



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:20 PM EDT

PDB ID : 3L75 / pdb_00003l75
Title : Cytochrome BC1 complex from chicken with fenamidone bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-28
Resolution : 2.79 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:

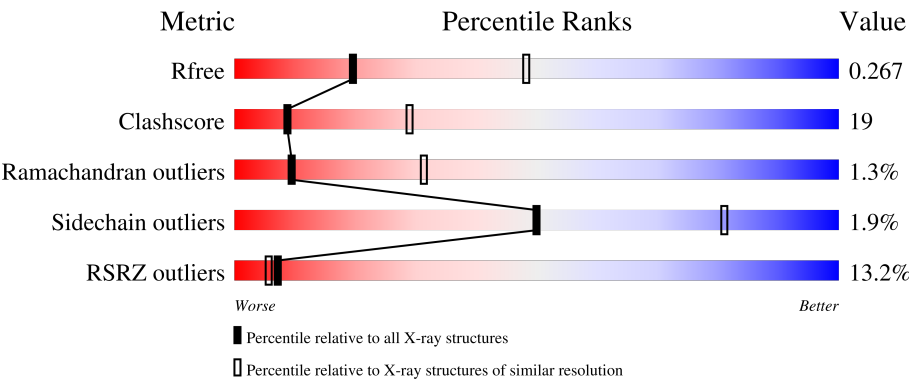
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	-	-
12	UNL	P	3048	-	-	-	X
16	AZI	C	2011	-	X	-	-
16	AZI	P	3011	-	X	-	-
17	BOG	D	2091	-	-	-	X
18	HEC	D	501	X	-	-	-
18	HEC	Q	501	X	-	-	-
20	FES	R	501	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			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 5, RIESKE IRONSULFUR PROTEIN, 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
			1512	952	262	292	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	78	Total	C	N	O	0	0	0
			654	428	116	110			

- 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			

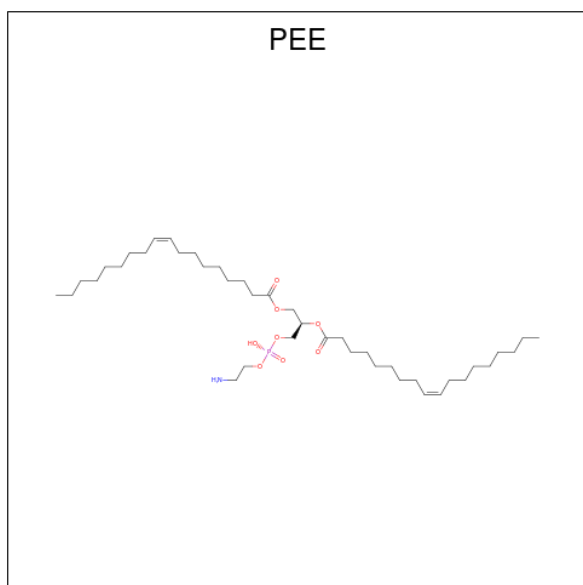
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			288	172	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

- Molecule 10 is a protein called 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
			50	40	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

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

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

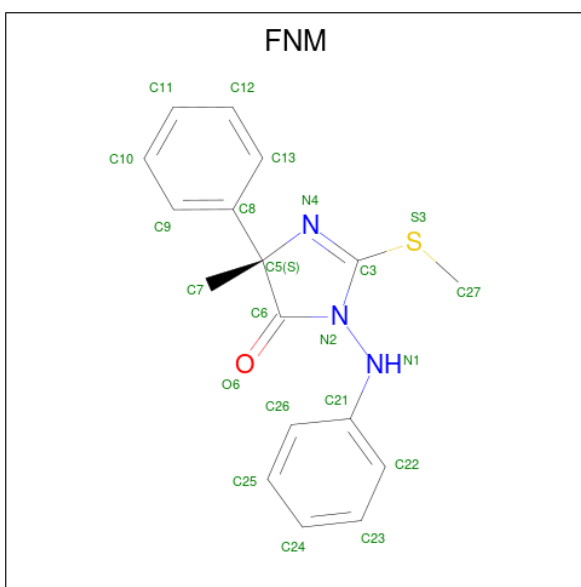
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	3	Total O 5 5	0	0
12	D	1	Total O 2 2	0	0
12	P	5	Total O 7 7	0	0
12	R	1	Total O 1 1	0	0

- # HEM

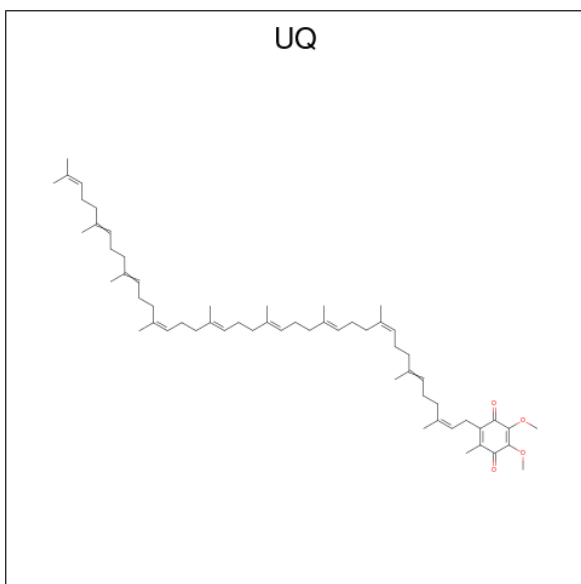
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	S	0	0
			22	17	3	1	1		
14	P	1	Total	C	N	O	S	0	0
			22	17	3	1	1		

- Molecule 15 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



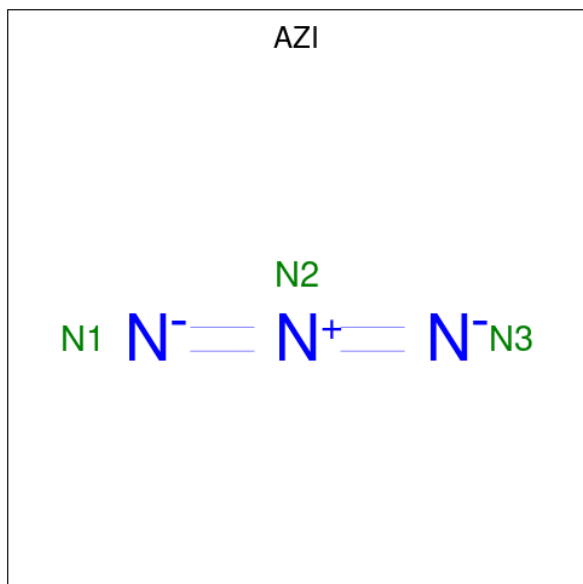
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			19	15	4		

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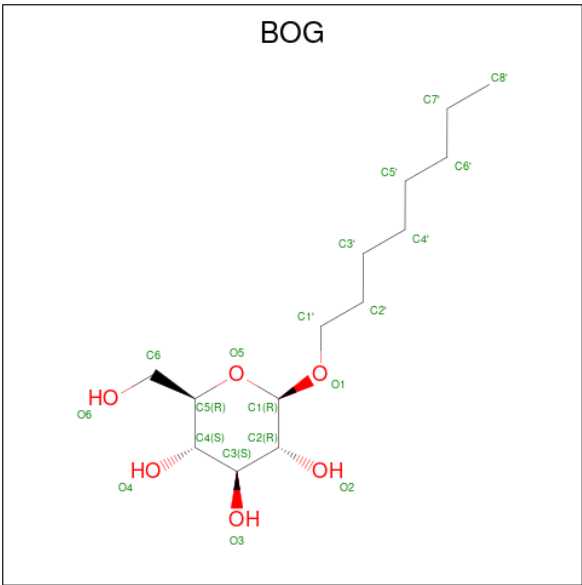
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 16 is AZIDE ION (CCD ID: AZI) (formula: N_3).



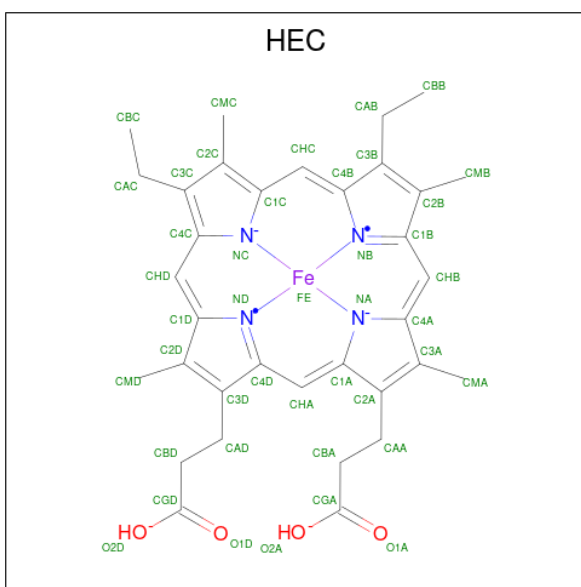
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	N	0	0
			3	3		
16	P	1	Total	N	0	0
			3	3		

- Molecule 17 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



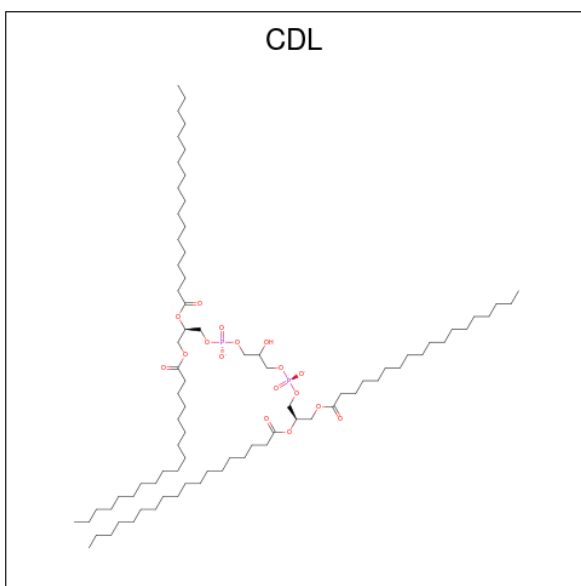
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			12	10	2		
17	D	1	Total	C	O	0	0
			20	14	6		
17	D	1	Total	C	O	0	0
			20	14	6		
17	P	1	Total	C	O	0	0
			19	13	6		
17	Q	1	Total	C	O	0	0
			20	14	6		
17	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



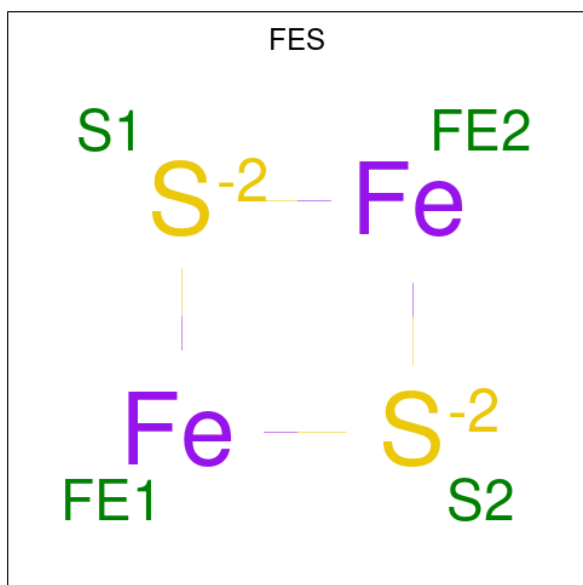
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total 42	C 23	O 17	P 2	0	0
19	G	1	Total 40	C 21	O 17	P 2	0	0

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

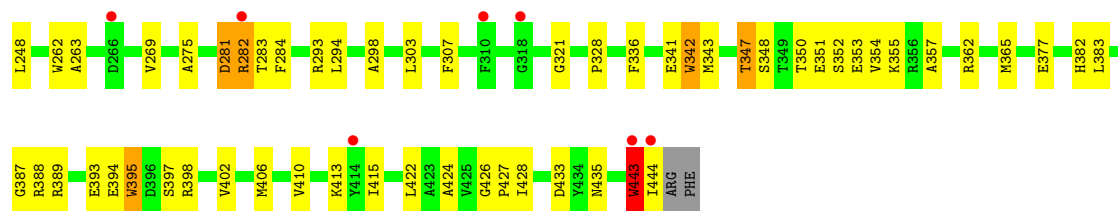
- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



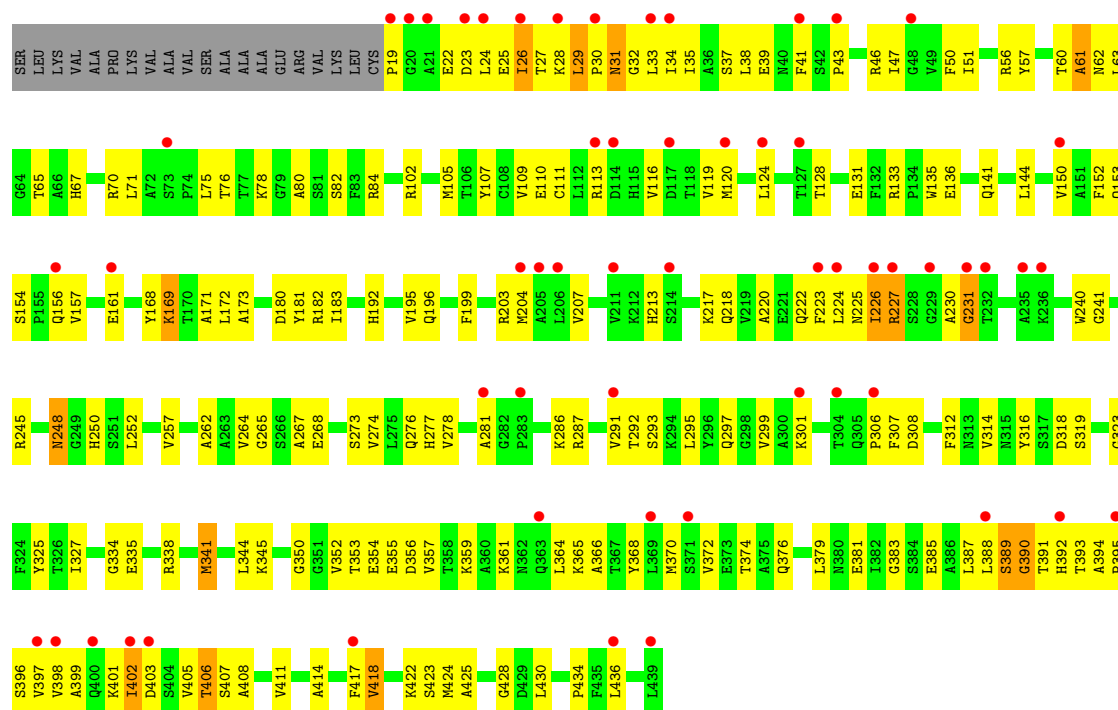
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	E	1	Total	Fe	S	0	0
			4	2	2		
20	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 21 is water.

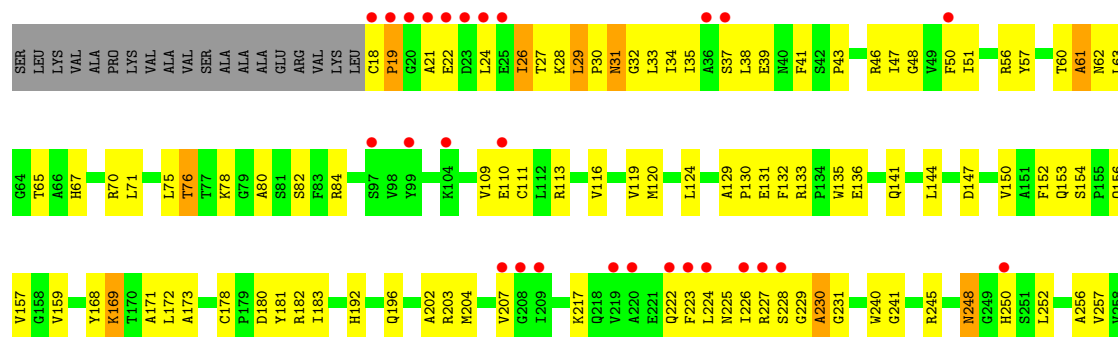
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	O	0	0
			2	2		
21	C	9	Total	O	0	0
			9	9		
21	E	3	Total	O	0	0
			3	3		
21	P	10	Total	O	0	0
			10	10		
21	R	4	Total	O	0	0
			4	4		

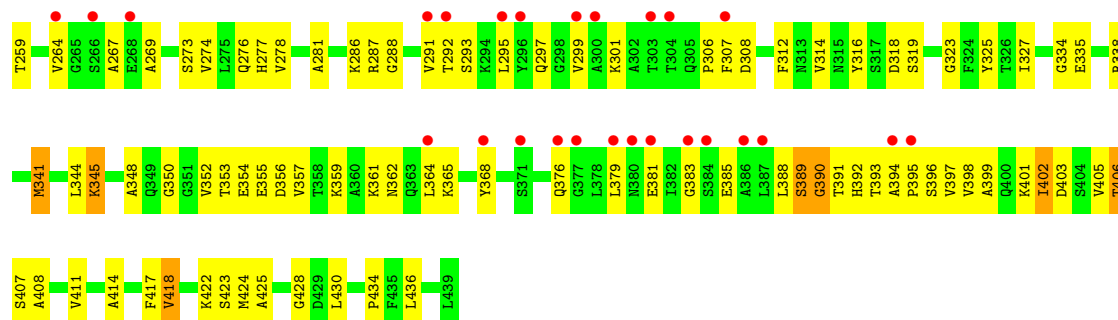


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

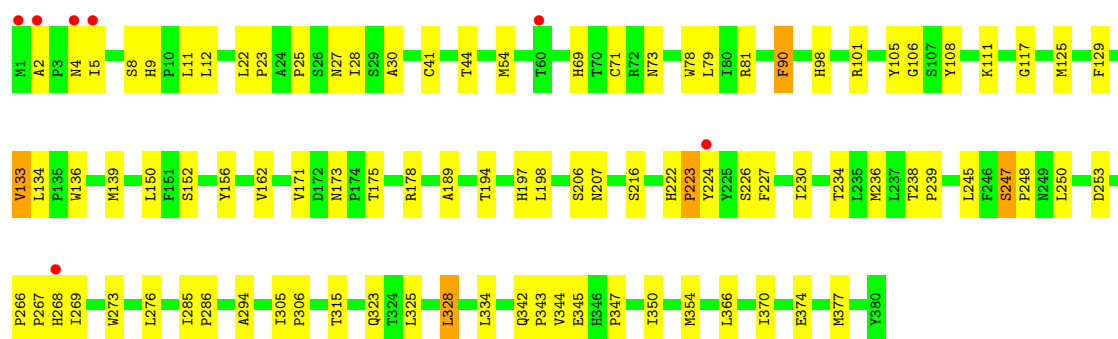
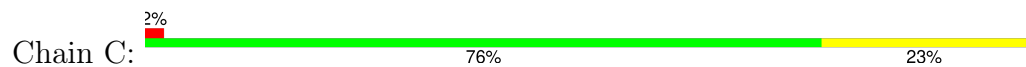


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

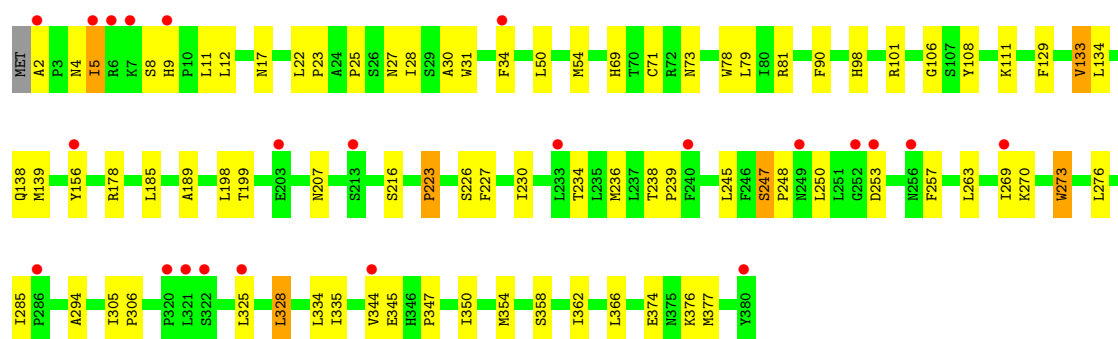
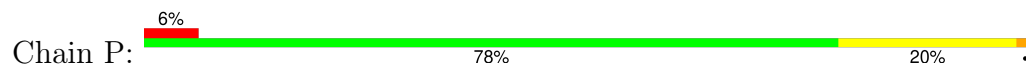




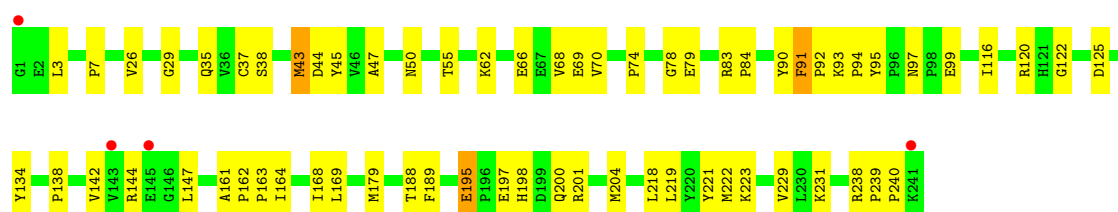
• Molecule 3: CYTOCHROME B



• Molecule 3: CYTOCHROME B

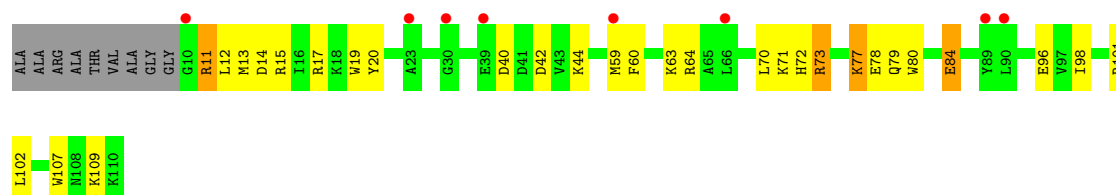


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

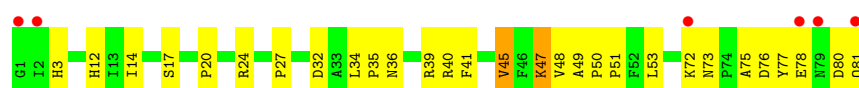




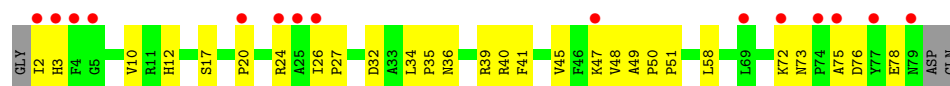
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



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



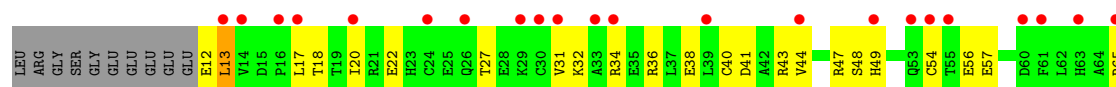
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

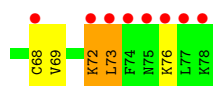


- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

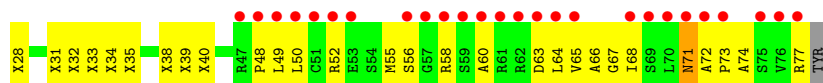


- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

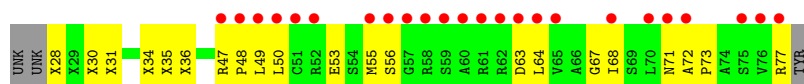




● Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



● 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	172.28Å 182.14Å 241.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.78 – 2.79 58.78 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.6 (58.78-2.79) 97.6 (58.78-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.275 0.236 , 0.267	Depositor DCC
R_{free} test set	3613 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32691	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: CDL, UQ, PEE, BOG, AZI, FES, FNM, UNL, HEC, HEM

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	0.52	0/3511	0.97	13/4757 (0.3%)
1	N	0.49	0/3508	0.98	12/4753 (0.3%)
2	B	0.45	0/3196	0.95	8/4334 (0.2%)
2	O	0.48	0/3202	0.99	11/4343 (0.3%)
3	C	0.62	0/3119	1.01	16/4270 (0.4%)
3	P	0.55	0/3114	0.99	14/4263 (0.3%)
4	D	0.58	0/1956	1.01	9/2658 (0.3%)
4	Q	0.48	0/1956	0.98	10/2658 (0.4%)
5	E	0.47	0/1547	0.94	5/2103 (0.2%)
5	R	0.45	0/1545	0.90	7/2098 (0.3%)
6	F	0.59	0/911	0.90	1/1219 (0.1%)
6	S	0.48	0/911	0.89	1/1219 (0.1%)
7	G	0.57	0/698	1.03	3/946 (0.3%)
7	T	0.45	0/676	1.01	3/918 (0.3%)
8	H	0.51	0/582	0.88	0/779
8	U	0.38	0/561	0.88	1/751 (0.1%)
9	I	0.52	0/218	1.00	1/293 (0.3%)
9	V	0.53	0/218	0.94	2/293 (0.7%)
10	J	0.51	0/508	0.89	1/682 (0.1%)
10	W	0.47	0/490	0.87	1/660 (0.2%)
All	All	0.51	0/32427	0.97	119/43997 (0.3%)

There are no bond length outliers.

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	227	ARG	N-CA-C	9.96	125.81	110.36
3	C	111	LYS	N-CA-C	9.20	122.46	111.33
2	O	18	CYS	CA-C-N	8.91	128.97	119.89
2	O	18	CYS	C-N-CA	8.91	128.97	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	ILE	CB-CA-C	-8.12	104.81	111.71
3	P	111	LYS	N-CA-C	8.10	120.83	111.11
3	P	207	ASN	N-CA-C	-7.73	99.38	110.59
1	N	415	ILE	N-CA-C	7.34	118.38	111.48
1	A	415	ILE	N-CA-C	7.25	118.29	111.48
1	N	415	ILE	CB-CA-C	-7.12	105.66	111.71
6	S	109	LYS	N-CA-C	-7.11	104.23	113.12
2	O	169	LYS	N-CA-C	-6.92	105.11	113.97
3	C	27	ASN	N-CA-C	6.86	120.33	112.57
1	N	226	ASP	N-CA-C	-6.77	104.14	112.88
5	E	143	GLY	N-CA-C	6.77	125.50	115.08
3	P	27	ASN	N-CA-C	6.76	120.21	112.57
1	A	348	SER	N-CA-C	6.72	120.83	111.56
1	A	66	GLY	N-CA-C	6.57	120.32	111.72
4	Q	91	PHE	CA-C-N	6.54	126.50	119.76
4	Q	91	PHE	C-N-CA	6.54	126.50	119.76
1	N	21	ASN	N-CA-C	-6.50	105.32	113.18
3	C	207	ASN	N-CA-C	-6.47	100.32	110.36
5	E	176	ALA	CA-C-N	6.45	127.90	119.84
5	E	176	ALA	C-N-CA	6.45	127.90	119.84
2	B	141	GLN	CA-C-N	-6.45	112.98	119.56
2	B	141	GLN	C-N-CA	-6.45	112.98	119.56
2	B	267	ALA	N-CA-C	-6.44	104.90	112.89
7	T	47	LYS	N-CA-C	-6.42	105.10	113.12
4	D	95	TYR	CA-C-N	6.40	126.32	119.28
4	D	95	TYR	C-N-CA	6.40	126.32	119.28
4	Q	95	TYR	CA-C-N	6.39	126.31	119.28
4	Q	95	TYR	C-N-CA	6.39	126.31	119.28
4	D	91	PHE	CA-C-N	6.38	126.33	119.76
4	D	91	PHE	C-N-CA	6.38	126.33	119.76
2	O	230	ALA	N-CA-C	-6.36	104.67	112.88
2	O	141	GLN	CA-C-N	-6.35	113.08	119.56
2	O	141	GLN	C-N-CA	-6.35	113.08	119.56
1	N	348	SER	N-CA-C	6.35	120.93	112.30
2	B	169	LYS	N-CA-C	-6.30	105.91	113.97
1	N	189	HIS	N-CA-C	6.25	121.43	113.55
1	A	189	HIS	N-CA-C	6.17	121.33	113.55
7	G	47	LYS	N-CA-C	-6.14	105.45	113.12
3	P	189	ALA	N-CA-C	-6.05	104.77	111.36
1	N	32	GLN	N-CA-C	5.96	117.17	109.72
1	N	263	ALA	N-CA-C	5.94	120.06	112.34
4	D	195	GLU	CA-C-N	5.90	125.58	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	195	GLU	C-N-CA	5.90	125.58	119.56
10	W	14	PHE	N-CA-C	5.88	120.29	113.18
10	J	14	PHE	N-CA-C	5.87	120.28	113.18
3	C	133	VAL	CB-CA-C	-5.86	104.14	112.22
1	A	263	ALA	N-CA-C	5.85	119.95	112.34
3	P	257	PHE	N-CA-C	-5.85	105.73	112.92
2	O	61	ALA	N-CA-C	5.83	117.64	111.28
3	C	206	SER	N-CA-C	5.82	118.22	110.53
4	Q	45	TYR	N-CA-C	5.82	120.01	113.02
1	N	347	THR	N-CA-C	5.80	120.86	113.55
7	G	12	HIS	N-CA-C	5.75	119.50	111.74
6	F	89	TYR	N-CA-C	5.68	118.25	111.71
4	D	45	TYR	N-CA-C	5.65	119.87	112.92
4	Q	116	ILE	N-CA-C	5.64	116.37	110.62
5	E	81	ILE	N-CA-C	5.63	113.72	108.15
3	P	134	LEU	N-CA-C	5.62	121.19	113.77
5	R	17	ASP	N-CA-C	5.61	119.75	113.01
1	A	148	VAL	N-CA-C	-5.61	105.05	110.72
7	T	12	HIS	N-CA-C	5.61	119.31	111.74
4	D	7	PRO	N-CA-C	5.61	115.86	110.47
1	A	347	THR	N-CA-C	5.60	120.61	113.55
3	P	328	LEU	N-CA-C	-5.59	105.09	111.07
1	N	66	GLY	N-CA-C	5.56	119.01	111.72
2	B	180	ASP	N-CA-C	5.52	117.30	111.28
3	C	189	ALA	N-CA-C	-5.48	105.47	111.82
4	D	116	ILE	N-CA-C	5.47	116.85	110.62
9	I	74	ALA	N-CA-C	-5.43	101.69	110.32
2	O	19	PRO	N-CA-C	5.41	119.72	111.11
3	C	224	TYR	N-CA-C	5.41	117.62	111.02
4	Q	195	GLU	CA-C-N	5.40	126.59	119.84
4	Q	195	GLU	C-N-CA	5.40	126.59	119.84
2	B	345	LYS	N-CA-C	-5.39	105.10	110.97
3	C	175	THR	N-CA-C	-5.34	105.12	111.69
3	C	173	ASN	CA-C-N	-5.33	114.17	119.56
3	C	173	ASN	C-N-CA	-5.33	114.17	119.56
5	R	158	CYS	CA-C-N	5.33	125.41	119.87
5	R	158	CYS	C-N-CA	5.33	125.41	119.87
2	B	61	ALA	N-CA-C	5.33	117.84	111.71
3	C	90	PHE	N-CA-C	-5.32	105.59	111.71
1	A	32	GLN	CA-C-N	5.31	124.98	119.56
1	A	32	GLN	C-N-CA	5.31	124.98	119.56
3	P	185	LEU	N-CA-C	5.28	117.84	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	328	LEU	N-CA-C	-5.25	105.45	111.07
5	E	17	ASP	N-CA-C	5.24	119.30	113.01
3	P	226	SER	N-CA-C	-5.24	105.65	111.36
1	N	148	VAL	N-CA-C	-5.23	105.44	110.72
1	A	272	VAL	N-CA-C	-5.22	105.45	110.72
3	P	273	TRP	N-CA-C	5.21	117.63	111.33
1	A	428	ILE	N-CA-C	5.20	120.16	109.34
3	P	247	SER	CA-C-N	5.20	125.25	119.32
3	P	247	SER	C-N-CA	5.20	125.25	119.32
7	T	10	VAL	N-CA-C	5.19	115.38	108.11
7	G	53	LEU	N-CA-C	-5.17	105.54	111.07
2	B	372	VAL	N-CA-C	5.14	117.12	112.29
3	C	134	LEU	N-CA-C	5.14	121.16	109.81
1	N	244	ARG	N-CA-C	5.13	117.61	109.24
2	O	180	ASP	N-CA-C	5.12	116.55	111.07
3	C	226	SER	N-CA-C	-5.12	105.78	111.36
5	R	174	GLY	CA-C-N	5.12	124.73	119.56
5	R	174	GLY	C-N-CA	5.12	124.73	119.56
4	Q	155	GLY	N-CA-C	-5.12	108.99	115.08
2	O	345	LYS	N-CA-C	-5.11	105.40	110.97
3	P	133	VAL	CB-CA-C	-5.10	105.18	112.22
1	A	32	GLN	N-CA-C	5.08	116.99	109.62
3	C	247	SER	CA-C-N	5.08	125.36	119.47
3	C	247	SER	C-N-CA	5.08	125.36	119.47
5	R	145	VAL	N-CA-C	5.06	113.41	107.89
5	R	143	GLY	N-CA-C	5.06	122.88	114.48
8	U	73	LEU	N-CA-C	5.05	119.70	111.37
4	Q	7	PRO	N-CA-C	5.04	115.31	110.47
9	V	47	ARG	CA-C-N	5.03	126.12	119.84
9	V	47	ARG	C-N-CA	5.03	126.12	119.84
3	P	5	ILE	N-CA-C	5.00	116.32	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	141	0
1	N	3437	0	3349	148	0
2	B	3141	0	3142	200	0
2	O	3147	0	3146	187	0
3	C	3017	0	3063	78	0
3	P	3012	0	3058	70	0
4	D	1898	0	1846	52	0
4	Q	1898	0	1846	51	0
5	E	1513	0	1478	70	0
5	R	1512	0	1476	100	0
6	F	891	0	893	23	0
6	S	891	0	893	30	0
7	G	676	0	659	26	0
7	T	654	0	641	25	0
8	H	574	0	548	18	0
8	U	553	0	535	24	0
9	I	288	0	254	45	0
9	V	278	0	252	32	0
10	J	497	0	490	11	0
10	W	479	0	478	14	0
11	A	21	0	13	1	0
11	C	98	0	147	0	0
11	N	5	0	0	0	0
11	P	98	0	147	1	0
12	A	1	0	0	0	0
12	C	5	0	0	0	0
12	D	2	0	0	0	0
12	P	7	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	5	0
13	P	86	0	60	5	0
14	C	22	0	17	5	0
14	P	22	0	17	4	0
15	C	19	0	17	3	0
15	P	19	0	17	2	0
16	C	3	0	0	0	0
16	P	3	0	0	0	0
17	C	12	0	18	0	0
17	D	40	0	56	3	0
17	P	19	0	24	1	0
17	Q	40	0	56	1	0
18	D	43	0	30	1	0
18	Q	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	42	0	28	2	0
19	G	40	0	24	1	0
19	Q	42	0	28	3	0
19	T	40	0	24	1	0
20	E	4	0	0	1	0
20	R	4	0	0	2	0
21	A	2	0	0	0	0
21	C	9	0	0	1	0
21	E	3	0	0	0	0
21	P	10	0	0	1	0
21	R	4	0	0	0	0
All	All	32691	0	32213	1210	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 19.

All (1210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:THR:HG22	2:O:355:GLU:H	1.16	1.11
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.33	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.20	1.06
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.38	1.03
1:N:178:THR:HG22	1:N:180:ALA:H	1.22	1.02
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.62	1.00
1:A:343:MET:O	1:A:347:THR:HG22	1.62	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.24	0.99
1:N:343:MET:O	1:N:347:THR:HG22	1.63	0.98
2:B:76:THR:HG22	2:B:82:SER:H	1.25	0.97
4:D:47:ALA:H	4:D:50:ASN:HD22	1.11	0.95
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.47	0.95
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.49	0.94
1:N:206:LYS:H	1:N:206:LYS:HD2	1.32	0.94
1:A:344:ARG:NH1	1:A:344:ARG:HB2	1.82	0.93
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.49	0.93
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.49	0.91
1:N:206:LYS:H	1:N:206:LYS:CD	1.84	0.91
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.56	0.88
1:A:178:THR:HB	1:A:181:ASP:OD1	1.74	0.87
9:I:71:ASN:HD22	9:I:71:ASN:H	1.19	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.55	0.87
1:N:178:THR:HB	1:N:181:ASP:OD1	1.75	0.85
2:B:27:THR:HG22	2:B:28:LYS:H	1.39	0.85
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.74	0.85
9:I:32:UNK:N	9:I:73:PRO:HG2	1.93	0.83
1:A:281:ASP:CG	9:I:33:UNK:HB1	2.03	0.83
9:I:64:LEU:HD12	9:I:77:ARG:O	1.78	0.83
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.59	0.83
1:N:282:ARG:HH21	9:V:36:UNK:CB	1.91	0.82
4:D:47:ALA:H	4:D:50:ASN:ND2	1.76	0.82
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.62	0.82
5:R:101:ARG:HH22	5:R:127:VAL:HG11	1.45	0.81
2:O:76:THR:HG22	2:O:82:SER:H	1.43	0.81
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.44	0.81
5:E:134:ILE:HB	5:E:185:TYR:CE2	2.15	0.81
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.61	0.81
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.64	0.80
1:N:22:GLY:O	1:N:193:PRO:HA	1.82	0.80
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.64	0.80
5:R:188:VAL:HG11	5:R:192:LEU:HD12	1.62	0.80
1:N:205:HIS:HB3	1:N:206:LYS:NZ	1.97	0.80
2:B:153:GLN:HE22	9:I:34:UNK:CG	1.95	0.79
9:I:71:ASN:HD22	9:I:71:ASN:N	1.79	0.79
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.45	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.46	0.79
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.63	0.78
2:B:153:GLN:HE22	9:I:34:UNK:HG2	1.48	0.78
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.48	0.78
2:O:192:HIS:O	2:O:196:GLN:HG3	1.83	0.78
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.64	0.77
2:O:62:ASN:O	2:O:65:THR:HG22	1.83	0.77
2:B:22:GLU:HG2	2:B:39:GLU:HB3	1.66	0.77
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.50	0.77
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.67	0.76
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.02	0.76
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.66	0.76
1:N:49:ASN:HD22	1:N:51:LYS:H	1.32	0.76
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.66	0.76
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.68	0.75
1:N:362:ARG:O	1:N:365:MET:HG2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:238:THR:HB	3:P:239:PRO:HD3	1.69	0.75
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.53	0.74
2:O:248:ASN:HD22	2:O:248:ASN:C	1.95	0.74
10:W:40:ASP:O	10:W:44:GLU:HG3	1.87	0.74
3:C:30:ALA:HB1	19:D:2003:CDL:H111	1.69	0.74
2:B:27:THR:HG22	2:B:28:LYS:N	2.01	0.74
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.01	0.74
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.23	0.73
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.69	0.73
2:B:248:ASN:C	2:B:248:ASN:HD22	1.96	0.73
2:B:47:ILE:HD13	2:B:120:MET:CE	2.18	0.73
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.06	0.73
2:B:76:THR:HG22	2:B:82:SER:N	2.03	0.73
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.18	0.73
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.18	0.73
3:P:247:SER:OG	3:P:250:LEU:HB2	1.89	0.72
2:B:227:ARG:HA	2:B:227:ARG:NE	2.04	0.72
1:A:362:ARG:O	1:A:365:MET:HG2	1.89	0.72
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.04	0.72
1:N:49:ASN:ND2	1:N:51:LYS:H	1.86	0.72
3:P:101:ARG:C	3:P:101:ARG:HD2	2.14	0.72
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.71	0.72
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.25	0.71
7:T:73:ASN:HB3	7:T:76:ASP:OD2	1.89	0.71
2:B:156:GLN:HE22	9:I:77:ARG:C	1.98	0.71
2:O:76:THR:HG22	2:O:82:SER:HB2	1.72	0.71
1:A:49:ASN:HD22	1:A:51:LYS:H	1.38	0.71
3:C:238:THR:HB	3:C:239:PRO:HD3	1.73	0.71
8:U:47:ARG:HD3	8:U:48:SER:H	1.54	0.71
2:O:297:GLN:O	2:O:301:LYS:HG3	1.91	0.71
3:P:9:HIS:HD2	3:P:12:LEU:H	1.37	0.71
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.31	0.71
10:J:40:ASP:O	10:J:44:GLU:HG3	1.90	0.70
2:B:264:VAL:HG23	2:B:316:TYR:C	2.16	0.70
1:A:178:THR:HG22	1:A:180:ALA:N	2.03	0.70
2:O:376:GLN:HE22	9:V:77:ARG:NH2	1.89	0.70
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.55	0.70
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.22	0.70
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.15	0.70
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.73	0.70
3:C:328:LEU:HD23	7:G:51:PRO:HB3	1.72	0.70
2:O:47:ILE:HD13	2:O:120:MET:CE	2.21	0.69
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.73	0.69
3:C:269:ILE:HD12	5:R:160:CYS:SG	2.33	0.69
4:D:164:ILE:O	4:D:179:MET:HE2	1.92	0.69
3:P:30:ALA:HB1	19:Q:3003:CDL:H111	1.75	0.69
5:R:101:ARG:HG2	5:R:105:GLU:OE1	1.93	0.69
7:G:73:ASN:HB3	7:G:76:ASP:OD2	1.92	0.69
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.58	0.69
2:B:153:GLN:NE2	9:I:34:UNK:HG1	2.09	0.68
8:U:27:THR:O	8:U:31:VAL:HG23	1.93	0.68
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.58	0.68
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.34	0.68
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.58	0.68
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.74	0.68
1:N:187:ASP:O	1:N:191:LYS:HE3	1.94	0.68
3:C:139:MET:HE3	3:C:253:ASP:OD2	1.93	0.68
3:C:9:HIS:HD2	3:C:12:LEU:H	1.41	0.68
1:N:49:ASN:HD22	1:N:49:ASN:C	2.02	0.68
2:B:192:HIS:O	2:B:196:GLN:HG3	1.94	0.67
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.56	0.67
2:B:297:GLN:O	2:B:301:LYS:HG3	1.93	0.67
8:U:47:ARG:HG3	8:U:49:HIS:H	1.59	0.67
2:O:252:LEU:HD13	9:V:55:MET:HE3	1.75	0.67
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.29	0.67
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.75	0.67
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.77	0.67
1:N:178:THR:HG22	1:N:180:ALA:N	2.03	0.67
2:O:27:THR:HG22	2:O:28:LYS:N	2.07	0.67
1:A:350:THR:HG22	1:A:352:SER:H	1.59	0.67
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.59	0.67
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.10	0.67
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.77	0.66
3:P:139:MET:HE3	3:P:253:ASP:OD2	1.95	0.66
5:R:129:LYS:HB3	5:R:131:GLU:OE1	1.95	0.66
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.77	0.66
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.66
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.77	0.66
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:407:SER:O	2:O:411:VAL:HG23	1.95	0.66
2:O:154:SER:O	2:O:157:VAL:HG12	1.96	0.66
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.78	0.66
2:O:399:ALA:O	2:O:402:ILE:HG22	1.96	0.66
1:N:19:LEU:O	1:N:21:ASN:N	2.29	0.66
3:C:344:VAL:O	3:C:345:GLU:HG3	1.95	0.65
9:I:28:UNK:HA	9:I:72:ALA:HB2	1.77	0.65
4:Q:241:LYS:HE3	4:Q:241:LYS:HA	1.78	0.65
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.77	0.65
5:E:163:SER:OG	5:E:175:PRO:HD2	1.96	0.65
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.26	0.65
2:B:381:GLU:OE1	2:B:381:GLU:HA	1.96	0.65
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.78	0.65
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.78	0.65
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.60	0.65
9:I:31:UNK:C	9:I:73:PRO:HG2	2.27	0.65
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.32	0.65
4:Q:164:ILE:O	4:Q:179:MET:HE2	1.97	0.65
5:R:147:ILE:HG22	5:R:148:ALA:N	2.12	0.65
5:R:10:PHE:O	5:R:14:ARG:HG3	1.96	0.64
1:A:222:THR:OG1	1:A:225:GLU:HG3	1.96	0.64
2:O:31:ASN:ND2	2:O:33:LEU:H	1.94	0.64
2:O:381:GLU:HA	2:O:381:GLU:OE1	1.97	0.64
1:N:350:THR:HG22	1:N:352:SER:H	1.61	0.64
5:R:116:LYS:HA	5:R:116:LYS:HE2	1.79	0.64
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.11	0.64
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.32	0.64
1:N:21:ASN:HB2	1:N:218:GLY:O	1.97	0.64
2:B:27:THR:HG21	2:B:217:LYS:HE3	1.81	0.63
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.63	0.63
1:N:222:THR:OG1	1:N:225:GLU:HG3	1.98	0.63
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.32	0.63
3:P:269:ILE:HG23	14:P:3001:FNM:H23	1.81	0.63
1:A:49:ASN:ND2	1:A:51:LYS:H	1.96	0.63
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.81	0.63
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.63
3:P:273:TRP:HA	3:P:276:LEU:HD12	1.79	0.63
1:A:350:THR:HB	1:A:353:GLU:HG3	1.81	0.63
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.80	0.63
1:A:77:LYS:HE3	2:B:359:LYS:NZ	2.14	0.63
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.81	0.63
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.79	0.63
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.81	0.62
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.80	0.62
5:R:164:HIS:HB2	5:R:173:LYS:HB3	1.80	0.62
1:A:187:ASP:O	1:A:191:LYS:HE3	1.98	0.62
2:O:402:ILE:C	2:O:402:ILE:HD13	2.24	0.62
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.00	0.62
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.00	0.62
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.24	0.62
2:B:389:SER:O	2:B:391:THR:HG23	1.99	0.62
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.64	0.62
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.40	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.34	0.62
5:R:142:LEU:HD12	5:R:161:HIS:CE1	2.35	0.62
7:T:41:PHE:O	7:T:45:VAL:HG23	1.99	0.62
5:R:190:ASP:O	5:R:191:ASP:HB2	2.00	0.62
2:B:31:ASN:ND2	2:B:33:LEU:H	1.98	0.62
1:N:205:HIS:HB3	1:N:206:LYS:HZ1	1.65	0.62
3:P:377:MET:HE1	6:S:19:TRP:HZ3	1.65	0.62
2:B:113:ARG:O	2:B:116:VAL:HG23	2.00	0.61
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.65	0.61
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.81	0.61
5:E:171:ILE:HG12	5:E:176:ALA:O	2.00	0.61
7:G:41:PHE:O	7:G:45:VAL:HG23	2.00	0.61
1:N:77:LYS:HE3	2:O:359:LYS:NZ	2.15	0.61
1:A:49:ASN:HD22	1:A:49:ASN:C	2.08	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.36	0.61
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.63	0.61
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.66	0.61
5:R:82:PRO:HD2	5:R:85:LYS:CD	2.30	0.61
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.00	0.61
2:B:402:ILE:HD13	2:B:402:ILE:C	2.26	0.61
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.35	0.61
2:O:388:LEU:O	2:O:389:SER:HB3	1.99	0.61
9:I:71:ASN:N	9:I:71:ASN:ND2	2.40	0.61
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.82	0.61
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.61
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.35	0.61
8:H:27:THR:O	8:H:31:VAL:HG23	2.01	0.60
3:P:347:PRO:O	3:P:350:ILE:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.16	0.60
8:H:40:CYS:O	8:H:44:VAL:HG23	2.02	0.60
1:N:347:THR:HG21	1:N:444:ILE:C	2.26	0.60
9:V:34:UNK:N	9:V:35:UNK:N	2.48	0.60
2:B:38:LEU:HD12	2:B:39:GLU:N	2.17	0.60
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.24	0.60
4:D:47:ALA:N	4:D:50:ASN:HD22	1.92	0.60
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.81	0.60
5:R:188:VAL:HB	5:R:192:LEU:HB2	1.82	0.60
1:A:7:THR:HG21	2:B:113:ARG:CD	2.31	0.60
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.32	0.60
2:B:156:GLN:NE2	9:I:77:ARG:C	2.60	0.60
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.82	0.60
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.84	0.60
2:O:124:LEU:HD21	2:O:223:PHE:HB3	1.82	0.60
5:R:52:LYS:HD3	5:R:52:LYS:C	2.27	0.60
5:R:131:GLU:CD	5:R:131:GLU:H	2.10	0.60
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.83	0.59
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.84	0.59
3:C:101:ARG:HD2	3:C:101:ARG:C	2.26	0.59
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.85	0.59
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.70	0.59
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.83	0.59
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.44	0.59
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.17	0.59
2:B:399:ALA:O	2:B:402:ILE:HG22	2.03	0.59
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.38	0.59
3:C:377:MET:HE1	6:F:19:TRP:HZ3	1.66	0.59
4:Q:241:LYS:OXT	4:Q:241:LYS:HG3	2.03	0.59
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.38	0.59
9:V:31:UNK:C	9:V:73:PRO:HG2	2.32	0.59
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.37	0.59
2:O:38:LEU:HD12	2:O:39:GLU:N	2.17	0.59
1:A:170:THR:HG22	1:A:171:THR:N	2.18	0.59
2:O:335:GLU:HA	2:O:338:ARG:HH12	1.68	0.59
2:O:385:GLU:OE1	2:O:392:HIS:HA	2.02	0.59
3:C:269:ILE:HG23	14:C:2001:FNM:H23	1.83	0.59
2:O:306:PRO:HG2	9:V:50:LEU:O	2.03	0.59
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.91	0.58
6:S:12:LEU:HB3	6:S:13:MET:HE2	1.85	0.58
2:B:43:PRO:O	2:B:113:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ILE:O	2:B:226:ILE:HG23	2.02	0.58
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.85	0.58
2:B:388:LEU:O	2:B:389:SER:HB3	2.02	0.58
1:N:350:THR:HB	1:N:353:GLU:HG3	1.85	0.58
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.85	0.58
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.28	0.58
2:O:353:THR:HG22	2:O:354:GLU:N	2.18	0.58
3:C:41:CYS:SG	3:C:90:PHE:CD2	2.96	0.58
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.33	0.58
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.84	0.58
2:O:353:THR:HG22	2:O:355:GLU:N	2.01	0.58
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.44	0.58
5:E:160:CYS:SG	3:P:269:ILE:HD12	2.44	0.58
7:G:72:LYS:HG2	8:H:56:GLU:OE2	2.03	0.58
1:N:205:HIS:HB3	1:N:206:LYS:HZ2	1.68	0.58
3:P:328:LEU:HD23	7:T:51:PRO:HB3	1.86	0.58
9:V:30:UNK:HG3	9:V:31:UNK:N	2.18	0.58
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.34	0.58
5:R:122:HIS:O	5:R:125:ASP:HB2	2.04	0.58
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.85	0.58
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.86	0.58
4:D:200:GLN:NE2	17:D:2091:BOG:H5	2.19	0.58
6:F:13:MET:HE2	6:F:16:ILE:HD12	1.85	0.58
1:N:383:LEU:O	1:N:387:GLY:HA2	2.03	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.39	0.58
5:R:82:PRO:HD2	5:R:85:LYS:HD2	1.86	0.58
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.03	0.57
5:E:77:LYS:HE2	5:E:80:ASP:OD2	2.04	0.57
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.37	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.33	0.57
10:W:55:ILE:CG2	10:W:59:TYR:HE1	2.16	0.57
2:B:353:THR:HG22	2:B:354:GLU:N	2.18	0.57
10:J:55:ILE:CG2	10:J:59:TYR:HE1	2.17	0.57
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.37	0.57
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.86	0.57
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.28	0.57
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.39	0.57
6:S:11:ARG:O	6:S:15:ARG:HG3	2.05	0.57
3:C:245:LEU:O	4:D:201:ARG:HD2	2.04	0.57
5:E:103:GLN:O	5:E:107:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:LYS:HD2	1:N:206:LYS:N	2.13	0.57
2:B:292:THR:HG22	2:B:292:THR:O	2.05	0.57
2:O:338:ARG:HB2	2:O:338:ARG:HH11	1.70	0.57
2:O:353:THR:HB	2:O:356:ASP:CG	2.29	0.57
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.87	0.57
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.18	0.57
2:B:414:ALA:O	2:B:418:VAL:HG23	2.05	0.57
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.87	0.57
2:B:407:SER:O	2:B:411:VAL:HG23	2.05	0.57
3:C:247:SER:OG	3:C:250:LEU:HB2	2.05	0.57
2:B:385:GLU:OE1	2:B:392:HIS:HA	2.04	0.56
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.87	0.56
10:W:4:ALA:O	10:W:8:GLN:HG3	2.05	0.56
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.87	0.56
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.87	0.56
1:N:161:THR:HG21	1:N:235:ARG:H	1.70	0.56
1:A:219:VAL:HG12	1:A:220:SER:N	2.20	0.56
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.70	0.56
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.36	0.56
2:B:353:THR:HB	2:B:356:ASP:CG	2.30	0.56
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.45	0.56
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.86	0.56
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.32	0.56
5:R:126:ARG:HB3	5:R:182:VAL:HG21	1.88	0.56
1:A:15:ASN:O	1:A:26:ALA:HA	2.05	0.56
2:O:389:SER:O	2:O:391:THR:HG23	2.05	0.56
6:S:13:MET:HE2	6:S:13:MET:N	2.20	0.56
2:B:341:MET:CE	2:B:417:PHE:HE2	2.17	0.56
1:N:190:PHE:C	1:N:195:MET:HE2	2.31	0.56
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.88	0.56
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.87	0.56
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.41	0.56
2:O:414:ALA:O	2:O:418:VAL:HG23	2.06	0.56
2:B:76:THR:HG22	2:B:82:SER:HB2	1.88	0.56
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.87	0.56
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.40	0.56
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.71	0.56
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.87	0.55
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.31	0.55
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	1.88	0.55
19:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:308:ASP:OD2	9:V:56:SER:HA	2.05	0.55
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.88	0.55
3:C:129:PHE:CE1	14:C:2001:FNM:H27B	2.42	0.55
1:A:350:THR:HG22	1:A:351:GLU:N	2.21	0.55
2:B:27:THR:CG2	2:B:28:LYS:H	2.14	0.55
2:B:338:ARG:HH11	2:B:338:ARG:HB2	1.72	0.55
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.89	0.55
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.54	0.55
2:O:341:MET:CE	2:O:417:PHE:HE2	2.17	0.55
7:T:48:VAL:O	7:T:51:PRO:HD2	2.05	0.55
2:B:124:LEU:HD21	2:B:223:PHE:HB3	1.88	0.55
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.42	0.55
9:I:38:UNK:O	9:I:39:UNK:C	2.55	0.55
1:N:106:MET:C	1:N:106:MET:HE2	2.32	0.55
1:A:106:MET:HE2	1:A:107:PRO:HA	1.89	0.55
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.72	0.55
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.41	0.55
5:E:85:LYS:HG2	5:E:86:ASN:N	2.22	0.55
1:A:106:MET:HE2	1:A:106:MET:C	2.31	0.55
2:B:225:ASN:O	2:B:226:ILE:C	2.48	0.55
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.21	0.55
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.42	0.55
3:P:270:LYS:O	3:P:270:LYS:HG3	2.07	0.55
5:R:74:ILE:HD11	5:R:96:LEU:HD23	1.88	0.55
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.89	0.55
1:A:190:PHE:C	1:A:195:MET:HE2	2.31	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.71	0.55
1:N:15:ASN:O	1:N:26:ALA:HA	2.07	0.55
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.37	0.55
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.88	0.55
1:A:4:TYR:HE2	1:A:396:ASP:OD2	1.90	0.55
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.42	0.55
2:O:150:VAL:O	2:O:153:GLN:HG3	2.07	0.55
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.42	0.55
5:E:190:ASP:CG	5:E:191:ASP:H	2.15	0.55
1:N:350:THR:HG22	1:N:351:GLU:N	2.22	0.55
5:R:128:LYS:O	5:R:129:LYS:HG3	2.07	0.55
1:A:106:MET:N	1:A:107:PRO:HD2	2.22	0.54
5:E:52:LYS:C	5:E:52:LYS:HD3	2.31	0.54
7:G:48:VAL:O	7:G:51:PRO:HD2	2.07	0.54
1:N:398:ARG:HH11	1:N:398:ARG:HG2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:126:ARG:H	5:R:126:ARG:HD3	1.72	0.54
2:B:368:TYR:HE1	2:B:381:GLU:OE2	1.90	0.54
1:N:170:THR:HG22	1:N:171:THR:N	2.21	0.54
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.41	0.54
5:R:137:GLY:O	5:R:145:VAL:HG22	2.07	0.54
1:A:106:MET:HE2	1:A:106:MET:O	2.08	0.54
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.08	0.54
2:O:225:ASN:O	2:O:226:ILE:C	2.50	0.54
2:O:292:THR:HG22	2:O:292:THR:O	2.08	0.54
2:O:368:TYR:HE1	2:O:381:GLU:OE2	1.91	0.54
5:R:109:GLU:C	5:R:111:GLU:H	2.15	0.54
5:R:122:HIS:HB3	5:R:125:ASP:OD1	2.08	0.54
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.89	0.54
5:E:119:ASP:OD2	5:E:179:ASN:ND2	2.40	0.54
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.23	0.54
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.90	0.54
5:R:85:LYS:HG2	5:R:86:ASN:N	2.21	0.54
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.37	0.54
9:I:71:ASN:H	9:I:71:ASN:ND2	1.94	0.54
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.22	0.54
2:B:335:GLU:HA	2:B:338:ARG:HH12	1.72	0.54
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.89	0.54
8:U:47:ARG:CD	8:U:48:SER:H	2.21	0.54
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.90	0.54
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.36	0.54
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.43	0.54
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.37	0.54
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.54
1:A:239:SER:HB2	7:G:17:SER:O	2.08	0.54
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.38	0.54
5:E:177:PRO:HB2	5:E:178:TYR:CD1	2.43	0.54
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.54	0.54
4:Q:195:GLU:HG3	4:Q:198:HIS:HB2	1.89	0.54
2:B:150:VAL:O	2:B:153:GLN:HG3	2.08	0.54
1:A:217:SER:O	1:A:218:GLY:C	2.51	0.53
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.43	0.53
2:B:227:ARG:HA	2:B:227:ARG:HE	1.72	0.53
1:N:106:MET:N	1:N:107:PRO:HD2	2.23	0.53
3:P:9:HIS:CD2	3:P:11:LEU:H	2.26	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.42	0.53
5:R:115:SER:O	5:R:116:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:TRP:CD2	4:D:197:GLU:HG3	2.44	0.53
1:N:49:ASN:ND2	1:N:49:ASN:C	2.66	0.53
2:O:248:ASN:ND2	2:O:250:HIS:H	2.06	0.53
5:E:165:TYR:HA	5:E:170:ARG:O	2.08	0.53
5:R:134:ILE:HD11	5:R:193:VAL:HG21	1.89	0.53
2:B:46:ARG:HH11	2:B:110:GLU:HG3	1.73	0.53
1:N:53:ASN:H	1:N:173:ASN:ND2	2.07	0.53
8:U:12:GLU:O	8:U:13:LEU:HB2	2.08	0.53
1:N:90:THR:O	1:N:167:VAL:HG11	2.09	0.53
2:O:46:ARG:HH11	2:O:110:GLU:HG3	1.72	0.53
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.91	0.53
2:O:76:THR:HG22	2:O:82:SER:CB	2.38	0.53
3:C:273:TRP:HA	3:C:276:LEU:HD12	1.90	0.53
19:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.42	0.53
8:U:40:CYS:O	8:U:44:VAL:HG23	2.07	0.53
1:A:383:LEU:O	1:A:387:GLY:HA2	2.09	0.52
2:B:306:PRO:HA	9:I:52:ARG:CG	2.38	0.52
3:P:376:LYS:O	6:S:17:ARG:NH1	2.40	0.52
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.91	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.73	0.52
2:B:128:THR:HG21	2:B:224:LEU:HD23	1.92	0.52
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.39	0.52
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.73	0.52
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.38	0.52
2:B:78:LYS:HA	2:B:131:GLU:OE2	2.09	0.52
8:H:65:ARG:O	8:H:69:VAL:HG23	2.10	0.52
1:N:170:THR:HG22	1:N:172:GLU:H	1.74	0.52
2:O:31:ASN:HD22	2:O:32:GLY:N	2.07	0.52
2:O:46:ARG:HD2	2:O:110:GLU:OE2	2.09	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
5:R:190:ASP:O	5:R:191:ASP:CB	2.58	0.52
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.74	0.52
3:C:347:PRO:O	3:C:350:ILE:HG22	2.09	0.52
1:N:112:LEU:O	1:N:116:VAL:HG23	2.09	0.52
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.44	0.52
11:A:2008:PEE:H13	3:C:222:HIS:HE1	1.73	0.52
3:C:150:LEU:HD23	5:R:142:LEU:HD21	1.92	0.52
5:E:113:ASP:OD1	5:E:116:LYS:HG2	2.10	0.52
9:I:49:LEU:O	9:I:50:LEU:HD23	2.10	0.52
2:O:156:GLN:HE22	9:V:77:ARG:C	2.17	0.52
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.17	0.52
5:E:155:GLY:HA3	5:E:166:ASP:C	2.35	0.52
5:E:83:GLU:HG2	5:E:102:THR:HA	1.92	0.52
9:I:64:LEU:HA	9:I:77:ARG:O	2.10	0.52
3:P:198:LEU:HD13	15:P:3002:UQ:HM52	1.91	0.52
4:Q:97:ASN:OD1	4:Q:99:GLU:HB2	2.10	0.52
2:O:76:THR:HG23	2:O:136:GLU:CD	2.35	0.52
2:O:203:ARG:HD2	2:O:230:ALA:O	2.10	0.52
2:O:273:SER:O	2:O:276:GLN:HB3	2.10	0.52
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.10	0.52
1:A:307:PHE:CD1	1:A:307:PHE:C	2.88	0.52
2:B:264:VAL:HG23	2:B:316:TYR:O	2.10	0.52
6:F:78:GLU:H	6:F:78:GLU:CD	2.17	0.52
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.10	0.52
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.92	0.52
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.10	0.51
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.74	0.51
1:N:206:LYS:H	1:N:206:LYS:CE	2.23	0.51
2:O:335:GLU:HA	2:O:338:ARG:NH1	2.24	0.51
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.92	0.51
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.45	0.51
2:B:307:PHE:CD1	2:B:308:ASP:N	2.79	0.51
2:B:318:ASP:O	2:B:319:SER:HB2	2.09	0.51
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.46	0.51
1:N:387:GLY:O	1:N:388:ARG:HB3	2.09	0.51
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.25	0.51
3:P:344:VAL:O	3:P:345:GLU:HG3	2.09	0.51
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.46	0.51
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.78	0.51
3:C:9:HIS:CD2	3:C:11:LEU:H	2.28	0.51
8:H:43:ARG:O	8:H:47:ARG:HG3	2.10	0.51
1:A:344:ARG:HB2	1:A:344:ARG:CZ	2.40	0.51
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.45	0.51
1:N:307:PHE:CD1	1:N:307:PHE:C	2.89	0.51
8:U:65:ARG:O	8:U:68:CYS:HB3	2.09	0.51
9:V:64:LEU:HD12	9:V:77:ARG:C	2.36	0.51
2:B:248:ASN:ND2	2:B:250:HIS:H	2.08	0.51
5:E:74:ILE:HD11	5:E:96:LEU:HD23	1.92	0.51
1:A:106:MET:HG3	1:A:203:ILE:HG21	1.93	0.51
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.41	0.51
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LYS:O	2:B:365:LYS:HG3	2.10	0.51
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.45	0.51
6:S:78:GLU:CD	6:S:78:GLU:H	2.19	0.51
10:W:49:GLY:N	10:W:54:HIS:ND1	2.59	0.51
2:B:27:THR:CG2	2:B:28:LYS:N	2.72	0.51
5:E:133:VAL:HG13	5:E:133:VAL:O	2.11	0.51
2:O:287:ARG:HD3	9:V:53:GLU:HG2	1.92	0.51
5:R:83:GLU:HG2	5:R:102:THR:CG2	2.23	0.51
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.92	0.51
1:N:106:MET:HE2	1:N:107:PRO:HA	1.92	0.51
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.93	0.51
2:O:31:ASN:HD22	2:O:31:ASN:C	2.19	0.51
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.50	0.51
1:A:49:ASN:ND2	1:A:49:ASN:C	2.69	0.51
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.93	0.51
2:B:274:VAL:O	2:B:278:VAL:HG23	2.11	0.51
2:B:341:MET:HE2	2:B:341:MET:HA	1.92	0.51
1:N:19:LEU:C	1:N:21:ASN:H	2.19	0.51
2:O:308:ASP:OD2	9:V:55:MET:O	2.29	0.51
2:O:422:LYS:O	2:O:436:LEU:HD21	2.11	0.51
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.11	0.51
10:W:60:GLU:C	10:W:60:GLU:CD	2.79	0.51
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.93	0.50
2:B:31:ASN:HD22	2:B:32:GLY:N	2.08	0.50
1:N:206:LYS:HA	1:N:209:VAL:CG1	2.41	0.50
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.93	0.50
10:J:4:ALA:O	10:J:8:GLN:HG3	2.11	0.50
1:N:106:MET:CE	1:N:110:VAL:HG21	2.41	0.50
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.93	0.50
5:R:84:GLY:N	5:R:100:HIS:O	2.44	0.50
1:A:21:ASN:HB3	1:A:219:VAL:HG22	1.92	0.50
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.93	0.50
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.10	0.50
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.78	0.50
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.46	0.50
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.41	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.26	0.50
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.93	0.50
5:R:116:LYS:O	5:R:117:LEU:HD23	2.11	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.93	0.50
3:C:216:SER:HB3	6:F:59:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.46	0.50
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.50
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.46	0.50
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.93	0.50
3:P:98:HIS:CD2	13:P:502:HEM:NC	2.79	0.50
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.94	0.50
2:B:273:SER:O	2:B:276:GLN:HB3	2.11	0.50
2:O:291:VAL:C	2:O:293:SER:H	2.19	0.50
1:A:380:GLY:O	1:A:384:LEU:HB2	2.12	0.50
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.47	0.50
2:B:308:ASP:OD2	9:I:56:SER:HA	2.11	0.50
2:O:26:ILE:HG12	2:O:26:ILE:O	2.11	0.50
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.46	0.50
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.94	0.50
2:B:424:MET:HG2	2:B:425:ALA:N	2.27	0.50
1:N:209:VAL:O	1:N:212:ALA:HB3	2.11	0.50
2:O:361:LYS:O	2:O:365:LYS:HG3	2.11	0.50
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.27	0.50
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.92	0.49
1:A:23:LEU:HD23	1:A:24:ARG:N	2.26	0.49
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.93	0.49
1:N:410:VAL:O	1:N:413:LYS:HB3	2.11	0.49
2:O:307:PHE:CD1	2:O:308:ASP:N	2.80	0.49
5:R:101:ARG:HB3	5:R:105:GLU:HB2	1.93	0.49
1:N:219:VAL:HG12	1:N:220:SER:N	2.26	0.49
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.93	0.49
9:V:67:GLY:O	9:V:68:ILE:HD13	2.13	0.49
9:I:67:GLY:O	9:I:68:ILE:HD13	2.12	0.49
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.47	0.49
3:P:156:TYR:CD2	3:P:156:TYR:N	2.79	0.49
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.94	0.49
1:A:138:LEU:HD11	1:A:174:ILE:HD12	1.95	0.49
1:A:156:THR:HA	5:E:7:VAL:HG21	1.93	0.49
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.12	0.49
2:B:389:SER:O	2:B:390:GLY:C	2.56	0.49
1:N:138:LEU:HD11	1:N:174:ILE:HD12	1.95	0.49
1:N:156:THR:HA	5:R:7:VAL:HG21	1.94	0.49
2:O:274:VAL:O	2:O:278:VAL:HG23	2.13	0.49
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.94	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
2:O:113:ARG:O	2:O:116:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.94	0.49
4:Q:235:MET:HE1	6:S:63:LYS:HG2	1.94	0.49
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.13	0.49
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.43	0.49
2:B:262:ALA:HB2	2:B:268:GLU:HG2	1.94	0.49
1:N:191:LYS:N	1:N:195:MET:HE2	2.27	0.49
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.49
1:A:281:ASP:OD1	9:I:33:UNK:HB1	2.13	0.49
2:B:102:ARG:HH22	2:B:161:GLU:HA	1.76	0.49
2:B:257:VAL:O	2:B:323:GLY:HA3	2.13	0.49
1:A:23:LEU:HD23	1:A:23:LEU:C	2.38	0.49
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.47	0.49
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.49
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.95	0.49
8:H:72:LYS:HD2	8:H:72:LYS:N	2.27	0.49
1:N:178:THR:CG2	1:N:179:ARG:N	2.75	0.49
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.78	0.49
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.37	0.49
5:R:77:LYS:HA	5:R:191:ASP:O	2.13	0.49
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.48	0.49
1:A:106:MET:CE	1:A:110:VAL:HG21	2.43	0.48
1:A:281:ASP:OD1	1:A:281:ASP:C	2.55	0.48
2:B:335:GLU:HA	2:B:338:ARG:NH1	2.28	0.48
2:B:389:SER:O	2:B:391:THR:N	2.46	0.48
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.94	0.48
4:D:231:LYS:O	6:F:71:LYS:HE3	2.13	0.48
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.48
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.43	0.48
10:W:14:PHE:N	10:W:14:PHE:CD2	2.80	0.48
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.48	0.48
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.94	0.48
3:P:90:PHE:CZ	3:P:236:MET:HB3	2.48	0.48
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.48	0.48
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.94	0.48
3:C:344:VAL:C	3:C:345:GLU:HG3	2.37	0.48
8:H:11:GLU:CD	8:H:11:GLU:H	2.20	0.48
2:B:291:VAL:C	2:B:293:SER:H	2.21	0.48
2:B:402:ILE:HG23	2:B:403:ASP:N	2.28	0.48
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.95	0.48
1:N:49:ASN:HD22	1:N:51:LYS:N	2.05	0.48
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:318:ASP:O	2:O:319:SER:HB2	2.13	0.48
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.94	0.48
5:R:101:ARG:HH22	5:R:127:VAL:CG1	2.19	0.48
2:B:110:GLU:O	2:B:111:CYS:HB3	2.13	0.48
3:C:216:SER:CB	6:F:59:MET:HE2	2.44	0.48
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.94	0.48
2:O:248:ASN:HD22	2:O:250:HIS:H	1.61	0.48
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.94	0.48
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.96	0.48
1:A:75:PHE:HZ	1:A:86:PHE:HE2	1.61	0.48
3:C:54:MET:HG2	3:P:178:ARG:HA	1.95	0.48
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.96	0.48
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.78	0.48
2:B:422:LYS:O	2:B:436:LEU:HD21	2.14	0.48
1:N:26:ALA:O	1:N:198:ALA:HA	2.14	0.48
2:O:78:LYS:HA	2:O:131:GLU:OE2	2.14	0.48
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.94	0.48
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.78	0.48
1:A:351:GLU:O	1:A:354:VAL:HG22	2.13	0.48
5:E:82:PRO:HD2	5:E:85:LYS:HD3	1.95	0.48
5:E:134:ILE:HD11	5:E:193:VAL:HG21	1.96	0.48
8:H:32:LYS:O	8:H:36:ARG:HG3	2.14	0.48
1:N:206:LYS:CA	1:N:209:VAL:HG12	2.43	0.48
2:O:67:HIS:O	2:O:70:ARG:HB3	2.14	0.48
2:O:76:THR:HG22	2:O:82:SER:N	2.20	0.48
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.26	0.48
3:P:2:ALA:CB	3:P:8:SER:HB3	2.40	0.48
5:R:109:GLU:C	5:R:111:GLU:N	2.72	0.48
10:W:20:PHE:O	10:W:24:VAL:HG23	2.14	0.48
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.96	0.48
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.43	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.31	0.48
3:P:71:CYS:SG	3:P:81:ARG:HD2	2.54	0.48
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.14	0.48
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.14	0.48
19:Q:3003:CDL:H511	7:T:26:ILE:HG21	1.96	0.48
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.43	0.48
3:C:323:GLN:OE1	7:G:47:LYS:HD3	2.14	0.48
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.94	0.48
5:E:41:ALA:O	5:E:45:VAL:HG23	2.14	0.48
7:G:40:ARG:HD2	19:G:2004:CDL:OA4	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:394:GLU:O	1:N:397:SER:HB3	2.13	0.48
3:P:34:PHE:HB2	21:P:381:HOH:O	2.13	0.48
6:S:98:ILE:O	6:S:102:LEU:HG	2.14	0.48
1:A:240:GLU:CD	1:A:242:ARG:HE	2.21	0.47
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.44	0.47
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.13	0.47
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	1.95	0.47
5:R:155:GLY:HA3	5:R:166:ASP:C	2.39	0.47
9:V:28:UNK:HA	9:V:72:ALA:HB2	1.94	0.47
1:A:233:ARG:HH12	1:A:316:ASP:HB2	1.80	0.47
2:B:60:THR:HG23	2:B:61:ALA:N	2.29	0.47
1:N:21:ASN:CB	1:N:219:VAL:HA	2.44	0.47
1:N:239:SER:HB2	7:T:17:SER:O	2.14	0.47
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.49	0.47
5:R:165:TYR:HA	5:R:170:ARG:O	2.14	0.47
1:A:136:GLN:O	1:A:140:GLU:HG3	2.13	0.47
2:B:60:THR:CG2	2:B:61:ALA:N	2.76	0.47
2:B:76:THR:CG2	2:B:82:SER:HB2	2.45	0.47
8:H:18:THR:O	8:H:22:GLU:HG3	2.14	0.47
1:N:53:ASN:N	1:N:173:ASN:ND2	2.62	0.47
2:O:341:MET:CE	2:O:341:MET:HA	2.44	0.47
2:O:353:THR:CG2	2:O:354:GLU:N	2.77	0.47
5:R:147:ILE:HG22	5:R:148:ALA:H	1.78	0.47
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.97	0.47
2:O:248:ASN:C	2:O:248:ASN:ND2	2.67	0.47
2:O:295:LEU:O	2:O:299:VAL:HG23	2.14	0.47
3:P:78:TRP:CD2	4:Q:197:GLU:HG3	2.49	0.47
3:P:129:PHE:CD1	14:P:3001:FNM:H27B	2.49	0.47
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.97	0.47
7:T:36:ASN:O	7:T:40:ARG:HG3	2.14	0.47
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.96	0.47
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.44	0.47
2:O:399:ALA:C	2:O:402:ILE:HG22	2.39	0.47
1:A:394:GLU:O	1:A:397:SER:HB3	2.15	0.47
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.96	0.47
2:O:338:ARG:HB2	2:O:338:ARG:NH1	2.28	0.47
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.49	0.47
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.97	0.47
1:A:387:GLY:O	1:A:388:ARG:HB3	2.13	0.47
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.30	0.47
2:B:248:ASN:C	2:B:248:ASN:ND2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:THR:OG1	2:B:408:ALA:HB3	2.15	0.47
4:D:70:VAL:HG21	4:D:83:ARG:NH1	2.28	0.47
5:E:102:THR:O	5:E:106:ILE:HG13	2.14	0.47
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.49	0.47
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.50	0.47
1:N:75:PHE:HZ	1:N:86:PHE:HE2	1.61	0.47
1:N:443:TRP:O	1:N:444:ILE:CB	2.63	0.47
2:O:202:ALA:HB3	2:O:229:GLY:O	2.14	0.47
2:O:389:SER:O	2:O:390:GLY:C	2.58	0.47
5:R:78:LEU:HD13	5:R:132:TRP:CE2	2.50	0.47
8:U:65:ARG:O	8:U:69:VAL:HG23	2.15	0.47
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.97	0.47
2:B:46:ARG:HG3	2:B:110:GLU:HG2	1.96	0.47
1:A:350:THR:CG2	1:A:351:GLU:N	2.77	0.47
2:B:341:MET:CE	2:B:341:MET:HA	2.45	0.47
2:B:353:THR:CG2	2:B:354:GLU:N	2.78	0.47
3:C:156:TYR:N	3:C:156:TYR:CD2	2.81	0.47
4:Q:167:GLU:CG	8:U:13:LEU:HD13	2.45	0.47
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.50	0.47
2:B:312:PHE:CE2	2:B:314:VAL:HG23	2.50	0.47
3:C:269:ILE:O	3:C:269:ILE:HG22	2.14	0.47
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.97	0.47
6:F:59:MET:HE3	6:F:59:MET:HA	1.97	0.47
10:J:49:GLY:N	10:J:54:HIS:ND1	2.63	0.47
13:P:502:HEM:HMC2	13:P:502:HEM:HBC2	1.97	0.47
5:R:113:ASP:OD2	5:R:116:LYS:HG3	2.14	0.47
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.50	0.47
2:B:26:ILE:O	2:B:26:ILE:HG12	2.16	0.46
2:B:385:GLU:C	2:B:387:LEU:H	2.23	0.46
3:C:152:SER:HB3	3:C:162:VAL:HG21	1.96	0.46
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.15	0.46
1:A:21:ASN:HA	1:A:219:VAL:HG13	1.98	0.46
1:A:240:GLU:HA	1:A:422:LEU:O	2.14	0.46
1:A:304:CYS:HB2	1:A:325:VAL:O	2.15	0.46
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.97	0.46
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.48	0.46
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.97	0.46
8:H:65:ARG:O	8:H:68:CYS:HB3	2.16	0.46
1:N:106:MET:HE2	1:N:106:MET:O	2.14	0.46
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.50	0.46
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:338:ARG:HH11	2:O:338:ARG:CB	2.28	0.46
4:Q:200:GLN:NE2	17:Q:3091:BOG:H3	2.29	0.46
5:R:118:ARG:HB2	5:R:171:ILE:CG2	2.45	0.46
1:A:103:SER:HB3	1:A:202:GLY:O	2.15	0.46
5:E:189:GLY:O	5:E:190:ASP:C	2.59	0.46
2:O:393:THR:HG23	2:O:397:VAL:HB	1.97	0.46
5:R:101:ARG:NH2	5:R:127:VAL:HG11	2.22	0.46
1:A:410:VAL:O	1:A:413:LYS:HB3	2.15	0.46
1:N:77:LYS:HE3	2:O:359:LYS:HZ1	1.80	0.46
2:O:27:THR:CG2	2:O:28:LYS:H	2.21	0.46
2:O:76:THR:CG2	2:O:82:SER:HB2	2.43	0.46
7:T:75:ALA:HA	7:T:78:GLU:HG3	1.97	0.46
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.97	0.46
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.97	0.46
2:O:19:PRO:HB3	2:O:41:PHE:CE2	2.50	0.46
8:U:72:LYS:N	8:U:72:LYS:HD2	2.29	0.46
1:A:178:THR:CG2	1:A:179:ARG:N	2.79	0.46
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.97	0.46
3:C:268:HIS:HB3	21:C:1288:HOH:O	2.14	0.46
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.15	0.46
1:N:105:ASP:O	1:N:106:MET:C	2.59	0.46
5:R:78:LEU:HB3	5:R:132:TRP:CH2	2.50	0.46
5:R:146:PRO:HB2	5:R:156:TYR:HB3	1.97	0.46
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.81	0.46
8:H:54:CYS:HA	8:H:57:GLU:OE2	2.16	0.46
2:O:267:ALA:C	2:O:269:ALA:H	2.24	0.46
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.46
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.16	0.46
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.16	0.46
1:N:382:HIS:HB3	1:N:388:ARG:O	2.16	0.46
2:O:341:MET:HA	2:O:341:MET:HE2	1.96	0.46
3:P:216:SER:HB3	6:S:59:MET:HE2	1.98	0.46
1:A:49:ASN:HD22	1:A:51:LYS:N	2.08	0.46
1:A:105:ASP:O	1:A:106:MET:C	2.59	0.46
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.98	0.46
3:C:198:LEU:HD21	13:C:502:HEM:CMA	2.45	0.46
6:F:13:MET:HE2	6:F:13:MET:HA	1.97	0.46
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.97	0.46
2:O:327:ILE:HG22	9:V:55:MET:CE	2.46	0.46
3:P:269:ILE:O	3:P:269:ILE:HG22	2.14	0.46
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:32:LYS:O	8:U:36:ARG:HG3	2.16	0.46
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.49	0.46
2:B:393:THR:HG23	2:B:397:VAL:HB	1.97	0.46
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.98	0.46
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.51	0.46
1:N:106:MET:HE3	1:N:208:LEU:HD12	1.98	0.46
2:O:353:THR:HB	2:O:356:ASP:OD1	2.16	0.46
6:S:96:GLU:OE2	6:S:96:GLU:HA	2.16	0.46
2:B:327:ILE:CG2	9:I:55:MET:HE3	2.47	0.45
4:D:195:GLU:HG3	4:D:198:HIS:HB2	1.97	0.45
1:N:7:THR:HG21	2:O:113:ARG:CD	2.44	0.45
1:N:351:GLU:O	1:N:354:VAL:HG22	2.16	0.45
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.15	0.45
5:R:126:ARG:NH2	5:R:170:ARG:HG3	2.30	0.45
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.30	0.45
9:V:31:UNK:O	9:V:73:PRO:HG2	2.16	0.45
1:A:280:TYR:CG	1:A:281:ASP:N	2.84	0.45
4:D:97:ASN:OD1	4:D:99:GLU:HB2	2.16	0.45
5:E:73:LYS:HB3	5:E:195:VAL:O	2.16	0.45
2:O:402:ILE:HG23	2:O:403:ASP:H	1.81	0.45
3:P:17:ASN:HB2	17:P:2010:BOG:O3	2.15	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.16	0.45
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.46	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.34	0.45
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.98	0.45
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.52	0.45
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.47	0.45
2:O:50:PHE:C	2:O:51:ILE:HG13	2.41	0.45
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.51	0.45
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.81	0.45
5:R:134:ILE:CD1	5:R:193:VAL:HG21	2.46	0.45
1:A:4:TYR:CE2	1:A:396:ASP:OD2	2.69	0.45
2:B:76:THR:HG22	2:B:82:SER:CB	2.46	0.45
1:N:23:LEU:HD23	1:N:24:ARG:N	2.31	0.45
1:N:294:LEU:HB2	1:N:341:GLU:HG3	1.99	0.45
2:O:424:MET:HG2	2:O:425:ALA:N	2.30	0.45
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.17	0.45
2:B:31:ASN:HD22	2:B:31:ASN:C	2.23	0.45
1:N:350:THR:HG22	1:N:352:SER:N	2.31	0.45
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.46	0.45
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:VAL:O	2:B:120:MET:HB2	2.16	0.45
2:B:218:GLN:O	2:B:222:GLN:HG3	2.16	0.45
2:B:353:THR:HB	2:B:356:ASP:OD1	2.16	0.45
5:R:71:LEU:HD13	5:R:92:ARG:HD3	1.98	0.45
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.16	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.17	0.45
1:A:191:LYS:N	1:A:195:MET:HE2	2.31	0.45
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.17	0.45
2:B:195:VAL:O	2:B:199:PHE:HB2	2.16	0.45
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.99	0.45
2:B:338:ARG:HB2	2:B:338:ARG:NH1	2.31	0.45
2:B:357:VAL:O	2:B:361:LYS:HG3	2.16	0.45
3:C:79:LEU:HD22	4:D:204:MET:HE1	1.97	0.45
4:D:238:ARG:HD2	7:G:14:ILE:HD12	1.97	0.45
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.97	0.45
2:O:31:ASN:ND2	2:O:31:ASN:C	2.74	0.45
2:B:24:LEU:HG	2:B:24:LEU:O	2.17	0.45
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.52	0.45
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.99	0.45
8:H:10:GLU:HB2	8:H:11:GLU:OE2	2.16	0.45
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.32	0.45
2:O:397:VAL:O	2:O:401:LYS:HG2	2.16	0.45
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.47	0.45
1:A:370:ASP:O	2:B:374:THR:HG22	2.17	0.45
2:B:46:ARG:HE	2:B:376:GLN:HA	1.82	0.45
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.97	0.45
1:N:136:GLN:O	1:N:140:GLU:HG3	2.17	0.45
1:A:168:GLU:H	1:A:168:GLU:CD	2.25	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.45
2:B:327:ILE:HG22	9:I:55:MET:HE3	1.99	0.45
3:C:198:LEU:HD21	13:C:502:HEM:C3A	2.52	0.45
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.47	0.45
5:E:77:LYS:C	5:E:79:SER:H	2.25	0.45
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.99	0.45
1:N:62:LEU:C	1:N:64:PHE:H	2.23	0.45
1:N:161:THR:HG21	1:N:235:ARG:N	2.32	0.45
2:O:116:VAL:O	2:O:120:MET:HB2	2.17	0.45
5:R:91:TRP:O	5:R:92:ARG:C	2.60	0.45
5:R:147:ILE:CG2	5:R:148:ALA:N	2.80	0.45
1:A:89:TYR:CD1	1:A:89:TYR:C	2.95	0.44
1:A:242:ARG:O	7:G:14:ILE:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PHE:C	2:B:51:ILE:HG13	2.42	0.44
2:B:67:HIS:O	2:B:70:ARG:HB3	2.16	0.44
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.53	0.44
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.47	0.44
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.99	0.44
1:A:3:THR:OG1	1:A:6:GLN:HG3	2.17	0.44
2:B:350:GLY:C	2:B:352:VAL:H	2.25	0.44
2:B:399:ALA:C	2:B:402:ILE:HG22	2.43	0.44
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.17	0.44
4:D:62:LYS:O	4:D:66:GLU:HG3	2.17	0.44
4:D:161:ALA:O	4:D:162:PRO:C	2.60	0.44
5:E:10:PHE:O	5:E:14:ARG:HG3	2.17	0.44
3:P:79:LEU:HD22	4:Q:204:MET:HE1	1.99	0.44
1:A:170:THR:CG2	1:A:171:THR:N	2.81	0.44
2:O:62:ASN:O	2:O:65:THR:CG2	2.62	0.44
2:O:406:THR:OG1	2:O:408:ALA:HB3	2.17	0.44
3:P:358:SER:O	3:P:362:ILE:HG13	2.18	0.44
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.53	0.44
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.81	0.44
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.31	0.44
3:C:305:ILE:HB	3:C:306:PRO:HD3	2.00	0.44
7:G:24:ARG:HB2	7:G:27:PRO:HB3	2.00	0.44
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.46	0.44
5:R:133:VAL:HG13	5:R:133:VAL:O	2.17	0.44
2:B:248:ASN:HD22	2:B:250:HIS:H	1.65	0.44
1:N:23:LEU:HD23	1:N:23:LEU:C	2.42	0.44
1:N:350:THR:CG2	1:N:351:GLU:N	2.80	0.44
2:O:60:THR:CG2	2:O:61:ALA:N	2.80	0.44
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.82	0.44
2:B:312:PHE:CZ	2:B:314:VAL:CG2	3.01	0.44
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.98	0.44
2:O:110:GLU:O	2:O:111:CYS:HB3	2.17	0.44
5:R:112:VAL:O	5:R:113:ASP:C	2.60	0.44
1:A:53:ASN:H	1:A:173:ASN:ND2	2.16	0.44
2:B:19:PRO:HB2	2:B:41:PHE:CE1	2.52	0.44
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.52	0.44
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.99	0.44
5:R:109:GLU:HB3	5:R:123:ASP:HB2	2.00	0.44
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.53	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.44
7:G:80:ASP:O	7:G:81:GLN:OXT	2.36	0.44
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.48	0.44
4:Q:95:TYR:HA	4:Q:96:PRO:HD3	1.85	0.44
5:R:177:PRO:HB2	5:R:178:TYR:CE1	2.53	0.44
4:D:120:ARG:HH21	18:D:501:HEC:CGA	2.31	0.44
5:R:124:LEU:HA	5:R:127:VAL:CG2	2.48	0.44
5:R:163:SER:HA	5:R:174:GLY:HA3	2.00	0.44
7:T:40:ARG:HD2	19:T:3004:CDL:OA4	2.18	0.44
2:B:218:GLN:HG2	2:B:222:GLN:OE1	2.18	0.43
1:N:143:ASN:ND2	9:V:48:PRO:HD2	2.27	0.43
2:O:24:LEU:O	2:O:24:LEU:HG	2.18	0.43
2:O:276:GLN:HG2	2:O:281:ALA:HB2	2.00	0.43
3:P:25:PRO:HB2	3:P:28:ILE:HG23	2.00	0.43
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.17	0.43
2:B:402:ILE:HG23	2:B:403:ASP:H	1.81	0.43
4:D:3:LEU:HD11	7:G:72:LYS:HE3	2.00	0.43
9:I:32:UNK:N	9:I:73:PRO:CG	2.74	0.43
1:N:168:GLU:CD	1:N:168:GLU:H	2.26	0.43
2:O:389:SER:O	2:O:391:THR:N	2.51	0.43
3:P:101:ARG:NH2	13:P:502:HEM:HBD2	2.32	0.43
5:R:146:PRO:CB	5:R:156:TYR:HB3	2.48	0.43
1:A:272:VAL:O	1:A:275:ALA:HB3	2.18	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.61	0.43
5:E:185:TYR:CB	5:E:195:VAL:HG22	2.47	0.43
6:F:96:GLU:HA	6:F:96:GLU:OE2	2.18	0.43
7:G:75:ALA:HA	7:G:78:GLU:HG3	1.99	0.43
2:O:60:THR:HG23	2:O:61:ALA:N	2.33	0.43
5:R:193:VAL:HG13	5:R:193:VAL:O	2.18	0.43
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.89	0.43
3:C:178:ARG:HA	3:P:54:MET:HG2	1.99	0.43
4:D:138:PRO:HB3	8:H:58:LEU:HD22	2.00	0.43
5:E:19:MET:HE2	5:E:19:MET:HB2	1.86	0.43
5:E:74:ILE:HD11	5:E:96:LEU:CD2	2.48	0.43
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.43
9:I:64:LEU:HD12	9:I:77:ARG:C	2.41	0.43
2:O:286:LYS:C	2:O:288:GLY:H	2.27	0.43
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.51	0.43
2:B:397:VAL:O	2:B:401:LYS:HG2	2.18	0.43
5:E:193:VAL:O	5:E:193:VAL:HG13	2.19	0.43
9:I:58:ARG:HA	9:I:58:ARG:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.48	0.43
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.43
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.99	0.43
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.01	0.43
2:B:366:ALA:O	2:B:370:MET:HG3	2.19	0.43
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.54	0.43
4:D:35:GLN:NE2	4:D:169:LEU:HD12	2.34	0.43
10:J:20:PHE:O	10:J:24:VAL:HG23	2.19	0.43
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.47	0.43
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	2.00	0.43
5:R:136:VAL:O	5:R:138:VAL:N	2.43	0.43
1:A:350:THR:HG22	1:A:352:SER:N	2.28	0.43
2:B:31:ASN:ND2	2:B:31:ASN:C	2.76	0.43
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.43
3:C:105:TYR:O	3:C:315:THR:HG22	2.18	0.43
3:C:234:THR:HG21	4:D:219:LEU:HD12	2.01	0.43
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.18	0.43
1:N:206:LYS:O	1:N:209:VAL:HG12	2.17	0.43
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.99	0.43
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.18	0.43
5:R:112:VAL:O	5:R:113:ASP:O	2.36	0.43
6:S:59:MET:HE3	6:S:59:MET:HA	2.00	0.43
8:U:17:LEU:HD13	8:U:73:LEU:HD22	2.00	0.43
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.49	0.43
3:C:117:GLY:O	13:C:502:HEM:HMC3	2.19	0.43
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.00	0.43
3:C:354:MET:HE2	3:C:354:MET:HA	2.01	0.43
1:N:240:GLU:HA	1:N:422:LEU:O	2.19	0.43
2:O:350:GLY:C	2:O:352:VAL:H	2.27	0.43
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.00	0.43
5:R:161:HIS:HB2	20:R:501:FES:S1	2.58	0.43
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.54	0.43
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.19	0.43
1:A:106:MET:HE3	1:A:208:LEU:HD12	2.00	0.43
3:C:377:MET:HE2	6:F:20:TYR:CB	2.46	0.43
1:N:269:VAL:HG22	1:N:406:MET:HE2	2.00	0.43
1:N:281:ASP:OD1	1:N:281:ASP:C	2.61	0.43
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.01	0.43
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.43
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.34	0.43
5:E:91:TRP:O	5:E:92:ARG:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:VAL:HA	1:N:196:VAL:O	2.19	0.43
3:P:133:VAL:HG22	14:P:3001:FNM:H27	2.01	0.43
5:R:71:LEU:HD13	5:R:92:ARG:NH1	2.34	0.43
5:R:117:LEU:O	5:R:118:ARG:C	2.62	0.43
1:A:62:LEU:HD11	1:A:127:ILE:HG12	2.00	0.42
2:B:230:ALA:O	2:B:231:GLY:C	2.61	0.42
5:E:55:VAL:O	5:E:59:ILE:HG12	2.19	0.42
5:E:97:PHE:CE2	5:E:137:GLY:HA3	2.54	0.42
5:E:161:HIS:HB2	20:E:501:FES:S1	2.59	0.42
2:O:402:ILE:O	2:O:405:VAL:HG23	2.19	0.42
3:P:101:ARG:C	3:P:101:ARG:CD	2.87	0.42
3:P:129:PHE:CE1	14:P:3001:FNM:H27B	2.54	0.42
2:B:394:ALA:HB3	2:B:397:VAL:HG23	2.01	0.42
3:C:247:SER:N	3:C:248:PRO:HD3	2.34	0.42
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	2.00	0.42
4:D:200:GLN:CD	17:D:2091:BOG:H5	2.44	0.42
2:O:47:ILE:HG22	2:O:48:GLY:N	2.34	0.42
2:O:312:PHE:CE2	2:O:314:VAL:HG23	2.54	0.42
5:R:85:LYS:O	5:R:99:ARG:HG3	2.20	0.42
2:B:399:ALA:CA	2:B:402:ILE:HG22	2.50	0.42
7:G:77:TYR:O	8:H:47:ARG:NH1	2.52	0.42
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.01	0.42
1:A:328:PRO:HB3	1:A:427:PRO:HB2	2.02	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.76	0.42
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.85	0.42
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.82	0.42
8:H:57:GLU:H	8:H:57:GLU:CD	2.27	0.42
10:J:14:PHE:CD2	10:J:14:PHE:N	2.85	0.42
1:N:62:LEU:C	1:N:64:PHE:N	2.77	0.42
9:V:28:UNK:CB	9:V:71:ASN:ND2	2.83	0.42
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.27	0.42
2:B:28:LYS:O	2:B:28:LYS:HG2	2.18	0.42
5:E:134:ILE:CD1	5:E:193:VAL:HG21	2.50	0.42
9:I:65:VAL:HG12	9:I:66:ALA:N	2.34	0.42
1:N:240:GLU:CD	1:N:242:ARG:HE	2.27	0.42
2:O:245:ARG:HB3	2:O:430:LEU:CD1	2.49	0.42
3:P:350:ILE:O	3:P:354:MET:HG2	2.19	0.42
7:T:24:ARG:HB2	7:T:27:PRO:HB3	2.01	0.42
8:U:18:THR:O	8:U:22:GLU:HG3	2.19	0.42
5:E:191:ASP:OD1	5:E:191:ASP:O	2.38	0.42
7:G:45:VAL:O	7:G:49:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.55	0.42
1:N:137:GLU:O	1:N:141:MET:HG3	2.20	0.42
2:O:24:LEU:HD12	2:O:37:SER:O	2.18	0.42
3:P:216:SER:CB	6:S:59:MET:HE2	2.49	0.42
5:R:63:SER:O	5:R:64:ALA:C	2.62	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.54	0.42
6:S:40:ASP:O	6:S:44:LYS:HG3	2.18	0.42
6:S:71:LYS:O	6:S:72:HIS:HB2	2.18	0.42
7:T:72:LYS:HZ2	8:U:56:GLU:HB3	1.84	0.42
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.54	0.42
1:A:62:LEU:C	1:A:64:PHE:H	2.28	0.42
2:O:129:ALA:N	2:O:130:PRO:CD	2.83	0.42
2:O:395:PRO:HA	2:O:398:VAL:HG12	2.00	0.42
3:P:198:LEU:HD21	13:P:502:HEM:CMA	2.49	0.42
8:U:34:ARG:O	8:U:38:GLU:HG3	2.20	0.42
2:B:84:ARG:HD2	6:S:107:TRP:HZ3	1.85	0.42
3:C:269:ILE:CG2	14:C:2001:FNM:H23	2.48	0.42
3:C:285:ILE:HA	3:C:286:PRO:HD2	1.92	0.42
5:E:189:GLY:O	5:E:192:LEU:N	2.52	0.42
1:N:206:LYS:CD	1:N:206:LYS:N	2.64	0.42
2:O:357:VAL:O	2:O:361:LYS:HG3	2.20	0.42
7:T:72:LYS:HE3	8:U:56:GLU:HB2	2.02	0.42
10:W:52:TRP:O	10:W:56:LYS:HB2	2.19	0.42
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.50	0.42
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.80	0.42
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.54	0.42
5:E:163:SER:HA	5:E:174:GLY:HA3	2.01	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.53	0.42
2:O:257:VAL:O	2:O:323:GLY:HA3	2.19	0.42
2:O:264:VAL:HG23	2:O:316:TYR:C	2.44	0.42
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.55	0.42
7:T:72:LYS:CG	8:U:56:GLU:OE2	2.51	0.42
1:A:161:THR:HG21	1:A:235:ARG:H	1.83	0.42
2:B:26:ILE:HA	2:B:35:ILE:O	2.19	0.42
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.55	0.42
6:F:71:LYS:O	6:F:72:HIS:HB2	2.20	0.42
9:I:38:UNK:O	9:I:40:UNK:N	2.52	0.42
1:N:158:PHE:O	1:N:164:ALA:HB2	2.20	0.42
2:O:43:PRO:C	2:O:113:ARG:HG3	2.44	0.42
4:Q:79:GLU:OE2	4:Q:79:GLU:HA	2.20	0.42
5:R:73:LYS:HB3	5:R:195:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:LEU:C	1:N:21:ASN:N	2.78	0.41
1:N:123:GLU:OE1	1:N:123:GLU:HA	2.20	0.41
1:N:170:THR:CG2	1:N:171:THR:N	2.83	0.41
2:O:307:PHE:CD1	2:O:307:PHE:C	2.98	0.41
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.84	0.41
3:P:344:VAL:C	3:P:345:GLU:HG3	2.44	0.41
1:A:105:ASP:C	1:A:107:PRO:HD2	2.45	0.41
2:B:22:GLU:HG3	2:B:23:ASP:H	1.84	0.41
5:R:139:CYS:C	5:R:141:HIS:H	2.28	0.41
1:A:228:VAL:O	1:A:228:VAL:HG13	2.20	0.41
2:B:385:GLU:C	2:B:387:LEU:N	2.76	0.41
2:B:394:ALA:C	2:B:396:SER:H	2.28	0.41
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.02	0.41
3:C:194:THR:O	3:C:197:HIS:HB3	2.21	0.41
4:D:68:VAL:HG12	4:D:69:GLU:N	2.35	0.41
1:N:402:VAL:HG22	1:N:406:MET:HE2	2.01	0.41
2:O:63:LEU:HB2	2:O:182:ARG:HD3	2.02	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.75	0.41
4:Q:195:GLU:HG3	4:Q:195:GLU:O	2.20	0.41
5:R:73:LYS:HG2	5:R:196:GLY:HA3	2.01	0.41
10:W:48:GLU:HA	10:W:54:HIS:CE1	2.55	0.41
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.54	0.41
1:A:144:ASP:CG	1:A:147:ASN:HD22	2.29	0.41
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.82	0.41
2:B:295:LEU:O	2:B:299:VAL:HG23	2.20	0.41
1:N:284:PHE:CE2	9:V:71:ASN:O	2.73	0.41
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.03	0.41
5:R:141:HIS:HB3	20:R:501:FES:S2	2.61	0.41
5:R:176:ALA:HA	5:R:177:PRO:HD2	1.95	0.41
1:A:90:THR:O	1:A:167:VAL:HG11	2.21	0.41
1:A:233:ARG:NH1	1:A:316:ASP:HB2	2.34	0.41
1:A:294:LEU:HB2	1:A:341:GLU:HG3	2.02	0.41
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.51	0.41
2:B:398:VAL:HG13	2:B:399:ALA:N	2.35	0.41
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.84	0.41
1:N:140:GLU:CG	9:V:50:LEU:HD12	2.49	0.41
2:O:34:ILE:HD13	2:O:390:GLY:CA	2.51	0.41
5:R:75:GLU:HG2	5:R:194:VAL:HG22	2.02	0.41
6:S:77:LYS:O	6:S:77:LYS:HG2	2.19	0.41
1:A:316:ASP:OD1	1:A:316:ASP:N	2.51	0.41
4:D:38:SER:O	4:D:94:PRO:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:VAL:O	4:D:142:VAL:HG23	2.21	0.41
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.54	0.41
2:O:132:PHE:HB2	2:O:192:HIS:CE1	2.56	0.41
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.47	0.41
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	2.03	0.41
2:B:306:PRO:HA	9:I:52:ARG:HG2	2.02	0.41
3:C:133:VAL:HG22	14:C:2001:FNM:H27	2.02	0.41
2:O:178:CYS:SG	2:O:183:ILE:HD13	2.61	0.41
2:O:359:LYS:O	2:O:362:ASN:HB2	2.21	0.41
3:C:377:MET:HE2	6:F:20:TYR:CG	2.56	0.41
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.55	0.41
4:D:204:MET:HG2	17:D:2009:BOG:H5	2.02	0.41
5:E:85:LYS:O	5:E:99:ARG:HG3	2.21	0.41
5:E:185:TYR:HB3	5:E:195:VAL:HG22	2.02	0.41
6:F:13:MET:CE	6:F:16:ILE:HD12	2.51	0.41
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.51	0.41
1:A:281:ASP:OD2	9:I:33:UNK:HB1	2.20	0.41
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.03	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.03	0.41
2:B:84:ARG:HD2	6:S:107:TRP:CZ3	2.56	0.41
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.36	0.41
3:C:223:PRO:HB2	3:C:227:PHE:HD2	1.85	0.41
4:D:162:PRO:HA	4:D:163:PRO:HD2	2.01	0.41
1:N:14:THR:OG1	1:N:389:ARG:HG2	2.21	0.41
1:N:89:TYR:CD1	1:N:89:TYR:C	2.99	0.41
1:N:228:VAL:O	1:N:228:VAL:HG13	2.21	0.41
2:O:57:TYR:CD1	2:O:57:TYR:N	2.89	0.41
2:O:147:ASP:O	2:O:150:VAL:HG22	2.20	0.41
2:O:222:GLN:O	2:O:223:PHE:HD2	2.04	0.41
2:O:345:LYS:O	2:O:348:ALA:N	2.52	0.41
2:O:394:ALA:C	2:O:396:SER:H	2.29	0.41
3:P:31:TRP:CH2	11:P:3007:PEE:H20	2.55	0.41
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.34	0.41
4:D:74:PRO:HA	4:D:79:GLU:O	2.20	0.41
5:E:71:LEU:HD13	5:E:92:ARG:HD3	2.02	0.41
8:H:51:GLU:HA	8:H:51:GLU:OE1	2.20	0.41
1:N:18:THR:HG23	1:N:24:ARG:HG3	2.02	0.41
1:N:57:TYR:HA	1:N:90:THR:HG21	2.03	0.41
1:N:328:PRO:HB3	1:N:427:PRO:HB2	2.03	0.41
2:O:67:HIS:CD2	2:O:67:HIS:C	2.98	0.41
10:W:26:LEU:O	10:W:30:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:CG1	1:A:220:SER:N	2.84	0.40
2:B:38:LEU:HD12	2:B:39:GLU:H	1.85	0.40
2:B:109:VAL:HG21	2:B:119:VAL:HG12	2.02	0.40
14:C:2001:FNM:H13	14:C:2001:FNM:H7B	1.85	0.40
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.85	0.40
10:J:5:LEU:HD23	10:J:5:LEU:HA	1.95	0.40
6:S:12:LEU:HB3	6:S:13:MET:CE	2.50	0.40
6:S:79:GLN:HE21	6:S:79:GLN:HB3	1.68	0.40
10:W:56:LYS:HE2	10:W:56:LYS:HB3	1.86	0.40
2:B:394:ALA:C	2:B:396:SER:N	2.78	0.40
3:C:350:ILE:O	3:C:354:MET:HG2	2.21	0.40
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.03	0.40
4:D:218:LEU:CD2	5:E:39:VAL:HG13	2.51	0.40
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	2.03	0.40
6:S:84:GLU:H	6:S:84:GLU:CD	2.29	0.40
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.21	0.40
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.57	0.40
4:D:223:LYS:HD3	4:D:223:LYS:C	2.46	0.40
5:E:84:GLY:N	5:E:100:HIS:O	2.47	0.40
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.89	0.40
1:N:354:VAL:O	1:N:355:LYS:C	2.64	0.40
2:O:256:ALA:HB2	2:O:325:TYR:CD1	2.57	0.40
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.51	0.40
2:B:307:PHE:CD1	2:B:307:PHE:C	2.99	0.40
2:B:395:PRO:C	2:B:398:VAL:HG12	2.47	0.40
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.93	0.40
6:F:84:GLU:H	6:F:84:GLU:CD	2.28	0.40
1:N:293:ARG:HE	1:N:293:ARG:HB3	1.71	0.40
3:P:377:MET:HE1	6:S:19:TRP:CZ3	2.52	0.40
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.36	0.40
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.87	0.40
3:C:342:GLN:HB3	3:C:343:PRO:HD2	2.04	0.40
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.03	0.40
4:D:122:GLY:O	4:D:125:ASP:HB2	2.22	0.40
7:G:41:PHE:O	7:G:45:VAL:CG2	2.67	0.40
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.85	0.40
2:O:21:ALA:O	2:O:22:GLU:HB2	2.21	0.40
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.22	0.40
5:R:147:ILE:HG13	5:R:157:TYR:O	2.22	0.40
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	412 (93%)	23 (5%)	6 (1%)	9	30
1	N	440/446 (99%)	411 (93%)	22 (5%)	7 (2%)	7	27
2	B	419/441 (95%)	374 (89%)	35 (8%)	10 (2%)	4	17
2	O	420/441 (95%)	372 (89%)	41 (10%)	7 (2%)	7	25
3	C	378/380 (100%)	364 (96%)	14 (4%)	0	100	100
3	P	377/380 (99%)	360 (96%)	17 (4%)	0	100	100
4	D	239/241 (99%)	228 (95%)	11 (5%)	0	100	100
4	Q	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
5	E	194/196 (99%)	170 (88%)	18 (9%)	6 (3%)	3	12
5	R	192/196 (98%)	156 (81%)	28 (15%)	8 (4%)	2	7
6	F	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	12	38
6	S	99/110 (90%)	91 (92%)	6 (6%)	2 (2%)	6	21
7	G	79/81 (98%)	69 (87%)	10 (13%)	0	100	100
7	T	76/81 (94%)	68 (90%)	8 (10%)	0	100	100
8	H	68/77 (88%)	62 (91%)	6 (9%)	0	100	100
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	8	28
9	I	29/47 (62%)	26 (90%)	2 (7%)	1 (3%)	3	11
9	V	29/47 (62%)	24 (83%)	5 (17%)	0	100	100
10	J	59/61 (97%)	55 (93%)	3 (5%)	1 (2%)	7	25
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	3	11
All	All	4000/4160 (96%)	3673 (92%)	275 (7%)	52 (1%)	9	31

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG

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Mol	Chain	Res	Type
2	B	26	ILE
2	B	226	ILE
2	B	227	ARG
2	B	389	SER
5	E	188	VAL
5	E	190	ASP
1	N	20	ASP
1	N	282	ARG
2	O	26	ILE
2	O	228	SER
2	O	389	SER
5	R	113	ASP
5	R	191	ASP
8	U	13	LEU
1	A	218	GLY
2	B	171	ALA
2	B	390	GLY
5	E	137	GLY
1	N	218	GLY
2	O	171	ALA
2	O	390	GLY
5	R	137	GLY
5	R	147	ILE
5	R	189	GLY
1	A	72	CYS
1	A	443	TRP
6	F	77	LYS
1	N	72	CYS
1	N	262	TRP
1	N	443	TRP
5	R	149	ASN
1	A	262	TRP
5	R	110	ALA
6	S	77	LYS
10	W	56	LYS
2	B	29	LEU
5	E	141	HIS
10	J	56	LYS
6	S	11	ARG
10	W	61	ALA
2	B	220	ALA
2	B	231	GLY

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Mol	Chain	Res	Type
2	O	29	LEU
5	E	189	GLY
1	A	71	PRO
2	B	265	GLY
5	E	120	PRO
2	O	231	GLY
9	I	48	PRO
1	N	71	PRO
5	R	188	VAL

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%)	357 (98%)	8 (2%)	45	78
1	N	365/368 (99%)	353 (97%)	12 (3%)	33	69
2	B	332/347 (96%)	326 (98%)	6 (2%)	51	82
2	O	333/347 (96%)	325 (98%)	8 (2%)	43	77
3	C	328/329 (100%)	323 (98%)	5 (2%)	57	84
3	P	328/329 (100%)	324 (99%)	4 (1%)	63	87
4	D	200/200 (100%)	198 (99%)	2 (1%)	68	88
4	Q	200/200 (100%)	197 (98%)	3 (2%)	57	84
5	E	166/166 (100%)	166 (100%)	0	100	100
5	R	165/166 (99%)	164 (99%)	1 (1%)	78	92
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	60
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	51
7	G	71/71 (100%)	70 (99%)	1 (1%)	59	85
7	T	69/71 (97%)	68 (99%)	1 (1%)	59	85
8	H	65/71 (92%)	64 (98%)	1 (2%)	57	84
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	83
9	I	23/26 (88%)	22 (96%)	1 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	80
10	W	47/49 (96%)	46 (98%)	1 (2%)	47	79
All	All	3378/3446 (98%)	3313 (98%)	65 (2%)	50	81

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	90	THR
1	A	106	MET
1	A	108	LYS
1	A	228	VAL
1	A	281	ASP
1	A	342	TRP
1	A	443	TRP
2	B	31	ASN
2	B	248	ASN
2	B	341	MET
2	B	402	ILE
2	B	406	THR
2	B	418	VAL
3	C	5	ILE
3	C	44	THR
3	C	125	MET
3	C	223	PRO
3	C	334	LEU
4	D	37	CYS
4	D	43	MET
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
6	F	84	GLU
7	G	45	VAL
8	H	72	LYS
9	I	71	ASN
10	J	60	GLU
1	N	3	THR
1	N	18	THR
1	N	29	GLU
1	N	49	ASN

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Mol	Chain	Res	Type
1	N	90	THR
1	N	106	MET
1	N	108	LYS
1	N	206	LYS
1	N	281	ASP
1	N	342	TRP
1	N	395	TRP
1	N	443	TRP
2	O	31	ASN
2	O	76	THR
2	O	248	ASN
2	O	259	THR
2	O	341	MET
2	O	402	ILE
2	O	406	THR
2	O	418	VAL
3	P	5	ILE
3	P	199	THR
3	P	223	PRO
3	P	334	LEU
4	Q	43	MET
4	Q	172	ASP
4	Q	241	LYS
5	R	125	ASP
6	S	14	ASP
6	S	64	ARG
6	S	70	LEU
6	S	73	ARG
6	S	84	GLU
7	T	2	ILE
8	U	72	LYS
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	118	GLN
1	A	147	ASN
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	308	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	192	HIS
2	B	247	GLN
2	B	248	ASN
2	B	305	GLN
2	B	315	ASN
2	B	329	GLN
2	B	332	HIS
2	B	343	GLN
2	B	376	GLN
3	C	9	HIS
3	C	55	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	71	GLN
4	D	148	HIS
4	D	225	HIS
5	E	164	HIS
5	E	186	GLN
6	F	72	HIS
6	F	79	GLN
7	G	12	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
8	H	71	HIS
9	I	71	ASN
1	N	10	ASN
1	N	32	GLN
1	N	49	ASN
1	N	53	ASN
1	N	118	GLN
1	N	143	ASN

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Mol	Chain	Res	Type
1	N	147	ASN
1	N	173	ASN
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	192	HIS
2	O	247	GLN
2	O	248	ASN
2	O	305	GLN
2	O	329	GLN
2	O	332	HIS
2	O	343	GLN
2	O	376	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	332	ASN
3	P	342	GLN
3	P	379	ASN
4	Q	35	GLN
4	Q	50	ASN
4	Q	71	GLN
4	Q	148	HIS
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
5	R	164	HIS
6	S	79	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	79	ASN
8	U	71	HIS
8	U	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 11 are unknown - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
11	PEE	P	3007	-	47,47,50	1.38	5 (10%)	50,52,55	0.77	2 (4%)
19	CDL	G	2004	-	39,39,99	1.21	3 (7%)	45,51,111	1.10	3 (6%)
16	AZI	P	3011	-	2,2,2	3.11	2 (100%)	0,1,1	-	-
17	BOG	P	2010	-	18,18,20	1.10	3 (16%)	22,22,25	0.57	0
17	BOG	C	3010	-	11,11,20	1.08	2 (18%)	10,11,25	0.97	1 (10%)
14	FNM	P	3001	-	24,24,24	1.84	4 (16%)	24,34,34	1.73	2 (8%)
13	HEM	C	501	3	50,50,50	1.39	4 (8%)	67,82,82	1.44	10 (14%)
17	BOG	D	2091	-	20,20,20	1.12	2 (10%)	25,25,25	1.00	1 (4%)
13	HEM	C	502	3	50,50,50	1.57	8 (16%)	67,82,82	1.46	11 (16%)
14	FNM	C	2001	-	24,24,24	1.81	3 (12%)	24,34,34	1.89	3 (12%)
17	BOG	Q	3091	-	20,20,20	1.14	2 (10%)	25,25,25	0.90	1 (4%)
11	PEE	A	2008	-	20,20,50	1.71	4 (20%)	23,25,55	0.65	0
19	CDL	T	3004	-	39,39,99	1.22	3 (7%)	45,51,111	1.10	2 (4%)
18	HEC	D	501	4	50,50,50	1.23	6 (12%)	68,82,82	1.62	15 (22%)
17	BOG	D	2009	-	20,20,20	0.98	1 (5%)	25,25,25	0.93	2 (8%)
13	HEM	P	501	3	50,50,50	1.44	5 (10%)	67,82,82	1.21	4 (5%)
15	UQ	P	3002	-	19,19,63	2.46	10 (52%)	24,26,79	1.05	2 (8%)
13	HEM	P	502	3	50,50,50	1.53	4 (8%)	67,82,82	1.24	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BOG	Q	3009	-	20,20,20	0.94	1 (5%)	25,25,25	0.85	1 (4%)
11	PEE	P	3005	-	49,49,50	1.48	9 (18%)	52,54,55	0.83	3 (5%)
20	FES	E	501	5	0,4,4	-	-	-	-	-
11	PEE	C	2005	-	49,49,50	1.48	9 (18%)	52,54,55	0.83	2 (3%)
16	AZI	C	2011	-	2,2,2	2.74	2 (100%)	0,1,1	-	-
11	PEE	N	3008	-	4,4,50	3.65	4 (100%)	6,6,55	0.63	0
19	CDL	Q	3003	-	41,41,99	1.20	2 (4%)	47,53,111	1.07	4 (8%)
11	PEE	C	2007	-	47,47,50	1.32	6 (12%)	50,52,55	0.80	3 (6%)
20	FES	R	501	5	0,4,4	-	-	-	-	-
19	CDL	D	2003	-	41,41,99	1.15	1 (2%)	47,53,111	1.07	4 (8%)
18	HEC	Q	501	4	50,50,50	1.09	2 (4%)	68,82,82	1.52	13 (19%)
15	UQ	C	2002	-	19,19,63	2.63	10 (52%)	24,26,79	1.10	2 (8%)

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
11	PEE	P	3007	-	-	24/51/51/54	-
19	CDL	G	2004	-	-	21/49/49/110	-
17	BOG	P	2010	-	-	1/6/26/31	0/1/1/1
17	BOG	C	3010	-	-	5/9/9/31	-
14	FNM	P	3001	-	-	2/12/31/31	0/3/3/3
13	HEM	C	501	3	-	2/14/54/54	-
17	BOG	D	2091	-	-	6/11/31/31	0/1/1/1
13	HEM	C	502	3	-	6/14/54/54	-
14	FNM	C	2001	-	-	2/12/31/31	0/3/3/3
17	BOG	Q	3091	-	-	4/11/31/31	0/1/1/1
11	PEE	A	2008	-	-	10/24/24/54	-
19	CDL	T	3004	-	-	22/49/49/110	-
18	HEC	D	501	4	1/1/3/7	9/14/54/54	-
17	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
13	HEM	P	501	3	-	2/14/54/54	-
15	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
13	HEM	P	502	3	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BOG	Q	3009	-	-	6/11/31/31	0/1/1/1
11	PEE	P	3005	-	-	29/53/53/54	-
20	FES	E	501	5	-	-	0/1/1/1
11	PEE	C	2005	-	-	28/53/53/54	-
19	CDL	Q	3003	-	-	24/51/51/110	-
11	PEE	C	2007	-	-	24/51/51/54	-
20	FES	R	501	5	-	-	0/1/1/1
19	CDL	D	2003	-	-	26/51/51/110	-
18	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
15	UQ	C	2002	-	-	3/11/35/87	0/1/1/1

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	2001	FNM	C3-N4	6.99	1.34	1.28
14	P	3001	FNM	C3-N4	6.60	1.33	1.28
13	P	502	HEM	CBB-CAB	5.30	1.55	1.30
15	C	2002	UQ	C6-C5	5.09	1.44	1.35
15	C	2002	UQ	C7-C6	5.03	1.60	1.51
11	N	3008	PEE	P-O1P	4.91	1.62	1.50
15	P	3002	UQ	C7-C6	4.89	1.60	1.51
18	D	501	HEC	C4D-C3D	4.85	1.53	1.45
15	P	3002	UQ	C6-C5	4.72	1.43	1.35
13	C	502	HEM	CBB-CAB	4.67	1.52	1.30
13	P	501	HEM	CBB-CAB	4.62	1.52	1.30
13	C	502	HEM	C4D-C3D	4.53	1.52	1.45
13	P	502	HEM	CBC-CAC	4.44	1.51	1.30
13	P	501	HEM	CBC-CAC	4.35	1.51	1.30
11	C	2007	PEE	C39-C38	4.24	1.55	1.31
11	P	3007	PEE	C39-C38	4.20	1.55	1.31
11	P	3005	PEE	C39-C38	4.19	1.55	1.31
11	C	2005	PEE	C39-C38	4.17	1.55	1.31
13	C	501	HEM	CBB-CAB	4.15	1.50	1.30
13	P	502	HEM	C4D-C3D	4.00	1.51	1.45
13	C	501	HEM	CBC-CAC	3.90	1.49	1.30
15	C	2002	UQ	C6-C1	3.86	1.57	1.46
13	C	502	HEM	CBC-CAC	3.85	1.48	1.30
13	C	501	HEM	CAB-C3B	-3.82	1.37	1.47
15	P	3002	UQ	C6-C1	3.65	1.56	1.46
11	N	3008	PEE	P-O4P	3.60	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	3011	AZI	N1-N2	-3.57	1.15	1.23
11	P	3007	PEE	C21-C22	-3.49	1.34	1.51
13	P	501	HEM	CAB-C3B	-3.43	1.38	1.47
11	C	2007	PEE	C21-C22	-3.37	1.35	1.51
11	C	2005	PEE	O2-C10	3.30	1.43	1.34
11	P	3005	PEE	C21-C22	-3.29	1.35	1.51
11	C	2005	PEE	C21-C22	-3.27	1.35	1.51
11	P	3005	PEE	O2-C10	3.25	1.43	1.34
11	A	2008	PEE	O3-C30	3.25	1.42	1.33
11	C	2005	PEE	P-O1P	3.25	1.62	1.50
11	P	3005	PEE	P-O1P	3.20	1.61	1.50
11	C	2005	PEE	O3-C30	3.16	1.42	1.33
15	C	2002	UQ	O3-C3	3.15	1.44	1.36
11	A	2008	PEE	O2-C10	3.12	1.43	1.34
11	A	2008	PEE	P-O1P	3.11	1.61	1.50
11	N	3008	PEE	P-O3P	3.10	1.63	1.54
16	C	2011	AZI	N1-N2	-3.06	1.16	1.23
11	P	3007	PEE	P-O1P	3.03	1.61	1.50
13	C	502	HEM	CAB-C3B	-3.02	1.39	1.47
11	P	3007	PEE	O3-C30	3.02	1.42	1.33
15	C	2002	UQ	CM5-C5	2.98	1.56	1.50
11	C	2007	PEE	P-O1P	2.94	1.61	1.50
15	C	2002	UQ	O2-C2	2.93	1.43	1.36
11	P	3005	PEE	O3-C30	2.93	1.41	1.33
15	P	3002	UQ	O3-C3	2.87	1.43	1.36
15	C	2002	UQ	C2-C1	2.84	1.57	1.48
18	Q	501	HEC	C4B-NB	-2.81	1.35	1.40
11	P	3007	PEE	O2-C10	2.80	1.42	1.34
15	P	3002	UQ	CM5-C5	2.77	1.56	1.50
15	C	2002	UQ	C5-C4	2.72	1.56	1.47
13	C	502	HEM	C3B-C4B	2.68	1.50	1.44
11	C	2007	PEE	O3-C30	2.65	1.41	1.33
15	P	3002	UQ	C7-C8	2.64	1.54	1.50
13	P	502	HEM	CAB-C3B	-2.60	1.40	1.47
14	P	3001	FNM	C3-N2	-2.58	1.33	1.38
16	P	3011	AZI	N3-N2	-2.57	1.17	1.23
11	N	3008	PEE	P-O2P	2.56	1.62	1.54
17	C	3010	BOG	C2-C1	2.54	1.57	1.50
19	T	3004	CDL	O1-C1	2.53	1.50	1.43
14	C	2001	FNM	C3-N2	-2.52	1.33	1.38
15	P	3002	UQ	C2-C1	2.50	1.56	1.48
13	C	501	HEM	CAC-C3C	-2.49	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	2007	PEE	O2-C10	2.48	1.41	1.34
15	P	3002	UQ	O2-C2	2.48	1.42	1.36
17	D	2091	BOG	O5-C1	2.48	1.48	1.41
17	Q	3091	BOG	C4-C5	2.47	1.58	1.53
14	P	3001	FNM	C26-C21	2.46	1.43	1.39
17	Q	3091	BOG	O5-C1	2.45	1.48	1.41
11	C	2005	PEE	C31-C30	2.45	1.57	1.50
14	C	2001	FNM	C6-N2	-2.44	1.35	1.38
18	D	501	HEC	C1D-ND	-2.41	1.36	1.40
15	P	3002	UQ	C5-C4	2.41	1.55	1.47
18	D	501	HEC	C1D-C2D	2.39	1.49	1.44
17	D	2091	BOG	C4-C5	2.39	1.58	1.53
13	C	502	HEM	CAC-C3C	-2.39	1.41	1.47
16	C	2011	AZI	N3-N2	-2.38	1.18	1.23
13	C	502	HEM	CHD-C4C	-2.37	1.33	1.38
18	D	501	HEC	CHD-C4C	-2.36	1.34	1.39
17	C	3010	BOG	O5-C1	2.34	1.45	1.40
15	C	2002	UQ	C3-C4	2.33	1.55	1.48
18	D	501	HEC	C1C-C2C	2.32	1.48	1.43
11	P	3005	PEE	C11-C10	2.32	1.57	1.50
19	G	2004	CDL	O1-C1	2.31	1.50	1.43
19	G	2004	CDL	CA3-CA4	2.29	1.58	1.50
15	C	2002	UQ	C7-C8	2.27	1.54	1.50
17	P	2010	BOG	C4-C5	2.26	1.57	1.53
17	D	2009	BOG	O5-C1	2.26	1.47	1.41
19	Q	3003	CDL	O1-C1	2.25	1.49	1.43
11	P	3005	PEE	C31-C30	2.22	1.57	1.50
11	C	2005	PEE	C11-C10	2.21	1.57	1.50
13	C	502	HEM	FE-NB	-2.21	1.88	1.94
11	P	3005	PEE	C3-C2	2.21	1.57	1.50
15	P	3002	UQ	C3-C4	2.21	1.55	1.48
17	P	2010	BOG	C1-C2	2.20	1.57	1.52
19	T	3004	CDL	CA3-CA4	2.20	1.57	1.50
13	P	501	HEM	CAC-C3C	-2.19	1.41	1.47
17	Q	3009	BOG	O5-C1	2.18	1.47	1.41
13	P	501	HEM	CHD-C1D	-2.11	1.34	1.39
11	C	2005	PEE	C1-C2	2.10	1.57	1.50
18	D	501	HEC	CMB-C2B	2.08	1.55	1.50
19	T	3004	CDL	OA8-CA6	-2.08	1.40	1.45
11	P	3005	PEE	C1-C2	2.08	1.57	1.50
19	Q	3003	CDL	OA2-CA2	-2.07	1.36	1.44
19	G	2004	CDL	OA6-CA5	2.07	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	2003	CDL	O1-C1	2.06	1.49	1.43
17	P	2010	BOG	O5-C1	2.04	1.47	1.42
11	C	2005	PEE	C3-C2	2.04	1.57	1.50
11	A	2008	PEE	C3-C2	2.03	1.57	1.50
18	Q	501	HEC	C3C-C2C	-2.02	1.33	1.38
14	P	3001	FNM	C6-N2	-2.01	1.35	1.38
11	C	2007	PEE	C3-C2	2.00	1.57	1.50

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	2001	FNM	C27-S3-C3	7.71	110.67	100.43
14	P	3001	FNM	C27-S3-C3	6.94	109.64	100.43
13	C	502	HEM	CAD-C3D-C4D	5.47	134.23	124.70
18	D	501	HEC	CAD-C3D-C4D	4.96	133.34	124.70
13	P	502	HEM	CAD-C3D-C4D	4.33	132.25	124.70
17	D	2091	BOG	C1'-O1-C1	3.91	120.36	113.68
14	P	3001	FNM	C21-N1-N2	3.90	123.42	116.20
18	Q	501	HEC	CAA-C2A-C1A	3.85	132.67	124.85
14	C	2001	FNM	C21-N1-N2	3.82	123.27	116.20
13	C	501	HEM	C3B-C2B-C1B	-3.76	103.59	106.41
18	Q	501	HEC	CAD-C3D-C4D	3.74	131.22	124.70
18	Q	501	HEC	CAC-C3C-C2C	3.64	132.64	126.89
18	D	501	HEC	CAA-C2A-C1A	3.56	132.10	124.85
18	Q	501	HEC	CAA-C2A-C3A	-3.55	121.22	127.87
13	P	501	HEM	C3B-C2B-C1B	-3.54	103.75	106.41
18	Q	501	HEC	CAC-C3C-C4C	-3.54	120.04	124.91
18	D	501	HEC	CAA-C2A-C3A	-3.48	121.35	127.87
15	C	2002	UQ	C8-C7-C6	3.43	120.53	112.08
17	D	2009	BOG	C1'-O1-C1	3.40	119.48	113.68
18	D	501	HEC	CBA-CAA-C2A	3.38	121.89	112.53
18	Q	501	HEC	CBA-CAA-C2A	3.36	121.83	112.53
13	C	501	HEM	C2D-C1D-ND	3.33	113.76	109.90
19	T	3004	CDL	CB4-OB6-CB5	-3.28	109.94	117.80
19	G	2004	CDL	CB4-OB6-CB5	-3.22	110.08	117.80
15	P	3002	UQ	C8-C7-C6	3.21	119.98	112.08
17	Q	3091	BOG	C1'-O1-C1	3.17	119.10	113.68
13	C	501	HEM	CAD-C3D-C4D	3.16	130.21	124.70
13	C	502	HEM	C3B-C4B-NB	3.12	111.71	109.47
13	C	502	HEM	C3D-C4D-ND	3.05	113.52	110.17
18	D	501	HEC	CAD-C3D-C2D	-2.94	122.36	127.87
17	Q	3009	BOG	C1'-O1-C1	2.94	118.70	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	502	HEM	C4D-ND-C1D	-2.93	101.74	105.21
18	Q	501	HEC	CMC-C2C-C1C	2.90	129.84	125.42
13	C	501	HEM	CAD-C3D-C2D	-2.89	122.45	127.87
13	P	501	HEM	C2D-C1D-ND	2.83	113.17	109.90
18	D	501	HEC	C2D-C1D-ND	2.83	113.09	109.84
18	D	501	HEC	CAC-C3C-C2C	2.82	131.35	126.89
13	P	502	HEM	C3B-C4B-NB	2.82	111.49	109.47
11	P	3005	PEE	C22-C21-C20	2.80	127.33	113.86
13	P	501	HEM	CAD-C3D-C4D	2.78	129.54	124.70
11	C	2007	PEE	C22-C21-C20	2.77	127.15	113.86
11	C	2005	PEE	C22-C21-C20	2.76	127.12	113.86
13	C	502	HEM	C4D-C3D-C2D	-2.75	102.89	106.89
11	P	3007	PEE	C22-C21-C20	2.74	127.03	113.86
13	C	501	HEM	C3B-C4B-NB	2.72	111.42	109.47
13	C	502	HEM	CAD-C3D-C2D	-2.69	122.83	127.87
18	Q	501	HEC	CMB-C2B-C1B	2.69	129.24	125.03
13	P	502	HEM	CAD-C3D-C2D	-2.63	122.95	127.87
19	D	2003	CDL	CB4-OB6-CB5	-2.61	111.54	117.80
13	P	502	HEM	C4C-C3C-C2C	-2.61	104.55	106.81
18	D	501	HEC	CMD-C2D-C1D	2.61	129.11	125.03
18	Q	501	HEC	CAB-C3B-C4B	-2.60	121.41	124.79
13	P	502	HEM	C2D-C1D-ND	2.58	112.89	109.90
18	D	501	HEC	CMC-C2C-C1C	2.58	129.35	125.42
13	C	502	HEM	C2D-C1D-ND	2.54	112.83	109.90
19	Q	3003	CDL	CB4-OB6-CB5	-2.53	111.74	117.80
14	C	2001	FNM	O6-C6-C5	2.53	128.42	126.00
18	D	501	HEC	CAB-C3B-C4B	-2.50	121.53	124.79
11	C	2005	PEE	C21-C22-C23	2.48	126.91	114.37
15	C	2002	UQ	C7-C6-C1	-2.46	115.66	118.52
11	P	3005	PEE	C21-C22-C23	2.44	126.71	114.37
11	C	2007	PEE	C21-C22-C23	2.38	126.42	114.37
19	D	2003	CDL	CA6-OA8-CA7	-2.37	111.24	117.08
17	C	3010	BOG	C1'-O1-C1	2.35	118.91	113.81
13	P	502	HEM	C2A-C1A-NA	2.34	112.75	110.15
15	P	3002	UQ	C7-C6-C1	-2.32	115.81	118.52
11	P	3007	PEE	C21-C22-C23	2.28	125.87	114.37
13	C	501	HEM	CBD-CAD-C3D	2.27	118.81	112.53
13	C	501	HEM	C4D-ND-C1D	-2.26	102.53	105.21
13	C	501	HEM	C2B-C1B-NB	2.26	112.44	109.84
19	Q	3003	CDL	CA6-OA8-CA7	-2.26	111.52	117.08
19	Q	3003	CDL	CA4-OA6-CA5	-2.26	112.40	117.80
13	C	501	HEM	CHD-C1D-C2D	-2.23	121.50	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	2004	CDL	CA4-OA6-CA5	-2.23	112.46	117.80
18	D	501	HEC	C3C-C4C-NC	2.21	112.60	110.15
18	D	501	HEC	CMB-C2B-C1B	2.19	128.45	125.03
13	C	502	HEM	C2B-C1B-NB	2.17	112.33	109.84
19	D	2003	CDL	CA6-CA4-CA3	-2.17	106.73	111.78
18	D	501	HEC	CAB-C3B-C2B	2.16	131.52	127.56
18	Q	501	HEC	C2D-C1D-ND	2.15	112.31	109.84
13	C	502	HEM	CHC-C1C-NC	-2.14	122.13	124.45
13	P	501	HEM	C2B-C1B-NB	2.13	112.29	109.84
18	Q	501	HEC	CAD-C3D-C2D	-2.13	123.88	127.87
13	C	502	HEM	C4C-C3C-C2C	-2.12	104.98	106.81
13	P	502	HEM	C2B-C1B-NB	2.11	112.26	109.84
13	C	501	HEM	CHD-C4C-C3C	-2.09	121.68	125.21
13	C	502	HEM	CHA-C4D-ND	-2.08	121.79	124.37
11	C	2007	PEE	O3-C3-C2	2.08	114.38	108.40
18	D	501	HEC	C4D-C3D-C2D	-2.07	103.88	106.89
11	P	3005	PEE	O3-C3-C2	2.06	114.34	108.40
19	Q	3003	CDL	CA6-CA4-CA3	-2.06	106.99	111.78
17	D	2009	BOG	O1-C1-C2	2.04	111.37	108.27
19	D	2003	CDL	CA4-OA6-CA5	-2.04	112.92	117.80
18	Q	501	HEC	CAB-C3B-C2B	2.03	131.28	127.56
18	D	501	HEC	CAC-C3C-C4C	-2.03	122.12	124.91
18	Q	501	HEC	CHA-C1A-NA	-2.02	122.25	124.45
19	T	3004	CDL	CA4-OA6-CA5	-2.02	112.97	117.80
19	G	2004	CDL	OB6-CB4-CB3	2.02	115.57	108.34

All (2) chirality outliers are listed below:

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

All (276) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C1-O3P-P-O1P
11	A	2008	PEE	C1-O3P-P-O4P
11	C	2005	PEE	C11-C10-O2-C2
11	C	2005	PEE	C4-O4P-P-O3P
11	C	2005	PEE	C4-O4P-P-O2P
11	C	2005	PEE	C4-O4P-P-O1P
11	P	3005	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
11	P	3005	PEE	C4-O4P-P-O3P
11	P	3005	PEE	C4-O4P-P-O2P
11	P	3005	PEE	C4-O4P-P-O1P
15	C	2002	UQ	C12-C11-C9-C10
17	D	2091	BOG	O5-C1-O1-C1'
17	Q	3009	BOG	C2-C1-O1-C1'
18	D	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
19	D	2003	CDL	CB2-C1-CA2-OA2
19	D	2003	CDL	CA2-OA2-PA1-OA3
19	D	2003	CDL	CA2-OA2-PA1-OA4
19	D	2003	CDL	CA2-OA2-PA1-OA5
19	D	2003	CDL	CB2-OB2-PB2-OB3
19	D	2003	CDL	CB2-OB2-PB2-OB5
19	G	2004	CDL	O1-C1-CA2-OA2
19	G	2004	CDL	CA2-OA2-PA1-OA4
19	G	2004	CDL	CA3-OA5-PA1-OA2
19	G	2004	CDL	CA3-OA5-PA1-OA3
19	Q	3003	CDL	CA2-OA2-PA1-OA3
19	Q	3003	CDL	CA2-OA2-PA1-OA4
19	Q	3003	CDL	CA2-OA2-PA1-OA5
19	Q	3003	CDL	CB2-OB2-PB2-OB3
19	T	3004	CDL	O1-C1-CA2-OA2
19	T	3004	CDL	CA3-OA5-PA1-OA3
11	P	3005	PEE	O5-C30-O3-C3
11	C	2005	PEE	O5-C30-O3-C3
19	G	2004	CDL	OB9-CB7-OB8-CB6
19	T	3004	CDL	OB9-CB7-OB8-CB6
19	D	2003	CDL	C31-CA7-OA8-CA6
19	Q	3003	CDL	C31-CA7-OA8-CA6
11	C	2005	PEE	O4-C10-O2-C2
11	P	3005	PEE	O4-C10-O2-C2
19	G	2004	CDL	OB7-CB5-OB6-CB4
19	T	3004	CDL	OB7-CB5-OB6-CB4
11	C	2005	PEE	C31-C30-O3-C3
11	P	3005	PEE	C31-C30-O3-C3
19	T	3004	CDL	C51-CB5-OB6-CB4
19	G	2004	CDL	C71-CB7-OB8-CB6
19	T	3004	CDL	C71-CB7-OB8-CB6
11	P	3007	PEE	C17-C18-C19-C20
18	D	501	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	D	2003	CDL	OA9-CA7-OA8-CA6
18	D	501	HEC	C4B-C3B-CAB-CBB
19	D	2003	CDL	O1-C1-CA2-OA2
19	Q	3003	CDL	O1-C1-CA2-OA2
17	D	2009	BOG	C4-C5-C6-O6
19	G	2004	CDL	C51-CB5-OB6-CB4
19	Q	3003	CDL	OA9-CA7-OA8-CA6
17	D	2091	BOG	O5-C5-C6-O6
11	C	2007	PEE	C17-C18-C19-C20
19	G	2004	CDL	CB2-C1-CA2-OA2
19	Q	3003	CDL	CB2-C1-CA2-OA2
19	T	3004	CDL	CB2-C1-CA2-OA2
19	D	2003	CDL	C71-CB7-OB8-CB6
19	Q	3003	CDL	C71-CB7-OB8-CB6
17	D	2091	BOG	C4-C5-C6-O6
17	Q	3091	BOG	C2-C1-O1-C1'
17	D	2009	BOG	O5-C5-C6-O6
18	Q	501	HEC	C4C-C3C-CAC-CBC
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
18	Q	501	HEC	C2B-C3B-CAB-CBB
17	Q	3009	BOG	O1-C1'-C2'-C3'
19	Q	3003	CDL	OB9-CB7-OB8-CB6
18	D	501	HEC	C4C-C3C-CAC-CBC
17	Q	3009	BOG	O5-C1-O1-C1'
17	Q	3091	BOG	O5-C1-O1-C1'
18	Q	501	HEC	C4B-C3B-CAB-CBB
19	D	2003	CDL	OB9-CB7-OB8-CB6
18	D	501	HEC	C2B-C3B-CAB-CBB
19	G	2004	CDL	C11-CA5-OA6-CA4
19	T	3004	CDL	C11-CA5-OA6-CA4
11	P	3007	PEE	C12-C13-C14-C15
19	T	3004	CDL	OA7-CA5-OA6-CA4
19	D	2003	CDL	CB7-C71-C72-C73
19	Q	3003	CDL	CB7-C71-C72-C73
11	C	2005	PEE	C33-C34-C35-C36
17	C	3010	BOG	C3'-C4'-C5'-C6'
19	G	2004	CDL	CB5-C51-C52-C53
19	T	3004	CDL	CB5-C51-C52-C53
11	P	3005	PEE	C10-C11-C12-C13
11	C	2007	PEE	C12-C13-C14-C15
19	G	2004	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C10-C11-C12-C13
11	P	3005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C10-C11-C12-C13
11	P	3005	PEE	C33-C34-C35-C36
11	C	2005	PEE	C10-C11-C12-C13
11	C	2005	PEE	C30-C31-C32-C33
11	C	2005	PEE	C14-C15-C16-C17
11	A	2008	PEE	C31-C30-O3-C3
11	C	2007	PEE	C34-C35-C36-C37
17	P	2010	BOG	C3'-C4'-C5'-C6'
11	P	3007	PEE	C34-C35-C36-C37
11	P	3005	PEE	C14-C15-C16-C17
17	D	2009	BOG	C3'-C4'-C5'-C6'
11	A	2008	PEE	C11-C10-O2-C2
11	A	2008	PEE	O4-C10-O2-C2
15	C	2002	UQ	C5-C6-C7-C8
15	P	3002	UQ	C5-C6-C7-C8
11	P	3005	PEE	C37-C38-C39-C40
17	C	3010	BOG	C4'-C5'-C6'-C7'
15	C	2002	UQ	C1-C6-C7-C8
15	P	3002	UQ	C1-C6-C7-C8
18	D	501	HEC	C2C-C3C-CAC-CBC
11	P	3007	PEE	C40-C41-C42-C43
11	P	3005	PEE	C40-C41-C42-C43
11	C	2007	PEE	C40-C41-C42-C43
11	C	2005	PEE	C17-C18-C19-C20
11	P	3005	PEE	C17-C18-C19-C20
11	P	3005	PEE	C11-C12-C13-C14
11	A	2008	PEE	O5-C30-O3-C3
17	Q	3009	BOG	C2'-C3'-C4'-C5'
11	C	2005	PEE	C19-C20-C21-C22
11	P	3005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C11-C12-C13-C14
11	A	2008	PEE	O3P-C1-C2-C3
11	C	2005	PEE	C11-C12-C13-C14
11	C	2005	PEE	C40-C41-C42-C43
13	C	502	HEM	C4D-C3D-CAD-CBD
13	P	502	HEM	C4D-C3D-CAD-CBD
19	G	2004	CDL	CA3-CA4-CA6-OA8
19	T	3004	CDL	CA3-CA4-CA6-OA8
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C39-C40-C41-C42
11	P	3007	PEE	C14-C15-C16-C17
17	D	2009	BOG	C2'-C3'-C4'-C5'
11	C	2007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C11-C12-C13-C14
14	P	3001	FNM	N4-C5-C8-C13
17	Q	3009	BOG	C1'-C2'-C3'-C4'
11	P	3007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C39-C40-C41-C42
11	P	3007	PEE	C15-C16-C17-C18
11	P	3005	PEE	O3P-C1-C2-O2
19	Q	3003	CDL	C71-C72-C73-C74
11	P	3007	PEE	C32-C33-C34-C35
11	C	2007	PEE	C14-C15-C16-C17
11	P	3005	PEE	C20-C21-C22-C23
11	C	2005	PEE	C20-C21-C22-C23
19	D	2003	CDL	C71-C72-C73-C74
17	C	3010	BOG	C2'-C1'-O1-C1
11	C	2007	PEE	C32-C33-C34-C35
11	P	3005	PEE	O3P-C1-C2-C3
11	C	2005	PEE	C37-C38-C39-C40
11	C	2005	PEE	O3P-C1-C2-O2
19	G	2004	CDL	OB5-CB3-CB4-OB6
19	D	2003	CDL	OA6-CA4-CA6-OA8
19	Q	3003	CDL	OA6-CA4-CA6-OA8
17	Q	3091	BOG	O1-C1'-C2'-C3'
17	D	2091	BOG	C1'-C2'-C3'-C4'
17	Q	3091	BOG	C3'-C4'-C5'-C6'
11	C	2005	PEE	C12-C13-C14-C15
17	C	3010	BOG	O1-C1'-C2'-C3'
11	C	2005	PEE	O3P-C1-C2-C3
11	P	3005	PEE	C12-C13-C14-C15
19	D	2003	CDL	CB5-C51-C52-C53
19	Q	3003	CDL	CB5-C51-C52-C53
11	A	2008	PEE	O3P-C1-C2-O2
13	P	502	HEM	C2D-C3D-CAD-CBD
11	C	2005	PEE	C21-C22-C23-C24
17	D	2091	BOG	C2'-C1'-O1-C1
11	P	3005	PEE	C21-C22-C23-C24
11	P	3007	PEE	C43-C44-C45-C46
19	Q	3003	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
19	T	3004	CDL	OB5-CB3-CB4-OB6
11	C	2005	PEE	C35-C36-C37-C38
11	P	3005	PEE	C35-C36-C37-C38
19	Q	3003	CDL	C51-CB5-OB6-CB4
19	G	2004	CDL	OA6-CA4-CA6-OA8
19	T	3004	CDL	OA6-CA4-CA6-OA8
19	Q	3003	CDL	OB7-CB5-OB6-CB4
14	C	2001	FNM	N4-C5-C8-C9
14	C	2001	FNM	N4-C5-C8-C13
14	P	3001	FNM	N4-C5-C8-C9
19	D	2003	CDL	CA3-OA5-PA1-OA2
19	D	2003	CDL	CA3-OA5-PA1-OA4
19	G	2004	CDL	CA2-OA2-PA1-OA5
19	G	2004	CDL	CA3-OA5-PA1-OA4
19	G	2004	CDL	CB2-OB2-PB2-OB3
19	G	2004	CDL	CB3-OB5-PB2-OB4
19	Q	3003	CDL	CA3-OA5-PA1-OA2
19	Q	3003	CDL	CA3-OA5-PA1-OA4
19	T	3004	CDL	CA2-OA2-PA1-OA5
19	T	3004	CDL	CA3-OA5-PA1-OA2
19	T	3004	CDL	CA3-OA5-PA1-OA4
19	T	3004	CDL	CB2-OB2-PB2-OB3
19	T	3004	CDL	CB3-OB5-PB2-OB2
19	T	3004	CDL	CB3-OB5-PB2-OB4
11	P	3005	PEE	C15-C16-C17-C18
18	Q	501	HEC	C2C-C3C-CAC-CBC
11	A	2008	PEE	O5-C30-C31-C32
11	C	2007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C43-C44-C45-C46
11	C	2005	PEE	C15-C16-C17-C18
11	A	2008	PEE	O3-C30-C31-C32
11	C	2007	PEE	C19-C20-C21-C22
19	D	2003	CDL	OB5-CB3-CB4-OB6
13	C	502	HEM	C2D-C3D-CAD-CBD
17	Q	3009	BOG	C3'-C4'-C5'-C6'
19	D	2003	CDL	OB7-CB5-OB6-CB4
13	P	502	HEM	CAA-CBA-CGA-O1A
11	P	3007	PEE	C33-C34-C35-C36
11	P	3005	PEE	C42-C43-C44-C45
13	P	502	HEM	CAA-CBA-CGA-O2A
13	C	502	HEM	CAA-CBA-CGA-O1A
11	C	2005	PEE	C1-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
11	P	3005	PEE	C1-C2-O2-C10
11	C	2005	PEE	C13-C14-C15-C16
11	P	3005	PEE	C13-C14-C15-C16
13	C	502	HEM	CAA-CBA-CGA-O2A
13	P	502	HEM	CAD-CBD-CGD-O1D
18	D	501	HEC	C4D-C3D-CAD-CBD
19	T	3004	CDL	C1-CB2-OB2-PB2
17	C	3010	BOG	C1'-C2'-C3'-C4'
11	C	2007	PEE	C31-C32-C33-C34
13	C	501	HEM	CAA-CBA-CGA-O1A
13	P	502	HEM	CAD-CBD-CGD-O2D
19	D	2003	CDL	C51-CB5-OB6-CB4
13	C	501	HEM	CAA-CBA-CGA-O2A
18	D	501	HEC	CAD-CBD-CGD-O2D
18	Q	501	HEC	CAD-CBD-CGD-O2D
13	C	502	HEM	CAD-CBD-CGD-O2D
13	P	501	HEM	CAA-CBA-CGA-O1A
11	P	3007	PEE	C31-C32-C33-C34
19	G	2004	CDL	OB5-CB3-CB4-CB6
11	P	3005	PEE	C36-C37-C38-C39
19	G	2004	CDL	C1-CB2-OB2-PB2
13	C	502	HEM	CAD-CBD-CGD-O1D
11	C	2005	PEE	C42-C43-C44-C45
11	C	2007	PEE	C16-C17-C18-C19
13	P	501	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C38-C39-C40-C41
11	P	3005	PEE	C38-C39-C40-C41
11	P	3007	PEE	C16-C17-C18-C19
11	P	3007	PEE	C38-C39-C40-C41
11	P	3007	PEE	C19-C20-C21-C22
18	D	501	HEC	CAD-CBD-CGD-O1D
11	C	2005	PEE	C36-C37-C38-C39
18	Q	501	HEC	CAD-CBD-CGD-O1D
19	D	2003	CDL	CA3-CA4-CA6-OA8
19	Q	3003	CDL	CA3-CA4-CA6-OA8
11	C	2007	PEE	C18-C19-C20-C21
11	C	2005	PEE	C38-C39-C40-C41
11	P	3007	PEE	C18-C19-C20-C21
11	C	2007	PEE	O2-C10-C11-C12
19	D	2003	CDL	OB5-CB3-CB4-CB6
19	Q	3003	CDL	OB5-CB3-CB4-CB6
19	T	3004	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O2-C10-C11-C12
11	P	3007	PEE	O3-C30-C31-C32
11	C	2007	PEE	O3-C30-C31-C32
19	T	3004	CDL	C31-CA7-OA8-CA6
19	D	2003	CDL	C72-C71-CB7-OB8
19	D	2003	CDL	C12-C11-CA5-OA6
19	Q	3003	CDL	C12-C11-CA5-OA6
11	C	2007	PEE	O4-C10-C11-C12
11	P	3007	PEE	O5-C30-C31-C32
11	P	3007	PEE	O4-C10-C11-C12
17	D	2091	BOG	C2'-C3'-C4'-C5'
19	D	2003	CDL	C52-C51-CB5-OB6
19	Q	3003	CDL	C52-C51-CB5-OB6
19	Q	3003	CDL	C72-C71-CB7-OB8
11	P	3005	PEE	C22-C23-C24-C25
11	C	2007	PEE	O5-C30-C31-C32
19	D	2003	CDL	C72-C71-CB7-OB9

There are no ring outliers.

21 monomers are involved in 42 short contacts:

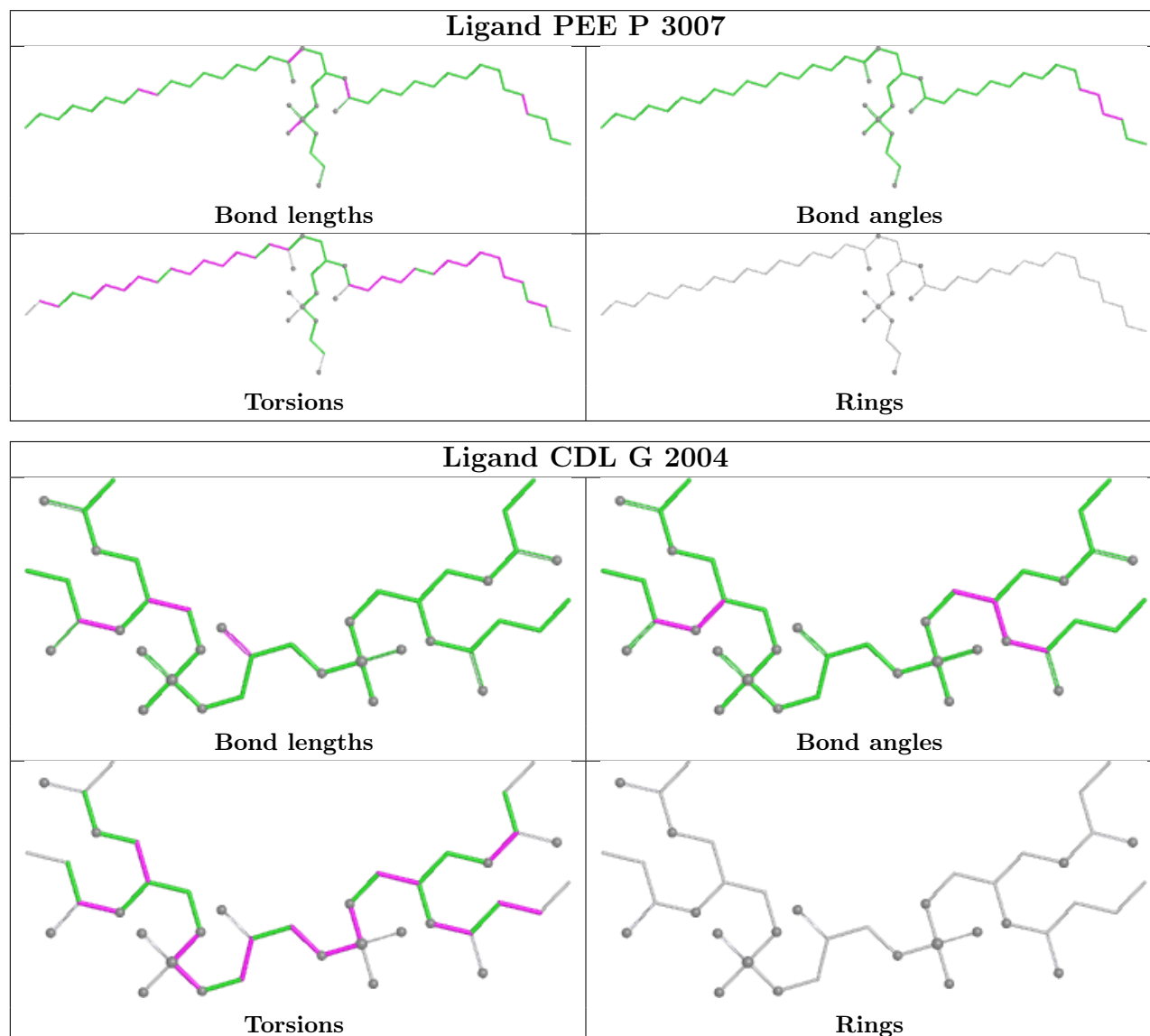
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	3007	PEE	1	0
19	G	2004	CDL	1	0
17	P	2010	BOG	1	0
14	P	3001	FNM	4	0
13	C	501	HEM	1	0
17	D	2091	BOG	2	0
13	C	502	HEM	4	0
14	C	2001	FNM	5	0
17	Q	3091	BOG	1	0
11	A	2008	PEE	1	0
19	T	3004	CDL	1	0
18	D	501	HEC	1	0
17	D	2009	BOG	1	0
13	P	501	HEM	1	0
15	P	3002	UQ	2	0
13	P	502	HEM	4	0
20	E	501	FES	1	0
19	Q	3003	CDL	3	0
20	R	501	FES	2	0
19	D	2003	CDL	2	0

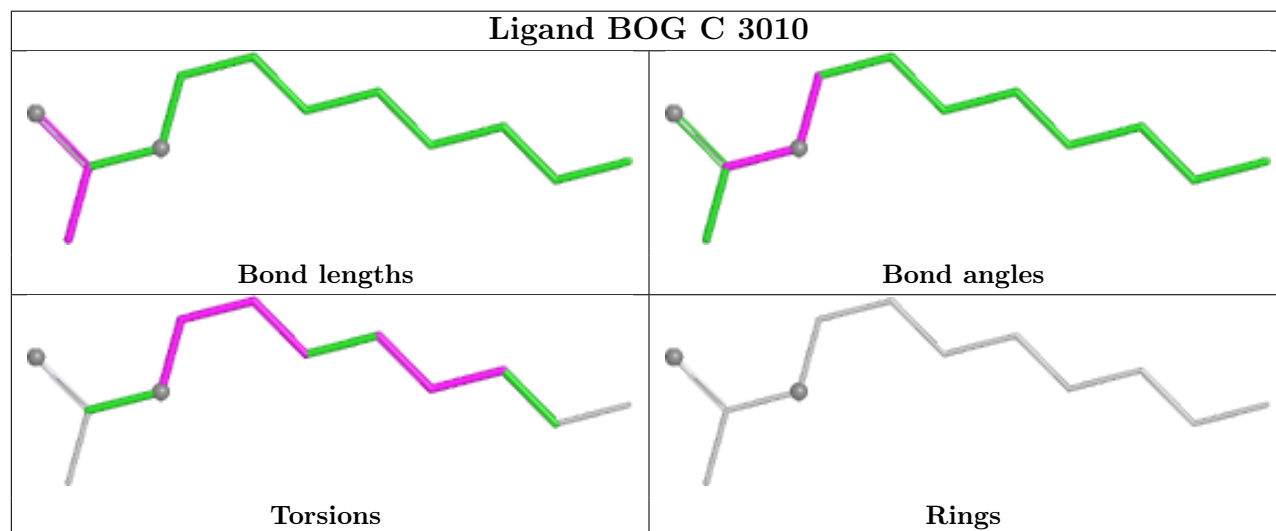
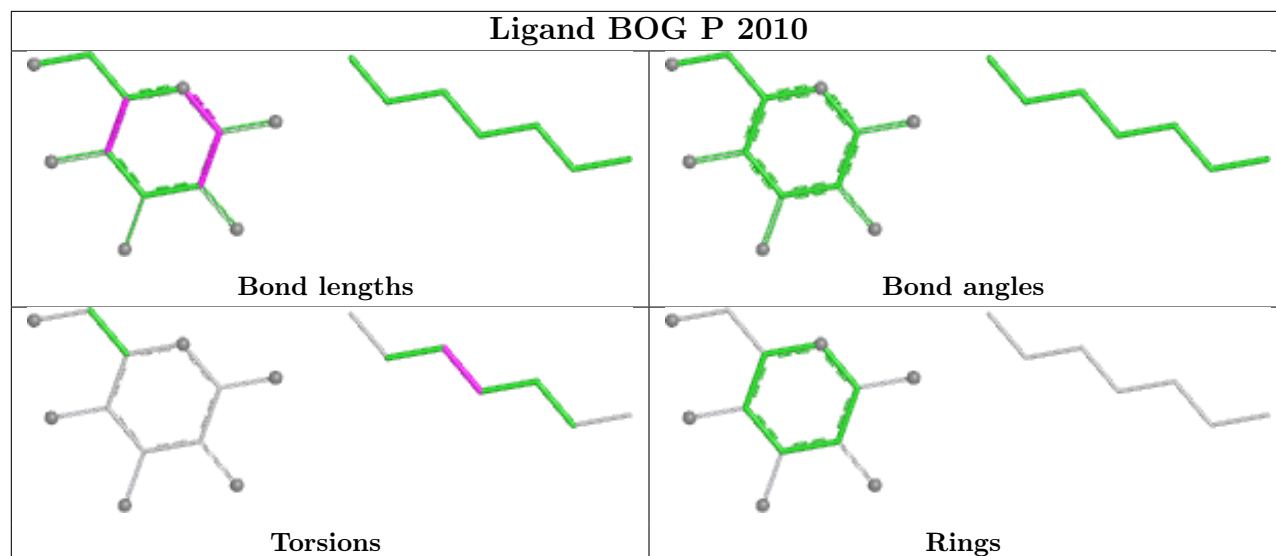
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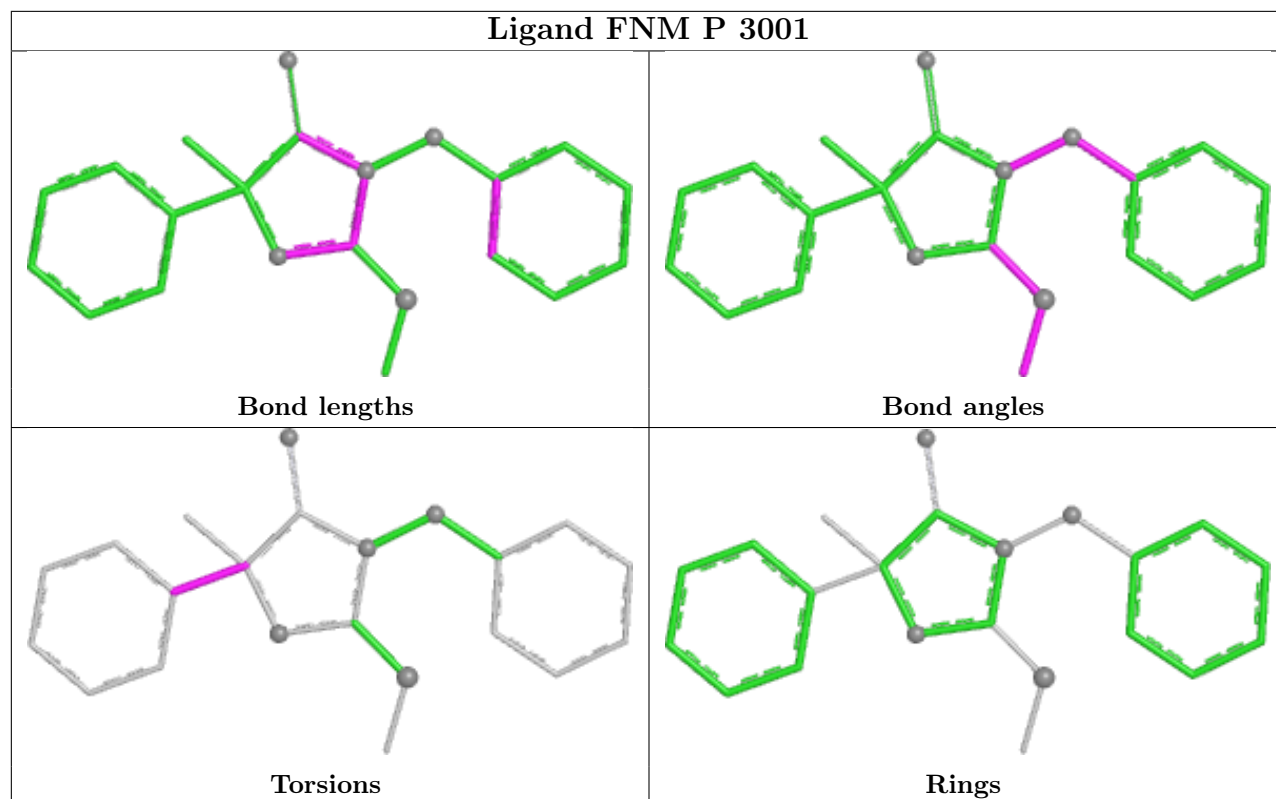
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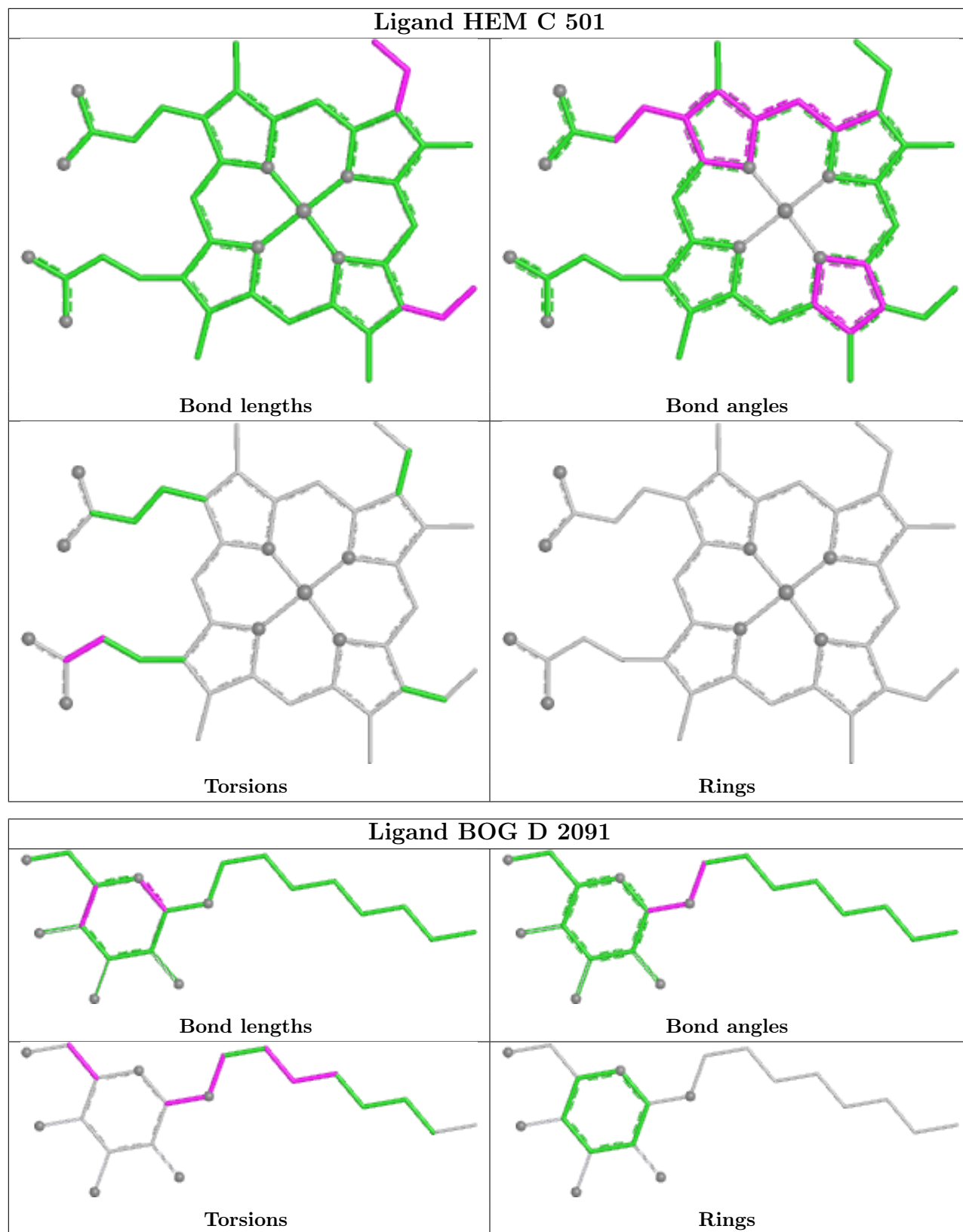
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	2002	UQ	3	0

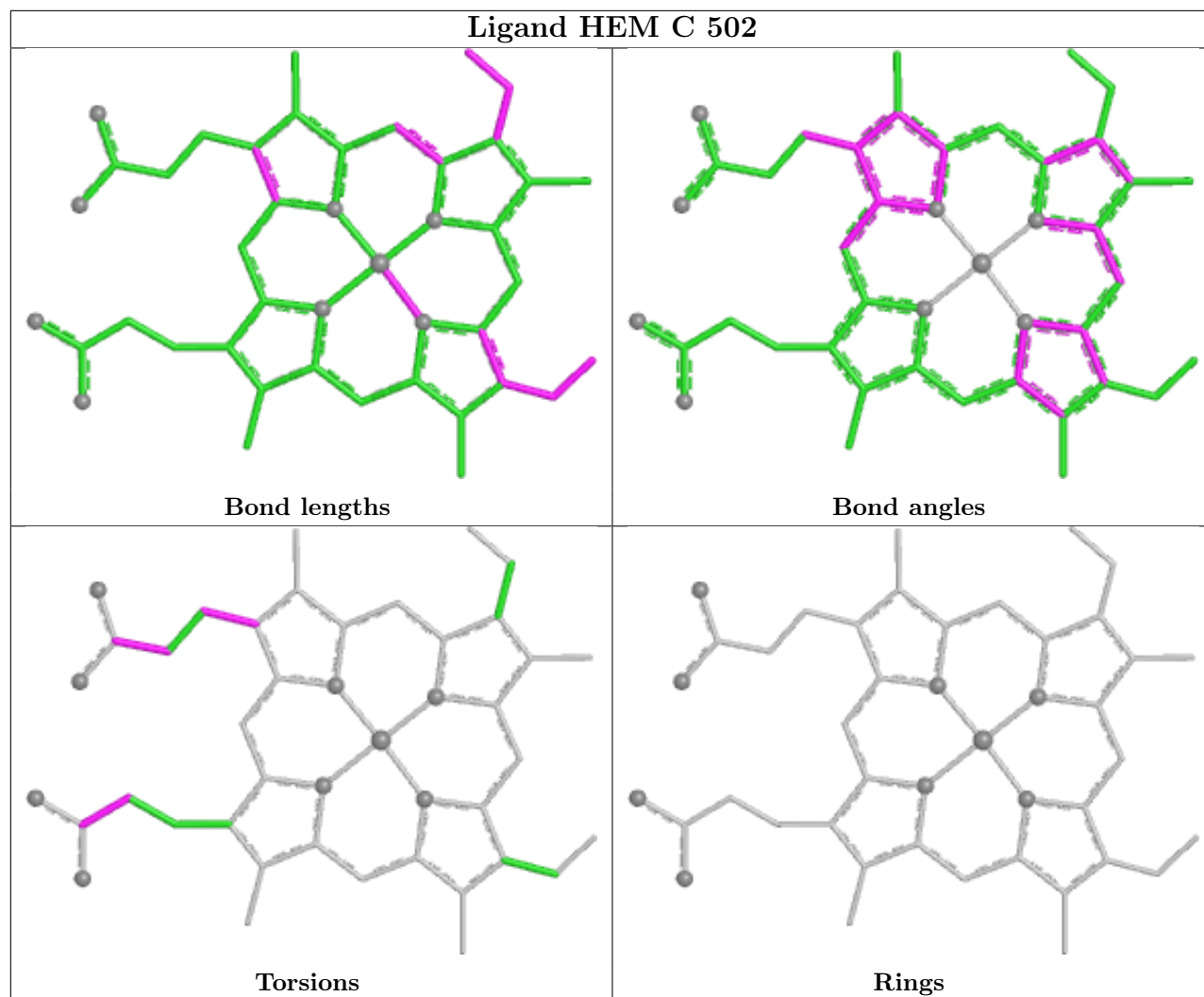
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

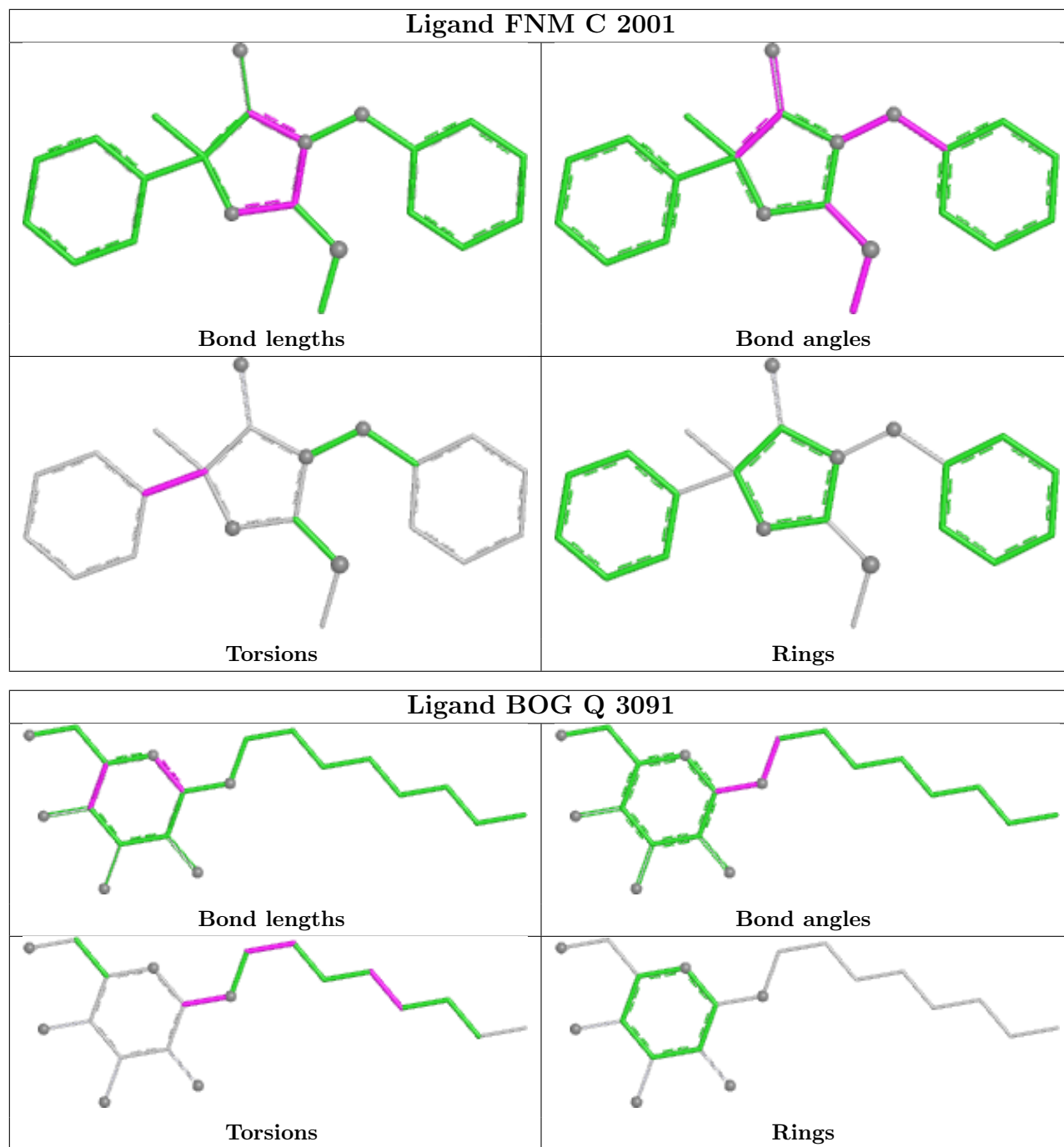


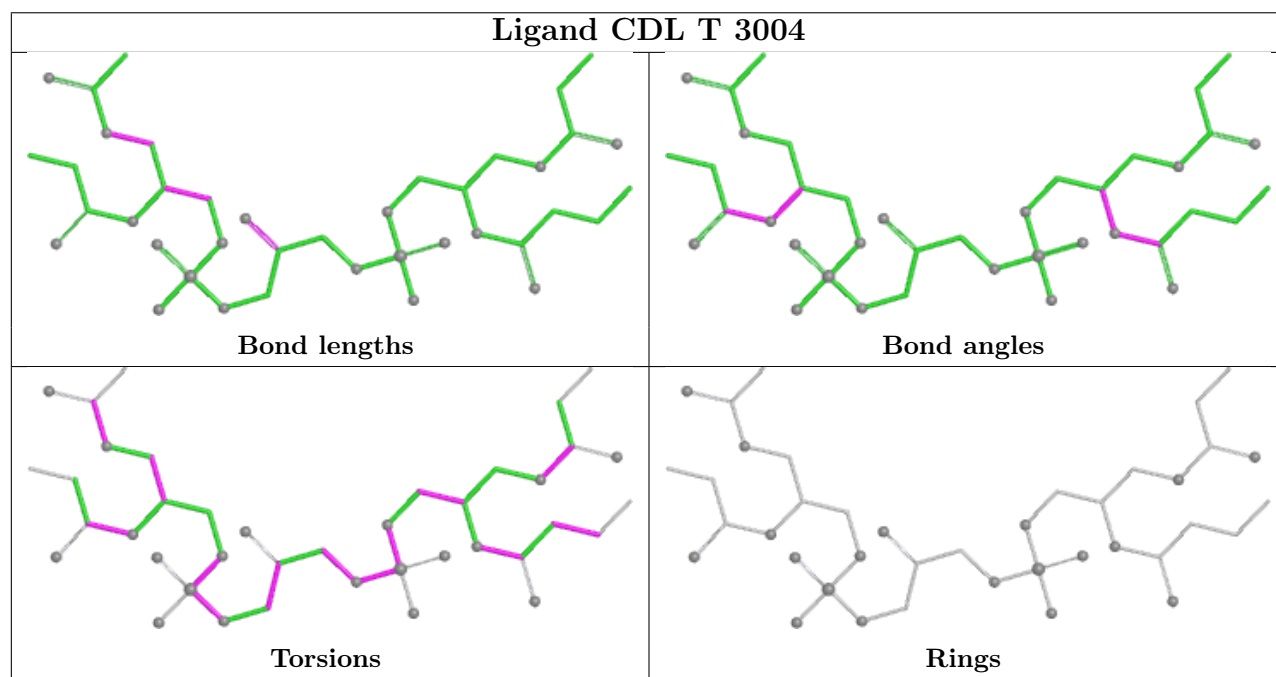
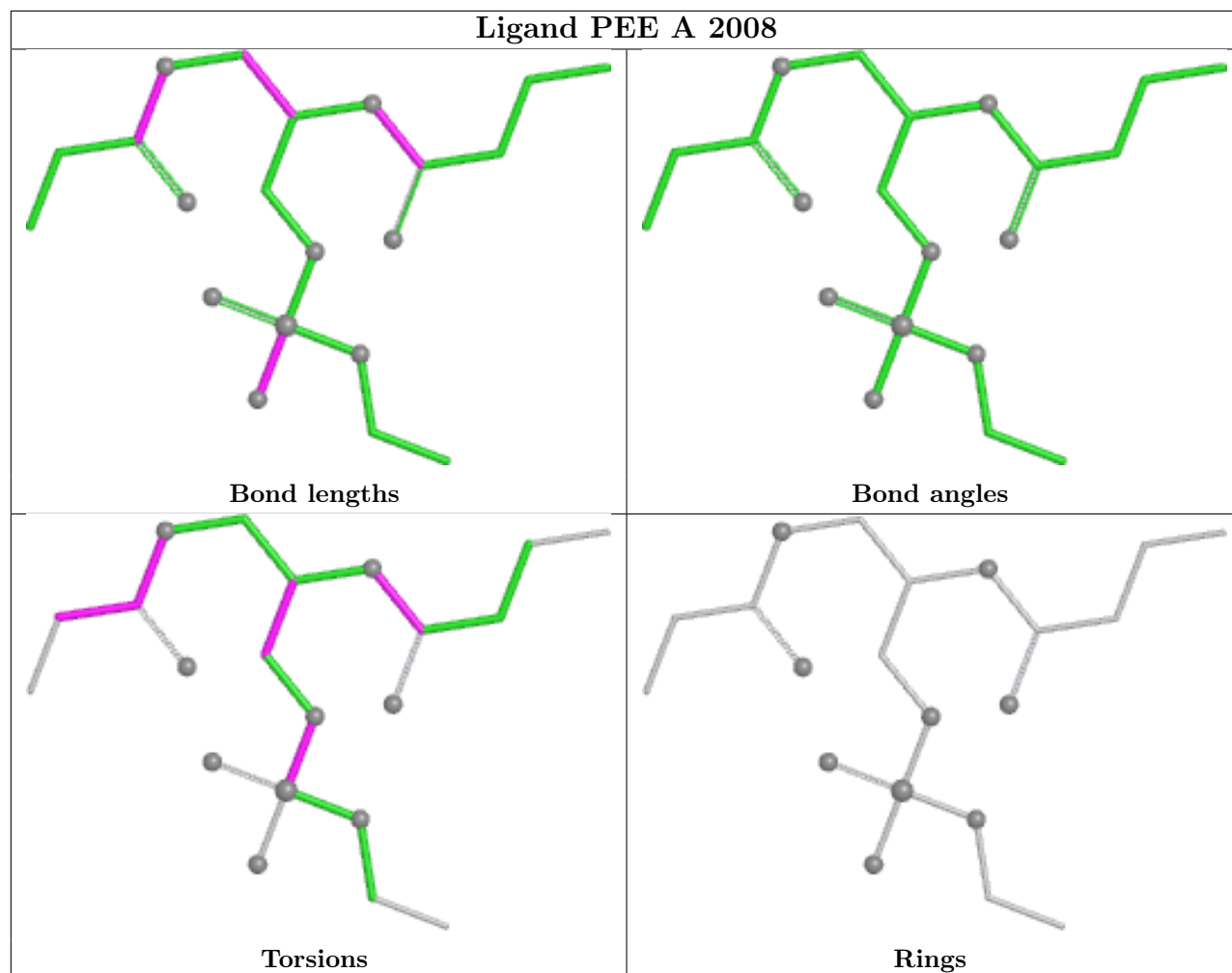




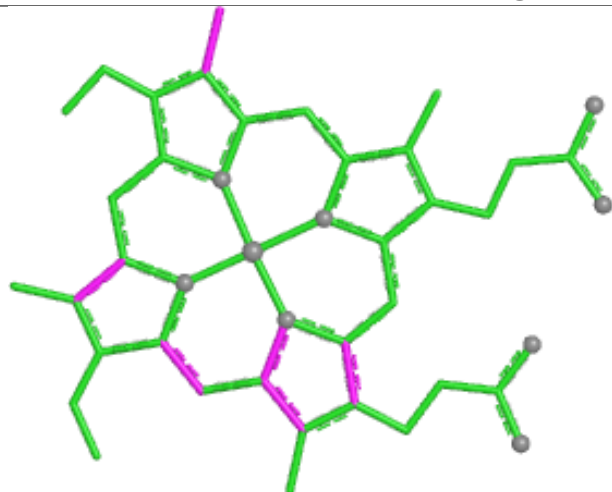




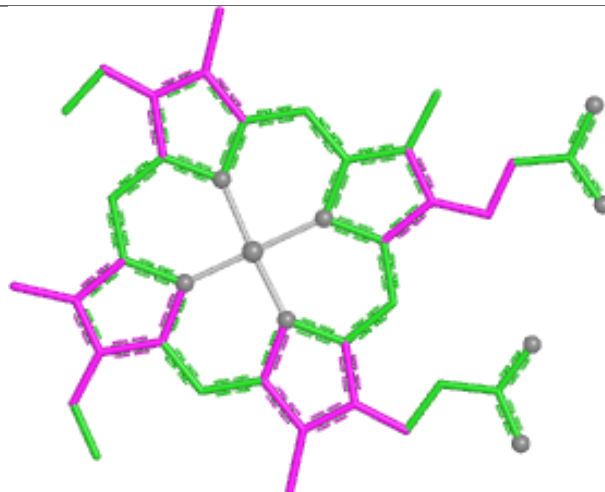




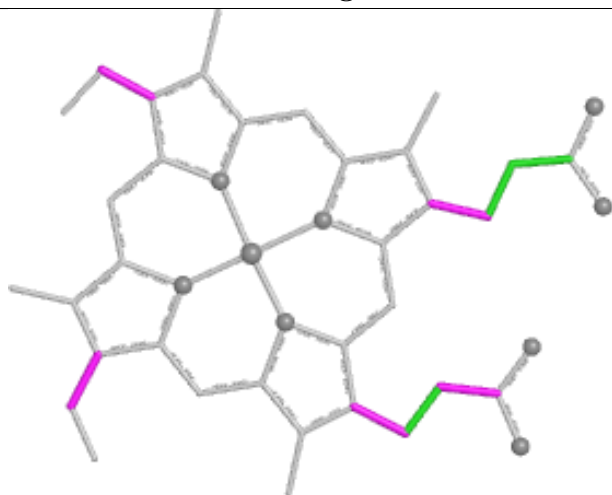
Ligand HEC D 501



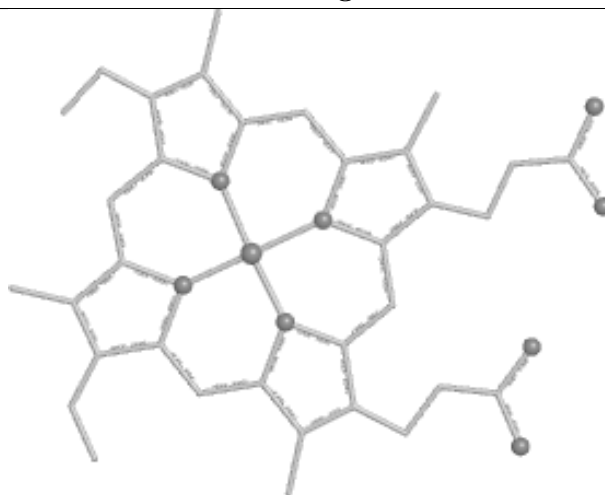
Bond lengths



Bond angles

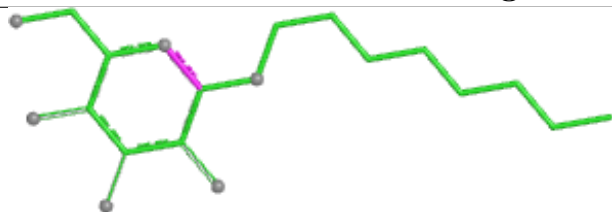


Torsions

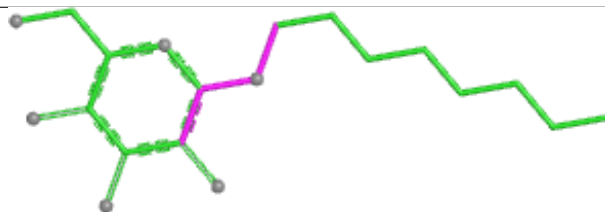


Rings

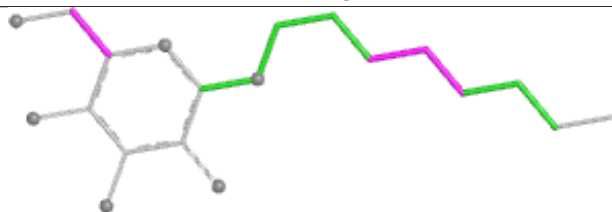
Ligand BOG D 2009



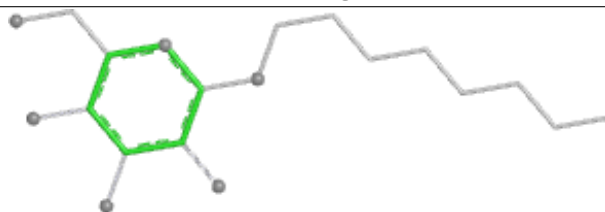
Bond lengths



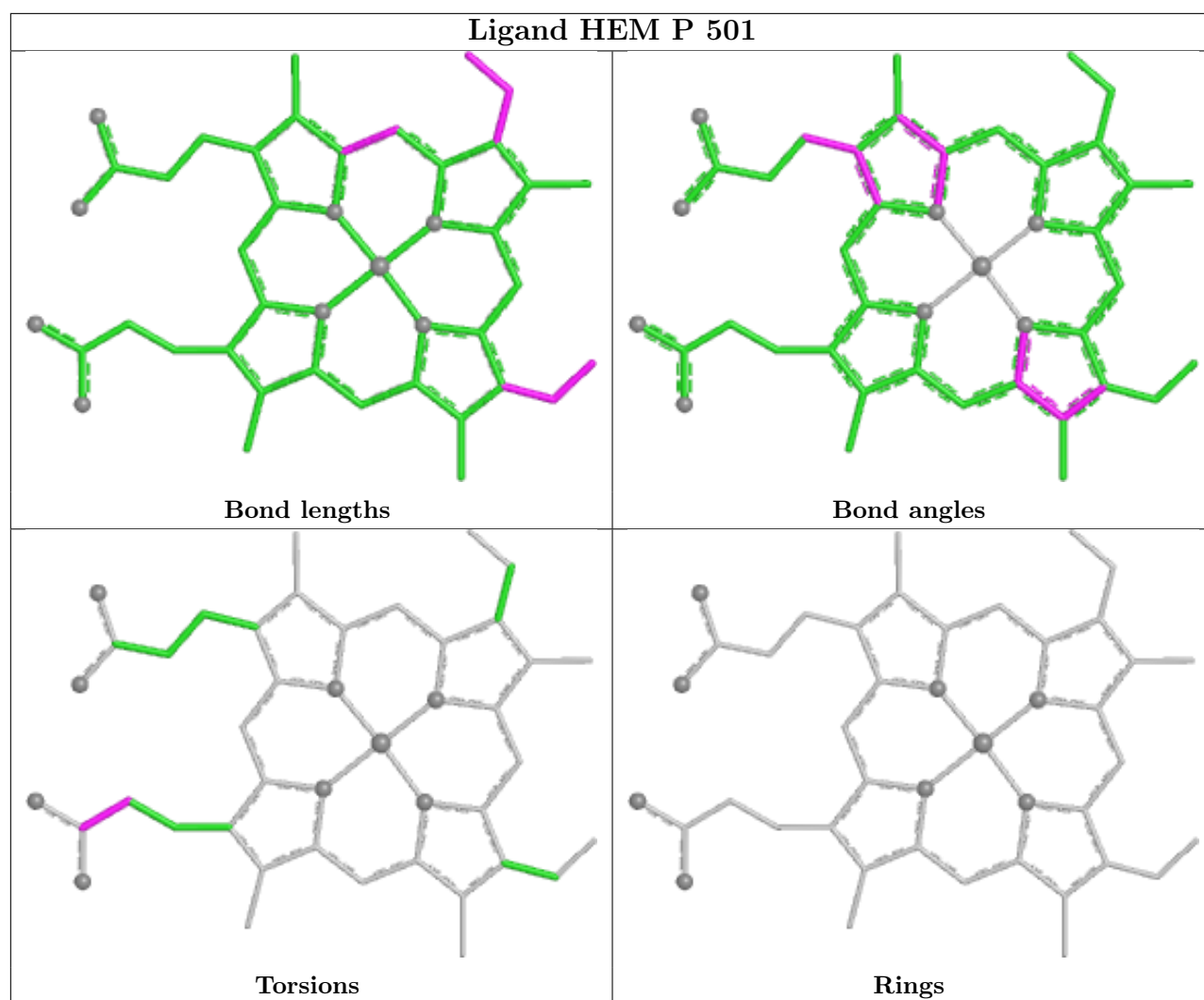
Bond angles

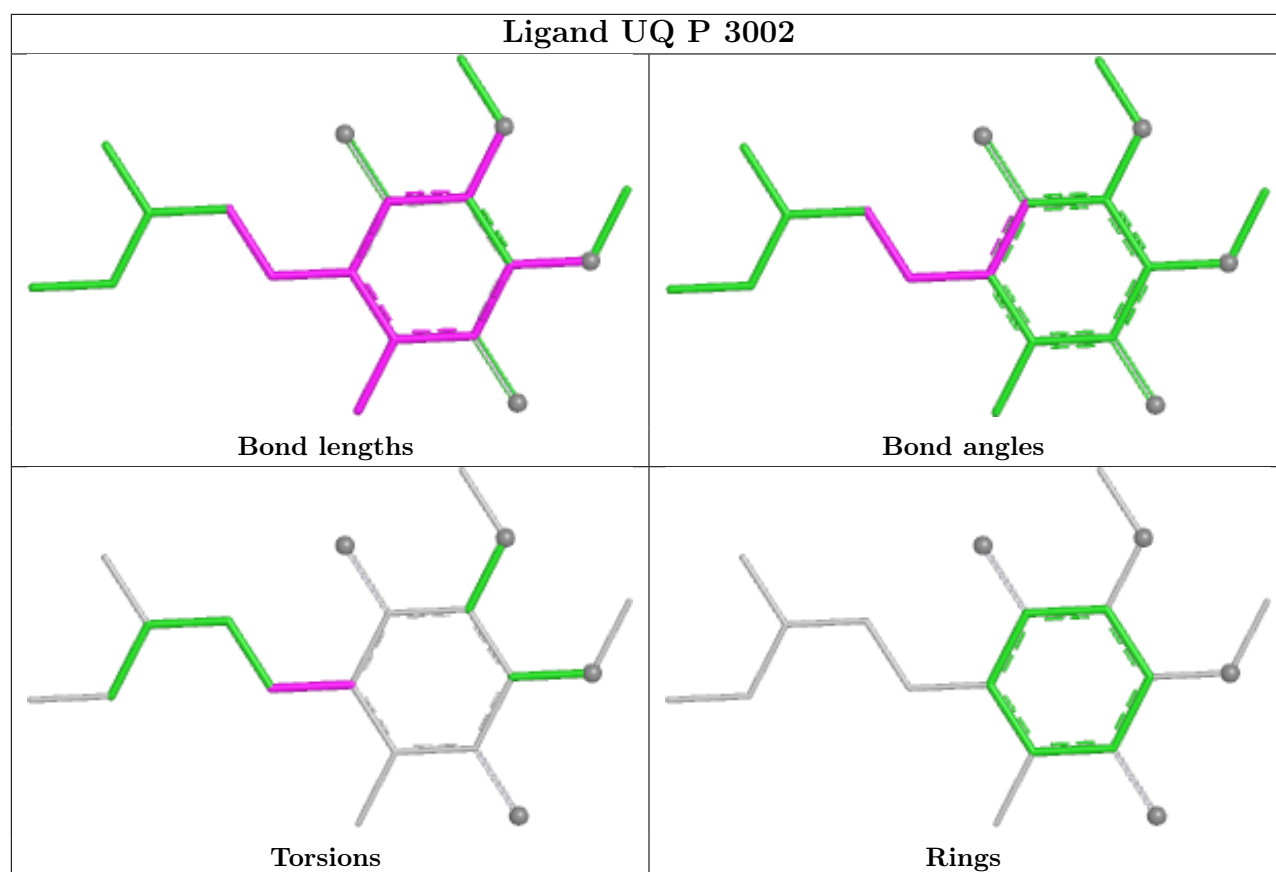


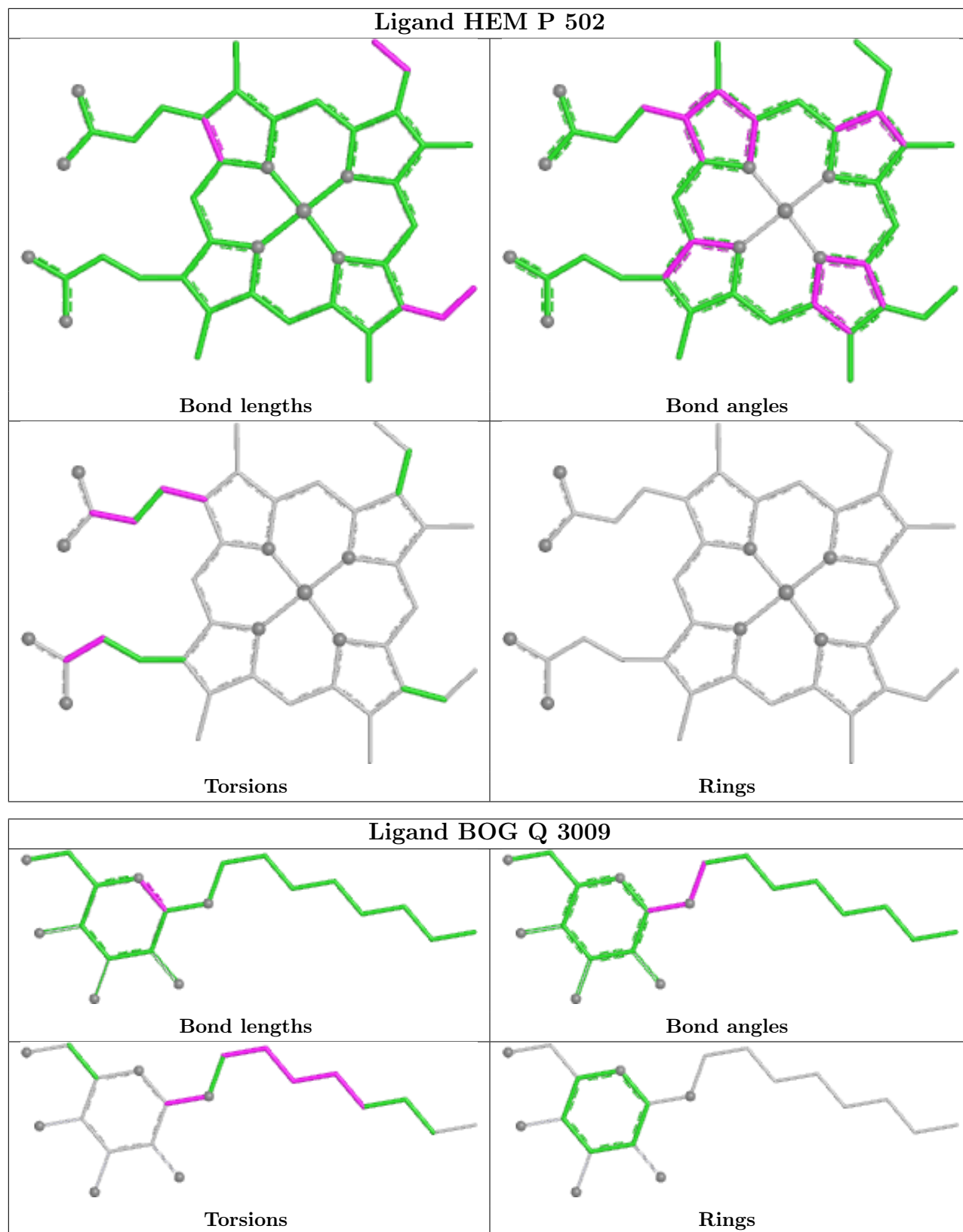
Torsions

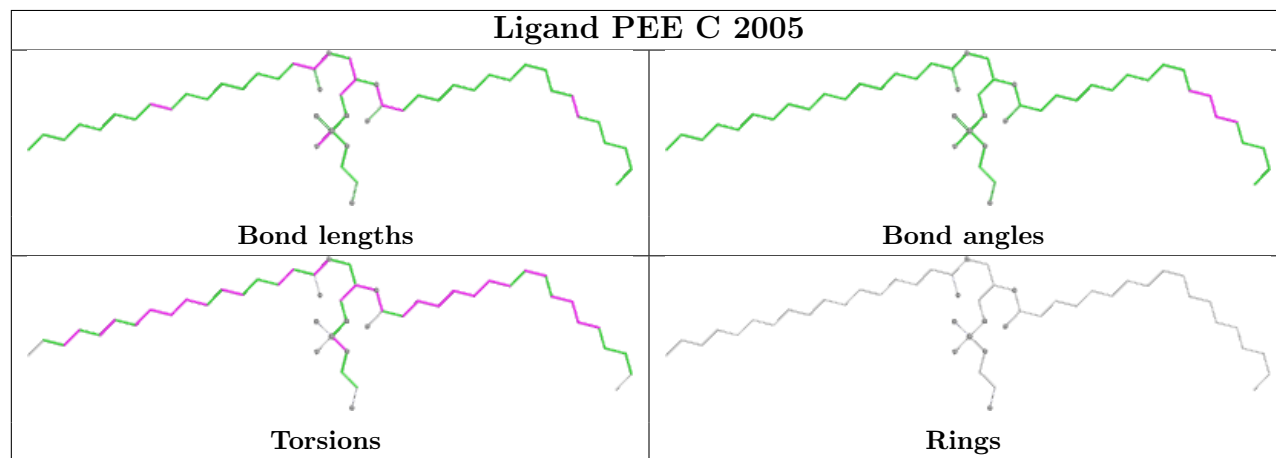
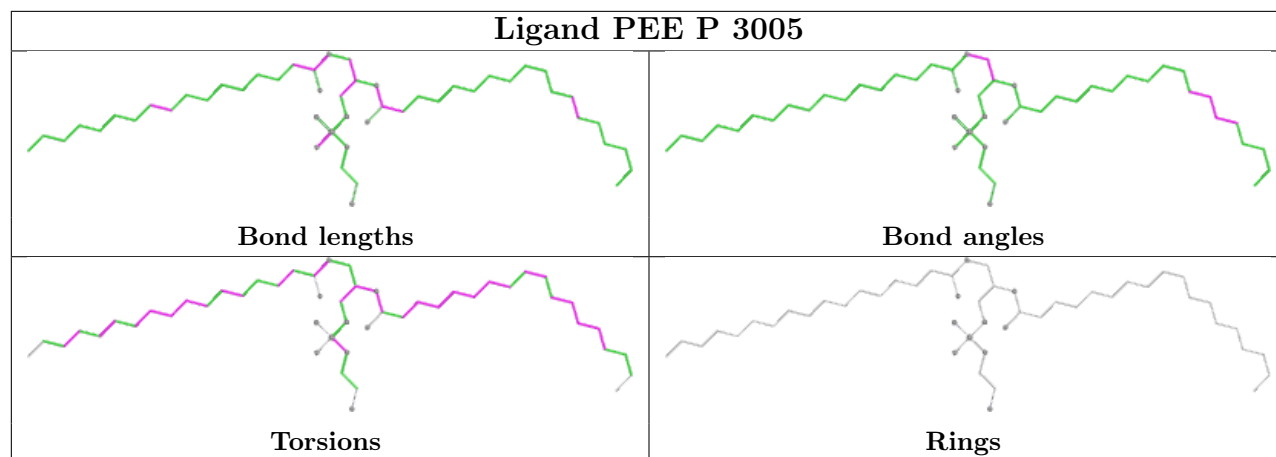


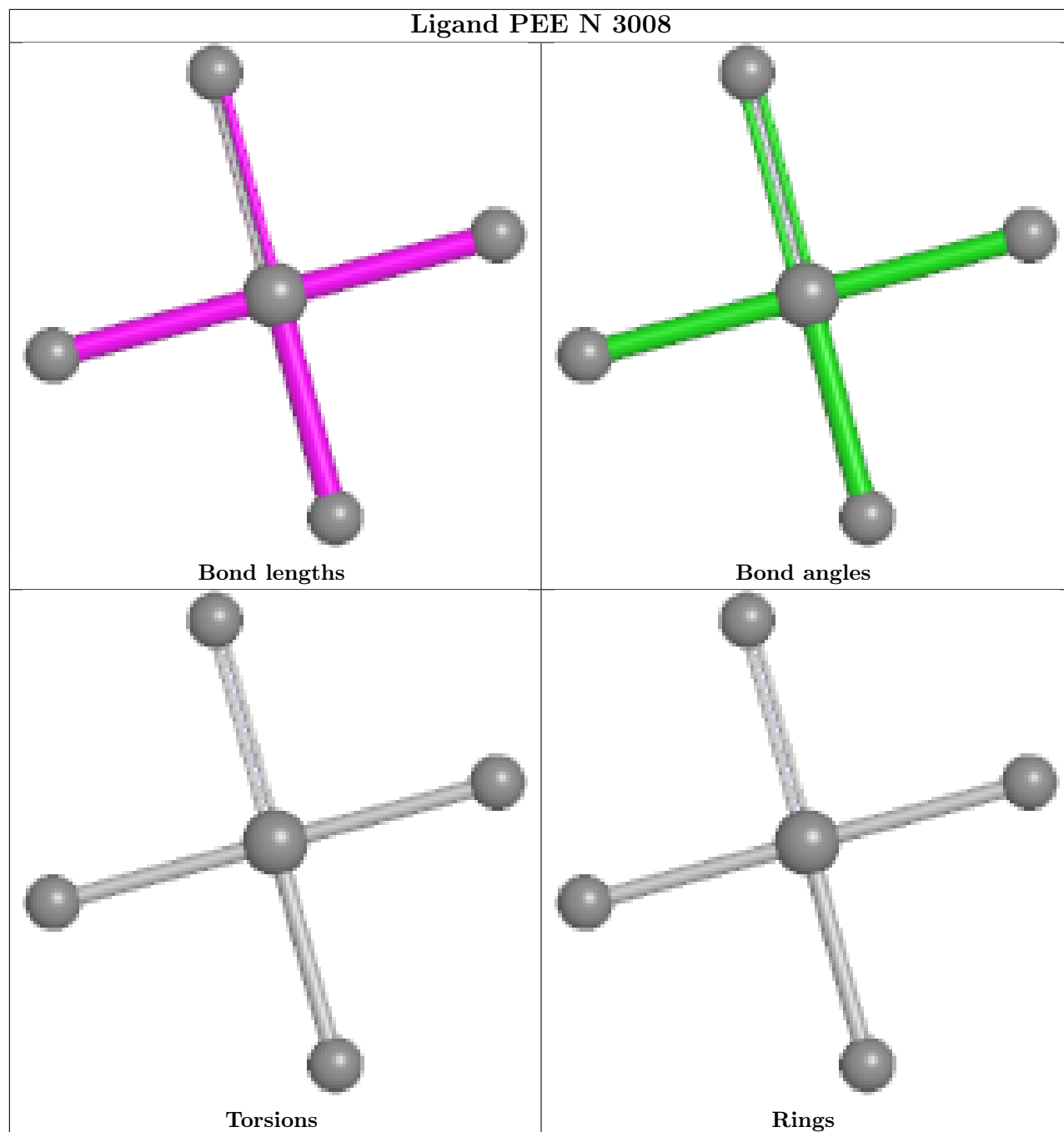
Rings

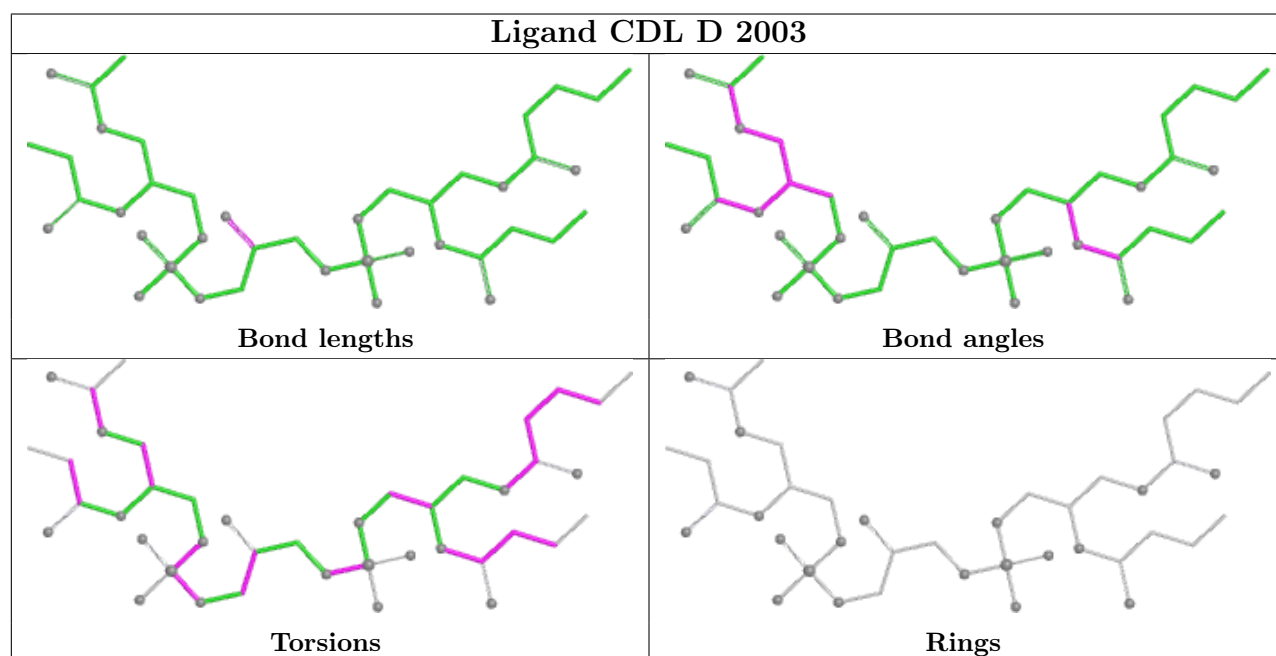
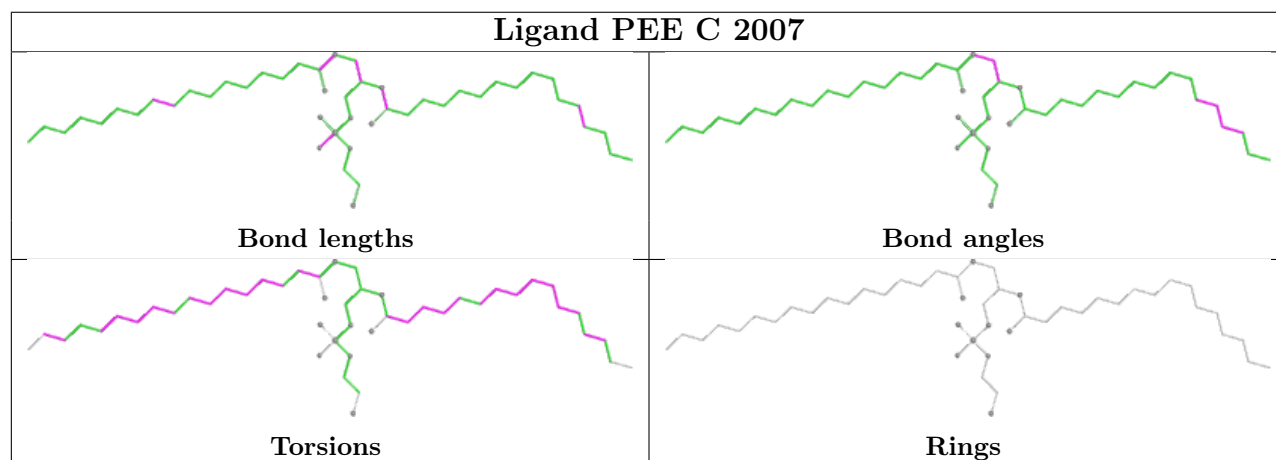
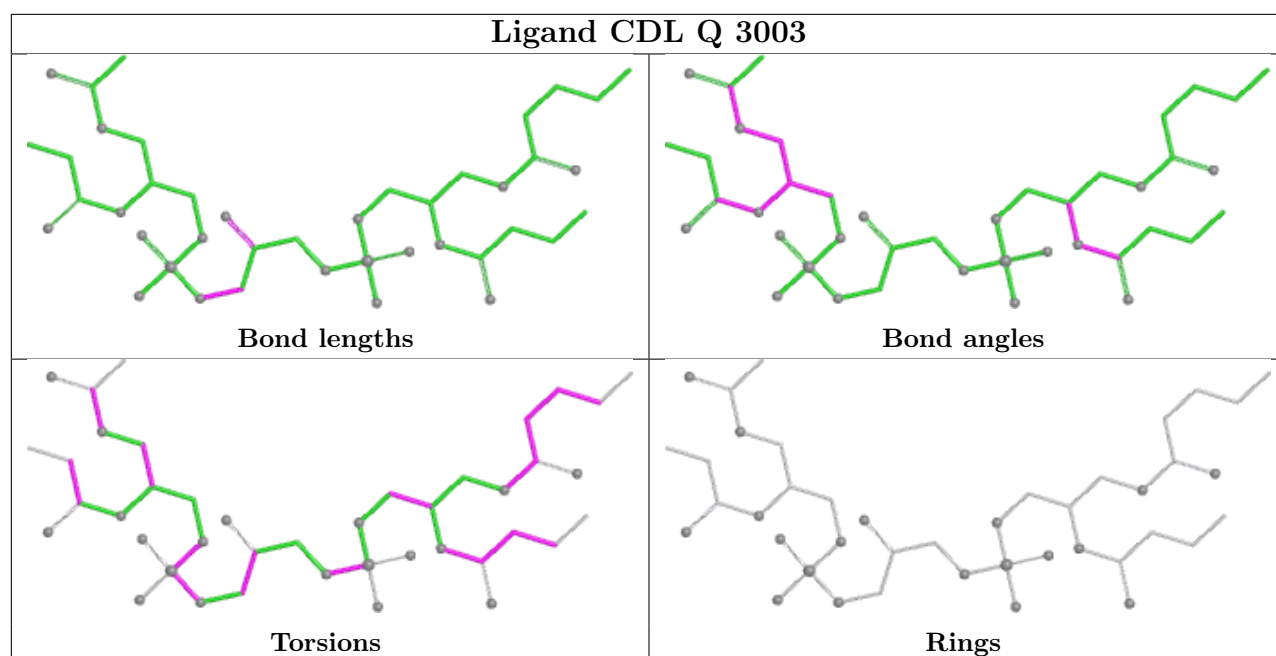


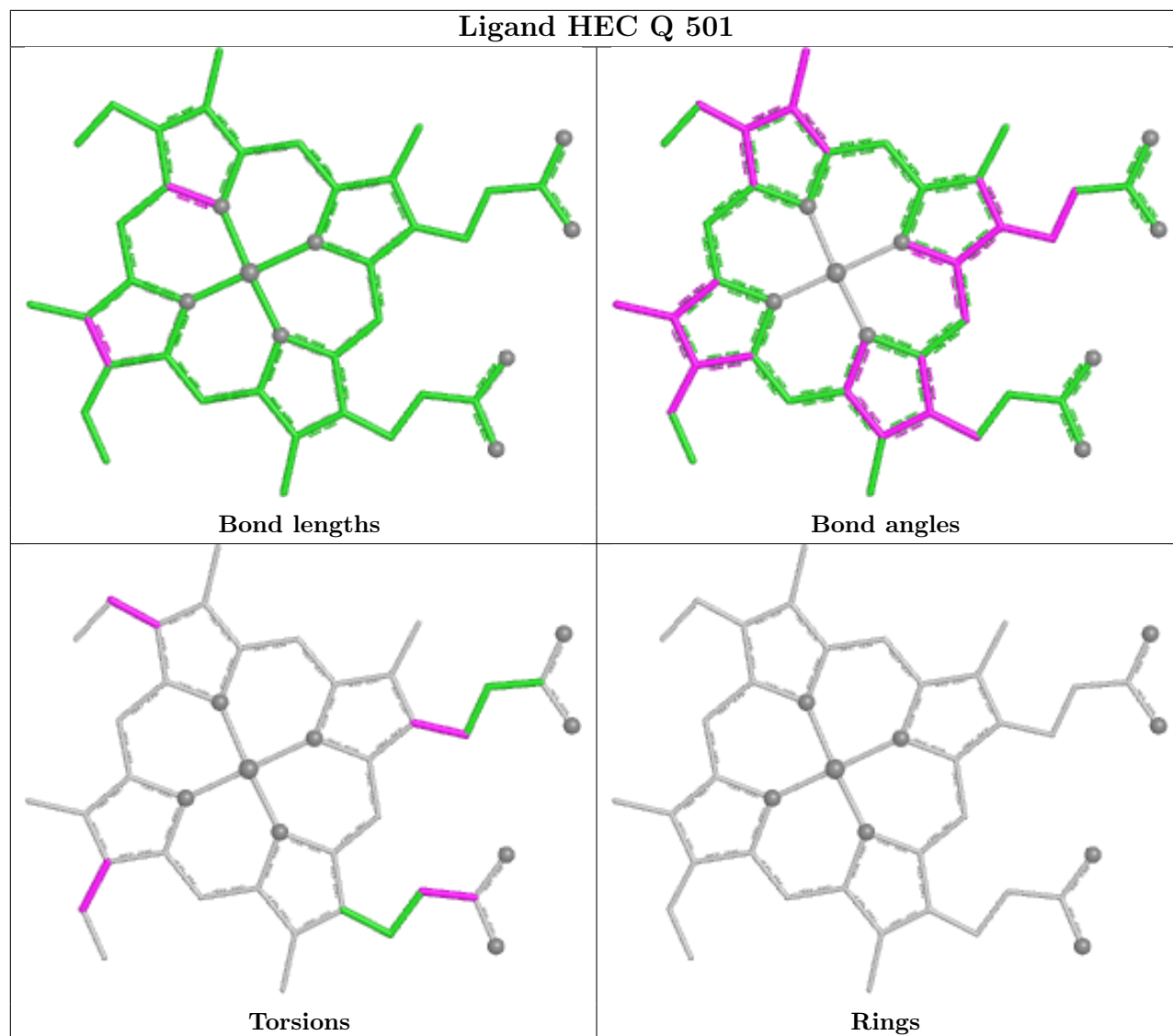


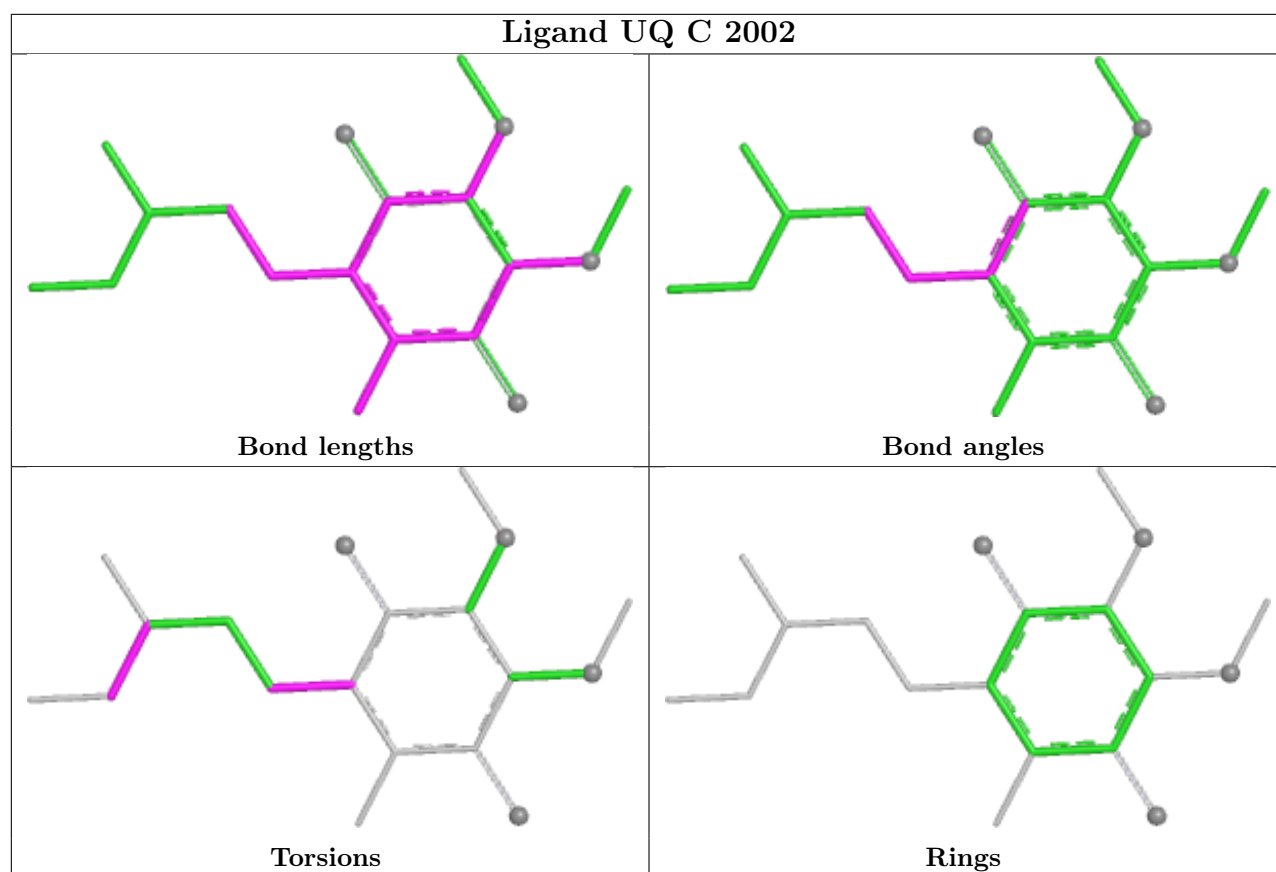












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.52	20 (4%) 38 30	29, 61, 87, 104	0
1	N	442/446 (99%)	0.94	45 (10%) 12 9	39, 69, 95, 104	0
2	B	421/441 (95%)	1.05	57 (13%) 7 5	50, 78, 116, 141	0
2	O	422/441 (95%)	0.95	53 (12%) 8 6	37, 74, 106, 120	0
3	C	380/380 (100%)	-0.11	7 (1%) 67 58	21, 39, 73, 109	0
3	P	379/380 (99%)	0.52	23 (6%) 27 20	30, 62, 84, 96	0
4	D	241/241 (100%)	-0.14	4 (1%) 69 60	30, 42, 78, 94	0
4	Q	241/241 (100%)	0.84	25 (10%) 11 8	50, 69, 99, 119	0
5	E	196/196 (100%)	1.24	57 (29%) 1 1	38, 80, 108, 113	0
5	R	196/196 (100%)	2.86	115 (58%) 0 0	42, 99, 140, 144	127 (64%)
6	F	101/110 (91%)	-0.17	2 (1%) 65 56	29, 42, 60, 96	0
6	S	101/110 (91%)	0.79	8 (7%) 18 13	55, 68, 111, 135	0
7	G	81/81 (100%)	0.44	6 (7%) 20 15	32, 52, 93, 108	0
7	T	78/81 (96%)	1.22	15 (19%) 3 2	48, 82, 144, 161	0
8	H	70/77 (90%)	0.41	4 (5%) 29 22	39, 59, 84, 123	0
8	U	67/77 (87%)	2.03	30 (44%) 0 0	96, 115, 133, 140	0
9	I	31/47 (65%)	3.40	26 (83%) 0 0	81, 105, 125, 126	0
9	V	31/47 (65%)	3.76	24 (77%) 0 0	69, 109, 142, 145	0
10	J	61/61 (100%)	0.33	2 (3%) 49 39	44, 60, 92, 130	0
10	W	60/61 (98%)	1.04	9 (15%) 5 4	56, 77, 99, 111	0
All	All	4042/4160 (97%)	0.81	532 (13%) 7 6	21, 65, 110, 161	127 (3%)

All (532) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	12.5
5	R	195	VAL	10.8
5	R	194	VAL	10.5
5	R	124	LEU	10.0
5	R	133	VAL	10.0
5	R	193	VAL	10.0
5	R	192	LEU	9.6
1	A	444	ILE	9.5
5	R	130	PRO	8.9
5	R	188	VAL	8.8
5	R	148	ALA	8.7
5	R	147	ILE	8.6
5	R	114	VAL	8.3
9	V	61	ARG	8.0
5	R	129	LYS	7.4
5	R	112	VAL	7.4
5	R	132	TRP	7.3
5	R	98	VAL	7.3
5	R	183	PRO	7.2
5	R	185	TYR	7.1
5	R	127	VAL	7.0
7	G	1	GLY	6.9
5	R	184	THR	6.9
5	R	87	VAL	6.9
5	R	110	ALA	6.8
9	V	77	ARG	6.8
5	R	74	ILE	6.6
9	I	61	ARG	6.6
9	V	62	ARG	6.4
10	W	62	SER	6.4
9	I	63	ASP	6.4
5	R	186	GLN	6.3
9	V	76	VAL	6.2
5	R	196	GLY	6.1
5	R	86	ASN	6.0
2	B	226	ILE	5.9
5	R	128	LYS	5.9
7	T	2	ILE	5.8
5	R	109	GLU	5.7
2	O	23	ASP	5.7
2	O	226	ILE	5.6
5	R	97	PHE	5.6
9	V	47	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
5	R	117	LEU	5.4
2	O	21	ALA	5.4
2	B	19	PRO	5.4
2	O	371	SER	5.4
5	E	110	ALA	5.4
5	R	187	PHE	5.4
1	N	318	GLY	5.3
5	E	188	VAL	5.1
5	R	104	ALA	5.1
5	R	89	PHE	5.1
5	R	136	VAL	5.0
5	R	145	VAL	5.0
9	V	49	LEU	5.0
8	U	54	CYS	5.0
9	I	53	GLU	5.0
5	R	126	ARG	4.9
5	R	106	ILE	4.9
5	R	93	GLY	4.8
5	R	94	LYS	4.8
9	I	56	SER	4.8
5	R	181	GLU	4.7
7	G	2	ILE	4.7
1	A	2	ALA	4.7
2	O	384	SER	4.7
8	H	9	GLU	4.6
2	B	120	MET	4.6
9	I	57	GLY	4.6
5	R	138	VAL	4.6
5	R	156	TYR	4.6
9	V	59	SER	4.6
9	I	62	ARG	4.6
5	R	146	PRO	4.6
5	R	150	SER	4.6
5	R	96	LEU	4.5
9	V	64	LEU	4.5
5	R	174	GLY	4.5
5	E	187	PHE	4.5
5	R	189	GLY	4.5
2	O	223	PHE	4.4
2	B	21	ALA	4.4
4	Q	9	ALA	4.4
5	R	71	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
9	I	49	LEU	4.4
5	R	172	ARG	4.4
9	I	75	SER	4.4
9	V	56	SER	4.4
2	O	207	VAL	4.4
5	E	133	VAL	4.4
2	B	124	LEU	4.4
5	R	99	ARG	4.4
2	B	20	GLY	4.4
2	B	402	ILE	4.4
5	E	117	LEU	4.3
9	I	64	LEU	4.3
9	I	72	ALA	4.3
2	O	383	GLY	4.3
8	U	78	LYS	4.2
2	O	380	ASN	4.2
4	Q	180	SER	4.2
5	R	72	SER	4.2
5	R	154	GLY	4.2
10	W	61	ALA	4.2
5	R	82	PRO	4.1
1	N	444	ILE	4.1
5	R	173	LYS	4.1
9	I	77	ARG	4.1
1	A	4	TYR	4.1
2	O	368	TYR	4.1
5	R	92	ARG	4.1
5	R	182	VAL	4.1
5	E	115	SER	4.0
8	U	24	CYS	4.0
10	W	63	GLU	4.0
9	I	51	CYS	4.0
2	B	205	ALA	4.0
9	I	47	ARG	3.9
2	B	235	ALA	3.9
6	S	10	GLY	3.9
5	R	91	TRP	3.9
9	V	50	LEU	3.9
1	A	219	VAL	3.9
9	I	71	ASN	3.9
5	R	78	LEU	3.9
1	A	443	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	365	MET	3.8
5	R	120	PRO	3.8
9	V	70	LEU	3.8
5	R	178	TYR	3.7
5	R	180	LEU	3.7
2	O	104	LYS	3.7
8	U	76	LYS	3.7
5	E	74	ILE	3.7
5	R	76	ILE	3.7
5	R	151	GLY	3.7
5	E	178	TYR	3.7
5	E	114	VAL	3.7
2	O	224	LEU	3.7
2	O	20	GLY	3.7
7	T	75	ALA	3.7
1	N	219	VAL	3.7
1	N	443	TRP	3.6
5	R	167	ALA	3.6
5	R	88	ALA	3.6
7	T	77	TYR	3.6
9	V	60	ALA	3.6
8	U	73	LEU	3.6
5	E	91	TRP	3.6
4	Q	2	GLU	3.6
2	B	236	LYS	3.6
9	V	71	ASN	3.6
2	B	223	PHE	3.6
2	O	24	LEU	3.6
5	R	73	LYS	3.6
8	U	26	GLN	3.5
5	E	118	ARG	3.5
5	R	134	ILE	3.5
1	A	226	ASP	3.5
5	R	95	PRO	3.5
8	U	16	PRO	3.5
5	E	124	LEU	3.5
5	R	80	ASP	3.5
5	R	113	ASP	3.5
3	C	2	ALA	3.5
1	N	57	TYR	3.5
7	T	72	LYS	3.5
1	A	73	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	O	268	GLU	3.5
2	B	291	VAL	3.5
8	U	30	CYS	3.4
9	V	52	ARG	3.4
5	R	108	GLN	3.4
2	O	291	VAL	3.4
2	O	19	PRO	3.4
4	Q	1	GLY	3.4
2	O	292	THR	3.4
5	E	192	LEU	3.4
7	T	79	ASN	3.4
1	A	300	GLU	3.3
5	R	153	PHE	3.3
2	B	439	LEU	3.3
5	R	149	ASN	3.3
5	R	160	CYS	3.3
5	R	102	THR	3.3
5	R	155	GLY	3.3
1	N	75	PHE	3.3
9	I	50	LEU	3.3
5	E	148	ALA	3.3
9	V	57	GLY	3.2
5	R	118	ARG	3.2
9	I	52	ARG	3.2
2	B	224	LEU	3.2
5	E	90	LYS	3.2
5	R	116	LYS	3.2
2	O	376	GLN	3.2
5	R	176	ALA	3.2
5	E	147	ILE	3.2
5	E	193	VAL	3.2
5	R	90	LYS	3.2
1	A	392	LEU	3.2
8	U	39	LEU	3.2
9	V	48	PRO	3.2
3	C	1	MET	3.1
7	G	72	LYS	3.1
3	P	203	GLU	3.1
4	D	145	GLU	3.1
2	O	18	CYS	3.1
5	R	157	TYR	3.1
5	E	116	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
9	I	60	ALA	3.1
5	R	159	PRO	3.1
10	J	61	ALA	3.1
5	R	161	HIS	3.1
10	W	8	GLN	3.1
8	U	29	LYS	3.1
3	P	325	LEU	3.0
5	R	131	GLU	3.0
1	N	69	LYS	3.0
2	B	204	MET	3.0
5	E	89	PHE	3.0
5	E	101	ARG	3.0
5	R	81	ILE	3.0
7	T	24	ARG	3.0
4	Q	139	ALA	3.0
9	V	72	ALA	3.0
2	O	50	PHE	3.0
2	B	392	HIS	3.0
5	E	122	HIS	3.0
5	E	167	ALA	3.0
1	N	190	PHE	3.0
2	B	417	PHE	3.0
9	V	58	ARG	3.0
2	B	26	ILE	3.0
2	O	299	VAL	3.0
7	T	3	HIS	2.9
5	E	128	LYS	2.9
5	E	156	TYR	2.9
5	R	123	ASP	2.9
4	Q	143	VAL	2.9
2	O	381	GLU	2.9
8	U	75	ASN	2.9
5	E	93	GLY	2.9
4	Q	142	VAL	2.9
4	Q	3	LEU	2.9
4	Q	169	LEU	2.9
2	B	34	ILE	2.9
5	R	119	ASP	2.9
6	S	89	TYR	2.9
5	E	71	LEU	2.9
9	I	73	PRO	2.9
5	E	185	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
7	T	47	LYS	2.9
1	N	310	PHE	2.9
2	O	227	ARG	2.8
5	R	115	SER	2.8
5	E	190	ASP	2.8
9	I	58	ARG	2.8
5	E	73	LYS	2.8
2	B	33	LEU	2.8
2	O	36	ALA	2.8
3	P	2	ALA	2.8
1	N	216	PHE	2.8
5	R	122	HIS	2.8
8	H	22	GLU	2.8
5	E	82	PRO	2.8
8	U	65	ARG	2.8
5	R	168	SER	2.8
2	O	387	LEU	2.8
5	R	135	LEU	2.8
3	P	380	TYR	2.8
9	I	76	VAL	2.8
1	N	218	GLY	2.8
5	R	142	LEU	2.8
1	N	185	TYR	2.8
4	Q	87	ILE	2.7
5	E	129	LYS	2.7
8	U	72	LYS	2.7
2	B	231	GLY	2.7
2	B	113	ARG	2.7
5	E	99	ARG	2.7
8	U	34	ARG	2.7
9	I	70	LEU	2.7
5	R	101	ARG	2.7
1	N	228	VAL	2.7
5	E	184	THR	2.7
1	A	69	LYS	2.7
1	N	19	LEU	2.7
5	R	162	GLY	2.7
9	I	69	SER	2.7
1	N	64	PHE	2.7
8	U	55	THR	2.7
1	N	266	ASP	2.7
2	B	403	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	130	PRO	2.7
2	O	99	TYR	2.6
9	V	51	CYS	2.6
10	W	5	LEU	2.6
5	E	149	ASN	2.6
4	Q	175	THR	2.6
4	Q	171	TYR	2.6
5	R	165	TYR	2.6
1	N	168	GLU	2.6
5	E	196	GLY	2.6
2	O	395	PRO	2.6
2	O	110	GLU	2.6
5	E	109	GLU	2.6
1	N	180	ALA	2.6
4	Q	137	PRO	2.6
4	Q	141	VAL	2.6
5	E	98	VAL	2.6
8	U	44	VAL	2.6
1	N	85	HIS	2.6
7	G	78	GLU	2.6
3	P	252	GLY	2.6
8	U	68	CYS	2.6
1	N	26	ALA	2.6
1	N	229	PRO	2.6
6	S	23	ALA	2.6
7	T	25	ALA	2.6
5	E	72	SER	2.5
5	R	125	ASP	2.5
2	B	24	LEU	2.5
3	P	6	ARG	2.5
2	O	250	HIS	2.5
2	O	22	GLU	2.5
1	A	22	GLY	2.5
1	N	54	GLY	2.5
1	N	160	GLY	2.5
2	B	43	PRO	2.5
5	E	119	ASP	2.5
5	E	106	ILE	2.5
5	R	164	HIS	2.5
3	P	156	TYR	2.5
5	E	75	GLU	2.5
5	R	137	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	395	PRO	2.5
5	R	177	PRO	2.5
4	D	143	VAL	2.5
9	V	55	MET	2.5
2	B	117	ASP	2.5
5	R	111	GLU	2.5
2	O	296	TYR	2.5
2	B	229	GLY	2.5
4	D	1	GLY	2.5
1	N	209	VAL	2.5
2	O	386	ALA	2.5
5	E	132	TRP	2.5
6	S	66	LEU	2.5
2	O	208	GLY	2.5
2	B	30	PRO	2.5
7	T	74	PRO	2.5
2	B	150	VAL	2.5
2	B	41	PHE	2.5
2	O	300	ALA	2.5
7	T	4	PHE	2.5
8	U	74	PHE	2.5
3	P	269	ILE	2.4
3	P	213	SER	2.4
2	B	114	ASP	2.4
4	Q	69	GLU	2.4
1	A	33	PRO	2.4
5	E	157	TYR	2.4
3	C	4	ASN	2.4
5	E	96	LEU	2.4
5	R	107	ASN	2.4
3	C	268	HIS	2.4
3	P	286	PRO	2.4
5	R	85	LYS	2.4
1	N	116	VAL	2.4
2	O	220	ALA	2.4
1	N	3	THR	2.4
3	C	5	ILE	2.4
4	Q	5	LEU	2.4
1	A	21	ASN	2.4
5	R	190	ASP	2.4
5	R	121	GLN	2.4
5	E	87	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	5	ILE	2.4
3	P	9	HIS	2.4
2	O	228	SER	2.4
2	O	266	SER	2.4
2	B	281	ALA	2.4
8	U	13	LEU	2.3
8	U	77	LEU	2.3
2	B	73	SER	2.3
1	A	193	PRO	2.3
4	Q	176	PRO	2.3
2	B	48	GLY	2.3
5	E	121	GLN	2.3
8	U	14	VAL	2.3
1	N	86	PHE	2.3
2	O	394	ALA	2.3
8	U	61	PHE	2.3
7	T	69	LEU	2.3
8	U	17	LEU	2.3
1	N	223	TYR	2.3
8	H	71	HIS	2.3
1	N	82	MET	2.3
9	I	59	SER	2.3
7	T	20	PRO	2.3
2	O	264	VAL	2.3
1	N	122	LEU	2.3
5	E	134	ILE	2.3
1	N	18	THR	2.3
4	D	241	LYS	2.3
4	Q	173	ASP	2.3
5	R	175	PRO	2.3
2	B	211	VAL	2.3
1	N	170	THR	2.3
2	B	232	THR	2.3
2	O	304	THR	2.3
5	R	83	GLU	2.3
5	E	86	ASN	2.3
2	B	23	ASP	2.3
2	B	306	PRO	2.3
3	P	253	ASP	2.3
8	U	60	ASP	2.3
2	B	156	GLN	2.3
1	N	121	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	209	ILE	2.2
2	B	161	GLU	2.2
1	N	282	ARG	2.2
7	G	81	GLN	2.2
1	N	230	ILE	2.2
3	P	34	PHE	2.2
9	V	68	ILE	2.2
2	B	127	THR	2.2
6	S	39	GLU	2.2
1	N	414	TYR	2.2
2	B	227	ARG	2.2
9	I	48	PRO	2.2
2	B	363	GLN	2.2
2	O	37	SER	2.2
2	O	377	GLY	2.2
7	T	5	GLY	2.2
2	B	369	LEU	2.2
4	Q	130	LEU	2.2
5	E	138	VAL	2.2
5	E	173	LYS	2.2
2	O	307	PHE	2.2
1	N	28	GLU	2.2
5	R	75	GLU	2.2
8	H	10	GLU	2.2
4	Q	7	PRO	2.2
2	O	222	GLN	2.2
5	R	103	GLN	2.2
8	U	53	GLN	2.2
1	N	112	LEU	2.2
2	B	436	LEU	2.2
2	B	398	VAL	2.2
3	P	344	VAL	2.2
5	E	136	VAL	2.2
5	R	100	HIS	2.2
4	Q	119	ALA	2.2
5	R	70	ALA	2.2
10	J	63	GLU	2.2
3	C	224	TYR	2.2
5	R	77	LYS	2.2
2	O	379	LEU	2.2
5	E	174	GLY	2.2
1	A	81	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	322	SER	2.2
9	V	75	SER	2.2
3	P	240	PHE	2.2
8	U	33	ALA	2.1
5	R	105	GLU	2.1
2	B	283	PRO	2.1
3	P	7	LYS	2.1
3	P	256	ASN	2.1
6	F	87	LYS	2.1
2	B	206	LEU	2.1
4	Q	121	HIS	2.1
2	B	214	SER	2.1
5	E	194	VAL	2.1
7	T	26	ILE	2.1
1	A	227	ALA	2.1
10	W	12	ALA	2.1
1	N	50	GLU	2.1
5	E	102	THR	2.1
1	N	108	LYS	2.1
2	B	301	LYS	2.1
1	N	182	LEU	2.1
1	N	201	GLY	2.1
9	V	65	VAL	2.1
2	O	97	SER	2.1
2	O	303	THR	2.1
2	B	28	LYS	2.1
3	P	320	PRO	2.1
5	E	120	PRO	2.1
1	N	23	LEU	2.1
6	S	90	LEU	2.1
7	G	79	ASN	2.1
8	U	49	HIS	2.1
5	E	112	VAL	2.1
8	U	20	ILE	2.1
9	I	68	ILE	2.1
10	W	55	ILE	2.1
1	A	86	PHE	2.1
5	R	24	SER	2.1
1	N	233	ARG	2.1
10	W	4	ALA	2.1
1	A	224	LYS	2.1
6	S	59	MET	2.1

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Mol	Chain	Res	Type	RSRZ
5	R	26	GLN	2.1
2	O	364	LEU	2.1
3	P	233	LEU	2.1
4	Q	174	GLY	2.1
6	S	30	GLY	2.1
1	N	174	ILE	2.1
2	O	219	VAL	2.1
2	B	371	SER	2.0
5	R	29	SER	2.0
10	W	11	SER	2.0
2	B	304	THR	2.0
3	C	60	THR	2.0
2	B	388	LEU	2.0
2	O	295	LEU	2.0
3	P	321	LEU	2.0
8	U	63	HIS	2.0
2	B	397	VAL	2.0
8	U	31	VAL	2.0
2	O	25	GLU	2.0
4	Q	241	LYS	2.0
6	F	110	LYS	2.0
1	A	217	SER	2.0
5	R	25	SER	2.0
4	Q	138	PRO	2.0
2	B	400	GLN	2.0
3	P	249	ASN	2.0
9	I	65	VAL	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.

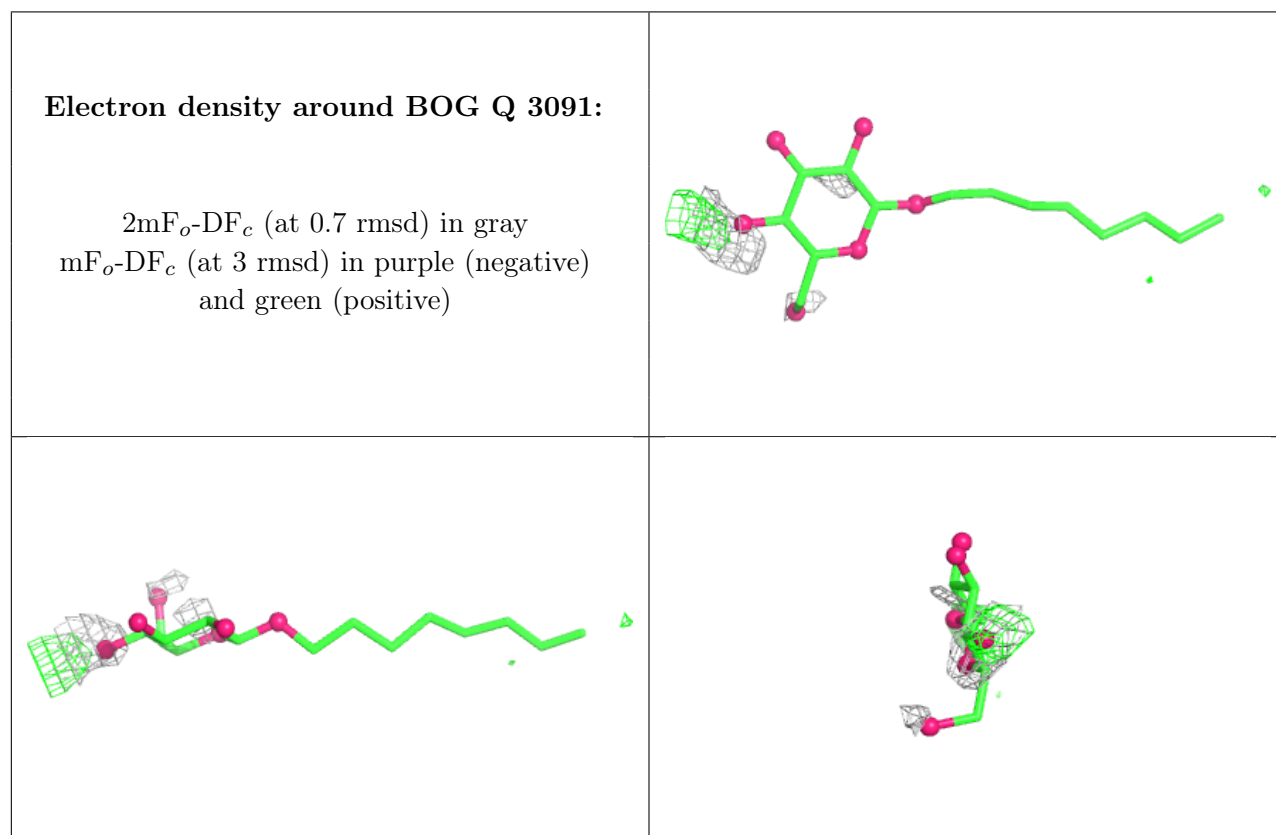
6.4 Ligands [i](#)

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.

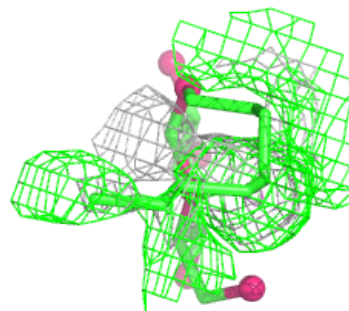
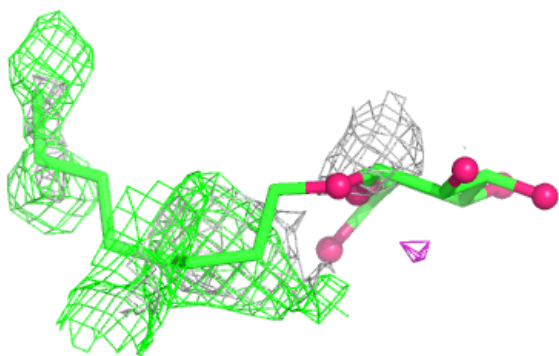
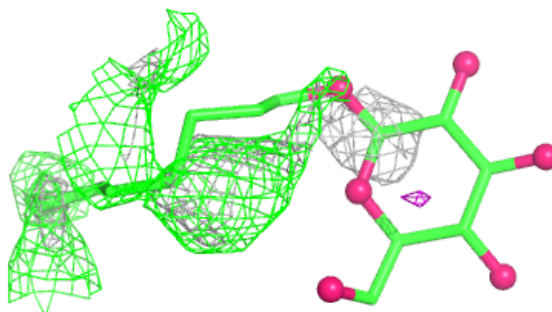
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	BOG	Q	3091	20/20	0.53	0.34	178,186,187,187	0
12	UNL	P	3048	2/-	0.54	0.88	92,92,92,95	0
17	BOG	D	2091	20/20	0.72	0.50	177,189,190,190	0
12	UNL	D	2012	2/-	0.78	0.21	59,59,59,60	0
12	UNL	C	2048	2/-	0.78	0.37	62,62,62,63	0
17	BOG	P	2010	19/20	0.79	0.35	102,183,184,184	0
19	CDL	T	3004	40/100	0.79	0.23	94,97,106,107	0
19	CDL	Q	3003	42/100	0.81	0.26	119,124,137,138	0
19	CDL	D	2003	42/100	0.81	0.22	81,93,97,98	0
11	PEE	A	2008	21/51	0.82	0.24	95,113,116,118	0
12	UNL	P	3046	2/-	0.86	0.17	85,85,85,85	0
15	UQ	C	2002	19/63	0.86	0.27	85,87,89,89	0
12	UNL	P	3014	1/-	0.87	0.17	55,55,55,55	0
19	CDL	G	2004	40/100	0.87	0.17	60,70,85,86	0
11	PEE	C	2005	50/51	0.87	0.25	83,93,101,104	0
16	AZI	C	2011	3/3	0.87	0.25	68,68,69,71	0
15	UQ	P	3002	19/63	0.88	0.33	138,141,143,143	0
11	PEE	N	3008	5/51	0.88	0.11	88,88,89,89	0
11	PEE	P	3005	50/51	0.88	0.26	74,100,105,105	0
17	BOG	Q	3009	20/20	0.90	0.17	71,79,81,82	0
11	PEE	P	3007	48/51	0.90	0.24	76,90,105,106	0
17	BOG	C	3010	12/20	0.90	0.26	94,96,97,98	0
12	UNL	C	2047	1/-	0.91	0.09	34,34,34,34	0
17	BOG	D	2009	20/20	0.91	0.13	56,63,65,67	0
12	UNL	C	2046	2/-	0.92	0.22	87,87,87,91	0
12	UNL	P	3013	1/-	0.92	0.29	56,56,56,56	0
12	UNL	A	3015	1/-	0.92	0.15	48,48,48,48	0
12	UNL	P	3047	1/-	0.94	0.09	47,47,47,47	0
16	AZI	P	3011	3/3	0.94	0.20	74,74,76,77	0
14	FNM	P	3001	22/22	0.95	0.11	49,53,59,62	0
20	FES	R	501	4/4	0.95	0.17	106,106,106,107	4
18	HEC	Q	501	43/43	0.96	0.10	47,55,64,66	0
12	UNL	R	3012	1/-	0.96	0.19	38,38,38,38	0
11	PEE	C	2007	48/51	0.96	0.14	41,52,81,82	0
20	FES	E	501	4/4	0.97	0.08	83,84,85,86	0
14	FNM	C	2001	22/22	0.97	0.07	38,40,42,44	0
13	HEM	P	502	43/43	0.98	0.07	34,40,55,62	0
18	HEC	D	501	43/43	0.98	0.07	23,30,35,37	0
13	HEM	P	501	43/43	0.98	0.09	40,43,54,58	0
13	HEM	C	501	43/43	0.99	0.07	23,31,38,43	0
13	HEM	C	502	43/43	0.99	0.06	23,26,33,39	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.

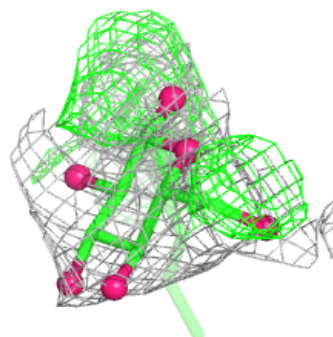
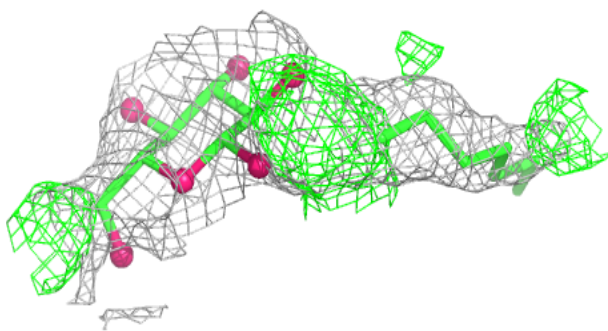
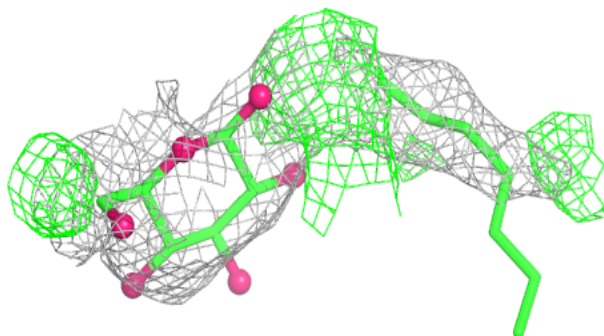


Electron density around BOG D 2091:

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

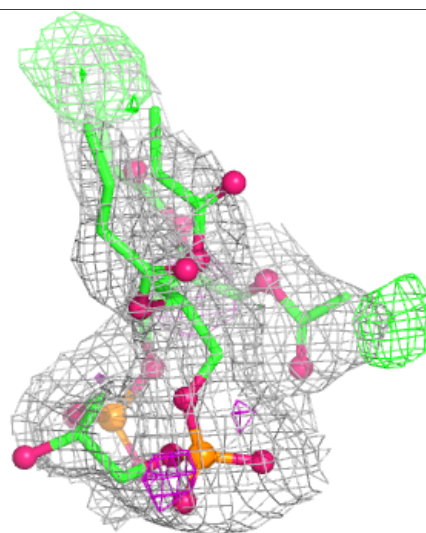
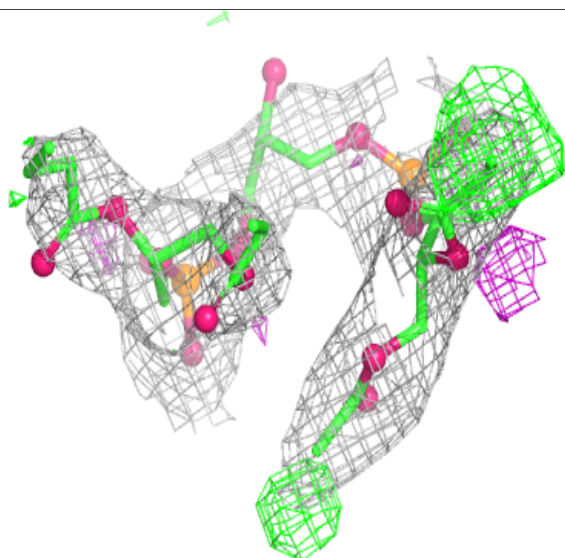
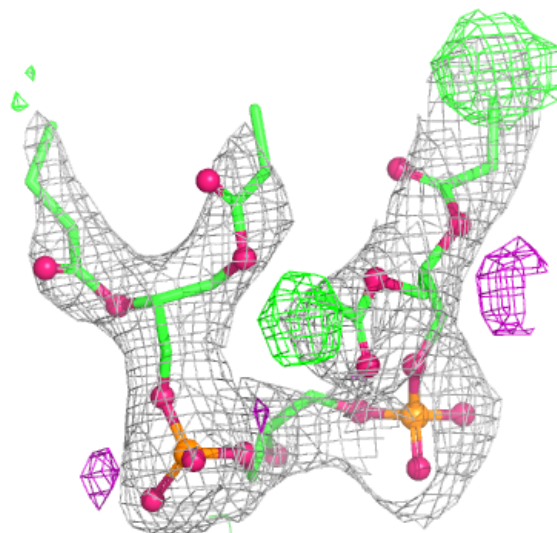
**Electron density around BOG P 2010:**

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



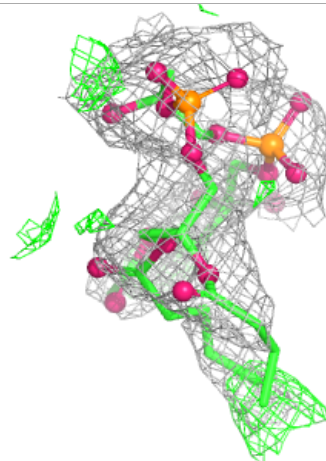
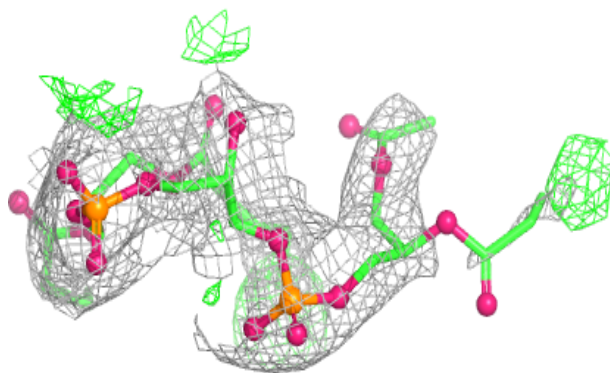
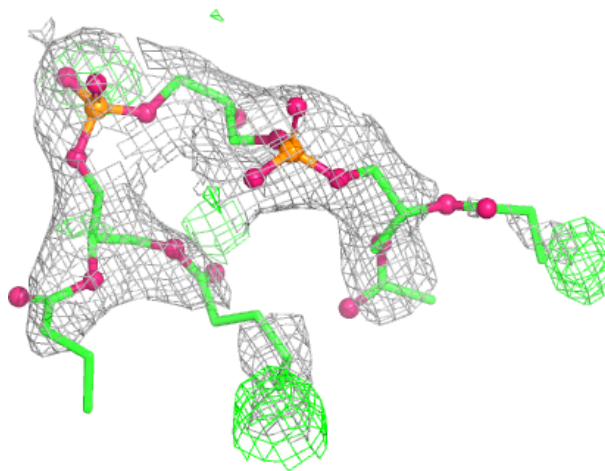
Electron density around CDL T 3004:

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



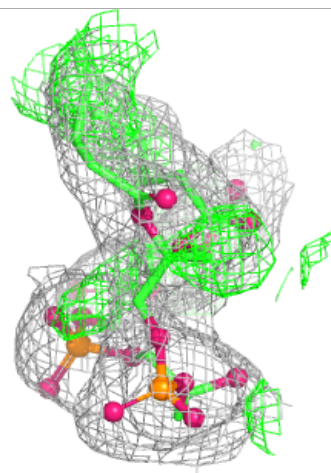
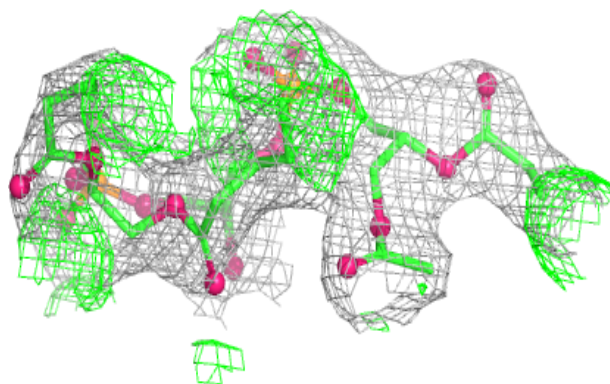
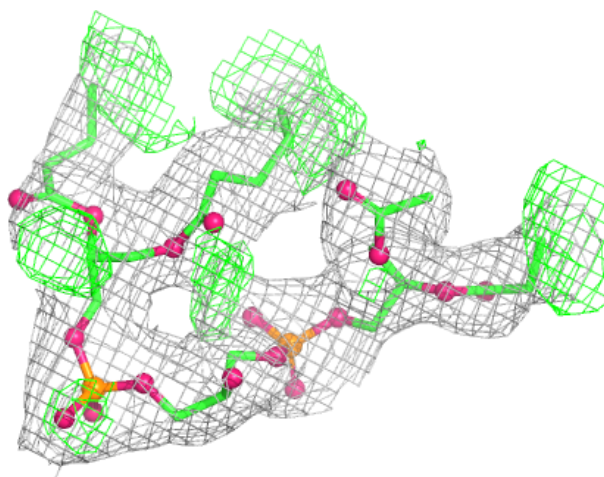
Electron density around CDL Q 3003:

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



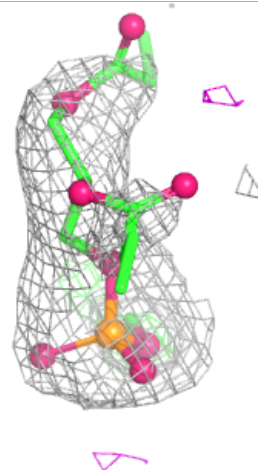
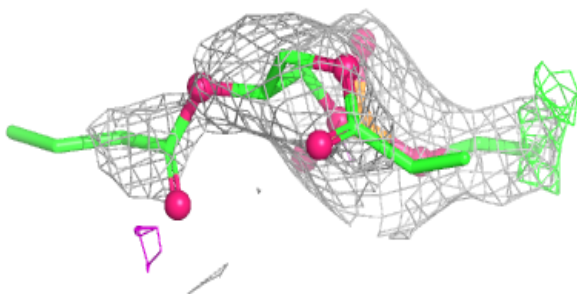
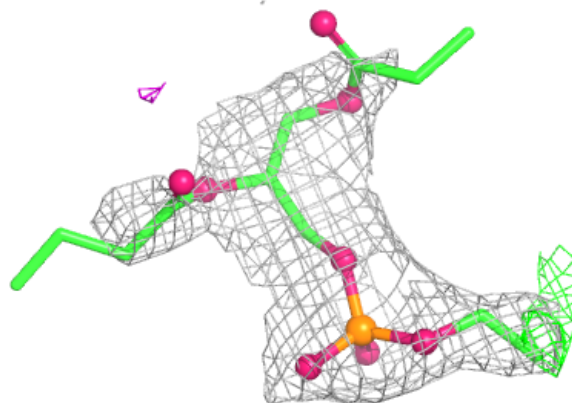
Electron density around CDL D 2003:

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



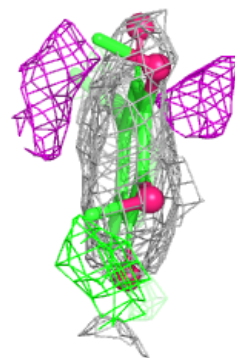
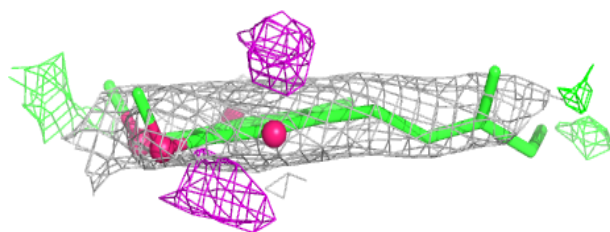
Electron density around PEE A 2008:

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



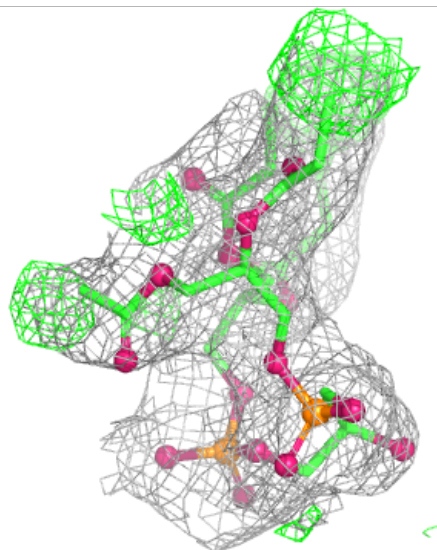
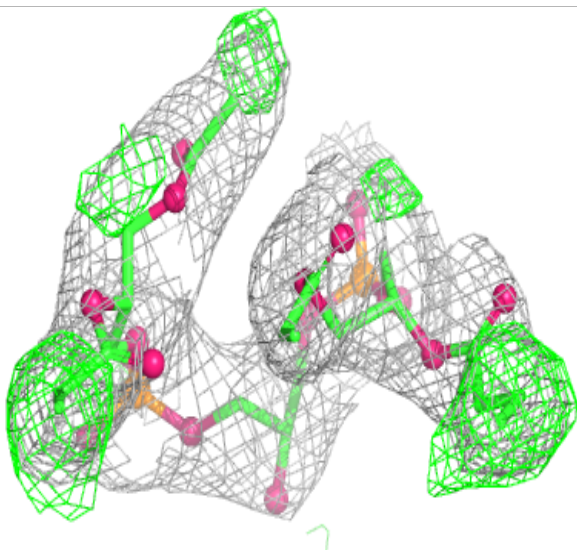
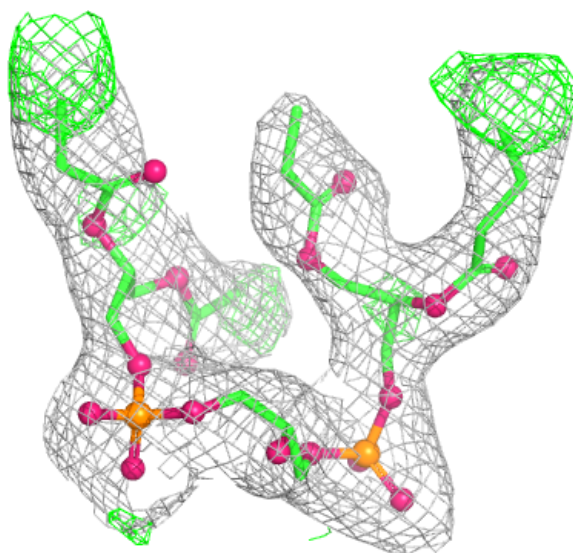
Electron density around UQ C 2002:

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



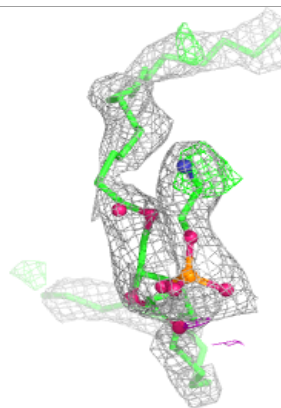
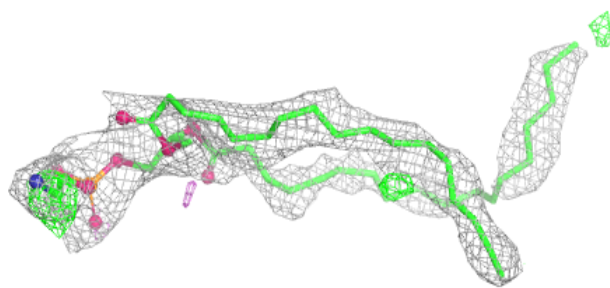
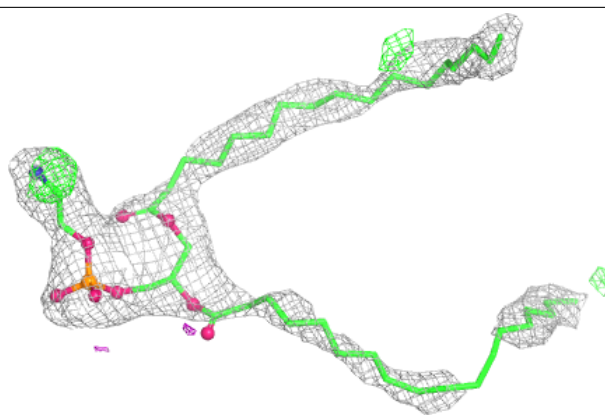
Electron density around CDL G 2004:

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

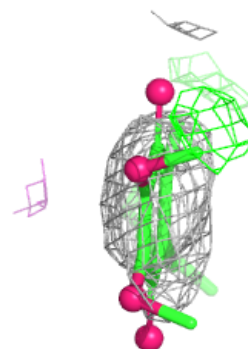
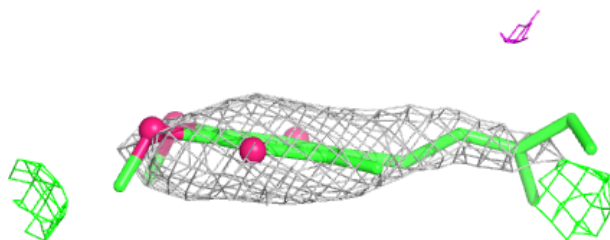
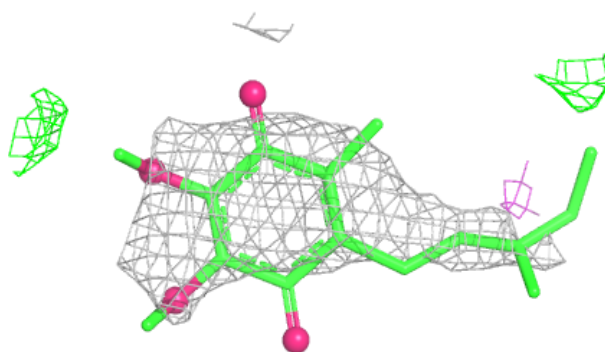


Electron density around PEE C 2005:

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

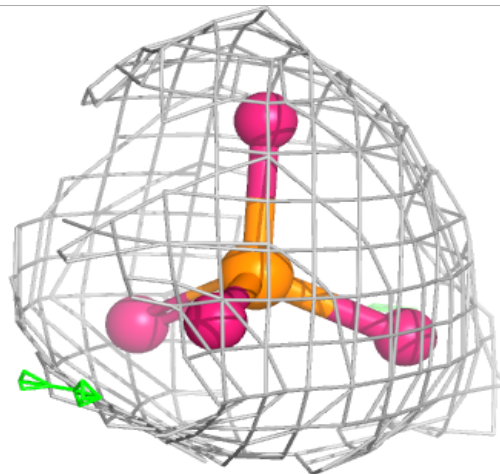
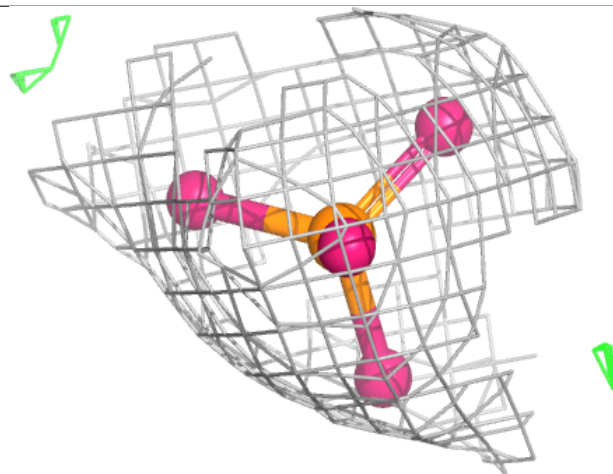
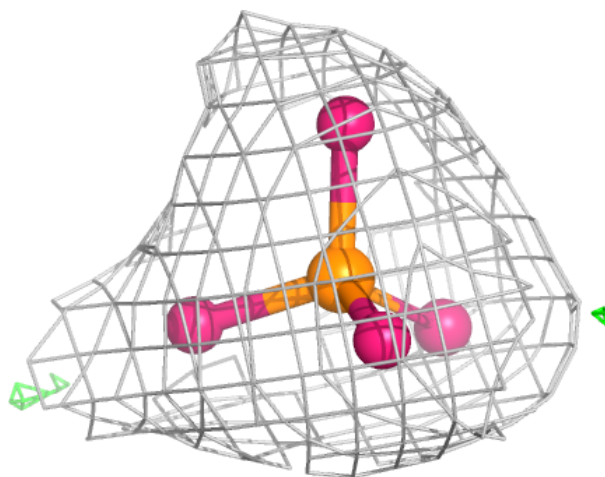
**Electron density around UQ P 3002:**

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



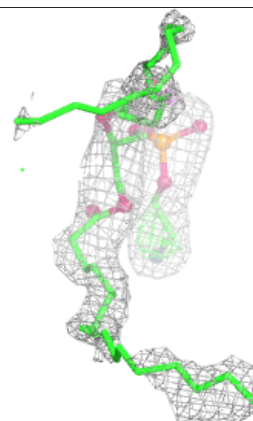
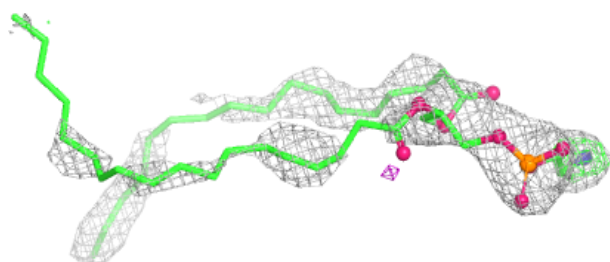
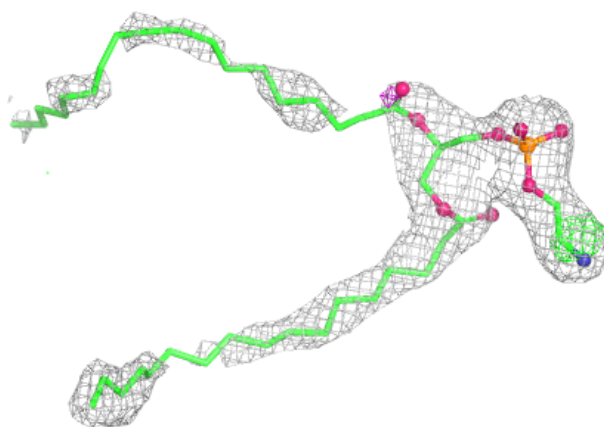
Electron density around PEE N 3008:

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

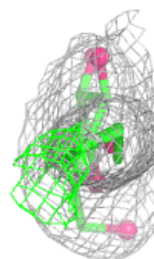
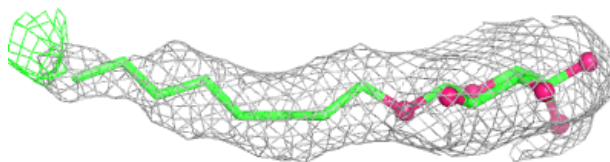
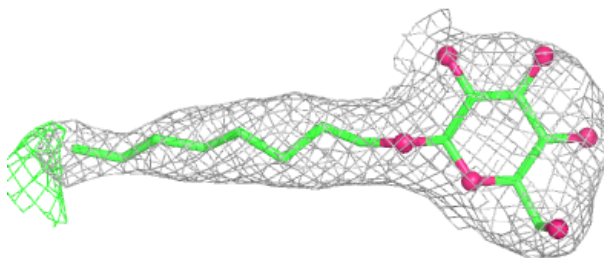


Electron density around PEE P 3005:

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and green (positive)

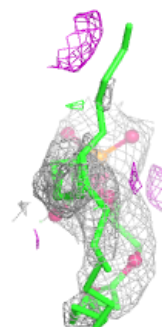
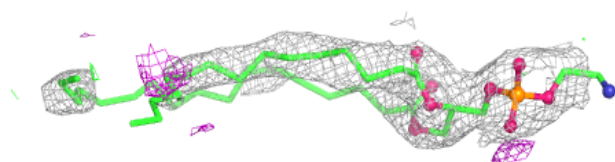
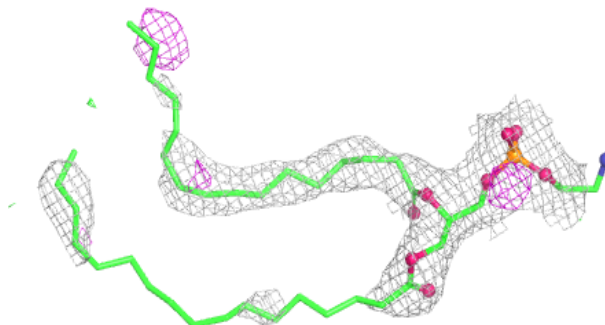
**Electron density around BOG Q 3009:**

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

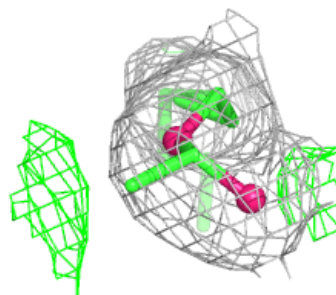
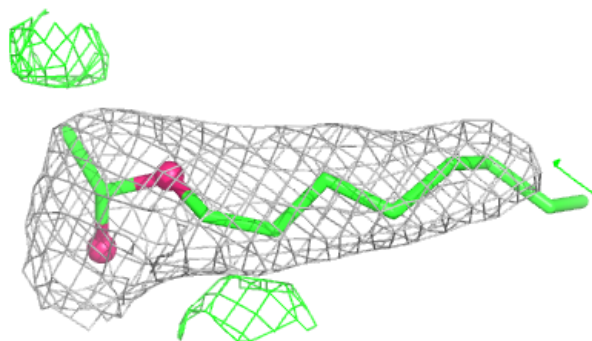
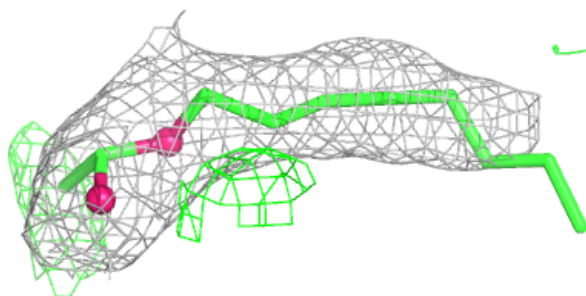


Electron density around PEE P 3007:

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

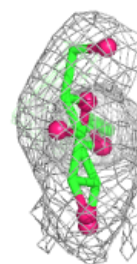
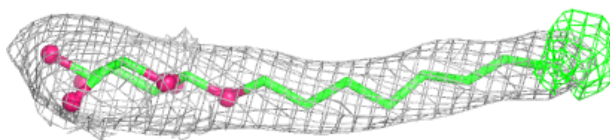
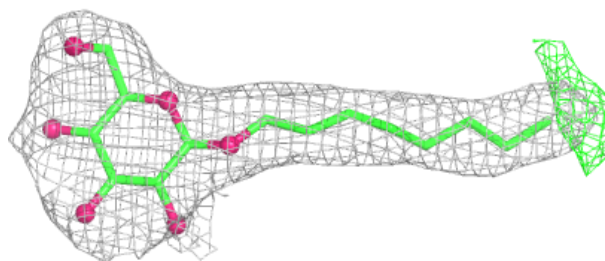
**Electron density around BOG C 3010:**

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

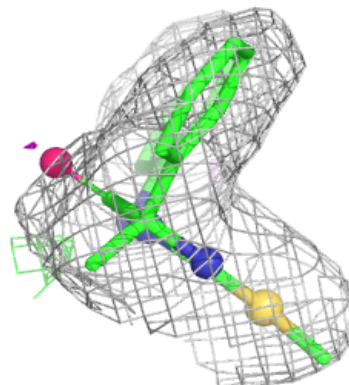
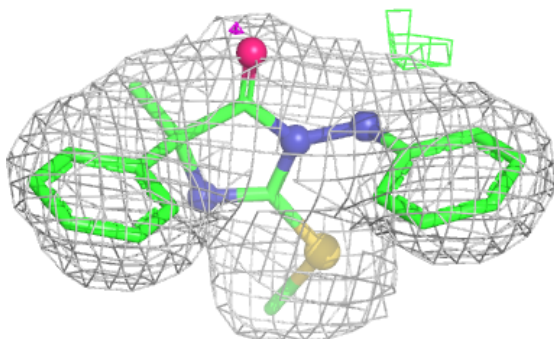
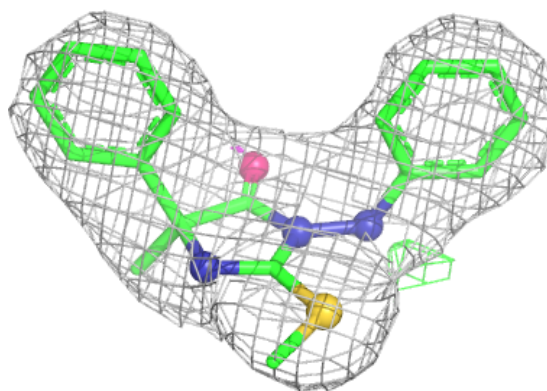


Electron density around BOG D 2009:

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

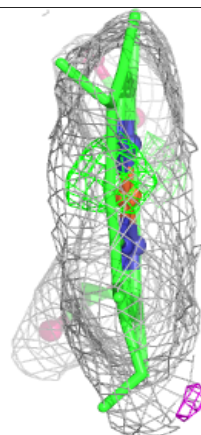
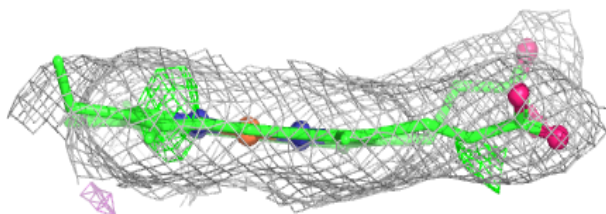
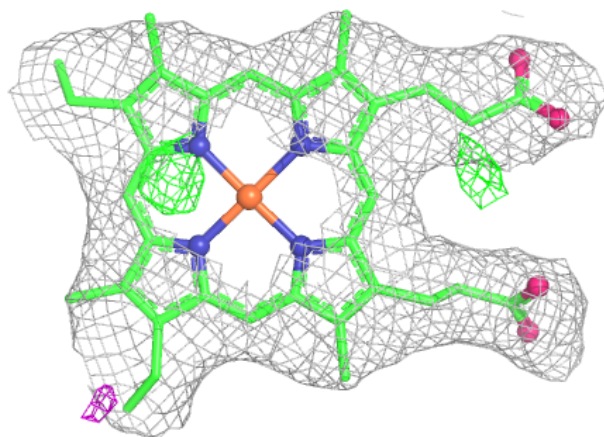
**Electron density around FNM P 3001:**

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

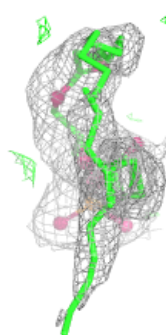
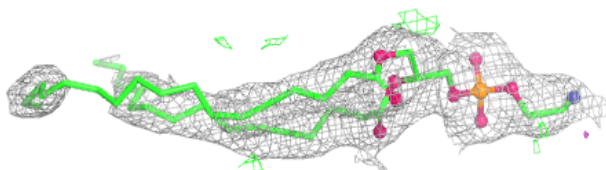
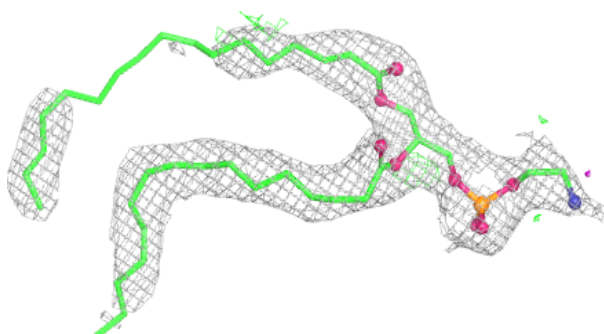


Electron density around HEC Q 501:

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

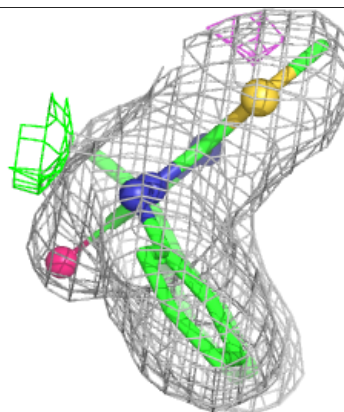
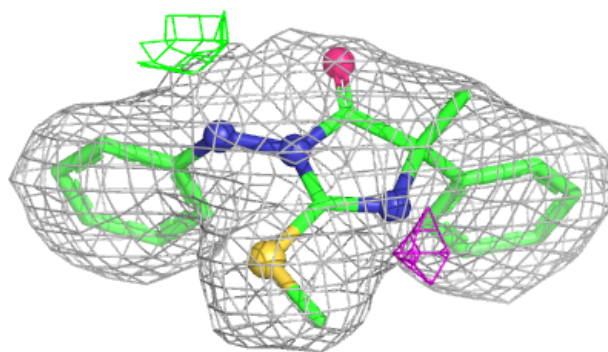
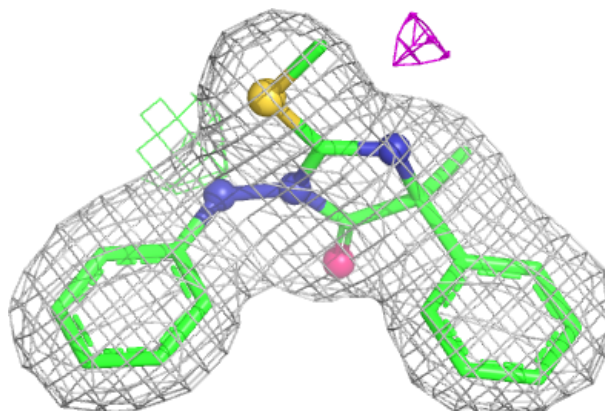
**Electron density around PEE C 2007:**

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



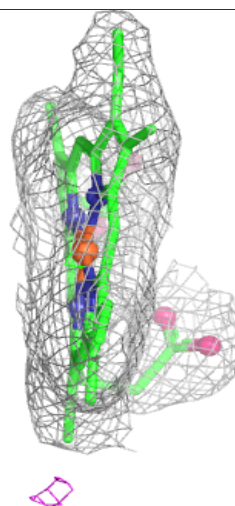
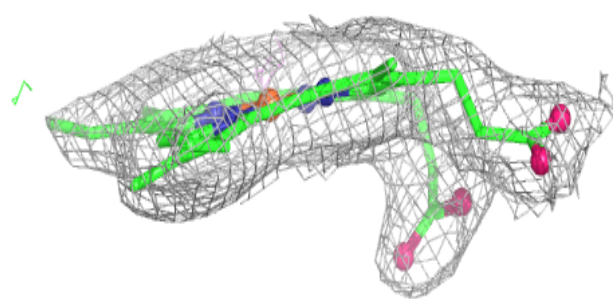
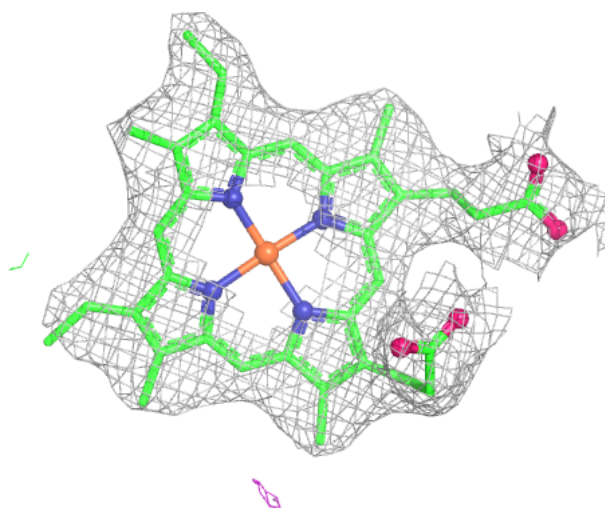
Electron density around FNM C 2001:

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



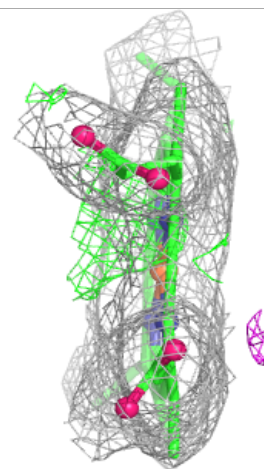
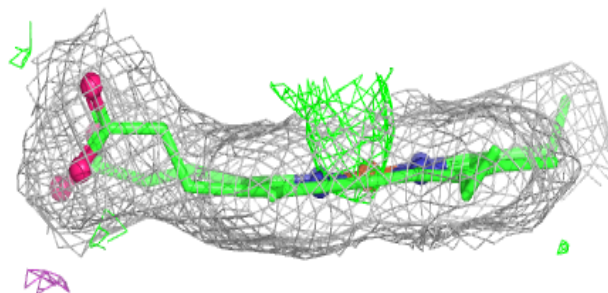
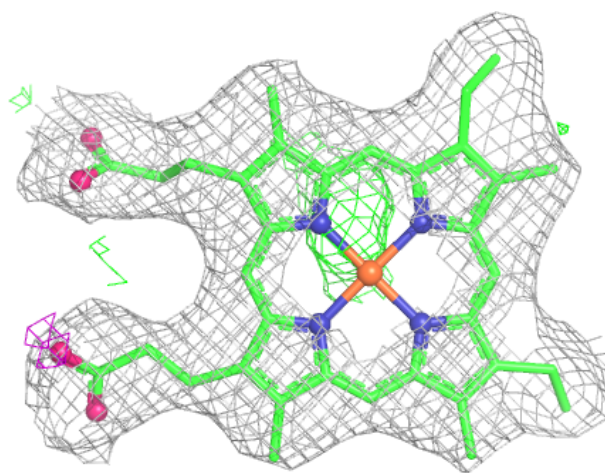
Electron density around HEM P 502:

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



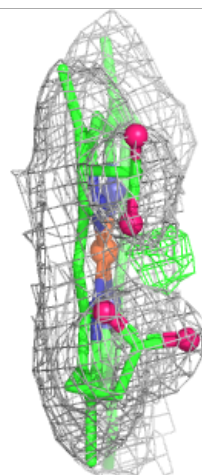
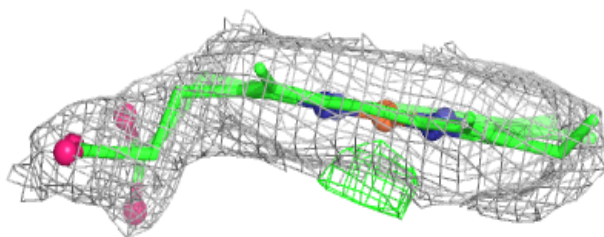
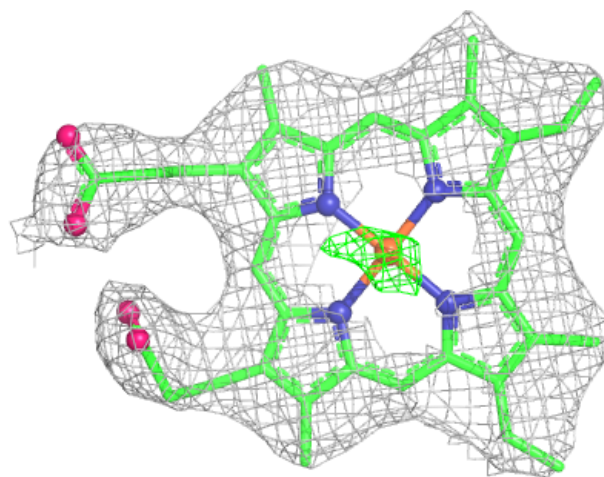
Electron density around HEC D 501:

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



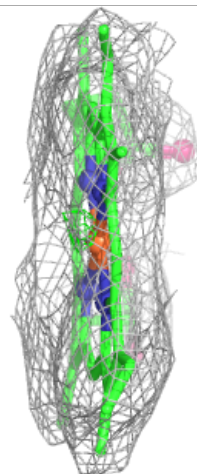
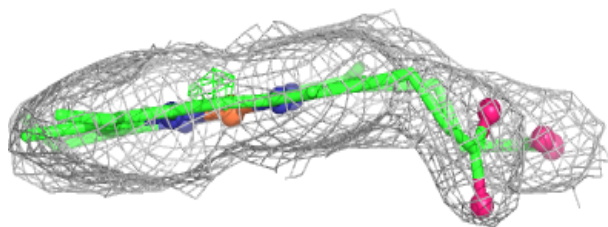
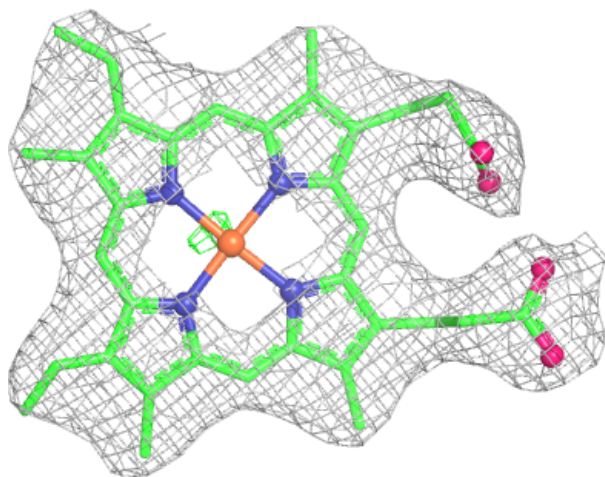
Electron density around HEM P 501:

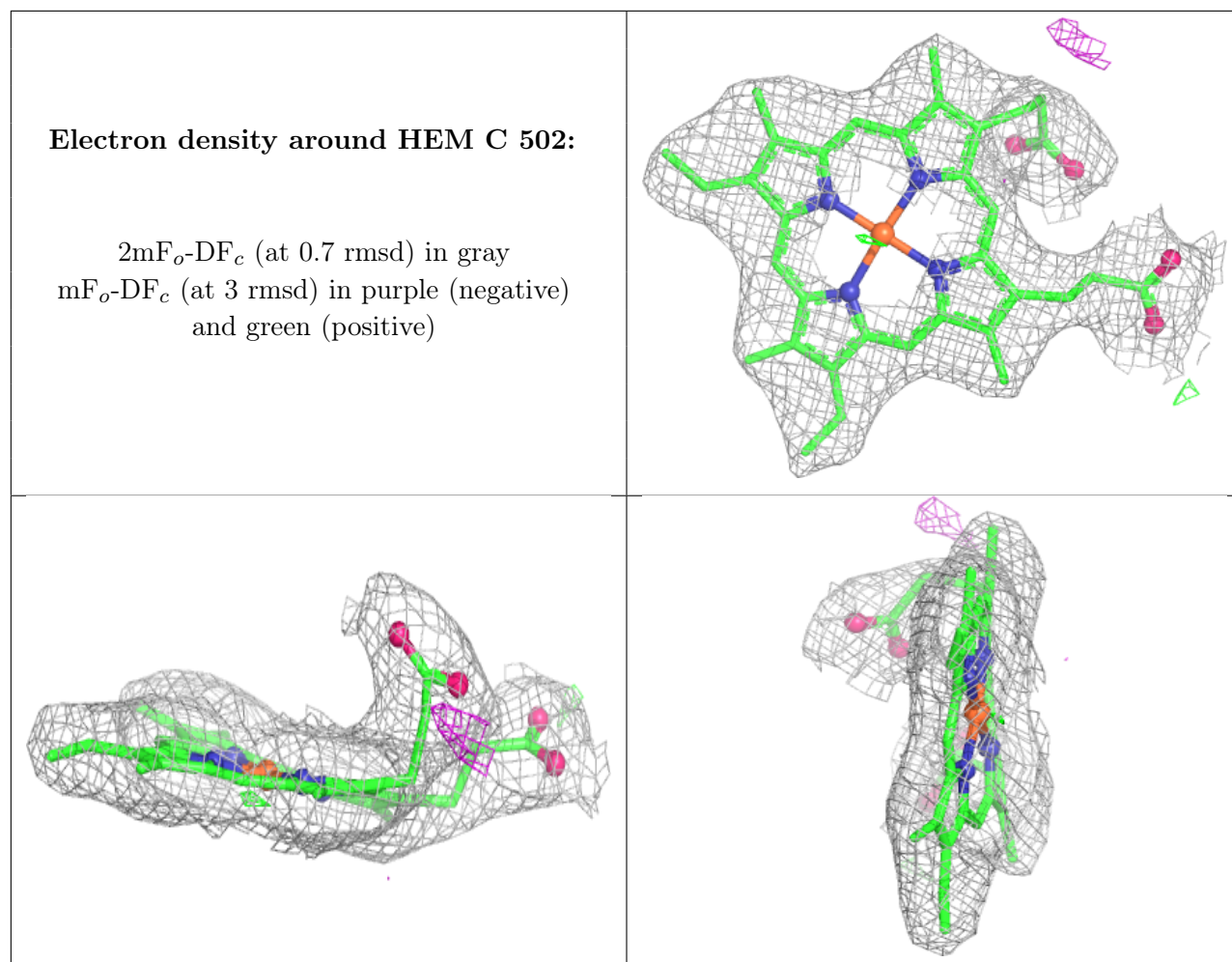
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.