



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:46 PM UTC

PDB ID : 3L72 / pdb_00003l72
Title : Chicken cytochrome BC1 complex with kresoxim-I-dimethyl bound
Authors : Huang, L.; Zhang, Z.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 3.06 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

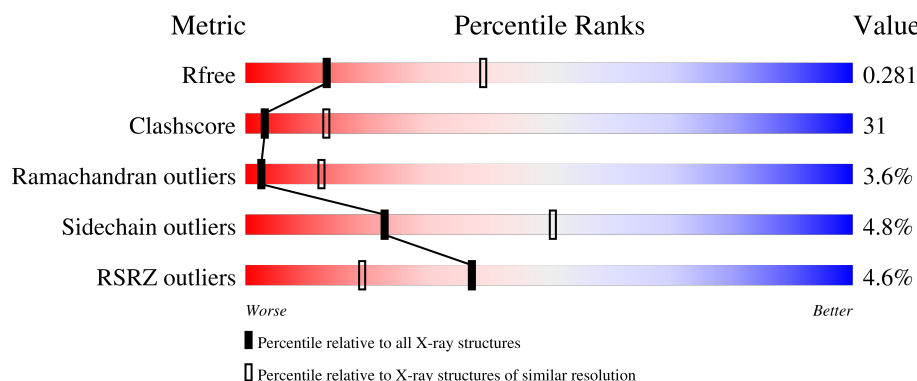
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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.



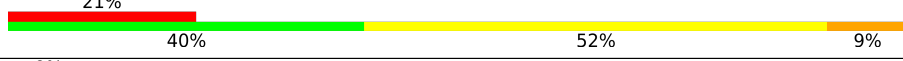
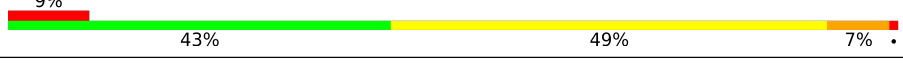
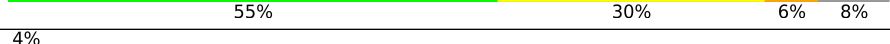
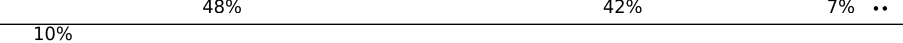
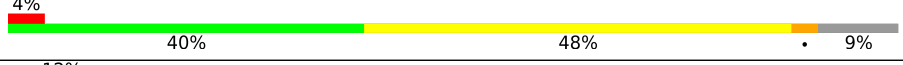
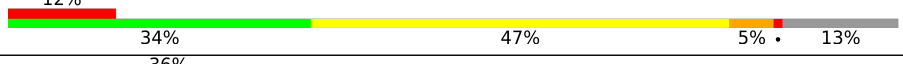
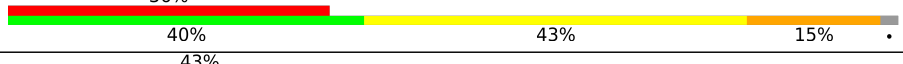
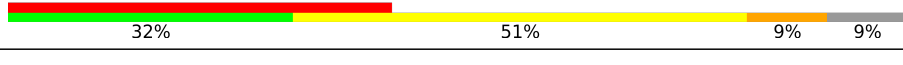
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	48% 46% 5%
1	N	446	4% 44% 48% 7% •
2	B	441	2% 37% 50% 7% • 5%
2	O	441	3% 42% 47% 7% •
3	C	380	2% 51% 44% 5%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PEE	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 32648 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	421	Total	C	N	O	S	0	0	0
			3137	1970	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL.

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

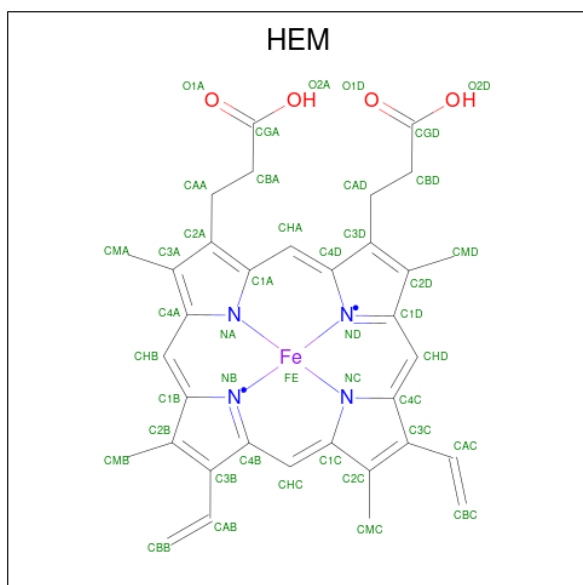
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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.

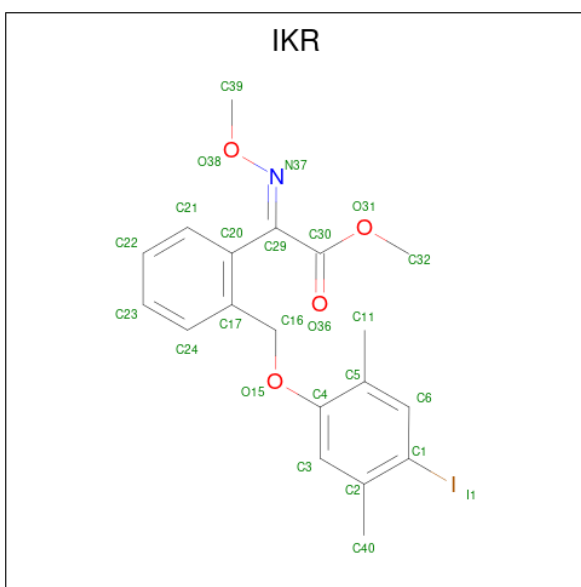
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total 497	C 321	N 87	O 89	0	0	0
10	W	60	Total 479	C 311	N 86	O 82	0	0	1

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



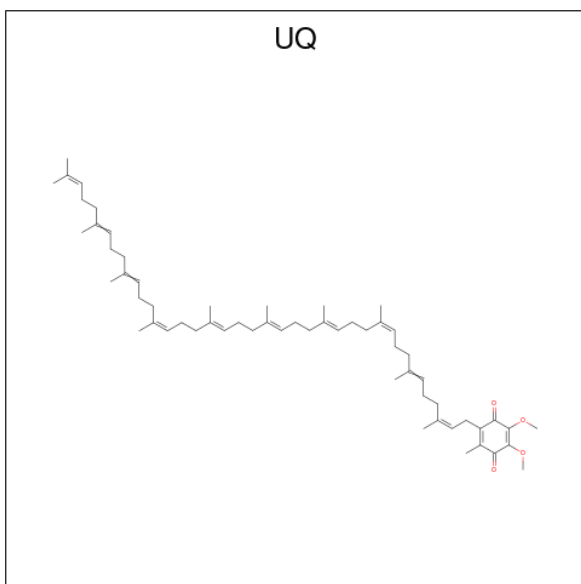
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 12 is methyl (2E)-{2-[(4-iodo-2,5-dimethylphenoxy)methyl]phenyl}(methoxyimino)ethanoate (CCD ID: IKR) (formula: C₁₉H₂₀INO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
12	P	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

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



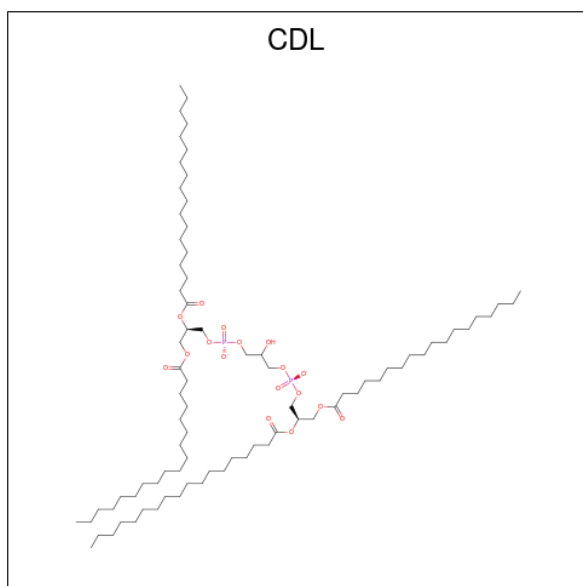
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			19	15	4		

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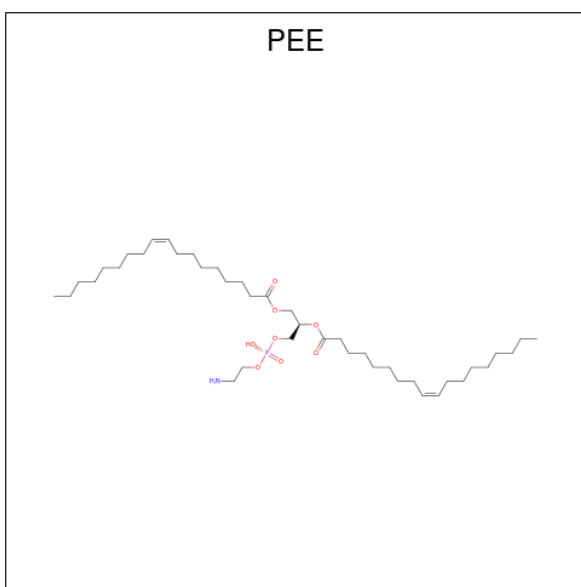
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



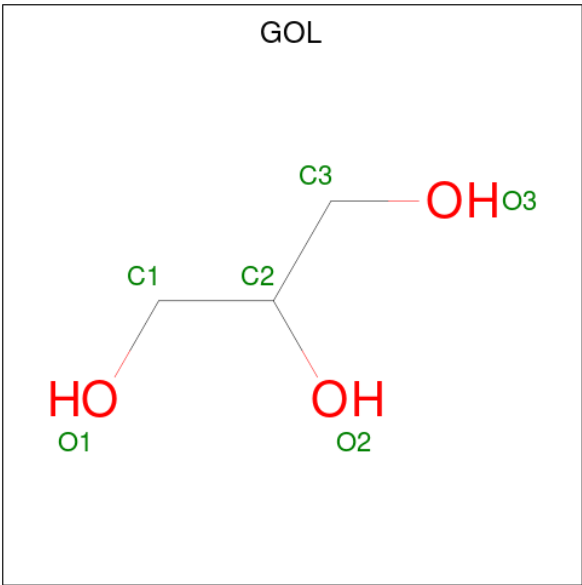
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			40	21	17	2		
14	D	1	Total	C	O	P	0	0
			42	23	17	2		
14	P	1	Total	C	O	P	0	0
			40	21	17	2		
14	Q	1	Total	C	O	P	0	0
			42	23	17	2		

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



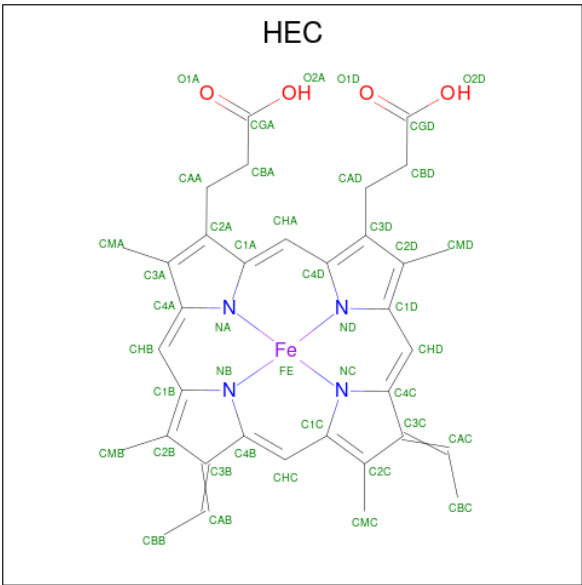
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	P	1	Total	O	P			0	0
			5	4	1				
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

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

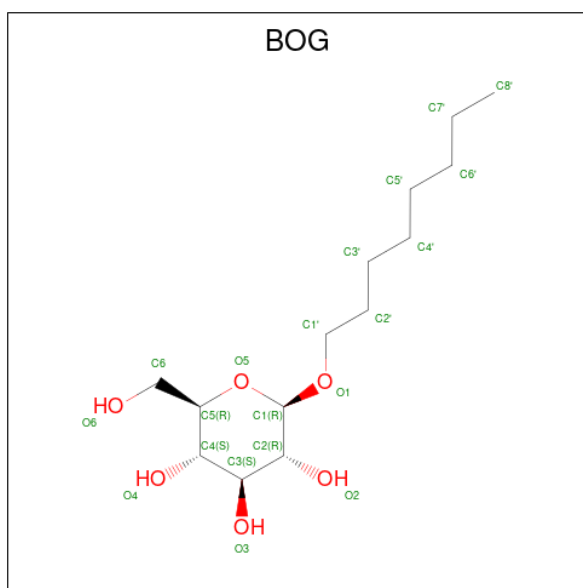


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

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

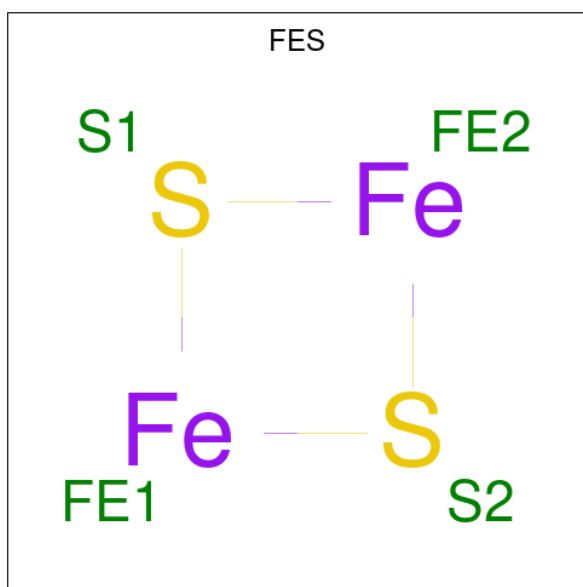


- Molecule 18 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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		

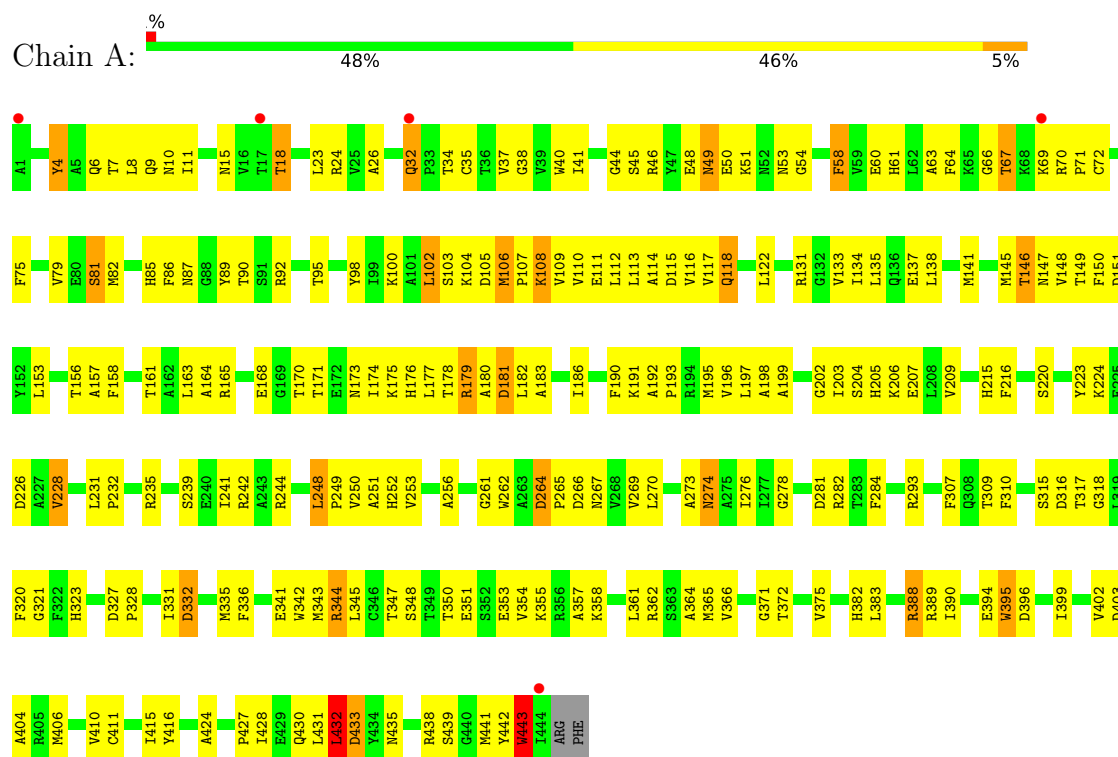
- Molecule 20 is water.

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	8	Total	O	0	0
			8	8		
20	R	1	Total	O	0	0
			1	1		

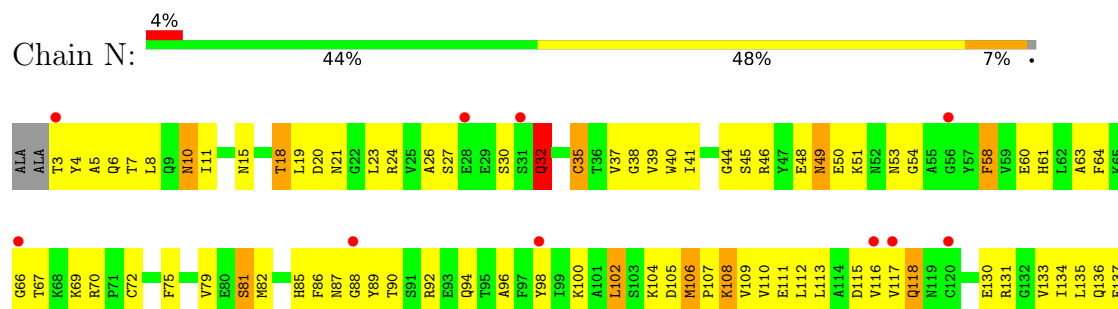
3 Residue-property plots

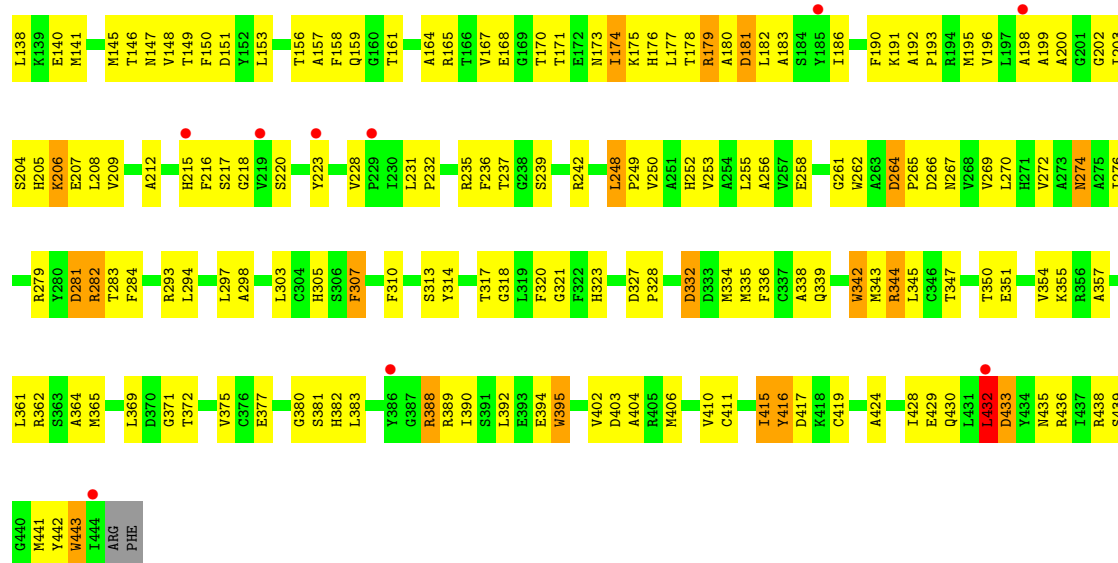
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

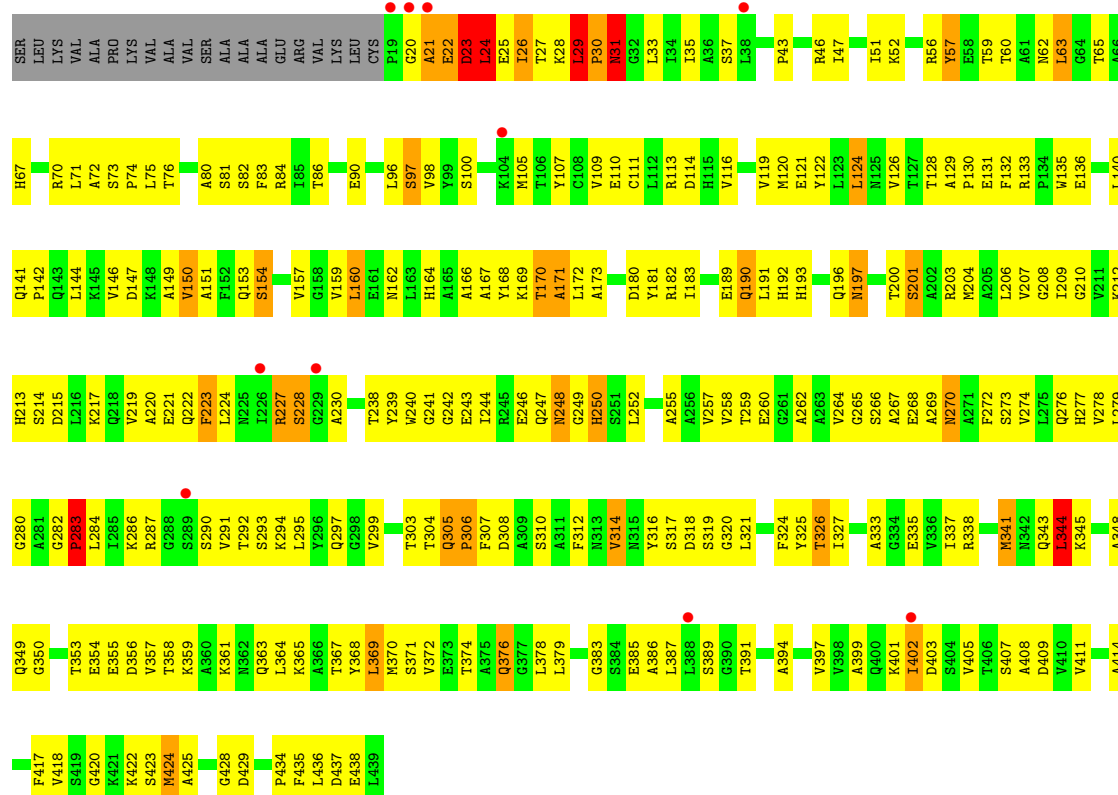


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

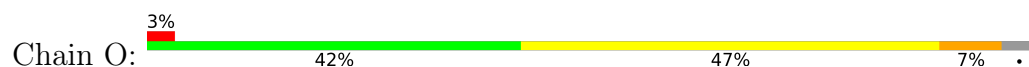


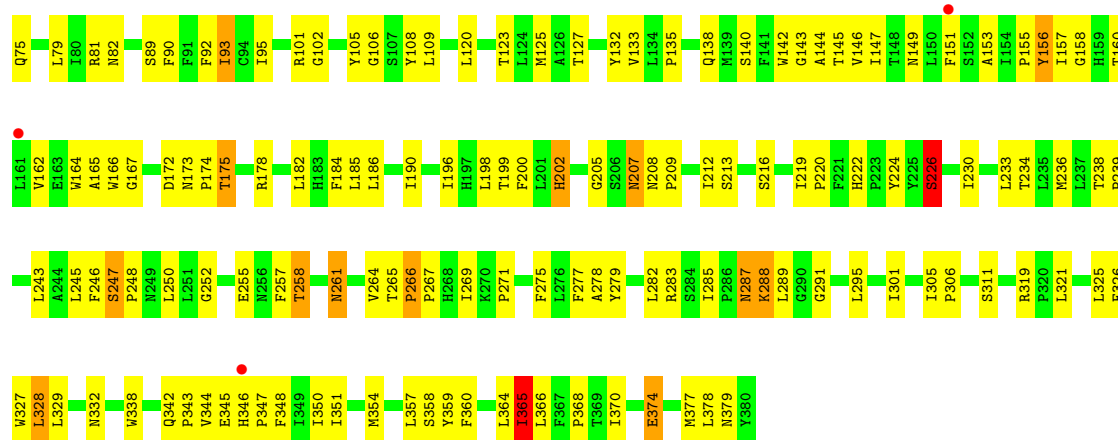


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2



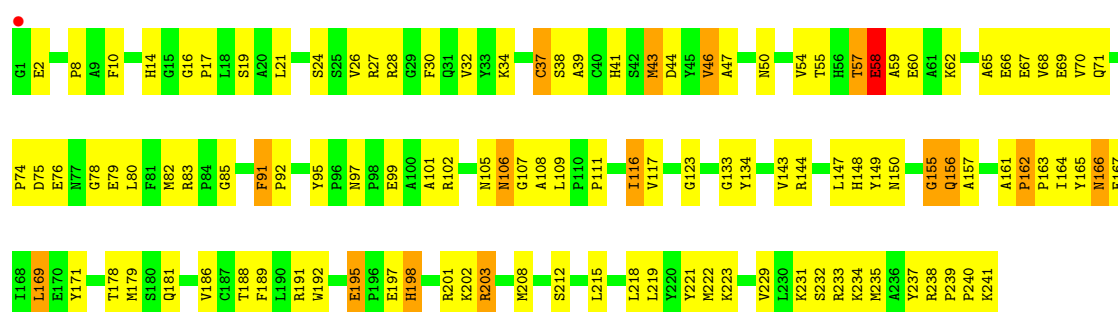
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2





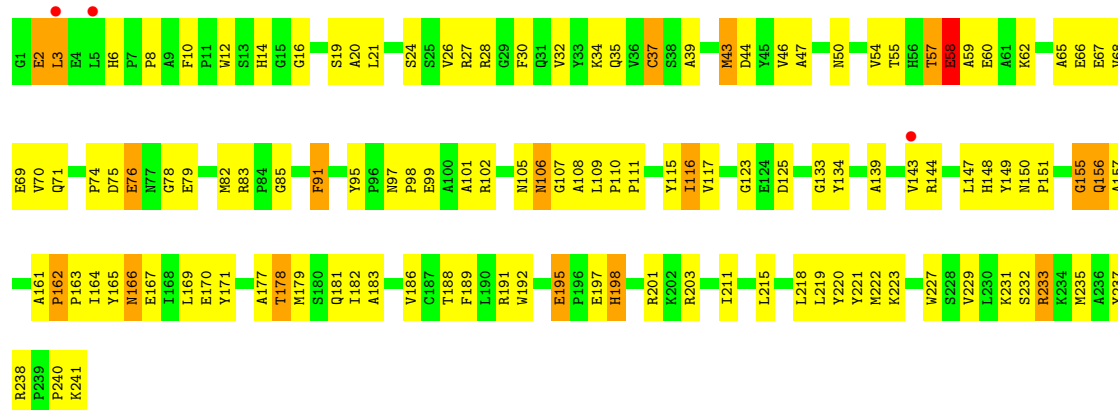
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D: 52% 41% 6%



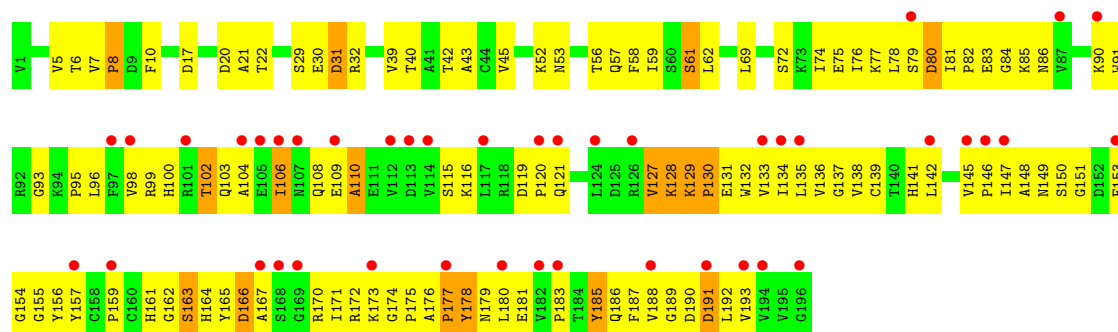
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q: 49% 44% 7%

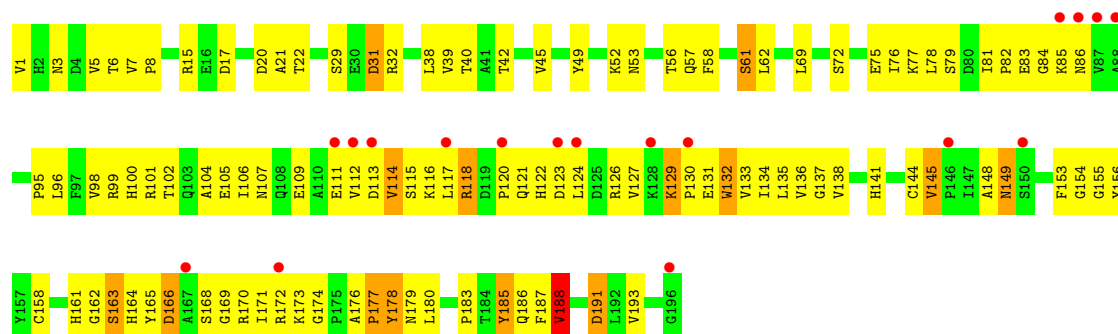


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL

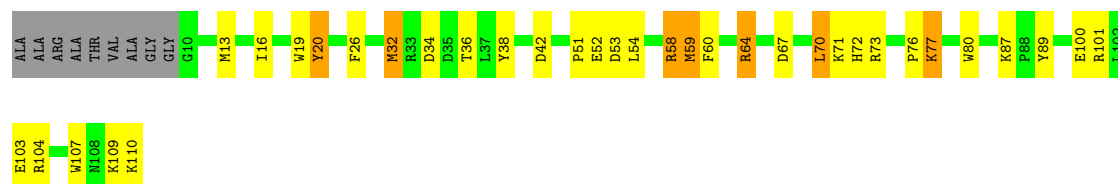
Chain E: 21% 40% 52% 9%



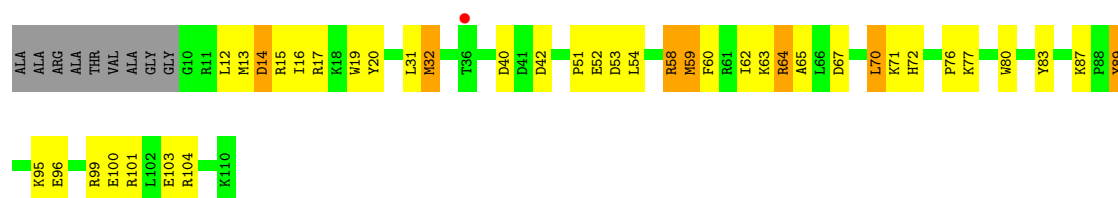
- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



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

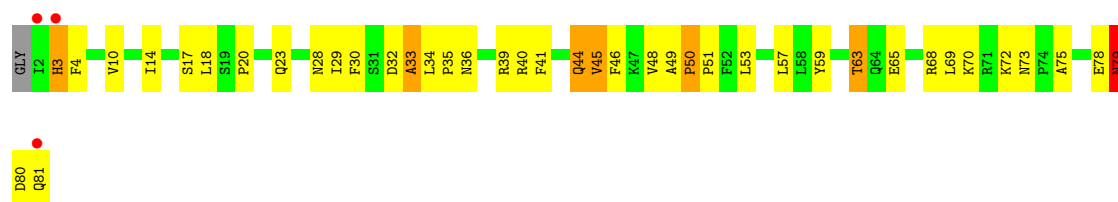


- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



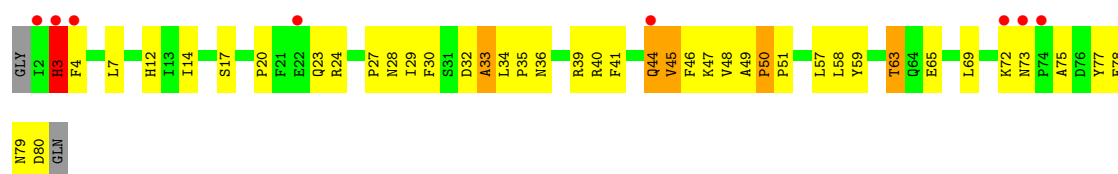
● Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



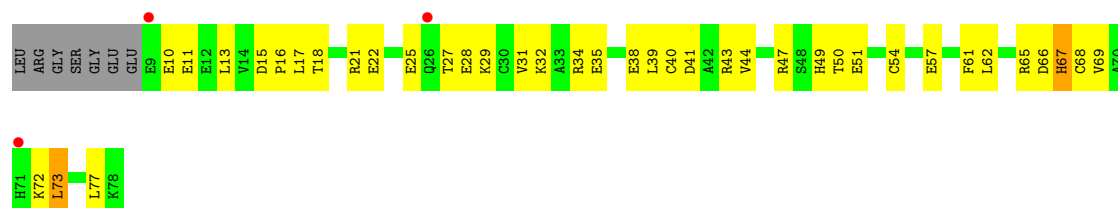
● Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T: 



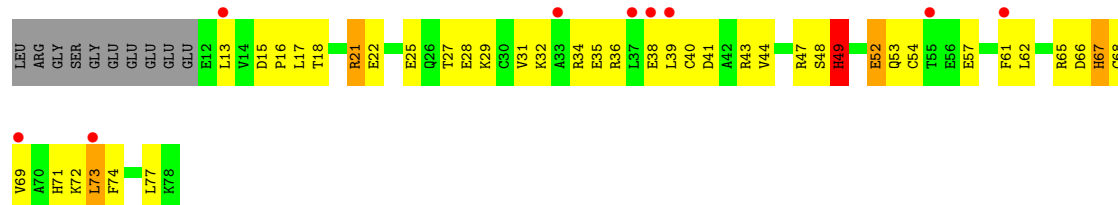
● Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H: 



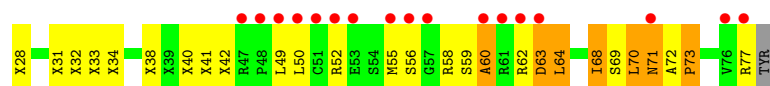
● Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U: 

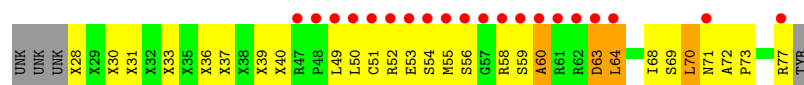


● Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

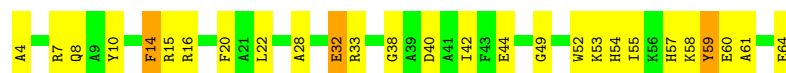
Chain I: 



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	172.61Å 181.55Å 241.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.93 – 3.06 28.93 – 3.06	Depositor EDS
% Data completeness (in resolution range)	93.8 (28.93-3.06) 93.7 (28.93-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.294 0.252 , 0.281	Depositor DCC
R_{free} test set	2766 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32648	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/3518	1.04	24/4767 (0.5%)
1	N	0.53	0/3508	1.04	22/4753 (0.5%)
2	B	0.49	0/3191	1.04	21/4326 (0.5%)
2	O	0.52	0/3202	1.06	14/4343 (0.3%)
3	C	0.62	0/3119	1.06	20/4270 (0.5%)
3	P	0.56	0/3114	1.04	24/4263 (0.6%)
4	D	0.56	0/1956	1.07	14/2658 (0.5%)
4	Q	0.49	0/1956	1.04	13/2658 (0.5%)
5	E	0.47	0/1547	0.94	4/2103 (0.2%)
5	R	0.48	0/1543	0.96	4/2098 (0.2%)
6	F	0.57	0/911	1.00	4/1219 (0.3%)
6	S	0.47	0/911	1.00	4/1219 (0.3%)
7	G	0.59	0/694	1.04	1/941 (0.1%)
7	T	0.58	0/684	1.06	3/929 (0.3%)
8	H	0.54	0/582	1.00	2/779 (0.3%)
8	U	0.43	0/561	0.92	1/751 (0.1%)
9	I	0.62	0/218	1.01	0/293
9	V	0.62	0/218	1.01	0/293
10	J	0.55	0/508	0.97	1/682 (0.1%)
10	W	0.50	0/490	0.97	1/660 (0.2%)
All	All	0.53	0/32431	1.03	177/44005 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1

There are no bond length outliers.

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	226	SER	N-CA-C	-9.84	100.11	111.03
3	P	226	SER	N-CA-C	-9.49	100.50	111.03
2	O	225	ASN	N-CA-C	8.85	124.05	112.72
10	J	14	PHE	N-CA-C	8.56	122.82	112.38
2	O	227	ARG	N-CA-C	8.28	121.87	109.95
10	W	14	PHE	N-CA-C	8.26	122.46	112.38
5	E	17	ASP	N-CA-C	7.54	119.50	111.28
1	N	347	THR	N-CA-C	7.52	123.36	114.04
6	S	15	ARG	N-CA-C	-7.29	104.52	113.41
1	A	32	GLN	N-CA-C	7.28	118.53	109.57
4	Q	116	ILE	N-CA-C	7.28	118.00	110.36
8	H	13	LEU	N-CA-C	7.26	120.77	109.96
3	P	257	PHE	N-CA-C	-7.19	103.61	112.88
3	C	261	ASN	CA-C-N	7.18	126.86	119.82
3	C	261	ASN	C-N-CA	7.18	126.86	119.82
7	T	78	GLU	N-CA-C	-7.16	104.97	113.21
5	R	17	ASP	N-CA-C	7.15	119.98	111.33
4	D	116	ILE	N-CA-C	7.14	117.86	110.36
3	C	207	ASN	N-CA-C	-7.10	100.55	110.35
1	N	32	GLN	CA-C-N	7.09	126.70	119.19
1	N	32	GLN	C-N-CA	7.09	126.70	119.19
3	P	207	ASN	N-CA-C	-7.02	101.47	110.53
1	N	264	ASP	CA-C-N	6.93	126.63	119.56
1	N	264	ASP	C-N-CA	6.93	126.63	119.56
1	A	347	THR	N-CA-C	6.85	122.54	114.04
5	E	129	LYS	CA-C-N	6.81	128.35	119.84
5	E	129	LYS	C-N-CA	6.81	128.35	119.84
1	N	66	GLY	N-CA-C	6.76	120.58	111.72
6	S	14	ASP	N-CA-C	-6.72	105.05	113.18
1	N	151	ASP	N-CA-C	-6.72	103.88	111.14
2	B	267	ALA	N-CA-C	-6.67	103.93	111.14
1	A	66	GLY	N-CA-C	6.58	120.34	111.72
1	N	432	LEU	N-CA-C	6.58	118.21	108.60
1	A	432	LEU	N-CA-C	6.55	118.72	108.96
1	A	4	TYR	N-CA-C	-6.54	104.07	111.07
4	D	44	ASP	N-CA-C	6.54	120.85	112.34
5	R	129	LYS	CA-C-N	6.53	126.76	119.32
5	R	129	LYS	C-N-CA	6.53	126.76	119.32
1	A	32	GLN	CA-C-N	6.45	126.03	119.19
1	A	32	GLN	C-N-CA	6.45	126.03	119.19
1	A	264	ASP	CA-C-N	6.44	126.13	119.56
1	A	264	ASP	C-N-CA	6.44	126.13	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	248	LEU	CA-C-N	6.43	125.66	118.97
1	N	248	LEU	C-N-CA	6.43	125.66	118.97
4	D	91	PHE	CA-C-N	6.41	126.17	119.76
4	D	91	PHE	C-N-CA	6.41	126.17	119.76
1	N	32	GLN	N-CA-C	6.37	117.41	109.57
2	B	326	THR	N-CA-C	6.31	119.18	108.90
1	A	264	ASP	N-CA-C	6.30	118.66	109.71
1	N	179	ARG	N-CA-C	-6.28	103.71	111.75
3	P	261	ASN	CA-C-N	6.22	126.34	119.87
3	P	261	ASN	C-N-CA	6.22	126.34	119.87
3	P	205	GLY	N-CA-C	-6.18	104.85	112.33
3	C	147	ILE	N-CA-C	6.17	116.29	110.30
3	P	252	GLY	N-CA-C	6.16	119.92	111.54
3	C	265	THR	CA-C-N	-6.15	115.23	119.66
3	C	265	THR	C-N-CA	-6.15	115.23	119.66
3	C	266	PRO	CA-C-N	6.13	127.51	119.84
3	C	266	PRO	C-N-CA	6.13	127.51	119.84
6	F	109	LYS	N-CA-C	-6.12	104.16	111.69
4	Q	6	HIS	CA-C-N	6.12	124.12	119.66
4	Q	6	HIS	C-N-CA	6.12	124.12	119.66
3	C	257	PHE	N-CA-C	-6.11	104.33	112.94
2	O	326	THR	N-CA-C	6.10	119.06	108.76
3	P	72	ARG	N-CA-C	6.08	118.87	111.82
4	D	178	THR	N-CA-C	-6.02	103.00	110.41
1	A	58	PHE	N-CA-C	-6.00	104.87	111.82
2	O	226	ILE	N-CA-C	-6.00	100.84	108.93
2	B	230	ALA	N-CA-C	-5.99	105.54	114.64
1	N	416	TYR	N-CA-C	5.97	119.25	110.30
3	P	143	GLY	N-CA-C	-5.94	105.30	112.49
7	T	47	LYS	N-CA-C	-5.93	105.71	113.12
5	E	106	ILE	N-CA-C	-5.92	106.97	113.43
4	D	58	GLU	N-CA-C	-5.92	104.91	111.36
2	B	197	ASN	N-CA-C	5.92	118.69	111.82
3	C	185	LEU	N-CA-C	5.92	118.87	111.24
8	H	51	GLU	N-CA-C	-5.90	106.05	113.18
3	C	252	GLY	N-CA-C	5.89	119.56	111.54
4	Q	195	GLU	CA-C-N	5.88	127.19	119.84
4	Q	195	GLU	C-N-CA	5.88	127.19	119.84
4	Q	58	GLU	N-CA-C	-5.87	104.96	111.36
4	D	155	GLY	N-CA-C	-5.87	107.58	115.21
4	Q	67	GLU	N-CA-C	-5.81	106.27	113.19
1	N	58	PHE	N-CA-C	-5.79	105.05	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	44	ASP	N-CA-C	5.79	119.87	112.34
3	C	378	LEU	N-CA-C	-5.79	106.22	113.28
3	P	185	LEU	N-CA-C	5.78	118.70	111.24
1	A	118	GLN	N-CA-C	5.78	117.38	111.14
1	A	179	ARG	N-CA-C	-5.77	104.36	111.75
2	O	197	ASN	N-CA-C	5.73	118.46	111.82
2	B	227	ARG	N-CA-C	5.69	122.92	110.80
3	P	93	ILE	N-CA-C	-5.69	104.32	110.23
3	C	328	LEU	N-CA-C	-5.68	105.00	111.14
3	C	205	GLY	N-CA-C	-5.66	105.48	112.33
2	O	180	ASP	N-CA-C	5.65	117.89	111.11
1	N	332	ASP	N-CA-C	5.64	117.11	111.07
2	O	369	LEU	N-CA-C	5.64	117.43	111.28
3	P	265	THR	CA-C-N	-5.63	115.61	119.66
3	P	265	THR	C-N-CA	-5.63	115.61	119.66
1	A	332	ASP	N-CA-C	5.61	117.07	111.07
3	P	147	ILE	N-CA-C	5.58	115.71	110.30
3	P	167	GLY	N-CA-C	-5.57	106.50	115.08
1	N	272	VAL	N-CA-C	-5.57	105.08	110.42
2	B	180	ASP	N-CA-C	5.55	117.77	111.11
2	B	369	LEU	N-CA-C	5.53	117.31	111.28
3	P	247	SER	CA-C-N	5.52	125.61	119.32
3	P	247	SER	C-N-CA	5.52	125.61	119.32
1	A	256	ALA	N-CA-C	5.51	117.22	108.79
1	A	416	TYR	N-CA-C	5.51	118.56	110.30
4	D	41	HIS	N-CA-C	5.50	117.48	108.52
6	S	32	MET	N-CA-C	-5.50	102.62	110.59
2	B	29	LEU	N-CA-C	5.49	121.95	109.81
1	A	151	ASP	N-CA-C	-5.48	105.22	111.14
2	O	230	ALA	N-CA-C	-5.45	106.63	113.72
8	U	21	ARG	N-CA-C	-5.44	105.43	111.36
3	P	328	LEU	N-CA-C	-5.44	105.43	111.36
2	B	344	LEU	N-CA-C	-5.41	106.81	113.41
4	Q	155	GLY	N-CA-C	-5.41	108.18	115.21
2	B	305	GLN	CA-C-N	5.40	126.59	119.84
2	B	305	GLN	C-N-CA	5.40	126.59	119.84
1	N	35	CYS	N-CA-C	5.36	114.92	107.73
2	B	150	VAL	N-CA-C	-5.35	105.50	110.53
2	O	373	GLU	N-CA-C	-5.35	105.49	112.23
3	C	143	GLY	N-CA-C	-5.32	106.32	112.50
2	O	100	SER	N-CA-C	5.32	117.17	108.76
3	C	21	ASP	N-CA-C	-5.32	106.02	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	132	TRP	N-CA-C	5.32	117.08	108.41
4	D	203	ARG	N-CA-C	-5.31	105.57	111.36
6	F	26	PHE	N-CA-C	-5.30	106.81	113.28
2	B	310	SER	N-CA-C	5.29	116.32	108.86
3	P	378	LEU	N-CA-C	-5.28	106.84	113.28
2	O	264	VAL	N-CA-C	-5.27	102.04	109.63
4	D	67	GLU	N-CA-C	-5.27	106.92	113.19
1	N	27	SER	N-CA-C	5.27	116.53	108.52
4	D	195	GLU	CA-C-N	5.27	126.42	119.84
4	D	195	GLU	C-N-CA	5.27	126.42	119.84
4	Q	57	THR	N-CA-C	-5.26	103.44	110.55
4	Q	91	PHE	CA-C-N	5.26	125.02	119.76
4	Q	91	PHE	C-N-CA	5.26	125.02	119.76
3	C	27	ASN	N-CA-C	5.23	120.31	113.30
7	T	44	GLN	N-CA-C	5.23	118.13	111.69
3	P	27	ASN	N-CA-C	5.23	120.31	113.30
1	N	415	ILE	CB-CA-C	-5.23	105.63	111.80
2	B	223	PHE	N-CA-C	5.22	119.65	113.12
1	A	248	LEU	CA-C-N	5.22	126.36	119.84
1	A	248	LEU	C-N-CA	5.22	126.36	119.84
2	B	100	SER	N-CA-C	5.20	116.97	108.76
1	A	431	LEU	CA-C-N	-5.19	113.36	121.87
1	A	431	LEU	C-N-CA	-5.19	113.36	121.87
7	G	44	GLN	N-CA-C	5.19	118.08	111.69
2	B	129	ALA	N-CA-C	5.19	121.27	109.81
6	F	32	MET	N-CA-C	-5.17	103.09	110.59
2	O	282	GLY	CA-C-N	5.16	126.29	119.84
2	O	282	GLY	C-N-CA	5.16	126.29	119.84
2	B	282	GLY	CA-C-N	5.15	126.28	119.84
2	B	282	GLY	C-N-CA	5.15	126.28	119.84
1	A	348	SER	N-CA-C	5.15	120.32	112.54
3	C	274	TYR	N-CA-C	5.14	119.31	113.19
3	P	266	PRO	CA-C-N	5.14	126.27	119.84
3	P	266	PRO	C-N-CA	5.14	126.27	119.84
6	S	89	TYR	N-CA-C	5.14	117.78	111.82
1	N	419	CYS	N-CA-C	-5.14	102.10	109.24
1	N	256	ALA	N-CA-C	5.14	116.65	108.79
4	D	57	THR	N-CA-C	-5.10	103.66	110.55
3	C	314	ARG	N-CA-C	5.09	116.63	111.14
4	D	80	LEU	N-CA-C	-5.07	103.99	110.53
1	A	331	ILE	CB-CA-C	-5.07	105.39	111.88
2	B	428	GLY	N-CA-C	-5.06	103.80	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	GLN	N-CA-C	5.06	118.23	111.75
1	N	118	GLN	N-CA-C	5.06	116.60	111.14
3	P	365	ILE	N-CA-C	5.05	116.22	111.48
2	B	23	ASP	N-CA-C	5.05	121.55	110.80
6	F	38	TYR	N-CA-C	-5.03	102.83	110.28
3	P	29	SER	N-CA-C	5.03	116.45	109.31
4	Q	178	THR	N-CA-C	-5.03	104.22	110.41
1	A	278	GLY	N-CA-C	5.02	120.41	111.73
2	O	344	LEU	N-CA-C	-5.02	107.29	113.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	20	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3362	200	0
1	N	3437	0	3349	227	0
2	B	3137	0	3131	281	0
2	O	3147	0	3146	270	0
3	C	3017	0	3063	165	0
3	P	3012	0	3058	177	0
4	D	1898	0	1846	100	0
4	Q	1898	0	1846	124	0
5	E	1513	0	1478	129	0
5	R	1509	0	1474	133	0
6	F	891	0	893	37	0
6	S	891	0	893	52	0
7	G	672	0	653	51	0
7	T	662	0	645	47	0
8	H	574	0	548	39	0
8	U	553	0	535	46	0
9	I	287	0	251	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	277	0	251	45	0
10	J	497	0	490	22	0
10	W	479	0	478	29	0
11	C	86	0	60	8	0
11	P	86	0	60	5	0
12	C	25	0	20	4	0
12	P	25	0	20	3	0
13	C	19	0	17	5	0
13	P	19	0	17	2	0
14	C	40	0	24	1	0
14	D	42	0	28	0	0
14	P	40	0	24	2	0
14	Q	42	0	28	2	0
15	C	70	0	85	1	0
15	E	50	0	77	0	0
15	P	54	0	72	2	0
15	R	50	0	77	1	0
16	C	6	0	8	0	0
16	P	6	0	8	2	0
17	D	43	0	30	1	0
17	Q	43	0	30	1	0
18	D	33	0	39	1	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	8	0	0	1	0
20	R	1	0	0	0	0
All	All	32648	0	32164	2020	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 31.

All (2020) 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	1.26	1.14
5:E:127:VAL:HG12	5:E:128:LYS:H	1.15	1.09
2:O:76:THR:HG22	2:O:82:SER:H	1.14	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.36	1.04
2:B:76:THR:HG22	2:B:82:SER:H	1.17	1.03
3:C:125:MET:HE2	12:C:2001:IKR:I1	2.30	1.02
2:O:353:THR:HG22	2:O:355:GLU:H	1.24	1.02
2:B:353:THR:HG22	2:B:355:GLU:H	1.24	1.00
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.26	1.00
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.41	1.00
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.22	0.99
3:P:40:VAL:HA	3:P:43:MET:HE3	1.44	0.99
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.45	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.26	0.97
1:N:102:LEU:H	1:N:102:LEU:HD12	1.31	0.95
2:B:270:ASN:HD22	2:B:270:ASN:H	1.01	0.94
7:G:41:PHE:O	7:G:45:VAL:HG23	1.68	0.94
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.47	0.94
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.33	0.93
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.50	0.93
1:A:102:LEU:HD12	1:A:102:LEU:H	1.33	0.93
7:T:41:PHE:O	7:T:45:VAL:HG23	1.69	0.93
3:P:125:MET:HE2	12:P:3001:IKR:I1	2.39	0.92
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.32	0.92
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.52	0.92
1:A:178:THR:HG22	1:A:180:ALA:H	1.31	0.92
4:D:57:THR:HG22	4:D:59:ALA:H	1.34	0.91
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.52	0.91
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.06	0.90
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.52	0.90
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.53	0.90
2:O:76:THR:CG2	2:O:82:SER:H	1.85	0.90
2:B:76:THR:CG2	2:B:82:SER:H	1.85	0.89
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.03	0.89
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.73	0.89
1:N:170:THR:HG22	1:N:171:THR:H	1.37	0.89
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.55	0.88
4:D:2:GLU:HB3	7:G:70:LYS:HE2	1.54	0.88
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.22	0.88
5:R:118:ARG:O	5:R:120:PRO:HD3	1.74	0.87
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.38	0.87
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.74	0.86
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.56	0.86
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.57	0.85
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.56	0.85
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.93	0.84
6:F:32:MET:CE	6:F:87:LYS:HG2	2.07	0.84
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.59	0.84
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.60	0.83
5:E:83:GLU:HG2	5:E:102:THR:HA	1.59	0.83
4:D:231:LYS:O	6:F:71:LYS:HE3	1.78	0.83
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.13	0.83
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.59	0.83
4:D:47:ALA:H	4:D:50:ASN:HD22	1.22	0.82
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.79	0.82
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.79	0.82
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.45	0.82
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.44	0.82
3:C:125:MET:CE	12:C:2001:IKR:I1	2.97	0.82
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.62	0.81
9:I:64:LEU:HD12	9:I:77:ARG:C	2.05	0.81
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.46	0.81
8:U:32:LYS:O	8:U:36:ARG:HG3	1.79	0.81
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.15	0.81
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.46	0.81
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.47	0.80
2:O:150:VAL:O	2:O:153:GLN:HG3	1.81	0.80
4:D:164:ILE:O	4:D:179:MET:HE2	1.82	0.80
2:O:248:ASN:C	2:O:248:ASN:HD22	1.89	0.80
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.46	0.80
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.63	0.80
5:E:127:VAL:HG12	5:E:128:LYS:N	1.96	0.80
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.65	0.79
2:B:150:VAL:O	2:B:153:GLN:HG3	1.81	0.79
2:O:76:THR:HG22	2:O:82:SER:N	1.94	0.79
5:R:112:VAL:HG21	5:R:170:ARG:NH2	1.97	0.79
2:O:324:PHE:HE2	2:O:341:MET:HE3	1.48	0.79
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.63	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.63	0.78
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.83	0.78
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.65	0.78
5:R:117:LEU:HD11	5:R:172:ARG:NH1	1.98	0.78
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ASP:O	1:N:109:VAL:HG23	1.84	0.78
2:O:207:VAL:HG12	2:O:208:GLY:H	1.49	0.78
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.66	0.78
2:O:222:GLN:O	2:O:222:GLN:HG2	1.84	0.78
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.64	0.77
2:O:62:ASN:O	2:O:65:THR:HG22	1.84	0.77
2:B:207:VAL:HG12	2:B:208:GLY:H	1.49	0.77
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.63	0.77
2:B:57:TYR:HE2	2:B:203:ARG:HH22	1.29	0.77
2:B:76:THR:HG22	2:B:82:SER:N	1.96	0.77
5:E:78:LEU:HD12	5:E:190:ASP:O	1.85	0.77
1:A:112:LEU:O	1:A:116:VAL:HG23	1.84	0.77
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.66	0.77
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.50	0.77
3:C:120:LEU:HD13	11:C:502:HEM:HAB	1.65	0.76
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.50	0.76
1:N:182:LEU:O	1:N:186:ILE:HG13	1.86	0.76
8:U:43:ARG:HD2	8:U:47:ARG:NH2	1.99	0.76
1:A:170:THR:HG22	1:A:171:THR:H	1.49	0.76
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.67	0.76
1:A:50:GLU:HB2	1:A:165:ARG:NH2	2.00	0.76
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.68	0.76
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.21	0.76
6:F:59:MET:HA	6:F:59:MET:HE3	1.68	0.76
2:O:57:TYR:HE2	2:O:203:ARG:HH22	1.32	0.76
2:O:192:HIS:O	2:O:196:GLN:HG3	1.85	0.76
3:P:125:MET:CE	12:P:3001:IKR:I1	3.04	0.76
3:P:9:HIS:O	3:P:13:LYS:HB3	1.86	0.75
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.47	0.75
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.66	0.75
2:O:283:PRO:HG2	9:V:56:SER:HB2	1.67	0.75
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.02	0.75
2:B:270:ASN:H	2:B:270:ASN:ND2	1.78	0.75
1:N:170:THR:HG22	1:N:171:THR:N	2.01	0.75
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.22	0.75
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.69	0.75
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.69	0.75
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.68	0.75
7:G:81:GLN:HA	8:H:47:ARG:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:221:GLU:HG3	2:O:222:GLN:H	1.52	0.74
9:I:70:LEU:HD23	9:I:71:ASN:N	2.02	0.74
3:P:138:GLN:HB2	3:P:255:GLU:O	1.87	0.74
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.53	0.74
1:N:35:CYS:HA	1:N:372:THR:HG21	1.69	0.74
2:O:397:VAL:O	2:O:401:LYS:HG2	1.87	0.74
3:P:101:ARG:HD2	3:P:101:ARG:C	2.12	0.74
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.52	0.74
2:B:169:LYS:O	2:B:170:THR:HG23	1.87	0.74
6:F:107:TRP:O	6:F:110:LYS:HB3	1.88	0.74
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.69	0.74
10:W:57:HIS:HA	10:W:60:GLU:HG2	1.69	0.74
2:B:248:ASN:C	2:B:248:ASN:HD22	1.94	0.73
1:A:182:LEU:O	1:A:186:ILE:HG13	1.88	0.73
3:C:22:LEU:HD21	13:C:2002:UQ:HM32	1.68	0.73
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.70	0.73
1:A:206:LYS:O	1:A:209:VAL:HG12	1.88	0.73
2:B:270:ASN:HD22	2:B:270:ASN:N	1.82	0.73
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.71	0.73
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.22	0.73
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.73
2:O:47:ILE:HD13	2:O:120:MET:CE	2.19	0.73
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.19	0.73
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.71	0.73
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.24	0.73
7:G:65:GLU:O	7:G:69:LEU:HG	1.87	0.73
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.69	0.73
7:T:29:ILE:O	7:T:33:ALA:HB3	1.88	0.73
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.70	0.72
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.70	0.72
3:C:9:HIS:O	3:C:13:LYS:HB3	1.89	0.72
3:C:377:MET:HE2	6:F:20:TYR:CG	2.24	0.72
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.54	0.72
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.14	0.72
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.71	0.72
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.04	0.72
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.03	0.72
3:C:50:LEU:O	3:C:54:MET:HG3	1.90	0.72
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.55	0.72
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.05	0.72
1:N:206:LYS:O	1:N:209:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:112:LEU:O	1:N:116:VAL:HG23	1.89	0.72
6:F:32:MET:HE3	6:F:87:LYS:CG	2.19	0.72
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.25	0.72
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.25	0.71
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.55	0.71
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.72	0.71
9:V:64:LEU:HD12	9:V:77:ARG:C	2.15	0.71
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.58	0.71
2:B:306:PRO:HA	9:I:52:ARG:CG	2.19	0.71
5:E:106:ILE:O	5:E:110:ALA:HB3	1.90	0.71
7:G:80:ASP:HB3	8:H:50:THR:HA	1.72	0.71
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.71	0.71
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.90	0.71
14:P:3004:CDL:OA4	7:T:40:ARG:HD2	1.89	0.71
15:C:2007:PEE:H7	7:G:44:GLN:HE21	1.54	0.71
7:G:29:ILE:O	7:G:33:ALA:HB3	1.91	0.71
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.56	0.71
6:S:13:MET:HA	6:S:16:ILE:HB	1.72	0.71
2:B:47:ILE:HD13	2:B:120:MET:CE	2.21	0.71
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.73	0.71
3:C:101:ARG:HD2	3:C:101:ARG:C	2.15	0.71
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.06	0.71
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.73	0.71
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.05	0.71
4:Q:164:ILE:O	4:Q:179:MET:HE2	1.92	0.70
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.74	0.70
5:R:120:PRO:O	5:R:121:GLN:HG3	1.90	0.70
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.57	0.70
2:O:422:LYS:O	2:O:436:LEU:HD21	1.91	0.70
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.26	0.70
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.73	0.70
5:R:112:VAL:HG21	5:R:170:ARG:HH22	1.54	0.70
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.54	0.70
3:P:245:LEU:O	4:Q:201:ARG:HD3	1.91	0.70
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.73	0.70
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.57	0.70
4:Q:222:MET:HE3	5:R:40:THR:OG1	1.92	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.22	0.70
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.72	0.70
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.21	0.70
5:R:77:LYS:HA	5:R:191:ASP:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.26	0.69
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.25	0.69
3:P:238:THR:HB	3:P:239:PRO:HD3	1.74	0.69
1:A:178:THR:HB	1:A:181:ASP:OD1	1.92	0.69
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.73	0.69
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.59	0.69
2:B:264:VAL:HG23	2:B:316:TYR:C	2.18	0.69
2:B:397:VAL:O	2:B:401:LYS:HG2	1.91	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.73	0.69
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.07	0.69
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.75	0.69
4:D:47:ALA:H	4:D:50:ASN:ND2	1.90	0.69
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.75	0.69
1:N:50:GLU:HB2	1:N:165:ARG:NH2	2.08	0.69
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.08	0.69
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.27	0.69
2:O:238:THR:HG22	2:O:239:TYR:N	2.09	0.68
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.56	0.68
5:E:106:ILE:C	5:E:110:ALA:HB3	2.19	0.68
5:E:190:ASP:C	5:E:192:LEU:H	2.00	0.68
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.58	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
2:O:248:ASN:ND2	2:O:250:HIS:H	1.92	0.68
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.58	0.68
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.22	0.68
2:O:96:LEU:HB3	9:V:70:LEU:HD22	1.76	0.68
2:O:154:SER:O	2:O:157:VAL:HG12	1.94	0.68
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.27	0.68
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.28	0.68
2:B:238:THR:HG22	2:B:239:TYR:H	1.59	0.68
1:A:170:THR:HG22	1:A:171:THR:N	2.08	0.68
3:P:40:VAL:CA	3:P:43:MET:HE3	2.22	0.68
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.59	0.67
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.24	0.67
6:S:95:LYS:O	6:S:99:ARG:HG3	1.95	0.67
1:A:50:GLU:HB2	1:A:165:ARG:HH21	1.56	0.67
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.23	0.67
2:O:27:THR:HG22	2:O:28:LYS:N	2.09	0.67
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.76	0.67
15:P:3007:PEE:H7	7:T:44:GLN:HE21	1.59	0.67
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:GLN:HB2	3:C:255:GLU:O	1.95	0.67
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.76	0.67
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.29	0.67
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.77	0.67
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.30	0.67
5:R:117:LEU:HD11	5:R:172:ARG:HH11	1.58	0.67
3:P:50:LEU:O	3:P:54:MET:HG3	1.96	0.66
5:R:177:PRO:HG2	5:R:178:TYR:H	1.59	0.66
10:J:38:GLY:O	10:J:42:ILE:HG13	1.95	0.66
2:O:361:LYS:O	2:O:365:LYS:HG3	1.94	0.66
10:W:49:GLY:N	10:W:54:HIS:ND1	2.44	0.66
2:B:374:THR:HG22	2:B:376:GLN:H	1.61	0.66
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.30	0.66
8:U:27:THR:O	8:U:31:VAL:HG23	1.96	0.66
4:D:57:THR:HG22	4:D:59:ALA:N	2.10	0.66
3:P:49:GLY:C	11:P:501:HEM:HAC	2.21	0.66
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.77	0.66
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.78	0.66
7:T:65:GLU:O	7:T:69:LEU:HG	1.95	0.66
2:O:169:LYS:O	2:O:170:THR:HG23	1.96	0.66
7:T:77:TYR:C	7:T:79:ASN:H	2.04	0.66
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.13	0.66
3:C:238:THR:HB	3:C:239:PRO:HD3	1.78	0.66
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.31	0.66
2:O:31:ASN:HD22	2:O:31:ASN:N	1.93	0.66
2:B:283:PRO:HG2	9:I:56:SER:HB2	1.77	0.65
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.76	0.65
2:O:325:TYR:HD1	9:V:60:ALA:CB	2.09	0.65
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.79	0.65
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.61	0.65
5:E:165:TYR:HA	5:E:170:ARG:O	1.96	0.65
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.78	0.65
2:O:238:THR:HG22	2:O:239:TYR:H	1.60	0.65
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.77	0.65
10:J:49:GLY:N	10:J:54:HIS:ND1	2.45	0.65
2:O:166:ALA:HB1	2:O:242:GLY:O	1.97	0.65
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.10	0.65
1:A:35:CYS:HA	1:A:372:THR:HG21	1.77	0.65
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.32	0.65
1:N:371:GLY:O	1:N:375:VAL:HG23	1.95	0.65
5:E:116:LYS:H	5:E:116:LYS:HD2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.79	0.65
3:P:173:ASN:N	3:P:174:PRO:HD2	2.12	0.65
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.11	0.64
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.61	0.64
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.33	0.64
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.80	0.64
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.77	0.64
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.31	0.64
2:B:238:THR:HG22	2:B:239:TYR:N	2.11	0.64
3:C:173:ASN:N	3:C:174:PRO:HD2	2.12	0.64
9:I:71:ASN:HD22	9:I:71:ASN:H	1.44	0.64
2:B:325:TYR:HD1	9:I:60:ALA:HB3	1.61	0.64
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.79	0.64
1:A:117:VAL:HG23	1:A:118:GLN:N	2.12	0.64
2:B:192:HIS:O	2:B:196:GLN:HG3	1.98	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.97	0.64
10:W:38:GLY:O	10:W:42:ILE:HG13	1.97	0.64
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.32	0.64
5:E:69:LEU:O	5:E:72:SER:HB3	1.97	0.64
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.97	0.64
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.79	0.64
1:N:178:THR:HB	1:N:181:ASP:OD1	1.98	0.64
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.21	0.64
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.80	0.64
4:D:102:ARG:NH1	4:D:107:GLY:O	2.31	0.64
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.28	0.64
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.79	0.64
2:O:402:ILE:HD13	2:O:402:ILE:C	2.23	0.64
1:N:49:ASN:ND2	1:N:51:LYS:H	1.95	0.63
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.63	0.63
2:O:325:TYR:HD2	2:O:326:THR:N	1.96	0.63
6:S:59:MET:HA	6:S:59:MET:HE3	1.78	0.63
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.26	0.63
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.63	0.63
1:N:332:ASP:HB2	1:N:430:GLN:HG2	1.81	0.63
2:O:56:ARG:HA	2:O:171:ALA:O	1.97	0.63
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.81	0.63
2:B:295:LEU:O	2:B:299:VAL:HG23	1.98	0.63
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.27	0.63
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.28	0.63
5:E:96:LEU:HD12	5:E:135:LEU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.13	0.63
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.80	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.32	0.63
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.64	0.63
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.61	0.63
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.34	0.63
1:A:249:PRO:HG2	1:A:250:VAL:H	1.64	0.63
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.33	0.63
2:B:422:LYS:O	2:B:436:LEU:HD21	1.97	0.63
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.64	0.63
2:O:56:ARG:HH11	2:O:56:ARG:HG3	1.64	0.63
2:O:359:LYS:O	2:O:363:GLN:HG3	1.99	0.63
2:B:57:TYR:CD1	2:B:57:TYR:N	2.67	0.63
1:N:161:THR:HG21	1:N:235:ARG:H	1.62	0.63
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.34	0.62
2:O:399:ALA:O	2:O:402:ILE:HG22	1.99	0.62
9:I:32:UNK:N	9:I:73:PRO:HG2	2.14	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.34	0.62
5:E:187:PHE:C	5:E:189:GLY:H	2.07	0.62
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.81	0.62
2:B:166:ALA:HB1	2:B:242:GLY:O	1.99	0.62
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.81	0.62
9:V:70:LEU:HD23	9:V:71:ASN:N	2.13	0.62
3:C:377:MET:HE2	6:F:20:TYR:CB	2.30	0.62
2:O:417:PHE:O	2:O:422:LYS:HE3	1.99	0.62
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.81	0.62
1:N:249:PRO:HG2	1:N:250:VAL:H	1.62	0.62
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.64	0.62
8:H:40:CYS:O	8:H:44:VAL:HG23	2.00	0.62
3:P:67:VAL:HG12	16:P:3011:GOL:H31	1.82	0.62
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.35	0.62
5:R:96:LEU:HD12	5:R:135:LEU:O	2.00	0.62
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.81	0.62
2:B:417:PHE:O	2:B:422:LYS:HE3	1.99	0.61
2:O:424:MET:HG2	2:O:425:ALA:N	2.15	0.61
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.22	0.61
2:B:21:ALA:O	2:B:22:GLU:HB2	1.99	0.61
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.82	0.61
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.30	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.35	0.61
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:165:TYR:HA	5:R:170:ARG:O	2.00	0.61
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.61
2:O:219:VAL:O	2:O:223:PHE:HB2	1.99	0.61
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.00	0.61
1:A:191:LYS:O	1:A:195:MET:HG3	1.99	0.61
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.83	0.61
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.15	0.61
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.65	0.61
3:P:70:THR:HA	3:P:74:VAL:HG23	1.82	0.61
5:R:129:LYS:HB3	5:R:131:GLU:OE1	1.99	0.61
3:C:347:PRO:O	3:C:350:ILE:HG22	2.01	0.61
14:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.01	0.61
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.40	0.61
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.30	0.61
2:O:374:THR:HG22	2:O:376:GLN:H	1.65	0.61
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.66	0.61
2:O:338:ARG:HG3	2:O:338:ARG:NH1	2.16	0.61
5:R:69:LEU:O	5:R:72:SER:HB3	2.00	0.61
3:P:199:THR:HA	18:P:2010:BOG:O1	2.01	0.61
3:C:127:THR:HG21	11:C:501:HEM:HBB2	1.82	0.61
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.83	0.61
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.83	0.61
2:O:325:TYR:HD1	9:V:60:ALA:HB3	1.64	0.61
1:A:178:THR:HG22	1:A:179:ARG:N	2.14	0.60
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.36	0.60
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.16	0.60
1:N:307:PHE:CD1	1:N:307:PHE:C	2.78	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.36	0.60
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.83	0.60
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.82	0.60
3:P:9:HIS:HD2	3:P:12:LEU:H	1.49	0.60
9:V:59:SER:O	9:V:60:ALA:C	2.43	0.60
5:R:148:ALA:HB2	5:R:156:TYR:CD2	2.36	0.60
2:B:292:THR:O	2:B:292:THR:HG22	2.02	0.60
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.84	0.60
5:E:131:GLU:H	5:E:131:GLU:CD	2.09	0.60
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.37	0.60
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.84	0.60
2:B:399:ALA:O	2:B:402:ILE:HG22	2.01	0.60
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.36	0.60
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:TYR:HD2	2:B:326:THR:N	1.99	0.60
2:O:295:LEU:O	2:O:299:VAL:HG23	2.02	0.60
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.16	0.60
1:A:406:MET:O	1:A:410:VAL:HG23	2.01	0.60
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.82	0.60
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.37	0.60
2:B:201:SER:OG	2:B:228:SER:HA	2.00	0.60
3:C:377:MET:CE	6:F:20:TYR:HB2	2.32	0.60
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.67	0.60
1:A:106:MET:C	1:A:106:MET:HE2	2.26	0.59
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.28	0.59
8:H:18:THR:O	8:H:22:GLU:HG3	2.02	0.59
2:B:31:ASN:HD22	2:B:31:ASN:N	2.00	0.59
3:C:49:GLY:C	11:C:501:HEM:HAC	2.26	0.59
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.02	0.59
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.84	0.59
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.36	0.59
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.67	0.59
9:V:30:UNK:HG3	9:V:31:UNK:N	2.17	0.59
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.33	0.59
5:E:52:LYS:C	5:E:52:LYS:HD3	2.27	0.59
8:H:27:THR:HG22	8:H:29:LYS:H	1.68	0.59
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.41	0.59
1:N:178:THR:HG22	1:N:179:ARG:N	2.17	0.59
3:P:377:MET:HE2	6:S:20:TYR:CG	2.37	0.59
8:U:62:LEU:O	8:U:66:ASP:HB2	2.02	0.59
1:A:156:THR:HA	5:E:7:VAL:HG21	1.84	0.59
1:A:371:GLY:O	1:A:375:VAL:HG23	2.02	0.59
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.67	0.59
1:A:332:ASP:HB2	1:A:430:GLN:HG2	1.83	0.59
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.37	0.59
3:P:22:LEU:HD21	13:P:3002:UQ:HM32	1.84	0.59
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.28	0.59
2:B:140:LEU:C	2:B:142:PRO:HD2	2.28	0.59
2:B:248:ASN:ND2	2:B:250:HIS:H	2.01	0.59
2:B:402:ILE:HD13	2:B:402:ILE:C	2.27	0.59
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.36	0.59
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.17	0.59
2:B:424:MET:HG2	2:B:425:ALA:N	2.17	0.59
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.33	0.59
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:32:MET:HE3	6:S:87:LYS:HB2	1.84	0.59
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.50	0.59
3:C:9:HIS:HD2	3:C:12:LEU:H	1.50	0.59
1:N:317:THR:HG23	1:N:318:GLY:N	2.18	0.59
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.03	0.59
5:R:187:PHE:O	5:R:188:VAL:HG13	2.03	0.59
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.67	0.59
2:O:248:ASN:HD22	2:O:249:GLY:N	2.00	0.59
10:W:14:PHE:N	10:W:14:PHE:CD2	2.69	0.59
2:B:97:SER:HB3	9:I:69:SER:HA	1.85	0.58
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.38	0.58
2:O:239:TYR:HE2	2:O:241:GLY:CA	2.16	0.58
1:A:64:PHE:HA	1:A:75:PHE:HE2	1.68	0.58
2:B:327:ILE:HD11	9:I:58:ARG:O	2.04	0.58
2:O:71:LEU:O	2:O:74:PRO:HD2	2.02	0.58
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.03	0.58
5:R:82:PRO:O	5:R:100:HIS:HB3	2.03	0.58
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.84	0.58
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.18	0.58
3:P:31:TRP:O	3:P:101:ARG:HG3	2.03	0.58
3:C:245:LEU:O	4:D:201:ARG:HD3	2.03	0.58
9:I:63:ASP:CG	9:I:64:LEU:H	2.12	0.58
1:N:406:MET:O	1:N:410:VAL:HG23	2.03	0.58
1:N:439:SER:HA	1:N:442:TYR:CE2	2.38	0.58
8:U:28:GLU:O	8:U:32:LYS:HG3	2.04	0.58
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.32	0.58
1:A:362:ARG:O	1:A:365:MET:HG2	2.03	0.58
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.86	0.58
4:D:37:CYS:C	4:D:39:ALA:H	2.09	0.58
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.33	0.58
8:H:27:THR:O	8:H:31:VAL:HG23	2.02	0.58
2:O:207:VAL:HG12	2:O:208:GLY:N	2.18	0.58
1:A:106:MET:HE2	1:A:106:MET:O	2.04	0.58
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.85	0.58
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.18	0.58
2:B:207:VAL:HG12	2:B:208:GLY:N	2.18	0.58
1:A:307:PHE:CD1	1:A:307:PHE:C	2.81	0.58
2:B:262:ALA:O	2:B:320:GLY:HA3	2.03	0.58
4:Q:24:SER:OG	10:W:55:ILE:HG21	2.04	0.58
5:E:102:THR:HB	5:E:103:GLN:OE1	2.03	0.58
1:N:38:GLY:HA3	1:N:98:TYR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:140:LEU:C	2:O:142:PRO:HD2	2.29	0.58
3:P:142:TRP:O	3:P:146:VAL:HG23	2.03	0.58
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.39	0.58
1:N:106:MET:HE2	1:N:106:MET:C	2.29	0.58
2:O:292:THR:O	2:O:292:THR:HG22	2.02	0.58
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.38	0.58
10:W:56:LYS:HG2	10:W:60:GLU:OE1	2.03	0.58
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.85	0.57
3:P:127:THR:HG21	11:P:501:HEM:HBB2	1.85	0.57
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.85	0.57
8:U:40:CYS:O	8:U:44:VAL:HG23	2.03	0.57
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.69	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.85	0.57
2:B:26:ILE:HG12	2:B:26:ILE:O	2.03	0.57
8:H:34:ARG:HD2	8:H:38:GLU:OE2	2.05	0.57
9:I:31:UNK:C	9:I:73:PRO:HG2	2.33	0.57
1:N:342:TRP:O	1:N:345:LEU:HB2	2.03	0.57
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.70	0.57
3:P:145:THR:O	3:P:149:ASN:HB2	2.04	0.57
4:Q:147:LEU:C	4:Q:148:HIS:HD2	2.13	0.57
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.67	0.57
2:B:407:SER:O	2:B:411:VAL:HG23	2.04	0.57
5:E:29:SER:HA	5:E:32:ARG:NH2	2.19	0.57
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.35	0.57
1:N:117:VAL:HG23	1:N:118:GLN:N	2.20	0.57
5:R:52:LYS:C	5:R:52:LYS:HD3	2.30	0.57
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.87	0.57
5:E:136:VAL:O	5:E:138:VAL:N	2.36	0.57
2:O:248:ASN:C	2:O:248:ASN:ND2	2.59	0.57
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.87	0.57
1:A:105:ASP:O	1:A:109:VAL:HG23	2.04	0.57
2:B:259:THR:HG22	2:B:260:GLU:N	2.19	0.57
8:H:10:GLU:O	8:H:11:GLU:HG3	2.04	0.57
1:N:50:GLU:HB2	1:N:165:ARG:HH21	1.67	0.57
2:O:57:TYR:N	2:O:57:TYR:CD1	2.73	0.57
2:O:97:SER:HB3	9:V:69:SER:HA	1.85	0.57
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.40	0.57
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.33	0.57
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.69	0.57
2:B:46:ARG:HG3	2:B:379:LEU:HD22	1.87	0.57
3:C:162:VAL:C	3:C:164:TRP:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.40	0.57
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.86	0.57
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.40	0.57
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.40	0.57
5:R:29:SER:HA	5:R:32:ARG:NH2	2.19	0.57
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.20	0.57
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.19	0.57
3:P:287:ASN:O	3:P:288:LYS:C	2.46	0.57
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.53	0.57
7:T:80:ASP:HB3	8:U:47:ARG:NH1	2.14	0.57
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.34	0.56
3:C:287:ASN:O	3:C:288:LYS:C	2.48	0.56
5:R:118:ARG:NH2	5:R:174:GLY:O	2.38	0.56
2:B:71:LEU:O	2:B:74:PRO:HD2	2.05	0.56
2:B:76:THR:HG22	2:B:81:SER:HA	1.87	0.56
4:D:71:GLN:HG3	4:D:82:MET:HE1	1.86	0.56
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.31	0.56
8:H:62:LEU:O	8:H:66:ASP:HB2	2.05	0.56
3:P:236:MET:O	3:P:239:PRO:HD2	2.05	0.56
3:P:347:PRO:O	3:P:350:ILE:HG22	2.04	0.56
5:R:78:LEU:HB3	5:R:132:TRP:HZ2	1.65	0.56
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.40	0.56
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.86	0.56
2:B:239:TYR:HE2	2:B:241:GLY:CA	2.18	0.56
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.88	0.56
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.88	0.56
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.87	0.56
3:C:70:THR:HA	3:C:74:VAL:HG23	1.87	0.56
3:C:329:LEU:O	3:C:332:ASN:HB3	2.05	0.56
7:G:81:GLN:HA	8:H:47:ARG:CG	2.34	0.56
2:O:156:GLN:NE2	9:V:77:ARG:C	2.63	0.56
3:P:329:LEU:O	3:P:332:ASN:HB3	2.04	0.56
8:U:18:THR:O	8:U:22:GLU:HG3	2.04	0.56
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.87	0.56
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.71	0.56
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.88	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
3:C:247:SER:OG	3:C:250:LEU:HB2	2.06	0.56
1:A:137:GLU:O	1:A:141:MET:HG3	2.05	0.56
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.40	0.56
3:C:246:PHE:C	3:C:248:PRO:HD3	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:136:VAL:O	5:R:138:VAL:N	2.38	0.56
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.41	0.56
3:P:246:PHE:C	3:P:248:PRO:HD3	2.31	0.56
10:W:60:GLU:O	10:W:61:ALA:HB2	2.06	0.56
3:C:350:ILE:HG23	3:C:351:ILE:N	2.21	0.56
5:E:178:TYR:H	5:E:178:TYR:HD1	1.54	0.56
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.05	0.56
10:W:40:ASP:O	10:W:44:GLU:HG3	2.05	0.56
2:B:341:MET:HE2	2:B:341:MET:HA	1.88	0.56
3:C:222:HIS:HA	3:C:226:SER:OG	2.06	0.56
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.20	0.56
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.40	0.56
1:N:137:GLU:O	1:N:141:MET:HG3	2.06	0.56
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.88	0.56
2:O:357:VAL:O	2:O:361:LYS:HG3	2.06	0.56
2:O:414:ALA:O	2:O:418:VAL:HG23	2.06	0.56
2:B:23:ASP:OD1	2:B:24:LEU:N	2.39	0.56
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.21	0.56
1:N:64:PHE:HA	1:N:75:PHE:HE2	1.71	0.56
1:N:170:THR:CG2	1:N:171:THR:H	2.15	0.56
2:O:27:THR:CG2	2:O:28:LYS:N	2.69	0.56
3:P:61:SER:O	3:P:62:LEU:HD23	2.06	0.56
6:S:32:MET:HE3	6:S:87:LYS:H	1.69	0.56
6:S:100:GLU:O	6:S:103:GLU:HB3	2.05	0.56
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.41	0.55
2:O:407:SER:O	2:O:411:VAL:HG23	2.06	0.55
5:R:29:SER:HA	5:R:32:ARG:HH21	1.71	0.55
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.22	0.55
6:S:58:ARG:HG3	6:S:89:TYR:OH	2.06	0.55
2:B:306:PRO:HB3	9:I:52:ARG:N	2.21	0.55
6:F:104:ARG:HA	2:O:83:PHE:CE2	2.41	0.55
1:N:281:ASP:OD2	9:V:33:UNK:HB1	2.07	0.55
4:Q:71:GLN:HG3	4:Q:82:MET:HE1	1.88	0.55
8:U:21:ARG:HH11	8:U:21:ARG:HG3	1.71	0.55
1:A:327:ASP:HB3	1:A:328:PRO:HD2	1.87	0.55
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.89	0.55
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.88	0.55
5:E:133:VAL:O	5:E:133:VAL:HG13	2.06	0.55
3:P:198:LEU:HD21	11:P:502:HEM:HMA3	1.88	0.55
3:P:247:SER:OG	3:P:250:LEU:HB2	2.07	0.55
4:D:62:LYS:O	4:D:66:GLU:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.06	0.55
1:N:87:ASN:CG	1:N:88:GLY:H	2.14	0.55
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.21	0.55
2:O:325:TYR:CD1	9:V:60:ALA:N	2.75	0.55
6:S:12:LEU:C	6:S:14:ASP:H	2.12	0.55
1:A:49:ASN:ND2	1:A:51:LYS:H	2.05	0.55
1:A:117:VAL:HG23	1:A:118:GLN:H	1.70	0.55
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.89	0.55
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.41	0.55
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.42	0.55
2:O:306:PRO:CG	9:V:51:CYS:HA	2.37	0.55
2:O:308:ASP:CG	9:V:56:SER:HA	2.31	0.55
3:P:162:VAL:C	3:P:164:TRP:H	2.14	0.55
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.42	0.55
4:D:223:LYS:C	4:D:223:LYS:HD3	2.32	0.55
5:E:147:ILE:O	5:E:156:TYR:HA	2.06	0.55
4:Q:197:GLU:O	4:Q:198:HIS:C	2.50	0.55
4:D:197:GLU:O	4:D:198:HIS:C	2.50	0.55
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.37	0.55
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.07	0.55
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.89	0.55
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.88	0.55
4:Q:211:ILE:HG12	10:W:35:PHE:CZ	2.42	0.55
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.37	0.55
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.14	0.55
3:C:236:MET:O	3:C:239:PRO:HD2	2.06	0.55
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.89	0.55
8:U:43:ARG:O	8:U:47:ARG:HG3	2.06	0.55
4:D:97:ASN:HB2	4:D:99:GLU:OE1	2.06	0.55
4:D:222:MET:HE1	5:E:40:THR:HG23	1.89	0.55
2:O:259:THR:HG22	2:O:260:GLU:N	2.20	0.55
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.37	0.55
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.07	0.55
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.07	0.55
7:T:29:ILE:O	7:T:34:LEU:HG	2.07	0.55
1:A:40:TRP:CZ3	1:A:198:ALA:HB3	2.43	0.55
1:A:178:THR:CG2	1:A:179:ARG:N	2.69	0.55
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.07	0.55
2:O:56:ARG:NH1	2:O:56:ARG:HG3	2.22	0.55
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.72	0.55
1:A:281:ASP:OD2	1:A:284:PHE:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:VAL:O	2:B:361:LYS:HG3	2.06	0.54
8:H:28:GLU:O	8:H:32:LYS:HG3	2.07	0.54
10:J:14:PHE:CD2	10:J:14:PHE:N	2.71	0.54
1:N:63:ALA:O	1:N:116:VAL:HG13	2.07	0.54
5:R:133:VAL:O	5:R:133:VAL:HG13	2.07	0.54
2:B:28:LYS:O	2:B:29:LEU:O	2.25	0.54
13:C:2002:UQ:H8	13:C:2002:UQ:HM51	1.90	0.54
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.89	0.54
1:N:61:HIS:NE2	2:O:287:ARG:NE	2.55	0.54
3:P:222:HIS:HA	3:P:226:SER:OG	2.06	0.54
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.39	0.54
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.47	0.54
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.71	0.54
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.42	0.54
5:E:127:VAL:CG1	5:E:128:LYS:H	1.99	0.54
7:G:59:TYR:O	7:G:63:THR:HB	2.07	0.54
1:N:58:PHE:HB3	1:N:182:LEU:HD21	1.88	0.54
2:O:402:ILE:HD13	2:O:402:ILE:O	2.06	0.54
4:D:65:ALA:O	4:D:85:GLY:HA3	2.07	0.54
5:E:155:GLY:HA3	5:E:166:ASP:O	2.08	0.54
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.71	0.54
1:N:417:ASP:O	1:N:438:ARG:NH2	2.40	0.54
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.88	0.54
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.23	0.54
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.72	0.54
5:E:109:GLU:HB2	5:E:167:ALA:HB3	1.89	0.54
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.90	0.54
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.88	0.54
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.89	0.54
2:O:181:TYR:CE1	2:O:182:ARG:CG	2.90	0.54
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.90	0.54
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.32	0.54
3:C:120:LEU:HD13	11:C:502:HEM:CAB	2.35	0.54
3:C:142:TRP:O	3:C:146:VAL:HG23	2.08	0.54
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.56	0.54
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.08	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.89	0.54
1:N:178:THR:CG2	1:N:179:ARG:N	2.70	0.54
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.23	0.54
2:B:248:ASN:C	2:B:248:ASN:ND2	2.62	0.54
8:H:35:GLU:O	8:H:39:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:162:ASN:O	2:O:244:ILE:HD12	2.08	0.54
3:P:23:PRO:HG3	7:T:4:PHE:CD1	2.43	0.54
3:P:155:PRO:O	3:P:156:TYR:HB2	2.08	0.54
5:R:141:HIS:HB3	19:R:501:FES:S2	2.48	0.54
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.22	0.54
2:B:365:LYS:O	2:B:369:LEU:HG	2.08	0.54
3:C:332:ASN:ND2	3:C:358:SER:OG	2.41	0.54
1:N:362:ARG:O	1:N:365:MET:HG2	2.07	0.54
5:R:178:TYR:N	5:R:178:TYR:CD1	2.75	0.54
8:U:27:THR:HG22	8:U:29:LYS:H	1.73	0.54
1:A:342:TRP:O	1:A:345:LEU:HB2	2.08	0.54
5:E:130:PRO:HG2	5:E:131:GLU:H	1.73	0.54
2:O:105:MET:HE2	2:O:107:TYR:HE1	1.73	0.54
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.43	0.54
4:Q:235:MET:HE2	6:S:64:ARG:HA	1.89	0.54
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.72	0.54
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.89	0.54
1:A:242:ARG:O	7:G:14:ILE:HA	2.07	0.53
2:B:31:ASN:N	2:B:31:ASN:ND2	2.54	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.22	0.53
9:I:63:ASP:O	9:I:64:LEU:HB2	2.07	0.53
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.38	0.53
3:P:377:MET:HE2	6:S:20:TYR:CB	2.38	0.53
2:B:312:PHE:HE1	9:I:62:ARG:O	1.91	0.53
3:C:172:ASP:C	3:C:174:PRO:HD2	2.32	0.53
4:D:222:MET:CE	5:E:40:THR:HG23	2.38	0.53
9:I:49:LEU:O	9:I:50:LEU:HD23	2.09	0.53
9:I:55:MET:O	9:I:58:ARG:HB2	2.07	0.53
2:O:46:ARG:HG3	2:O:46:ARG:O	2.07	0.53
5:R:148:ALA:O	5:R:149:ASN:HB2	2.09	0.53
8:U:34:ARG:HD2	8:U:38:GLU:OE2	2.09	0.53
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.37	0.53
5:E:29:SER:HA	5:E:32:ARG:HH21	1.74	0.53
6:F:13:MET:HE2	6:F:13:MET:HA	1.90	0.53
1:N:351:GLU:O	1:N:354:VAL:HG22	2.08	0.53
1:N:239:SER:HB2	7:T:17:SER:O	2.08	0.53
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.43	0.53
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.90	0.53
2:B:312:PHE:CE1	9:I:62:ARG:O	2.61	0.53
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.23	0.53
8:H:10:GLU:C	8:H:11:GLU:HG3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.72	0.53
5:R:78:LEU:HB2	5:R:191:ASP:HA	1.91	0.53
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.09	0.53
1:A:102:LEU:HD13	1:A:105:ASP:OD2	2.09	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
2:B:110:GLU:O	2:B:111:CYS:HB3	2.09	0.53
2:B:248:ASN:HD22	2:B:249:GLY:N	2.06	0.53
2:B:359:LYS:O	2:B:363:GLN:HG3	2.07	0.53
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.43	0.53
1:N:32:GLN:OE1	2:O:373:GLU:HG2	2.08	0.53
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.90	0.53
5:R:76:ILE:O	5:R:193:VAL:HG12	2.08	0.53
5:R:126:ARG:NH2	5:R:169:GLY:O	2.40	0.53
8:U:52:GLU:HG3	8:U:53:GLN:N	2.24	0.53
1:A:7:THR:O	1:A:11:ILE:HG13	2.09	0.53
3:C:23:PRO:HG3	7:G:4:PHE:CE1	2.44	0.53
3:C:34:PHE:HB2	20:C:381:HOH:O	2.08	0.53
6:F:53:ASP:OD1	6:F:54:LEU:N	2.42	0.53
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.44	0.53
4:Q:235:MET:CE	6:S:64:ARG:HA	2.39	0.53
5:E:187:PHE:C	5:E:189:GLY:N	2.66	0.53
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.44	0.53
5:E:163:SER:HA	5:E:174:GLY:HA3	1.90	0.53
2:O:221:GLU:HG3	2:O:222:GLN:N	2.24	0.53
5:R:98:VAL:HG22	5:R:134:ILE:HG12	1.90	0.53
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.90	0.52
2:B:70:ARG:HG3	2:B:98:VAL:CG1	2.39	0.52
4:Q:220:TYR:CE2	14:Q:3003:CDL:H722	2.44	0.52
5:R:79:SER:OG	5:R:191:ASP:HB2	2.08	0.52
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.24	0.52
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.91	0.52
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.52
1:N:276:ILE:HG12	1:N:357:ALA:HB2	1.90	0.52
2:O:166:ALA:HB1	2:O:242:GLY:C	2.34	0.52
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.52
2:B:239:TYR:HD1	2:B:260:GLU:OE1	1.91	0.52
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.08	0.52
3:C:285:ILE:HB	3:C:291:GLY:HA2	1.90	0.52
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.43	0.52
4:Q:16:GLY:CA	4:Q:19:SER:OG	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.91	0.52
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.74	0.52
2:B:333:ALA:O	2:B:337:ILE:HG13	2.09	0.52
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.09	0.52
2:O:424:MET:HE1	2:O:434:PRO:O	2.10	0.52
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.44	0.52
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.45	0.52
3:C:9:HIS:CD2	3:C:11:LEU:H	2.27	0.52
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.90	0.52
2:B:303:THR:HA	2:B:335:GLU:OE1	2.08	0.52
3:C:279:TYR:O	3:C:283:ARG:HG3	2.09	0.52
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.44	0.52
2:O:274:VAL:O	2:O:278:VAL:HG23	2.10	0.52
3:P:354:MET:HE2	3:P:354:MET:HA	1.92	0.52
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.34	0.52
7:T:28:ASN:HB2	7:T:32:ASP:HB3	1.91	0.52
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.24	0.52
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.40	0.52
5:E:58:PHE:O	5:E:61:SER:HB3	2.09	0.52
5:E:95:PRO:HG2	5:E:145:VAL:HG11	1.90	0.52
1:N:7:THR:O	1:N:11:ILE:HG13	2.10	0.52
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.38	0.52
2:O:156:GLN:HE22	9:V:77:ARG:C	2.18	0.52
2:O:303:THR:HA	2:O:335:GLU:OE1	2.09	0.52
3:P:9:HIS:CD2	3:P:12:LEU:H	2.27	0.52
5:E:84:GLY:CA	5:E:102:THR:HG23	2.39	0.52
1:N:87:ASN:CG	1:N:88:GLY:N	2.68	0.52
1:N:117:VAL:HG23	1:N:118:GLN:H	1.74	0.52
1:N:133:VAL:O	1:N:137:GLU:HG3	2.10	0.52
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.92	0.52
2:O:76:THR:HG22	2:O:81:SER:HA	1.92	0.52
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.91	0.52
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.40	0.52
1:A:317:THR:HG23	1:A:318:GLY:N	2.25	0.52
2:B:274:VAL:O	2:B:278:VAL:HG23	2.10	0.52
3:C:9:HIS:CD2	3:C:12:LEU:H	2.27	0.52
3:C:23:PRO:HG3	7:G:4:PHE:CD1	2.45	0.52
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.45	0.52
1:N:45:SER:HA	1:N:48:GLU:HG3	1.92	0.52
2:O:96:LEU:HD12	2:O:97:SER:N	2.25	0.52
2:O:341:MET:HE2	2:O:341:MET:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:THR:HB	2:B:356:ASP:CG	2.35	0.52
3:C:92:PHE:O	3:C:95:ILE:HG22	2.10	0.52
8:H:21:ARG:O	8:H:25:GLU:HG3	2.10	0.52
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.91	0.52
1:N:23:LEU:HA	1:N:192:ALA:O	2.10	0.52
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.44	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.52
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.39	0.51
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.22	0.51
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.40	0.51
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.45	0.51
2:O:305:GLN:HB3	2:O:306:PRO:HD2	1.92	0.51
8:U:35:GLU:O	8:U:39:LEU:HG	2.09	0.51
4:D:240:PRO:O	4:D:241:LYS:C	2.53	0.51
1:N:81:SER:HB3	2:O:359:LYS:HD3	1.93	0.51
1:N:281:ASP:HB3	9:V:33:UNK:HB2	1.91	0.51
3:P:120:LEU:HD13	11:P:502:HEM:HAB	1.91	0.51
3:C:365:ILE:O	3:C:368:PRO:HG2	2.09	0.51
1:N:4:TYR:HB2	2:O:114:ASP:OD1	2.11	0.51
5:R:169:GLY:O	5:R:179:ASN:HB3	2.11	0.51
6:S:58:ARG:HG3	6:S:58:ARG:HH11	1.76	0.51
2:B:46:ARG:HG3	2:B:46:ARG:O	2.10	0.51
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.51
2:O:170:THR:O	2:O:172:LEU:N	2.43	0.51
2:O:290:SER:C	2:O:297:GLN:HE21	2.19	0.51
3:P:182:LEU:O	3:P:186:LEU:HG	2.10	0.51
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.91	0.51
5:E:189:GLY:O	5:E:192:LEU:O	2.28	0.51
6:F:58:ARG:HG3	6:F:89:TYR:OH	2.11	0.51
5:E:76:ILE:O	5:E:193:VAL:HG12	2.11	0.51
5:E:139:CYS:SG	5:E:176:ALA:HB2	2.50	0.51
8:H:43:ARG:HD2	8:H:47:ARG:NH2	2.26	0.51
2:O:46:ARG:HG3	2:O:379:LEU:HD22	1.91	0.51
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.93	0.51
3:P:172:ASP:C	3:P:174:PRO:HD2	2.36	0.51
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.46	0.51
1:A:133:VAL:O	1:A:137:GLU:HG3	2.10	0.51
1:A:147:ASN:C	1:A:149:THR:N	2.68	0.51
2:B:215:ASP:O	2:B:219:VAL:HG23	2.11	0.51
1:N:106:MET:CG	1:N:203:ILE:HD13	2.39	0.51
1:A:61:HIS:NE2	2:B:287:ARG:NE	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:O	1:A:108:LYS:HG3	2.11	0.51
1:A:281:ASP:OD2	9:I:33:UNK:HG2	2.11	0.51
4:D:57:THR:HG22	4:D:58:GLU:N	2.26	0.51
2:O:239:TYR:C	2:O:239:TYR:CD2	2.89	0.51
3:P:23:PRO:HG3	7:T:4:PHE:CE1	2.46	0.51
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.45	0.51
1:A:23:LEU:HD23	1:A:24:ARG:N	2.26	0.51
2:B:56:ARG:HA	2:B:171:ALA:O	2.11	0.51
2:B:124:LEU:O	2:B:128:THR:HG23	2.10	0.51
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.93	0.51
2:B:270:ASN:ND2	2:B:270:ASN:N	2.49	0.51
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.75	0.51
3:C:5:ILE:O	3:C:5:ILE:HG22	2.11	0.51
5:E:109:GLU:CB	5:E:167:ALA:HB3	2.41	0.51
5:E:171:ILE:HG12	5:E:176:ALA:O	2.10	0.51
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.93	0.51
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.22	0.51
9:V:55:MET:HA	9:V:58:ARG:HG3	1.92	0.51
2:B:325:TYR:C	2:B:325:TYR:CD2	2.88	0.51
2:B:372:VAL:O	2:B:372:VAL:HG12	2.11	0.51
1:N:106:MET:HE2	1:N:106:MET:O	2.11	0.51
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.92	0.51
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.46	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.46	0.51
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.26	0.51
1:A:75:PHE:O	1:A:79:VAL:HG23	2.11	0.50
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.47	0.50
2:B:290:SER:C	2:B:297:GLN:HE21	2.19	0.50
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.46	0.50
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.36	0.50
2:O:268:GLU:HG2	2:O:268:GLU:O	2.10	0.50
2:O:279:LEU:O	2:O:295:LEU:HB3	2.11	0.50
2:O:325:TYR:C	2:O:325:TYR:CD2	2.89	0.50
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.44	0.50
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.92	0.50
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.46	0.50
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.47	0.50
2:B:21:ALA:O	2:B:22:GLU:CB	2.60	0.50
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.50
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.40	0.50
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.46	0.50
1:N:147:ASN:C	1:N:149:THR:N	2.68	0.50
2:O:26:ILE:O	2:O:26:ILE:HG12	2.10	0.50
4:Q:26:VAL:CG2	4:Q:188:THR:HG22	2.41	0.50
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.29	0.50
8:U:21:ARG:O	8:U:25:GLU:HG3	2.12	0.50
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.77	0.50
2:B:239:TYR:C	2:B:239:TYR:CD2	2.88	0.50
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.41	0.50
4:Q:99:GLU:H	4:Q:99:GLU:CD	2.19	0.50
4:Q:148:HIS:N	4:Q:148:HIS:CD2	2.79	0.50
6:S:32:MET:CE	6:S:87:LYS:H	2.23	0.50
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.93	0.50
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.46	0.50
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.74	0.50
4:D:143:VAL:HG21	4:D:149:TYR:HB2	1.94	0.50
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.93	0.50
1:N:281:ASP:C	1:N:281:ASP:OD1	2.55	0.50
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.93	0.50
13:C:2002:UQ:HM51	13:C:2002:UQ:C8	2.41	0.50
4:D:26:VAL:CG2	4:D:188:THR:HG22	2.42	0.50
5:R:53:ASN:O	5:R:56:THR:HB	2.10	0.50
6:S:13:MET:CA	6:S:16:ILE:HB	2.41	0.50
2:B:189:GLU:O	2:B:190:GLN:C	2.54	0.50
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.93	0.50
7:G:36:ASN:O	7:G:40:ARG:HG3	2.12	0.50
1:N:102:LEU:HD13	1:N:105:ASP:OD2	2.11	0.50
1:N:436:ARG:NH1	3:P:220:PRO:HB2	2.26	0.50
2:O:62:ASN:O	2:O:65:THR:CG2	2.57	0.50
4:Q:221:TYR:CE2	5:R:39:VAL:HG21	2.47	0.50
5:R:114:VAL:O	5:R:114:VAL:HG12	2.12	0.50
5:R:155:GLY:HA3	5:R:166:ASP:O	2.11	0.50
6:S:16:ILE:O	6:S:19:TRP:HB3	2.12	0.50
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.50
3:C:271:PRO:HB2	3:C:275:PHE:HB2	1.94	0.50
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.27	0.50
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.11	0.50
2:B:146:VAL:HG12	2:B:147:ASP:N	2.27	0.50
3:C:145:THR:O	3:C:149:ASN:HB2	2.12	0.50
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.10	0.50
4:D:148:HIS:CD2	4:D:148:HIS:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:GLY:N	5:E:102:THR:HG23	2.26	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.50
1:N:112:LEU:O	1:N:113:LEU:C	2.55	0.50
1:N:158:PHE:O	1:N:164:ALA:HB2	2.12	0.50
1:N:354:VAL:HG23	1:N:355:LYS:N	2.26	0.50
3:P:184:PHE:O	3:P:184:PHE:HD2	1.95	0.50
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.47	0.50
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.12	0.49
4:D:99:GLU:CD	4:D:99:GLU:H	2.20	0.49
9:I:32:UNK:N	9:I:73:PRO:CG	2.75	0.49
3:P:89:SER:O	3:P:90:PHE:C	2.55	0.49
3:P:142:TRP:HB3	3:P:269:ILE:HD13	1.94	0.49
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.12	0.49
4:Q:203:ARG:HD3	18:Q:3009:BOG:O6	2.12	0.49
1:A:103:SER:HB3	1:A:202:GLY:O	2.12	0.49
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.49
2:O:31:ASN:N	2:O:31:ASN:ND2	2.60	0.49
2:O:67:HIS:O	2:O:70:ARG:HB3	2.13	0.49
3:P:9:HIS:CD2	3:P:11:LEU:H	2.31	0.49
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.94	0.49
2:B:96:LEU:HB3	9:I:70:LEU:HD22	1.94	0.49
2:B:181:TYR:CE1	2:B:182:ARG:CG	2.95	0.49
4:D:148:HIS:CE1	4:D:161:ALA:HB2	2.48	0.49
5:E:185:TYR:O	5:E:186:GLN:HB3	2.12	0.49
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.12	0.49
2:O:333:ALA:O	2:O:337:ILE:HG13	2.12	0.49
3:P:332:ASN:ND2	3:P:358:SER:OG	2.43	0.49
6:S:13:MET:HA	6:S:16:ILE:HD12	1.93	0.49
1:A:23:LEU:HA	1:A:192:ALA:O	2.13	0.49
2:B:424:MET:HE1	2:B:434:PRO:O	2.12	0.49
1:N:242:ARG:O	7:T:14:ILE:HA	2.12	0.49
1:N:361:LEU:O	1:N:364:ALA:HB3	2.12	0.49
2:O:325:TYR:HD2	2:O:325:TYR:C	2.20	0.49
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.30	0.49
4:Q:70:VAL:CG2	4:Q:83:ARG:CZ	2.90	0.49
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.12	0.49
2:B:252:LEU:HD13	9:I:55:MET:HE3	1.94	0.49
2:B:325:TYR:HD2	2:B:325:TYR:C	2.21	0.49
5:E:84:GLY:N	5:E:100:HIS:O	2.40	0.49
5:E:98:VAL:HG22	5:E:134:ILE:HG12	1.95	0.49
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:PHE:O	7:G:35:PRO:HD3	2.11	0.49
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.28	0.49
1:N:37:VAL:HG12	1:N:199:ALA:HA	1.95	0.49
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.48	0.49
2:O:272:PHE:O	2:O:276:GLN:N	2.44	0.49
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.95	0.49
2:O:353:THR:HB	2:O:356:ASP:CG	2.38	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.95	0.49
4:Q:181:GLN:CA	8:U:77:LEU:HD22	2.42	0.49
7:T:30:PHE:CD2	7:T:34:LEU:HD12	2.47	0.49
8:U:73:LEU:HD12	8:U:73:LEU:O	2.12	0.49
1:A:63:ALA:O	1:A:116:VAL:HG13	2.12	0.49
1:A:293:ARG:HD3	1:A:344:ARG:NH1	2.27	0.49
4:D:147:LEU:C	4:D:148:HIS:HD2	2.21	0.49
1:N:212:ALA:O	1:N:216:PHE:HB2	2.13	0.49
1:N:293:ARG:O	1:N:297:LEU:HG	2.13	0.49
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.95	0.49
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.77	0.49
1:A:37:VAL:HG12	1:A:199:ALA:HA	1.93	0.49
2:O:306:PRO:HB3	9:V:52:ARG:N	2.27	0.49
10:W:60:GLU:O	10:W:60:GLU:HG3	2.12	0.49
1:A:161:THR:HG21	1:A:235:ARG:H	1.78	0.49
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.93	0.49
2:B:62:ASN:O	2:B:65:THR:CG2	2.60	0.49
2:B:325:TYR:HD1	9:I:60:ALA:CB	2.26	0.49
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.77	0.49
1:N:19:LEU:C	1:N:21:ASN:H	2.21	0.49
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.43	0.49
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.49
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.20	0.49
9:V:64:LEU:CD1	9:V:77:ARG:C	2.85	0.49
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.38	0.49
2:B:73:SER:OG	2:B:74:PRO:HD3	2.13	0.49
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.78	0.49
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.77	0.49
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.95	0.49
1:N:10:ASN:OD1	2:O:19:PRO:HD2	2.13	0.49
1:N:223:TYR:H	1:N:223:TYR:HD2	1.61	0.49
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.42	0.49
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.95	0.49
3:P:151:PHE:C	3:P:153:ALA:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HB2	1:A:192:ALA:HB1	1.94	0.48
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.94	0.48
1:A:223:TYR:H	1:A:223:TYR:HD2	1.60	0.48
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.48
3:P:285:ILE:HB	3:P:291:GLY:HA2	1.95	0.48
6:S:96:GLU:OE1	6:S:99:ARG:NH2	2.46	0.48
1:A:15:ASN:O	1:A:26:ALA:HA	2.13	0.48
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.95	0.48
2:B:46:ARG:CD	2:B:110:GLU:HG2	2.44	0.48
2:B:147:ASP:O	2:B:150:VAL:HG22	2.13	0.48
3:C:125:MET:HE1	12:C:2001:IKR:I1	2.82	0.48
4:D:57:THR:HB	4:D:60:GLU:HG3	1.93	0.48
4:D:70:VAL:CG2	4:D:83:ARG:CZ	2.91	0.48
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.28	0.48
6:S:12:LEU:C	6:S:14:ASP:N	2.71	0.48
7:T:59:TYR:O	7:T:63:THR:HB	2.14	0.48
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.53	0.48
3:C:2:ALA:HB1	3:C:3:PRO:HD2	1.96	0.48
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.48
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.48	0.48
2:O:306:PRO:HB3	9:V:51:CYS:C	2.39	0.48
3:P:70:THR:HA	3:P:74:VAL:CG2	2.43	0.48
4:Q:35:GLN:NE2	4:Q:169:LEU:HD12	2.28	0.48
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.43	0.48
2:B:24:LEU:HG	2:B:24:LEU:O	2.13	0.48
3:C:207:ASN:ND2	3:C:208:ASN:H	2.11	0.48
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.45	0.48
7:T:46:PHE:O	7:T:50:PRO:HG2	2.13	0.48
8:U:34:ARG:HB2	8:U:61:PHE:CE1	2.48	0.48
4:D:37:CYS:C	4:D:39:ALA:N	2.67	0.48
1:N:108:LYS:HG3	1:N:108:LYS:O	2.12	0.48
2:O:345:LYS:O	2:O:349:GLN:HG3	2.13	0.48
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.28	0.48
5:R:20:ASP:C	5:R:22:THR:H	2.22	0.48
8:U:48:SER:O	8:U:49:HIS:ND1	2.45	0.48
1:A:18:THR:HG23	1:A:24:ARG:HG3	1.94	0.48
2:B:150:VAL:CG2	2:B:151:ALA:N	2.76	0.48
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.14	0.48
6:F:13:MET:HE2	6:F:16:ILE:HD12	1.94	0.48
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.48	0.48
1:N:45:SER:HA	1:N:48:GLU:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:46:ARG:CD	2:O:110:GLU:HG2	2.44	0.48
2:O:287:ARG:HA	9:V:53:GLU:HG3	1.95	0.48
2:O:294:LYS:NZ	2:O:356:ASP:OD2	2.41	0.48
3:P:5:ILE:O	3:P:5:ILE:HG22	2.14	0.48
3:P:271:PRO:HD2	3:P:279:TYR:CD2	2.48	0.48
1:A:38:GLY:HA3	1:A:98:TYR:HA	1.95	0.48
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.77	0.48
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.43	0.48
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.96	0.48
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.48	0.48
3:C:101:ARG:C	3:C:101:ARG:CD	2.87	0.48
3:C:166:TRP:HA	3:C:175:THR:HG23	1.96	0.48
4:D:34:LYS:O	4:D:34:LYS:HG2	2.12	0.48
5:E:77:LYS:HE2	5:E:79:SER:OG	2.14	0.48
6:F:58:ARG:HG3	6:F:58:ARG:HH11	1.77	0.48
10:J:40:ASP:O	10:J:44:GLU:HG3	2.13	0.48
4:Q:97:ASN:HB2	4:Q:99:GLU:OE1	2.13	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:B:290:SER:O	2:B:297:GLN:HG2	2.14	0.48
4:D:47:ALA:N	4:D:50:ASN:HD22	2.03	0.48
5:E:161:HIS:HB2	19:E:501:FES:S1	2.54	0.48
2:O:193:HIS:O	2:O:197:ASN:ND2	2.46	0.48
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.78	0.48
1:A:53:ASN:N	1:A:173:ASN:HD22	2.11	0.48
1:A:170:THR:CG2	1:A:171:THR:H	2.23	0.48
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.49	0.48
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.96	0.48
2:B:167:ALA:C	2:B:168:TYR:CD1	2.92	0.48
3:C:142:TRP:HB3	3:C:269:ILE:HD13	1.95	0.48
1:N:15:ASN:O	1:N:26:ALA:HA	2.14	0.48
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.49	0.48
2:O:37:SER:HB3	2:O:213:HIS:CG	2.48	0.48
4:Q:76:GLU:H	4:Q:76:GLU:CD	2.21	0.48
5:R:178:TYR:N	5:R:178:TYR:HD1	2.11	0.48
6:S:53:ASP:OD1	6:S:54:LEU:N	2.46	0.48
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.29	0.48
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.23	0.48
3:C:9:HIS:HB3	3:C:12:LEU:HB2	1.95	0.48
5:E:175:PRO:O	5:E:176:ALA:C	2.55	0.48
8:H:34:ARG:HB2	8:H:61:PHE:CE1	2.49	0.48
2:O:124:LEU:HD23	2:O:124:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:CA	1:A:195:MET:HE2	2.45	0.47
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.39	0.47
3:C:156:TYR:C	3:C:158:GLY:H	2.22	0.47
3:C:350:ILE:CG2	3:C:351:ILE:N	2.77	0.47
4:D:16:GLY:CA	4:D:19:SER:OG	2.62	0.47
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.18	0.47
7:G:80:ASP:O	7:G:81:GLN:C	2.57	0.47
9:I:59:SER:O	9:I:60:ALA:C	2.56	0.47
1:N:94:GLN:NE2	1:N:381:SER:OG	2.37	0.47
1:N:253:VAL:HG11	1:N:335:MET:HE2	1.96	0.47
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.44	0.47
3:P:132:TYR:O	3:P:135:PRO:HD2	2.14	0.47
3:P:138:GLN:O	3:P:142:TRP:HD1	1.97	0.47
7:T:30:PHE:O	7:T:35:PRO:HD3	2.14	0.47
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.96	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.49	0.47
5:E:178:TYR:N	5:E:178:TYR:CD1	2.82	0.47
6:F:71:LYS:O	6:F:72:HIS:HB2	2.14	0.47
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.13	0.47
1:N:49:ASN:CG	1:N:51:LYS:H	2.22	0.47
1:N:53:ASN:N	1:N:173:ASN:HD22	2.12	0.47
1:N:382:HIS:HB3	1:N:388:ARG:O	2.13	0.47
1:N:402:VAL:HG22	1:N:406:MET:CE	2.36	0.47
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.48	0.47
2:O:150:VAL:CG2	2:O:151:ALA:N	2.77	0.47
3:P:261:ASN:HD21	3:P:264:VAL:HG23	1.78	0.47
5:R:78:LEU:HD13	5:R:132:TRP:HE1	1.76	0.47
2:B:105:MET:HE2	2:B:107:TYR:CE1	2.48	0.47
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.96	0.47
2:O:146:VAL:HG12	2:O:147:ASP:N	2.28	0.47
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.95	0.47
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.44	0.47
1:A:170:THR:CG2	1:A:171:THR:N	2.78	0.47
2:B:279:LEU:O	2:B:295:LEU:HB3	2.13	0.47
3:C:31:TRP:O	3:C:101:ARG:HG3	2.14	0.47
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.95	0.47
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.49	0.47
5:E:82:PRO:O	5:E:100:HIS:HB3	2.14	0.47
2:O:122:TYR:O	2:O:126:VAL:HG23	2.15	0.47
2:O:225:ASN:O	2:O:227:ARG:HG2	2.15	0.47
4:Q:2:GLU:O	4:Q:3:LEU:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:LYS:O	4:Q:34:LYS:HG2	2.11	0.47
4:Q:65:ALA:O	4:Q:85:GLY:HA3	2.14	0.47
7:T:72:LYS:NZ	8:U:52:GLU:OE2	2.47	0.47
1:A:102:LEU:H	1:A:102:LEU:CD1	2.10	0.47
2:B:157:VAL:HG22	2:B:157:VAL:O	2.14	0.47
10:J:44:GLU:OE2	10:J:53:LYS:NZ	2.42	0.47
2:O:167:ALA:C	2:O:168:TYR:CD1	2.93	0.47
3:P:182:LEU:HA	3:P:182:LEU:HD23	1.58	0.47
5:R:95:PRO:HG2	5:R:145:VAL:CG1	2.45	0.47
2:B:57:TYR:N	2:B:57:TYR:HD1	2.11	0.47
2:B:122:TYR:O	2:B:126:VAL:HG23	2.15	0.47
2:B:162:ASN:O	2:B:244:ILE:HD12	2.15	0.47
2:B:166:ALA:HB1	2:B:242:GLY:C	2.39	0.47
2:B:243:GLU:OE1	2:B:436:LEU:HB3	2.14	0.47
2:B:286:LYS:HE2	2:B:287:ARG:NH2	2.29	0.47
3:C:19:LEU:C	3:C:20:ILE:HG13	2.39	0.47
4:D:109:LEU:O	4:D:111:PRO:HD3	2.14	0.47
2:O:43:PRO:O	2:O:113:ARG:HG3	2.13	0.47
2:O:259:THR:OG1	2:O:422:LYS:HG3	2.14	0.47
3:P:350:ILE:HG23	3:P:351:ILE:N	2.29	0.47
4:Q:66:GLU:C	4:Q:68:VAL:H	2.23	0.47
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.14	0.47
2:B:83:PHE:CE2	6:S:104:ARG:HA	2.49	0.47
3:C:151:PHE:C	3:C:153:ALA:H	2.22	0.47
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.97	0.47
4:D:203:ARG:HD3	18:D:2009:BOG:O6	2.15	0.47
5:E:20:ASP:C	5:E:22:THR:H	2.23	0.47
8:H:44:VAL:HG13	8:H:50:THR:HG21	1.95	0.47
1:N:23:LEU:HB2	1:N:192:ALA:HB1	1.97	0.47
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.40	0.47
2:O:110:GLU:O	2:O:111:CYS:HB3	2.13	0.47
2:O:290:SER:O	2:O:297:GLN:HG2	2.15	0.47
2:O:372:VAL:O	2:O:372:VAL:HG12	2.14	0.47
3:P:30:ALA:C	3:P:32:TRP:H	2.23	0.47
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.15	0.47
4:Q:235:MET:HE1	6:S:63:LYS:C	2.40	0.47
5:R:101:ARG:HA	5:R:105:GLU:OE1	2.15	0.47
6:S:71:LYS:O	6:S:72:HIS:HB2	2.14	0.47
1:A:310:PHE:C	1:A:310:PHE:CD2	2.93	0.47
1:A:354:VAL:HG23	1:A:355:LYS:N	2.28	0.47
3:C:30:ALA:C	3:C:32:TRP:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:OD1	2:O:18:CYS:N	2.47	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.14	0.47
3:P:16:ASN:OD1	3:P:21:ASP:OD1	2.32	0.47
3:P:30:ALA:HB1	14:Q:3003:CDL:H111	1.97	0.47
1:A:6:GLN:C	1:A:8:LEU:N	2.72	0.47
1:A:244:ARG:NE	7:G:10:VAL:HB	2.29	0.47
1:A:439:SER:HA	1:A:442:TYR:CE2	2.49	0.47
3:C:151:PHE:HB2	3:C:162:VAL:CG2	2.44	0.47
3:C:182:LEU:O	3:C:186:LEU:HG	2.15	0.47
4:D:167:GLU:C	4:D:169:LEU:N	2.73	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.50	0.47
1:N:46:ARG:HD3	1:N:231:LEU:HD13	1.95	0.47
2:O:73:SER:OG	2:O:74:PRO:HD3	2.15	0.47
3:P:133:VAL:HG22	3:P:144:ALA:HB2	1.96	0.47
4:Q:167:GLU:C	4:Q:169:LEU:N	2.71	0.47
5:R:185:TYR:N	5:R:185:TYR:CD2	2.83	0.47
1:A:180:ALA:O	1:A:183:ALA:HB3	2.15	0.47
1:A:206:LYS:O	1:A:207:GLU:C	2.57	0.47
2:B:86:THR:O	2:B:90:GLU:HG3	2.14	0.47
2:B:345:LYS:O	2:B:349:GLN:HG3	2.15	0.47
3:C:164:TRP:CZ2	5:R:62:LEU:HD12	2.50	0.47
3:C:202:HIS:NE2	13:C:2002:UQ:O4	2.44	0.47
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.23	0.47
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.22	0.47
5:R:185:TYR:N	5:R:185:TYR:HD2	2.12	0.47
7:T:48:VAL:HG12	7:T:49:ALA:N	2.30	0.47
9:V:63:ASP:OD1	9:V:63:ASP:N	2.48	0.47
10:W:20:PHE:O	10:W:24:VAL:HG23	2.15	0.47
2:B:124:LEU:HD23	2:B:124:LEU:C	2.39	0.46
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.30	0.46
3:C:354:MET:HE2	3:C:354:MET:HA	1.97	0.46
1:N:180:ALA:O	1:N:183:ALA:HB3	2.15	0.46
2:O:239:TYR:HE2	2:O:241:GLY:HA2	1.79	0.46
3:P:9:HIS:HB3	3:P:12:LEU:HB2	1.98	0.46
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.97	0.46
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.97	0.46
5:R:100:HIS:CD2	5:R:131:GLU:HB2	2.50	0.46
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.29	0.46
1:A:7:THR:HG21	2:B:113:ARG:CD	2.43	0.46
1:N:60:GLU:CD	1:N:90:THR:HG22	2.40	0.46
3:P:101:ARG:C	3:P:101:ARG:CD	2.86	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:LEU:HD21	11:C:502:HEM:CMA	2.45	0.46
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.33	0.46
4:D:235:MET:CE	6:F:64:ARG:HA	2.45	0.46
5:E:163:SER:H	5:E:175:PRO:HD2	1.79	0.46
1:N:140:GLU:OE2	9:V:50:LEU:N	2.45	0.46
1:N:146:THR:O	1:N:150:PHE:HD1	1.98	0.46
2:O:239:TYR:C	2:O:239:TYR:HD2	2.23	0.46
2:O:424:MET:HG2	2:O:425:ALA:H	1.79	0.46
3:P:40:VAL:O	3:P:44:THR:OG1	2.33	0.46
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.45	0.46
5:R:83:GLU:HG2	5:R:100:HIS:CD2	2.51	0.46
7:G:48:VAL:HG12	7:G:49:ALA:N	2.31	0.46
1:N:249:PRO:HG2	1:N:250:VAL:N	2.31	0.46
2:O:47:ILE:HG22	2:O:48:GLY:N	2.29	0.46
2:O:227:ARG:O	2:O:228:SER:O	2.33	0.46
2:O:353:THR:HB	2:O:356:ASP:OD1	2.15	0.46
2:O:385:GLU:HB3	2:O:391:THR:O	2.15	0.46
3:P:6:ARG:HG2	3:P:16:ASN:CB	2.45	0.46
3:P:198:LEU:HD13	13:P:3002:UQ:HM52	1.96	0.46
4:Q:167:GLU:C	4:Q:169:LEU:H	2.22	0.46
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.98	0.46
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.45	0.46
2:B:307:PHE:CD1	2:B:308:ASP:N	2.83	0.46
3:C:89:SER:O	3:C:90:PHE:C	2.58	0.46
3:C:117:GLY:O	11:C:502:HEM:HMC3	2.15	0.46
3:C:121:LEU:O	3:C:125:MET:HG3	2.16	0.46
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.38	0.46
5:E:62:LEU:HD12	3:P:164:TRP:CZ2	2.51	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
1:N:344:ARG:HG3	1:N:344:ARG:NH1	2.26	0.46
2:O:259:THR:O	2:O:260:GLU:C	2.59	0.46
3:P:13:LYS:O	3:P:17:ASN:HB2	2.15	0.46
3:P:123:THR:CG2	3:P:190:ILE:HG13	2.46	0.46
4:Q:32:VAL:HG11	4:Q:186:VAL:HB	1.98	0.46
4:Q:167:GLU:HG3	8:U:13:LEU:HD12	1.97	0.46
10:W:52:TRP:O	10:W:56:LYS:HB2	2.15	0.46
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.50	0.46
1:A:192:ALA:N	1:A:193:PRO:HD2	2.30	0.46
3:C:162:VAL:C	3:C:164:TRP:N	2.74	0.46
4:D:148:HIS:ND1	4:D:161:ALA:HA	2.30	0.46
6:F:100:GLU:O	6:F:104:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ASP:O	8:H:17:LEU:N	2.49	0.46
1:N:269:VAL:HG21	1:N:410:VAL:HG21	1.98	0.46
1:N:281:ASP:OD2	1:N:284:PHE:HE1	1.99	0.46
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.50	0.46
2:O:291:VAL:C	2:O:293:SER:H	2.24	0.46
3:P:364:LEU:O	3:P:368:PRO:HG3	2.15	0.46
4:Q:186:VAL:O	4:Q:189:PHE:HB3	2.14	0.46
5:R:58:PHE:O	5:R:61:SER:HB3	2.15	0.46
6:S:51:PRO:HD2	6:S:54:LEU:HD12	1.98	0.46
1:A:146:THR:O	1:A:150:PHE:HD1	1.99	0.46
2:B:131:GLU:O	2:B:132:PHE:C	2.57	0.46
2:B:239:TYR:C	2:B:239:TYR:HD2	2.24	0.46
2:B:385:GLU:HB3	2:B:391:THR:O	2.16	0.46
2:B:402:ILE:HD13	2:B:402:ILE:O	2.16	0.46
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.51	0.46
4:D:150:ASN:O	4:D:156:GLN:HA	2.15	0.46
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.15	0.46
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.51	0.46
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.98	0.46
5:R:100:HIS:HB2	5:R:132:TRP:CZ3	2.51	0.46
5:R:120:PRO:O	5:R:121:GLN:CG	2.62	0.46
5:E:188:VAL:HG12	5:E:188:VAL:O	2.16	0.46
8:H:15:ASP:C	8:H:17:LEU:N	2.73	0.46
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.75	0.46
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.42	0.46
3:P:123:THR:HG21	3:P:190:ILE:HG13	1.97	0.46
5:R:163:SER:OG	5:R:176:ALA:HB2	2.16	0.46
6:S:32:MET:HE3	6:S:87:LYS:CB	2.46	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.15	0.46
2:B:368:TYR:O	2:B:371:SER:HB2	2.16	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.98	0.46
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.98	0.46
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.83	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.16	0.46
3:C:134:LEU:HD21	3:C:180:PHE:HA	1.98	0.46
4:D:66:GLU:C	4:D:68:VAL:H	2.24	0.46
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.30	0.46
4:D:235:MET:HE2	6:F:64:ARG:HA	1.97	0.46
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.36	0.46
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.51	0.46
1:N:106:MET:CE	1:N:110:VAL:CG2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:145:MET:CB	1:N:252:HIS:CD2	2.99	0.46
2:O:124:LEU:O	2:O:128:THR:HG23	2.16	0.46
5:R:118:ARG:O	5:R:120:PRO:CD	2.56	0.46
9:V:63:ASP:O	9:V:64:LEU:HB2	2.16	0.46
1:A:351:GLU:O	1:A:354:VAL:HG22	2.16	0.45
2:B:170:THR:O	2:B:172:LEU:N	2.49	0.45
2:B:265:GLY:O	2:B:266:SER:C	2.58	0.45
3:C:13:LYS:O	3:C:17:ASN:HB2	2.16	0.45
3:C:22:LEU:CD2	13:C:2002:UQ:HM32	2.43	0.45
6:F:51:PRO:O	6:F:52:GLU:C	2.58	0.45
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.45
1:N:191:LYS:O	1:N:195:MET:HG3	2.16	0.45
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.51	0.45
2:O:252:LEU:HD11	9:V:49:LEU:HB2	1.97	0.45
3:P:92:PHE:O	3:P:95:ILE:HG22	2.16	0.45
3:P:271:PRO:HB2	3:P:275:PHE:HB2	1.97	0.45
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.16	0.45
4:Q:165:TYR:O	4:Q:166:ASN:C	2.60	0.45
5:R:109:GLU:OE2	5:R:168:SER:HB2	2.17	0.45
5:R:171:ILE:HG21	5:R:177:PRO:O	2.16	0.45
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.99	0.45
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.79	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.45
2:B:385:GLU:C	2:B:387:LEU:H	2.25	0.45
3:C:6:ARG:HG2	3:C:16:ASN:CB	2.46	0.45
3:C:98:HIS:CD2	11:C:502:HEM:NC	2.83	0.45
3:C:231:LEU:O	3:C:235:LEU:HG	2.16	0.45
4:D:117:VAL:O	4:D:123:GLY:HA2	2.16	0.45
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	0.45
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.16	0.45
2:O:408:ALA:O	2:O:409:ASP:C	2.59	0.45
3:P:6:ARG:O	3:P:13:LYS:HA	2.16	0.45
3:P:151:PHE:HB2	3:P:162:VAL:CG2	2.46	0.45
5:R:77:LYS:HE3	5:R:191:ASP:OD2	2.16	0.45
5:R:100:HIS:HA	5:R:131:GLU:O	2.16	0.45
5:R:109:GLU:CD	5:R:123:ASP:HB2	2.41	0.45
5:R:116:LYS:O	5:R:117:LEU:HD23	2.16	0.45
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.45	0.45
2:B:71:LEU:HD22	9:I:68:ILE:HG13	1.98	0.45
3:C:16:ASN:OD1	3:C:21:ASP:OD1	2.34	0.45
3:C:82:ASN:HD22	3:C:82:ASN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:167:GLU:C	4:D:169:LEU:H	2.25	0.45
9:I:38:UNK:C	9:I:40:UNK:N	2.76	0.45
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.34	0.45
1:N:79:VAL:O	1:N:82:MET:HG2	2.16	0.45
1:N:191:LYS:C	1:N:193:PRO:HD2	2.41	0.45
2:O:157:VAL:O	2:O:157:VAL:HG22	2.16	0.45
3:P:4:ASN:C	3:P:6:ARG:H	2.24	0.45
3:P:166:TRP:HA	3:P:175:THR:HG23	1.99	0.45
3:P:377:MET:HE2	6:S:20:TYR:CD1	2.51	0.45
6:S:100:GLU:O	6:S:104:ARG:HG3	2.17	0.45
1:A:343:MET:HE3	1:A:441:MET:HA	1.98	0.45
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.99	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.32	0.45
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.99	0.45
9:I:33:UNK:O	9:I:34:UNK:O	2.34	0.45
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.17	0.45
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.98	0.45
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.51	0.45
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.52	0.45
3:P:344:VAL:O	3:P:345:GLU:HG3	2.16	0.45
4:Q:161:ALA:O	4:Q:162:PRO:C	2.59	0.45
5:R:161:HIS:HB2	19:R:501:FES:S1	2.57	0.45
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.15	0.45
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.85	0.45
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.47	0.45
4:Q:233:ARG:O	6:S:71:LYS:NZ	2.49	0.45
8:U:65:ARG:O	8:U:69:VAL:HG23	2.17	0.45
10:W:10:TYR:HE2	10:W:15:ARG:HD2	1.81	0.45
1:A:85:HIS:CE1	2:B:370:MET:HE1	2.52	0.45
1:A:274:ASN:ND2	1:A:309:THR:HB	2.32	0.45
5:E:171:ILE:HG21	5:E:177:PRO:O	2.16	0.45
9:I:71:ASN:N	9:I:71:ASN:HD22	2.09	0.45
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.30	0.45
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.52	0.45
1:N:90:THR:O	1:N:167:VAL:HG11	2.15	0.45
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.44	0.45
1:N:354:VAL:HG11	1:N:404:ALA:HA	1.99	0.45
2:O:31:ASN:HD22	2:O:31:ASN:H	1.62	0.45
2:O:70:ARG:HG3	2:O:98:VAL:CG1	2.47	0.45
2:O:403:ASP:C	2:O:405:VAL:H	2.25	0.45
3:P:162:VAL:C	3:P:164:TRP:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:47:ALA:N	4:Q:50:ASN:HD22	2.02	0.45
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.99	0.45
9:V:70:LEU:HD23	9:V:70:LEU:C	2.42	0.45
2:B:206:LEU:O	2:B:206:LEU:HG	2.16	0.45
2:B:424:MET:HG2	2:B:425:ALA:H	1.81	0.45
10:J:20:PHE:CD1	10:J:20:PHE:C	2.94	0.45
1:N:30:SER:O	1:N:202:GLY:HA2	2.15	0.45
1:N:106:MET:CE	1:N:110:VAL:HG21	2.47	0.45
1:N:131:ARG:NH2	1:N:177:LEU:O	2.50	0.45
3:P:338:TRP:NE1	7:T:59:TYR:HE1	2.15	0.45
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.47	0.45
1:A:106:MET:CG	1:A:203:ILE:HD13	2.46	0.45
1:A:251:ALA:HB2	1:A:427:PRO:HG2	1.99	0.45
1:A:269:VAL:HG21	1:A:410:VAL:HG21	1.98	0.45
3:C:147:ILE:HG13	12:C:2001:IKR:H16A	1.99	0.45
4:D:161:ALA:O	4:D:162:PRO:C	2.60	0.45
5:E:191:ASP:OD2	5:E:191:ASP:N	2.49	0.45
7:G:68:ARG:NH2	7:G:69:LEU:HD21	2.31	0.45
8:H:40:CYS:O	8:H:41:ASP:C	2.59	0.45
1:N:19:LEU:O	1:N:21:ASN:N	2.50	0.45
1:N:147:ASN:O	1:N:149:THR:N	2.50	0.45
2:O:307:PHE:CD1	2:O:308:ASP:N	2.85	0.45
3:P:101:ARG:HD2	3:P:102:GLY:N	2.32	0.45
3:P:207:ASN:ND2	3:P:208:ASN:H	2.15	0.45
5:R:102:THR:O	5:R:106:ILE:HG13	2.16	0.45
8:U:15:ASP:C	8:U:17:LEU:N	2.73	0.45
1:A:249:PRO:HG2	1:A:250:VAL:N	2.29	0.45
2:B:135:TRP:O	2:B:136:GLU:C	2.59	0.45
2:B:146:VAL:O	2:B:149:ALA:N	2.50	0.45
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.99	0.45
5:E:78:LEU:HD11	5:E:187:PHE:HE2	1.80	0.45
3:P:151:PHE:C	3:P:153:ALA:N	2.73	0.45
1:A:191:LYS:C	1:A:195:MET:HE2	2.41	0.44
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.52	0.44
3:C:75:GLN:HA	3:C:75:GLN:OE1	2.17	0.44
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.76	0.44
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.52	0.44
1:N:282:ARG:NH2	9:V:37:UNK:N	2.65	0.44
1:N:310:PHE:C	1:N:310:PHE:CD2	2.95	0.44
2:O:86:THR:O	2:O:90:GLU:HG3	2.17	0.44
2:O:168:TYR:HE2	2:O:172:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.77	0.44
3:P:261:ASN:ND2	3:P:264:VAL:HG23	2.32	0.44
4:Q:54:VAL:HG11	4:Q:192:TRP:HE1	1.82	0.44
4:Q:147:LEU:C	4:Q:148:HIS:CD2	2.92	0.44
7:T:36:ASN:O	7:T:40:ARG:HG3	2.15	0.44
2:B:27:THR:HG22	2:B:28:LYS:N	2.32	0.44
2:B:150:VAL:HG23	2:B:151:ALA:N	2.32	0.44
3:C:158:GLY:O	3:C:160:THR:N	2.50	0.44
4:D:43:MET:CE	4:D:189:PHE:CZ	2.98	0.44
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.27	0.44
2:O:25:GLU:HB2	2:O:213:HIS:ND1	2.32	0.44
2:O:26:ILE:HA	2:O:35:ILE:O	2.17	0.44
3:P:278:ALA:HB1	3:P:295:LEU:HD13	1.98	0.44
4:Q:46:VAL:HB	4:Q:91:PHE:CE2	2.53	0.44
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.47	0.44
8:U:67:HIS:C	8:U:67:HIS:ND1	2.75	0.44
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.52	0.44
4:D:24:SER:OG	10:J:55:ILE:HG21	2.17	0.44
4:D:222:MET:HE3	5:E:40:THR:OG1	2.17	0.44
10:J:52:TRP:O	10:J:53:LYS:C	2.61	0.44
1:N:58:PHE:HA	1:N:134:ILE:HD11	1.98	0.44
1:N:134:ILE:HG21	1:N:174:ILE:CG1	2.47	0.44
2:O:286:LYS:HE2	2:O:287:ARG:NH2	2.33	0.44
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	2.00	0.44
5:R:102:THR:C	5:R:104:ALA:N	2.74	0.44
1:A:106:MET:CE	1:A:110:VAL:CG2	2.95	0.44
1:A:402:VAL:HG22	1:A:406:MET:CE	2.34	0.44
2:B:43:PRO:O	2:B:113:ARG:HG3	2.17	0.44
2:B:72:ALA:HB1	2:B:75:LEU:HD12	2.00	0.44
2:B:268:GLU:HG2	2:B:272:PHE:HE1	1.81	0.44
3:C:158:GLY:C	3:C:160:THR:N	2.75	0.44
4:D:165:TYR:O	4:D:166:ASN:C	2.59	0.44
1:N:82:MET:CE	1:N:105:ASP:HB3	2.48	0.44
2:O:31:ASN:ND2	2:O:31:ASN:H	2.15	0.44
2:O:374:THR:HG22	2:O:376:GLN:HB3	1.99	0.44
3:P:92:PHE:O	3:P:93:ILE:C	2.61	0.44
3:P:175:THR:O	3:P:178:ARG:HG2	2.17	0.44
3:P:319:ARG:HB3	3:P:374:GLU:OE1	2.17	0.44
7:T:44:GLN:O	7:T:45:VAL:C	2.60	0.44
1:A:45:SER:OG	1:A:92:ARG:HA	2.18	0.44
1:A:403:ASP:O	1:A:404:ALA:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLU:C	2:B:387:LEU:N	2.76	0.44
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.98	0.44
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.99	0.44
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.17	0.44
5:R:79:SER:OG	5:R:191:ASP:CB	2.65	0.44
1:A:147:ASN:O	1:A:148:VAL:C	2.59	0.44
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.44
3:C:278:ALA:HB1	3:C:295:LEU:HD13	1.99	0.44
4:D:17:PRO:O	4:D:202:LYS:HD3	2.17	0.44
17:D:501:HEC:HHA	17:D:501:HEC:HBA1	2.00	0.44
1:N:145:MET:HE2	1:N:145:MET:N	2.32	0.44
1:N:429:GLU:CD	7:T:7:LEU:HB2	2.42	0.44
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.52	0.44
4:Q:27:ARG:HH22	4:Q:60:GLU:CD	2.25	0.44
5:R:53:ASN:O	5:R:57:GLN:HG3	2.17	0.44
10:W:60:GLU:O	10:W:61:ALA:CB	2.65	0.44
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.17	0.44
1:A:261:GLY:O	1:A:262:TRP:C	2.61	0.44
2:B:62:ASN:O	2:B:63:LEU:C	2.61	0.44
3:C:158:GLY:C	3:C:160:THR:H	2.26	0.44
4:D:43:MET:HG3	4:D:46:VAL:HG23	1.99	0.44
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.33	0.44
1:N:192:ALA:N	1:N:193:PRO:HD2	2.32	0.44
3:P:33:ASN:HB3	20:P:386:HOH:O	2.16	0.44
3:P:279:TYR:O	3:P:282:LEU:HB3	2.18	0.44
6:S:40:ASP:C	6:S:40:ASP:OD1	2.60	0.44
10:W:20:PHE:CD1	10:W:20:PHE:C	2.95	0.44
1:A:9:GLN:C	1:A:11:ILE:H	2.25	0.44
1:A:177:LEU:HD22	1:A:181:ASP:HB2	2.00	0.44
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.33	0.44
2:B:146:VAL:O	2:B:147:ASP:C	2.61	0.44
2:B:403:ASP:C	2:B:405:VAL:H	2.25	0.44
3:C:254:PRO:C	3:C:256:ASN:H	2.26	0.44
3:C:366:LEU:O	3:C:367:PHE:C	2.60	0.44
4:D:2:GLU:CB	7:G:70:LYS:HE2	2.39	0.44
4:D:218:LEU:HD13	5:E:43:ALA:N	2.33	0.44
5:E:53:ASN:O	5:E:57:GLN:HG3	2.18	0.44
5:E:153:PHE:C	5:E:155:GLY:H	2.26	0.44
7:G:28:ASN:HB2	7:G:32:ASP:HB3	1.98	0.44
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.42	0.44
2:O:275:LEU:HD12	2:O:275:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.52	0.44
5:R:113:ASP:O	5:R:115:SER:N	2.51	0.44
5:R:136:VAL:HG23	5:R:183:PRO:HD3	2.00	0.44
6:S:13:MET:O	6:S:17:ARG:HG3	2.18	0.44
9:V:39:UNK:O	9:V:40:UNK:C	2.66	0.44
1:A:176:HIS:O	1:A:177:LEU:C	2.61	0.44
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.23	0.44
2:B:238:THR:CG2	2:B:239:TYR:N	2.80	0.44
3:C:184:PHE:HD2	3:C:184:PHE:O	2.01	0.44
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.27	0.44
1:N:48:GLU:CD	1:N:54:GLY:H	2.25	0.44
3:P:31:TRP:NE1	15:P:3007:PEE:O4	2.51	0.44
3:P:75:GLN:OE1	3:P:75:GLN:HA	2.18	0.44
8:U:34:ARG:O	8:U:34:ARG:HD3	2.17	0.44
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.53	0.43
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.99	0.43
2:B:46:ARG:HD3	2:B:110:GLU:HG2	1.99	0.43
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.33	0.43
2:B:272:PHE:O	2:B:273:SER:C	2.61	0.43
1:N:178:THR:C	1:N:180:ALA:N	2.75	0.43
1:N:206:LYS:O	1:N:208:LEU:N	2.51	0.43
2:O:59:THR:HG22	2:O:60:THR:N	2.33	0.43
2:O:383:GLY:O	2:O:384:SER:C	2.61	0.43
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.18	0.43
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.58	0.43
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.36	0.43
1:A:411:CYS:HB3	1:A:415:ILE:HD12	1.99	0.43
2:B:81:SER:C	2:B:83:PHE:N	2.74	0.43
2:B:350:GLY:H	2:B:411:VAL:HG11	1.82	0.43
2:B:408:ALA:O	2:B:409:ASP:C	2.60	0.43
3:C:18:SER:HB2	3:C:202:HIS:CE1	2.48	0.43
3:C:358:SER:O	3:C:359:TYR:C	2.61	0.43
5:E:106:ILE:O	5:E:106:ILE:HG22	2.18	0.43
7:G:46:PHE:O	7:G:50:PRO:HG2	2.18	0.43
8:H:15:ASP:O	8:H:16:PRO:C	2.60	0.43
1:N:135:LEU:CD2	1:N:174:ILE:HG21	2.48	0.43
2:O:50:PHE:C	2:O:51:ILE:HG13	2.44	0.43
2:O:135:TRP:O	2:O:136:GLU:C	2.61	0.43
2:O:306:PRO:HB3	9:V:51:CYS:HA	1.99	0.43
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.53	0.43
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	2.00	0.43
5:R:15:ARG:NH1	5:R:32:ARG:HB3	2.33	0.43
8:U:72:LYS:O	8:U:74:PHE:N	2.51	0.43
1:A:48:GLU:CD	1:A:54:GLY:H	2.26	0.43
2:B:338:ARG:O	2:B:341:MET:HB2	2.18	0.43
3:C:6:ARG:O	3:C:13:LYS:HA	2.19	0.43
3:C:364:LEU:O	3:C:368:PRO:HG3	2.19	0.43
4:D:16:GLY:N	4:D:19:SER:OG	2.50	0.43
4:D:106:ASN:C	4:D:108:ALA:H	2.25	0.43
4:D:155:GLY:C	4:D:157:ALA:H	2.26	0.43
4:D:238:ARG:CZ	5:E:5:VAL:HG22	2.49	0.43
9:I:28:UNK:N	9:I:72:ALA:HB2	2.33	0.43
1:N:281:ASP:CB	9:V:33:UNK:HB2	2.49	0.43
2:O:168:TYR:HB2	2:O:173:ALA:CB	2.43	0.43
2:O:225:ASN:O	2:O:227:ARG:CG	2.65	0.43
3:P:34:PHE:CD1	3:P:37:LEU:HD12	2.54	0.43
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.33	0.43
4:Q:178:THR:HG21	8:U:16:PRO:HD2	2.01	0.43
4:Q:231:LYS:HD3	6:S:71:LYS:HA	2.00	0.43
2:B:435:PHE:O	2:B:438:GLU:N	2.52	0.43
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.48	0.43
5:E:100:HIS:CD2	5:E:131:GLU:HB2	2.53	0.43
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.53	0.43
9:I:33:UNK:HG2	9:I:73:PRO:HB3	2.00	0.43
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.99	0.43
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.18	0.43
2:O:164:HIS:O	2:O:173:ALA:HA	2.19	0.43
2:O:365:LYS:O	2:O:369:LEU:HG	2.17	0.43
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.99	0.43
3:P:261:ASN:ND2	3:P:264:VAL:CG2	2.81	0.43
5:R:69:LEU:O	5:R:72:SER:CB	2.67	0.43
9:V:49:LEU:O	9:V:50:LEU:HD23	2.19	0.43
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.43
1:A:87:ASN:OD1	2:B:286:LYS:HD2	2.18	0.43
1:A:112:LEU:O	1:A:113:LEU:C	2.60	0.43
1:A:239:SER:HB2	7:G:17:SER:O	2.18	0.43
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.48	0.43
2:B:353:THR:HB	2:B:356:ASP:OD1	2.18	0.43
3:C:41:CYS:SG	3:C:91:PHE:HA	2.58	0.43
3:C:133:VAL:HG22	3:C:144:ALA:HB2	2.01	0.43
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:GLU:HG3	5:E:75:GLU:O	2.17	0.43
5:E:119:ASP:O	5:E:121:GLN:N	2.52	0.43
5:E:141:HIS:HB2	5:E:176:ALA:CA	2.49	0.43
1:N:23:LEU:HD23	1:N:24:ARG:N	2.33	0.43
1:N:159:GLN:NE2	1:N:237:THR:HG21	2.33	0.43
2:O:312:PHE:O	2:O:322:PHE:HA	2.18	0.43
5:R:75:GLU:O	5:R:75:GLU:HG3	2.18	0.43
1:A:131:ARG:NH2	1:A:177:LEU:O	2.52	0.43
2:B:28:LYS:O	2:B:28:LYS:HG2	2.18	0.43
2:B:70:ARG:HG3	2:B:98:VAL:HG12	1.99	0.43
2:B:191:LEU:O	2:B:192:HIS:C	2.61	0.43
3:C:82:ASN:O	3:C:83:LEU:C	2.61	0.43
3:C:380:TYR:OH	6:F:34:ASP:OD1	2.33	0.43
4:D:27:ARG:O	4:D:30:PHE:HB3	2.18	0.43
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.89	0.43
7:G:32:ASP:C	7:G:35:PRO:HD2	2.43	0.43
9:I:33:UNK:HG3	9:I:73:PRO:HB3	2.01	0.43
1:N:236:PHE:CB	1:N:258:GLU:OE1	2.66	0.43
2:O:306:PRO:HB3	9:V:51:CYS:CA	2.49	0.43
2:O:309:ALA:HA	2:O:325:TYR:O	2.18	0.43
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.47	0.43
5:R:107:ASN:C	5:R:109:GLU:N	2.76	0.43
5:R:148:ALA:O	5:R:149:ASN:CB	2.66	0.43
6:S:70:LEU:C	6:S:70:LEU:HD12	2.43	0.43
7:T:77:TYR:C	7:T:79:ASN:N	2.72	0.43
1:A:103:SER:O	1:A:106:MET:HB2	2.18	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.83	0.43
1:A:241:ILE:O	1:A:241:ILE:HG23	2.19	0.43
2:B:385:GLU:O	2:B:387:LEU:N	2.51	0.43
3:C:36:SER:O	3:C:40:VAL:HG23	2.18	0.43
5:E:59:ILE:HD13	5:E:59:ILE:HA	1.82	0.43
5:E:162:GLY:O	5:E:163:SER:C	2.62	0.43
8:H:43:ARG:HG3	8:H:44:VAL:N	2.33	0.43
10:J:32:GLU:O	10:J:33:ARG:C	2.62	0.43
1:N:50:GLU:O	1:N:50:GLU:HG2	2.18	0.43
2:O:131:GLU:O	2:O:132:PHE:C	2.60	0.43
2:O:402:ILE:C	2:O:402:ILE:CD1	2.92	0.43
3:P:64:PHE:CE1	16:P:3011:GOL:H12	2.53	0.43
3:P:344:VAL:C	3:P:345:GLU:HG3	2.43	0.43
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.52	0.43
1:A:147:ASN:O	1:A:149:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.84	0.43
6:F:16:ILE:O	6:F:19:TRP:HB3	2.19	0.43
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.54	0.43
1:N:145:MET:HE2	1:N:145:MET:H	1.84	0.43
1:N:394:GLU:O	1:N:395:TRP:C	2.62	0.43
2:O:76:THR:HG23	2:O:82:SER:HB2	2.00	0.43
2:O:109:VAL:CG2	2:O:119:VAL:HG12	2.47	0.43
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.18	0.43
5:R:135:LEU:HD13	5:R:180:LEU:HD12	2.00	0.43
2:B:255:ALA:O	2:B:325:TYR:HA	2.19	0.43
3:C:19:LEU:O	3:C:20:ILE:HG13	2.18	0.43
2:O:221:GLU:C	2:O:223:PHE:H	2.26	0.43
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.31	0.43
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.54	0.43
5:R:148:ALA:HB2	5:R:156:TYR:CE2	2.53	0.43
5:R:153:PHE:CE2	5:R:172:ARG:NE	2.87	0.43
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.49	0.43
1:A:266:ASP:O	1:A:267:ASN:C	2.62	0.43
2:B:325:TYR:CD1	9:I:60:ALA:CB	3.02	0.43
3:C:175:THR:O	3:C:178:ARG:HG2	2.18	0.43
3:C:367:PHE:N	3:C:368:PRO:HD2	2.34	0.43
1:N:147:ASN:O	1:N:148:VAL:C	2.61	0.43
1:N:411:CYS:HB3	1:N:415:ILE:HD12	2.01	0.43
2:O:258:VAL:HG21	2:O:321:LEU:HD22	2.01	0.43
5:R:29:SER:CA	5:R:32:ARG:HH21	2.32	0.43
5:R:109:GLU:C	5:R:111:GLU:N	2.74	0.43
5:R:122:HIS:C	5:R:124:LEU:H	2.26	0.43
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.49	0.43
2:B:26:ILE:HA	2:B:35:ILE:O	2.18	0.42
2:B:59:THR:HG22	2:B:60:THR:N	2.33	0.42
2:B:355:GLU:O	2:B:358:THR:HB	2.19	0.42
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.01	0.42
3:C:37:LEU:O	3:C:41:CYS:HB2	2.18	0.42
3:C:212:ILE:O	3:C:213:SER:C	2.61	0.42
5:E:75:GLU:HA	5:E:193:VAL:O	2.18	0.42
5:E:156:TYR:CD1	5:E:156:TYR:N	2.87	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.41	0.42
8:H:72:LYS:O	8:H:73:LEU:C	2.61	0.42
1:N:45:SER:OG	1:N:92:ARG:HA	2.19	0.42
3:P:82:ASN:HD22	3:P:82:ASN:N	2.15	0.42
3:P:133:VAL:HA	3:P:140:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:266:PRO:HA	3:P:267:PRO:HD3	1.84	0.42
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.84	0.42
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.52	0.42
1:A:341:GLU:HA	1:A:344:ARG:HB2	2.01	0.42
2:B:209:ILE:HG22	2:B:210:GLY:N	2.33	0.42
3:C:151:PHE:C	3:C:153:ALA:N	2.74	0.42
5:E:100:HIS:HD2	5:E:131:GLU:HB2	1.84	0.42
1:N:176:HIS:O	1:N:177:LEU:C	2.62	0.42
1:N:403:ASP:O	1:N:404:ALA:C	2.62	0.42
2:O:81:SER:C	2:O:83:PHE:N	2.74	0.42
2:O:146:VAL:O	2:O:147:ASP:C	2.62	0.42
2:O:350:GLY:H	2:O:411:VAL:HG11	1.84	0.42
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.19	0.42
3:P:27:ASN:O	3:P:28:ILE:C	2.59	0.42
4:Q:143:VAL:HG21	4:Q:149:TYR:HB2	2.01	0.42
8:U:43:ARG:HG3	8:U:44:VAL:N	2.34	0.42
1:A:204:SER:O	1:A:205:HIS:C	2.61	0.42
2:B:246:GLU:O	2:B:246:GLU:HG2	2.19	0.42
2:B:424:MET:HB2	2:B:436:LEU:HD13	2.01	0.42
2:O:150:VAL:HG23	2:O:151:ALA:N	2.34	0.42
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.01	0.42
3:P:379:ASN:HA	6:S:17:ARG:HH12	1.85	0.42
4:Q:155:GLY:C	4:Q:157:ALA:H	2.27	0.42
5:R:153:PHE:C	5:R:155:GLY:H	2.27	0.42
1:A:153:LEU:O	1:A:156:THR:HG22	2.18	0.42
2:B:259:THR:O	2:B:260:GLU:C	2.62	0.42
3:C:263:LEU:C	3:C:264:VAL:HG23	2.45	0.42
1:N:44:GLY:HA3	1:N:92:ARG:O	2.19	0.42
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.42
1:N:135:LEU:HD23	1:N:135:LEU:HA	1.86	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.42
2:O:325:TYR:HB3	9:V:59:SER:HB3	2.01	0.42
3:P:172:ASP:OD1	3:P:173:ASN:N	2.40	0.42
11:P:502:HEM:HBB2	11:P:502:HEM:HMB1	2.00	0.42
4:Q:37:CYS:C	4:Q:39:ALA:N	2.76	0.42
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.34	0.42
1:A:90:THR:HB	1:A:95:THR:HG23	2.01	0.42
1:A:315:SER:OG	1:A:316:ASP:N	2.52	0.42
3:C:249:ASN:O	3:C:250:LEU:C	2.61	0.42
5:E:147:ILE:HD11	5:E:159:PRO:HG3	2.01	0.42
7:G:30:PHE:O	7:G:35:PRO:CD	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:41:UNK:O	9:I:42:UNK:C	2.67	0.42
1:N:269:VAL:O	1:N:270:LEU:C	2.62	0.42
3:P:212:ILE:O	3:P:213:SER:C	2.63	0.42
5:R:83:GLU:HA	5:R:100:HIS:O	2.19	0.42
5:R:122:HIS:C	5:R:124:LEU:N	2.77	0.42
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.33	0.42
8:U:15:ASP:O	8:U:17:LEU:N	2.52	0.42
2:B:193:HIS:O	2:B:197:ASN:ND2	2.53	0.42
3:C:284:SER:O	3:C:286:PRO:HD3	2.18	0.42
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.54	0.42
1:N:313:SER:O	1:N:314:TYR:CD2	2.72	0.42
2:O:46:ARG:HD3	2:O:110:GLU:HG2	2.02	0.42
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.55	0.42
3:P:224:TYR:HB3	4:Q:227:TRP:CZ2	2.54	0.42
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.55	0.42
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	2.01	0.42
5:R:39:VAL:O	5:R:42:THR:HB	2.20	0.42
6:S:80:TRP:N	6:S:80:TRP:CD1	2.86	0.42
1:A:171:THR:O	1:A:175:LYS:HG3	2.20	0.42
2:B:141:GLN:N	2:B:142:PRO:HD2	2.33	0.42
2:B:189:GLU:O	2:B:191:LEU:N	2.53	0.42
3:C:123:THR:CG2	3:C:190:ILE:HG13	2.49	0.42
4:D:76:GLU:O	4:Q:99:GLU:HB3	2.20	0.42
1:N:24:ARG:NH2	1:N:193:PRO:O	2.53	0.42
1:N:383:LEU:HD23	1:N:388:ARG:HA	2.02	0.42
2:O:22:GLU:HG3	2:O:23:ASP:H	1.84	0.42
2:O:280:GLY:HA3	2:O:293:SER:OG	2.20	0.42
3:P:81:ARG:C	3:P:81:ARG:HD3	2.45	0.42
3:P:287:ASN:O	3:P:289:LEU:N	2.53	0.42
3:P:346:HIS:CG	3:P:347:PRO:HA	2.54	0.42
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.50	0.42
4:Q:16:GLY:HA3	4:Q:19:SER:OG	2.19	0.42
4:Q:16:GLY:N	4:Q:19:SER:OG	2.53	0.42
6:S:31:LEU:HD21	6:S:65:ALA:HB2	2.01	0.42
8:U:65:ARG:O	8:U:68:CYS:HB3	2.19	0.42
10:W:4:ALA:O	10:W:8:GLN:HG3	2.19	0.42
1:A:45:SER:HA	1:A:48:GLU:CD	2.44	0.42
1:A:191:LYS:C	1:A:193:PRO:HD2	2.45	0.42
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.52	0.42
1:A:365:MET:HG3	1:A:366:VAL:N	2.33	0.42
2:B:291:VAL:C	2:B:293:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.54	0.42
5:E:130:PRO:C	5:E:132:TRP:H	2.27	0.42
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.47	0.42
1:N:136:GLN:OE1	9:V:50:LEU:HD13	2.20	0.42
2:O:146:VAL:O	2:O:149:ALA:N	2.53	0.42
2:O:353:THR:HG22	2:O:354:GLU:N	2.34	0.42
7:T:29:ILE:C	7:T:33:ALA:HB3	2.44	0.42
10:W:59:TYR:CD1	10:W:59:TYR:N	2.87	0.42
1:A:24:ARG:NH2	1:A:193:PRO:O	2.53	0.42
2:B:220:ALA:O	2:B:224:LEU:HB2	2.20	0.42
3:C:4:ASN:C	3:C:6:ARG:H	2.26	0.42
4:D:32:VAL:HG11	4:D:186:VAL:HB	2.01	0.42
8:H:34:ARG:O	8:H:38:GLU:HG3	2.20	0.42
1:N:298:ALA:HA	1:N:303:LEU:HD12	2.02	0.42
2:O:355:GLU:O	2:O:358:THR:HB	2.20	0.42
2:O:385:GLU:C	2:O:387:LEU:N	2.77	0.42
2:O:385:GLU:C	2:O:387:LEU:H	2.28	0.42
4:Q:179:MET:O	4:Q:182:ILE:HB	2.19	0.42
1:A:106:MET:CE	1:A:110:VAL:HG21	2.49	0.42
1:A:310:PHE:CD2	1:A:310:PHE:O	2.73	0.42
3:C:38:LEU:HA	3:C:38:LEU:HD23	1.83	0.42
3:C:61:SER:O	3:C:62:LEU:HD23	2.20	0.42
3:C:276:LEU:HB2	3:C:337:THR:HG23	2.02	0.42
3:C:297:ALA:O	3:C:301:ILE:HB	2.20	0.42
4:D:234:LYS:HD2	5:E:8:PRO:HB2	2.01	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.55	0.42
7:G:44:GLN:O	7:G:45:VAL:C	2.63	0.42
1:N:156:THR:HG23	1:N:157:ALA:N	2.35	0.42
1:N:279:ARG:HA	1:N:307:PHE:CE1	2.55	0.42
2:O:215:ASP:O	2:O:219:VAL:HG23	2.19	0.42
3:P:165:ALA:O	3:P:178:ARG:HD2	2.19	0.42
5:R:78:LEU:N	5:R:191:ASP:O	2.53	0.42
5:R:102:THR:OG1	5:R:105:GLU:HG3	2.20	0.42
8:U:40:CYS:O	8:U:41:ASP:C	2.63	0.42
3:C:40:VAL:O	3:C:44:THR:OG1	2.38	0.41
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.02	0.41
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.95	0.41
5:E:52:LYS:C	5:E:52:LYS:CD	2.93	0.41
5:E:104:ALA:O	5:E:108:GLN:HB3	2.19	0.41
7:G:78:GLU:C	7:G:79:ASN:CG	2.88	0.41
7:G:80:ASP:HB3	8:H:50:THR:CA	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:6:GLN:C	1:N:8:LEU:N	2.73	0.41
3:P:277:PHE:CD1	3:P:277:PHE:C	2.98	0.41
3:P:377:MET:CE	6:S:20:TYR:HB2	2.45	0.41
4:Q:222:MET:HE1	5:R:40:THR:HG23	2.00	0.41
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	2.01	0.41
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.55	0.41
1:A:117:VAL:CG2	1:A:118:GLN:N	2.80	0.41
1:A:156:THR:HG23	1:A:157:ALA:N	2.34	0.41
2:B:51:ILE:HG22	2:B:52:LYS:N	2.35	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.54	0.41
5:E:189:GLY:O	5:E:192:LEU:N	2.53	0.41
1:N:255:LEU:O	1:N:321:GLY:HA3	2.21	0.41
1:N:261:GLY:HA2	1:N:317:THR:O	2.19	0.41
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.41
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.41
4:Q:235:MET:HE1	6:S:64:ARG:N	2.35	0.41
8:U:72:LYS:O	8:U:73:LEU:C	2.63	0.41
1:A:104:LYS:O	1:A:107:PRO:HD2	2.20	0.41
1:A:106:MET:HB3	1:A:107:PRO:HD3	2.01	0.41
1:A:186:ILE:HG13	1:A:186:ILE:H	1.64	0.41
2:B:239:TYR:HE2	2:B:241:GLY:HA2	1.84	0.41
3:C:70:THR:HA	3:C:74:VAL:CG2	2.49	0.41
3:C:254:PRO:C	3:C:256:ASN:N	2.76	0.41
3:C:277:PHE:CG	3:C:278:ALA:N	2.88	0.41
5:E:82:PRO:HG2	5:E:85:LYS:HB2	2.01	0.41
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.19	0.41
8:H:65:ARG:O	8:H:68:CYS:HB3	2.21	0.41
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.41
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.34	0.41
1:N:39:VAL:HG13	1:N:39:VAL:O	2.20	0.41
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.02	0.41
1:N:294:LEU:HD11	1:N:334:MET:HE1	2.02	0.41
2:O:81:SER:O	2:O:82:SER:C	2.63	0.41
3:P:125:MET:HE1	12:P:3001:IKR:I1	2.89	0.41
3:P:365:ILE:O	3:P:368:PRO:HG2	2.20	0.41
7:T:57:LEU:O	7:T:58:LEU:C	2.63	0.41
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.36	0.41
1:A:90:THR:HA	1:A:95:THR:HA	2.02	0.41
2:B:319:SER:OG	2:B:320:GLY:N	2.53	0.41
2:B:355:GLU:O	2:B:358:THR:N	2.53	0.41
2:B:372:VAL:HG13	2:B:378:LEU:CA	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:336:LEU:HG	3:C:355:ALA:HB1	2.02	0.41
3:C:344:VAL:C	3:C:345:GLU:HG3	2.45	0.41
5:E:30:GLU:HB2	10:J:7:ARG:HG2	2.01	0.41
1:N:136:GLN:O	1:N:140:GLU:HG3	2.21	0.41
1:N:153:LEU:O	1:N:156:THR:HG22	2.20	0.41
1:N:307:PHE:HA	1:N:323:HIS:O	2.20	0.41
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.47	0.41
2:O:238:THR:CG2	2:O:239:TYR:H	2.31	0.41
5:R:156:TYR:CD1	5:R:156:TYR:N	2.87	0.41
1:A:44:GLY:HA3	1:A:92:ARG:O	2.20	0.41
1:A:58:PHE:HA	1:A:134:ILE:HD11	2.01	0.41
2:B:59:THR:O	2:B:60:THR:C	2.64	0.41
2:B:71:LEU:HD11	2:B:144:LEU:HD23	2.02	0.41
2:B:209:ILE:CG2	2:B:210:GLY:N	2.83	0.41
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.55	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.86	0.41
4:D:37:CYS:O	4:D:39:ALA:N	2.52	0.41
9:I:70:LEU:HD23	9:I:70:LEU:C	2.45	0.41
1:N:106:MET:HB3	1:N:107:PRO:CD	2.50	0.41
1:N:171:THR:O	1:N:175:LYS:HG3	2.21	0.41
1:N:338:ALA:O	1:N:339:GLN:C	2.62	0.41
2:O:27:THR:CG2	2:O:28:LYS:H	2.32	0.41
2:O:59:THR:C	2:O:61:ALA:N	2.78	0.41
2:O:225:ASN:O	2:O:226:ILE:C	2.63	0.41
2:O:338:ARG:O	2:O:341:MET:HB2	2.21	0.41
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.54	0.41
3:P:350:ILE:O	3:P:354:MET:HG2	2.21	0.41
1:A:81:SER:HB3	2:B:359:LYS:HD3	2.02	0.41
1:A:281:ASP:C	1:A:281:ASP:OD1	2.63	0.41
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.20	0.41
2:B:278:VAL:O	2:B:294:LYS:HG3	2.20	0.41
3:C:130:VAL:HG23	3:C:131:GLY:N	2.35	0.41
3:C:287:ASN:O	3:C:289:LEU:N	2.53	0.41
2:O:97:SER:HB3	9:V:69:SER:CB	2.51	0.41
3:P:79:LEU:CD2	5:R:57:GLN:NE2	2.84	0.41
3:P:138:GLN:HG2	3:P:258:THR:HG22	2.03	0.41
3:P:230:ILE:HG21	15:R:3005:PEE:H22	2.02	0.41
4:Q:66:GLU:C	4:Q:68:VAL:N	2.77	0.41
5:R:84:GLY:N	5:R:102:THR:HG23	2.36	0.41
1:A:382:HIS:HB3	1:A:388:ARG:O	2.20	0.41
2:B:37:SER:HB3	2:B:213:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:THR:CG2	2:B:239:TYR:H	2.31	0.41
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.36	0.41
3:C:11:LEU:HA	3:C:14:MET:HG3	2.02	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CG	2.55	0.41
5:E:53:ASN:O	5:E:56:THR:HB	2.19	0.41
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.85	0.41
8:H:67:HIS:ND1	8:H:67:HIS:C	2.78	0.41
1:N:45:SER:HA	1:N:48:GLU:CG	2.50	0.41
1:N:261:GLY:O	1:N:262:TRP:C	2.62	0.41
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.55	0.41
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.35	0.41
6:S:76:PRO:O	6:S:77:LYS:C	2.62	0.41
1:A:358:LYS:HE3	1:A:399:ILE:O	2.21	0.41
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.38	0.41
2:B:259:THR:CG2	2:B:260:GLU:N	2.82	0.41
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.20	0.41
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.35	0.41
1:N:269:VAL:HG22	1:N:406:MET:CE	2.51	0.41
1:N:274:ASN:HD22	1:N:274:ASN:HA	1.59	0.41
1:N:343:MET:HE3	1:N:441:MET:HA	2.03	0.41
2:O:105:MET:HE2	2:O:107:TYR:CE1	2.55	0.41
2:O:212:LYS:HG2	2:O:214:SER:OG	2.20	0.41
2:O:287:ARG:NH1	2:O:287:ARG:HG3	2.36	0.41
3:P:326:PHE:O	3:P:329:LEU:HB3	2.21	0.41
4:Q:106:ASN:C	4:Q:108:ALA:H	2.28	0.41
1:A:23:LEU:HD23	1:A:23:LEU:C	2.46	0.41
1:A:228:VAL:HG13	1:A:228:VAL:O	2.21	0.41
1:A:270:LEU:O	1:A:273:ALA:HB3	2.21	0.41
1:A:394:GLU:O	1:A:395:TRP:C	2.63	0.41
2:B:67:HIS:CD2	2:B:67:HIS:C	2.99	0.41
2:B:81:SER:O	2:B:82:SER:C	2.64	0.41
2:B:164:HIS:O	2:B:173:ALA:HA	2.21	0.41
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.68	0.41
3:C:173:ASN:N	3:C:174:PRO:CD	2.83	0.41
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.35	0.41
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.56	0.41
4:D:208:MET:O	4:D:212:SER:HB2	2.21	0.41
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.86	0.41
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.95	0.41
7:G:30:PHE:CD2	7:G:34:LEU:HD12	2.56	0.41
7:G:72:LYS:CE	8:H:57:GLU:OE1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:204:SER:O	1:N:205:HIS:C	2.63	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:62:ASN:O	2:O:63:LEU:C	2.64	0.41
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.96	0.41
2:O:141:GLN:N	2:O:142:PRO:HD2	2.36	0.41
2:O:272:PHE:O	2:O:273:SER:C	2.63	0.41
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.51	0.41
3:P:120:LEU:HD23	3:P:120:LEU:HA	1.95	0.41
3:P:196:ILE:HG22	3:P:200:PHE:CE2	2.56	0.41
3:P:357:LEU:HD12	3:P:357:LEU:HA	1.92	0.41
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.89	0.41
4:Q:148:HIS:CE1	4:Q:161:ALA:HB2	2.56	0.41
4:Q:161:ALA:O	4:Q:163:PRO:N	2.53	0.41
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.91	0.41
5:R:162:GLY:O	5:R:163:SER:C	2.63	0.41
6:S:51:PRO:O	6:S:52:GLU:C	2.64	0.41
10:W:44:GLU:OE2	10:W:53:LYS:NZ	2.50	0.41
1:A:45:SER:HA	1:A:48:GLU:HG3	2.02	0.41
1:A:46:ARG:HD3	1:A:231:LEU:HD13	2.03	0.41
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.20	0.41
2:B:56:ARG:HH22	2:B:318:ASP:CG	2.29	0.41
2:B:120:MET:O	2:B:121:GLU:C	2.64	0.41
2:B:402:ILE:O	2:B:405:VAL:HG23	2.21	0.41
7:G:53:LEU:O	7:G:57:LEU:HG	2.21	0.41
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.50	0.41
1:N:85:HIS:CE1	2:O:370:MET:HE1	2.55	0.41
1:N:104:LYS:O	1:N:107:PRO:HD2	2.21	0.41
2:O:206:LEU:HG	2:O:206:LEU:O	2.21	0.41
3:P:19:LEU:C	3:P:20:ILE:HG13	2.46	0.41
1:A:106:MET:HB3	1:A:107:PRO:CD	2.52	0.40
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.87	0.40
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.56	0.40
2:B:212:LYS:HG2	2:B:214:SER:OG	2.21	0.40
3:C:46:ILE:HA	11:C:501:HEM:HMC2	2.01	0.40
3:C:323:GLN:O	3:C:326:PHE:HB3	2.21	0.40
3:C:344:VAL:O	3:C:345:GLU:HG3	2.22	0.40
4:D:148:HIS:CE1	4:D:161:ALA:CB	3.04	0.40
5:E:29:SER:CA	5:E:32:ARG:HH21	2.34	0.40
5:E:157:TYR:O	5:E:159:PRO:HD3	2.21	0.40
6:F:76:PRO:O	6:F:77:LYS:C	2.63	0.40
6:F:103:GLU:O	6:F:104:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:266:ASP:O	1:N:267:ASN:C	2.64	0.40
2:O:306:PRO:CB	9:V:51:CYS:HA	2.51	0.40
3:P:198:LEU:HD23	3:P:198:LEU:HA	1.90	0.40
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.84	0.40
9:V:49:LEU:HD22	9:V:54:SER:O	2.21	0.40
3:C:277:PHE:CD1	3:C:277:PHE:C	2.99	0.40
6:F:100:GLU:O	6:F:103:GLU:HB3	2.21	0.40
8:H:65:ARG:O	8:H:69:VAL:HG23	2.21	0.40
1:N:159:GLN:HE21	1:N:237:THR:HB	1.87	0.40
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.35	0.40
3:P:31:TRP:HE1	14:P:3004:CDL:H1	1.86	0.40
3:P:238:THR:CB	3:P:239:PRO:HD3	2.48	0.40
4:Q:238:ARG:NH1	5:R:5:VAL:HG22	2.36	0.40
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.61	0.40
5:R:166:ASP:OD1	5:R:168:SER:N	2.47	0.40
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.02	0.40
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.03	0.40
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.51	0.40
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.49	0.40
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.85	0.40
1:N:206:LYS:C	1:N:208:LEU:N	2.80	0.40
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.87	0.40
3:P:36:SER:O	3:P:40:VAL:HG23	2.21	0.40
7:T:30:PHE:O	7:T:35:PRO:CD	2.69	0.40
1:A:156:THR:CG2	1:A:157:ALA:N	2.84	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.94	0.40
1:A:253:VAL:HG11	1:A:335:MET:HE2	2.04	0.40
1:A:261:GLY:HA2	1:A:317:THR:O	2.21	0.40
1:A:361:LEU:O	1:A:364:ALA:HB3	2.22	0.40
2:B:353:THR:HG22	2:B:354:GLU:N	2.36	0.40
2:B:437:ASP:O	2:B:437:ASP:OD1	2.39	0.40
3:C:123:THR:HG21	3:C:190:ILE:HG13	2.03	0.40
5:E:136:VAL:HG21	5:E:181:GLU:HG2	2.04	0.40
1:N:6:GLN:O	1:N:7:THR:C	2.63	0.40
1:N:39:VAL:HA	1:N:196:VAL:O	2.22	0.40
1:N:177:LEU:HD22	1:N:181:ASP:HB2	2.03	0.40
3:P:158:GLY:C	3:P:160:THR:N	2.77	0.40
3:P:245:LEU:HA	3:P:245:LEU:HD23	1.80	0.40
3:P:350:ILE:CG2	3:P:351:ILE:N	2.84	0.40
4:Q:105:ASN:O	4:Q:106:ASN:CB	2.69	0.40
1:A:4:TYR:OH	1:A:396:ASP:OD2	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:C	1:A:106:MET:H	2.30	0.40
2:B:280:GLY:HA3	2:B:293:SER:OG	2.21	0.40
2:B:316:TYR:O	2:B:317:SER:C	2.65	0.40
4:D:116:ILE:CG2	4:D:117:VAL:N	2.85	0.40
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.57	0.40
1:N:35:CYS:HB2	1:N:200:ALA:O	2.21	0.40
1:N:104:LYS:C	1:N:106:MET:H	2.28	0.40
5:R:170:ARG:HG2	5:R:179:ASN:CG	2.46	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%)	391 (88%)	44 (10%)	7 (2%)	7	26
1	N	440/446 (99%)	380 (86%)	49 (11%)	11 (2%)	4	17
2	B	419/441 (95%)	337 (80%)	62 (15%)	20 (5%)	2	9
2	O	420/441 (95%)	351 (84%)	57 (14%)	12 (3%)	3	16
3	C	378/380 (100%)	332 (88%)	37 (10%)	9 (2%)	4	18
3	P	377/380 (99%)	322 (85%)	47 (12%)	8 (2%)	5	21
4	D	239/241 (99%)	212 (89%)	19 (8%)	8 (3%)	3	13
4	Q	239/241 (99%)	213 (89%)	15 (6%)	11 (5%)	2	9
5	E	194/196 (99%)	142 (73%)	32 (16%)	20 (10%)	0	2
5	R	194/196 (99%)	158 (81%)	23 (12%)	13 (7%)	1	4
6	F	99/110 (90%)	89 (90%)	9 (9%)	1 (1%)	12	37
6	S	99/110 (90%)	88 (89%)	10 (10%)	1 (1%)	12	37
7	G	78/81 (96%)	63 (81%)	11 (14%)	4 (5%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	77/81 (95%)	60 (78%)	13 (17%)	4 (5%)	1	8
8	H	68/77 (88%)	57 (84%)	10 (15%)	1 (2%)	8	28
8	U	65/77 (84%)	48 (74%)	14 (22%)	3 (5%)	2	9
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0	0
9	V	29/47 (62%)	23 (79%)	3 (10%)	3 (10%)	0	2
10	J	59/61 (97%)	46 (78%)	12 (20%)	1 (2%)	7	25
10	W	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1	4
All	All	4003/4160 (96%)	3377 (84%)	481 (12%)	145 (4%)	2	12

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA
2	B	22	GLU
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	227	ARG
2	B	228	SER
2	B	283	PRO
3	C	287	ASN
5	E	102	THR
5	E	115	SER
5	E	127	VAL
5	E	128	LYS
5	E	149	ASN
5	E	150	SER
5	E	177	PRO
7	G	79	ASN
9	I	63	ASP
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
2	O	283	PRO
3	P	287	ASN
4	Q	3	LEU
5	R	118	ARG
5	R	137	GLY

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Mol	Chain	Res	Type
5	R	177	PRO
8	U	49	HIS
9	V	63	ASP
10	W	61	ALA
1	A	433	ASP
2	B	31	ASN
2	B	63	LEU
2	B	201	SER
2	B	221	GLU
2	B	269	ALA
2	B	420	GLY
5	E	130	PRO
5	E	137	GLY
5	E	151	GLY
5	E	163	SER
5	E	166	ASP
7	G	45	VAL
8	H	73	LEU
1	N	20	ASP
1	N	206	LYS
1	N	207	GLU
1	N	218	GLY
1	N	282	ARG
2	O	201	SER
4	Q	198	HIS
5	R	8	PRO
5	R	21	ALA
5	R	154	GLY
5	R	163	SER
5	R	166	ASP
5	R	188	VAL
6	S	83	TYR
7	T	3	HIS
7	T	33	ALA
7	T	45	VAL
8	U	73	LEU
1	A	282	ARG
1	A	388	ARG
2	B	30	PRO
2	B	386	ALA
3	C	159	HIS
3	C	288	LYS

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Mol	Chain	Res	Type
4	D	166	ASN
4	D	198	HIS
4	D	233	ARG
5	E	21	ALA
5	E	146	PRO
7	G	33	ALA
9	I	64	LEU
1	N	5	ALA
2	O	24	LEU
2	O	63	LEU
2	O	222	GLN
3	P	288	LYS
4	Q	2	GLU
4	Q	20	ALA
5	R	114	VAL
5	R	149	ASN
5	R	191	ASP
8	U	52	GLU
9	V	60	ALA
9	V	64	LEU
10	W	17	THR
2	B	389	SER
3	C	202	HIS
4	D	106	ASN
4	D	133	GLY
4	D	156	GLN
5	E	120	PRO
5	E	191	ASP
6	F	77	LYS
9	I	73	PRO
10	J	32	GLU
1	N	72	CYS
1	N	81	SER
1	N	388	ARG
3	P	156	TYR
3	P	202	HIS
4	Q	156	GLN
4	Q	162	PRO
4	Q	166	ASN
4	Q	233	ARG
10	W	32	GLU
10	W	33	ARG

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Mol	Chain	Res	Type
1	A	72	CYS
3	C	156	TYR
4	D	162	PRO
5	E	154	GLY
7	G	50	PRO
9	I	60	ALA
2	O	384	SER
2	O	389	SER
3	P	5	ILE
4	Q	133	GLY
4	Q	177	ALA
5	R	127	VAL
7	T	50	PRO
1	A	71	PRO
1	A	81	SER
1	A	443	TRP
2	B	190	GLN
3	C	3	PRO
4	D	38	SER
5	E	80	ASP
5	E	110	ALA
1	N	217	SER
3	P	157	ILE
4	Q	106	ASN
3	C	5	ILE
5	E	8	PRO
2	O	19	PRO
3	C	20	ILE
3	P	20	ILE
3	P	3	PRO
2	B	20	GLY
3	C	209	PRO
2	O	420	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	343 (94%)	22 (6%)	17	43
1	N	365/368 (99%)	343 (94%)	22 (6%)	17	43
2	B	331/347 (95%)	307 (93%)	24 (7%)	13	36
2	O	333/347 (96%)	312 (94%)	21 (6%)	16	41
3	C	328/329 (100%)	319 (97%)	9 (3%)	39	64
3	P	328/329 (100%)	319 (97%)	9 (3%)	39	64
4	D	200/200 (100%)	193 (96%)	7 (4%)	32	59
4	Q	200/200 (100%)	194 (97%)	6 (3%)	36	62
5	E	166/166 (100%)	160 (96%)	6 (4%)	31	58
5	R	165/166 (99%)	158 (96%)	7 (4%)	26	54
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	53
6	S	93/96 (97%)	89 (96%)	4 (4%)	26	53
7	G	71/71 (100%)	68 (96%)	3 (4%)	26	54
7	T	70/71 (99%)	68 (97%)	2 (3%)	37	62
8	H	65/71 (92%)	63 (97%)	2 (3%)	35	61
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	50
9	I	23/26 (88%)	20 (87%)	3 (13%)	4	15
9	V	23/26 (88%)	21 (91%)	2 (9%)	9	30
10	J	49/49 (100%)	45 (92%)	4 (8%)	10	32
10	W	47/49 (96%)	45 (96%)	2 (4%)	26	53
All	All	3378/3446 (98%)	3216 (95%)	162 (5%)	23	50

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	18	THR
1	A	32	GLN
1	A	34	THR
1	A	49	ASN
1	A	67	THR
1	A	102	LEU
1	A	106	MET
1	A	108	LYS
1	A	146	THR
1	A	174	ILE

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Mol	Chain	Res	Type
1	A	181	ASP
1	A	220	SER
1	A	226	ASP
1	A	228	VAL
1	A	248	LEU
1	A	274	ASN
1	A	344	ARG
1	A	350	THR
1	A	395	TRP
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	24	LEU
2	B	31	ASN
2	B	57	TYR
2	B	97	SER
2	B	114	ASP
2	B	124	LEU
2	B	154	SER
2	B	160	LEU
2	B	170	THR
2	B	248	ASN
2	B	250	HIS
2	B	270	ASN
2	B	283	PRO
2	B	304	THR
2	B	306	PRO
2	B	314	VAL
2	B	341	MET
2	B	343	GLN
2	B	344	LEU
2	B	367	THR
2	B	376	GLN
2	B	402	ILE
2	B	424	MET
3	C	14	MET
3	C	44	THR
3	C	175	THR
3	C	216	SER
3	C	223	PRO
3	C	226	SER
3	C	243	LEU

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Mol	Chain	Res	Type
3	C	365	ILE
3	C	374	GLU
4	D	37	CYS
4	D	43	MET
4	D	46	VAL
4	D	58	GLU
4	D	69	GLU
4	D	169	LEU
4	D	215	LEU
5	E	6	THR
5	E	31	ASP
5	E	61	SER
5	E	80	ASP
5	E	178	TYR
5	E	185	TYR
6	F	58	ARG
6	F	59	MET
6	F	64	ARG
6	F	70	LEU
7	G	3	HIS
7	G	63	THR
7	G	79	ASN
8	H	49	HIS
8	H	67	HIS
9	I	68	ILE
9	I	70	LEU
9	I	71	ASN
10	J	16	ARG
10	J	22	LEU
10	J	59	TYR
10	J	64	GLU
1	N	3	THR
1	N	10	ASN
1	N	18	THR
1	N	32	GLN
1	N	49	ASN
1	N	102	LEU
1	N	106	MET
1	N	108	LYS
1	N	174	ILE
1	N	181	ASP
1	N	220	SER

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Mol	Chain	Res	Type
1	N	228	VAL
1	N	248	LEU
1	N	274	ASN
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	344	ARG
1	N	350	THR
1	N	395	TRP
1	N	432	LEU
1	N	443	TRP
2	O	22	GLU
2	O	31	ASN
2	O	57	TYR
2	O	97	SER
2	O	114	ASP
2	O	124	LEU
2	O	154	SER
2	O	160	LEU
2	O	248	ASN
2	O	250	HIS
2	O	260	GLU
2	O	283	PRO
2	O	304	THR
2	O	314	VAL
2	O	341	MET
2	O	343	GLN
2	O	344	LEU
2	O	367	THR
2	O	376	GLN
2	O	402	ILE
2	O	424	MET
3	P	44	THR
3	P	175	THR
3	P	216	SER
3	P	226	SER
3	P	243	LEU
3	P	258	THR
3	P	283	ARG
3	P	365	ILE
3	P	374	GLU
4	Q	37	CYS

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Mol	Chain	Res	Type
4	Q	43	MET
4	Q	58	GLU
4	Q	69	GLU
4	Q	76	GLU
4	Q	215	LEU
5	R	6	THR
5	R	31	ASP
5	R	61	SER
5	R	145	VAL
5	R	178	TYR
5	R	185	TYR
5	R	188	VAL
6	S	58	ARG
6	S	59	MET
6	S	64	ARG
6	S	70	LEU
7	T	3	HIS
7	T	63	THR
8	U	49	HIS
8	U	67	HIS
8	U	71	HIS
9	V	68	ILE
9	V	70	LEU
10	W	22	LEU
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	49	ASN
1	A	118	GLN
1	A	159	GLN
1	A	173	ASN
1	A	176	HIS
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
1	A	368	GLN
1	A	435	ASN
2	B	31	ASN
2	B	153	GLN

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Mol	Chain	Res	Type
2	B	156	GLN
2	B	197	ASN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	69	HIS
3	C	73	ASN
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
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	28	ASN
7	G	44	GLN
7	G	73	ASN
8	H	71	HIS
8	H	75	ASN
9	I	71	ASN
1	N	6	GLN
1	N	10	ASN
1	N	49	ASN
1	N	118	GLN
1	N	159	GLN
1	N	274	ASN
1	N	289	HIS

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Mol	Chain	Res	Type
1	N	308	GLN
1	N	339	GLN
1	N	368	GLN
1	N	435	ASN
2	O	31	ASN
2	O	156	GLN
2	O	197	ASN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	363	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	6	HIS
4	Q	35	GLN
4	Q	50	ASN
4	Q	105	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	26	GLN
5	R	57	GLN
5	R	164	HIS
5	R	186	GLN
6	S	72	HIS
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
14	CDL	C	2004	-	39,39,99	1.23	2 (5%)	45,51,111	1.13	4 (8%)
18	BOG	D	2091	-	13,13,20	1.47	4 (30%)	18,18,25	1.19	2 (11%)
18	BOG	D	2009	-	20,20,20	1.08	1 (5%)	25,25,25	0.92	1 (4%)
18	BOG	Q	3009	-	20,20,20	1.13	3 (15%)	25,25,25	1.01	2 (8%)
12	IKR	P	3001	-	26,26,26	1.54	6 (23%)	33,35,35	1.59	6 (18%)
13	UQ	P	3002	-	19,19,63	2.57	10 (52%)	24,26,79	1.43	3 (12%)
15	PEE	P	3007	-	48,48,50	1.42	5 (10%)	51,53,55	0.78	2 (3%)
11	HEM	P	502	3	50,50,50	1.54	7 (14%)	67,82,82	1.47	7 (10%)
16	GOL	P	3011	-	5,5,5	1.39	0	5,5,5	0.63	0
13	UQ	C	2002	-	19,19,63	2.65	10 (52%)	24,26,79	1.43	3 (12%)
15	PEE	R	3005	-	49,49,50	1.62	11 (22%)	52,54,55	0.89	3 (5%)
11	HEM	C	502	3	50,50,50	1.52	9 (18%)	67,82,82	1.65	10 (14%)
11	HEM	C	501	3	50,50,50	1.35	6 (12%)	67,82,82	1.39	10 (14%)
14	CDL	Q	3003	-	41,41,99	1.22	2 (4%)	47,53,111	1.07	2 (4%)
18	BOG	P	2010	-	12,12,20	1.44	4 (33%)	17,17,25	0.59	0
15	PEE	C	2008	-	20,20,50	1.86	6 (30%)	23,25,55	0.66	0
19	FES	R	501	5	0,4,4	-	-	-	-	-
18	BOG	Q	3091	-	13,13,20	1.56	3 (23%)	18,18,25	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	GOL	C	2011	-	5,5,5	1.63	1 (20%)	5,5,5	0.80	0
12	IKR	C	2001	-	26,26,26	1.77	8 (30%)	33,35,35	1.53	6 (18%)
15	PEE	C	2007	-	48,48,50	1.44	6 (12%)	51,53,55	0.81	2 (3%)
11	HEM	P	501	3	50,50,50	1.43	6 (12%)	67,82,82	1.37	8 (11%)
14	CDL	P	3004	-	39,39,99	1.26	3 (7%)	45,51,111	1.14	4 (8%)
15	PEE	P	3008	-	4,4,50	3.67	4 (100%)	6,6,55	0.63	0
14	CDL	D	2003	-	41,41,99	1.22	2 (4%)	47,53,111	1.08	2 (4%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
15	PEE	E	2005	-	49,49,50	1.54	10 (20%)	52,54,55	0.87	3 (5%)
17	HEC	Q	501	4	46,50,50	1.62	4 (8%)	58,82,82	2.27	9 (15%)
17	HEC	D	501	4	46,50,50	1.78	10 (21%)	58,82,82	2.46	13 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	C	2004	-	-	22/49/49/110	-
18	BOG	D	2091	-	-	3/4/24/31	0/1/1/1
18	BOG	D	2009	-	-	5/11/31/31	0/1/1/1
18	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
12	IKR	P	3001	-	-	0/18/18/18	0/2/2/2
13	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
15	PEE	P	3007	-	-	26/52/52/54	-
11	HEM	P	502	3	-	9/14/54/54	-
16	GOL	P	3011	-	-	3/4/4/4	-
13	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
15	PEE	R	3005	-	-	22/53/53/54	-
11	HEM	C	502	3	-	8/14/54/54	-
11	HEM	C	501	3	-	8/14/54/54	-
14	CDL	Q	3003	-	-	14/51/51/110	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
15	PEE	C	2008	-	-	9/24/24/54	-
19	FES	R	501	5	-	-	0/1/1/1
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
16	GOL	C	2011	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
15	PEE	C	2007	-	-	26/52/52/54	-
11	HEM	P	501	3	-	9/14/54/54	-
14	CDL	P	3004	-	-	20/49/49/110	-
14	CDL	D	2003	-	-	15/51/51/110	-
19	FES	E	501	5	-	-	0/1/1/1
15	PEE	E	2005	-	-	27/53/53/54	-
17	HEC	Q	501	4	-	10/14/54/54	-
17	HEC	D	501	4	-	10/14/54/54	-

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	CAC-C3C	5.80	1.53	1.35
17	D	501	HEC	CAB-C3B	5.74	1.53	1.35
17	Q	501	HEC	CAB-C3B	5.37	1.52	1.35
17	D	501	HEC	CAC-C3C	5.06	1.51	1.35
15	P	3008	PEE	P-O1P	4.98	1.62	1.50
13	P	3002	UQ	C7-C6	4.94	1.60	1.51
13	P	3002	UQ	C6-C5	4.90	1.44	1.35
13	C	2002	UQ	C6-C5	4.61	1.43	1.35
11	P	501	HEM	CBC-CAC	4.61	1.52	1.30
13	C	2002	UQ	C7-C6	4.59	1.59	1.51
11	C	501	HEM	CBC-CAC	4.58	1.52	1.30
11	P	502	HEM	CBB-CAB	4.57	1.52	1.30
11	P	501	HEM	CBB-CAB	4.55	1.52	1.30
11	C	502	HEM	CBB-CAB	4.41	1.51	1.30
15	C	2007	PEE	C39-C38	4.21	1.55	1.31
15	P	3007	PEE	C39-C38	4.20	1.55	1.31
15	R	3005	PEE	C39-C38	4.15	1.55	1.31
15	E	2005	PEE	C39-C38	4.14	1.55	1.31
11	C	502	HEM	CBC-CAC	4.13	1.50	1.30
11	P	502	HEM	CBC-CAC	4.05	1.49	1.30
13	C	2002	UQ	C6-C1	4.00	1.57	1.46
13	C	2002	UQ	O3-C3	3.87	1.46	1.36
15	R	3005	PEE	O2-C10	3.84	1.45	1.34
12	C	2001	IKR	C40-C2	3.69	1.57	1.51
13	P	3002	UQ	C6-C1	3.67	1.56	1.46
11	C	501	HEM	CBB-CAB	3.58	1.47	1.30
15	C	2008	PEE	O2-C10	3.47	1.44	1.34
13	P	3002	UQ	O3-C3	3.45	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	2005	PEE	O2-C10	3.40	1.43	1.34
15	P	3008	PEE	P-O3P	3.39	1.64	1.54
15	P	3007	PEE	C21-C22	-3.38	1.35	1.51
15	P	3008	PEE	P-O4P	3.35	1.64	1.54
15	E	2005	PEE	O3-C30	3.31	1.43	1.33
11	C	501	HEM	CAB-C3B	-3.28	1.38	1.47
15	R	3005	PEE	C11-C10	3.27	1.60	1.50
15	R	3005	PEE	O3-C30	3.25	1.42	1.33
15	R	3005	PEE	P-O1P	3.23	1.62	1.50
15	C	2007	PEE	O3-C30	3.23	1.42	1.33
15	C	2008	PEE	P-O1P	3.22	1.62	1.50
15	R	3005	PEE	C21-C22	-3.20	1.35	1.51
15	P	3007	PEE	O3-C30	3.19	1.42	1.33
17	D	501	HEC	C3B-C2B	-3.17	1.30	1.41
12	C	2001	IKR	C24-C17	3.14	1.44	1.39
15	C	2007	PEE	P-O1P	3.14	1.61	1.50
15	C	2008	PEE	O3-C30	3.14	1.42	1.33
11	P	502	HEM	CAC-C3C	-3.14	1.39	1.47
11	P	502	HEM	CAB-C3B	-3.13	1.39	1.47
11	C	502	HEM	CAB-C3B	-3.13	1.39	1.47
15	E	2005	PEE	C21-C22	-3.12	1.36	1.51
17	D	501	HEC	C1D-ND	-3.12	1.33	1.39
12	P	3001	IKR	C40-C2	3.10	1.56	1.51
15	E	2005	PEE	P-O1P	3.09	1.61	1.50
12	C	2001	IKR	C21-C20	3.09	1.44	1.39
15	C	2007	PEE	C21-C22	-3.08	1.36	1.51
12	C	2001	IKR	C3-C4	3.01	1.44	1.38
13	C	2002	UQ	C3-C4	3.00	1.57	1.48
15	P	3007	PEE	P-O1P	2.97	1.61	1.50
15	E	2005	PEE	C11-C10	2.95	1.59	1.50
11	P	501	HEM	CAC-C3C	-2.94	1.39	1.47
13	C	2002	UQ	O2-C2	2.94	1.43	1.36
15	P	3007	PEE	O2-C10	2.93	1.42	1.34
11	P	501	HEM	CAB-C3B	-2.90	1.39	1.47
13	C	2002	UQ	C2-C1	2.88	1.57	1.48
12	P	3001	IKR	C3-C4	2.87	1.43	1.38
15	C	2007	PEE	O2-C10	2.87	1.42	1.34
11	C	502	HEM	C3B-C4B	2.80	1.50	1.44
12	P	3001	IKR	C24-C17	2.78	1.44	1.39
18	Q	3091	BOG	O5-C1	2.76	1.48	1.41
13	P	3002	UQ	C5-C4	2.76	1.56	1.47
13	P	3002	UQ	C2-C1	2.70	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	501	HEM	CAC-C3C	-2.69	1.40	1.47
18	Q	3091	BOG	C4-C5	2.69	1.58	1.53
17	Q	501	HEC	C3B-C2B	-2.68	1.32	1.41
11	C	502	HEM	CAC-C3C	-2.67	1.40	1.47
12	C	2001	IKR	C1-I1	-2.63	2.04	2.10
13	P	3002	UQ	C3-C4	2.63	1.56	1.48
15	E	2005	PEE	C31-C30	2.61	1.58	1.50
18	D	2091	BOG	O5-C1	2.60	1.48	1.41
12	P	3001	IKR	C21-C20	2.58	1.43	1.39
13	C	2002	UQ	C5-C4	2.57	1.56	1.47
13	C	2002	UQ	C7-C8	2.56	1.54	1.50
11	P	502	HEM	C1B-C2B	2.56	1.49	1.44
13	P	3002	UQ	C7-C8	2.52	1.54	1.50
15	P	3008	PEE	P-O2P	2.50	1.61	1.54
17	D	501	HEC	C3C-C2C	-2.47	1.32	1.41
15	R	3005	PEE	C31-C30	2.44	1.57	1.50
13	P	3002	UQ	CM5-C5	2.44	1.55	1.50
13	C	2002	UQ	CM5-C5	2.43	1.55	1.50
15	C	2008	PEE	C11-C10	2.43	1.57	1.50
18	Q	3009	BOG	O5-C1	2.43	1.48	1.41
18	D	2091	BOG	C4-C5	2.42	1.58	1.53
14	P	3004	CDL	O1-C1	2.40	1.50	1.43
13	P	3002	UQ	O2-C2	2.40	1.42	1.36
14	C	2004	CDL	O1-C1	2.38	1.50	1.43
17	Q	501	HEC	C1D-ND	-2.35	1.35	1.39
11	C	502	HEM	C4D-C3D	2.34	1.49	1.45
17	D	501	HEC	C4C-NC	-2.34	1.35	1.39
14	C	2004	CDL	CB3-CB4	2.34	1.58	1.50
14	D	2003	CDL	O1-C1	2.32	1.50	1.43
16	C	2011	GOL	O2-C2	2.32	1.50	1.43
15	C	2008	PEE	C1-C2	2.32	1.58	1.50
11	P	502	HEM	CMB-C2B	2.29	1.55	1.50
18	Q	3091	BOG	O5-C5	2.29	1.50	1.44
11	C	502	HEM	C1B-C2B	2.28	1.49	1.44
14	D	2003	CDL	OA6-CA5	2.28	1.40	1.34
15	R	3005	PEE	C3-C2	2.26	1.57	1.50
14	P	3004	CDL	CB3-CB4	2.26	1.57	1.50
18	P	2010	BOG	O5-C1	2.25	1.48	1.42
18	P	2010	BOG	C4-C5	2.25	1.57	1.53
12	C	2001	IKR	C22-C21	2.25	1.42	1.38
11	P	502	HEM	C3B-C4B	2.24	1.49	1.44
17	D	501	HEC	CHD-C1D	-2.23	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Q	3003	CDL	O1-C1	2.23	1.49	1.43
11	C	502	HEM	C1C-NC	-2.23	1.35	1.39
18	D	2009	BOG	O5-C1	2.23	1.47	1.41
17	D	501	HEC	C1B-NB	-2.22	1.35	1.39
11	C	501	HEM	CMC-C2C	2.22	1.55	1.50
15	R	3005	PEE	P-O4P	2.22	1.68	1.59
17	D	501	HEC	C3D-C2D	-2.20	1.33	1.38
17	D	501	HEC	C1C-C2C	2.20	1.48	1.43
18	P	2010	BOG	C1-C2	2.19	1.57	1.52
15	E	2005	PEE	P-O4P	2.16	1.67	1.59
18	P	2010	BOG	C4-C3	2.15	1.57	1.52
12	C	2001	IKR	C2-C1	2.15	1.42	1.39
15	R	3005	PEE	C1-C2	2.14	1.57	1.50
15	C	2008	PEE	C3-C2	2.13	1.57	1.50
14	Q	3003	CDL	OA6-CA5	2.13	1.40	1.34
18	Q	3009	BOG	C1-C2	2.12	1.58	1.52
11	P	501	HEM	CHA-C4D	-2.12	1.34	1.38
11	C	502	HEM	C3C-C2C	-2.11	1.32	1.37
18	Q	3009	BOG	C4-C5	2.11	1.57	1.53
12	P	3001	IKR	C1-I1	-2.10	2.05	2.10
11	P	501	HEM	CMD-C2D	2.10	1.55	1.50
15	C	2007	PEE	C31-C30	2.10	1.56	1.50
12	C	2001	IKR	C20-C17	2.09	1.43	1.40
18	D	2091	BOG	C1-C2	2.08	1.58	1.52
15	R	3005	PEE	O2-C2	2.07	1.51	1.46
15	E	2005	PEE	C3-C2	2.04	1.57	1.50
15	E	2005	PEE	C1-C2	2.01	1.57	1.50
14	P	3004	CDL	OB8-CB7	2.00	1.39	1.33
18	D	2091	BOG	C4-C3	2.00	1.57	1.52
11	C	501	HEM	CHA-C4D	-2.00	1.34	1.38
12	P	3001	IKR	C20-C17	2.00	1.43	1.40

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CBC-CAC-C3C	-11.88	103.68	127.43
17	Q	501	HEC	CBC-CAC-C3C	-11.68	104.10	127.43
17	D	501	HEC	CBB-CAB-C3B	-6.60	114.25	127.43
11	C	502	HEM	C3B-C2B-C1B	-6.50	101.53	106.41
17	Q	501	HEC	CBB-CAB-C3B	-6.32	114.81	127.43
11	P	502	HEM	C3B-C2B-C1B	-6.21	101.75	106.41
12	P	3001	IKR	C40-C2-C1	5.03	127.00	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CMC-C2C-C1C	4.86	132.82	125.42
13	C	2002	UQ	C8-C7-C6	4.78	123.86	112.08
12	C	2001	IKR	C40-C2-C1	4.71	126.77	123.40
13	P	3002	UQ	C8-C7-C6	4.63	123.50	112.08
11	C	502	HEM	CMB-C2B-C1B	4.61	132.24	125.03
17	Q	501	HEC	CAA-C2A-C1A	4.44	133.87	124.85
17	D	501	HEC	CAA-C2A-C1A	4.32	133.63	124.85
17	D	501	HEC	CAA-C2A-C3A	-4.08	120.22	127.87
11	C	502	HEM	C2B-C1B-NB	3.97	114.41	109.84
18	Q	3009	BOG	C1'-O1-C1	3.94	120.41	113.68
11	P	501	HEM	C3B-C2B-C1B	-3.88	103.50	106.41
11	P	502	HEM	CMB-C2B-C1B	3.70	130.81	125.03
18	D	2091	BOG	C1'-O1-C1	3.68	118.86	113.26
11	C	501	HEM	C3B-C4B-NB	3.64	112.08	109.47
13	P	3002	UQ	C7-C6-C1	-3.64	114.29	118.52
11	C	501	HEM	CBA-CAA-C2A	-3.61	102.54	112.53
18	D	2009	BOG	C1'-O1-C1	3.55	119.74	113.68
18	Q	3091	BOG	C1'-O1-C1	3.54	118.64	113.26
17	Q	501	HEC	CAA-C2A-C3A	-3.54	121.24	127.87
13	C	2002	UQ	C7-C6-C1	-3.54	114.41	118.52
17	Q	501	HEC	CMC-C2C-C1C	3.51	130.76	125.42
12	P	3001	IKR	C40-C2-C3	-3.44	113.52	119.57
11	P	502	HEM	C2B-C1B-NB	3.30	113.64	109.84
11	P	501	HEM	C3B-C4B-NB	3.28	111.83	109.47
11	C	501	HEM	CAD-C3D-C4D	3.26	130.39	124.70
17	D	501	HEC	CAD-C3D-C4D	3.19	131.18	124.94
14	P	3004	CDL	CB4-OB6-CB5	-3.15	110.25	117.80
12	C	2001	IKR	C40-C2-C3	-3.15	114.02	119.57
14	C	2004	CDL	CB4-OB6-CB5	-3.09	110.40	117.80
11	P	501	HEM	CAD-C3D-C4D	3.03	129.97	124.70
11	P	501	HEM	C2B-C1B-NB	2.89	113.17	109.84
15	E	2005	PEE	C22-C21-C20	2.89	127.77	113.86
17	D	501	HEC	CMB-C2B-C1B	2.87	129.78	125.42
15	R	3005	PEE	C22-C21-C20	2.84	127.52	113.86
11	P	501	HEM	CBA-CAA-C2A	-2.82	104.73	112.53
11	P	502	HEM	CAD-C3D-C2D	-2.78	122.66	127.87
14	D	2003	CDL	CB4-OB6-CB5	-2.75	111.21	117.80
15	C	2007	PEE	C22-C21-C20	2.74	127.04	113.86
18	D	2091	BOG	O1-C1-C2	2.70	111.26	108.14
14	P	3004	CDL	CA6-CA4-CA3	-2.69	105.50	111.78
17	Q	501	HEC	CAD-C3D-C4D	2.69	130.19	124.94
11	P	501	HEM	C2D-C1D-ND	2.68	113.01	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	2004	CDL	CA4-OA6-CA5	-2.68	111.38	117.80
11	C	502	HEM	CMC-C2C-C1C	2.68	129.44	124.73
17	Q	501	HEC	CBA-CAA-C2A	2.68	119.93	112.53
12	P	3001	IKR	O31-C30-O36	2.67	128.62	123.50
11	C	502	HEM	CAD-C3D-C2D	-2.65	122.91	127.87
11	C	501	HEM	CAD-C3D-C2D	-2.64	122.92	127.87
15	C	2007	PEE	C21-C22-C23	2.63	127.69	114.37
11	P	502	HEM	CAD-C3D-C4D	2.59	129.21	124.70
11	C	502	HEM	CAD-C3D-C4D	2.55	129.14	124.70
11	P	501	HEM	CAD-C3D-C2D	-2.54	123.11	127.87
15	P	3007	PEE	C22-C21-C20	2.52	125.97	113.86
11	C	501	HEM	C3B-C2B-C1B	-2.52	104.52	106.41
15	E	2005	PEE	C21-C22-C23	2.52	127.09	114.37
12	C	2001	IKR	O31-C30-O36	2.51	128.31	123.50
18	Q	3091	BOG	O1-C1-C2	2.50	111.03	108.14
15	P	3007	PEE	C21-C22-C23	2.50	126.98	114.37
15	R	3005	PEE	C21-C22-C23	2.49	126.94	114.37
14	Q	3003	CDL	CB4-OB6-CB5	-2.48	111.85	117.80
14	C	2004	CDL	CA6-CA4-CA3	-2.43	106.11	111.78
14	D	2003	CDL	CA6-CA4-CA3	-2.43	106.12	111.78
11	C	501	HEM	C3C-C2C-C1C	-2.41	104.76	107.05
17	D	501	HEC	CMC-C2C-C3C	-2.40	120.90	126.55
12	P	3001	IKR	O31-C30-C29	-2.39	109.19	111.75
17	D	501	HEC	C2A-C1A-NA	2.39	112.63	110.32
11	C	502	HEM	C4A-C3A-C2A	-2.39	104.08	106.82
12	C	2001	IKR	O31-C30-C29	-2.39	109.20	111.75
11	C	501	HEM	C3D-C4D-ND	2.34	112.74	110.17
14	Q	3003	CDL	CA6-CA4-CA3	-2.34	106.34	111.78
17	Q	501	HEC	C3D-C4D-ND	2.32	112.72	110.15
14	P	3004	CDL	CA4-OA6-CA5	-2.31	112.26	117.80
14	P	3004	CDL	OB6-CB4-CB3	2.30	116.58	108.34
11	C	502	HEM	C4A-NA-C1A	-2.28	102.11	105.82
14	C	2004	CDL	OB6-CB4-CB3	2.26	116.45	108.34
12	C	2001	IKR	C2-C1-I1	-2.24	118.93	120.69
12	P	3001	IKR	O15-C4-C5	2.23	119.73	114.94
11	P	502	HEM	C4C-C3C-C2C	-2.22	104.89	106.81
11	C	501	HEM	C2B-C1B-NB	2.22	112.39	109.84
17	Q	501	HEC	C1A-C2A-C3A	-2.22	104.19	107.11
12	C	2001	IKR	O15-C4-C5	2.20	119.67	114.94
12	P	3001	IKR	C6-C1-C2	-2.18	120.57	122.20
13	P	3002	UQ	C10-C9-C8	-2.17	118.05	123.63
15	R	3005	PEE	O3-C3-C2	2.17	114.66	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	2002	UQ	C10-C9-C8	-2.15	118.11	123.63
17	D	501	HEC	CHC-C4B-NB	-2.13	122.13	124.45
11	P	501	HEM	C1D-C2D-C3D	-2.12	104.75	106.98
11	C	501	HEM	C4D-ND-C1D	-2.11	102.71	105.21
11	C	502	HEM	C2D-C1D-ND	2.11	112.34	109.90
17	D	501	HEC	C4B-NB-C1B	-2.10	102.40	105.82
11	C	501	HEM	C2D-C1D-ND	2.07	112.30	109.90
11	P	502	HEM	CHB-C4A-C3A	-2.07	121.42	127.43
15	E	2005	PEE	O3-C3-C2	2.07	114.36	108.40
17	D	501	HEC	CBA-CAA-C2A	2.06	118.22	112.53
18	Q	3009	BOG	O1-C1-C2	2.05	111.39	108.27
11	C	502	HEM	C1B-NB-C4B	-2.04	102.80	105.21
17	D	501	HEC	C3D-C4D-ND	2.03	112.41	110.15

There are no chirality outliers.

All (266) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	2002	UQ	C1-C6-C7-C8
13	C	2002	UQ	C5-C6-C7-C8
13	C	2002	UQ	C12-C11-C9-C8
13	C	2002	UQ	C12-C11-C9-C10
13	P	3002	UQ	C1-C6-C7-C8
13	P	3002	UQ	C5-C6-C7-C8
13	P	3002	UQ	C12-C11-C9-C8
13	P	3002	UQ	C12-C11-C9-C10
14	C	2004	CDL	CB2-C1-CA2-OA2
14	C	2004	CDL	CB3-OB5-PB2-OB3
14	C	2004	CDL	C51-CB5-OB6-CB4
14	D	2003	CDL	CA2-OA2-PA1-OA4
14	D	2003	CDL	CA2-OA2-PA1-OA5
14	P	3004	CDL	CB2-C1-CA2-OA2
14	P	3004	CDL	CA2-C1-CB2-OB2
14	P	3004	CDL	CB3-OB5-PB2-OB3
14	P	3004	CDL	C51-CB5-OB6-CB4
14	Q	3003	CDL	CA2-OA2-PA1-OA4
14	Q	3003	CDL	CA2-OA2-PA1-OA5
15	C	2007	PEE	C1-O3P-P-O2P
15	C	2007	PEE	C1-O3P-P-O1P
15	C	2007	PEE	C4-O4P-P-O3P
15	C	2007	PEE	C4-O4P-P-O2P
15	C	2007	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
15	C	2007	PEE	O4P-C4-C5-N
15	C	2008	PEE	C4-O4P-P-O3P
15	C	2008	PEE	C4-O4P-P-O2P
15	C	2008	PEE	C4-O4P-P-O1P
15	E	2005	PEE	C11-C10-O2-C2
15	E	2005	PEE	C1-O3P-P-O2P
15	E	2005	PEE	C1-O3P-P-O1P
15	E	2005	PEE	C1-O3P-P-O4P
15	E	2005	PEE	O4P-C4-C5-N
15	P	3007	PEE	C1-O3P-P-O2P
15	P	3007	PEE	C1-O3P-P-O1P
15	P	3007	PEE	C4-O4P-P-O3P
15	P	3007	PEE	C4-O4P-P-O2P
15	P	3007	PEE	C4-O4P-P-O1P
15	P	3007	PEE	O4P-C4-C5-N
15	R	3005	PEE	C11-C10-O2-C2
15	R	3005	PEE	C1-O3P-P-O2P
15	R	3005	PEE	C1-O3P-P-O1P
15	R	3005	PEE	C1-O3P-P-O4P
15	R	3005	PEE	O4P-C4-C5-N
16	C	2011	GOL	O1-C1-C2-C3
16	P	3011	GOL	O1-C1-C2-C3
17	D	501	HEC	C3A-C2A-CAA-CBA
17	D	501	HEC	C2B-C3B-CAB-CBB
17	D	501	HEC	C4B-C3B-CAB-CBB
17	D	501	HEC	C2C-C3C-CAC-CBC
17	D	501	HEC	C4C-C3C-CAC-CBC
17	Q	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C2B-C3B-CAB-CBB
17	Q	501	HEC	C4B-C3B-CAB-CBB
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
14	D	2003	CDL	C31-CA7-OA8-CA6
14	Q	3003	CDL	C31-CA7-OA8-CA6
15	C	2008	PEE	O5-C30-O3-C3
14	C	2004	CDL	OB9-CB7-OB8-CB6
14	P	3004	CDL	OB9-CB7-OB8-CB6
15	E	2005	PEE	O5-C30-O3-C3
15	R	3005	PEE	O5-C30-O3-C3
14	D	2003	CDL	OA9-CA7-OA8-CA6
15	E	2005	PEE	O4-C10-O2-C2
15	R	3005	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
15	C	2008	PEE	C31-C30-O3-C3
15	E	2005	PEE	C31-C30-O3-C3
15	R	3005	PEE	C31-C30-O3-C3
14	Q	3003	CDL	OA9-CA7-OA8-CA6
14	C	2004	CDL	C31-CA7-OA8-CA6
14	P	3004	CDL	C31-CA7-OA8-CA6
14	C	2004	CDL	C71-CB7-OB8-CB6
14	P	3004	CDL	C71-CB7-OB8-CB6
17	Q	501	HEC	C1A-C2A-CAA-CBA
14	C	2004	CDL	OB7-CB5-OB6-CB4
14	P	3004	CDL	OB7-CB5-OB6-CB4
14	C	2004	CDL	O1-C1-CA2-OA2
14	P	3004	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
14	C	2004	CDL	OA9-CA7-OA8-CA6
17	D	501	HEC	C1A-C2A-CAA-CBA
14	D	2003	CDL	C71-CB7-OB8-CB6
14	Q	3003	CDL	C71-CB7-OB8-CB6
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'
14	D	2003	CDL	OB9-CB7-OB8-CB6
18	D	2091	BOG	O5-C1-O1-C1'
14	P	3004	CDL	OA9-CA7-OA8-CA6
18	Q	3009	BOG	O1-C1'-C2'-C3'
18	D	2009	BOG	O1-C1'-C2'-C3'
15	R	3005	PEE	C30-C31-C32-C33
14	Q	3003	CDL	OB9-CB7-OB8-CB6
15	E	2005	PEE	C30-C31-C32-C33
15	C	2007	PEE	C17-C18-C19-C20
15	P	3007	PEE	C17-C18-C19-C20
14	C	2004	CDL	C11-CA5-OA6-CA4
14	C	2004	CDL	OA7-CA5-OA6-CA4
14	P	3004	CDL	C11-CA5-OA6-CA4
14	P	3004	CDL	OA7-CA5-OA6-CA4
15	C	2008	PEE	C10-C11-C12-C13
15	C	2007	PEE	C10-C11-C12-C13
14	C	2004	CDL	CA2-C1-CB2-OB2
15	P	3007	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	R	3005	PEE	C35-C36-C37-C38
15	R	3005	PEE	C22-C23-C24-C25
15	E	2005	PEE	C22-C23-C24-C25
15	P	3007	PEE	C20-C21-C22-C23
15	R	3005	PEE	C34-C35-C36-C37
15	E	2005	PEE	C20-C21-C22-C23
14	Q	3003	CDL	CB7-C71-C72-C73
15	C	2007	PEE	C20-C21-C22-C23
15	C	2007	PEE	C15-C16-C17-C18
15	C	2007	PEE	C35-C36-C37-C38
15	E	2005	PEE	C35-C36-C37-C38
15	P	3007	PEE	C15-C16-C17-C18
15	P	3007	PEE	C35-C36-C37-C38
15	E	2005	PEE	C34-C35-C36-C37
15	P	3007	PEE	C33-C34-C35-C36
15	C	2007	PEE	C33-C34-C35-C36
15	R	3005	PEE	C20-C21-C22-C23
14	D	2003	CDL	CB7-C71-C72-C73
15	C	2007	PEE	O3P-C1-C2-O2
15	P	3007	PEE	O3P-C1-C2-O2
16	C	2011	GOL	O1-C1-C2-O2
16	P	3011	GOL	O1-C1-C2-O2
15	P	3007	PEE	C39-C40-C41-C42
15	P	3007	PEE	C40-C41-C42-C43
15	R	3005	PEE	C11-C12-C13-C14
11	C	502	HEM	C4D-C3D-CAD-CBD
14	C	2004	CDL	CA3-CA4-CA6-OA8
14	P	3004	CDL	CA3-CA4-CA6-OA8
18	Q	3009	BOG	C2'-C3'-C4'-C5'
15	E	2005	PEE	C11-C12-C13-C14
15	C	2007	PEE	C40-C41-C42-C43
15	E	2005	PEE	O3P-C1-C2-O2
14	D	2003	CDL	OA6-CA4-CA6-OA8
14	Q	3003	CDL	OA6-CA4-CA6-OA8
14	P	3004	CDL	O1-C1-CB2-OB2
15	C	2007	PEE	C11-C12-C13-C14
15	C	2007	PEE	C39-C40-C41-C42
18	D	2009	BOG	C2'-C3'-C4'-C5'
15	R	3005	PEE	C42-C43-C44-C45
15	E	2005	PEE	C43-C44-C45-C46
15	R	3005	PEE	C43-C44-C45-C46
15	C	2007	PEE	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	C11-C12-C13-C14
15	P	3007	PEE	C43-C44-C45-C46
14	D	2003	CDL	CA3-CA4-CA6-OA8
14	Q	3003	CDL	CA3-CA4-CA6-OA8
14	Q	3003	CDL	C71-C72-C73-C74
14	D	2003	CDL	C71-C72-C73-C74
14	C	2004	CDL	OB5-CB3-CB4-OB6
14	P	3004	CDL	OB5-CB3-CB4-OB6
16	C	2011	GOL	O2-C2-C3-O3
16	P	3011	GOL	O2-C2-C3-O3
15	C	2007	PEE	O3P-C1-C2-C3
15	C	2008	PEE	O3P-C1-C2-C3
15	P	3007	PEE	O3P-C1-C2-C3
11	C	501	HEM	C3D-CAD-CBD-CGD
11	C	501	HEM	C2B-C3B-CAB-CBB
11	C	501	HEM	C2C-C3C-CAC-CBC
11	C	502	HEM	C2B-C3B-CAB-CBB
11	C	502	HEM	C2C-C3C-CAC-CBC
11	P	501	HEM	C2C-C3C-CAC-CBC
11	P	502	HEM	C2B-C3B-CAB-CBB
11	P	502	HEM	C2C-C3C-CAC-CBC
15	E	2005	PEE	C42-C43-C44-C45
15	R	3005	PEE	O3P-C1-C2-O2
15	C	2008	PEE	O2-C2-C3-O3
15	R	3005	PEE	C39-C40-C41-C42
11	P	502	HEM	C4D-C3D-CAD-CBD
15	E	2005	PEE	C39-C40-C41-C42
14	C	2004	CDL	OB5-CB3-CB4-CB6
17	Q	501	HEC	C4C-C3C-CAC-CBC
14	C	2004	CDL	CA3-OA5-PA1-OA2
14	C	2004	CDL	CA3-OA5-PA1-OA3
14	C	2004	CDL	CB3-OB5-PB2-OB2
14	C	2004	CDL	CB3-OB5-PB2-OB4
14	P	3004	CDL	CA3-OA5-PA1-OA3
14	P	3004	CDL	CB3-OB5-PB2-OB2
14	P	3004	CDL	CB3-OB5-PB2-OB4
15	C	2007	PEE	C1-O3P-P-O4P
15	E	2005	PEE	C4-O4P-P-O2P
15	P	3007	PEE	C1-O3P-P-O4P
17	Q	501	HEC	C2C-C3C-CAC-CBC
14	P	3004	CDL	OB5-CB3-CB4-CB6
14	Q	3003	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	C21-C22-C23-C24
14	C	2004	CDL	OA6-CA4-CA6-OA8
14	P	3004	CDL	OA6-CA4-CA6-OA8
15	C	2008	PEE	C1-C2-C3-O3
15	C	2007	PEE	C21-C22-C23-C24
15	C	2007	PEE	C41-C42-C43-C44
11	P	501	HEM	C3D-CAD-CBD-CGD
15	C	2007	PEE	C34-C35-C36-C37
15	E	2005	PEE	C1-C2-O2-C10
15	R	3005	PEE	C1-C2-O2-C10
14	C	2004	CDL	O1-C1-CB2-OB2
11	P	502	HEM	CAA-CBA-CGA-O1A
11	P	502	HEM	CAA-CBA-CGA-O2A
15	E	2005	PEE	C36-C37-C38-C39
11	C	502	HEM	CAA-CBA-CGA-O1A
11	C	502	HEM	CAA-CBA-CGA-O2A
15	E	2005	PEE	C14-C15-C16-C17
15	R	3005	PEE	C14-C15-C16-C17
15	P	3007	PEE	C41-C42-C43-C44
11	P	501	HEM	CAA-CBA-CGA-O2A
14	D	2003	CDL	OA5-CA3-CA4-OA6
15	R	3005	PEE	C41-C42-C43-C44
11	P	501	HEM	CAA-CBA-CGA-O1A
18	D	2009	BOG	C1'-C2'-C3'-C4'
17	D	501	HEC	CAA-CBA-CGA-O2A
15	E	2005	PEE	C40-C41-C42-C43
14	Q	3003	CDL	OA5-CA3-CA4-CA6
11	P	501	HEM	CAD-CBD-CGD-O2D
15	R	3005	PEE	C36-C37-C38-C39
11	P	502	HEM	CAD-CBD-CGD-O1D
11	P	502	HEM	CAD-CBD-CGD-O2D
11	P	501	HEM	C2B-C3B-CAB-CBB
11	C	501	HEM	CAD-CBD-CGD-O2D
14	C	2004	CDL	CB5-C51-C52-C53
11	P	501	HEM	CAD-CBD-CGD-O1D
17	D	501	HEC	CAA-CBA-CGA-O1A
11	C	501	HEM	C4B-C3B-CAB-CBB
11	C	502	HEM	C4B-C3B-CAB-CBB
11	P	501	HEM	C4B-C3B-CAB-CBB
11	P	501	HEM	C4C-C3C-CAC-CBC
11	P	502	HEM	C4B-C3B-CAB-CBB
11	P	502	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	C	501	HEM	CAD-CBD-CGD-O1D
15	E	2005	PEE	C41-C42-C43-C44
11	C	502	HEM	CAD-CBD-CGD-O2D
17	D	501	HEC	CAD-CBD-CGD-O2D
11	C	501	HEM	CAA-CBA-CGA-O1A
14	D	2003	CDL	OA5-CA3-CA4-CA6
14	D	2003	CDL	OB5-CB3-CB4-CB6
14	Q	3003	CDL	OB5-CB3-CB4-CB6
15	E	2005	PEE	O3P-C1-C2-C3
11	C	501	HEM	CAA-CBA-CGA-O2A
17	Q	501	HEC	CAD-CBD-CGD-O2D
11	C	502	HEM	CAD-CBD-CGD-O1D
18	D	2091	BOG	C4-C5-C6-O6
17	Q	501	HEC	CAA-CBA-CGA-O2A
15	E	2005	PEE	C23-C24-C25-C26
15	P	3007	PEE	C34-C35-C36-C37
17	D	501	HEC	CAD-CBD-CGD-O1D
17	Q	501	HEC	CAD-CBD-CGD-O1D
15	C	2007	PEE	O2-C10-C11-C12
15	P	3007	PEE	O3-C30-C31-C32
15	C	2007	PEE	O3-C30-C31-C32
15	P	3007	PEE	O2-C10-C11-C12
18	Q	3009	BOG	C1'-C2'-C3'-C4'
14	D	2003	CDL	C12-C11-CA5-OA6
17	Q	501	HEC	CAA-CBA-CGA-O1A
14	Q	3003	CDL	OB5-CB3-CB4-OB6
15	C	2007	PEE	O4-C10-C11-C12
15	C	2007	PEE	O5-C30-C31-C32
15	P	3007	PEE	O5-C30-C31-C32
15	E	2005	PEE	C31-C32-C33-C34
14	D	2003	CDL	C72-C71-CB7-OB8
15	P	3007	PEE	O4-C10-C11-C12

There are no ring outliers.

22 monomers are involved in 47 short contacts:

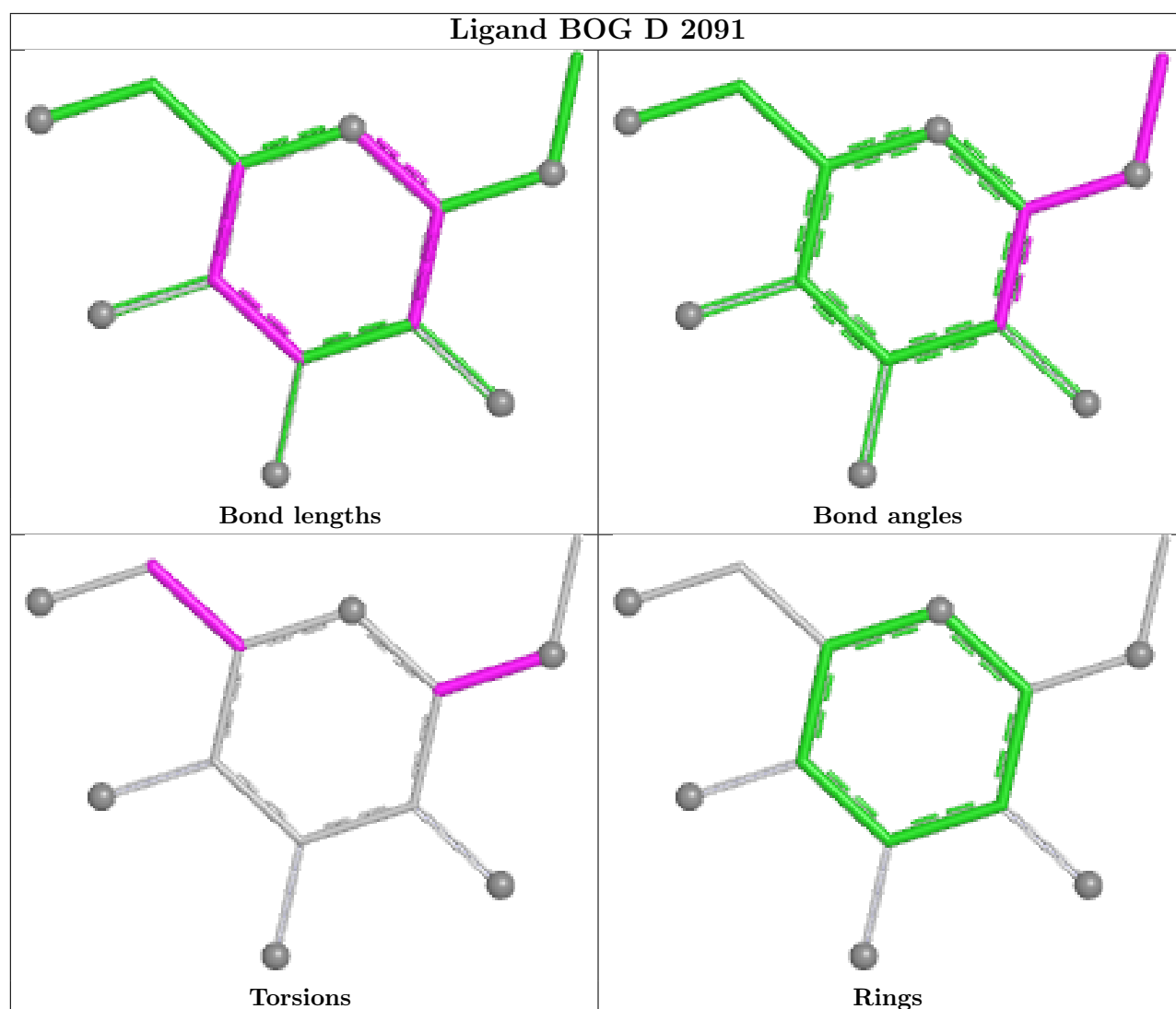
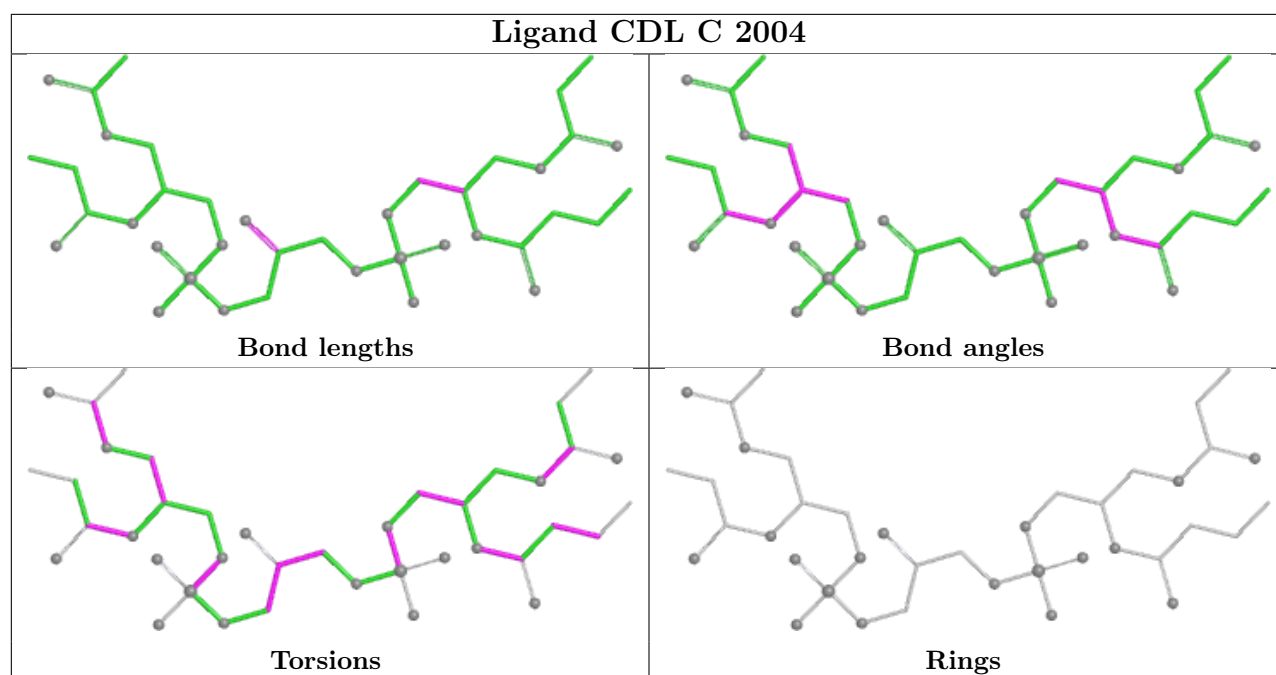
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2004	CDL	1	0
18	D	2009	BOG	1	0
18	Q	3009	BOG	1	0
12	P	3001	IKR	3	0
13	P	3002	UQ	2	0

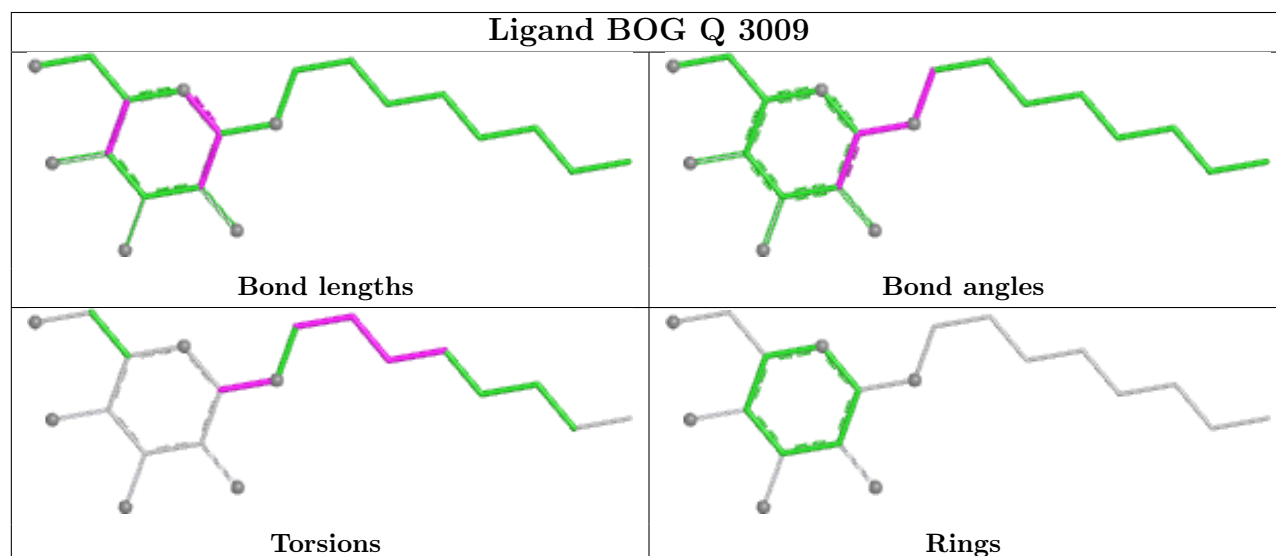
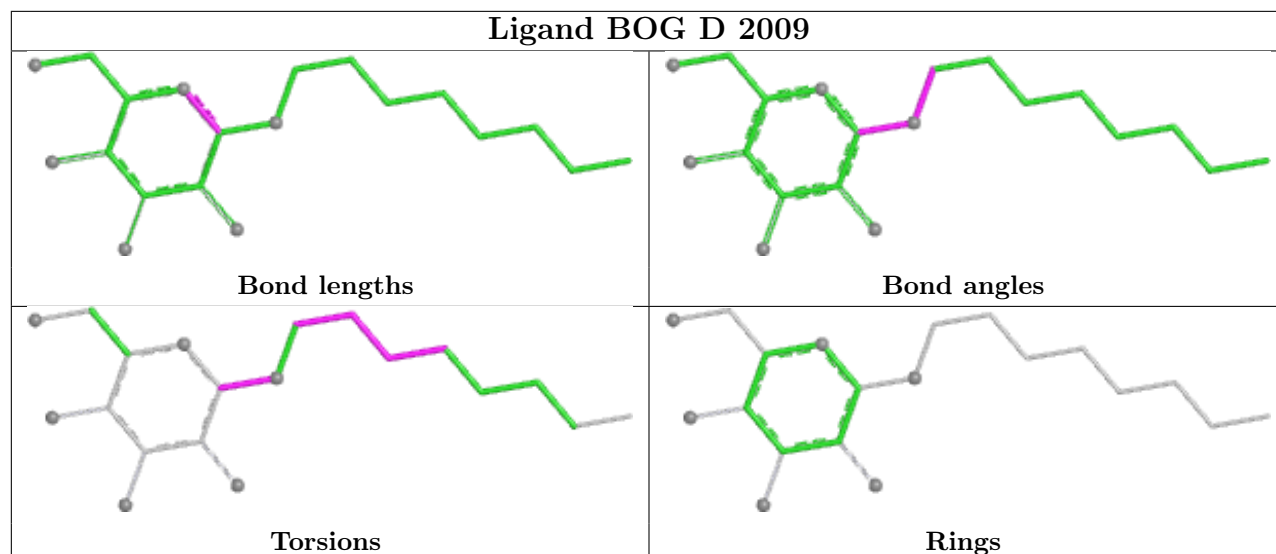
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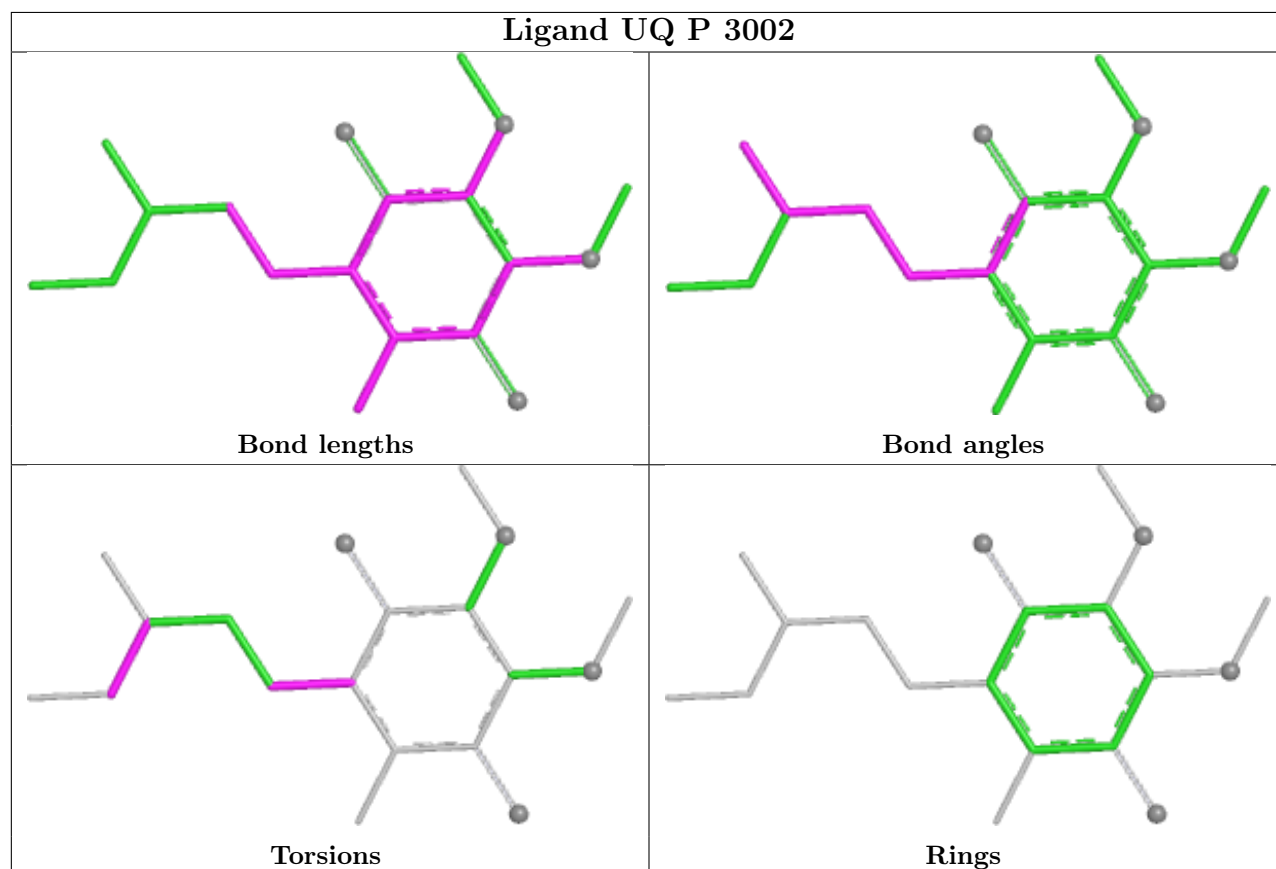
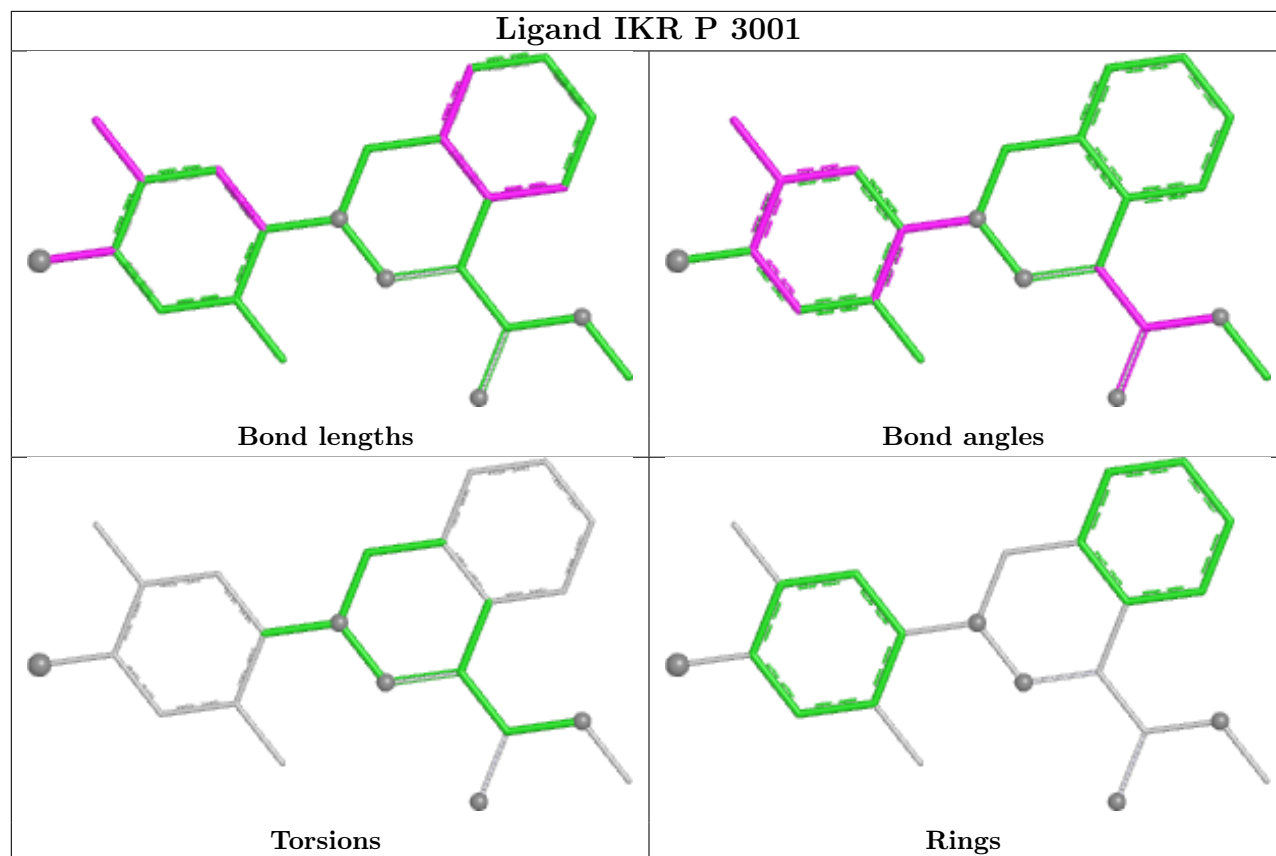
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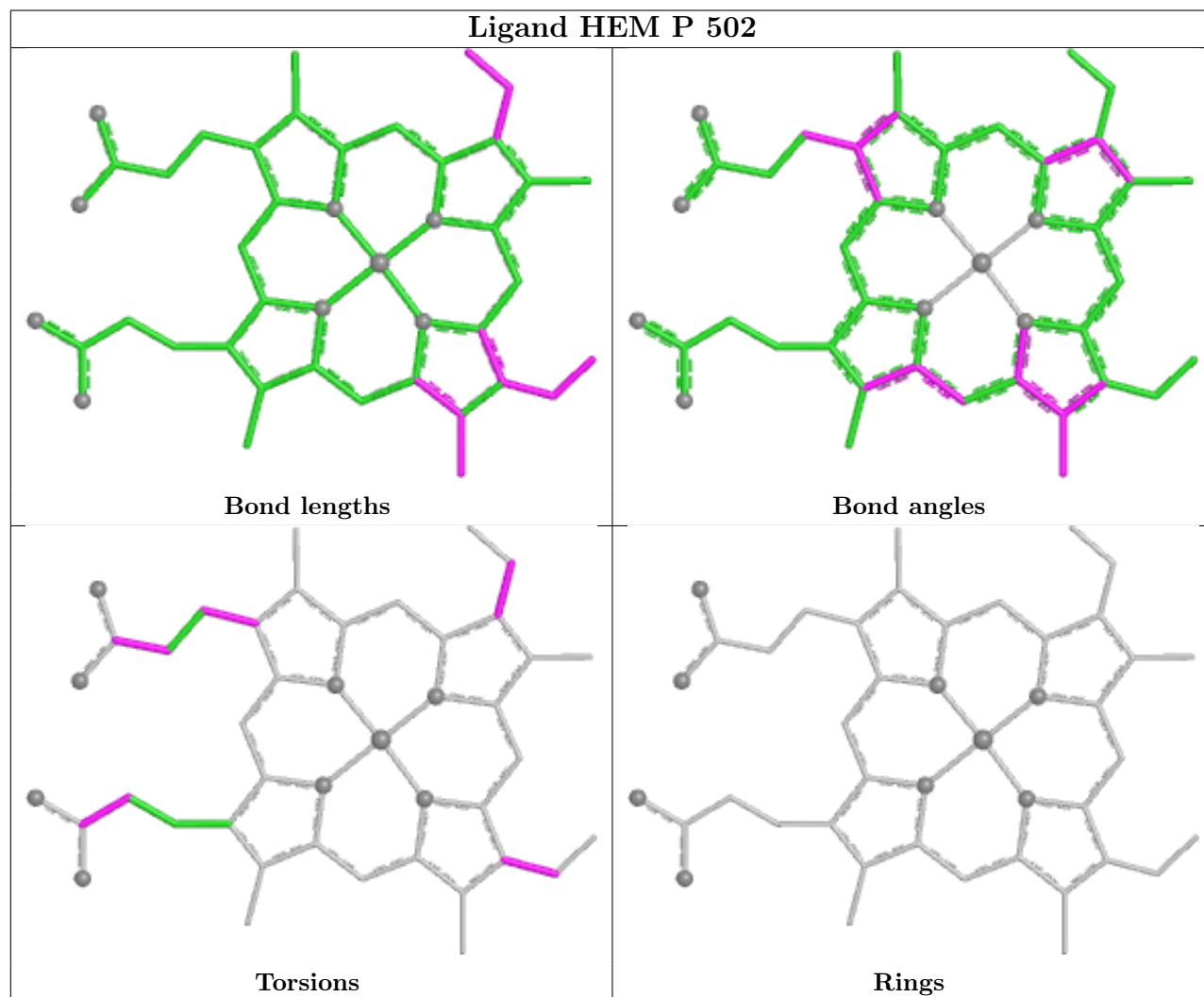
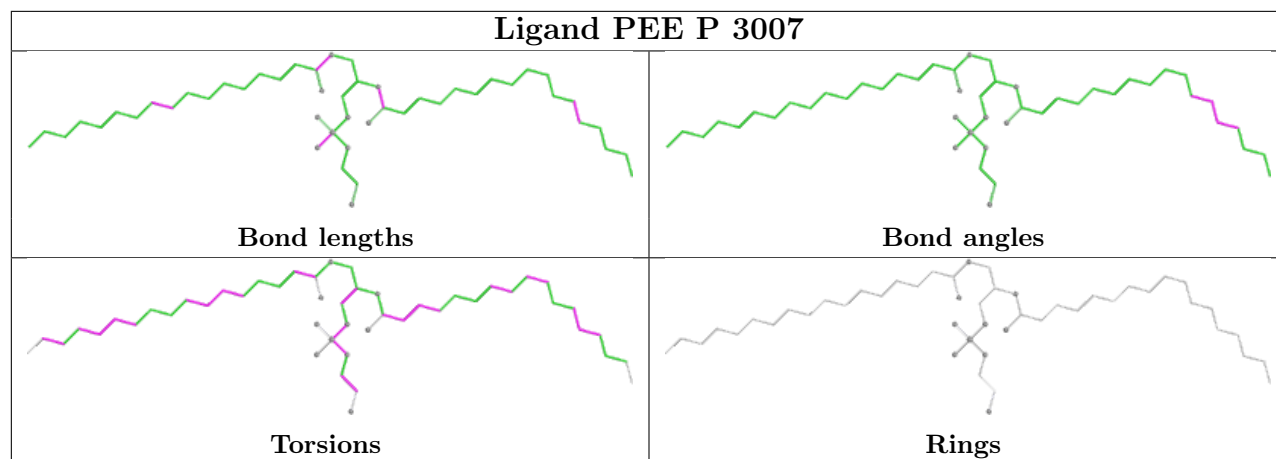
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	3007	PEE	2	0
11	P	502	HEM	3	0
16	P	3011	GOL	2	0
13	C	2002	UQ	5	0
15	R	3005	PEE	1	0
11	C	502	HEM	5	0
11	C	501	HEM	3	0
14	Q	3003	CDL	2	0
18	P	2010	BOG	1	0
19	R	501	FES	2	0
12	C	2001	IKR	4	0
15	C	2007	PEE	1	0
11	P	501	HEM	2	0
14	P	3004	CDL	2	0
19	E	501	FES	2	0
17	Q	501	HEC	1	0
17	D	501	HEC	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.

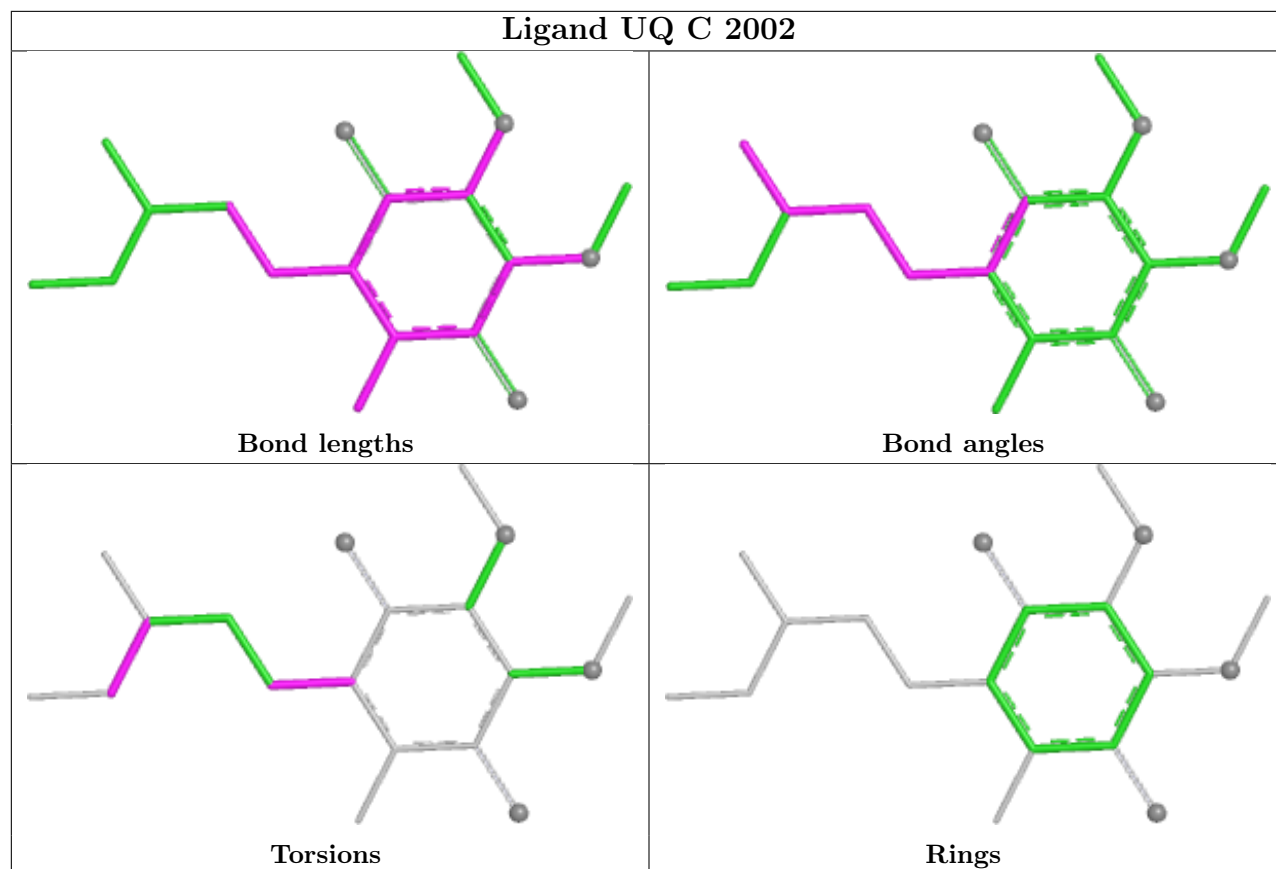




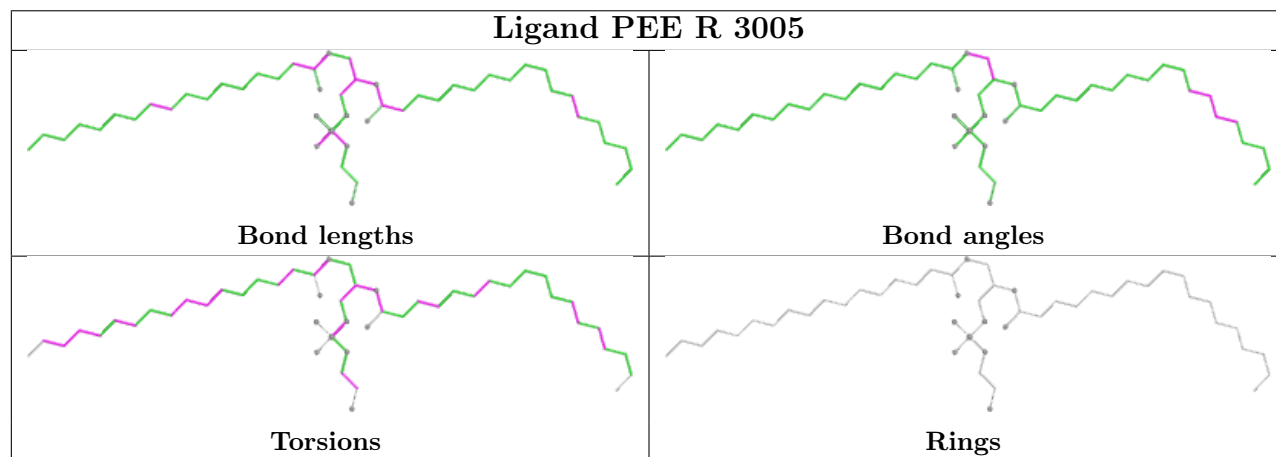


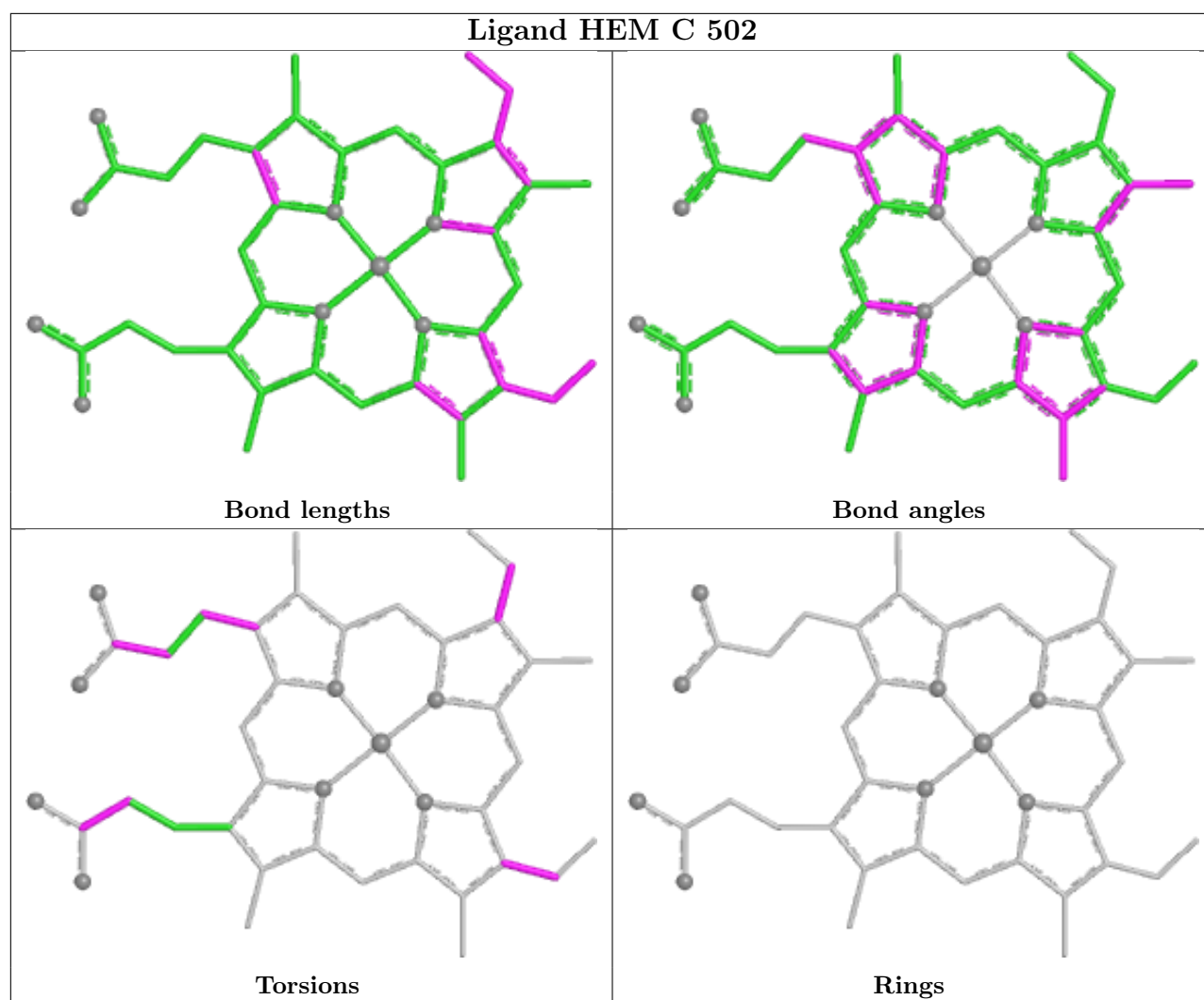


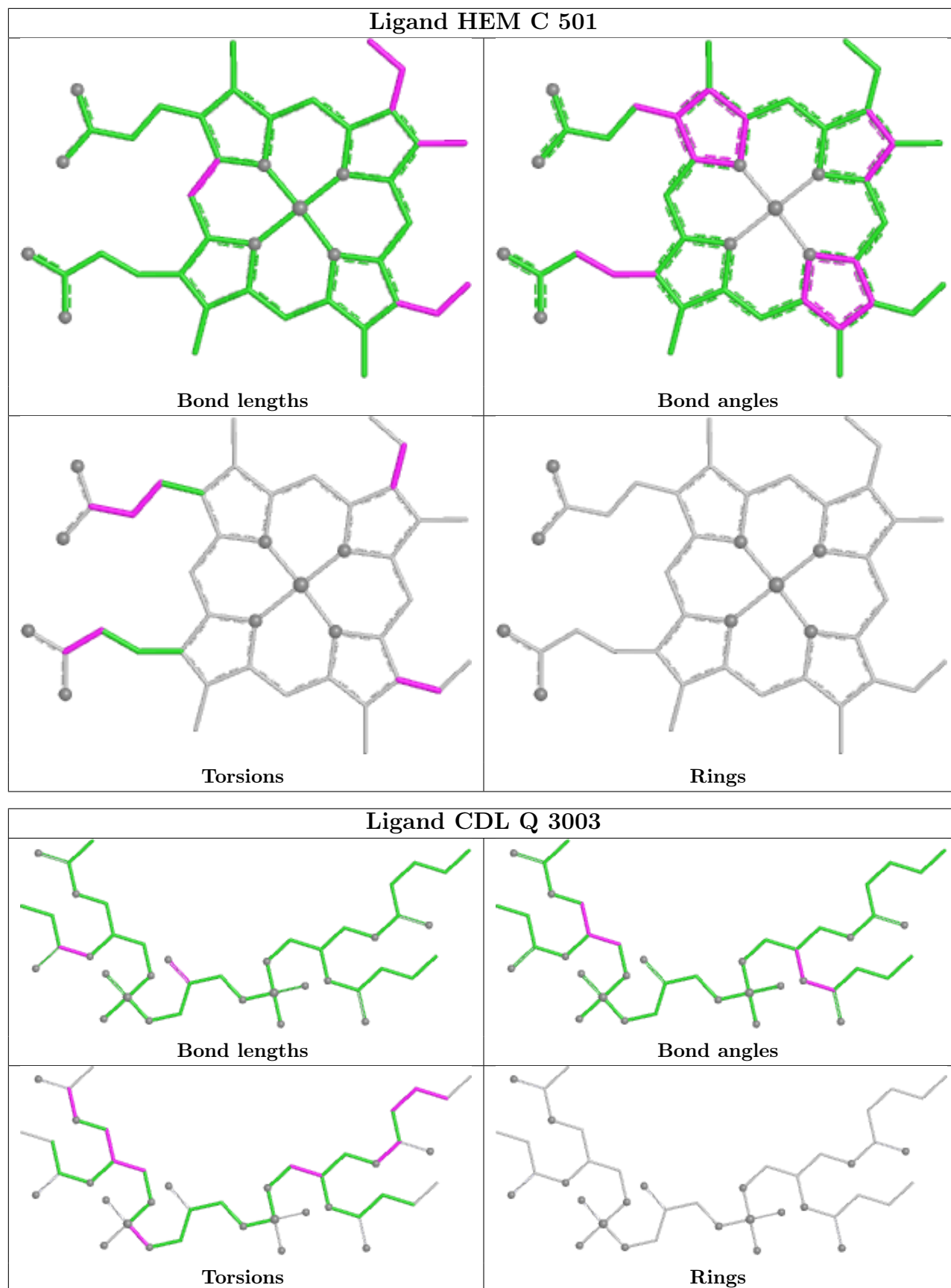
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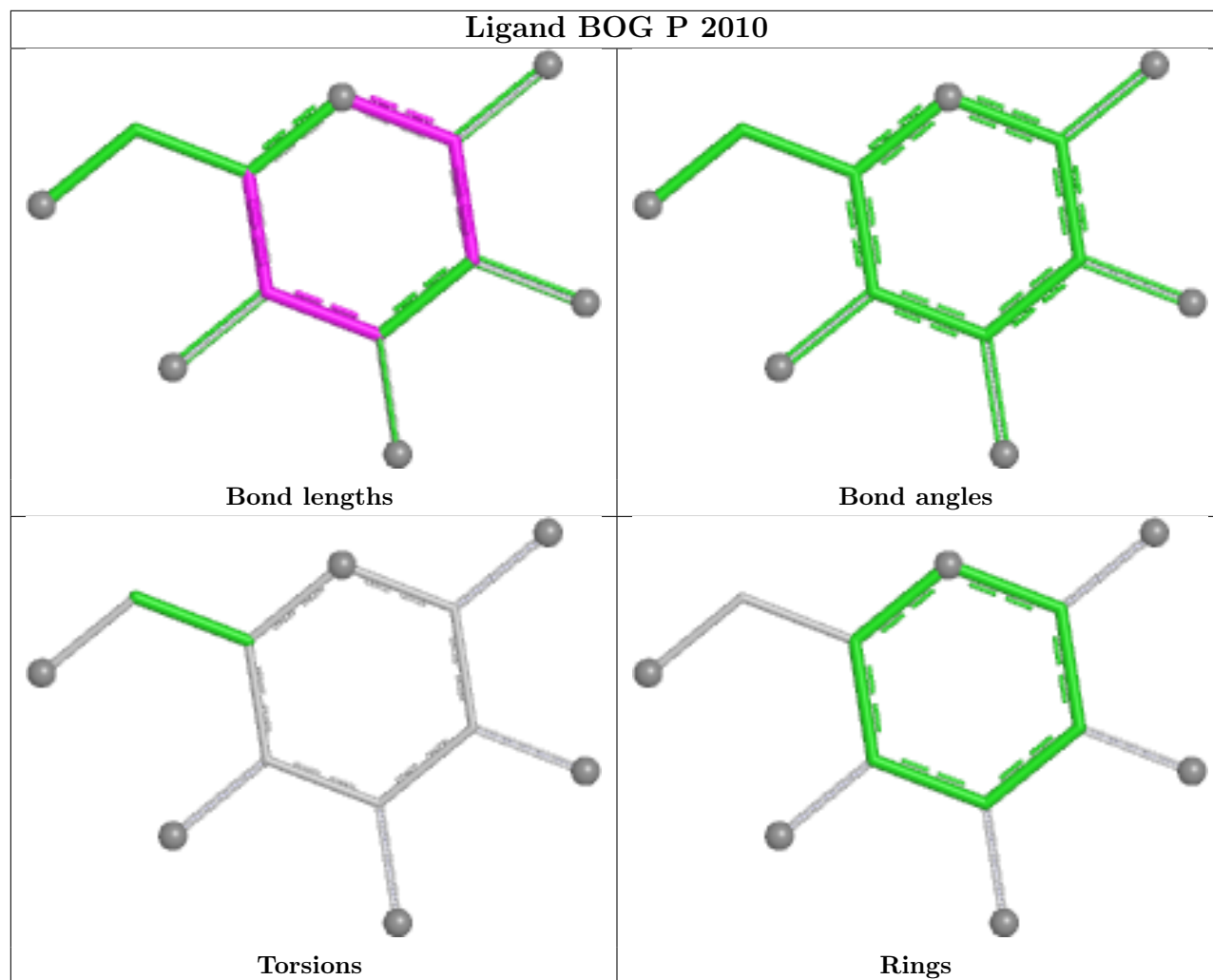
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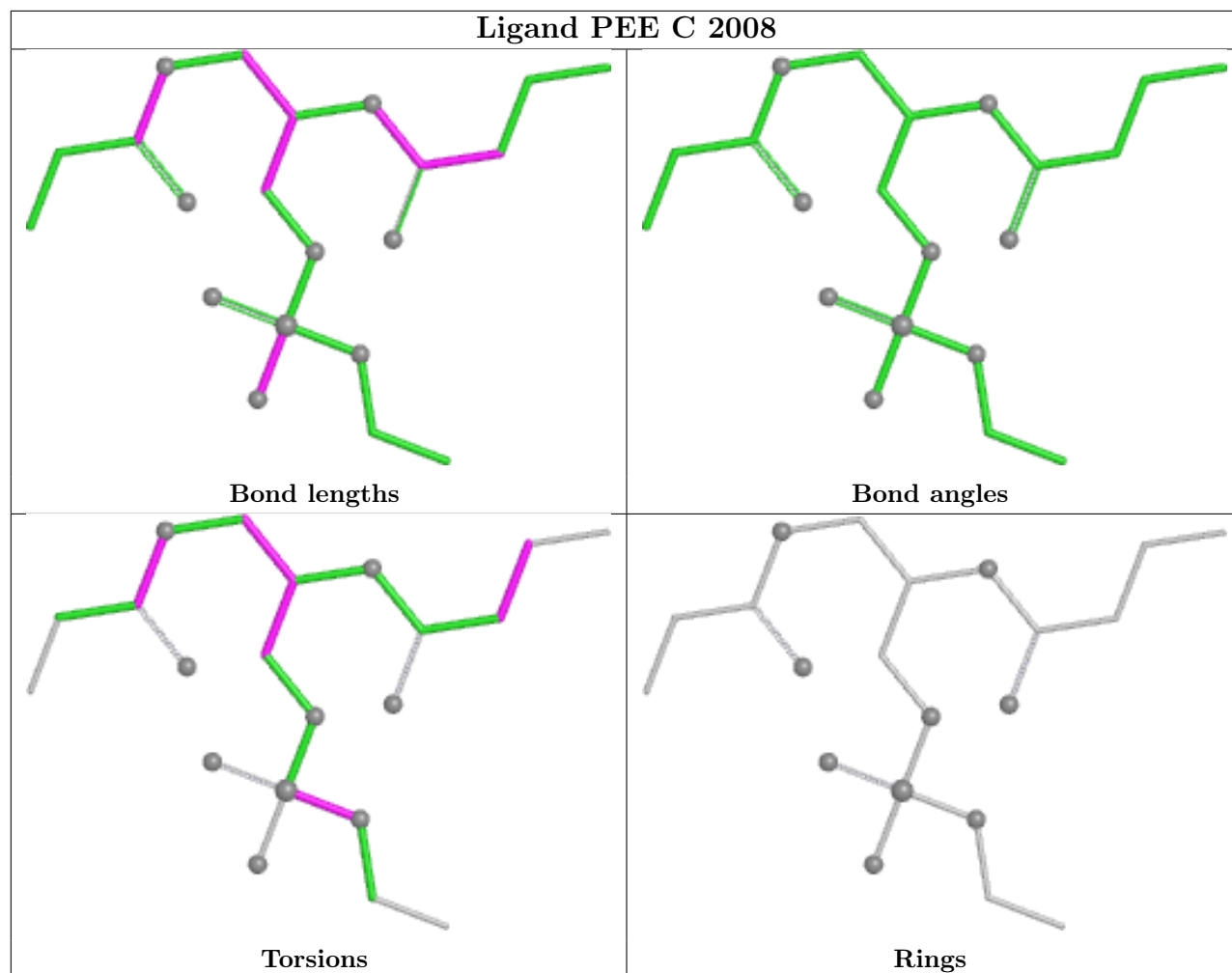




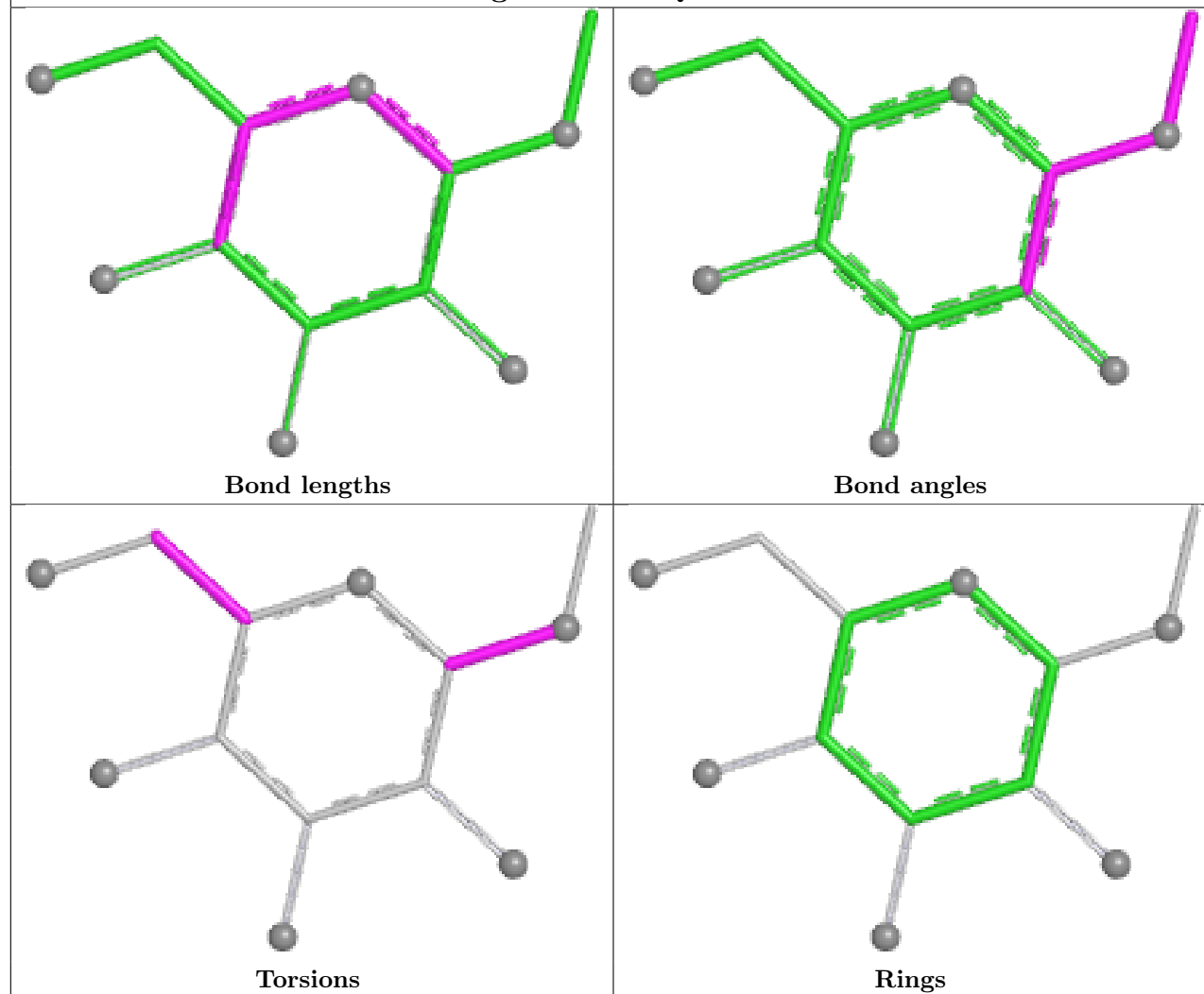


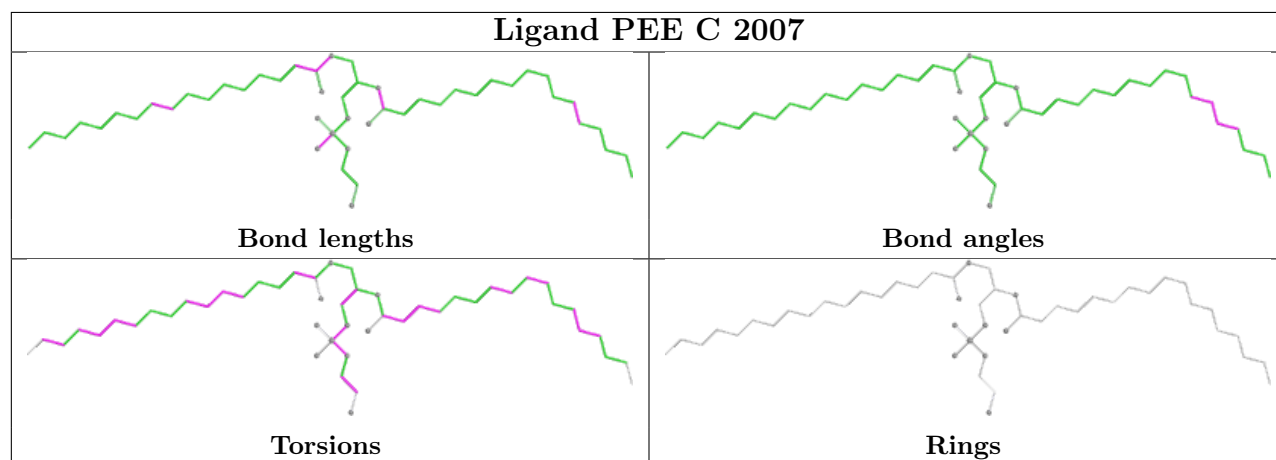
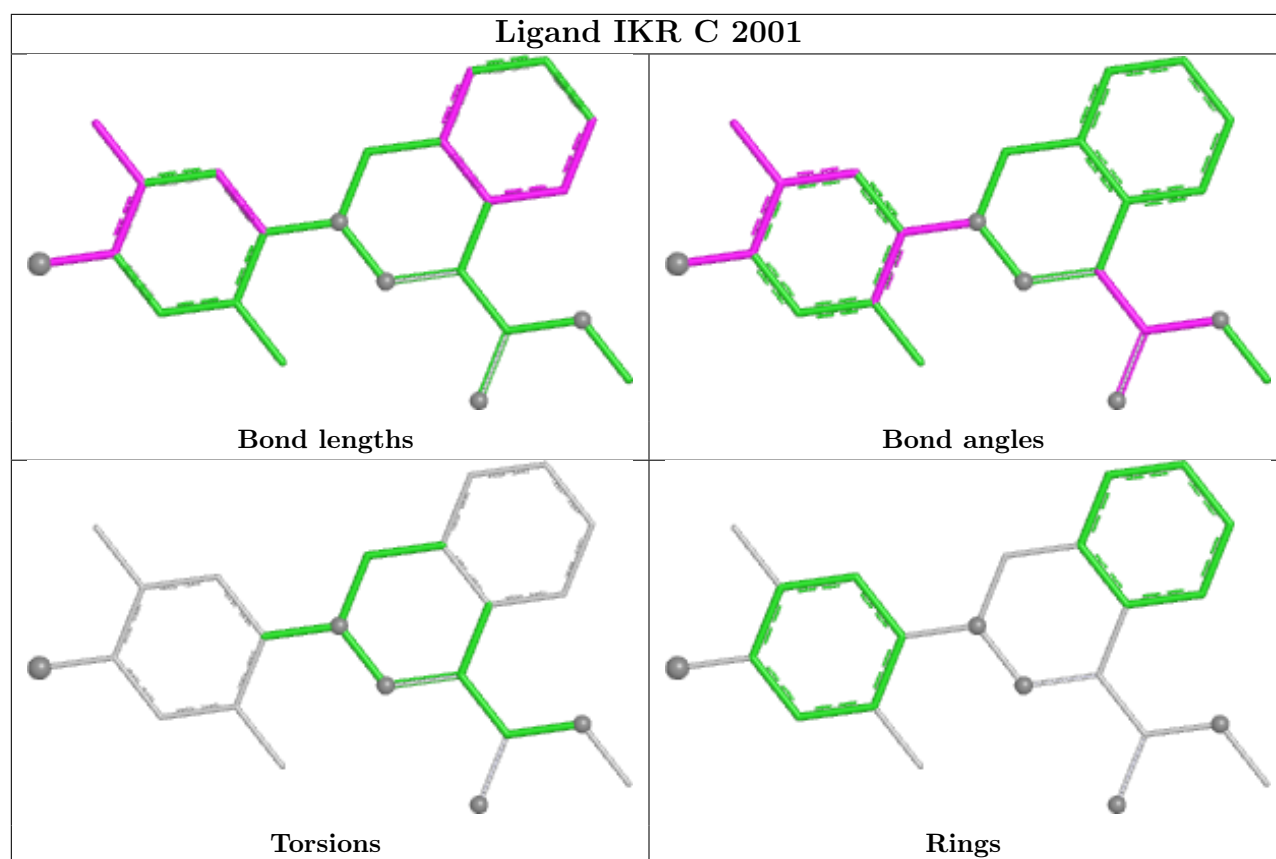
Ligand BOG P 2010

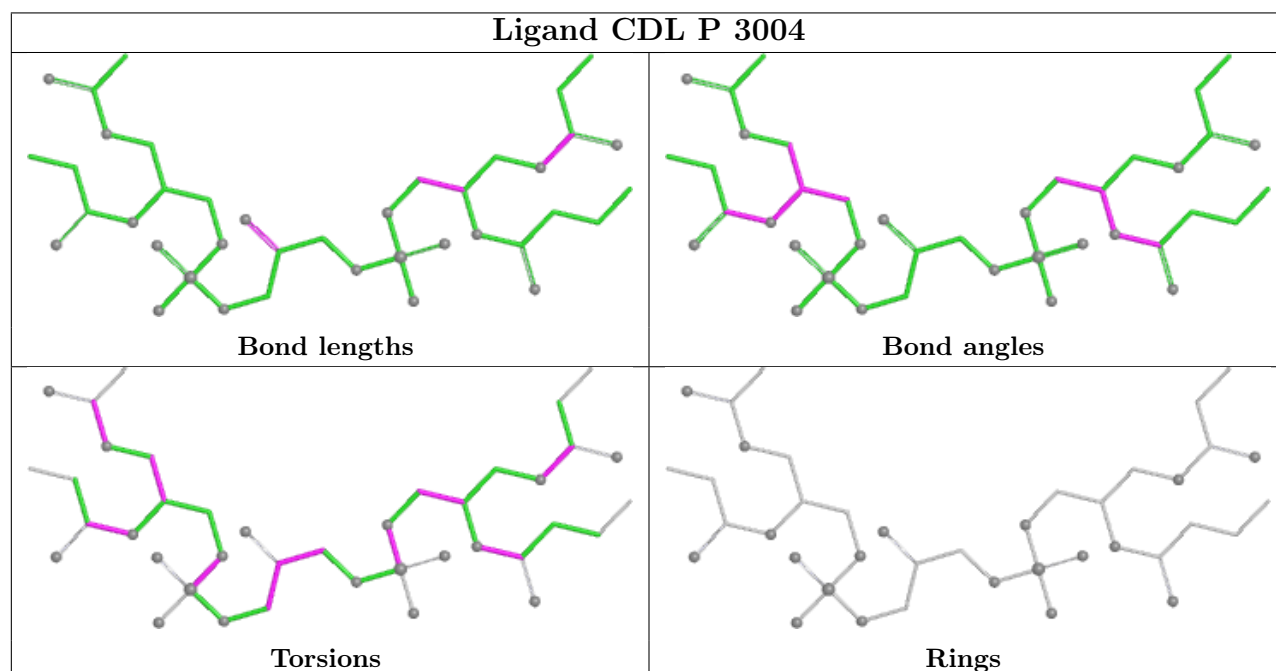
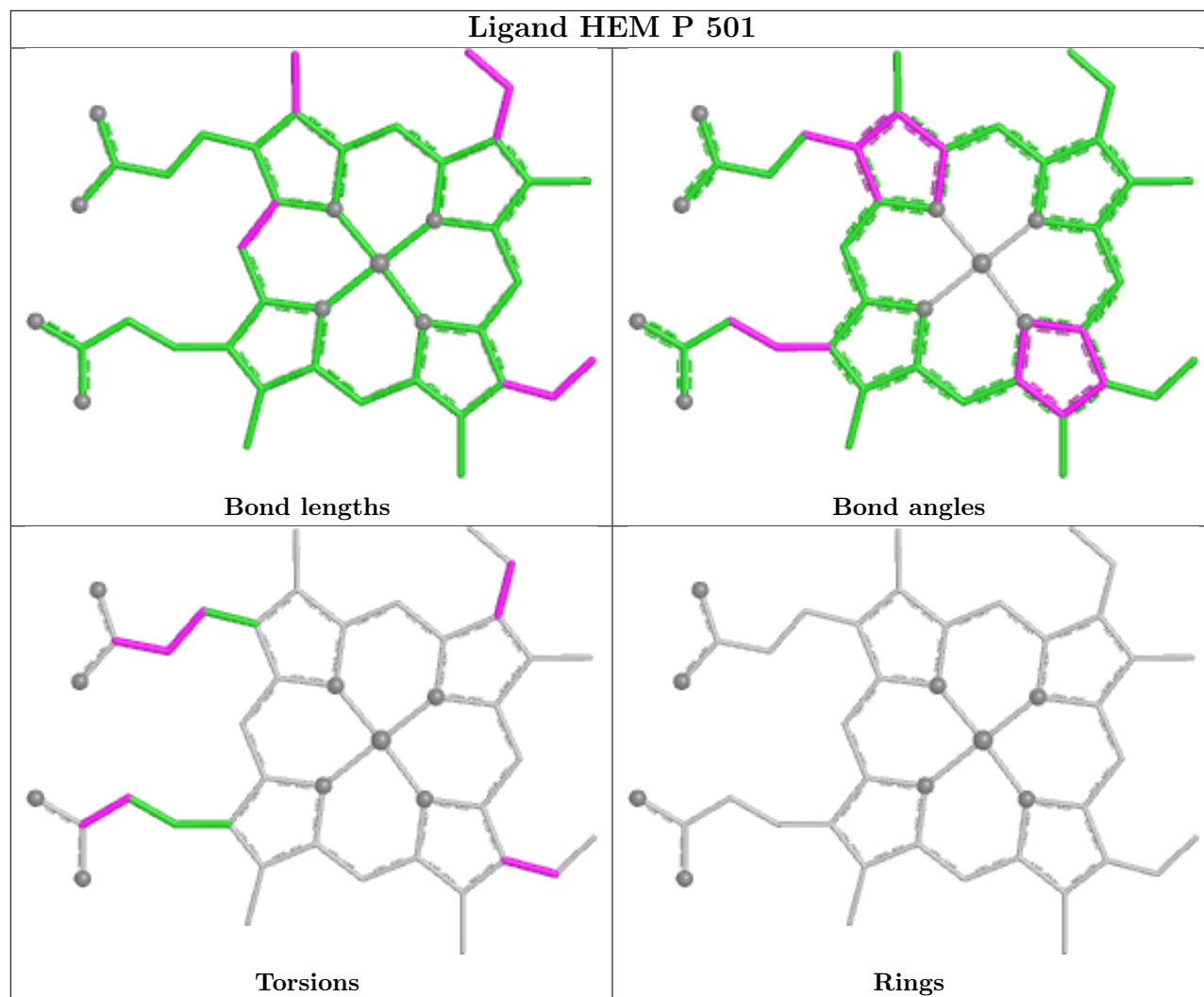


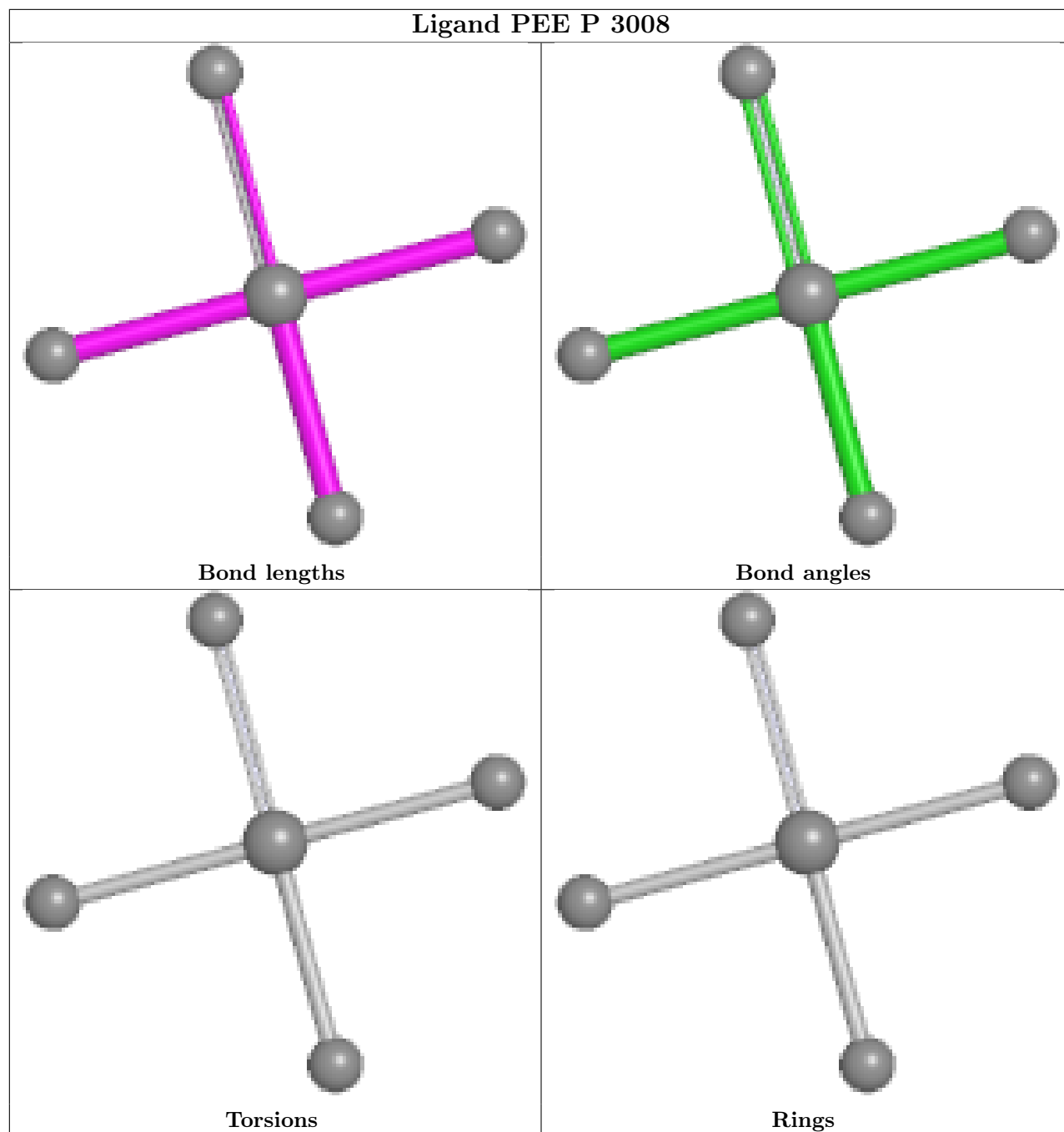


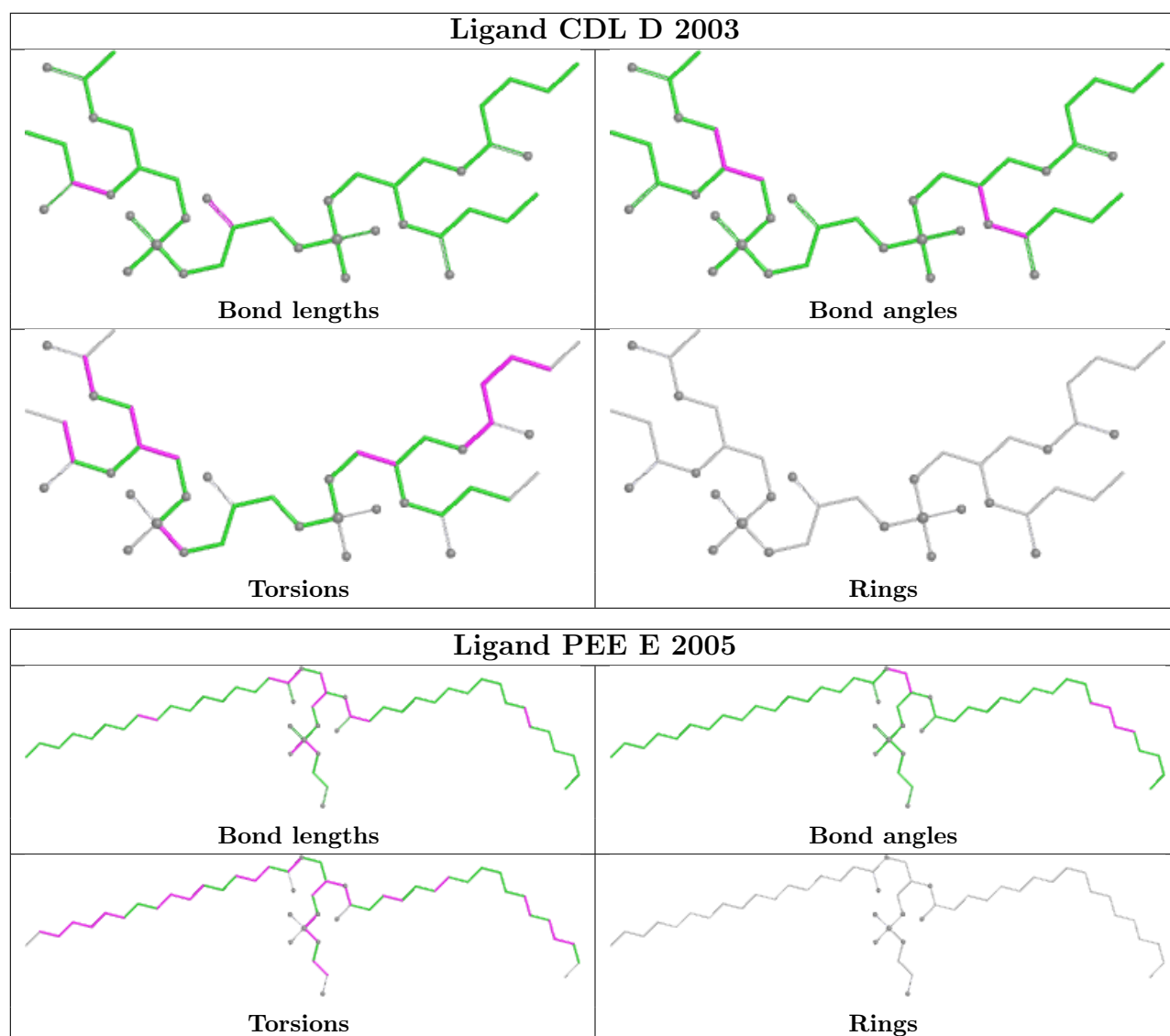
Ligand BOG Q 3091

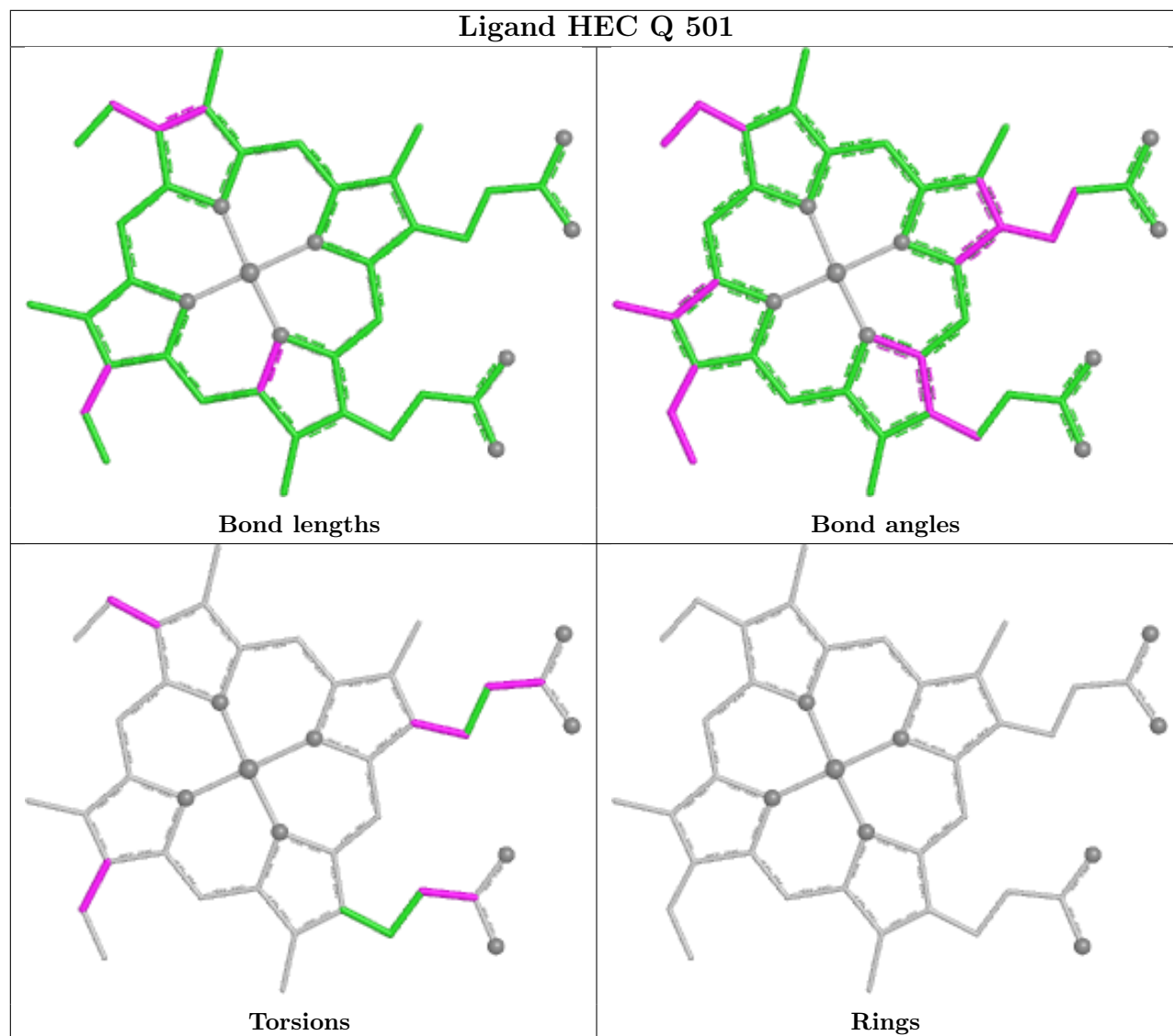


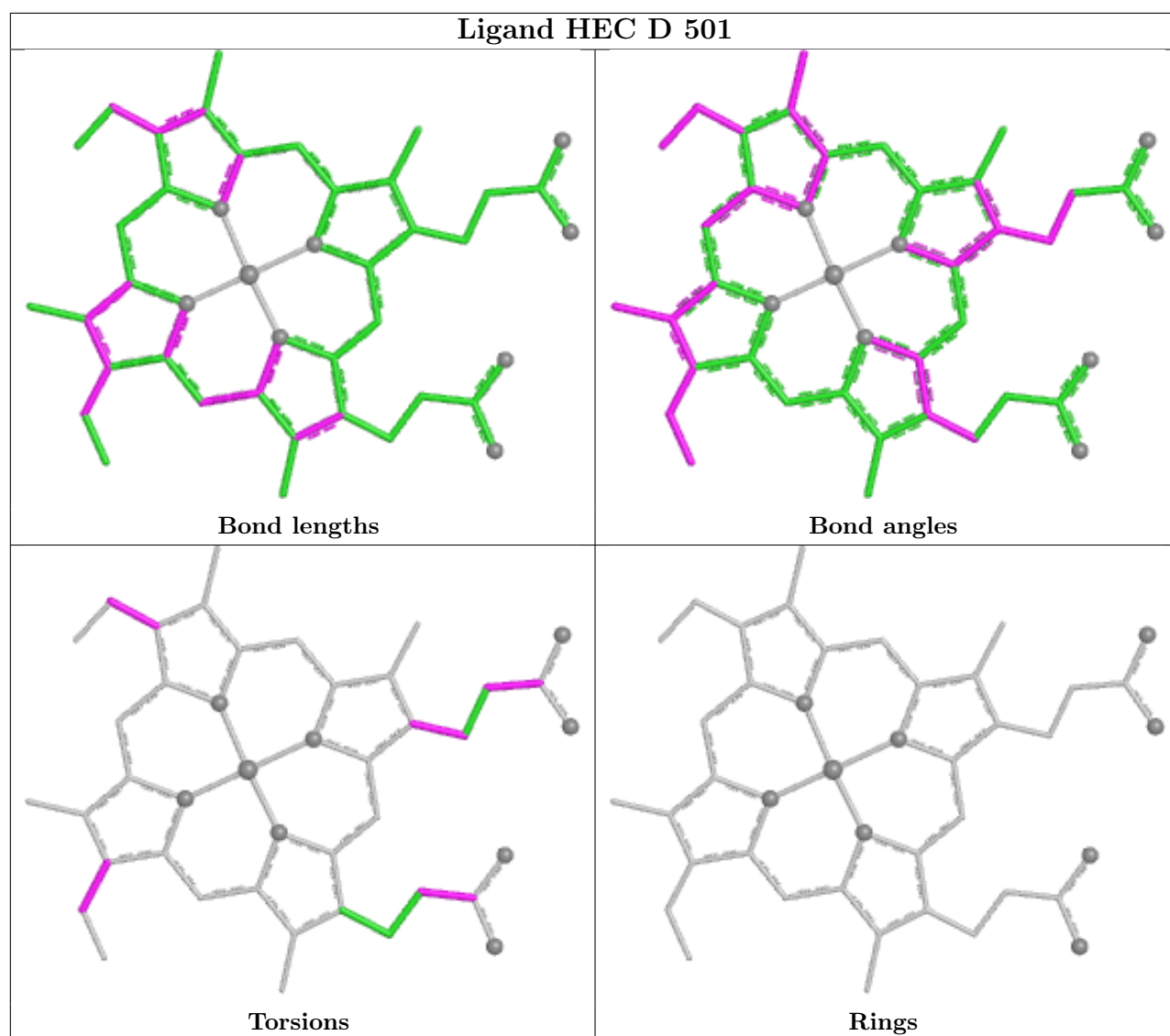












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/446 (99%)	0.18	5 (1%) 78 57	39, 74, 106, 125	0
1	N	442/446 (99%)	0.44	19 (4%) 40 21	43, 79, 111, 119	0
2	B	421/441 (95%)	0.51	10 (2%) 59 37	63, 90, 121, 156	0
2	O	422/441 (95%)	0.42	15 (3%) 46 25	50, 85, 115, 134	0
3	C	380/380 (100%)	-0.38	6 (1%) 70 47	23, 45, 98, 135	0
3	P	379/380 (99%)	0.06	4 (1%) 78 57	32, 68, 104, 128	0
4	D	241/241 (100%)	-0.36	1 (0%) 88 75	37, 51, 89, 114	0
4	Q	241/241 (100%)	0.39	3 (1%) 76 55	55, 85, 118, 130	0
5	E	196/196 (100%)	0.97	42 (21%) 2 1	39, 124, 158, 164	125 (63%)
5	R	196/196 (100%)	0.79	18 (9%) 14 8	51, 94, 138, 157	0
6	F	101/110 (91%)	-0.43	0 100 100	38, 52, 70, 90	0
6	S	101/110 (91%)	0.39	1 (0%) 79 59	62, 84, 126, 151	0
7	G	80/81 (98%)	0.07	3 (3%) 44 24	39, 61, 118, 127	0
7	T	79/81 (97%)	0.80	8 (10%) 12 6	55, 91, 154, 161	0
8	H	70/77 (90%)	0.15	3 (4%) 40 21	52, 74, 95, 133	0
8	U	67/77 (87%)	1.10	9 (13%) 7 4	103, 131, 152, 157	0
9	I	31/47 (65%)	2.61	17 (54%) 0 0	92, 128, 164, 167	0
9	V	31/47 (65%)	2.69	20 (64%) 0 0	87, 119, 167, 170	0
10	J	61/61 (100%)	-0.10	0 100 100	46, 63, 107, 143	0
10	W	60/61 (98%)	0.25	1 (1%) 69 46	65, 83, 120, 129	0
All	All	4043/4160 (97%)	0.30	185 (4%) 37 19	23, 77, 131, 170	125 (3%)

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	56	SER	7.9
9	I	51	CYS	7.4
9	V	63	ASP	6.6
9	I	63	ASP	5.9
2	O	226	ILE	5.1
9	V	61	ARG	5.1
9	I	50	LEU	5.0
5	E	113	ASP	4.9
9	I	61	ARG	4.9
9	V	59	SER	4.8
5	E	106	ILE	4.8
9	I	47	ARG	4.8
5	E	120	PRO	4.5
9	I	53	GLU	4.3
1	A	444	ILE	4.3
7	G	2	ILE	4.2
5	E	168	SER	4.2
9	V	47	ARG	4.2
9	I	49	LEU	4.1
9	V	49	LEU	4.0
5	E	98	VAL	4.0
7	T	2	ILE	3.9
7	T	73	ASN	3.8
5	R	113	ASP	3.8
2	B	19	PRO	3.8
9	V	57	GLY	3.7
8	H	9	GLU	3.7
5	E	114	VAL	3.7
5	R	124	LEU	3.7
5	R	167	ALA	3.6
5	E	109	GLU	3.5
9	V	50	LEU	3.5
3	C	4	ASN	3.5
9	I	55	MET	3.5
5	E	142	LEU	3.5
2	O	224	LEU	3.4
5	E	117	LEU	3.4
5	E	135	LEU	3.4
5	E	167	ALA	3.3
9	I	56	SER	3.2
9	V	60	ALA	3.2
9	I	48	PRO	3.2
9	I	57	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	20	GLY	3.1
3	C	7	LYS	3.1
3	C	8	SER	3.1
1	N	88	GLY	3.1
9	V	52	ARG	3.1
9	V	62	ARG	3.1
5	E	133	VAL	3.1
2	O	19	PRO	3.1
7	T	74	PRO	3.1
4	Q	3	LEU	3.0
5	E	180	LEU	3.0
9	I	52	ARG	3.0
5	R	112	VAL	3.0
5	R	111	GLU	3.0
5	E	107	ASN	3.0
5	E	134	ILE	3.0
5	E	188	VAL	2.9
5	R	120	PRO	2.9
3	P	346	HIS	2.9
9	V	53	GLU	2.9
5	E	101	ARG	2.9
2	O	20	GLY	2.9
5	E	87	VAL	2.8
1	N	386	TYR	2.8
5	R	130	PRO	2.8
3	P	151	PHE	2.7
5	E	121	GLN	2.7
5	E	147	ILE	2.7
9	V	55	MET	2.7
1	N	198	ALA	2.7
8	U	61	PHE	2.7
1	A	69	LYS	2.7
2	O	335	GLU	2.7
5	E	112	VAL	2.7
2	O	232	THR	2.6
9	V	51	CYS	2.6
2	O	386	ALA	2.6
5	R	88	ALA	2.6
8	U	55	THR	2.6
5	R	117	LEU	2.6
2	B	226	ILE	2.6
1	N	3	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	9	HIS	2.6
9	V	54	SER	2.6
2	O	21	ALA	2.6
5	E	145	VAL	2.6
5	E	124	LEU	2.6
5	E	194	VAL	2.6
5	E	157	TYR	2.5
7	G	81	GLN	2.5
1	N	432	LEU	2.5
9	V	48	PRO	2.5
9	V	58	ARG	2.5
8	U	37	LEU	2.5
2	B	229	GLY	2.5
5	E	191	ASP	2.5
1	A	17	THR	2.5
8	U	73	LEU	2.5
5	R	123	ASP	2.5
5	E	90	LYS	2.5
8	H	71	HIS	2.5
3	P	7	LYS	2.4
5	R	128	LYS	2.4
9	V	77	ARG	2.4
9	I	76	VAL	2.4
5	E	97	PHE	2.4
5	R	150	SER	2.4
5	E	183	PRO	2.4
5	R	86	ASN	2.4
4	Q	143	VAL	2.4
1	N	31	SER	2.4
2	O	384	SER	2.4
7	T	3	HIS	2.3
9	I	71	ASN	2.3
7	T	44	GLN	2.3
1	N	219	VAL	2.3
5	R	146	PRO	2.3
1	N	56	GLY	2.3
2	B	402	ILE	2.3
1	A	1	ALA	2.3
3	P	161	LEU	2.3
8	U	39	LEU	2.3
9	V	64	LEU	2.3
8	H	26	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	105	GLU	2.3
3	C	10	PRO	2.3
1	N	120	CYS	2.3
5	E	153	PHE	2.3
2	B	21	ALA	2.3
2	B	289	SER	2.3
9	I	77	ARG	2.3
2	O	371	SER	2.2
1	A	32	GLN	2.2
1	N	229	PRO	2.2
2	B	388	LEU	2.2
5	E	169	GLY	2.2
7	T	4	PHE	2.2
6	S	36	THR	2.2
2	O	350	GLY	2.2
8	U	33	ALA	2.2
5	R	85	LYS	2.2
5	R	172	ARG	2.2
10	W	17	THR	2.2
1	N	116	VAL	2.2
5	E	79	SER	2.2
8	U	13	LEU	2.2
5	E	173	LYS	2.2
9	V	71	ASN	2.2
2	B	38	LEU	2.1
2	O	229	GLY	2.1
5	E	177	PRO	2.1
2	O	332	HIS	2.1
5	E	182	VAL	2.1
5	E	193	VAL	2.1
1	N	444	ILE	2.1
9	I	60	ALA	2.1
4	D	1	GLY	2.1
7	T	22	GLU	2.1
1	N	28	GLU	2.1
1	N	66	GLY	2.1
5	E	159	PRO	2.1
5	E	196	GLY	2.1
8	U	38	GLU	2.1
2	O	233	SER	2.1
5	R	87	VAL	2.1
2	B	104	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
7	T	72	LYS	2.1
5	E	126	ARG	2.1
5	R	196	GLY	2.1
5	E	146	PRO	2.1
9	I	62	ARG	2.0
1	N	185	TYR	2.0
1	N	117	VAL	2.0
8	U	69	VAL	2.0
1	N	215	HIS	2.0
7	G	3	HIS	2.0
5	E	104	ALA	2.0
1	N	98	TYR	2.0
1	N	223	TYR	2.0
2	O	344	LEU	2.0
4	Q	5	LEU	2.0
3	C	5	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	BOG	Q	3091	13/20	0.47	0.36	194,197,197,198	0
15	PEE	C	2008	21/51	0.52	0.29	132,138,141,142	0
18	BOG	D	2091	13/20	0.61	0.32	167,171,171,171	0
15	PEE	P	3008	5/51	0.71	0.15	140,140,140,140	0
14	CDL	P	3004	40/100	0.73	0.23	111,116,122,123	0
18	BOG	P	2010	12/20	0.75	0.30	162,165,167,167	0
14	CDL	Q	3003	42/100	0.78	0.27	120,141,152,153	0

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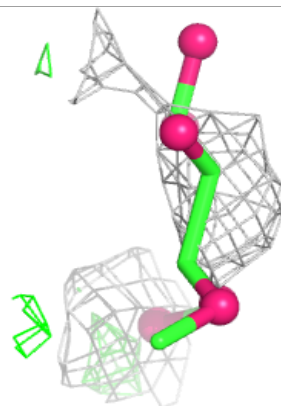
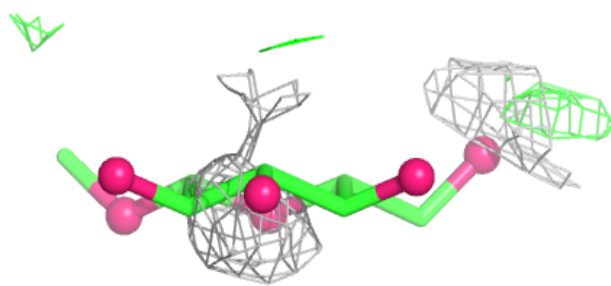
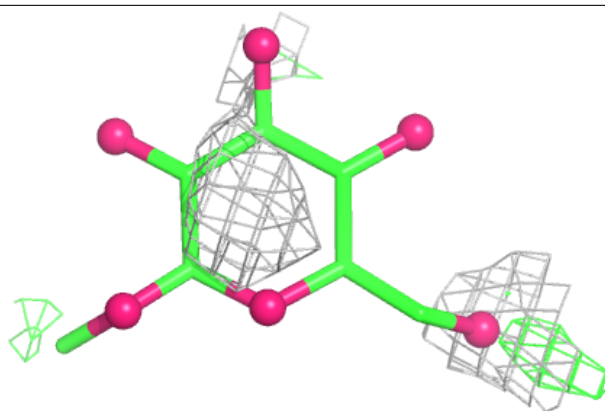
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	PEE	R	3005	50/51	0.79	0.28	80,99,106,107	0
14	CDL	D	2003	42/100	0.79	0.27	112,121,125,126	0
14	CDL	C	2004	40/100	0.83	0.16	72,82,99,101	0
15	PEE	E	2005	50/51	0.87	0.24	79,91,105,106	0
18	BOG	Q	3009	20/20	0.88	0.18	71,99,102,102	0
13	UQ	C	2002	19/63	0.90	0.22	85,89,90,90	0
15	PEE	P	3007	49/51	0.90	0.21	68,91,107,109	0
16	GOL	C	2011	6/6	0.91	0.16	54,56,58,60	0
18	BOG	D	2009	20/20	0.91	0.13	51,76,80,81	0
13	UQ	P	3002	19/63	0.91	0.26	97,111,114,115	0
15	PEE	C	2007	49/51	0.93	0.16	49,59,88,90	0
16	GOL	P	3011	6/6	0.94	0.20	79,79,79,80	0
19	FES	E	501	4/4	0.94	0.08	151,151,152,152	4
17	HEC	Q	501	43/43	0.97	0.10	68,71,76,78	0
17	HEC	D	501	43/43	0.98	0.07	38,42,46,48	0
12	IKR	P	3001	25/25	0.98	0.10	66,67,76,78	0
11	HEM	P	501	43/43	0.98	0.08	46,50,57,60	0
11	HEM	P	502	43/43	0.98	0.08	40,47,59,62	0
19	FES	R	501	4/4	0.98	0.04	88,90,91,91	0
11	HEM	C	501	43/43	0.99	0.06	30,37,43,45	0
11	HEM	C	502	43/43	0.99	0.06	24,31,37,44	0
12	IKR	C	2001	25/25	0.99	0.06	38,40,44,54	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.

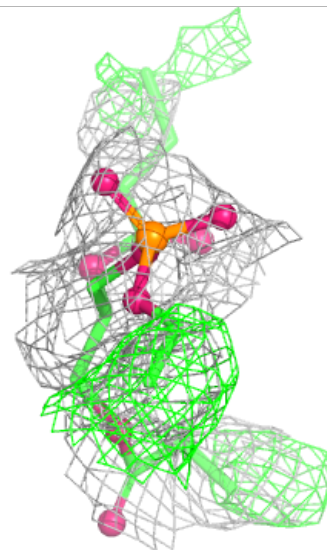
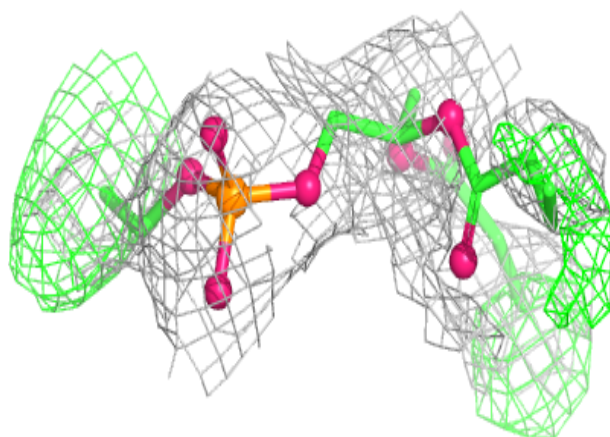
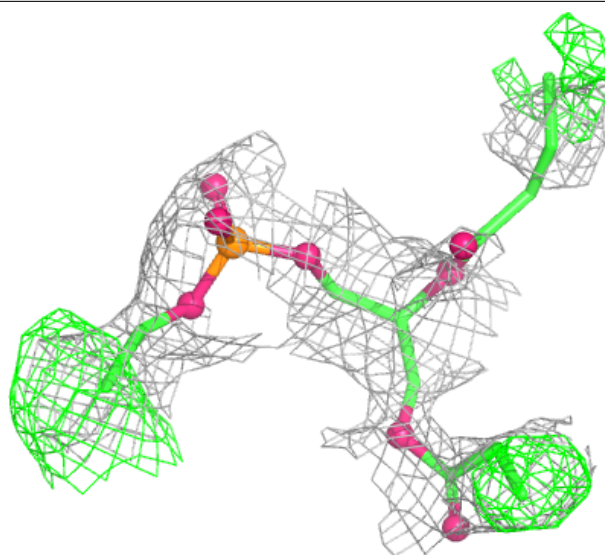
Electron density around BOG Q 3091:

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



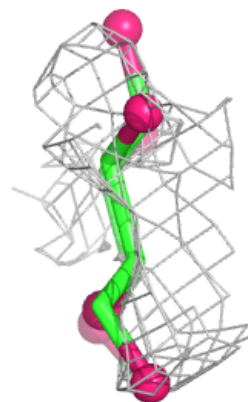
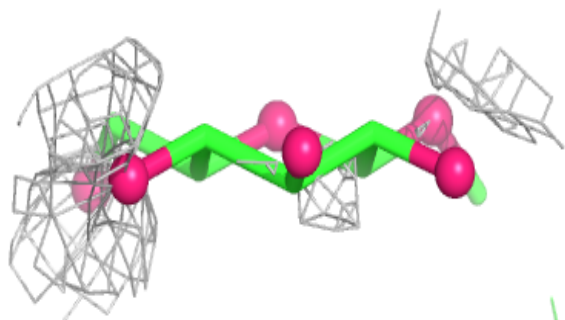
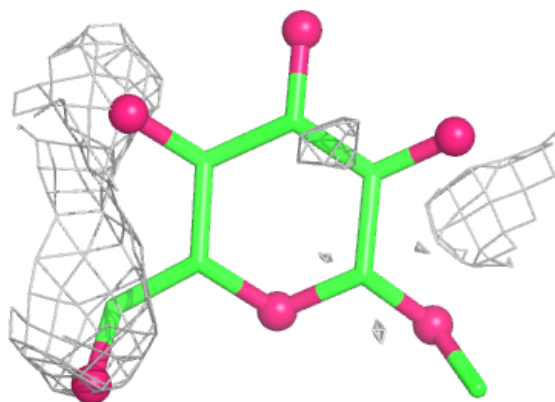
Electron density around PEE C 2008:

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



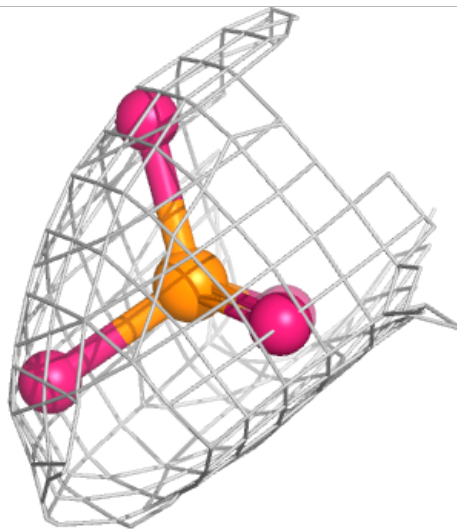
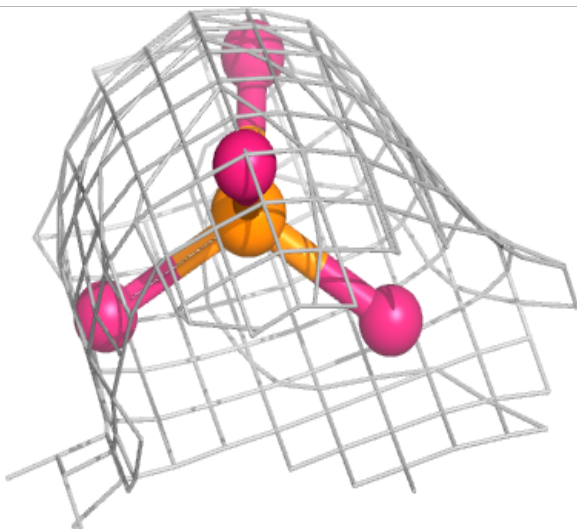
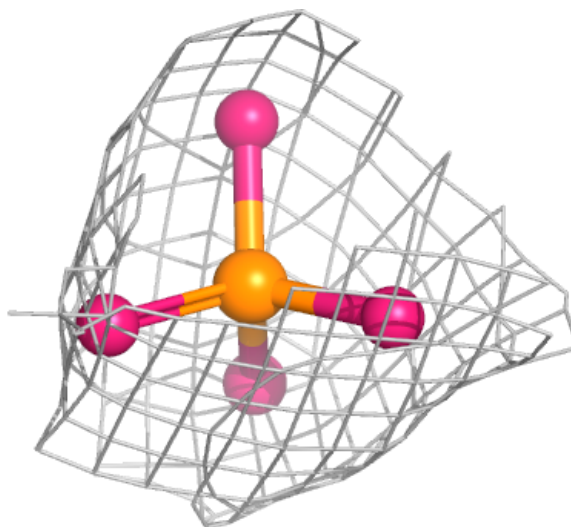
Electron density around BOG D 2091:

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and green (positive)



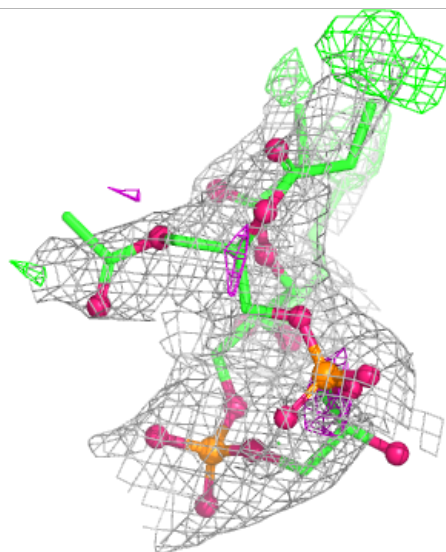
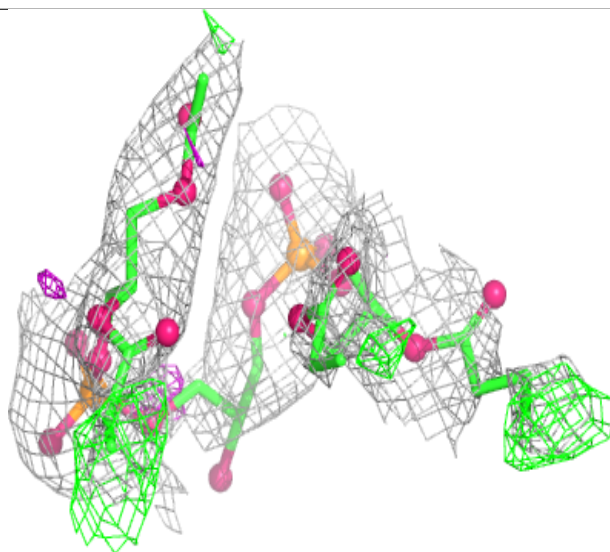
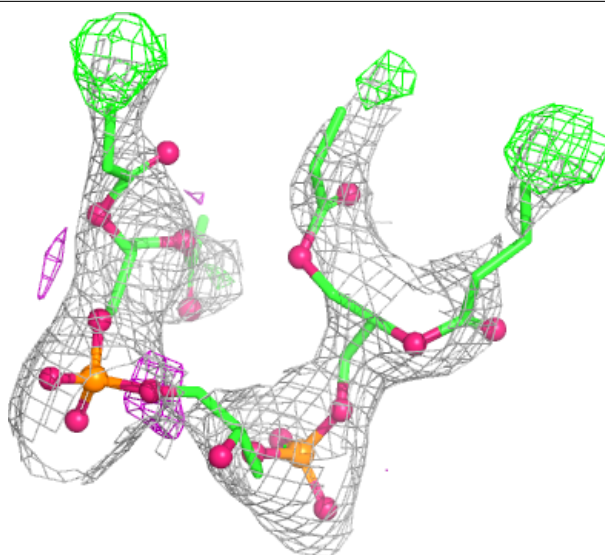
Electron density around PEE P 3008:

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and green (positive)



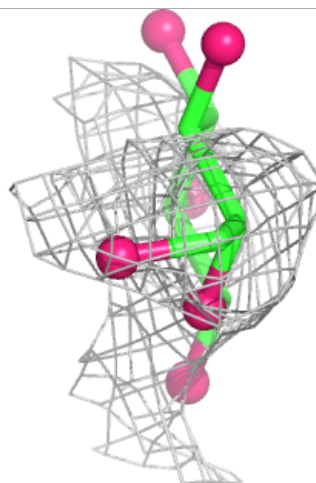
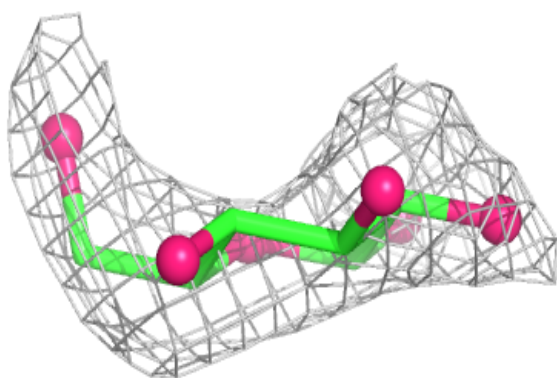
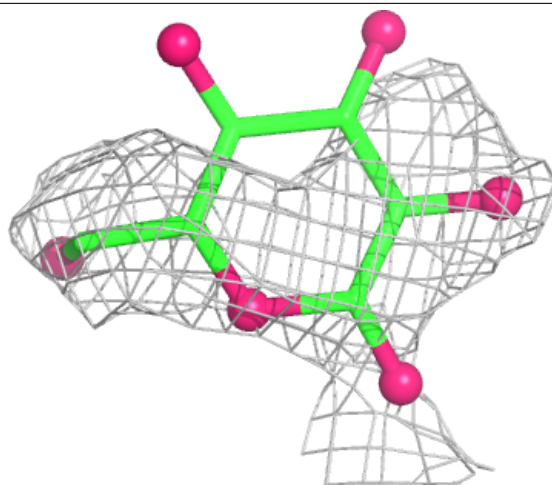
Electron density around CDL P 3004:

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and green (positive)



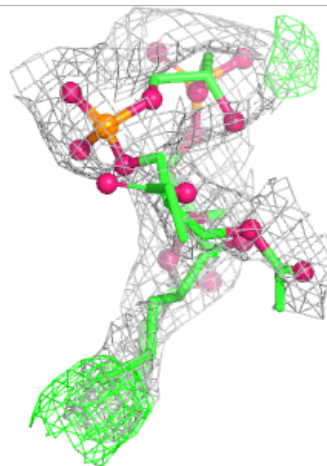
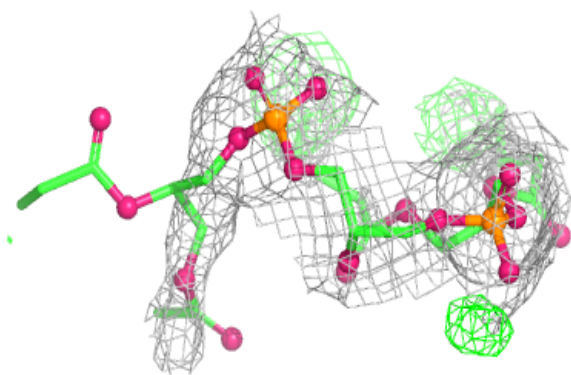
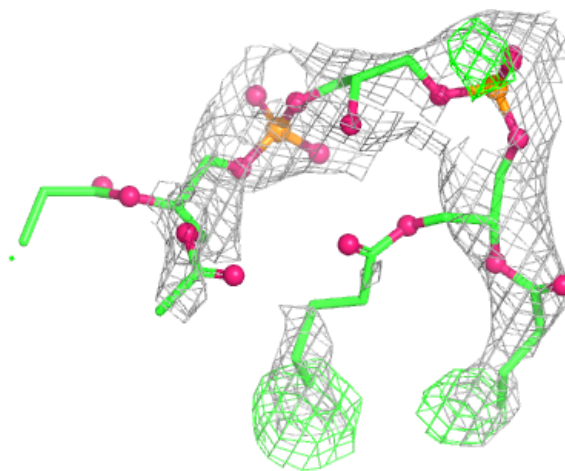
Electron density around BOG P 2010:

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and green (positive)



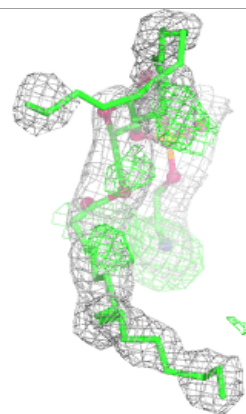
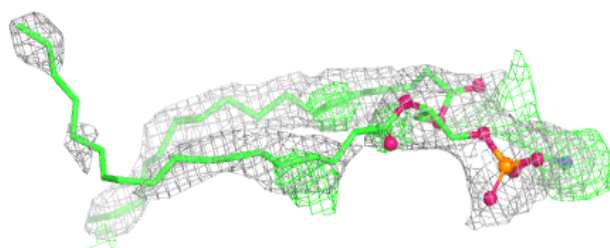
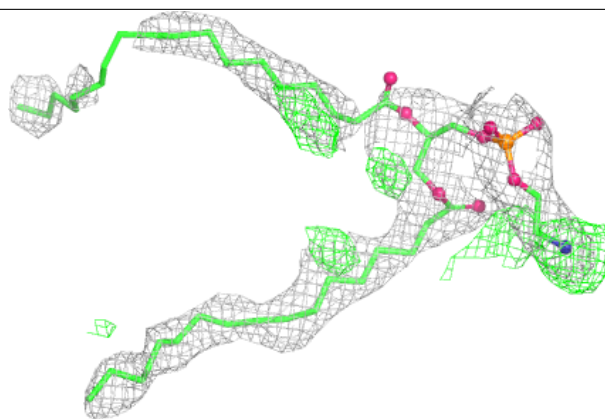
Electron density around CDL Q 3003:

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



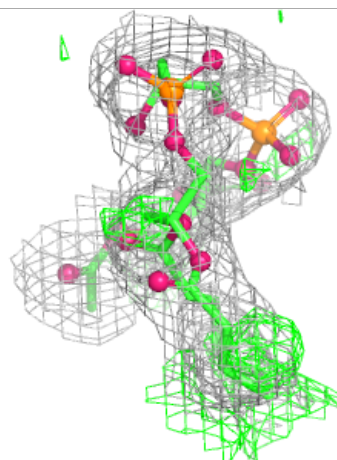
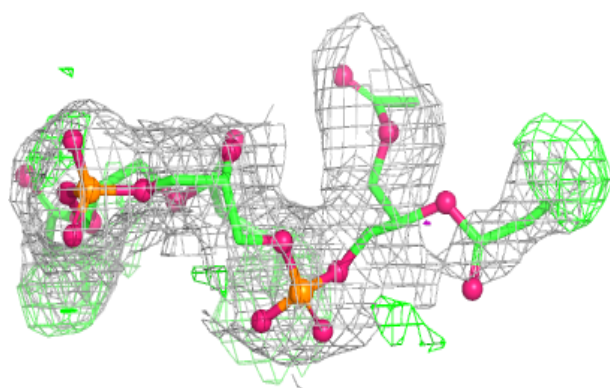
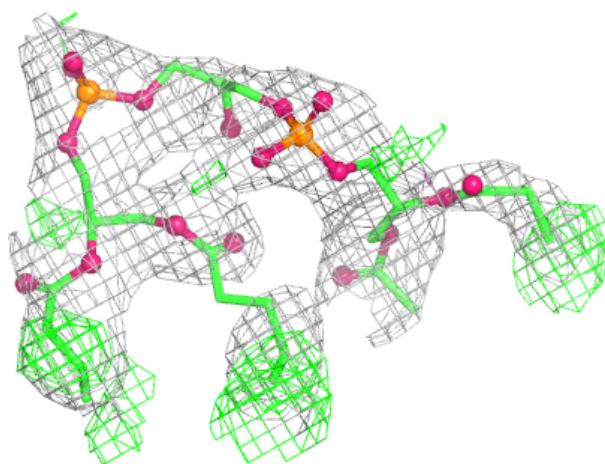
Electron density around PEE R 3005:

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and green (positive)



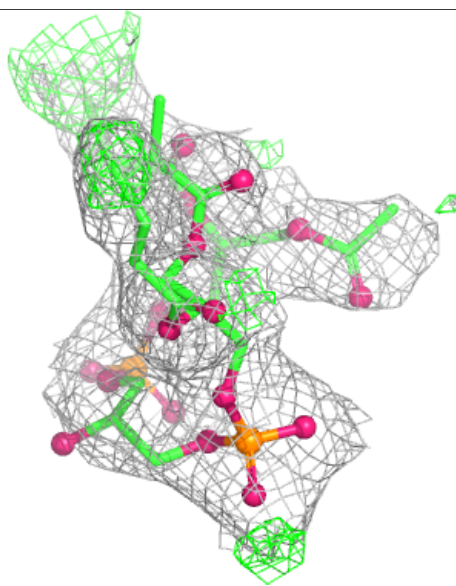
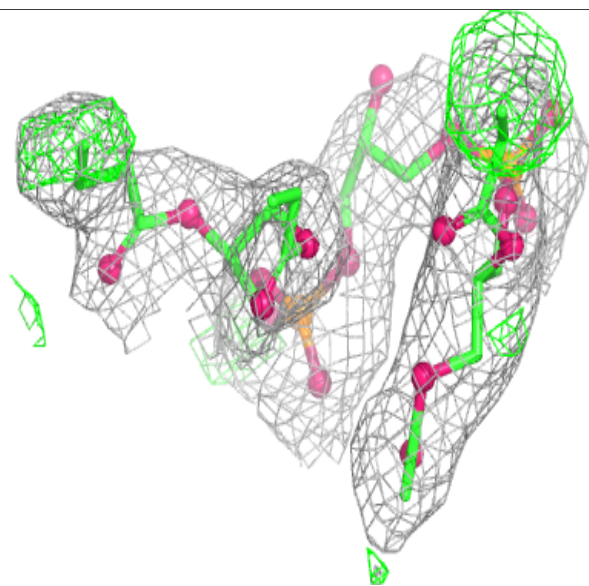
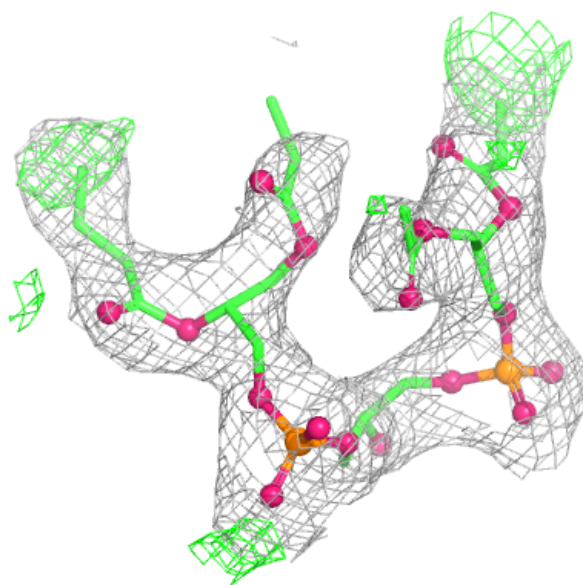
Electron density around CDL D 2003:

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



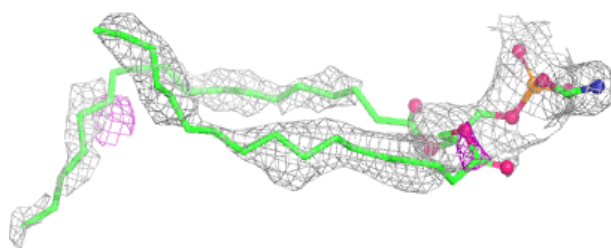
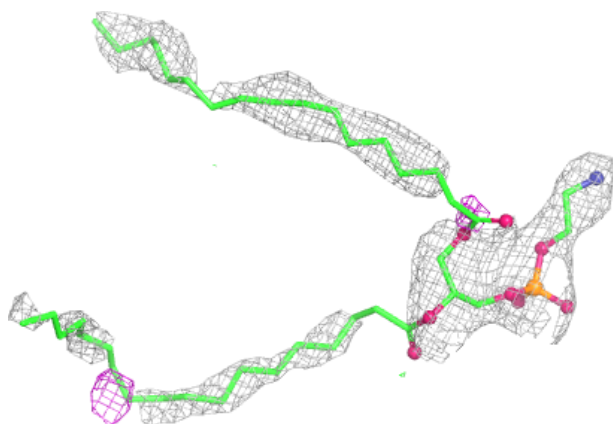
Electron density around CDL C 2004:

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

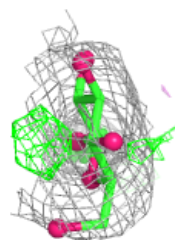
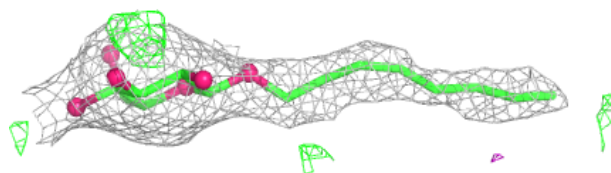
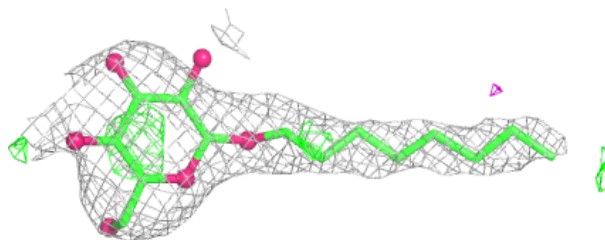


Electron density around PEE E 2005:

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

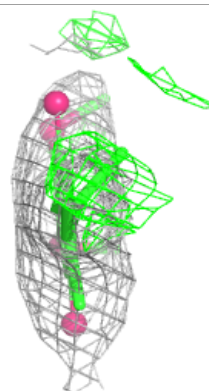
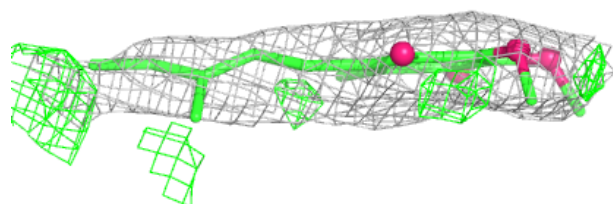
**Electron density around BOG Q 3009:**

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

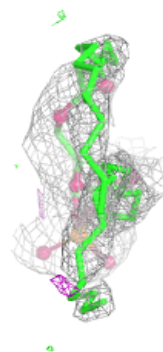
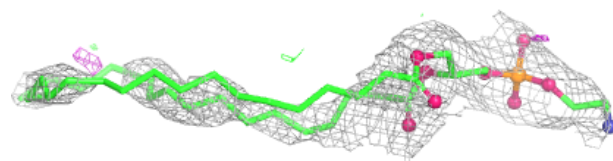


Electron density around UQ C 2002:

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

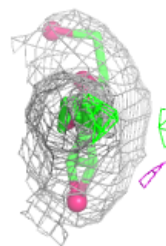
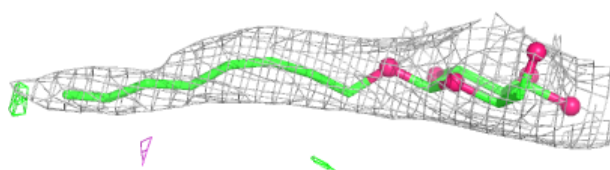
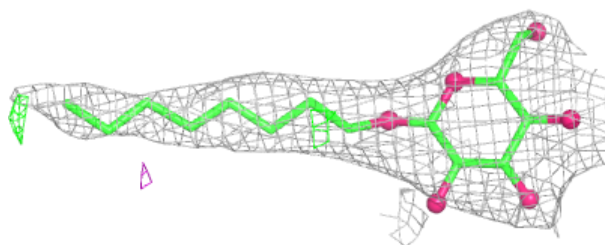
**Electron density around PEE P 3007:**

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

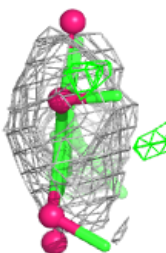
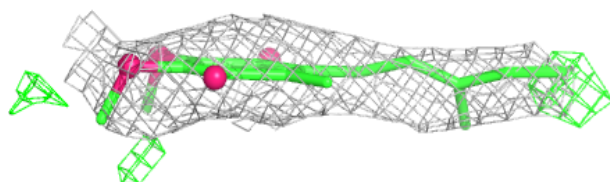
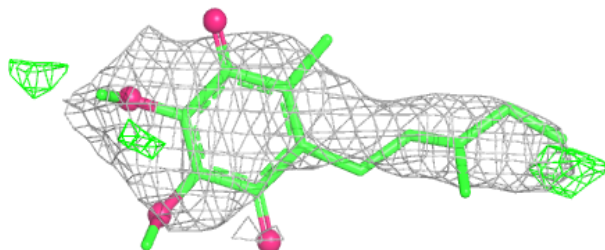


Electron density around BOG D 2009:

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

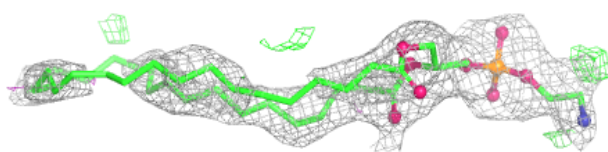
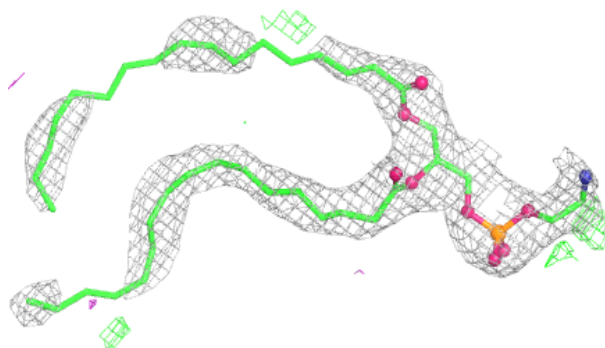
**Electron density around UQ P 3002:**

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

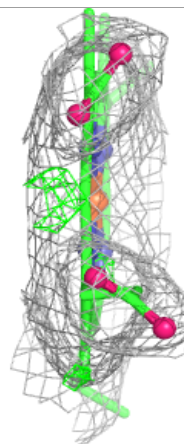
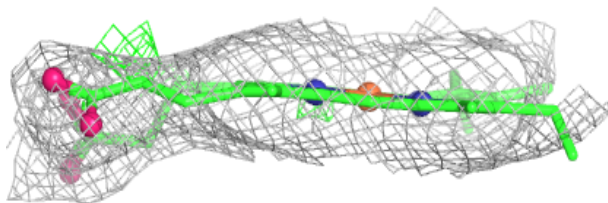
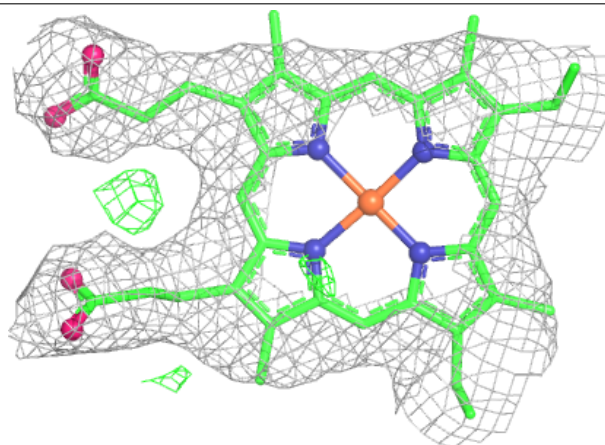


Electron density around PEE C 2007:

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

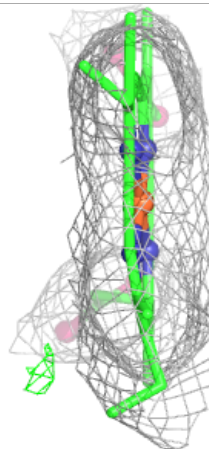
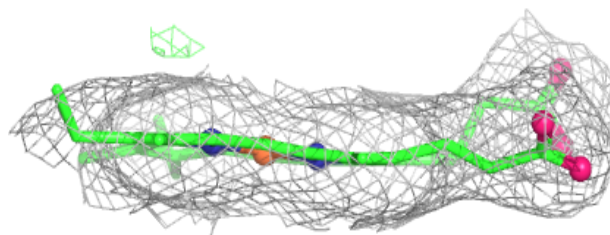
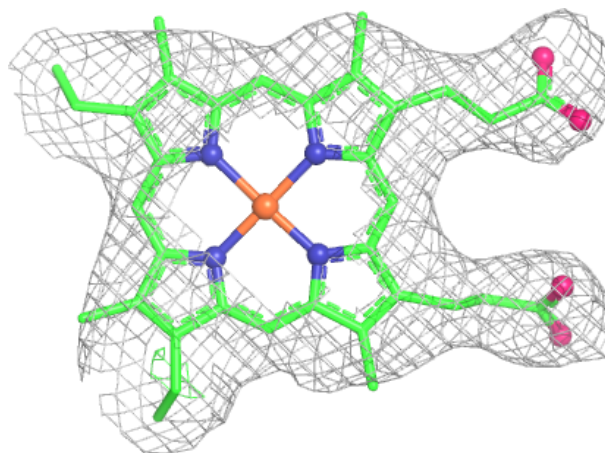
**Electron density around HEC Q 501:**

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



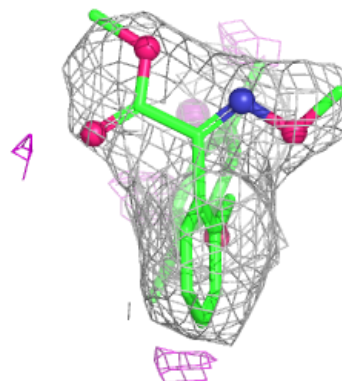
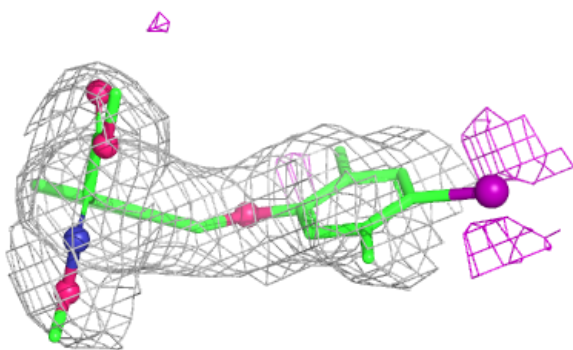
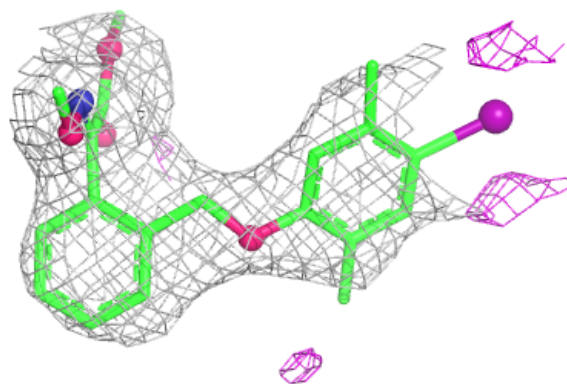
Electron density around HEC D 501:

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



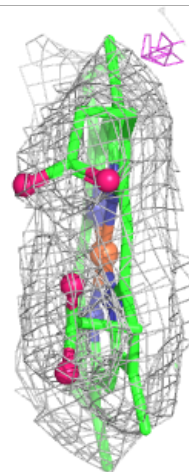
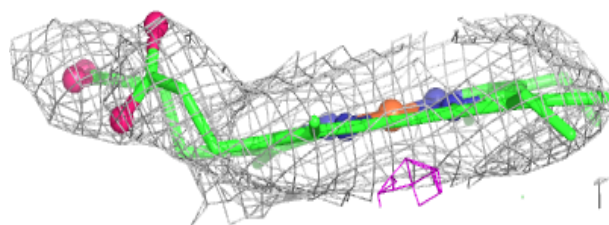
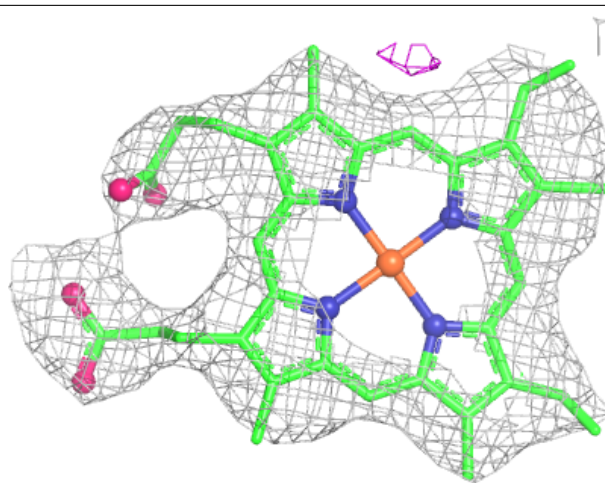
Electron density around IKR P 3001:

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



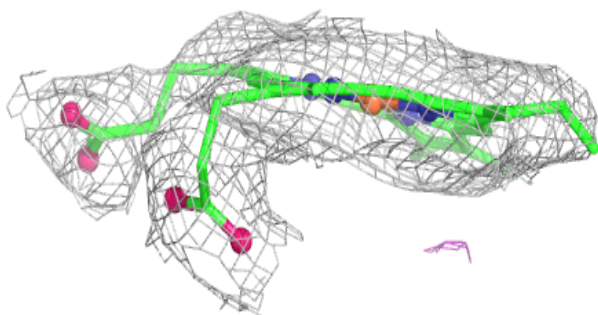
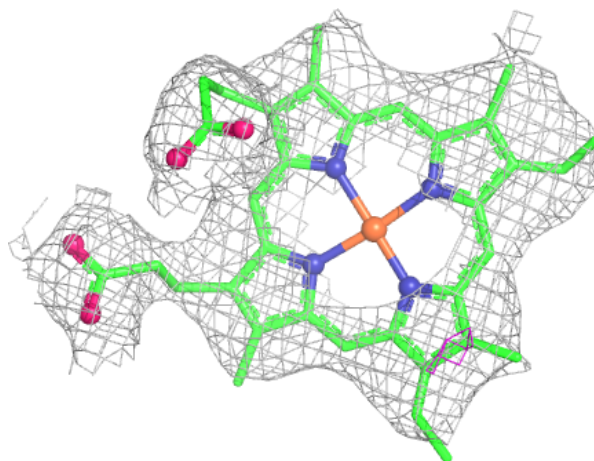
Electron density around HEM P 501:

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



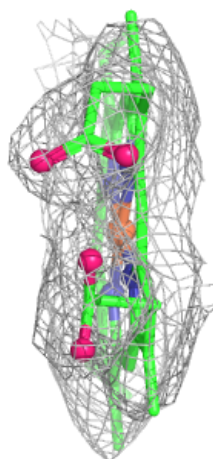
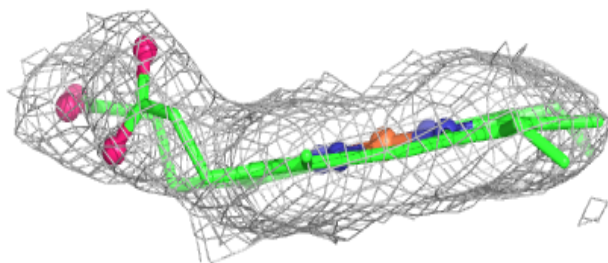
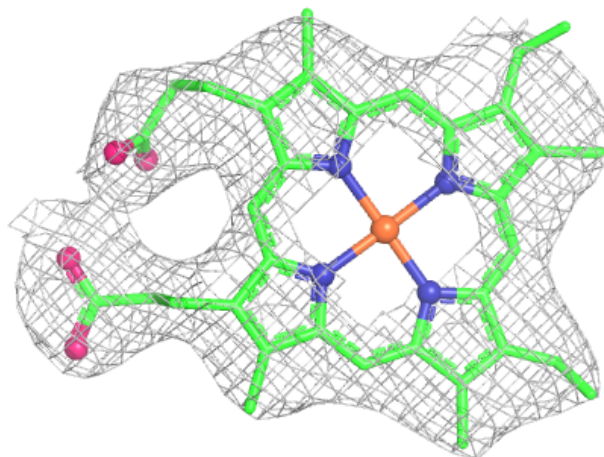
Electron density around HEM P 502:

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



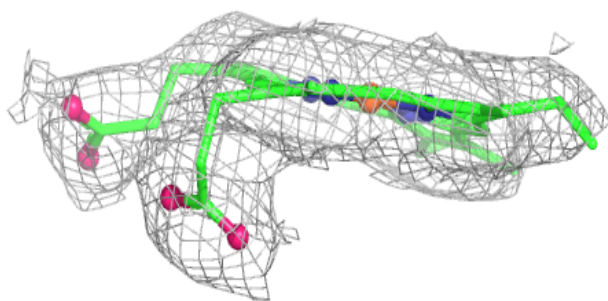
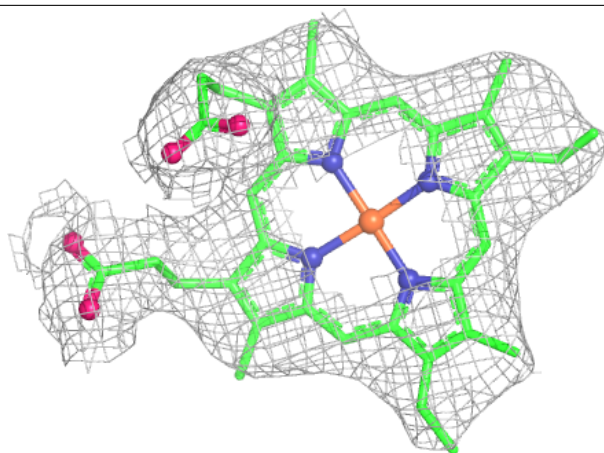
Electron density around HEM C 501:

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



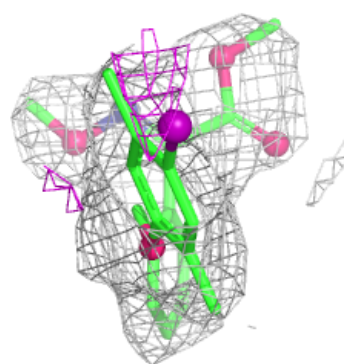
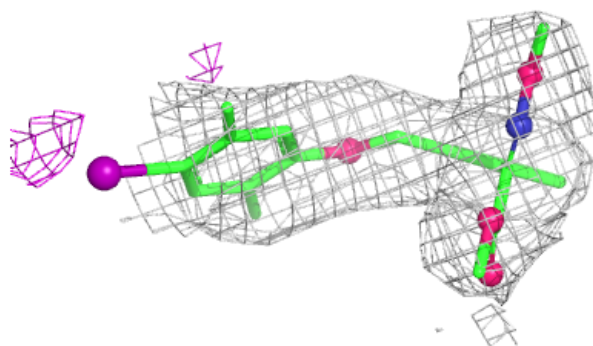
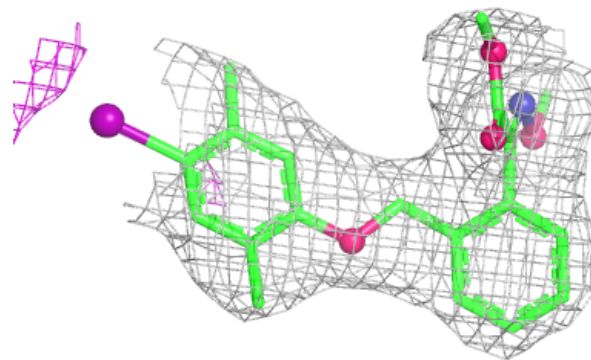
Electron density around HEM C 502:

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



Electron density around IKR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.