



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:10 AM UTC

PDB ID : 3L74 / pdb_00003L74
Title : Cytochrome BC1 complex from chicken with famoxadone bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-28
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

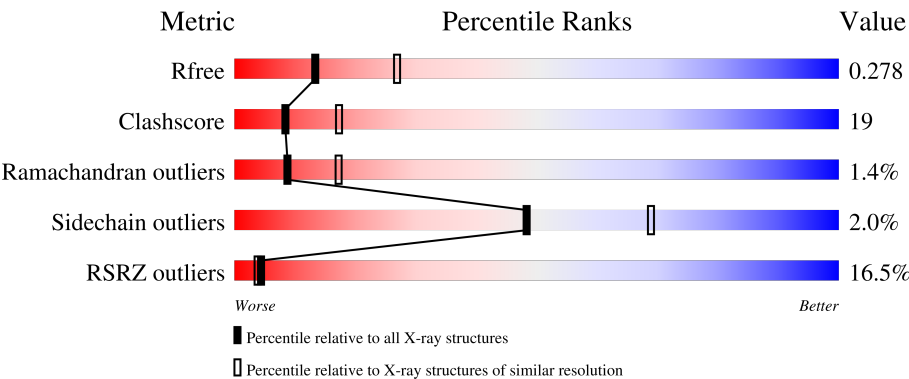
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.76 Å.

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



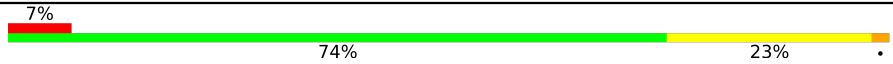
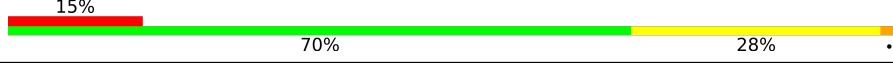
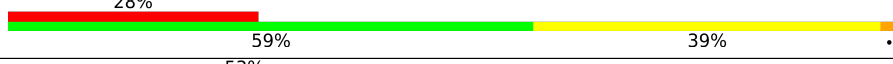
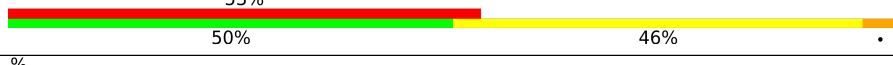
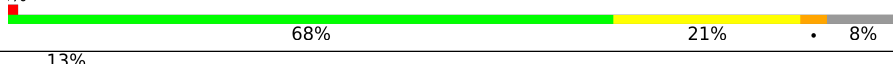
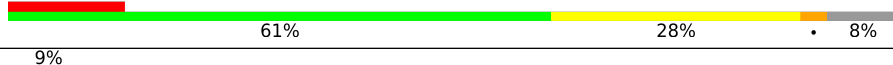
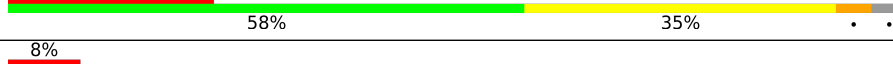
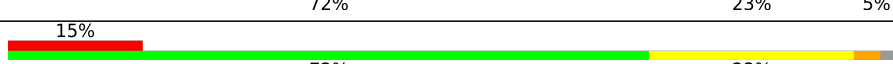
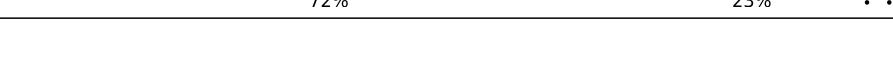
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	446	7% 59% 38% ..
1	N	446	21% 57% 38% ..
2	B	441	20% 52% 39% 5%
2	O	441	15% 54% 37% 5%
3	C	380	2% 74% 24% .

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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
17	BOG	P	2010	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32703 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			

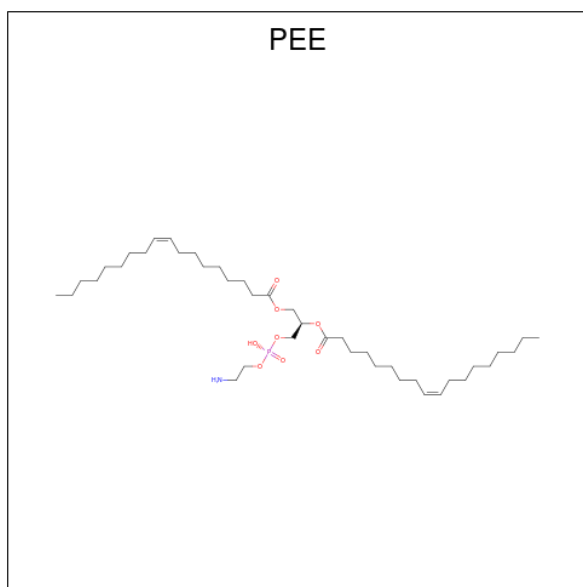
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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	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	C	1	Total	C	O	P		0	0
			21	12	8	1			
11	N	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

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

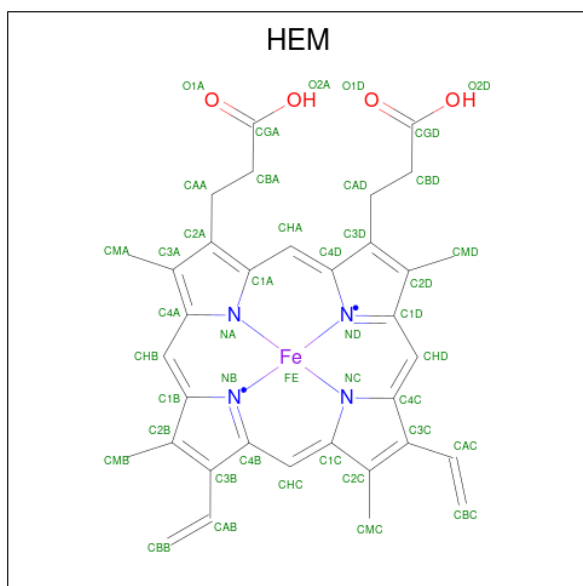
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total 1 O 1	0	0

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

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



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

- Molecule 14 is FAMOXADONE (CCD ID: FMX) (formula: $C_{22}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total 28	C 22	N 2	O 4	0	0
14	P	1	Total 28	C 22	N 2	O 4	0	0

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



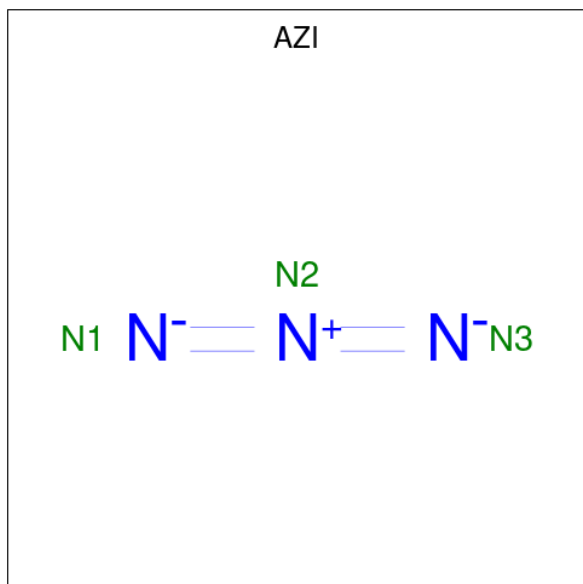
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			19	15	4		

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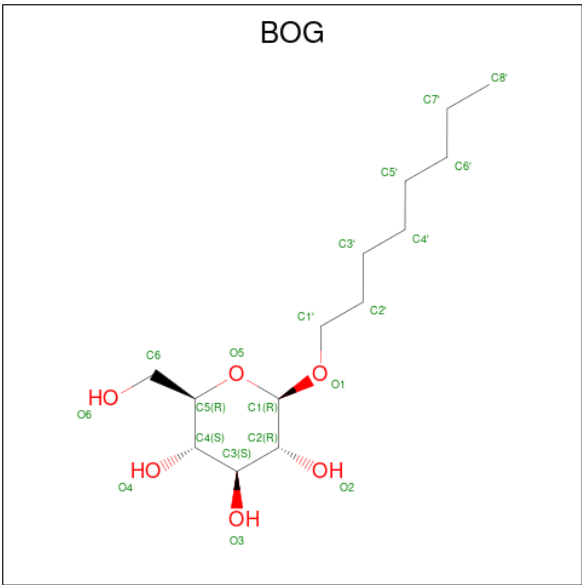
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 16 is AZIDE ION (CCD ID: AZI) (formula: N₃).



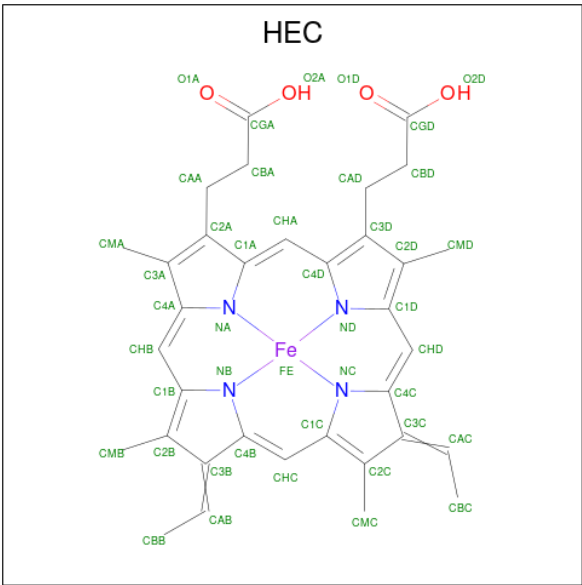
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	N	0	0
			3	3		
16	P	1	Total	N	0	0
			3	3		

- Molecule 17 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



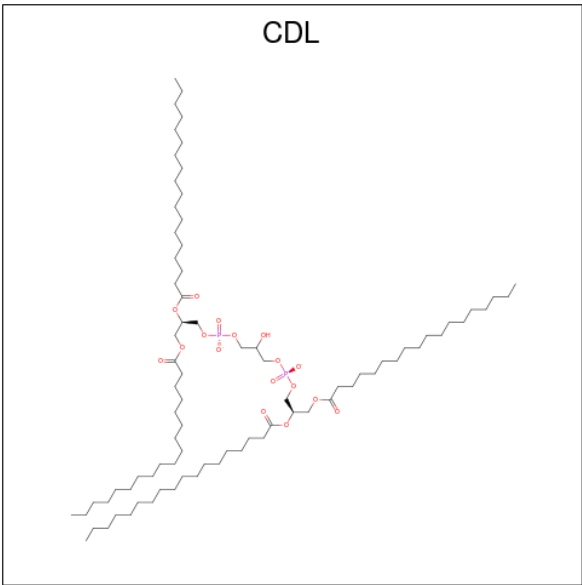
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			12	10	2		
17	D	1	Total	C	O	0	0
			20	14	6		
17	D	1	Total	C	O	0	0
			20	14	6		
17	P	1	Total	C	O	0	0
			19	13	6		
17	Q	1	Total	C	O	0	0
			20	14	6		
17	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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: $C_{81}H_{156}O_{17}P_2$).



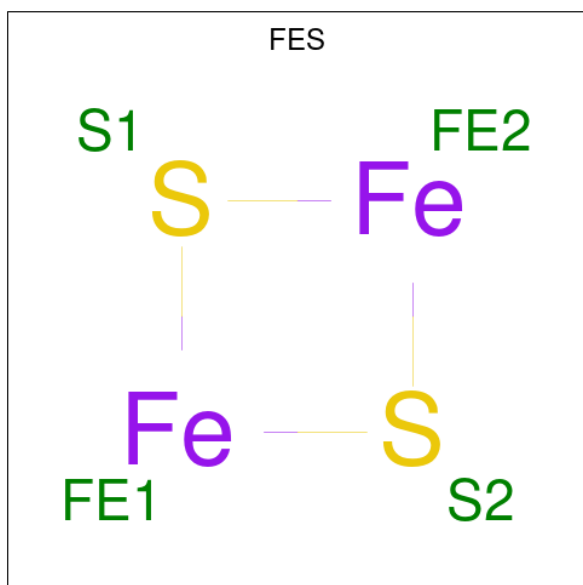
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			42	23	17	2		
19	G	1	Total	C	O	P	0	0
			40	21	17	2		

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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		

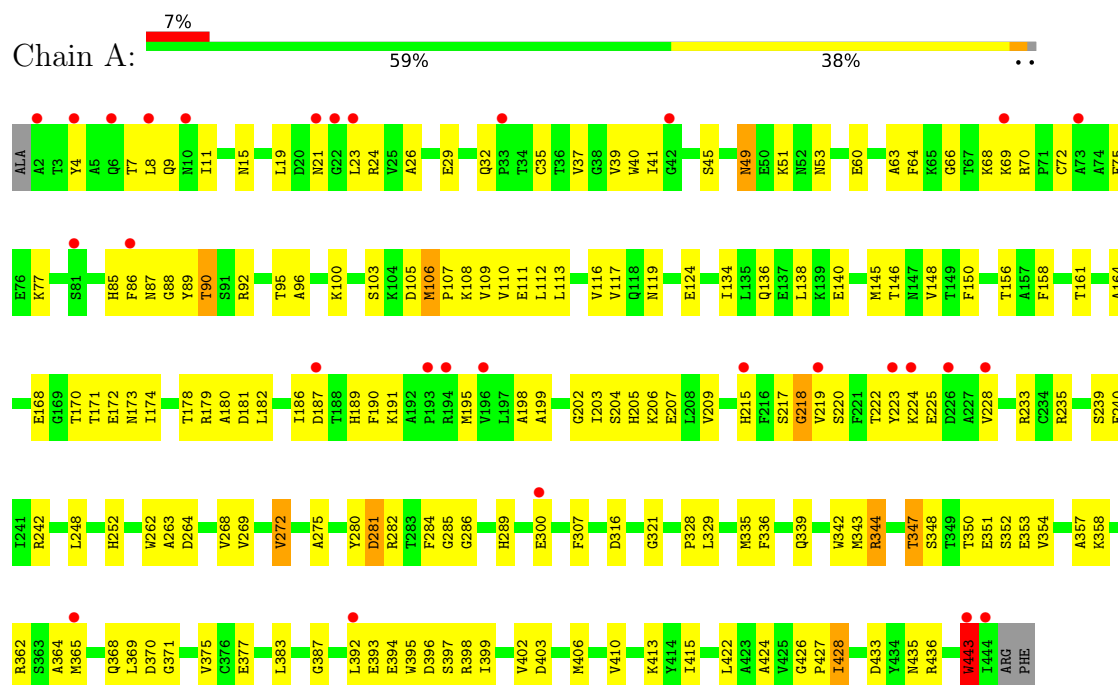
- Molecule 21 is water.

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	1	Total	O	0	0
			1	1		
21	P	12	Total	O	0	0
			12	12		
21	R	4	Total	O	0	0
			4	4		

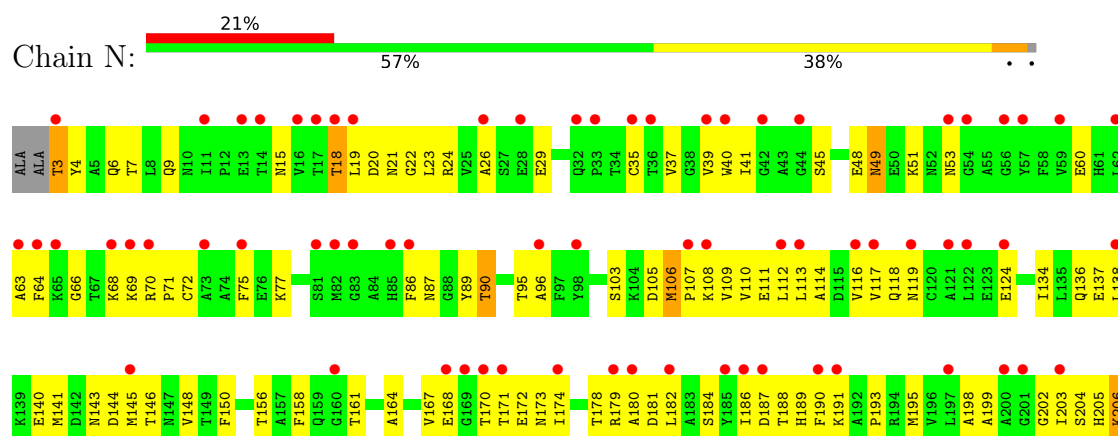
3 Residue-property plots [i](#)

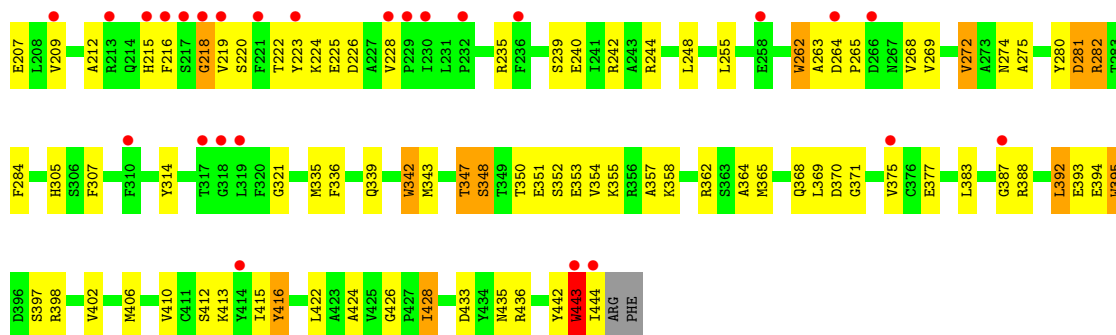
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

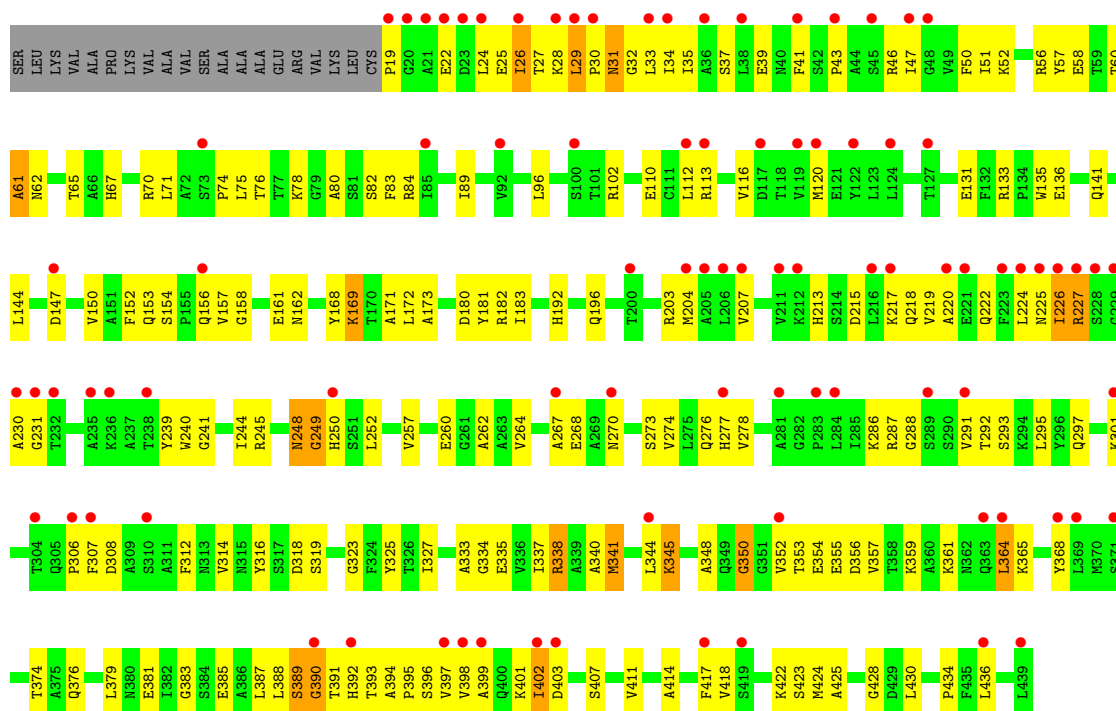


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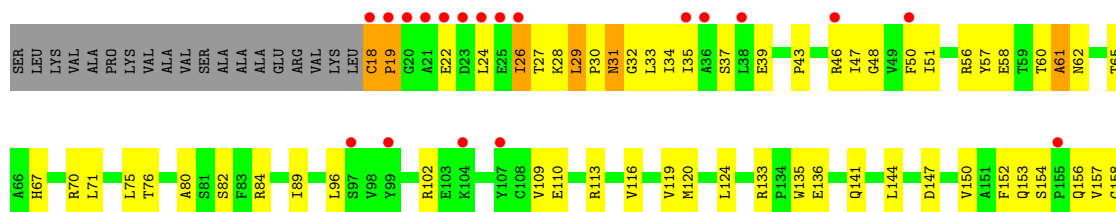


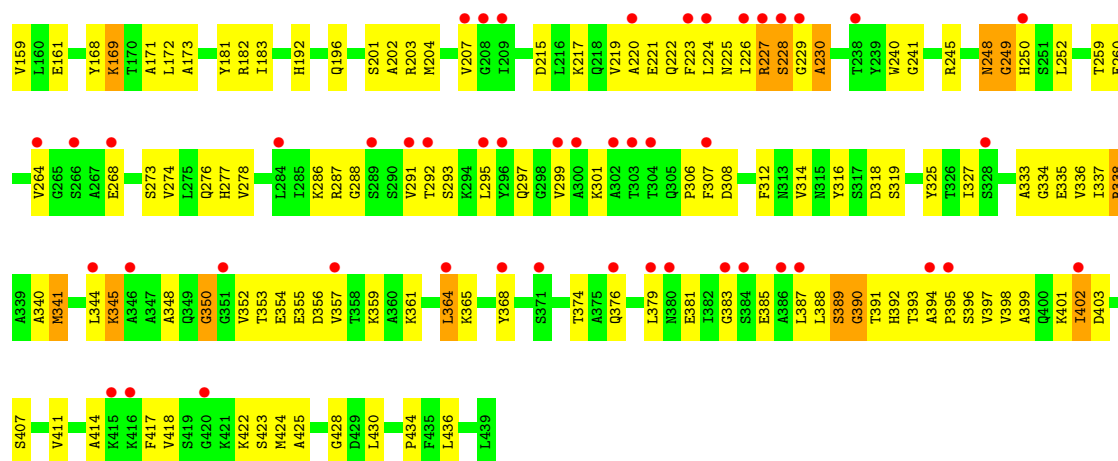


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

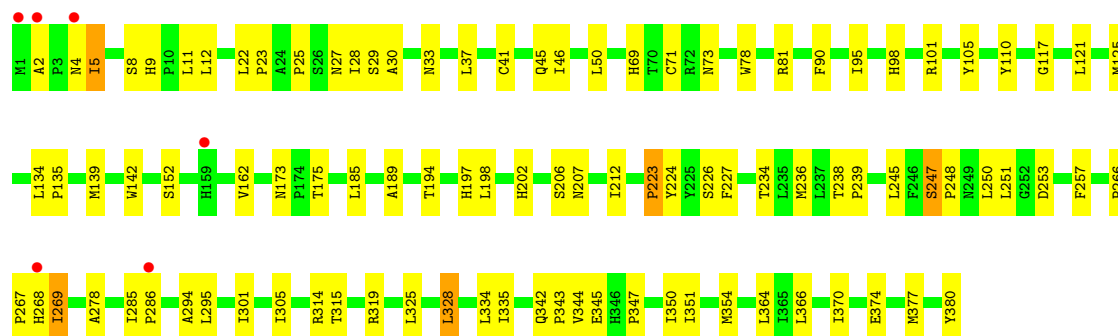
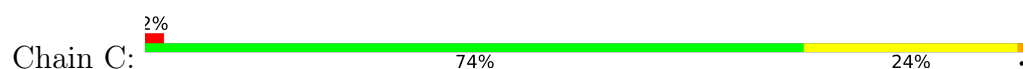


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

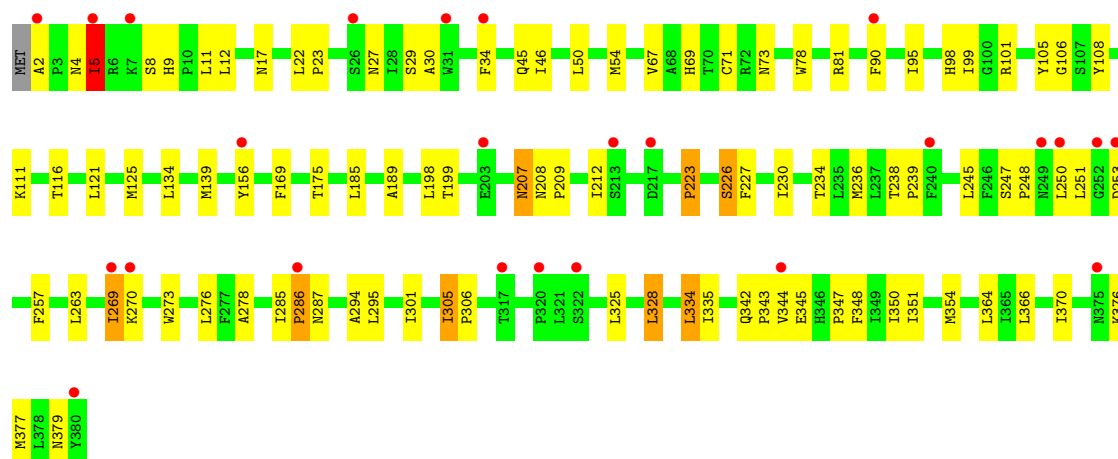
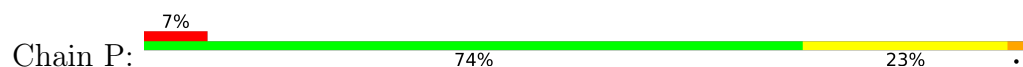




• Molecule 3: CYTOCHROME B

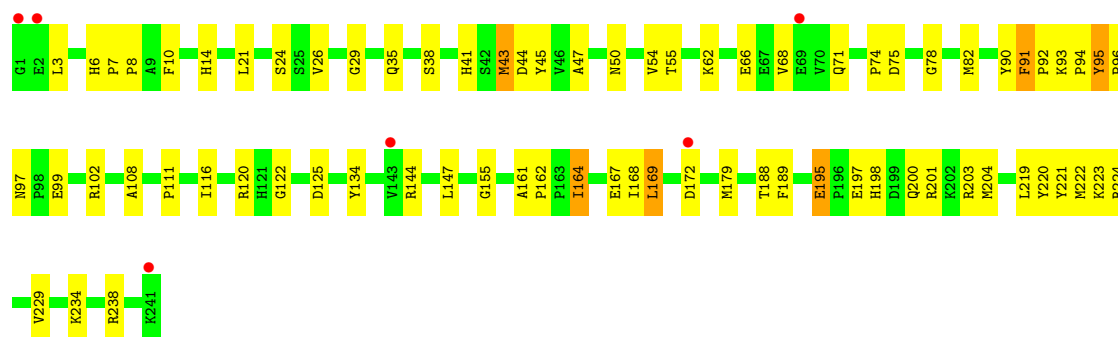


• Molecule 3: CYTOCHROME B

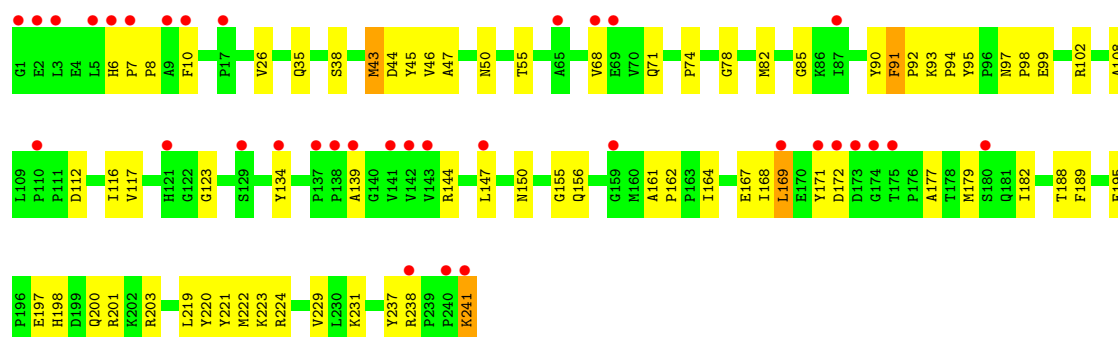


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

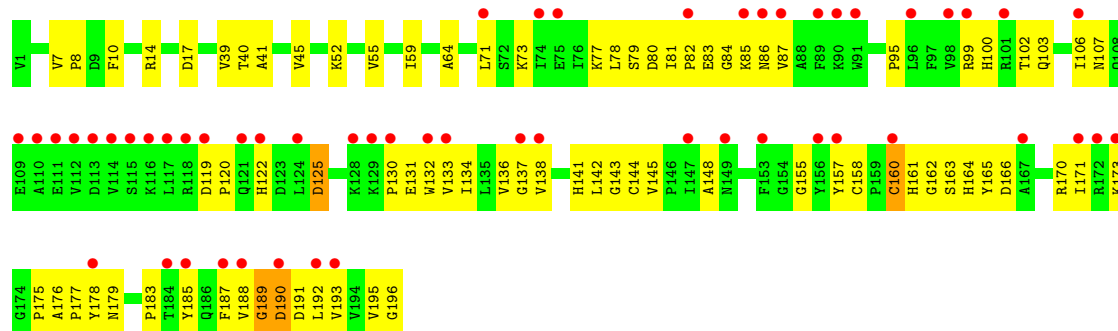




• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

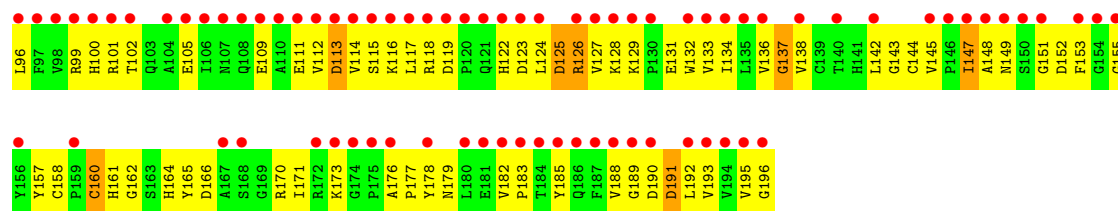


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL

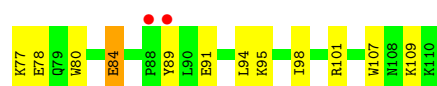




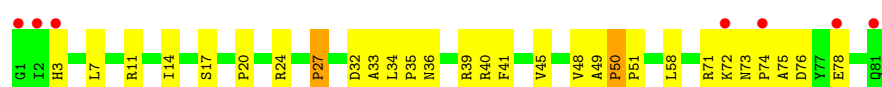
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



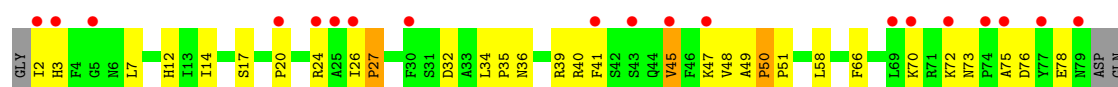
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



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



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

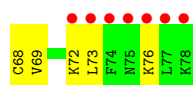


• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

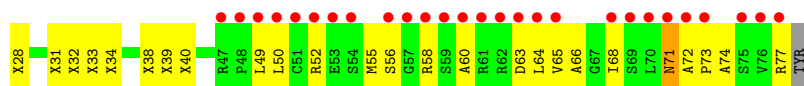




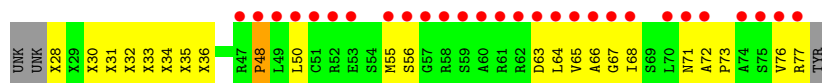
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



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



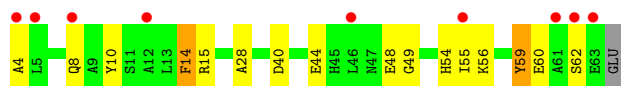
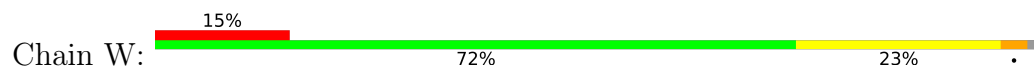
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.89Å 181.69Å 240.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.66 – 2.76 58.66 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.0 (58.66-2.76) 98.0 (58.66-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.286 0.248 , 0.278	Depositor DCC
R_{free} test set	3886 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32703	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: PEE, HEM, BOG, UNL, FMX, AZI, FES, UQ, CDL, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3511	0.97	15/4757 (0.3%)
1	N	0.48	0/3508	0.99	15/4753 (0.3%)
2	B	0.44	0/3196	0.93	8/4334 (0.2%)
2	O	0.47	0/3202	0.97	12/4343 (0.3%)
3	C	0.62	1/3119 (0.0%)	1.02	18/4270 (0.4%)
3	P	0.55	1/3114 (0.0%)	0.99	16/4263 (0.4%)
4	D	0.57	0/1956	1.03	14/2658 (0.5%)
4	Q	0.46	0/1956	1.00	12/2658 (0.5%)
5	E	0.47	0/1547	0.92	6/2103 (0.3%)
5	R	0.44	0/1545	0.90	4/2098 (0.2%)
6	F	0.61	0/911	0.94	2/1219 (0.2%)
6	S	0.45	0/911	0.93	3/1219 (0.2%)
7	G	0.54	0/698	1.05	3/946 (0.3%)
7	T	0.45	0/676	1.02	5/918 (0.5%)
8	H	0.51	0/582	0.89	1/779 (0.1%)
8	U	0.37	0/561	0.87	1/751 (0.1%)
9	I	0.49	0/218	1.01	1/293 (0.3%)
9	V	0.51	0/218	0.92	0/293
10	J	0.49	0/508	0.87	1/682 (0.1%)
10	W	0.49	0/490	0.85	1/660 (0.2%)
All	All	0.51	2/32427 (0.0%)	0.97	138/43997 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	125	MET	SD-CE	5.98	1.94	1.79
3	P	125	MET	SD-CE	5.30	1.92	1.79

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	18	CYS	CA-C-N	10.00	130.09	119.89
2	O	18	CYS	C-N-CA	10.00	130.09	119.89
2	O	227	ARG	N-CA-C	9.98	125.83	110.36
1	N	415	ILE	N-CA-C	8.84	119.16	111.56
1	N	428	ILE	N-CA-C	8.46	119.44	111.91
1	A	415	ILE	N-CA-C	8.18	119.17	111.48
5	E	143	GLY	N-CA-C	7.83	126.18	115.30
1	A	415	ILE	CB-CA-C	-7.46	105.37	111.71
3	C	27	ASN	N-CA-C	7.44	121.20	112.72
1	N	226	ASP	N-CA-C	-7.43	103.52	112.59
3	P	111	LYS	N-CA-C	7.25	119.81	111.11
1	A	66	GLY	N-CA-C	7.21	121.17	111.72
4	Q	91	PHE	CA-C-N	7.19	127.16	119.76
4	Q	91	PHE	C-N-CA	7.19	127.16	119.76
3	C	207	ASN	N-CA-C	-7.14	99.29	110.36
1	A	347	THR	N-CA-C	7.05	122.44	113.55
3	P	207	ASN	N-CA-C	-7.04	99.45	110.36
4	D	91	PHE	CA-C-N	7.03	127.42	119.83
4	D	91	PHE	C-N-CA	7.03	127.42	119.83
1	N	347	THR	N-CA-C	6.86	122.19	113.55
6	S	109	LYS	N-CA-C	-6.84	104.57	113.12
4	D	45	TYR	N-CA-C	6.75	121.13	113.02
3	P	27	ASN	N-CA-C	6.75	120.82	112.59
4	Q	45	TYR	N-CA-C	6.62	120.97	113.02
10	J	14	PHE	N-CA-C	6.55	121.01	112.89
9	I	74	ALA	N-CA-C	-6.42	101.02	110.52
2	B	267	ALA	N-CA-C	-6.36	104.78	112.54
7	G	7	LEU	N-CA-C	6.35	118.08	111.03
3	C	110	TYR	N-CA-C	-6.34	100.11	109.62
4	D	6	HIS	CA-C-N	6.31	124.27	119.66
4	D	6	HIS	C-N-CA	6.31	124.27	119.66
2	O	19	PRO	N-CA-C	6.30	121.12	111.11
3	P	305	ILE	CB-CA-C	-6.28	107.73	113.70
1	N	66	GLY	N-CA-C	6.26	119.92	111.72
3	C	226	SER	N-CA-C	-6.24	104.40	111.14
3	C	328	LEU	N-CA-C	-6.23	104.41	111.07
3	C	175	THR	N-CA-C	-6.21	104.06	111.69
10	W	14	PHE	N-CA-C	6.20	120.58	112.89
5	R	143	GLY	N-CA-C	6.11	123.71	114.61
3	C	305	ILE	CB-CA-C	-6.10	107.90	113.70
1	N	415	ILE	CB-CA-C	-6.10	105.65	111.44
4	D	95	TYR	CA-C-N	6.07	125.69	119.56
4	D	95	TYR	C-N-CA	6.07	125.69	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	6	HIS	CA-C-N	6.06	124.08	119.66
4	Q	6	HIS	C-N-CA	6.06	124.08	119.66
3	P	328	LEU	N-CA-C	-6.03	104.62	111.14
2	O	230	ALA	N-CA-C	-5.95	105.33	113.30
2	O	169	LYS	N-CA-C	-5.95	106.36	113.97
7	T	50	PRO	N-CA-C	5.91	117.91	110.70
2	B	61	ALA	N-CA-C	5.91	117.72	111.28
4	Q	95	TYR	CA-C-N	5.84	125.46	119.56
4	Q	95	TYR	C-N-CA	5.84	125.46	119.56
5	E	17	ASP	N-CA-C	5.84	120.01	113.01
7	G	50	PRO	N-CA-C	5.82	117.80	110.70
3	C	224	TYR	N-CA-C	5.81	117.30	110.97
2	O	141	GLN	CA-C-N	-5.80	113.64	119.56
2	O	141	GLN	C-N-CA	-5.80	113.64	119.56
3	C	185	LEU	N-CA-C	5.78	117.45	111.03
3	P	189	ALA	N-CA-C	-5.73	105.11	111.36
2	B	345	LYS	N-CA-C	-5.72	104.68	111.03
3	C	189	ALA	N-CA-C	-5.71	105.20	111.82
3	P	185	LEU	N-CA-C	5.66	117.25	111.14
3	P	257	PHE	N-CA-C	-5.64	105.60	112.88
5	R	17	ASP	N-CA-C	5.64	119.78	113.01
2	B	169	LYS	N-CA-C	-5.64	106.76	113.97
4	D	116	ILE	N-CA-C	5.60	116.33	110.62
3	P	226	SER	N-CA-C	-5.59	105.10	111.14
4	D	155	GLY	N-CA-C	-5.59	108.43	115.08
4	Q	155	GLY	N-CA-C	-5.58	108.44	115.08
8	H	73	LEU	N-CA-C	5.57	120.56	111.37
8	U	73	LEU	N-CA-C	5.57	120.56	111.37
4	D	7	PRO	N-CA-C	5.54	115.78	110.47
3	P	134	LEU	N-CA-C	5.54	120.45	113.25
4	Q	112	ASP	N-CA-C	-5.52	102.71	110.50
3	C	173	ASN	CA-C-N	-5.52	113.99	119.56
3	C	173	ASN	C-N-CA	-5.52	113.99	119.56
1	A	348	SER	N-CA-C	5.48	119.12	111.56
4	Q	7	PRO	N-CA-C	5.48	115.73	110.47
4	Q	116	ILE	N-CA-C	5.44	116.17	110.62
2	B	249	GLY	N-CA-C	5.40	122.55	115.36
4	D	24	SER	N-CA-C	-5.40	105.39	111.28
7	T	7	LEU	N-CA-C	5.39	117.02	111.03
4	D	195	GLU	CA-C-N	5.37	125.69	119.47
4	D	195	GLU	C-N-CA	5.37	125.69	119.47
6	S	89	TYR	N-CA-C	5.36	117.87	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ALA	N-CA-C	5.33	119.28	112.34
3	C	251	LEU	N-CA-C	5.33	119.79	113.28
2	B	180	ASP	N-CA-C	5.33	116.77	111.07
1	N	244	ARG	N-CA-C	5.33	117.92	109.24
1	N	263	ALA	N-CA-C	5.31	119.25	112.34
3	C	257	PHE	N-CA-C	-5.31	106.39	112.92
7	T	12	HIS	N-CA-C	5.30	118.90	111.74
2	B	141	GLN	CA-C-N	-5.28	114.17	119.56
2	B	141	GLN	C-N-CA	-5.28	114.17	119.56
6	F	89	TYR	N-CA-C	5.28	117.78	111.71
1	A	32	GLN	CA-C-N	5.28	124.94	119.56
1	A	32	GLN	C-N-CA	5.28	124.94	119.56
1	A	428	ILE	N-CA-C	5.27	120.31	109.34
4	Q	85	GLY	N-CA-C	5.24	118.09	112.33
4	D	164	ILE	N-CA-C	5.23	116.26	108.46
3	P	29	SER	N-CA-C	5.23	116.74	109.31
6	F	74	ILE	N-CA-C	-5.22	102.45	108.82
1	N	189	HIS	N-CA-C	5.21	120.12	113.55
7	G	11	ARG	N-CA-C	5.21	117.91	109.06
3	P	116	THR	N-CA-C	-5.21	105.78	111.82
2	O	249	GLY	N-CA-C	5.20	122.29	115.47
3	P	175	THR	N-CA-C	-5.20	105.52	111.14
3	C	314	ARG	N-CA-C	5.20	116.75	111.14
7	T	45	VAL	N-CA-C	5.18	116.53	110.62
3	P	5	ILE	N-CA-C	5.17	116.52	110.62
7	T	47	LYS	N-CA-C	-5.17	105.81	112.68
1	N	392	LEU	N-CA-C	-5.16	105.83	111.82
2	O	61	ALA	N-CA-C	5.16	117.57	111.33
1	N	348	SER	N-CA-C	5.16	119.31	112.30
2	O	221	GLU	N-CA-C	5.16	117.30	111.11
3	P	67	VAL	N-CA-C	-5.16	105.38	111.00
3	C	247	SER	CA-C-N	5.16	125.45	119.47
3	C	247	SER	C-N-CA	5.16	125.45	119.47
5	R	15	ARG	N-CA-C	-5.16	103.23	110.50
1	N	416	TYR	N-CA-C	5.15	118.02	110.30
5	E	145	VAL	CA-C-N	5.13	124.89	119.76
5	E	145	VAL	C-N-CA	5.13	124.89	119.76
1	N	412	SER	N-CA-C	-5.12	105.70	111.28
3	C	206	SER	N-CA-C	5.11	117.27	110.53
5	E	125	ASP	N-CA-C	-5.10	107.11	113.38
2	O	345	LYS	N-CA-C	-5.09	105.42	110.97
6	S	32	MET	N-CA-C	-5.08	103.98	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	VAL	N-CA-C	-5.06	105.61	110.72
5	E	160	CYS	N-CA-C	5.06	116.48	110.97
1	A	189	HIS	N-CA-C	5.05	119.92	113.55
5	R	160	CYS	N-CA-C	5.04	116.47	110.97
1	N	305	HIS	N-CA-C	-5.04	106.97	113.23
1	A	264	ASP	CA-C-N	5.01	124.79	119.28
1	A	264	ASP	C-N-CA	5.01	124.79	119.28
1	A	272	VAL	N-CA-C	-5.01	105.82	110.53
1	A	329	LEU	N-CA-C	5.01	119.03	113.02
1	N	272	VAL	N-CA-C	-5.01	105.82	110.53
3	P	251	LEU	N-CA-C	5.01	119.39	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	147	0
1	N	3437	0	3349	166	0
2	B	3141	0	3142	204	0
2	O	3147	0	3146	191	0
3	C	3017	0	3063	81	0
3	P	3012	0	3058	83	0
4	D	1898	0	1846	56	0
4	Q	1898	0	1846	56	0
5	E	1513	0	1478	65	0
5	R	1512	0	1476	88	0
6	F	891	0	893	19	0
6	S	891	0	893	29	0
7	G	676	0	659	27	0
7	T	654	0	641	25	0
8	H	574	0	548	14	0
8	U	553	0	535	18	0
9	I	288	0	253	43	0
9	V	278	0	253	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	497	0	490	14	0
10	W	479	0	478	11	0
11	A	50	0	77	0	0
11	C	69	0	83	0	0
11	N	55	0	77	0	0
11	P	48	0	70	0	0
12	A	1	0	0	0	0
12	C	5	0	0	0	0
12	E	2	0	0	0	0
12	P	7	0	0	0	0
12	Q	1	0	0	0	0
13	C	86	0	60	8	0
13	P	86	0	60	7	0
14	C	28	0	18	2	0
14	P	28	0	18	2	0
15	C	19	0	17	5	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	2	0
18	Q	43	0	30	0	0
19	D	42	0	28	2	0
19	G	40	0	24	2	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	1	0
21	A	2	0	0	0	0
21	C	9	0	0	2	0
21	E	1	0	0	0	0
21	P	12	0	0	2	0
21	R	4	0	0	0	0
All	All	32703	0	32215	1242	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 (1242) 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)
1:A:344:ARG:HH11	1:A:344:ARG:HB2	1.04	1.10
1:A:344:ARG:HB2	1:A:344:ARG:NH1	1.69	1.08
1:N:178:THR:HG22	1:N:180:ALA:H	1.18	1.08
2:B:76:THR:HG22	2:B:82:SER:H	1.13	1.07
1:A:178:THR:HG22	1:A:180:ALA:H	1.20	1.04
2:B:353:THR:HG22	2:B:355:GLU:H	1.20	1.01
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.59	1.00
2:O:353:THR:HG22	2:O:355:GLU:H	1.18	1.00
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.38	1.00
1:N:206:LYS:H	1:N:206:LYS:HD2	1.28	0.98
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.45	0.97
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.44	0.97
1:A:343:MET:O	1:A:347:THR:HG22	1.63	0.96
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.47	0.96
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.44	0.95
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.14	0.95
2:B:27:THR:HG22	2:B:28:LYS:H	1.29	0.95
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.46	0.94
1:N:343:MET:O	1:N:347:THR:HG22	1.64	0.94
4:D:47:ALA:H	4:D:50:ASN:HD22	1.18	0.92
1:N:206:LYS:H	1:N:206:LYS:CD	1.83	0.91
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.50	0.91
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.52	0.90
2:O:76:THR:HG22	2:O:82:SER:H	1.34	0.90
2:O:335:GLU:HA	2:O:338:ARG:HH12	1.35	0.89
1:A:281:ASP:CG	9:I:33:UNK:HB1	1.98	0.88
9:I:64:LEU:HD12	9:I:77:ARG:O	1.73	0.88
2:O:376:GLN:HE22	9:V:77:ARG:NH2	1.72	0.88
2:O:27:THR:HG22	2:O:28:LYS:H	1.36	0.88
2:O:376:GLN:HE22	9:V:77:ARG:HH22	1.23	0.86
1:A:178:THR:HB	1:A:181:ASP:OD1	1.76	0.86
2:B:335:GLU:HA	2:B:338:ARG:HH12	1.39	0.85
2:B:22:GLU:HG2	2:B:39:GLU:HB3	1.57	0.85
5:E:134:ILE:HB	5:E:185:TYR:CE2	2.12	0.84
2:O:338:ARG:HB2	2:O:338:ARG:HH11	1.44	0.82
1:N:49:ASN:HD22	1:N:51:LYS:H	1.26	0.82
1:A:178:THR:HG22	1:A:180:ALA:N	1.94	0.82
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.60	0.82
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.62	0.82
2:O:248:ASN:HD22	2:O:248:ASN:C	1.88	0.81
1:N:178:THR:HB	1:N:181:ASP:OD1	1.81	0.81
2:B:248:ASN:C	2:B:248:ASN:HD22	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:101:ARG:HH22	5:R:127:VAL:HG11	1.44	0.80
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.11	0.80
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.63	0.80
3:C:69:HIS:CD2	3:C:73:ASN:HD22	1.99	0.80
1:N:178:THR:HG22	1:N:180:ALA:N	1.95	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
2:B:264:VAL:HG23	2:B:316:TYR:C	2.08	0.79
2:B:27:THR:HG22	2:B:28:LYS:N	1.96	0.79
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.23	0.78
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.65	0.78
1:N:350:THR:HG22	1:N:352:SER:H	1.49	0.78
2:B:338:ARG:HH11	2:B:338:ARG:HB2	1.48	0.78
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.63	0.78
9:I:71:ASN:HD22	9:I:71:ASN:H	1.27	0.78
2:O:31:ASN:ND2	2:O:33:LEU:H	1.80	0.78
2:B:153:GLN:HE22	9:I:34:UNK:CG	1.97	0.77
1:A:350:THR:HG22	1:A:352:SER:H	1.49	0.77
4:D:47:ALA:H	4:D:50:ASN:ND2	1.81	0.77
1:N:49:ASN:ND2	1:N:51:LYS:H	1.81	0.77
1:A:362:ARG:O	1:A:365:MET:HG2	1.84	0.77
2:B:31:ASN:ND2	2:B:33:LEU:H	1.81	0.77
1:N:22:GLY:O	1:N:193:PRO:HA	1.85	0.77
3:P:101:ARG:C	3:P:101:ARG:HD2	2.10	0.77
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.32	0.77
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.66	0.77
5:R:190:ASP:O	5:R:191:ASP:HB2	1.85	0.77
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.48	0.76
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.65	0.76
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.67	0.76
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.08	0.76
9:I:32:UNK:N	9:I:73:PRO:HG2	1.99	0.76
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.65	0.76
2:B:153:GLN:HE22	9:I:34:UNK:HG2	1.48	0.76
2:O:192:HIS:O	2:O:196:GLN:HG3	1.84	0.76
1:N:362:ARG:O	1:N:365:MET:HG2	1.85	0.76
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.67	0.76
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.26	0.75
2:O:27:THR:HG22	2:O:28:LYS:N	2.01	0.75
1:A:49:ASN:HD22	1:A:51:LYS:H	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:LEU:O	1:N:21:ASN:N	2.19	0.75
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.50	0.75
1:A:344:ARG:HH11	1:A:344:ARG:CB	1.94	0.75
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.21	0.74
3:P:269:ILE:HG23	14:P:3001:FMX:H231	1.68	0.74
3:P:238:THR:HB	3:P:239:PRO:HD3	1.69	0.74
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.70	0.74
2:B:76:THR:HG22	2:B:82:SER:N	1.98	0.74
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.70	0.73
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.69	0.73
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.70	0.73
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.70	0.73
1:N:205:HIS:HB3	1:N:206:LYS:NZ	2.04	0.73
2:O:353:THR:HG22	2:O:355:GLU:N	2.01	0.73
7:T:73:ASN:HB3	7:T:76:ASP:OD2	1.89	0.73
3:C:328:LEU:HD23	7:G:51:PRO:HB3	1.70	0.73
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.88	0.73
9:I:71:ASN:HD22	9:I:71:ASN:N	1.87	0.72
2:B:47:ILE:HD13	2:B:120:MET:CE	2.19	0.72
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.52	0.72
3:C:238:THR:HB	3:C:239:PRO:HD3	1.71	0.72
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.55	0.72
4:Q:241:LYS:HE3	4:Q:241:LYS:HA	1.71	0.72
2:B:227:ARG:HA	2:B:227:ARG:NE	2.05	0.72
2:O:47:ILE:HD13	2:O:120:MET:CE	2.20	0.72
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.72	0.72
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.20	0.71
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.72	0.71
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.24	0.71
7:G:48:VAL:O	7:G:51:PRO:HD2	1.89	0.71
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.71	0.71
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.05	0.71
1:A:49:ASN:ND2	1:A:51:LYS:H	1.89	0.71
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.55	0.70
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.04	0.70
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.73	0.70
5:R:10:PHE:O	5:R:14:ARG:HG3	1.91	0.70
2:O:335:GLU:HA	2:O:338:ARG:NH1	2.06	0.70
5:R:101:ARG:HG2	5:R:105:GLU:OE1	1.91	0.69
1:N:398:ARG:HH11	1:N:398:ARG:HG2	1.56	0.69
5:R:188:VAL:HG11	5:R:192:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:UNK:HA	9:I:72:ALA:HB2	1.75	0.69
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.57	0.69
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.06	0.69
1:N:282:ARG:HH21	9:V:36:UNK:CB	2.05	0.69
6:S:12:LEU:HB3	6:S:13:MET:HE2	1.74	0.69
8:U:47:ARG:HG3	8:U:49:HIS:H	1.58	0.69
3:C:245:LEU:O	4:D:201:ARG:HD2	1.92	0.69
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.75	0.68
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.76	0.68
2:B:389:SER:O	2:B:391:THR:HG23	1.92	0.68
1:N:9:GLN:HG2	1:N:393:GLU:OE2	1.93	0.68
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.59	0.68
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.75	0.68
13:P:502:HEM:HMC2	13:P:502:HEM:HBC2	1.75	0.68
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.75	0.68
3:C:101:ARG:HD2	3:C:101:ARG:C	2.18	0.68
5:R:116:LYS:HA	5:R:116:LYS:HE2	1.76	0.68
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.75	0.68
3:C:269:ILE:HD12	5:R:160:CYS:SG	2.33	0.68
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.08	0.68
2:B:113:ARG:O	2:B:116:VAL:HG23	1.93	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.28	0.68
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.29	0.68
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.29	0.68
1:A:103:SER:HB3	1:A:202:GLY:O	1.94	0.68
2:B:27:THR:HG21	2:B:217:LYS:HE3	1.76	0.67
3:P:328:LEU:HD23	7:T:51:PRO:HB3	1.76	0.67
2:O:297:GLN:O	2:O:301:LYS:HG3	1.93	0.67
8:H:18:THR:O	8:H:22:GLU:HG3	1.96	0.66
1:N:178:THR:CG2	1:N:180:ALA:H	2.04	0.66
1:A:222:THR:OG1	1:A:225:GLU:HG3	1.94	0.66
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.61	0.66
1:A:350:THR:HB	1:A:353:GLU:HG3	1.77	0.66
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.29	0.66
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.59	0.66
2:B:297:GLN:O	2:B:301:LYS:HG3	1.95	0.66
2:O:252:LEU:HD13	9:V:55:MET:HE3	1.78	0.66
4:D:204:MET:HG2	17:D:2009:BOG:H5	1.78	0.66
7:G:73:ASN:HB3	7:G:76:ASP:OD2	1.95	0.66
7:T:48:VAL:O	7:T:51:PRO:HD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:34:UNK:N	9:V:35:UNK:N	2.44	0.66
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.78	0.65
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.26	0.65
1:N:222:THR:OG1	1:N:225:GLU:HG3	1.96	0.65
3:C:41:CYS:SG	3:C:90:PHE:CD2	2.88	0.65
2:O:31:ASN:C	2:O:31:ASN:HD22	2.05	0.65
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.78	0.65
3:C:354:MET:HE2	3:C:354:MET:HA	1.79	0.65
1:A:178:THR:CG2	1:A:180:ALA:H	2.04	0.65
9:I:31:UNK:C	9:I:73:PRO:HG2	2.27	0.65
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.31	0.65
2:B:335:GLU:HA	2:B:338:ARG:NH1	2.10	0.65
2:B:27:THR:CG2	2:B:28:LYS:H	2.05	0.65
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.79	0.65
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.78	0.64
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.32	0.64
2:O:407:SER:O	2:O:411:VAL:HG23	1.97	0.64
5:R:82:PRO:HD2	5:R:85:LYS:CD	2.27	0.64
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.79	0.64
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.78	0.64
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.61	0.64
2:O:43:PRO:O	2:O:113:ARG:HG3	1.97	0.64
7:T:75:ALA:HA	7:T:78:GLU:HG3	1.80	0.64
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.32	0.64
3:C:377:MET:HE1	6:F:19:TRP:HZ3	1.62	0.64
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.10	0.64
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.78	0.64
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.80	0.64
7:G:75:ALA:HA	7:G:78:GLU:HG3	1.80	0.64
3:P:9:HIS:HD2	3:P:12:LEU:H	1.43	0.64
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.13	0.64
2:O:338:ARG:HB2	2:O:338:ARG:NH1	2.12	0.64
2:B:353:THR:HG22	2:B:355:GLU:N	2.03	0.64
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.79	0.64
1:A:7:THR:HG21	2:B:113:ARG:CD	2.27	0.64
1:A:106:MET:HE2	1:A:107:PRO:HA	1.80	0.64
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.63	0.64
3:C:344:VAL:O	3:C:345:GLU:HG3	1.98	0.64
2:O:389:SER:O	2:O:391:THR:HG23	1.97	0.64
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.79	0.63
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.32	0.63
2:B:31:ASN:HD22	2:B:31:ASN:C	2.04	0.63
1:N:350:THR:HB	1:N:353:GLU:HG3	1.79	0.63
1:A:170:THR:HG22	1:A:171:THR:N	2.12	0.63
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.34	0.63
5:R:122:HIS:O	5:R:125:ASP:HB2	1.99	0.63
1:A:9:GLN:HG2	1:A:393:GLU:OE2	1.97	0.63
2:B:43:PRO:O	2:B:113:ARG:HG3	1.98	0.63
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.61	0.63
3:P:354:MET:HA	3:P:354:MET:HE2	1.80	0.63
3:P:247:SER:OG	3:P:250:LEU:HB2	1.99	0.63
3:P:350:ILE:O	3:P:354:MET:HG2	1.99	0.63
10:J:40:ASP:O	10:J:44:GLU:HG3	1.99	0.63
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.33	0.63
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.81	0.63
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.80	0.62
1:A:77:LYS:HE3	2:B:359:LYS:NZ	2.14	0.62
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.62
1:N:187:ASP:O	1:N:191:LYS:HE3	1.98	0.62
2:O:399:ALA:O	2:O:402:ILE:HG22	1.99	0.62
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.81	0.62
2:B:192:HIS:O	2:B:196:GLN:HG3	1.99	0.62
3:C:30:ALA:HB1	19:D:2003:CDL:H111	1.80	0.62
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.63	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.35	0.62
1:N:170:THR:HG22	1:N:171:THR:N	2.15	0.62
1:N:190:PHE:C	1:N:195:MET:HE2	2.25	0.62
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.62
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.14	0.62
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.65	0.62
5:E:77:LYS:HE2	5:E:80:ASP:OD2	2.00	0.62
2:O:31:ASN:HD22	2:O:32:GLY:N	1.98	0.62
2:O:338:ARG:HH11	2:O:338:ARG:CB	2.12	0.62
7:G:41:PHE:O	7:G:45:VAL:HG23	1.98	0.62
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.80	0.62
2:B:31:ASN:HD22	2:B:32:GLY:N	1.98	0.61
3:P:377:MET:HE1	6:S:19:TRP:HZ3	1.64	0.61
10:W:40:ASP:O	10:W:44:GLU:HG3	2.00	0.61
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.82	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.36	0.61
2:B:156:GLN:HE22	9:I:77:ARG:C	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.83	0.61
2:B:353:THR:HB	2:B:356:ASP:CG	2.25	0.61
2:B:402:ILE:HD13	2:B:402:ILE:C	2.26	0.61
2:O:203:ARG:HD2	2:O:230:ALA:O	1.99	0.61
1:N:112:LEU:O	1:N:116:VAL:HG23	2.01	0.61
7:T:41:PHE:O	7:T:45:VAL:HG23	2.00	0.61
1:A:190:PHE:C	1:A:195:MET:HE2	2.26	0.61
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.83	0.61
1:N:49:ASN:HD22	1:N:49:ASN:C	2.09	0.61
5:E:177:PRO:HB2	5:E:178:TYR:CD1	2.35	0.60
1:A:15:ASN:O	1:A:26:ALA:HA	2.01	0.60
4:D:164:ILE:O	4:D:179:MET:HE2	2.00	0.60
8:U:27:THR:O	8:U:31:VAL:HG23	2.01	0.60
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.01	0.60
3:C:269:ILE:HG23	14:C:2001:FMX:H231	1.82	0.60
2:O:381:GLU:HA	2:O:381:GLU:OE1	2.01	0.60
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.83	0.60
5:R:188:VAL:HB	5:R:192:LEU:HB2	1.83	0.60
4:Q:97:ASN:OD1	4:Q:99:GLU:HB2	2.02	0.60
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.83	0.60
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.35	0.60
2:B:306:PRO:HA	9:I:52:ARG:CG	2.31	0.60
2:O:46:ARG:HH11	2:O:110:GLU:HG3	1.65	0.60
2:B:46:ARG:HH11	2:B:110:GLU:HG3	1.65	0.60
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.83	0.60
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.35	0.60
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.32	0.60
2:B:292:THR:HG22	2:B:292:THR:O	2.01	0.60
10:W:55:ILE:CG2	10:W:59:TYR:HE1	2.15	0.60
2:B:153:GLN:NE2	9:I:34:UNK:HG1	2.17	0.60
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.37	0.60
1:N:103:SER:HB3	1:N:202:GLY:O	2.02	0.59
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.84	0.59
2:O:402:ILE:C	2:O:402:ILE:HD13	2.26	0.59
3:C:9:HIS:HD2	3:C:12:LEU:H	1.50	0.59
5:R:129:LYS:HB3	5:R:131:GLU:OE1	2.02	0.59
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.42	0.59
2:O:113:ARG:O	2:O:116:VAL:HG23	2.02	0.59
2:O:422:LYS:O	2:O:436:LEU:HD21	2.03	0.59
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.84	0.59
1:N:206:LYS:HA	1:N:209:VAL:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:410:VAL:O	1:N:413:LYS:HB3	2.02	0.59
1:A:49:ASN:HD22	1:A:51:LYS:N	2.01	0.59
1:A:187:ASP:O	1:A:191:LYS:HE3	2.02	0.59
2:B:262:ALA:HB2	2:B:268:GLU:HG2	1.84	0.59
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.85	0.59
1:N:15:ASN:O	1:N:26:ALA:HA	2.03	0.59
5:R:147:ILE:HG22	5:R:148:ALA:N	2.18	0.59
1:A:145:MET:HE2	1:A:145:MET:HA	1.84	0.59
3:P:71:CYS:SG	3:P:81:ARG:HD2	2.43	0.59
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.84	0.59
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.43	0.59
7:G:71:ARG:NH1	8:H:56:GLU:OE1	2.33	0.59
2:O:248:ASN:C	2:O:248:ASN:ND2	2.60	0.59
5:R:101:ARG:HH22	5:R:127:VAL:CG1	2.16	0.59
8:H:65:ARG:O	8:H:69:VAL:HG23	2.03	0.59
2:B:338:ARG:HB2	2:B:338:ARG:NH1	2.17	0.58
2:O:156:GLN:HE22	9:V:77:ARG:C	2.11	0.58
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.03	0.58
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.28	0.58
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.85	0.58
2:O:248:ASN:ND2	2:O:250:HIS:H	2.01	0.58
1:N:21:ASN:HB2	1:N:218:GLY:O	2.04	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.03	0.58
8:U:47:ARG:HD3	8:U:48:SER:H	1.68	0.58
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.33	0.58
1:N:347:THR:HG21	1:N:444:ILE:C	2.27	0.58
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.04	0.58
1:N:145:MET:HE2	1:N:145:MET:HA	1.86	0.58
2:O:150:VAL:O	2:O:153:GLN:HG3	2.04	0.58
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.86	0.58
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.86	0.58
1:A:350:THR:HG22	1:A:352:SER:N	2.18	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.39	0.58
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.39	0.58
6:S:59:MET:HE3	6:S:59:MET:HA	1.85	0.58
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.38	0.58
1:A:272:VAL:O	1:A:275:ALA:HB3	2.04	0.57
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.86	0.57
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.86	0.57
1:N:191:LYS:N	1:N:195:MET:HE2	2.18	0.57
2:B:226:ILE:O	2:B:226:ILE:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ASN:ND2	2:B:250:HIS:H	2.03	0.57
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.70	0.57
5:E:82:PRO:HD2	5:E:85:LYS:HD3	1.84	0.57
1:A:49:ASN:HD22	1:A:49:ASN:C	2.11	0.57
2:B:341:MET:CE	2:B:417:PHE:HE2	2.17	0.57
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.57
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.87	0.57
1:N:77:LYS:HE3	2:O:359:LYS:NZ	2.18	0.57
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.18	0.57
2:O:353:THR:HB	2:O:356:ASP:CG	2.28	0.57
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.57
2:O:341:MET:CE	2:O:417:PHE:HE2	2.18	0.57
2:B:422:LYS:O	2:B:436:LEU:HD21	2.05	0.57
4:D:200:GLN:NE2	17:D:2091:BOG:H5	2.19	0.57
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.19	0.57
2:O:308:ASP:OD2	9:V:55:MET:O	2.21	0.57
2:O:361:LYS:O	2:O:365:LYS:HG3	2.03	0.57
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.86	0.57
3:P:90:PHE:CZ	3:P:236:MET:HB3	2.39	0.57
10:W:4:ALA:O	10:W:8:GLN:HG3	2.04	0.57
2:O:273:SER:O	2:O:276:GLN:HB3	2.04	0.57
2:B:52:LYS:HE2	2:B:388:LEU:HD23	1.86	0.57
1:N:106:MET:HE2	1:N:107:PRO:HA	1.86	0.57
2:O:154:SER:O	2:O:157:VAL:HG12	2.04	0.57
2:O:225:ASN:O	2:O:226:ILE:C	2.47	0.57
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.86	0.57
6:F:59:MET:HE3	6:F:59:MET:HA	1.87	0.57
10:J:55:ILE:CG2	10:J:59:TYR:HE1	2.17	0.57
2:O:357:VAL:O	2:O:361:LYS:HG3	2.05	0.57
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.56
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.88	0.56
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.53	0.56
3:P:101:ARG:HD2	3:P:101:ARG:O	2.06	0.56
2:B:338:ARG:HH11	2:B:338:ARG:CB	2.18	0.56
9:I:49:LEU:O	9:I:50:LEU:HD23	2.05	0.56
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.88	0.56
5:R:126:ARG:HB3	5:R:182:VAL:HG21	1.87	0.56
1:A:106:MET:HG3	1:A:203:ILE:HG21	1.87	0.56
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.71	0.56
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.20	0.56
2:B:225:ASN:O	2:B:226:ILE:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:MET:HE2	1:N:106:MET:C	2.30	0.56
1:N:383:LEU:O	1:N:387:GLY:HA2	2.05	0.56
2:O:308:ASP:OD2	9:V:56:SER:HA	2.06	0.56
7:G:40:ARG:HD2	19:G:2004:CDL:OA4	2.04	0.56
1:N:394:GLU:O	1:N:397:SER:HB3	2.06	0.56
2:O:376:GLN:NE2	9:V:77:ARG:NH2	2.47	0.56
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.86	0.56
5:E:83:GLU:HG2	5:E:102:THR:HA	1.88	0.56
5:E:155:GLY:HA3	5:E:166:ASP:C	2.31	0.56
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.87	0.56
2:B:273:SER:O	2:B:276:GLN:HB3	2.06	0.56
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.87	0.56
5:R:52:LYS:HD3	5:R:52:LYS:C	2.30	0.56
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.06	0.56
1:A:307:PHE:CD1	1:A:307:PHE:C	2.83	0.56
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.69	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.04	0.56
1:N:49:ASN:HD22	1:N:51:LYS:N	1.98	0.56
2:O:306:PRO:HG2	9:V:50:LEU:O	2.06	0.56
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.87	0.56
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.71	0.55
4:D:47:ALA:N	4:D:50:ASN:HD22	1.98	0.55
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.88	0.55
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.40	0.55
4:Q:222:MET:HE3	5:R:40:THR:OG1	2.06	0.55
5:R:115:SER:O	5:R:116:LYS:HG2	2.05	0.55
5:R:126:ARG:H	5:R:126:ARG:HD3	1.71	0.55
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.89	0.55
5:E:160:CYS:SG	3:P:269:ILE:HD12	2.47	0.55
3:C:344:VAL:O	3:C:344:VAL:HG23	2.07	0.55
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.89	0.55
8:H:40:CYS:O	8:H:44:VAL:HG23	2.06	0.55
3:P:30:ALA:HB1	19:Q:3003:CDL:H111	1.89	0.55
7:T:40:ARG:HD2	19:T:3004:CDL:OA4	2.06	0.55
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.45	0.55
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.07	0.55
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.21	0.55
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.07	0.55
2:B:31:ASN:ND2	2:B:31:ASN:C	2.63	0.55
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.88	0.55
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.42	0.55
8:U:18:THR:O	8:U:22:GLU:HG3	2.05	0.55
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.18	0.55
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.37	0.55
1:A:106:MET:HE2	1:A:106:MET:C	2.32	0.55
4:D:47:ALA:HA	4:D:90:TYR:HA	1.89	0.55
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.88	0.55
7:G:72:LYS:HG2	8:H:56:GLU:OE2	2.07	0.55
3:P:95:ILE:O	3:P:99:ILE:HG13	2.07	0.55
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.35	0.54
2:O:353:THR:HG22	2:O:354:GLU:N	2.22	0.54
3:P:198:LEU:HD21	13:P:502:HEM:HMA3	1.89	0.54
5:R:78:LEU:HD13	5:R:132:TRP:CE2	2.42	0.54
2:B:26:ILE:HG12	2:B:26:ILE:O	2.07	0.54
5:E:10:PHE:O	5:E:14:ARG:HG3	2.07	0.54
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.89	0.54
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.90	0.54
2:O:202:ALA:HB3	2:O:229:GLY:O	2.07	0.54
1:N:205:HIS:HB3	1:N:206:LYS:HZ2	1.70	0.54
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.96	0.54
2:B:60:THR:CG2	2:B:61:ALA:N	2.71	0.54
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.41	0.54
5:R:190:ASP:O	5:R:191:ASP:CB	2.55	0.54
1:A:21:ASN:HB3	1:A:219:VAL:HG22	1.89	0.54
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.43	0.54
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.42	0.54
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.41	0.54
2:O:31:ASN:ND2	2:O:31:ASN:C	2.65	0.54
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.90	0.54
1:A:191:LYS:N	1:A:195:MET:HE2	2.23	0.54
1:A:383:LEU:O	1:A:387:GLY:HA2	2.08	0.54
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.42	0.54
2:B:227:ARG:HA	2:B:227:ARG:HE	1.72	0.54
2:B:361:LYS:O	2:B:365:LYS:HG3	2.08	0.54
3:C:268:HIS:HB3	21:C:1288:HOH:O	2.07	0.54
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.89	0.54
2:B:156:GLN:NE2	9:I:77:ARG:C	2.66	0.54
5:E:171:ILE:HG12	5:E:176:ALA:O	2.08	0.54
9:I:71:ASN:N	9:I:71:ASN:ND2	2.48	0.54
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.88	0.54
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:286:PRO:HA	21:P:1285:HOH:O	2.08	0.54
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.41	0.54
2:B:353:THR:HG22	2:B:354:GLU:N	2.23	0.54
3:C:198:LEU:HD21	13:C:502:HEM:HMA3	1.90	0.54
1:N:350:THR:HG22	1:N:352:SER:N	2.19	0.54
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.48	0.54
10:W:60:GLU:C	10:W:60:GLU:CD	2.76	0.54
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.33	0.53
1:N:206:LYS:HD2	1:N:206:LYS:N	2.11	0.53
2:B:399:ALA:O	2:B:402:ILE:HG22	2.09	0.53
4:D:35:GLN:NE2	4:D:169:LEU:HD12	2.23	0.53
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.73	0.53
4:Q:43:MET:HE2	4:Q:91:PHE:HE2	1.71	0.53
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.89	0.53
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.36	0.53
2:B:407:SER:O	2:B:411:VAL:HG23	2.09	0.53
5:R:155:GLY:HA3	5:R:166:ASP:C	2.33	0.53
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.43	0.53
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.44	0.53
2:O:60:THR:CG2	2:O:61:ALA:N	2.71	0.53
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.44	0.53
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.43	0.53
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.53
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.43	0.53
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.39	0.53
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.44	0.53
4:Q:195:GLU:HG3	4:Q:198:HIS:HB2	1.90	0.53
9:V:31:UNK:C	9:V:73:PRO:HG2	2.38	0.53
2:O:385:GLU:OE1	2:O:392:HIS:HA	2.09	0.53
3:P:9:HIS:CD2	3:P:11:LEU:H	2.27	0.53
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.09	0.53
1:A:394:GLU:O	1:A:397:SER:HB3	2.09	0.53
4:Q:241:LYS:OXT	4:Q:241:LYS:HG3	2.07	0.53
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.09	0.53
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.44	0.53
2:B:157:VAL:HG13	2:B:158:GLY:N	2.24	0.53
2:B:248:ASN:C	2:B:248:ASN:ND2	2.60	0.53
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.44	0.53
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.34	0.53
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.09	0.52
8:U:65:ARG:O	8:U:69:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:393:THR:HG23	2:O:397:VAL:HB	1.90	0.52
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.09	0.52
1:A:219:VAL:HG12	1:A:220:SER:N	2.24	0.52
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.75	0.52
2:B:393:THR:HG23	2:B:397:VAL:HB	1.90	0.52
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.44	0.52
1:N:21:ASN:CB	1:N:219:VAL:HA	2.39	0.52
1:N:146:THR:O	1:N:150:PHE:HD1	1.92	0.52
1:N:443:TRP:O	1:N:444:ILE:CB	2.56	0.52
2:O:26:ILE:HG12	2:O:26:ILE:O	2.07	0.52
2:O:33:LEU:HD22	2:O:224:LEU:HD12	1.92	0.52
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.77	0.52
3:P:34:PHE:HB2	21:P:381:HOH:O	2.09	0.52
9:I:38:UNK:O	9:I:39:UNK:C	2.57	0.52
1:N:205:HIS:HB3	1:N:206:LYS:HZ1	1.74	0.52
2:B:274:VAL:O	2:B:278:VAL:HG23	2.10	0.52
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.90	0.52
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.44	0.52
1:A:106:MET:N	1:A:107:PRO:HD2	2.25	0.52
9:I:65:VAL:HG12	9:I:66:ALA:N	2.24	0.52
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.38	0.52
4:Q:38:SER:O	4:Q:94:PRO:HG3	2.09	0.52
2:B:388:LEU:O	2:B:389:SER:HB3	2.10	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.91	0.52
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.91	0.52
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.92	0.52
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.09	0.52
5:R:136:VAL:O	5:R:138:VAL:N	2.42	0.52
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.10	0.52
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.10	0.52
5:E:73:LYS:HB3	5:E:195:VAL:O	2.10	0.52
5:E:103:GLN:O	5:E:107:ASN:ND2	2.43	0.52
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.45	0.52
1:N:7:THR:HG21	2:O:113:ARG:CD	2.39	0.52
3:P:344:VAL:O	3:P:345:GLU:HG3	2.10	0.52
3:P:347:PRO:O	3:P:350:ILE:HG22	2.10	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
5:R:114:VAL:HG13	5:R:122:HIS:HD2	1.75	0.52
6:S:13:MET:HE2	6:S:13:MET:N	2.24	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.75	0.51
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.92	0.51
3:C:269:ILE:CG2	14:C:2001:FMX:H231	2.40	0.51
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.51
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.91	0.51
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.45	0.51
1:A:138:LEU:HD11	1:A:174:ILE:HD12	1.92	0.51
2:O:27:THR:HG21	2:O:217:LYS:HE3	1.93	0.51
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.51
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.40	0.51
2:B:248:ASN:HD22	2:B:249:GLY:N	2.07	0.51
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.45	0.51
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.92	0.51
5:E:190:ASP:CG	5:E:191:ASP:H	2.19	0.51
2:O:264:VAL:HG23	2:O:316:TYR:C	2.36	0.51
5:R:101:ARG:CZ	5:R:133:VAL:HB	2.41	0.51
10:J:49:GLY:N	10:J:54:HIS:ND1	2.58	0.51
5:R:142:LEU:HD12	5:R:161:HIS:CE1	2.46	0.51
1:A:351:GLU:O	1:A:354:VAL:HG22	2.10	0.51
2:B:312:PHE:CE2	2:B:314:VAL:HG23	2.45	0.51
3:C:344:VAL:C	3:C:345:GLU:HG3	2.35	0.51
6:F:13:MET:HE2	6:F:16:ILE:HD12	1.91	0.51
1:N:106:MET:N	1:N:107:PRO:HD2	2.25	0.51
1:A:146:THR:O	1:A:150:PHE:HD1	1.93	0.51
2:B:385:GLU:OE1	2:B:392:HIS:HA	2.11	0.51
8:H:27:THR:O	8:H:31:VAL:HG23	2.11	0.51
1:N:268:VAL:O	1:N:272:VAL:HG23	2.10	0.51
2:O:62:ASN:O	2:O:65:THR:HG22	2.10	0.51
4:D:203:ARG:HD3	10:J:40:ASP:OD1	2.11	0.51
3:P:269:ILE:O	3:P:269:ILE:HG22	2.09	0.51
3:P:376:LYS:O	6:S:17:ARG:NH1	2.44	0.51
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.41	0.51
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.92	0.51
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.92	0.51
2:O:286:LYS:C	2:O:288:GLY:H	2.19	0.51
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.11	0.51
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.45	0.51
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.92	0.51
4:D:238:ARG:HD2	7:G:14:ILE:HD12	1.93	0.51
18:D:501:HEC:HMC1	18:D:501:HEC:HBC3	1.93	0.51
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.93	0.51
1:A:23:LEU:HD23	1:A:24:ARG:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.92	0.50
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.76	0.50
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.40	0.50
2:O:388:LEU:O	2:O:389:SER:HB3	2.09	0.50
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.92	0.50
8:H:11:GLU:CD	8:H:11:GLU:H	2.19	0.50
5:R:114:VAL:HG13	5:R:122:HIS:CD2	2.47	0.50
2:B:24:LEU:HD12	2:B:37:SER:O	2.11	0.50
3:C:105:TYR:O	3:C:315:THR:HG22	2.11	0.50
4:D:38:SER:O	4:D:94:PRO:HG3	2.12	0.50
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.93	0.50
2:O:76:THR:HG23	2:O:136:GLU:CD	2.36	0.50
1:A:410:VAL:O	1:A:413:LYS:HB3	2.11	0.50
2:B:333:ALA:O	2:B:337:ILE:HG13	2.12	0.50
5:E:83:GLU:HA	5:E:100:HIS:CG	2.46	0.50
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.46	0.50
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.42	0.50
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.94	0.50
4:D:41:HIS:HE1	4:D:111:PRO:HD2	1.76	0.50
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.94	0.50
4:D:71:GLN:HE21	4:D:82:MET:CE	2.25	0.50
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.93	0.50
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.46	0.50
2:B:264:VAL:HG23	2:B:316:TYR:O	2.11	0.50
4:D:97:ASN:OD1	4:D:99:GLU:HB2	2.12	0.50
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.42	0.50
2:O:67:HIS:O	2:O:70:ARG:HB3	2.11	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.27	0.50
3:C:285:ILE:CD1	3:C:294:ALA:HB2	2.42	0.50
5:E:163:SER:OG	5:E:175:PRO:HD2	2.12	0.50
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.44	0.50
1:N:335:MET:HG3	1:N:339:GLN:HE21	1.76	0.50
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.47	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.50
1:A:242:ARG:O	7:G:14:ILE:HA	2.11	0.49
5:E:165:TYR:HA	5:E:170:ARG:O	2.11	0.49
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.47	0.49
6:S:11:ARG:O	6:S:15:ARG:HG3	2.12	0.49
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.27	0.49
2:B:308:ASP:OD2	9:I:56:SER:HA	2.11	0.49
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:ILE:O	3:C:354:MET:HG2	2.11	0.49
1:N:138:LEU:HD11	1:N:174:ILE:HD12	1.95	0.49
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.41	0.49
2:O:274:VAL:O	2:O:278:VAL:HG23	2.12	0.49
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.77	0.49
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.49
1:A:268:VAL:O	1:A:272:VAL:HG23	2.12	0.49
2:B:307:PHE:CD1	2:B:308:ASP:N	2.81	0.49
1:N:63:ALA:O	1:N:116:VAL:HG13	2.13	0.49
1:N:161:THR:HG21	1:N:235:ARG:H	1.77	0.49
2:O:156:GLN:NE2	9:V:77:ARG:C	2.69	0.49
9:V:30:UNK:HG3	9:V:31:UNK:N	2.27	0.49
2:B:19:PRO:HB2	2:B:41:PHE:CE1	2.47	0.49
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.47	0.49
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.94	0.49
1:A:134:ILE:HG22	1:A:174:ILE:HD13	1.95	0.49
4:D:222:MET:CE	5:E:40:THR:HG23	2.43	0.49
3:P:198:LEU:HD13	15:P:3002:UQ:HM52	1.94	0.49
9:V:65:VAL:HG12	9:V:66:ALA:N	2.27	0.49
1:A:358:LYS:HE3	1:A:399:ILE:O	2.13	0.49
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.49
8:U:12:GLU:O	8:U:13:LEU:HB2	2.12	0.49
1:A:239:SER:HB2	7:G:17:SER:O	2.13	0.49
1:A:281:ASP:OD1	9:I:33:UNK:HB1	2.11	0.49
10:J:4:ALA:O	10:J:8:GLN:HG3	2.13	0.49
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.27	0.49
1:N:170:THR:HG22	1:N:172:GLU:H	1.78	0.49
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.95	0.49
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.95	0.49
4:D:220:TYR:O	4:D:224:ARG:HG2	2.12	0.49
2:O:248:ASN:HD22	2:O:249:GLY:N	2.09	0.49
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.28	0.49
5:E:102:THR:O	5:E:106:ILE:HG13	2.13	0.49
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.94	0.49
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.48	0.49
1:A:23:LEU:HD23	1:A:23:LEU:C	2.38	0.48
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.95	0.48
2:B:60:THR:HG23	2:B:61:ALA:N	2.28	0.48
13:C:502:HEM:HBD1	21:C:386:HOH:O	2.11	0.48
19:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.45	0.48
1:N:134:ILE:HG22	1:N:174:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.94	0.48
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.94	0.48
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.93	0.48
4:D:54:VAL:HG22	17:D:2091:BOG:H5'2	1.96	0.48
5:E:52:LYS:C	5:E:52:LYS:HD3	2.38	0.48
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.43	0.48
1:N:53:ASN:H	1:N:173:ASN:ND2	2.11	0.48
1:A:112:LEU:O	1:A:116:VAL:HG23	2.13	0.48
3:C:9:HIS:CD2	3:C:11:LEU:H	2.31	0.48
2:O:312:PHE:CE2	2:O:314:VAL:HG23	2.47	0.48
5:R:117:LEU:O	5:R:118:ARG:C	2.56	0.48
2:B:286:LYS:C	2:B:288:GLY:H	2.21	0.48
1:N:206:LYS:CA	1:N:209:VAL:HG12	2.41	0.48
1:A:106:MET:HE2	1:A:106:MET:O	2.13	0.48
10:J:55:ILE:HG22	10:J:59:TYR:CE1	2.44	0.48
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.77	0.48
2:O:60:THR:HG23	2:O:61:ALA:N	2.28	0.48
5:R:161:HIS:HB2	20:R:501:FES:S1	2.53	0.48
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.96	0.48
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.27	0.48
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.43	0.48
2:B:318:ASP:O	2:B:319:SER:HB2	2.11	0.48
3:C:247:SER:OG	3:C:250:LEU:HB2	2.13	0.48
3:P:269:ILE:CG2	14:P:3001:FMX:H231	2.42	0.48
5:R:109:GLU:C	5:R:111:GLU:H	2.22	0.48
8:U:65:ARG:O	8:U:68:CYS:HB3	2.13	0.48
1:A:370:ASP:O	2:B:374:THR:HG22	2.14	0.48
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.13	0.48
5:E:161:HIS:HB2	20:E:501:FES:S1	2.53	0.48
3:P:5:ILE:CG2	3:P:12:LEU:HD12	2.44	0.48
5:R:131:GLU:CD	5:R:131:GLU:H	2.22	0.48
6:S:51:PRO:HD2	6:S:54:LEU:HD12	1.95	0.48
2:B:26:ILE:HA	2:B:35:ILE:O	2.13	0.48
2:B:257:VAL:O	2:B:323:GLY:HA3	2.14	0.48
2:B:385:GLU:C	2:B:387:LEU:H	2.22	0.48
9:I:64:LEU:HD12	9:I:77:ARG:C	2.37	0.48
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.29	0.48
1:A:280:TYR:CG	1:A:281:ASP:N	2.82	0.48
1:N:19:LEU:C	1:N:21:ASN:H	2.22	0.48
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.78	0.48
4:D:197:GLU:O	4:D:198:HIS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:LEU:HD12	2:O:37:SER:O	2.13	0.48
2:O:147:ASP:O	2:O:150:VAL:HG22	2.14	0.48
3:P:379:ASN:HA	6:S:17:ARG:HH12	1.77	0.48
4:Q:238:ARG:HD2	7:T:14:ILE:HD12	1.96	0.48
2:B:218:GLN:HG2	2:B:222:GLN:OE1	2.14	0.47
3:C:45:GLN:HB3	13:C:501:HEM:HAB	1.95	0.47
1:N:49:ASN:ND2	1:N:49:ASN:C	2.72	0.47
1:N:219:VAL:HG12	1:N:220:SER:N	2.28	0.47
2:O:307:PHE:CD1	2:O:308:ASP:N	2.82	0.47
3:P:98:HIS:CD2	13:P:502:HEM:NC	2.82	0.47
6:S:40:ASP:O	6:S:44:LYS:HG3	2.13	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.15	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.49	0.47
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.29	0.47
5:E:133:VAL:HG13	5:E:133:VAL:O	2.14	0.47
9:I:64:LEU:HA	9:I:77:ARG:O	2.14	0.47
1:N:272:VAL:O	1:N:275:ALA:HB3	2.14	0.47
2:O:58:GLU:HG2	2:O:65:THR:HG22	1.95	0.47
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	1.96	0.47
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.29	0.47
2:B:402:ILE:HG23	2:B:403:ASP:N	2.29	0.47
3:C:325:LEU:HD22	3:C:370:ILE:HG13	1.94	0.47
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.50	0.47
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.96	0.47
7:G:71:ARG:HD3	8:H:56:GLU:CD	2.39	0.47
1:N:21:ASN:HB2	1:N:219:VAL:HA	1.96	0.47
1:N:209:VAL:O	1:N:212:ALA:HB3	2.15	0.47
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.45	0.47
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.95	0.47
10:W:49:GLY:N	10:W:54:HIS:ND1	2.63	0.47
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.44	0.47
1:A:371:GLY:O	1:A:375:VAL:HG23	2.14	0.47
5:E:77:LYS:HE2	5:E:80:ASP:CG	2.39	0.47
1:N:23:LEU:HD23	1:N:24:ARG:N	2.29	0.47
1:N:124:GLU:OE1	1:N:179:ARG:HG3	2.15	0.47
5:R:113:ASP:OD2	5:R:116:LYS:HG3	2.14	0.47
2:B:291:VAL:C	2:B:293:SER:H	2.22	0.47
3:C:5:ILE:CG2	3:C:12:LEU:HD12	2.45	0.47
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.15	0.47
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.95	0.47
6:F:84:GLU:H	6:F:84:GLU:CD	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:LYS:O	6:F:110:LYS:HB2	2.14	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.96	0.47
1:N:106:MET:HE2	1:N:106:MET:O	2.14	0.47
1:N:228:VAL:O	1:N:228:VAL:HG13	2.15	0.47
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.96	0.47
2:O:57:TYR:CD1	2:O:57:TYR:N	2.83	0.47
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.50	0.47
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.97	0.47
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.14	0.47
2:B:345:LYS:O	2:B:348:ALA:N	2.48	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.29	0.47
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.15	0.47
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.95	0.47
2:O:291:VAL:C	2:O:293:SER:H	2.22	0.47
4:D:168:ILE:HG12	4:D:168:ILE:O	2.15	0.47
2:O:159:VAL:HG21	2:O:325:TYR:HE1	1.80	0.47
5:R:124:LEU:HA	5:R:127:VAL:CG2	2.44	0.47
6:S:94:LEU:O	6:S:98:ILE:HG13	2.15	0.47
1:A:21:ASN:HA	1:A:219:VAL:HG13	1.97	0.47
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.32	0.47
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.97	0.47
3:C:69:HIS:HD2	3:C:73:ASN:ND2	2.08	0.47
5:E:189:GLY:O	5:E:190:ASP:C	2.58	0.47
3:P:247:SER:N	3:P:248:PRO:HD3	2.30	0.47
4:Q:35:GLN:NE2	4:Q:169:LEU:HD12	2.30	0.47
1:A:37:VAL:HG22	1:A:109:VAL:HG11	1.97	0.46
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.45	0.46
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.97	0.46
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.97	0.46
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.14	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.46
10:W:48:GLU:HA	10:W:54:HIS:CE1	2.51	0.46
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.82	0.46
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.97	0.46
1:N:369:LEU:HD12	1:N:392:LEU:HD21	1.97	0.46
2:O:345:LYS:O	2:O:348:ALA:N	2.48	0.46
3:P:17:ASN:HB2	17:P:2010:BOG:O3	2.16	0.46
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.15	0.46
5:R:147:ILE:HG13	5:R:157:TYR:O	2.16	0.46
1:A:281:ASP:OD1	1:A:281:ASP:C	2.58	0.46
2:B:102:ARG:HH22	2:B:161:GLU:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:ND2	1:A:49:ASN:C	2.73	0.46
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.96	0.46
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.97	0.46
6:F:40:ASP:O	6:F:44:LYS:HG3	2.15	0.46
1:N:53:ASN:N	1:N:173:ASN:ND2	2.63	0.46
3:P:101:ARG:C	3:P:101:ARG:CD	2.81	0.46
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.44	0.46
1:A:63:ALA:O	1:A:116:VAL:HG13	2.16	0.46
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.16	0.46
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.30	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.16	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.51	0.46
10:J:59:TYR:O	10:J:61:ALA:N	2.45	0.46
19:Q:3003:CDL:H511	7:T:26:ILE:HG21	1.97	0.46
1:A:217:SER:O	1:A:218:GLY:C	2.58	0.46
2:B:424:MET:HG2	2:B:425:ALA:N	2.29	0.46
3:C:101:ARG:HD2	3:C:101:ARG:O	2.16	0.46
3:C:117:GLY:O	13:C:502:HEM:HMC3	2.15	0.46
2:O:353:THR:CG2	2:O:354:GLU:N	2.79	0.46
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.98	0.46
4:Q:161:ALA:O	4:Q:162:PRO:C	2.59	0.46
1:A:45:SER:OG	1:A:92:ARG:HA	2.16	0.46
2:B:78:LYS:HA	2:B:131:GLU:OE2	2.16	0.46
2:B:350:GLY:C	2:B:352:VAL:H	2.23	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.15	0.46
5:E:189:GLY:O	5:E:192:LEU:N	2.48	0.46
1:N:49:ASN:ND2	1:N:51:LYS:N	2.58	0.46
3:P:139:MET:HE3	3:P:253:ASP:OD2	2.16	0.46
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.46	0.46
1:A:168:GLU:H	1:A:168:GLU:CD	2.23	0.46
2:B:62:ASN:O	2:B:65:THR:HG22	2.16	0.46
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.46
1:N:77:LYS:HE3	2:O:359:LYS:HZ1	1.81	0.46
1:N:178:THR:CG2	1:N:179:ARG:N	2.79	0.46
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.98	0.46
6:S:84:GLU:CD	6:S:84:GLU:H	2.24	0.46
1:A:75:PHE:HZ	1:A:86:PHE:HE2	1.64	0.46
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.97	0.46
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.51	0.46
1:N:184:SER:O	1:N:188:THR:OG1	2.28	0.46
1:N:351:GLU:O	1:N:354:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:347:PRO:O	3:P:351:ILE:HG13	2.16	0.46
2:B:50:PHE:C	2:B:51:ILE:HG13	2.40	0.46
2:B:327:ILE:HG22	9:I:55:MET:HE3	1.97	0.46
2:B:389:SER:O	2:B:390:GLY:C	2.58	0.46
4:D:3:LEU:HD11	7:G:72:LYS:CE	2.46	0.46
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.46	0.46
2:O:402:ILE:HG23	2:O:403:ASP:H	1.81	0.46
3:C:101:ARG:C	3:C:101:ARG:CD	2.88	0.45
2:O:26:ILE:HA	2:O:35:ILE:O	2.16	0.45
1:A:124:GLU:OE1	1:A:179:ARG:HG3	2.16	0.45
2:B:19:PRO:O	2:B:41:PHE:HE1	1.98	0.45
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.52	0.45
1:N:106:MET:CE	1:N:110:VAL:HG21	2.47	0.45
2:O:31:ASN:HD22	2:O:33:LEU:H	1.61	0.45
19:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.49	0.45
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.51	0.45
5:R:109:GLU:C	5:R:111:GLU:N	2.75	0.45
5:R:113:ASP:HB3	5:R:116:LYS:HG3	1.99	0.45
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.98	0.45
6:F:13:MET:HE2	6:F:13:MET:HA	1.97	0.45
1:N:350:THR:HG22	1:N:351:GLU:N	2.31	0.45
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.46	0.45
3:P:45:GLN:HB3	13:P:501:HEM:HAB	1.99	0.45
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.51	0.45
1:A:68:LYS:HD2	1:A:119:ASN:HB3	1.98	0.45
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.84	0.45
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.85	0.45
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.52	0.45
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.99	0.45
4:D:120:ARG:HH21	18:D:501:HEC:CGA	2.30	0.45
3:P:270:LYS:O	3:P:270:LYS:HG3	2.16	0.45
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.99	0.45
1:A:289:HIS:CD2	2:B:83:PHE:HD1	2.34	0.45
4:D:234:LYS:HD2	5:E:8:PRO:HB2	1.98	0.45
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.33	0.45
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.52	0.45
3:C:50:LEU:HD23	13:C:501:HEM:HBC1	1.98	0.45
3:P:344:VAL:C	3:P:345:GLU:HG3	2.41	0.45
5:R:73:LYS:HB3	5:R:195:VAL:O	2.16	0.45
1:A:136:GLN:O	1:A:140:GLU:HG3	2.17	0.45
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:HE	2:B:376:GLN:HA	1.81	0.45
2:B:397:VAL:O	2:B:401:LYS:HG2	2.17	0.45
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.17	0.45
1:N:23:LEU:HD23	1:N:23:LEU:C	2.42	0.45
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.47	0.45
2:O:327:ILE:HG22	9:V:55:MET:CE	2.47	0.45
3:P:69:HIS:HD2	3:P:73:ASN:ND2	2.11	0.45
5:R:55:VAL:O	5:R:59:ILE:HG12	2.17	0.45
5:R:99:ARG:NH2	5:R:149:ASN:OD1	2.49	0.45
1:A:106:MET:HE2	1:A:107:PRO:CA	2.46	0.45
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.47	0.45
1:A:205:HIS:O	1:A:209:VAL:HG12	2.16	0.45
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.47	0.45
1:N:206:LYS:H	1:N:206:LYS:CE	2.27	0.45
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.82	0.45
2:O:215:ASP:O	2:O:219:VAL:HG23	2.17	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.17	0.45
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.98	0.45
1:A:4:TYR:HE2	1:A:396:ASP:OD2	2.00	0.45
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.17	0.45
2:O:157:VAL:HG13	2:O:158:GLY:N	2.31	0.45
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.47	0.45
3:P:334:LEU:HD23	3:P:334:LEU:HA	1.75	0.45
9:V:64:LEU:HD12	9:V:77:ARG:C	2.42	0.45
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.99	0.44
3:C:234:THR:HG21	4:D:219:LEU:CD1	2.47	0.44
5:E:84:GLY:N	5:E:100:HIS:O	2.45	0.44
2:O:222:GLN:O	2:O:223:PHE:HD2	2.00	0.44
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.00	0.44
4:Q:71:GLN:HE21	4:Q:82:MET:CE	2.30	0.44
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.18	0.44
8:U:47:ARG:CD	8:U:48:SER:H	2.30	0.44
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.44
2:B:215:ASP:O	2:B:219:VAL:HG23	2.16	0.44
2:B:308:ASP:OD2	9:I:55:MET:O	2.36	0.44
5:E:85:LYS:HG2	5:E:86:ASN:N	2.33	0.44
1:N:158:PHE:O	1:N:164:ALA:HB2	2.16	0.44
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.47	0.44
1:A:170:THR:CG2	1:A:171:THR:N	2.77	0.44
5:E:41:ALA:O	5:E:45:VAL:HG23	2.16	0.44
3:P:350:ILE:HG23	3:P:351:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.53	0.44
1:A:156:THR:HA	5:E:7:VAL:HG21	2.00	0.44
4:D:62:LYS:O	4:D:66:GLU:HG3	2.18	0.44
1:N:75:PHE:HZ	1:N:86:PHE:HE2	1.65	0.44
2:O:333:ALA:O	2:O:337:ILE:HG13	2.17	0.44
3:P:285:ILE:CD1	3:P:294:ALA:HB2	2.46	0.44
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.51	0.44
5:R:41:ALA:O	5:R:45:VAL:HG23	2.18	0.44
8:U:40:CYS:O	8:U:44:VAL:HG23	2.17	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
1:A:350:THR:HG22	1:A:351:GLU:N	2.33	0.44
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.53	0.44
2:B:57:TYR:N	2:B:57:TYR:CD1	2.86	0.44
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.18	0.44
2:B:157:VAL:CG1	2:B:158:GLY:N	2.80	0.44
2:B:353:THR:CG2	2:B:354:GLU:N	2.81	0.44
3:C:347:PRO:O	3:C:350:ILE:HG22	2.17	0.44
2:O:399:ALA:C	2:O:402:ILE:HG22	2.42	0.44
3:P:344:VAL:O	3:P:344:VAL:HG23	2.17	0.44
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.99	0.44
9:V:65:VAL:O	9:V:76:VAL:HG23	2.16	0.44
2:B:218:GLN:O	2:B:222:GLN:HG3	2.17	0.44
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.47	0.44
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.99	0.44
2:B:230:ALA:O	2:B:231:GLY:C	2.59	0.44
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.86	0.44
10:J:60:GLU:O	10:J:61:ALA:HB3	2.18	0.44
1:A:240:GLU:CD	1:A:242:ARG:HE	2.25	0.44
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.99	0.44
6:F:78:GLU:H	6:F:78:GLU:CD	2.25	0.44
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.53	0.44
2:O:18:CYS:HA	2:O:19:PRO:HD2	1.74	0.44
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	2.00	0.44
5:R:85:LYS:HG2	5:R:86:ASN:N	2.33	0.44
2:B:116:VAL:O	2:B:120:MET:HB2	2.18	0.44
3:C:202:HIS:NE2	15:C:2002:UQ:O4	2.42	0.44
5:E:55:VAL:O	5:E:59:ILE:HG12	2.18	0.44
5:E:119:ASP:OD2	5:E:179:ASN:ND2	2.51	0.44
1:N:95:THR:HG22	1:N:96:ALA:N	2.33	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.90	0.44
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.43	0.44
5:R:128:LYS:O	5:R:129:LYS:HG3	2.18	0.44
9:V:28:UNK:HA	9:V:72:ALA:HB2	2.00	0.44
9:V:65:VAL:HB	9:V:77:ARG:HD3	1.99	0.44
2:B:43:PRO:C	2:B:113:ARG:HG3	2.43	0.43
2:B:89:ILE:HD13	2:B:96:LEU:HB2	2.00	0.43
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.32	0.43
1:N:223:TYR:OH	1:N:224:LYS:HE3	2.17	0.43
2:O:47:ILE:HG22	2:O:48:GLY:N	2.33	0.43
5:R:147:ILE:HG22	5:R:148:ALA:H	1.81	0.43
2:B:71:LEU:O	2:B:74:PRO:HD2	2.18	0.43
2:B:152:PHE:HA	2:B:157:VAL:CG1	2.46	0.43
5:E:136:VAL:O	5:E:138:VAL:N	2.47	0.43
8:H:57:GLU:H	8:H:57:GLU:CD	2.26	0.43
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.18	0.43
2:O:43:PRO:C	2:O:113:ARG:HG3	2.42	0.43
2:O:76:THR:HG22	2:O:82:SER:N	2.17	0.43
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.98	0.43
2:O:389:SER:O	2:O:390:GLY:C	2.61	0.43
3:P:335:ILE:HD13	7:T:58:LEU:HD23	2.00	0.43
7:T:36:ASN:O	7:T:40:ARG:HG3	2.18	0.43
1:A:95:THR:HG22	1:A:96:ALA:N	2.33	0.43
1:A:106:MET:CE	1:A:110:VAL:HG21	2.49	0.43
2:O:259:THR:O	2:O:260:GLU:C	2.61	0.43
5:R:177:PRO:HB2	5:R:178:TYR:CE1	2.54	0.43
1:A:85:HIS:HB2	1:A:100:LYS:HB2	2.00	0.43
1:A:89:TYR:CD1	1:A:89:TYR:C	2.95	0.43
2:B:286:LYS:C	2:B:288:GLY:N	2.77	0.43
2:B:368:TYR:HE1	2:B:381:GLU:OE2	2.02	0.43
2:O:286:LYS:C	2:O:288:GLY:N	2.75	0.43
4:Q:167:GLU:C	4:Q:169:LEU:N	2.76	0.43
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.47	0.43
3:C:198:LEU:HD13	15:C:2002:UQ:HM52	2.00	0.43
3:C:247:SER:N	3:C:248:PRO:HD3	2.33	0.43
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.43
6:F:71:LYS:O	6:F:72:HIS:HB2	2.19	0.43
2:O:245:ARG:HB3	2:O:430:LEU:CD1	2.48	0.43
5:R:73:LYS:HG2	5:R:196:GLY:HA3	2.01	0.43
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.48	0.43
5:R:133:VAL:HG13	5:R:133:VAL:O	2.18	0.43
1:A:240:GLU:HA	1:A:422:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:HD11	2:B:340:ALA:HB1	2.01	0.43
4:D:222:MET:HE3	5:E:40:THR:HG23	2.01	0.43
9:I:71:ASN:H	9:I:71:ASN:ND2	2.02	0.43
1:N:284:PHE:CE2	9:V:71:ASN:O	2.71	0.43
3:C:152:SER:HB3	3:C:162:VAL:HG21	2.00	0.43
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.54	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.72	0.43
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.49	0.43
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.01	0.43
5:R:84:GLY:N	5:R:100:HIS:O	2.52	0.43
6:S:78:GLU:CD	6:S:78:GLU:H	2.27	0.43
2:B:312:PHE:CZ	2:B:314:VAL:CG2	3.02	0.43
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.54	0.43
8:H:32:LYS:O	8:H:36:ARG:HG3	2.19	0.43
1:N:191:LYS:CA	1:N:195:MET:HE2	2.49	0.43
1:N:248:LEU:HD12	1:N:426:GLY:HA2	2.01	0.43
3:C:25:PRO:HB2	3:C:28:ILE:HG23	2.00	0.43
3:C:78:TRP:CD2	4:D:197:GLU:HG3	2.54	0.43
5:E:191:ASP:OD1	5:E:191:ASP:O	2.37	0.43
1:N:37:VAL:HG22	1:N:109:VAL:HG11	2.01	0.43
2:O:397:VAL:O	2:O:401:LYS:HG2	2.18	0.43
4:Q:200:GLN:NE2	17:Q:3091:BOG:H3	2.33	0.43
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.18	0.43
6:S:70:LEU:HD12	6:S:70:LEU:C	2.44	0.43
9:I:38:UNK:C	9:I:40:UNK:N	2.80	0.43
1:N:137:GLU:O	1:N:141:MET:HG3	2.19	0.43
1:N:168:GLU:CD	1:N:168:GLU:H	2.26	0.43
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.19	0.43
5:R:74:ILE:HD11	5:R:96:LEU:HD23	2.01	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.54	0.43
5:R:137:GLY:O	5:R:145:VAL:HG22	2.19	0.43
1:A:182:LEU:O	1:A:186:ILE:HG13	2.19	0.42
2:B:58:GLU:HG2	2:B:65:THR:HG22	2.00	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.54	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.80	0.42
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.47	0.42
5:R:124:LEU:HA	5:R:127:VAL:HG22	2.01	0.42
5:R:165:TYR:HA	5:R:170:ARG:O	2.18	0.42
1:A:64:PHE:CE2	1:A:86:PHE:CE1	3.07	0.42
1:A:161:THR:HG21	1:A:235:ARG:H	1.83	0.42
2:B:273:SER:HB3	2:B:364:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.85	0.42
5:E:77:LYS:CE	5:E:80:ASP:OD2	2.65	0.42
2:O:31:ASN:HD21	2:O:33:LEU:H	1.61	0.42
2:O:156:GLN:O	2:O:159:VAL:HG22	2.19	0.42
3:P:377:MET:HE2	6:S:20:TYR:HB2	2.02	0.42
5:R:122:HIS:HB3	5:R:125:ASP:OD1	2.19	0.42
5:R:171:ILE:HG23	5:R:171:ILE:O	2.18	0.42
9:V:67:GLY:O	9:V:68:ILE:HD13	2.20	0.42
1:A:178:THR:CG2	1:A:179:ARG:N	2.81	0.42
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.85	0.42
3:C:269:ILE:O	3:C:269:ILE:HG22	2.19	0.42
5:E:164:HIS:HB2	5:E:173:LYS:HB3	2.01	0.42
2:O:89:ILE:HD13	2:O:96:LEU:HB2	2.00	0.42
2:O:222:GLN:O	2:O:222:GLN:HG2	2.17	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.49	0.42
2:B:270:ASN:O	2:B:274:VAL:HG23	2.19	0.42
3:C:334:LEU:HD23	3:C:334:LEU:HA	1.86	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.20	0.42
1:N:90:THR:O	1:N:167:VAL:HG11	2.19	0.42
1:N:106:MET:HE2	1:N:107:PRO:CA	2.49	0.42
1:N:140:GLU:HG3	9:V:50:LEU:HD12	2.02	0.42
1:N:350:THR:CG2	1:N:351:GLU:N	2.83	0.42
1:N:398:ARG:HH11	1:N:398:ARG:CG	2.25	0.42
1:A:87:ASN:CG	1:A:88:GLY:H	2.27	0.42
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.50	0.42
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.42
3:C:95:ILE:HD13	3:C:121:LEU:HD13	2.01	0.42
4:D:102:ARG:HA	4:D:108:ALA:O	2.19	0.42
4:D:122:GLY:O	4:D:125:ASP:HB2	2.18	0.42
1:N:206:LYS:CD	1:N:206:LYS:N	2.63	0.42
2:O:34:ILE:HD13	2:O:390:GLY:CA	2.50	0.42
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.54	0.42
1:A:269:VAL:HG22	1:A:406:MET:HE2	2.01	0.42
2:B:29:LEU:HB3	2:B:30:PRO:HD2	2.00	0.42
2:B:399:ALA:CA	2:B:402:ILE:HG22	2.50	0.42
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.85	0.42
1:N:239:SER:HB2	7:T:17:SER:O	2.20	0.42
2:O:31:ASN:HD21	2:O:33:LEU:CB	2.33	0.42
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.42
2:O:424:MET:HG2	2:O:425:ALA:N	2.34	0.42
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:164:HIS:HB2	5:R:173:LYS:HB3	2.02	0.42
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.85	0.42
3:C:194:THR:O	3:C:197:HIS:HB3	2.20	0.42
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.55	0.42
7:G:45:VAL:O	7:G:49:ALA:HB3	2.20	0.42
1:N:370:ASP:O	2:O:374:THR:HG22	2.20	0.42
2:O:295:LEU:HD11	2:O:340:ALA:HB1	2.01	0.42
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	2.01	0.42
3:C:335:ILE:HD13	7:G:58:LEU:HD23	2.01	0.42
5:E:71:LEU:HD11	3:P:169:PHE:CE1	2.55	0.42
6:F:20:TYR:O	6:F:21:TYR:C	2.62	0.42
1:N:240:GLU:HA	1:N:422:LEU:O	2.20	0.42
2:O:157:VAL:CG1	2:O:158:GLY:N	2.82	0.42
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.01	0.42
2:O:201:SER:OG	2:O:228:SER:HA	2.20	0.42
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.01	0.42
5:R:109:GLU:HB3	5:R:123:ASP:HB2	2.02	0.42
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.20	0.42
2:B:71:LEU:HD12	2:B:144:LEU:HD23	2.02	0.42
2:B:84:ARG:HD2	6:S:107:TRP:CZ3	2.55	0.42
2:B:162:ASN:O	2:B:244:ILE:HD12	2.20	0.42
3:C:380:TYR:CZ	6:F:37:LEU:HD21	2.55	0.42
4:D:54:VAL:HG12	4:D:55:THR:HG23	2.02	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.42
2:O:299:VAL:HG11	2:O:336:VAL:HG13	2.00	0.42
3:P:208:ASN:HB2	3:P:209:PRO:HD2	2.02	0.42
5:R:101:ARG:HB3	5:R:105:GLU:HB2	2.02	0.42
6:S:13:MET:HB3	6:S:17:ARG:HE	1.84	0.42
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.76	0.42
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.47	0.42
2:B:385:GLU:C	2:B:387:LEU:N	2.76	0.42
4:D:167:GLU:C	4:D:169:LEU:N	2.76	0.42
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.50	0.42
2:O:318:ASP:O	2:O:319:SER:HB2	2.20	0.42
2:O:414:ALA:O	2:O:418:VAL:HG23	2.20	0.42
5:R:112:VAL:O	5:R:113:ASP:C	2.63	0.42
6:S:12:LEU:HB3	6:S:13:MET:CE	2.45	0.42
8:U:32:LYS:O	8:U:36:ARG:HG3	2.20	0.42
1:A:26:ALA:O	1:A:198:ALA:HA	2.20	0.41
1:A:284:PHE:O	1:A:285:GLY:C	2.63	0.41
4:D:195:GLU:HG3	4:D:198:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:ASN:HD22	1:N:274:ASN:HA	1.65	0.41
2:O:31:ASN:HD21	2:O:33:LEU:HB3	1.85	0.41
3:P:207:ASN:ND2	3:P:208:ASN:H	2.18	0.41
3:P:345:GLU:O	3:P:348:PHE:HB2	2.19	0.41
1:A:233:ARG:HH12	1:A:316:ASP:HB2	1.85	0.41
2:B:24:LEU:HD23	2:B:392:HIS:CE1	2.55	0.41
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.82	0.41
1:N:4:TYR:O	1:N:7:THR:OG1	2.32	0.41
4:Q:167:GLU:CG	8:U:13:LEU:HD13	2.50	0.41
6:S:52:GLU:HG3	6:S:56:ASN:ND2	2.34	0.41
1:A:77:LYS:HE3	2:B:359:LYS:HZ1	1.85	0.41
2:B:31:ASN:HD21	2:B:33:LEU:H	1.60	0.41
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.48	0.41
2:B:394:ALA:C	2:B:396:SER:H	2.27	0.41
10:J:14:PHE:CD2	10:J:14:PHE:N	2.87	0.41
10:J:38:GLY:O	10:J:42:ILE:HG13	2.20	0.41
1:N:242:ARG:O	7:T:14:ILE:HA	2.20	0.41
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.29	0.41
2:O:102:ARG:HH22	2:O:161:GLU:HA	1.86	0.41
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.49	0.41
7:T:66:PHE:CE2	7:T:70:LYS:HE3	2.56	0.41
1:A:170:THR:HG22	1:A:171:THR:H	1.83	0.41
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.20	0.41
2:B:307:PHE:HA	9:I:55:MET:HE1	2.01	0.41
5:E:132:TRP:CB	5:E:187:PHE:HZ	2.33	0.41
8:H:11:GLU:O	8:H:12:GLU:HB2	2.20	0.41
9:I:55:MET:O	9:I:58:ARG:HG2	2.20	0.41
1:N:68:LYS:HD2	1:N:119:ASN:HB3	2.02	0.41
2:O:385:GLU:C	2:O:387:LEU:H	2.28	0.41
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.85	0.41
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.21	0.41
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.01	0.41
1:A:285:GLY:O	1:A:286:GLY:C	2.64	0.41
2:B:337:ILE:HD12	2:B:434:PRO:HD2	2.01	0.41
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.01	0.41
2:O:46:ARG:HD2	2:O:110:GLU:OE2	2.20	0.41
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.36	0.41
2:O:248:ASN:HD22	2:O:250:HIS:H	1.68	0.41
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.19	0.41
4:Q:167:GLU:C	4:Q:169:LEU:H	2.27	0.41
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:SER:O	2:B:391:THR:N	2.54	0.41
4:D:161:ALA:O	4:D:162:PRO:C	2.63	0.41
1:N:19:LEU:C	1:N:21:ASN:N	2.78	0.41
2:O:368:TYR:HE1	2:O:381:GLU:OE2	2.03	0.41
3:P:156:TYR:CD2	3:P:156:TYR:N	2.88	0.41
3:P:273:TRP:HA	3:P:276:LEU:HD12	2.02	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.50	0.41
1:A:362:ARG:HB2	2:B:112:LEU:HD11	2.03	0.41
2:B:224:LEU:HD23	2:B:224:LEU:HA	1.90	0.41
2:B:307:PHE:H	9:I:52:ARG:HG2	1.86	0.41
3:C:139:MET:HE3	3:C:253:ASP:OD2	2.21	0.41
5:E:171:ILE:HG23	5:E:171:ILE:O	2.21	0.41
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.86	0.41
1:N:358:LYS:O	1:N:362:ARG:HG3	2.21	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.46	0.41
2:O:350:GLY:C	2:O:352:VAL:H	2.25	0.41
3:P:226:SER:O	3:P:230:ILE:HG13	2.20	0.41
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.85	0.41
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.56	0.41
3:C:301:ILE:CD1	3:C:364:LEU:HD21	2.50	0.41
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.92	0.41
1:N:45:SER:HA	1:N:48:GLU:HG3	2.03	0.41
2:O:225:ASN:O	2:O:227:ARG:N	2.53	0.41
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.47	0.41
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.20	0.41
6:S:77:LYS:HE2	6:S:77:LYS:HB3	1.83	0.41
9:V:32:UNK:O	9:V:33:UNK:C	2.68	0.41
1:A:105:ASP:O	1:A:106:MET:C	2.64	0.41
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	2.03	0.41
3:C:37:LEU:CD1	3:C:236:MET:HG3	2.51	0.41
3:C:342:GLN:HB3	3:C:343:PRO:HD2	2.03	0.41
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.55	0.41
4:D:14:HIS:HB3	4:D:21:LEU:HA	2.03	0.41
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.03	0.41
4:D:71:GLN:HB2	4:D:82:MET:HE1	2.03	0.41
4:D:223:LYS:C	4:D:223:LYS:HD3	2.46	0.41
10:J:56:LYS:O	10:J:60:GLU:HB2	2.20	0.41
1:N:89:TYR:CD1	1:N:89:TYR:C	2.99	0.41
1:N:105:ASP:O	1:N:106:MET:C	2.64	0.41
1:N:262:TRP:CD1	1:N:314:TYR:C	2.99	0.41
1:N:436:ARG:HD2	1:N:436:ARG:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:307:PHE:CD1	2:O:307:PHE:C	2.99	0.41
3:P:54:MET:SD	5:R:62:LEU:HD21	2.61	0.41
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.56	0.41
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.86	0.41
4:Q:197:GLU:O	4:Q:198:HIS:C	2.62	0.41
5:R:118:ARG:HB2	5:R:171:ILE:CG2	2.50	0.41
5:R:151:GLY:C	5:R:153:PHE:H	2.29	0.41
6:S:77:LYS:O	6:S:77:LYS:HG2	2.21	0.41
2:B:307:PHE:CD1	2:B:307:PHE:C	2.99	0.41
5:E:106:ILE:HG21	5:E:130:PRO:HB3	2.02	0.41
5:E:193:VAL:HG13	5:E:193:VAL:O	2.21	0.41
1:N:182:LEU:O	1:N:186:ILE:HG13	2.21	0.41
1:N:280:TYR:CG	1:N:281:ASP:N	2.89	0.41
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.49	0.41
3:P:285:ILE:C	3:P:287:ASN:H	2.29	0.41
3:C:2:ALA:HB3	3:C:8:SER:HB3	2.02	0.40
7:G:24:ARG:HB2	7:G:27:PRO:HB3	2.04	0.40
8:H:10:GLU:HB2	8:H:11:GLU:OE2	2.21	0.40
1:N:387:GLY:O	1:N:388:ARG:HB3	2.20	0.40
2:O:394:ALA:C	2:O:396:SER:H	2.29	0.40
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	2.03	0.40
5:R:193:VAL:HG13	5:R:193:VAL:O	2.20	0.40
2:B:46:ARG:HG3	2:B:110:GLU:HG2	2.04	0.40
3:C:30:ALA:O	3:C:33:ASN:HB2	2.20	0.40
3:C:347:PRO:O	3:C:351:ILE:HG13	2.20	0.40
1:N:371:GLY:O	1:N:375:VAL:HG23	2.21	0.40
2:O:268:GLU:HG2	2:O:268:GLU:O	2.21	0.40
8:U:12:GLU:HG2	8:U:13:LEU:N	2.36	0.40
2:B:399:ALA:C	2:B:402:ILE:HG22	2.47	0.40
5:E:77:LYS:C	5:E:79:SER:H	2.29	0.40
8:H:65:ARG:O	8:H:68:CYS:HB3	2.22	0.40
1:N:26:ALA:O	1:N:198:ALA:HA	2.22	0.40
2:O:109:VAL:HG21	2:O:119:VAL:CG1	2.51	0.40
1:A:328:PRO:HB3	1:A:427:PRO:HB2	2.04	0.40
3:C:29:SER:HB2	19:G:2004:CDL:OB4	2.21	0.40
1:N:354:VAL:O	1:N:355:LYS:C	2.64	0.40
10:W:14:PHE:CD2	10:W:14:PHE:N	2.84	0.40
1:A:7:THR:O	1:A:11:ILE:HG13	2.22	0.40
1:A:300:GLU:HA	1:A:300:GLU:OE1	2.21	0.40
1:A:350:THR:CG2	1:A:351:GLU:N	2.84	0.40
1:A:364:ALA:O	1:A:368:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:LEU:N	3:C:135:PRO:HD2	2.36	0.40
5:E:78:LEU:HD13	5:E:132:TRP:CE2	2.56	0.40
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.03	0.40
1:N:144:ASP:O	1:N:148:VAL:HG23	2.21	0.40
1:N:364:ALA:O	1:N:368:GLN:HG3	2.21	0.40
2:O:124:LEU:HD21	2:O:223:PHE:HB3	2.04	0.40
2:O:399:ALA:HA	2:O:402:ILE:CG2	2.52	0.40
3:P:69:HIS:CD2	3:P:73:ASN:ND2	2.81	0.40
3:P:98:HIS:HD2	13:P:502:HEM:C1C	2.40	0.40
5:R:63:SER:O	5:R:64:ALA:C	2.65	0.40
5:R:116:LYS:O	5:R:117:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	415 (94%)	21 (5%)	5 (1%)	11	22
1	N	440/446 (99%)	413 (94%)	21 (5%)	6 (1%)	9	17
2	B	419/441 (95%)	370 (88%)	40 (10%)	9 (2%)	5	11
2	O	420/441 (95%)	374 (89%)	38 (9%)	8 (2%)	6	12
3	C	378/380 (100%)	363 (96%)	14 (4%)	1 (0%)	36	56
3	P	377/380 (99%)	361 (96%)	15 (4%)	1 (0%)	36	56
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	30	50
5	E	194/196 (99%)	174 (90%)	13 (7%)	7 (4%)	2	4
5	R	192/196 (98%)	163 (85%)	22 (12%)	7 (4%)	2	4
6	F	99/110 (90%)	94 (95%)	4 (4%)	1 (1%)	12	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	G	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	18
7	T	76/81 (94%)	69 (91%)	7 (9%)	0	100	100
8	H	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	8	15
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	8	15
9	I	29/47 (62%)	25 (86%)	4 (14%)	0	100	100
9	V	29/47 (62%)	25 (86%)	3 (10%)	1 (3%)	3	5
10	J	59/61 (97%)	54 (92%)	3 (5%)	2 (3%)	3	5
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	3	5
All	All	4000/4160 (96%)	3688 (92%)	258 (6%)	54 (1%)	9	17

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
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	171	ALA
2	O	228	SER
2	O	389	SER
5	R	113	ASP
5	R	191	ASP
1	A	218	GLY
2	B	171	ALA
2	B	390	GLY
5	E	137	GLY
1	N	218	GLY
5	R	137	GLY
5	R	189	GLY
8	U	13	LEU
1	A	72	CYS
1	N	72	CYS

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Mol	Chain	Res	Type
1	N	262	TRP
9	V	48	PRO
1	A	262	TRP
2	B	220	ALA
5	E	64	ALA
5	E	120	PRO
5	E	141	HIS
8	H	12	GLU
10	J	56	LYS
2	O	350	GLY
5	R	152	ASP
10	W	62	SER
1	A	443	TRP
7	G	33	ALA
10	J	60	GLU
1	N	443	TRP
2	O	220	ALA
2	O	390	GLY
4	Q	177	ALA
10	W	56	LYS
2	B	29	LEU
6	F	77	LYS
3	P	286	PRO
5	E	189	GLY
2	B	350	GLY
5	R	8	PRO
3	C	286	PRO
2	O	29	LEU
5	R	147	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	365/368 (99%)	357 (98%)	8 (2%)	45 67
1	N	365/368 (99%)	352 (96%)	13 (4%)	31 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	332/347 (96%)	326 (98%)	6 (2%)	51	71
2	O	333/347 (96%)	327 (98%)	6 (2%)	51	71
3	C	328/329 (100%)	325 (99%)	3 (1%)	70	82
3	P	328/329 (100%)	323 (98%)	5 (2%)	57	74
4	D	200/200 (100%)	197 (98%)	3 (2%)	57	74
4	Q	200/200 (100%)	196 (98%)	4 (2%)	48	69
5	E	166/166 (100%)	166 (100%)	0	100	100
5	R	165/166 (99%)	163 (99%)	2 (1%)	63	78
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	47
6	S	93/96 (97%)	89 (96%)	4 (4%)	26	47
7	G	71/71 (100%)	70 (99%)	1 (1%)	59	75
7	T	69/71 (97%)	67 (97%)	2 (3%)	37	61
8	H	65/71 (92%)	63 (97%)	2 (3%)	35	59
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	73
9	I	23/26 (88%)	22 (96%)	1 (4%)	26	47
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	69
10	W	47/49 (96%)	46 (98%)	1 (2%)	47	67
All	All	3378/3446 (98%)	3311 (98%)	67 (2%)	48	69

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	49	ASN
1	A	90	THR
1	A	106	MET
1	A	108	LYS
1	A	281	ASP
1	A	344	ARG
1	A	443	TRP
2	B	31	ASN
2	B	248	ASN
2	B	338	ARG
2	B	341	MET
2	B	364	LEU

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Mol	Chain	Res	Type
2	B	402	ILE
3	C	5	ILE
3	C	223	PRO
3	C	269	ILE
4	D	43	MET
4	D	169	LEU
4	D	172	ASP
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
6	F	84	GLU
7	G	27	PRO
8	H	27	THR
8	H	72	LYS
9	I	71	ASN
10	J	64	GLU
1	N	3	THR
1	N	18	THR
1	N	29	GLU
1	N	49	ASN
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	348	SER
1	N	395	TRP
1	N	443	TRP
2	O	31	ASN
2	O	248	ASN
2	O	338	ARG
2	O	341	MET
2	O	364	LEU
2	O	402	ILE
3	P	5	ILE
3	P	199	THR
3	P	223	PRO
3	P	269	ILE
3	P	334	LEU
4	Q	43	MET
4	Q	169	LEU

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Mol	Chain	Res	Type
4	Q	172	ASP
4	Q	241	LYS
5	R	125	ASP
5	R	126	ARG
6	S	64	ARG
6	S	70	LEU
6	S	73	ARG
6	S	84	GLU
7	T	2	ILE
7	T	27	PRO
8	U	72	LYS
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	61	HIS
1	A	118	GLN
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	115	HIS
2	B	153	GLN
2	B	156	GLN
2	B	192	HIS
2	B	248	ASN
2	B	276	GLN
2	B	305	GLN
2	B	315	ASN
2	B	329	GLN
2	B	343	GLN
3	C	9	HIS
3	C	55	HIS
3	C	69	HIS
3	C	82	ASN
3	C	86	ASN
3	C	207	ASN
3	C	268	HIS

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Mol	Chain	Res	Type
3	C	332	ASN
3	C	342	GLN
3	C	346	HIS
4	D	31	GLN
4	D	35	GLN
4	D	50	ASN
4	D	71	GLN
4	D	148	HIS
4	D	156	GLN
4	D	200	GLN
4	D	225	HIS
5	E	3	ASN
5	E	57	GLN
6	F	72	HIS
6	F	79	GLN
7	G	12	HIS
7	G	23	GLN
7	G	79	ASN
8	H	71	HIS
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	271	HIS
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	311	ASN
1	N	339	GLN
2	O	31	ASN
2	O	115	HIS
2	O	156	GLN
2	O	192	HIS
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	305	GLN
2	O	329	GLN
2	O	343	GLN
2	O	349	GLN

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Mol	Chain	Res	Type
2	O	376	GLN
3	P	9	HIS
3	P	55	HIS
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	268	HIS
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	71	GLN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	108	GLN
6	S	79	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	79	ASN
8	U	71	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
14	FMX	C	2001	-	30,31,31	1.25	2 (6%)	36,44,44	1.18	3 (8%)
16	AZI	C	2011	-	2,2,2	2.88	2 (100%)	0,1,1	-	-
15	UQ	C	2002	-	19,19,63	2.57	10 (52%)	24,26,79	1.00	2 (8%)
17	BOG	Q	3009	-	20,20,20	0.95	1 (5%)	25,25,25	0.86	1 (4%)
11	PEE	N	3005	-	49,49,50	1.44	9 (18%)	52,54,55	0.82	3 (5%)
16	AZI	P	3011	-	2,2,2	3.31	2 (100%)	0,1,1	-	-
11	PEE	N	3008	-	4,4,50	3.75	4 (100%)	6,6,55	0.58	0
11	PEE	C	2007	-	47,47,50	1.33	7 (14%)	50,52,55	0.81	3 (6%)
17	BOG	Q	3091	-	20,20,20	1.11	2 (10%)	25,25,25	0.89	1 (4%)
19	CDL	G	2004	-	39,39,99	1.20	2 (5%)	45,51,111	1.06	3 (6%)
14	FMX	P	3001	-	30,31,31	1.17	2 (6%)	36,44,44	1.17	3 (8%)
13	HEM	C	502	3	50,50,50	1.68	7 (14%)	67,82,82	1.53	10 (14%)
19	CDL	Q	3003	-	41,41,99	1.19	2 (4%)	47,53,111	1.07	3 (6%)
17	BOG	D	2009	-	20,20,20	1.01	1 (5%)	25,25,25	0.89	2 (8%)
11	PEE	P	3007	-	47,47,50	1.36	5 (10%)	50,52,55	0.78	2 (4%)
20	FES	E	501	5	0,4,4	-	-	-	-	-
19	CDL	D	2003	-	41,41,99	1.18	1 (2%)	47,53,111	1.07	4 (8%)
18	HEC	D	501	4	46,50,50	1.59	5 (10%)	58,82,82	2.08	8 (13%)
11	PEE	A	2005	-	49,49,50	1.46	9 (18%)	52,54,55	0.83	3 (5%)
17	BOG	C	3010	-	11,11,20	1.07	2 (18%)	10,11,25	1.02	1 (10%)
20	FES	R	501	5	0,4,4	-	-	-	-	-
13	HEM	P	501	3	50,50,50	1.35	4 (8%)	67,82,82	1.27	5 (7%)
17	BOG	P	2010	-	18,18,20	1.07	3 (16%)	22,22,25	0.57	0
15	UQ	P	3002	-	19,19,63	2.43	10 (52%)	24,26,79	1.06	2 (8%)
13	HEM	C	501	3	50,50,50	1.43	6 (12%)	67,82,82	1.48	9 (13%)
17	BOG	D	2091	-	20,20,20	1.11	2 (10%)	25,25,25	1.02	1 (4%)
13	HEM	P	502	3	50,50,50	1.43	4 (8%)	67,82,82	1.22	5 (7%)
19	CDL	T	3004	-	39,39,99	1.20	3 (7%)	45,51,111	1.07	3 (6%)
11	PEE	C	2008	-	20,20,50	1.66	5 (25%)	23,25,55	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	HEC	Q	501	4	46,50,50	1.72	9 (19%)	58,82,82	2.01	9 (15%)

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
14	FMX	C	2001	-	-	4/14/33/33	0/4/4/4
15	UQ	C	2002	-	-	2/11/35/87	0/1/1/1
17	BOG	Q	3009	-	-	6/11/31/31	0/1/1/1
11	PEE	N	3005	-	-	31/53/53/54	-
11	PEE	C	2007	-	-	22/51/51/54	-
17	BOG	Q	3091	-	-	5/11/31/31	0/1/1/1
19	CDL	G	2004	-	-	23/49/49/110	-
14	FMX	P	3001	-	-	2/14/33/33	0/4/4/4
13	HEM	C	502	3	-	6/14/54/54	-
19	CDL	Q	3003	-	-	21/51/51/110	-
17	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
11	PEE	P	3007	-	-	22/51/51/54	-
20	FES	E	501	5	-	-	0/1/1/1
19	CDL	D	2003	-	-	22/51/51/110	-
18	HEC	D	501	4	-	9/14/54/54	-
11	PEE	A	2005	-	-	30/53/53/54	-
17	BOG	C	3010	-	-	4/9/9/31	-
20	FES	R	501	5	-	-	0/1/1/1
13	HEM	P	501	3	-	4/14/54/54	-
17	BOG	P	2010	-	-	1/6/26/31	0/1/1/1
15	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
13	HEM	C	501	3	-	4/14/54/54	-
17	BOG	D	2091	-	-	7/11/31/31	0/1/1/1
13	HEM	P	502	3	-	6/14/54/54	-
19	CDL	T	3004	-	-	25/49/49/110	-
11	PEE	C	2008	-	-	10/24/24/54	-
18	HEC	Q	501	4	-	10/14/54/54	-

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	501	HEC	CAC-C3C	6.10	1.54	1.35
18	D	501	HEC	CAC-C3C	5.73	1.53	1.35
13	P	502	HEM	CBB-CAB	5.37	1.56	1.30
18	D	501	HEC	CAB-C3B	5.14	1.51	1.35
11	N	3008	PEE	P-O1P	5.10	1.62	1.50
18	Q	501	HEC	CAB-C3B	5.08	1.51	1.35
15	C	2002	UQ	C6-C5	5.08	1.44	1.35
13	C	502	HEM	CBB-CAB	5.01	1.54	1.30
15	P	3002	UQ	C6-C5	4.83	1.43	1.35
13	C	502	HEM	C4D-C3D	4.83	1.53	1.45
15	P	3002	UQ	C7-C6	4.78	1.60	1.51
13	P	502	HEM	CBC-CAC	4.67	1.52	1.30
13	C	501	HEM	CBC-CAC	4.62	1.52	1.30
15	C	2002	UQ	C7-C6	4.51	1.59	1.51
13	C	502	HEM	CBC-CAC	4.51	1.52	1.30
11	C	2007	PEE	C39-C38	4.24	1.55	1.31
11	A	2005	PEE	C39-C38	4.21	1.55	1.31
13	P	501	HEM	CBC-CAC	4.20	1.50	1.30
13	P	501	HEM	CBB-CAB	4.20	1.50	1.30
11	P	3007	PEE	C39-C38	4.15	1.55	1.31
11	N	3005	PEE	C39-C38	4.12	1.55	1.31
13	C	501	HEM	CAB-C3B	-4.08	1.36	1.47
15	C	2002	UQ	C6-C1	3.82	1.57	1.46
13	C	501	HEM	CBB-CAB	3.76	1.48	1.30
16	P	3011	AZI	N1-N2	-3.71	1.15	1.23
11	N	3008	PEE	P-O4P	3.64	1.65	1.54
15	P	3002	UQ	C6-C1	3.62	1.56	1.46
13	C	502	HEM	CAB-C3B	-3.57	1.37	1.47
11	P	3007	PEE	C21-C22	-3.44	1.34	1.51
13	P	501	HEM	CAB-C3B	-3.39	1.38	1.47
14	P	3001	FMX	C3-N2	-3.37	1.35	1.43
11	N	3005	PEE	C21-C22	-3.36	1.35	1.51
14	C	2001	FMX	C3-N2	-3.34	1.35	1.43
11	C	2007	PEE	C21-C22	-3.31	1.35	1.51
11	N	3008	PEE	P-O3P	3.28	1.64	1.54
15	C	2002	UQ	O3-C3	3.28	1.44	1.36
11	C	2008	PEE	O3-C30	3.27	1.42	1.33
11	A	2005	PEE	C21-C22	-3.24	1.35	1.51
11	A	2005	PEE	O2-C10	3.24	1.43	1.34
13	P	502	HEM	C4D-C3D	3.23	1.50	1.45
18	D	501	HEC	C4D-C3D	3.22	1.51	1.44
11	A	2005	PEE	P-O1P	3.17	1.61	1.50
11	N	3005	PEE	O2-C10	3.15	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	3005	PEE	P-O1P	3.15	1.61	1.50
16	C	2011	AZI	N1-N2	-3.12	1.16	1.23
15	C	2002	UQ	CM5-C5	3.07	1.57	1.50
11	C	2007	PEE	P-O1P	3.04	1.61	1.50
11	P	3007	PEE	P-O1P	3.01	1.61	1.50
18	Q	501	HEC	C4B-NB	-2.99	1.34	1.39
11	C	2008	PEE	O2-C10	2.97	1.42	1.34
11	P	3007	PEE	O3-C30	2.95	1.42	1.33
15	C	2002	UQ	C2-C1	2.91	1.57	1.48
11	A	2005	PEE	O3-C30	2.88	1.41	1.33
15	P	3002	UQ	O3-C3	2.88	1.43	1.36
16	P	3011	AZI	N3-N2	-2.86	1.17	1.23
11	C	2008	PEE	P-O1P	2.83	1.60	1.50
15	C	2002	UQ	O2-C2	2.82	1.43	1.36
18	Q	501	HEC	C1C-NC	-2.76	1.34	1.39
14	C	2001	FMX	C6-N2	-2.74	1.34	1.38
13	C	501	HEM	CAC-C3C	-2.71	1.40	1.47
15	P	3002	UQ	CM5-C5	2.70	1.56	1.50
11	N	3005	PEE	O3-C30	2.68	1.41	1.33
11	P	3007	PEE	O2-C10	2.68	1.41	1.34
11	C	2007	PEE	O3-C30	2.63	1.41	1.33
13	C	502	HEM	CAC-C3C	-2.61	1.40	1.47
16	C	2011	AZI	N3-N2	-2.60	1.17	1.23
15	C	2002	UQ	C5-C4	2.57	1.56	1.47
15	P	3002	UQ	C2-C1	2.51	1.56	1.48
11	N	3008	PEE	P-O2P	2.50	1.61	1.54
17	C	3010	BOG	C2-C1	2.46	1.57	1.50
17	D	2091	BOG	O5-C1	2.45	1.48	1.41
18	Q	501	HEC	C3B-C2B	-2.45	1.32	1.41
15	P	3002	UQ	O2-C2	2.45	1.42	1.36
15	P	3002	UQ	C5-C4	2.43	1.55	1.47
19	T	3004	CDL	O1-C1	2.41	1.50	1.43
11	A	2005	PEE	C31-C30	2.41	1.57	1.50
13	C	501	HEM	C3C-C4C	-2.41	1.41	1.46
13	P	502	HEM	CAB-C3B	-2.40	1.41	1.47
17	Q	3091	BOG	C4-C5	2.40	1.58	1.53
15	P	3002	UQ	C7-C8	2.39	1.54	1.50
17	C	3010	BOG	O5-C1	2.39	1.45	1.40
17	Q	3091	BOG	O5-C1	2.38	1.48	1.41
13	C	502	HEM	C3B-C4B	2.38	1.49	1.44
15	C	2002	UQ	C3-C4	2.36	1.55	1.48
17	D	2091	BOG	C4-C5	2.34	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	2007	PEE	O2-C10	2.34	1.40	1.34
17	D	2009	BOG	O5-C1	2.33	1.47	1.41
18	D	501	HEC	C1C-C2C	2.32	1.48	1.43
18	Q	501	HEC	CHC-C1C	-2.27	1.34	1.39
19	G	2004	CDL	O1-C1	2.25	1.49	1.43
15	P	3002	UQ	C3-C4	2.24	1.55	1.48
11	N	3005	PEE	C11-C10	2.22	1.57	1.50
11	N	3005	PEE	C1-C2	2.22	1.57	1.50
11	A	2005	PEE	C11-C10	2.21	1.57	1.50
19	Q	3003	CDL	O1-C1	2.21	1.49	1.43
11	N	3005	PEE	C3-C2	2.18	1.57	1.50
18	Q	501	HEC	C3C-C2C	-2.18	1.33	1.41
19	T	3004	CDL	CA3-CA4	2.17	1.57	1.50
11	N	3005	PEE	C31-C30	2.16	1.57	1.50
11	A	2005	PEE	C3-C2	2.16	1.57	1.50
18	D	501	HEC	C3B-C2B	-2.16	1.33	1.41
17	P	2010	BOG	C4-C5	2.15	1.57	1.53
19	T	3004	CDL	OA8-CA6	-2.15	1.40	1.45
17	Q	3009	BOG	O5-C1	2.11	1.47	1.41
13	P	501	HEM	CMB-C2B	2.08	1.55	1.50
15	C	2002	UQ	C7-C8	2.08	1.53	1.50
17	P	2010	BOG	O5-C1	2.08	1.48	1.42
17	P	2010	BOG	C1-C2	2.07	1.57	1.52
14	P	3001	FMX	C26-C21	2.07	1.42	1.39
18	Q	501	HEC	CHC-C4B	-2.06	1.34	1.38
11	A	2005	PEE	C1-C2	2.06	1.57	1.50
19	G	2004	CDL	OA6-CA5	2.05	1.40	1.34
11	C	2007	PEE	C3-C2	2.04	1.57	1.50
18	Q	501	HEC	C2A-C3A	-2.04	1.32	1.36
11	C	2008	PEE	C3-C2	2.04	1.57	1.50
13	C	502	HEM	CHD-C4C	-2.04	1.34	1.38
11	C	2008	PEE	C1-C2	2.04	1.57	1.50
19	D	2003	CDL	O1-C1	2.04	1.49	1.43
13	C	501	HEM	C1C-NC	-2.02	1.35	1.39
19	Q	3003	CDL	OA2-CA2	-2.02	1.36	1.44
11	C	2007	PEE	C31-C30	2.00	1.56	1.50

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	501	HEC	CBB-CAB-C3B	-9.10	109.25	127.43
18	Q	501	HEC	CBB-CAB-C3B	-8.93	109.58	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	501	HEC	CBC-CAC-C3C	-6.54	114.36	127.43
18	Q	501	HEC	CBC-CAC-C3C	-6.44	114.56	127.43
13	C	502	HEM	CAD-C3D-C4D	5.43	134.16	124.70
13	C	501	HEM	CAD-C3D-C4D	5.13	133.63	124.70
18	D	501	HEC	CAA-C2A-C3A	-4.88	118.72	127.87
18	Q	501	HEC	CAA-C2A-C3A	-4.66	119.15	127.87
13	C	502	HEM	C3B-C4B-NB	4.31	112.56	109.47
18	Q	501	HEC	CAA-C2A-C1A	4.25	133.50	124.85
18	D	501	HEC	CAA-C2A-C1A	4.21	133.42	124.85
17	D	2091	BOG	C1'-O1-C1	4.12	120.72	113.68
14	P	3001	FMX	C21-N1-N2	4.11	123.80	116.20
13	P	502	HEM	CAD-C3D-C4D	4.07	131.80	124.70
14	C	2001	FMX	C21-N1-N2	4.07	123.73	116.20
13	C	501	HEM	CAD-C3D-C2D	-3.98	120.41	127.87
13	P	501	HEM	CAD-C3D-C4D	3.86	131.42	124.70
13	P	501	HEM	C3B-C2B-C1B	-3.51	103.78	106.41
13	P	502	HEM	C3B-C4B-NB	3.48	111.97	109.47
13	C	501	HEM	C3B-C2B-C1B	-3.37	103.88	106.41
18	D	501	HEC	CAD-C3D-C4D	3.32	131.43	124.94
15	P	3002	UQ	C8-C7-C6	3.26	120.10	112.08
13	C	502	HEM	C2D-C1D-ND	3.19	113.59	109.90
19	T	3004	CDL	CB4-OB6-CB5	-3.09	110.41	117.80
17	Q	3091	BOG	C1'-O1-C1	3.07	118.92	113.68
18	D	501	HEC	CMC-C2C-C1C	3.06	130.08	125.42
19	G	2004	CDL	CB4-OB6-CB5	-3.03	110.54	117.80
13	P	502	HEM	C4C-C3C-C2C	-3.02	104.20	106.81
13	P	502	HEM	CAD-C3D-C2D	-3.00	122.26	127.87
17	Q	3009	BOG	C1'-O1-C1	2.97	118.76	113.68
17	D	2009	BOG	C1'-O1-C1	2.96	118.73	113.68
15	C	2002	UQ	C8-C7-C6	2.95	119.34	112.08
13	C	501	HEM	CBD-CAD-C3D	2.90	120.55	112.53
14	P	3001	FMX	O4-C5-C7	2.88	110.33	106.54
13	P	501	HEM	CAD-C3D-C2D	-2.84	122.56	127.87
13	C	502	HEM	CAD-C3D-C2D	-2.80	122.62	127.87
11	N	3005	PEE	C22-C21-C20	2.79	127.28	113.86
11	C	2007	PEE	C22-C21-C20	2.77	127.19	113.86
11	A	2005	PEE	C22-C21-C20	2.77	127.15	113.86
18	Q	501	HEC	CMC-C2C-C1C	2.74	129.59	125.42
11	P	3007	PEE	C22-C21-C20	2.74	127.03	113.86
18	Q	501	HEC	CAD-C3D-C4D	2.70	130.22	124.94
13	C	502	HEM	C3D-C4D-ND	2.69	113.12	110.17
13	C	502	HEM	C4C-C3C-C2C	-2.69	104.48	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	HEM	C2D-C1D-ND	2.62	112.93	109.90
13	P	501	HEM	C2B-C1B-NB	2.61	112.84	109.84
14	C	2001	FMX	O4-C5-C7	2.59	109.95	106.54
19	D	2003	CDL	CB4-OB6-CB5	-2.59	111.60	117.80
17	C	3010	BOG	C1'-O1-C1	2.57	119.40	113.81
15	P	3002	UQ	C7-C6-C1	-2.53	115.57	118.52
13	C	502	HEM	C4D-C3D-C2D	-2.53	103.21	106.89
19	Q	3003	CDL	CB4-OB6-CB5	-2.52	111.75	117.80
13	P	502	HEM	C2D-C1D-ND	2.52	112.81	109.90
18	Q	501	HEC	CMB-C2B-C1B	2.51	129.24	125.42
11	A	2005	PEE	C21-C22-C23	2.47	126.87	114.37
14	C	2001	FMX	C15-O14-C11	-2.47	113.15	118.78
13	C	502	HEM	CHD-C1D-C2D	-2.44	121.17	125.03
11	N	3005	PEE	C21-C22-C23	2.42	126.59	114.37
18	Q	501	HEC	CBA-CAA-C2A	2.41	119.20	112.53
11	C	2007	PEE	C21-C22-C23	2.41	126.55	114.37
13	C	502	HEM	C4D-ND-C1D	-2.39	102.38	105.21
13	C	501	HEM	CHC-C1C-NC	-2.35	121.90	124.45
13	C	501	HEM	C4D-ND-C1D	-2.34	102.43	105.21
19	Q	3003	CDL	CA4-OA6-CA5	-2.33	112.23	117.80
11	P	3007	PEE	C21-C22-C23	2.32	126.09	114.37
19	D	2003	CDL	CA6-OA8-CA7	-2.28	111.46	117.08
17	D	2009	BOG	O1-C1-C2	2.25	111.69	108.27
15	C	2002	UQ	C7-C6-C1	-2.24	115.92	118.52
19	Q	3003	CDL	CA6-OA8-CA7	-2.23	111.59	117.08
13	C	501	HEM	C3B-C4B-NB	2.19	111.04	109.47
14	P	3001	FMX	C15-O14-C11	-2.18	113.79	118.78
18	Q	501	HEC	CHA-C1A-NA	-2.16	122.10	124.45
19	G	2004	CDL	CA4-OA6-CA5	-2.13	112.69	117.80
11	C	2007	PEE	O3-C3-C2	2.13	114.55	108.40
11	N	3005	PEE	O3-C3-C2	2.13	114.52	108.40
19	D	2003	CDL	CA4-OA6-CA5	-2.11	112.75	117.80
18	D	501	HEC	O2A-CGA-CBA	2.11	120.66	114.00
13	P	501	HEM	CMD-C2D-C1D	2.10	128.32	125.03
19	D	2003	CDL	CA6-CA4-CA3	-2.08	106.93	111.78
13	C	502	HEM	C2B-C1B-NB	2.06	112.21	109.84
19	G	2004	CDL	CB6-CB4-CB3	-2.05	107.00	111.78
11	A	2005	PEE	O3-C3-C2	2.05	114.31	108.40
19	T	3004	CDL	CA4-OA6-CA5	-2.04	112.92	117.80
18	D	501	HEC	O1A-CGA-CBA	-2.03	116.65	123.09
13	C	501	HEM	C2B-C1B-NB	2.03	112.17	109.84
19	T	3004	CDL	CB6-CB4-CB3	-2.02	107.06	111.78

There are no chirality outliers.

All (282) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2005	PEE	C11-C10-O2-C2
11	A	2005	PEE	C4-O4P-P-O3P
11	A	2005	PEE	C4-O4P-P-O2P
11	A	2005	PEE	C4-O4P-P-O1P
11	A	2005	PEE	O4P-C4-C5-N
11	C	2008	PEE	C1-O3P-P-O1P
11	C	2008	PEE	C1-O3P-P-O4P
11	N	3005	PEE	C11-C10-O2-C2
11	N	3005	PEE	C4-O4P-P-O3P
11	N	3005	PEE	C4-O4P-P-O2P
11	N	3005	PEE	C4-O4P-P-O1P
11	N	3005	PEE	O4P-C4-C5-N
11	P	3007	PEE	O4P-C4-C5-N
17	D	2091	BOG	O5-C1-O1-C1'
18	D	501	HEC	C3A-C2A-CAA-CBA
18	D	501	HEC	C2B-C3B-CAB-CBB
18	D	501	HEC	C4B-C3B-CAB-CBB
18	D	501	HEC	C2C-C3C-CAC-CBC
18	D	501	HEC	C4C-C3C-CAC-CBC
18	Q	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C2B-C3B-CAB-CBB
18	Q	501	HEC	C4B-C3B-CAB-CBB
18	Q	501	HEC	C2C-C3C-CAC-CBC
18	Q	501	HEC	C4C-C3C-CAC-CBC
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	CB3-OB5-PB2-OB2
19	G	2004	CDL	CB3-OB5-PB2-OB3
19	Q	3003	CDL	CB2-C1-CA2-OA2
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	Q	3003	CDL	CB2-OB2-PB2-OB5
19	T	3004	CDL	O1-C1-CA2-OA2
19	T	3004	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
11	N	3005	PEE	O5-C30-O3-C3
11	A	2005	PEE	O5-C30-O3-C3
19	G	2004	CDL	OB9-CB7-OB8-CB6
19	T	3004	CDL	OB9-CB7-OB8-CB6
11	A	2005	PEE	O4-C10-O2-C2
11	N	3005	PEE	O4-C10-O2-C2
11	A	2005	PEE	C31-C30-O3-C3
11	N	3005	PEE	C31-C30-O3-C3
19	D	2003	CDL	C31-CA7-OA8-CA6
19	Q	3003	CDL	C31-CA7-OA8-CA6
19	G	2004	CDL	C71-CB7-OB8-CB6
19	T	3004	CDL	C71-CB7-OB8-CB6
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
18	Q	501	HEC	C1A-C2A-CAA-CBA
17	D	2009	BOG	C4-C5-C6-O6
19	D	2003	CDL	O1-C1-CA2-OA2
19	G	2004	CDL	O1-C1-CA2-OA2
19	Q	3003	CDL	O1-C1-CA2-OA2
19	G	2004	CDL	C51-CB5-OB6-CB4
19	T	3004	CDL	C51-CB5-OB6-CB4
17	Q	3091	BOG	O5-C1-O1-C1'
17	D	2009	BOG	O5-C5-C6-O6
19	T	3004	CDL	OB7-CB5-OB6-CB4
19	G	2004	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
19	D	2003	CDL	OA9-CA7-OA8-CA6
17	Q	3091	BOG	C2-C1-O1-C1'
19	D	2003	CDL	OB9-CB7-OB8-CB6
19	Q	3003	CDL	OB9-CB7-OB8-CB6
19	G	2004	CDL	OB7-CB5-OB6-CB4
19	Q	3003	CDL	OA9-CA7-OA8-CA6
19	D	2003	CDL	CB7-C71-C72-C73
19	Q	3003	CDL	CB7-C71-C72-C73
17	Q	3009	BOG	O5-C1-O1-C1'
17	D	2091	BOG	O5-C5-C6-O6
17	D	2091	BOG	C4-C5-C6-O6
11	A	2005	PEE	C37-C38-C39-C40
11	C	2007	PEE	C37-C38-C39-C40
11	N	3005	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C37-C38-C39-C40
17	Q	3009	BOG	O1-C1'-C2'-C3'
18	D	501	HEC	C1A-C2A-CAA-CBA
11	C	2008	PEE	C31-C30-O3-C3
17	Q	3009	BOG	C2-C1-O1-C1'
19	T	3004	CDL	OA7-CA5-OA6-CA4
19	G	2004	CDL	C11-CA5-OA6-CA4
19	T	3004	CDL	C11-CA5-OA6-CA4
11	N	3005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C10-C11-C12-C13
11	A	2005	PEE	C14-C15-C16-C17
17	C	3010	BOG	C2'-C1'-O1-C1
17	P	2010	BOG	C3'-C4'-C5'-C6'
11	C	2008	PEE	C11-C10-O2-C2
11	C	2008	PEE	O5-C30-O3-C3
19	G	2004	CDL	CB5-C51-C52-C53
19	T	3004	CDL	CB5-C51-C52-C53
11	A	2005	PEE	C30-C31-C32-C33
17	C	3010	BOG	C3'-C4'-C5'-C6'
11	C	2007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C34-C35-C36-C37
11	N	3005	PEE	C14-C15-C16-C17
11	N	3005	PEE	C40-C41-C42-C43
11	P	3007	PEE	C34-C35-C36-C37
11	A	2005	PEE	C40-C41-C42-C43
18	D	501	HEC	C4D-C3D-CAD-CBD
11	P	3007	PEE	C12-C13-C14-C15
11	A	2005	PEE	C11-C12-C13-C14
11	C	2007	PEE	C21-C22-C23-C24
11	N	3005	PEE	C11-C12-C13-C14
11	P	3007	PEE	C40-C41-C42-C43
19	G	2004	CDL	OA7-CA5-OA6-CA4
11	P	3007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C40-C41-C42-C43
11	C	2008	PEE	O4-C10-O2-C2
11	A	2005	PEE	C10-C11-C12-C13
11	N	3005	PEE	C10-C11-C12-C13
15	P	3002	UQ	C5-C6-C7-C8
11	N	3005	PEE	C33-C34-C35-C36
15	C	2002	UQ	C1-C6-C7-C8
15	P	3002	UQ	C1-C6-C7-C8
11	A	2005	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
17	C	3010	BOG	C4'-C5'-C6'-C7'
11	P	3007	PEE	C39-C40-C41-C42
11	C	2007	PEE	C12-C13-C14-C15
11	P	3007	PEE	C11-C12-C13-C14
11	P	3007	PEE	C14-C15-C16-C17
17	Q	3009	BOG	C2'-C3'-C4'-C5'
13	P	502	HEM	C4D-C3D-CAD-CBD
11	C	2007	PEE	C14-C15-C16-C17
11	A	2005	PEE	C19-C20-C21-C22
11	C	2007	PEE	C39-C40-C41-C42
11	N	3005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C35-C36-C37-C38
11	A	2005	PEE	O3P-C1-C2-C3
11	C	2008	PEE	O3P-C1-C2-C3
11	N	3005	PEE	O3P-C1-C2-C3
11	C	2007	PEE	C11-C12-C13-C14
13	C	502	HEM	C4D-C3D-CAD-CBD
19	T	3004	CDL	C31-CA7-OA8-CA6
19	T	3004	CDL	CA3-CA4-CA6-OA8
17	D	2009	BOG	C3'-C4'-C5'-C6'
11	A	2005	PEE	C35-C36-C37-C38
11	C	2007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C35-C36-C37-C38
11	A	2005	PEE	C20-C21-C22-C23
11	N	3005	PEE	C20-C21-C22-C23
17	D	2009	BOG	C2'-C3'-C4'-C5'
11	P	3007	PEE	C15-C16-C17-C18
11	P	3007	PEE	C32-C33-C34-C35
13	P	502	HEM	C2D-C3D-CAD-CBD
19	Q	3003	CDL	C71-C72-C73-C74
11	N	3005	PEE	C35-C36-C37-C38
19	D	2003	CDL	C71-C72-C73-C74
19	G	2004	CDL	C31-CA7-OA8-CA6
11	C	2007	PEE	C32-C33-C34-C35
19	G	2004	CDL	CA3-CA4-CA6-OA8
11	A	2005	PEE	C12-C13-C14-C15
19	D	2003	CDL	OA6-CA4-CA6-OA8
19	Q	3003	CDL	OA6-CA4-CA6-OA8
19	T	3004	CDL	OA6-CA4-CA6-OA8
17	Q	3091	BOG	C3'-C4'-C5'-C6'
17	D	2091	BOG	C1'-C2'-C3'-C4'
11	N	3005	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
13	C	502	HEM	C2D-C3D-CAD-CBD
15	C	2002	UQ	C5-C6-C7-C8
19	D	2003	CDL	CB5-C51-C52-C53
11	C	2008	PEE	O3P-C1-C2-O2
19	D	2003	CDL	OB5-CB3-CB4-OB6
11	P	3007	PEE	C43-C44-C45-C46
11	A	2005	PEE	C17-C18-C19-C20
11	N	3005	PEE	C17-C18-C19-C20
11	N	3005	PEE	C42-C43-C44-C45
19	G	2004	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C43-C44-C45-C46
11	A	2005	PEE	C42-C43-C44-C45
17	D	2091	BOG	C2'-C1'-O1-C1
17	Q	3009	BOG	C1'-C2'-C3'-C4'
11	N	3005	PEE	C24-C25-C26-C27
11	A	2005	PEE	C21-C22-C23-C24
11	A	2005	PEE	C24-C25-C26-C27
11	C	2007	PEE	C33-C34-C35-C36
19	T	3004	CDL	OA9-CA7-OA8-CA6
11	A	2005	PEE	O3P-C1-C2-O2
11	N	3005	PEE	O3P-C1-C2-O2
19	Q	3003	CDL	OB5-CB3-CB4-OB6
19	Q	3003	CDL	CB5-C51-C52-C53
11	P	3007	PEE	C33-C34-C35-C36
11	C	2007	PEE	O4P-C4-C5-N
19	G	2004	CDL	CA3-OA5-PA1-OA2
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	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
17	C	3010	BOG	C1'-C2'-C3'-C4'
11	N	3005	PEE	C22-C23-C24-C25
11	A	2005	PEE	C43-C44-C45-C46
19	T	3004	CDL	OB6-CB4-CB6-OB8
11	N	3005	PEE	C21-C22-C23-C24
19	D	2003	CDL	CA3-CA4-CA6-OA8
19	Q	3003	CDL	CA3-CA4-CA6-OA8
11	P	3007	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
13	C	501	HEM	C2B-C3B-CAB-CBB
19	T	3004	CDL	OB5-CB3-CB4-OB6
19	G	2004	CDL	OA9-CA7-OA8-CA6
19	G	2004	CDL	OB6-CB4-CB6-OB8
11	A	2005	PEE	C22-C23-C24-C25
19	Q	3003	CDL	OB7-CB5-OB6-CB4
13	C	502	HEM	CAA-CBA-CGA-O1A
11	N	3005	PEE	C43-C44-C45-C46
19	D	2003	CDL	OB7-CB5-OB6-CB4
13	P	502	HEM	CAD-CBD-CGD-O1D
13	C	502	HEM	CAA-CBA-CGA-O2A
17	Q	3091	BOG	C2'-C3'-C4'-C5'
13	C	502	HEM	CAD-CBD-CGD-O2D
19	G	2004	CDL	OB5-CB3-CB4-OB6
11	C	2008	PEE	O3-C30-C31-C32
11	C	2007	PEE	C20-C21-C22-C23
19	G	2004	CDL	C1-CB2-OB2-PB2
13	P	502	HEM	CAA-CBA-CGA-O2A
13	C	502	HEM	CAD-CBD-CGD-O1D
13	P	502	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAA-CBA-CGA-O1A
17	Q	3091	BOG	O1-C1'-C2'-C3'
19	T	3004	CDL	C1-CB2-OB2-PB2
11	C	2008	PEE	O5-C30-C31-C32
19	Q	3003	CDL	C51-CB5-OB6-CB4
19	D	2003	CDL	C52-C51-CB5-OB6
13	C	501	HEM	CAA-CBA-CGA-O1A
13	P	501	HEM	CAA-CBA-CGA-O2A
19	D	2003	CDL	OB5-CB3-CB4-CB6
19	D	2003	CDL	C51-CB5-OB6-CB4
19	Q	3003	CDL	C52-C51-CB5-OB6
11	A	2005	PEE	C36-C37-C38-C39
13	P	501	HEM	CAA-CBA-CGA-O1A
18	D	501	HEC	CAD-CBD-CGD-O2D
11	N	3005	PEE	C15-C16-C17-C18
13	C	501	HEM	CAA-CBA-CGA-O2A
18	Q	501	HEC	CAD-CBD-CGD-O2D
13	P	501	HEM	C2B-C3B-CAB-CBB
11	N	3005	PEE	C1-C2-O2-C10
18	Q	501	HEC	CAD-CBD-CGD-O1D
18	D	501	HEC	CAD-CBD-CGD-O1D
13	C	501	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	P	501	HEM	C4B-C3B-CAB-CBB
11	N	3005	PEE	C36-C37-C38-C39
17	Q	3009	BOG	C4'-C5'-C6'-C7'
11	P	3007	PEE	O3-C30-C31-C32
19	Q	3003	CDL	OB5-CB3-CB4-CB6
11	A	2005	PEE	C38-C39-C40-C41
11	C	2007	PEE	C38-C39-C40-C41
11	P	3007	PEE	C38-C39-C40-C41
11	P	3007	PEE	O2-C10-C11-C12
11	N	3005	PEE	C38-C39-C40-C41
11	C	2007	PEE	O3-C30-C31-C32
11	C	2007	PEE	O2-C10-C11-C12
18	Q	501	HEC	CAA-CBA-CGA-O2A
19	T	3004	CDL	CB3-CB4-CB6-OB8
14	C	2001	FMX	C6-C5-C8-C9
14	C	2001	FMX	C6-C5-C8-C13
11	A	2005	PEE	C1-C2-O2-C10
19	T	3004	CDL	C12-C11-CA5-OA6
11	P	3007	PEE	O5-C30-C31-C32
11	P	3007	PEE	O4-C10-C11-C12
11	C	2007	PEE	O5-C30-C31-C32
14	C	2001	FMX	O4-C5-C8-C9
14	C	2001	FMX	O4-C5-C8-C13
14	P	3001	FMX	O4-C5-C8-C9
14	P	3001	FMX	O4-C5-C8-C13
18	Q	501	HEC	CAA-CBA-CGA-O1A
11	C	2007	PEE	O4-C10-C11-C12
19	G	2004	CDL	CB3-CB4-CB6-OB8
19	D	2003	CDL	C72-C71-CB7-OB8
17	D	2091	BOG	C2'-C3'-C4'-C5'
19	T	3004	CDL	OB5-CB3-CB4-CB6
17	D	2091	BOG	C3'-C4'-C5'-C6'

There are no ring outliers.

19 monomers are involved in 43 short contacts:

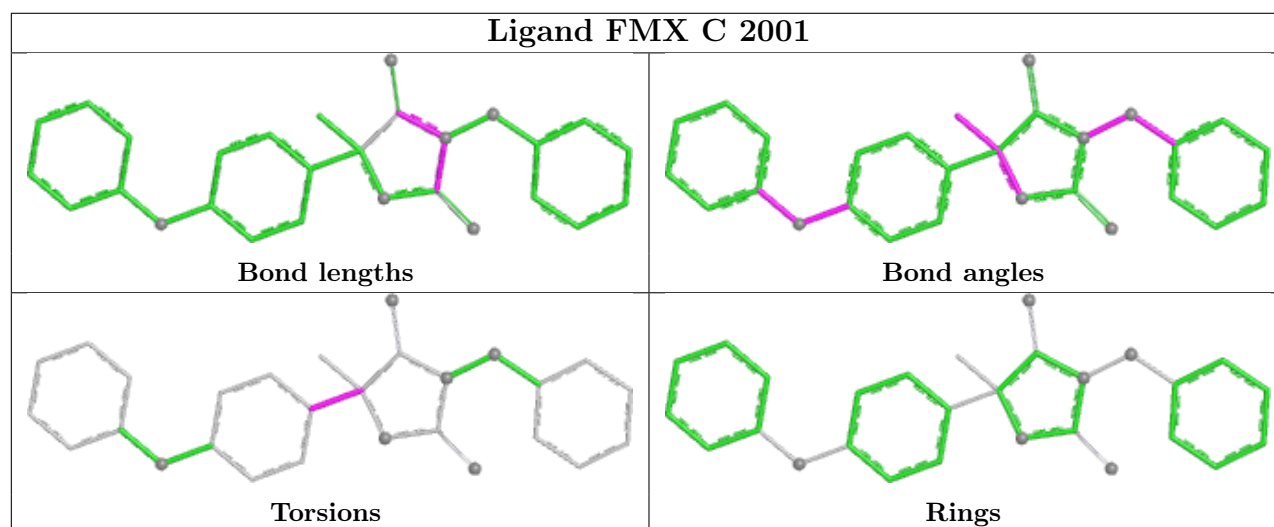
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2001	FMX	2	0
15	C	2002	UQ	5	0
17	Q	3091	BOG	1	0
19	G	2004	CDL	2	0
14	P	3001	FMX	2	0

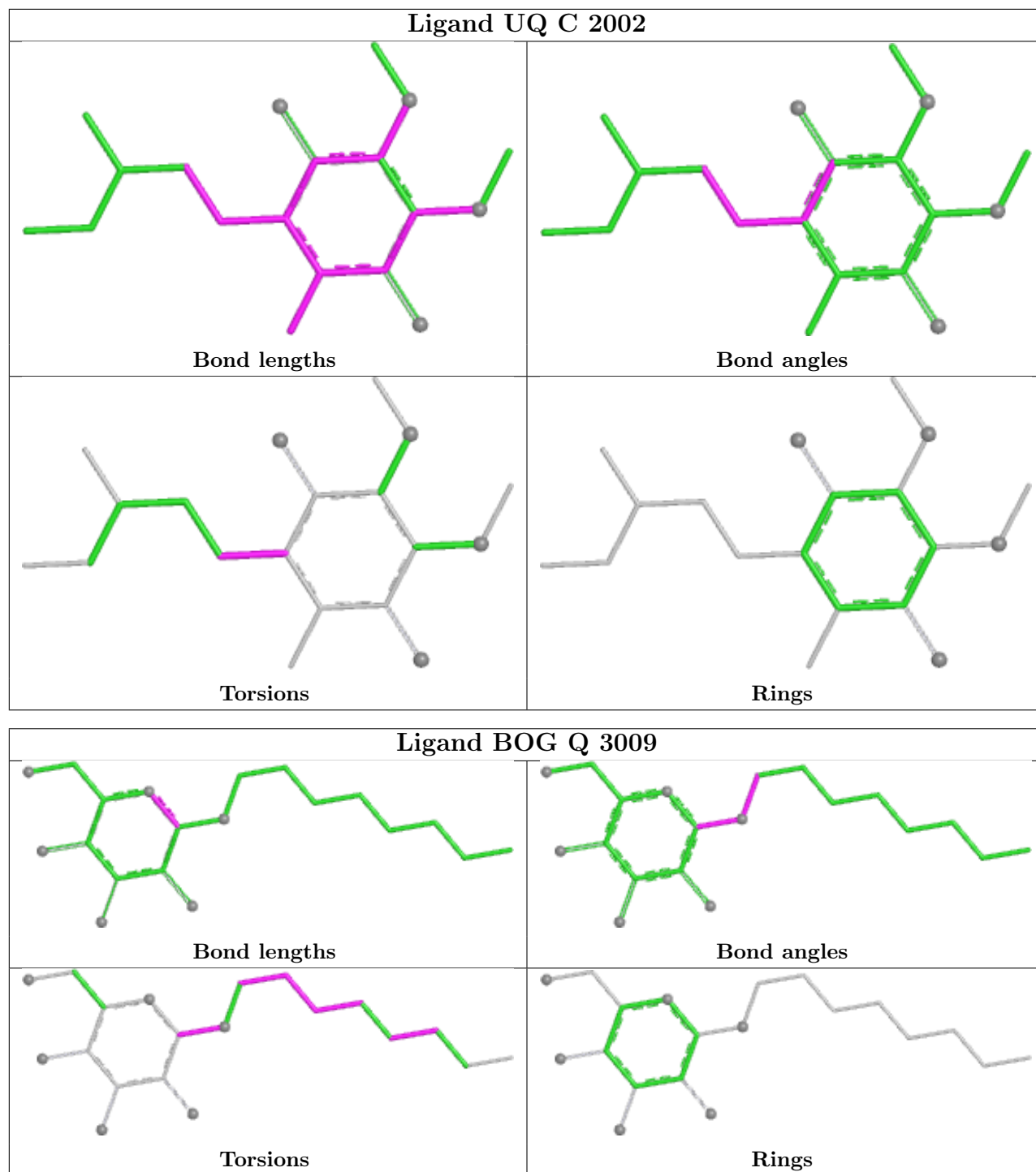
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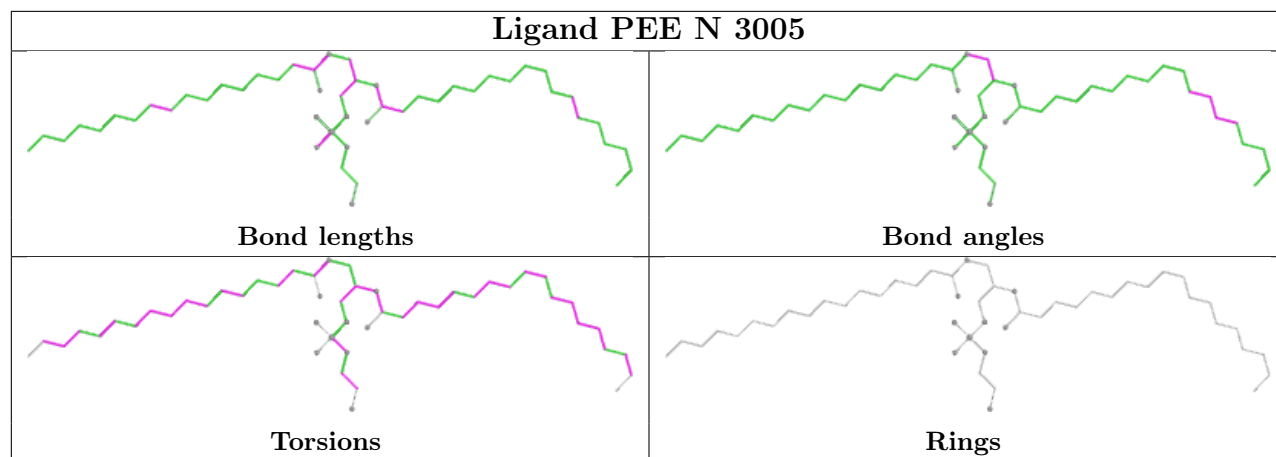
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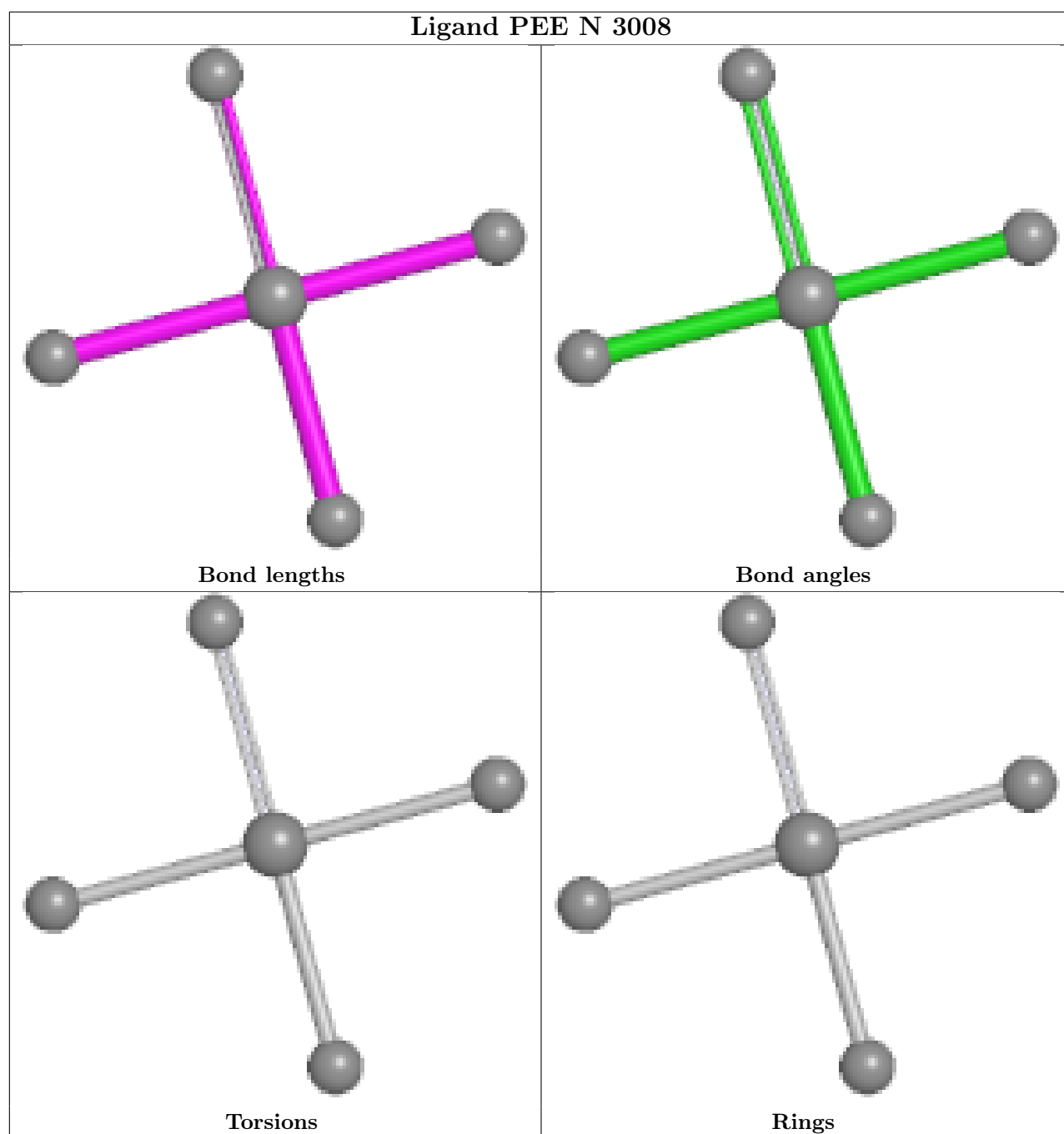
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	502	HEM	4	0
19	Q	3003	CDL	3	0
17	D	2009	BOG	1	0
20	E	501	FES	1	0
19	D	2003	CDL	2	0
18	D	501	HEC	2	0
20	R	501	FES	1	0
13	P	501	HEM	3	0
17	P	2010	BOG	1	0
15	P	3002	UQ	2	0
13	C	501	HEM	4	0
17	D	2091	BOG	2	0
13	P	502	HEM	4	0
19	T	3004	CDL	1	0

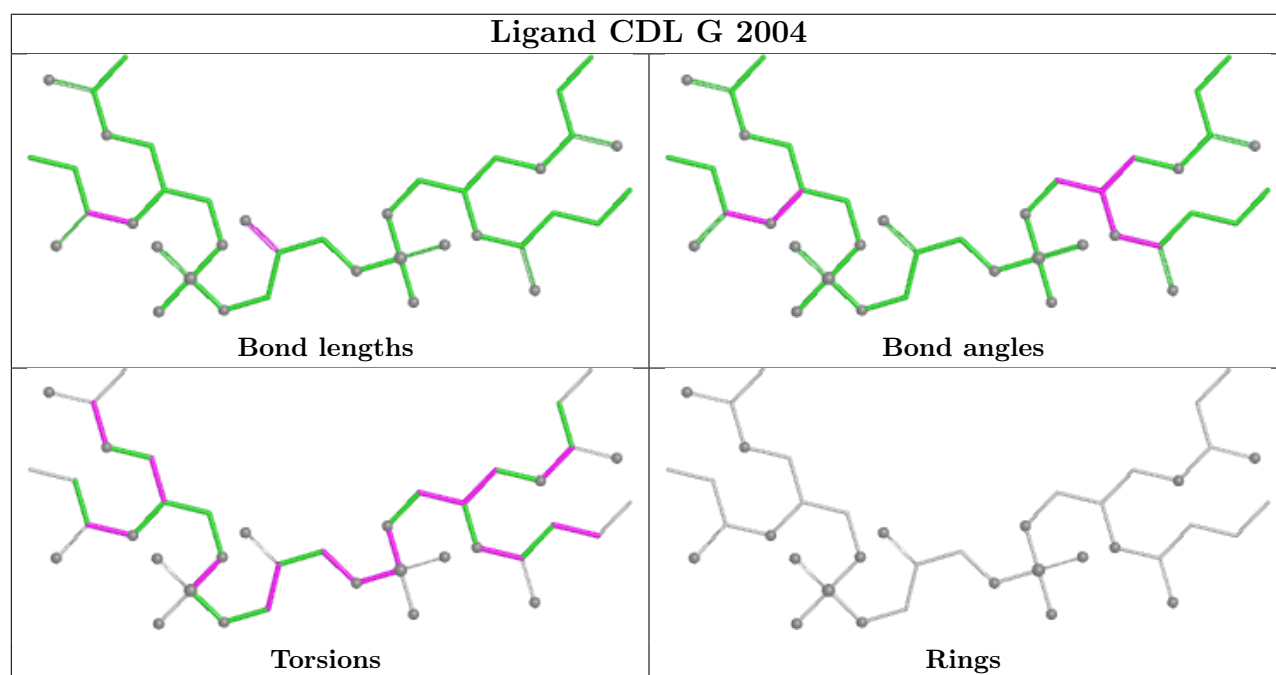
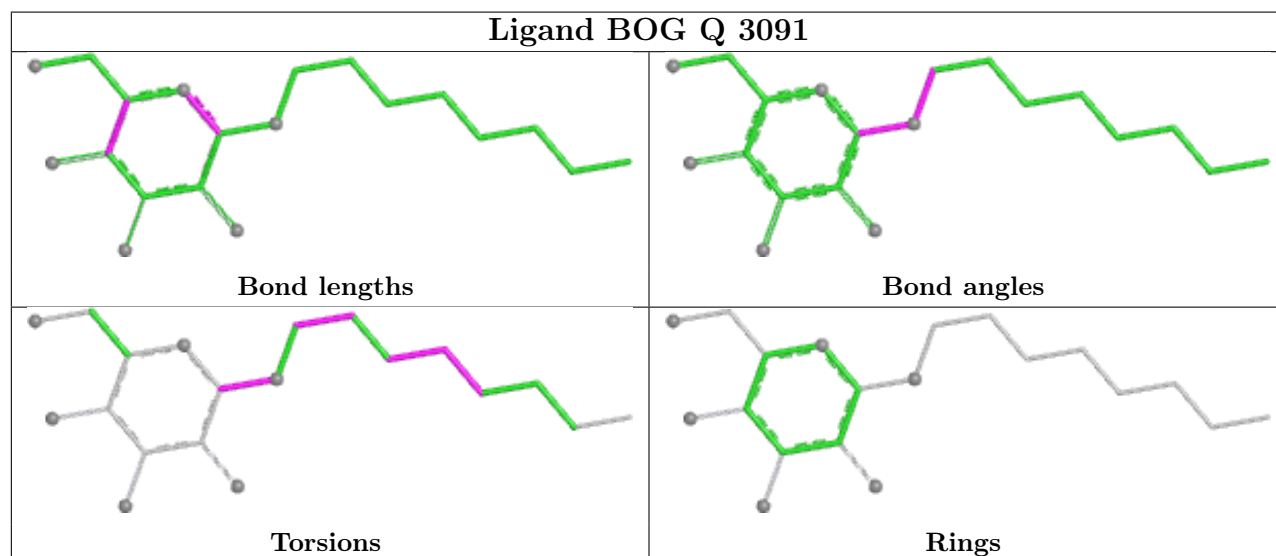
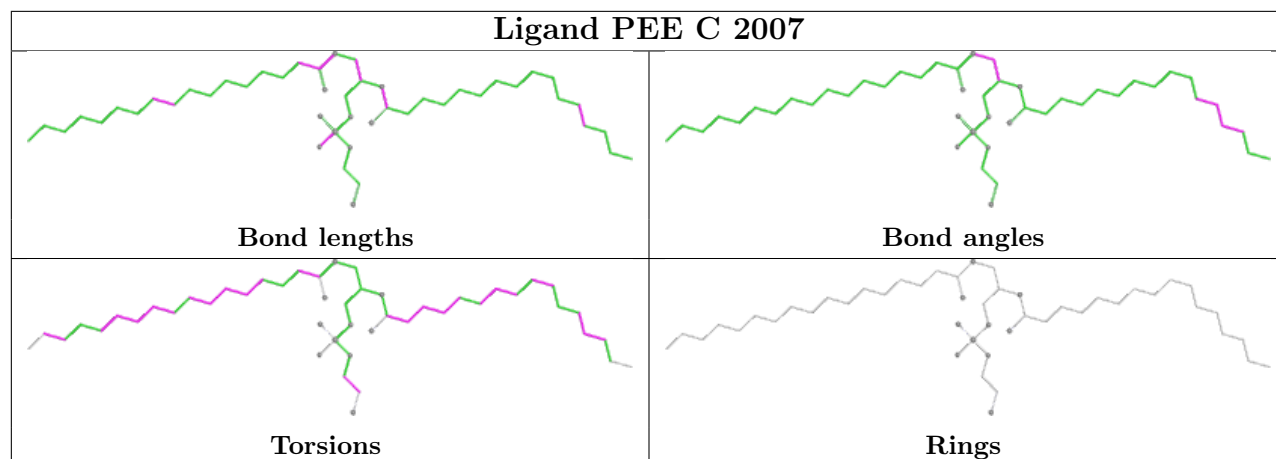
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



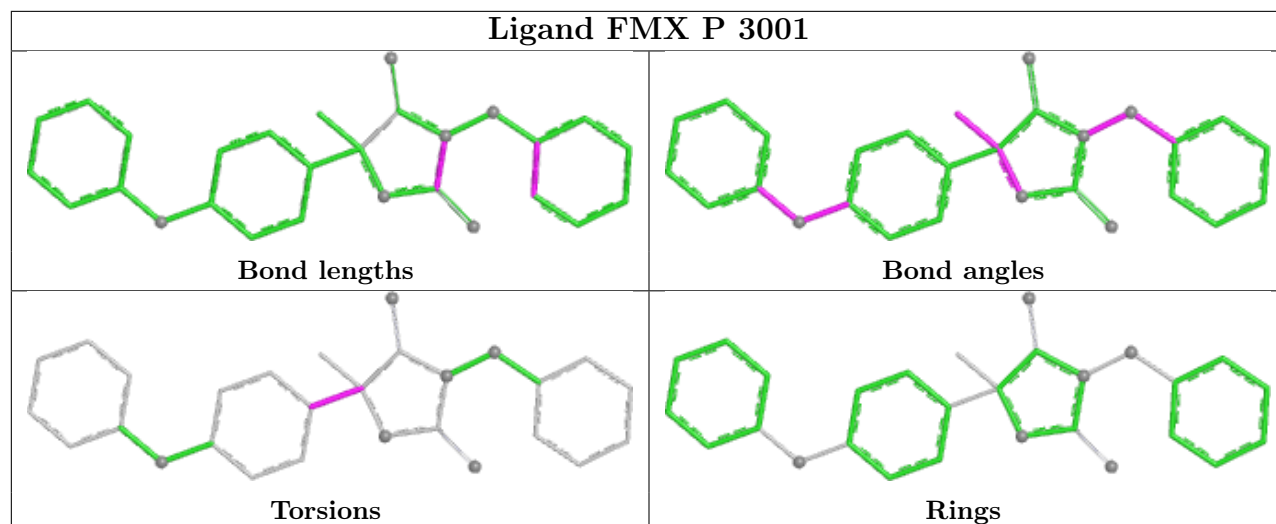




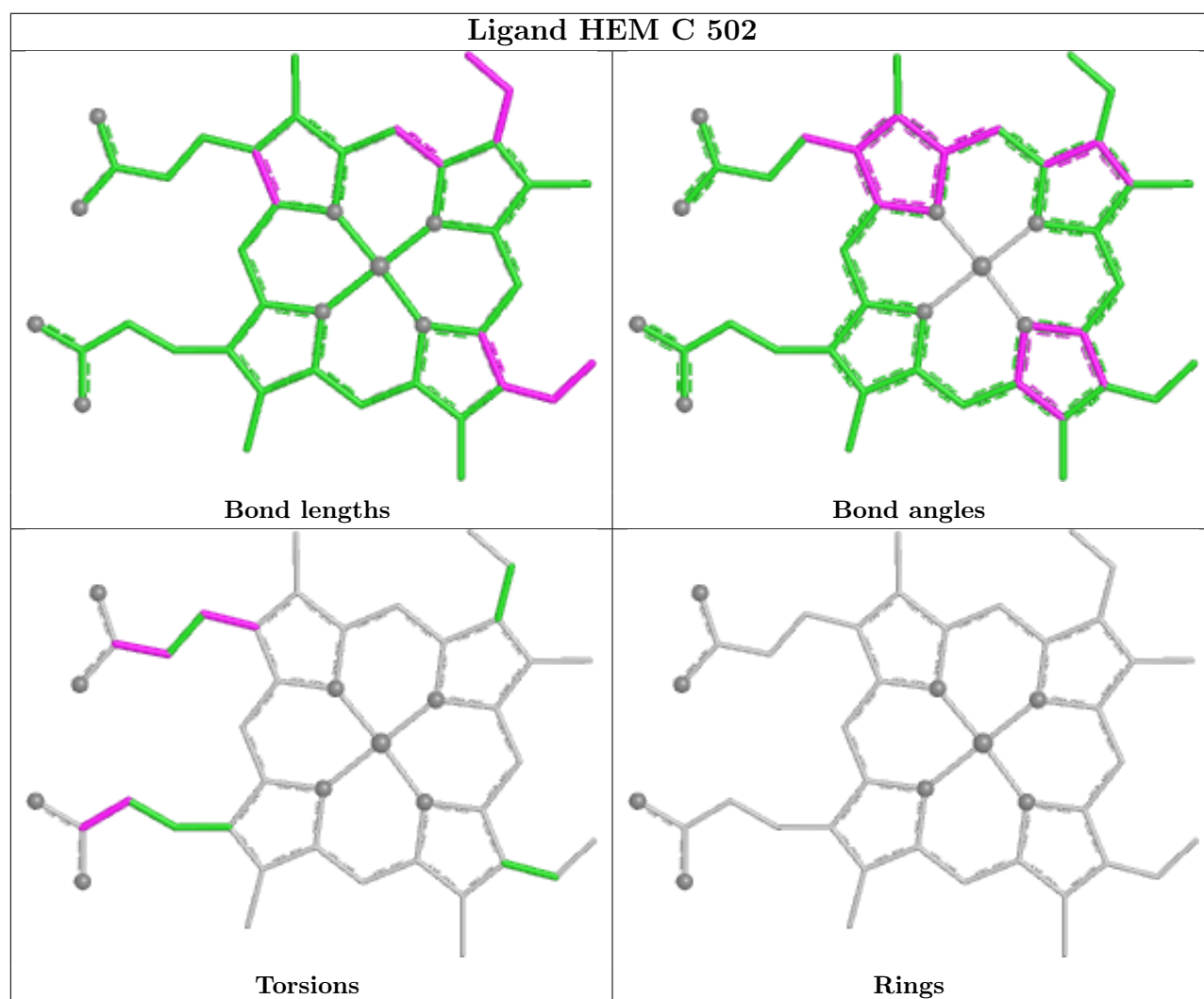


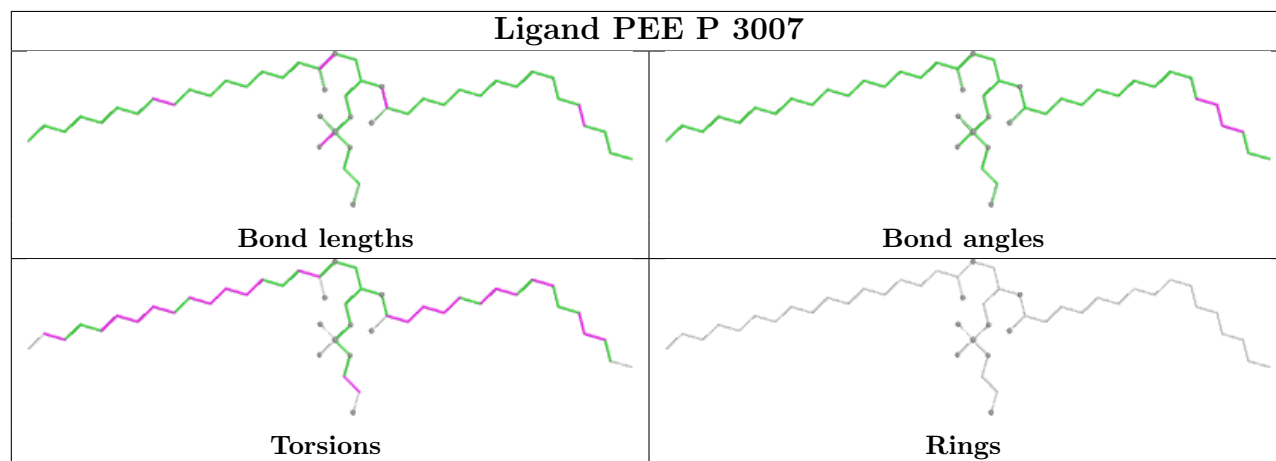
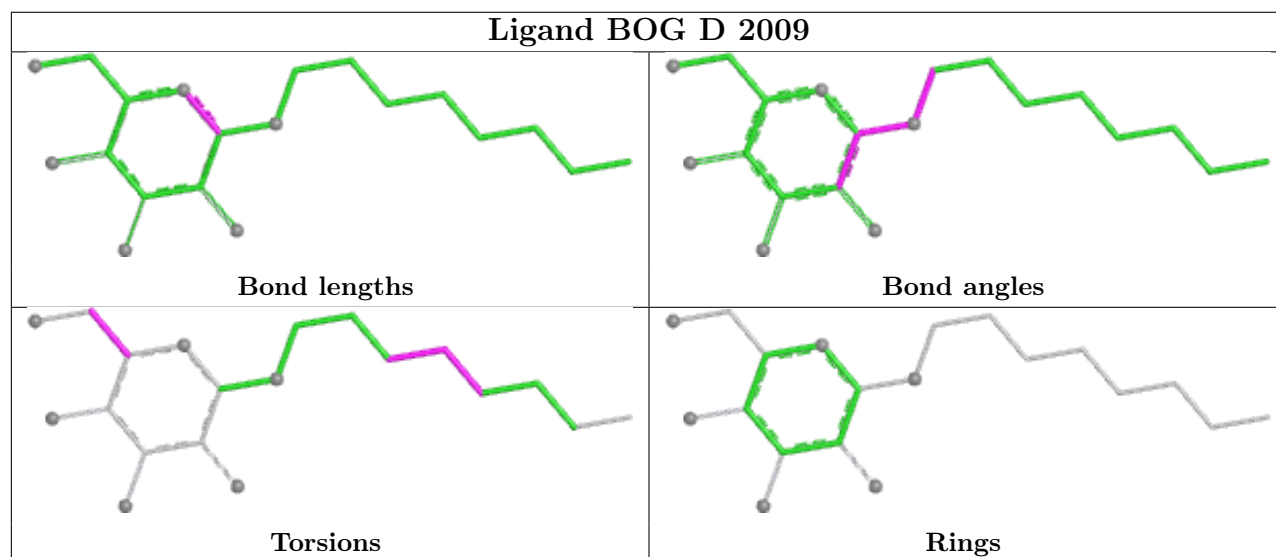
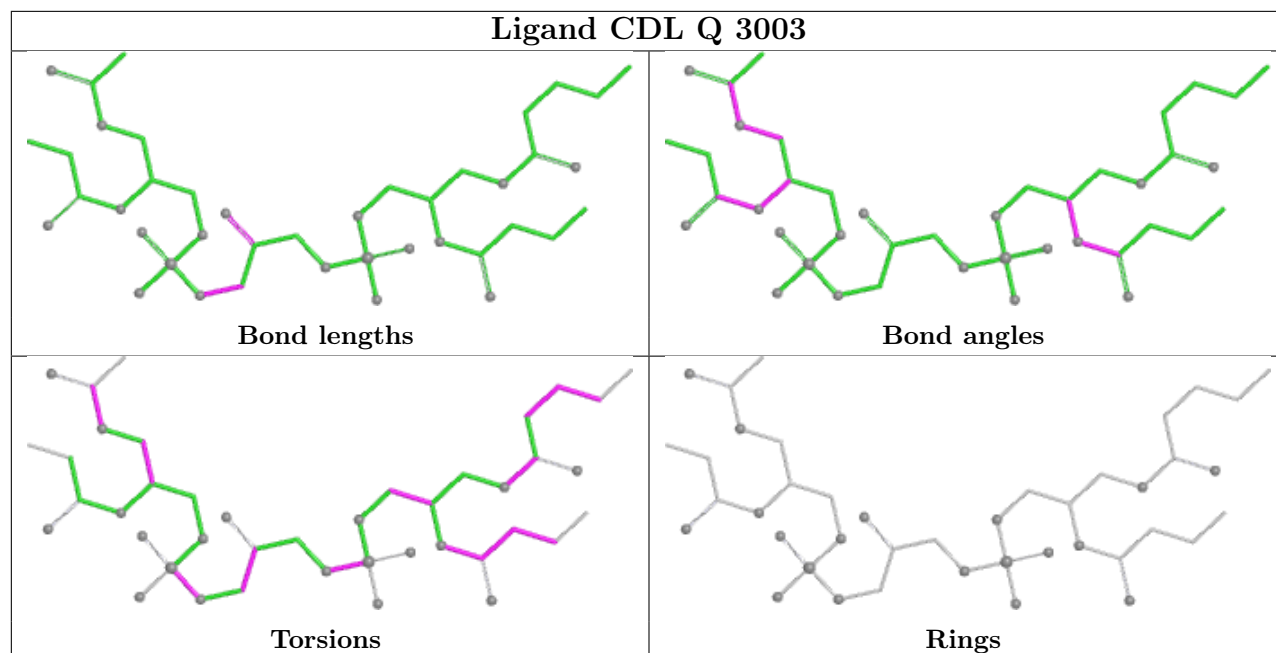


Ligand FMX P 3001

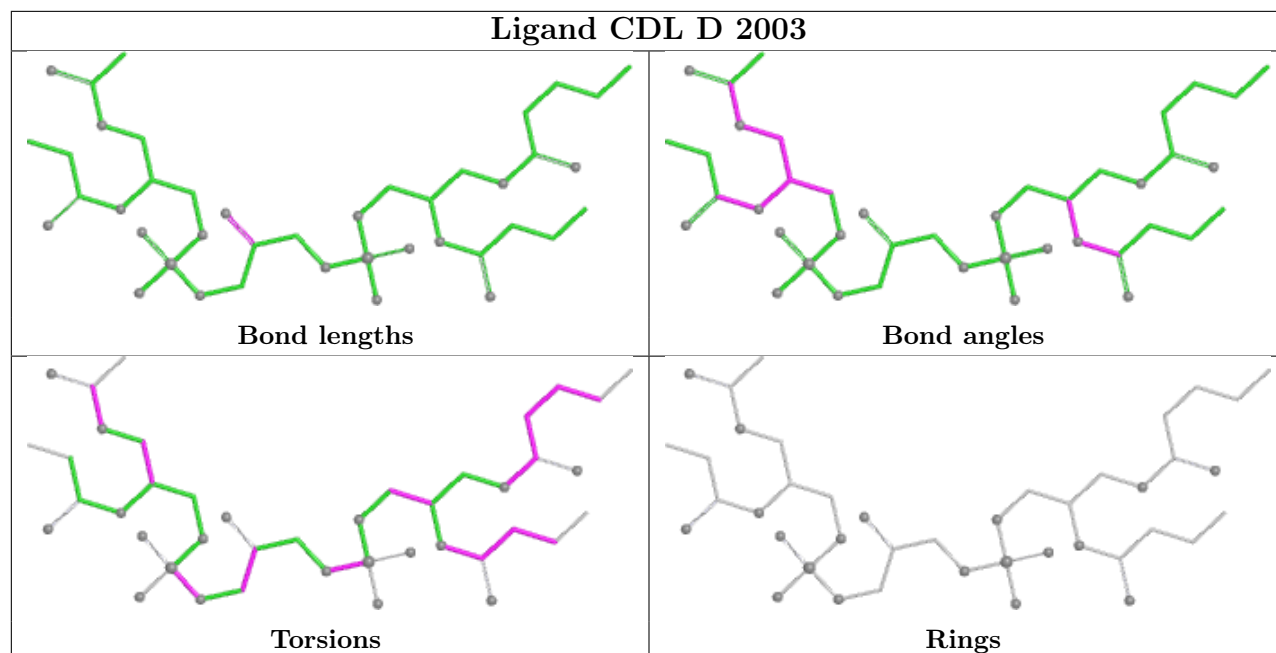


Ligand HEM C 502

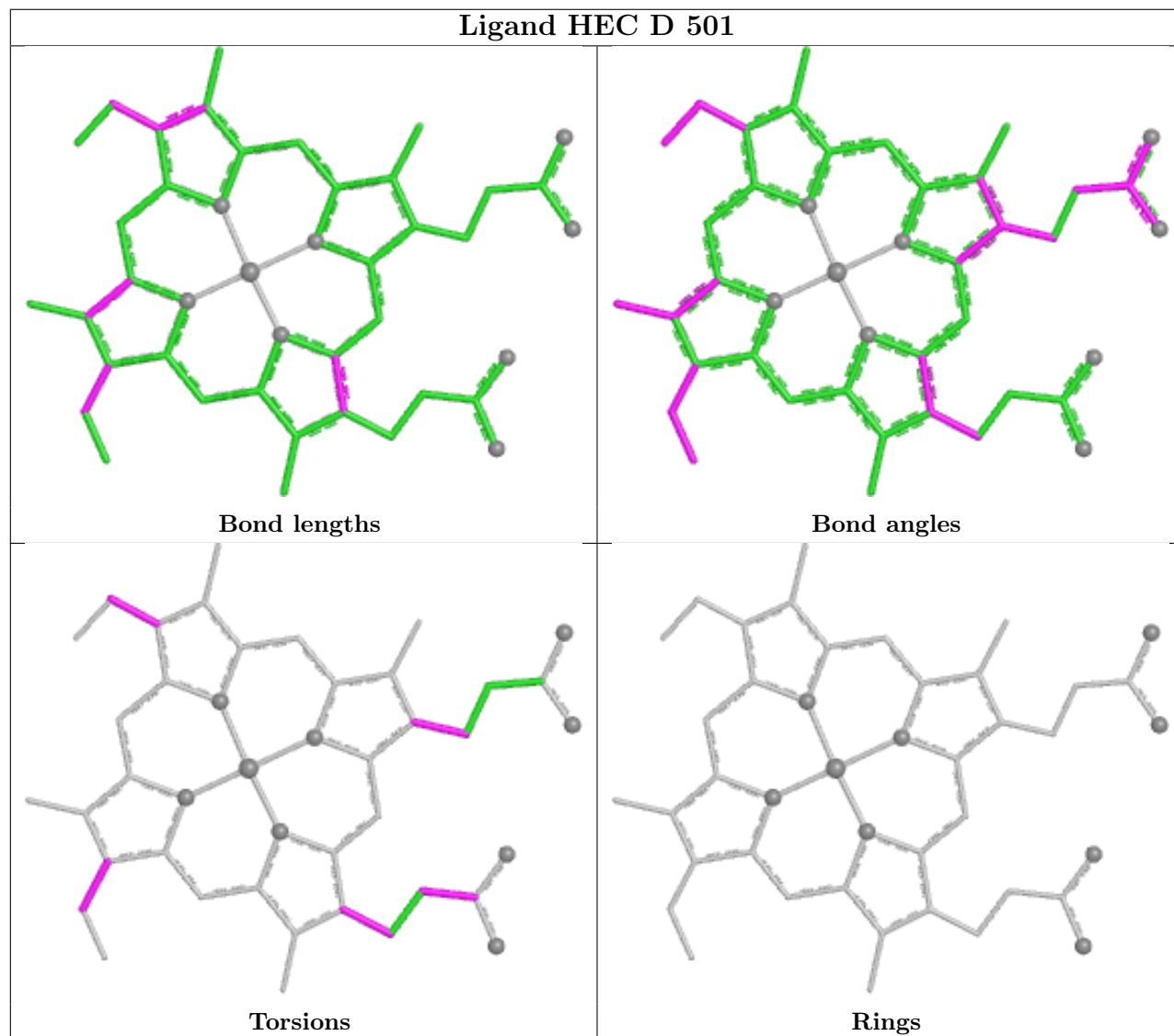


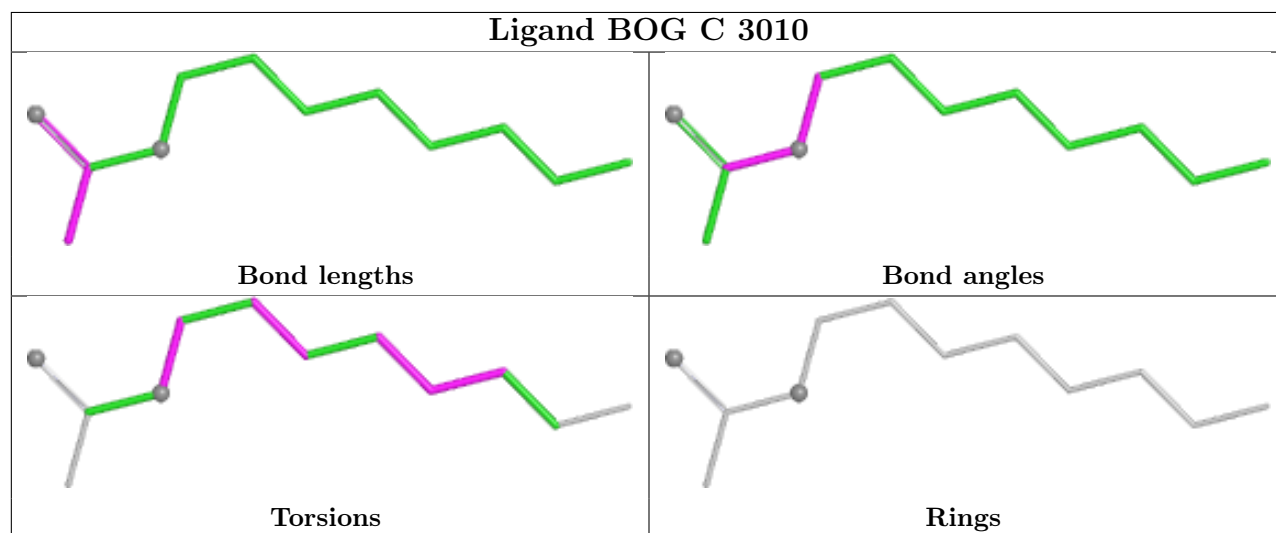
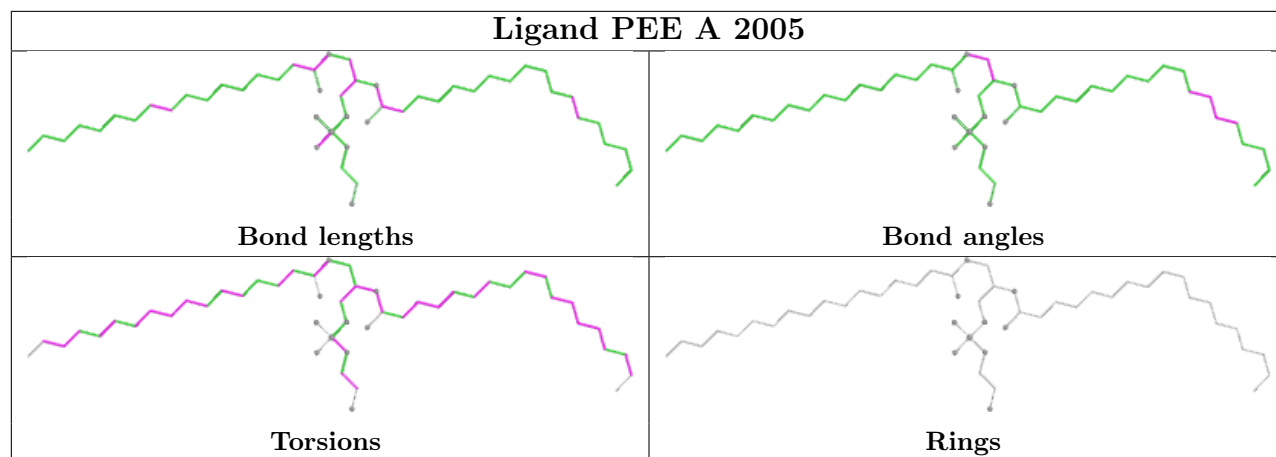


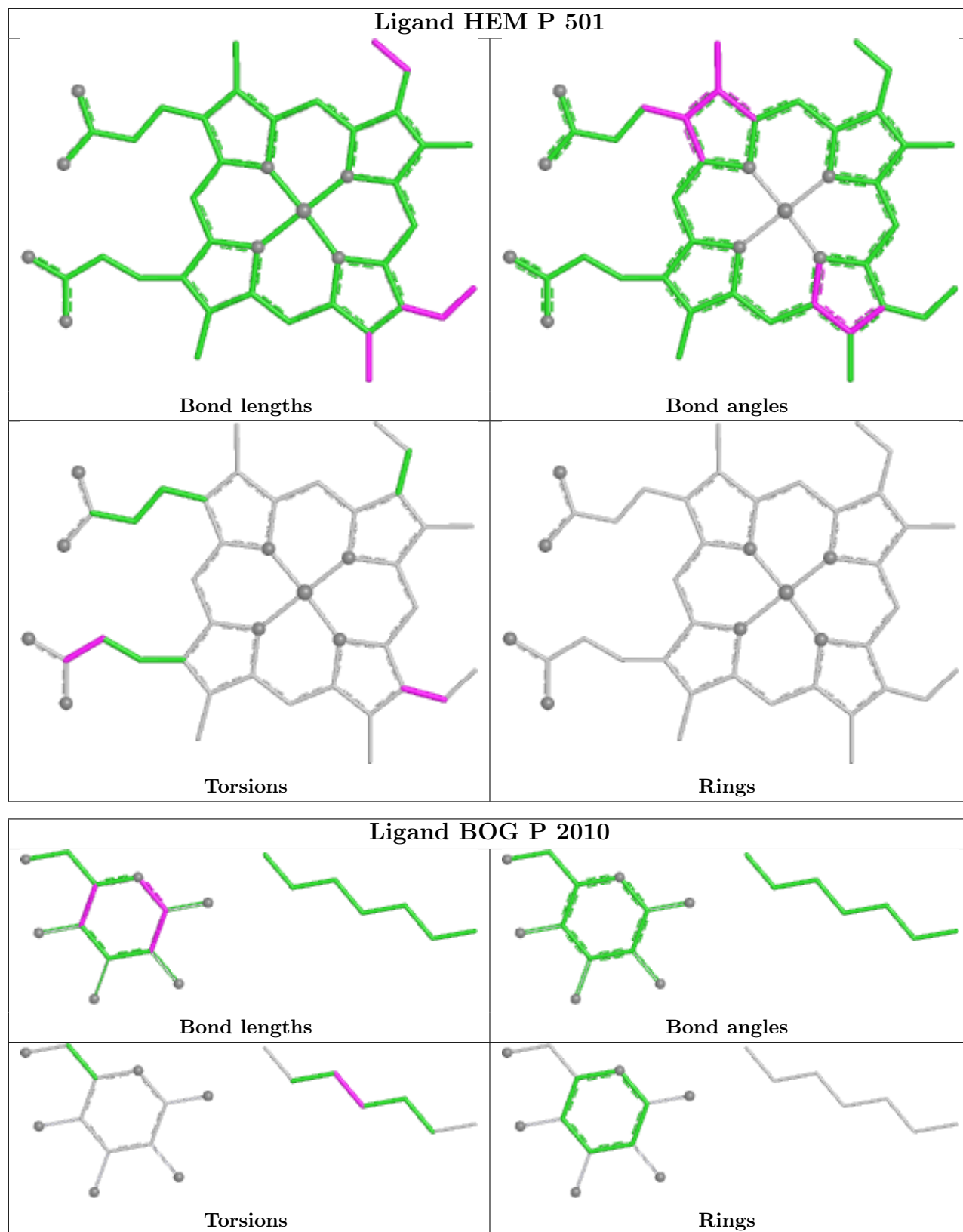
Ligand CDL D 2003

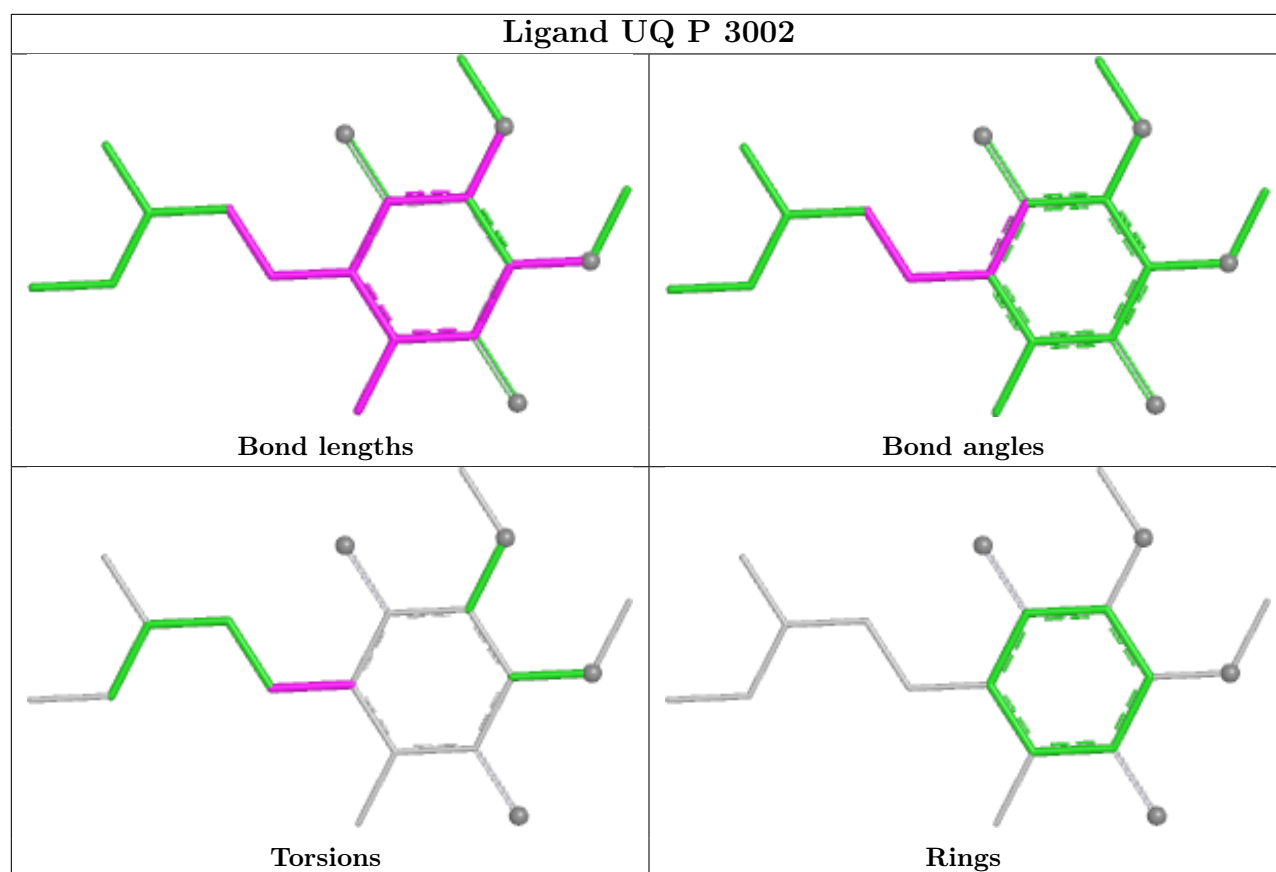


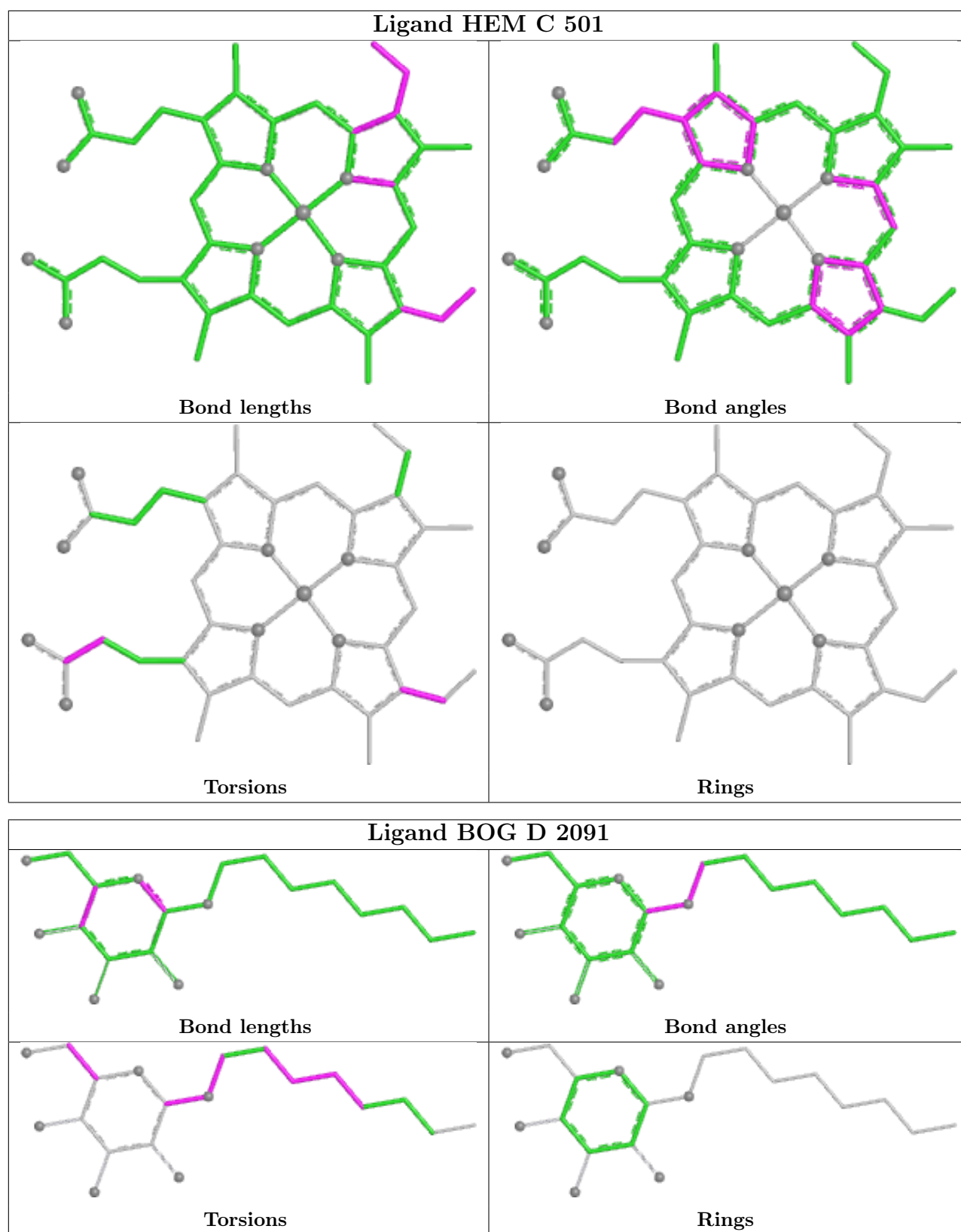
Ligand HEC D 501

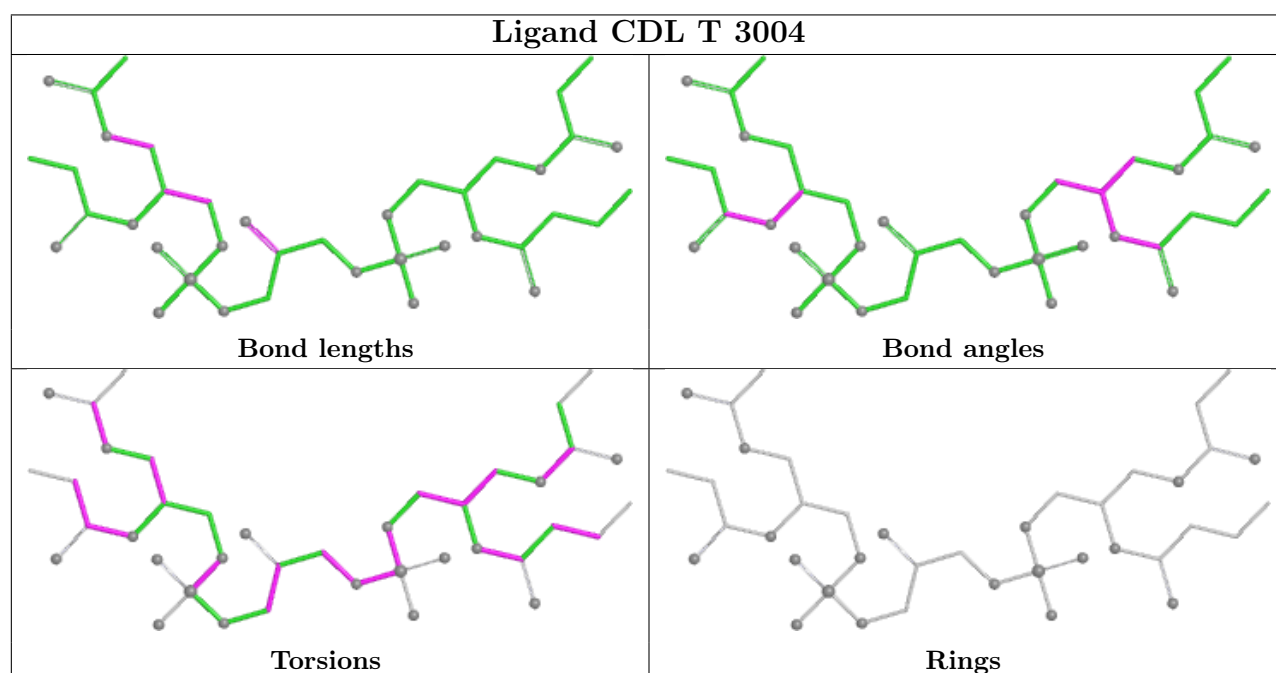
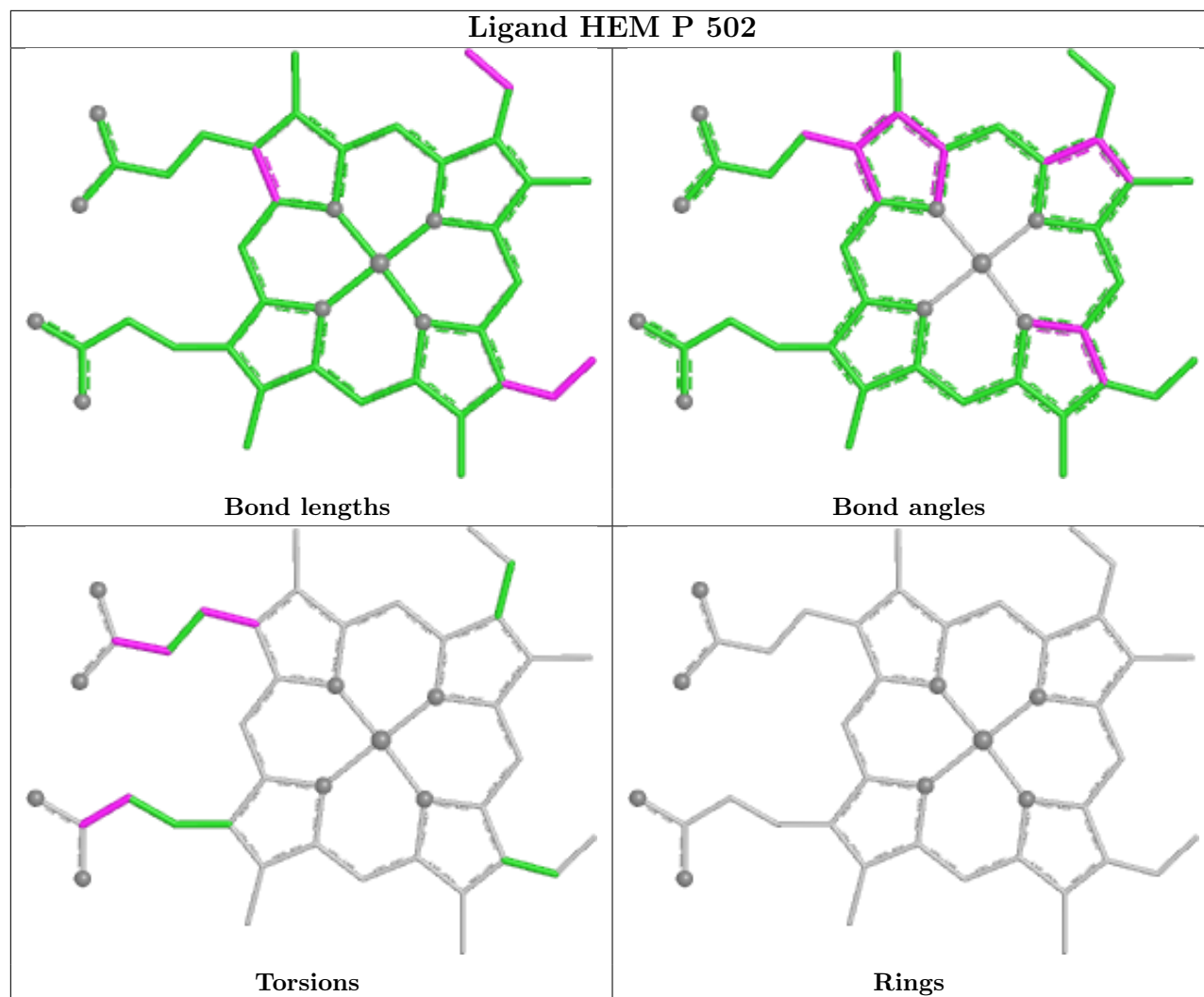


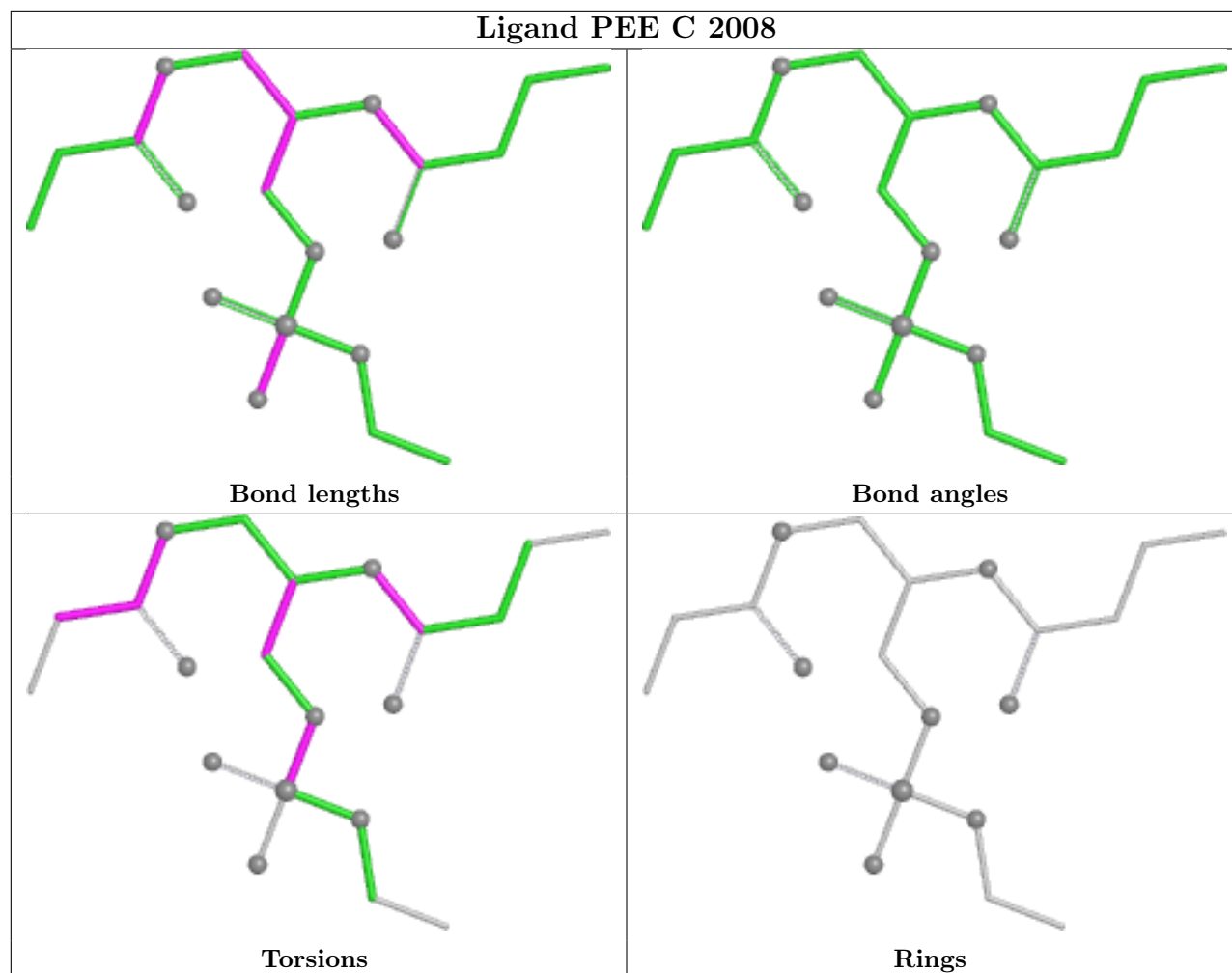


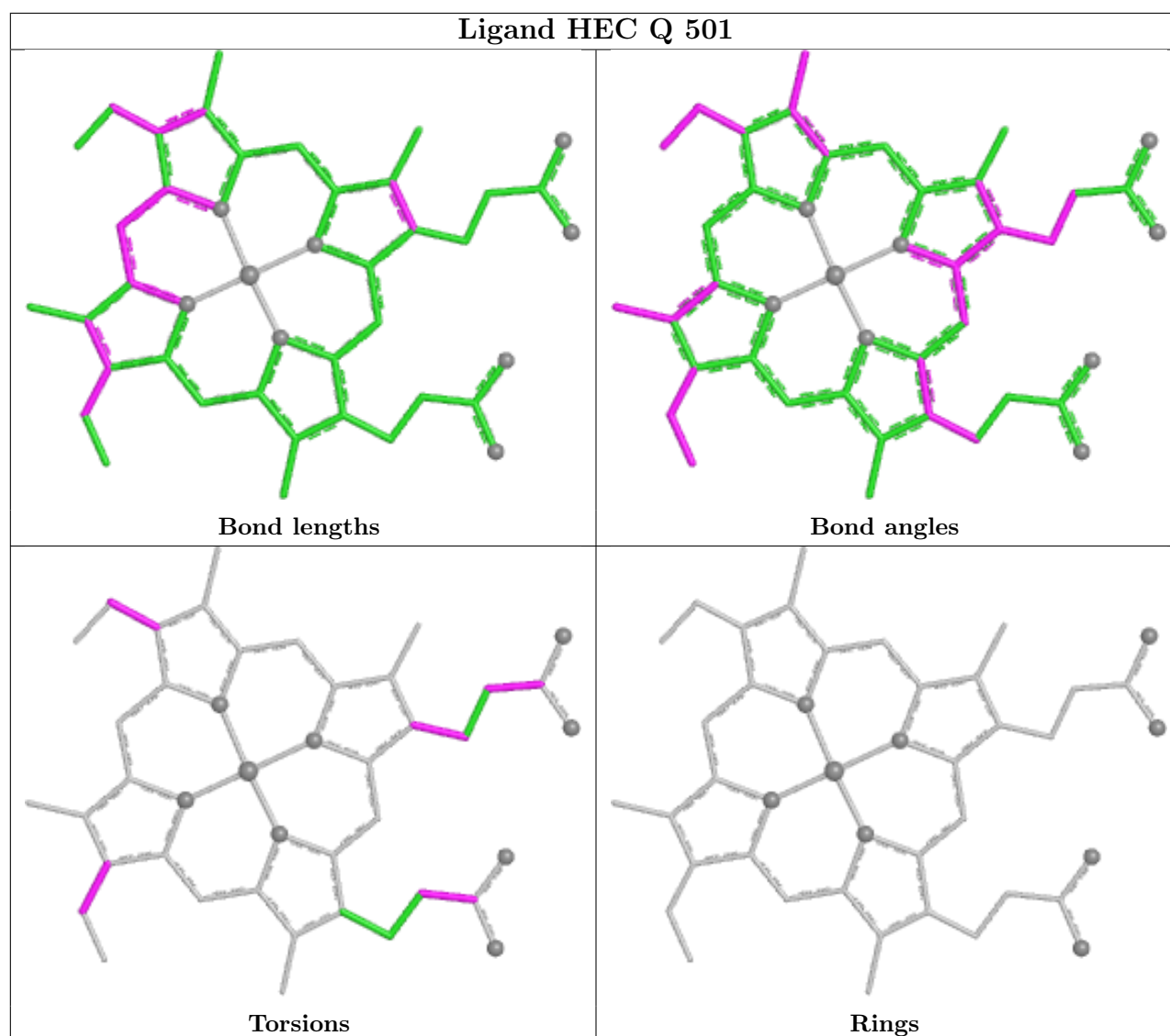












5.7 Other polymers [i](#)

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%)	0.66	29 (6%) 25 24	29, 57, 82, 98	0
1	N	442/446 (99%)	1.21	95 (21%) 2 2	33, 64, 89, 98	0
2	B	421/441 (95%)	1.30	89 (21%) 2 2	44, 74, 109, 136	0
2	O	422/441 (95%)	1.13	67 (15%) 5 4	32, 69, 100, 114	0
3	C	380/380 (100%)	-0.15	6 (1%) 70 69	18, 33, 63, 102	0
3	P	379/380 (99%)	0.66	25 (6%) 24 24	26, 56, 76, 85	0
4	D	241/241 (100%)	-0.14	6 (2%) 58 56	25, 36, 70, 88	0
4	Q	241/241 (100%)	1.07	35 (14%) 6 5	39, 65, 91, 114	0
5	E	196/196 (100%)	1.27	54 (27%) 1 1	33, 76, 107, 114	0
5	R	196/196 (100%)	2.56	104 (53%) 0 0	32, 98, 147, 152	0
6	F	101/110 (91%)	-0.19	1 (0%) 79 79	19, 35, 54, 85	0
6	S	101/110 (91%)	1.10	14 (13%) 6 5	52, 65, 106, 131	0
7	G	81/81 (100%)	0.44	7 (8%) 16 16	28, 46, 82, 97	0
7	T	78/81 (96%)	1.59	19 (24%) 2 1	43, 77, 139, 156	0
8	H	70/77 (90%)	0.56	6 (8%) 16 16	34, 51, 75, 115	0
8	U	67/77 (87%)	2.45	42 (62%) 0 0	87, 108, 130, 134	0
9	I	31/47 (65%)	3.80	27 (87%) 0 0	80, 102, 120, 121	0
9	V	31/47 (65%)	3.91	28 (90%) 0 0	65, 105, 136, 138	0
10	J	61/61 (100%)	0.44	5 (8%) 17 18	40, 53, 85, 124	0
10	W	60/61 (98%)	1.24	9 (15%) 5 5	52, 70, 96, 105	0
All	All	4042/4160 (97%)	0.94	668 (16%) 4 4	18, 61, 107, 156	0

All (668) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	195	VAL	9.6
5	R	194	VAL	9.2
9	V	63	ASP	9.0
5	R	114	VAL	8.8
5	R	193	VAL	8.2
9	I	61	ARG	8.1
9	V	61	ARG	7.9
1	A	444	ILE	7.9
5	R	124	LEU	7.8
5	R	192	LEU	7.8
5	R	112	VAL	7.7
5	R	148	ALA	7.7
9	I	63	ASP	7.0
5	R	188	VAL	6.8
9	V	77	ARG	6.8
2	B	226	ILE	6.7
5	R	147	ILE	6.7
5	E	110	ALA	6.5
5	R	133	VAL	6.4
5	R	110	ALA	6.3
5	R	183	PRO	6.3
2	O	21	ALA	6.3
5	R	87	VAL	6.3
7	T	2	ILE	6.2
2	B	19	PRO	6.1
4	Q	180	SER	6.1
5	R	129	LYS	6.1
9	V	62	ARG	6.0
7	G	1	GLY	6.0
5	R	130	PRO	6.0
5	R	184	THR	6.0
5	R	98	VAL	5.9
9	I	53	GLU	5.8
5	E	188	VAL	5.8
8	H	9	GLU	5.8
9	V	76	VAL	5.7
5	R	127	VAL	5.7
5	R	185	TYR	5.6
5	R	117	LEU	5.6
1	N	318	GLY	5.6
5	R	74	ILE	5.6
2	O	226	ILE	5.6
5	R	187	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
5	R	128	LYS	5.5
7	G	2	ILE	5.5
2	B	402	ILE	5.5
8	U	76	LYS	5.4
5	R	94	LYS	5.4
7	T	72	LYS	5.3
10	W	62	SER	5.3
5	R	89	PHE	5.3
9	I	56	SER	5.3
5	R	93	GLY	5.3
9	V	49	LEU	5.3
5	R	136	VAL	5.2
5	R	97	PHE	5.2
5	R	186	GLN	5.0
9	V	47	ARG	5.0
10	W	61	ALA	5.0
5	R	86	ASN	5.0
5	R	196	GLY	5.0
9	I	62	ARG	4.9
9	I	77	ARG	4.9
5	R	132	TRP	4.9
9	I	57	GLY	4.9
5	E	115	SER	4.9
2	O	371	SER	4.9
8	U	54	CYS	4.8
8	U	26	GLN	4.8
5	E	90	LYS	4.7
5	R	71	LEU	4.7
2	O	383	GLY	4.7
5	R	80	ASP	4.7
7	T	77	TYR	4.7
5	R	106	ILE	4.6
5	E	117	LEU	4.6
1	A	219	VAL	4.6
2	B	124	LEU	4.6
9	V	59	SER	4.6
5	R	96	LEU	4.5
9	V	50	LEU	4.5
3	C	1	MET	4.5
9	V	56	SER	4.5
9	I	51	CYS	4.5
5	R	181	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	235	ALA	4.5
2	B	120	MET	4.5
2	O	23	ASP	4.5
9	I	47	ARG	4.4
5	R	145	VAL	4.4
2	B	20	GLY	4.4
5	E	122	HIS	4.4
4	Q	1	GLY	4.4
9	V	72	ALA	4.4
2	O	20	GLY	4.4
9	I	64	LEU	4.3
5	E	89	PHE	4.3
9	V	64	LEU	4.3
5	R	126	ARG	4.3
5	R	95	PRO	4.3
5	R	189	GLY	4.3
5	E	111	GLU	4.3
9	I	50	LEU	4.2
9	I	72	ALA	4.2
9	I	49	LEU	4.2
9	V	48	PRO	4.2
2	O	368	TYR	4.2
1	A	443	TRP	4.2
2	B	205	ALA	4.1
4	Q	9	ALA	4.1
8	U	78	LYS	4.1
9	V	70	LEU	4.1
2	O	19	PRO	4.1
5	R	174	GLY	4.1
1	N	219	VAL	4.1
9	I	70	LEU	4.1
9	V	71	ASN	4.1
2	B	21	ALA	4.0
10	J	61	ALA	4.0
1	A	226	ASP	4.0
2	O	224	LEU	4.0
5	R	118	ARG	4.0
9	I	60	ALA	4.0
1	N	75	PHE	4.0
2	B	223	PHE	4.0
2	O	223	PHE	4.0
1	N	229	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	4.0
2	O	18	CYS	4.0
1	A	2	ALA	4.0
2	B	33	LEU	4.0
2	O	384	SER	3.9
2	O	104	LYS	3.9
5	E	187	PHE	3.9
1	N	57	TYR	3.8
9	I	75	SER	3.8
3	C	2	ALA	3.8
5	R	104	ALA	3.8
6	S	10	GLY	3.8
8	U	77	LEU	3.8
1	N	54	GLY	3.8
5	R	116	LYS	3.8
9	I	71	ASN	3.8
5	R	113	ASP	3.7
7	T	79	ASN	3.7
9	V	60	ALA	3.7
5	R	138	VAL	3.7
1	N	230	ILE	3.7
5	R	172	ARG	3.7
9	V	52	ARG	3.7
5	R	109	GLU	3.7
2	B	224	LEU	3.7
2	O	386	ALA	3.7
1	A	4	TYR	3.7
5	R	150	SER	3.7
7	T	75	ALA	3.6
5	R	72	SER	3.6
1	N	190	PHE	3.6
2	O	207	VAL	3.6
5	E	114	VAL	3.6
8	U	39	LEU	3.6
5	R	156	TYR	3.6
5	E	133	VAL	3.6
2	O	380	ASN	3.6
5	R	91	TRP	3.6
1	N	69	LYS	3.6
5	R	180	LEU	3.6
7	G	72	LYS	3.6
8	U	30	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
7	T	24	ARG	3.5
8	U	75	ASN	3.5
4	Q	5	LEU	3.5
8	H	71	HIS	3.5
2	O	292	THR	3.5
4	Q	139	ALA	3.5
7	T	74	PRO	3.5
8	U	74	PHE	3.5
4	Q	3	LEU	3.5
5	R	92	ARG	3.5
2	B	229	GLY	3.5
8	U	16	PRO	3.5
4	Q	142	VAL	3.5
5	E	124	LEU	3.5
8	U	73	LEU	3.5
2	B	281	ALA	3.5
8	U	29	LYS	3.4
5	E	190	ASP	3.4
5	R	146	PRO	3.4
6	S	23	ALA	3.4
2	O	268	GLU	3.4
1	N	19	LEU	3.4
10	W	8	GLN	3.4
3	C	268	HIS	3.4
2	O	227	ARG	3.4
3	P	344	VAL	3.4
4	Q	143	VAL	3.4
5	R	178	TYR	3.4
5	E	116	LYS	3.4
7	T	20	PRO	3.4
5	R	135	LEU	3.4
1	N	444	ILE	3.4
4	Q	87	ILE	3.4
5	E	147	ILE	3.4
2	B	232	THR	3.4
2	B	283	PRO	3.4
8	U	65	ARG	3.4
9	I	76	VAL	3.4
5	R	115	SER	3.3
2	B	24	LEU	3.3
9	I	52	ARG	3.3
2	B	231	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	O	250	HIS	3.3
8	U	44	VAL	3.3
5	R	173	LYS	3.3
2	B	41	PHE	3.3
5	R	99	ARG	3.3
5	R	88	ALA	3.3
5	E	74	ILE	3.3
2	B	439	LEU	3.2
2	B	291	VAL	3.2
1	N	266	ASP	3.2
5	R	82	PRO	3.2
10	W	63	GLU	3.2
5	R	79	SER	3.2
8	U	34	ARG	3.2
9	V	58	ARG	3.2
9	I	48	PRO	3.2
1	N	310	PHE	3.2
5	E	193	VAL	3.2
4	Q	141	VAL	3.2
2	O	24	LEU	3.1
5	R	111	GLU	3.1
3	P	320	PRO	3.1
7	T	3	HIS	3.1
1	N	64	PHE	3.1
2	O	291	VAL	3.1
8	U	15	ASP	3.1
4	Q	69	GLU	3.1
2	O	395	PRO	3.1
3	P	5	ILE	3.1
9	I	69	SER	3.1
2	O	387	LEU	3.1
5	E	192	LEU	3.1
1	A	33	PRO	3.1
1	N	443	TRP	3.1
3	P	2	ALA	3.1
1	A	69	LYS	3.1
8	U	37	LEU	3.1
5	E	113	ASP	3.1
10	J	63	GLU	3.1
9	I	73	PRO	3.1
1	A	22	GLY	3.1
2	O	36	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
9	I	58	ARG	3.1
2	O	376	GLN	3.0
1	N	218	GLY	3.0
1	A	73	ALA	3.0
1	A	365	MET	3.0
5	R	176	ALA	3.0
2	B	29	LEU	3.0
2	O	38	LEU	3.0
2	B	117	ASP	3.0
5	R	26	GLN	3.0
2	O	304	THR	3.0
5	R	154	GLY	3.0
5	E	128	LYS	3.0
5	E	129	LYS	3.0
1	N	180	ALA	3.0
2	O	344	LEU	3.0
1	N	223	TYR	3.0
1	N	187	ASP	3.0
1	N	82	MET	3.0
2	B	113	ARG	3.0
8	U	55	THR	3.0
5	R	142	LEU	2.9
8	U	24	CYS	2.9
2	B	204	MET	2.9
4	Q	171	TYR	2.9
9	V	55	MET	2.9
2	B	26	ILE	2.9
2	B	230	ALA	2.9
2	O	302	ALA	2.9
5	E	112	VAL	2.9
4	Q	7	PRO	2.9
2	B	270	ASN	2.9
5	E	156	TYR	2.9
2	B	34	ILE	2.9
1	N	116	VAL	2.9
7	T	47	LYS	2.9
10	J	64	GLU	2.9
5	E	130	PRO	2.9
5	R	134	ILE	2.9
2	B	392	HIS	2.9
9	V	53	GLU	2.9
5	R	29	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	209	ILE	2.9
5	E	106	ILE	2.9
2	O	229	GLY	2.9
2	B	417	PHE	2.9
5	R	182	VAL	2.9
5	R	120	PRO	2.8
5	E	118	ARG	2.8
8	U	53	GLN	2.8
7	T	43	SER	2.8
5	R	149	ASN	2.8
1	N	182	LEU	2.8
5	E	167	ALA	2.8
1	N	28	GLU	2.8
3	C	4	ASN	2.8
4	D	1	GLY	2.8
5	E	185	TYR	2.8
1	N	16	VAL	2.8
1	N	39	VAL	2.8
5	R	76	ILE	2.8
9	V	75	SER	2.8
1	N	169	GLY	2.8
4	Q	175	THR	2.8
1	N	185	TYR	2.8
1	N	258	GLU	2.8
2	O	296	TYR	2.8
4	Q	2	GLU	2.8
1	N	85	HIS	2.8
1	N	121	ALA	2.8
1	N	209	VAL	2.8
5	E	178	TYR	2.8
1	N	112	LEU	2.7
2	B	238	THR	2.7
3	P	317	THR	2.7
2	B	306	PRO	2.7
8	U	72	LYS	2.7
1	A	10	ASN	2.7
1	N	160	GLY	2.7
1	N	201	GLY	2.7
1	N	124	GLU	2.7
5	E	184	THR	2.7
5	R	27	THR	2.7
1	N	108	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	O	107	TYR	2.7
5	R	73	LYS	2.7
5	E	96	LEU	2.7
1	N	387	GLY	2.7
1	N	216	PHE	2.7
8	U	31	VAL	2.7
2	B	212	LYS	2.7
4	Q	17	PRO	2.7
10	W	5	LEU	2.7
2	O	25	GLU	2.7
3	P	322	SER	2.7
5	E	149	ASN	2.7
4	Q	10	PHE	2.7
1	A	193	PRO	2.7
1	N	232	PRO	2.7
2	B	43	PRO	2.7
2	B	403	ASP	2.7
1	A	6	GLN	2.6
6	S	59	MET	2.6
2	B	369	LEU	2.6
4	Q	147	LEU	2.6
8	U	43	ARG	2.6
5	E	109	GLU	2.6
5	R	151	GLY	2.6
6	S	30	GLY	2.6
9	V	67	GLY	2.6
2	B	228	SER	2.6
2	O	50	PHE	2.6
2	O	394	ALA	2.6
9	I	59	SER	2.6
4	Q	138	PRO	2.6
5	R	108	GLN	2.6
1	N	174	ILE	2.6
3	P	269	ILE	2.6
9	V	68	ILE	2.6
1	N	122	LEU	2.6
2	B	227	ARG	2.6
4	D	241	LYS	2.6
5	R	153	PHE	2.6
8	U	50	THR	2.6
2	B	363	GLN	2.6
2	O	402	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
6	S	66	LEU	2.6
8	U	13	LEU	2.6
5	E	99	ARG	2.6
5	R	90	LYS	2.6
5	R	155	GLY	2.6
1	N	18	THR	2.6
2	O	266	SER	2.6
5	R	121	GLN	2.6
7	G	81	GLN	2.6
2	B	216	LEU	2.6
2	O	284	LEU	2.6
2	B	236	LYS	2.6
2	B	267	ALA	2.6
2	B	127	THR	2.5
9	I	54	SER	2.5
5	R	78	LEU	2.5
2	B	277	HIS	2.5
2	O	22	GLU	2.5
5	R	105	GLU	2.5
1	N	56	GLY	2.5
2	B	30	PRO	2.5
2	B	119	VAL	2.5
3	P	286	PRO	2.5
8	U	61	PHE	2.5
8	U	19	THR	2.5
1	N	68	LYS	2.5
2	O	99	TYR	2.5
6	S	89	TYR	2.5
1	N	117	VAL	2.5
1	N	86	PHE	2.5
1	A	21	ASN	2.5
2	O	303	THR	2.5
8	U	17	LEU	2.5
2	B	221	GLU	2.5
3	P	380	TYR	2.5
2	O	300	ALA	2.5
5	R	102	THR	2.5
4	Q	241	LYS	2.5
9	V	51	CYS	2.5
5	E	101	ARG	2.5
6	S	12	LEU	2.5
9	I	68	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	119	ASP	2.5
2	O	208	GLY	2.5
6	S	29	TYR	2.5
9	V	57	GLY	2.5
4	Q	137	PRO	2.5
2	B	352	VAL	2.5
3	P	90	PHE	2.5
6	S	11	ARG	2.4
2	B	364	LEU	2.4
2	O	228	SER	2.4
2	O	289	SER	2.4
2	B	23	ASP	2.4
7	G	3	HIS	2.4
1	N	13	GLU	2.4
1	N	107	PRO	2.4
2	O	415	LYS	2.4
2	O	416	LYS	2.4
9	V	74	ALA	2.4
5	R	101	ARG	2.4
8	U	21	ARG	2.4
1	N	62	LEU	2.4
6	S	34	ASP	2.4
1	N	168	GLU	2.4
1	A	42	GLY	2.4
1	N	42	GLY	2.4
6	F	10	GLY	2.4
1	A	223	TYR	2.4
1	N	228	VAL	2.4
2	B	92	VAL	2.4
2	B	211	VAL	2.4
2	B	397	VAL	2.4
4	Q	68	VAL	2.4
6	S	55	TYR	2.4
1	N	73	ALA	2.4
2	B	284	LEU	2.4
5	R	81	ILE	2.4
5	E	85	LYS	2.4
1	N	83	GLY	2.4
1	N	200	ALA	2.4
3	P	34	PHE	2.4
2	B	436	LEU	2.4
4	Q	121	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
5	R	122	HIS	2.4
2	B	100	SER	2.4
2	B	371	SER	2.4
3	P	217	ASP	2.4
5	R	119	ASP	2.4
1	N	375	VAL	2.4
10	W	12	ALA	2.4
3	P	156	TYR	2.3
1	N	170	THR	2.3
1	N	317	THR	2.3
8	U	18	THR	2.3
1	N	119	ASN	2.3
5	R	123	ASP	2.3
7	T	70	LYS	2.3
5	E	132	TRP	2.3
2	B	48	GLY	2.3
2	O	351	GLY	2.3
4	Q	174	GLY	2.3
2	B	36	ALA	2.3
7	T	30	PHE	2.3
7	T	41	PHE	2.3
2	O	379	LEU	2.3
8	U	42	ALA	2.3
10	W	4	ALA	2.3
1	N	14	THR	2.3
8	U	49	HIS	2.3
1	N	65	LYS	2.3
2	B	28	LYS	2.3
3	P	270	LYS	2.3
5	R	77	LYS	2.3
7	G	78	GLU	2.3
2	B	73	SER	2.3
3	P	31	TRP	2.3
2	O	46	ARG	2.3
8	U	36	ARG	2.3
1	N	63	ALA	2.3
1	N	319	LEU	2.3
2	B	220	ALA	2.3
2	O	220	ALA	2.3
8	H	13	LEU	2.3
4	Q	134	TYR	2.3
2	B	22	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	69	GLU	2.3
1	A	81	SER	2.3
4	Q	238	ARG	2.3
5	E	91	TRP	2.3
2	B	390	GLY	2.3
5	E	87	VAL	2.3
8	U	14	VAL	2.3
2	B	112	LEU	2.3
4	Q	169	LEU	2.3
7	T	26	ILE	2.3
8	U	33	ALA	2.3
2	O	238	THR	2.3
5	R	85	LYS	2.3
1	N	98	TYR	2.3
5	E	157	TYR	2.3
1	N	53	ASN	2.3
1	N	264	ASP	2.3
2	B	147	ASP	2.3
1	N	138	LEU	2.3
2	O	295	LEU	2.3
3	P	250	LEU	2.3
10	W	46	LEU	2.3
1	N	35	CYS	2.2
2	O	35	ILE	2.2
1	N	191	LYS	2.2
1	N	36	THR	2.2
8	U	25	GLU	2.2
1	N	70	ARG	2.2
2	O	97	SER	2.2
3	P	253	ASP	2.2
2	B	344	LEU	2.2
9	I	65	VAL	2.2
9	V	65	VAL	2.2
1	N	221	PHE	2.2
3	P	240	PHE	2.2
10	W	55	ILE	2.2
8	H	10	GLU	2.2
4	Q	172	ASP	2.2
5	R	168	SER	2.2
1	N	197	LEU	2.2
2	O	364	LEU	2.2
5	E	71	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	S	37	LEU	2.2
1	A	228	VAL	2.2
1	N	236	PHE	2.2
2	O	346	ALA	2.2
5	R	167	ALA	2.2
5	R	75	GLU	2.2
8	U	40	CYS	2.2
10	J	7	ARG	2.2
2	B	368	TYR	2.2
5	E	86	ASN	2.2
2	O	155	PRO	2.2
1	N	32	GLN	2.2
1	A	224	LYS	2.2
1	N	145	MET	2.2
1	A	86	PHE	2.2
1	N	11	ILE	2.2
2	O	307	PHE	2.2
5	E	171	ILE	2.2
1	N	26	ALA	2.2
2	B	399	ALA	2.2
5	E	121	GLN	2.2
2	B	301	LYS	2.2
4	Q	159	GLY	2.2
1	N	81	SER	2.2
3	P	213	SER	2.2
1	N	203	ILE	2.2
1	N	215	HIS	2.2
2	B	47	ILE	2.2
3	C	159	HIS	2.2
4	D	143	VAL	2.2
5	E	138	VAL	2.2
10	J	62	SER	2.2
5	E	153	PHE	2.2
4	Q	65	ALA	2.1
7	T	25	ALA	2.1
9	V	66	ALA	2.1
4	D	2	GLU	2.1
2	B	156	GLN	2.1
5	R	107	ASN	2.1
4	Q	173	ASP	2.1
5	R	28	SER	2.1
2	B	307	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
8	U	64	ALA	2.1
1	N	33	PRO	2.1
3	C	286	PRO	2.1
4	Q	240	PRO	2.1
5	E	82	PRO	2.1
5	R	175	PRO	2.1
1	A	392	LEU	2.1
2	B	122	TYR	2.1
2	O	420	GLY	2.1
7	T	5	GLY	2.1
2	B	398	VAL	2.1
2	O	299	VAL	2.1
7	T	45	VAL	2.1
2	B	310	SER	2.1
3	P	26	SER	2.1
4	Q	129	SER	2.1
3	P	203	GLU	2.1
1	N	3	THR	2.1
8	U	27	THR	2.1
6	S	88	PRO	2.1
2	B	206	LEU	2.1
2	B	225	ASN	2.1
2	B	250	HIS	2.1
3	P	252	GLY	2.1
8	U	23	HIS	2.1
2	O	357	VAL	2.1
8	U	20	ILE	2.1
4	D	172	ASP	2.1
1	N	96	ALA	2.1
1	N	217	SER	2.1
2	B	45	SER	2.1
2	B	289	SER	2.1
8	U	48	SER	2.1
1	N	213	ARG	2.1
8	H	28	GLU	2.1
2	B	217	LYS	2.1
7	G	74	PRO	2.1
2	B	38	LEU	2.1
3	P	375	ASN	2.1
4	Q	6	HIS	2.1
2	B	85	ILE	2.1
2	O	264	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	179	ARG	2.0
5	E	172	ARG	2.0
5	R	190	ASP	2.0
2	B	419	SER	2.0
2	O	328	SER	2.0
5	E	173	LYS	2.0
1	N	40	TRP	2.0
2	B	304	THR	2.0
4	Q	110	PRO	2.0
1	A	215	HIS	2.0
3	P	249	ASN	2.0
5	R	100	HIS	2.0
1	N	44	GLY	2.0
2	O	26	ILE	2.0
1	A	196	VAL	2.0
1	N	59	VAL	2.0
5	E	160	CYS	2.0
6	S	21	TYR	2.0
1	A	194	ARG	2.0
1	A	187	ASP	2.0
5	E	75	GLU	2.0
3	P	7	LYS	2.0
1	N	17	THR	2.0
1	N	171	THR	2.0
2	B	200	THR	2.0
5	R	140	THR	2.0
5	R	159	PRO	2.0
1	A	8	LEU	2.0
1	A	23	LEU	2.0
1	N	113	LEU	2.0
7	T	69	LEU	2.0
1	N	186	ILE	2.0
5	E	137	GLY	2.0
8	H	75	ASN	2.0
2	B	207	VAL	2.0
5	E	98	VAL	2.0
1	N	414	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	UNL	P	3048	2/-	0.39	0.88	93,93,93,95	0
17	BOG	Q	3091	20/20	0.48	0.39	172,179,180,180	0
17	BOG	D	2091	20/20	0.65	0.54	171,182,183,184	0
17	BOG	P	2010	19/20	0.73	0.43	97,177,178,178	0
12	UNL	P	3046	2/-	0.77	0.27	85,85,85,86	0
12	UNL	C	2048	2/-	0.78	0.31	41,41,41,45	0
19	CDL	T	3004	40/100	0.78	0.27	85,89,100,101	0
19	CDL	Q	3003	42/100	0.81	0.28	114,118,123,124	0
11	PEE	C	2008	21/51	0.82	0.24	89,103,110,111	0
19	CDL	D	2003	42/100	0.82	0.20	60,75,87,88	0
15	UQ	C	2002	19/63	0.83	0.29	80,84,86,86	0
12	UNL	P	3047	1/-	0.85	0.12	45,45,45,45	0
12	UNL	P	3014	1/-	0.85	0.19	55,55,55,55	0
12	UNL	E	2012	2/-	0.86	0.20	51,51,51,51	0
11	PEE	N	3005	50/51	0.86	0.27	64,92,98,98	0
15	UQ	P	3002	19/63	0.86	0.36	132,136,138,138	0
12	UNL	Q	3012	1/-	0.87	0.20	33,33,33,33	0
19	CDL	G	2004	40/100	0.87	0.17	48,63,77,78	0
17	BOG	Q	3009	20/20	0.87	0.19	69,80,83,84	0
11	PEE	N	3008	5/51	0.87	0.11	74,74,75,76	0
17	BOG	D	2009	20/20	0.88	0.14	47,57,61,61	0
12	UNL	P	3013	1/-	0.88	0.29	72,72,72,72	0
11	PEE	A	2005	50/51	0.88	0.25	74,85,89,90	0
12	UNL	C	2046	2/-	0.89	0.21	78,78,78,80	0
14	FMX	P	3001	28/28	0.90	0.17	55,65,70,71	0
11	PEE	P	3007	48/51	0.90	0.23	71,83,98,100	0
14	FMX	C	2001	28/28	0.91	0.14	31,49,61,62	0
16	AZI	C	2011	3/3	0.91	0.20	62,62,63,64	0
17	BOG	C	3010	12/20	0.91	0.22	78,81,83,84	0
12	UNL	A	3015	1/-	0.94	0.06	45,45,45,45	0
12	UNL	C	2047	1/-	0.95	0.12	28,28,28,28	0
16	AZI	P	3011	3/3	0.95	0.17	66,66,68,68	0

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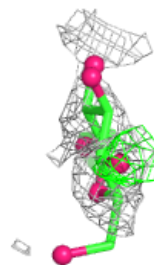
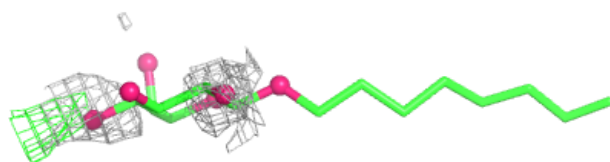
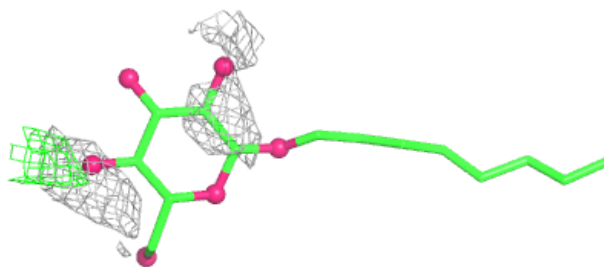
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	PEE	C	2007	48/51	0.95	0.14	33,49,72,72	0
18	HEC	Q	501	43/43	0.96	0.11	40,49,58,60	0
20	FES	E	501	4/4	0.97	0.07	72,73,74,74	0
20	FES	R	501	4/4	0.97	0.14	85,85,86,86	0
13	HEM	P	502	43/43	0.98	0.07	32,38,50,56	0
18	HEC	D	501	43/43	0.98	0.07	14,25,29,32	0
13	HEM	P	501	43/43	0.98	0.09	37,41,52,56	0
13	HEM	C	501	43/43	0.99	0.07	17,27,37,40	0
13	HEM	C	502	43/43	0.99	0.06	15,20,28,32	0

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

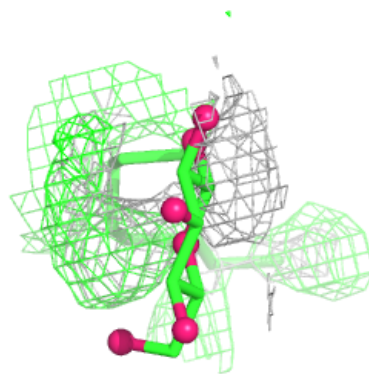
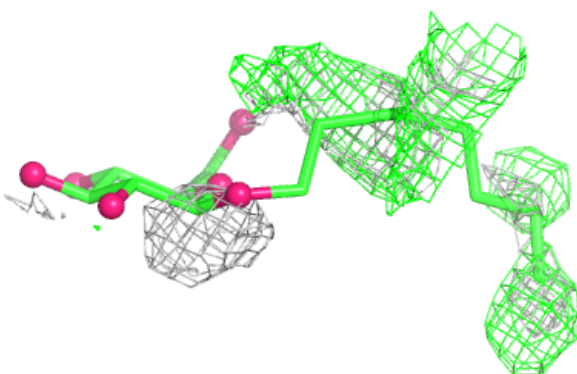
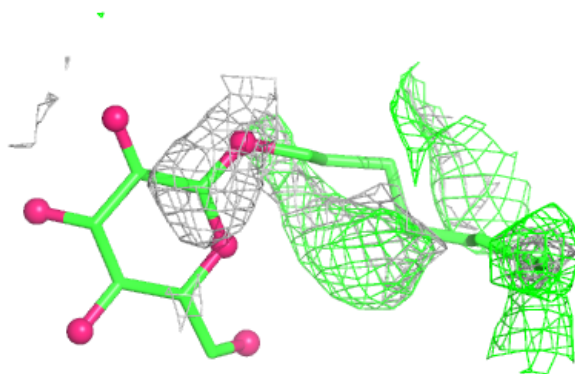
Electron density around BOG Q 3091:

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

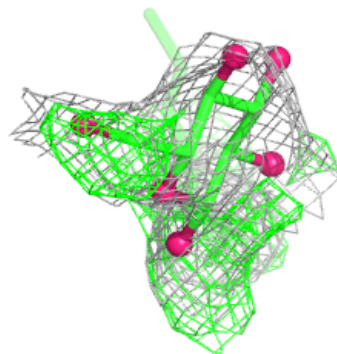
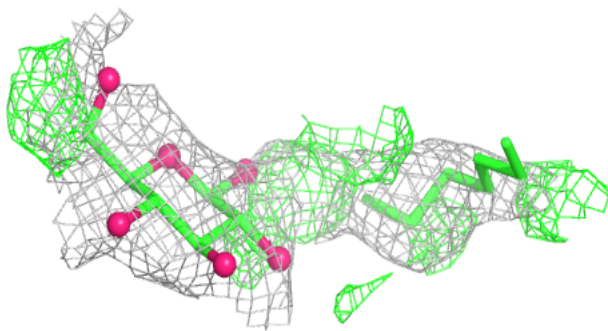
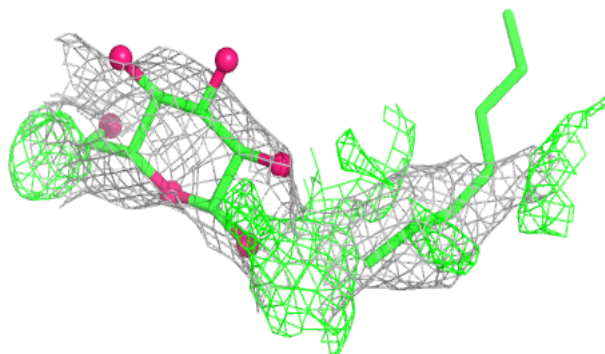


Electron density around BOG D 2091:

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

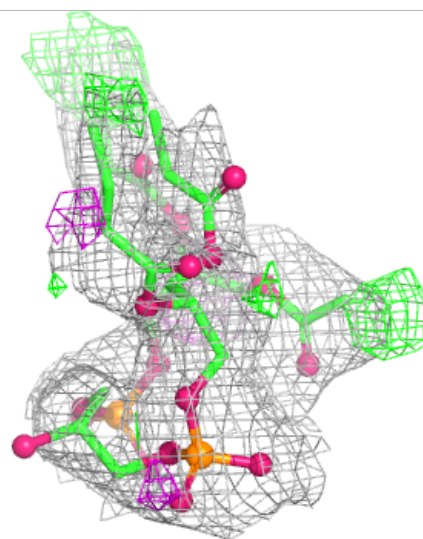
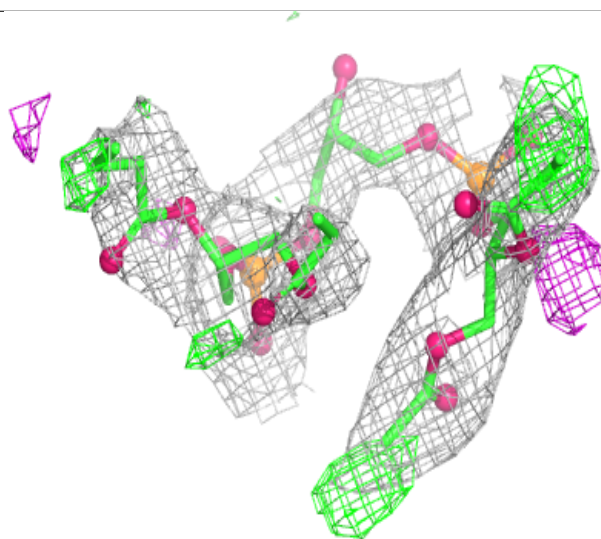
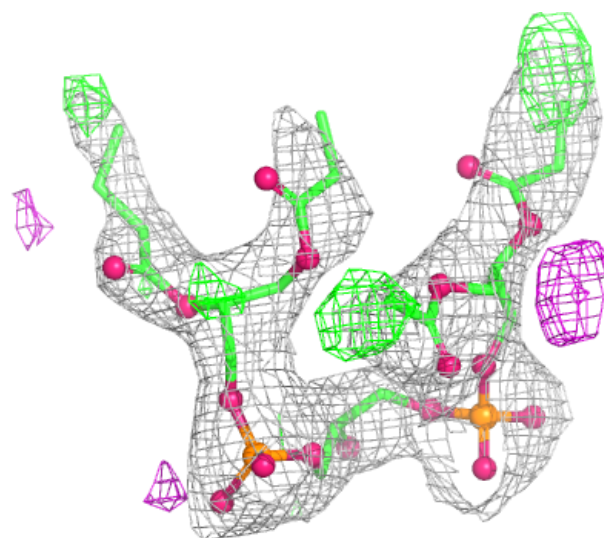
**Electron density around BOG P 2010:**

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



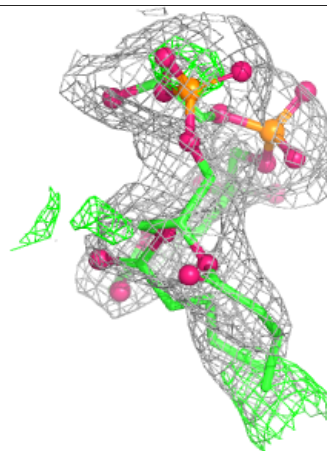
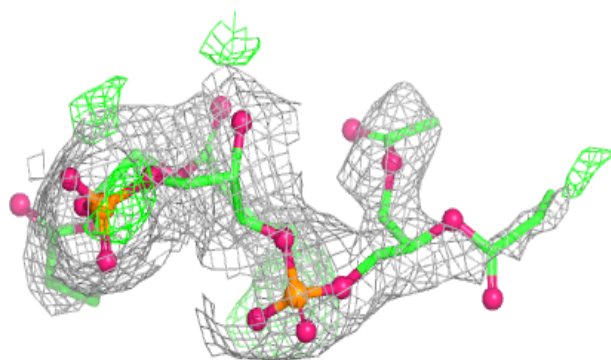
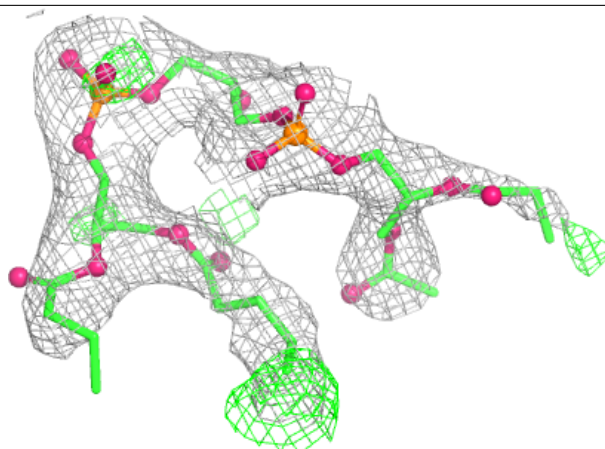
Electron density around CDL T 3004:

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



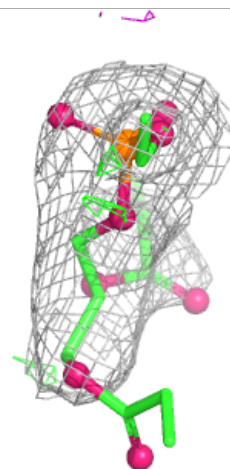
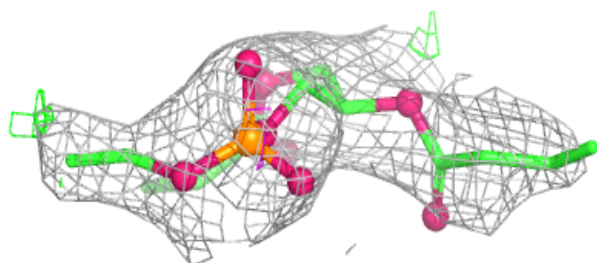
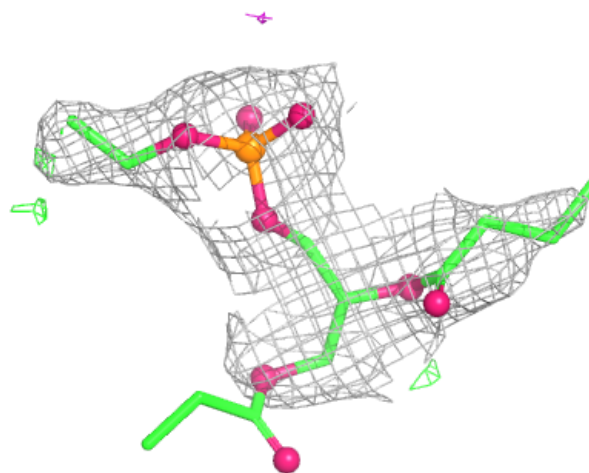
Electron density around CDL Q 3003:

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



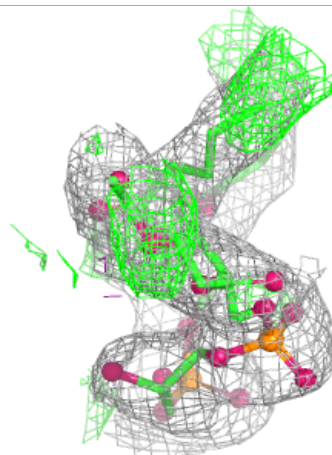
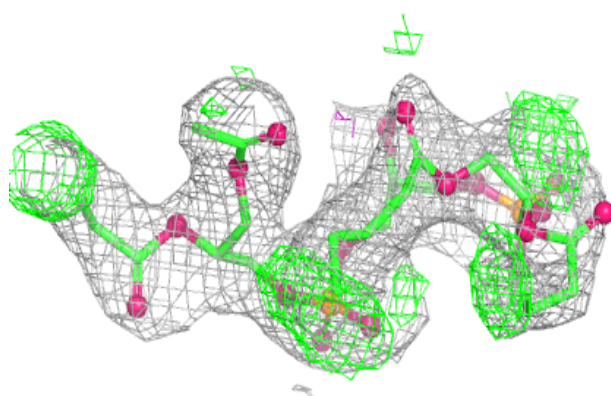
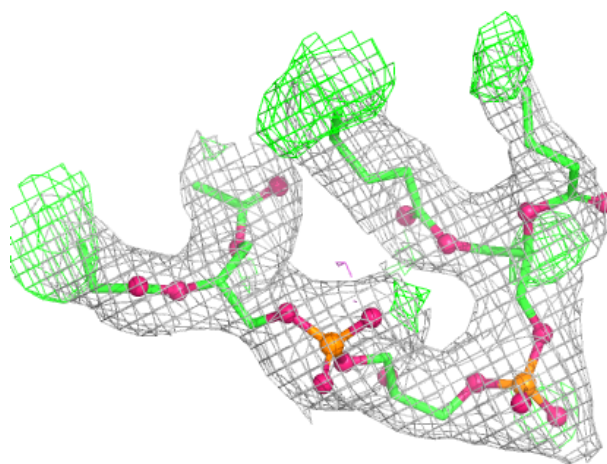
Electron density around PEE C 2008:

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



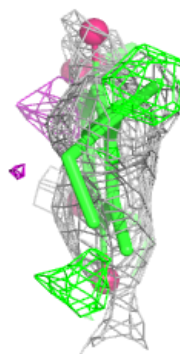
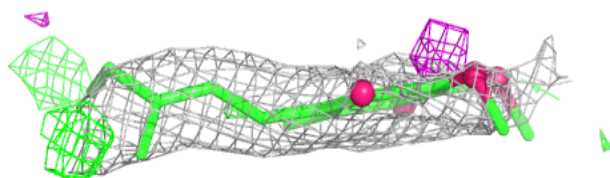
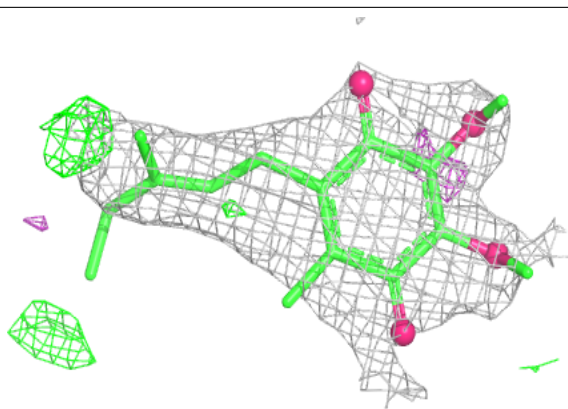
Electron density around CDL D 2003:

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

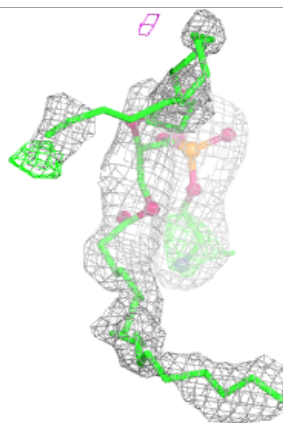
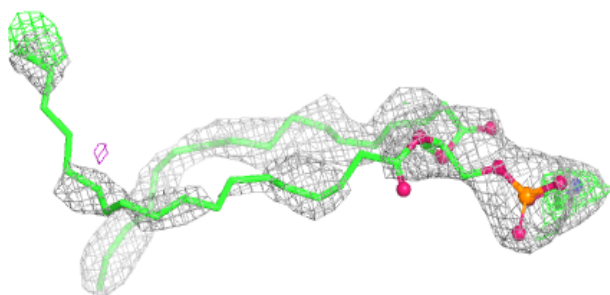
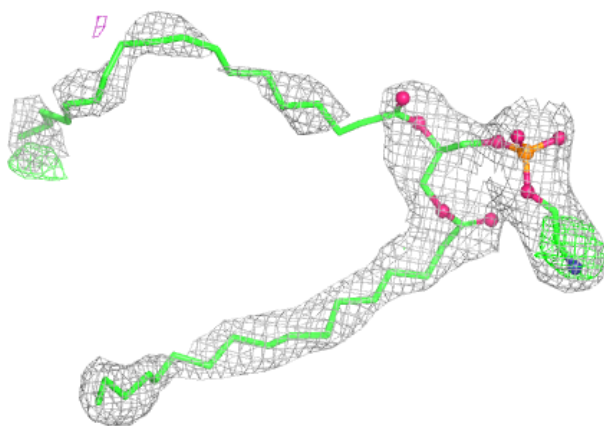


Electron density around UQ C 2002:

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

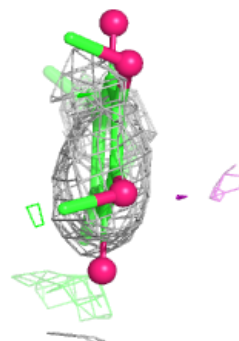
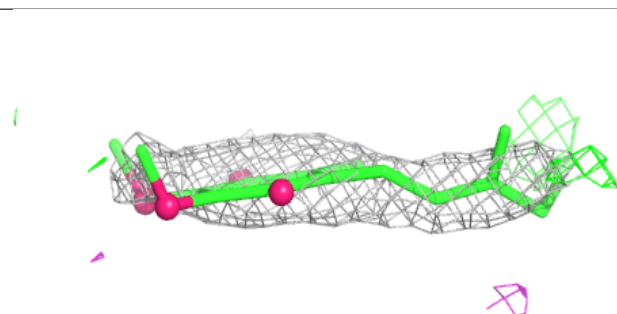
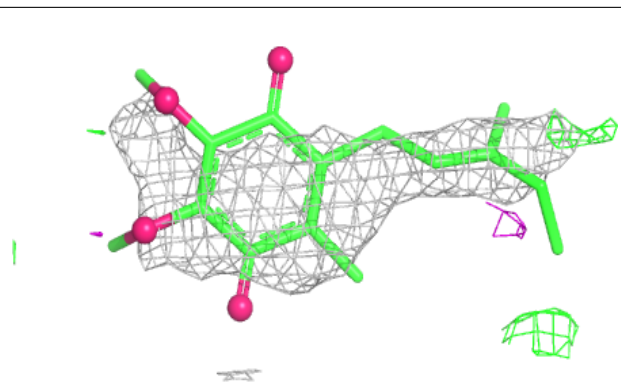
**Electron density around PEE N 3005:**

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



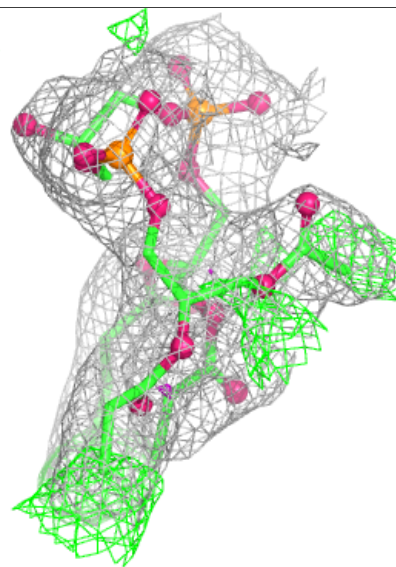
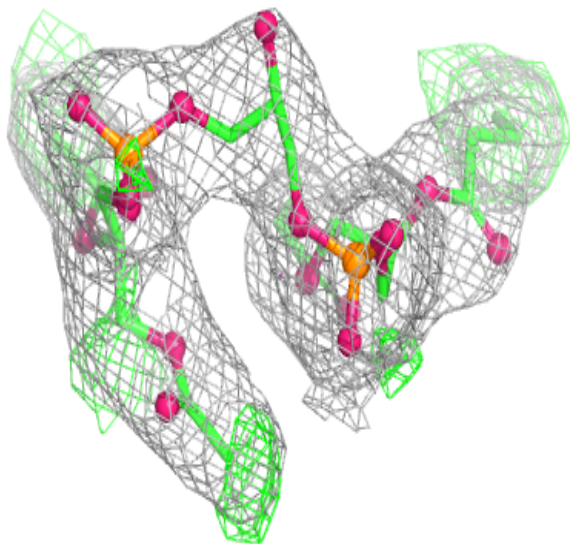
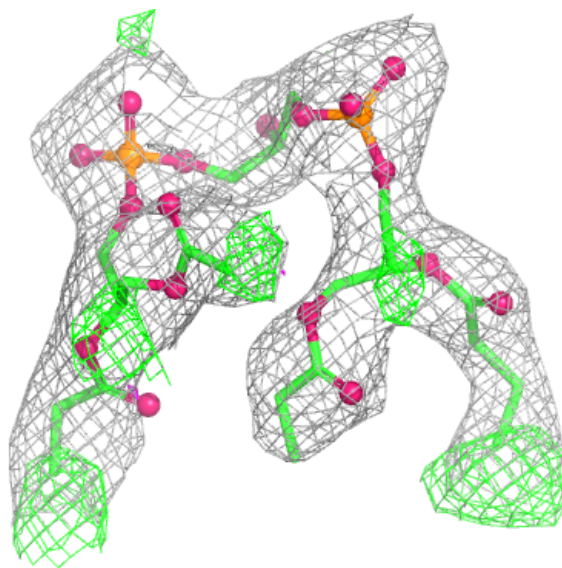
Electron density around UQ P 3002:

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



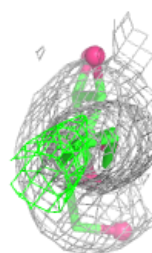
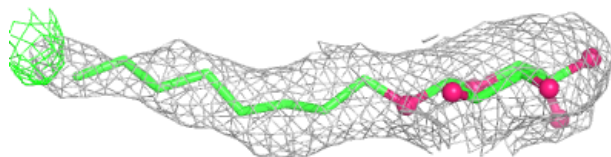
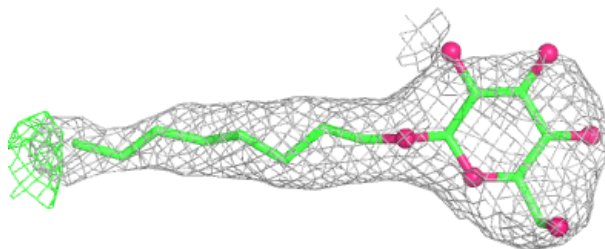
Electron density around CDL G 2004:

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



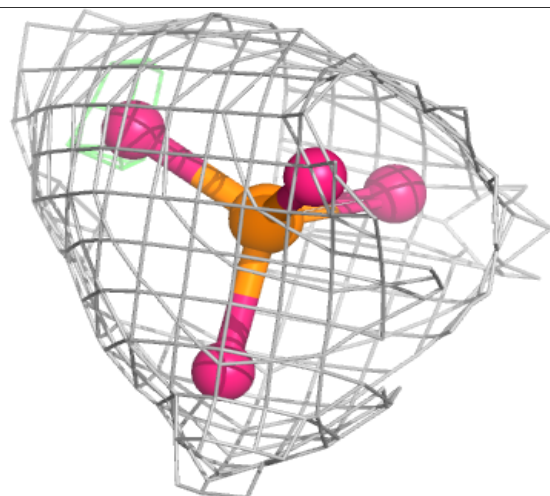
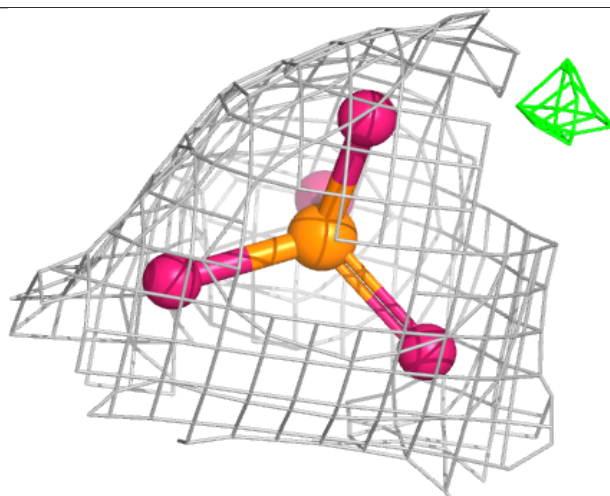
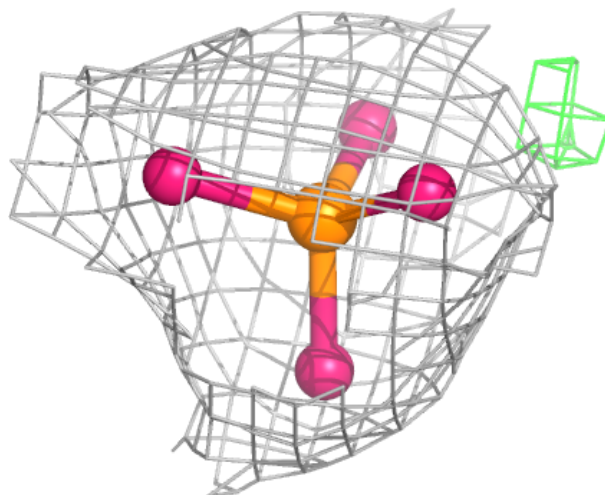
Electron density around BOG Q 3009:

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



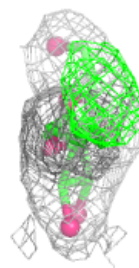
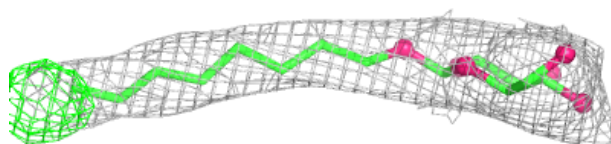
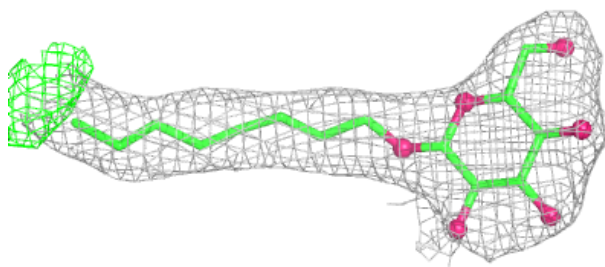
Electron density around PEE N 3008:

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

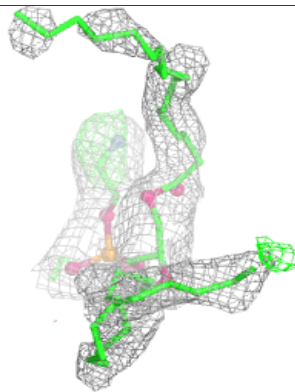
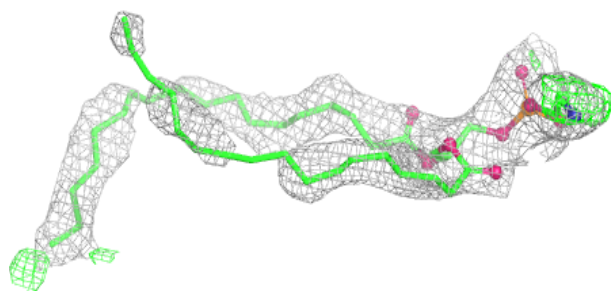
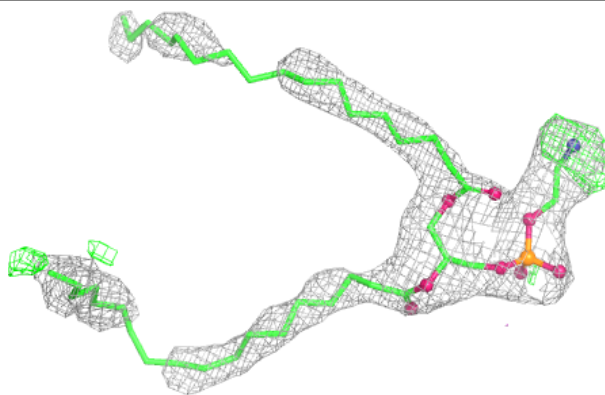


Electron density around BOG D 2009:

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

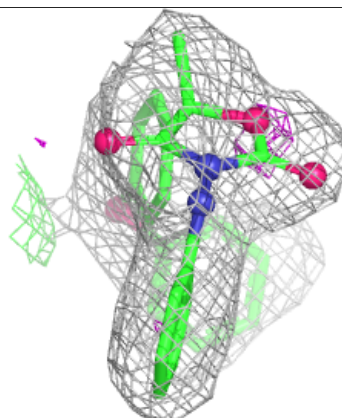
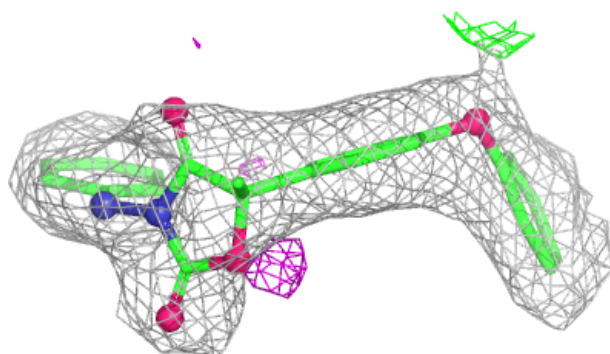
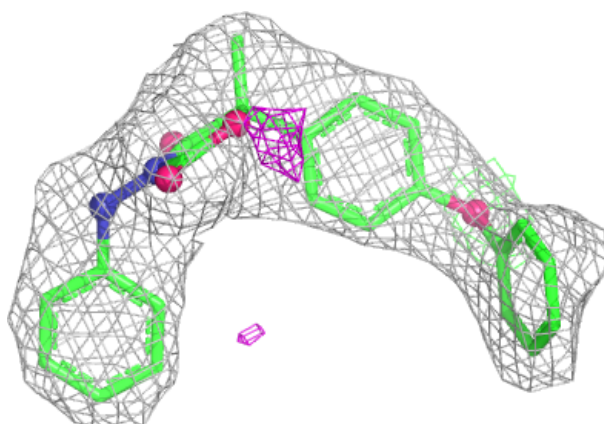
**Electron density around PEE A 2005:**

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

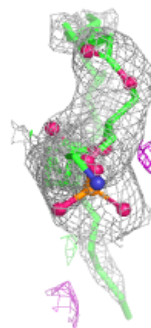
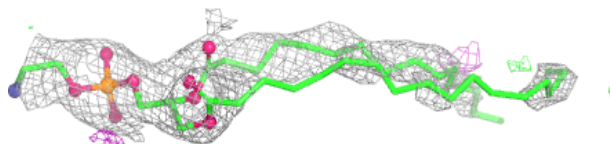
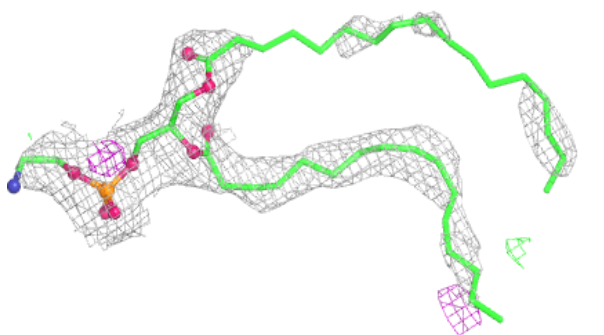


Electron density around FMX P 3001:

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

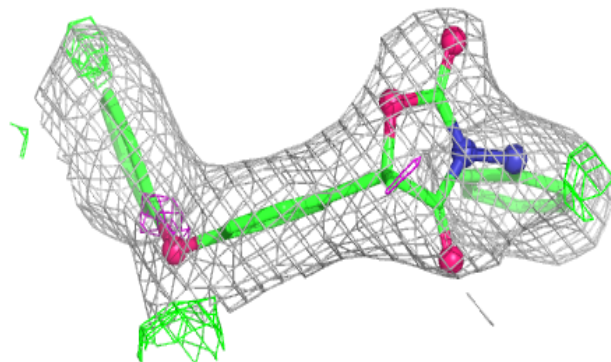
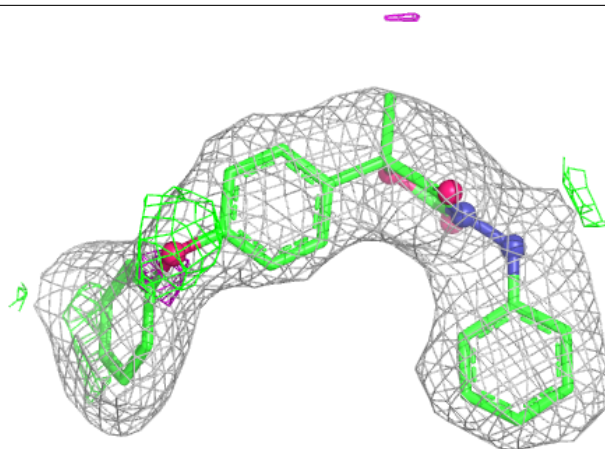
**Electron density around PEE P 3007:**

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



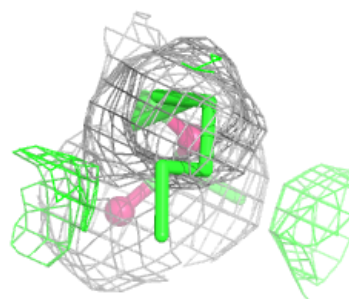
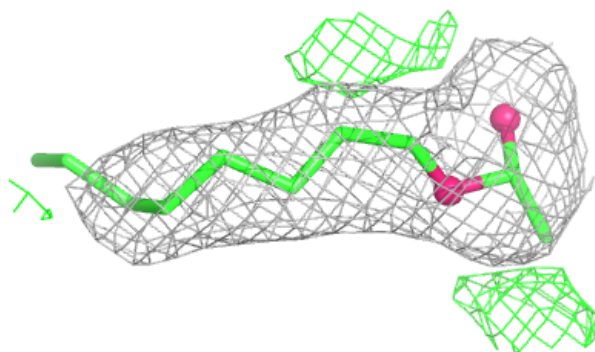
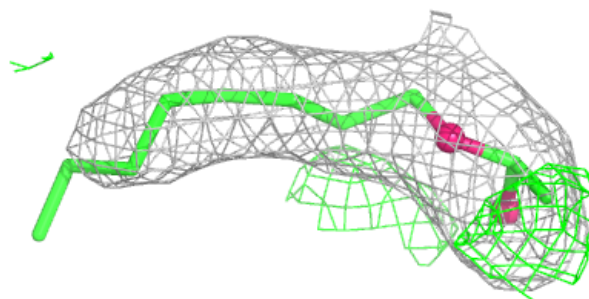
Electron density around FMX C 2001:

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

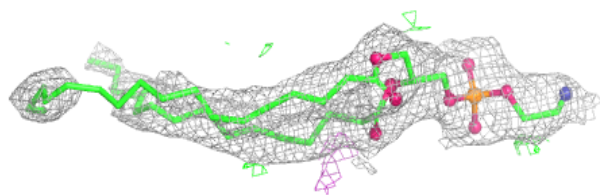
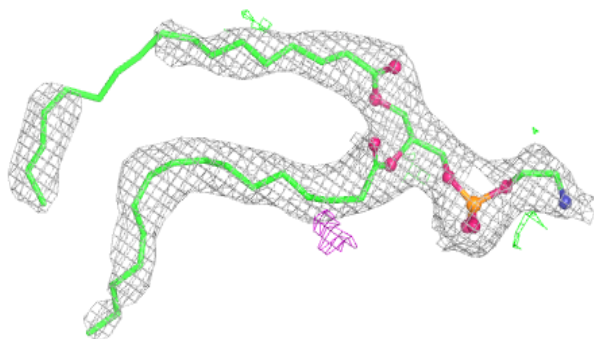


Electron density around BOG C 3010:

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

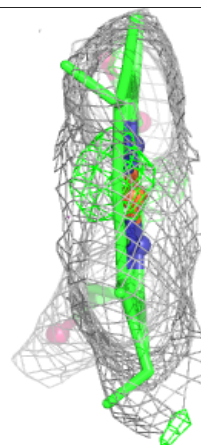
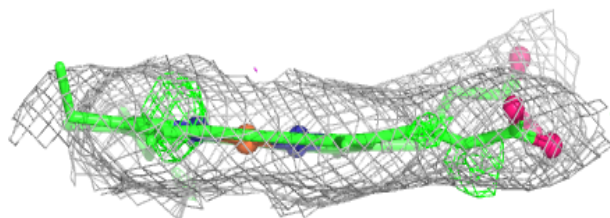
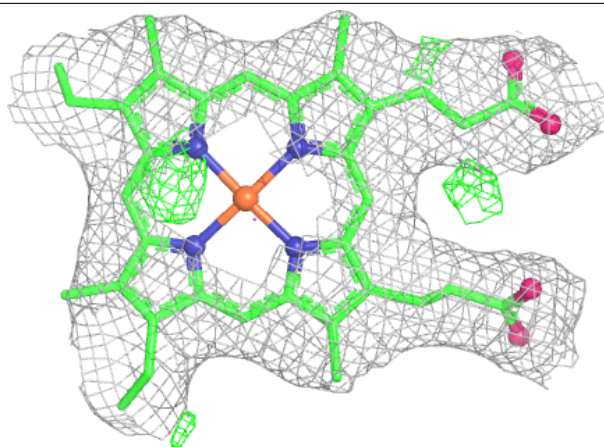
**Electron density around PEE C 2007:**

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



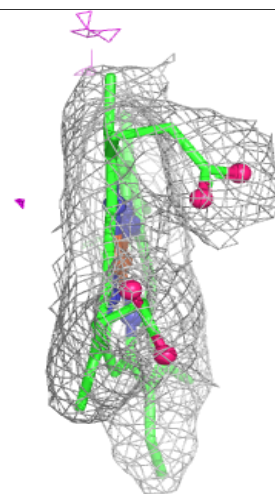
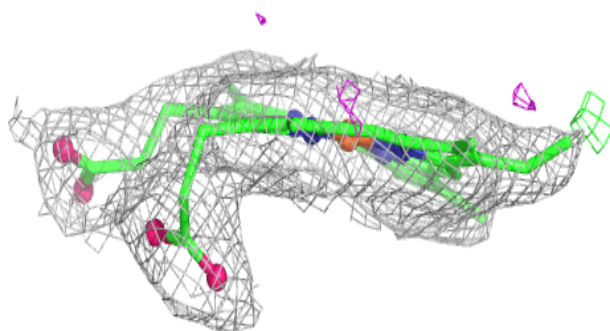
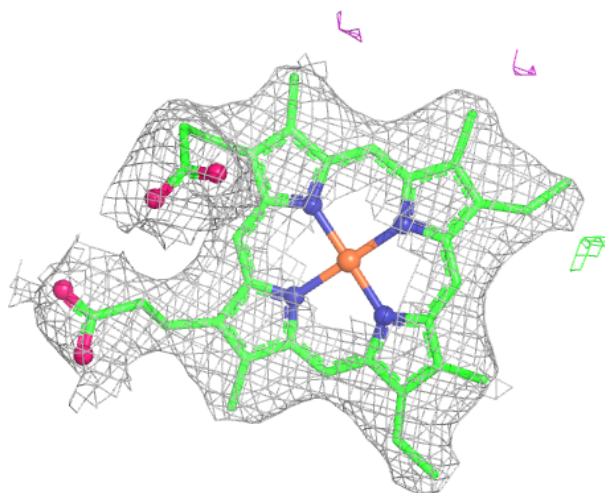
Electron density around HEC Q 501:

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



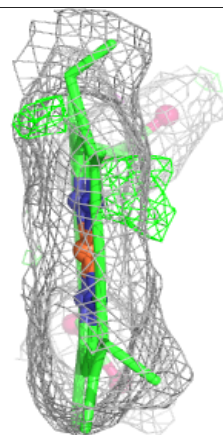
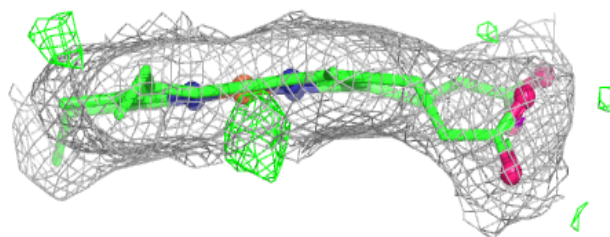
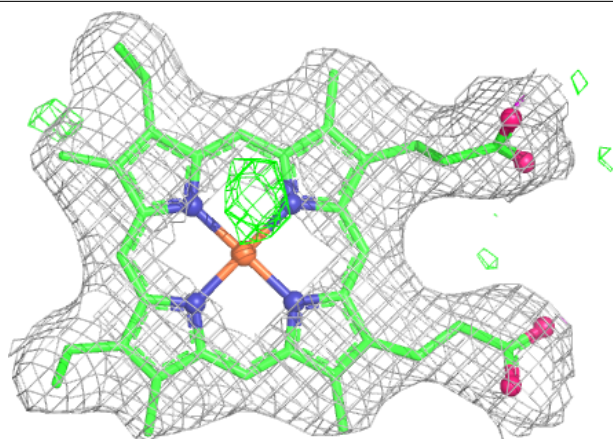
Electron density around HEM P 502:

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



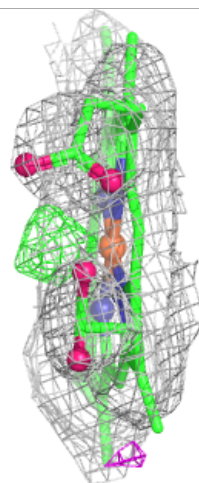
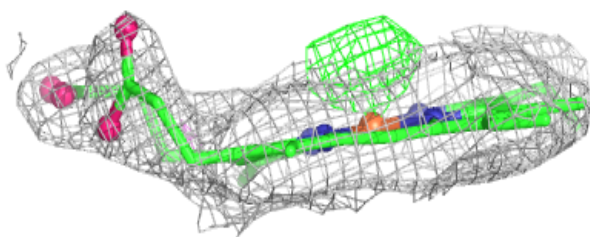
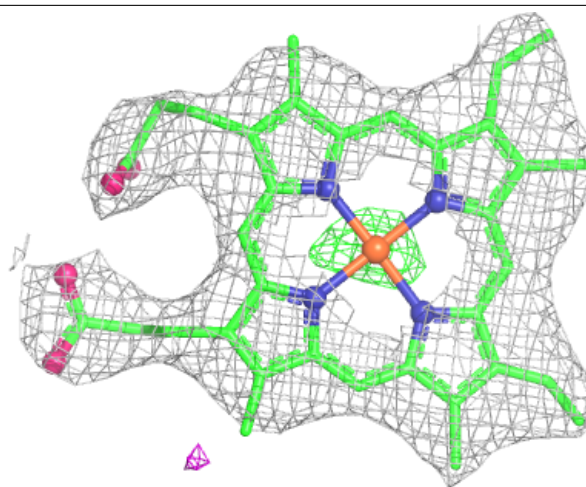
Electron density around HEC D 501:

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



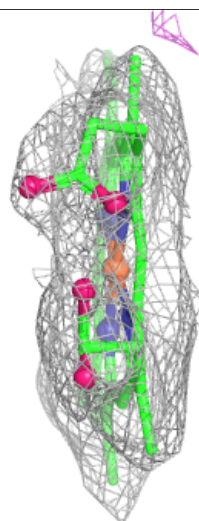
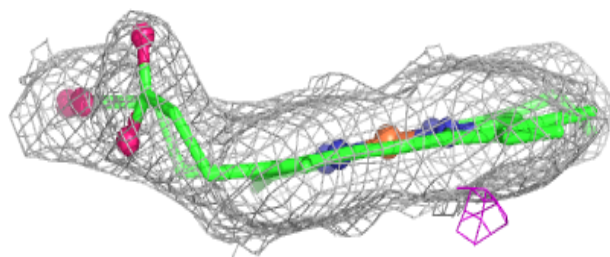
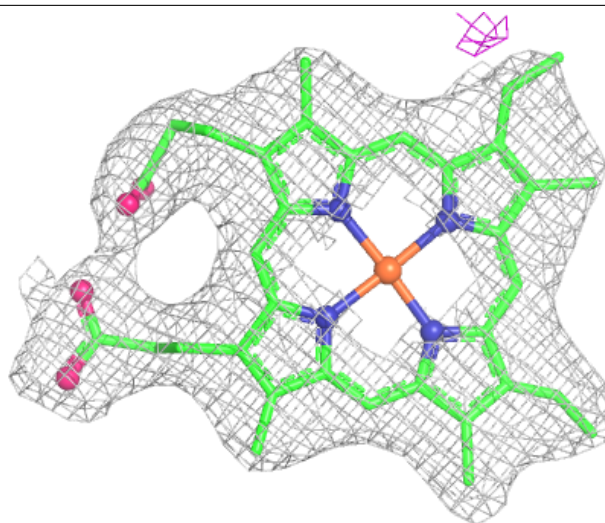
Electron density around HEM P 501:

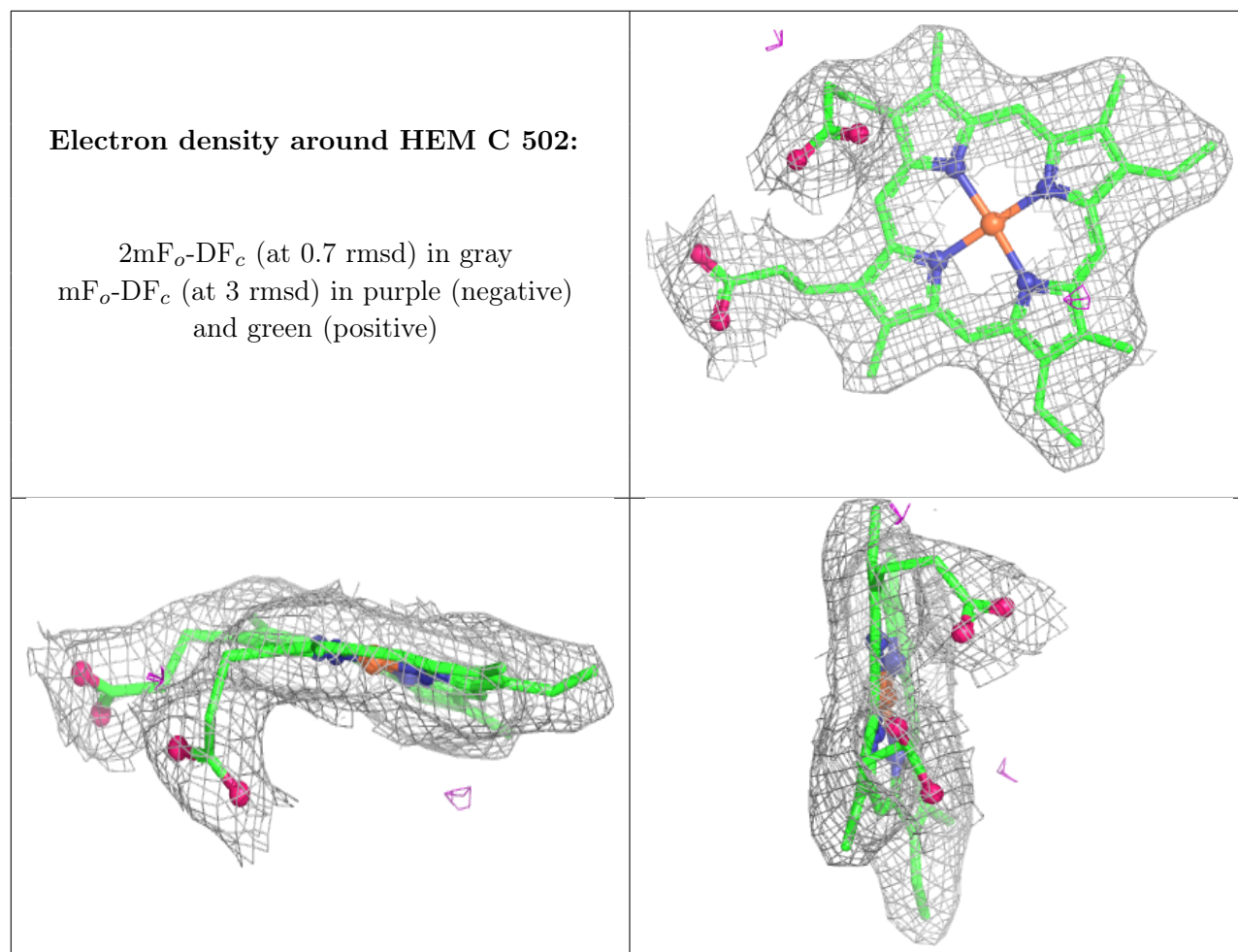
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.