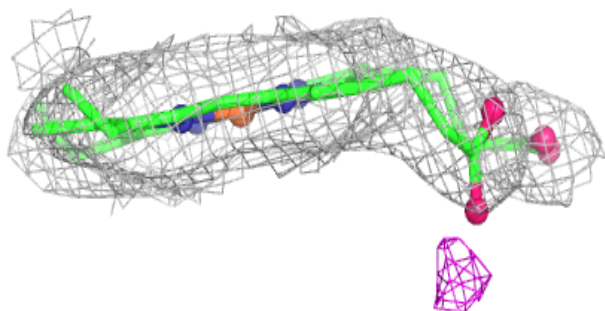
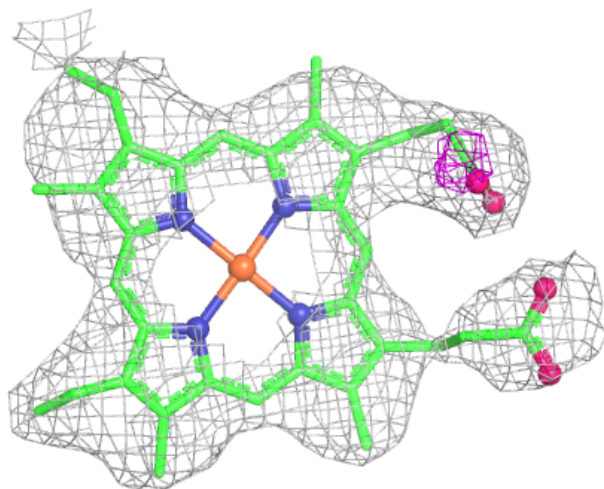
Electron density around HEC D 501:

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



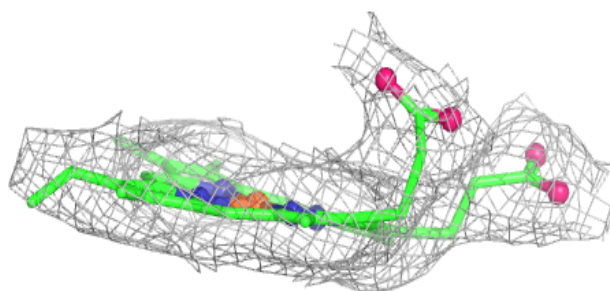
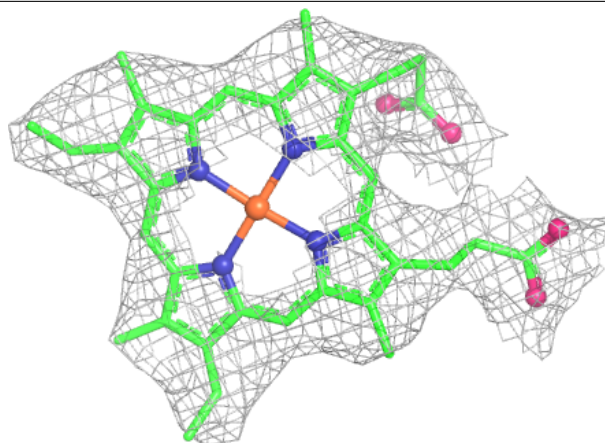
Electron density around HEM P 501:

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



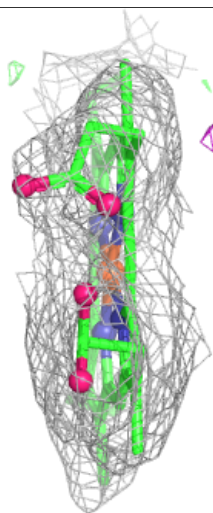
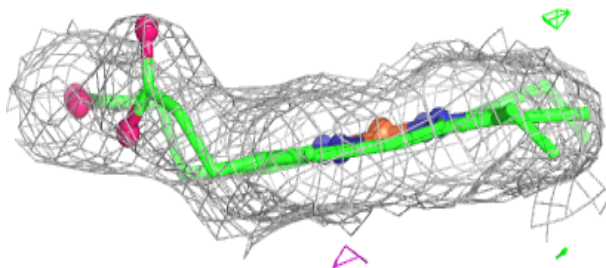
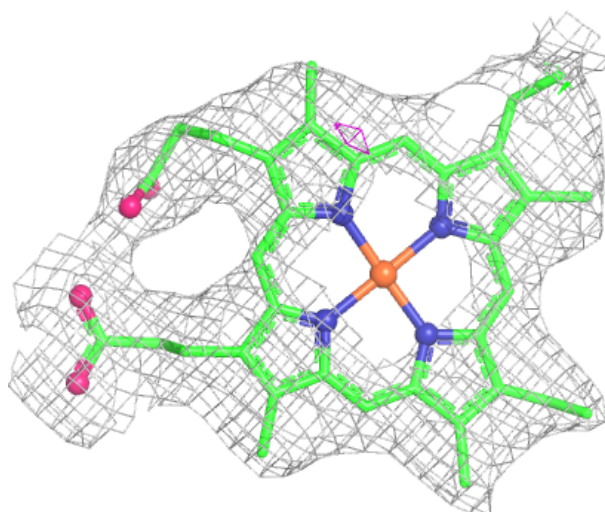
Electron density around HEM P 502:

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



Electron density around HEM C 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.