



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:37 PM UTC

PDB ID : 3L73 / pdb_00003L73
Title : Cytochrome BC1 complex from chicken with triazolone inhibitor
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

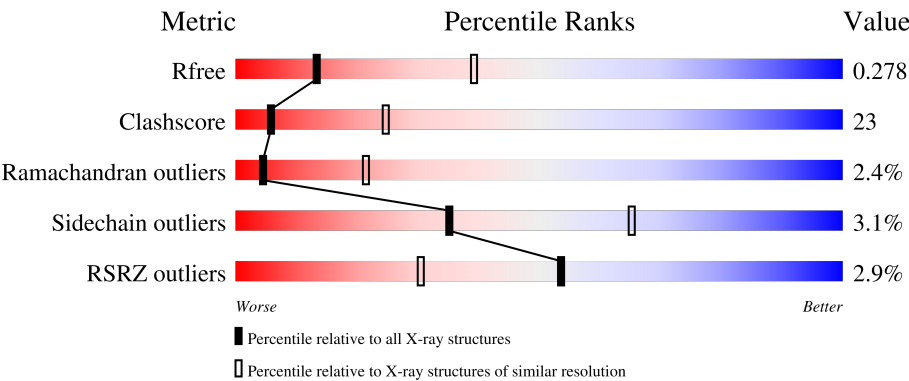
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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.



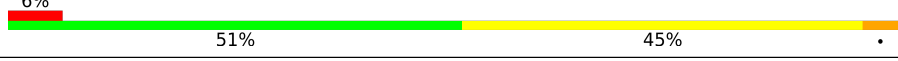
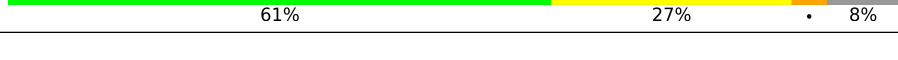
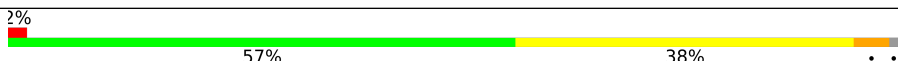
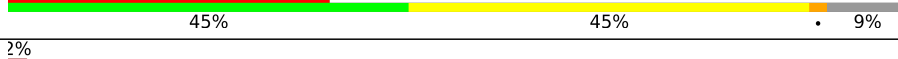
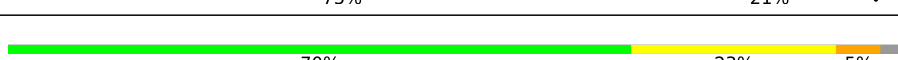
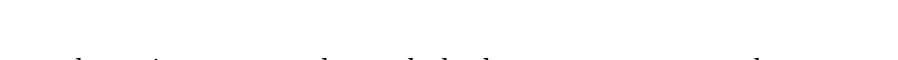
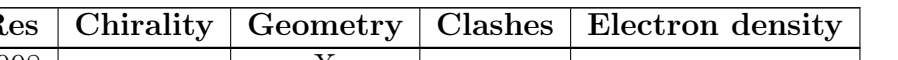
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	% 59%38%..
1	N	446	2% 54%41%..
2	B	441	2% 44%44%6%5%
2	O	441	% 49%41%5%..
3	C	380	% 68%29%. .

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

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

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

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

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

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 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
			1509	950	263	290	6			

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

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

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

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

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

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

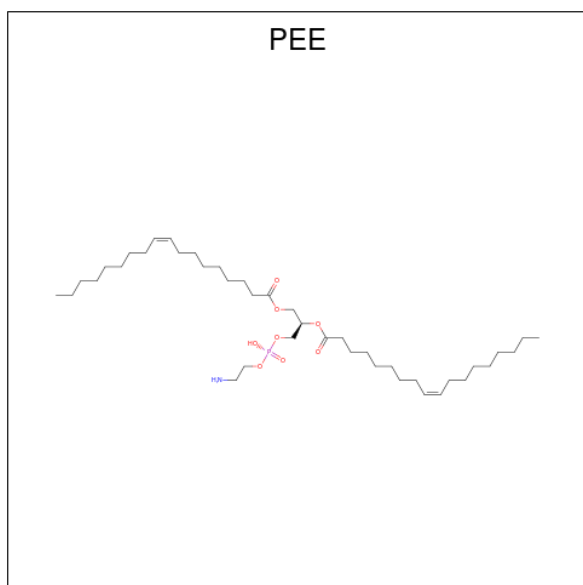
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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

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

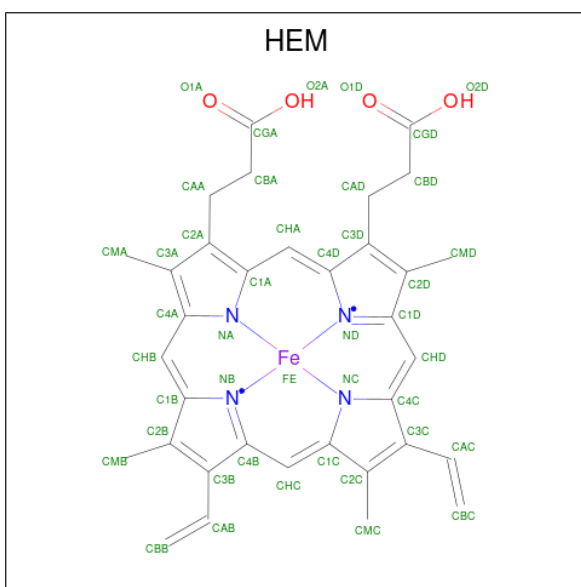
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

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



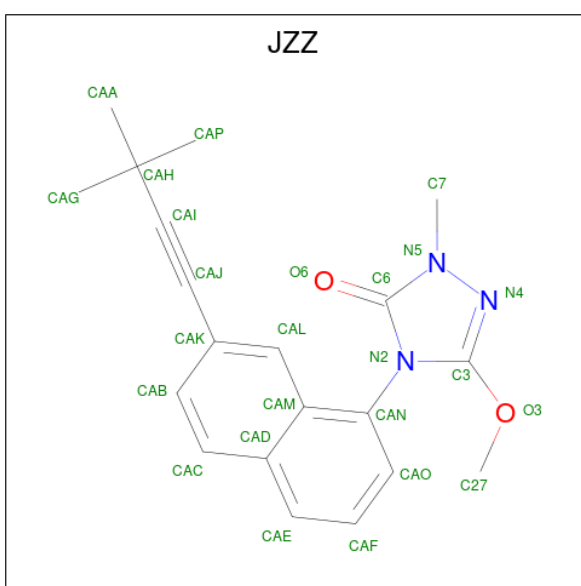
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	P	0	0
			21	12	8	1		
11	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	E	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	P	1	Total	O	P		0	0
			5	4	1			
11	R	1	Total	C	N	O	P	0
			50	40	1	8	1	

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



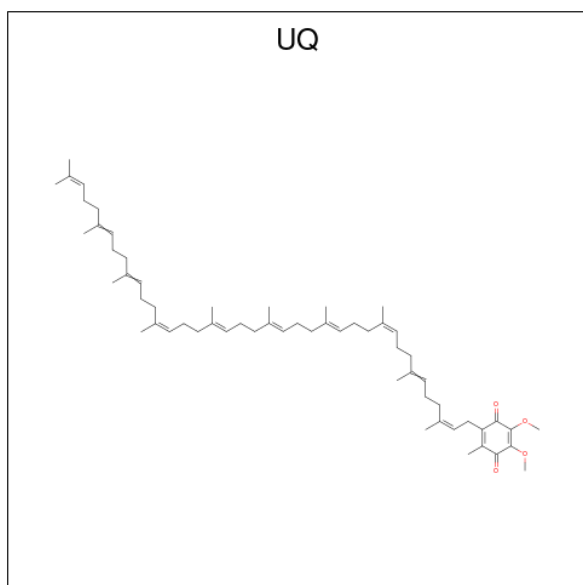
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is 4-[7-(3,3-dimethylbut-1-yn-1-yl)naphthalen-1-yl]-5-methoxy-2-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one (CCD ID: JZZ) (formula: $C_{20}H_{21}N_3O_2$).



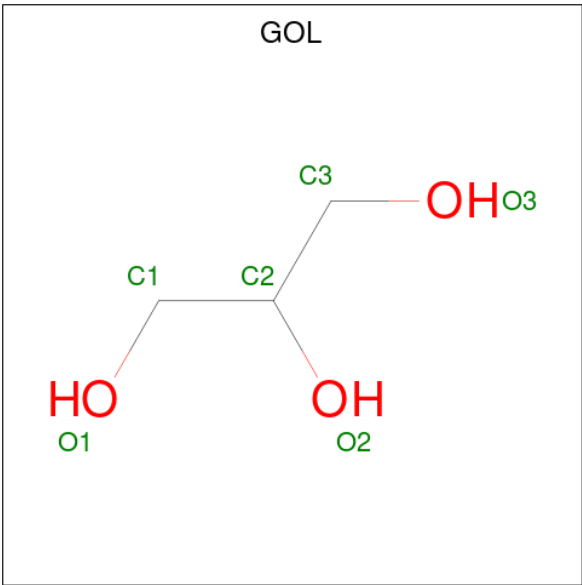
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			25	20	3	2		
13	P	1	Total	C	N	O	0	0
			25	20	3	2		

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



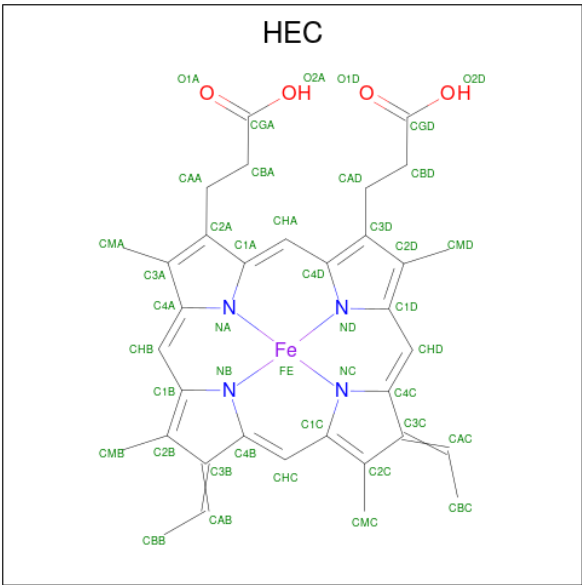
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

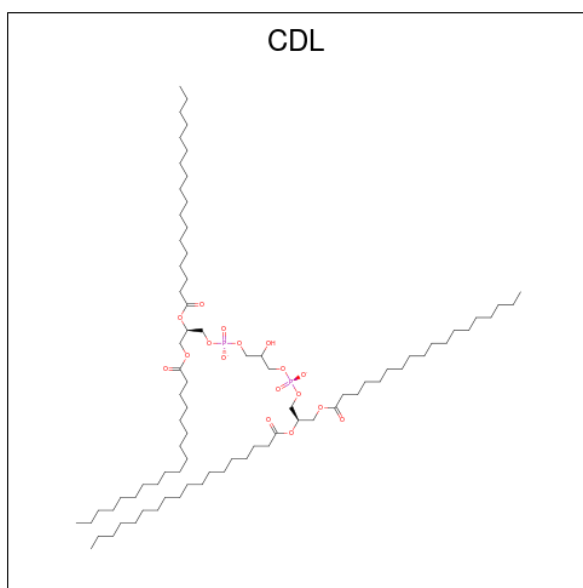


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			6	3	3		
15	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

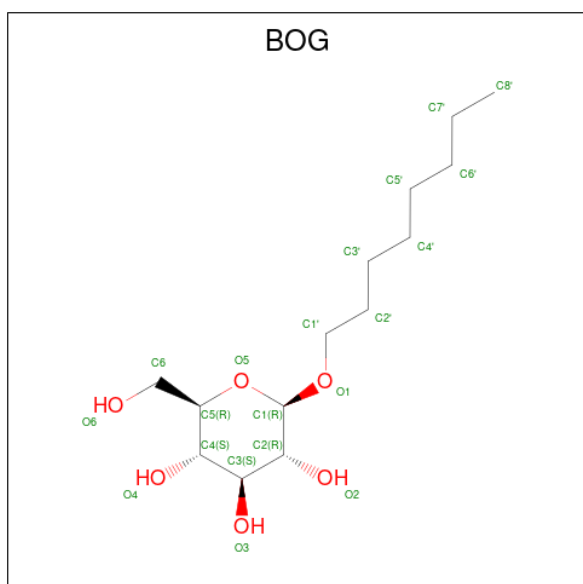


- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



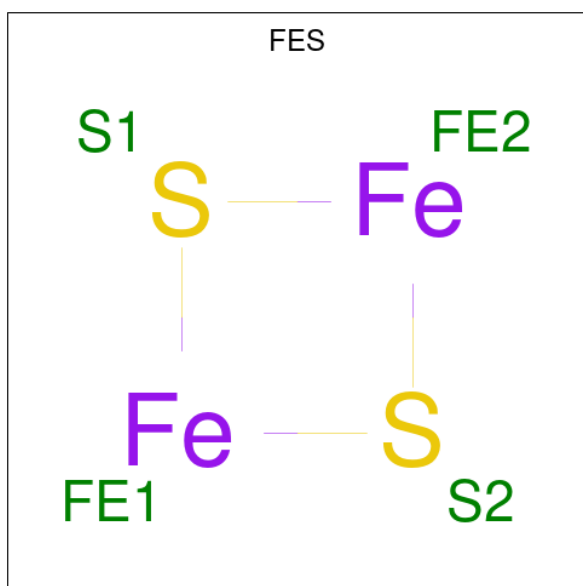
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

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



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 20 is water.

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

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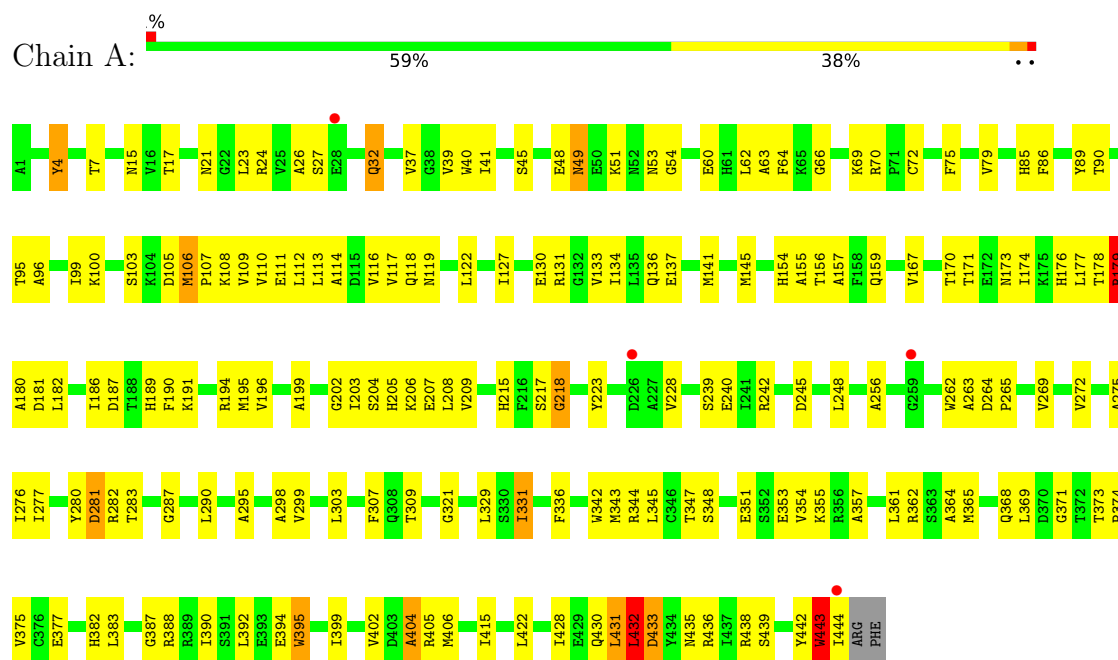
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	R	1	Total	O	0	0
			1	1		

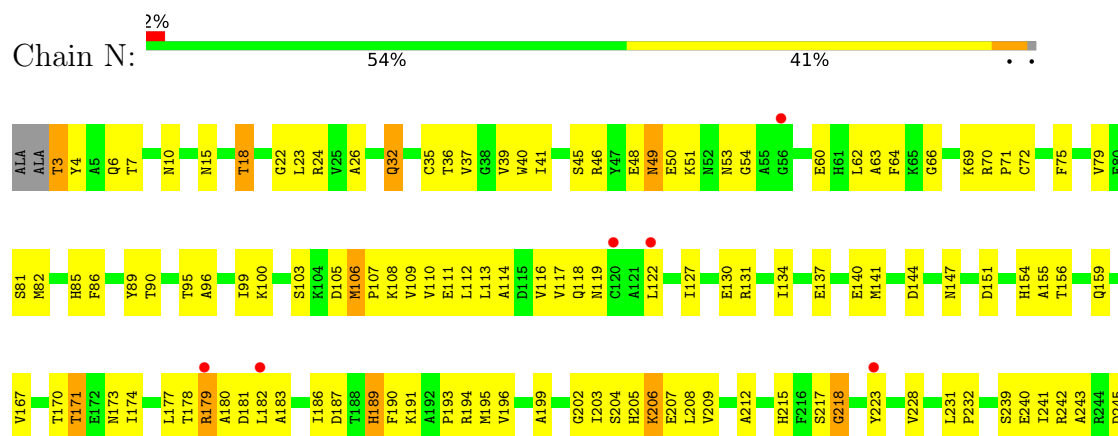
3 Residue-property plots

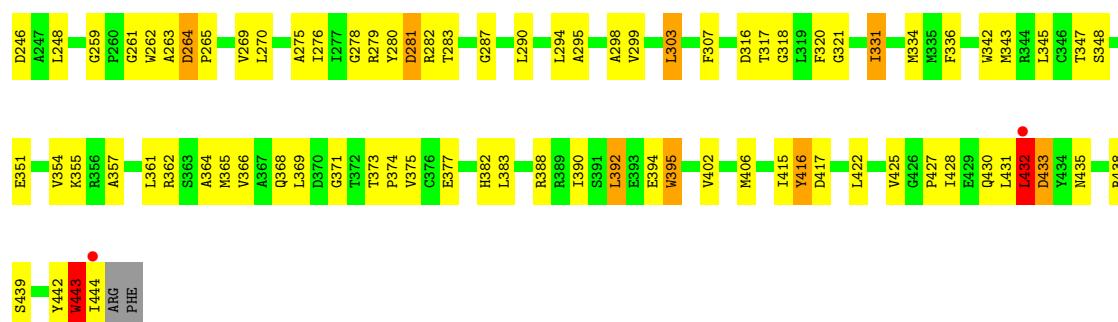
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

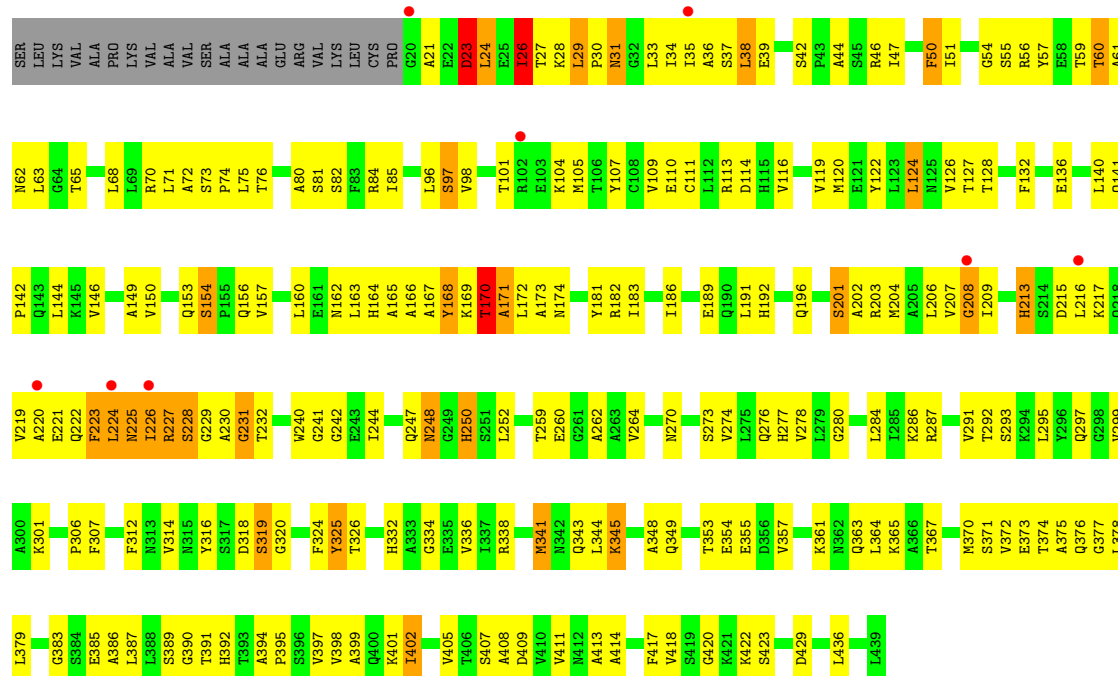
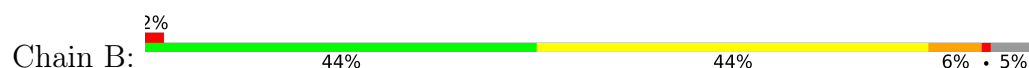


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

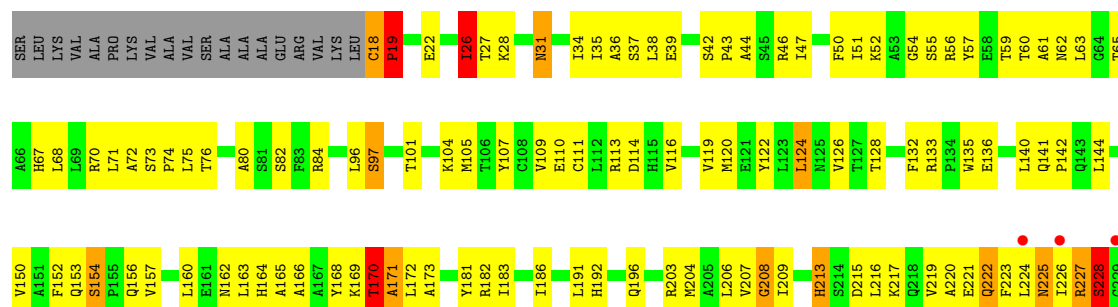


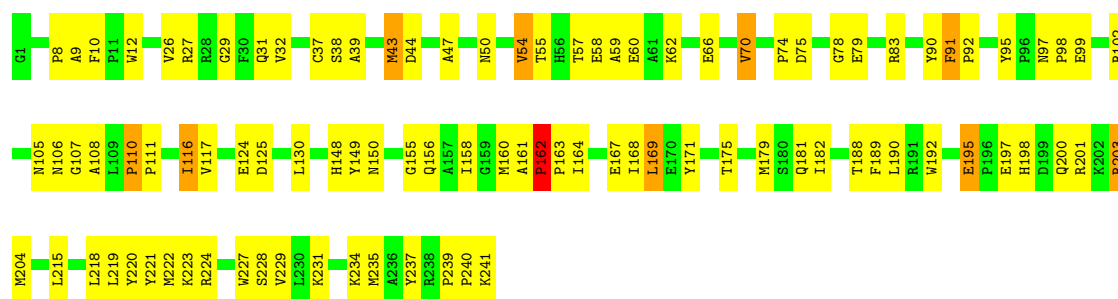


● Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

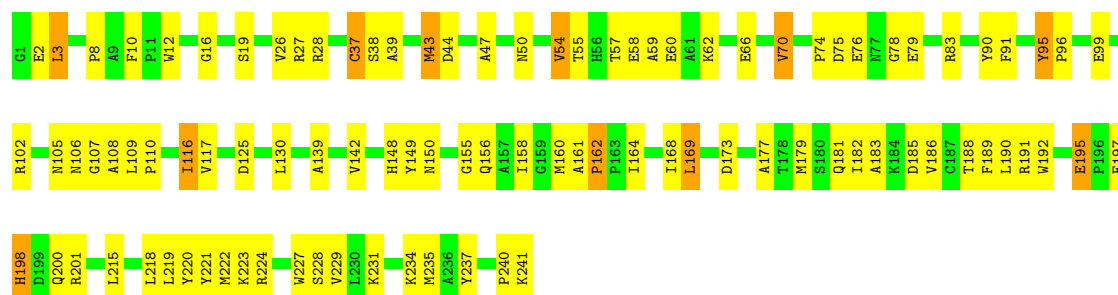


● Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

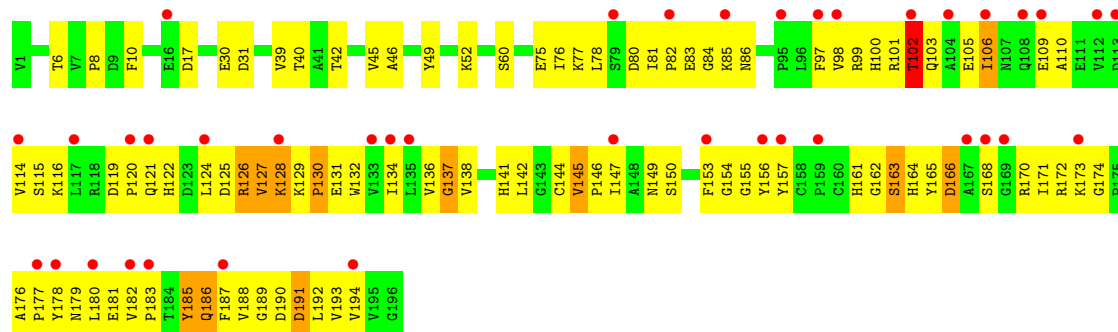




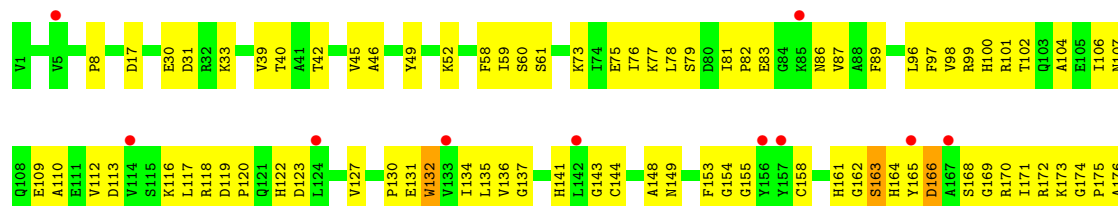
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



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

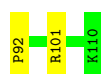
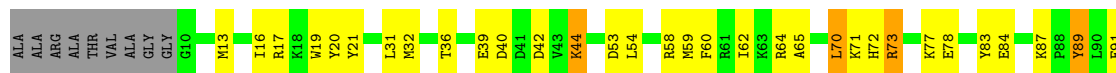


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL





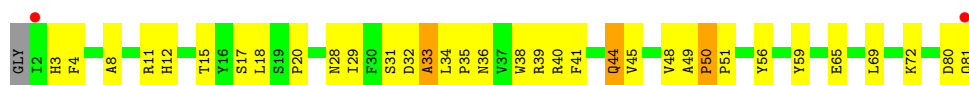
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



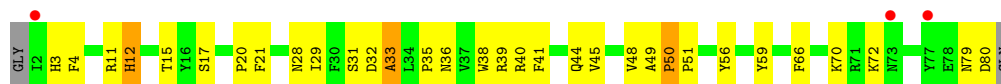
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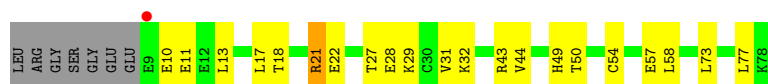
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



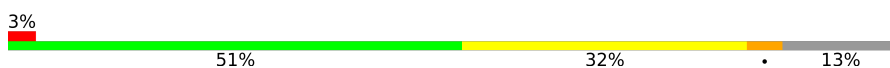
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

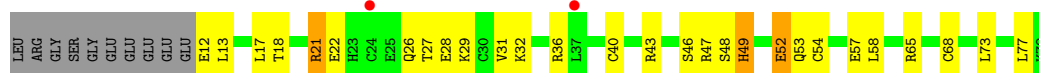


- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

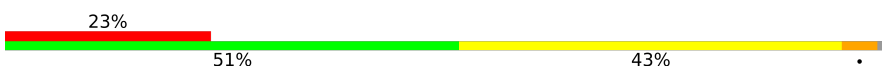


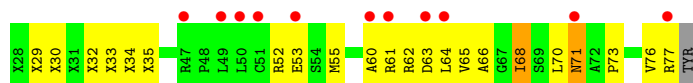
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U: 



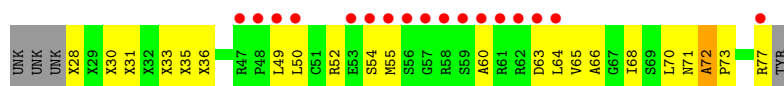
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I: 



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

Chain V: 



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

Chain J: 



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

Chain W: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.50Å 182.93Å 241.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 3.04 24.97 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.97-3.04) 99.5 (24.97-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.293 0.246 , 0.278	Depositor DCC
R_{free} test set	3273 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32645	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/3518	1.07	22/4767 (0.5%)
1	N	0.51	0/3508	1.05	25/4753 (0.5%)
2	B	0.49	0/3187	1.00	14/4321 (0.3%)
2	O	0.51	0/3202	1.01	8/4343 (0.2%)
3	C	0.69	1/3119 (0.0%)	1.07	24/4270 (0.6%)
3	P	0.59	0/3114	1.05	23/4263 (0.5%)
4	D	0.62	1/1956 (0.1%)	1.08	14/2658 (0.5%)
4	Q	0.50	0/1956	1.04	12/2658 (0.5%)
5	E	0.50	0/1547	0.94	6/2103 (0.3%)
5	R	0.47	0/1543	0.95	5/2098 (0.2%)
6	F	0.61	0/911	0.95	2/1219 (0.2%)
6	S	0.48	0/911	0.96	4/1219 (0.3%)
7	G	0.59	0/694	1.07	4/941 (0.4%)
7	T	0.49	0/684	1.04	2/929 (0.2%)
8	H	0.55	0/582	0.94	0/779
8	U	0.41	0/561	0.95	2/751 (0.3%)
9	I	0.64	0/218	0.93	0/293
9	V	0.56	0/218	1.04	2/293 (0.7%)
10	J	0.55	0/508	0.96	3/682 (0.4%)
10	W	0.50	0/490	0.92	2/660 (0.3%)
All	All	0.55	2/32427 (0.0%)	1.03	174/44000 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	204	MET	SD-CE	5.50	1.93	1.79
3	C	54	MET	SD-CE	5.03	1.92	1.79

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	227	ARG	N-CA-C	10.71	122.85	108.07
1	N	32	GLN	CA-C-N	10.54	130.21	119.56
1	N	32	GLN	C-N-CA	10.54	130.21	119.56
1	A	32	GLN	CA-C-N	9.64	129.41	119.19
1	A	32	GLN	C-N-CA	9.64	129.41	119.19
1	A	32	GLN	N-CA-C	8.65	120.82	109.83
1	A	248	LEU	CA-C-N	8.52	128.09	119.24
1	A	248	LEU	C-N-CA	8.52	128.09	119.24
4	Q	116	ILE	N-CA-C	8.49	118.57	110.42
3	P	365	ILE	N-CA-C	8.46	118.83	111.56
1	N	32	GLN	N-CA-C	8.10	120.12	109.83
3	P	205	GLY	N-CA-C	-8.06	102.58	112.33
3	C	365	ILE	N-CA-C	7.64	118.13	111.56
2	O	226	ILE	N-CA-C	-7.62	98.64	108.93
4	D	116	ILE	N-CA-C	7.44	117.56	110.42
3	C	247	SER	CA-C-N	7.42	128.07	119.47
3	C	247	SER	C-N-CA	7.42	128.07	119.47
3	P	185	LEU	N-CA-C	7.30	119.13	111.03
4	Q	195	GLU	CA-C-N	7.19	127.81	119.47
4	Q	195	GLU	C-N-CA	7.19	127.81	119.47
4	D	44	ASP	N-CA-C	7.17	120.93	111.75
1	N	415	ILE	N-CA-C	7.15	117.71	111.56
3	P	247	SER	CA-C-N	7.12	127.44	119.32
3	P	247	SER	C-N-CA	7.12	127.44	119.32
1	N	263	ALA	N-CA-C	7.10	119.88	111.71
7	T	12	HIS	N-CA-C	7.06	121.20	112.58
2	B	230	ALA	N-CA-C	-7.01	103.99	114.64
1	A	263	ALA	N-CA-C	6.96	119.72	111.71
3	C	147	ILE	N-CA-C	6.96	117.75	110.72
1	A	415	ILE	N-CA-C	6.95	117.53	111.56
1	N	348	SER	N-CA-C	6.94	119.29	110.61
4	D	162	PRO	CA-C-N	6.92	126.52	119.19
4	D	162	PRO	C-N-CA	6.92	126.52	119.19
4	D	195	GLU	CA-C-N	6.90	127.18	119.32
4	D	195	GLU	C-N-CA	6.90	127.18	119.32
7	G	12	HIS	N-CA-C	6.86	120.95	112.58
4	D	155	GLY	N-CA-C	-6.83	106.56	114.69
1	A	66	GLY	N-CA-C	6.81	120.72	112.48
3	C	205	GLY	N-CA-C	-6.80	102.75	112.81
3	P	147	ILE	N-CA-C	6.71	117.50	110.72
1	N	66	GLY	N-CA-C	6.62	120.49	112.48
3	C	134	LEU	N-CA-C	6.59	121.82	113.25
10	W	13	LEU	N-CA-C	6.56	121.20	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	145	VAL	N-CA-C	6.55	114.03	107.55
1	A	348	SER	N-CA-C	6.50	118.08	110.41
1	A	415	ILE	CB-CA-C	-6.44	105.32	111.44
5	E	182	VAL	CA-C-N	6.41	126.59	120.31
5	E	182	VAL	C-N-CA	6.41	126.59	120.31
4	Q	162	PRO	CA-C-N	6.36	125.93	119.19
4	Q	162	PRO	C-N-CA	6.36	125.93	119.19
10	J	14	PHE	N-CA-C	6.36	120.87	113.18
5	E	106	ILE	N-CA-C	-6.36	105.03	112.98
2	O	225	ASN	N-CA-C	6.33	121.84	114.62
3	C	328	LEU	N-CA-C	-6.33	104.31	111.14
2	B	375	ALA	N-CA-C	-6.32	104.39	111.28
3	C	207	ASN	N-CA-C	-6.31	101.44	110.59
4	Q	44	ASP	N-CA-C	6.30	119.82	111.75
3	P	116	THR	N-CA-C	-6.29	104.43	111.28
1	A	432	LEU	N-CA-C	6.16	118.14	108.96
2	O	375	ALA	N-CA-C	-6.15	104.57	111.28
10	J	13	LEU	N-CA-C	6.15	120.63	111.96
3	P	378	LEU	N-CA-C	-6.15	105.42	113.17
3	C	378	LEU	N-CA-C	-6.13	105.44	113.17
1	N	119	ASN	N-CA-C	6.12	120.34	112.26
3	P	134	LEU	N-CA-C	6.09	121.17	113.25
1	N	415	ILE	CB-CA-C	-6.08	105.67	111.44
3	P	110	TYR	N-CA-C	-6.06	103.01	110.65
4	D	110	PRO	CA-C-N	6.04	126.38	119.92
4	D	110	PRO	C-N-CA	6.04	126.38	119.92
6	S	15	ARG	N-CA-C	-6.03	104.91	112.93
3	C	185	LEU	N-CA-C	6.02	118.74	111.40
1	N	248	LEU	CA-C-N	6.00	125.48	119.24
1	N	248	LEU	C-N-CA	6.00	125.48	119.24
5	R	182	VAL	CA-C-N	6.00	126.19	120.31
5	R	182	VAL	C-N-CA	6.00	126.19	120.31
3	C	90	PHE	N-CA-C	-5.97	104.77	111.28
2	O	213	HIS	N-CA-C	5.94	118.52	111.33
3	P	226	SER	N-CA-C	-5.94	104.81	111.28
2	O	170	THR	N-CA-C	5.93	116.07	108.24
7	G	50	PRO	N-CA-C	5.93	117.93	110.70
1	A	119	ASN	N-CA-C	5.92	120.21	111.87
3	C	261	ASN	CA-C-N	5.90	125.58	119.56
3	C	261	ASN	C-N-CA	5.90	125.58	119.56
3	P	143	GLY	N-CA-C	-5.90	105.35	112.49
5	E	17	ASP	N-CA-C	5.89	119.73	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	THR	N-CA-C	5.89	121.12	113.88
10	W	14	PHE	N-CA-C	5.85	120.25	113.18
6	S	89	TYR	N-CA-C	5.82	119.20	111.75
3	C	226	SER	N-CA-C	-5.75	105.01	111.28
2	B	223	PHE	N-CA-C	5.75	120.00	112.13
3	P	257	PHE	N-CA-C	-5.74	105.58	112.59
1	A	331	ILE	CB-CA-C	-5.74	104.63	111.97
3	P	27	ASN	N-CA-C	5.70	119.54	112.59
7	T	50	PRO	N-CA-C	5.70	117.65	110.70
1	N	347	THR	N-CA-C	5.69	120.88	113.88
1	A	428	ILE	N-CA-C	5.68	121.17	109.34
6	F	89	TYR	N-CA-C	5.67	119.01	111.75
1	N	428	ILE	N-CA-C	5.66	121.11	109.34
1	A	179	ARG	N-CA-C	-5.66	104.49	111.33
3	C	143	GLY	N-CA-C	-5.63	105.68	112.49
1	N	432	LEU	N-CA-C	5.63	117.35	108.96
2	B	213	HIS	N-CA-C	5.62	118.14	111.33
2	B	127	THR	N-CA-C	5.60	118.31	111.82
5	E	126	ARG	N-CA-C	5.56	116.50	107.32
2	B	227	ARG	N-CA-C	5.56	118.46	109.79
5	R	17	ASP	N-CA-C	5.55	119.31	112.54
3	C	305	ILE	CB-CA-C	-5.52	108.46	113.70
1	A	431	LEU	CA-C-N	-5.51	112.84	121.87
1	A	431	LEU	C-N-CA	-5.51	112.84	121.87
4	Q	95	TYR	CA-C-N	5.51	125.03	119.19
4	Q	95	TYR	C-N-CA	5.51	125.03	119.19
3	P	207	ASN	N-CA-C	-5.49	102.62	110.59
1	N	179	ARG	N-CA-C	-5.48	104.70	111.33
3	P	319	ARG	CA-C-N	5.48	125.30	119.28
3	P	319	ARG	C-N-CA	5.48	125.30	119.28
2	B	174	ASN	CA-C-N	5.47	125.42	119.78
2	B	174	ASN	C-N-CA	5.47	125.42	119.78
4	D	223	LYS	N-CA-C	-5.46	105.23	111.07
3	C	110	TYR	N-CA-C	-5.46	103.78	110.65
3	C	289	LEU	N-CA-C	5.46	117.31	111.36
6	S	109	LYS	N-CA-C	-5.45	104.75	111.40
3	C	72	ARG	N-CA-C	5.44	119.09	112.23
1	N	331	ILE	CB-CA-C	-5.42	105.04	111.97
4	D	91	PHE	CA-C-N	5.40	125.66	119.83
4	D	91	PHE	C-N-CA	5.40	125.66	119.83
3	P	107	SER	N-CA-C	-5.40	105.56	111.82
3	P	328	LEU	N-CA-C	-5.39	105.48	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	THR	N-CA-C	-5.38	102.50	110.46
2	B	345	LYS	N-CA-C	-5.37	105.34	111.14
1	A	4	TYR	N-CA-C	-5.36	105.44	111.28
8	U	48	SER	N-CA-C	5.36	117.31	110.61
3	P	261	ASN	CA-C-N	5.35	125.02	119.56
3	P	261	ASN	C-N-CA	5.35	125.02	119.56
1	N	259	GLY	CA-C-N	5.34	125.03	119.64
1	N	259	GLY	C-N-CA	5.34	125.03	119.64
3	C	27	ASN	N-CA-C	5.33	119.10	112.59
2	O	345	LYS	N-CA-C	-5.32	105.39	111.14
1	A	256	ALA	N-CA-C	5.30	117.12	109.07
7	G	44	GLN	N-CA-C	5.29	119.74	113.12
2	B	23	ASP	N-CA-C	5.29	122.07	110.80
4	D	95	TYR	CA-C-N	5.29	124.61	118.85
4	D	95	TYR	C-N-CA	5.29	124.61	118.85
1	A	329	LEU	N-CA-C	5.28	119.35	113.02
2	B	326	THR	N-CA-C	5.27	117.66	108.76
4	Q	91	PHE	CA-C-N	5.26	125.17	119.76
4	Q	91	PHE	C-N-CA	5.26	125.17	119.76
1	N	303	LEU	N-CA-C	5.25	117.91	111.82
2	B	413	ALA	N-CA-C	-5.22	104.84	111.11
3	C	319	ARG	CA-C-N	5.22	125.27	119.32
3	C	319	ARG	C-N-CA	5.22	125.27	119.32
1	N	278	GLY	N-CA-C	5.21	120.56	111.50
2	O	228	SER	N-CA-C	5.21	121.89	110.80
8	U	46	SER	N-CA-C	5.20	118.48	112.97
9	V	72	ALA	CA-C-N	5.20	125.12	119.76
9	V	72	ALA	C-N-CA	5.20	125.12	119.76
4	Q	155	GLY	N-CA-C	-5.20	108.51	114.69
2	B	168	TYR	N-CA-C	5.19	116.17	108.86
3	C	111	LYS	N-CA-C	5.18	121.82	110.80
5	R	143	GLY	N-CA-C	5.16	125.42	113.18
5	R	132	TRP	N-CA-C	5.15	116.79	108.34
1	N	392	LEU	N-CA-C	-5.13	105.69	111.28
10	J	54	HIS	N-CA-C	5.13	116.68	111.14
6	F	39	GLU	N-CA-C	5.12	117.43	108.52
3	C	109	LEU	N-CA-C	-5.12	107.10	113.19
1	N	416	TYR	N-CA-C	5.09	117.93	110.30
1	N	151	ASP	N-CA-C	-5.08	105.65	111.14
4	Q	173	ASP	N-CA-C	-5.06	106.35	112.88
7	G	8	ALA	N-CA-C	5.06	116.76	109.07
6	S	14	ASP	N-CA-C	-5.05	107.18	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	264	ASP	N-CA-C	5.04	116.91	109.50
2	B	170	THR	N-CA-C	5.03	114.47	107.73
1	N	189	HIS	N-CA-C	5.03	119.41	113.12
3	P	272	GLU	N-CA-C	-5.03	103.90	110.53
3	P	209	PRO	N-CA-C	5.00	121.06	113.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3362	150	0
1	N	3437	0	3349	171	0
2	B	3133	0	3130	232	0
2	O	3147	0	3146	221	0
3	C	3017	0	3063	96	0
3	P	3012	0	3058	102	0
4	D	1898	0	1846	82	0
4	Q	1898	0	1846	78	0
5	E	1513	0	1478	113	0
5	R	1509	0	1474	109	0
6	F	891	0	893	25	0
6	S	891	0	893	35	0
7	G	672	0	653	32	0
7	T	662	0	645	33	0
8	H	574	0	548	20	0
8	U	553	0	535	26	0
9	I	287	0	249	30	0
9	V	277	0	250	33	0
10	J	497	0	490	17	0
10	W	479	0	478	21	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	P	54	0	72	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	50	0	77	1	0
12	C	86	0	60	6	0
12	P	86	0	60	5	0
13	C	25	0	21	2	0
13	P	25	0	21	7	0
14	C	19	0	17	2	0
14	P	19	0	17	3	0
15	C	6	0	8	1	0
15	P	6	0	8	1	0
16	D	43	0	30	0	0
16	Q	43	0	30	1	0
17	D	42	0	28	3	0
17	G	40	0	24	5	0
17	Q	42	0	28	1	0
17	T	40	0	24	5	0
18	D	33	0	39	2	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	0	0
20	R	1	0	0	0	0
All	All	32645	0	32162	1496	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 23.

All (1496) 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.21	1.16
9:V:35:UNK:HG3	9:V:36:UNK:H	1.22	1.05
2:B:353:THR:HG22	2:B:355:GLU:H	1.19	1.04
2:O:76:THR:HG22	2:O:82:SER:H	1.22	1.04
2:O:353:THR:HG22	2:O:355:GLU:H	1.21	1.04
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.44	0.99
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.26	0.98
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.48	0.95
2:B:76:THR:HG22	2:B:82:SER:H	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.34	0.93
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.84	0.92
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.30	0.92
4:D:47:ALA:H	4:D:50:ASN:HD22	1.13	0.91
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.16	0.91
1:A:178:THR:HG22	1:A:180:ALA:H	1.36	0.91
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.33	0.91
1:N:178:THR:HG22	1:N:180:ALA:H	1.36	0.91
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.01	0.91
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.52	0.89
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.54	0.87
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.87
7:T:41:PHE:O	7:T:45:VAL:HG23	1.74	0.87
5:E:127:VAL:HG12	5:E:128:LYS:H	1.39	0.86
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.89	0.86
2:O:154:SER:O	2:O:157:VAL:HG12	1.75	0.86
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.57	0.86
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.11	0.86
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.76	0.85
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.42	0.85
2:B:154:SER:O	2:B:157:VAL:HG12	1.77	0.85
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.59	0.85
3:P:9:HIS:HD2	3:P:12:LEU:H	1.25	0.85
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.12	0.84
7:G:41:PHE:O	7:G:45:VAL:HG23	1.79	0.83
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.13	0.83
4:D:231:LYS:O	6:F:71:LYS:HE3	1.79	0.83
3:C:9:HIS:HD2	3:C:12:LEU:H	1.24	0.83
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.60	0.82
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.60	0.82
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.61	0.82
2:B:47:ILE:HD13	2:B:120:MET:CE	2.10	0.82
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.61	0.82
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.80	0.82
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.63	0.81
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.63	0.81
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.62	0.80
1:N:170:THR:HG22	1:N:171:THR:H	1.47	0.80
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.62	0.80
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.17	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.64	0.79
9:I:70:LEU:HD23	9:I:71:ASN:H	1.45	0.79
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.62	0.79
1:A:402:VAL:HA	1:A:406:MET:HE2	1.64	0.79
4:D:57:THR:HB	4:D:60:GLU:HG3	1.65	0.79
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.18	0.78
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.19	0.78
2:O:219:VAL:O	2:O:223:PHE:HB2	1.84	0.78
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.65	0.78
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.66	0.78
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.66	0.77
1:N:187:ASP:O	1:N:191:LYS:HE3	1.85	0.77
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.67	0.77
2:O:27:THR:HG22	2:O:28:LYS:N	2.00	0.77
2:O:47:ILE:HD13	2:O:120:MET:CE	2.13	0.77
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.66	0.77
4:D:57:THR:HG22	4:D:59:ALA:H	1.49	0.77
1:N:112:LEU:O	1:N:116:VAL:HG23	1.84	0.77
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.85	0.77
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.66	0.77
2:O:422:LYS:O	2:O:436:LEU:HD21	1.82	0.77
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.48	0.76
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.66	0.76
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.50	0.76
1:A:295:ALA:O	1:A:299:VAL:HG23	1.86	0.76
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.66	0.76
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.65	0.76
1:N:402:VAL:HA	1:N:406:MET:HE2	1.68	0.76
1:A:103:SER:HB3	1:A:202:GLY:O	1.87	0.75
1:N:10:ASN:HD21	2:O:18:CYS:N	1.83	0.75
1:N:295:ALA:O	1:N:299:VAL:HG23	1.85	0.75
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.21	0.75
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.04	0.75
4:D:164:ILE:O	4:D:179:MET:HE2	1.87	0.75
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.52	0.75
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.69	0.75
2:O:221:GLU:HG3	2:O:222:GLN:H	1.50	0.75
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.74
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.68	0.74
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.69	0.74
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ASP:O	1:N:109:VAL:HG23	1.87	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.22	0.74
2:O:156:GLN:HE22	9:V:77:ARG:C	1.95	0.74
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.86	0.74
2:B:422:LYS:O	2:B:436:LEU:HD21	1.87	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.70	0.74
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.87	0.74
1:A:178:THR:HB	1:A:181:ASP:OD1	1.87	0.73
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.51	0.73
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.89	0.73
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.89	0.73
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.70	0.73
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.07	0.73
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.24	0.73
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.71	0.72
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.71	0.72
2:O:248:ASN:HD22	2:O:248:ASN:C	1.97	0.72
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.71	0.72
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.54	0.72
5:E:190:ASP:C	5:E:192:LEU:H	1.95	0.72
2:B:38:LEU:HD12	2:B:39:GLU:N	2.05	0.72
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.19	0.72
2:O:338:ARG:HG3	2:O:338:ARG:NH1	1.98	0.72
2:O:192:HIS:O	2:O:196:GLN:HG3	1.90	0.72
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.71	0.72
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.25	0.72
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.70	0.72
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.72	0.72
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.90	0.72
2:B:122:TYR:O	2:B:126:VAL:HG23	1.90	0.72
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.71	0.71
1:N:170:THR:HG22	1:N:171:THR:N	2.05	0.71
2:B:31:ASN:HD22	2:B:31:ASN:N	1.88	0.71
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.20	0.71
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.71	0.71
4:Q:222:MET:HE3	5:R:40:THR:OG1	1.90	0.71
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.71	0.71
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.53	0.71
2:B:27:THR:HG22	2:B:28:LYS:N	2.06	0.71
10:W:60:GLU:O	10:W:60:GLU:HG2	1.89	0.71
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:361:LYS:O	2:O:365:LYS:HG3	1.92	0.70
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.04	0.70
4:D:62:LYS:O	4:D:66:GLU:HG3	1.91	0.70
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.55	0.70
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.21	0.70
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.06	0.70
3:P:238:THR:HB	3:P:239:PRO:HD3	1.73	0.70
6:S:91:GLU:O	6:S:95:LYS:HG3	1.91	0.70
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.26	0.70
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.74	0.70
4:D:47:ALA:H	4:D:50:ASN:ND2	1.89	0.70
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.74	0.70
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.57	0.69
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.07	0.69
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.74	0.69
6:F:13:MET:HA	6:F:13:MET:HE2	1.75	0.69
3:P:216:SER:HB3	6:S:59:MET:HE2	1.72	0.69
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.74	0.69
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.75	0.69
4:Q:164:ILE:O	4:Q:179:MET:HE2	1.92	0.69
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.58	0.69
1:N:49:ASN:HD21	1:N:51:LYS:HE3	1.57	0.69
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.56	0.69
2:B:306:PRO:HA	9:I:52:ARG:CG	2.22	0.69
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.74	0.69
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.75	0.68
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.73	0.68
1:A:187:ASP:O	1:A:191:LYS:HE3	1.93	0.68
2:B:150:VAL:O	2:B:153:GLN:HG3	1.94	0.68
1:N:178:THR:HB	1:N:181:ASP:OD1	1.93	0.68
2:B:164:HIS:O	2:B:173:ALA:HA	1.94	0.68
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.28	0.68
1:A:49:ASN:HD21	1:A:51:LYS:HE3	1.59	0.68
7:T:29:ILE:O	7:T:33:ALA:HB3	1.93	0.68
2:B:202:ALA:HB3	2:B:229:GLY:O	1.94	0.68
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.58	0.68
1:N:402:VAL:HG22	1:N:406:MET:CE	2.23	0.68
5:R:102:THR:O	5:R:106:ILE:HG13	1.94	0.68
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.75	0.68
2:B:399:ALA:O	2:B:402:ILE:HG22	1.94	0.68
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:127:VAL:HG12	5:E:128:LYS:N	2.08	0.68
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.74	0.68
2:O:399:ALA:O	2:O:402:ILE:HG22	1.94	0.68
1:A:112:LEU:O	1:A:116:VAL:HG23	1.93	0.68
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.75	0.68
1:A:170:THR:HG22	1:A:171:THR:H	1.59	0.68
5:E:86:ASN:OD1	5:E:99:ARG:HB2	1.94	0.68
2:O:341:MET:CE	2:O:417:PHE:HE2	2.06	0.67
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.29	0.67
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.76	0.67
1:A:343:MET:HB3	1:A:444:ILE:HA	1.75	0.67
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.77	0.67
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.75	0.67
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.59	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.10	0.67
1:A:137:GLU:O	1:A:141:MET:HG3	1.95	0.67
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.41	0.67
3:C:238:THR:HB	3:C:239:PRO:HD3	1.75	0.67
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.22	0.67
1:N:178:THR:HG22	1:N:179:ARG:N	2.09	0.66
1:A:178:THR:HG22	1:A:179:ARG:N	2.09	0.66
9:I:70:LEU:HD23	9:I:71:ASN:N	2.10	0.66
1:N:371:GLY:O	1:N:375:VAL:HG23	1.96	0.66
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.35	0.66
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.61	0.66
2:B:248:ASN:C	2:B:248:ASN:HD22	2.03	0.66
2:O:122:TYR:O	2:O:126:VAL:HG23	1.94	0.66
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.78	0.66
2:B:318:ASP:O	2:B:319:SER:HB2	1.96	0.66
8:H:28:GLU:O	8:H:32:LYS:HG3	1.96	0.66
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.78	0.66
2:B:361:LYS:O	2:B:365:LYS:HG3	1.96	0.66
1:A:105:ASP:O	1:A:109:VAL:HG23	1.96	0.66
9:V:70:LEU:HD23	9:V:71:ASN:N	2.12	0.66
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.29	0.65
1:N:182:LEU:O	1:N:186:ILE:HG13	1.96	0.65
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.96	0.65
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.11	0.65
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.31	0.65
2:O:156:GLN:NE2	9:V:77:ARG:C	2.54	0.65
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:28:GLU:O	8:U:32:LYS:HG3	1.96	0.65
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.76	0.65
1:N:106:MET:O	1:N:110:VAL:HG23	1.96	0.65
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.31	0.65
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.32	0.65
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.32	0.65
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.12	0.65
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.32	0.65
3:C:377:MET:HE2	6:F:20:TYR:CG	2.32	0.65
5:R:86:ASN:OD1	5:R:99:ARG:HB2	1.97	0.65
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.12	0.65
5:E:109:GLU:OE2	5:E:153:PHE:HB3	1.95	0.65
9:V:64:LEU:HD12	9:V:77:ARG:O	1.97	0.65
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.78	0.65
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.32	0.65
8:U:18:THR:O	8:U:22:GLU:HG3	1.95	0.65
2:B:27:THR:HG22	2:B:28:LYS:H	1.61	0.64
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.77	0.64
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.32	0.64
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.32	0.64
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.78	0.64
9:V:35:UNK:HG3	9:V:36:UNK:N	2.04	0.64
2:B:215:ASP:O	2:B:219:VAL:HG23	1.97	0.64
5:E:155:GLY:HA3	5:E:166:ASP:O	1.98	0.64
1:N:103:SER:HB3	1:N:202:GLY:O	1.97	0.64
2:O:318:ASP:O	2:O:319:SER:HB2	1.98	0.64
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.78	0.64
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.61	0.64
3:C:101:ARG:HD2	3:C:101:ARG:C	2.22	0.64
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.32	0.64
7:T:79:ASN:O	7:T:80:ASP:HB2	1.98	0.64
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.33	0.64
7:G:29:ILE:O	7:G:33:ALA:HB3	1.98	0.64
5:R:169:GLY:O	5:R:179:ASN:HB3	1.97	0.64
3:P:147:ILE:HD11	13:P:3001:JZZ:CAB	2.27	0.64
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.33	0.64
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.33	0.63
5:E:163:SER:HA	5:E:174:GLY:HA3	1.80	0.63
2:O:38:LEU:HD12	2:O:39:GLU:N	2.13	0.63
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.63	0.63
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.33	0.63
3:C:81:ARG:HH22	15:C:2011:GOL:H11	1.63	0.63
2:B:341:MET:HE2	2:B:341:MET:HA	1.81	0.63
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.23	0.63
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.27	0.63
2:B:252:LEU:HD13	9:I:55:MET:HE3	1.80	0.63
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.79	0.63
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.14	0.63
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.32	0.63
2:O:273:SER:O	2:O:276:GLN:HB3	1.99	0.63
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.63
2:O:31:ASN:N	2:O:31:ASN:HD22	1.97	0.63
6:S:95:LYS:O	6:S:99:ARG:HG3	1.99	0.63
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.34	0.62
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.64	0.62
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.63	0.62
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.63	0.62
1:A:371:GLY:O	1:A:375:VAL:HG23	1.98	0.62
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.99	0.62
5:E:187:PHE:C	5:E:189:GLY:H	2.06	0.62
1:N:45:SER:HA	1:N:48:GLU:HG3	1.81	0.62
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.62
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.25	0.62
2:O:150:VAL:O	2:O:153:GLN:HG3	1.99	0.62
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.34	0.62
1:A:388:ARG:NH2	1:A:390:ILE:HG12	2.14	0.62
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.62
2:B:341:MET:CE	2:B:417:PHE:HE2	2.08	0.62
1:N:382:HIS:HB3	1:N:388:ARG:O	1.99	0.62
1:N:178:THR:CG2	1:N:179:ARG:N	2.63	0.62
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.81	0.62
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.30	0.62
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.82	0.62
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.30	0.62
3:P:199:THR:HA	18:P:2010:BOG:O1	2.00	0.62
1:N:137:GLU:O	1:N:141:MET:HG3	1.99	0.61
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.82	0.61
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.15	0.61
9:I:34:UNK:HG3	9:I:35:UNK:N	2.14	0.61
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.36	0.61
2:B:192:HIS:O	2:B:196:GLN:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.80	0.61
5:E:130:PRO:HG2	5:E:131:GLU:H	1.65	0.61
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.65	0.61
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.81	0.61
1:N:7:THR:HG21	2:O:113:ARG:CD	2.30	0.61
2:O:62:ASN:O	2:O:65:THR:HG22	2.00	0.61
5:R:155:GLY:HA3	5:R:166:ASP:O	2.00	0.61
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.16	0.61
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.35	0.61
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.82	0.61
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.82	0.61
5:E:106:ILE:C	5:E:110:ALA:HB3	2.26	0.61
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.27	0.61
1:A:178:THR:CG2	1:A:179:ARG:N	2.64	0.61
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.46	0.61
3:P:92:PHE:O	3:P:95:ILE:HG22	2.01	0.61
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.48	0.61
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.82	0.60
2:B:292:THR:HG22	2:B:292:THR:O	2.01	0.60
5:R:165:TYR:HA	5:R:170:ARG:O	2.01	0.60
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.31	0.60
2:B:31:ASN:H	2:B:31:ASN:ND2	1.99	0.60
3:C:147:ILE:HD11	13:C:2001:JZZ:CAB	2.30	0.60
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.60
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.83	0.60
2:O:215:ASP:O	2:O:219:VAL:HG23	2.00	0.60
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.30	0.60
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.17	0.60
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.83	0.60
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.01	0.60
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.32	0.60
2:B:201:SER:OG	2:B:228:SER:HA	2.02	0.60
2:B:372:VAL:HG12	2:B:372:VAL:O	2.01	0.60
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.84	0.60
3:P:52:LEU:HD13	12:P:501:HEM:HBD1	1.84	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.02	0.60
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.37	0.60
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.84	0.60
4:D:222:MET:HE3	5:E:40:THR:OG1	2.02	0.60
2:O:164:HIS:O	2:O:173:ALA:HA	2.02	0.60
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.82	0.60
2:O:76:THR:HG22	2:O:82:SER:N	2.05	0.60
8:U:27:THR:O	8:U:31:VAL:HG23	2.02	0.60
4:D:37:CYS:C	4:D:39:ALA:H	2.10	0.60
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.67	0.60
9:I:33:UNK:HG2	9:I:73:PRO:CB	2.27	0.60
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.84	0.60
5:E:84:GLY:N	5:E:102:THR:HG23	2.17	0.60
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.01	0.60
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.66	0.60
2:O:357:VAL:O	2:O:361:LYS:HG3	2.02	0.60
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.67	0.60
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.36	0.59
8:H:18:THR:O	8:H:22:GLU:HG3	2.02	0.59
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.02	0.59
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.84	0.59
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.27	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.84	0.59
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.36	0.59
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.59
1:N:388:ARG:NH2	1:N:390:ILE:HG12	2.17	0.59
2:O:170:THR:O	2:O:172:LEU:N	2.36	0.59
7:T:40:ARG:HB3	17:T:3004:CDL:HA32	1.84	0.59
1:A:182:LEU:O	1:A:186:ILE:HG13	2.03	0.59
1:N:90:THR:O	1:N:167:VAL:HG11	2.02	0.59
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.84	0.59
1:A:106:MET:O	1:A:110:VAL:HG23	2.03	0.59
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.66	0.59
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.37	0.59
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.18	0.59
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.31	0.59
8:H:27:THR:O	8:H:31:VAL:HG23	2.03	0.59
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.84	0.59
5:E:116:LYS:HD2	5:E:116:LYS:N	2.18	0.59
9:I:29:UNK:O	9:I:30:UNK:HB2	2.02	0.59
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.85	0.59
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.68	0.59
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.23	0.59
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.84	0.59
9:V:70:LEU:HD23	9:V:71:ASN:H	1.67	0.59
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:325:TYR:HD1	9:V:60:ALA:HB3	1.68	0.58
2:O:372:VAL:HG12	2:O:372:VAL:O	2.03	0.58
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.02	0.58
2:O:27:THR:CG2	2:O:28:LYS:H	2.15	0.58
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.86	0.58
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.85	0.58
2:B:169:LYS:O	2:B:170:THR:HG23	2.02	0.58
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.84	0.58
3:C:9:HIS:CD2	3:C:12:LEU:H	2.15	0.58
1:N:361:LEU:O	1:N:364:ALA:HB3	2.03	0.58
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.38	0.58
9:V:49:LEU:HD22	9:V:54:SER:O	2.04	0.58
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.85	0.58
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.86	0.58
2:B:357:VAL:O	2:B:361:LYS:HG3	2.03	0.58
5:E:84:GLY:N	5:E:100:HIS:O	2.36	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.03	0.58
2:O:402:ILE:C	2:O:402:ILE:HD13	2.29	0.58
1:A:7:THR:HG21	2:B:113:ARG:CD	2.33	0.58
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.68	0.58
5:R:52:LYS:HD3	5:R:52:LYS:C	2.29	0.58
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.86	0.58
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.38	0.58
5:E:165:TYR:HA	5:E:170:ARG:O	2.03	0.58
1:N:269:VAL:HG22	1:N:406:MET:HE3	1.85	0.58
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.69	0.58
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.85	0.58
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.69	0.58
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.85	0.58
2:B:225:ASN:O	2:B:226:ILE:C	2.47	0.57
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.86	0.57
2:B:26:ILE:HG12	2:B:26:ILE:O	2.02	0.57
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.84	0.57
1:N:15:ASN:O	1:N:26:ALA:HA	2.05	0.57
2:O:417:PHE:O	2:O:422:LYS:HE3	2.04	0.57
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.86	0.57
4:D:57:THR:HG22	4:D:58:GLU:N	2.19	0.57
5:E:52:LYS:C	5:E:52:LYS:HD3	2.29	0.57
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.05	0.57
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.84	0.57
2:B:156:GLN:HE22	9:I:77:ARG:C	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.38	0.57
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.86	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.19	0.57
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.86	0.57
5:E:189:GLY:O	5:E:192:LEU:N	2.38	0.57
2:O:52:LYS:O	2:O:203:ARG:NH2	2.23	0.57
2:B:28:LYS:O	2:B:29:LEU:O	2.22	0.57
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.39	0.57
1:A:95:THR:HG22	1:A:96:ALA:N	2.20	0.57
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.85	0.57
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.86	0.57
3:C:92:PHE:O	3:C:95:ILE:HG22	2.04	0.56
5:E:190:ASP:C	5:E:192:LEU:N	2.63	0.56
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.05	0.56
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.70	0.56
3:C:345:GLU:C	3:C:349:ILE:HG13	2.30	0.56
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.19	0.56
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.30	0.56
3:P:377:MET:HE2	6:S:20:TYR:CG	2.39	0.56
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.40	0.56
5:E:187:PHE:C	5:E:189:GLY:N	2.63	0.56
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.40	0.56
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.71	0.56
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.19	0.56
2:B:189:GLU:OE1	2:B:189:GLU:N	2.39	0.56
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.70	0.56
1:N:276:ILE:HG12	1:N:357:ALA:HB2	1.86	0.56
1:N:362:ARG:O	1:N:365:MET:HG2	2.05	0.56
3:P:236:MET:O	3:P:239:PRO:HD2	2.06	0.56
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.86	0.56
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.88	0.56
2:B:23:ASP:OD1	2:B:24:LEU:N	2.39	0.56
5:R:106:ILE:O	5:R:109:GLU:HB3	2.06	0.56
2:B:31:ASN:N	2:B:31:ASN:ND2	2.49	0.56
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.41	0.56
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.05	0.56
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.56
2:O:27:THR:CG2	2:O:28:LYS:N	2.69	0.56
2:O:221:GLU:C	2:O:223:PHE:H	2.13	0.56
3:P:40:VAL:HA	3:P:43:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.38	0.56
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.88	0.56
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.87	0.56
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.36	0.56
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.69	0.56
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.88	0.56
2:B:312:PHE:HE1	9:I:62:ARG:O	1.89	0.56
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.33	0.56
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.41	0.56
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.36	0.56
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.44	0.55
1:N:269:VAL:CG2	1:N:406:MET:HE3	2.35	0.55
1:N:281:ASP:O	1:N:283:THR:N	2.39	0.55
5:R:185:TYR:O	5:R:186:GLN:HB3	2.06	0.55
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.06	0.55
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.71	0.55
2:O:150:VAL:HA	2:O:153:GLN:HG3	1.88	0.55
5:R:79:SER:OG	5:R:191:ASP:HB2	2.06	0.55
2:B:374:THR:HG22	2:B:376:GLN:H	1.71	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.87	0.55
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.88	0.55
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.41	0.55
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.20	0.55
2:O:374:THR:HG22	2:O:376:GLN:H	1.72	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.41	0.55
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.07	0.55
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.37	0.55
2:B:225:ASN:O	2:B:227:ARG:N	2.40	0.55
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.89	0.55
1:N:205:HIS:O	1:N:208:LEU:HB3	2.06	0.55
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.22	0.55
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.41	0.55
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.20	0.55
2:O:169:LYS:O	2:O:170:THR:HG23	2.07	0.55
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.15	0.55
1:A:15:ASN:O	1:A:26:ALA:HA	2.07	0.55
1:A:48:GLU:CD	1:A:54:GLY:H	2.15	0.55
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.89	0.55
2:O:124:LEU:HD23	2:O:124:LEU:C	2.32	0.55
2:O:345:LYS:O	2:O:349:GLN:HG3	2.07	0.55
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.22	0.55
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.14	0.55
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.88	0.55
2:O:264:VAL:HG12	2:O:265:GLY:N	2.22	0.55
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.37	0.54
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.89	0.54
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.74	0.54
2:B:417:PHE:O	2:B:422:LYS:HE3	2.07	0.54
4:D:47:ALA:HA	4:D:90:TYR:HA	1.88	0.54
5:E:77:LYS:HG3	5:E:191:ASP:O	2.06	0.54
2:B:170:THR:O	2:B:172:LEU:N	2.40	0.54
1:A:106:MET:O	1:A:106:MET:HE2	2.07	0.54
2:B:374:THR:HB	2:B:377:GLY:H	1.72	0.54
1:N:317:THR:HG23	1:N:318:GLY:N	2.23	0.54
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.08	0.54
1:A:402:VAL:HG22	1:A:406:MET:CE	2.38	0.54
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.54
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.54
1:A:430:GLN:HG3	7:G:4:PHE:O	2.08	0.54
3:P:49:GLY:C	12:P:501:HEM:HAC	2.33	0.54
1:A:280:TYR:CG	1:A:281:ASP:N	2.76	0.54
7:G:36:ASN:O	7:G:40:ARG:HG3	2.08	0.54
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.89	0.54
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.71	0.54
2:O:332:HIS:O	2:O:336:VAL:HG23	2.07	0.54
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.90	0.54
2:B:402:ILE:HD13	2:B:402:ILE:C	2.32	0.54
3:C:271:PRO:HG2	3:C:276:LEU:HD23	1.90	0.54
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.90	0.54
1:N:156:THR:HA	1:N:159:GLN:HB3	1.90	0.54
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.89	0.54
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.22	0.54
1:A:191:LYS:N	1:A:195:MET:HE2	2.22	0.53
1:A:272:VAL:O	1:A:275:ALA:HB3	2.09	0.53
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.08	0.53
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.71	0.53
6:S:16:ILE:O	6:S:19:TRP:HB3	2.08	0.53
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.89	0.53
1:A:388:ARG:HH22	1:A:390:ILE:HG12	1.73	0.53
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.43	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:217:LYS:O	2:O:221:GLU:HG2	2.09	0.53
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.89	0.53
6:S:70:LEU:HD12	6:S:70:LEU:C	2.33	0.53
1:N:209:VAL:O	1:N:212:ALA:HB3	2.08	0.53
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.73	0.53
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.09	0.53
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.91	0.53
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.43	0.53
4:Q:37:CYS:C	4:Q:39:ALA:H	2.17	0.53
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.41	0.53
1:A:217:SER:O	1:A:218:GLY:C	2.52	0.53
1:N:430:GLN:HG3	7:T:4:PHE:O	2.08	0.53
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.90	0.53
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.91	0.53
7:G:40:ARG:HB3	17:G:2004:CDL:HA32	1.91	0.53
1:N:22:GLY:O	1:N:193:PRO:HA	2.07	0.53
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.09	0.53
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.44	0.53
5:R:170:ARG:HA	5:R:179:ASN:CB	2.38	0.53
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.72	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.23	0.53
6:F:40:ASP:O	6:F:44:LYS:HG3	2.09	0.53
1:N:131:ARG:NH2	1:N:177:LEU:O	2.41	0.53
1:N:186:ILE:HG23	1:N:190:PHE:HD1	1.74	0.53
2:O:259:THR:HG22	2:O:260:GLU:N	2.24	0.53
1:A:90:THR:O	1:A:167:VAL:HG11	2.09	0.53
1:A:191:LYS:CA	1:A:195:MET:HE2	2.39	0.53
2:B:57:TYR:N	2:B:57:TYR:CD1	2.76	0.53
2:B:280:GLY:HA3	2:B:293:SER:OG	2.07	0.53
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.72	0.53
3:C:130:VAL:HG23	3:C:183:HIS:HB2	1.91	0.53
3:C:326:PHE:O	3:C:330:VAL:HG23	2.09	0.53
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.89	0.53
2:O:105:MET:HE2	2:O:107:TYR:HE1	1.73	0.53
4:Q:2:GLU:O	4:Q:3:LEU:O	2.27	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.44	0.53
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.23	0.53
2:B:76:THR:HG22	2:B:82:SER:N	2.14	0.53
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.44	0.53
2:O:54:GLY:C	2:O:56:ARG:H	2.17	0.53
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:173:ASN:N	3:P:174:PRO:HD2	2.24	0.53
6:S:40:ASP:O	6:S:44:LYS:HG3	2.09	0.52
7:T:36:ASN:O	7:T:40:ARG:HG3	2.09	0.52
4:D:239:PRO:C	4:D:241:LYS:H	2.17	0.52
2:O:295:LEU:O	2:O:299:VAL:HG23	2.09	0.52
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.26	0.52
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.52
3:C:49:GLY:C	12:C:501:HEM:HAC	2.34	0.52
3:C:216:SER:HB3	6:F:59:MET:HE2	1.91	0.52
3:C:236:MET:O	3:C:239:PRO:HD2	2.08	0.52
11:P:3007:PEE:H50	17:T:3004:CDL:H712	1.91	0.52
1:A:130:GLU:O	1:A:134:ILE:HG13	2.10	0.52
2:B:96:LEU:HD12	2:B:97:SER:N	2.25	0.52
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.90	0.52
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.42	0.52
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.39	0.52
7:T:40:ARG:HD2	17:T:3004:CDL:OA4	2.10	0.52
5:E:75:GLU:HA	5:E:193:VAL:O	2.09	0.52
2:O:225:ASN:O	2:O:227:ARG:HG3	2.09	0.52
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.25	0.52
1:A:204:SER:HB3	1:A:207:GLU:HG3	1.92	0.52
2:B:50:PHE:N	2:B:50:PHE:CD1	2.77	0.52
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.68	0.52
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.91	0.52
2:B:297:GLN:O	2:B:301:LYS:HG3	2.09	0.52
10:W:49:GLY:N	10:W:54:HIS:ND1	2.58	0.52
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.17	0.52
2:B:54:GLY:C	2:B:56:ARG:H	2.18	0.52
5:E:136:VAL:O	5:E:138:VAL:N	2.41	0.52
3:P:138:GLN:HB2	3:P:255:GLU:O	2.10	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.91	0.52
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.75	0.52
5:E:147:ILE:HG22	5:E:149:ASN:H	1.74	0.52
6:S:91:GLU:CG	6:S:95:LYS:HE3	2.37	0.52
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.40	0.52
9:V:64:LEU:HD12	9:V:77:ARG:C	2.35	0.52
1:A:75:PHE:O	1:A:79:VAL:HG23	2.10	0.52
2:B:264:VAL:HG23	2:B:316:TYR:C	2.35	0.52
2:B:27:THR:CG2	2:B:28:LYS:N	2.73	0.51
2:B:325:TYR:HD1	9:I:60:ALA:HB3	1.76	0.51
2:O:397:VAL:O	2:O:401:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:131:GLU:OE1	5:R:131:GLU:N	2.40	0.51
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.92	0.51
2:B:207:VAL:HG12	2:B:208:GLY:H	1.76	0.51
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.92	0.51
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.39	0.51
6:F:32:MET:CE	6:F:87:LYS:HG2	2.40	0.51
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.23	0.51
3:P:9:HIS:CD2	3:P:12:LEU:H	2.16	0.51
5:R:141:HIS:HB3	19:R:501:FES:S2	2.50	0.51
5:R:186:GLN:O	5:R:193:VAL:HG23	2.10	0.51
2:B:28:LYS:HG3	2:B:34:ILE:HG12	1.91	0.51
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.92	0.51
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.40	0.51
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.25	0.51
2:B:345:LYS:O	2:B:349:GLN:HG3	2.09	0.51
3:C:245:LEU:O	4:D:201:ARG:HD2	2.10	0.51
2:O:341:MET:HE2	2:O:341:MET:HA	1.91	0.51
3:P:132:TYR:O	3:P:135:PRO:HD2	2.11	0.51
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.75	0.51
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.93	0.51
5:R:76:ILE:O	5:R:193:VAL:HG12	2.10	0.51
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.26	0.51
3:C:207:ASN:ND2	3:C:208:ASN:H	2.08	0.51
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.92	0.51
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.11	0.51
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.10	0.51
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.46	0.51
2:B:42:SER:C	2:B:44:ALA:H	2.19	0.51
2:B:307:PHE:H	9:I:52:ARG:HG2	1.74	0.51
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.41	0.51
5:E:185:TYR:O	5:E:186:GLN:HB3	2.09	0.51
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.45	0.51
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.93	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.44	0.51
10:J:10:TYR:HE2	10:J:15:ARG:HD2	1.74	0.51
2:O:140:LEU:C	2:O:142:PRO:HD2	2.36	0.51
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.46	0.51
3:C:347:PRO:O	3:C:350:ILE:HG22	2.11	0.51
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.93	0.51
2:O:345:LYS:HG2	2:O:418:VAL:HG11	1.93	0.51
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:LEU:C	2:B:142:PRO:HD2	2.36	0.50
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.42	0.50
2:O:31:ASN:N	2:O:31:ASN:ND2	2.59	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
2:B:295:LEU:O	2:B:299:VAL:HG23	2.11	0.50
2:O:141:GLN:N	2:O:142:PRO:HD2	2.27	0.50
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.94	0.50
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.24	0.50
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.42	0.50
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.94	0.50
2:B:150:VAL:HA	2:B:153:GLN:HG3	1.92	0.50
17:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.26	0.50
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.40	0.50
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.42	0.50
1:A:223:TYR:H	1:A:223:TYR:HD2	1.59	0.50
12:C:502:HEM:HMB1	12:C:502:HEM:HBB2	1.92	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.50
4:D:227:TRP:O	4:D:228:SER:C	2.52	0.50
5:E:189:GLY:O	5:E:192:LEU:O	2.29	0.50
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.92	0.50
1:N:354:VAL:HG23	1:N:355:LYS:N	2.25	0.50
2:O:57:TYR:CD1	2:O:57:TYR:N	2.79	0.50
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.94	0.50
10:W:7:ARG:CB	10:W:7:ARG:HH11	2.25	0.50
3:C:132:TYR:O	3:C:135:PRO:HD2	2.12	0.50
3:C:173:ASN:N	3:C:174:PRO:HD2	2.26	0.50
4:D:57:THR:HG22	4:D:59:ALA:N	2.23	0.50
1:N:279:ARG:HH22	9:V:30:UNK:C	2.24	0.50
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.25	0.50
5:R:163:SER:H	5:R:175:PRO:HD2	1.76	0.50
1:A:45:SER:HA	1:A:48:GLU:HG3	1.92	0.50
3:C:52:LEU:HD13	12:C:501:HEM:HBD1	1.94	0.50
4:D:37:CYS:O	4:D:39:ALA:N	2.44	0.50
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.50
1:N:106:MET:CE	1:N:110:VAL:HG21	2.41	0.50
1:N:223:TYR:H	1:N:223:TYR:HD2	1.58	0.50
10:W:10:TYR:HE2	10:W:15:ARG:HD2	1.75	0.50
1:N:4:TYR:CB	2:O:114:ASP:OD2	2.59	0.50
1:N:439:SER:HA	1:N:442:TYR:CE2	2.46	0.50
3:P:101:ARG:C	3:P:101:ARG:CD	2.83	0.50
9:V:31:UNK:C	9:V:73:PRO:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.12	0.50
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.44	0.50
2:B:141:GLN:N	2:B:142:PRO:HD2	2.27	0.50
5:E:121:GLN:CB	5:E:170:ARG:HD3	2.40	0.50
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.94	0.50
3:P:377:MET:HE2	6:S:20:TYR:CD1	2.47	0.50
1:A:89:TYR:O	1:A:95:THR:HG23	2.12	0.49
1:A:239:SER:HB2	7:G:17:SER:O	2.12	0.49
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.47	0.49
1:N:48:GLU:CD	1:N:54:GLY:H	2.21	0.49
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.27	0.49
3:P:223:PRO:O	3:P:227:PHE:HD2	1.94	0.49
1:A:307:PHE:CD1	1:A:307:PHE:C	2.90	0.49
3:C:286:PRO:O	3:C:287:ASN:CB	2.60	0.49
1:N:307:PHE:CD1	1:N:307:PHE:C	2.89	0.49
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.44	0.49
3:P:50:LEU:O	3:P:54:MET:HG3	2.12	0.49
5:R:178:TYR:N	5:R:178:TYR:CD1	2.80	0.49
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.93	0.49
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.75	0.49
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.47	0.49
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.47	0.49
1:A:106:MET:HE2	1:A:106:MET:C	2.38	0.49
1:A:382:HIS:HB3	1:A:388:ARG:O	2.12	0.49
5:E:76:ILE:O	5:E:193:VAL:HG12	2.13	0.49
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.94	0.49
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.37	0.49
2:O:26:ILE:HG12	2:O:26:ILE:O	2.11	0.49
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.41	0.49
3:P:246:PHE:C	3:P:248:PRO:HD3	2.37	0.49
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.27	0.49
1:A:354:VAL:HG23	1:A:355:LYS:N	2.26	0.49
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.37	0.49
2:B:38:LEU:HD12	2:B:38:LEU:C	2.36	0.49
1:N:63:ALA:O	1:N:116:VAL:HG13	2.12	0.49
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.42	0.49
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.93	0.49
2:O:222:GLN:O	2:O:222:GLN:HG2	2.12	0.49
2:O:280:GLY:HA3	2:O:293:SER:OG	2.12	0.49
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.28	0.49
2:O:353:THR:HG22	2:O:354:GLU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.49
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.47	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.49
2:B:338:ARG:NH1	2:B:338:ARG:CG	2.74	0.49
5:E:122:HIS:O	5:E:125:ASP:HB2	2.11	0.49
1:N:364:ALA:O	1:N:368:GLN:HG3	2.12	0.49
2:O:209:ILE:HD12	2:O:379:LEU:HB2	1.94	0.49
3:P:147:ILE:HD11	13:P:3001:JZZ:HAB	1.95	0.49
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.78	0.49
4:D:102:ARG:HA	4:D:108:ALA:O	2.12	0.49
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.47	0.49
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.13	0.49
8:U:27:THR:HG22	8:U:29:LYS:H	1.77	0.49
1:A:387:GLY:O	1:A:388:ARG:HB3	2.13	0.49
2:B:385:GLU:O	2:B:387:LEU:N	2.46	0.49
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.43	0.49
5:E:147:ILE:O	5:E:156:TYR:HA	2.13	0.49
5:E:155:GLY:HA3	5:E:166:ASP:C	2.38	0.49
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.53	0.49
4:Q:148:HIS:N	4:Q:148:HIS:CD2	2.81	0.49
1:A:23:LEU:HD23	1:A:24:ARG:N	2.28	0.48
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.47	0.48
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.48	0.48
3:P:347:PRO:O	3:P:350:ILE:HG22	2.13	0.48
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.95	0.48
2:B:59:THR:O	2:B:61:ALA:N	2.45	0.48
3:C:246:PHE:C	3:C:248:PRO:HD3	2.37	0.48
2:O:96:LEU:HD12	2:O:97:SER:N	2.28	0.48
3:P:155:PRO:O	3:P:156:TYR:HB2	2.13	0.48
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.78	0.48
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.95	0.48
2:B:124:LEU:C	2:B:124:LEU:HD23	2.38	0.48
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.77	0.48
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.28	0.48
4:D:148:HIS:CD2	4:D:148:HIS:N	2.82	0.48
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.96	0.48
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.95	0.48
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.96	0.48
5:R:161:HIS:HB2	19:R:501:FES:S1	2.53	0.48
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.78	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:LYS:N	1:N:195:MET:HE2	2.29	0.48
5:R:82:PRO:O	5:R:100:HIS:HB3	2.13	0.48
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.28	0.48
2:B:27:THR:CG2	2:B:28:LYS:H	2.26	0.48
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.79	0.48
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.79	0.48
5:R:166:ASP:OD1	5:R:168:SER:N	2.45	0.48
1:A:133:VAL:O	1:A:136:GLN:HB2	2.14	0.48
4:D:37:CYS:C	4:D:39:ALA:N	2.72	0.48
4:D:220:TYR:O	4:D:224:ARG:HG2	2.13	0.48
1:N:351:GLU:O	1:N:354:VAL:HG22	2.12	0.48
2:O:221:GLU:O	2:O:223:PHE:N	2.46	0.48
2:O:414:ALA:O	2:O:418:VAL:HG23	2.14	0.48
17:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.29	0.48
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.47	0.48
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.95	0.48
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.48
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.96	0.48
5:E:102:THR:C	5:E:103:GLN:HG3	2.39	0.48
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.95	0.48
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.14	0.48
4:Q:169:LEU:CD2	4:Q:182:ILE:HD11	2.44	0.48
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.29	0.48
6:S:13:MET:O	6:S:17:ARG:HG3	2.14	0.48
5:E:97:PHE:O	5:E:134:ILE:HA	2.13	0.48
1:N:32:GLN:HE22	2:O:373:GLU:HA	1.79	0.48
5:R:75:GLU:HA	5:R:193:VAL:O	2.14	0.48
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.14	0.48
2:B:104:LYS:HD2	2:B:104:LYS:C	2.39	0.48
1:N:45:SER:HA	1:N:48:GLU:CG	2.44	0.48
2:O:338:ARG:O	2:O:341:MET:HB2	2.14	0.48
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.48	0.48
3:P:125:MET:HE2	13:P:3001:JZZ:HAGA	1.95	0.48
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.28	0.48
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.96	0.48
1:A:365:MET:HE3	1:A:392:LEU:HD22	1.95	0.48
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.13	0.48
6:F:53:ASP:OD1	6:F:54:LEU:N	2.46	0.48
7:G:28:ASN:HB3	7:G:31:SER:OG	2.14	0.48
1:N:240:GLU:HA	1:N:422:LEU:O	2.14	0.48
2:O:73:SER:N	2:O:74:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.79	0.48
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.95	0.48
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.95	0.47
2:B:162:ASN:O	2:B:244:ILE:HD12	2.14	0.47
2:B:206:LEU:CD2	2:B:220:ALA:HB2	2.43	0.47
5:E:83:GLU:C	5:E:85:LYS:H	2.22	0.47
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.28	0.47
9:I:71:ASN:H	9:I:71:ASN:HD22	1.61	0.47
1:N:394:GLU:O	1:N:395:TRP:C	2.57	0.47
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.96	0.47
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.45	0.47
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.49	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.96	0.47
1:A:287:GLY:O	1:A:290:LEU:HG	2.14	0.47
1:A:362:ARG:O	1:A:365:MET:HG2	2.14	0.47
2:B:110:GLU:O	2:B:111:CYS:HB3	2.14	0.47
2:B:124:LEU:CD1	2:B:223:PHE:HB3	2.42	0.47
2:B:262:ALA:O	2:B:320:GLY:HA3	2.14	0.47
2:B:332:HIS:O	2:B:336:VAL:HG23	2.13	0.47
3:C:50:LEU:O	3:C:54:MET:HG3	2.15	0.47
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.47
2:O:46:ARG:HD2	2:O:110:GLU:CG	2.44	0.47
2:O:110:GLU:O	2:O:111:CYS:HB3	2.13	0.47
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.14	0.47
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.96	0.47
1:N:53:ASN:N	1:N:173:ASN:ND2	2.62	0.47
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.77	0.47
5:R:162:GLY:O	5:R:163:SER:C	2.56	0.47
1:A:205:HIS:O	1:A:208:LEU:HB3	2.15	0.47
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.97	0.47
3:C:37:LEU:O	3:C:41:CYS:HB2	2.14	0.47
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.96	0.47
5:E:188:VAL:HG12	5:E:188:VAL:O	2.15	0.47
1:N:36:THR:HG21	1:N:373:THR:HA	1.96	0.47
1:N:90:THR:O	1:N:90:THR:HG23	2.15	0.47
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.40	0.47
2:O:54:GLY:C	2:O:56:ARG:N	2.72	0.47
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.43	0.47
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.95	0.47
7:T:56:TYR:O	7:T:59:TYR:HB3	2.14	0.47
1:A:364:ALA:O	1:A:368:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:VAL:HG12	2:B:208:GLY:N	2.29	0.47
2:B:248:ASN:C	2:B:248:ASN:ND2	2.71	0.47
5:E:52:LYS:C	5:E:52:LYS:CD	2.88	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.95	0.47
1:A:281:ASP:O	1:A:283:THR:N	2.47	0.47
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.43	0.47
2:B:353:THR:HG22	2:B:354:GLU:N	2.29	0.47
5:E:101:ARG:HA	5:E:105:GLU:OE1	2.14	0.47
6:F:32:MET:HE3	6:F:87:LYS:HE2	1.97	0.47
1:N:154:HIS:O	1:N:156:THR:N	2.48	0.47
1:N:388:ARG:HH22	1:N:390:ILE:HG12	1.78	0.47
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.97	0.47
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.50	0.47
6:F:16:ILE:O	6:F:19:TRP:HB3	2.14	0.47
1:N:106:MET:O	1:N:106:MET:HE2	2.14	0.47
2:O:252:LEU:HD13	9:V:55:MET:HE3	1.96	0.47
3:P:275:PHE:CG	13:P:3001:JZZ:HAGB	2.50	0.47
3:P:345:GLU:C	3:P:349:ILE:HG13	2.38	0.47
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.97	0.47
5:R:155:GLY:HA3	5:R:166:ASP:C	2.39	0.47
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.77	0.47
8:U:32:LYS:O	8:U:36:ARG:HG3	2.15	0.47
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.44	0.47
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.80	0.47
10:J:59:TYR:CD1	10:J:59:TYR:N	2.82	0.47
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.43	0.47
2:B:345:LYS:HG2	2:B:418:VAL:CG1	2.45	0.47
4:D:57:THR:CG2	4:D:58:GLU:N	2.78	0.47
8:H:50:THR:HG23	8:H:50:THR:O	2.14	0.47
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.95	0.47
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.50	0.47
2:O:248:ASN:C	2:O:248:ASN:ND2	2.67	0.47
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.50	0.47
3:P:365:ILE:HG22	3:P:366:LEU:HD23	1.96	0.47
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.50	0.47
5:E:162:GLY:O	5:E:163:SER:C	2.58	0.47
7:G:80:ASP:O	7:G:81:GLN:C	2.58	0.47
10:J:56:LYS:HB3	10:J:56:LYS:HE2	1.72	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.15	0.47
5:R:83:GLU:CD	5:R:102:THR:HA	2.39	0.47
2:B:70:ARG:HG3	2:B:98:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ARG:O	2:B:341:MET:HB2	2.15	0.46
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.82	0.46
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.50	0.46
1:N:144:ASP:OD2	1:N:147:ASN:ND2	2.47	0.46
2:O:291:VAL:C	2:O:293:SER:H	2.23	0.46
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.97	0.46
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.30	0.46
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.50	0.46
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.46
9:V:33:UNK:HA	9:V:73:PRO:HB3	1.97	0.46
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.50	0.46
2:B:59:THR:C	2:B:61:ALA:N	2.71	0.46
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.96	0.46
5:E:191:ASP:OD2	5:E:191:ASP:N	2.48	0.46
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.14	0.46
12:P:502:HEM:HBB2	12:P:502:HEM:CMB	2.45	0.46
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.45	0.46
3:C:19:LEU:C	3:C:20:ILE:HG13	2.41	0.46
8:U:22:GLU:O	8:U:26:GLN:HG2	2.16	0.46
2:B:54:GLY:C	2:B:56:ARG:N	2.73	0.46
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.30	0.46
4:D:235:MET:HB3	7:G:15:THR:HG22	1.97	0.46
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.77	0.46
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.50	0.46
5:R:186:GLN:NE2	5:R:187:PHE:O	2.48	0.46
1:A:351:GLU:O	1:A:354:VAL:HG22	2.16	0.46
3:C:234:THR:HG21	4:D:219:LEU:CD1	2.45	0.46
3:C:286:PRO:O	3:C:287:ASN:HB2	2.15	0.46
5:E:106:ILE:O	5:E:106:ILE:HG22	2.15	0.46
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.50	0.46
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.45	0.46
5:E:161:HIS:HB2	19:E:501:FES:S1	2.56	0.46
6:F:84:GLU:H	6:F:84:GLU:CD	2.23	0.46
8:H:27:THR:HG22	8:H:29:LYS:H	1.81	0.46
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.97	0.46
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.98	0.46
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.15	0.46
10:W:60:GLU:O	10:W:61:ALA:HB2	2.14	0.46
5:E:115:SER:HB2	5:E:116:LYS:HD2	1.97	0.46
7:G:65:GLU:O	7:G:69:LEU:HG	2.16	0.46
3:P:5:ILE:O	3:P:5:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:79:GLU:OE2	4:Q:79:GLU:HA	2.16	0.46
10:W:56:LYS:O	10:W:60:GLU:HB3	2.15	0.46
1:A:156:THR:HA	1:A:159:GLN:HB3	1.97	0.46
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.31	0.46
3:C:101:ARG:C	3:C:101:ARG:CD	2.89	0.46
3:C:245:LEU:O	4:D:201:ARG:CD	2.64	0.46
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.79	0.46
5:E:144:CYS:HB2	19:E:501:FES:S2	2.56	0.46
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.96	0.46
1:N:294:LEU:HD11	1:N:334:MET:CE	2.45	0.46
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.46	0.46
2:O:207:VAL:HG12	2:O:208:GLY:H	1.81	0.46
2:O:334:GLY:O	2:O:338:ARG:HG2	2.15	0.46
5:R:97:PHE:O	5:R:134:ILE:HA	2.16	0.46
5:R:118:ARG:NH1	5:R:174:GLY:O	2.48	0.46
1:A:114:ALA:O	1:A:118:GLN:HB2	2.16	0.46
1:A:404:ALA:O	1:A:405:ARG:C	2.59	0.46
2:B:274:VAL:O	2:B:278:VAL:HG23	2.16	0.46
3:C:269:ILE:HG22	3:C:269:ILE:O	2.16	0.46
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.41	0.46
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.49	0.46
3:P:245:LEU:O	4:Q:201:ARG:CD	2.64	0.46
10:W:59:TYR:N	10:W:59:TYR:CD1	2.83	0.46
3:C:5:ILE:O	3:C:5:ILE:HG22	2.16	0.46
6:F:70:LEU:C	6:F:70:LEU:HD12	2.40	0.46
2:O:385:GLU:O	2:O:387:LEU:N	2.48	0.46
5:R:130:PRO:C	5:R:132:TRP:H	2.24	0.46
5:R:177:PRO:HG2	5:R:178:TYR:HD1	1.81	0.46
5:R:185:TYR:HD2	5:R:185:TYR:N	2.14	0.46
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.72	0.45
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.46	0.45
2:O:31:ASN:ND2	2:O:31:ASN:H	2.13	0.45
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.45
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.97	0.45
2:B:24:LEU:HD12	2:B:37:SER:O	2.16	0.45
4:D:169:LEU:C	4:D:169:LEU:HD23	2.40	0.45
5:E:127:VAL:CG1	5:E:128:LYS:H	2.12	0.45
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.99	0.45
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.96	0.45
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.97	0.45
2:B:397:VAL:O	2:B:401:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:239:PRO:C	4:D:241:LYS:N	2.74	0.45
1:N:180:ALA:O	1:N:183:ALA:HB3	2.16	0.45
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.45
7:T:66:PHE:CE2	7:T:70:LYS:HE3	2.52	0.45
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.51	0.45
1:A:106:MET:N	1:A:107:PRO:HD2	2.32	0.45
2:B:81:SER:O	2:B:85:ILE:HG13	2.17	0.45
2:B:105:MET:HE2	2:B:107:TYR:CE1	2.48	0.45
3:C:31:TRP:CH2	17:G:2004:CDL:H512	2.51	0.45
8:H:58:LEU:O	8:H:58:LEU:HD12	2.15	0.45
1:N:245:ASP:OD1	7:T:11:ARG:NE	2.41	0.45
2:O:38:LEU:HD12	2:O:38:LEU:C	2.41	0.45
2:O:227:ARG:HB3	2:O:228:SER:H	1.47	0.45
4:Q:99:GLU:CD	4:Q:99:GLU:H	2.24	0.45
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.31	0.45
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.32	0.45
2:B:395:PRO:O	2:B:398:VAL:HG12	2.17	0.45
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.79	0.45
5:E:125:ASP:C	5:E:126:ARG:HG3	2.42	0.45
2:O:67:HIS:O	2:O:70:ARG:HB3	2.17	0.45
2:O:162:ASN:O	2:O:244:ILE:HD12	2.17	0.45
2:O:367:THR:HA	2:O:370:MET:HE3	1.98	0.45
3:P:101:ARG:HD2	3:P:101:ARG:O	2.16	0.45
3:P:286:PRO:O	3:P:287:ASN:CB	2.64	0.45
5:R:134:ILE:HD12	5:R:185:TYR:HE1	1.80	0.45
1:A:170:THR:CG2	1:A:171:THR:N	2.79	0.45
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.99	0.45
2:O:76:THR:CG2	2:O:82:SER:H	2.10	0.45
5:R:163:SER:OG	5:R:176:ALA:HB2	2.17	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.35	0.45
2:B:325:TYR:C	2:B:325:TYR:CD2	2.95	0.45
9:I:65:VAL:HG12	9:I:66:ALA:N	2.31	0.45
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.81	0.45
2:O:104:LYS:HD2	2:O:104:LYS:C	2.42	0.45
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.45
3:P:81:ARG:O	3:P:81:ARG:HD3	2.17	0.45
3:P:275:PHE:CD2	13:P:3001:JZZ:HAGB	2.52	0.45
7:T:40:ARG:CB	17:T:3004:CDL:HA32	2.45	0.45
3:C:287:ASN:O	3:C:288:LYS:C	2.58	0.45
4:D:169:LEU:CD2	4:D:182:ILE:HD11	2.47	0.45
5:E:171:ILE:HG12	5:E:176:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:280:TYR:CG	1:N:281:ASP:N	2.85	0.45
2:O:248:ASN:HD22	2:O:249:GLY:N	2.15	0.45
3:P:350:ILE:O	3:P:354:MET:HG2	2.16	0.45
4:Q:197:GLU:O	4:Q:198:HIS:C	2.59	0.45
5:R:76:ILE:HD13	5:R:89:PHE:CE1	2.52	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.52	0.45
1:A:190:PHE:C	1:A:195:MET:HE2	2.42	0.45
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.98	0.45
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.46	0.45
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.51	0.45
4:D:234:LYS:HD2	5:E:8:PRO:HB2	1.99	0.45
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.52	0.45
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.45
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.97	0.45
4:Q:227:TRP:O	4:Q:228:SER:C	2.58	0.45
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.57	0.45
5:R:179:ASN:O	5:R:180:LEU:C	2.60	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.17	0.45
2:O:59:THR:C	2:O:61:ALA:N	2.73	0.45
2:O:370:MET:C	2:O:372:VAL:H	2.25	0.45
4:Q:240:PRO:O	4:Q:241:LYS:C	2.59	0.45
5:R:148:ALA:O	5:R:149:ASN:HB2	2.16	0.45
5:R:185:TYR:N	5:R:185:TYR:CD2	2.85	0.45
1:A:106:MET:CE	1:A:110:VAL:HG21	2.47	0.44
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.52	0.44
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.41	0.44
1:N:53:ASN:N	1:N:173:ASN:HD22	2.14	0.44
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.99	0.44
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.98	0.44
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.99	0.44
2:B:370:MET:C	2:B:372:VAL:H	2.25	0.44
4:D:200:GLN:HB2	18:D:2091:BOG:H3	1.99	0.44
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.46	0.44
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.00	0.44
3:P:75:GLN:HB2	5:R:61:SER:HA	1.98	0.44
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.99	0.44
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.53	0.44
1:A:23:LEU:HD23	1:A:23:LEU:C	2.42	0.44
2:B:31:ASN:HD22	2:B:31:ASN:H	1.58	0.44
3:C:127:THR:O	3:C:130:VAL:HG22	2.18	0.44
5:E:82:PRO:HG2	5:E:85:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:VAL:HG23	5:E:181:GLU:O	2.17	0.44
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.80	0.44
1:N:243:ALA:O	1:N:425:VAL:HA	2.17	0.44
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.43	0.44
2:O:76:THR:HG23	2:O:82:SER:HB2	1.99	0.44
3:P:263:LEU:C	3:P:264:VAL:HG23	2.42	0.44
3:P:271:PRO:HG2	3:P:276:LEU:HD23	2.00	0.44
4:Q:220:TYR:CZ	4:Q:224:ARG:HD3	2.52	0.44
2:B:209:ILE:HD12	2:B:379:LEU:HB2	2.00	0.44
3:C:147:ILE:HD11	13:C:2001:JZZ:HAB	1.98	0.44
1:N:239:SER:HB2	7:T:17:SER:O	2.17	0.44
2:O:206:LEU:HG	2:O:216:LEU:HD11	1.99	0.44
2:O:297:GLN:O	2:O:301:LYS:HG3	2.17	0.44
5:R:76:ILE:HD13	5:R:89:PHE:CD1	2.52	0.44
5:R:76:ILE:HD12	5:R:98:VAL:HG21	2.00	0.44
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.33	0.44
5:R:184:THR:O	5:R:185:TYR:HB3	2.17	0.44
1:A:53:ASN:N	1:A:173:ASN:ND2	2.65	0.44
3:C:138:GLN:HB2	3:C:255:GLU:O	2.18	0.44
5:E:150:SER:OG	5:E:157:TYR:HB3	2.18	0.44
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.30	0.44
2:O:169:LYS:CG	2:O:240:TRP:HB2	2.47	0.44
2:O:374:THR:HB	2:O:377:GLY:H	1.81	0.44
4:Q:234:LYS:HD2	5:R:8:PRO:HB2	2.00	0.44
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.16	0.44
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.47	0.44
1:N:85:HIS:HB2	1:N:100:LYS:HB2	2.00	0.44
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.99	0.44
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.53	0.44
1:A:21:ASN:OD1	1:A:21:ASN:N	2.47	0.44
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.82	0.44
2:B:24:LEU:HG	2:B:24:LEU:O	2.17	0.44
2:B:71:LEU:HD12	2:B:144:LEU:HD23	2.00	0.44
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.48	0.44
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.47	0.44
3:C:272:GLU:O	3:C:273:TRP:C	2.56	0.44
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.48	0.44
1:N:383:LEU:HD23	1:N:388:ARG:HA	1.98	0.44
1:N:402:VAL:HA	1:N:406:MET:CE	2.44	0.44
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.00	0.44
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:12:GLU:HG2	8:U:13:LEU:N	2.33	0.44
1:A:269:VAL:HG22	1:A:406:MET:HE3	1.99	0.44
3:C:160:THR:O	3:C:161:LEU:C	2.61	0.44
2:O:407:SER:O	2:O:411:VAL:HG23	2.17	0.44
1:A:53:ASN:N	1:A:173:ASN:HD22	2.16	0.44
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.33	0.44
1:A:373:THR:HB	1:A:374:PRO:CD	2.47	0.44
2:B:167:ALA:C	2:B:168:TYR:CD1	2.96	0.44
5:E:178:TYR:HD1	5:E:178:TYR:H	1.66	0.44
1:N:154:HIS:C	1:N:156:THR:H	2.26	0.44
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.26	0.44
5:R:107:ASN:C	5:R:109:GLU:N	2.70	0.44
2:B:166:ALA:HB1	2:B:242:GLY:C	2.44	0.43
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.99	0.43
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.18	0.43
3:C:34:PHE:HB2	20:C:381:HOH:O	2.18	0.43
4:D:31:GLN:O	4:D:32:VAL:C	2.61	0.43
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.33	0.43
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.53	0.43
1:N:170:THR:CG2	1:N:171:THR:H	2.23	0.43
2:O:163:LEU:C	2:O:165:ALA:N	2.76	0.43
3:P:287:ASN:O	3:P:288:LYS:C	2.61	0.43
5:R:122:HIS:O	5:R:123:ASP:C	2.60	0.43
10:W:56:LYS:HE2	10:W:56:LYS:HB3	1.63	0.43
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.00	0.43
1:A:394:GLU:O	1:A:395:TRP:C	2.60	0.43
3:C:263:LEU:O	3:C:264:VAL:CG2	2.66	0.43
5:E:130:PRO:HG2	5:E:131:GLU:OE1	2.18	0.43
2:O:59:THR:O	2:O:61:ALA:N	2.51	0.43
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.34	0.43
8:U:58:LEU:HD12	8:U:58:LEU:O	2.18	0.43
10:W:10:TYR:CD2	10:W:10:TYR:C	2.96	0.43
2:B:407:SER:O	2:B:411:VAL:HG23	2.18	0.43
3:C:30:ALA:HB1	17:D:2003:CDL:H111	1.99	0.43
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.53	0.43
5:E:115:SER:CB	5:E:116:LYS:HD2	2.49	0.43
1:N:106:MET:HE2	1:N:106:MET:C	2.43	0.43
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.43
3:P:189:ALA:O	3:P:193:ILE:HG13	2.17	0.43
3:P:207:ASN:ND2	3:P:208:ASN:H	2.16	0.43
4:Q:109:LEU:HD12	4:Q:110:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.01	0.43
2:B:42:SER:C	2:B:44:ALA:N	2.74	0.43
2:B:76:THR:CG2	2:B:82:SER:H	2.16	0.43
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.43
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.48	0.43
3:C:366:LEU:O	3:C:367:PHE:C	2.61	0.43
4:D:27:ARG:NH1	4:D:55:THR:O	2.50	0.43
5:E:187:PHE:O	5:E:189:GLY:N	2.50	0.43
1:N:206:LYS:N	1:N:206:LYS:HD3	2.34	0.43
16:Q:501:HEC:CMB	16:Q:501:HEC:HBB3	2.49	0.43
5:R:116:LYS:O	5:R:117:LEU:HD23	2.19	0.43
1:A:176:HIS:O	1:A:177:LEU:C	2.61	0.43
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.54	0.43
1:N:190:PHE:C	1:N:195:MET:HE2	2.43	0.43
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.99	0.43
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.49	0.43
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.82	0.43
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.48	0.43
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.99	0.43
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.45	0.43
3:C:277:PHE:CG	3:C:278:ALA:N	2.86	0.43
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.93	0.43
17:D:2003:CDL:HB22	7:G:40:ARG:HH21	1.84	0.43
1:N:154:HIS:C	1:N:156:THR:N	2.74	0.43
2:O:50:PHE:C	2:O:51:ILE:HG13	2.43	0.43
2:O:54:GLY:O	2:O:56:ARG:N	2.51	0.43
2:O:225:ASN:C	2:O:227:ARG:HG3	2.44	0.43
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.83	0.43
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.44	0.43
7:T:28:ASN:HB3	7:T:31:SER:OG	2.19	0.43
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.01	0.43
5:E:171:ILE:O	5:E:171:ILE:HG23	2.18	0.43
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.53	0.43
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.18	0.43
1:N:106:MET:N	1:N:107:PRO:HD2	2.34	0.43
2:O:306:PRO:HA	9:V:52:ARG:CG	2.48	0.43
1:A:277:ILE:HD11	1:A:345:LEU:HD11	2.01	0.43
2:B:399:ALA:C	2:B:402:ILE:HG22	2.44	0.43
3:C:263:LEU:C	3:C:264:VAL:HG23	2.43	0.43
3:C:350:ILE:HG23	3:C:351:ILE:N	2.33	0.43
5:E:153:PHE:C	5:E:155:GLY:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:45:SER:HA	1:N:48:GLU:CD	2.44	0.43
1:N:206:LYS:O	1:N:207:GLU:C	2.61	0.43
4:Q:169:LEU:HD22	4:Q:182:ILE:HD11	2.01	0.43
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.84	0.43
2:B:150:VAL:C	2:B:153:GLN:HG3	2.44	0.43
2:B:166:ALA:HB1	2:B:242:GLY:O	2.18	0.43
5:E:129:LYS:HB2	5:E:132:TRP:HB2	2.01	0.43
9:I:70:LEU:CD2	9:I:71:ASN:N	2.79	0.43
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.40	0.43
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.88	0.43
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.83	0.43
4:D:171:TYR:CD1	4:D:175:THR:HB	2.54	0.43
3:P:156:TYR:N	3:P:156:TYR:CD2	2.87	0.43
6:S:84:GLU:CD	6:S:84:GLU:H	2.26	0.43
1:A:275:ALA:HB3	1:A:357:ALA:HB1	2.00	0.42
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.54	0.42
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.84	0.42
4:D:240:PRO:O	4:D:241:LYS:C	2.61	0.42
5:E:75:GLU:HB3	5:E:194:VAL:HG22	2.00	0.42
5:E:81:ILE:HG22	5:E:100:HIS:HB2	2.01	0.42
10:J:10:TYR:CD2	10:J:10:TYR:C	2.97	0.42
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.37	0.42
2:O:395:PRO:O	2:O:398:VAL:HG12	2.19	0.42
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.19	0.42
6:S:91:GLU:HB3	6:S:92:PRO:HD3	2.01	0.42
1:A:382:HIS:HE1	1:A:390:ILE:HB	1.85	0.42
2:B:408:ALA:O	2:B:409:ASP:C	2.63	0.42
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.76	0.42
4:D:197:GLU:O	4:D:198:HIS:C	2.60	0.42
7:G:40:ARG:HD2	17:G:2004:CDL:OA4	2.19	0.42
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.19	0.42
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.19	0.42
2:O:160:LEU:HB2	9:V:64:LEU:HD22	2.01	0.42
3:P:125:MET:CE	13:P:3001:JZZ:HAGA	2.49	0.42
3:P:130:VAL:HG23	3:P:183:HIS:HB2	2.01	0.42
8:U:73:LEU:HD12	8:U:73:LEU:O	2.19	0.42
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.19	0.42
1:A:245:ASP:OD1	7:G:11:ARG:NE	2.47	0.42
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.01	0.42
11:C:2007:PEE:H50	17:G:2004:CDL:H712	2.01	0.42
5:E:166:ASP:OD1	5:E:168:SER:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:MET:HG3	1:N:366:VAL:N	2.33	0.42
2:O:50:PHE:CD1	2:O:50:PHE:N	2.88	0.42
6:S:60:PHE:O	6:S:64:ARG:HB2	2.19	0.42
9:V:65:VAL:HG12	9:V:66:ALA:N	2.33	0.42
1:A:178:THR:CG2	1:A:179:ARG:H	2.31	0.42
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.54	0.42
8:H:43:ARG:NH1	8:H:43:ARG:HG2	2.34	0.42
1:N:106:MET:CG	1:N:203:ILE:HD13	2.46	0.42
1:N:287:GLY:O	1:N:290:LEU:HG	2.19	0.42
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.01	0.42
2:O:68:LEU:HD23	2:O:186:ILE:HG21	2.00	0.42
3:P:272:GLU:O	3:P:273:TRP:C	2.62	0.42
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.45	0.42
5:R:101:ARG:HH21	5:R:130:PRO:HA	1.84	0.42
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.67	0.42
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.54	0.42
1:A:369:LEU:HD11	1:A:392:LEU:HD21	2.02	0.42
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.54	0.42
3:C:365:ILE:HG22	3:C:366:LEU:HD23	2.01	0.42
4:D:218:LEU:HD11	5:E:42:THR:HG22	2.01	0.42
10:J:42:ILE:HG22	10:J:46:LEU:HD12	2.02	0.42
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.80	0.42
1:N:95:THR:HG22	1:N:96:ALA:N	2.34	0.42
1:N:369:LEU:HD11	1:N:392:LEU:HD21	2.00	0.42
2:O:259:THR:CG2	2:O:260:GLU:N	2.82	0.42
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.54	0.42
1:A:62:LEU:HD11	1:A:127:ILE:HG12	2.01	0.42
1:A:156:THR:HG23	1:A:157:ALA:N	2.35	0.42
1:A:361:LEU:O	1:A:364:ALA:HB3	2.19	0.42
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.55	0.42
2:B:270:ASN:O	2:B:274:VAL:HG23	2.19	0.42
2:B:334:GLY:O	2:B:338:ARG:HG2	2.20	0.42
3:C:182:LEU:HD23	3:C:182:LEU:HA	1.86	0.42
4:D:161:ALA:O	4:D:162:PRO:C	2.61	0.42
5:E:127:VAL:O	5:E:128:LYS:HB2	2.20	0.42
1:N:89:TYR:O	1:N:95:THR:HG23	2.20	0.42
1:N:382:HIS:HE1	1:N:390:ILE:HB	1.84	0.42
3:P:92:PHE:HA	3:P:95:ILE:HG22	2.02	0.42
3:P:131:GLY:HA3	3:P:183:HIS:CE1	2.54	0.42
5:R:81:ILE:HG12	5:R:87:VAL:CG2	2.49	0.42
5:R:100:HIS:HD2	5:R:131:GLU:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:HIS:C	1:A:156:THR:N	2.76	0.42
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.00	0.42
2:B:50:PHE:N	2:B:50:PHE:HD1	2.18	0.42
2:B:231:GLY:O	2:B:232:THR:C	2.62	0.42
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.31	0.42
3:P:286:PRO:O	3:P:287:ASN:HB2	2.19	0.42
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.81	0.42
2:B:96:LEU:HD12	2:B:96:LEU:C	2.44	0.42
2:B:163:LEU:C	2:B:165:ALA:N	2.74	0.42
3:C:37:LEU:HD21	3:C:233:LEU:HA	2.01	0.42
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.34	0.42
4:D:98:PRO:HG2	4:D:99:GLU:OE1	2.20	0.42
5:E:149:ASN:N	5:E:149:ASN:HD22	2.17	0.42
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.54	0.42
1:N:204:SER:O	1:N:205:HIS:C	2.62	0.42
1:N:417:ASP:O	1:N:438:ARG:NH2	2.53	0.42
2:O:96:LEU:HB3	9:V:70:LEU:HD22	2.01	0.42
2:O:325:TYR:C	2:O:325:TYR:CD2	2.98	0.42
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.54	0.42
7:T:48:VAL:O	7:T:51:PRO:HD2	2.19	0.42
9:V:52:ARG:HG3	9:V:52:ARG:NH1	2.33	0.42
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.68	0.42
2:B:76:THR:HG23	2:B:82:SER:HB2	2.02	0.42
4:D:150:ASN:O	4:D:156:GLN:HA	2.20	0.42
1:N:113:LEU:O	1:N:116:VAL:N	2.49	0.42
2:O:166:ALA:HB1	2:O:242:GLY:O	2.20	0.42
2:O:222:GLN:O	2:O:223:PHE:CD2	2.73	0.42
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.84	0.42
5:R:52:LYS:C	5:R:52:LYS:CD	2.93	0.42
5:R:58:PHE:O	5:R:59:ILE:C	2.63	0.42
6:S:58:ARG:HD2	6:S:89:TYR:OH	2.20	0.42
2:B:341:MET:HA	2:B:341:MET:CE	2.46	0.42
2:B:385:GLU:HB3	2:B:391:THR:O	2.20	0.42
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.87	0.42
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.49	0.42
4:D:102:ARG:HG2	4:D:102:ARG:NH1	2.35	0.42
5:E:126:ARG:C	5:E:127:VAL:HG23	2.45	0.42
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.60	0.42
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.82	0.42
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.53	0.42
1:A:89:TYR:CD1	1:A:89:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:HIS:O	1:A:156:THR:N	2.53	0.41
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.02	0.41
2:B:325:TYR:C	2:B:325:TYR:HD2	2.27	0.41
1:N:6:GLN:O	1:N:7:THR:C	2.62	0.41
2:O:42:SER:C	2:O:44:ALA:H	2.28	0.41
3:P:18:SER:CB	3:P:202:HIS:HE1	2.32	0.41
3:P:75:GLN:O	3:P:76:TYR:HB2	2.20	0.41
3:P:132:TYR:HD2	13:P:3001:JZZ:H27A	1.85	0.41
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.49	0.41
5:R:76:ILE:HB	5:R:193:VAL:CG1	2.50	0.41
8:U:52:GLU:HG2	8:U:53:GLN:N	2.33	0.41
10:W:42:ILE:HG22	10:W:46:LEU:HD12	2.02	0.41
1:A:27:SER:HA	1:A:199:ALA:O	2.20	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.38	0.41
2:B:163:LEU:C	2:B:165:ALA:H	2.29	0.41
2:B:287:ARG:HB3	9:I:53:GLU:HG3	2.02	0.41
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.85	0.41
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.54	0.41
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.56	0.41
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.54	0.41
7:G:56:TYR:O	7:G:59:TYR:HB3	2.20	0.41
1:N:261:GLY:HA2	1:N:317:THR:O	2.20	0.41
3:P:235:LEU:HA	3:P:235:LEU:HD23	1.84	0.41
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.45	0.41
2:B:54:GLY:O	2:B:56:ARG:N	2.53	0.41
2:B:345:LYS:HG2	2:B:418:VAL:HG11	2.01	0.41
1:N:37:VAL:HG23	1:N:113:LEU:HD11	2.02	0.41
2:O:56:ARG:HA	2:O:171:ALA:O	2.20	0.41
2:O:248:ASN:ND2	2:O:250:HIS:H	2.18	0.41
3:P:25:PRO:HB2	3:P:28:ILE:HG23	2.03	0.41
3:P:31:TRP:CH2	17:T:3004:CDL:H512	2.54	0.41
3:P:277:PHE:CG	3:P:278:ALA:N	2.87	0.41
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.20	0.41
5:R:153:PHE:C	5:R:155:GLY:H	2.28	0.41
7:T:35:PRO:O	7:T:38:TRP:HB3	2.19	0.41
1:A:202:GLY:C	1:A:203:ILE:HG13	2.44	0.41
2:B:59:THR:C	2:B:61:ALA:H	2.28	0.41
3:C:233:LEU:O	3:C:237:LEU:HB2	2.20	0.41
3:C:247:SER:N	3:C:248:PRO:HD3	2.34	0.41
3:C:339:ILE:HD13	3:C:339:ILE:HA	1.92	0.41
4:D:169:LEU:HD22	4:D:182:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:131:GLU:H	5:E:131:GLU:CD	2.28	0.41
5:E:178:TYR:N	5:E:178:TYR:CD1	2.89	0.41
5:E:179:ASN:O	5:E:180:LEU:C	2.62	0.41
8:H:10:GLU:C	8:H:11:GLU:HG3	2.45	0.41
8:H:43:ARG:HG2	8:H:43:ARG:HH11	1.86	0.41
1:N:79:VAL:O	1:N:82:MET:HG2	2.20	0.41
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.89	0.41
5:R:73:LYS:HB3	5:R:196:GLY:O	2.20	0.41
8:U:65:ARG:O	8:U:68:CYS:HB3	2.20	0.41
2:B:59:THR:HG22	2:B:60:THR:N	2.35	0.41
2:B:153:GLN:NE2	9:I:34:UNK:HB1	2.35	0.41
2:B:206:LEU:HG	2:B:206:LEU:O	2.20	0.41
2:B:385:GLU:C	2:B:387:LEU:N	2.79	0.41
1:N:114:ALA:O	1:N:118:GLN:HB2	2.20	0.41
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.41
2:O:166:ALA:HB1	2:O:242:GLY:C	2.45	0.41
2:O:206:LEU:HG	2:O:206:LEU:O	2.19	0.41
4:Q:16:GLY:N	4:Q:19:SER:OG	2.54	0.41
4:Q:218:LEU:HD11	5:R:42:THR:HG22	2.01	0.41
5:R:171:ILE:N	5:R:179:ASN:OD1	2.46	0.41
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.49	0.41
2:B:50:PHE:C	2:B:51:ILE:HG13	2.44	0.41
2:B:128:THR:O	2:B:226:ILE:HD11	2.20	0.41
2:B:153:GLN:HE22	9:I:34:UNK:HB1	1.85	0.41
4:D:9:ALA:HA	4:D:125:ASP:OD1	2.20	0.41
4:D:99:GLU:H	4:D:99:GLU:CD	2.28	0.41
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.54	0.41
1:N:373:THR:HB	1:N:374:PRO:CD	2.51	0.41
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.56	0.41
3:P:172:ASP:OD1	3:P:173:ASN:N	2.51	0.41
5:R:171:ILE:HB	5:R:178:TYR:O	2.20	0.41
1:A:133:VAL:O	1:A:137:GLU:HG3	2.20	0.41
2:B:146:VAL:O	2:B:149:ALA:N	2.53	0.41
2:B:223:PHE:O	2:B:225:ASN:N	2.54	0.41
3:C:172:ASP:HB3	3:C:174:PRO:HD2	2.02	0.41
4:D:169:LEU:HD23	4:D:169:LEU:O	2.20	0.41
4:D:239:PRO:HG2	4:D:241:LYS:HB2	2.02	0.41
2:O:18:CYS:CB	2:O:19:PRO:CD	2.93	0.41
2:O:35:ILE:O	2:O:213:HIS:HE1	2.03	0.41
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.50	0.41
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:32:MET:O	6:S:35:ASP:HB2	2.20	0.41
1:A:240:GLU:HA	1:A:422:LEU:O	2.21	0.41
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.51	0.41
2:B:207:VAL:HG21	2:B:383:GLY:HA3	2.03	0.41
3:C:292:VAL:O	3:C:293:LEU:C	2.63	0.41
4:D:158:ILE:HG12	4:D:160:MET:H	1.85	0.41
6:F:31:LEU:HD21	6:F:65:ALA:HB2	2.03	0.41
2:O:43:PRO:O	2:O:113:ARG:HG3	2.20	0.41
2:O:207:VAL:HG12	2:O:208:GLY:N	2.36	0.41
1:A:32:GLN:HE22	2:B:373:GLU:HA	1.85	0.41
1:A:439:SER:HA	1:A:442:TYR:CE2	2.56	0.41
2:B:72:ALA:C	2:B:74:PRO:HD2	2.45	0.41
2:B:385:GLU:C	2:B:387:LEU:H	2.29	0.41
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.86	0.41
5:E:137:GLY:O	5:E:145:VAL:HG13	2.20	0.41
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.69	0.41
6:F:21:TYR:CG	6:F:83:TYR:HD1	2.39	0.41
6:F:71:LYS:O	6:F:72:HIS:HB2	2.21	0.41
7:G:34:LEU:HB2	7:G:35:PRO:HD3	2.03	0.41
1:N:217:SER:O	1:N:218:GLY:C	2.63	0.41
2:O:150:VAL:C	2:O:153:GLN:HG3	2.45	0.41
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.89	0.41
4:Q:169:LEU:HD23	4:Q:169:LEU:O	2.20	0.41
5:R:96:LEU:HD21	5:R:195:VAL:HG21	2.01	0.41
10:W:52:TRP:O	10:W:56:LYS:HB2	2.20	0.41
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.51	0.41
2:B:35:ILE:HD11	2:B:220:ALA:HB3	2.03	0.41
2:B:73:SER:N	2:B:74:PRO:HD2	2.36	0.41
3:C:223:PRO:O	3:C:227:PHE:HD2	2.04	0.41
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.54	0.41
9:I:61:ARG:C	9:I:62:ARG:HG3	2.46	0.41
1:N:206:LYS:C	1:N:208:LEU:N	2.79	0.41
2:O:274:VAL:O	2:O:278:VAL:HG23	2.21	0.41
2:O:399:ALA:O	2:O:402:ILE:CG2	2.68	0.41
2:O:399:ALA:C	2:O:402:ILE:HG22	2.45	0.41
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.21	0.41
5:R:109:GLU:CD	5:R:123:ASP:HB2	2.46	0.41
6:S:13:MET:C	6:S:15:ARG:H	2.28	0.41
1:A:134:ILE:HG21	1:A:174:ILE:HD13	2.02	0.40
1:A:154:HIS:C	1:A:156:THR:H	2.29	0.40
2:B:84:ARG:HG3	6:S:107:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:O	2:B:292:THR:CG2	2.68	0.40
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.36	0.40
3:P:89:SER:O	3:P:90:PHE:C	2.64	0.40
4:Q:95:TYR:HA	4:Q:96:PRO:HD3	1.87	0.40
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.56	0.40
6:S:40:ASP:OD1	6:S:40:ASP:C	2.64	0.40
2:B:259:THR:CG2	2:B:260:GLU:N	2.84	0.40
11:E:2005:PEE:H13	11:E:2005:PEE:H8	2.03	0.40
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.38	0.40
1:N:373:THR:N	1:N:374:PRO:HD2	2.36	0.40
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.36	0.40
5:R:171:ILE:HG12	5:R:176:ALA:O	2.21	0.40
11:R:3005:PEE:H8	11:R:3005:PEE:H13	2.03	0.40
1:A:269:VAL:CG2	1:A:406:MET:HE3	2.52	0.40
1:A:395:TRP:O	1:A:399:ILE:HG13	2.20	0.40
2:B:59:THR:O	2:B:60:THR:C	2.65	0.40
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.57	0.40
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.03	0.40
2:O:37:SER:CB	2:O:213:HIS:ND1	2.69	0.40
2:O:207:VAL:HG21	2:O:383:GLY:HA3	2.03	0.40
3:P:64:PHE:CE1	15:P:3011:GOL:H12	2.56	0.40
3:P:120:LEU:HD23	3:P:120:LEU:HA	1.80	0.40
1:A:145:MET:HE2	1:A:145:MET:N	2.37	0.40
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.50	0.40
3:C:98:HIS:CE1	12:C:502:HEM:NA	2.89	0.40
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.20	0.40
4:D:102:ARG:HB3	4:D:107:GLY:HA2	2.02	0.40
5:E:10:PHE:CB	7:G:18:LEU:HD11	2.51	0.40
7:G:35:PRO:O	7:G:38:TRP:HB3	2.22	0.40
7:G:40:ARG:CB	17:G:2004:CDL:HA32	2.52	0.40
1:N:246:ASP:HA	1:N:427:PRO:HB3	2.03	0.40
2:O:18:CYS:O	2:O:19:PRO:C	2.65	0.40
2:O:62:ASN:O	2:O:63:LEU:C	2.64	0.40
2:O:181:TYR:CD1	2:O:182:ARG:HG3	2.55	0.40
2:O:231:GLY:O	2:O:232:THR:C	2.63	0.40
3:P:182:LEU:HD23	3:P:182:LEU:HA	1.85	0.40
4:Q:28:ARG:HE	4:Q:185:ASP:CG	2.29	0.40
5:R:106:ILE:HG21	5:R:130:PRO:HB3	2.04	0.40
5:R:171:ILE:O	5:R:171:ILE:HG23	2.22	0.40
6:S:51:PRO:O	6:S:52:GLU:C	2.64	0.40
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ALA:O	1:A:116:VAL:HG13	2.21	0.40
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.36	0.40
3:C:101:ARG:HD2	3:C:101:ARG:O	2.21	0.40
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.57	0.40
4:D:203:ARG:NH1	18:D:2091:BOG:O3	2.54	0.40
5:E:83:GLU:C	5:E:102:THR:HG23	2.46	0.40
5:E:126:ARG:O	5:E:127:VAL:CG2	2.69	0.40
1:N:23:LEU:HD23	1:N:24:ARG:N	2.37	0.40
1:N:342:TRP:O	1:N:345:LEU:HB2	2.21	0.40
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.56	0.40
8:U:52:GLU:CG	8:U:53:GLN:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/446 (99%)	388 (88%)	46 (10%)	8 (2%)	6	28
1	N	440/446 (99%)	386 (88%)	45 (10%)	9 (2%)	6	25
2	B	418/441 (95%)	342 (82%)	56 (13%)	20 (5%)	2	9
2	O	420/441 (95%)	355 (84%)	51 (12%)	14 (3%)	3	15
3	C	378/380 (100%)	347 (92%)	28 (7%)	3 (1%)	16	46
3	P	377/380 (99%)	345 (92%)	26 (7%)	6 (2%)	7	30
4	D	239/241 (99%)	215 (90%)	22 (9%)	2 (1%)	16	46
4	Q	239/241 (99%)	213 (89%)	22 (9%)	4 (2%)	7	29
5	E	194/196 (99%)	150 (77%)	31 (16%)	13 (7%)	1	4
5	R	194/196 (99%)	156 (80%)	26 (13%)	12 (6%)	1	6
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	99/110 (90%)	89 (90%)	10 (10%)	0	100	100
7	G	78/81 (96%)	68 (87%)	9 (12%)	1 (1%)	9	35
7	T	77/81 (95%)	66 (86%)	10 (13%)	1 (1%)	9	35
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100	100
8	U	65/77 (84%)	59 (91%)	4 (6%)	2 (3%)	3	16
9	I	29/47 (62%)	26 (90%)	2 (7%)	1 (3%)	3	14
9	V	29/47 (62%)	25 (86%)	4 (14%)	0	100	100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
10	W	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	29
All	All	4002/4160 (96%)	3500 (88%)	405 (10%)	97 (2%)	4	21

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	433	ASP
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
2	B	231	GLY
3	C	287	ASN
5	E	80	ASP
5	E	102	THR
5	E	127	VAL
5	E	128	LYS
1	N	282	ARG
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
8	U	49	HIS
10	W	61	ALA
1	A	72	CYS

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Mol	Chain	Res	Type
1	A	218	GLY
2	B	224	LEU
2	B	371	SER
2	B	386	ALA
4	D	38	SER
5	E	130	PRO
5	E	163	SER
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	262	TRP
2	O	222	GLN
2	O	231	GLY
2	O	371	SER
2	O	386	ALA
5	R	137	GLY
5	R	154	GLY
5	R	163	SER
5	R	185	TYR
8	U	52	GLU
1	A	155	ALA
1	A	262	TRP
2	B	60	THR
2	B	221	GLU
2	B	222	GLN
5	E	137	GLY
5	E	166	ASP
1	N	72	CYS
1	N	155	ALA
2	O	319	SER
4	Q	38	SER
4	Q	177	ALA
5	R	127	VAL
5	R	186	GLN
5	R	191	ASP
2	B	55	SER
2	B	389	SER
2	B	420	GLY
1	N	81	SER
1	N	443	TRP
2	O	19	PRO
2	O	55	SER

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Mol	Chain	Res	Type
2	O	60	THR
3	P	156	TYR
3	P	274	TYR
4	Q	198	HIS
5	R	166	ASP
5	R	190	ASP
7	T	33	ALA
1	A	443	TRP
2	B	201	SER
5	E	120	PRO
5	E	154	GLY
5	E	186	GLN
7	G	33	ALA
1	N	206	LYS
2	O	389	SER
3	P	3	PRO
5	R	113	ASP
1	A	404	ALA
2	B	319	SER
3	C	3	PRO
5	R	120	PRO
3	C	264	VAL
3	P	157	ILE
2	B	208	GLY
2	O	208	GLY
3	P	264	VAL
4	D	162	PRO
9	I	76	VAL
2	O	420	GLY
5	R	177	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	365/368 (99%)	356 (98%)	9 (2%)	42 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	365/368 (99%)	352 (96%)	13 (4%)	31	62
2	B	331/347 (95%)	314 (95%)	17 (5%)	21	52
2	O	333/347 (96%)	316 (95%)	17 (5%)	21	52
3	C	328/329 (100%)	324 (99%)	4 (1%)	63	79
3	P	328/329 (100%)	324 (99%)	4 (1%)	63	79
4	D	200/200 (100%)	194 (97%)	6 (3%)	36	66
4	Q	200/200 (100%)	194 (97%)	6 (3%)	36	66
5	E	166/166 (100%)	162 (98%)	4 (2%)	43	70
5	R	165/166 (99%)	162 (98%)	3 (2%)	51	74
6	F	93/96 (97%)	88 (95%)	5 (5%)	20	50
6	S	93/96 (97%)	87 (94%)	6 (6%)	15	44
7	G	71/71 (100%)	71 (100%)	0	100	100
7	T	70/71 (99%)	70 (100%)	0	100	100
8	H	65/71 (92%)	63 (97%)	2 (3%)	35	65
8	U	63/71 (89%)	61 (97%)	2 (3%)	34	64
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	33
9	V	23/26 (88%)	22 (96%)	1 (4%)	26	57
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	73
10	W	47/49 (96%)	45 (96%)	2 (4%)	26	57
All	All	3378/3446 (98%)	3274 (97%)	104 (3%)	35	65

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	106	MET
1	A	108	LYS
1	A	179	ARG
1	A	228	VAL
1	A	281	ASP
1	A	395	TRP
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	26	ILE

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Mol	Chain	Res	Type
2	B	31	ASN
2	B	38	LEU
2	B	50	PHE
2	B	97	SER
2	B	124	LEU
2	B	154	SER
2	B	170	THR
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	325	TYR
2	B	341	MET
2	B	343	GLN
2	B	367	THR
2	B	402	ILE
3	C	81	ARG
3	C	146	VAL
3	C	216	SER
3	C	328	LEU
4	D	43	MET
4	D	54	VAL
4	D	70	VAL
4	D	130	LEU
4	D	169	LEU
4	D	203	ARG
5	E	6	THR
5	E	60	SER
5	E	102	THR
5	E	185	TYR
6	F	44	LYS
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
6	F	78	GLU
8	H	21	ARG
8	H	49	HIS
9	I	68	ILE
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	49	ASN

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Mol	Chain	Res	Type
1	N	50	GLU
1	N	106	MET
1	N	108	LYS
1	N	171	THR
1	N	228	VAL
1	N	241	ILE
1	N	281	ASP
1	N	395	TRP
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO
2	O	26	ILE
2	O	31	ASN
2	O	97	SER
2	O	124	LEU
2	O	154	SER
2	O	170	THR
2	O	248	ASN
2	O	250	HIS
2	O	260	GLU
2	O	325	TYR
2	O	341	MET
2	O	343	GLN
2	O	367	THR
2	O	402	ILE
2	O	418	VAL
3	P	81	ARG
3	P	146	VAL
3	P	216	SER
3	P	328	LEU
4	Q	37	CYS
4	Q	43	MET
4	Q	54	VAL
4	Q	70	VAL
4	Q	130	LEU
4	Q	169	LEU
5	R	60	SER
5	R	178	TYR
5	R	185	TYR
6	S	14	ASP
6	S	64	ARG

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Mol	Chain	Res	Type
6	S	70	LEU
6	S	73	ARG
6	S	78	GLU
6	S	84	GLU
8	U	21	ARG
8	U	49	HIS
9	V	68	ILE
10	W	59	TYR
10	W	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	173	ASN
1	A	176	HIS
1	A	214	GLN
1	A	274	ASN
1	A	289	HIS
1	A	301	HIS
1	A	308	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	17	ASN
3	C	69	HIS
3	C	73	ASN
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	35	GLN

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Mol	Chain	Res	Type
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	12	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
8	H	23	HIS
9	I	71	ASN
1	N	32	GLN
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	176	HIS
1	N	214	GLN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	435	ASN
2	O	31	ASN
2	O	156	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	329	GLN
2	O	342	ASN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
2	O	392	HIS
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS
3	P	73	ASN
3	P	82	ASN
3	P	149	ASN
3	P	207	ASN

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Mol	Chain	Res	Type
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	23	HIS
8	U	71	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
11	PEE	C	2007	-	48,48,50	1.47	7 (14%)	51,53,55	0.83	3 (5%)
11	PEE	A	2008	-	20,20,50	1.90	6 (30%)	23,25,55	0.69	0
12	HEM	P	502	3	50,50,50	1.43	5 (10%)	67,82,82	1.28	9 (13%)
14	UQ	C	2002	-	19,19,63	2.76	10 (52%)	24,26,79	1.33	3 (12%)
17	CDL	G	2004	-	39,39,99	1.22	2 (5%)	45,51,111	1.11	4 (8%)
18	BOG	D	2009	-	20,20,20	0.99	2 (10%)	25,25,25	0.87	2 (8%)
12	HEM	C	501	3	50,50,50	1.59	8 (16%)	67,82,82	1.43	9 (13%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
14	UQ	P	3002	-	19,19,63	2.63	10 (52%)	24,26,79	1.34	3 (12%)
16	HEC	Q	501	4	46,50,50	1.82	9 (19%)	58,82,82	2.12	7 (12%)
11	PEE	E	2005	-	49,49,50	1.57	10 (20%)	52,54,55	0.92	3 (5%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
17	CDL	T	3004	-	39,39,99	1.23	2 (5%)	45,51,111	1.13	4 (8%)
18	BOG	P	2010	-	12,12,20	1.46	4 (33%)	17,17,25	0.67	0
11	PEE	P	3007	-	48,48,50	1.43	6 (12%)	51,53,55	0.80	2 (3%)
12	HEM	P	501	3	50,50,50	1.48	4 (8%)	67,82,82	1.43	9 (13%)
17	CDL	Q	3003	-	41,41,99	1.22	3 (7%)	47,53,111	1.04	2 (4%)
13	JZZ	C	2001	-	27,27,27	2.25	7 (25%)	32,40,40	1.70	3 (9%)
13	JZZ	P	3001	-	27,27,27	2.29	7 (25%)	32,40,40	1.68	3 (9%)
15	GOL	P	3011	-	5,5,5	1.34	0	5,5,5	0.53	0
12	HEM	C	502	3	50,50,50	1.71	10 (20%)	67,82,82	1.34	9 (13%)
16	HEC	D	501	4	46,50,50	1.89	13 (28%)	58,82,82	2.33	14 (24%)
18	BOG	D	2091	-	13,13,20	1.36	2 (15%)	18,18,25	1.11	2 (11%)
18	BOG	Q	3009	-	20,20,20	0.97	1 (5%)	25,25,25	0.91	1 (4%)
15	GOL	C	2011	-	5,5,5	1.48	0	5,5,5	0.68	0
17	CDL	D	2003	-	41,41,99	1.23	2 (4%)	47,53,111	1.00	2 (4%)
11	PEE	P	3008	-	4,4,50	3.76	4 (100%)	6,6,55	0.65	0
11	PEE	R	3005	-	49,49,50	1.60	10 (20%)	52,54,55	0.92	3 (5%)
18	BOG	Q	3091	-	13,13,20	1.49	3 (23%)	18,18,25	1.19	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEE	C	2007	-	-	19/52/52/54	-
11	PEE	A	2008	-	-	11/24/24/54	-
12	HEM	P	502	3	-	6/14/54/54	-
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
17	CDL	G	2004	-	-	19/49/49/110	-
18	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
12	HEM	C	501	3	-	7/14/54/54	-
19	FES	R	501	5	-	-	0/1/1/1
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
16	HEC	Q	501	4	-	10/14/54/54	-
11	PEE	E	2005	-	-	25/53/53/54	-
19	FES	E	501	5	-	-	0/1/1/1
17	CDL	T	3004	-	-	19/49/49/110	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
11	PEE	P	3007	-	-	22/52/52/54	-
12	HEM	P	501	3	-	7/14/54/54	-
17	CDL	Q	3003	-	-	24/51/51/110	-
13	JZZ	C	2001	-	-	2/12/12/12	0/3/3/3
13	JZZ	P	3001	-	-	5/12/12/12	0/3/3/3
15	GOL	P	3011	-	-	3/4/4/4	-
12	HEM	C	502	3	-	5/14/54/54	-
16	HEC	D	501	4	-	9/14/54/54	-
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
18	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
15	GOL	C	2011	-	-	4/4/4/4	-
17	CDL	D	2003	-	-	22/51/51/110	-
11	PEE	R	3005	-	-	25/53/53/54	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	JZZ	N5-N4	-6.66	1.23	1.36
13	C	2001	JZZ	N5-N4	-6.38	1.24	1.36
16	Q	501	HEC	CAB-C3B	5.88	1.54	1.35
16	Q	501	HEC	CAC-C3C	5.74	1.53	1.35
12	C	501	HEM	CBC-CAC	5.49	1.56	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	CAB-C3B	5.47	1.52	1.35
14	C	2002	UQ	C6-C5	5.31	1.44	1.35
14	C	2002	UQ	C7-C6	5.17	1.60	1.51
14	P	3002	UQ	C7-C6	5.11	1.60	1.51
11	P	3008	PEE	P-O1P	5.10	1.62	1.50
16	D	501	HEC	CAC-C3C	4.97	1.51	1.35
13	P	3001	JZZ	CAN-N2	-4.87	1.33	1.45
14	P	3002	UQ	C6-C5	4.84	1.43	1.35
12	P	501	HEM	CBC-CAC	4.81	1.53	1.30
12	C	502	HEM	CBB-CAB	4.78	1.53	1.30
13	C	2001	JZZ	CAN-N2	-4.71	1.33	1.45
12	P	502	HEM	CBB-CAB	4.44	1.51	1.30
12	P	501	HEM	CBB-CAB	4.42	1.51	1.30
13	P	3001	JZZ	C3-N4	4.42	1.33	1.29
13	C	2001	JZZ	C3-N4	4.22	1.33	1.29
11	C	2007	PEE	C39-C38	4.21	1.55	1.31
11	P	3007	PEE	C39-C38	4.17	1.55	1.31
12	C	501	HEM	CBB-CAB	4.17	1.50	1.30
11	E	2005	PEE	C39-C38	4.12	1.55	1.31
11	R	3005	PEE	C39-C38	4.12	1.55	1.31
12	P	502	HEM	CBC-CAC	3.95	1.49	1.30
11	R	3005	PEE	O2-C10	3.92	1.45	1.34
12	C	502	HEM	CAC-C3C	-3.91	1.37	1.47
14	C	2002	UQ	C6-C1	3.77	1.57	1.46
14	P	3002	UQ	C6-C1	3.73	1.57	1.46
13	C	2001	JZZ	C6-N2	-3.71	1.32	1.40
12	P	502	HEM	CAC-C3C	-3.68	1.37	1.47
14	P	3002	UQ	O3-C3	3.60	1.45	1.36
11	E	2005	PEE	O3-C30	3.57	1.43	1.33
11	P	3008	PEE	P-O4P	3.57	1.65	1.54
11	E	2005	PEE	O2-C10	3.56	1.44	1.34
13	P	3001	JZZ	C6-N2	-3.51	1.33	1.40
11	C	2007	PEE	O3-C30	3.50	1.43	1.33
11	P	3008	PEE	P-O3P	3.46	1.64	1.54
11	P	3007	PEE	C21-C22	-3.44	1.34	1.51
16	D	501	HEC	CHD-C4C	-3.40	1.31	1.38
14	C	2002	UQ	O3-C3	3.38	1.44	1.36
11	P	3007	PEE	O3-C30	3.36	1.43	1.33
12	C	502	HEM	CBC-CAC	3.33	1.46	1.30
11	A	2008	PEE	O2-C10	3.32	1.43	1.34
11	R	3005	PEE	O3-C30	3.29	1.42	1.33
12	P	501	HEM	CAB-C3B	-3.28	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	502	HEM	CAB-C3B	-3.27	1.38	1.47
11	R	3005	PEE	P-O1P	3.27	1.62	1.50
11	A	2008	PEE	P-O1P	3.23	1.62	1.50
11	A	2008	PEE	O3-C30	3.21	1.42	1.33
11	E	2005	PEE	C21-C22	-3.16	1.36	1.51
11	C	2007	PEE	C21-C22	-3.16	1.36	1.51
11	R	3005	PEE	C21-C22	-3.15	1.36	1.51
11	E	2005	PEE	P-O1P	3.15	1.61	1.50
16	D	501	HEC	C3B-C2B	-3.10	1.30	1.41
11	C	2007	PEE	P-O1P	3.06	1.61	1.50
12	C	502	HEM	CAB-C3B	-3.06	1.39	1.47
11	P	3007	PEE	O2-C10	3.05	1.42	1.34
12	C	502	HEM	C4D-C3D	3.03	1.50	1.45
14	C	2002	UQ	C2-C1	3.03	1.57	1.48
12	C	502	HEM	C3B-C4B	3.01	1.50	1.44
16	D	501	HEC	C3C-C2C	-3.00	1.31	1.41
13	C	2001	JZZ	O3-C3	2.98	1.36	1.33
12	C	501	HEM	CAB-C3B	-2.98	1.39	1.47
14	C	2002	UQ	CM5-C5	2.97	1.56	1.50
12	C	502	HEM	C3C-C2C	-2.94	1.31	1.37
14	C	2002	UQ	O2-C2	2.92	1.43	1.36
12	P	501	HEM	CAC-C3C	-2.90	1.39	1.47
11	P	3007	PEE	P-O1P	2.89	1.60	1.50
14	P	3002	UQ	C7-C8	2.85	1.55	1.50
14	C	2002	UQ	C5-C4	2.84	1.57	1.47
16	D	501	HEC	C1D-ND	-2.82	1.34	1.39
11	C	2007	PEE	O2-C10	2.82	1.42	1.34
11	R	3005	PEE	C11-C10	2.80	1.58	1.50
16	D	501	HEC	CHD-C1D	-2.80	1.33	1.39
14	C	2002	UQ	C7-C8	2.78	1.54	1.50
13	P	3001	JZZ	O3-C3	2.77	1.36	1.33
14	P	3002	UQ	C2-C1	2.73	1.56	1.48
18	Q	3091	BOG	O5-C1	2.72	1.48	1.41
16	Q	501	HEC	C3B-C2B	-2.69	1.32	1.41
11	A	2008	PEE	C1-C2	2.67	1.59	1.50
14	P	3002	UQ	C5-C4	2.67	1.56	1.47
11	E	2005	PEE	C3-C2	2.64	1.59	1.50
13	P	3001	JZZ	CAJ-CAI	2.64	1.23	1.19
11	E	2005	PEE	C31-C30	2.62	1.58	1.50
14	P	3002	UQ	CM5-C5	2.61	1.56	1.50
13	C	2001	JZZ	C3-N2	-2.56	1.32	1.37
18	P	2010	BOG	C4-C5	2.56	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	O2-C2	2.56	1.42	1.36
16	D	501	HEC	C4A-C3A	2.54	1.50	1.45
18	D	2091	BOG	C4-C5	2.51	1.58	1.53
18	Q	3091	BOG	C4-C5	2.51	1.58	1.53
14	C	2002	UQ	C3-C4	2.50	1.56	1.48
14	P	3002	UQ	C3-C4	2.50	1.56	1.48
11	R	3005	PEE	O2-C2	2.49	1.52	1.46
11	E	2005	PEE	C11-C10	2.46	1.57	1.50
11	R	3005	PEE	C3-C2	2.44	1.58	1.50
16	D	501	HEC	C4C-NC	-2.43	1.35	1.39
11	R	3005	PEE	C31-C30	2.43	1.57	1.50
18	P	2010	BOG	C1-C2	2.41	1.57	1.52
11	P	3008	PEE	P-O2P	2.40	1.61	1.54
13	C	2001	JZZ	CAJ-CAI	2.39	1.22	1.19
16	Q	501	HEC	C3C-C2C	-2.39	1.33	1.41
11	R	3005	PEE	C1-C2	2.38	1.58	1.50
13	P	3001	JZZ	C3-N2	-2.37	1.33	1.37
18	D	2091	BOG	O5-C1	2.36	1.47	1.41
18	Q	3009	BOG	O5-C1	2.36	1.47	1.41
17	Q	3003	CDL	O1-C1	2.36	1.50	1.43
11	A	2008	PEE	C3-C2	2.36	1.58	1.50
18	D	2009	BOG	O5-C1	2.34	1.47	1.41
12	C	501	HEM	CMC-C2C	2.33	1.55	1.50
16	Q	501	HEC	C4C-NC	-2.33	1.35	1.39
17	T	3004	CDL	O1-C1	2.31	1.50	1.43
17	D	2003	CDL	O1-C1	2.30	1.50	1.43
16	D	501	HEC	C1A-C2A	2.29	1.49	1.45
12	C	501	HEM	CAC-C3C	-2.29	1.41	1.47
12	C	501	HEM	CHC-C1C	-2.29	1.33	1.38
11	C	2007	PEE	C31-C30	2.27	1.57	1.50
11	A	2008	PEE	C11-C10	2.26	1.57	1.50
16	D	501	HEC	C1B-NB	-2.24	1.35	1.39
17	G	2004	CDL	CB3-CB4	2.23	1.57	1.50
12	C	502	HEM	CHB-C4A	-2.21	1.34	1.39
11	E	2005	PEE	C1-C2	2.20	1.57	1.50
12	C	501	HEM	C1C-NC	-2.20	1.35	1.39
16	D	501	HEC	CHA-C1A	-2.18	1.34	1.38
11	P	3007	PEE	C31-C30	2.17	1.57	1.50
11	C	2007	PEE	C3-C2	2.16	1.57	1.50
17	G	2004	CDL	O1-C1	2.16	1.49	1.43
18	D	2009	BOG	C1-C2	2.15	1.58	1.52
17	D	2003	CDL	OA6-CA5	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	3004	CDL	CB3-CB4	2.14	1.57	1.50
17	Q	3003	CDL	CA3-CA4	2.14	1.57	1.50
16	Q	501	HEC	C1B-NB	-2.13	1.35	1.39
16	Q	501	HEC	C4D-ND	-2.11	1.35	1.39
18	Q	3091	BOG	O5-C5	2.09	1.49	1.44
16	D	501	HEC	C1D-C2D	2.09	1.48	1.43
12	C	502	HEM	C1C-C2C	2.09	1.49	1.45
18	P	2010	BOG	C4-C3	2.07	1.57	1.52
16	Q	501	HEC	C1D-ND	-2.04	1.35	1.39
18	P	2010	BOG	O5-C1	2.04	1.47	1.42
12	C	501	HEM	C2A-C3A	-2.03	1.33	1.38
12	P	502	HEM	C4D-C3D	2.03	1.48	1.45
17	Q	3003	CDL	OB2-CB2	-2.02	1.36	1.44
16	Q	501	HEC	CHA-C4D	-2.01	1.34	1.39
12	C	502	HEM	C1C-NC	-2.01	1.35	1.39
11	E	2005	PEE	O2-C2	2.00	1.51	1.46

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	CBB-CAB-C3B	-9.49	108.47	127.43
16	Q	501	HEC	CBB-CAB-C3B	-9.25	108.94	127.43
16	D	501	HEC	CBC-CAC-C3C	-8.84	109.76	127.43
16	Q	501	HEC	CBC-CAC-C3C	-8.60	110.24	127.43
13	C	2001	JZZ	N2-C6-N5	6.61	107.41	102.95
13	P	3001	JZZ	N2-C6-N5	6.20	107.13	102.95
13	P	3001	JZZ	C27-O3-C3	-4.99	108.90	116.19
16	Q	501	HEC	CAA-C2A-C1A	4.64	134.29	124.85
13	C	2001	JZZ	C27-O3-C3	-4.48	109.64	116.19
12	P	501	HEM	C3B-C4B-NB	4.38	112.61	109.47
14	C	2002	UQ	C8-C7-C6	4.26	122.58	112.08
14	P	3002	UQ	C8-C7-C6	4.26	122.58	112.08
16	D	501	HEC	CAA-C2A-C1A	4.21	133.41	124.85
16	Q	501	HEC	CAA-C2A-C3A	-4.20	120.00	127.87
16	D	501	HEC	CAA-C2A-C3A	-3.97	120.44	127.87
18	Q	3091	BOG	C1'-O1-C1	3.87	119.14	113.26
12	C	501	HEM	C3B-C4B-NB	3.86	112.24	109.47
12	P	502	HEM	CAD-C3D-C4D	3.86	131.42	124.70
13	P	3001	JZZ	C7-N5-N4	3.76	124.92	119.29
13	C	2001	JZZ	C7-N5-N4	3.62	124.70	119.29
12	C	502	HEM	CAD-C3D-C4D	3.47	130.75	124.70
18	Q	3009	BOG	C1'-O1-C1	3.43	119.53	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	3004	CDL	CB4-OB6-CB5	-3.43	109.60	117.80
18	D	2091	BOG	C1'-O1-C1	3.36	118.37	113.26
14	C	2002	UQ	C7-C6-C1	-3.34	114.63	118.52
12	C	502	HEM	C3B-C2B-C1B	-3.24	103.98	106.41
12	P	501	HEM	CAD-C3D-C4D	3.20	130.28	124.70
17	G	2004	CDL	CB4-OB6-CB5	-3.18	110.18	117.80
12	C	502	HEM	C2B-C1B-NB	3.16	113.47	109.84
12	C	501	HEM	CAD-C3D-C4D	3.15	130.19	124.70
14	P	3002	UQ	C7-C6-C1	-3.10	114.91	118.52
12	P	502	HEM	C3B-C2B-C1B	-3.07	104.10	106.41
16	Q	501	HEC	CMB-C2B-C1B	2.93	129.89	125.42
11	R	3005	PEE	C22-C21-C20	2.93	127.92	113.86
12	C	501	HEM	C2B-C1B-NB	2.91	113.19	109.84
18	D	2009	BOG	C1'-O1-C1	2.91	118.66	113.68
11	E	2005	PEE	C22-C21-C20	2.90	127.81	113.86
12	P	501	HEM	C2B-C1B-NB	2.87	113.14	109.84
11	C	2007	PEE	C22-C21-C20	2.81	127.35	113.86
12	C	501	HEM	CMA-C3A-C2A	2.77	131.50	125.62
16	D	501	HEC	CMD-C2D-C1D	2.77	129.64	125.42
12	C	501	HEM	CAD-C3D-C2D	-2.76	122.69	127.87
12	P	502	HEM	C2B-C1B-NB	2.76	113.01	109.84
12	C	501	HEM	C3B-C2B-C1B	-2.74	104.35	106.41
12	P	501	HEM	CAD-C3D-C2D	-2.72	122.77	127.87
12	C	501	HEM	C4C-C3C-C2C	-2.67	104.50	106.81
11	P	3007	PEE	C22-C21-C20	2.63	126.50	113.86
17	G	2004	CDL	CA4-OA6-CA5	-2.63	111.51	117.80
16	D	501	HEC	CHA-C1A-NA	-2.61	121.61	124.45
12	P	502	HEM	C3B-C4B-NB	2.60	111.33	109.47
16	Q	501	HEC	CMA-C3A-C4A	2.58	129.27	124.73
12	P	501	HEM	C2D-C1D-ND	2.57	112.88	109.90
16	D	501	HEC	CMB-C2B-C1B	2.57	129.34	125.42
12	C	501	HEM	CMD-C2D-C1D	2.57	129.05	125.03
12	C	502	HEM	C2A-C1A-NA	2.57	113.00	110.15
11	C	2007	PEE	C21-C22-C23	2.56	127.32	114.37
12	P	501	HEM	C4C-C3C-C2C	-2.55	104.61	106.81
18	D	2091	BOG	O1-C1-C2	2.54	111.07	108.14
12	C	502	HEM	C3D-C4D-ND	2.54	112.96	110.17
18	Q	3091	BOG	O1-C1-C2	2.53	111.06	108.14
11	E	2005	PEE	C21-C22-C23	2.50	127.02	114.37
17	T	3004	CDL	CA4-OA6-CA5	-2.48	111.85	117.80
11	R	3005	PEE	C21-C22-C23	2.48	126.89	114.37
11	E	2005	PEE	O3-C3-C2	2.45	115.46	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	CMA-C3A-C4A	2.45	129.03	124.73
16	D	501	HEC	C3D-C4D-ND	2.44	112.86	110.15
12	C	502	HEM	C3B-C4B-NB	2.43	111.22	109.47
11	P	3007	PEE	C21-C22-C23	2.43	126.66	114.37
17	T	3004	CDL	CA6-CA4-CA3	-2.42	106.14	111.78
12	P	502	HEM	C4A-NA-C1A	-2.38	101.94	105.82
16	D	501	HEC	C4B-NB-C1B	-2.37	101.95	105.82
11	R	3005	PEE	O3-C3-C2	2.36	115.19	108.40
16	D	501	HEC	CAD-C3D-C4D	2.30	129.43	124.94
12	P	501	HEM	C1B-NB-C4B	-2.30	102.49	105.21
18	D	2009	BOG	O1-C1-C2	2.28	111.73	108.27
17	D	2003	CDL	CB4-OB6-CB5	-2.26	112.38	117.80
12	P	501	HEM	C3B-C2B-C1B	-2.25	104.72	106.41
16	D	501	HEC	C2A-C1A-NA	2.24	112.48	110.32
17	D	2003	CDL	CA6-CA4-CA3	-2.22	106.61	111.78
12	P	502	HEM	CAD-C3D-C2D	-2.22	123.71	127.87
12	P	502	HEM	CMA-C3A-C4A	2.22	128.80	125.42
17	Q	3003	CDL	CB4-OB6-CB5	-2.21	112.51	117.80
11	C	2007	PEE	O3-C3-C2	2.19	114.72	108.40
17	G	2004	CDL	CA6-CA4-CA3	-2.18	106.69	111.78
12	C	502	HEM	C4A-NA-C1A	-2.18	102.26	105.82
17	Q	3003	CDL	CA6-CA4-CA3	-2.17	106.71	111.78
16	D	501	HEC	CHC-C4B-NB	-2.17	122.09	124.45
17	T	3004	CDL	OB6-CB4-CB3	2.17	116.12	108.34
12	C	501	HEM	CMA-C3A-C4A	-2.14	122.16	125.42
12	P	502	HEM	CHC-C4B-NB	-2.14	122.12	124.42
14	P	3002	UQ	C10-C9-C8	-2.10	118.22	123.63
12	C	502	HEM	CHB-C1B-C2B	-2.09	121.01	126.95
14	C	2002	UQ	C10-C9-C8	-2.08	118.29	123.63
12	P	502	HEM	C3A-C4A-NA	2.07	113.46	110.14
16	Q	501	HEC	CMC-C2C-C1C	2.06	128.55	125.42
17	G	2004	CDL	OB6-CB4-CB3	2.05	115.70	108.34
16	D	501	HEC	CMC-C2C-C1C	2.03	128.51	125.42
12	P	501	HEM	C4A-NA-C1A	-2.01	102.55	105.82
12	C	502	HEM	CMC-C2C-C1C	2.01	128.26	124.73

There are no chirality outliers.

All (266) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C4-O4P-P-O2P
11	E	2005	PEE	C4-O4P-P-O1P
11	P	3007	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C4-O4P-P-O2P
11	R	3005	PEE	C4-O4P-P-O1P
13	C	2001	JZZ	N2-C3-O3-C27
13	C	2001	JZZ	N4-C3-O3-C27
13	P	3001	JZZ	N2-C3-O3-C27
13	P	3001	JZZ	N4-C3-O3-C27
13	P	3001	JZZ	CAA-CAH-CAI-CAJ
13	P	3001	JZZ	CAP-CAH-CAI-CAJ
14	C	2002	UQ	C1-C6-C7-C8
14	C	2002	UQ	C5-C6-C7-C8
14	C	2002	UQ	C12-C11-C9-C8
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8
14	P	3002	UQ	C12-C11-C9-C8
15	C	2011	GOL	O1-C1-C2-C3
15	C	2011	GOL	C1-C2-C3-O3
15	P	3011	GOL	C1-C2-C3-O3
16	D	501	HEC	C2B-C3B-CAB-CBB
16	D	501	HEC	C4B-C3B-CAB-CBB
16	D	501	HEC	C2C-C3C-CAC-CBC
16	D	501	HEC	C4C-C3C-CAC-CBC
16	Q	501	HEC	C2B-C3B-CAB-CBB
16	Q	501	HEC	C4B-C3B-CAB-CBB
16	Q	501	HEC	C4C-C3C-CAC-CBC
17	D	2003	CDL	CA2-OA2-PA1-OA4
17	D	2003	CDL	CA2-OA2-PA1-OA5
17	D	2003	CDL	CB2-OB2-PB2-OB4
17	D	2003	CDL	CB2-OB2-PB2-OB5
17	D	2003	CDL	CB3-OB5-PB2-OB2
17	D	2003	CDL	CB3-OB5-PB2-OB4
17	G	2004	CDL	CA3-OA5-PA1-OA2
17	G	2004	CDL	CA3-OA5-PA1-OA3
17	G	2004	CDL	CA3-OA5-PA1-OA4
17	G	2004	CDL	CB3-OB5-PB2-OB2
17	G	2004	CDL	CB3-OB5-PB2-OB3
17	G	2004	CDL	CB3-OB5-PB2-OB4
17	G	2004	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
17	Q	3003	CDL	CA2-OA2-PA1-OA5
17	Q	3003	CDL	CB2-OB2-PB2-OB4
17	Q	3003	CDL	CB2-OB2-PB2-OB5
17	Q	3003	CDL	CB3-OB5-PB2-OB2
17	Q	3003	CDL	CB3-OB5-PB2-OB4
17	T	3004	CDL	O1-C1-CA2-OA2
17	T	3004	CDL	CA3-OA5-PA1-OA2
17	T	3004	CDL	CA3-OA5-PA1-OA4
17	T	3004	CDL	CB3-OB5-PB2-OB2
17	T	3004	CDL	CB3-OB5-PB2-OB3
17	T	3004	CDL	CB3-OB5-PB2-OB4
17	T	3004	CDL	C51-CB5-OB6-CB4
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
11	R	3005	PEE	O5-C30-O3-C3
17	G	2004	CDL	OB9-CB7-OB8-CB6
17	T	3004	CDL	OB9-CB7-OB8-CB6
11	E	2005	PEE	O5-C30-O3-C3
17	G	2004	CDL	OA9-CA7-OA8-CA6
17	T	3004	CDL	OA9-CA7-OA8-CA6
17	G	2004	CDL	C31-CA7-OA8-CA6
17	T	3004	CDL	C31-CA7-OA8-CA6
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	O4-C10-O2-C2
17	G	2004	CDL	OB7-CB5-OB6-CB4
17	T	3004	CDL	OB7-CB5-OB6-CB4
11	R	3005	PEE	C31-C30-O3-C3
17	G	2004	CDL	C71-CB7-OB8-CB6
17	T	3004	CDL	C71-CB7-OB8-CB6
16	Q	501	HEC	C3A-C2A-CAA-CBA
11	A	2008	PEE	C31-C30-O3-C3
11	E	2005	PEE	C31-C30-O3-C3
17	D	2003	CDL	C31-CA7-OA8-CA6
17	Q	3003	CDL	C31-CA7-OA8-CA6
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
11	A	2008	PEE	O5-C30-O3-C3
17	G	2004	CDL	O1-C1-CA2-OA2
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
18	Q	3091	BOG	O5-C5-C6-O6
16	Q	501	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	D	2091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	C4-C5-C6-O6
18	D	2009	BOG	C2-C1-O1-C1'
18	Q	3009	BOG	C2-C1-O1-C1'
17	D	2003	CDL	O1-C1-CA2-OA2
17	Q	3003	CDL	O1-C1-CA2-OA2
18	D	2091	BOG	O5-C1-O1-C1'
17	D	2003	CDL	OA9-CA7-OA8-CA6
17	Q	3003	CDL	OA9-CA7-OA8-CA6
17	Q	3003	CDL	CB7-C71-C72-C73
17	D	2003	CDL	CB7-C71-C72-C73
17	D	2003	CDL	C71-CB7-OB8-CB6
17	G	2004	CDL	C11-CA5-OA6-CA4
17	T	3004	CDL	C11-CA5-OA6-CA4
16	D	501	HEC	C3A-C2A-CAA-CBA
17	G	2004	CDL	OA7-CA5-OA6-CA4
17	T	3004	CDL	OA7-CA5-OA6-CA4
17	G	2004	CDL	CB2-C1-CA2-OA2
17	T	3004	CDL	CB2-C1-CA2-OA2
17	Q	3003	CDL	C71-CB7-OB8-CB6
18	Q	3009	BOG	O1-C1'-C2'-C3'
17	D	2003	CDL	OB9-CB7-OB8-CB6
17	D	2003	CDL	C51-CB5-OB6-CB4
17	Q	3003	CDL	C51-CB5-OB6-CB4
18	D	2009	BOG	O1-C1'-C2'-C3'
17	Q	3003	CDL	OB9-CB7-OB8-CB6
11	C	2007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C37-C38-C39-C40
15	C	2011	GOL	O2-C2-C3-O3
15	P	3011	GOL	O2-C2-C3-O3
17	D	2003	CDL	CB5-C51-C52-C53
17	Q	3003	CDL	CB5-C51-C52-C53
17	D	2003	CDL	OB7-CB5-OB6-CB4
11	P	3007	PEE	C10-C11-C12-C13
11	R	3005	PEE	C30-C31-C32-C33
11	E	2005	PEE	C34-C35-C36-C37
18	Q	3009	BOG	C1'-C2'-C3'-C4'
11	R	3005	PEE	C34-C35-C36-C37
11	P	3007	PEE	C37-C38-C39-C40
18	D	2009	BOG	C1'-C2'-C3'-C4'
17	Q	3003	CDL	OB7-CB5-OB6-CB4
11	A	2008	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C20-C21-C22-C23
11	E	2005	PEE	C11-C12-C13-C14
11	E	2005	PEE	C23-C24-C25-C26
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C35-C36-C37-C38
11	R	3005	PEE	C23-C24-C25-C26
11	R	3005	PEE	C41-C42-C43-C44
11	A	2008	PEE	O4-C10-O2-C2
11	E	2005	PEE	C41-C42-C43-C44
11	R	3005	PEE	C11-C12-C13-C14
15	C	2011	GOL	O1-C1-C2-O2
11	C	2007	PEE	C15-C16-C17-C18
11	P	3007	PEE	C15-C16-C17-C18
11	A	2008	PEE	O3P-C1-C2-C3
11	E	2005	PEE	O3P-C1-C2-C3
11	R	3005	PEE	O3P-C1-C2-C3
11	C	2007	PEE	C31-C32-C33-C34
11	P	3007	PEE	C31-C32-C33-C34
17	G	2004	CDL	CB5-C51-C52-C53
17	T	3004	CDL	CB5-C51-C52-C53
16	D	501	HEC	C1A-C2A-CAA-CBA
11	C	2007	PEE	C39-C40-C41-C42
11	C	2007	PEE	C20-C21-C22-C23
11	P	3007	PEE	C40-C41-C42-C43
11	C	2007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C40-C41-C42-C43
11	P	3007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C43-C44-C45-C46
11	P	3007	PEE	C43-C44-C45-C46
11	A	2008	PEE	O2-C2-C3-O3
11	E	2005	PEE	C35-C36-C37-C38
11	R	3005	PEE	C35-C36-C37-C38
11	R	3005	PEE	C20-C21-C22-C23
11	P	3007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C33-C34-C35-C36
17	D	2003	CDL	OB5-CB3-CB4-CB6
17	Q	3003	CDL	OB5-CB3-CB4-CB6
17	Q	3003	CDL	C71-C72-C73-C74
17	D	2003	CDL	C71-C72-C73-C74
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C20-C21-C22-C23
11	C	2007	PEE	C34-C35-C36-C37
11	R	3005	PEE	C39-C40-C41-C42
17	D	2003	CDL	OA6-CA4-CA6-OA8
17	Q	3003	CDL	OA6-CA4-CA6-OA8
11	E	2005	PEE	C21-C22-C23-C24
11	E	2005	PEE	C39-C40-C41-C42
11	R	3005	PEE	C21-C22-C23-C24
15	P	3011	GOL	O1-C1-C2-O2
11	P	3007	PEE	C42-C43-C44-C45
12	C	501	HEM	C2C-C3C-CAC-CBC
12	C	502	HEM	C2C-C3C-CAC-CBC
12	P	501	HEM	C2C-C3C-CAC-CBC
11	A	2008	PEE	C10-C11-C12-C13
11	R	3005	PEE	O3P-C1-C2-O2
17	D	2003	CDL	OB5-CB3-CB4-OB6
17	Q	3003	CDL	OB5-CB3-CB4-OB6
11	P	3007	PEE	C34-C35-C36-C37
12	C	501	HEM	C3D-CAD-CBD-CGD
12	P	501	HEM	C3D-CAD-CBD-CGD
11	A	2008	PEE	O3P-C1-C2-O2
11	E	2005	PEE	O3P-C1-C2-O2
11	P	3007	PEE	C39-C40-C41-C42
11	C	2007	PEE	C42-C43-C44-C45
13	P	3001	JZZ	CAG-CAH-CAI-CAJ
11	R	3005	PEE	C12-C13-C14-C15
11	C	2007	PEE	C4-O4P-P-O3P
11	R	3005	PEE	O4P-C4-C5-N
16	Q	501	HEC	C2C-C3C-CAC-CBC
17	Q	3003	CDL	CA2-OA2-PA1-OA4
17	Q	3003	CDL	CA3-OA5-PA1-OA2
17	T	3004	CDL	CA3-OA5-PA1-OA3
11	E	2005	PEE	C12-C13-C14-C15
11	P	3007	PEE	C13-C14-C15-C16
11	R	3005	PEE	C22-C23-C24-C25
11	C	2007	PEE	C13-C14-C15-C16
11	P	3007	PEE	C14-C15-C16-C17
11	A	2008	PEE	O3-C30-C31-C32
11	R	3005	PEE	C14-C15-C16-C17
11	E	2005	PEE	C14-C15-C16-C17
12	P	501	HEM	CAA-CBA-CGA-O2A
12	C	502	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C1-C2-O2-C10
11	R	3005	PEE	C1-C2-O2-C10
12	C	502	HEM	CAA-CBA-CGA-O2A
12	C	501	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAA-CBA-CGA-O2A
17	T	3004	CDL	C1-CB2-OB2-PB2
12	C	501	HEM	CAA-CBA-CGA-O2A
11	E	2005	PEE	C19-C20-C21-C22
11	E	2005	PEE	C22-C23-C24-C25
11	R	3005	PEE	C19-C20-C21-C22
12	P	501	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAA-CBA-CGA-O1A
11	A	2008	PEE	O5-C30-C31-C32
12	P	502	HEM	CAD-CBD-CGD-O2D
16	Q	501	HEC	CAA-CBA-CGA-O2A
11	R	3005	PEE	C43-C44-C45-C46
17	Q	3003	CDL	C12-C11-CA5-OA6
11	E	2005	PEE	C43-C44-C45-C46
12	P	502	HEM	CAD-CBD-CGD-O1D
11	C	2007	PEE	C38-C39-C40-C41
12	C	501	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	C2C-C3C-CAC-CBC
12	C	502	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAD-CBD-CGD-O2D
16	D	501	HEC	CAD-CBD-CGD-O2D
16	Q	501	HEC	CAD-CBD-CGD-O2D
16	Q	501	HEC	CAA-CBA-CGA-O1A
17	G	2004	CDL	C1-CB2-OB2-PB2
17	G	2004	CDL	OB5-CB3-CB4-OB6
17	T	3004	CDL	OB5-CB3-CB4-OB6
17	Q	3003	CDL	CA3-CA4-CA6-OA8
12	C	501	HEM	C4C-C3C-CAC-CBC
12	P	501	HEM	C4C-C3C-CAC-CBC
12	P	502	HEM	C4C-C3C-CAC-CBC
12	C	501	HEM	CAD-CBD-CGD-O1D
16	D	501	HEC	CAD-CBD-CGD-O1D
12	P	501	HEM	CAD-CBD-CGD-O1D
16	Q	501	HEC	CAD-CBD-CGD-O1D
11	P	3007	PEE	C38-C39-C40-C41
11	P	3007	PEE	O2-C10-C11-C12
11	C	2007	PEE	O2-C10-C11-C12

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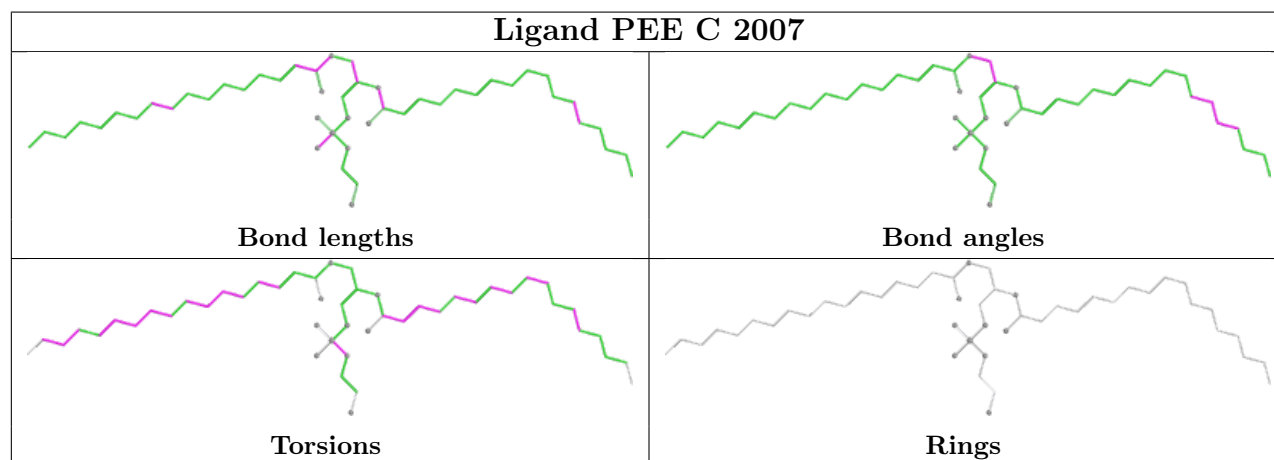
Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C12-C13-C14-C15
17	D	2003	CDL	C72-C71-CB7-OB8
11	A	2008	PEE	C1-C2-C3-O3
17	Q	3003	CDL	C72-C71-CB7-OB8
17	D	2003	CDL	C12-C11-CA5-OA6
11	C	2007	PEE	O4-C10-C11-C12
11	P	3007	PEE	O4-C10-C11-C12
17	D	2003	CDL	C72-C71-CB7-OB9
11	P	3007	PEE	O4-C10-O2-C2
17	Q	3003	CDL	C72-C71-CB7-OB9
11	E	2005	PEE	C10-C11-C12-C13
16	D	501	HEC	CAA-CBA-CGA-O2A

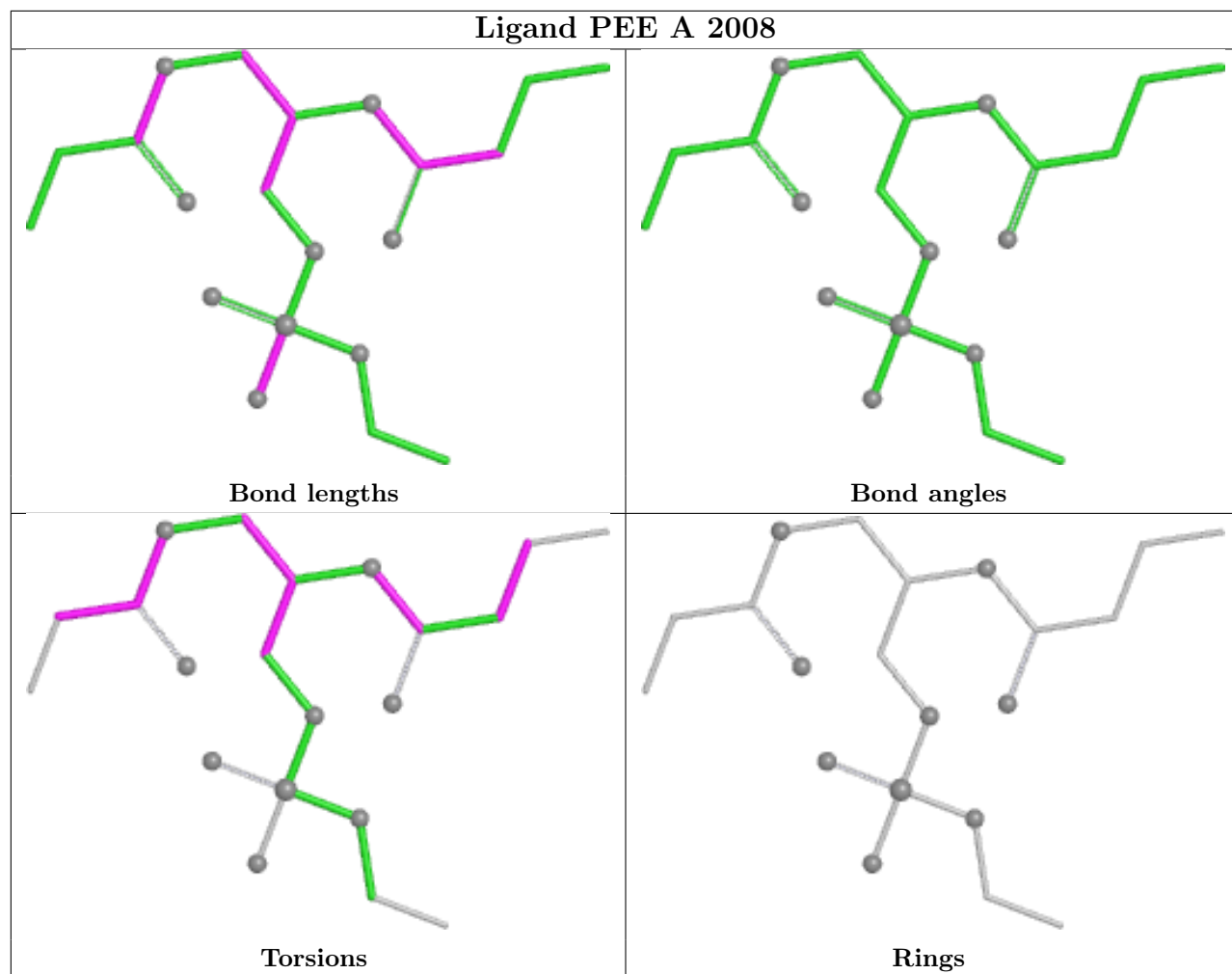
There are no ring outliers.

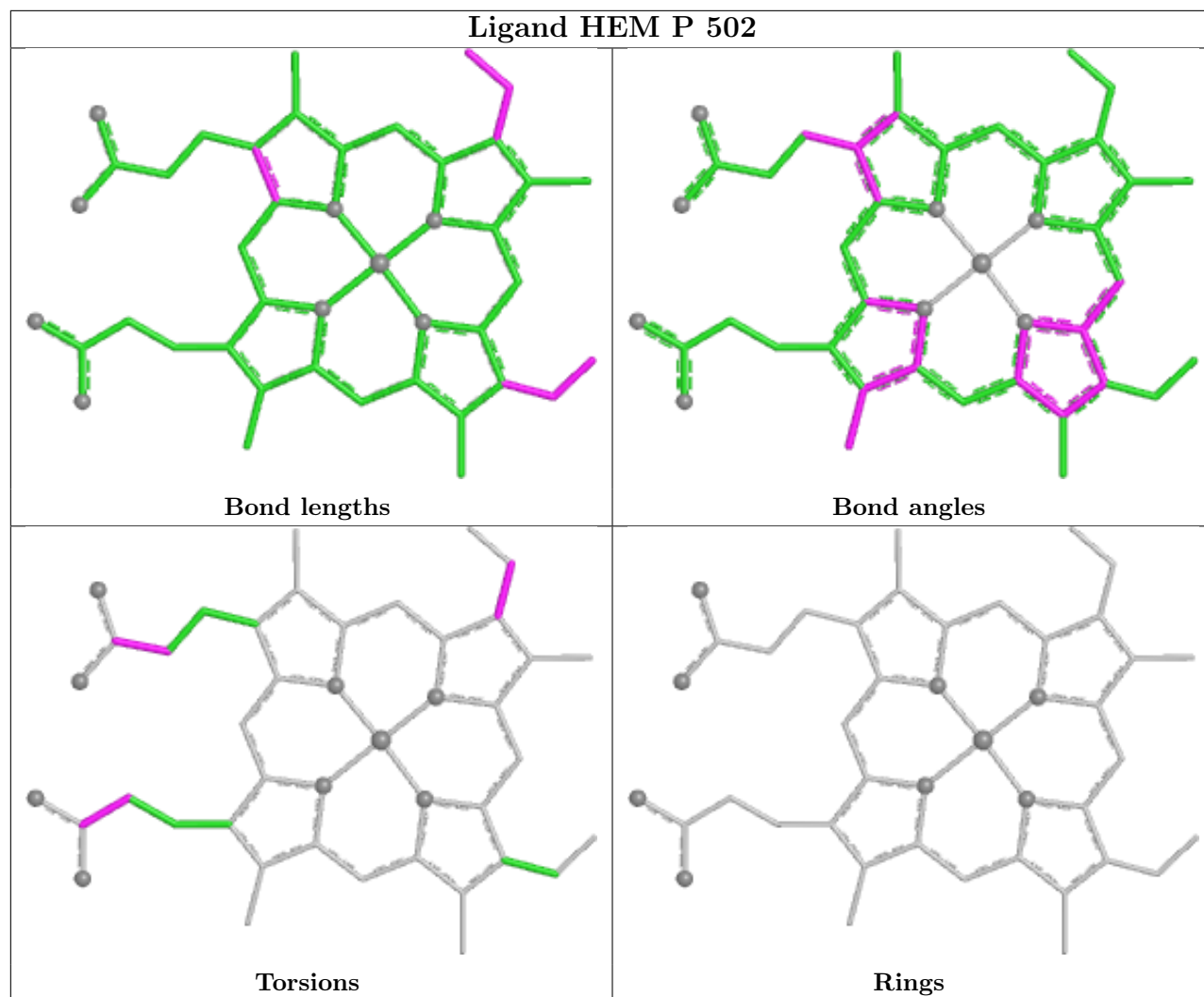
24 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	2007	PEE	4	0
12	P	502	HEM	3	0
14	C	2002	UQ	2	0
17	G	2004	CDL	5	0
12	C	501	HEM	2	0
19	R	501	FES	2	0
14	P	3002	UQ	3	0
16	Q	501	HEC	1	0
11	E	2005	PEE	1	0
19	E	501	FES	2	0
17	T	3004	CDL	5	0
18	P	2010	BOG	1	0
11	P	3007	PEE	4	0
12	P	501	HEM	2	0
17	Q	3003	CDL	1	0
13	C	2001	JZZ	2	0
13	P	3001	JZZ	7	0
15	P	3011	GOL	1	0
12	C	502	HEM	4	0
18	D	2091	BOG	2	0
15	C	2011	GOL	1	0
17	D	2003	CDL	3	0
11	R	3005	PEE	1	0
18	Q	3091	BOG	1	0

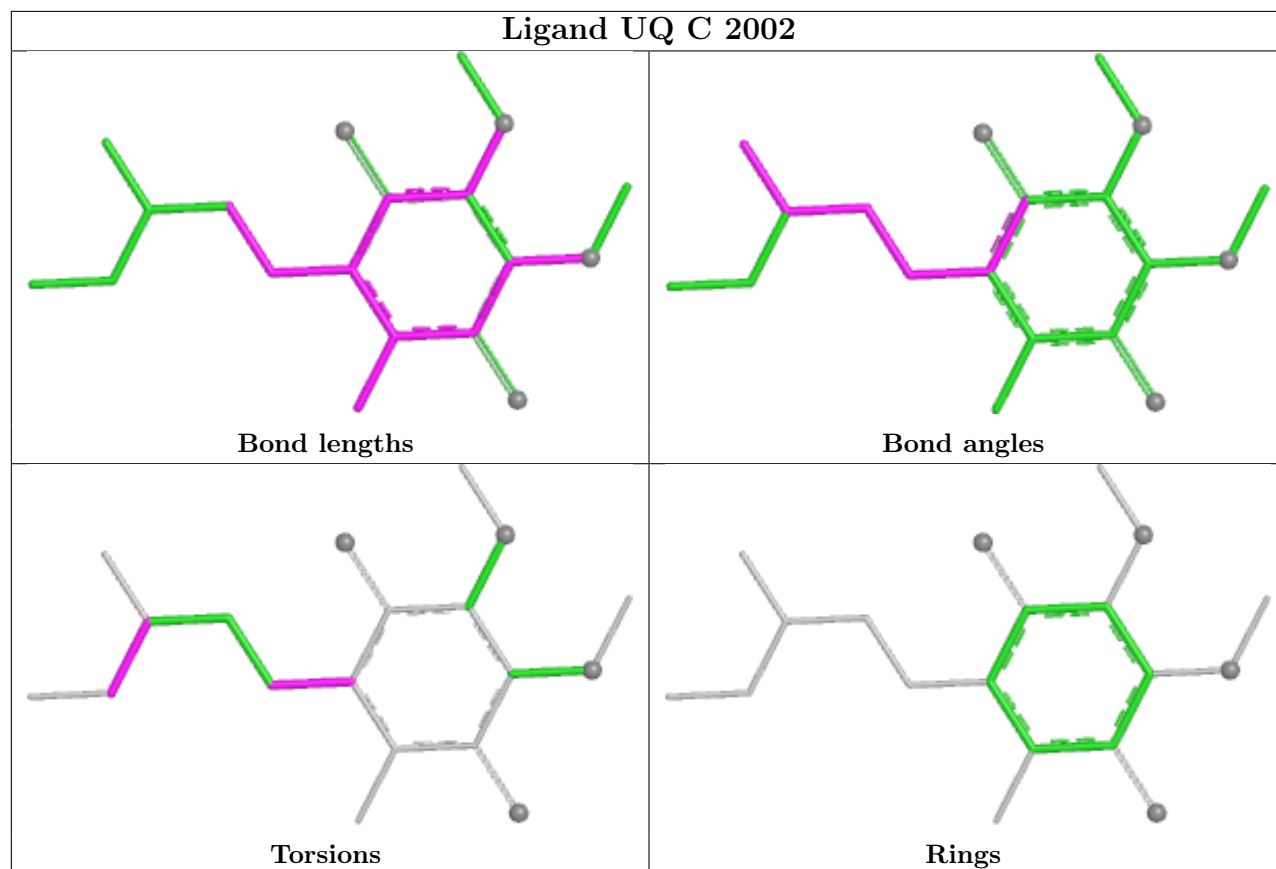
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



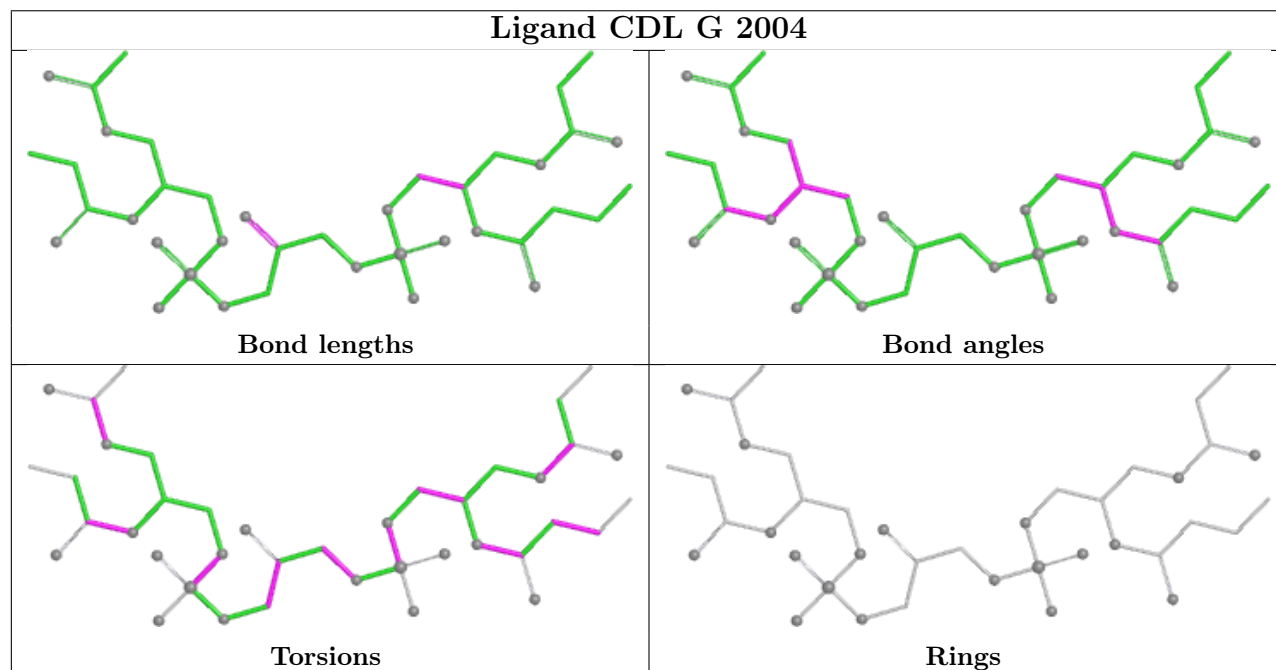




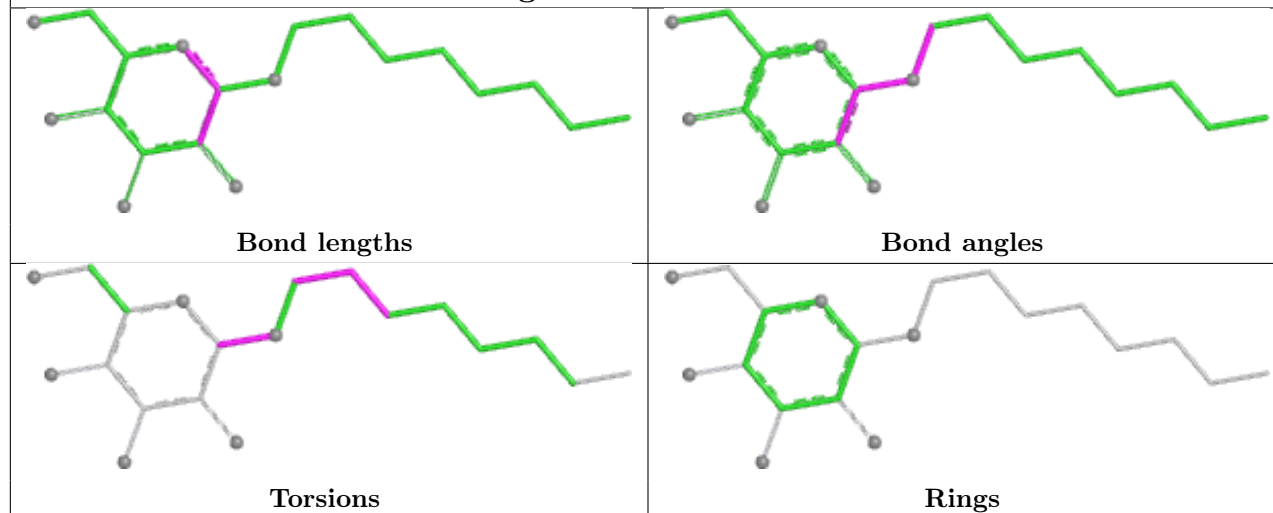
Ligand UQ C 2002



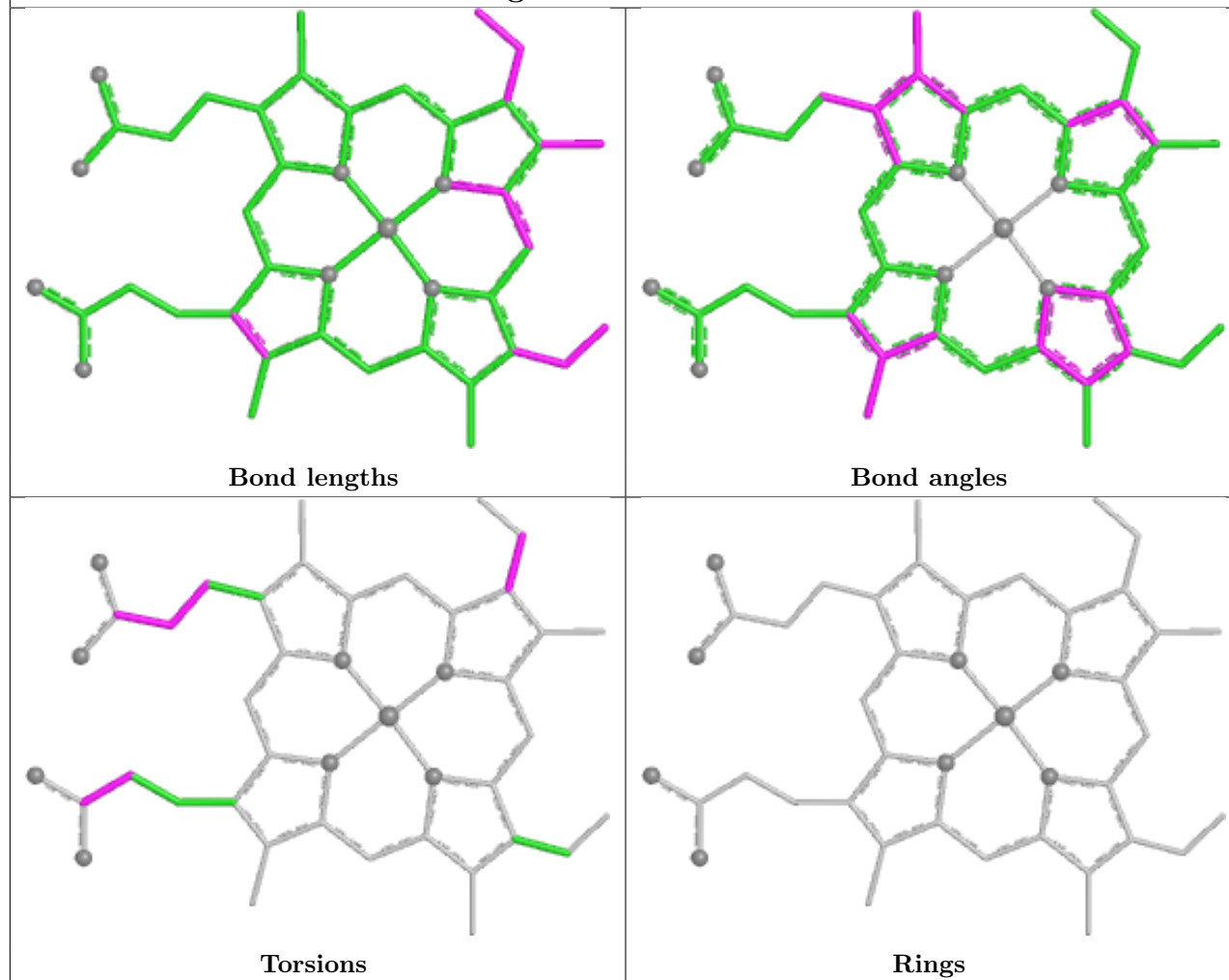
Ligand CDL G 2004

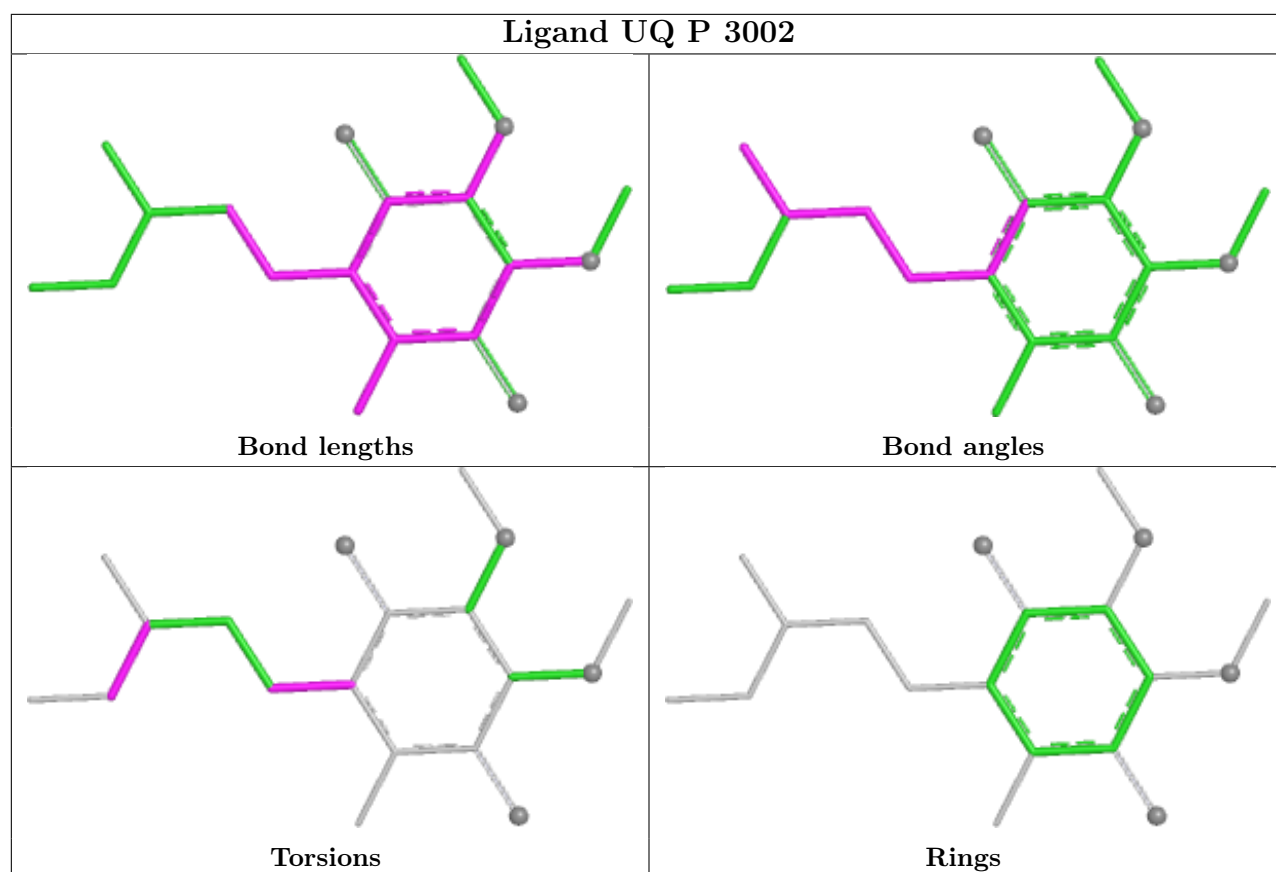


Ligand BOG D 2009

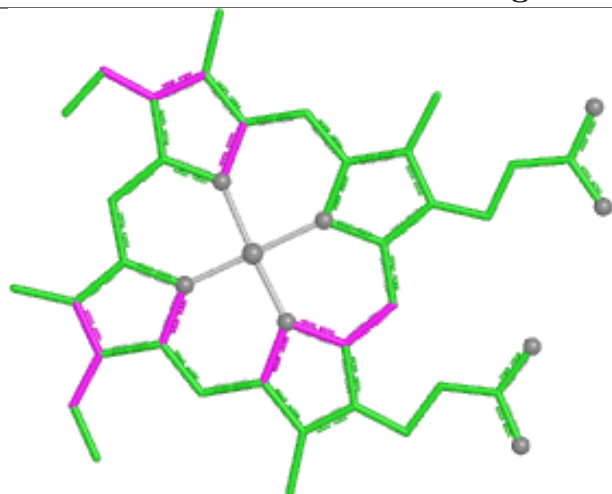


Ligand HEM C 501

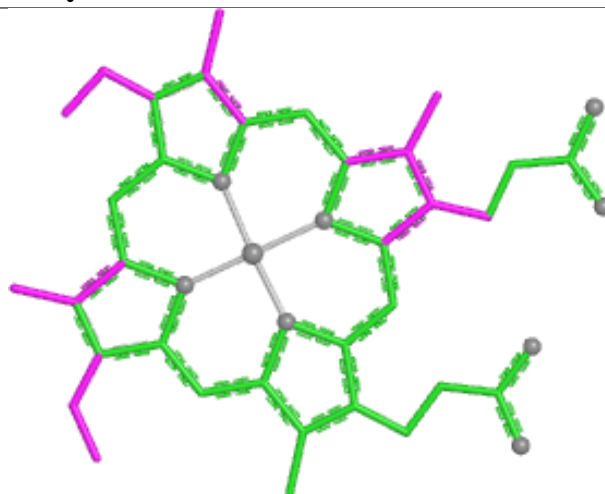




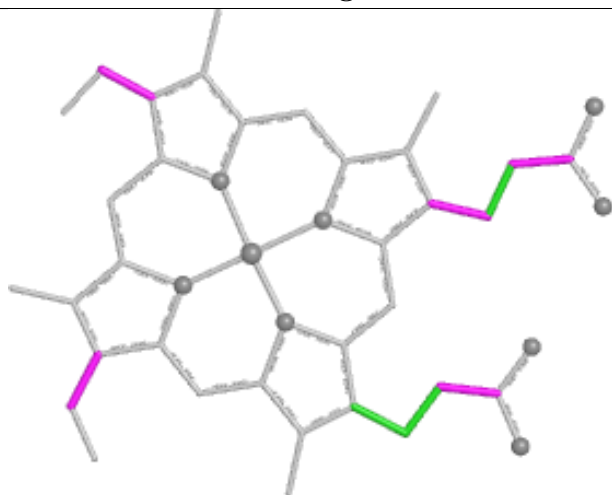
Ligand HEC Q 501



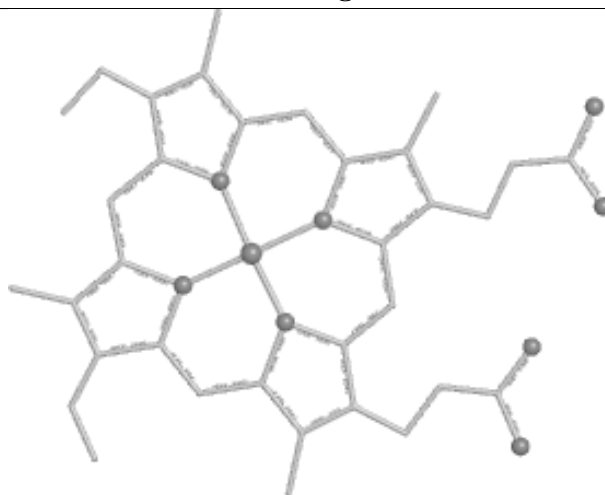
Bond lengths



Bond angles

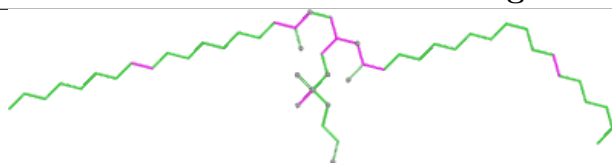


Torsions



Rings

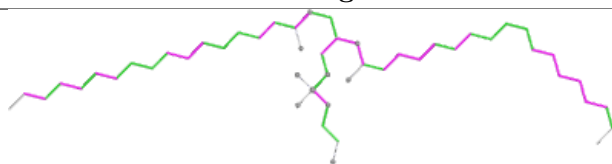
Ligand PEE E 2005



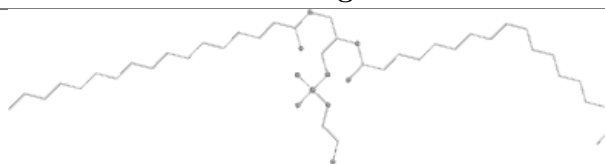
Bond lengths



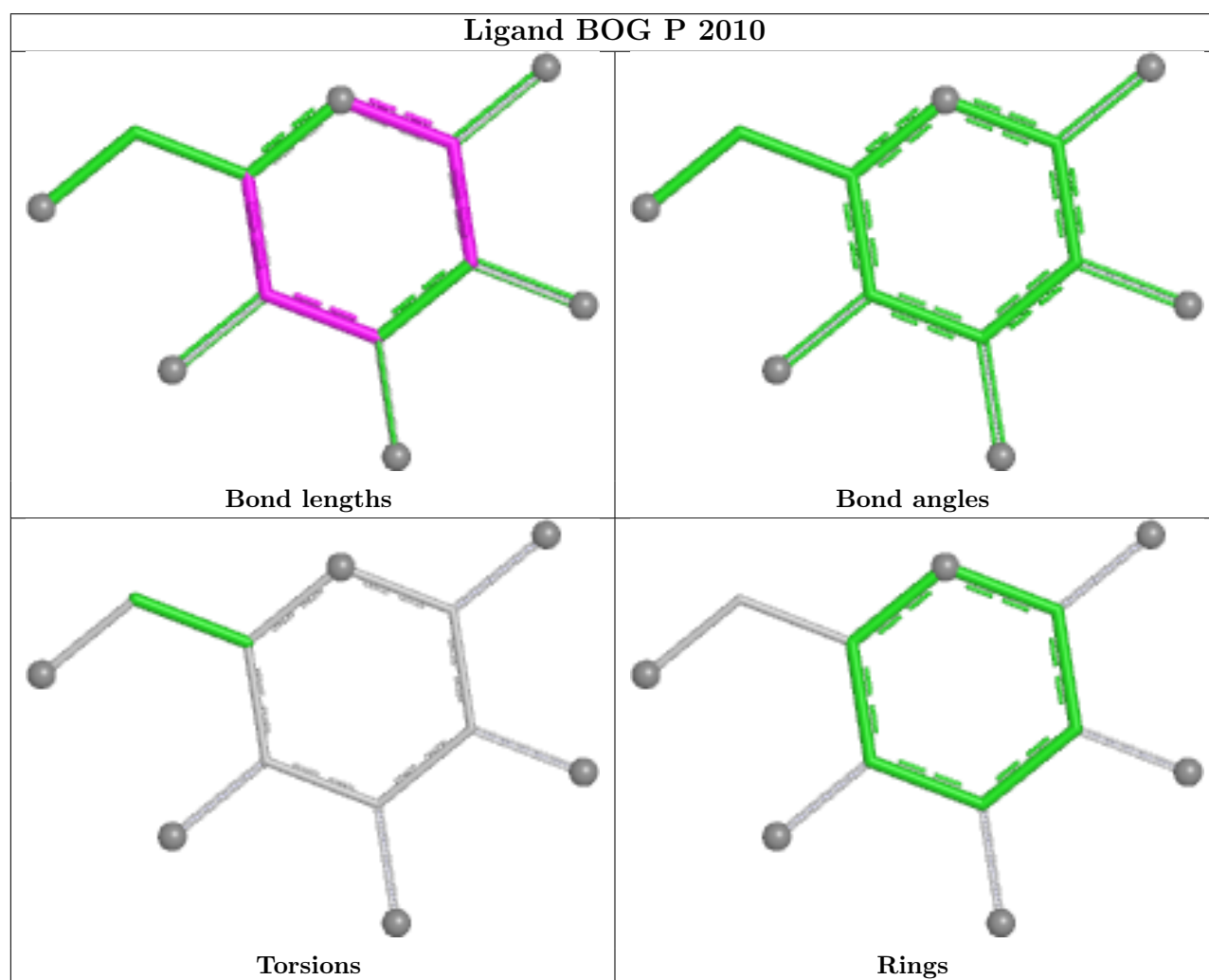
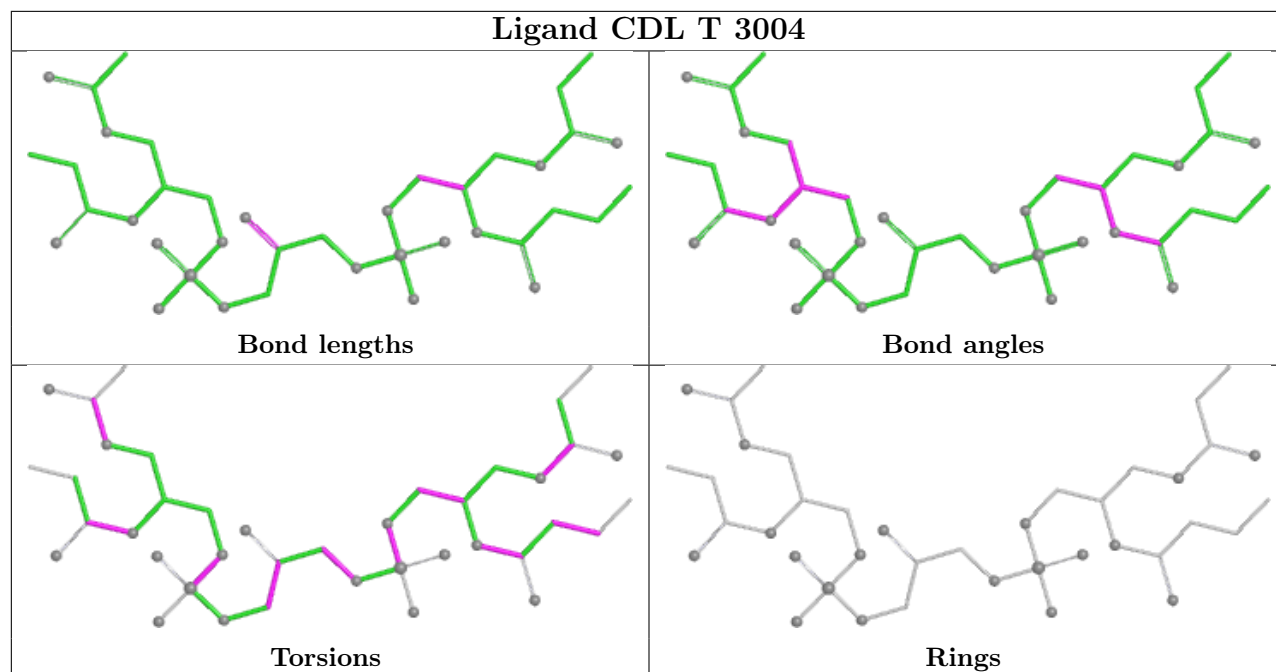
Bond angles

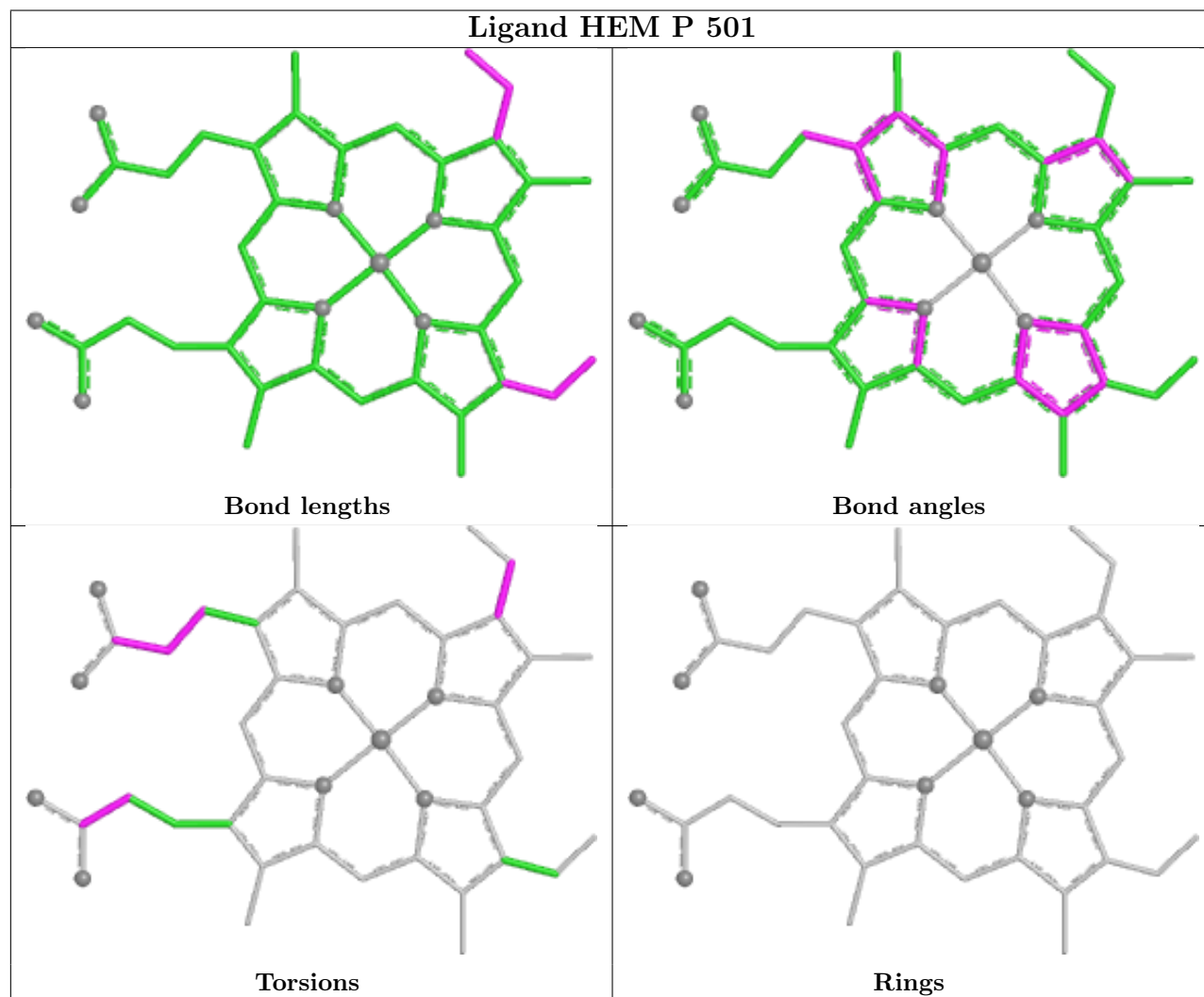
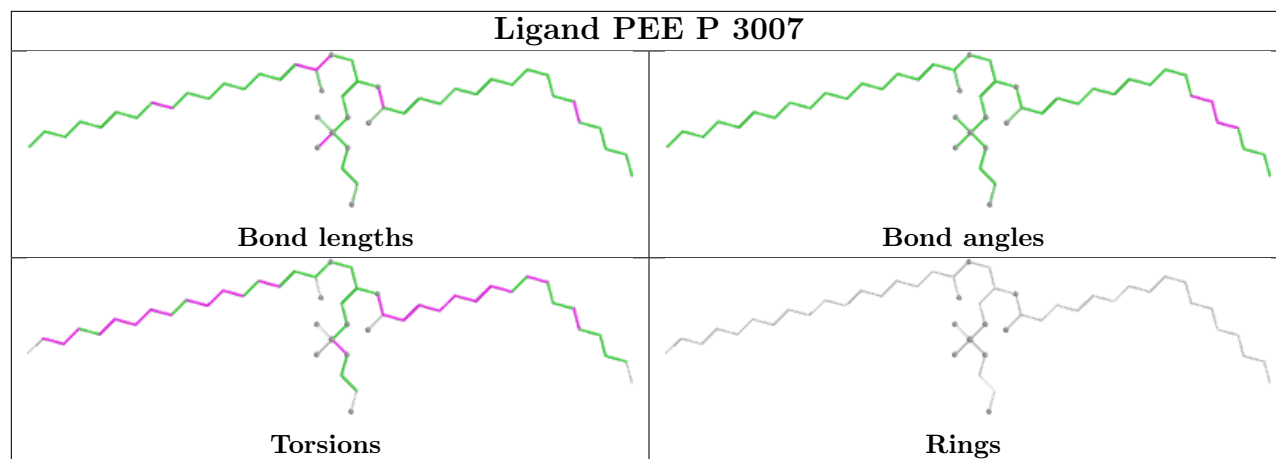


Torsions

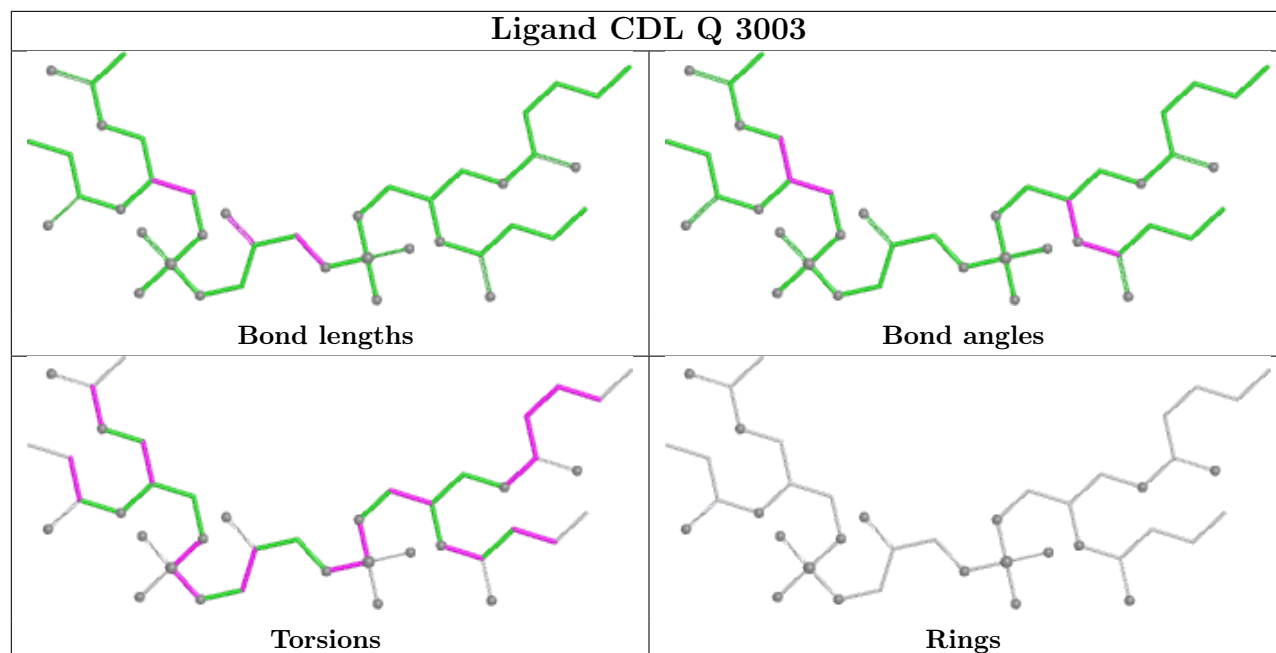


Rings

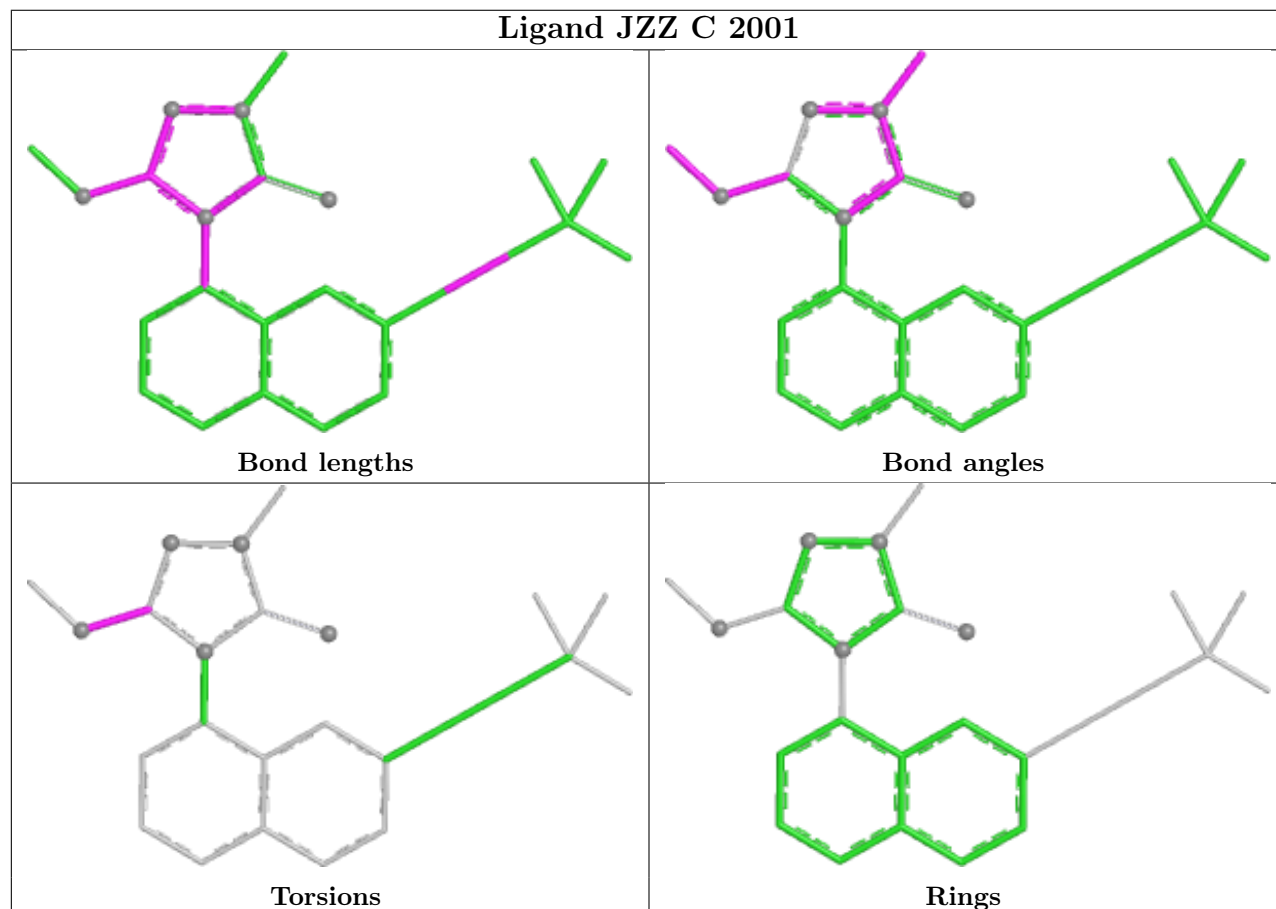


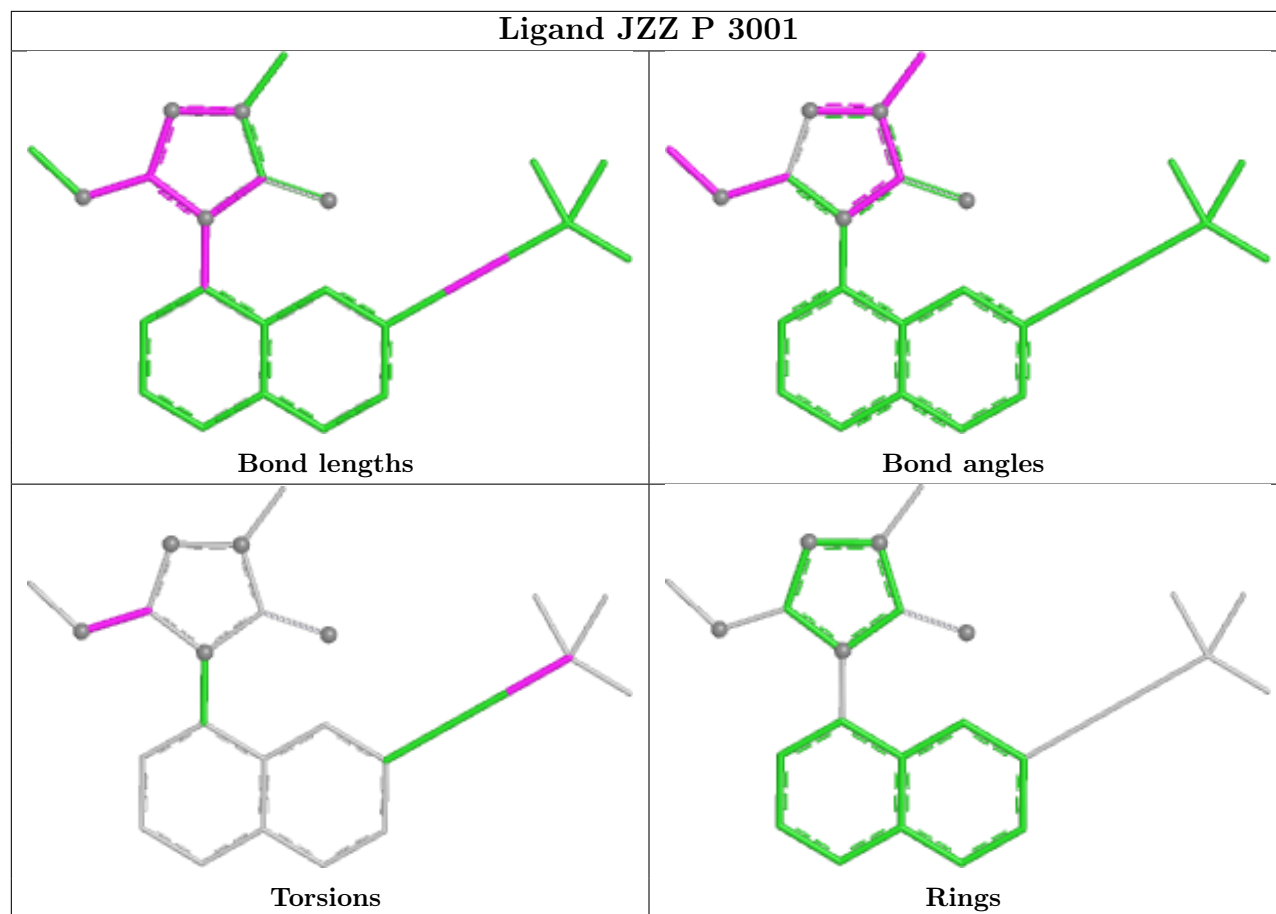


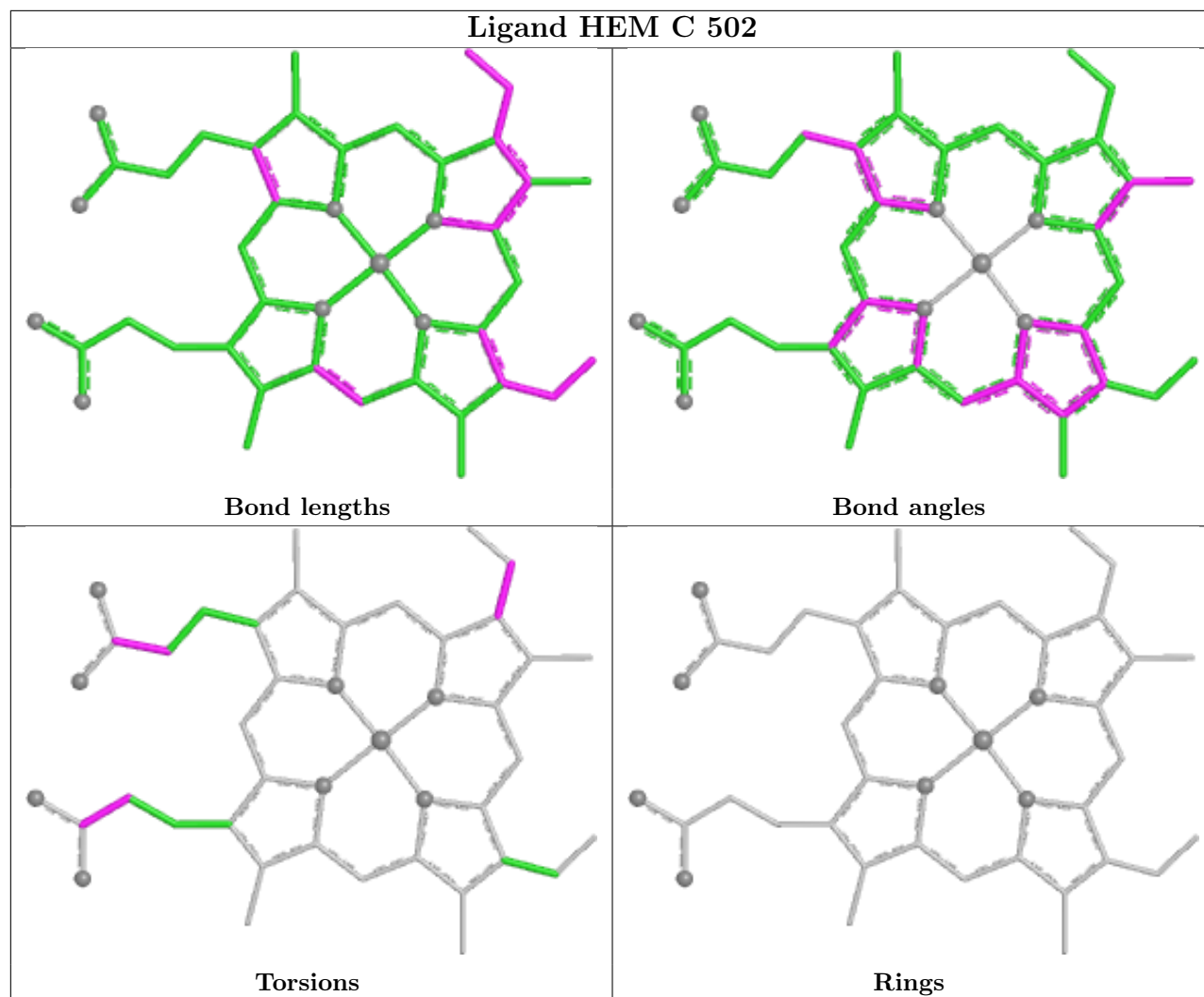
Ligand CDL Q 3003



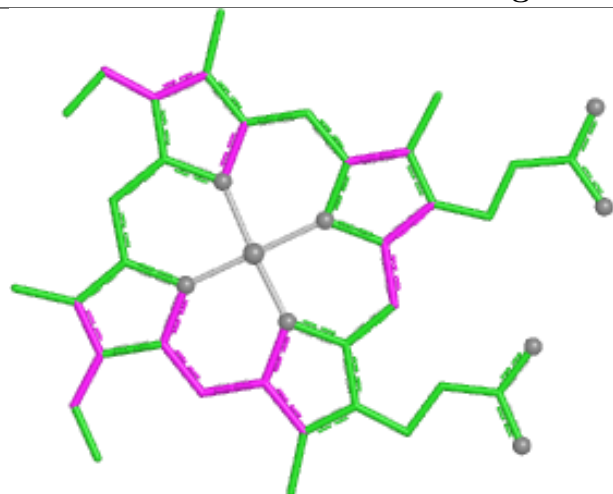
Ligand JZZ C 2001



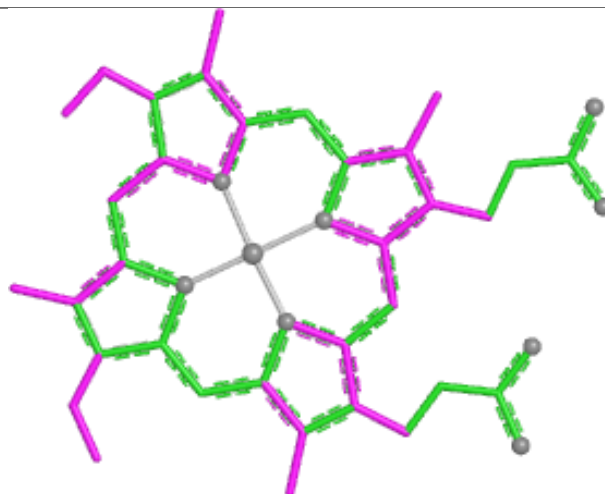




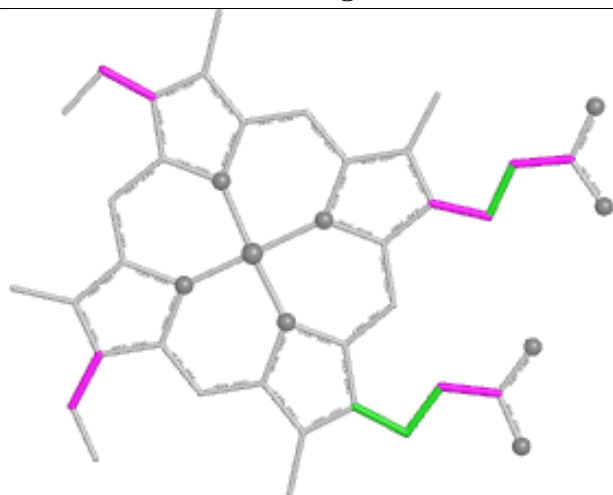
Ligand HEC D 501



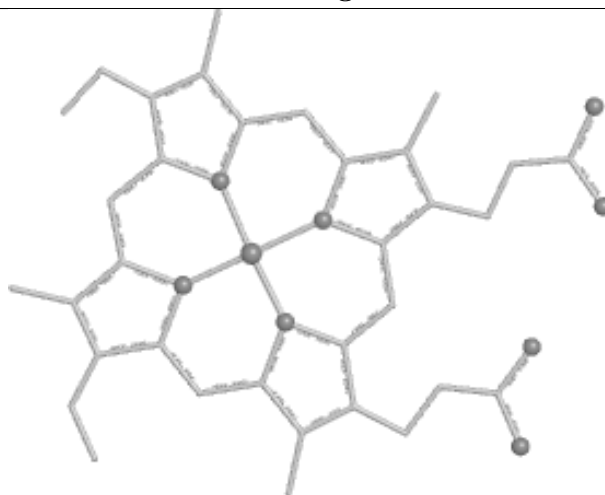
Bond lengths



Bond angles

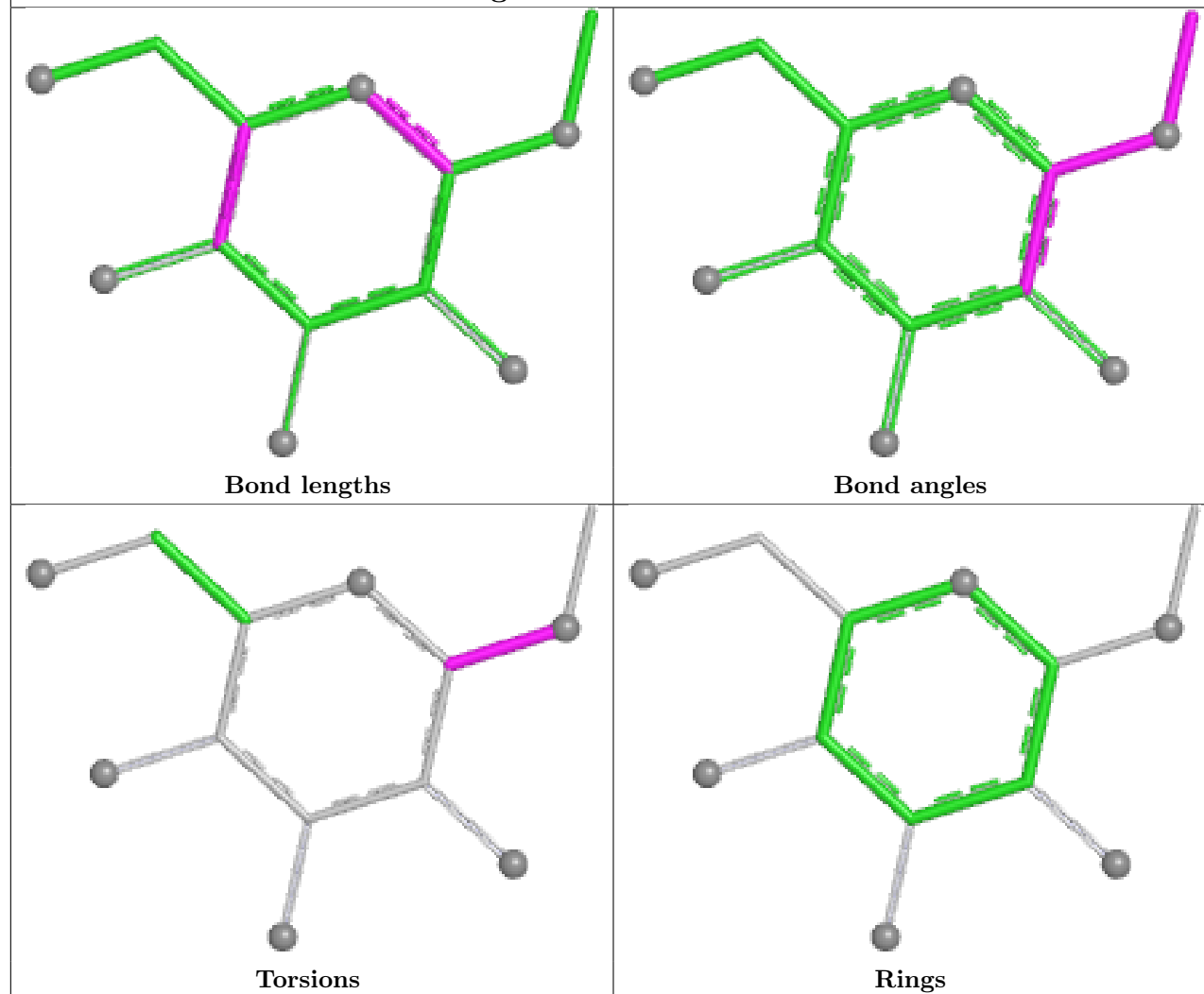


Torsions

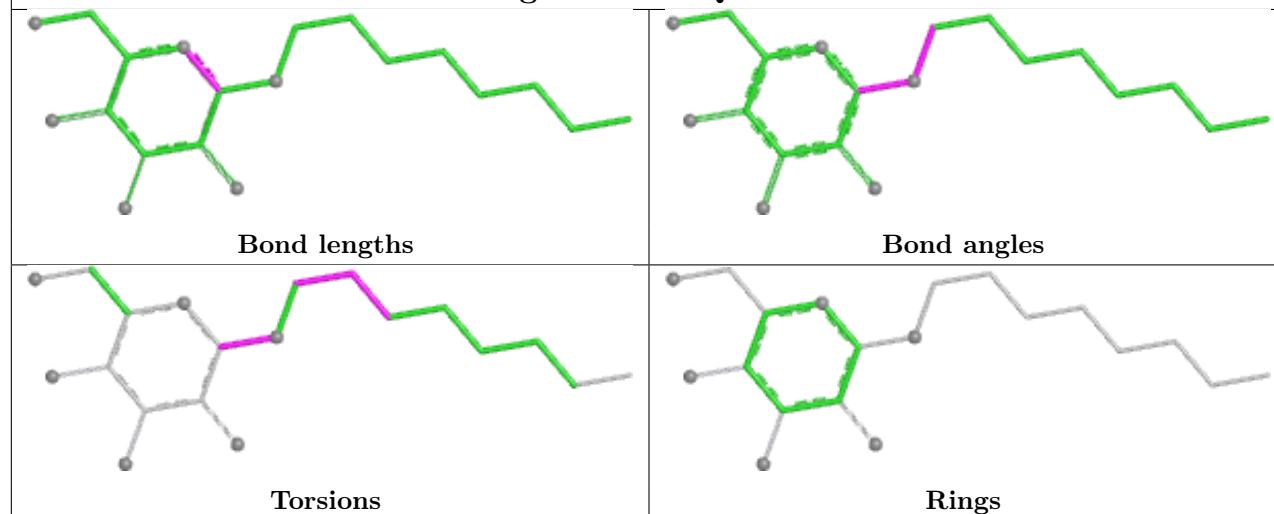


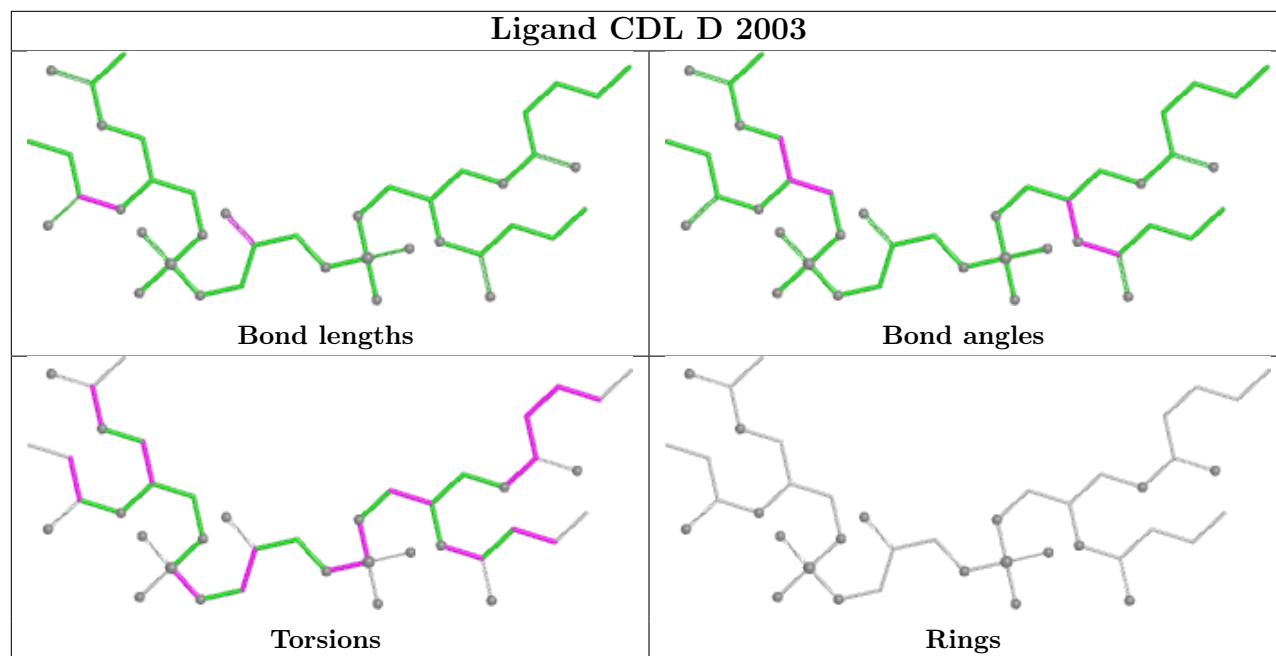
Rings

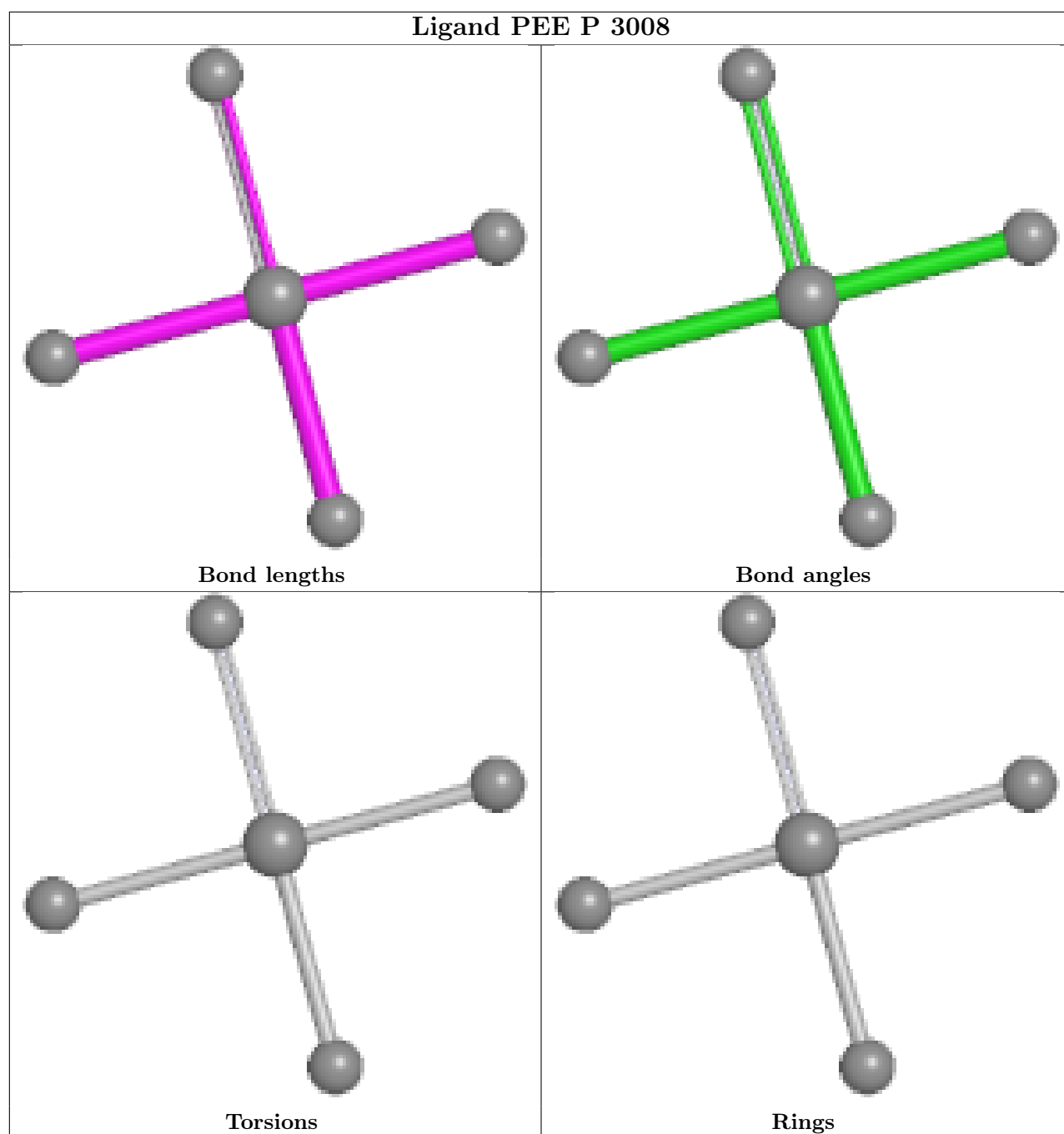
Ligand BOG D 2091

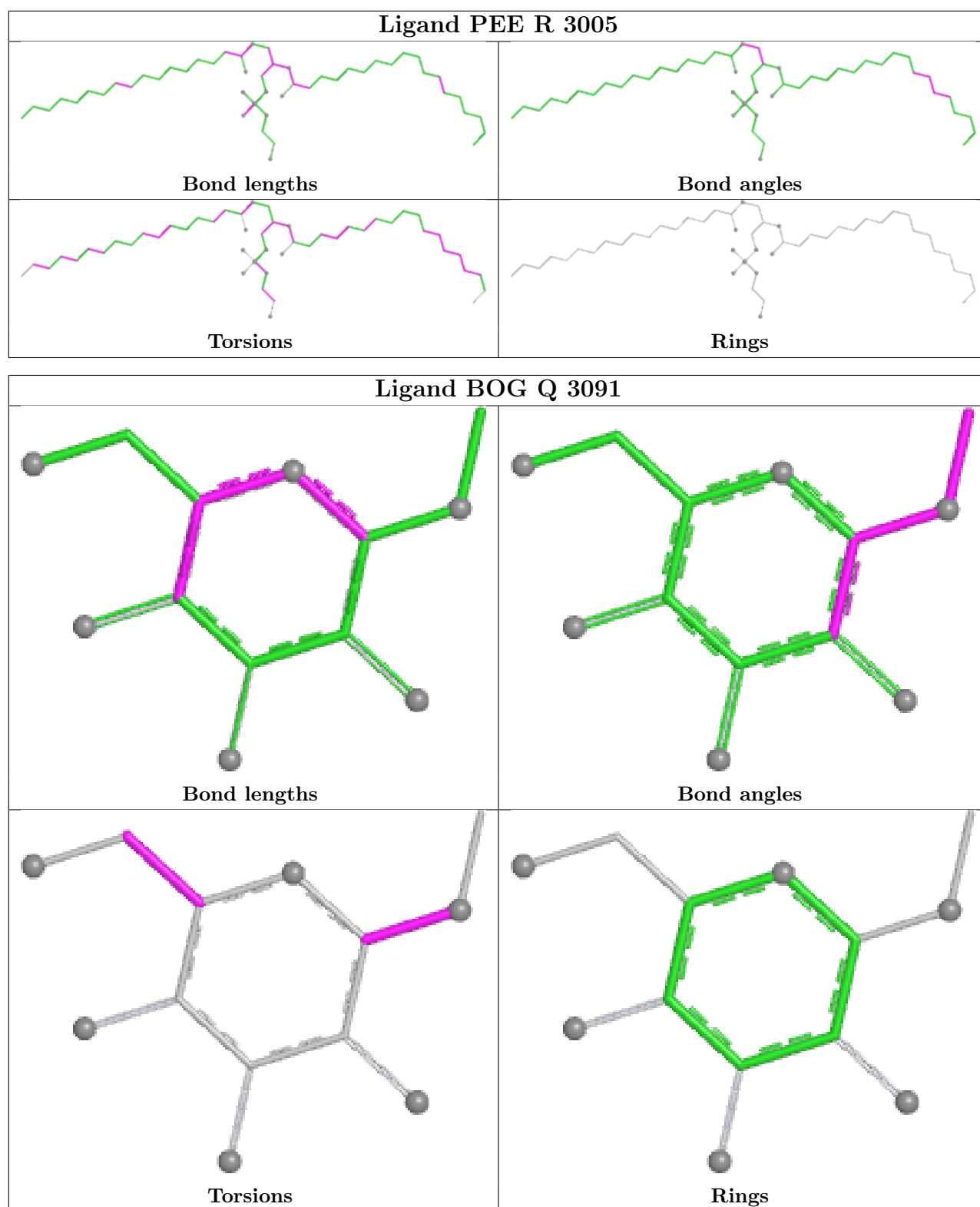


Ligand BOG Q 3009









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/446 (99%)	0.02	4 (0%) 81 60	49, 78, 110, 121	0
1	N	442/446 (99%)	0.20	8 (1%) 67 43	55, 88, 114, 124	0
2	B	420/441 (95%)	0.35	8 (1%) 66 42	66, 97, 130, 152	0
2	O	422/441 (95%)	0.26	6 (1%) 73 50	52, 92, 124, 143	0
3	C	380/380 (100%)	-0.47	3 (0%) 82 63	30, 51, 98, 137	0
3	P	379/380 (99%)	-0.12	3 (0%) 82 63	39, 75, 106, 134	0
4	D	241/241 (100%)	-0.43	0 100 100	42, 56, 102, 124	0
4	Q	241/241 (100%)	0.12	0 100 100	64, 88, 119, 136	0
5	E	196/196 (100%)	0.90	39 (19%) 3 2	47, 131, 157, 164	124 (63%)
5	R	196/196 (100%)	0.54	11 (5%) 30 15	60, 98, 139, 149	0
6	F	101/110 (91%)	-0.53	0 100 100	41, 59, 76, 111	0
6	S	101/110 (91%)	0.10	0 100 100	65, 84, 122, 139	0
7	G	80/81 (98%)	-0.21	2 (2%) 58 34	46, 64, 114, 128	0
7	T	79/81 (97%)	0.44	3 (3%) 44 24	62, 96, 159, 169	0
8	H	70/77 (90%)	-0.04	1 (1%) 73 50	50, 77, 102, 138	0
8	U	67/77 (87%)	0.76	2 (2%) 52 29	101, 131, 147, 150	0
9	I	31/47 (65%)	1.74	11 (35%) 1 1	90, 127, 152, 153	0
9	V	31/47 (65%)	2.09	17 (54%) 0 0	93, 128, 156, 160	0
10	J	61/61 (100%)	-0.23	1 (1%) 70 47	59, 72, 116, 156	0
10	W	60/61 (98%)	-0.10	0 100 100	71, 85, 121, 131	0
All	All	4042/4160 (97%)	0.11	119 (2%) 53 30	30, 82, 135, 169	124 (3%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	56	SER	6.8
9	V	63	ASP	6.0
5	E	106	ILE	5.6
5	E	112	VAL	4.8
9	I	63	ASP	4.6
9	I	61	ARG	4.5
9	I	47	ARG	4.5
5	E	180	LEU	4.3
9	V	59	SER	4.2
5	E	168	SER	4.1
2	O	226	ILE	4.1
2	B	20	GLY	4.0
5	E	167	ALA	3.9
2	B	226	ILE	3.9
5	E	135	LEU	3.8
5	E	120	PRO	3.7
5	E	169	GLY	3.7
3	C	4	ASN	3.7
7	G	2	ILE	3.6
1	A	444	ILE	3.5
5	E	109	GLU	3.5
1	N	444	ILE	3.5
9	V	57	GLY	3.4
5	E	147	ILE	3.4
5	E	183	PRO	3.4
8	H	9	GLU	3.3
9	I	49	LEU	3.2
7	T	2	ILE	3.2
5	E	133	VAL	3.2
1	A	226	ASP	3.1
5	R	124	LEU	3.0
1	N	223	TYR	3.0
5	E	134	ILE	3.0
9	V	58	ARG	3.0
5	E	113	ASP	2.9
5	R	165	TYR	2.9
9	I	51	CYS	2.8
3	P	380	TYR	2.8
5	E	177	PRO	2.8
9	V	47	ARG	2.8
5	E	173	LYS	2.8
9	I	77	ARG	2.7
7	G	81	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	187	PHE	2.7
5	E	178	TYR	2.7
3	C	155	PRO	2.6
5	R	196	GLY	2.6
10	J	64	GLU	2.6
9	V	77	ARG	2.6
9	V	54	SER	2.6
9	V	55	MET	2.5
5	R	157	TYR	2.5
9	V	49	LEU	2.5
5	R	167	ALA	2.5
5	R	156	TYR	2.5
3	C	380	TYR	2.5
5	E	98	VAL	2.5
9	V	61	ARG	2.5
2	O	229	GLY	2.5
9	V	50	LEU	2.4
1	N	432	LEU	2.4
2	B	224	LEU	2.4
9	I	50	LEU	2.4
5	E	159	PRO	2.4
2	O	296	TYR	2.4
3	P	2	ALA	2.4
5	E	104	ALA	2.4
9	V	48	PRO	2.4
5	E	124	LEU	2.4
9	V	53	GLU	2.3
5	E	114	VAL	2.3
5	E	85	LYS	2.3
5	E	182	VAL	2.3
2	B	35	ILE	2.3
8	U	24	CYS	2.3
9	V	64	LEU	2.3
9	I	53	GLU	2.3
5	E	153	PHE	2.3
5	E	194	VAL	2.3
5	R	114	VAL	2.3
5	R	85	LYS	2.3
7	T	73	ASN	2.3
9	I	60	ALA	2.2
9	V	60	ALA	2.2
5	R	133	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	224	LEU	2.2
8	U	37	LEU	2.2
9	I	64	LEU	2.2
5	E	97	PHE	2.2
5	E	102	THR	2.2
5	E	157	TYR	2.2
5	E	108	GLN	2.2
2	B	216	LEU	2.2
1	N	120	CYS	2.2
2	B	208	GLY	2.2
7	T	77	TYR	2.2
5	E	117	LEU	2.2
5	R	142	LEU	2.2
1	N	179	ARG	2.2
5	E	156	TYR	2.1
5	E	82	PRO	2.1
1	N	122	LEU	2.1
2	B	102	ARG	2.1
9	V	62	ARG	2.1
3	P	224	TYR	2.1
5	E	16	GLU	2.1
9	I	71	ASN	2.1
2	O	430	LEU	2.1
2	B	220	ALA	2.1
2	O	386	ALA	2.1
1	N	56	GLY	2.1
5	E	121	GLN	2.1
5	R	5	VAL	2.0
5	E	79	SER	2.0
5	E	95	PRO	2.0
1	A	28	GLU	2.0
1	A	259	GLY	2.0
5	E	128	LYS	2.0
1	N	182	LEU	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.

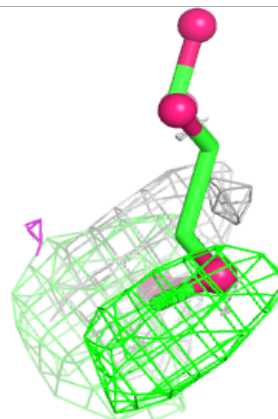
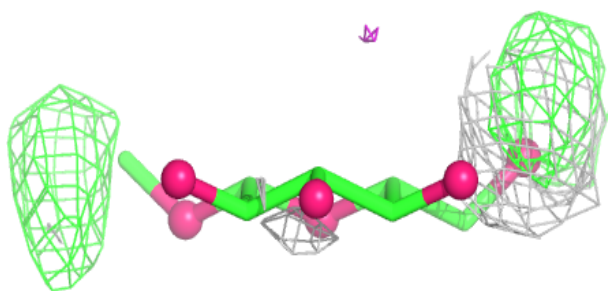
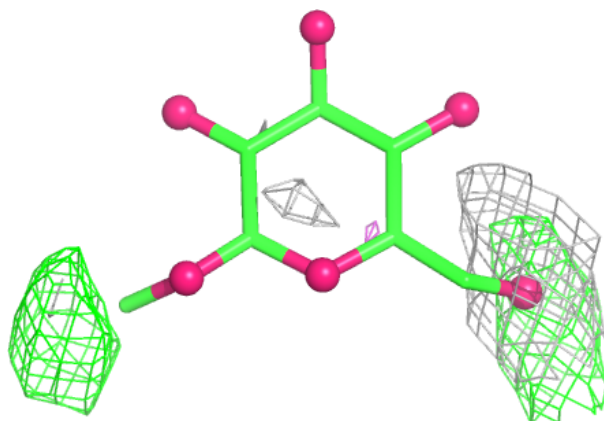
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	BOG	Q	3091	13/20	0.25	0.29	201,204,205,205	0
11	PEE	A	2008	21/51	0.50	0.26	139,142,145,145	0
18	BOG	P	2010	12/20	0.65	0.26	149,151,153,154	0
18	BOG	D	2091	13/20	0.67	0.33	215,217,218,218	0
11	PEE	P	3008	5/51	0.74	0.12	108,109,110,110	0
17	CDL	Q	3003	42/100	0.81	0.24	127,135,146,147	0
17	CDL	T	3004	40/100	0.82	0.17	104,109,120,121	0
11	PEE	R	3005	50/51	0.84	0.29	94,113,121,122	0
17	CDL	D	2003	42/100	0.85	0.21	94,105,109,110	0
14	UQ	P	3002	19/63	0.86	0.37	134,141,143,143	0
17	CDL	G	2004	40/100	0.88	0.14	72,83,101,103	0
14	UQ	C	2002	19/63	0.90	0.25	95,99,101,102	0
11	PEE	E	2005	50/51	0.90	0.21	88,101,111,112	0
11	PEE	P	3007	49/51	0.90	0.20	85,95,107,108	0
15	GOL	C	2011	6/6	0.91	0.30	90,90,91,91	0
19	FES	E	501	4/4	0.91	0.07	162,162,163,163	4
18	BOG	Q	3009	20/20	0.92	0.15	86,92,94,95	0
11	PEE	C	2007	49/51	0.92	0.17	53,73,95,96	0
18	BOG	D	2009	20/20	0.92	0.13	58,73,76,76	0
15	GOL	P	3011	6/6	0.93	0.20	90,91,93,95	0
13	JZZ	P	3001	25/25	0.95	0.12	74,76,79,80	0
13	JZZ	C	2001	25/25	0.96	0.08	45,49,51,51	0
16	HEC	Q	501	43/43	0.97	0.10	71,75,83,84	0
19	FES	R	501	4/4	0.97	0.04	100,101,102,102	0
12	HEM	P	501	43/43	0.98	0.09	51,55,62,67	0
12	HEM	P	502	43/43	0.98	0.07	42,52,65,70	0
12	HEM	C	501	43/43	0.99	0.08	30,42,53,55	0
12	HEM	C	502	43/43	0.99	0.07	31,37,47,52	0
16	HEC	D	501	43/43	0.99	0.07	39,45,50,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

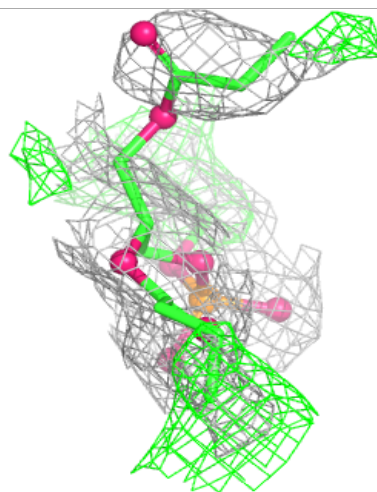
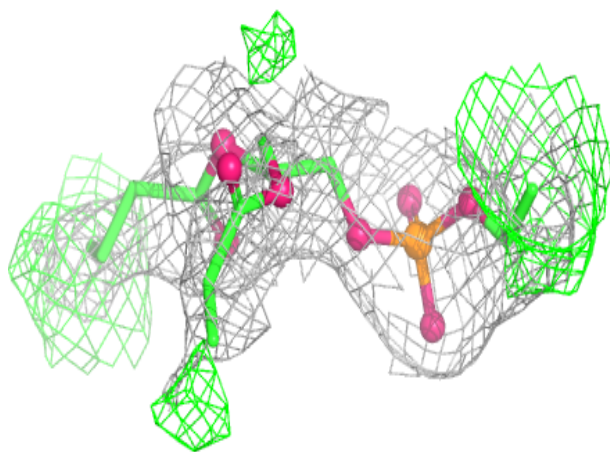
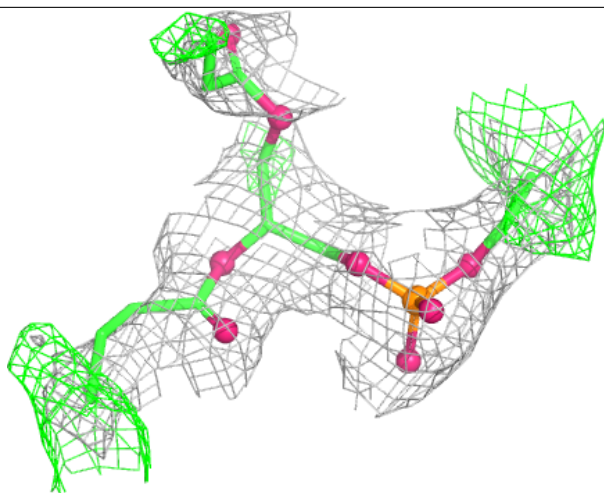
Electron density around BOG Q 3091:

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



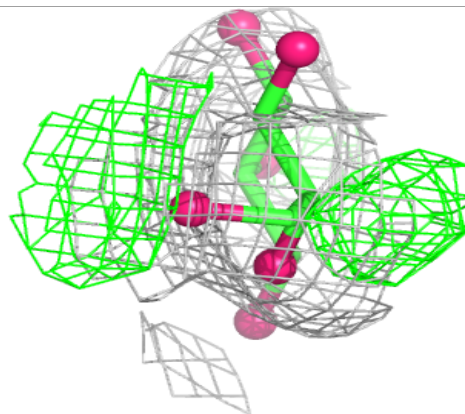
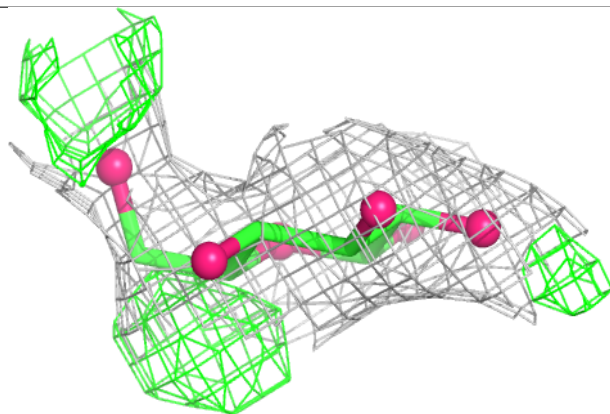
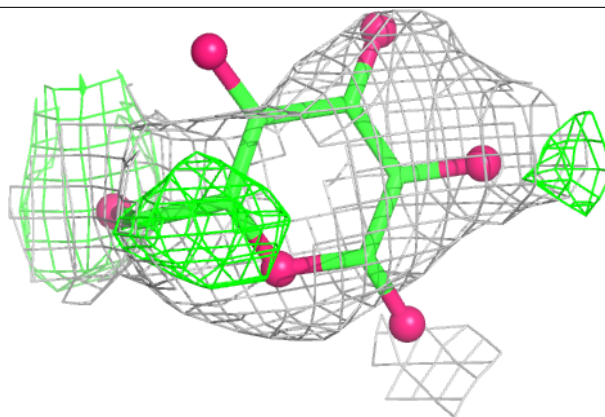
Electron density around PEE A 2008:

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



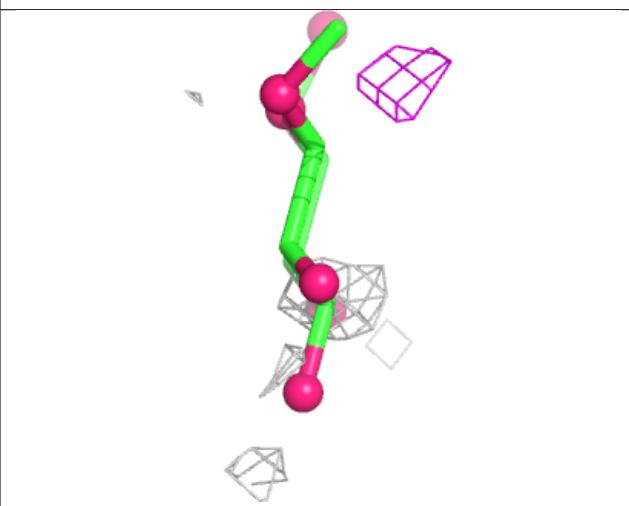
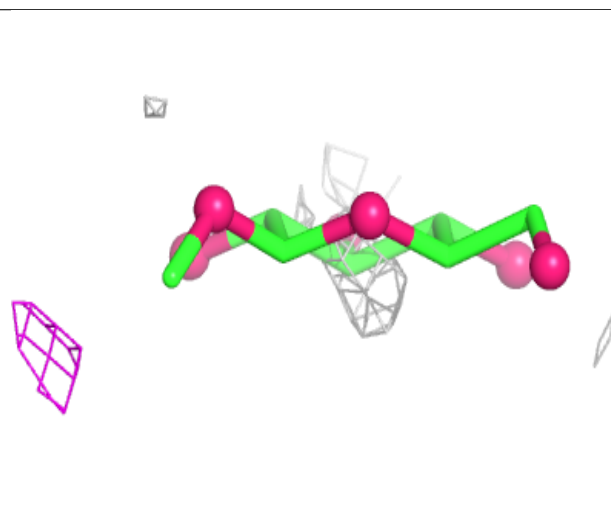
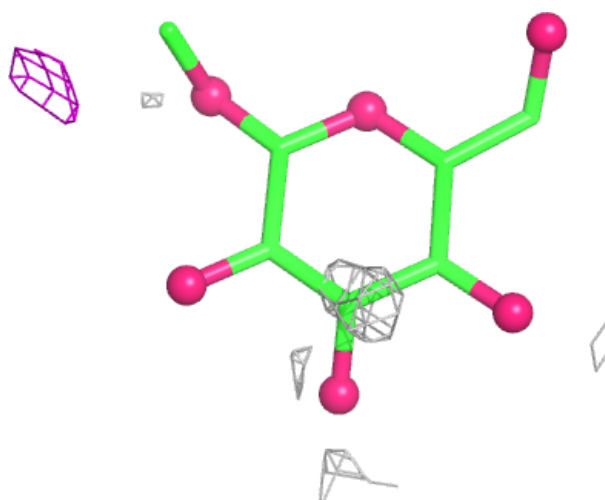
Electron density around BOG P 2010:

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



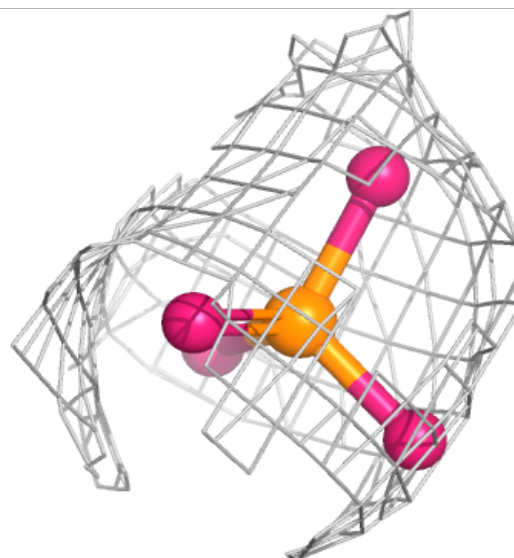
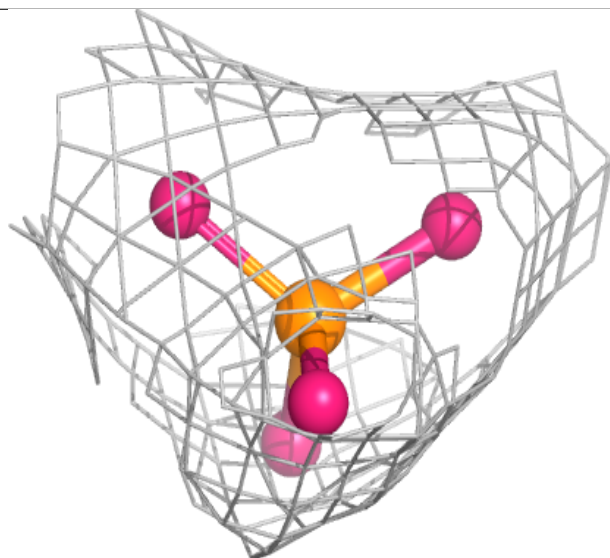
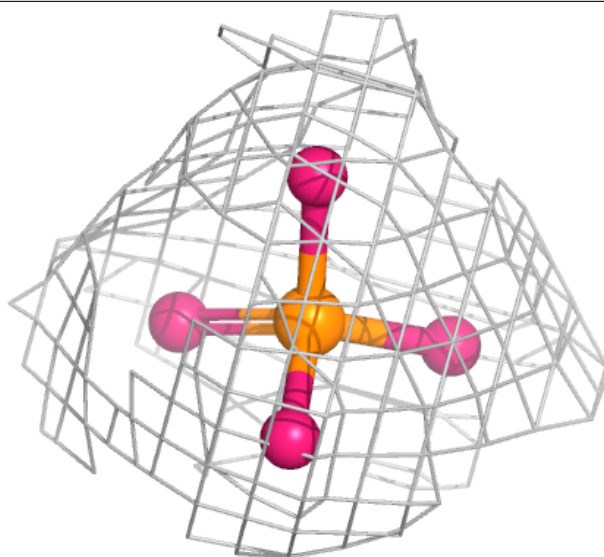
Electron density around BOG D 2091:

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



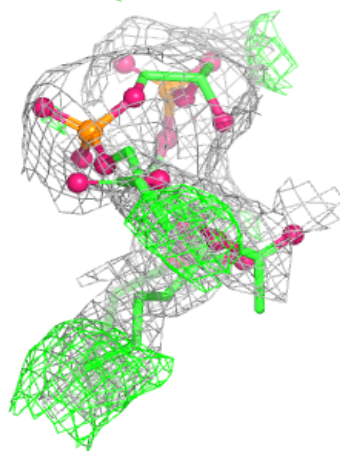
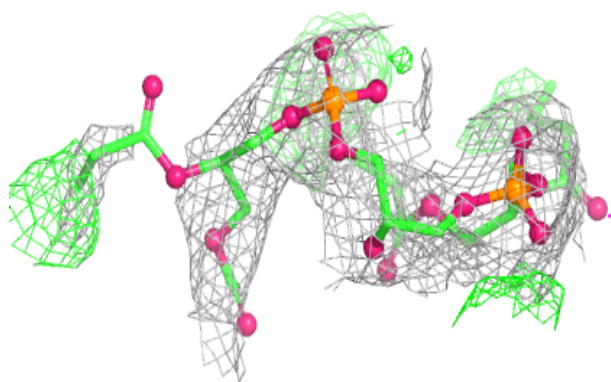
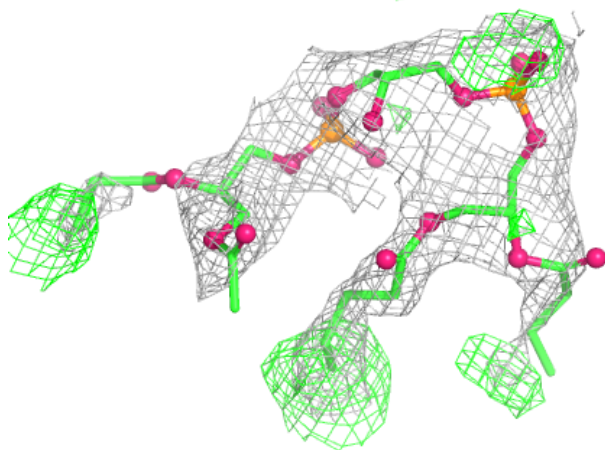
Electron density around PEE P 3008:

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and green (positive)



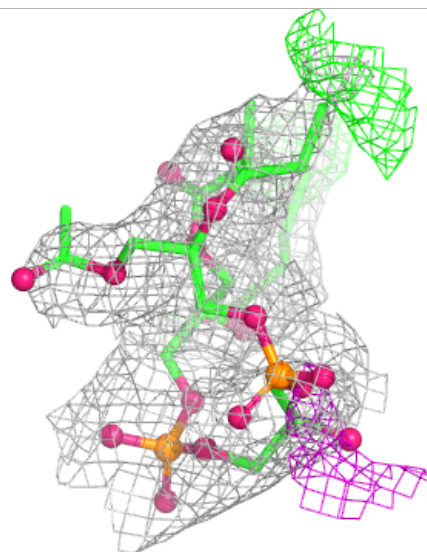
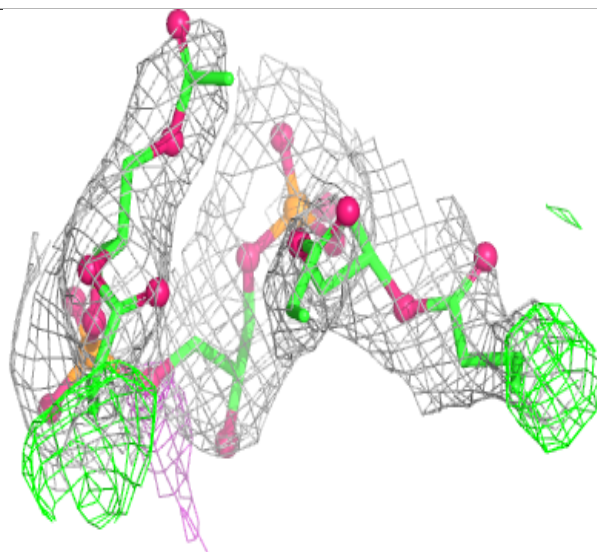
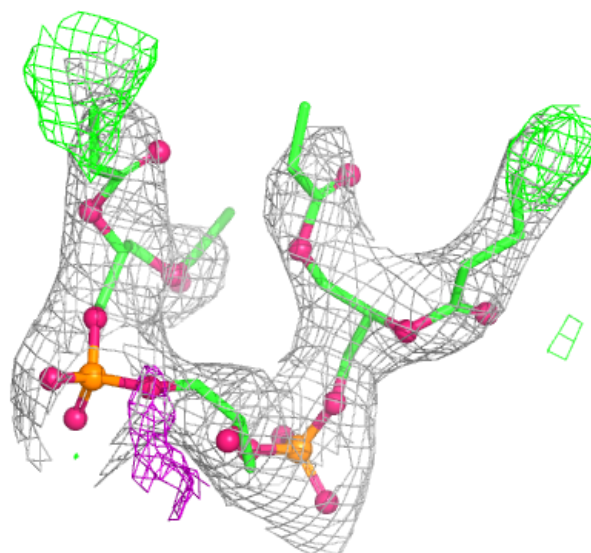
Electron density around CDL Q 3003:

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



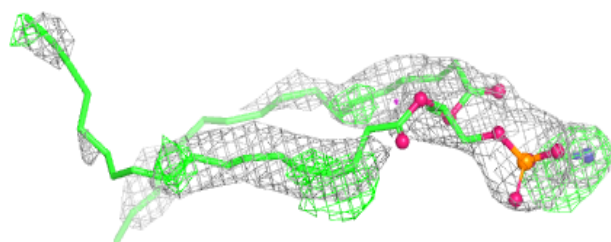
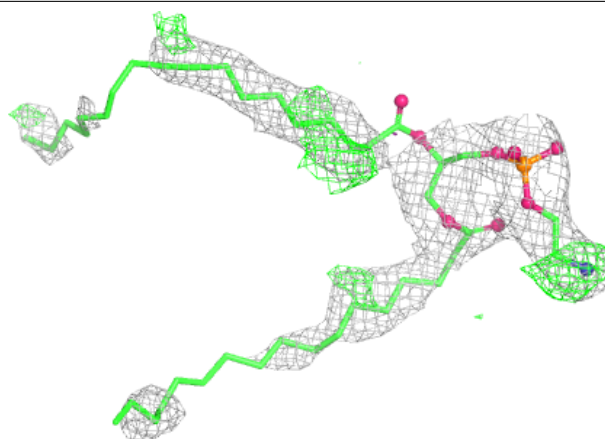
Electron density around CDL T 3004:

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



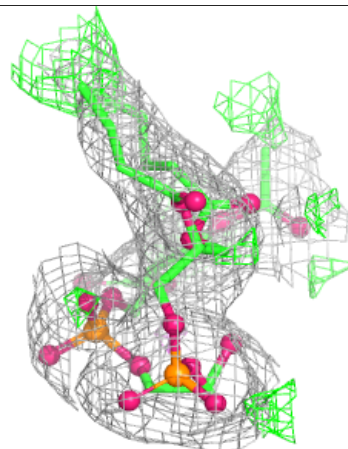
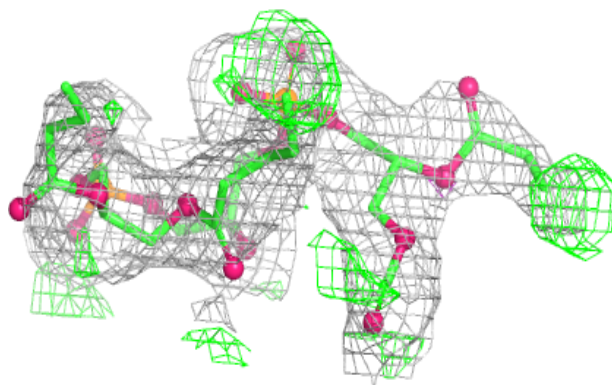
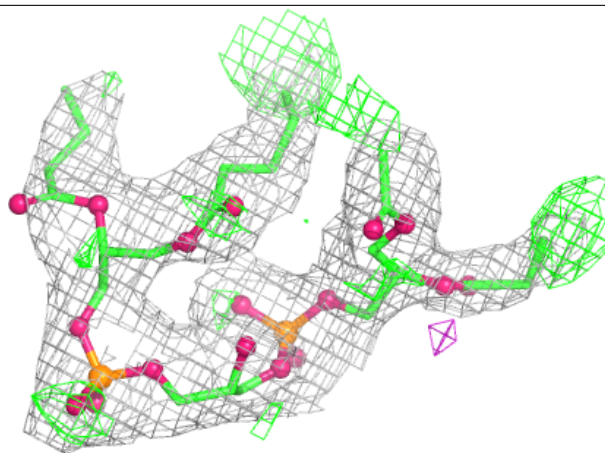
Electron density around PEE R 3005:

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

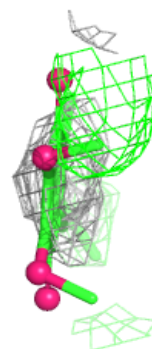
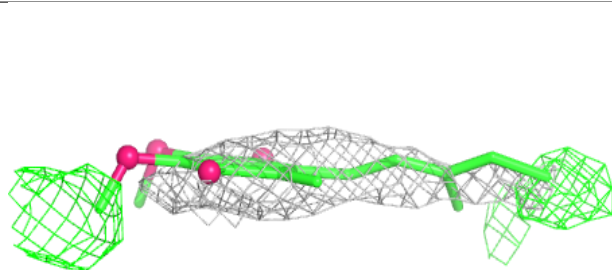
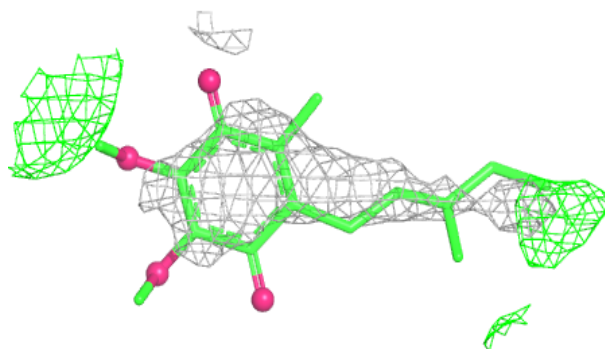


Electron density around CDL D 2003:

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

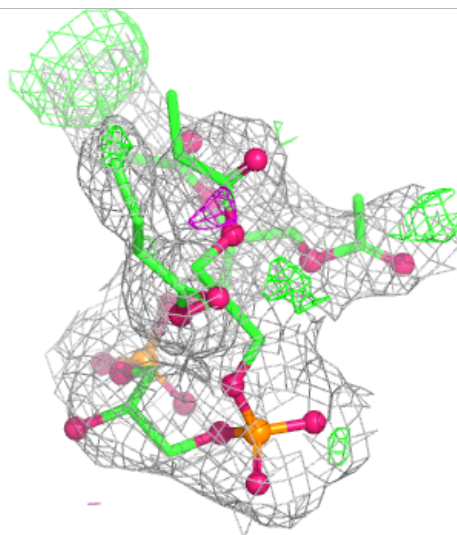
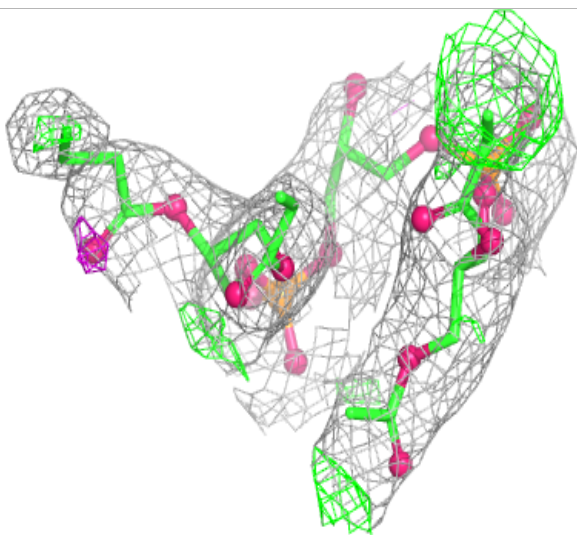
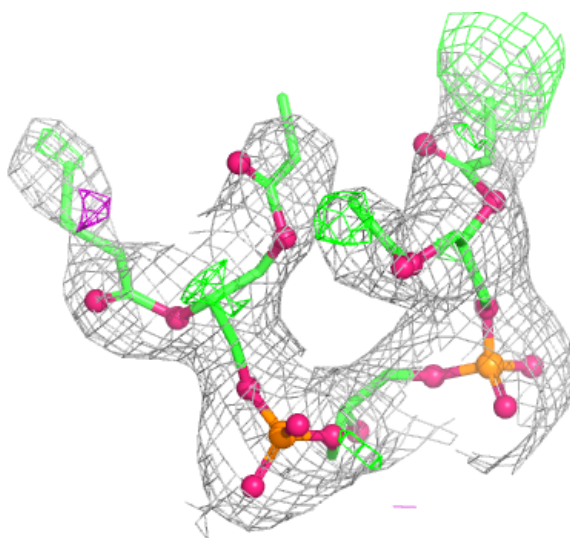
**Electron density around UQ P 3002:**

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and green (positive)



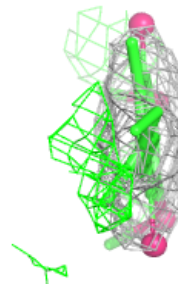
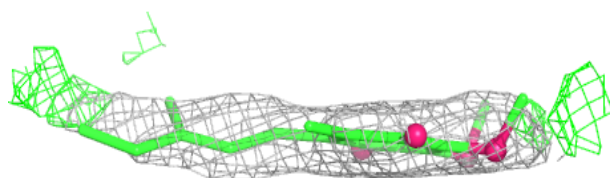
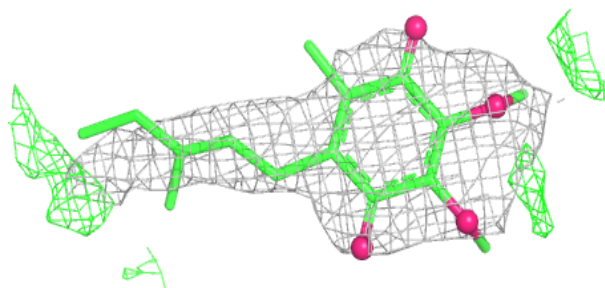
Electron density around CDL G 2004:

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

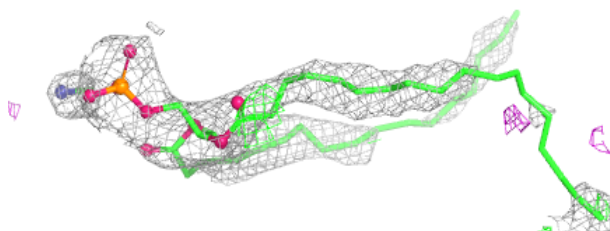
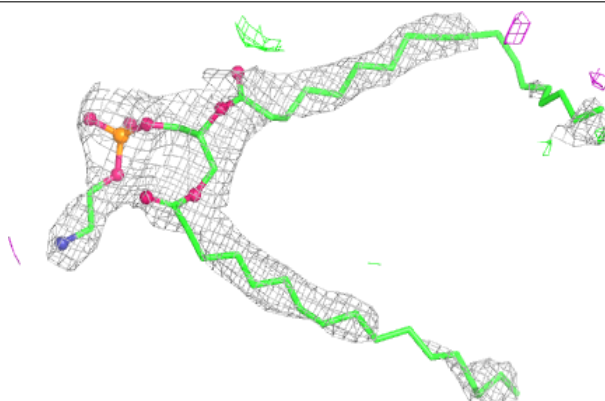


Electron density around UQ C 2002:

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and green (positive)

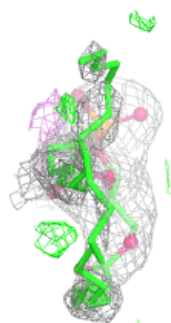
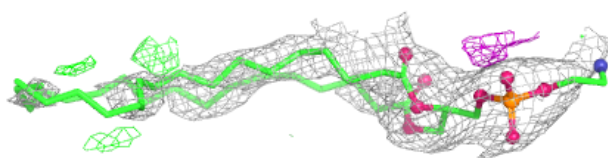
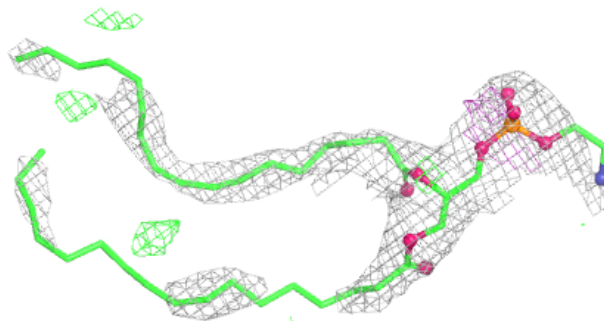
**Electron density around PEE E 2005:**

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and green (positive)

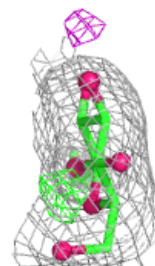
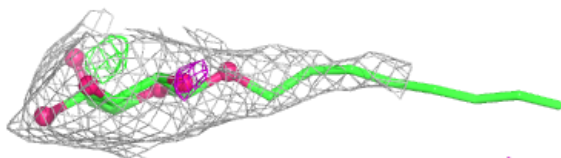
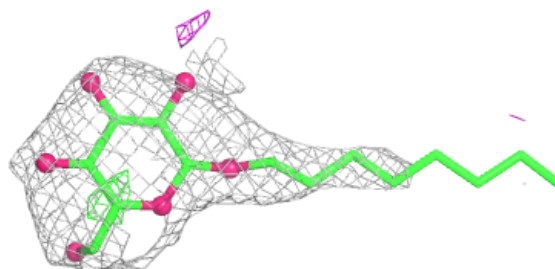


Electron density around PEE P 3007:

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and green (positive)

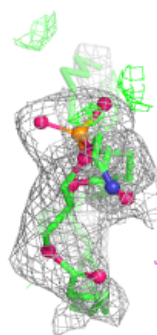
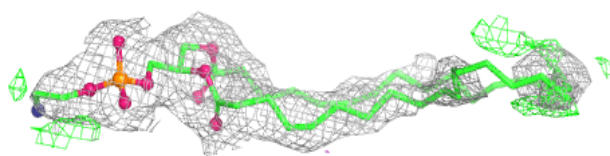
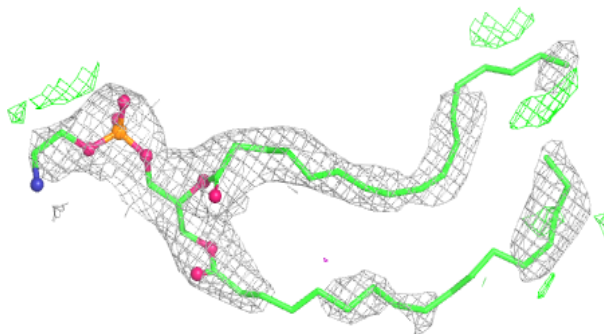
**Electron density around BOG Q 3009:**

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

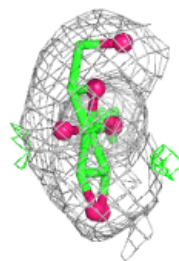
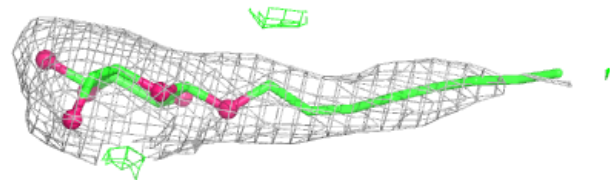
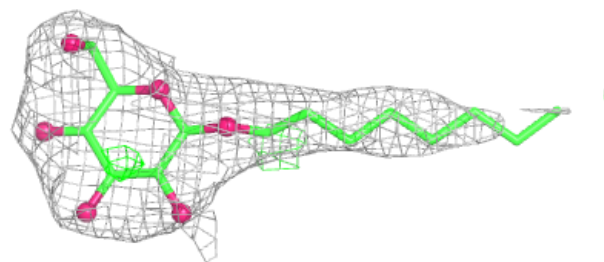


Electron density around PEE C 2007:

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

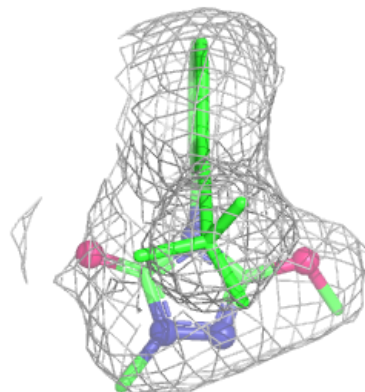
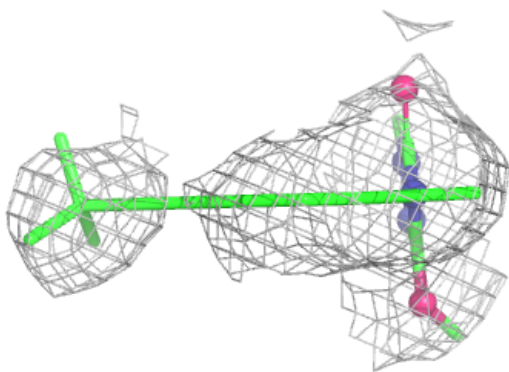
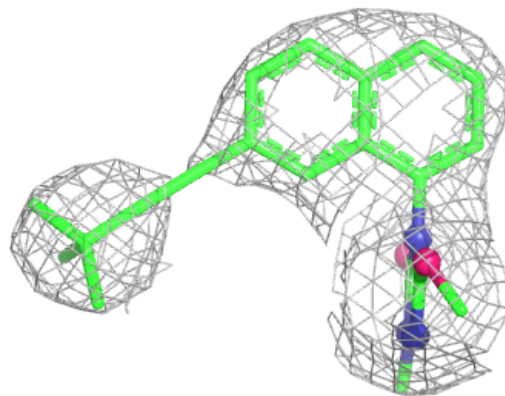
**Electron density around BOG D 2009:**

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

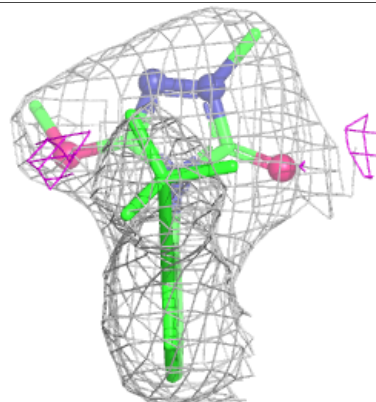
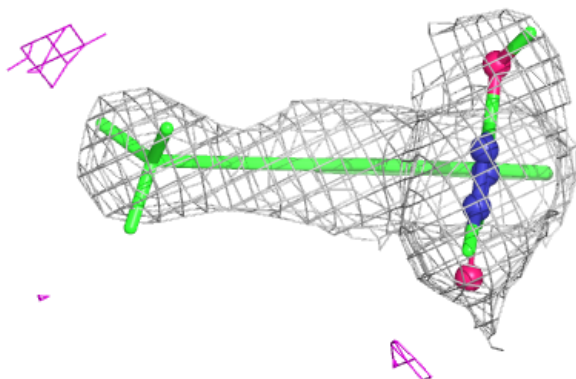
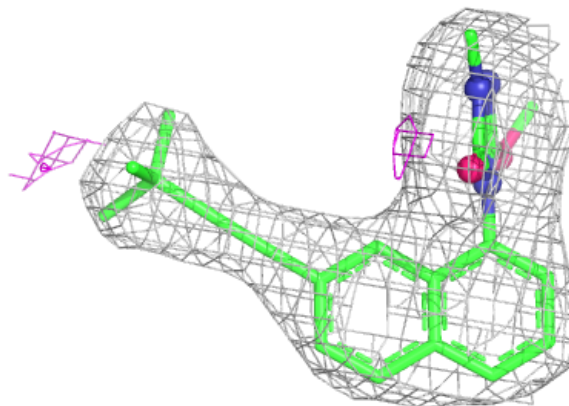


Electron density around JZZ P 3001:

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

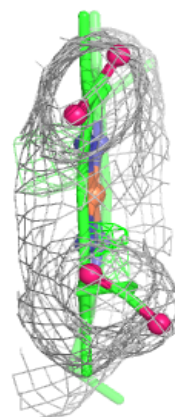
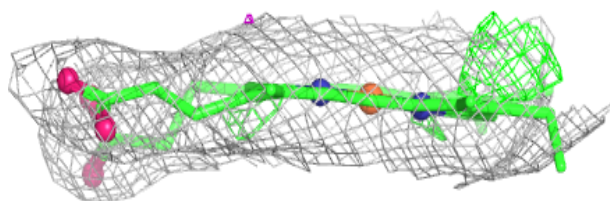
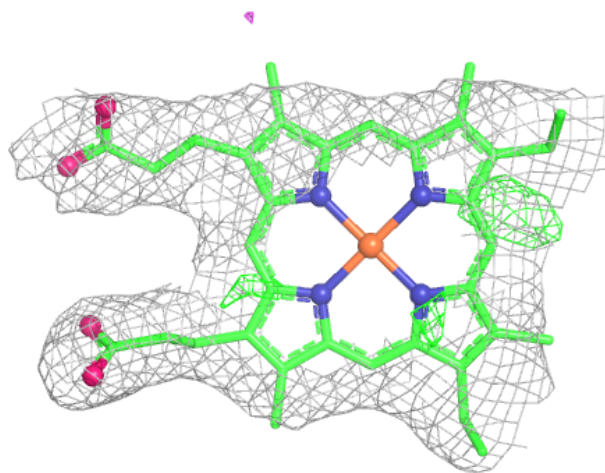
**Electron density around JZZ C 2001:**

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



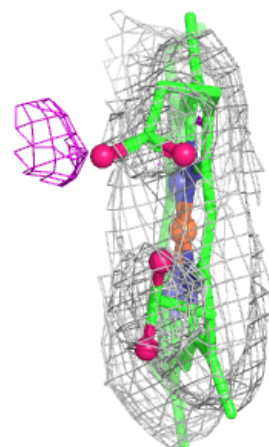
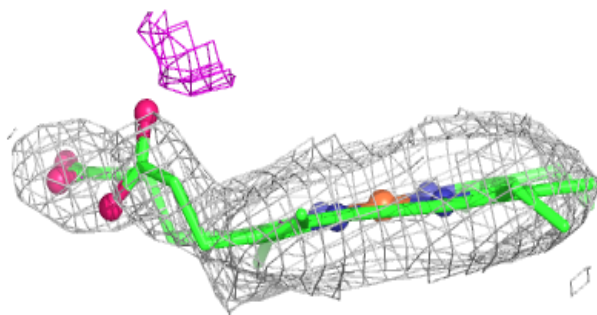
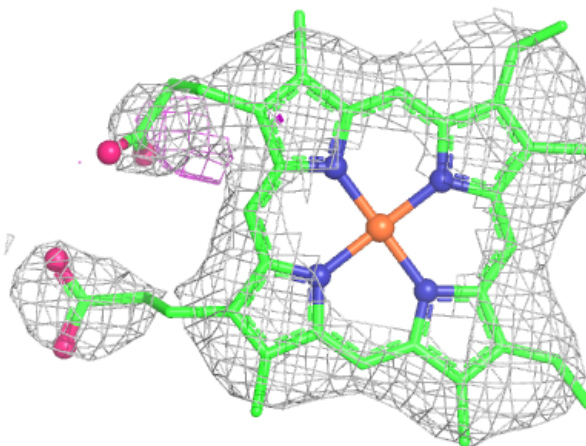
Electron density around HEC Q 501:

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



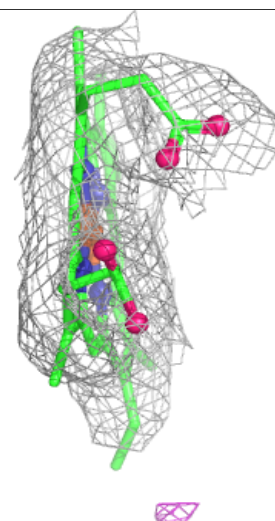
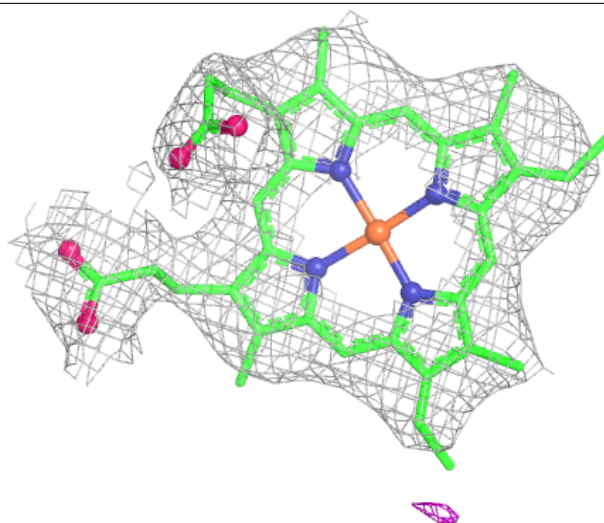
Electron density around HEM P 501:

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



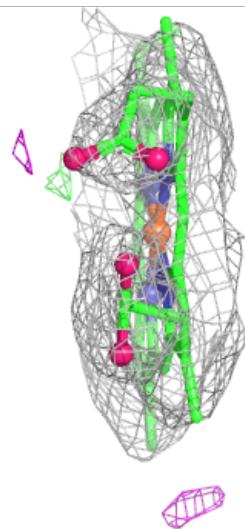
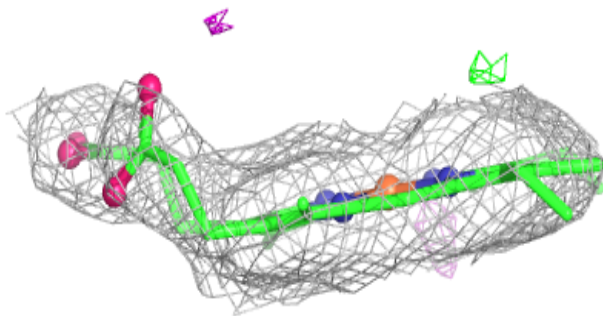
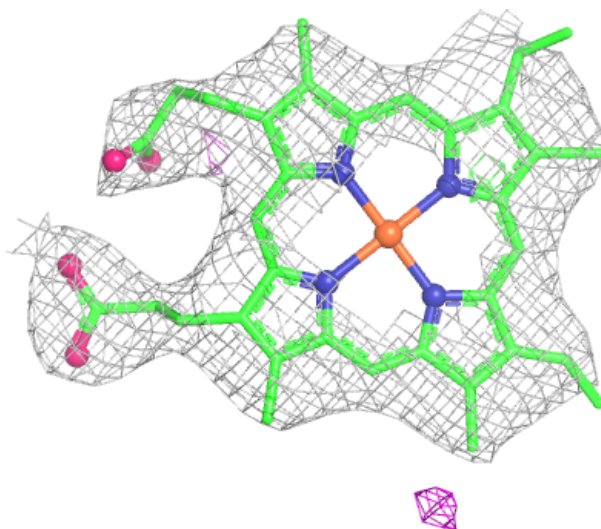
Electron density around HEM P 502:

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



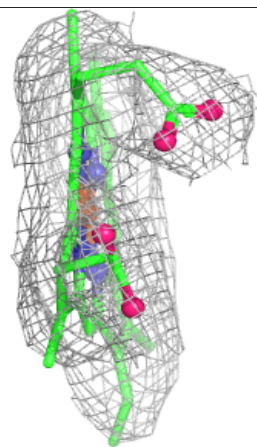
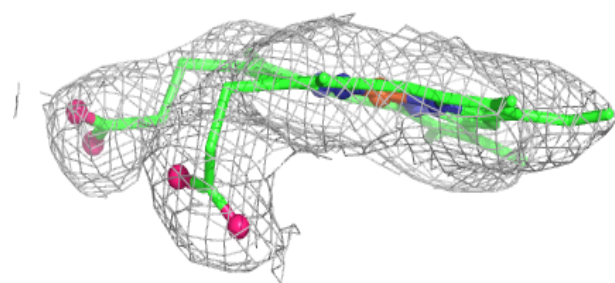
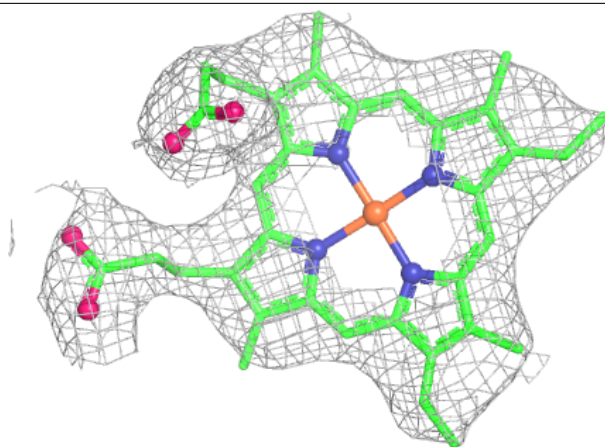
Electron density around HEM C 501:

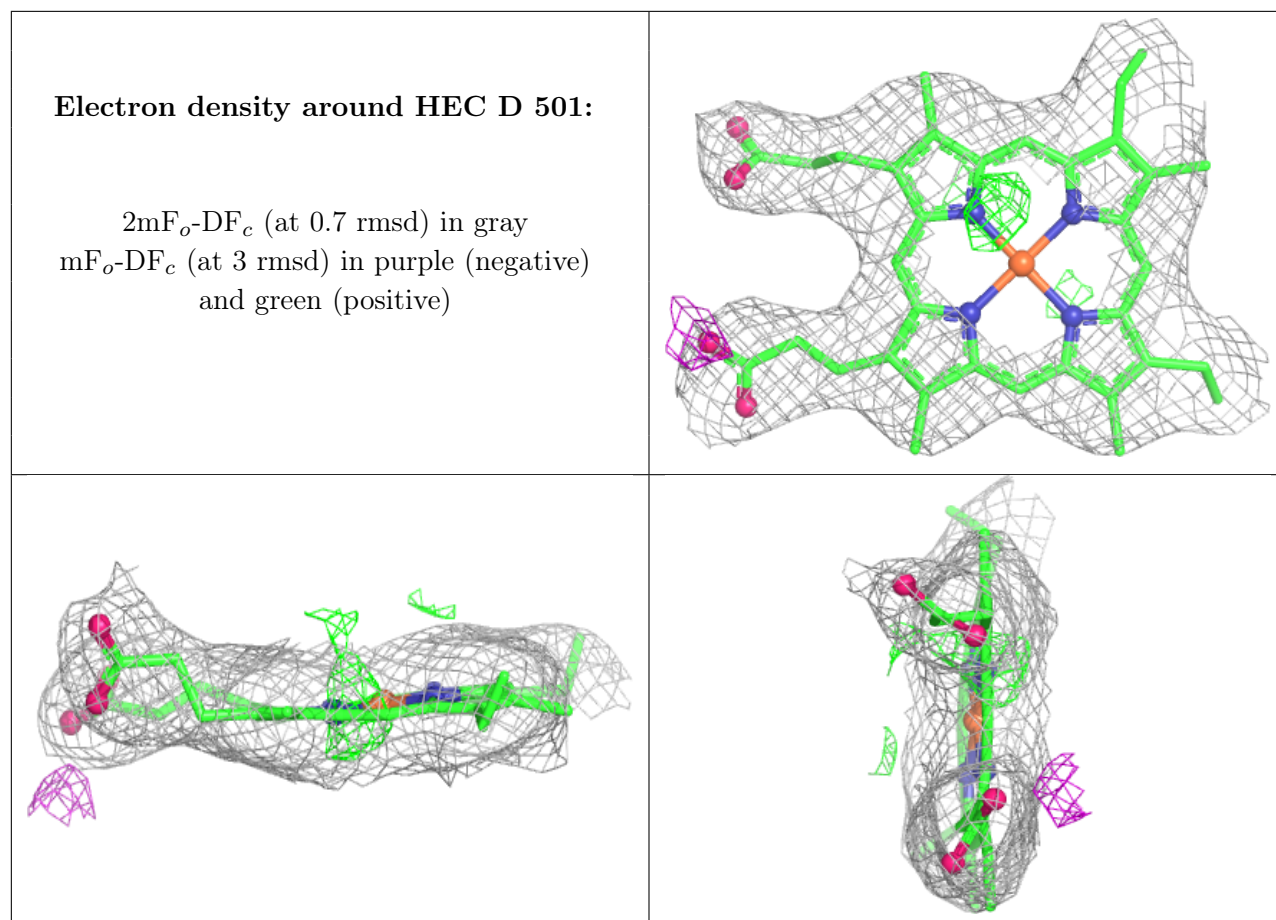
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.