



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:18 AM EDT

PDB ID : 3L70 / pdb_00003L70
Title : Cytochrome BC1 complex from chicken with trifloxystrobin bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

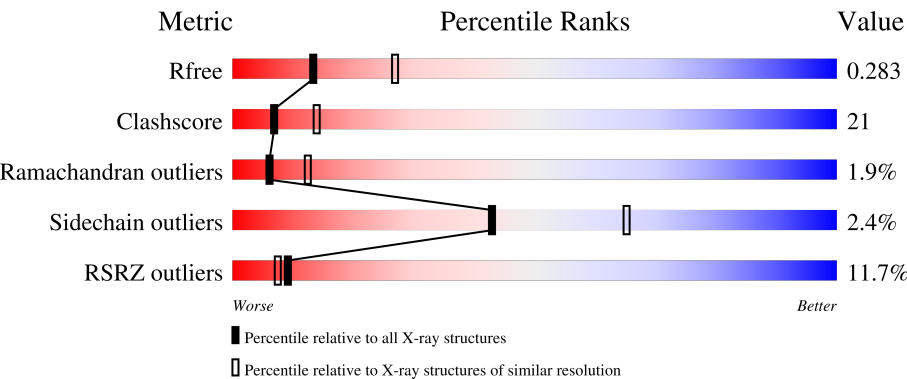
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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
11	PEE	N	3008	-	X	-	-
17	HEC	D	501	X	-	-	-
17	HEC	Q	501	X	-	-	-
18	BOG	D	2091	-	-	-	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 32653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	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 Mitochondrial cytochrome c1, heme protein.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

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

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	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 Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

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

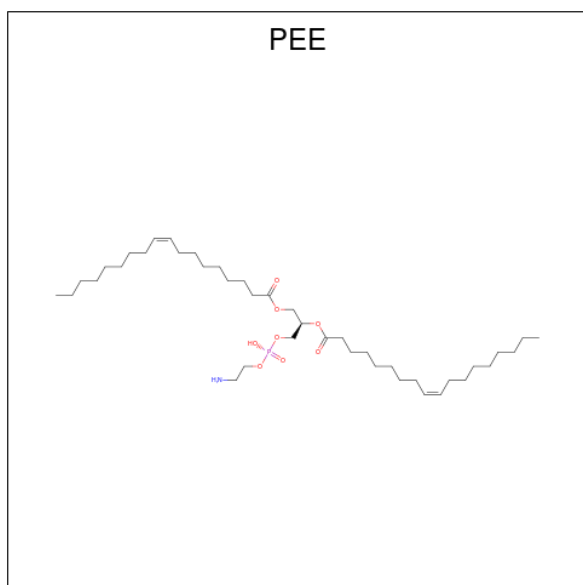
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

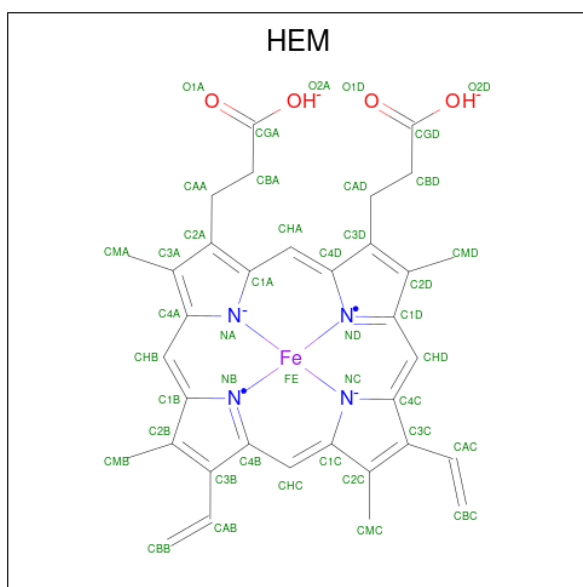
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

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



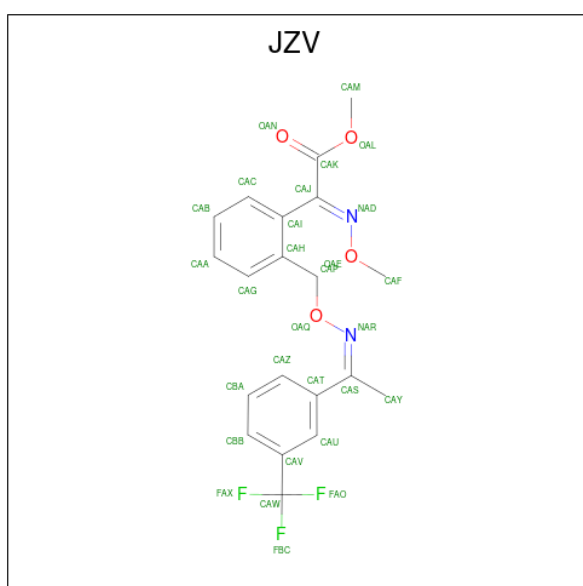
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	O	P		0	0
			21	12	8	1			
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

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



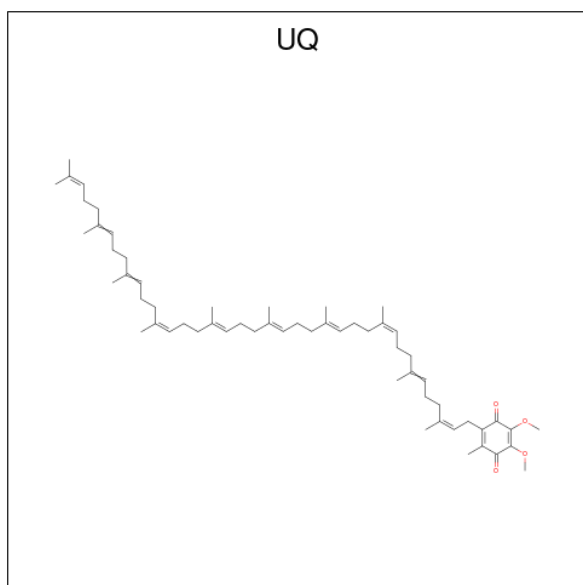
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is methyl (2E)-(methoxyimino)(2-{{[(1Z)-1-[3-(trifluoromethyl)phenyl]ethylidene}amino]oxy}methyl}phenyl)ethanoate (CCD ID: JZV) (formula: C₂₀H₁₉F₃N₂O₄).



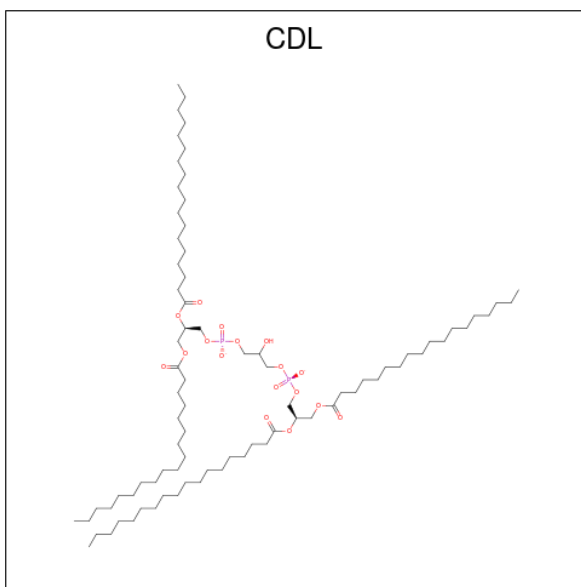
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	0	0
			29	20	3	2	4		
13	P	1	Total	C	F	N	O	0	0
			29	20	3	2	4		

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



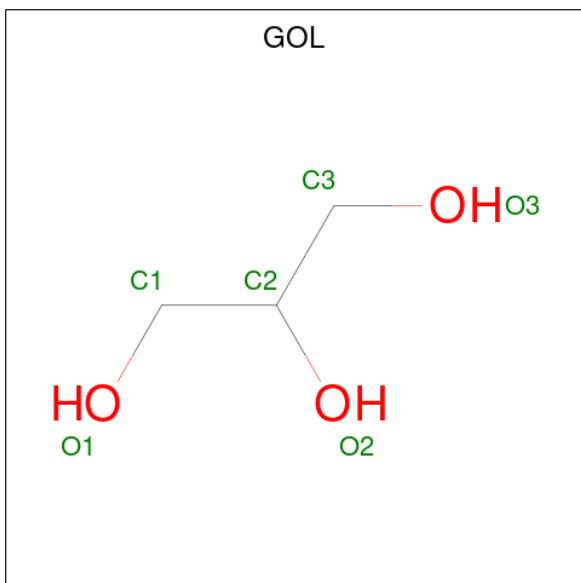
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



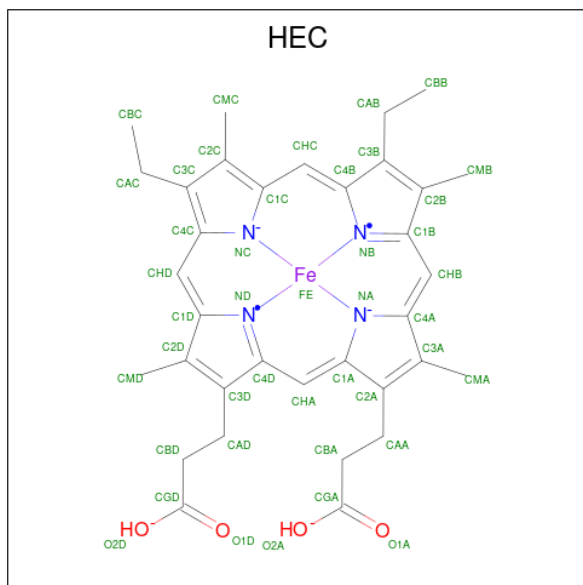
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			40	21	17	2		
15	D	1	Total	C	O	P	0	0
			42	23	17	2		
15	P	1	Total	C	O	P	0	0
			40	21	17	2		
15	Q	1	Total	C	O	P	0	0
			42	23	17	2		

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



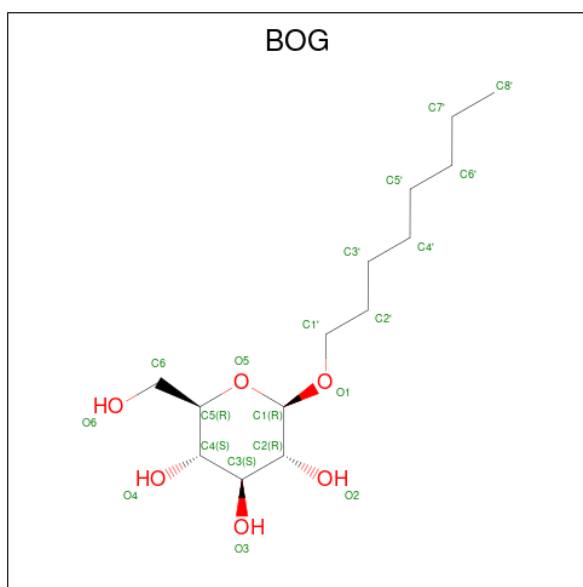
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

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



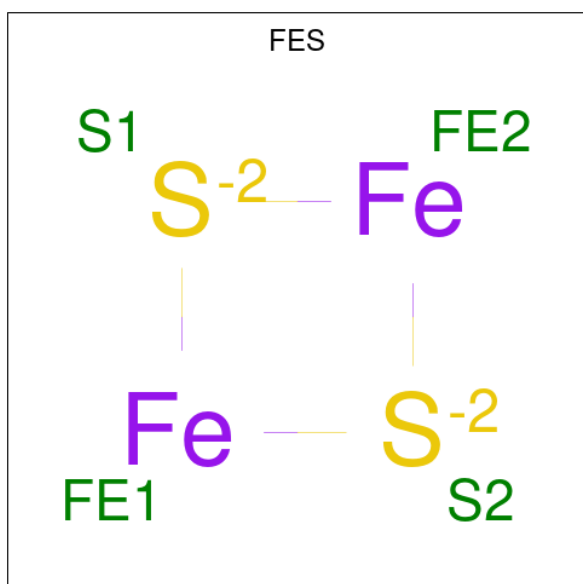
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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		
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		

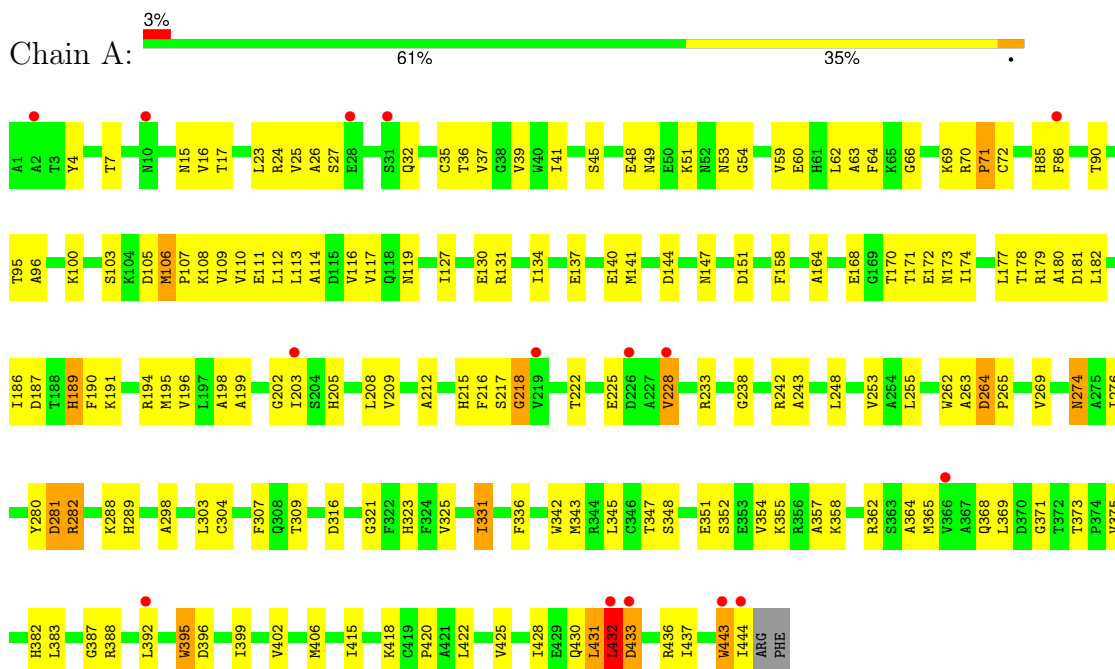
- Molecule 20 is water.

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		

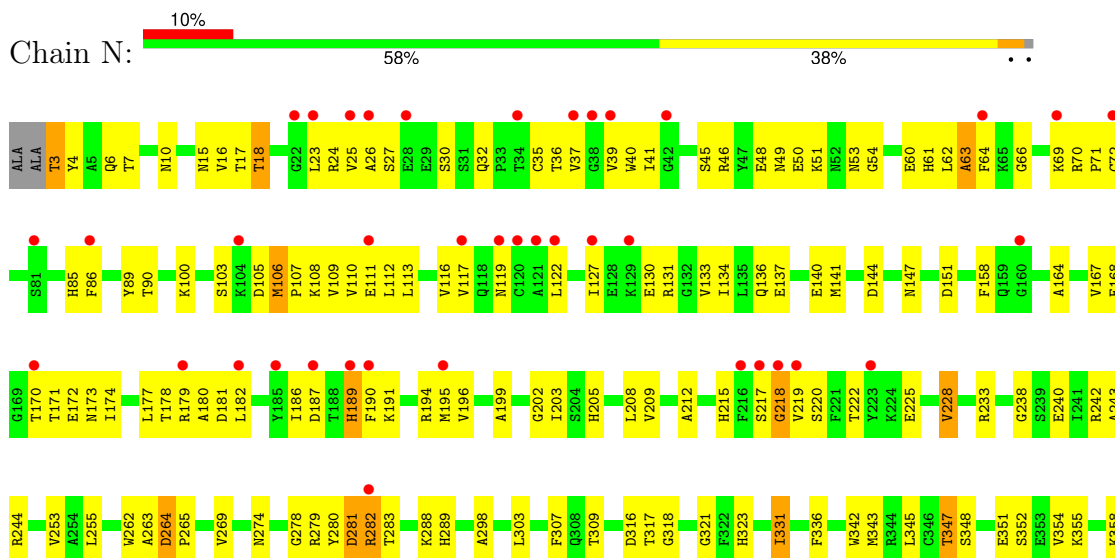
3 Residue-property plots

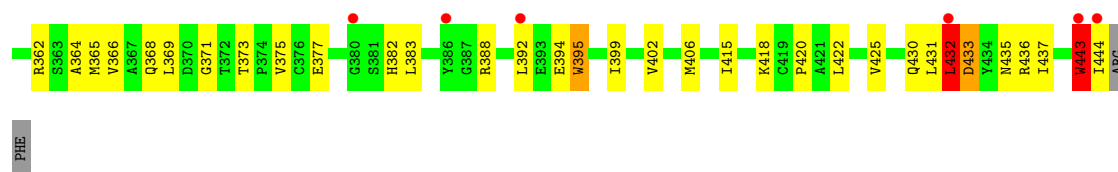
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

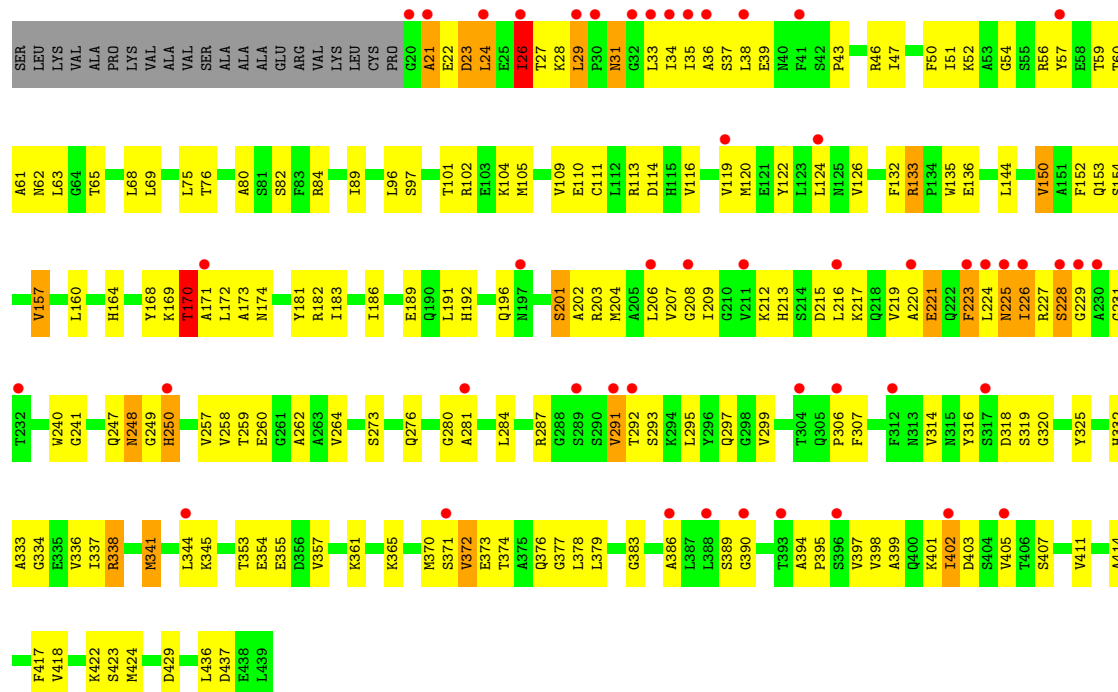


- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

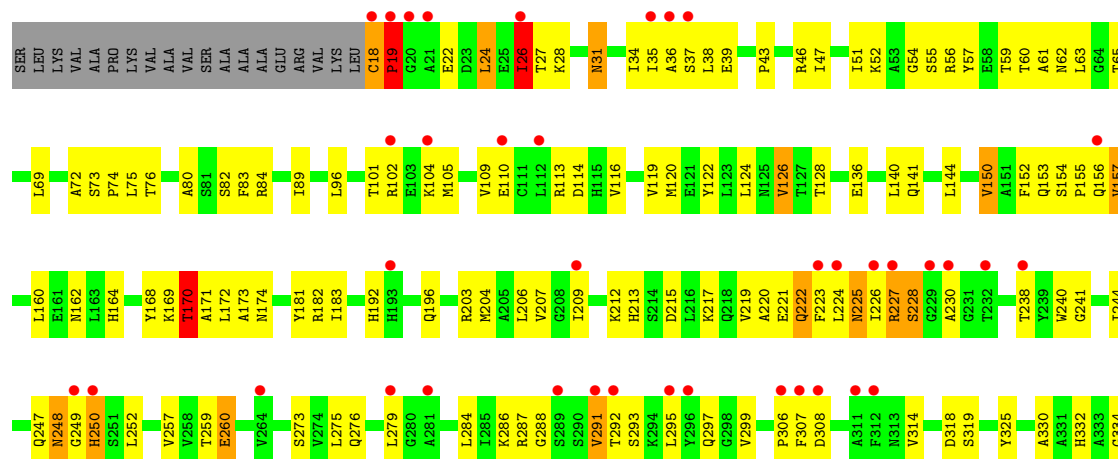


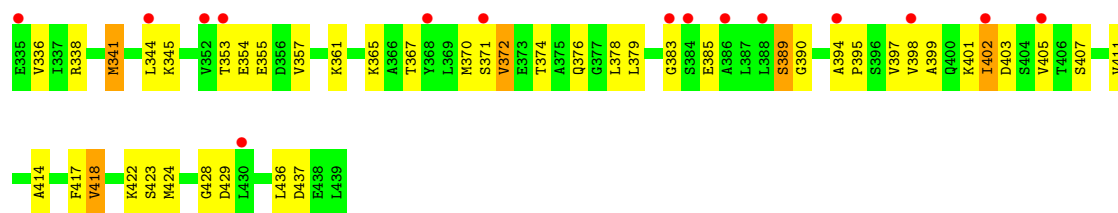


• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

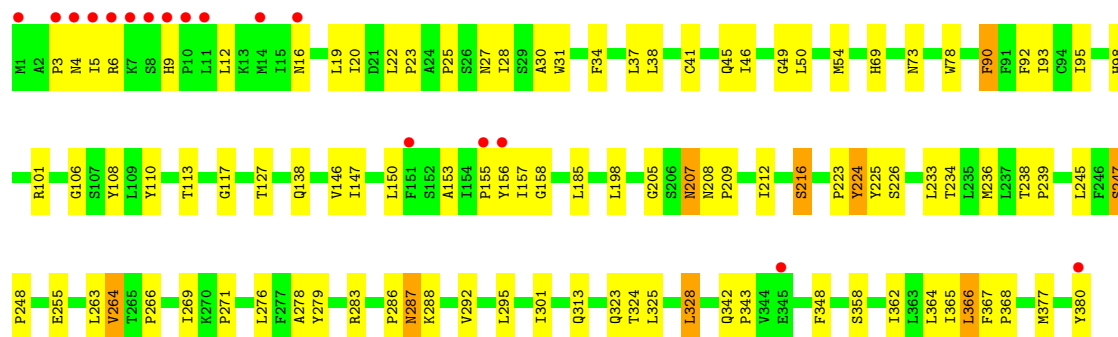
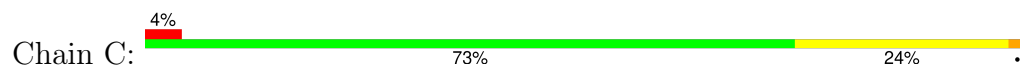


• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

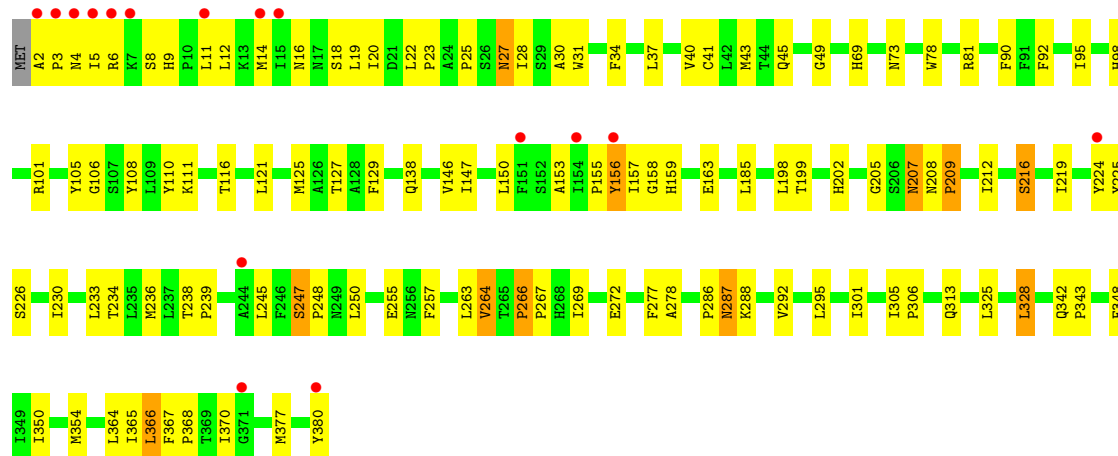




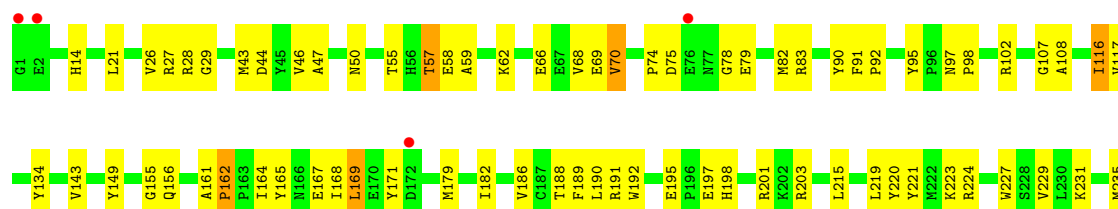
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b

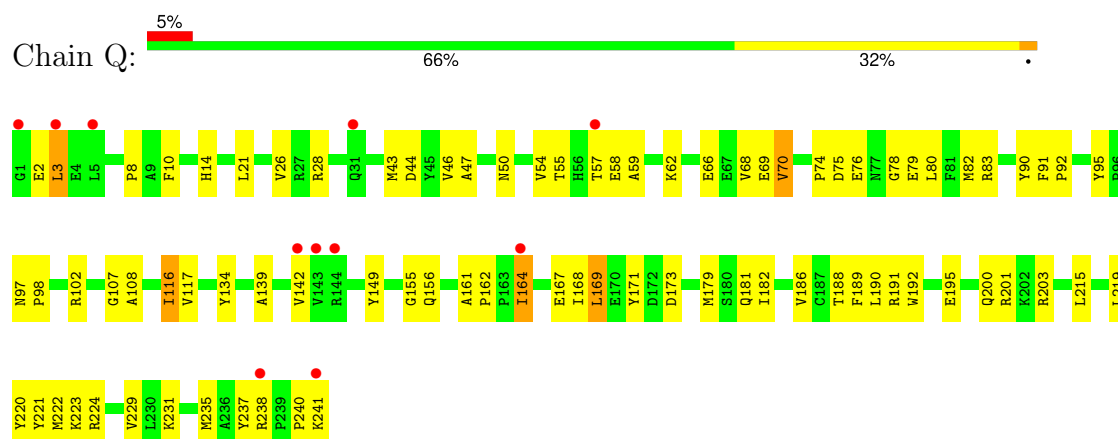


• Molecule 4: Mitochondrial cytochrome c1, heme protein

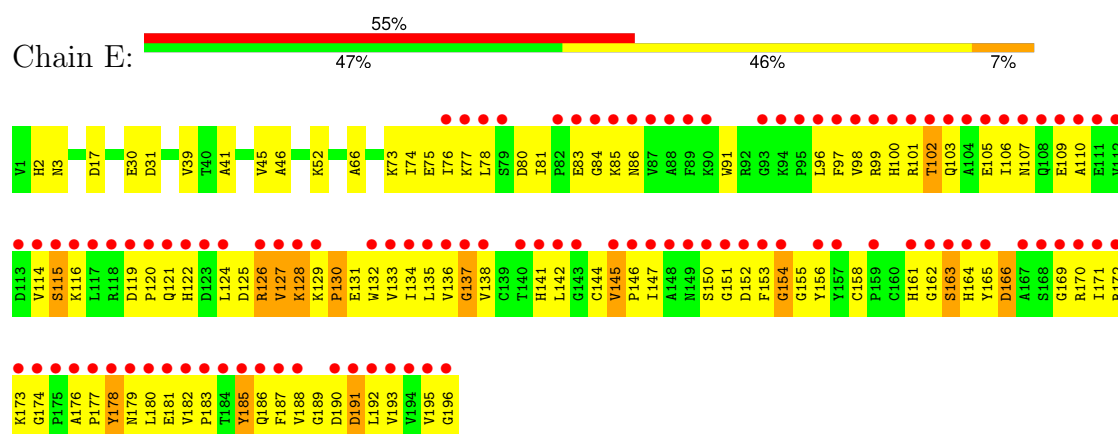




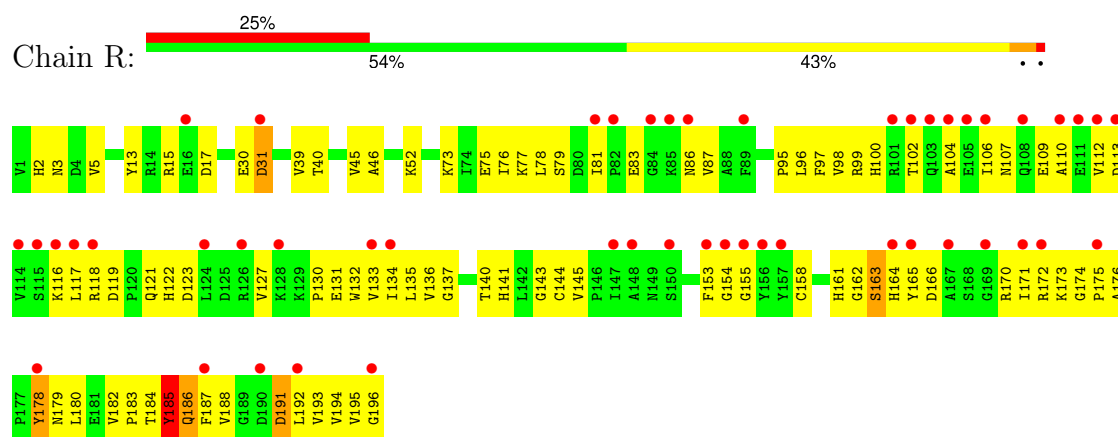
- Molecule 4: Mitochondrial cytochrome c1, heme protein



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

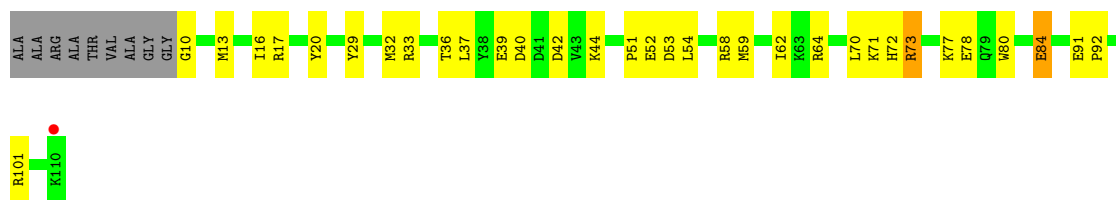


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

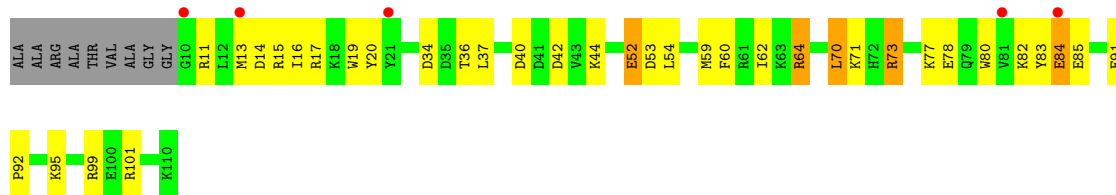


- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

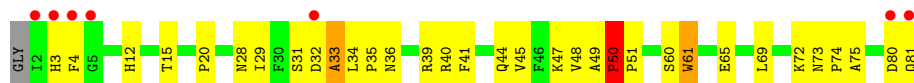




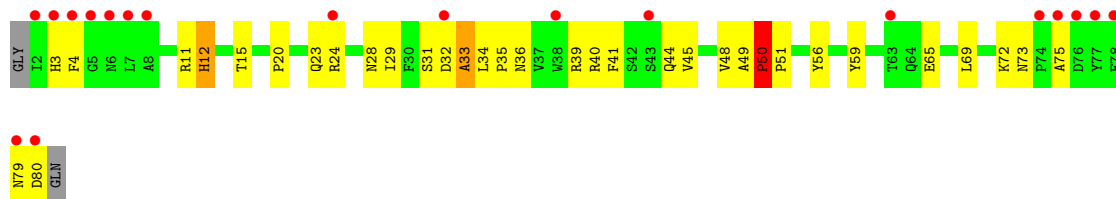
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

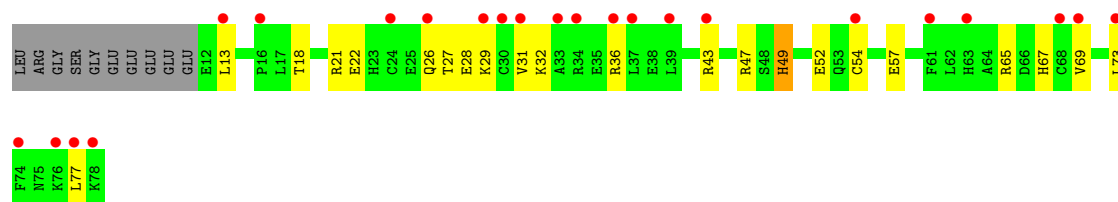


- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

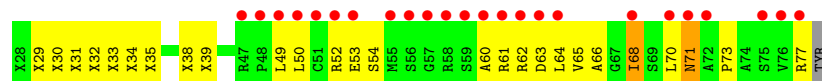
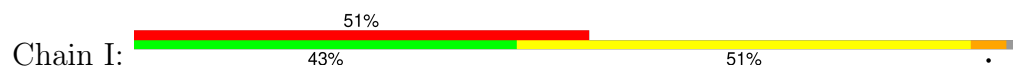


- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

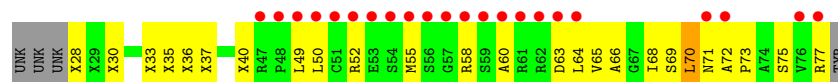




- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



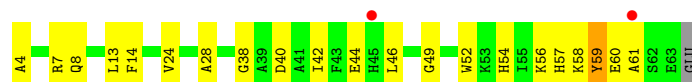
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 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	169.61Å 181.99Å 240.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.75 24.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.99-2.75) 99.2 (24.99-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.297 0.256 , 0.283	Depositor DCC
R_{free} test set	10214 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32653	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: HEM, GOL, UQ, FES, HEC, PEE, BOG, JZV, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/3518	1.02	22/4767 (0.5%)
1	N	0.49	0/3508	1.00	20/4753 (0.4%)
2	B	0.46	0/3187	0.96	8/4321 (0.2%)
2	O	0.49	0/3202	0.98	10/4343 (0.2%)
3	C	0.63	1/3119 (0.0%)	1.02	16/4270 (0.4%)
3	P	0.54	0/3114	1.01	19/4263 (0.4%)
4	D	0.60	0/1956	1.03	7/2658 (0.3%)
4	Q	0.47	0/1956	0.99	8/2658 (0.3%)
5	E	0.47	0/1547	0.90	4/2103 (0.2%)
5	R	0.45	0/1543	0.95	3/2098 (0.1%)
6	F	0.62	1/911 (0.1%)	0.91	1/1219 (0.1%)
6	S	0.47	0/911	0.91	1/1219 (0.1%)
7	G	0.54	0/694	1.03	2/941 (0.2%)
7	T	0.44	0/684	1.00	3/929 (0.3%)
8	H	0.51	0/582	0.91	2/779 (0.3%)
8	U	0.36	0/561	0.87	1/751 (0.1%)
9	I	0.58	0/218	0.92	0/293
9	V	0.55	0/218	1.02	1/293 (0.3%)
10	J	0.53	0/508	0.88	2/682 (0.3%)
10	W	0.48	0/490	0.88	2/660 (0.3%)
All	All	0.52	2/32427 (0.0%)	0.98	132/44000 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	266	PRO	CA-C	5.73	1.55	1.51
6	F	10	GLY	N-CA	5.15	1.53	1.45

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	227	ARG	N-CA-C	9.02	120.52	108.07
1	N	32	GLN	CA-C-N	8.61	128.34	119.56
1	N	32	GLN	C-N-CA	8.61	128.34	119.56
1	A	32	GLN	CA-C-N	8.47	128.20	119.56
1	A	32	GLN	C-N-CA	8.47	128.20	119.56
3	C	185	LEU	N-CA-C	8.37	120.32	111.03
3	P	185	LEU	N-CA-C	8.11	120.03	111.03
4	D	44	ASP	N-CA-C	7.82	121.75	111.75
1	A	432	LEU	N-CA-C	7.55	120.04	108.42
3	P	365	ILE	N-CA-C	7.51	118.02	111.56
1	N	432	LEU	N-CA-C	7.44	120.17	108.79
1	N	32	GLN	N-CA-C	7.40	118.97	109.72
4	Q	116	ILE	N-CA-C	7.39	118.12	110.36
1	A	428	ILE	N-CA-C	7.38	119.23	112.29
1	A	32	GLN	N-CA-C	7.33	118.88	109.72
5	R	143	GLY	N-CA-C	6.88	125.50	114.90
1	N	415	ILE	N-CA-C	6.82	117.43	111.56
4	Q	44	ASP	N-CA-C	6.75	120.38	111.75
2	O	157	VAL	N-CA-C	6.73	117.51	110.72
1	A	119	ASN	N-CA-C	6.72	121.35	111.87
4	D	116	ILE	N-CA-C	6.72	117.41	110.36
5	E	17	ASP	N-CA-C	6.66	120.50	112.38
3	C	365	ILE	N-CA-C	6.50	117.15	111.56
3	C	207	ASN	N-CA-C	-6.41	100.42	110.36
1	A	248	LEU	CA-C-N	6.38	126.13	119.05
1	A	248	LEU	C-N-CA	6.38	126.13	119.05
2	B	174	ASN	CA-C-N	6.38	126.35	119.78
2	B	174	ASN	C-N-CA	6.38	126.35	119.78
4	D	155	GLY	N-CA-C	-6.37	107.50	115.08
3	P	247	SER	CA-C-N	6.37	127.80	119.84
3	P	247	SER	C-N-CA	6.37	127.80	119.84
1	A	331	ILE	CB-CA-C	-6.36	103.74	111.88
8	U	73	LEU	N-CA-C	6.33	118.74	111.02
2	O	226	ILE	N-CA-C	-6.15	100.62	108.93
3	P	207	ASN	N-CA-C	-6.14	100.85	110.36
1	N	331	ILE	CB-CA-C	-6.13	104.12	111.97
2	O	126	VAL	N-CA-C	6.08	116.25	110.42
1	N	263	ALA	N-CA-C	6.06	118.66	111.33
1	N	119	ASN	N-CA-C	6.05	120.40	111.87
1	A	66	GLY	N-CA-C	6.04	119.79	112.48
1	A	263	ALA	N-CA-C	6.04	118.64	111.33
10	W	13	LEU	N-CA-C	6.04	120.72	112.68
1	N	348	SER	N-CA-C	6.01	118.13	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	110	TYR	N-CA-C	-5.99	100.63	109.62
7	T	50	PRO	N-CA-C	5.99	118.01	110.70
3	C	209	PRO	N-CA-C	5.97	121.61	113.84
1	A	415	ILE	N-CA-C	5.97	116.69	111.56
5	R	17	ASP	N-CA-C	5.95	119.64	112.38
4	D	95	TYR	CA-C-N	5.95	126.10	119.32
4	D	95	TYR	C-N-CA	5.95	126.10	119.32
3	C	205	GLY	N-CA-C	-5.94	104.02	112.81
3	C	247	SER	CA-C-N	5.94	127.26	119.84
3	C	247	SER	C-N-CA	5.94	127.26	119.84
8	H	73	LEU	N-CA-C	5.91	118.23	111.02
3	P	328	LEU	N-CA-C	-5.91	104.75	111.07
3	C	328	LEU	N-CA-C	-5.90	104.75	111.07
2	O	170	THR	N-CA-C	5.90	115.88	108.45
3	P	111	LYS	N-CA-C	5.90	121.10	111.37
2	B	157	VAL	N-CA-C	5.89	116.67	110.72
1	N	189	HIS	N-CA-C	5.88	120.96	113.55
9	V	70	LEU	N-CA-C	-5.87	106.28	113.50
1	N	264	ASP	N-CA-C	5.86	117.92	109.48
3	P	257	PHE	N-CA-C	-5.86	106.04	112.72
7	G	50	PRO	N-CA-C	5.85	117.83	110.70
1	A	189	HIS	N-CA-C	5.84	120.92	113.55
1	A	348	SER	N-CA-C	5.84	117.30	110.41
5	E	145	VAL	N-CA-C	5.81	113.30	107.55
1	N	347	THR	N-CA-C	5.80	121.02	113.88
4	Q	95	TYR	CA-C-N	5.77	125.46	119.05
4	Q	95	TYR	C-N-CA	5.77	125.46	119.05
3	C	366	LEU	N-CA-C	5.77	117.37	111.14
3	P	116	THR	N-CA-C	-5.76	105.00	111.28
3	P	366	LEU	N-CA-C	5.74	117.34	111.14
4	Q	155	GLY	N-CA-C	-5.73	108.26	115.08
1	A	431	LEU	N-CA-C	-5.64	100.49	109.96
10	J	13	LEU	N-CA-C	5.63	120.42	112.93
3	C	226	SER	N-CA-C	-5.62	105.16	111.28
2	O	174	ASN	CA-C-N	5.60	125.55	119.78
2	O	174	ASN	C-N-CA	5.60	125.55	119.78
3	C	113	THR	N-CA-C	-5.57	105.21	111.28
1	A	228	VAL	CA-C-N	5.57	125.84	119.83
1	A	228	VAL	C-N-CA	5.57	125.84	119.83
1	A	264	ASP	CA-C-N	5.55	125.39	119.28
1	A	264	ASP	C-N-CA	5.55	125.39	119.28
3	C	90	PHE	N-CA-C	-5.55	105.23	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	12	HIS	N-CA-C	5.54	119.33	112.24
3	C	110	TYR	N-CA-C	-5.49	101.39	109.62
2	B	133	ARG	CA-C-N	5.47	124.93	119.24
2	B	133	ARG	C-N-CA	5.47	124.93	119.24
3	P	266	PRO	CA-C-N	5.47	124.66	118.97
3	P	266	PRO	C-N-CA	5.47	124.66	118.97
2	O	225	ASN	N-CA-C	5.46	120.31	113.43
2	B	170	THR	N-CA-C	5.42	115.39	108.24
7	G	12	HIS	N-CA-C	5.38	119.15	112.58
1	A	347	THR	N-CA-C	5.35	120.82	113.97
4	D	162	PRO	CA-C-N	5.35	124.86	119.19
4	D	162	PRO	C-N-CA	5.35	124.86	119.19
3	C	27	ASN	N-CA-C	5.34	119.10	112.59
1	N	264	ASP	CA-C-N	5.33	125.15	119.28
1	N	264	ASP	C-N-CA	5.33	125.15	119.28
1	A	238	GLY	N-CA-C	-5.29	102.72	110.97
10	W	14	PHE	N-CA-C	5.28	119.72	113.28
1	N	66	GLY	N-CA-C	5.25	119.22	112.18
10	J	14	PHE	N-CA-C	5.25	119.68	113.28
3	P	272	GLU	N-CA-C	-5.24	103.57	110.43
3	C	93	ILE	N-CA-C	-5.21	105.41	110.42
1	N	238	GLY	N-CA-C	-5.19	102.88	110.97
8	H	50	THR	N-CA-C	5.18	117.18	108.73
7	T	23	GLN	N-CA-C	5.18	117.15	109.69
2	B	258	VAL	N-CA-C	5.18	115.14	108.82
6	F	39	GLU	N-CA-C	5.17	117.62	109.39
1	N	228	VAL	CA-C-N	5.17	125.42	119.83
1	N	228	VAL	C-N-CA	5.17	125.42	119.83
1	A	264	ASP	N-CA-C	5.17	116.93	109.48
4	Q	164	ILE	N-CA-C	5.15	117.25	108.86
2	B	223	PHE	N-CA-C	5.14	119.91	113.43
1	N	278	GLY	N-CA-C	5.13	120.43	111.50
3	C	224	TYR	N-CA-C	5.12	117.27	111.02
5	E	66	ALA	N-CA-C	5.12	117.53	111.33
3	P	27	ASN	N-CA-C	5.10	118.81	112.59
3	P	90	PHE	N-CA-C	-5.09	105.73	111.28
3	P	209	PRO	N-CA-C	5.08	120.51	113.65
3	P	205	GLY	N-CA-C	-5.07	104.20	112.83
3	P	226	SER	N-CA-C	-5.07	105.75	111.28
4	Q	173	ASP	N-CA-C	-5.07	106.51	113.30
2	O	141	GLN	CA-C-N	-5.05	114.87	119.82
2	O	141	GLN	C-N-CA	-5.05	114.87	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	80	LEU	N-CA-C	-5.04	103.74	110.55
5	R	15	ARG	N-CA-C	-5.04	103.75	110.55
5	E	126	ARG	N-CA-C	5.03	115.62	107.32
1	N	244	ARG	N-CA-C	5.03	117.43	109.24
6	S	15	ARG	N-CA-C	-5.01	106.02	112.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3362	136	0
1	N	3437	0	3349	153	0
2	B	3133	0	3130	190	0
2	O	3147	0	3146	196	0
3	C	3017	0	3063	82	0
3	P	3012	0	3058	104	0
4	D	1898	0	1846	63	0
4	Q	1898	0	1846	75	0
5	E	1513	0	1478	126	0
5	R	1509	0	1474	98	0
6	F	891	0	893	24	0
6	S	891	0	893	40	0
7	G	672	0	653	34	0
7	T	662	0	645	36	0
8	H	574	0	548	16	0
8	U	553	0	535	24	0
9	I	287	0	250	37	0
9	V	277	0	251	34	0
10	J	497	0	490	16	0
10	W	479	0	478	16	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	N	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	P	49	0	72	3	0
11	R	50	0	77	2	0
12	C	86	0	60	10	0
12	P	86	0	60	8	0
13	C	29	0	19	4	0
13	P	29	0	19	4	0
14	C	19	0	17	2	0
14	P	19	0	17	3	0
15	C	40	0	24	4	0
15	D	42	0	28	4	0
15	P	40	0	24	4	0
15	Q	42	0	28	3	0
16	C	6	0	8	0	0
16	P	6	0	8	0	0
17	D	43	0	30	0	0
17	Q	43	0	30	0	0
18	D	33	0	39	0	0
18	P	12	0	11	2	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
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	1	0
20	R	1	0	0	0	0
All	All	32653	0	32160	1376	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 21.

All (1376) 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)
9:V:35:UNK:HG3	9:V:36:UNK:H	1.05	1.14
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.15	1.13
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.34	1.07
2:B:76:THR:HG22	2:B:82:SER:H	1.18	1.07
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:O:353:THR:HG22	2:O:355:GLU:H	1.18	1.05
2:B:353:THR:HG22	2:B:355:GLU:H	1.19	1.03
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ILE:HG13	13:C:2001:JZV:HAP	1.44	0.99
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.28	0.99
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.78	0.99
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.42	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.25	0.98
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.97
1:A:178:THR:HG22	1:A:180:ALA:H	1.25	0.96
3:P:9:HIS:HD2	3:P:12:LEU:H	1.09	0.95
3:C:9:HIS:HD2	3:C:12:LEU:H	1.11	0.93
4:D:47:ALA:H	4:D:50:ASN:HD22	1.12	0.91
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.50	0.91
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.36	0.91
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.52	0.91
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.51	0.90
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.54	0.90
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.36	0.89
3:P:147:ILE:HG13	13:P:3001:JZV:HAP	1.50	0.88
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.54	0.88
9:I:32:UNK:N	9:I:73:PRO:HG2	1.89	0.88
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.37	0.88
7:T:41:PHE:O	7:T:45:VAL:HG23	1.75	0.87
3:P:238:THR:HB	3:P:239:PRO:HD3	1.56	0.86
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.56	0.86
2:O:27:THR:HG22	2:O:28:LYS:H	1.40	0.86
7:G:41:PHE:O	7:G:45:VAL:HG23	1.76	0.85
2:O:248:ASN:HD22	2:O:248:ASN:C	1.83	0.85
1:A:178:THR:HB	1:A:181:ASP:OD1	1.75	0.85
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.57	0.85
9:V:35:UNK:HG3	9:V:36:UNK:N	1.89	0.85
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.58	0.85
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.58	0.84
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.60	0.84
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.60	0.84
9:V:64:LEU:HD12	9:V:77:ARG:O	1.78	0.84
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.59	0.83
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.61	0.83
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.04	0.83
2:B:248:ASN:C	2:B:248:ASN:HD22	1.87	0.82
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.45	0.82
5:E:127:VAL:HG12	5:E:128:LYS:H	1.43	0.82
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.62	0.81
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.45	0.81
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.62	0.81
2:O:192:HIS:O	2:O:196:GLN:HG3	1.81	0.81
9:I:34:UNK:HG3	9:I:35:UNK:N	1.96	0.80
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.45	0.80
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.44	0.80
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.64	0.80
3:C:238:THR:HB	3:C:239:PRO:HD3	1.64	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.17	0.79
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.65	0.79
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.65	0.79
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
2:B:47:ILE:HD13	2:B:120:MET:CE	2.14	0.78
1:A:343:MET:HB3	1:A:444:ILE:HA	1.64	0.78
1:N:178:THR:HB	1:N:181:ASP:OD1	1.82	0.78
2:O:221:GLU:HG3	2:O:222:GLN:H	1.49	0.77
2:O:154:SER:O	2:O:157:VAL:HG12	1.85	0.77
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.66	0.77
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.49	0.77
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.66	0.77
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.19	0.76
3:P:101:ARG:C	3:P:101:ARG:HD2	2.09	0.76
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.11	0.76
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.86	0.76
4:D:57:THR:HG22	4:D:59:ALA:H	1.49	0.76
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.66	0.76
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.21	0.76
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.34	0.75
2:B:192:HIS:O	2:B:196:GLN:HG3	1.87	0.75
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.68	0.75
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.22	0.75
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.66	0.75
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.51	0.75
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.49	0.75
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.17	0.75
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.68	0.75
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.51	0.74
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.06	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.69	0.74
2:B:399:ALA:O	2:B:402:ILE:HG22	1.87	0.74
5:R:79:SER:OG	5:R:191:ASP:HB2	1.88	0.74
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.68	0.74
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.70	0.74
2:O:338:ARG:HG3	2:O:338:ARG:NH1	2.00	0.74
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.70	0.73
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.73
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.52	0.73
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.35	0.73
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.52	0.73
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.24	0.73
2:B:31:ASN:HD22	2:B:31:ASN:N	1.86	0.73
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.52	0.72
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.71	0.72
2:B:27:THR:HG22	2:B:28:LYS:H	1.53	0.72
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.54	0.72
1:N:170:THR:HG22	1:N:171:THR:N	2.03	0.72
1:N:10:ASN:HD21	2:O:18:CYS:N	1.88	0.72
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.24	0.72
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.23	0.72
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.05	0.72
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.70	0.72
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.25	0.72
5:E:52:LYS:C	5:E:52:LYS:HD3	2.14	0.72
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.88	0.72
5:E:84:GLY:N	5:E:102:THR:HG23	2.05	0.72
1:N:343:MET:HB3	1:N:444:ILE:HA	1.71	0.72
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.03	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.90	0.72
3:C:9:HIS:CD2	3:C:12:LEU:H	2.03	0.72
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.26	0.71
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.07	0.71
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.72	0.71
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.71	0.71
3:P:216:SER:HB3	6:S:59:MET:HE2	1.71	0.71
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.01	0.71
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.71	0.71
2:O:47:ILE:HD13	2:O:120:MET:CE	2.20	0.71
3:C:245:LEU:O	4:D:201:ARG:HD2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:CD2	3:P:12:LEU:H	2.01	0.71
2:O:399:ALA:O	2:O:402:ILE:HG22	1.90	0.70
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.06	0.70
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.72	0.70
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.71	0.70
2:O:225:ASN:O	2:O:227:ARG:HG3	1.90	0.70
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.15	0.70
2:B:202:ALA:HB3	2:B:229:GLY:O	1.91	0.70
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.71	0.70
4:Q:164:ILE:O	4:Q:179:MET:HE2	1.91	0.70
5:R:52:LYS:HD3	5:R:52:LYS:C	2.17	0.70
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.22	0.70
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.55	0.70
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.92	0.70
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.56	0.70
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.26	0.70
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.06	0.70
3:P:245:LEU:O	4:Q:201:ARG:HD2	1.91	0.69
1:A:106:MET:HE2	1:A:107:PRO:HA	1.75	0.69
3:C:101:ARG:HD2	3:C:101:ARG:C	2.17	0.69
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.28	0.69
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.74	0.69
5:E:190:ASP:C	5:E:192:LEU:H	1.98	0.69
4:D:47:ALA:H	4:D:50:ASN:ND2	1.89	0.68
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.93	0.68
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.27	0.68
1:N:15:ASN:O	1:N:26:ALA:HA	1.93	0.68
2:B:76:THR:HG22	2:B:82:SER:N	2.02	0.68
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.26	0.68
2:O:407:SER:O	2:O:411:VAL:HG23	1.94	0.68
2:B:27:THR:HG22	2:B:28:LYS:N	2.07	0.68
2:B:31:ASN:H	2:B:31:ASN:ND2	1.90	0.68
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.94	0.68
1:N:105:ASP:O	1:N:109:VAL:HG23	1.92	0.68
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.76	0.68
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.76	0.68
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.76	0.68
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.28	0.68
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.59	0.67
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.75	0.67
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:35:UNK:CG	9:V:36:UNK:H	1.89	0.67
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.75	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.08	0.67
4:D:57:THR:HG22	4:D:59:ALA:N	2.08	0.67
2:O:361:LYS:O	2:O:365:LYS:HG3	1.95	0.67
9:I:31:UNK:C	9:I:73:PRO:HG2	2.25	0.67
1:A:15:ASN:O	1:A:26:ALA:HA	1.95	0.67
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.75	0.67
2:B:225:ASN:O	2:B:227:ARG:N	2.28	0.67
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.77	0.67
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.30	0.67
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.10	0.67
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.75	0.66
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.29	0.66
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.11	0.66
4:D:62:LYS:O	4:D:66:GLU:HG3	1.95	0.66
9:I:70:LEU:HD23	9:I:71:ASN:N	2.10	0.66
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.59	0.66
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.31	0.66
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.78	0.66
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.96	0.66
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.26	0.66
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.10	0.66
3:P:40:VAL:HA	3:P:43:MET:HE3	1.76	0.66
15:P:3004:CDL:HA32	7:T:40:ARG:HB3	1.77	0.66
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.77	0.66
9:I:64:LEU:HD12	9:I:77:ARG:O	1.95	0.66
4:D:164:ILE:O	4:D:179:MET:HE2	1.94	0.66
2:B:62:ASN:O	2:B:65:THR:HG22	1.96	0.66
1:N:402:VAL:HG22	1:N:406:MET:CE	2.25	0.65
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.28	0.65
9:I:70:LEU:HD23	9:I:71:ASN:H	1.61	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.27	0.65
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.61	0.65
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.77	0.65
5:E:127:VAL:HG12	5:E:128:LYS:N	2.11	0.65
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.78	0.65
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.96	0.65
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.78	0.65
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.77	0.65
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.31	0.64
2:O:219:VAL:O	2:O:223:PHE:HB2	1.97	0.64
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.26	0.64
2:O:59:THR:HG22	2:O:61:ALA:H	1.62	0.64
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.78	0.64
12:P:502:HEM:HMC2	12:P:502:HEM:HBC2	1.79	0.64
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.12	0.64
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.12	0.64
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.80	0.64
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.78	0.64
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.27	0.64
2:O:273:SER:O	2:O:276:GLN:HB3	1.97	0.64
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.80	0.64
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.79	0.64
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.33	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.64
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.21	0.64
1:N:170:THR:HG22	1:N:172:GLU:H	1.62	0.64
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.13	0.64
9:V:70:LEU:HD23	9:V:71:ASN:N	2.14	0.64
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.12	0.63
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.32	0.63
1:A:178:THR:HG22	1:A:180:ALA:N	2.07	0.63
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.14	0.63
10:W:7:ARG:CB	10:W:7:ARG:HH11	2.11	0.63
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.79	0.63
5:E:78:LEU:HD12	5:E:190:ASP:O	1.98	0.63
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.79	0.63
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.81	0.63
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.11	0.63
2:B:38:LEU:HD12	2:B:39:GLU:N	2.14	0.63
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.63	0.63
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.99	0.63
3:P:236:MET:O	3:P:239:PRO:HD2	1.99	0.62
5:E:106:ILE:C	5:E:110:ALA:HB3	2.23	0.62
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.81	0.62
1:N:106:MET:HE2	1:N:107:PRO:HA	1.81	0.62
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.28	0.62
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.80	0.62
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.00	0.62
5:E:187:PHE:C	5:E:189:GLY:H	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.64	0.62
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.82	0.62
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.34	0.62
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.29	0.62
2:B:69:LEU:HD23	2:B:105:MET:HE1	1.82	0.62
2:O:217:LYS:O	2:O:221:GLU:HG2	1.99	0.62
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.34	0.62
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.81	0.62
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.29	0.62
1:A:7:THR:HG21	2:B:113:ARG:CD	2.30	0.62
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.25	0.62
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.00	0.62
2:O:353:THR:HG22	2:O:355:GLU:N	2.02	0.62
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.82	0.62
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.29	0.62
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.82	0.62
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.80	0.62
8:U:28:GLU:O	8:U:32:LYS:HG3	1.99	0.62
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.00	0.61
7:T:79:ASN:O	7:T:80:ASP:HB2	2.00	0.61
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.10	0.61
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.81	0.61
2:B:407:SER:O	2:B:411:VAL:HG23	2.00	0.61
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.61
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.80	0.61
2:B:353:THR:HG22	2:B:355:GLU:N	2.04	0.61
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.82	0.61
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.30	0.61
2:B:338:ARG:HH11	2:B:338:ARG:CG	2.10	0.61
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.36	0.61
1:N:182:LEU:O	1:N:186:ILE:HG13	2.01	0.61
2:B:292:THR:HG22	2:B:292:THR:O	2.00	0.61
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.61
2:B:248:ASN:C	2:B:248:ASN:ND2	2.59	0.61
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.83	0.61
8:H:18:THR:O	8:H:22:GLU:HG3	2.01	0.61
8:H:28:GLU:O	8:H:32:LYS:HG3	2.01	0.61
5:E:130:PRO:HG2	5:E:131:GLU:H	1.66	0.61
6:F:59:MET:HE3	6:F:59:MET:HA	1.83	0.60
9:V:64:LEU:HD12	9:V:77:ARG:C	2.26	0.60
2:B:215:ASP:O	2:B:219:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.16	0.60
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.37	0.60
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.67	0.60
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.01	0.60
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.83	0.60
2:B:96:LEU:H	9:I:70:LEU:HD22	1.66	0.60
1:N:371:GLY:O	1:N:375:VAL:HG23	2.01	0.60
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.81	0.60
1:A:23:LEU:HD23	1:A:24:ARG:N	2.17	0.60
2:O:402:ILE:C	2:O:402:ILE:HD13	2.27	0.60
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.83	0.60
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.69	0.60
2:O:27:THR:CG2	2:O:28:LYS:H	2.14	0.60
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.83	0.60
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.60
1:N:219:VAL:HG12	1:N:220:SER:N	2.16	0.60
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.65	0.60
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.84	0.60
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.83	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.37	0.60
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.37	0.60
5:R:117:LEU:HD11	5:R:172:ARG:NH1	2.16	0.59
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.84	0.59
1:N:178:THR:HG22	1:N:180:ALA:N	2.08	0.59
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.83	0.59
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.37	0.59
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.85	0.59
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.68	0.59
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.83	0.59
2:B:59:THR:HG22	2:B:61:ALA:H	1.66	0.59
1:N:269:VAL:HG22	1:N:406:MET:HE3	1.82	0.59
5:R:109:GLU:OE1	5:R:123:ASP:HB2	2.02	0.59
5:E:116:LYS:HD2	5:E:116:LYS:N	2.17	0.59
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.68	0.59
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.68	0.59
8:H:27:THR:O	8:H:31:VAL:HG23	2.02	0.59
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.84	0.59
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.02	0.59
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.84	0.59
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.36	0.59
1:A:106:MET:HE2	1:A:107:PRO:CA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:2004:CDL:HA32	7:G:40:ARG:HB3	1.85	0.59
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.15	0.59
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.84	0.59
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.85	0.59
5:R:171:ILE:HG12	5:R:176:ALA:O	2.02	0.59
8:U:27:THR:O	8:U:31:VAL:HG23	2.02	0.59
2:B:361:LYS:O	2:B:365:LYS:HG3	2.02	0.59
5:E:101:ARG:HA	5:E:105:GLU:OE1	2.03	0.59
5:E:163:SER:HA	5:E:174:GLY:HA3	1.85	0.59
5:R:76:ILE:O	5:R:193:VAL:HG12	2.03	0.59
6:S:59:MET:HE3	6:S:59:MET:HA	1.85	0.59
1:A:170:THR:HG22	1:A:172:GLU:H	1.68	0.58
3:P:34:PHE:HB2	20:P:381:HOH:O	2.03	0.58
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.84	0.58
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.86	0.58
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.17	0.58
5:E:147:ILE:O	5:E:156:TYR:HA	2.04	0.58
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.33	0.58
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.10	0.58
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.84	0.58
1:A:430:GLN:HG3	7:G:4:PHE:O	2.03	0.58
2:B:341:MET:CE	2:B:341:MET:HA	2.34	0.58
1:N:63:ALA:O	1:N:116:VAL:HG13	2.03	0.58
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.39	0.58
1:N:282:ARG:NH2	9:V:37:UNK:N	2.51	0.58
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.27	0.58
1:A:103:SER:HB3	1:A:202:GLY:O	2.04	0.58
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.67	0.58
2:O:422:LYS:O	2:O:436:LEU:HD21	2.02	0.58
8:U:27:THR:HG22	8:U:29:LYS:H	1.67	0.58
2:B:31:ASN:N	2:B:31:ASN:ND2	2.47	0.58
1:N:112:LEU:O	1:N:116:VAL:HG23	2.03	0.58
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.51	0.58
1:N:269:VAL:CG2	1:N:406:MET:HE3	2.33	0.58
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.85	0.58
1:A:371:GLY:O	1:A:375:VAL:HG23	2.04	0.58
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.03	0.58
1:A:402:VAL:HG22	1:A:406:MET:CE	2.34	0.58
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.86	0.58
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.84	0.58
2:O:414:ALA:O	2:O:418:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.34	0.58
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.34	0.58
5:E:76:ILE:O	5:E:193:VAL:HG12	2.04	0.58
3:P:313:GLN:HE21	6:S:36:THR:CB	2.17	0.58
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.34	0.57
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.03	0.57
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.86	0.57
2:O:332:HIS:O	2:O:336:VAL:HG23	2.03	0.57
2:O:341:MET:CE	2:O:417:PHE:HE2	2.15	0.57
2:O:215:ASP:O	2:O:219:VAL:HG23	2.04	0.57
3:P:377:MET:HE2	6:S:20:TYR:CD1	2.39	0.57
3:C:153:ALA:HB2	3:C:288:LYS:HG2	1.85	0.57
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.38	0.57
5:R:102:THR:O	5:R:106:ILE:HG13	2.04	0.57
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.39	0.57
1:A:274:ASN:ND2	1:A:309:THR:HB	2.20	0.57
2:B:341:MET:HA	2:B:341:MET:HE2	1.86	0.57
6:F:84:GLU:H	6:F:84:GLU:CD	2.12	0.57
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.40	0.57
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.04	0.57
3:C:147:ILE:CG1	13:C:2001:JZV:HAP	2.29	0.57
4:D:169:LEU:C	4:D:169:LEU:HD23	2.30	0.57
5:E:84:GLY:N	5:E:100:HIS:O	2.33	0.57
2:O:338:ARG:HH11	2:O:338:ARG:CG	2.09	0.57
1:A:178:THR:CG2	1:A:179:ARG:N	2.68	0.57
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.57
3:C:30:ALA:HB1	15:D:2003:CDL:H111	1.86	0.57
4:D:231:LYS:O	6:F:71:LYS:HE3	2.05	0.57
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.86	0.57
6:S:95:LYS:O	6:S:99:ARG:HG3	2.03	0.57
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.33	0.57
7:G:65:GLU:O	7:G:69:LEU:HG	2.04	0.57
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.87	0.57
2:O:292:THR:HG22	2:O:292:THR:O	2.02	0.57
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.05	0.57
1:A:364:ALA:O	1:A:368:GLN:HG3	2.05	0.57
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.20	0.57
4:Q:2:GLU:O	4:Q:3:LEU:O	2.22	0.57
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.86	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.05	0.56
1:N:364:ALA:O	1:N:368:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.87	0.56
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.86	0.56
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.40	0.56
5:R:186:GLN:O	5:R:193:VAL:HG23	2.04	0.56
2:B:31:ASN:HD22	2:B:31:ASN:H	1.48	0.56
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.28	0.56
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.45	0.56
1:N:36:THR:HG21	1:N:373:THR:HA	1.86	0.56
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.70	0.56
1:N:430:GLN:HG3	7:T:4:PHE:O	2.05	0.56
4:Q:169:LEU:HD22	4:Q:182:ILE:HD11	1.87	0.56
7:G:28:ASN:HB3	7:G:31:SER:OG	2.06	0.56
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.86	0.56
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.87	0.56
2:B:264:VAL:HG23	2:B:316:TYR:C	2.30	0.56
2:B:332:HIS:O	2:B:336:VAL:HG23	2.06	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.31	0.56
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.35	0.56
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.45	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.06	0.56
1:N:178:THR:CG2	1:N:179:ARG:N	2.68	0.56
5:R:106:ILE:O	5:R:109:GLU:HB3	2.05	0.56
1:A:269:VAL:HG22	1:A:406:MET:HE3	1.87	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.41	0.56
3:C:301:ILE:CD1	3:C:364:LEU:HD21	2.34	0.56
1:N:170:THR:CG2	1:N:171:THR:N	2.68	0.56
1:N:382:HIS:HB3	1:N:388:ARG:O	2.06	0.56
2:B:414:ALA:O	2:B:418:VAL:HG23	2.06	0.56
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.06	0.56
2:O:69:LEU:HD23	2:O:105:MET:HE1	1.86	0.56
1:N:279:ARG:HH22	9:V:30:UNK:C	2.19	0.56
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.68	0.56
2:B:28:LYS:O	2:B:29:LEU:O	2.24	0.56
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.88	0.56
1:N:187:ASP:O	1:N:191:LYS:HE3	2.06	0.56
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.70	0.56
6:S:53:ASP:OD1	6:S:54:LEU:N	2.39	0.56
2:O:38:LEU:HD12	2:O:39:GLU:N	2.21	0.55
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.87	0.55
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.89	0.55
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.20	0.55
2:B:23:ASP:OD1	2:B:24:LEU:N	2.38	0.55
2:B:201:SER:OG	2:B:228:SER:HA	2.07	0.55
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.07	0.55
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.71	0.55
2:O:150:VAL:O	2:O:153:GLN:HG3	2.06	0.55
15:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.07	0.55
4:Q:222:MET:HE3	5:R:40:THR:OG1	2.06	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.40	0.55
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.21	0.55
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.22	0.55
9:I:29:UNK:O	9:I:30:UNK:HB2	2.05	0.55
1:N:170:THR:HG22	1:N:171:THR:H	1.71	0.55
2:O:397:VAL:O	2:O:401:LYS:HG2	2.07	0.55
5:R:118:ARG:NH1	5:R:174:GLY:O	2.40	0.55
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.22	0.55
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.87	0.55
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.06	0.55
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.46	0.55
1:A:187:ASP:O	1:A:191:LYS:HE3	2.07	0.55
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.71	0.55
5:E:106:ILE:O	5:E:110:ALA:HB3	2.07	0.55
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.41	0.55
3:C:301:ILE:HD11	3:C:364:LEU:CD2	2.34	0.55
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.89	0.55
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.72	0.55
2:B:341:MET:CE	2:B:417:PHE:HE2	2.14	0.55
2:B:422:LYS:O	2:B:436:LEU:HD21	2.06	0.55
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.71	0.55
2:O:341:MET:CE	2:O:341:MET:HA	2.37	0.55
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.39	0.55
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.88	0.55
2:B:338:ARG:NH1	2:B:338:ARG:CG	2.69	0.55
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.89	0.55
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.42	0.55
15:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.22	0.55
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.89	0.55
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.88	0.55
3:C:286:PRO:O	3:C:287:ASN:HB2	2.08	0.54
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.07	0.54
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.22	0.54
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.68	0.54
1:N:106:MET:HE2	1:N:107:PRO:CA	2.37	0.54
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.37	0.54
2:O:31:ASN:N	2:O:31:ASN:HD22	2.05	0.54
8:U:18:THR:O	8:U:22:GLU:HG3	2.07	0.54
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.88	0.54
1:N:233:ARG:HH21	1:N:316:ASP:HB2	1.73	0.54
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.22	0.54
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.71	0.54
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.88	0.54
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.89	0.54
5:E:188:VAL:HG12	5:E:188:VAL:O	2.08	0.54
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.88	0.54
2:O:357:VAL:O	2:O:361:LYS:HG3	2.07	0.54
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.22	0.54
2:B:76:THR:CG2	2:B:82:SER:H	2.06	0.54
3:P:199:THR:HA	18:P:2010:BOG:O1	2.08	0.54
5:R:184:THR:O	5:R:185:TYR:HB3	2.07	0.54
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.54
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.33	0.54
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.89	0.54
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.38	0.54
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.90	0.54
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.37	0.54
6:F:53:ASP:OD1	6:F:54:LEU:N	2.39	0.54
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.42	0.54
2:O:374:THR:HG22	2:O:376:GLN:H	1.72	0.54
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.43	0.54
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.70	0.54
3:P:30:ALA:HB1	15:Q:3003:CDL:H111	1.90	0.54
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.43	0.53
5:E:84:GLY:CA	5:E:102:THR:HG23	2.38	0.53
1:N:23:LEU:HD23	1:N:24:ARG:N	2.23	0.53
1:N:209:VAL:O	1:N:212:ALA:HB3	2.07	0.53
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.91	0.53
15:P:3004:CDL:H712	11:P:3007:PEE:H50	1.90	0.53
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.28	0.53
2:B:24:LEU:HD12	2:B:37:SER:O	2.07	0.53
3:C:216:SER:HB3	6:F:59:MET:HE2	1.88	0.53
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.53
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.90	0.53
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.74	0.53
11:R:3005:PEE:H58	10:W:24:VAL:HG11	1.90	0.53
1:A:36:THR:HG21	1:A:373:THR:HA	1.91	0.53
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.73	0.53
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.88	0.53
2:O:252:LEU:HD13	9:V:55:MET:HE3	1.91	0.53
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.43	0.53
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.53
15:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.23	0.53
8:U:22:GLU:O	8:U:26:GLN:HG2	2.08	0.53
1:A:105:ASP:O	1:A:109:VAL:HG23	2.08	0.53
5:E:131:GLU:CD	5:E:131:GLU:H	2.17	0.53
2:O:372:VAL:HG12	2:O:372:VAL:O	2.08	0.53
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.74	0.53
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.38	0.53
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.90	0.53
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.39	0.53
5:E:165:TYR:HA	5:E:170:ARG:O	2.09	0.53
6:S:84:GLU:CD	6:S:84:GLU:H	2.15	0.53
3:C:45:GLN:CB	12:C:501:HEM:HAB	2.38	0.53
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.91	0.53
1:A:170:THR:CG2	1:A:171:THR:N	2.72	0.53
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.91	0.53
2:B:189:GLU:OE1	2:B:189:GLU:N	2.42	0.53
9:I:65:VAL:HG12	9:I:66:ALA:N	2.24	0.53
1:A:358:LYS:HE3	1:A:399:ILE:O	2.08	0.53
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.91	0.53
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.90	0.53
2:B:374:THR:HG22	2:B:376:GLN:H	1.74	0.53
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.90	0.53
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.90	0.53
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.91	0.53
5:R:131:GLU:OE1	5:R:131:GLU:N	2.40	0.53
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.91	0.52
1:N:7:THR:HG21	2:O:113:ARG:CD	2.38	0.52
2:O:248:ASN:C	2:O:248:ASN:ND2	2.56	0.52
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.39	0.52
10:W:52:TRP:O	10:W:56:LYS:HB2	2.09	0.52
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:ASP:C	2:B:437:ASP:OD1	2.52	0.52
8:H:27:THR:HG22	8:H:29:LYS:H	1.74	0.52
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.72	0.52
2:B:152:PHE:HA	2:B:157:VAL:CG1	2.40	0.52
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.90	0.52
1:N:48:GLU:CD	1:N:54:GLY:H	2.18	0.52
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.44	0.52
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.38	0.52
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.92	0.52
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.39	0.52
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.45	0.52
1:A:280:TYR:CG	1:A:281:ASP:N	2.78	0.52
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.09	0.52
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.92	0.52
3:C:313:GLN:HE21	6:F:36:THR:CB	2.22	0.52
4:D:47:ALA:HA	4:D:90:TYR:HA	1.91	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.91	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
2:B:372:VAL:HG12	2:B:372:VAL:O	2.09	0.52
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.90	0.52
3:P:286:PRO:O	3:P:287:ASN:HB2	2.09	0.52
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.40	0.52
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.92	0.52
1:A:106:MET:HE2	1:A:106:MET:C	2.34	0.52
1:A:217:SER:O	1:A:218:GLY:C	2.52	0.52
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.52
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.45	0.52
5:E:102:THR:O	5:E:103:GLN:HG3	2.10	0.52
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.44	0.52
1:N:317:THR:HG23	1:N:318:GLY:N	2.25	0.52
1:N:358:LYS:HE3	1:N:399:ILE:O	2.09	0.52
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.91	0.52
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.90	0.52
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.24	0.52
4:Q:161:ALA:O	4:Q:162:PRO:C	2.53	0.52
8:U:43:ARG:O	8:U:47:ARG:HG3	2.09	0.52
9:V:65:VAL:HG12	9:V:66:ALA:N	2.25	0.52
1:A:288:LYS:HE3	1:A:289:HIS:CE1	2.45	0.52
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.70	0.52
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.10	0.52
8:H:10:GLU:O	8:H:11:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:ASN:O	1:N:177:LEU:HG	2.10	0.52
1:N:217:SER:O	1:N:218:GLY:C	2.52	0.52
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.52
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.92	0.52
2:O:221:GLU:C	2:O:223:PHE:H	2.17	0.52
2:O:222:GLN:O	2:O:222:GLN:HG2	2.10	0.52
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.45	0.52
7:T:48:VAL:O	7:T:51:PRO:HD2	2.10	0.52
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.09	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.92	0.51
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.75	0.51
3:P:301:ILE:HD11	3:P:364:LEU:CD2	2.35	0.51
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.43	0.51
3:C:279:TYR:O	3:C:283:ARG:HG3	2.10	0.51
1:N:131:ARG:NH2	1:N:177:LEU:O	2.44	0.51
2:O:203:ARG:HD2	2:O:230:ALA:O	2.10	0.51
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.91	0.51
5:R:163:SER:H	5:R:175:PRO:HD2	1.75	0.51
6:S:91:GLU:O	6:S:95:LYS:HG3	2.09	0.51
4:D:169:LEU:HD22	4:D:182:ILE:HD11	1.92	0.51
1:N:45:SER:HA	1:N:48:GLU:HG3	1.92	0.51
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.92	0.51
4:Q:2:GLU:HB3	4:Q:3:LEU:HD12	1.91	0.51
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.92	0.51
10:W:40:ASP:O	10:W:44:GLU:HG3	2.09	0.51
1:A:140:GLU:OE2	9:I:49:LEU:HA	2.10	0.51
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.45	0.51
2:O:248:ASN:ND2	2:O:250:HIS:H	2.09	0.51
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.93	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.46	0.51
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.46	0.51
2:B:57:TYR:N	2:B:57:TYR:CD1	2.78	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.43	0.51
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.93	0.51
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.51
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.46	0.51
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.45	0.51
5:E:187:PHE:C	5:E:189:GLY:N	2.66	0.51
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.51
2:O:26:ILE:HG12	2:O:26:ILE:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:57:TYR:CD1	2:O:57:TYR:N	2.78	0.51
2:O:437:ASP:OD1	2:O:437:ASP:C	2.54	0.51
2:B:402:ILE:HG23	2:B:403:ASP:N	2.26	0.51
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.93	0.51
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.40	0.50
9:I:71:ASN:H	9:I:71:ASN:HD22	1.59	0.50
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.46	0.50
2:O:222:GLN:O	2:O:223:PHE:CD2	2.64	0.50
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.72	0.50
1:A:48:GLU:CD	1:A:54:GLY:H	2.19	0.50
9:I:49:LEU:HD22	9:I:54:SER:HB3	1.93	0.50
2:O:43:PRO:O	2:O:113:ARG:HG3	2.11	0.50
6:S:13:MET:HA	6:S:16:ILE:HD12	1.93	0.50
1:A:269:VAL:CG2	1:A:406:MET:HE3	2.42	0.50
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.40	0.50
1:N:106:MET:HE2	1:N:106:MET:C	2.36	0.50
1:N:368:GLN:O	1:N:369:LEU:HD23	2.12	0.50
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.41	0.50
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.92	0.50
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.75	0.50
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.41	0.50
3:C:207:ASN:ND2	3:C:208:ASN:H	2.10	0.50
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.94	0.50
1:N:17:THR:HG23	1:N:205:HIS:NE2	2.27	0.50
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.30	0.50
5:R:162:GLY:O	5:R:163:SER:C	2.53	0.50
5:R:165:TYR:HA	5:R:170:ARG:O	2.11	0.50
2:B:402:ILE:HG23	2:B:403:ASP:H	1.77	0.50
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.50
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.46	0.50
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.30	0.50
3:P:147:ILE:CG1	13:P:3001:JZV:HAP	2.32	0.50
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.94	0.50
5:E:101:ARG:NH2	5:E:130:PRO:O	2.45	0.50
5:E:190:ASP:C	5:E:192:LEU:N	2.67	0.50
3:P:45:GLN:HB3	12:P:501:HEM:HAB	1.94	0.50
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.41	0.50
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.93	0.50
2:B:225:ASN:O	2:B:226:ILE:C	2.54	0.50
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.92	0.50
3:P:101:ARG:C	3:P:101:ARG:CD	2.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.94	0.50
1:A:362:ARG:O	1:A:365:MET:HG2	2.11	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
2:B:395:PRO:O	2:B:398:VAL:HG12	2.11	0.50
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.94	0.50
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.41	0.50
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.30	0.50
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.42	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.94	0.50
1:A:106:MET:HE2	1:A:107:PRO:N	2.27	0.49
9:I:38:UNK:O	9:I:39:UNK:C	2.59	0.49
9:V:33:UNK:HA	9:V:73:PRO:HB3	1.94	0.49
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.94	0.49
1:N:158:PHE:O	1:N:164:ALA:HB2	2.12	0.49
5:R:178:TYR:N	5:R:178:TYR:CD1	2.80	0.49
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.93	0.49
3:C:377:MET:HE2	6:F:20:TYR:CG	2.47	0.49
2:O:76:THR:HG22	2:O:82:SER:N	2.02	0.49
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.94	0.49
2:O:334:GLY:O	2:O:338:ARG:HG2	2.12	0.49
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.37	0.49
3:C:19:LEU:C	3:C:20:ILE:HG13	2.36	0.49
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.41	0.49
2:O:52:LYS:O	2:O:203:ARG:NH2	2.38	0.49
4:Q:21:LEU:HD21	4:Q:191:ARG:HG3	1.93	0.49
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.49
2:B:26:ILE:HG12	2:B:26:ILE:O	2.12	0.49
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.94	0.49
7:G:80:ASP:O	7:G:81:GLN:C	2.55	0.49
3:P:138:GLN:HB2	3:P:255:GLU:O	2.12	0.49
3:P:238:THR:HB	3:P:239:PRO:CD	2.37	0.49
4:Q:43:MET:HE2	4:Q:91:PHE:HE2	1.75	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.52	0.49
2:B:402:ILE:O	2:B:405:VAL:HG23	2.13	0.49
1:N:362:ARG:O	1:N:365:MET:HG2	2.12	0.49
2:O:341:MET:HA	2:O:341:MET:HE2	1.93	0.49
3:P:159:HIS:O	3:P:163:GLU:HG3	2.13	0.49
3:P:301:ILE:CD1	3:P:364:LEU:HD21	2.36	0.49
7:T:28:ASN:HB3	7:T:31:SER:OG	2.13	0.49
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.49
5:E:106:ILE:O	5:E:106:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.28	0.49
6:S:40:ASP:O	6:S:44:LYS:HG3	2.13	0.49
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.31	0.49
2:B:397:VAL:O	2:B:401:LYS:HG2	2.13	0.49
3:C:34:PHE:HB2	20:C:381:HOH:O	2.12	0.49
3:C:263:LEU:O	3:C:264:VAL:CG2	2.61	0.49
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.11	0.49
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.48	0.49
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.94	0.49
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.76	0.49
3:C:138:GLN:HB2	3:C:255:GLU:O	2.13	0.49
4:D:21:LEU:HD21	4:D:191:ARG:HG3	1.94	0.49
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.73	0.49
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.13	0.49
1:A:173:ASN:O	1:A:177:LEU:HG	2.13	0.49
1:A:205:HIS:O	1:A:208:LEU:HB3	2.13	0.49
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.95	0.49
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.49
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.94	0.48
2:B:334:GLY:O	2:B:338:ARG:HG2	2.13	0.48
15:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.13	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.31	0.48
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.48	0.48
3:C:287:ASN:O	3:C:288:LYS:C	2.56	0.48
5:E:127:VAL:O	5:E:128:LYS:HB2	2.13	0.48
10:J:52:TRP:O	10:J:56:LYS:HB2	2.13	0.48
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.42	0.48
1:A:23:LEU:HD23	1:A:23:LEU:C	2.38	0.48
2:B:104:LYS:HD2	2:B:104:LYS:C	2.38	0.48
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.47	0.48
5:E:178:TYR:HD1	5:E:178:TYR:H	1.61	0.48
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.48
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.94	0.48
5:R:73:LYS:HB3	5:R:196:GLY:O	2.14	0.48
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.53	0.48
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.42	0.48
5:E:3:ASN:HD22	5:E:3:ASN:H	1.62	0.48
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.36	0.48
1:A:182:LEU:O	1:A:186:ILE:HG13	2.13	0.48
1:A:191:LYS:CA	1:A:195:MET:HE2	2.44	0.48
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:207:ASN:ND2	3:P:208:ASN:H	2.12	0.48
7:T:29:ILE:O	7:T:33:ALA:HB3	2.13	0.48
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.96	0.48
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.48	0.48
1:N:49:ASN:ND2	1:N:51:LYS:H	2.12	0.48
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.13	0.48
2:O:248:ASN:HD22	2:O:249:GLY:N	2.12	0.48
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.48	0.48
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.96	0.48
6:F:40:ASP:O	6:F:44:LYS:HG3	2.14	0.48
1:N:106:MET:HE2	1:N:107:PRO:N	2.28	0.48
3:P:156:TYR:C	3:P:158:GLY:H	2.19	0.48
6:F:13:MET:O	6:F:17:ARG:HG3	2.12	0.48
3:P:216:SER:CB	6:S:59:MET:HE2	2.43	0.48
6:S:16:ILE:O	6:S:19:TRP:HB3	2.14	0.48
10:W:49:GLY:N	10:W:54:HIS:ND1	2.61	0.48
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.42	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.14	0.48
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.49	0.48
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.48	0.48
5:E:185:TYR:O	5:E:186:GLN:HB3	2.14	0.48
2:O:164:HIS:O	2:O:173:ALA:HA	2.14	0.48
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.46	0.48
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.95	0.47
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.96	0.47
1:N:433:ASP:OD1	1:N:436:ARG:HG2	2.13	0.47
3:P:377:MET:HE2	6:S:20:TYR:CG	2.48	0.47
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.28	0.47
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.49	0.47
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.78	0.47
1:A:37:VAL:HG22	1:A:109:VAL:HG11	1.96	0.47
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.95	0.47
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.42	0.47
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.14	0.47
1:A:95:THR:HG22	1:A:96:ALA:N	2.28	0.47
1:A:178:THR:HG22	1:A:179:ARG:N	2.29	0.47
4:D:186:VAL:O	4:D:190:LEU:HG	2.14	0.47
4:D:220:TYR:O	4:D:224:ARG:HG2	2.14	0.47
5:E:83:GLU:C	5:E:85:LYS:H	2.22	0.47
5:E:102:THR:C	5:E:103:GLN:HG3	2.39	0.47
5:E:116:LYS:HD2	5:E:116:LYS:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:HIS:HB3	19:E:501:FES:S2	2.54	0.47
1:N:170:THR:CG2	1:N:171:THR:H	2.27	0.47
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.15	0.47
1:A:382:HIS:HB3	1:A:388:ARG:O	2.13	0.47
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.44	0.47
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.44	0.47
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.29	0.47
1:N:137:GLU:O	1:N:141:MET:HG3	2.13	0.47
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.14	0.47
5:E:178:TYR:N	5:E:178:TYR:CD1	2.83	0.47
8:H:43:ARG:O	8:H:47:ARG:HG3	2.15	0.47
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.14	0.47
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.14	0.47
3:C:49:GLY:C	12:C:501:HEM:HAC	2.40	0.47
5:E:77:LYS:HG3	5:E:191:ASP:O	2.13	0.47
9:I:34:UNK:CG	9:I:35:UNK:N	2.70	0.47
2:O:73:SER:N	2:O:74:PRO:HD2	2.29	0.47
2:O:89:ILE:HD13	2:O:96:LEU:HB2	1.95	0.47
2:O:295:LEU:O	2:O:299:VAL:HG23	2.14	0.47
2:O:395:PRO:O	2:O:398:VAL:HG12	2.14	0.47
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.77	0.47
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.96	0.47
3:C:117:GLY:O	12:C:502:HEM:HMC3	2.15	0.47
5:E:41:ALA:O	5:E:45:VAL:HG23	2.15	0.47
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.44	0.47
5:E:155:GLY:HA3	5:E:166:ASP:O	2.15	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.95	0.47
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.45	0.47
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.49	0.47
1:N:205:HIS:O	1:N:209:VAL:HG12	2.15	0.47
1:N:342:TRP:O	1:N:345:LEU:HB2	2.15	0.47
2:O:122:TYR:O	2:O:126:VAL:HG23	2.14	0.47
2:O:374:THR:HG22	2:O:376:GLN:N	2.29	0.47
2:O:402:ILE:HG23	2:O:403:ASP:N	2.29	0.47
3:P:49:GLY:C	12:P:501:HEM:HAC	2.40	0.47
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.47	0.47
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.50	0.47
1:A:144:ASP:OD2	1:A:147:ASN:ND2	2.47	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.15	0.47
3:C:101:ARG:C	3:C:101:ARG:CD	2.88	0.47
4:D:102:ARG:HA	4:D:108:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.44	0.47
1:N:178:THR:HG22	1:N:179:ARG:N	2.29	0.47
2:O:31:ASN:N	2:O:31:ASN:ND2	2.63	0.47
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.48	0.47
3:P:350:ILE:O	3:P:354:MET:HG2	2.15	0.47
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.29	0.47
5:E:136:VAL:O	5:E:138:VAL:N	2.44	0.47
9:I:61:ARG:C	9:I:62:ARG:HG3	2.40	0.47
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.40	0.47
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.94	0.47
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.45	0.47
2:B:122:TYR:O	2:B:126:VAL:HG23	2.15	0.47
3:C:37:LEU:O	3:C:41:CYS:HB2	2.15	0.47
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.45	0.47
5:E:130:PRO:C	5:E:132:TRP:H	2.22	0.47
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.97	0.47
2:O:59:THR:HG22	2:O:60:THR:N	2.30	0.47
3:P:101:ARG:HD2	3:P:101:ARG:O	2.15	0.47
3:P:155:PRO:O	3:P:156:TYR:HB2	2.15	0.47
4:Q:3:LEU:HD12	4:Q:3:LEU:N	2.29	0.47
7:T:80:ASP:OD1	8:U:47:ARG:HD3	2.14	0.47
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.50	0.46
5:E:162:GLY:O	5:E:163:SER:C	2.58	0.46
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.44	0.46
10:J:7:ARG:HH11	10:J:7:ARG:HB2	1.80	0.46
1:N:219:VAL:CG1	1:N:220:SER:N	2.78	0.46
3:P:247:SER:OG	3:P:250:LEU:HB2	2.15	0.46
3:P:287:ASN:O	3:P:288:LYS:C	2.58	0.46
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.96	0.46
2:B:54:GLY:C	2:B:56:ARG:H	2.22	0.46
6:F:71:LYS:O	6:F:72:HIS:HB2	2.15	0.46
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.98	0.46
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.51	0.46
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.97	0.46
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.50	0.46
10:W:4:ALA:O	10:W:8:GLN:HG3	2.15	0.46
2:B:207:VAL:HG12	2:B:208:GLY:N	2.30	0.46
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.30	0.46
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.51	0.46
1:N:130:GLU:O	1:N:134:ILE:HG13	2.16	0.46
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:403:ASP:C	2:O:405:VAL:H	2.23	0.46
15:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.48	0.46
5:R:185:TYR:O	5:R:186:GLN:HB3	2.15	0.46
2:O:259:THR:HG22	2:O:260:GLU:N	2.29	0.46
6:S:17:ARG:HG2	6:S:17:ARG:NH1	2.29	0.46
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.80	0.46
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.16	0.46
2:B:27:THR:CG2	2:B:28:LYS:H	2.24	0.46
3:C:247:SER:N	3:C:248:PRO:HD3	2.30	0.46
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.51	0.46
5:E:96:LEU:HD12	5:E:135:LEU:O	2.16	0.46
1:N:37:VAL:HG22	1:N:109:VAL:HG11	1.98	0.46
5:R:107:ASN:C	5:R:109:GLU:N	2.73	0.46
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.34	0.46
2:B:21:ALA:O	2:B:22:GLU:HB3	2.15	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.16	0.46
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.51	0.46
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.46	0.46
2:O:259:THR:CG2	2:O:260:GLU:N	2.79	0.46
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.43	0.46
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.97	0.46
4:Q:240:PRO:O	4:Q:241:LYS:C	2.59	0.46
5:R:179:ASN:O	5:R:180:LEU:C	2.59	0.46
1:A:49:ASN:ND2	1:A:51:LYS:H	2.14	0.46
1:A:402:VAL:HA	1:A:406:MET:HE2	1.98	0.46
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.16	0.46
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.80	0.46
1:N:23:LEU:HD23	1:N:23:LEU:C	2.41	0.46
1:N:288:LYS:HE3	1:N:289:HIS:CE1	2.51	0.46
2:O:307:PHE:H	9:V:52:ARG:HG2	1.81	0.46
1:A:45:SER:HA	1:A:48:GLU:CD	2.41	0.46
2:B:50:PHE:N	2:B:50:PHE:CD1	2.83	0.46
2:B:333:ALA:O	2:B:337:ILE:HG13	2.16	0.46
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.51	0.46
5:E:189:GLY:O	5:E:192:LEU:O	2.34	0.46
8:H:10:GLU:C	8:H:11:GLU:HG3	2.41	0.46
2:O:24:LEU:HD12	2:O:37:SER:O	2.15	0.46
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.41	0.46
5:R:109:GLU:HG2	5:R:123:ASP:HB2	1.97	0.46
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.64	0.46
1:A:368:GLN:O	1:A:369:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ASN:HD22	2:B:249:GLY:N	2.14	0.46
2:B:259:THR:CG2	2:B:260:GLU:N	2.78	0.46
5:E:133:VAL:O	5:E:133:VAL:HG13	2.16	0.46
10:J:40:ASP:O	10:J:44:GLU:HG3	2.15	0.46
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.80	0.46
2:O:385:GLU:O	2:O:389:SER:HB3	2.15	0.46
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.98	0.46
5:R:141:HIS:HB3	19:R:501:FES:S2	2.56	0.46
9:I:39:UNK:HA	9:V:40:UNK:O	2.16	0.45
1:N:354:VAL:HG23	1:N:355:LYS:N	2.30	0.45
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.31	0.45
3:P:153:ALA:CB	3:P:288:LYS:HG2	2.45	0.45
3:P:263:LEU:C	3:P:264:VAL:HG23	2.41	0.45
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.46	0.45
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.46	0.45
10:W:42:ILE:HG22	10:W:46:LEU:HD12	1.98	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.16	0.45
1:A:205:HIS:O	1:A:209:VAL:HG12	2.16	0.45
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.81	0.45
2:B:403:ASP:C	2:B:405:VAL:H	2.24	0.45
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.17	0.45
4:D:169:LEU:HD23	4:D:169:LEU:O	2.16	0.45
4:D:171:TYR:OH	4:D:182:ILE:HA	2.16	0.45
5:E:52:LYS:C	5:E:52:LYS:CD	2.85	0.45
6:F:32:MET:O	6:F:33:ARG:C	2.58	0.45
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.45
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.98	0.45
2:O:31:ASN:ND2	2:O:31:ASN:H	2.13	0.45
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.47	0.45
3:P:380:TYR:CZ	6:S:37:LEU:HD21	2.52	0.45
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.81	0.45
1:A:418:LYS:O	1:A:420:PRO:HD3	2.16	0.45
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.99	0.45
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.44	0.45
15:C:2004:CDL:H712	11:C:2007:PEE:H50	1.98	0.45
15:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.49	0.45
2:O:54:GLY:C	2:O:56:ARG:H	2.23	0.45
5:R:163:SER:HA	5:R:174:GLY:HA3	1.99	0.45
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.97	0.45
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:170:THR:O	2:O:172:LEU:N	2.50	0.45
2:O:367:THR:HA	2:O:370:MET:HE3	1.97	0.45
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.99	0.45
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.17	0.45
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.49	0.45
7:T:36:ASN:O	7:T:40:ARG:HG3	2.17	0.45
1:A:255:LEU:O	1:A:321:GLY:HA3	2.16	0.45
2:B:24:LEU:HD13	2:B:38:LEU:HB2	1.98	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.32	0.45
5:E:144:CYS:CB	5:E:158:CYS:SG	3.05	0.45
5:E:189:GLY:O	5:E:192:LEU:N	2.50	0.45
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.99	0.45
1:A:45:SER:HA	1:A:48:GLU:HG3	1.98	0.45
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.17	0.45
15:D:2003:CDL:H721	15:D:2003:CDL:HA61	1.98	0.45
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.32	0.45
10:W:38:GLY:O	10:W:42:ILE:HG13	2.16	0.45
2:B:27:THR:CG2	2:B:28:LYS:N	2.77	0.45
2:B:110:GLU:O	2:B:111:CYS:HB3	2.16	0.45
2:B:207:VAL:HG12	2:B:208:GLY:H	1.82	0.45
2:B:318:ASP:O	2:B:319:SER:HB2	2.16	0.45
3:C:328:LEU:HD12	3:C:328:LEU:HA	1.83	0.45
1:N:45:SER:HA	1:N:48:GLU:CD	2.42	0.45
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.99	0.45
2:O:75:LEU:HD11	2:O:140:LEU:HD22	1.97	0.45
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.17	0.45
9:V:69:SER:HB2	9:V:72:ALA:H	1.81	0.45
2:B:43:PRO:O	2:B:113:ARG:HG3	2.17	0.45
2:B:54:GLY:C	2:B:56:ARG:N	2.75	0.45
11:C:2007:PEE:H11	6:F:29:TYR:OH	2.17	0.45
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.46	0.45
5:E:127:VAL:CG1	5:E:128:LYS:H	2.15	0.45
2:O:225:ASN:C	2:O:227:ARG:HG3	2.42	0.45
3:P:263:LEU:O	3:P:264:VAL:CG2	2.65	0.45
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.52	0.45
6:S:82:LYS:O	6:S:83:TYR:C	2.59	0.45
7:T:56:TYR:O	7:T:59:TYR:HB3	2.17	0.45
1:A:27:SER:HA	1:A:199:ALA:O	2.16	0.45
3:C:50:LEU:O	3:C:54:MET:HG3	2.17	0.45
2:O:54:GLY:C	2:O:56:ARG:N	2.75	0.45
3:P:92:PHE:O	3:P:95:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:55:MET:HA	9:V:58:ARG:HG3	1.99	0.45
10:W:59:TYR:CD1	10:W:59:TYR:N	2.84	0.45
2:B:395:PRO:O	2:B:398:VAL:CG1	2.65	0.44
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.52	0.44
15:P:3004:CDL:HA32	7:T:40:ARG:CB	2.46	0.44
7:T:34:LEU:O	7:T:35:PRO:C	2.60	0.44
2:B:164:HIS:O	2:B:173:ALA:HA	2.17	0.44
5:E:73:LYS:HB2	5:E:195:VAL:O	2.16	0.44
1:N:255:LEU:O	1:N:321:GLY:HA3	2.17	0.44
3:P:19:LEU:C	3:P:20:ILE:HG13	2.42	0.44
3:P:266:PRO:HA	3:P:267:PRO:HD3	1.85	0.44
6:S:82:LYS:HD2	6:S:85:GLU:OE1	2.16	0.44
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.33	0.44
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.52	0.44
4:D:57:THR:CG2	4:D:58:GLU:N	2.79	0.44
6:F:77:LYS:HB3	6:F:77:LYS:HE2	1.81	0.44
3:P:28:ILE:HD11	3:P:225:TYR:CE2	2.52	0.44
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.43	0.44
5:R:178:TYR:N	5:R:178:TYR:HD1	2.15	0.44
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.80	0.44
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.99	0.44
9:I:68:ILE:HD13	9:I:68:ILE:HA	1.84	0.44
1:N:191:LYS:CA	1:N:195:MET:HE2	2.47	0.44
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.99	0.44
2:O:221:GLU:O	2:O:223:PHE:N	2.50	0.44
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.99	0.44
8:U:65:ARG:O	8:U:69:VAL:HG23	2.17	0.44
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.47	0.44
1:A:170:THR:HG22	1:A:171:THR:H	1.80	0.44
2:B:28:LYS:O	2:B:28:LYS:HG2	2.17	0.44
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.18	0.44
5:E:3:ASN:H	5:E:3:ASN:ND2	2.15	0.44
7:G:48:VAL:O	7:G:51:PRO:HD2	2.17	0.44
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.52	0.44
4:Q:169:LEU:CD2	4:Q:182:ILE:HD11	2.48	0.44
3:C:358:SER:O	3:C:362:ILE:HG13	2.16	0.44
5:R:75:GLU:O	5:R:75:GLU:HG3	2.17	0.44
5:R:102:THR:C	5:R:104:ALA:N	2.75	0.44
3:C:323:GLN:OE1	7:G:47:LYS:HD3	2.18	0.44
3:C:380:TYR:CZ	6:F:37:LEU:HD21	2.53	0.44
5:E:119:ASP:O	5:E:121:GLN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:161:HIS:HB2	19:E:501:FES:S1	2.58	0.44
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.47	0.44
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.99	0.44
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.53	0.44
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.99	0.44
5:R:133:VAL:O	5:R:133:VAL:HG13	2.17	0.44
1:A:63:ALA:O	1:A:116:VAL:HG13	2.18	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
5:E:171:ILE:O	5:E:171:ILE:HG23	2.17	0.44
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.98	0.44
1:N:168:GLU:CD	1:N:168:GLU:H	2.26	0.44
1:N:243:ALA:O	1:N:425:VAL:HA	2.17	0.44
1:N:365:MET:HG3	1:N:366:VAL:N	2.33	0.44
2:O:361:LYS:HD3	2:O:403:ASP:HA	2.00	0.44
3:P:14:MET:HE2	18:P:2010:BOG:O4	2.18	0.44
3:P:230:ILE:HG23	11:R:3005:PEE:H25	2.00	0.44
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.32	0.44
1:A:168:GLU:H	1:A:168:GLU:CD	2.26	0.44
2:B:59:THR:CG2	2:B:60:THR:N	2.80	0.44
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.39	0.44
3:C:263:LEU:C	3:C:264:VAL:HG23	2.43	0.44
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.55	0.43
1:A:191:LYS:N	1:A:195:MET:HE2	2.32	0.43
1:A:281:ASP:OD1	9:I:33:UNK:HB2	2.18	0.43
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.83	0.43
2:B:353:THR:HG22	2:B:354:GLU:N	2.32	0.43
4:D:143:VAL:HG21	4:D:149:TYR:HB2	1.99	0.43
5:E:73:LYS:HB3	5:E:196:GLY:O	2.17	0.43
5:E:97:PHE:O	5:E:134:ILE:HA	2.18	0.43
5:E:136:VAL:HG23	5:E:181:GLU:O	2.17	0.43
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.53	0.43
2:O:227:ARG:HB3	2:O:228:SER:H	1.48	0.43
3:P:377:MET:HE2	6:S:20:TYR:HB2	2.00	0.43
4:Q:169:LEU:HD22	4:Q:182:ILE:CD1	2.48	0.43
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.99	0.43
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.48	0.43
3:C:92:PHE:O	3:C:95:ILE:HG22	2.17	0.43
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.85	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.43	0.43
4:D:235:MET:HB3	7:G:15:THR:HG22	2.01	0.43
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:257:VAL:HG22	2:O:424:MET:HG3	2.00	0.43
3:P:121:LEU:O	3:P:125:MET:HG3	2.18	0.43
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.00	0.43
3:P:380:TYR:OH	6:S:34:ASP:OD1	2.32	0.43
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.17	0.43
3:C:46:ILE:HA	12:C:501:HEM:HMC2	2.00	0.43
5:E:125:ASP:C	5:E:126:ARG:HG3	2.44	0.43
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.01	0.43
9:I:71:ASN:N	9:I:71:ASN:HD22	2.16	0.43
4:Q:69:GLU:OE1	4:Q:82:MET:HB3	2.18	0.43
4:Q:181:GLN:HA	8:U:77:LEU:HD22	2.00	0.43
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.33	0.43
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.82	0.43
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.64	0.43
2:O:345:LYS:HG2	2:O:418:VAL:HG13	2.01	0.43
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.43
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.34	0.43
1:A:130:GLU:O	1:A:134:ILE:HG13	2.18	0.43
2:B:280:GLY:HA3	2:B:293:SER:OG	2.19	0.43
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.43
11:E:2005:PEE:H58	10:J:24:VAL:HG11	2.01	0.43
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.48	0.43
2:B:76:THR:HG23	2:B:82:SER:HB2	2.01	0.43
1:N:280:TYR:CG	1:N:281:ASP:N	2.85	0.43
2:O:402:ILE:HG23	2:O:403:ASP:H	1.83	0.43
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.53	0.43
5:R:3:ASN:H	5:R:3:ASN:HD22	1.66	0.43
5:R:170:ARG:HA	5:R:179:ASN:CB	2.45	0.43
6:S:70:LEU:HD12	6:S:70:LEU:C	2.43	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.61	0.43
1:N:205:HIS:O	1:N:208:LEU:HB3	2.18	0.43
1:N:274:ASN:ND2	1:N:309:THR:HB	2.34	0.43
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.83	0.43
2:B:170:THR:O	2:B:172:LEU:N	2.51	0.43
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.19	0.43
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.01	0.43
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.50	0.43
5:R:96:LEU:HD12	5:R:135:LEU:O	2.19	0.43
3:C:146:VAL:HG21	3:C:269:ILE:HG21	2.00	0.43
4:D:27:ARG:NH1	4:D:55:THR:O	2.52	0.43
5:E:52:LYS:HD3	5:E:52:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:162:ASN:O	2:O:244:ILE:HD12	2.18	0.43
3:P:129:PHE:CE1	13:P:3001:JZV:HAFB	2.54	0.43
3:P:367:PHE:N	3:P:368:PRO:HD2	2.34	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.54	0.43
8:U:32:LYS:O	8:U:36:ARG:HG3	2.19	0.43
8:U:67:HIS:C	8:U:67:HIS:HD1	2.27	0.43
1:A:140:GLU:OE2	9:I:50:LEU:N	2.41	0.43
3:C:155:PRO:O	3:C:157:ILE:N	2.50	0.43
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.54	0.43
12:C:502:HEM:HBC2	12:C:502:HEM:CMC	2.49	0.43
10:J:42:ILE:HG22	10:J:46:LEU:HD12	2.00	0.43
1:N:103:SER:HB3	1:N:202:GLY:O	2.19	0.43
2:O:73:SER:N	2:O:74:PRO:CD	2.82	0.43
2:O:156:GLN:HE22	9:V:77:ARG:C	2.27	0.43
2:O:221:GLU:HG3	2:O:222:GLN:N	2.26	0.43
3:P:277:PHE:CG	3:P:278:ALA:N	2.86	0.43
1:A:191:LYS:O	1:A:195:MET:HG3	2.18	0.42
2:B:56:ARG:HB2	2:B:102:ARG:O	2.19	0.42
4:D:161:ALA:O	4:D:162:PRO:C	2.62	0.42
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.54	0.42
5:E:137:GLY:O	5:E:145:VAL:HG13	2.19	0.42
9:I:31:UNK:O	9:I:32:UNK:O	2.37	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.42
1:N:436:ARG:HD2	1:N:436:ARG:HA	1.82	0.42
3:P:208:ASN:HB2	3:P:209:PRO:HD2	2.01	0.42
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.53	0.42
5:R:122:HIS:O	5:R:123:ASP:C	2.62	0.42
5:R:153:PHE:CD1	5:R:153:PHE:N	2.86	0.42
5:R:155:GLY:HA3	5:R:166:ASP:O	2.19	0.42
3:C:286:PRO:O	3:C:287:ASN:CB	2.67	0.42
4:D:69:GLU:OE1	4:D:82:MET:HB3	2.18	0.42
5:E:122:HIS:CE1	5:E:124:LEU:HB2	2.55	0.42
2:B:257:VAL:HG22	2:B:424:MET:HG3	2.01	0.42
2:B:345:LYS:HG2	2:B:418:VAL:HG13	2.02	0.42
4:D:116:ILE:HG23	4:D:117:VAL:N	2.33	0.42
5:E:179:ASN:O	5:E:180:LEU:C	2.60	0.42
1:N:90:THR:O	1:N:167:VAL:HG11	2.19	0.42
2:O:96:LEU:H	9:V:70:LEU:HD22	1.84	0.42
2:O:286:LYS:C	2:O:288:GLY:H	2.27	0.42
3:P:18:SER:CB	3:P:202:HIS:HE1	2.32	0.42
6:S:99:ARG:HH11	6:S:99:ARG:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:70:LEU:HD23	9:V:71:ASN:H	1.83	0.42
2:B:52:LYS:O	2:B:203:ARG:NH2	2.46	0.42
2:B:374:THR:HG22	2:B:376:GLN:N	2.33	0.42
5:E:105:GLU:C	5:E:107:ASN:H	2.24	0.42
5:E:191:ASP:OD2	5:E:191:ASP:N	2.52	0.42
8:H:40:CYS:O	8:H:44:VAL:HG23	2.18	0.42
1:N:27:SER:HA	1:N:199:ALA:O	2.19	0.42
1:A:16:VAL:HA	1:A:25:VAL:O	2.19	0.42
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.35	0.42
12:C:502:HEM:HBC2	12:C:502:HEM:HMC1	2.00	0.42
1:N:45:SER:HA	1:N:48:GLU:CG	2.49	0.42
1:N:144:ASP:OD2	1:N:147:ASN:ND2	2.52	0.42
1:N:418:LYS:O	1:N:420:PRO:HD3	2.19	0.42
2:O:227:ARG:O	2:O:228:SER:O	2.38	0.42
2:O:353:THR:HG22	2:O:354:GLU:N	2.35	0.42
3:P:5:ILE:O	3:P:5:ILE:HG22	2.20	0.42
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.48	0.42
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.20	0.42
4:Q:167:GLU:C	4:Q:169:LEU:N	2.75	0.42
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.84	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.64	0.42
2:B:22:GLU:O	2:B:23:ASP:OD2	2.38	0.42
7:G:34:LEU:O	7:G:35:PRO:C	2.60	0.42
2:O:209:ILE:HD11	2:O:379:LEU:N	2.35	0.42
4:Q:167:GLU:HG2	8:U:13:LEU:HD12	2.01	0.42
2:B:144:LEU:HB2	2:B:183:ILE:HD12	2.01	0.42
2:B:287:ARG:NH1	2:B:287:ARG:HG3	2.34	0.42
5:E:122:HIS:O	5:E:125:ASP:HB2	2.19	0.42
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.42
2:O:287:ARG:NH1	2:O:287:ARG:HG3	2.35	0.42
3:P:263:LEU:O	3:P:264:VAL:HG23	2.20	0.42
5:R:52:LYS:C	5:R:52:LYS:CD	2.87	0.42
1:A:17:THR:CG2	1:A:205:HIS:NE2	2.83	0.42
1:A:253:VAL:O	1:A:323:HIS:HA	2.20	0.42
2:B:28:LYS:HG3	2:B:34:ILE:HG12	2.02	0.42
2:B:292:THR:O	2:B:292:THR:CG2	2.66	0.42
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.01	0.42
5:E:75:GLU:HA	5:E:193:VAL:O	2.20	0.42
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.42
1:N:4:TYR:CB	2:O:114:ASP:OD2	2.67	0.42
1:A:233:ARG:HH21	1:A:316:ASP:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HD12	2:B:38:LEU:C	2.45	0.42
2:B:374:THR:HB	2:B:377:GLY:H	1.84	0.42
3:C:150:LEU:HB3	3:C:292:VAL:HG22	2.02	0.42
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.55	0.42
5:E:103:GLN:O	5:E:107:ASN:ND2	2.51	0.42
3:P:150:LEU:HB3	3:P:292:VAL:CG2	2.50	0.42
5:R:77:LYS:HE2	5:R:79:SER:CB	2.49	0.42
6:S:13:MET:O	6:S:17:ARG:HG3	2.19	0.42
10:W:57:HIS:HA	10:W:60:GLU:HB3	2.01	0.42
1:A:304:CYS:HB2	1:A:325:VAL:O	2.20	0.41
7:G:81:GLN:OXT	7:G:81:GLN:HG3	2.20	0.41
3:P:313:GLN:HE21	6:S:36:THR:HB	1.85	0.41
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.35	0.41
5:R:116:LYS:O	5:R:117:LEU:HD23	2.20	0.41
2:B:59:THR:C	2:B:61:ALA:N	2.75	0.41
15:C:2004:CDL:HA32	7:G:40:ARG:CB	2.50	0.41
7:G:29:ILE:O	7:G:33:ALA:HB3	2.19	0.41
8:H:50:THR:HG23	8:H:50:THR:O	2.19	0.41
1:N:30:SER:O	1:N:202:GLY:HA2	2.19	0.41
1:N:240:GLU:HA	1:N:422:LEU:O	2.20	0.41
2:O:371:SER:C	2:O:372:VAL:HG23	2.45	0.41
5:E:152:ASP:OD2	5:E:153:PHE:CE1	2.73	0.41
3:P:219:ILE:HD12	3:P:224:TYR:CG	2.55	0.41
5:R:184:THR:HG22	5:R:185:TYR:N	2.35	0.41
1:A:209:VAL:O	1:A:212:ALA:HB3	2.20	0.41
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.02	0.41
1:A:387:GLY:O	1:A:388:ARG:HB3	2.19	0.41
3:C:5:ILE:O	3:C:5:ILE:HG22	2.21	0.41
5:E:114:VAL:O	5:E:115:SER:C	2.63	0.41
2:O:275:LEU:HG	2:O:279:LEU:HD12	2.02	0.41
3:P:9:HIS:CD2	3:P:11:LEU:H	2.38	0.41
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.88	0.41
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.85	0.41
8:U:27:THR:HG22	8:U:29:LYS:N	2.33	0.41
3:C:150:LEU:HB3	3:C:292:VAL:CG2	2.50	0.41
10:J:56:LYS:HB3	10:J:56:LYS:HE2	1.77	0.41
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.80	0.41
1:N:281:ASP:CB	9:V:33:UNK:HB1	2.50	0.41
5:R:97:PHE:O	5:R:134:ILE:HA	2.21	0.41
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.35	0.41
6:F:51:PRO:HD2	6:F:54:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:ARG:O	8:H:69:VAL:HG23	2.20	0.41
2:O:154:SER:O	2:O:155:PRO:C	2.64	0.41
2:O:155:PRO:O	2:O:156:GLN:C	2.64	0.41
2:O:169:LYS:HD2	2:O:238:THR:HG21	2.02	0.41
2:O:306:PRO:HA	9:V:52:ARG:CG	2.51	0.41
2:O:307:PHE:CD1	2:O:308:ASP:N	2.88	0.41
2:O:395:PRO:O	2:O:398:VAL:CG1	2.69	0.41
6:S:91:GLU:HB3	6:S:92:PRO:HD3	2.03	0.41
2:B:399:ALA:O	2:B:402:ILE:CG2	2.65	0.41
1:N:16:VAL:HA	1:N:25:VAL:O	2.21	0.41
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.39	0.41
1:N:383:LEU:HD23	1:N:388:ARG:HA	2.02	0.41
2:O:72:ALA:C	2:O:74:PRO:HD2	2.45	0.41
5:R:13:TYR:O	7:T:24:ARG:HG3	2.21	0.41
1:A:26:ALA:O	1:A:198:ALA:HA	2.21	0.41
3:C:367:PHE:N	3:C:368:PRO:HD2	2.36	0.41
1:N:85:HIS:CE1	2:O:370:MET:HE1	2.55	0.41
3:P:146:VAL:HG21	3:P:269:ILE:HG21	2.03	0.41
13:P:3001:JZV:HAZ	13:P:3001:JZV:HAY	1.81	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.50	0.41
5:R:188:VAL:HG23	5:R:192:LEU:HB2	2.02	0.41
1:A:243:ALA:O	1:A:425:VAL:HA	2.20	0.41
1:A:342:TRP:O	1:A:345:LEU:HB2	2.20	0.41
2:B:262:ALA:O	2:B:320:GLY:HA3	2.20	0.41
2:B:399:ALA:HA	2:B:402:ILE:HG22	2.02	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.90	0.41
3:C:271:PRO:HG2	3:C:276:LEU:HD23	2.03	0.41
4:D:21:LEU:HD13	4:D:192:TRP:HB2	2.03	0.41
4:D:165:TYR:CZ	4:D:168:ILE:HG13	2.55	0.41
5:E:151:GLY:O	5:E:154:GLY:N	2.54	0.41
5:E:171:ILE:HG12	5:E:176:ALA:O	2.20	0.41
1:N:133:VAL:O	1:N:137:GLU:HG3	2.20	0.41
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.51	0.41
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.46	0.41
2:O:59:THR:CG2	2:O:60:THR:N	2.84	0.41
2:O:169:LYS:CG	2:O:240:TRP:HB2	2.49	0.41
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.21	0.41
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.36	0.41
2:O:318:ASP:O	2:O:319:SER:HB2	2.19	0.41
3:P:45:GLN:CB	12:P:501:HEM:HAB	2.51	0.41
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:156:TYR:N	3:P:156:TYR:CD2	2.89	0.41
3:P:286:PRO:O	3:P:287:ASN:CB	2.69	0.41
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.56	0.41
4:Q:70:VAL:CG2	4:Q:83:ARG:CZ	2.98	0.41
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.83	0.41
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.55	0.41
3:C:295:LEU:HD11	13:C:2001:JZV:HAZ	2.02	0.41
6:F:13:MET:HE2	6:F:16:ILE:HD12	2.03	0.41
2:O:72:ALA:HB1	2:O:75:LEU:HD12	2.03	0.41
3:P:37:LEU:O	3:P:41:CYS:HB2	2.20	0.41
3:P:81:ARG:HD3	3:P:81:ARG:C	2.46	0.41
5:R:95:PRO:HG2	5:R:145:VAL:CG1	2.51	0.41
1:A:4:TYR:HE2	1:A:396:ASP:OD2	2.04	0.40
1:A:140:GLU:HG2	9:I:50:LEU:HG	2.02	0.40
1:A:276:ILE:HG12	1:A:357:ALA:HB2	2.02	0.40
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.55	0.40
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.56	0.40
2:B:248:ASN:ND2	2:B:250:HIS:H	2.20	0.40
5:E:75:GLU:HG3	5:E:75:GLU:O	2.21	0.40
2:O:372:VAL:HG13	2:O:378:LEU:HA	2.03	0.40
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.02	0.40
5:R:134:ILE:HB	5:R:185:TYR:CE1	2.56	0.40
6:S:60:PHE:O	6:S:64:ARG:HB2	2.20	0.40
4:D:70:VAL:CG2	4:D:83:ARG:CZ	2.99	0.40
5:E:153:PHE:C	5:E:155:GLY:H	2.29	0.40
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.96	0.40
2:O:56:ARG:HB2	2:O:102:ARG:O	2.21	0.40
2:O:291:VAL:C	2:O:293:SER:H	2.30	0.40
1:A:170:THR:CG2	1:A:171:THR:H	2.33	0.40
1:A:354:VAL:HG23	1:A:355:LYS:N	2.35	0.40
3:C:324:THR:O	3:C:325:LEU:C	2.64	0.40
5:E:109:GLU:OE1	5:E:109:GLU:HA	2.21	0.40
5:E:115:SER:CB	5:E:116:LYS:HD2	2.52	0.40
7:G:60:SER:O	7:G:61:TRP:C	2.63	0.40
1:N:62:LEU:O	1:N:64:PHE:N	2.55	0.40
1:N:253:VAL:O	1:N:323:HIS:HA	2.20	0.40
1:N:343:MET:O	1:N:347:THR:HG23	2.21	0.40
2:O:124:LEU:HD23	2:O:124:LEU:C	2.46	0.40
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.36	0.40
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.83	0.40
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.52	0.40
5:R:121:GLN:O	5:R:170:ARG:NH1	2.45	0.40
13:C:2001:JZV:HAZ	13:C:2001:JZV:HAY	1.80	0.40
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.51	0.40
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.57	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.03	0.40
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.36	0.40
4:Q:79:GLU:OE2	4:Q:79:GLU:HA	2.22	0.40
5:R:106:ILE:HG21	5:R:130:PRO:HB3	2.02	0.40
5:R:194:VAL:O	5:R:194:VAL:HG12	2.21	0.40
8:U:67:HIS:C	8:U:67:HIS:ND1	2.79	0.40
2:B:217:LYS:HE2	2:B:221:GLU:OE2	2.21	0.40
2:B:276:GLN:HG2	2:B:281:ALA:HB2	2.03	0.40
2:B:370:MET:O	2:B:373:GLU:HG3	2.22	0.40
1:N:394:GLU:O	1:N:395:TRP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/446 (99%)	414 (94%)	22 (5%)	6 (1%)	9	17
1	N	440/446 (99%)	414 (94%)	19 (4%)	7 (2%)	7	14
2	B	418/441 (95%)	358 (86%)	46 (11%)	14 (3%)	3	5
2	O	420/441 (95%)	370 (88%)	40 (10%)	10 (2%)	4	9
3	C	378/380 (100%)	363 (96%)	10 (3%)	5 (1%)	9	18
3	P	377/380 (99%)	358 (95%)	14 (4%)	5 (1%)	9	18
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	30	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	194/196 (99%)	152 (78%)	28 (14%)	14 (7%)	1	1
5	R	194/196 (99%)	165 (85%)	22 (11%)	7 (4%)	2	4
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
6	S	99/110 (90%)	91 (92%)	8 (8%)	0	100	100
7	G	78/81 (96%)	69 (88%)	6 (8%)	3 (4%)	2	4
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	4	7
8	H	68/77 (88%)	64 (94%)	4 (6%)	0	100	100
8	U	65/77 (84%)	60 (92%)	3 (5%)	2 (3%)	3	6
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100	100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100	100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	14
All	All	4002/4160 (96%)	3659 (91%)	266 (7%)	77 (2%)	6	12

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
3	C	287	ASN
5	E	127	VAL
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
5	R	163	SER
8	U	52	GLU
10	W	61	ALA

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Mol	Chain	Res	Type
1	A	282	ARG
2	B	231	GLY
5	E	80	ASP
5	E	102	THR
5	E	115	SER
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	282	ARG
2	O	24	LEU
2	O	222	GLN
5	R	185	TYR
5	R	191	ASP
8	U	49	HIS
1	A	72	CYS
2	B	389	SER
5	E	137	GLY
1	N	63	ALA
1	N	72	CYS
1	N	262	TRP
1	N	433	ASP
2	O	372	VAL
2	O	389	SER
3	P	156	TYR
5	R	186	GLN
7	T	33	ALA
1	A	262	TRP
1	A	433	ASP
2	B	372	VAL
2	B	386	ALA
3	C	3	PRO
5	E	154	GLY
2	O	19	PRO
3	P	3	PRO
3	P	157	ILE
5	R	154	GLY
2	B	201	SER
2	B	221	GLU
2	B	371	SER
3	C	156	TYR
5	E	166	ASP
7	G	33	ALA

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Mol	Chain	Res	Type
1	N	443	TRP
5	E	120	PRO
5	E	150	SER
7	G	61	TRP
2	O	55	SER
2	O	330	ALA
3	C	158	GLY
1	A	71	PRO
3	C	264	VAL
5	R	137	GLY
3	P	264	VAL
5	R	127	VAL
7	T	50	PRO
7	G	50	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	355 (97%)	10 (3%)	39	62
1	N	365/368 (99%)	354 (97%)	11 (3%)	36	60
2	B	331/347 (95%)	319 (96%)	12 (4%)	31	55
2	O	333/347 (96%)	320 (96%)	13 (4%)	28	51
3	C	328/329 (100%)	326 (99%)	2 (1%)	78	88
3	P	328/329 (100%)	327 (100%)	1 (0%)	86	93
4	D	200/200 (100%)	196 (98%)	4 (2%)	48	69
4	Q	200/200 (100%)	197 (98%)	3 (2%)	57	74
5	E	166/166 (100%)	164 (99%)	2 (1%)	63	78
5	R	165/166 (99%)	162 (98%)	3 (2%)	51	71
6	F	93/96 (97%)	86 (92%)	7 (8%)	12	24
6	S	93/96 (97%)	87 (94%)	6 (6%)	15	29
7	G	71/71 (100%)	70 (99%)	1 (1%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	70/71 (99%)	70 (100%)	0	100	100
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	73
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	18
9	V	23/26 (88%)	21 (91%)	2 (9%)	9	18
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	69
10	W	47/49 (96%)	46 (98%)	1 (2%)	47	67
All	All	3378/3446 (98%)	3296 (98%)	82 (2%)	43	65

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	A	106	MET
1	A	108	LYS
1	A	228	VAL
1	A	274	ASN
1	A	281	ASP
1	A	352	SER
1	A	395	TRP
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	26	ILE
2	B	31	ASN
2	B	150	VAL
2	B	170	THR
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	291	VAL
2	B	338	ARG
2	B	341	MET
2	B	402	ILE
3	C	216	SER
3	C	223	PRO
4	D	57	THR
4	D	70	VAL
4	D	169	LEU
4	D	203	ARG

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Mol	Chain	Res	Type
5	E	178	TYR
5	E	185	TYR
6	F	52	GLU
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	50	PRO
9	I	68	ILE
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	50	GLU
1	N	106	MET
1	N	108	LYS
1	N	228	VAL
1	N	281	ASP
1	N	352	SER
1	N	395	TRP
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO
2	O	26	ILE
2	O	31	ASN
2	O	150	VAL
2	O	170	THR
2	O	248	ASN
2	O	250	HIS
2	O	260	GLU
2	O	291	VAL
2	O	341	MET
2	O	402	ILE
2	O	418	VAL
3	P	216	SER
4	Q	70	VAL
4	Q	169	LEU
4	Q	203	ARG
5	R	31	ASP

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Mol	Chain	Res	Type
5	R	178	TYR
5	R	185	TYR
6	S	52	GLU
6	S	64	ARG
6	S	70	LEU
6	S	73	ARG
6	S	78	GLU
6	S	84	GLU
8	U	49	HIS
9	V	68	ILE
9	V	75	SER
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	176	HIS
1	A	274	ASN
1	A	289	HIS
1	A	301	HIS
1	A	311	ASN
1	A	339	GLN
1	A	385	ASN
2	B	31	ASN
2	B	115	HIS
2	B	153	GLN
2	B	156	GLN
2	B	197	ASN
2	B	198	ASN
2	B	222	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	315	ASN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS

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Mol	Chain	Res	Type
3	C	17	ASN
3	C	55	HIS
3	C	69	HIS
3	C	73	ASN
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
4	D	225	HIS
5	E	3	ASN
5	E	53	ASN
5	E	57	GLN
5	E	121	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
5	E	179	ASN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	10	ASN
1	N	32	GLN
1	N	85	HIS
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	176	HIS
1	N	274	ASN
1	N	289	HIS
1	N	311	ASN
1	N	339	GLN
2	O	31	ASN
2	O	115	HIS
2	O	156	GLN
2	O	197	ASN
2	O	198	ASN
2	O	247	GLN
2	O	248	ASN

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Mol	Chain	Res	Type
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	342	ASN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS
3	P	17	ASN
3	P	27	ASN
3	P	69	HIS
3	P	73	ASN
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	107	ASN
5	R	121	GLN
5	R	164	HIS
5	R	186	GLN
6	S	72	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

29 ligands are modelled in this entry.

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$
18	BOG	P	2010	-	12,12,20	1.37	3 (25%)	17,17,25	0.58	0
15	CDL	C	2004	-	39,39,99	1.21	2 (5%)	45,51,111	1.12	4 (8%)
11	PEE	C	2007	-	48,48,50	1.46	7 (14%)	51,53,55	0.84	2 (3%)
16	GOL	C	2011	-	5,5,5	1.32	0	5,5,5	0.62	0
18	BOG	Q	3091	-	13,13,20	1.39	2 (15%)	18,18,25	1.15	2 (11%)
11	PEE	N	3008	-	4,4,50	3.72	4 (100%)	6,6,55	0.69	0
11	PEE	E	2005	-	49,49,50	1.57	11 (22%)	52,54,55	0.88	3 (5%)
12	HEM	P	501	3	50,50,50	1.44	4 (8%)	67,82,82	1.32	8 (11%)
16	GOL	P	3011	-	5,5,5	1.43	1 (20%)	5,5,5	0.67	0
19	FES	R	501	5	0,4,4	-	-	-	-	-
17	HEC	Q	501	4	50,50,50	1.20	5 (10%)	68,82,82	1.49	8 (11%)
12	HEM	C	501	3	50,50,50	1.47	6 (12%)	67,82,82	1.45	11 (16%)
11	PEE	P	3007	-	48,48,50	1.43	7 (14%)	51,53,55	0.81	2 (3%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
15	CDL	D	2003	-	41,41,99	1.21	4 (9%)	47,53,111	1.06	2 (4%)
18	BOG	D	2009	-	20,20,20	0.94	2 (10%)	25,25,25	0.83	2 (8%)
12	HEM	P	502	3	50,50,50	1.53	8 (16%)	67,82,82	1.42	8 (11%)
14	UQ	P	3002	-	19,19,63	2.64	10 (52%)	24,26,79	1.28	3 (12%)
18	BOG	D	2091	-	13,13,20	1.30	2 (15%)	18,18,25	1.11	2 (11%)
11	PEE	R	3005	-	49,49,50	1.55	10 (20%)	52,54,55	0.87	3 (5%)
13	JZV	C	2001	-	30,30,30	2.00	5 (16%)	41,41,41	3.47	11 (26%)
15	CDL	P	3004	-	39,39,99	1.22	2 (5%)	45,51,111	1.14	4 (8%)
18	BOG	Q	3009	-	20,20,20	0.97	1 (5%)	25,25,25	0.90	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	UQ	C	2002	-	19,19,63	2.67	10 (52%)	24,26,79	1.28	3 (12%)
17	HEC	D	501	4	50,50,50	1.18	4 (8%)	68,82,82	1.67	12 (17%)
11	PEE	A	2008	-	20,20,50	1.87	6 (30%)	23,25,55	0.69	0
15	CDL	Q	3003	-	41,41,99	1.21	2 (4%)	47,53,111	1.07	2 (4%)
13	JZV	P	3001	-	30,30,30	2.05	5 (16%)	41,41,41	3.58	11 (26%)
12	HEM	C	502	3	50,50,50	1.55	7 (14%)	67,82,82	1.65	13 (19%)

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
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
15	CDL	C	2004	-	-	21/49/49/110	-
11	PEE	C	2007	-	-	23/52/52/54	-
16	GOL	C	2011	-	-	4/4/4/4	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
11	PEE	E	2005	-	-	27/53/53/54	-
12	HEM	P	501	3	-	5/14/54/54	-
16	GOL	P	3011	-	-	3/4/4/4	-
19	FES	R	501	5	-	-	0/1/1/1
17	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
12	HEM	C	501	3	-	7/14/54/54	-
11	PEE	P	3007	-	-	26/52/52/54	-
19	FES	E	501	5	-	-	0/1/1/1
15	CDL	D	2003	-	-	22/51/51/110	-
18	BOG	D	2009	-	-	5/11/31/31	0/1/1/1
12	HEM	P	502	3	-	6/14/54/54	-
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
11	PEE	R	3005	-	-	27/53/53/54	-
13	JZV	C	2001	-	-	3/29/29/29	0/2/2/2
15	CDL	P	3004	-	-	21/49/49/110	-
18	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEC	D	501	4	1/1/3/7	9/14/54/54	-
11	PEE	A	2008	-	-	12/24/24/54	-
15	CDL	Q	3003	-	-	21/51/51/110	-
13	JZV	P	3001	-	-	3/29/29/29	0/2/2/2
12	HEM	C	502	3	-	5/14/54/54	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	JZV	CAT-CAS	-6.50	1.39	1.49
13	C	2001	JZV	CAT-CAS	-6.28	1.39	1.49
13	C	2001	JZV	CAI-CAJ	-5.27	1.39	1.48
13	P	3001	JZV	CAI-CAJ	-5.22	1.39	1.48
14	C	2002	UQ	C6-C5	5.18	1.44	1.35
14	P	3002	UQ	C7-C6	5.15	1.60	1.51
11	N	3008	PEE	P-O1P	5.07	1.62	1.50
14	C	2002	UQ	C7-C6	5.01	1.60	1.51
12	C	501	HEM	CBC-CAC	4.89	1.53	1.30
14	P	3002	UQ	C6-C5	4.84	1.43	1.35
12	P	501	HEM	CBC-CAC	4.62	1.52	1.30
11	C	2007	PEE	C39-C38	4.42	1.56	1.31
12	P	501	HEM	CBB-CAB	4.34	1.51	1.30
13	P	3001	JZV	CAS-NAR	4.31	1.33	1.28
11	P	3007	PEE	C39-C38	4.26	1.55	1.31
12	C	502	HEM	CBB-CAB	4.22	1.50	1.30
11	E	2005	PEE	C39-C38	4.16	1.55	1.31
11	R	3005	PEE	C39-C38	4.08	1.54	1.31
12	P	502	HEM	CBC-CAC	4.01	1.49	1.30
13	C	2001	JZV	CAS-NAR	3.98	1.33	1.28
12	C	502	HEM	CBC-CAC	3.93	1.49	1.30
12	P	502	HEM	CBB-CAB	3.82	1.48	1.30
14	P	3002	UQ	C6-C1	3.81	1.57	1.46
12	C	501	HEM	CBB-CAB	3.81	1.48	1.30
14	C	2002	UQ	C6-C1	3.74	1.57	1.46
11	R	3005	PEE	O2-C10	3.62	1.44	1.34
11	N	3008	PEE	P-O4P	3.55	1.65	1.54
11	E	2005	PEE	O3-C30	3.55	1.43	1.33
12	P	501	HEM	CAB-C3B	-3.47	1.38	1.47
11	P	3007	PEE	O3-C30	3.44	1.43	1.33
12	C	501	HEM	CAB-C3B	-3.42	1.38	1.47
11	C	2007	PEE	C21-C22	-3.41	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3007	PEE	C21-C22	-3.39	1.34	1.51
11	C	2007	PEE	O3-C30	3.39	1.43	1.33
11	A	2008	PEE	O2-C10	3.37	1.43	1.34
11	E	2005	PEE	O2-C10	3.35	1.43	1.34
14	P	3002	UQ	O3-C3	3.33	1.44	1.36
11	C	2007	PEE	P-O1P	3.33	1.62	1.50
11	R	3005	PEE	C21-C22	-3.29	1.35	1.51
11	A	2008	PEE	O3-C30	3.28	1.42	1.33
12	C	502	HEM	C4D-C3D	3.27	1.50	1.45
11	A	2008	PEE	P-O1P	3.27	1.62	1.50
11	N	3008	PEE	P-O3P	3.26	1.64	1.54
14	C	2002	UQ	O3-C3	3.25	1.44	1.36
11	R	3005	PEE	P-O1P	3.25	1.62	1.50
11	R	3005	PEE	O3-C30	3.24	1.42	1.33
11	E	2005	PEE	C21-C22	-3.24	1.35	1.51
11	E	2005	PEE	P-O1P	3.23	1.62	1.50
12	C	502	HEM	CAB-C3B	-3.22	1.38	1.47
13	C	2001	JZV	OAQ-NAR	-3.19	1.36	1.42
12	P	502	HEM	CAB-C3B	-3.13	1.39	1.47
13	P	3001	JZV	OAQ-NAR	-3.10	1.36	1.42
11	P	3007	PEE	P-O1P	3.05	1.61	1.50
13	P	3001	JZV	CAJ-NAD	3.01	1.33	1.29
14	C	2002	UQ	C2-C1	2.99	1.57	1.48
14	C	2002	UQ	CM5-C5	2.97	1.56	1.50
12	P	502	HEM	CAC-C3C	-2.97	1.39	1.47
14	P	3002	UQ	C7-C8	2.87	1.55	1.50
13	C	2001	JZV	CAJ-NAD	2.85	1.33	1.29
14	C	2002	UQ	O2-C2	2.83	1.43	1.36
17	Q	501	HEC	C1D-ND	-2.74	1.35	1.40
11	P	3007	PEE	O2-C10	2.74	1.42	1.34
14	P	3002	UQ	C2-C1	2.74	1.56	1.48
17	D	501	HEC	C4D-C3D	2.73	1.49	1.45
14	C	2002	UQ	C7-C8	2.72	1.54	1.50
11	C	2007	PEE	O2-C10	2.70	1.41	1.34
14	P	3002	UQ	CM5-C5	2.70	1.56	1.50
12	C	501	HEM	CAC-C3C	-2.68	1.40	1.47
14	P	3002	UQ	C5-C4	2.64	1.56	1.47
12	P	501	HEM	CAC-C3C	-2.64	1.40	1.47
14	P	3002	UQ	O2-C2	2.62	1.43	1.36
14	C	2002	UQ	C5-C4	2.59	1.56	1.47
14	P	3002	UQ	C3-C4	2.56	1.56	1.48
11	N	3008	PEE	P-O2P	2.56	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	2005	PEE	C31-C30	2.55	1.58	1.50
11	E	2005	PEE	C3-C2	2.51	1.58	1.50
18	Q	3091	BOG	O5-C1	2.48	1.48	1.41
12	C	502	HEM	CMB-C2B	2.46	1.55	1.50
17	D	501	HEC	CHD-C4C	-2.45	1.33	1.39
11	R	3005	PEE	C11-C10	2.45	1.57	1.50
18	P	2010	BOG	C4-C5	2.44	1.58	1.53
12	C	502	HEM	CAC-C3C	-2.40	1.41	1.47
11	E	2005	PEE	C1-C2	2.39	1.58	1.50
14	C	2002	UQ	C3-C4	2.39	1.55	1.48
11	C	2007	PEE	C31-C30	2.39	1.57	1.50
15	P	3004	CDL	O1-C1	2.38	1.50	1.43
11	A	2008	PEE	C3-C2	2.37	1.58	1.50
18	D	2091	BOG	C4-C5	2.36	1.58	1.53
11	R	3005	PEE	C31-C30	2.35	1.57	1.50
15	C	2004	CDL	O1-C1	2.35	1.50	1.43
18	Q	3091	BOG	C4-C5	2.34	1.58	1.53
11	R	3005	PEE	C3-C2	2.34	1.58	1.50
11	E	2005	PEE	C11-C10	2.33	1.57	1.50
17	D	501	HEC	C4C-NC	-2.31	1.35	1.39
12	P	502	HEM	C1C-NC	-2.30	1.35	1.39
18	D	2091	BOG	O5-C1	2.30	1.47	1.41
11	R	3005	PEE	C1-C2	2.30	1.58	1.50
15	D	2003	CDL	OA6-CA5	2.28	1.40	1.34
17	Q	501	HEC	C4C-NC	-2.28	1.35	1.39
17	Q	501	HEC	CHC-C4B	-2.27	1.33	1.38
11	P	3007	PEE	C31-C30	2.25	1.57	1.50
18	Q	3009	BOG	O5-C1	2.24	1.47	1.41
11	A	2008	PEE	C1-C2	2.22	1.57	1.50
11	A	2008	PEE	C11-C10	2.22	1.57	1.50
12	P	502	HEM	C4D-C3D	2.22	1.48	1.45
18	P	2010	BOG	C1-C2	2.22	1.57	1.52
11	R	3005	PEE	O2-C2	2.22	1.51	1.46
15	Q	3003	CDL	O1-C1	2.22	1.49	1.43
17	Q	501	HEC	C3C-C2C	-2.21	1.33	1.38
15	C	2004	CDL	CB3-CB4	2.17	1.57	1.50
15	D	2003	CDL	O1-C1	2.15	1.49	1.43
11	C	2007	PEE	C3-C2	2.13	1.57	1.50
11	E	2005	PEE	P-O4P	2.12	1.67	1.59
12	C	501	HEM	C4A-NA	-2.11	1.35	1.39
16	P	3011	GOL	O2-C2	2.09	1.49	1.43
17	D	501	HEC	C1D-ND	-2.08	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	2009	BOG	O5-C1	2.08	1.47	1.41
17	Q	501	HEC	C4B-NB	-2.08	1.36	1.40
15	P	3004	CDL	OB2-CB2	-2.07	1.36	1.44
12	P	502	HEM	C4B-NB	-2.05	1.34	1.38
11	E	2005	PEE	O2-C2	2.05	1.51	1.46
15	D	2003	CDL	OB8-CB7	2.04	1.39	1.33
11	P	3007	PEE	C3-C2	2.04	1.57	1.50
18	D	2009	BOG	C1-C2	2.03	1.58	1.52
12	C	502	HEM	CHD-C4C	-2.03	1.34	1.38
15	Q	3003	CDL	OB2-CB2	-2.02	1.37	1.44
12	P	502	HEM	C3B-C4B	2.02	1.48	1.44
15	D	2003	CDL	CA3-CA4	2.01	1.57	1.50
18	P	2010	BOG	O5-C1	2.00	1.47	1.42
12	C	501	HEM	C2A-C3A	-2.00	1.33	1.38

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	3001	JZV	OAQ-NAR-CAS	14.37	133.72	111.94
13	C	2001	JZV	OAQ-NAR-CAS	12.58	131.00	111.94
13	P	3001	JZV	CAT-CAS-NAR	8.27	133.75	115.30
13	C	2001	JZV	CAT-CAS-NAR	8.17	133.53	115.30
13	C	2001	JZV	CAY-CAS-NAR	-7.90	108.61	123.95
13	P	3001	JZV	OAE-NAD-CAJ	7.68	119.95	111.50
13	P	3001	JZV	CAY-CAS-NAR	-7.47	109.46	123.95
13	C	2001	JZV	OAE-NAD-CAJ	7.29	119.53	111.50
13	C	2001	JZV	OAL-CAK-CAJ	7.05	119.30	111.75
13	P	3001	JZV	OAL-CAK-CAJ	6.97	119.21	111.75
13	C	2001	JZV	CAP-OAQ-NAR	5.56	114.91	107.92
12	C	502	HEM	CAD-C3D-C4D	4.87	133.19	124.70
13	C	2001	JZV	OAQ-CAP-CAH	4.80	122.17	109.91
17	Q	501	HEC	CAA-C2A-C1A	4.73	134.46	124.85
12	C	502	HEM	C3B-C2B-C1B	-4.66	102.91	106.41
17	Q	501	HEC	CAA-C2A-C3A	-4.58	119.28	127.87
17	D	501	HEC	CAA-C2A-C1A	4.45	133.90	124.85
13	P	3001	JZV	CAP-OAQ-NAR	4.42	113.48	107.92
12	P	502	HEM	CAD-C3D-C4D	4.29	132.17	124.70
14	P	3002	UQ	C8-C7-C6	4.12	122.23	112.08
12	C	501	HEM	C3B-C4B-NB	4.05	112.38	109.47
14	C	2002	UQ	C8-C7-C6	4.05	122.06	112.08
17	D	501	HEC	CAA-C2A-C3A	-3.84	120.68	127.87
13	P	3001	JZV	OAQ-CAP-CAH	3.82	119.66	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	502	HEM	C3B-C2B-C1B	-3.74	103.60	106.41
12	P	501	HEM	CAD-C3D-C4D	3.73	131.20	124.70
18	Q	3091	BOG	C1'-O1-C1	3.67	118.83	113.26
17	D	501	HEC	CAD-C3D-C4D	3.61	130.99	124.70
12	P	502	HEM	C4C-C3C-C2C	-3.45	103.82	106.81
17	Q	501	HEC	CAC-C3C-C2C	3.44	132.34	126.89
12	C	502	HEM	C2D-C1D-ND	3.42	113.86	109.90
12	C	502	HEM	C2B-C1B-NB	3.42	113.78	109.84
18	D	2091	BOG	C1'-O1-C1	3.40	118.43	113.26
18	Q	3009	BOG	C1'-O1-C1	3.28	119.29	113.68
15	P	3004	CDL	CB4-OB6-CB5	-3.26	109.98	117.80
12	C	501	HEM	C2D-C1D-ND	3.24	113.65	109.90
12	P	501	HEM	CAD-C3D-C2D	-3.22	121.83	127.87
12	C	501	HEM	CAD-C3D-C4D	3.22	130.31	124.70
17	Q	501	HEC	CMB-C2B-C1B	3.21	130.06	125.03
14	C	2002	UQ	C7-C6-C1	-3.11	114.90	118.52
12	C	502	HEM	C4C-C3C-C2C	-3.11	104.12	106.81
17	D	501	HEC	CAC-C3C-C2C	3.10	131.79	126.89
12	P	501	HEM	C3B-C4B-NB	3.08	111.68	109.47
13	C	2001	JZV	OAN-CAK-CAJ	-3.04	119.51	123.53
15	C	2004	CDL	CA4-OA6-CA5	-3.03	110.55	117.80
15	C	2004	CDL	CB4-OB6-CB5	-3.03	110.56	117.80
12	C	502	HEM	C3B-C4B-NB	3.02	111.64	109.47
17	D	501	HEC	CMA-C3A-C4A	2.99	129.99	124.73
12	C	501	HEM	CAD-C3D-C2D	-2.99	122.27	127.87
14	P	3002	UQ	C7-C6-C1	-2.94	115.10	118.52
17	D	501	HEC	CMC-C2C-C1C	2.93	129.87	125.42
12	C	502	HEM	CAD-C3D-C2D	-2.91	122.42	127.87
12	P	502	HEM	C3B-C4B-NB	2.90	111.55	109.47
12	C	501	HEM	C3B-C2B-C1B	-2.90	104.23	106.41
17	Q	501	HEC	CAD-C3D-C4D	2.90	129.74	124.70
13	P	3001	JZV	CAP-CAH-CAI	2.86	126.23	122.06
15	P	3004	CDL	CA4-OA6-CA5	-2.85	110.99	117.80
11	E	2005	PEE	C22-C21-C20	2.83	127.44	113.86
17	D	501	HEC	C2D-C1D-ND	2.82	113.08	109.84
12	P	502	HEM	C2B-C1B-NB	2.81	113.07	109.84
11	R	3005	PEE	C22-C21-C20	2.80	127.34	113.86
12	C	502	HEM	C4D-ND-C1D	-2.80	101.89	105.21
11	C	2007	PEE	C22-C21-C20	2.79	127.27	113.86
17	Q	501	HEC	CAC-C3C-C4C	-2.78	121.09	124.91
12	P	501	HEM	C2D-C1D-ND	2.76	113.09	109.90
11	P	3007	PEE	C22-C21-C20	2.73	126.98	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	2007	PEE	C21-C22-C23	2.68	127.92	114.37
17	Q	501	HEC	CBA-CAA-C2A	2.66	119.88	112.53
12	C	502	HEM	C3D-C4D-ND	2.64	113.07	110.17
13	P	3001	JZV	CAM-OAL-CAK	-2.62	110.99	115.85
13	P	3001	JZV	CAP-CAH-CAG	-2.60	113.89	119.51
12	P	502	HEM	C2D-C1D-ND	2.58	112.89	109.90
17	D	501	HEC	CAB-C3B-C4B	-2.56	121.45	124.79
11	P	3007	PEE	C21-C22-C23	2.56	127.32	114.37
13	P	3001	JZV	OAN-CAK-CAJ	-2.56	120.15	123.53
12	C	501	HEM	CBD-CAD-C3D	2.55	119.58	112.53
17	D	501	HEC	CMD-C2D-C1D	2.54	129.01	125.03
12	C	502	HEM	C2A-C1A-NA	2.54	112.97	110.15
12	C	501	HEM	C3C-C2C-C1C	-2.54	104.64	107.05
18	D	2091	BOG	O1-C1-C2	2.51	111.04	108.14
18	Q	3091	BOG	O1-C1-C2	2.50	111.02	108.14
18	D	2009	BOG	C1'-O1-C1	2.49	117.94	113.68
11	E	2005	PEE	C21-C22-C23	2.48	126.90	114.37
15	D	2003	CDL	CB4-OB6-CB5	-2.47	111.87	117.80
12	P	502	HEM	CAD-C3D-C2D	-2.47	123.25	127.87
12	C	502	HEM	CAA-C2A-C1A	2.46	129.75	124.94
15	D	2003	CDL	CA6-CA4-CA3	-2.45	106.06	111.78
15	Q	3003	CDL	CB4-OB6-CB5	-2.44	111.95	117.80
15	P	3004	CDL	CA6-CA4-CA3	-2.41	106.16	111.78
11	R	3005	PEE	C21-C22-C23	2.41	126.55	114.37
12	C	501	HEM	CMD-C2D-C1D	2.40	128.79	125.03
13	C	2001	JZV	CAM-OAL-CAK	-2.38	111.44	115.85
13	C	2001	JZV	CAP-CAH-CAI	2.37	125.53	122.06
12	P	502	HEM	CAA-C2A-C1A	2.37	129.57	124.94
15	Q	3003	CDL	CA6-CA4-CA3	-2.36	106.28	111.78
11	E	2005	PEE	O3-C3-C2	2.35	115.16	108.40
11	R	3005	PEE	O3-C3-C2	2.33	115.11	108.40
12	C	502	HEM	C4D-C3D-C2D	-2.32	103.51	106.89
18	D	2009	BOG	O1-C1-C2	2.31	111.78	108.27
17	D	501	HEC	C2B-C1B-NB	2.30	112.56	109.90
12	P	501	HEM	CBD-CAD-C3D	2.30	118.89	112.53
12	P	501	HEM	CMD-C2D-C1D	2.27	128.59	125.03
12	P	501	HEM	C3C-C2C-C1C	-2.25	104.91	107.05
15	C	2004	CDL	CA6-CA4-CA3	-2.25	106.53	111.78
13	C	2001	JZV	CAP-CAH-CAG	-2.21	114.73	119.51
17	D	501	HEC	CAD-C3D-C2D	-2.20	123.74	127.87
14	C	2002	UQ	C10-C9-C8	-2.17	118.05	123.63
12	C	501	HEM	C2B-C1B-NB	2.17	112.33	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	3002	UQ	C10-C9-C8	-2.14	118.14	123.63
17	Q	501	HEC	CMA-C3A-C4A	2.13	128.47	124.73
17	D	501	HEC	CMB-C2B-C1B	2.11	128.32	125.03
12	C	501	HEM	CMB-C2B-C1B	2.08	128.28	125.03
12	P	501	HEM	CMB-C2B-C1B	2.07	128.27	125.03
15	P	3004	CDL	OB6-CB4-CB3	2.06	115.73	108.34
12	C	502	HEM	CHA-C4D-ND	-2.05	121.83	124.37
12	C	501	HEM	C4D-ND-C1D	-2.03	102.81	105.21
15	C	2004	CDL	OB6-CB4-CB3	2.01	115.56	108.34

All (2) chirality outliers are listed below:

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

All (277) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O3P
11	E	2005	PEE	C4-O4P-P-O2P
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	O4P-C4-C5-N
11	P	3007	PEE	C4-O4P-P-O3P
11	P	3007	PEE	C4-O4P-P-O2P
11	P	3007	PEE	C4-O4P-P-O1P
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C4-O4P-P-O2P
11	R	3005	PEE	C4-O4P-P-O1P
12	C	501	HEM	C2B-C3B-CAB-CBB
14	C	2002	UQ	C1-C6-C7-C8
14	C	2002	UQ	C5-C6-C7-C8
14	C	2002	UQ	C12-C11-C9-C8
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8
14	P	3002	UQ	C12-C11-C9-C8
15	C	2004	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
15	C	2004	CDL	CA3-OA5-PA1-OA2
15	C	2004	CDL	CA3-OA5-PA1-OA3
15	C	2004	CDL	CA3-OA5-PA1-OA4
15	C	2004	CDL	CB3-OB5-PB2-OB2
15	C	2004	CDL	CB3-OB5-PB2-OB3
15	C	2004	CDL	C51-CB5-OB6-CB4
15	D	2003	CDL	CA2-OA2-PA1-OA5
15	D	2003	CDL	CA3-OA5-PA1-OA2
15	D	2003	CDL	CA3-OA5-PA1-OA4
15	D	2003	CDL	OA6-CA4-CA6-OA8
15	D	2003	CDL	CB2-OB2-PB2-OB4
15	D	2003	CDL	CB2-OB2-PB2-OB5
15	D	2003	CDL	CB3-OB5-PB2-OB2
15	D	2003	CDL	CB3-OB5-PB2-OB4
15	P	3004	CDL	CB2-C1-CA2-OA2
15	P	3004	CDL	CA2-C1-CB2-OB2
15	P	3004	CDL	CA3-OA5-PA1-OA2
15	P	3004	CDL	CA3-OA5-PA1-OA3
15	P	3004	CDL	CA3-OA5-PA1-OA4
15	P	3004	CDL	CB3-OB5-PB2-OB2
15	P	3004	CDL	CB3-OB5-PB2-OB3
15	P	3004	CDL	C51-CB5-OB6-CB4
15	Q	3003	CDL	CA2-OA2-PA1-OA5
15	Q	3003	CDL	CA3-OA5-PA1-OA2
15	Q	3003	CDL	CA3-OA5-PA1-OA4
15	Q	3003	CDL	OA6-CA4-CA6-OA8
15	Q	3003	CDL	CB2-OB2-PB2-OB4
15	Q	3003	CDL	CB2-OB2-PB2-OB5
15	Q	3003	CDL	CB3-OB5-PB2-OB2
15	Q	3003	CDL	CB3-OB5-PB2-OB4
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	Q	501	HEC	C3A-C2A-CAA-CBA
18	Q	3009	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
11	R	3005	PEE	O5-C30-O3-C3
11	E	2005	PEE	O5-C30-O3-C3
15	C	2004	CDL	OB9-CB7-OB8-CB6
15	P	3004	CDL	OB9-CB7-OB8-CB6
11	A	2008	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	O4-C10-O2-C2
15	C	2004	CDL	OB7-CB5-OB6-CB4
15	P	3004	CDL	OB7-CB5-OB6-CB4
11	E	2005	PEE	C31-C30-O3-C3
11	R	3005	PEE	C31-C30-O3-C3
15	D	2003	CDL	C31-CA7-OA8-CA6
15	Q	3003	CDL	C31-CA7-OA8-CA6
15	C	2004	CDL	OA9-CA7-OA8-CA6
15	P	3004	CDL	OA9-CA7-OA8-CA6
11	A	2008	PEE	C31-C30-O3-C3
15	C	2004	CDL	C71-CB7-OB8-CB6
15	P	3004	CDL	C71-CB7-OB8-CB6
15	C	2004	CDL	C31-CA7-OA8-CA6
15	P	3004	CDL	C31-CA7-OA8-CA6
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
15	C	2004	CDL	O1-C1-CA2-OA2
15	P	3004	CDL	O1-C1-CA2-OA2
18	Q	3091	BOG	O5-C5-C6-O6
17	D	501	HEC	C4B-C3B-CAB-CBB
15	Q	3003	CDL	C71-CB7-OB8-CB6
15	D	2003	CDL	OA9-CA7-OA8-CA6
15	Q	3003	CDL	OA9-CA7-OA8-CA6
17	Q	501	HEC	C1A-C2A-CAA-CBA
15	D	2003	CDL	C71-CB7-OB8-CB6
18	D	2091	BOG	C2-C1-O1-C1'
18	D	2009	BOG	C2-C1-O1-C1'
15	D	2003	CDL	O1-C1-CA2-OA2
15	Q	3003	CDL	O1-C1-CA2-OA2
11	C	2007	PEE	C10-C11-C12-C13
11	P	3007	PEE	C10-C11-C12-C13
15	P	3004	CDL	C11-CA5-OA6-CA4
18	D	2091	BOG	O5-C1-O1-C1'
15	D	2003	CDL	CB7-C71-C72-C73
18	Q	3091	BOG	C4-C5-C6-O6
15	Q	3003	CDL	CB7-C71-C72-C73
15	D	2003	CDL	OB9-CB7-OB8-CB6
15	C	2004	CDL	C11-CA5-OA6-CA4
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
15	Q	3003	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
18	Q	3009	BOG	O1-C1'-C2'-C3'
17	D	501	HEC	C3A-C2A-CAA-CBA
18	D	2009	BOG	O1-C1'-C2'-C3'
15	C	2004	CDL	OA7-CA5-OA6-CA4
15	P	3004	CDL	OA7-CA5-OA6-CA4
17	Q	501	HEC	C2B-C3B-CAB-CBB
17	Q	501	HEC	C4B-C3B-CAB-CBB
12	C	502	HEM	C4D-C3D-CAD-CBD
16	C	2011	GOL	O1-C1-C2-O2
11	C	2007	PEE	C35-C36-C37-C38
11	R	3005	PEE	C34-C35-C36-C37
11	E	2005	PEE	C34-C35-C36-C37
11	P	3007	PEE	C40-C41-C42-C43
15	C	2004	CDL	CA2-C1-CB2-OB2
11	C	2007	PEE	C40-C41-C42-C43
18	D	2009	BOG	C1'-C2'-C3'-C4'
18	Q	3009	BOG	C1'-C2'-C3'-C4'
11	P	3007	PEE	C21-C22-C23-C24
15	D	2003	CDL	C51-CB5-OB6-CB4
15	Q	3003	CDL	C51-CB5-OB6-CB4
17	D	501	HEC	C1A-C2A-CAA-CBA
11	E	2005	PEE	C39-C40-C41-C42
11	P	3007	PEE	C20-C21-C22-C23
15	D	2003	CDL	OB7-CB5-OB6-CB4
11	P	3007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C15-C16-C17-C18
11	P	3007	PEE	C15-C16-C17-C18
11	P	3007	PEE	C35-C36-C37-C38
11	C	2007	PEE	C33-C34-C35-C36
15	Q	3003	CDL	OB7-CB5-OB6-CB4
11	C	2007	PEE	C20-C21-C22-C23
11	E	2005	PEE	C20-C21-C22-C23
16	C	2011	GOL	O2-C2-C3-O3
16	P	3011	GOL	O2-C2-C3-O3
11	R	3005	PEE	C39-C40-C41-C42
11	E	2005	PEE	O3P-C1-C2-C3
11	R	3005	PEE	O3P-C1-C2-C3
11	R	3005	PEE	C30-C31-C32-C33
12	P	502	HEM	C4D-C3D-CAD-CBD
15	D	2003	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
15	Q	3003	CDL	CA3-CA4-CA6-OA8
15	C	2004	CDL	O1-C1-CB2-OB2
11	R	3005	PEE	C20-C21-C22-C23
11	P	3007	PEE	C31-C32-C33-C34
13	P	3001	JZV	CAS-NAR-OAQ-CAP
15	C	2004	CDL	OB5-CB3-CB4-OB6
15	P	3004	CDL	OB5-CB3-CB4-OB6
11	P	3007	PEE	C11-C12-C13-C14
11	P	3007	PEE	C43-C44-C45-C46
11	E	2005	PEE	C30-C31-C32-C33
11	E	2005	PEE	C41-C42-C43-C44
15	D	2003	CDL	C71-C72-C73-C74
15	P	3004	CDL	O1-C1-CB2-OB2
11	C	2007	PEE	C31-C32-C33-C34
11	C	2007	PEE	C43-C44-C45-C46
15	Q	3003	CDL	C71-C72-C73-C74
17	D	501	HEC	C2B-C3B-CAB-CBB
11	C	2007	PEE	C34-C35-C36-C37
11	C	2007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C11-C12-C13-C14
11	E	2005	PEE	C23-C24-C25-C26
11	R	3005	PEE	C23-C24-C25-C26
11	A	2008	PEE	O3P-C1-C2-C3
15	D	2003	CDL	OB5-CB3-CB4-CB6
15	Q	3003	CDL	OB5-CB3-CB4-CB6
15	C	2004	CDL	CB5-C51-C52-C53
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10
11	C	2007	PEE	C42-C43-C44-C45
11	R	3005	PEE	C41-C42-C43-C44
11	A	2008	PEE	C11-C10-O2-C2
11	P	3007	PEE	C42-C43-C44-C45
11	A	2008	PEE	O2-C2-C3-O3
13	C	2001	JZV	CAS-NAR-OAQ-CAP
11	P	3007	PEE	C34-C35-C36-C37
11	E	2005	PEE	C10-C11-C12-C13
16	P	3011	GOL	O1-C1-C2-O2
11	E	2005	PEE	C43-C44-C45-C46
13	C	2001	JZV	CAY-CAS-NAR-OAQ
13	P	3001	JZV	CAY-CAS-NAR-OAQ
13	C	2001	JZV	CAT-CAS-NAR-OAQ
13	P	3001	JZV	CAT-CAS-NAR-OAQ

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Mol	Chain	Res	Type	Atoms
12	P	501	HEM	C2B-C3B-CAB-CBB
11	R	3005	PEE	C43-C44-C45-C46
11	A	2008	PEE	O4-C10-O2-C2
11	R	3005	PEE	O3P-C1-C2-O2
15	D	2003	CDL	OB5-CB3-CB4-OB6
15	Q	3003	CDL	OB5-CB3-CB4-OB6
12	C	501	HEM	C4B-C3B-CAB-CBB
11	R	3005	PEE	C31-C32-C33-C34
11	R	3005	PEE	C10-C11-C12-C13
11	A	2008	PEE	O3P-C1-C2-O2
11	E	2005	PEE	O3P-C1-C2-O2
12	P	502	HEM	C2D-C3D-CAD-CBD
11	E	2005	PEE	C31-C32-C33-C34
11	E	2005	PEE	C35-C36-C37-C38
11	E	2005	PEE	C11-C12-C13-C14
11	A	2008	PEE	C4-O4P-P-O2P
11	R	3005	PEE	O4P-C4-C5-N
15	C	2004	CDL	CB3-OB5-PB2-OB4
15	D	2003	CDL	CA2-OA2-PA1-OA4
15	P	3004	CDL	CB3-OB5-PB2-OB4
11	R	3005	PEE	C11-C12-C13-C14
11	R	3005	PEE	C19-C20-C21-C22
15	C	2004	CDL	OB5-CB3-CB4-CB6
15	P	3004	CDL	OB5-CB3-CB4-CB6
11	P	3007	PEE	C12-C13-C14-C15
11	A	2008	PEE	C10-C11-C12-C13
11	E	2005	PEE	C14-C15-C16-C17
11	C	2007	PEE	C12-C13-C14-C15
11	E	2005	PEE	C19-C20-C21-C22
11	R	3005	PEE	C14-C15-C16-C17
12	P	502	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAD-CBD-CGD-O1D
11	E	2005	PEE	C1-C2-O2-C10
11	R	3005	PEE	C1-C2-O2-C10
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAA-CBA-CGA-O2A
12	C	502	HEM	CAA-CBA-CGA-O2A
11	A	2008	PEE	O3-C30-C31-C32
12	P	502	HEM	CAA-CBA-CGA-O1A
11	R	3005	PEE	C35-C36-C37-C38
12	P	501	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	C	502	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAA-CBA-CGA-O1A
17	D	501	HEC	CAD-CBD-CGD-O2D
11	E	2005	PEE	C22-C23-C24-C25
11	E	2005	PEE	C37-C38-C39-C40
11	R	3005	PEE	C37-C38-C39-C40
12	C	501	HEM	CAA-CBA-CGA-O2A
11	P	3007	PEE	C38-C39-C40-C41
17	Q	501	HEC	CAA-CBA-CGA-O2A
11	A	2008	PEE	O5-C30-C31-C32
12	C	501	HEM	CAA-CBA-CGA-O1A
11	C	2007	PEE	C38-C39-C40-C41
11	E	2005	PEE	C40-C41-C42-C43
17	D	501	HEC	C2C-C3C-CAC-CBC
15	P	3004	CDL	CB5-C51-C52-C53
11	P	3007	PEE	C19-C20-C21-C22
17	D	501	HEC	CAD-CBD-CGD-O1D
17	Q	501	HEC	CAD-CBD-CGD-O2D
11	A	2008	PEE	C1-C2-C3-O3
12	P	501	HEM	C4B-C3B-CAB-CBB
11	R	3005	PEE	C22-C23-C24-C25
11	P	3007	PEE	O2-C10-C11-C12
17	Q	501	HEC	CAA-CBA-CGA-O1A
17	Q	501	HEC	CAD-CBD-CGD-O1D
11	C	2007	PEE	O2-C10-C11-C12
11	P	3007	PEE	C22-C23-C24-C25
12	C	501	HEM	CAD-CBD-CGD-O2D
17	D	501	HEC	CAA-CBA-CGA-O2A
11	P	3007	PEE	O5-C30-O3-C3
11	C	2007	PEE	O2-C2-C3-O3
11	P	3007	PEE	O2-C2-C3-O3
17	D	501	HEC	CAA-CBA-CGA-O1A
18	D	2009	BOG	C4'-C5'-C6'-C7'
11	C	2007	PEE	O4-C10-C11-C12
15	Q	3003	CDL	C72-C71-CB7-OB8
12	C	501	HEM	CAD-CBD-CGD-O1D
11	P	3007	PEE	O4-C10-C11-C12
11	P	3007	PEE	C31-C30-O3-C3
11	R	3005	PEE	C40-C41-C42-C43
12	C	501	HEM	C2C-C3C-CAC-CBC
12	P	501	HEM	C2C-C3C-CAC-CBC
18	Q	3009	BOG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C32-C33-C34-C35
15	D	2003	CDL	C72-C71-CB7-OB8

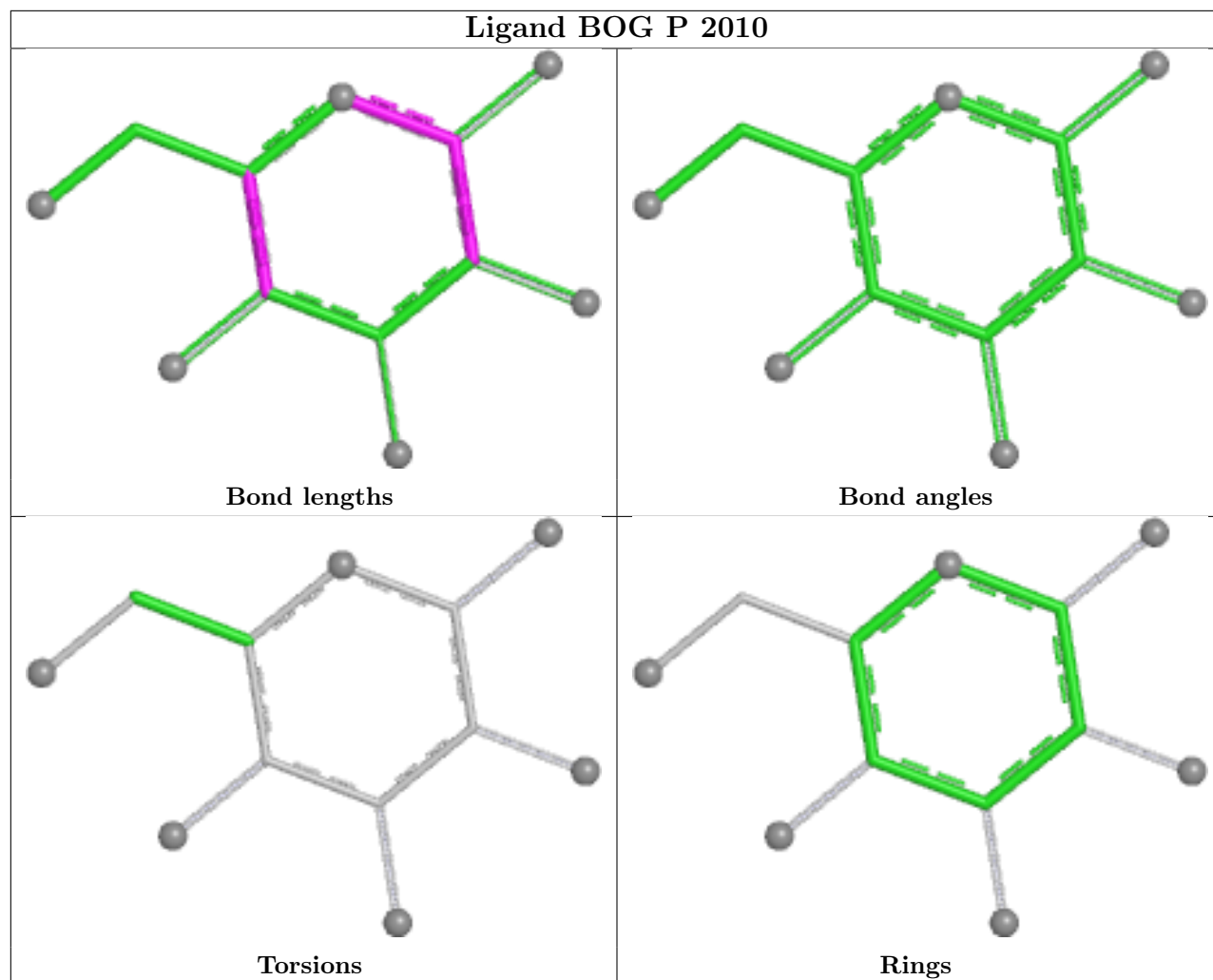
There are no ring outliers.

20 monomers are involved in 61 short contacts:

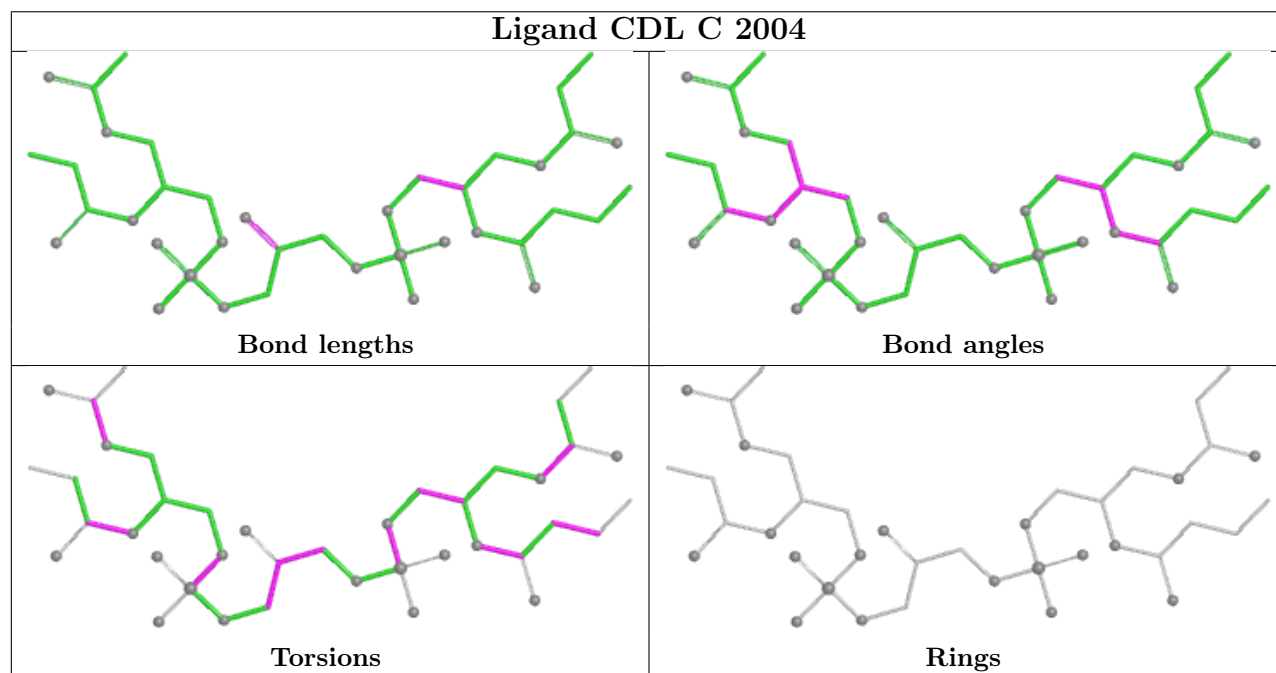
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	P	2010	BOG	2	0
15	C	2004	CDL	4	0
11	C	2007	PEE	4	0
18	Q	3091	BOG	1	0
11	E	2005	PEE	1	0
12	P	501	HEM	4	0
19	R	501	FES	2	0
12	C	501	HEM	5	0
11	P	3007	PEE	3	0
19	E	501	FES	2	0
15	D	2003	CDL	4	0
12	P	502	HEM	4	0
14	P	3002	UQ	3	0
11	R	3005	PEE	2	0
13	C	2001	JZV	4	0
15	P	3004	CDL	4	0
14	C	2002	UQ	2	0
15	Q	3003	CDL	3	0
13	P	3001	JZV	4	0
12	C	502	HEM	5	0

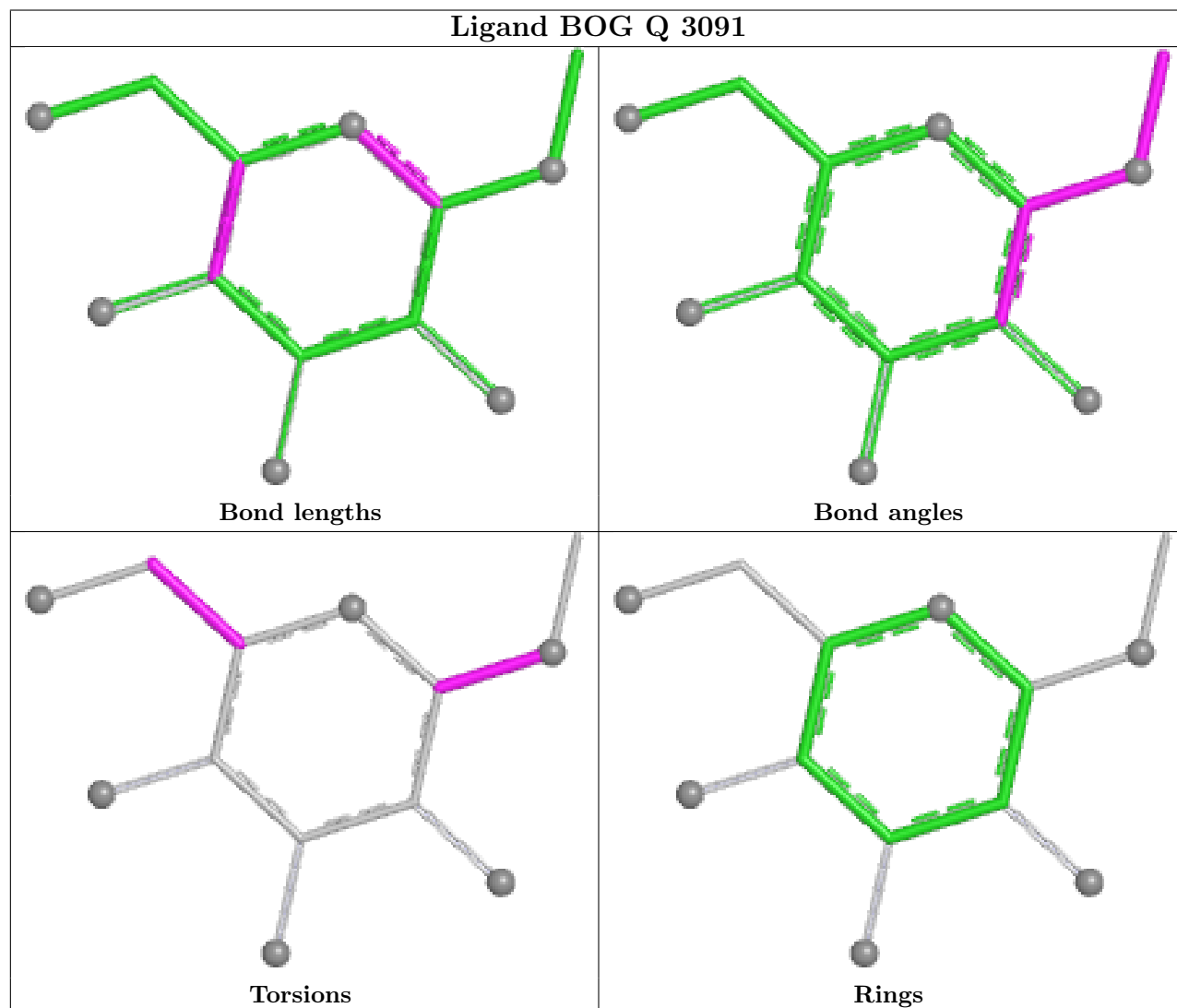
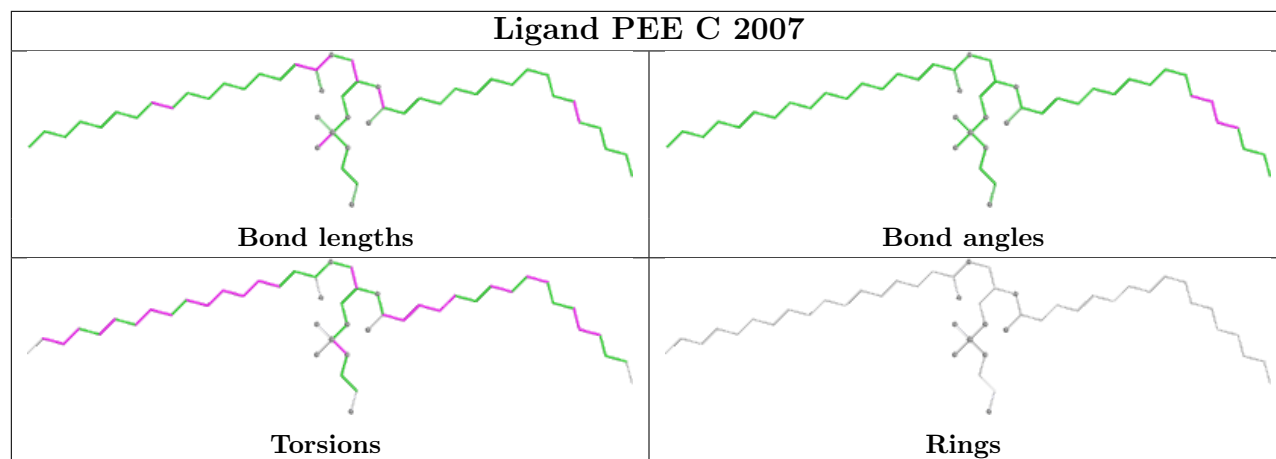
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

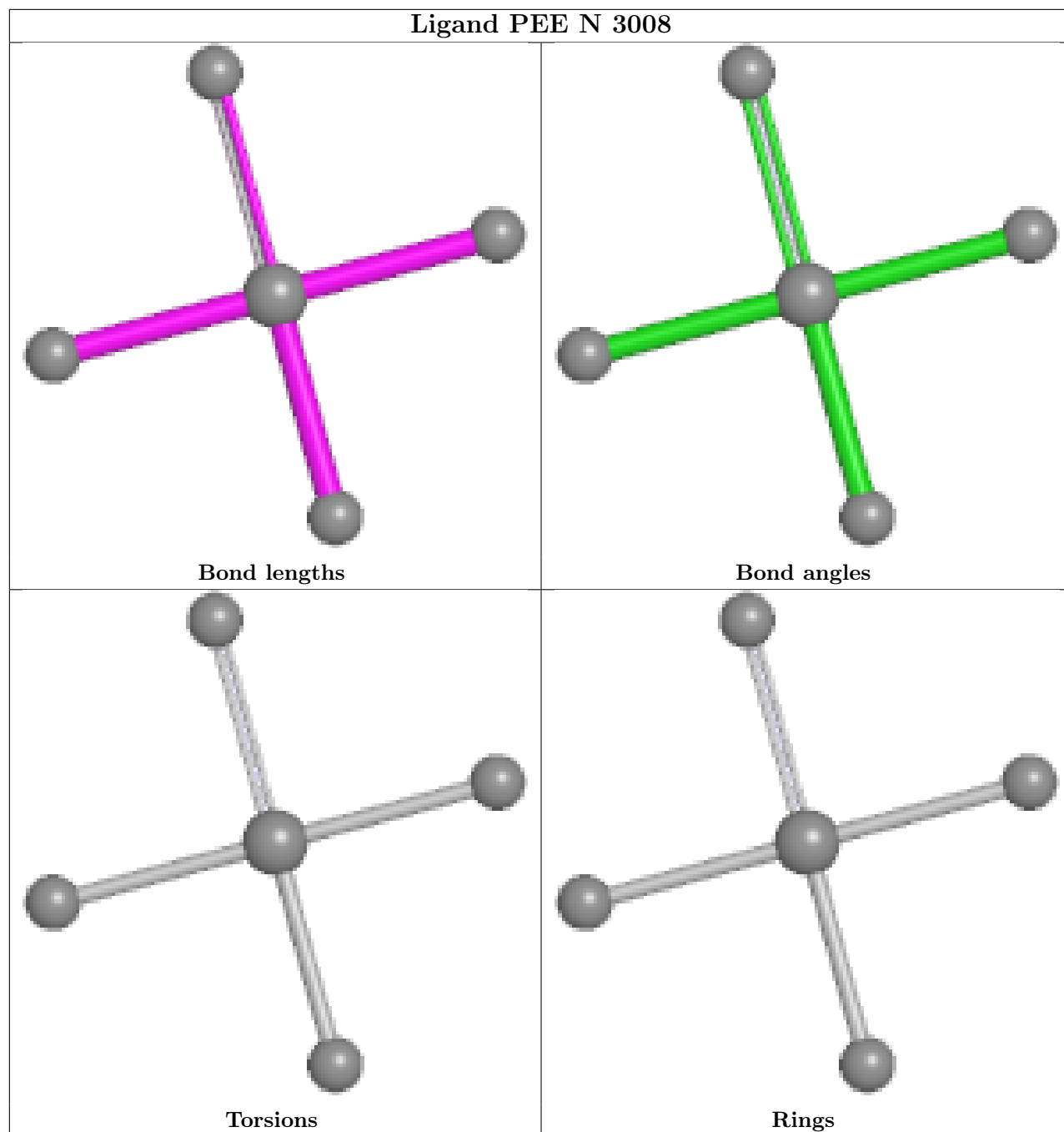
Ligand BOG P 2010

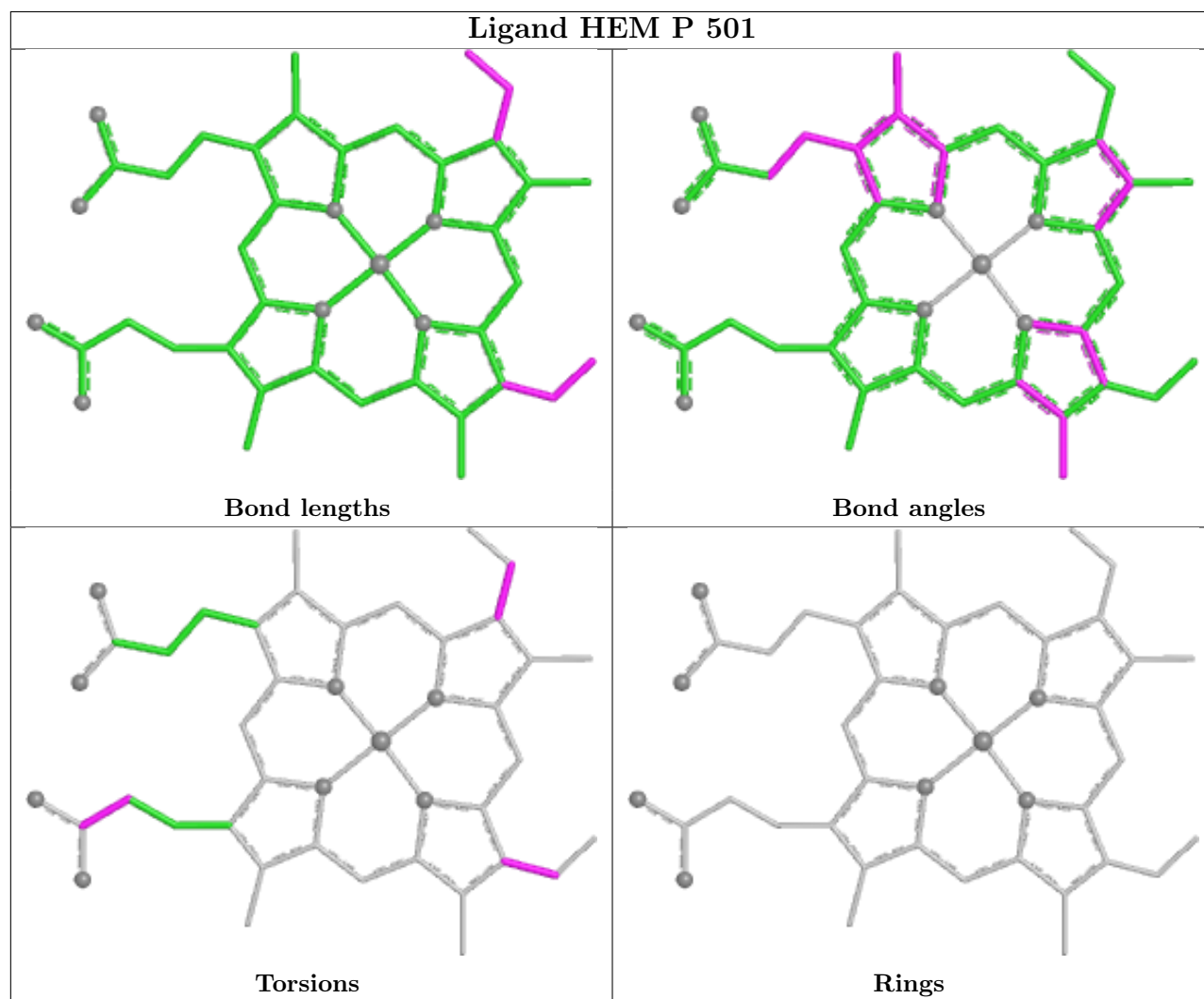
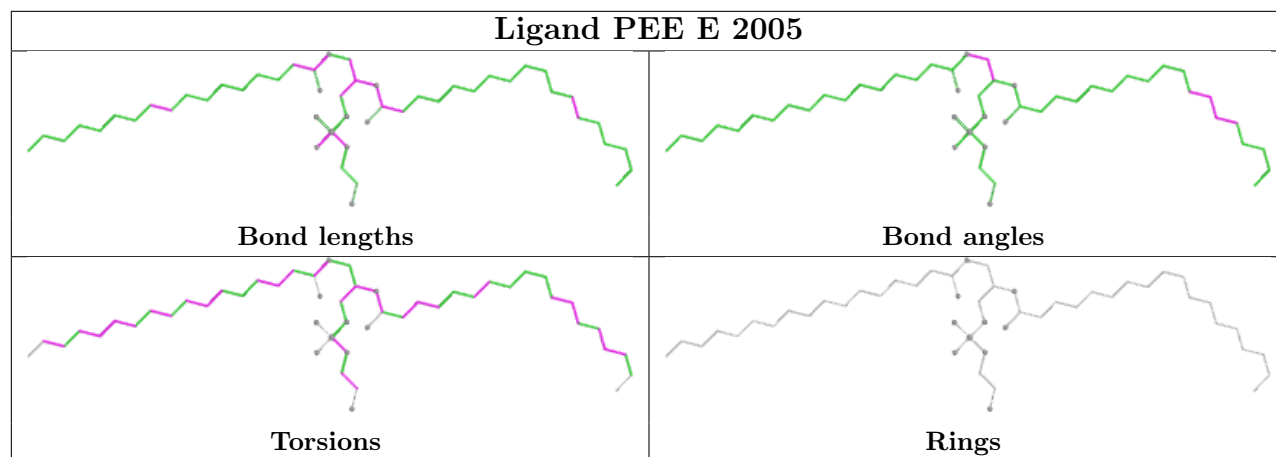


Ligand CDL C 2004

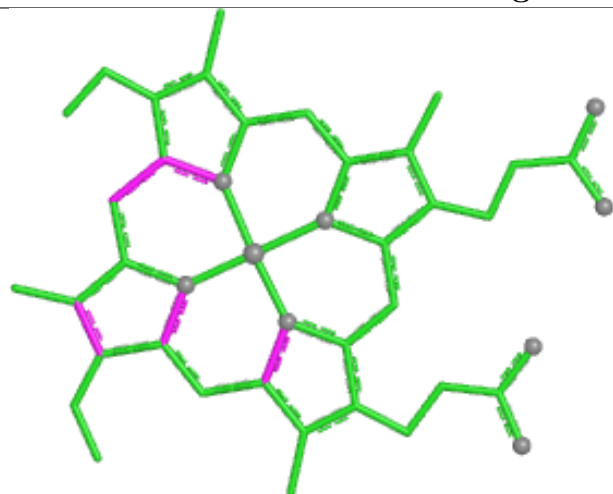




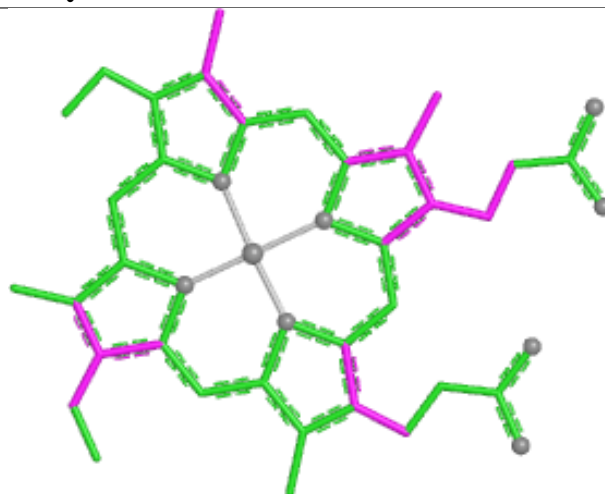




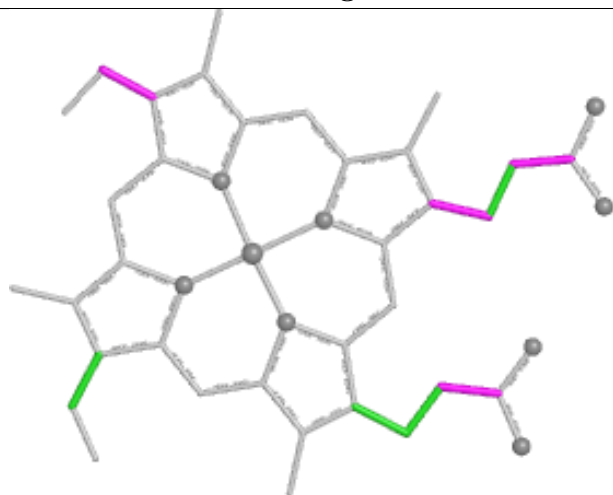
Ligand HEC Q 501



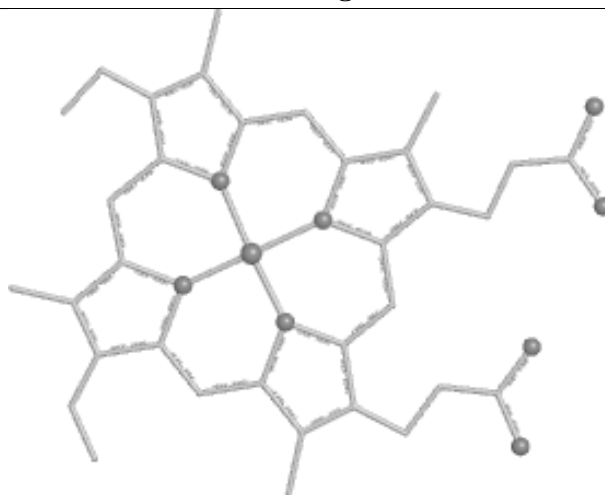
Bond lengths



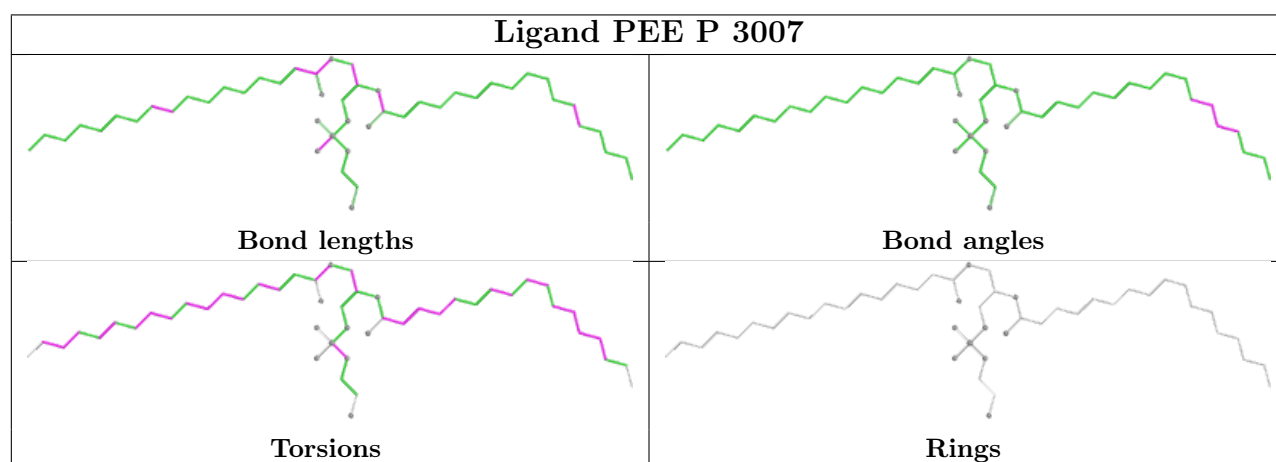
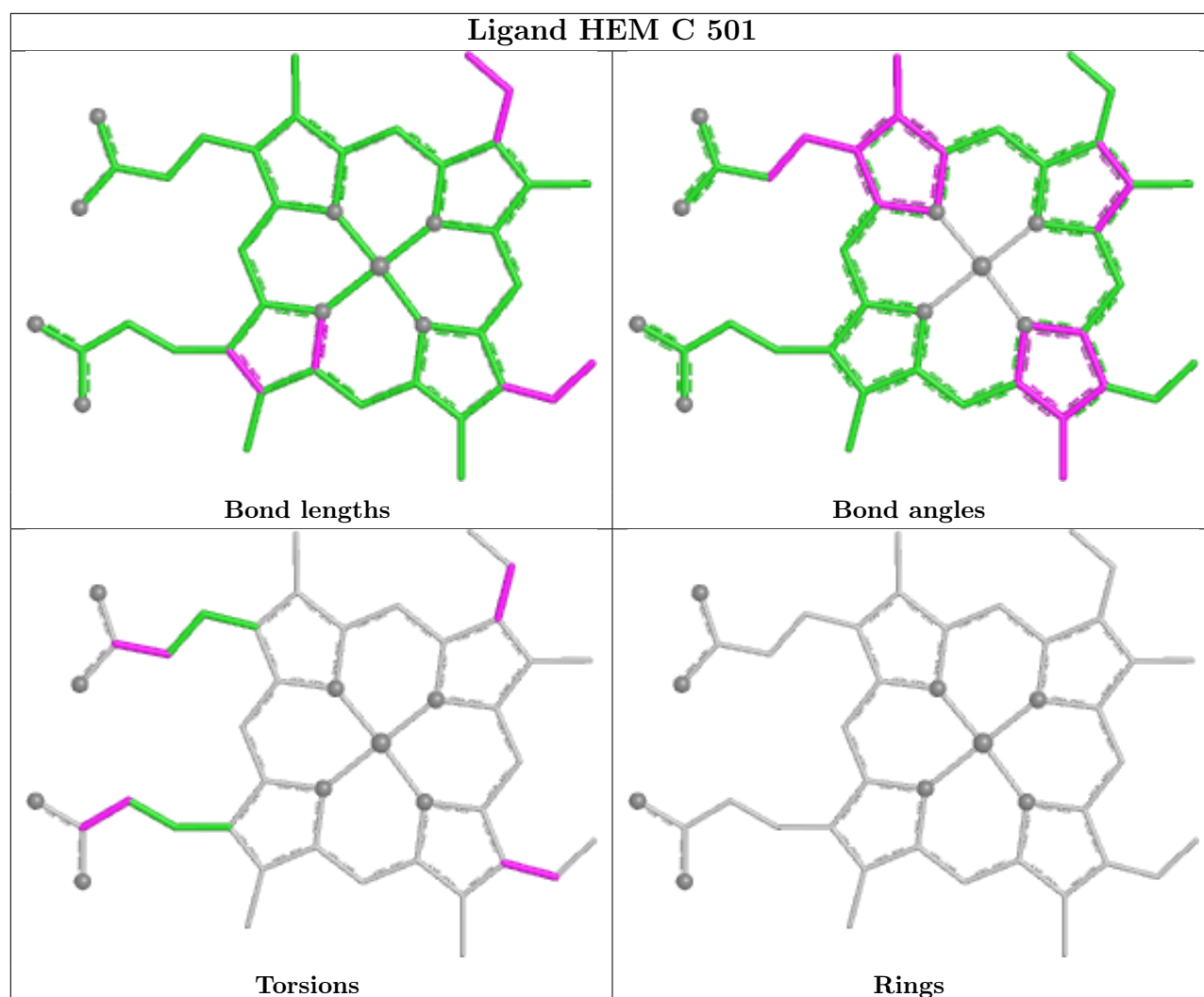
Bond angles

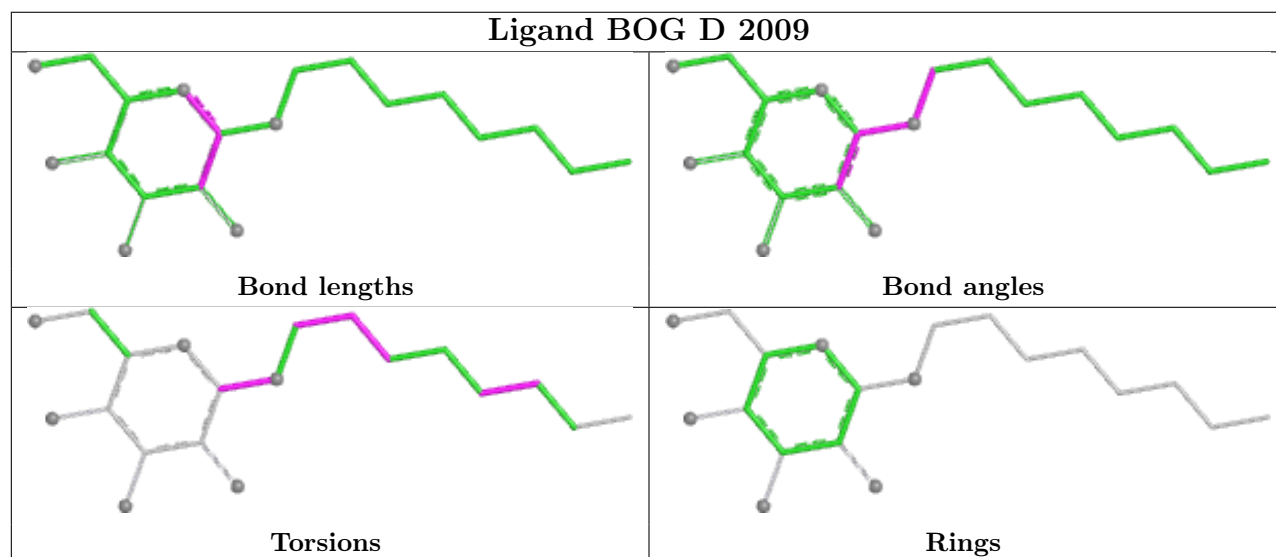
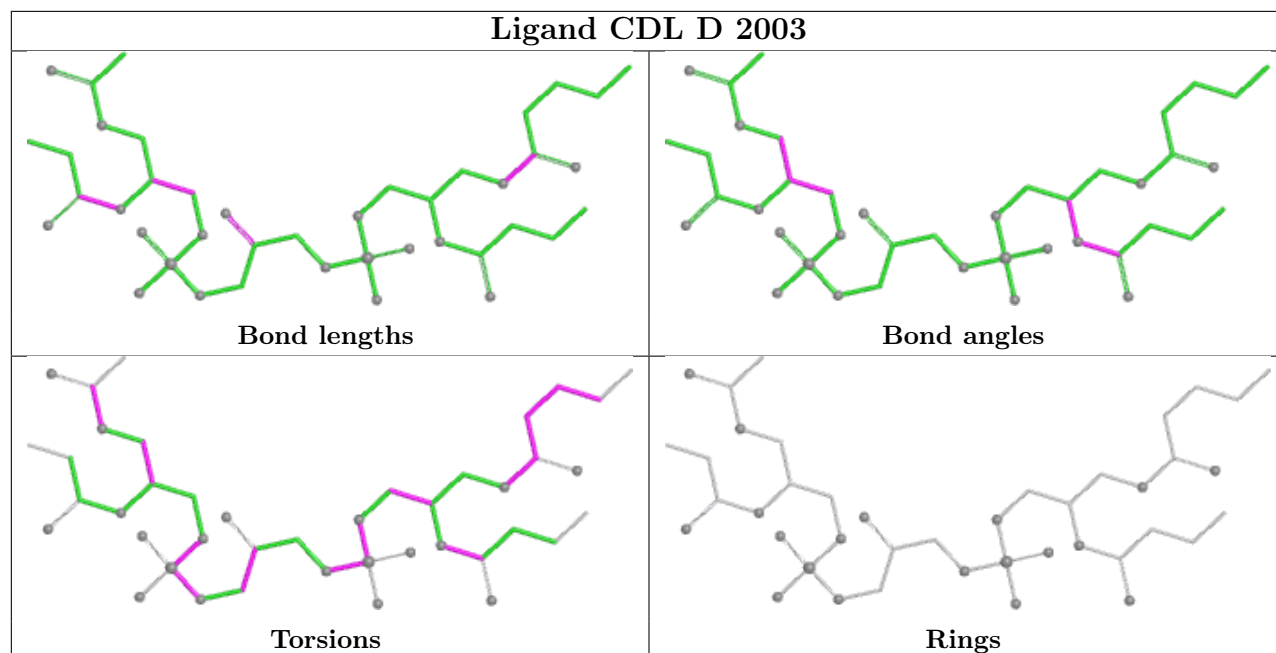


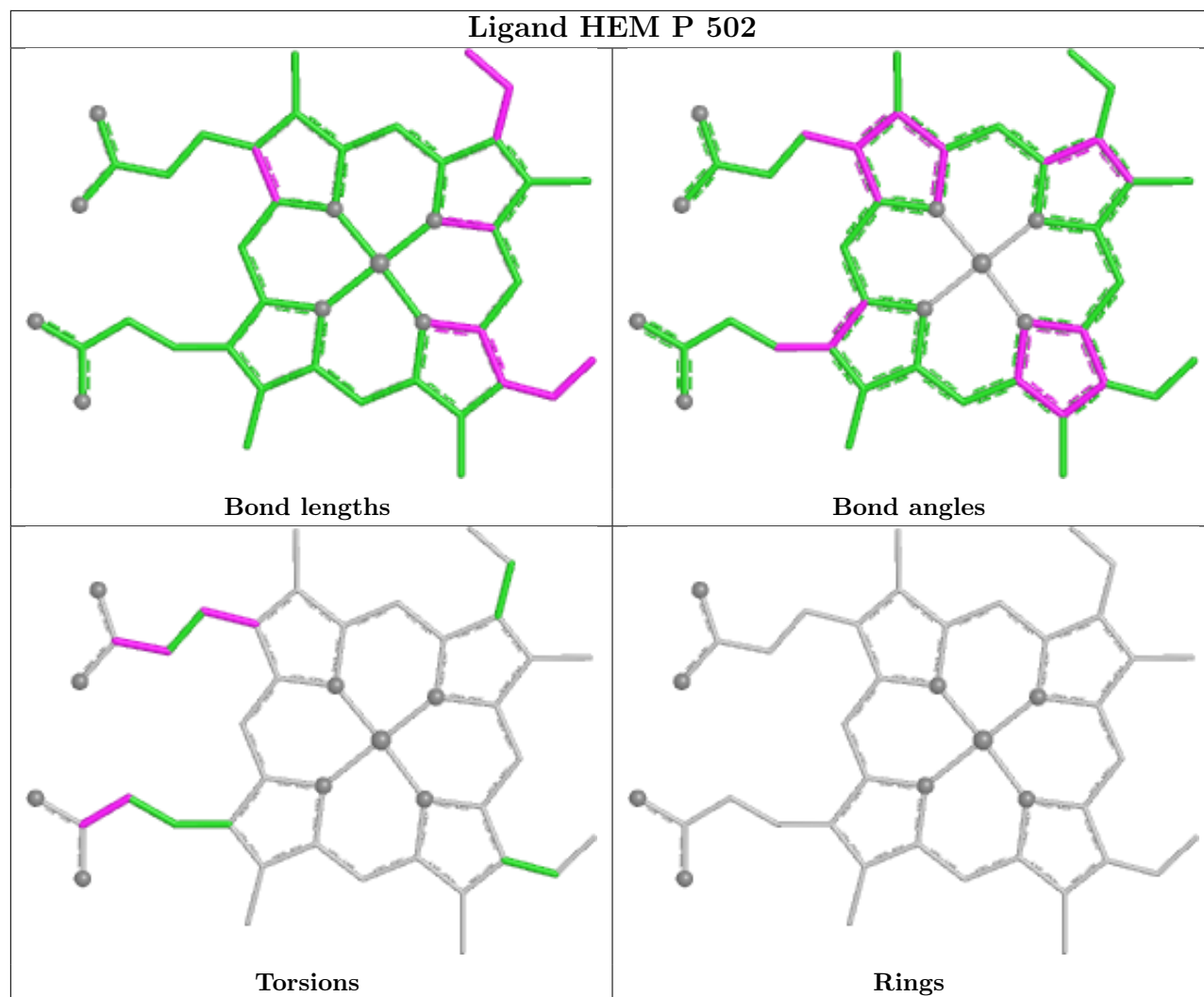
Torsions

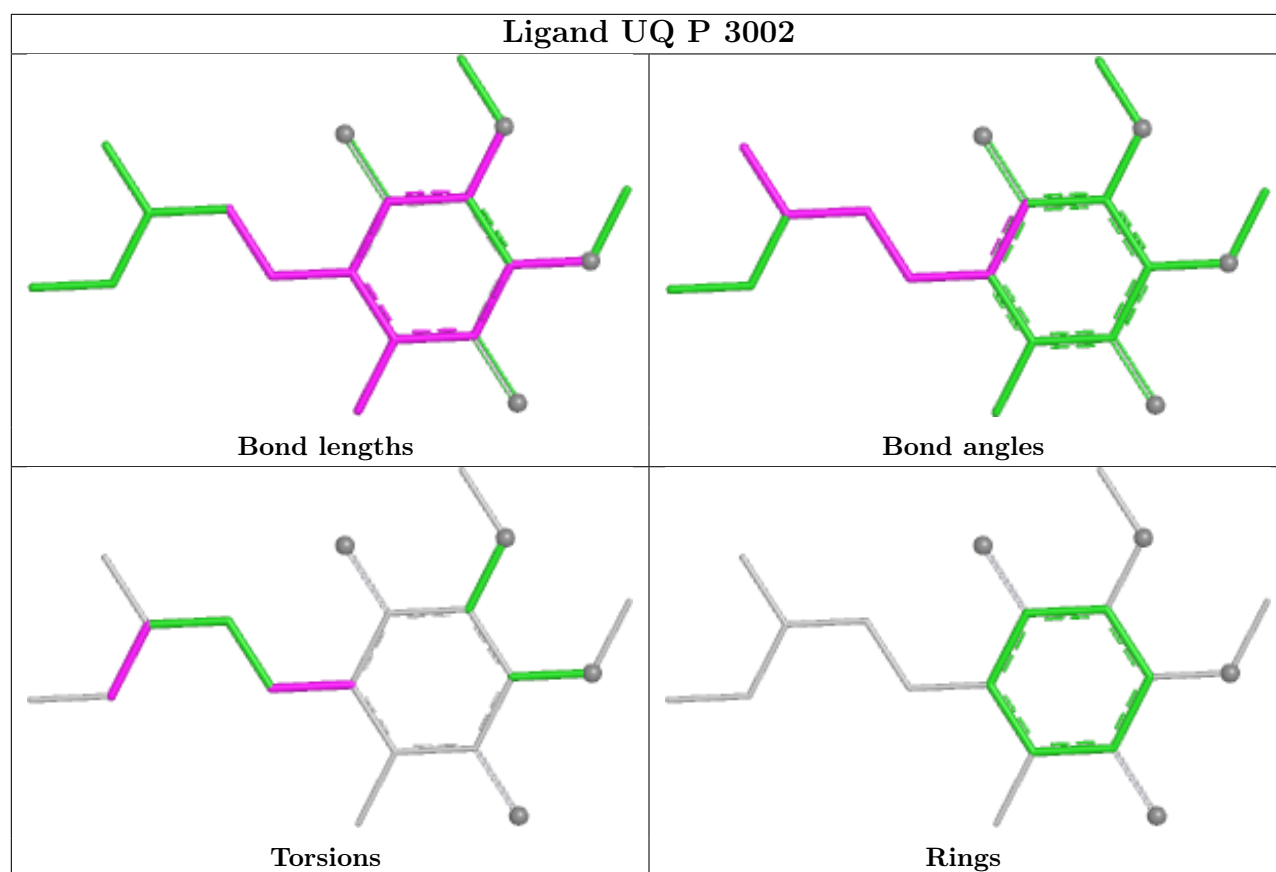


Rings

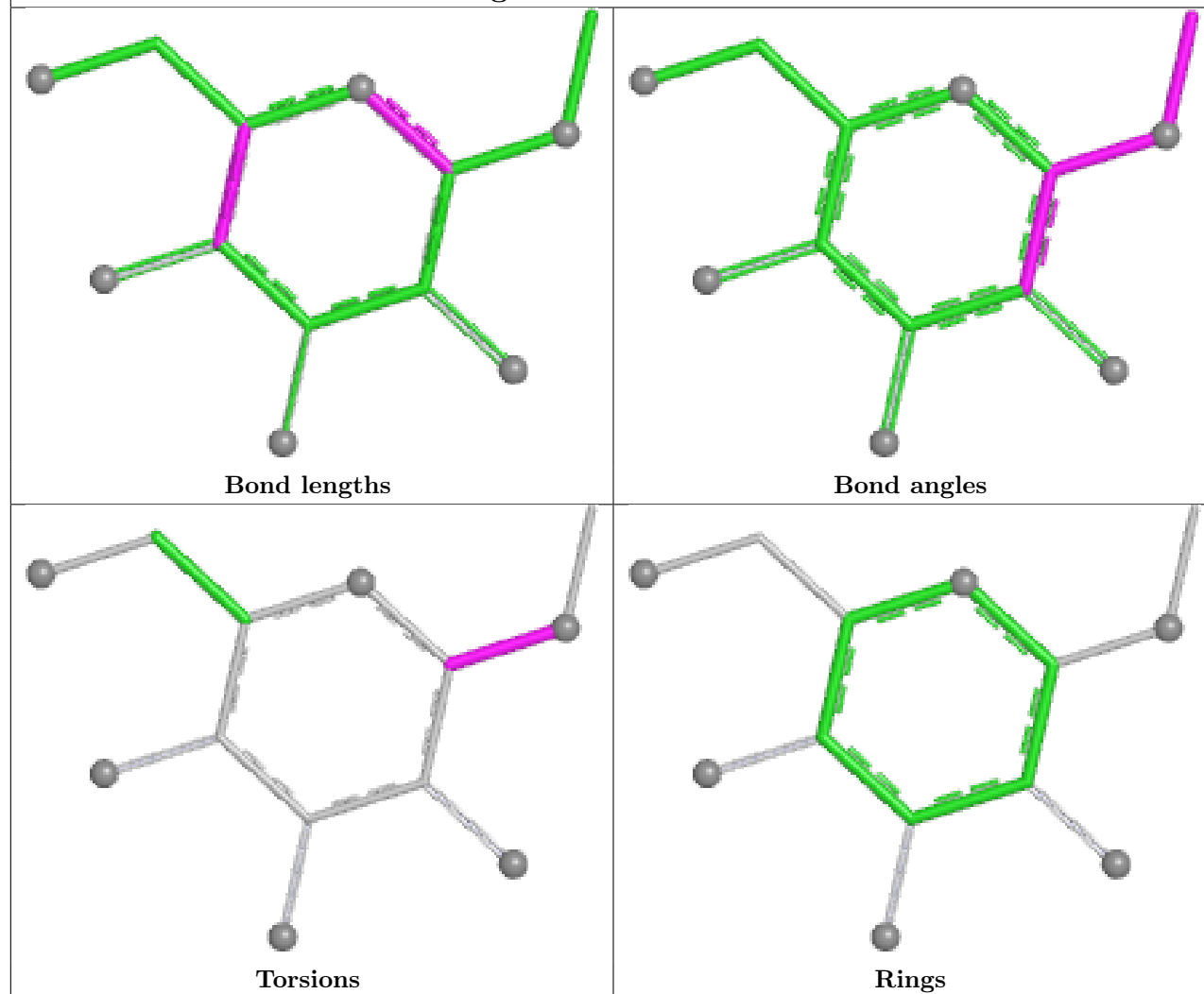




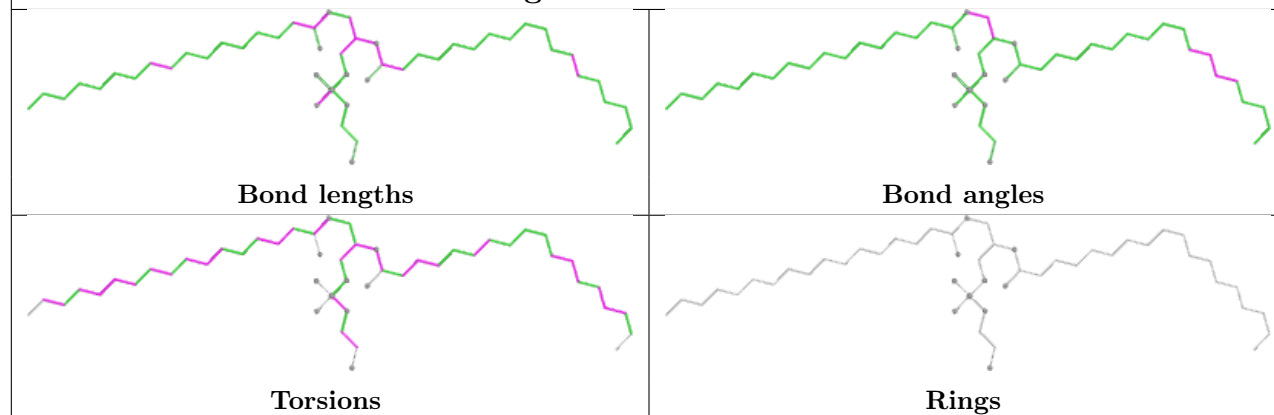


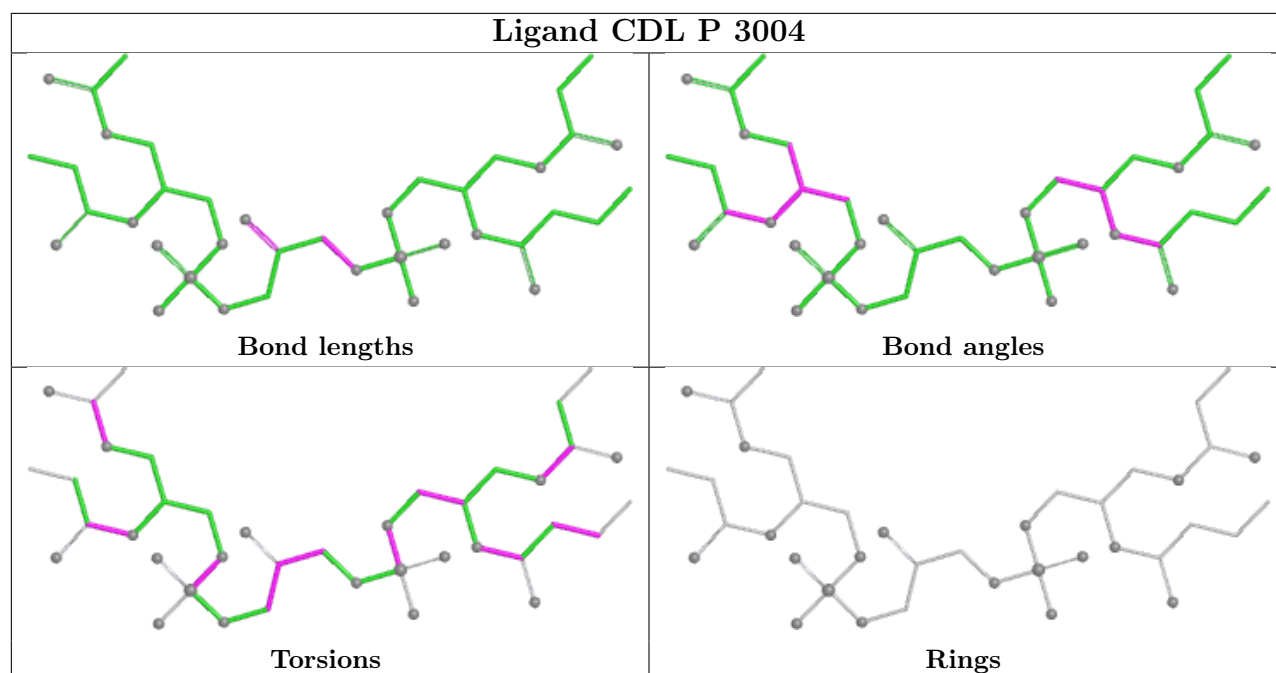
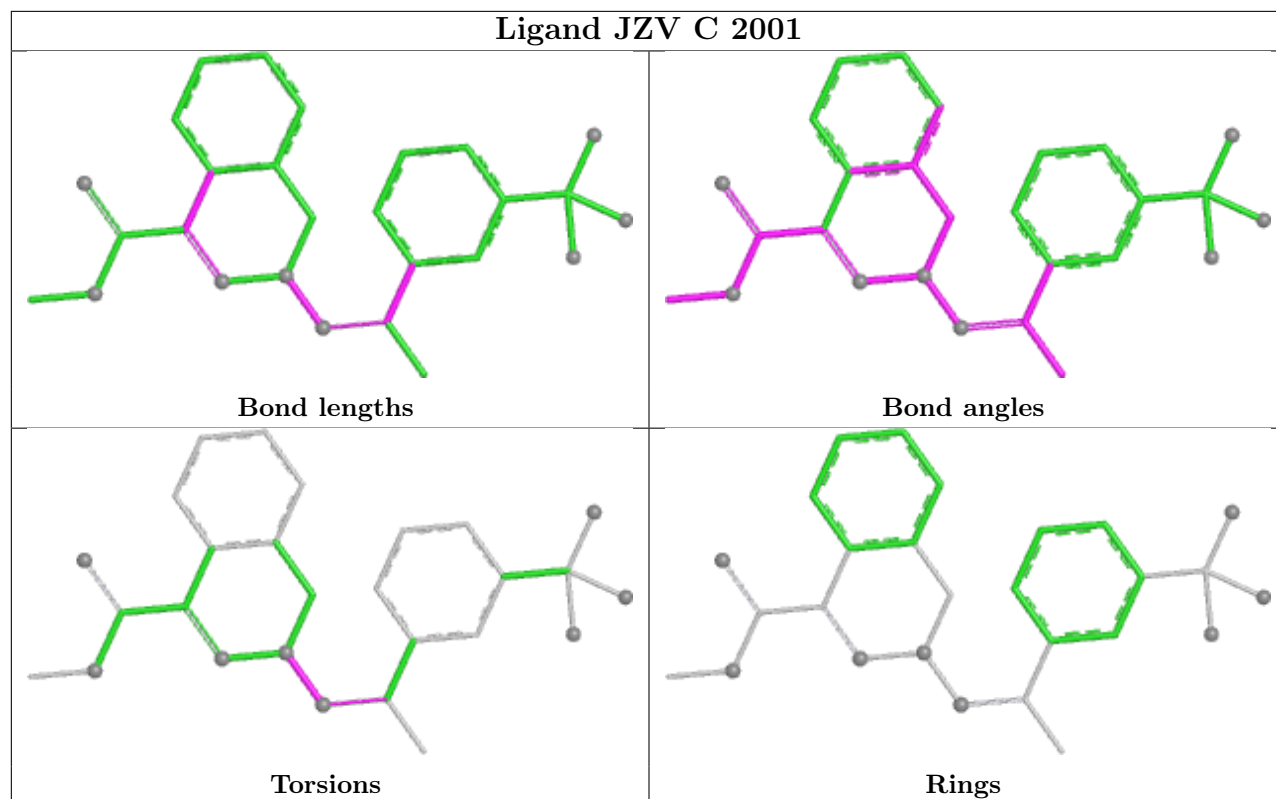


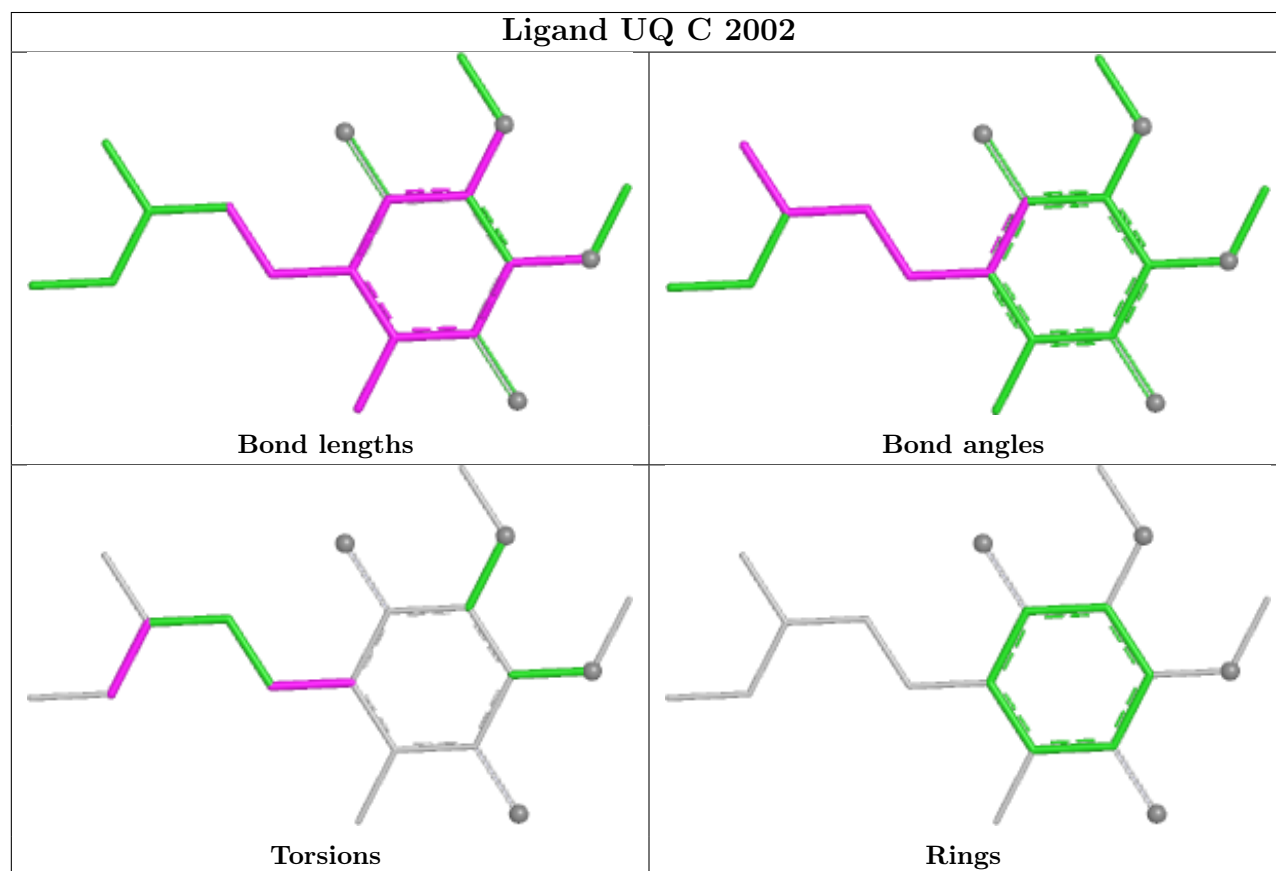
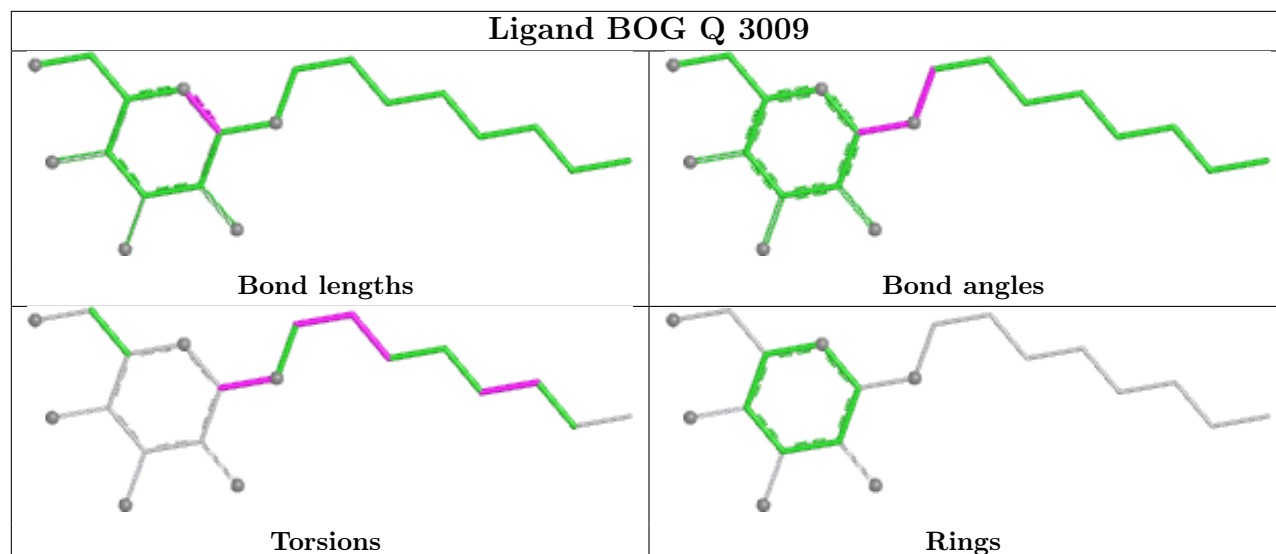
Ligand BOG D 2091

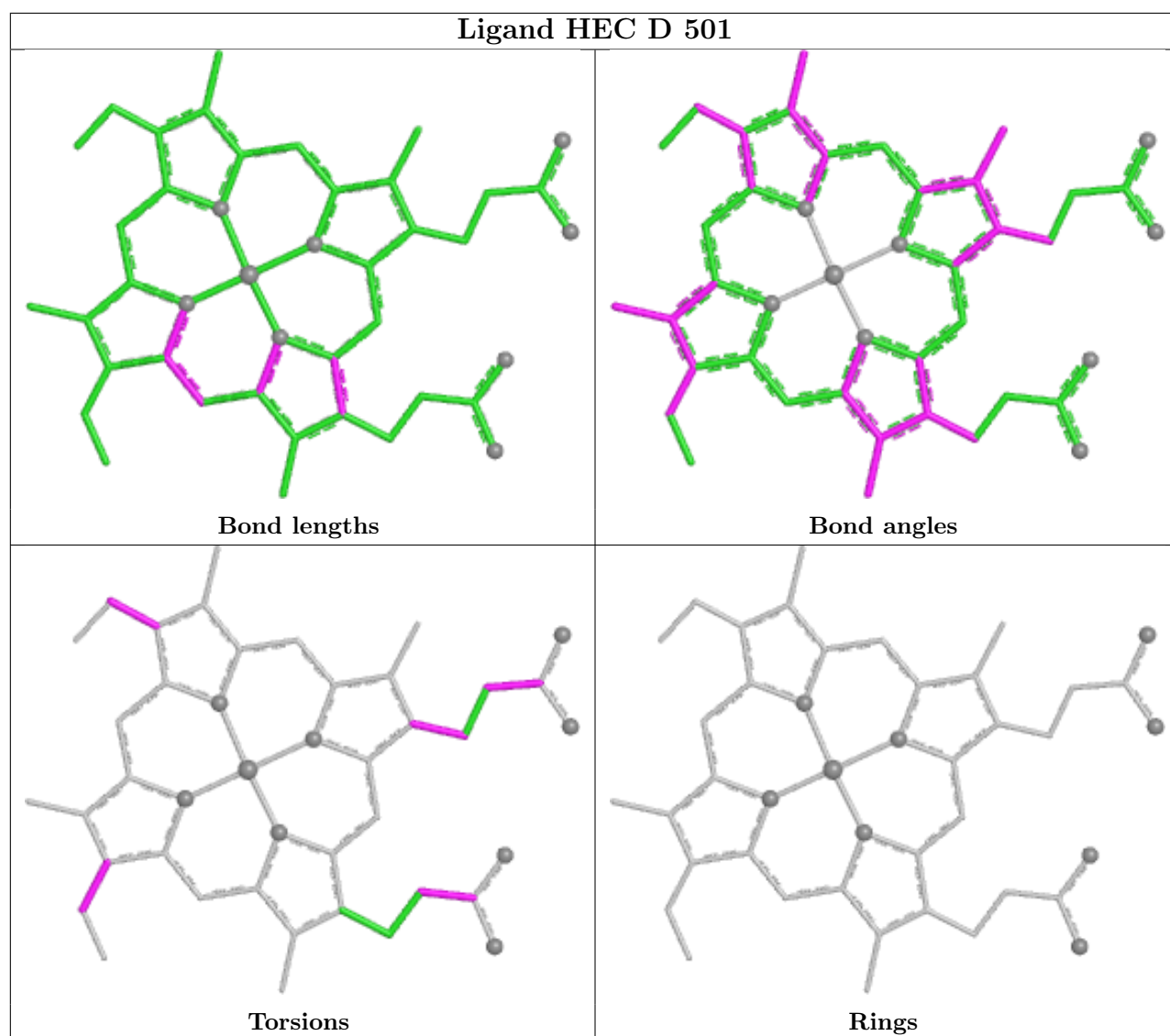


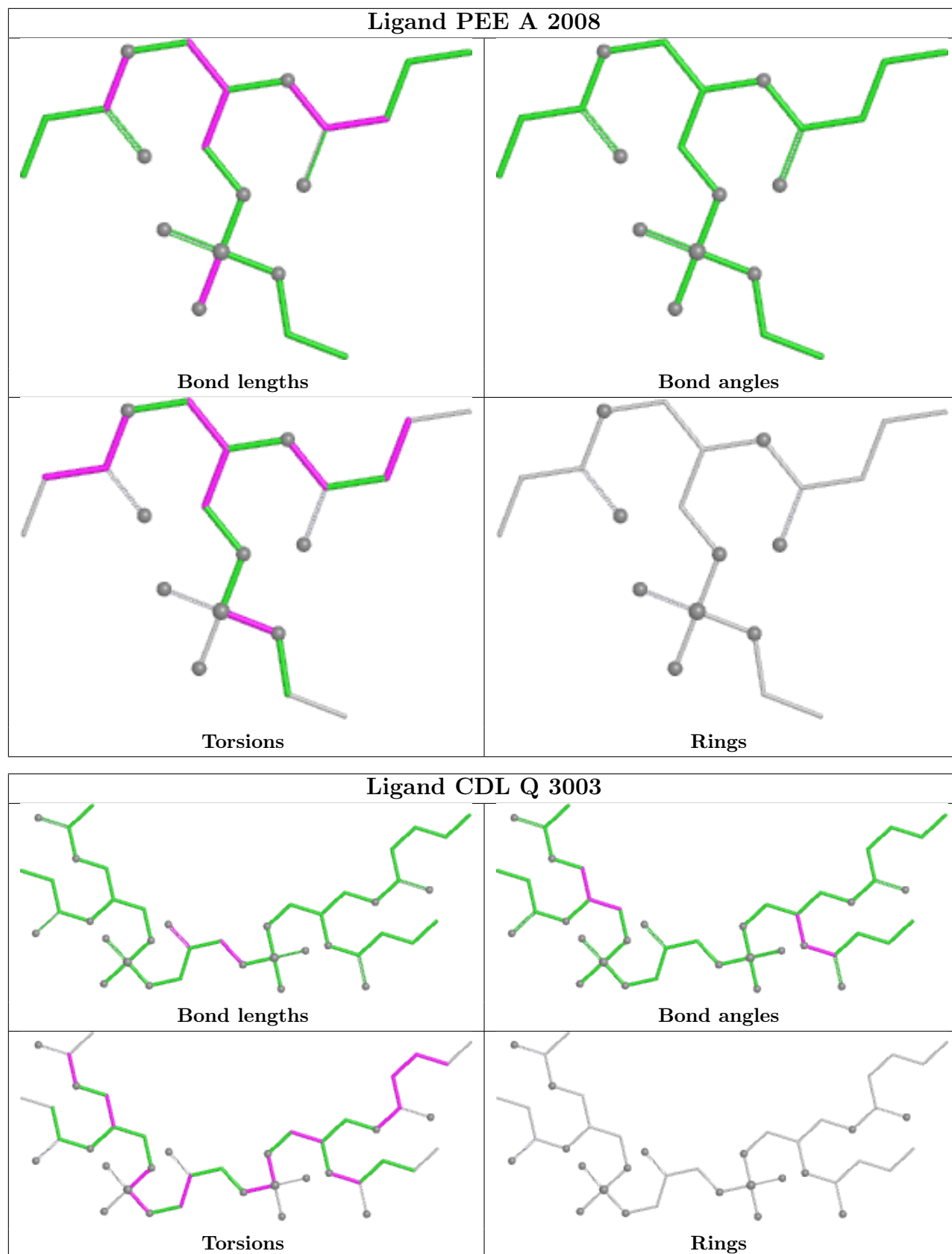
Ligand PEE R 3005

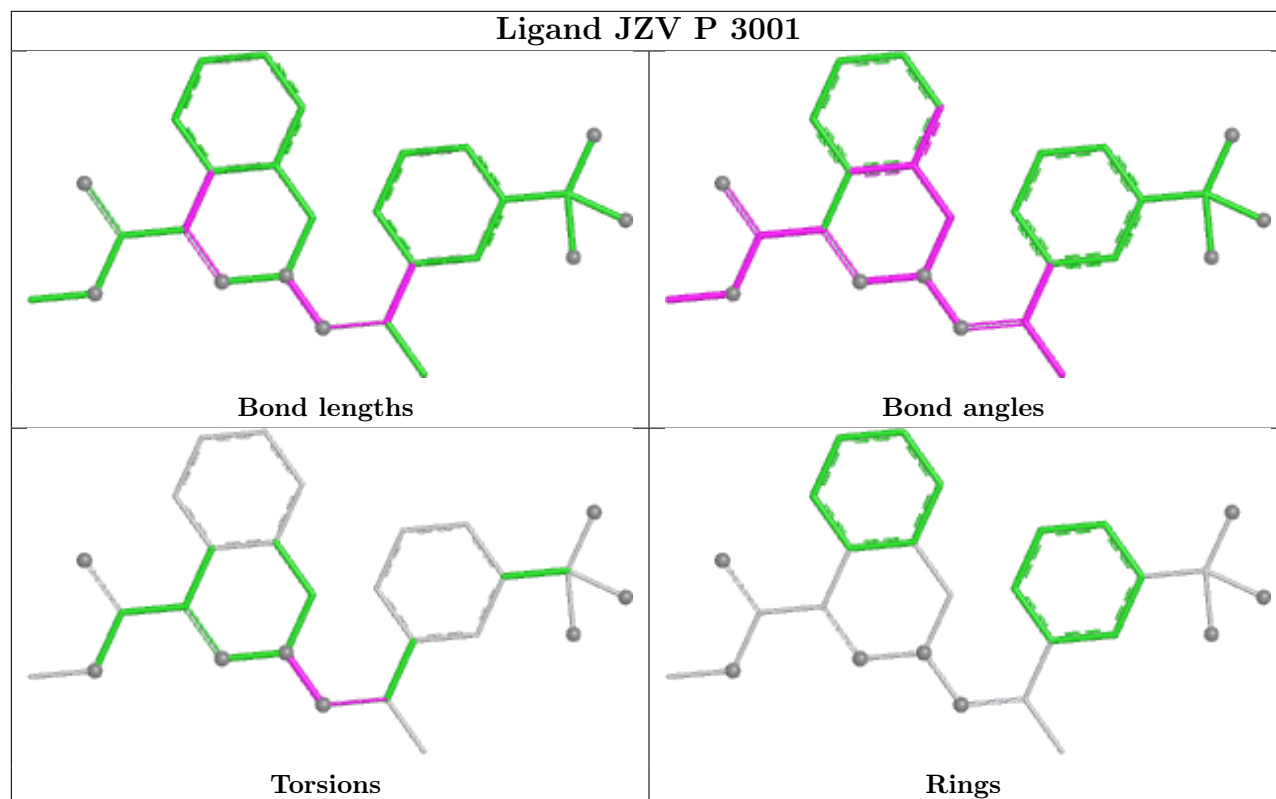


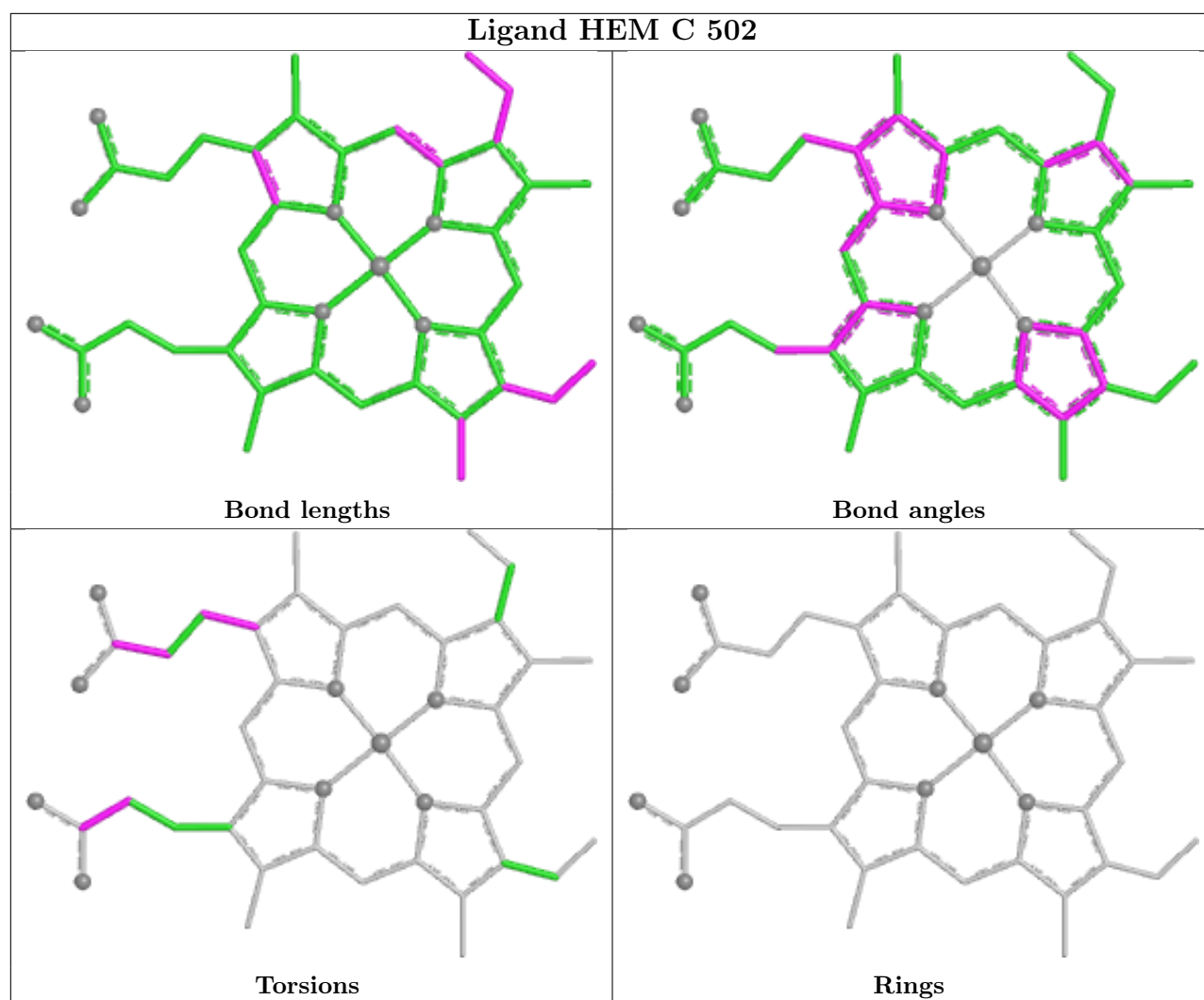












5.7 Other polymers [i](#)

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	444/446 (99%)	0.43	15 (3%)	48	46	32, 58, 86, 100	0
1	N	442/446 (99%)	0.89	45 (10%)	12	11	41, 68, 93, 100	0
2	B	420/441 (95%)	1.08	49 (11%)	9	7	48, 76, 111, 133	0
2	O	422/441 (95%)	1.01	53 (12%)	8	6	39, 74, 103, 122	0
3	C	380/380 (100%)	-0.11	17 (4%)	38	37	21, 39, 83, 123	0
3	P	379/380 (99%)	0.36	16 (4%)	40	39	29, 58, 88, 125	0
4	D	241/241 (100%)	-0.18	5 (2%)	63	61	29, 41, 81, 103	0
4	Q	241/241 (100%)	0.66	11 (4%)	37	36	46, 67, 97, 120	0
5	E	196/196 (100%)	2.14	107 (54%)	0	0	34, 125, 156, 163	0
5	R	196/196 (100%)	1.31	49 (25%)	2	1	40, 85, 129, 144	0
6	F	101/110 (91%)	-0.25	1 (0%)	79	79	26, 43, 61, 94	0
6	S	101/110 (91%)	0.66	5 (4%)	34	34	50, 65, 102, 121	0
7	G	80/81 (98%)	0.41	7 (8%)	15	15	33, 52, 97, 111	0
7	T	79/81 (97%)	1.33	19 (24%)	2	1	46, 78, 139, 149	0
8	H	70/77 (90%)	0.47	1 (1%)	73	73	34, 58, 80, 119	0
8	U	67/77 (87%)	1.82	23 (34%)	1	0	82, 108, 128, 130	0
9	I	31/47 (65%)	3.20	24 (77%)	0	0	72, 107, 133, 134	0
9	V	31/47 (65%)	3.23	22 (70%)	0	0	66, 107, 132, 136	0
10	J	61/61 (100%)	0.28	3 (4%)	35	34	43, 54, 95, 139	0
10	W	60/61 (98%)	0.67	2 (3%)	49	47	55, 68, 99, 107	0
All	All	4042/4160 (97%)	0.73	474 (11%)	9	7	21, 64, 121, 163	0

All (474) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	106	ILE	8.6
9	V	56	SER	8.2
5	E	120	PRO	7.8
2	B	226	ILE	7.5
1	N	444	ILE	7.3
5	E	180	LEU	7.3
9	V	63	ASP	7.2
9	I	47	ARG	6.9
9	I	61	ARG	6.7
5	E	124	LEU	6.7
5	E	143	GLY	6.6
5	E	167	ALA	6.1
7	G	2	ILE	6.0
5	E	147	ILE	6.0
7	T	2	ILE	5.9
8	H	9	GLU	5.9
5	E	98	VAL	5.9
5	E	168	SER	5.8
9	I	63	ASP	5.7
2	O	226	ILE	5.6
5	E	109	GLU	5.6
2	B	20	GLY	5.5
9	V	59	SER	5.5
9	V	61	ARG	5.5
5	E	112	VAL	5.5
5	E	121	GLN	5.4
9	I	49	LEU	5.4
5	E	177	PRO	5.3
5	E	157	TYR	5.3
5	E	187	PHE	5.2
5	E	117	LEU	5.2
1	A	444	ILE	5.2
5	E	97	PHE	5.1
5	E	173	LYS	5.0
2	O	21	ALA	4.9
9	V	50	LEU	4.9
5	E	169	GLY	4.9
9	I	51	CYS	4.8
3	C	4	ASN	4.8
9	I	77	ARG	4.8
5	E	182	VAL	4.8
9	V	49	LEU	4.7
5	E	135	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
5	E	142	LEU	4.7
5	E	178	TYR	4.7
3	P	2	ALA	4.7
5	R	124	LEU	4.6
5	E	79	SER	4.6
9	I	50	LEU	4.6
5	R	114	VAL	4.5
9	V	58	ARG	4.5
3	C	5	ILE	4.4
5	E	188	VAL	4.4
5	E	175	PRO	4.4
7	T	77	TYR	4.4
2	O	224	LEU	4.4
5	E	118	ARG	4.3
5	R	154	GLY	4.3
5	E	156	TYR	4.3
5	R	155	GLY	4.3
9	I	53	GLU	4.3
5	E	133	VAL	4.3
9	V	60	ALA	4.3
5	E	183	PRO	4.3
5	E	181	GLU	4.3
5	E	114	VAL	4.3
5	E	134	ILE	4.2
9	V	77	ARG	4.2
2	B	230	ALA	4.2
5	E	104	ALA	4.1
6	S	10	GLY	4.1
5	E	82	PRO	4.1
9	V	53	GLU	4.1
5	E	159	PRO	4.1
5	E	85	LYS	4.1
3	P	5	ILE	4.1
5	E	101	ARG	4.1
5	E	108	GLN	4.0
3	P	380	TYR	4.0
5	E	184	THR	4.0
7	G	81	GLN	4.0
5	E	185	TYR	4.0
4	Q	142	VAL	4.0
5	E	136	VAL	3.9
9	I	71	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	9	HIS	3.9
5	E	145	VAL	3.9
5	E	102	THR	3.9
9	V	52	ARG	3.9
10	J	61	ALA	3.9
1	A	432	LEU	3.8
9	I	64	LEU	3.8
1	N	38	GLY	3.8
5	E	87	VAL	3.8
5	R	196	GLY	3.8
5	E	150	SER	3.8
5	R	165	TYR	3.8
5	E	170	ARG	3.8
7	T	4	PHE	3.8
5	E	140	THR	3.7
5	R	147	ILE	3.7
5	E	110	ALA	3.7
5	E	194	VAL	3.7
5	E	153	PHE	3.7
5	E	138	VAL	3.7
2	O	371	SER	3.7
3	C	8	SER	3.7
2	B	224	LEU	3.6
2	O	296	TYR	3.6
1	N	190	PHE	3.6
5	E	192	LEU	3.6
3	C	7	LYS	3.6
5	E	128	LYS	3.6
4	D	1	GLY	3.6
5	E	111	GLU	3.6
9	V	55	MET	3.6
9	I	60	ALA	3.5
5	R	167	ALA	3.5
3	C	10	PRO	3.5
1	A	219	VAL	3.5
7	T	3	HIS	3.5
9	V	62	ARG	3.5
2	B	229	GLY	3.5
8	U	37	LEU	3.5
5	R	178	TYR	3.5
2	O	232	THR	3.5
5	E	107	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	3.5
3	C	156	TYR	3.4
5	E	171	ILE	3.4
5	E	193	VAL	3.4
5	E	122	HIS	3.4
5	R	106	ILE	3.4
5	R	104	ALA	3.4
5	E	149	ASN	3.4
1	N	185	TYR	3.4
5	R	133	VAL	3.4
5	E	174	GLY	3.3
8	U	61	PHE	3.3
9	I	76	VAL	3.3
3	C	380	TYR	3.3
1	N	432	LEU	3.3
9	I	52	ARG	3.3
1	A	10	ASN	3.3
5	E	172	ARG	3.3
5	R	156	TYR	3.3
9	I	70	LEU	3.3
2	O	383	GLY	3.3
4	Q	1	GLY	3.3
5	R	110	ALA	3.3
5	E	89	PHE	3.3
5	E	123	ASP	3.3
1	N	443	TRP	3.3
5	R	157	TYR	3.3
7	T	6	ASN	3.3
5	E	119	ASP	3.3
5	E	99	ARG	3.2
3	C	1	MET	3.2
1	A	443	TRP	3.2
2	B	30	PRO	3.2
7	T	74	PRO	3.2
2	B	208	GLY	3.2
9	I	56	SER	3.2
7	T	79	ASN	3.2
1	A	28	GLU	3.2
9	V	48	PRO	3.2
10	W	61	ALA	3.2
2	B	216	LEU	3.1
2	O	238	THR	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	162	GLY	3.1
5	R	115	SER	3.1
5	E	165	TYR	3.1
1	A	226	ASP	3.1
8	U	39	LEU	3.1
7	G	3	HIS	3.1
9	V	76	VAL	3.1
8	U	78	LYS	3.1
5	R	117	LEU	3.1
2	O	156	GLN	3.1
5	E	154	GLY	3.1
2	B	35	ILE	3.1
7	T	8	ALA	3.1
9	V	64	LEU	3.1
9	I	48	PRO	3.1
5	R	126	ARG	3.1
2	O	18	CYS	3.1
5	E	163	SER	3.1
5	E	96	LEU	3.0
3	P	4	ASN	3.0
2	B	292	THR	3.0
2	B	34	ILE	3.0
3	C	14	MET	3.0
4	Q	5	LEU	3.0
8	U	13	LEU	3.0
5	E	186	GLN	3.0
3	P	7	LYS	3.0
5	E	127	VAL	3.0
1	N	120	CYS	3.0
5	E	116	LYS	3.0
5	E	129	LYS	3.0
2	B	388	LEU	3.0
4	Q	241	LYS	3.0
5	R	116	LYS	3.0
1	N	223	TYR	3.0
7	T	24	ARG	3.0
5	R	148	ALA	3.0
2	O	405	VAL	3.0
5	E	100	HIS	2.9
5	R	128	LYS	2.9
8	U	68	CYS	2.9
5	E	152	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
5	R	171	ILE	2.9
2	O	307	PHE	2.9
3	C	3	PRO	2.9
5	E	84	GLY	2.9
9	V	57	GLY	2.9
2	B	24	LEU	2.9
4	Q	3	LEU	2.9
8	U	36	ARG	2.9
5	E	88	ALA	2.9
8	U	74	PHE	2.9
2	O	110	GLU	2.9
5	E	103	GLN	2.9
1	N	179	ARG	2.9
3	P	6	ARG	2.9
3	C	16	ASN	2.9
5	E	179	ASN	2.9
2	B	232	THR	2.9
1	N	129	LYS	2.9
8	U	76	LYS	2.9
2	O	291	VAL	2.9
5	R	105	GLU	2.8
9	V	71	ASN	2.8
5	E	196	GLY	2.8
2	B	21	ALA	2.8
1	N	39	VAL	2.8
2	B	312	PHE	2.8
5	E	146	PRO	2.8
1	A	31	SER	2.8
1	N	104	LYS	2.8
5	R	85	LYS	2.8
5	E	190	ASP	2.8
2	O	386	ALA	2.8
2	B	223	PHE	2.8
5	R	101	ARG	2.8
8	U	26	GLN	2.8
2	O	384	SER	2.8
2	O	295	LEU	2.8
2	O	344	LEU	2.8
3	C	11	LEU	2.8
2	O	353	THR	2.8
2	B	41	PHE	2.8
7	T	78	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	6	ARG	2.8
5	E	115	SER	2.8
2	B	33	LEU	2.8
7	T	76	ASP	2.8
7	T	80	ASP	2.8
10	W	45	HIS	2.8
2	O	335	GLU	2.8
9	I	72	ALA	2.8
3	P	3	PRO	2.7
8	U	54	CYS	2.7
9	I	59	SER	2.7
1	N	160	GLY	2.7
1	N	380	GLY	2.7
3	P	14	MET	2.7
6	S	13	MET	2.7
7	G	80	ASP	2.7
1	A	86	PHE	2.7
5	R	153	PHE	2.7
2	O	19	PRO	2.7
8	U	30	CYS	2.7
4	Q	164	ILE	2.7
9	V	54	SER	2.7
1	A	2	ALA	2.7
1	N	26	ALA	2.7
5	E	176	ALA	2.7
5	R	118	ARG	2.7
1	N	122	LEU	2.7
5	E	191	ASP	2.7
7	G	4	PHE	2.7
5	E	94	LYS	2.7
2	O	26	ILE	2.7
7	T	5	GLY	2.7
1	N	34	THR	2.7
3	P	156	TYR	2.6
10	J	63	GLU	2.6
2	O	230	ALA	2.6
4	Q	143	VAL	2.6
5	R	112	VAL	2.6
9	V	72	ALA	2.6
2	O	249	GLY	2.6
5	R	187	PHE	2.6
7	T	75	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	250	HIS	2.6
2	B	390	GLY	2.6
2	B	197	ASN	2.6
5	R	82	PRO	2.6
5	R	175	PRO	2.6
2	O	209	ILE	2.6
5	R	172	ARG	2.6
5	R	84	GLY	2.6
1	N	25	VAL	2.6
1	N	219	VAL	2.6
2	B	119	VAL	2.6
2	O	352	VAL	2.6
3	P	151	PHE	2.6
5	E	132	TRP	2.5
3	P	11	LEU	2.5
2	O	227	ARG	2.5
9	V	47	ARG	2.5
2	O	250	HIS	2.5
5	E	141	HIS	2.5
9	I	57	GLY	2.5
6	S	81	VAL	2.5
2	O	37	SER	2.5
2	B	36	ALA	2.5
8	U	24	CYS	2.5
2	O	289	SER	2.5
5	E	126	ARG	2.5
9	I	58	ARG	2.5
2	O	229	GLY	2.5
2	B	371	SER	2.5
2	O	430	LEU	2.5
4	D	2	GLU	2.5
1	N	22	GLY	2.5
8	U	16	PRO	2.5
2	O	279	LEU	2.4
1	N	217	SER	2.4
2	B	228	SER	2.4
5	R	164	HIS	2.4
5	R	190	ASP	2.4
7	G	32	ASP	2.4
2	O	20	GLY	2.4
1	N	69	LYS	2.4
5	E	77	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
5	R	89	PHE	2.4
3	C	345	GLU	2.4
5	E	137	GLY	2.4
5	E	148	ALA	2.4
5	R	134	ILE	2.4
2	O	193	HIS	2.4
1	N	72	CYS	2.4
5	E	105	GLU	2.4
7	G	5	GLY	2.4
5	R	103	GLN	2.4
1	N	386	TYR	2.4
2	B	281	ALA	2.4
9	I	62	ARG	2.4
1	N	127	ILE	2.4
2	B	225	ASN	2.4
9	I	55	MET	2.4
2	B	32	GLY	2.4
2	O	223	PHE	2.4
1	N	392	LEU	2.3
2	B	29	LEU	2.3
5	R	192	LEU	2.3
7	T	7	LEU	2.3
7	T	63	THR	2.3
5	E	83	GLU	2.3
1	N	187	ASP	2.3
5	R	169	GLY	2.3
1	N	37	VAL	2.3
1	N	117	VAL	2.3
1	N	64	PHE	2.3
2	O	312	PHE	2.3
3	P	15	ILE	2.3
3	P	224	TYR	2.3
4	Q	57	THR	2.3
5	E	161	HIS	2.3
2	B	317	SER	2.3
5	E	151	GLY	2.3
2	O	388	LEU	2.3
5	E	164	HIS	2.3
1	N	195	MET	2.3
2	B	206	LEU	2.3
1	N	121	ALA	2.3
2	B	26	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	386	ALA	2.3
2	O	36	ALA	2.3
6	S	21	TYR	2.3
5	R	31	ASP	2.3
8	U	69	VAL	2.3
2	B	220	ALA	2.2
8	U	33	ALA	2.2
6	S	84	GLU	2.2
4	D	172	ASP	2.2
7	T	43	SER	2.2
1	A	392	LEU	2.2
1	N	170	THR	2.2
2	O	368	TYR	2.2
5	R	86	ASN	2.2
1	N	218	GLY	2.2
2	O	308	ASP	2.2
8	U	29	LYS	2.2
1	A	203	ILE	2.2
2	O	402	ILE	2.2
2	B	171	ALA	2.2
1	N	111	GLU	2.2
2	O	306	PRO	2.2
1	N	23	LEU	2.2
2	B	344	LEU	2.2
4	D	241	LYS	2.2
8	U	73	LEU	2.2
1	A	366	VAL	2.2
5	R	111	GLU	2.2
2	B	304	THR	2.2
4	Q	144	ARG	2.2
4	Q	238	ARG	2.2
5	E	86	ASN	2.2
6	F	110	LYS	2.2
2	B	124	LEU	2.2
7	T	32	ASP	2.2
5	R	150	SER	2.2
2	B	402	ILE	2.2
1	N	216	PHE	2.2
2	O	281	ALA	2.1
4	D	76	GLU	2.1
8	U	34	ARG	2.1
9	V	51	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	155	PRO	2.1
2	O	104	LYS	2.1
4	Q	31	GLN	2.1
1	N	182	LEU	2.1
2	B	38	LEU	2.1
5	E	78	LEU	2.1
1	A	228	VAL	2.1
1	N	86	PHE	2.1
3	P	244	ALA	2.1
1	N	28	GLU	2.1
5	R	16	GLU	2.1
7	T	38	TRP	2.1
2	O	292	THR	2.1
5	R	108	GLN	2.1
2	O	112	LEU	2.1
8	U	77	LEU	2.1
3	P	371	GLY	2.1
5	R	81	ILE	2.1
8	U	63	HIS	2.1
8	U	31	VAL	2.1
2	B	289	SER	2.1
9	I	75	SER	2.1
2	O	394	ALA	2.1
10	J	64	GLU	2.1
1	N	119	ASN	2.1
2	B	57	TYR	2.1
5	E	76	ILE	2.1
3	C	151	PHE	2.1
2	B	396	SER	2.1
2	O	102	ARG	2.1
5	R	102	THR	2.1
2	B	306	PRO	2.1
1	N	189	HIS	2.1
5	E	93	GLY	2.1
2	B	211	VAL	2.1
2	O	398	VAL	2.1
1	A	433	ASP	2.0
1	N	282	ARG	2.0
5	R	113	ASP	2.0
1	N	81	SER	2.0
5	E	90	LYS	2.0
5	E	95	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	405	VAL	2.0
2	O	264	VAL	2.0
5	E	195	VAL	2.0
2	O	311	ALA	2.0
2	B	393	THR	2.0
1	N	42	GLY	2.0
2	O	35	ILE	2.0
3	P	154	ILE	2.0
9	I	68	ILE	2.0
2	B	291	VAL	2.0
8	U	43	ARG	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
18	BOG	Q	3091	13/20	0.29	0.35	183,186,187,187	0
11	PEE	A	2008	21/51	0.38	0.33	129,133,134,135	0
18	BOG	P	2010	12/20	0.54	0.29	135,137,138,138	0
18	BOG	D	2091	13/20	0.59	0.42	200,201,201,201	0
15	CDL	Q	3003	42/100	0.74	0.28	109,121,139,139	0
11	PEE	N	3008	5/51	0.75	0.16	110,111,112,112	0
11	PEE	P	3007	49/51	0.76	0.27	53,79,93,94	0
15	CDL	D	2003	42/100	0.78	0.24	82,92,106,108	0
15	CDL	P	3004	40/100	0.79	0.20	96,102,111,111	0
11	PEE	C	2007	49/51	0.80	0.24	43,58,70,73	0
11	PEE	R	3005	50/51	0.80	0.29	80,98,108,110	0
11	PEE	E	2005	50/51	0.84	0.24	68,89,95,97	0

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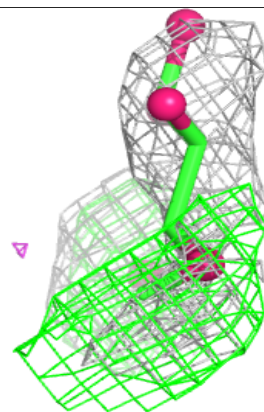
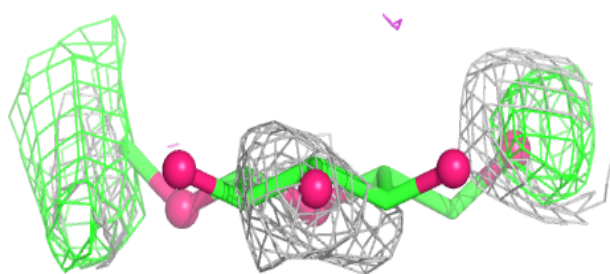
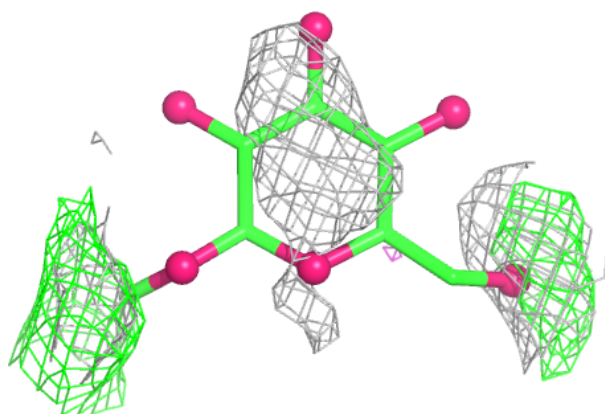
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	UQ	P	3002	19/63	0.84	0.36	119,124,125,126	0
16	GOL	P	3011	6/6	0.86	0.25	73,75,76,77	0
14	UQ	C	2002	19/63	0.86	0.27	88,90,90,91	0
13	JZV	P	3001	29/29	0.86	0.20	59,66,104,106	0
15	CDL	C	2004	40/100	0.86	0.17	66,80,91,93	0
18	BOG	Q	3009	20/20	0.89	0.15	62,75,77,78	0
19	FES	E	501	4/4	0.89	0.10	144,144,145,145	0
18	BOG	D	2009	20/20	0.90	0.12	53,59,62,64	0
16	GOL	C	2011	6/6	0.91	0.21	67,70,72,72	0
13	JZV	C	2001	29/29	0.91	0.14	38,46,86,87	0
17	HEC	Q	501	43/43	0.97	0.10	52,56,64,65	0
17	HEC	D	501	43/43	0.98	0.06	21,29,34,35	0
12	HEM	P	501	43/43	0.98	0.08	33,40,48,54	0
12	HEM	P	502	43/43	0.98	0.08	29,41,54,59	0
12	HEM	C	501	43/43	0.98	0.07	23,30,37,42	0
19	FES	R	501	4/4	0.98	0.05	74,76,77,78	0
12	HEM	C	502	43/43	0.99	0.07	24,27,35,41	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.

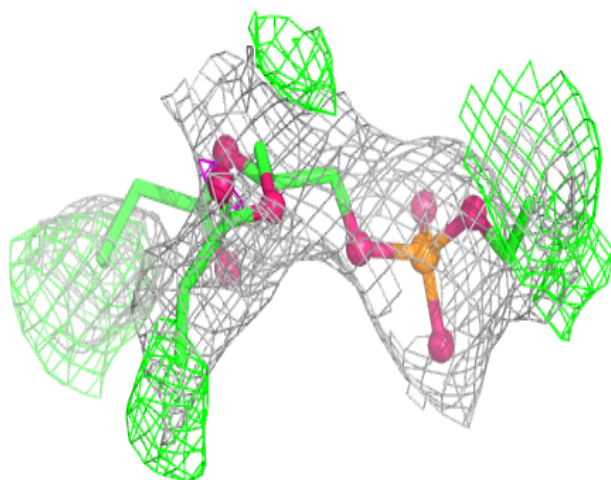
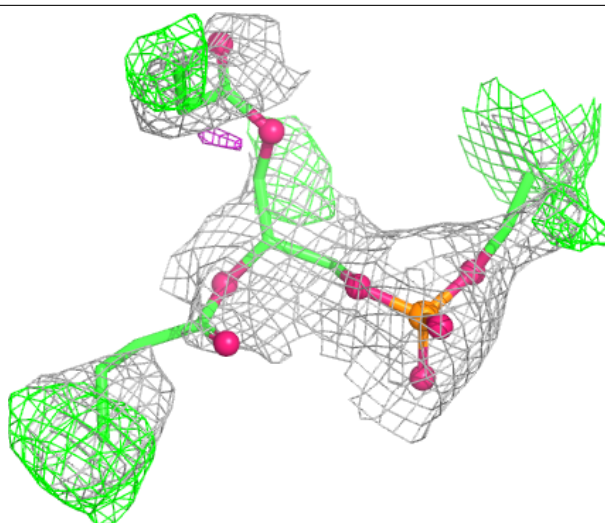
Electron density around BOG Q 3091:

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



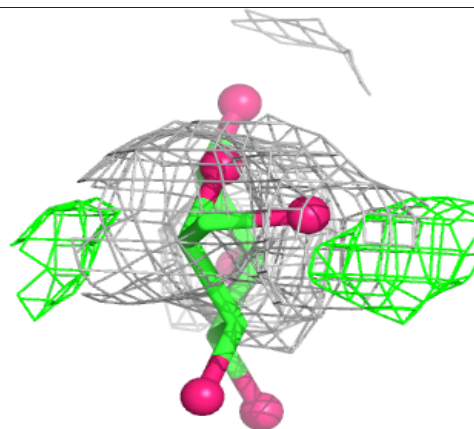
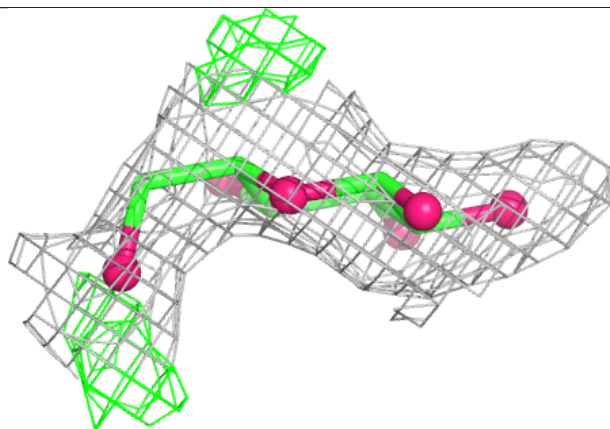
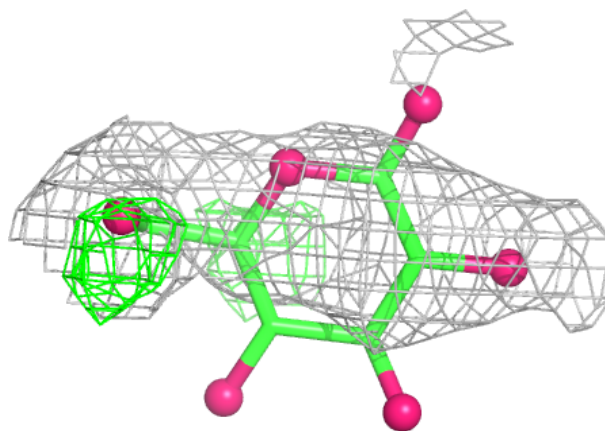
Electron density around PEE A 2008:

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



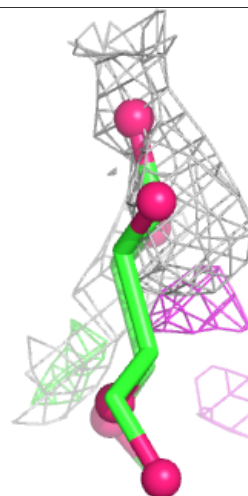
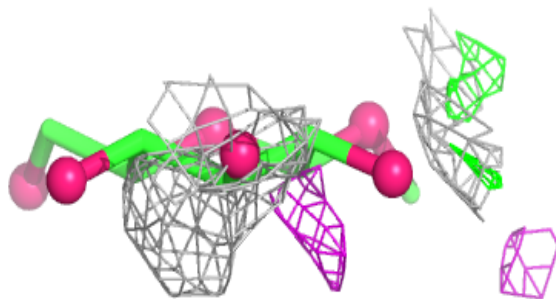
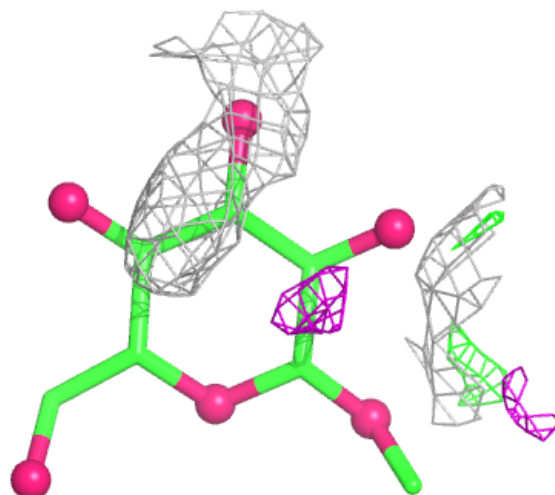
Electron density around BOG P 2010:

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



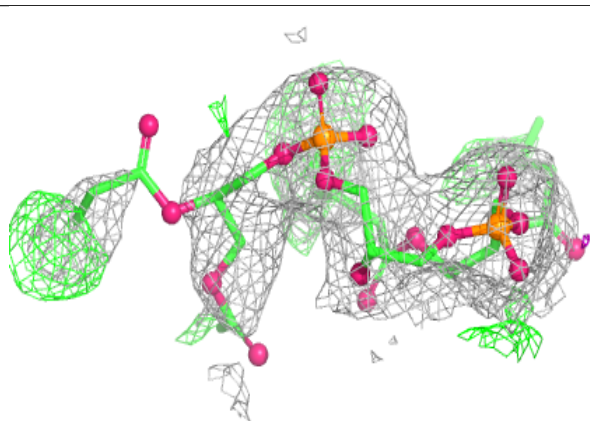
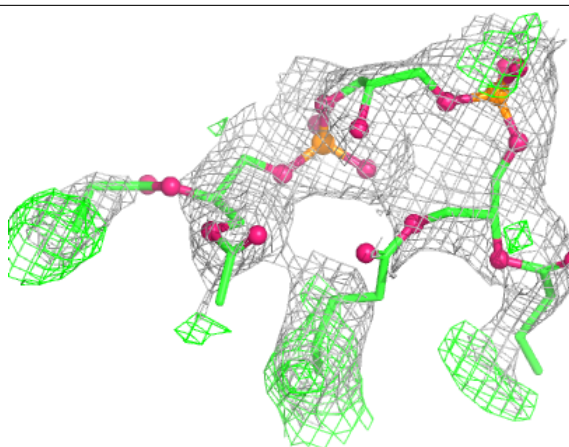
Electron density around BOG D 2091:

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



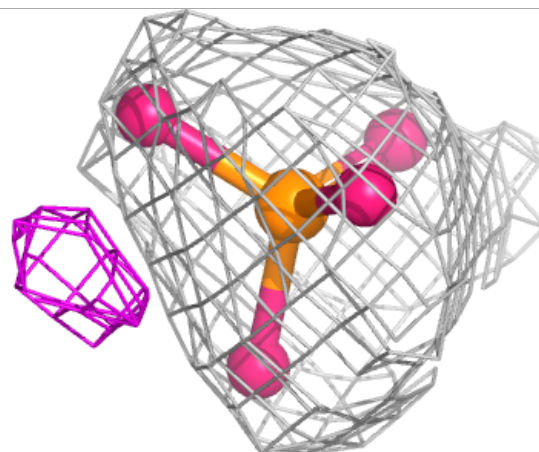
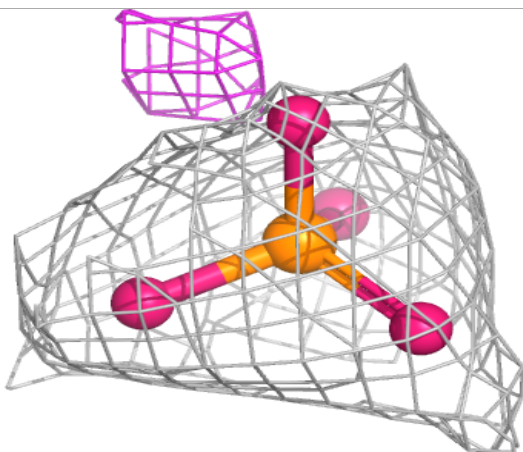
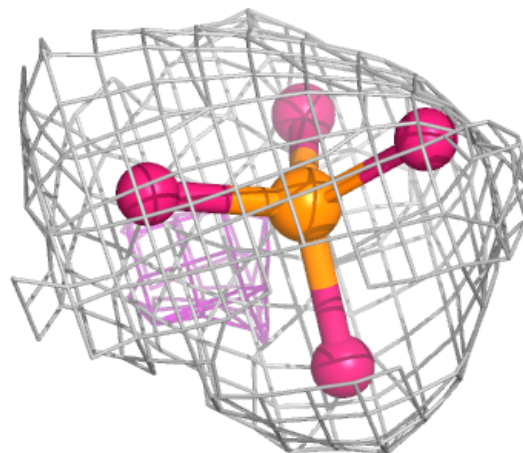
Electron density around CDL Q 3003:

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



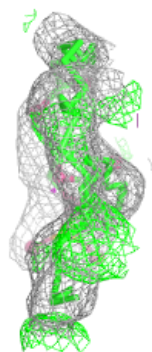
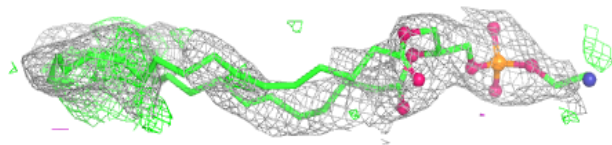
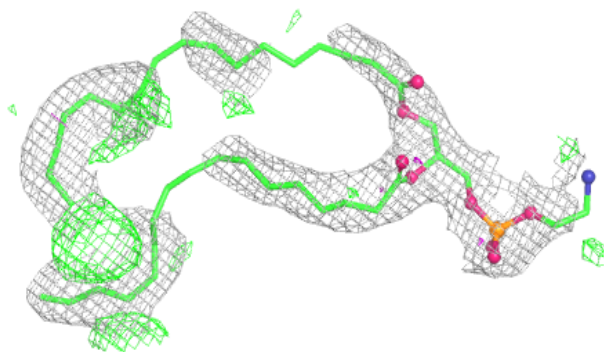
Electron density around PEE N 3008:

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



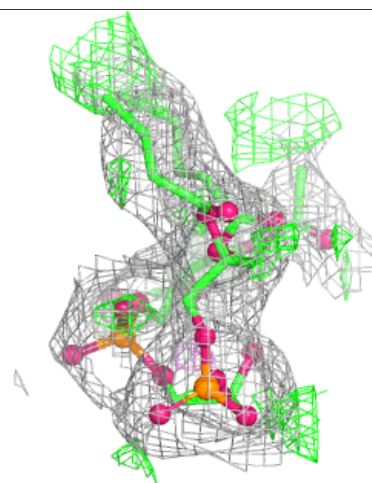
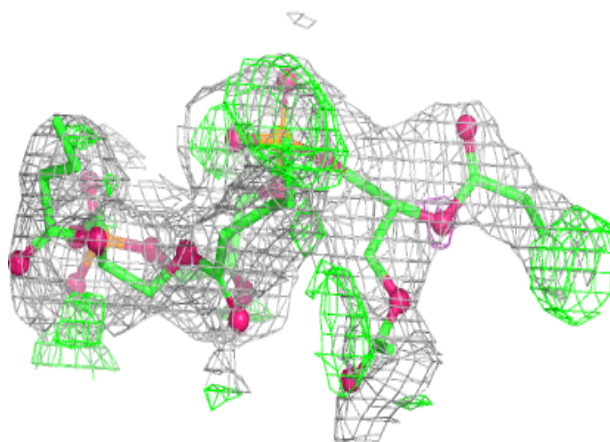
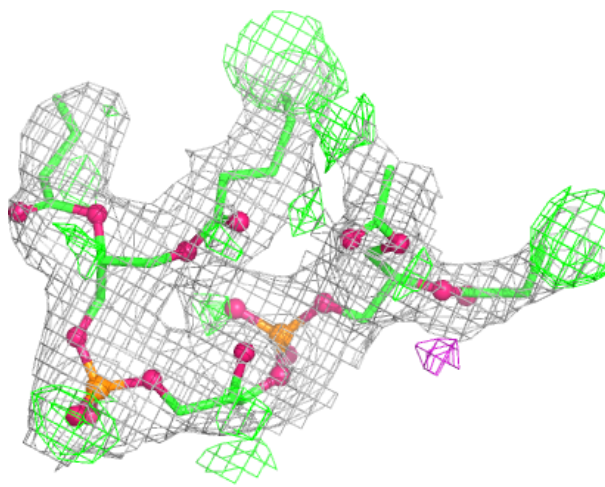
Electron density around PEE P 3007:

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



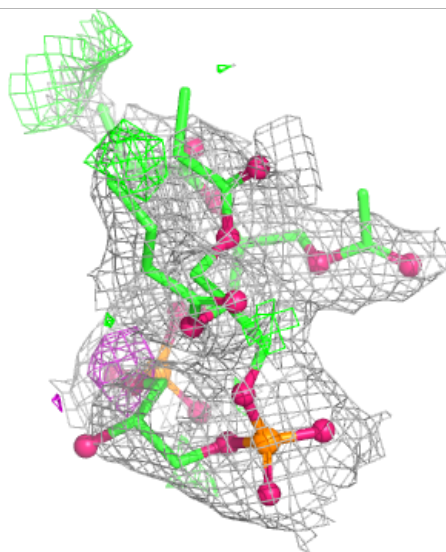
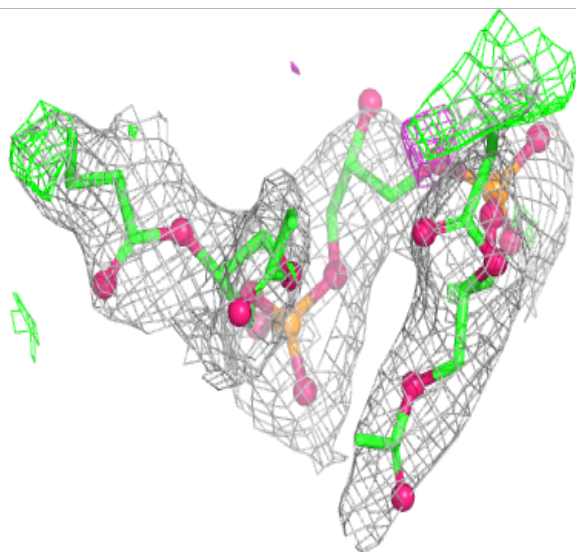
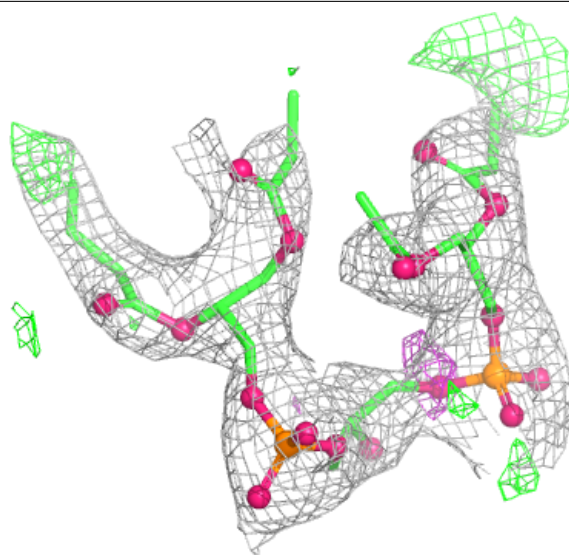
Electron density around CDL D 2003:

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



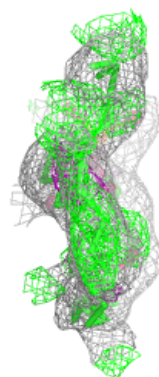
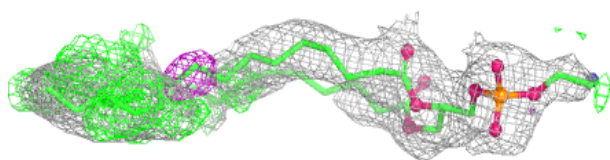
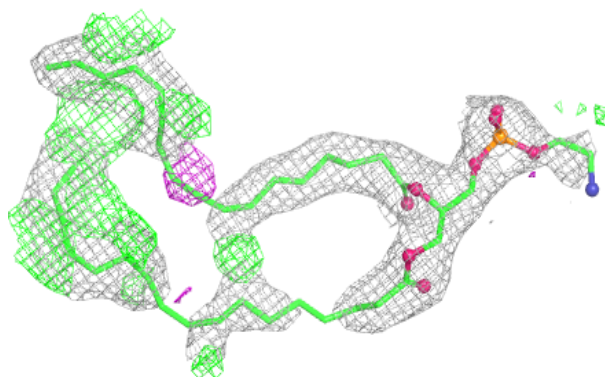
Electron density around CDL P 3004:

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

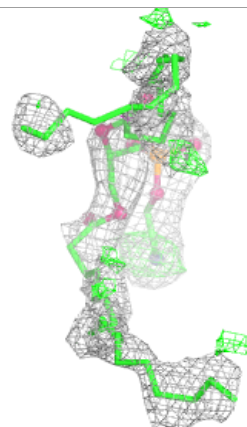
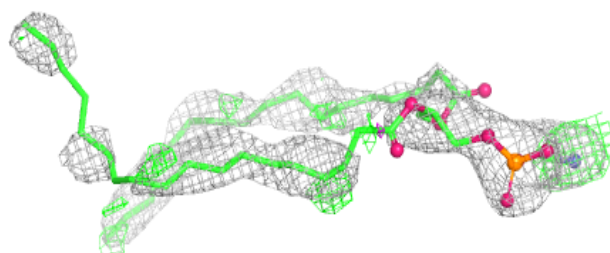
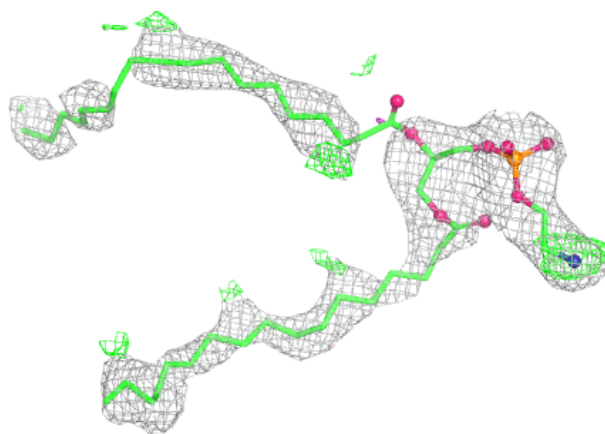


Electron density around PEE C 2007:

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and green (positive)

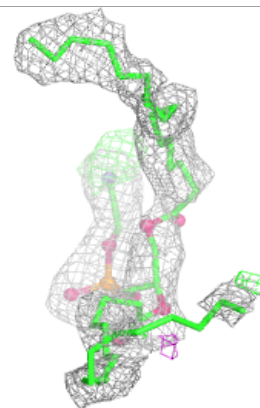
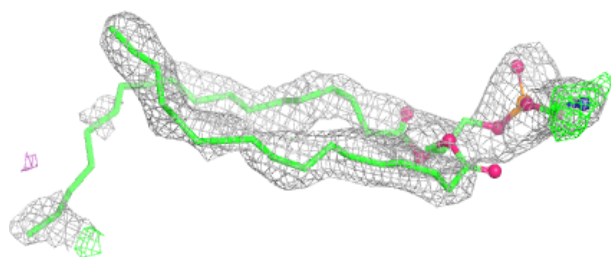
**Electron density around PEE R 3005:**

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

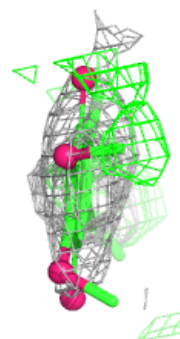
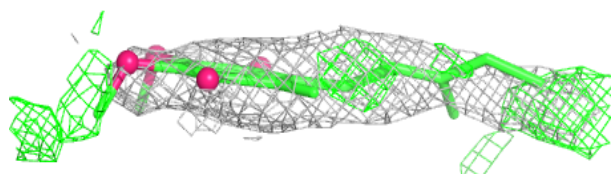
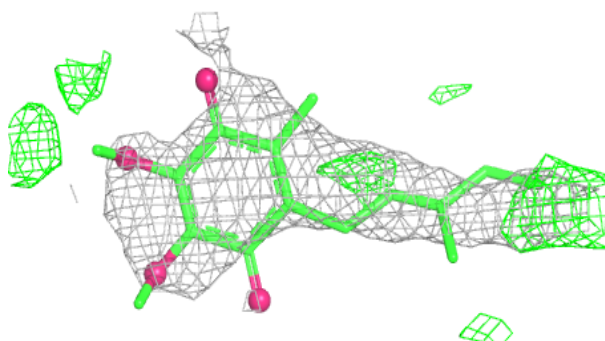


Electron density around PEE E 2005:

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

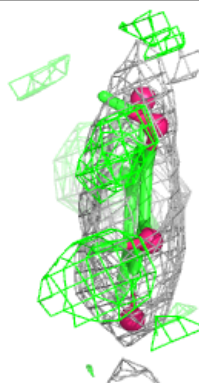
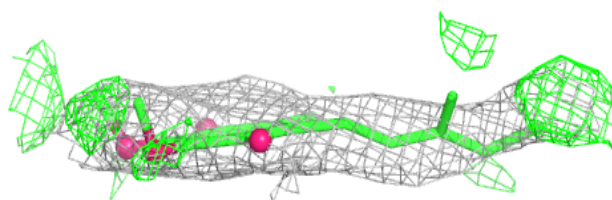
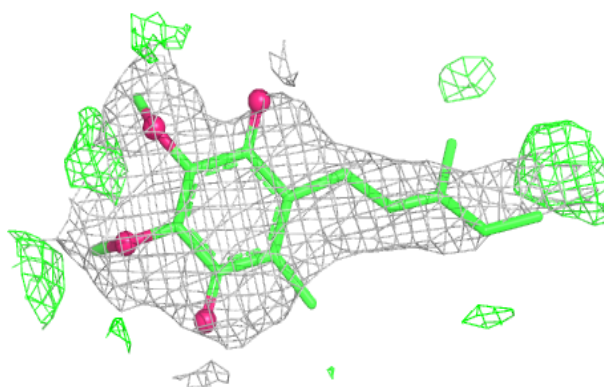
**Electron density around UQ P 3002:**

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

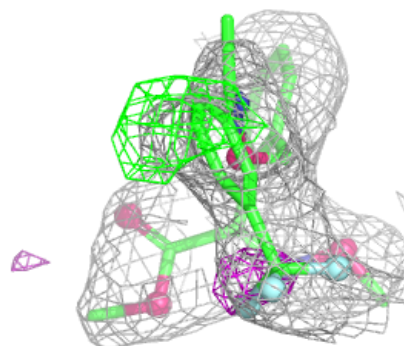
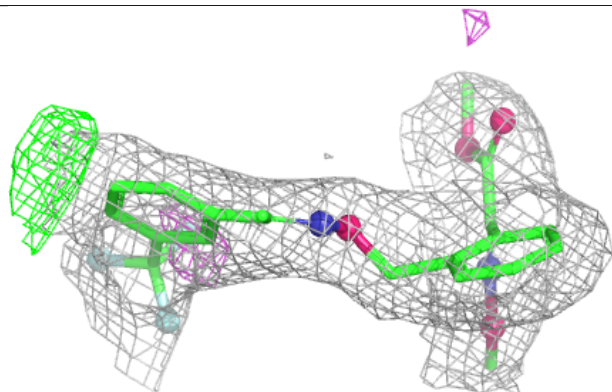
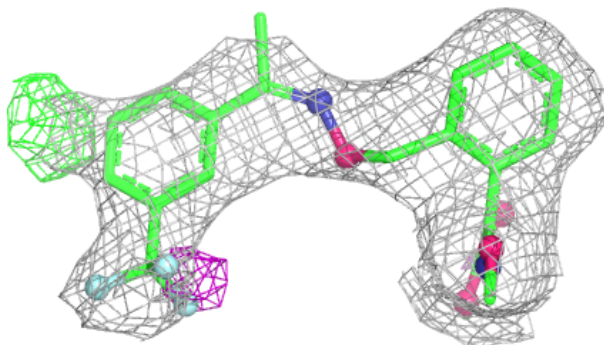


Electron density around UQ C 2002:

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

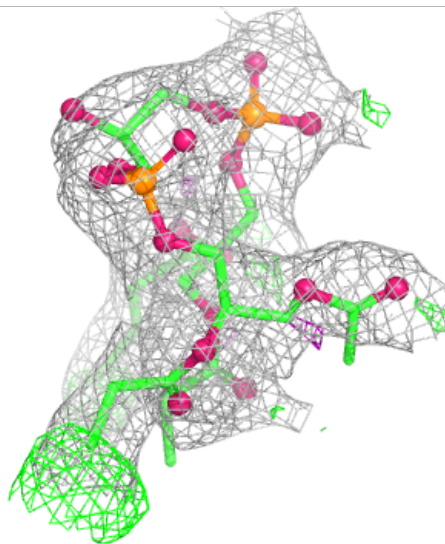
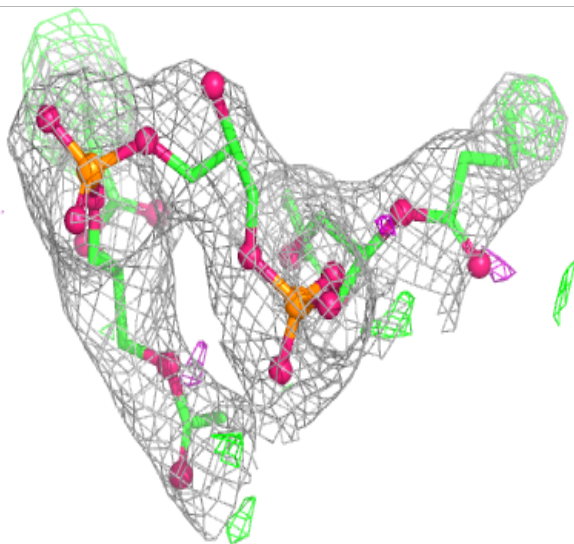
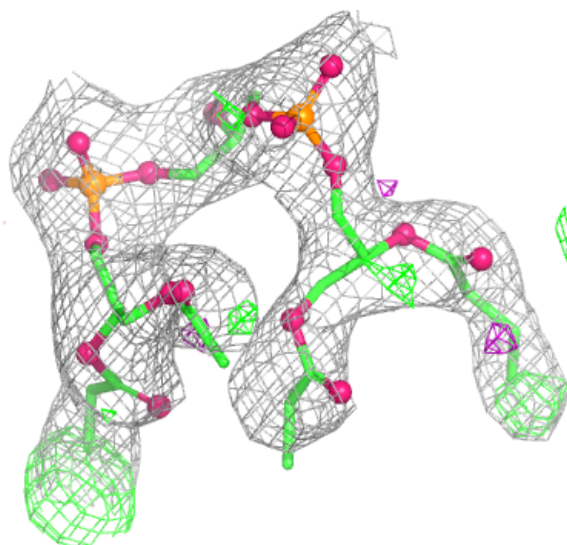
**Electron density around JZV P 3001:**

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



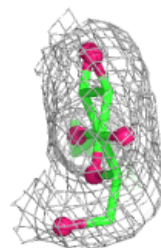
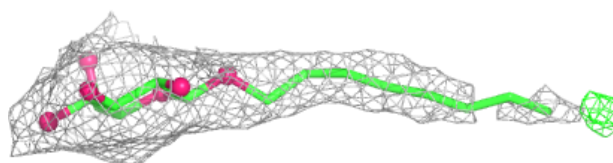
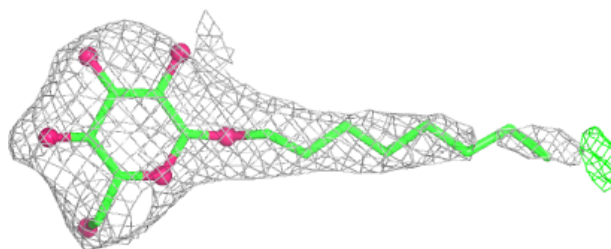
Electron density around CDL C 2004:

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

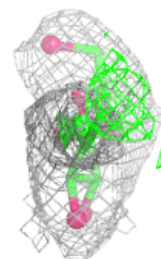
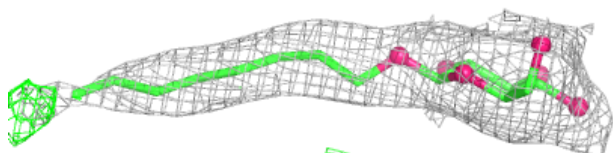


Electron density around BOG Q 3009:

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

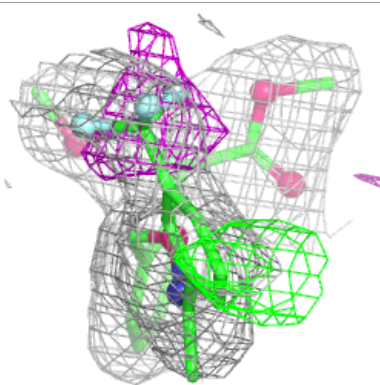
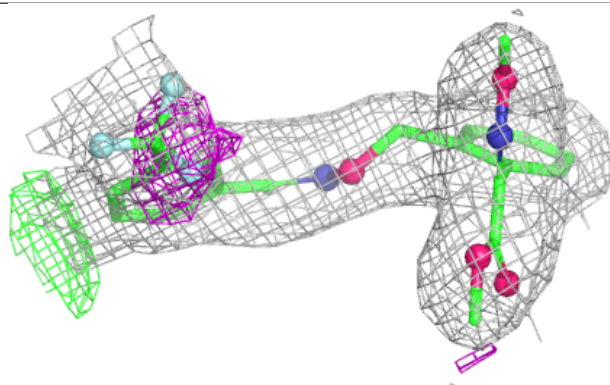
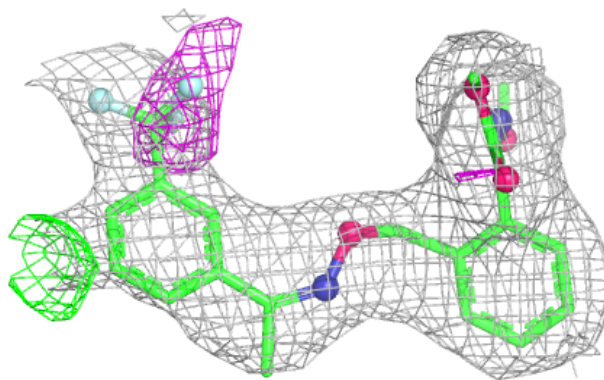
**Electron density around BOG D 2009:**

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and green (positive)

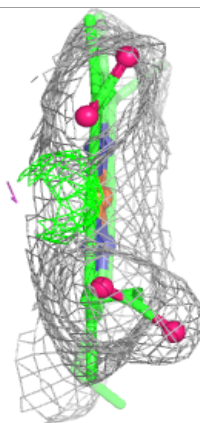
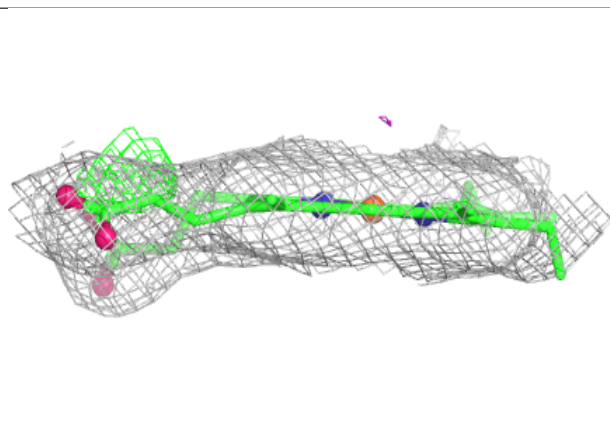
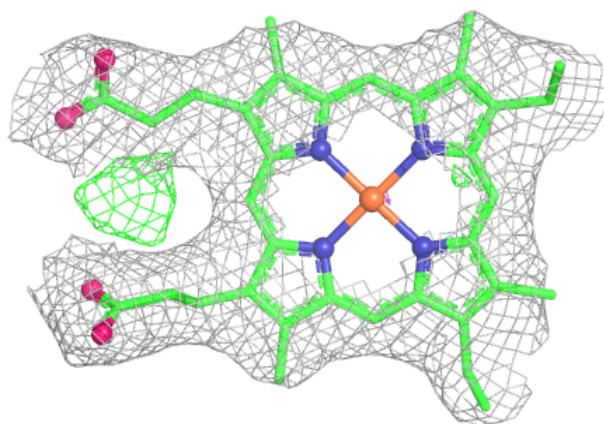


Electron density around JZV C 2001:

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

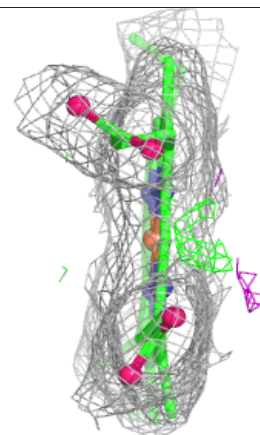
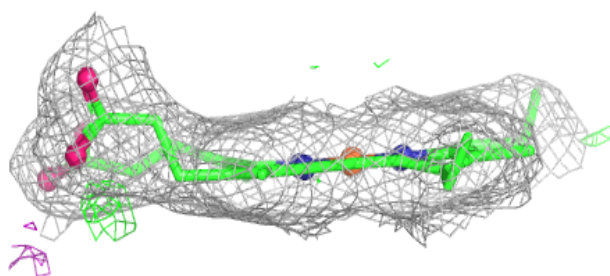
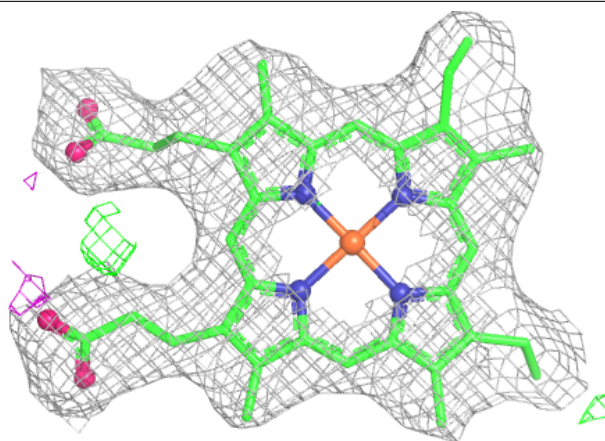
**Electron density around HEC Q 501:**

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



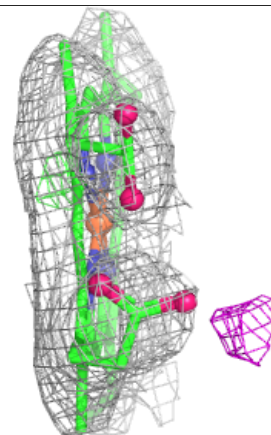
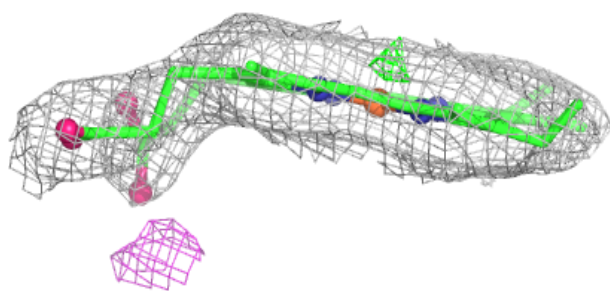
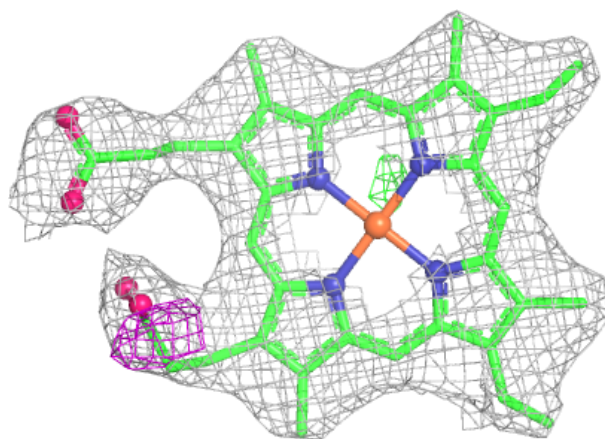
Electron density around HEC D 501:

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



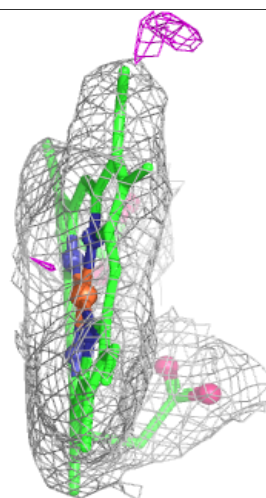
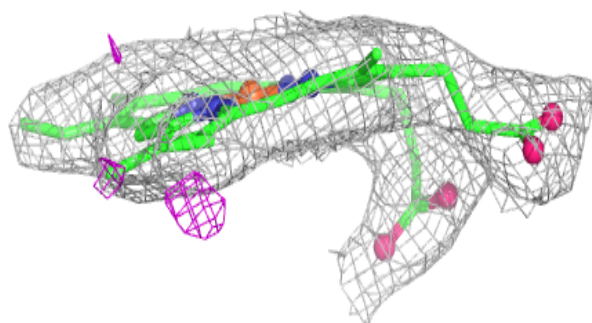
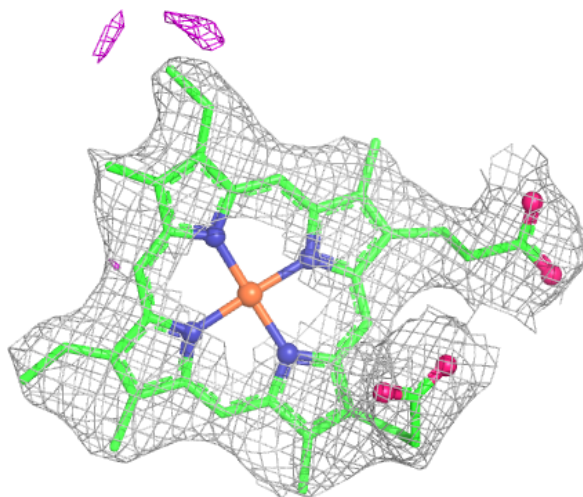
Electron density around HEM P 501:

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



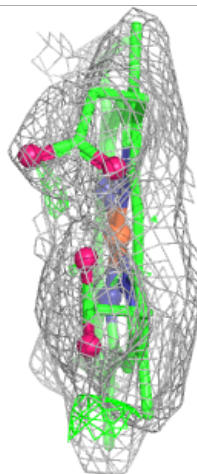
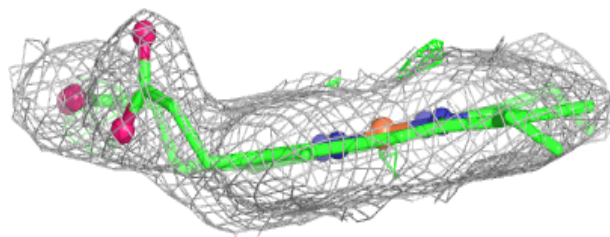
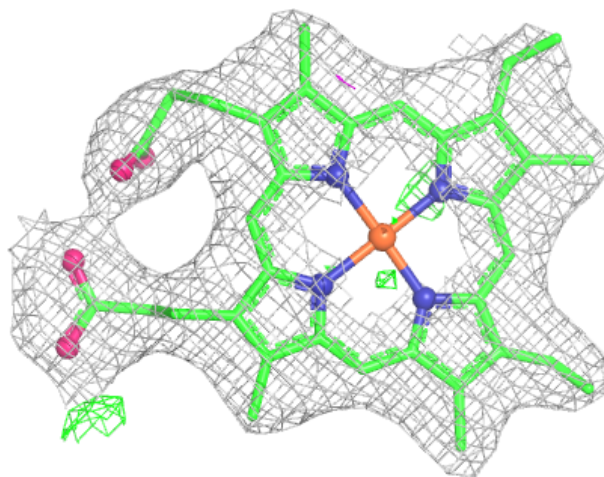
Electron density around HEM P 502:

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



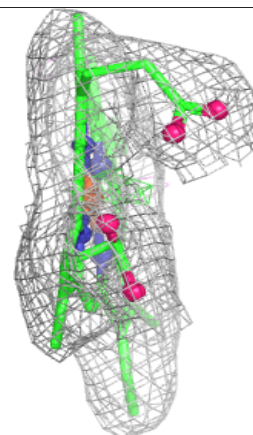
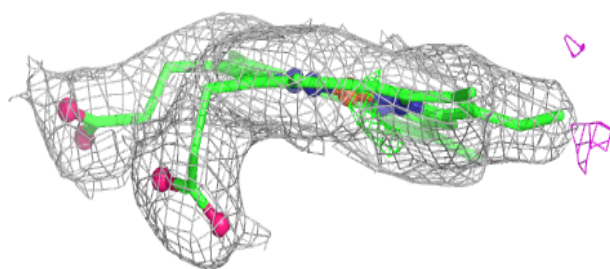
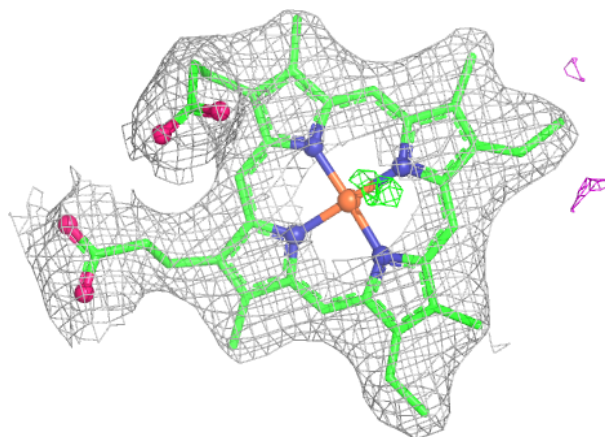
Electron density around HEM C 501:

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



Electron density around HEM C 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.