



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:27 PM EDT

PDB ID : 3CWB / pdb_00003cwb
Title : Chicken Cytochrome BC1 Complex inhibited by an iodinated analogue of the polyketide Crocacin-D
Authors : Huang, L.; Cromartie, T.; Viner, R.; Crowley, P.J.; Berry, E.A.
Deposited on : 2008-04-21
Resolution : 3.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

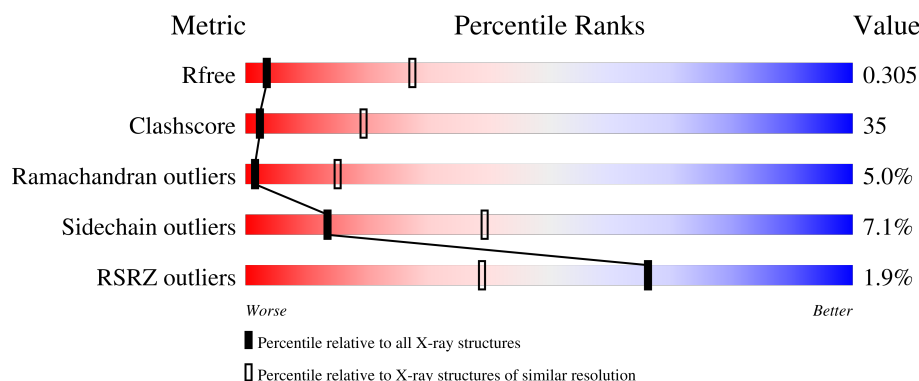
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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.



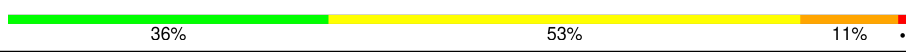
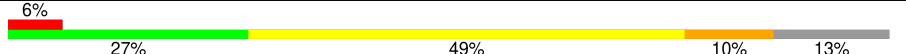
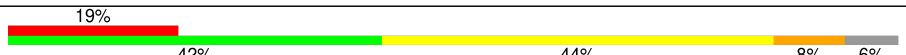
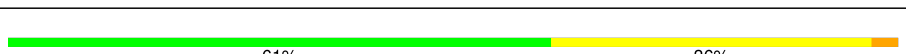
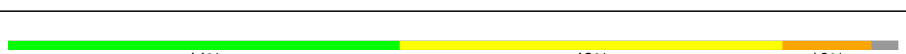
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	% 39% 50% 9% ..
1	N	446	% 41% 47% 10% ..
2	B	441	37% 49% 9% 5%
2	O	441	% 37% 50% 9% .
3	C	380	34% 56% 10% .

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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	52	
9	V	52	
10	J	61	
10	W	61	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEE	P	3008	-	X	-	-
13	AZI	C	2011	-	X	-	-
13	AZI	P	3011	-	X	-	-
17	HEC	D	501	X	-	-	-
17	HEC	Q	501	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32696 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN.

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
			1508	948	262	292	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			
6	S	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- 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			

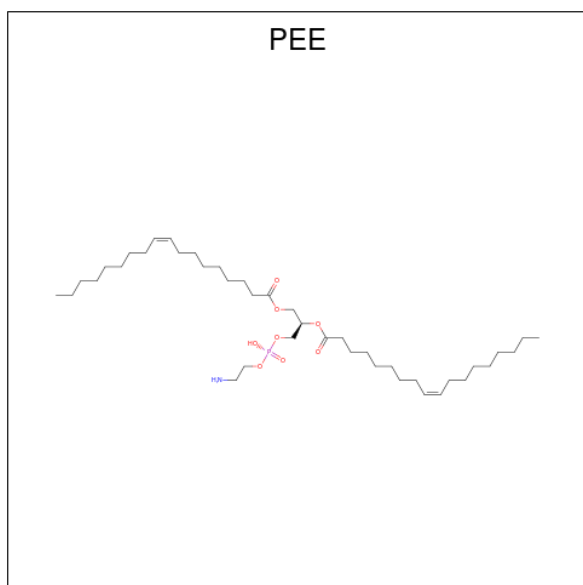
- Molecule 9 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	51	Total	C	N	O	S	0	0	2
			302	181	61	58	2			
9	V	49	Total	C	N	O	S	0	0	3
			292	176	59	55	2			

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

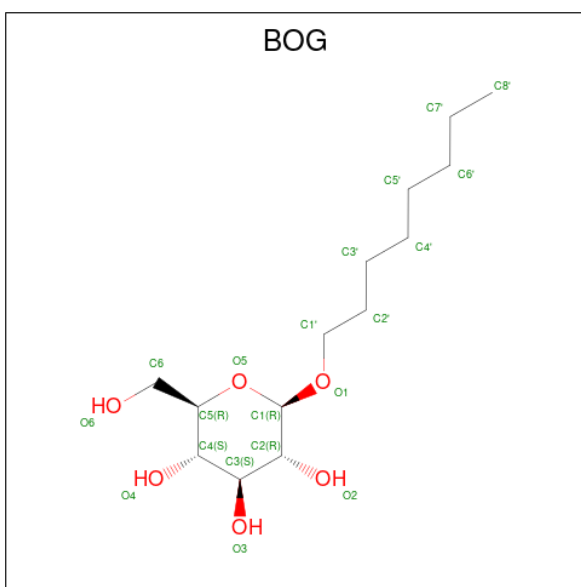
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

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



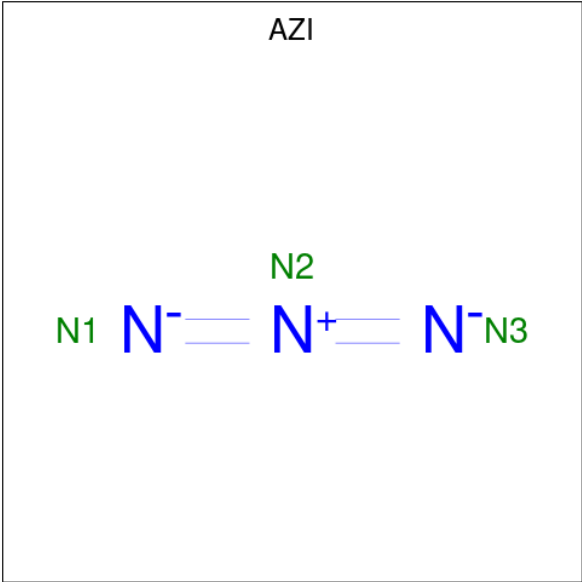
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	O	P		0	0
			21	12	8	1			
11	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	P	1	Total	O	P			0	0
			5	4	1				
11	W	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 12 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



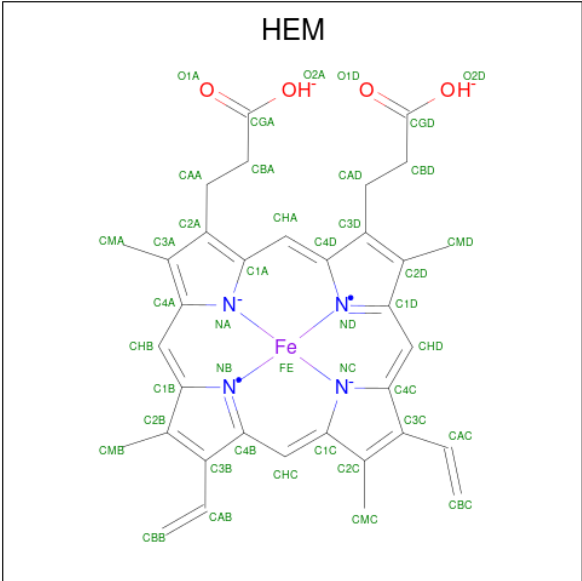
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			12	10	2		
12	D	1	Total	C	O	0	0
			20	14	6		
12	E	1	Total	C	O	0	0
			20	14	6		
12	P	1	Total	C	O	0	0
			19	13	6		
12	Q	1	Total	C	O	0	0
			20	14	6		
12	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 13 is AZIDE ION (CCD ID: AZI) (formula: N_3).



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

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



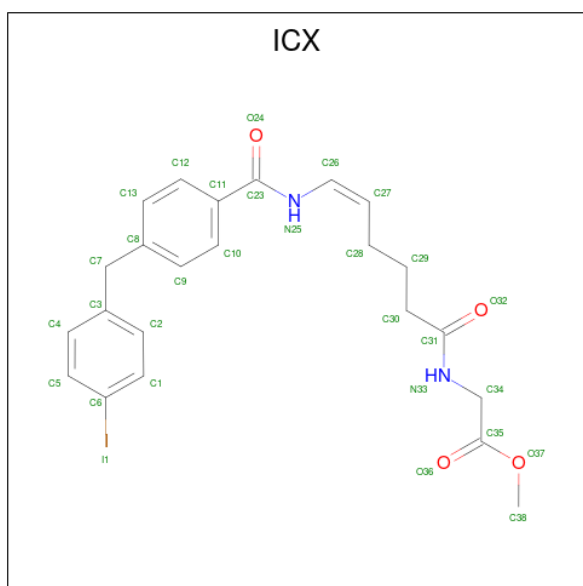
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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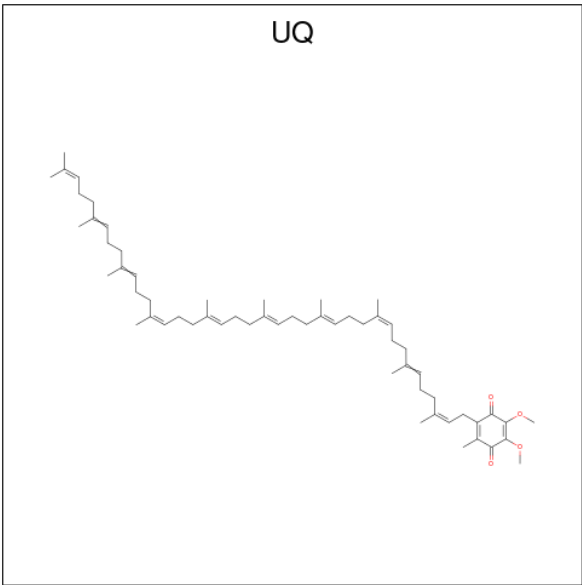
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is methyl N-[(5Z)-6-({[4-(4-iodobenzyl)phenyl]carbonyl}amino)hex-5-enoyl]glycinate (CCD ID: ICX) (formula: C₂₃H₂₅IN₂O₄).



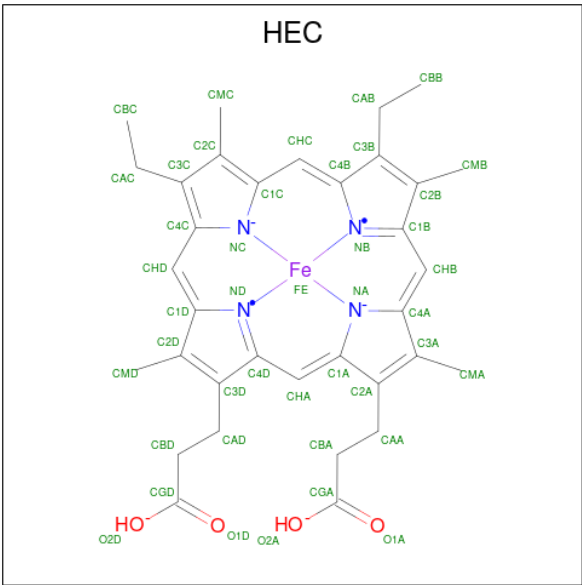
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	I	N	O	0	0
			30	23	1	2	4		
15	P	1	Total	C	I	N	O	0	0
			30	23	1	2	4		

- Molecule 16 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



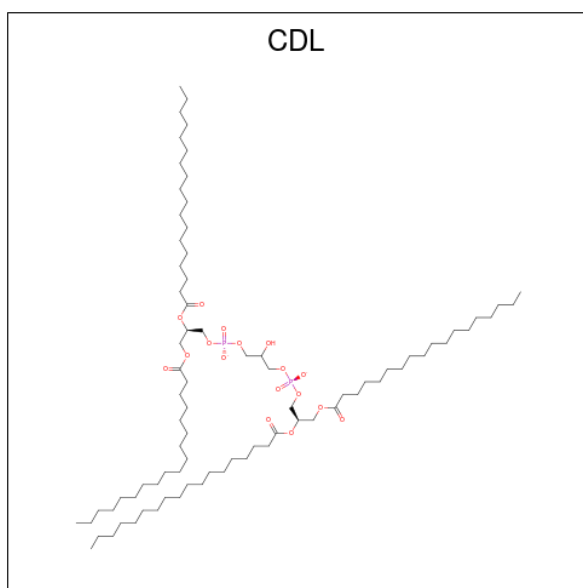
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			19	15	4		
16	P	1	Total	C	O	0	0
			19	15	4		

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



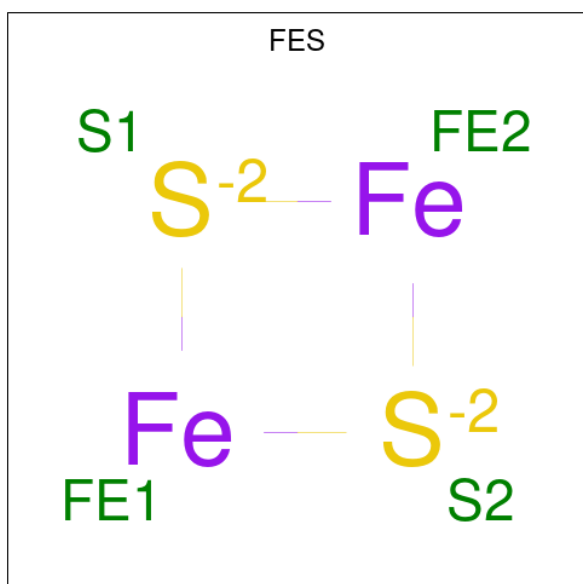
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
17	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- 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 UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	E	1	Total	O	0	0
			2	2		
20	P	2	Total	O	0	0
			2	2		
20	Q	1	Total	O	0	0
			1	1		

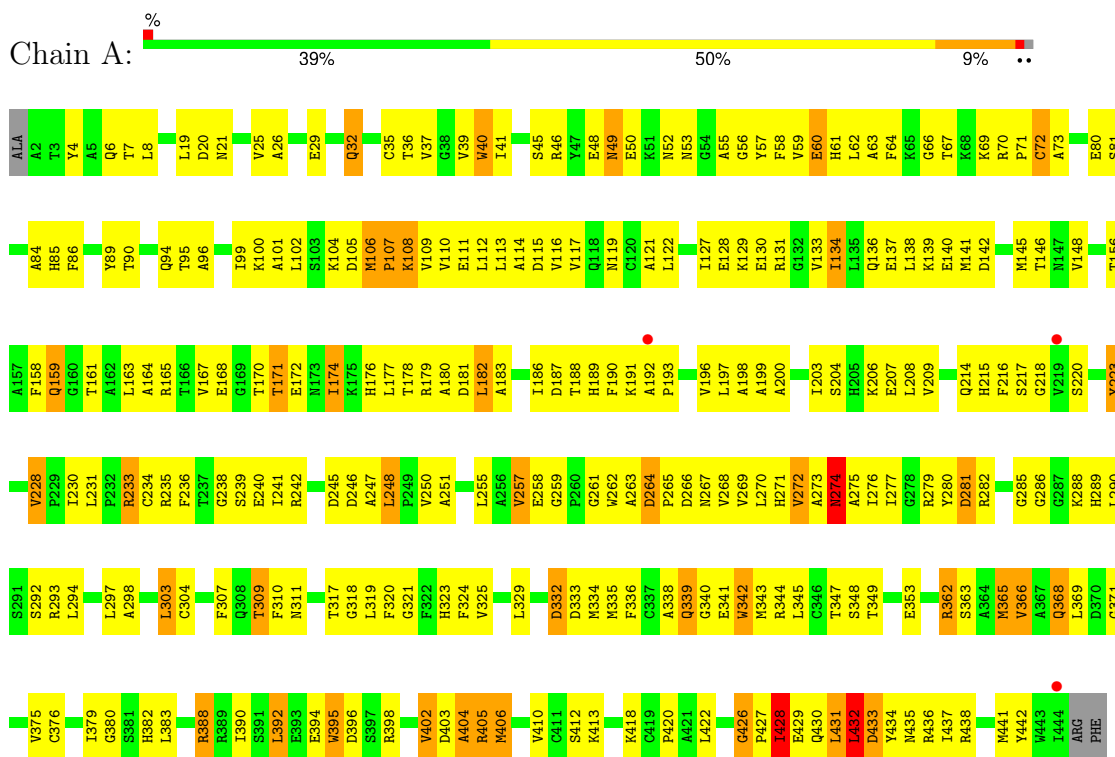
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	C	8	Total	O	0	0
			8	8		
21	P	7	Total	O	0	0
			7	7		
21	U	1	Total	O	0	0
			1	1		

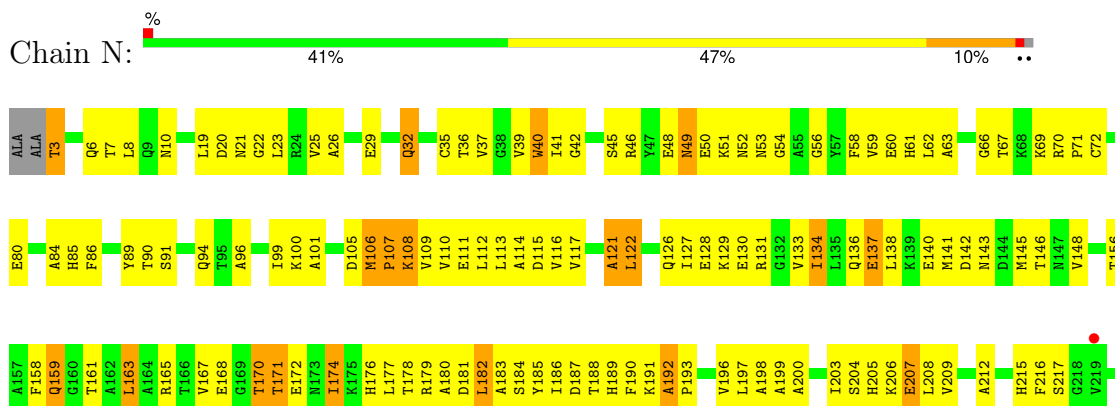
3 Residue-property plots

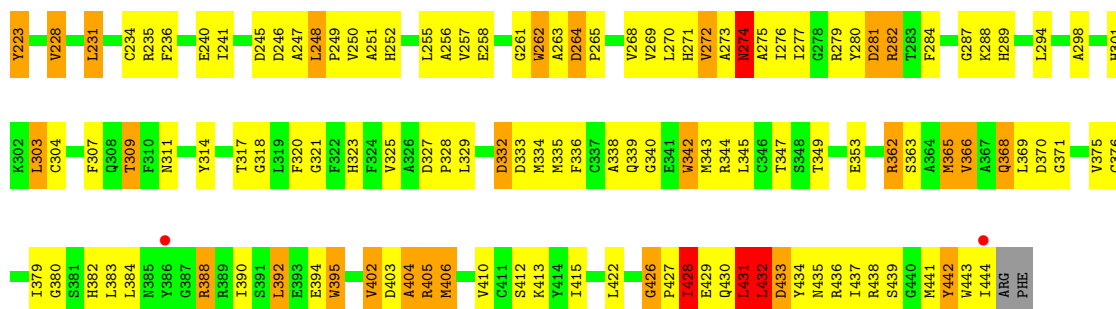
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



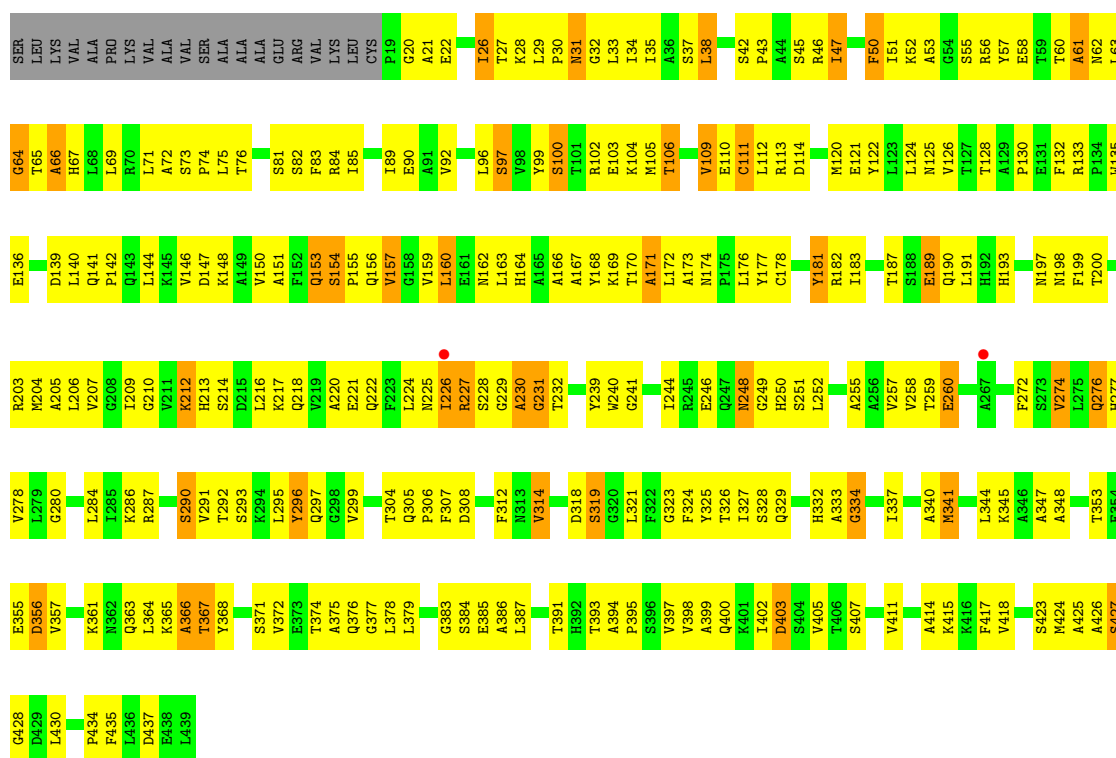
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I





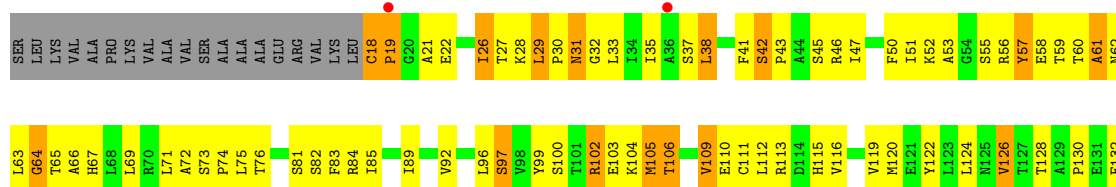
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

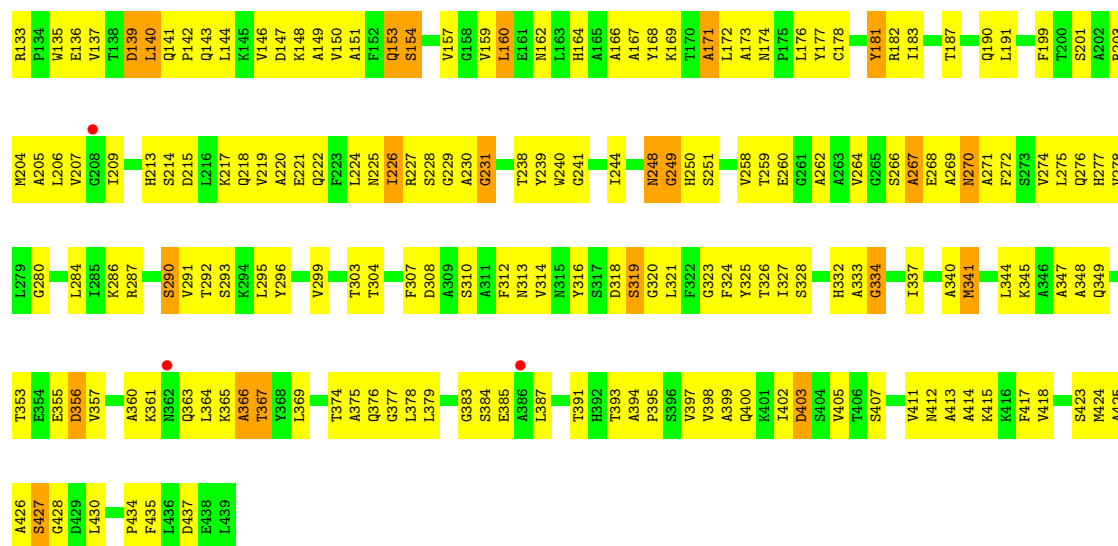
Chain B: 37% 49% 9% 5%



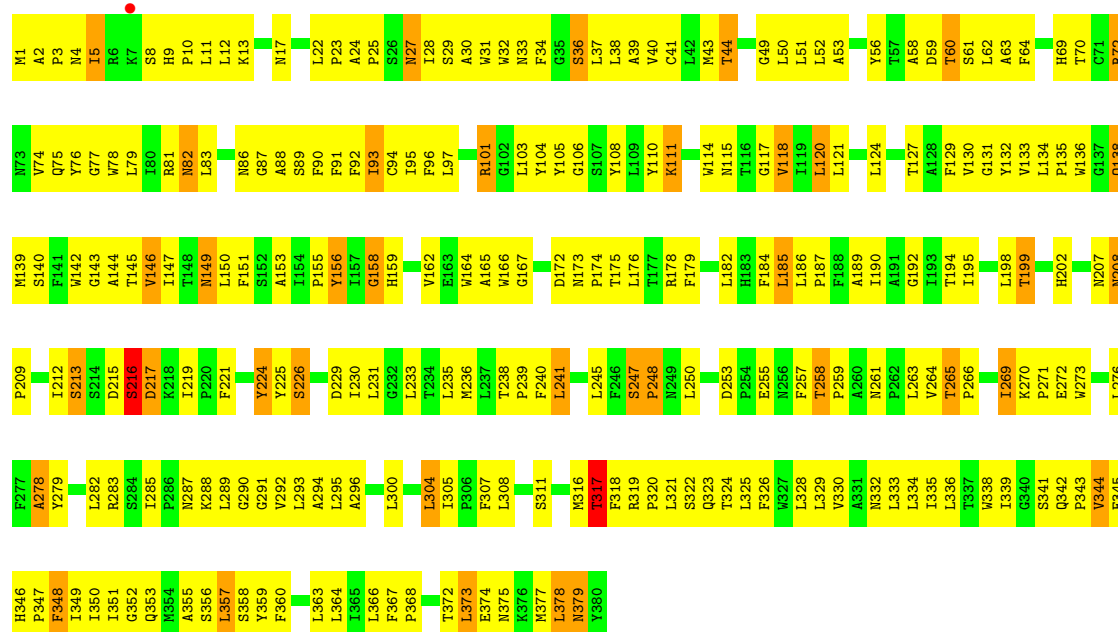
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain O: 37% 50% 9% 4%

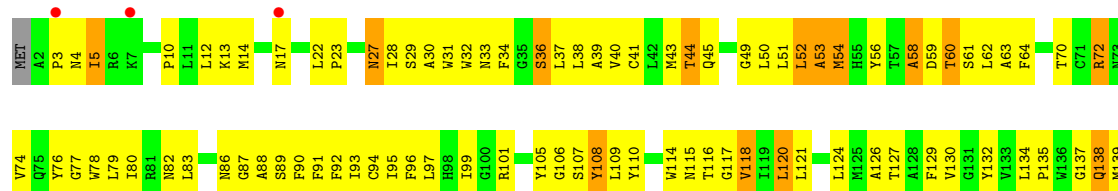


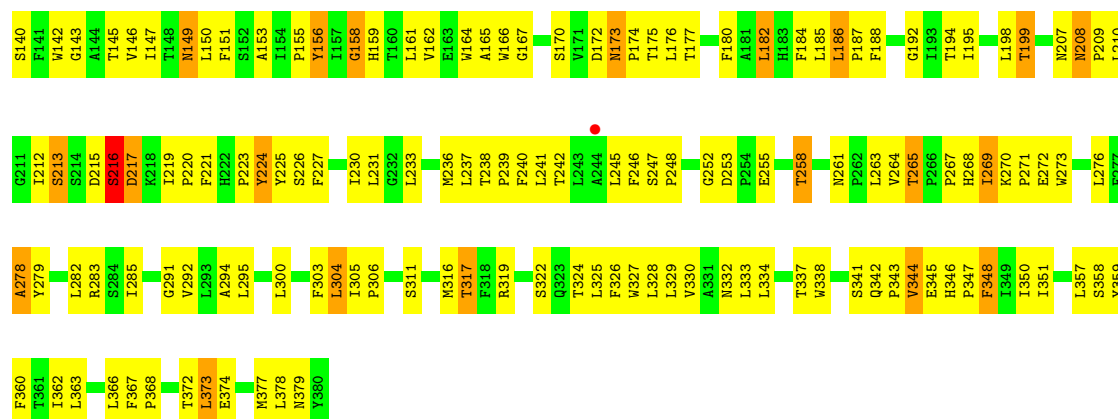


- Molecule 3: Cytochrome b



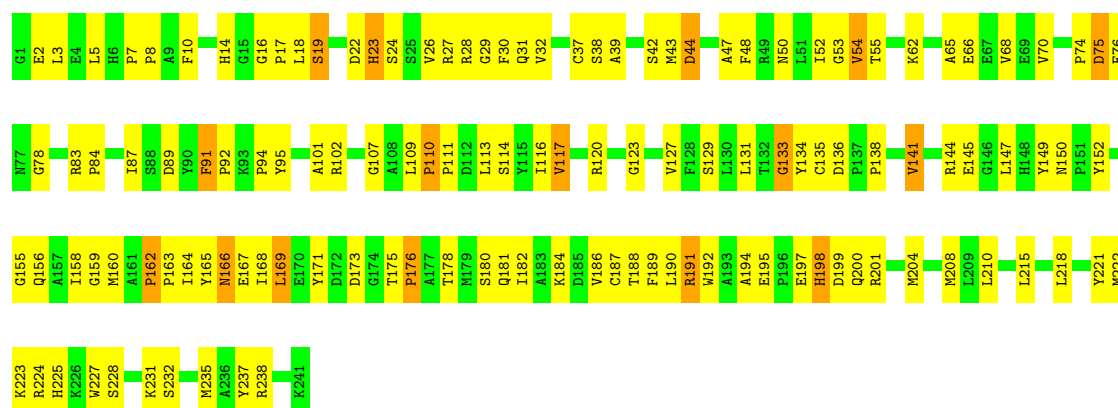
- Molecule 3: Cytochrome b





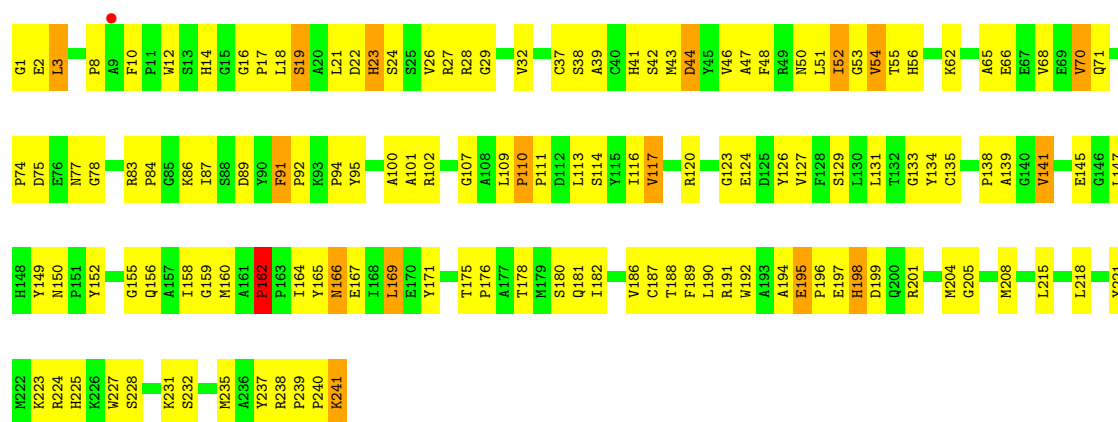
● Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D: 46% 48% 7%



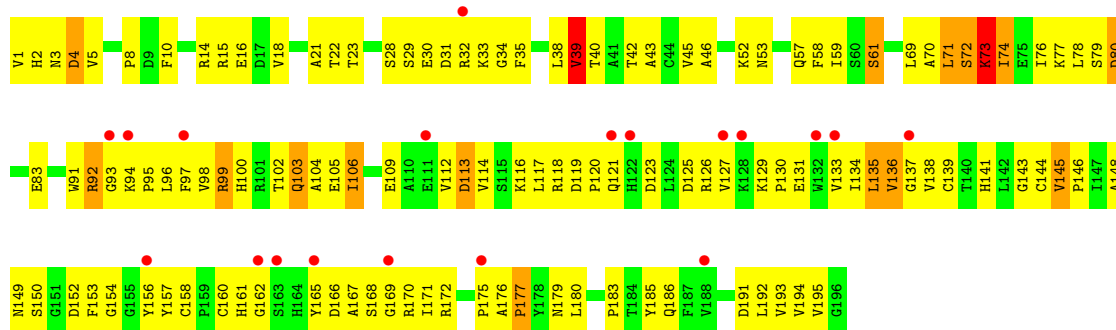
● Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q: 44% 49% 7%



● Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN

Chain E: 10% 37% 55% 8%



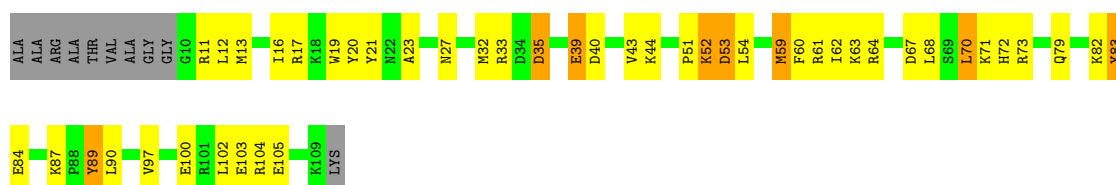
• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN

Chain R: 36% 53% 11%



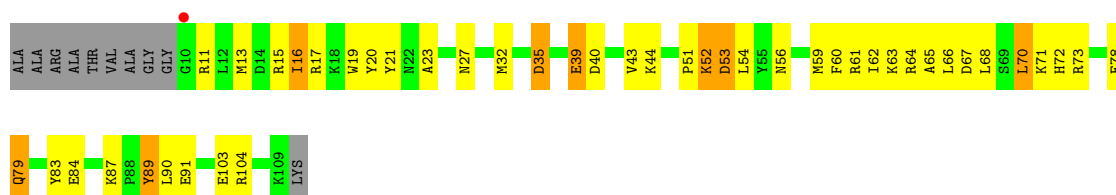
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain F: 49% 35% 7% 9%

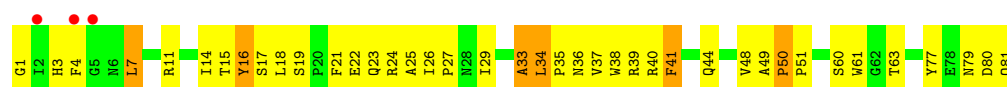


• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

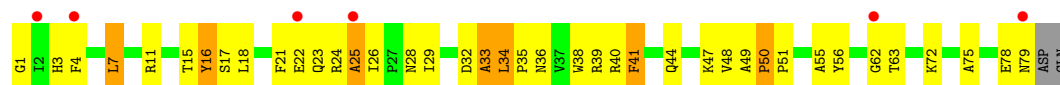
Chain S: 50% 34% 7% 9%



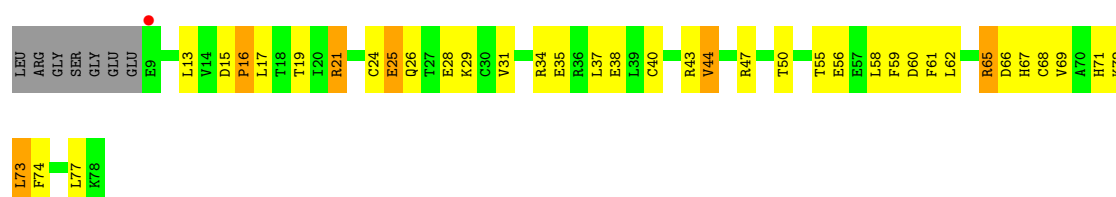
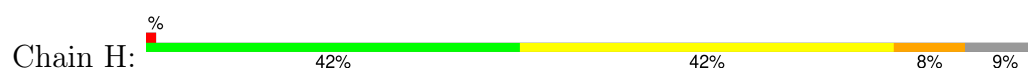
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



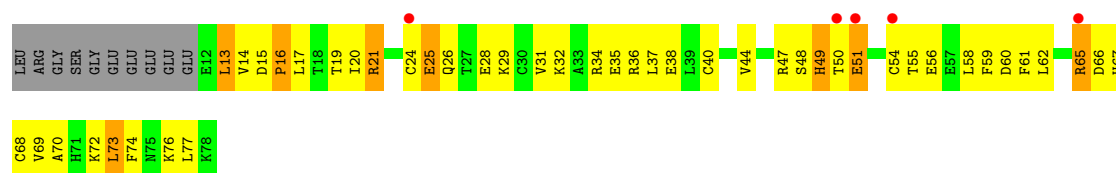
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



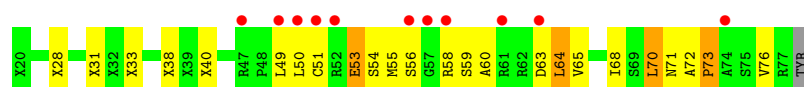
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



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

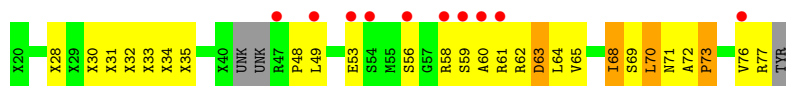


- Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence



- Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence

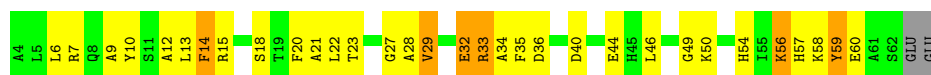




- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



- 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	174.78Å 182.66Å 242.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 3.51 21.98 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.8 (21.98-3.51) 98.5 (21.98-3.51)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.285 , 0.319 0.266 , 0.305	Depositor DCC
R_{free} test set	4918 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	32696	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	0/3511	1.11	32/4757 (0.7%)
1	N	0.63	0/3508	1.11	34/4753 (0.7%)
2	B	0.57	0/3196	1.04	15/4334 (0.3%)
2	O	0.59	0/3202	1.05	12/4343 (0.3%)
3	C	0.78	1/3122 (0.0%)	1.12	20/4273 (0.5%)
3	P	0.64	1/3114 (0.0%)	1.07	14/4263 (0.3%)
4	D	0.72	0/1956	1.16	18/2658 (0.7%)
4	Q	0.58	0/1956	1.12	15/2658 (0.6%)
5	E	0.55	0/1547	1.08	10/2103 (0.5%)
5	R	0.59	0/1542	1.13	11/2097 (0.5%)
6	F	0.74	0/901	1.03	5/1207 (0.4%)
6	S	0.58	0/901	0.96	4/1207 (0.3%)
7	G	0.69	0/698	1.06	3/946 (0.3%)
7	T	0.56	0/680	1.01	2/923 (0.2%)
8	H	0.63	0/582	0.96	3/779 (0.4%)
8	U	0.45	0/561	1.03	3/751 (0.4%)
9	I	0.67	0/218	1.16	0/293
9	V	0.71	0/218	1.07	1/293 (0.3%)
10	J	0.64	0/508	0.90	2/682 (0.3%)
10	W	0.58	0/489	0.87	2/658 (0.3%)
All	All	0.64	2/32410 (0.0%)	1.08	206/43978 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	54	MET	SD-CE	6.29	1.95	1.79
3	C	43	MET	SD-CE	5.11	1.92	1.79

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	143	GLY	N-CA-C	11.21	130.89	115.30
5	E	118	ARG	N-CA-C	-10.67	101.01	114.56
5	E	143	GLY	N-CA-C	10.55	128.92	115.21
2	O	18	CYS	CA-C-N	10.00	132.34	119.84
2	O	18	CYS	C-N-CA	10.00	132.34	119.84
1	A	66	GLY	N-CA-C	9.47	121.70	112.04
4	D	110	PRO	CA-C-N	9.12	129.20	119.90
4	D	110	PRO	C-N-CA	9.12	129.20	119.90
1	N	66	GLY	N-CA-C	8.43	120.63	112.04
1	N	433	ASP	N-CA-C	8.22	121.49	107.93
5	R	71	LEU	N-CA-C	8.18	120.33	110.19
1	A	426	GLY	CA-C-N	8.12	129.99	119.84
1	A	426	GLY	C-N-CA	8.12	129.99	119.84
1	N	426	GLY	CA-C-N	8.10	129.97	119.84
1	N	426	GLY	C-N-CA	8.10	129.97	119.84
1	A	433	ASP	N-CA-C	7.94	121.79	108.13
3	C	27	ASN	N-CA-C	7.89	122.66	112.41
2	B	251	SER	N-CA-C	7.62	120.47	111.71
3	P	27	ASN	N-CA-C	7.56	122.24	112.41
4	D	162	PRO	CA-C-N	7.28	126.91	119.56
4	D	162	PRO	C-N-CA	7.28	126.91	119.56
1	A	264	ASP	CA-C-N	7.27	127.44	119.87
1	A	264	ASP	C-N-CA	7.27	127.44	119.87
4	Q	195	GLU	CA-C-N	7.24	128.89	119.84
4	Q	195	GLU	C-N-CA	7.24	128.89	119.84
3	C	269	ILE	N-CA-C	7.21	118.25	107.51
3	C	72	ARG	N-CA-C	7.16	119.16	111.36
4	D	164	ILE	N-CA-C	7.16	120.53	108.86
4	Q	110	PRO	CA-C-N	7.15	127.19	119.90
4	Q	110	PRO	C-N-CA	7.15	127.19	119.90
8	U	49	HIS	N-CA-C	-7.13	95.61	110.80
3	C	110	TYR	N-CA-C	-7.12	98.93	109.62
2	O	349	GLN	N-CA-C	7.11	118.57	108.54
1	N	412	SER	N-CA-C	-7.08	103.49	111.07
5	R	125	ASP	N-CA-C	-7.08	104.77	113.41
5	R	39	VAL	N-CA-C	-7.04	103.47	110.30
6	F	39	GLU	N-CA-C	7.01	120.72	108.52
4	D	91	PHE	CA-C-N	6.98	126.74	119.76
4	D	91	PHE	C-N-CA	6.98	126.74	119.76
3	P	72	ARG	N-CA-C	6.95	118.93	111.36
3	P	269	ILE	N-CA-C	6.94	117.85	107.51
2	O	251	SER	N-CA-C	6.88	119.62	111.71
1	N	248	LEU	CA-C-N	6.83	126.63	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	248	LEU	C-N-CA	6.83	126.63	119.05
3	C	278	ALA	N-CA-C	-6.81	103.54	110.97
1	N	432	LEU	N-CA-C	6.78	123.91	112.99
3	C	226	SER	N-CA-C	-6.76	104.00	111.36
3	P	226	SER	N-CA-C	-6.73	103.95	111.28
10	J	20	PHE	N-CA-C	-6.67	103.70	110.97
3	C	185	LEU	N-CA-C	6.65	119.51	111.40
1	A	402	VAL	N-CA-C	6.64	118.33	109.37
3	C	378	LEU	N-CA-C	-6.63	105.09	113.72
1	A	220	SER	N-CA-C	6.62	120.31	110.52
1	A	412	SER	N-CA-C	-6.60	104.00	111.07
1	N	272	VAL	N-CA-C	-6.57	103.92	110.62
5	E	129	LYS	CA-C-N	6.55	128.03	119.84
5	E	129	LYS	C-N-CA	6.55	128.03	119.84
6	S	53	ASP	N-CA-C	6.50	118.05	110.97
1	N	303	LEU	N-CA-C	6.49	118.35	111.28
1	A	348	SER	N-CA-C	6.47	118.05	110.41
4	Q	164	ILE	N-CA-C	6.46	119.39	108.86
1	A	432	LEU	N-CA-C	6.44	123.36	112.99
3	P	378	LEU	N-CA-C	-6.42	105.38	113.72
1	N	368	GLN	N-CA-C	-6.38	104.98	112.89
3	C	101	ARG	N-CA-C	-6.37	104.26	111.07
2	B	21	ALA	N-CA-C	6.35	119.06	108.96
5	R	59	ILE	N-CA-C	6.35	117.09	110.62
1	N	347	THR	N-CA-C	6.27	121.81	114.04
5	R	85	LYS	N-CA-C	6.26	118.46	109.14
1	A	368	GLN	N-CA-C	-6.25	105.14	112.89
6	S	39	GLU	N-CA-C	6.20	119.31	108.52
7	T	24	ARG	N-CA-C	6.19	119.98	110.20
1	N	415	ILE	N-CA-C	6.15	116.85	111.56
3	P	185	LEU	N-CA-C	6.14	119.16	111.24
7	G	24	ARG	N-CA-C	6.14	119.17	109.96
1	N	189	HIS	N-CA-C	6.13	120.79	113.12
7	T	47	LYS	N-CA-C	-6.12	106.35	113.88
1	A	442	TYR	N-CA-C	6.05	118.35	108.55
10	W	20	PHE	N-CA-C	-6.04	104.39	110.97
4	Q	162	PRO	CA-C-N	5.97	125.59	119.56
4	Q	162	PRO	C-N-CA	5.97	125.59	119.56
4	D	7	PRO	CA-C-N	5.97	127.31	119.84
4	D	7	PRO	C-N-CA	5.97	127.31	119.84
3	C	224	TYR	N-CA-C	5.96	117.44	111.07
1	N	192	ALA	N-CA-C	5.95	122.96	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	263	ALA	N-CA-C	5.94	118.24	111.11
1	A	432	LEU	CA-C-N	-5.91	112.52	121.86
1	A	432	LEU	C-N-CA	-5.91	112.52	121.86
8	H	21	ARG	N-CA-C	-5.87	105.01	111.82
4	D	195	GLU	CA-C-N	5.87	127.17	119.84
4	D	195	GLU	C-N-CA	5.87	127.17	119.84
2	O	153	GLN	N-CA-C	-5.85	105.64	112.89
3	C	266	PRO	CA-C-N	5.83	125.20	118.85
3	C	266	PRO	C-N-CA	5.83	125.20	118.85
3	P	273	TRP	N-CA-C	5.83	120.98	111.37
1	A	231	LEU	N-CA-C	5.81	118.72	110.24
5	R	124	LEU	N-CA-C	5.81	120.23	113.20
5	R	129	LYS	CA-C-N	5.79	127.08	119.84
5	R	129	LYS	C-N-CA	5.79	127.08	119.84
6	F	35	ASP	N-CA-C	-5.79	105.32	112.90
2	B	227	ARG	N-CA-C	5.76	117.76	110.33
1	A	303	LEU	N-CA-C	5.75	117.55	111.28
1	N	415	ILE	CB-CA-C	-5.74	105.98	111.44
1	N	32	GLN	CA-C-N	5.74	125.44	119.64
1	N	32	GLN	C-N-CA	5.74	125.44	119.64
1	A	248	LEU	CA-C-N	5.73	125.41	119.05
1	A	248	LEU	C-N-CA	5.73	125.41	119.05
1	N	264	ASP	CA-C-N	5.73	125.83	119.87
1	N	264	ASP	C-N-CA	5.73	125.83	119.87
4	Q	155	GLY	N-CA-C	-5.72	107.89	114.69
1	A	272	VAL	N-CA-C	-5.71	105.16	110.53
4	D	155	GLY	N-CA-C	-5.71	107.89	114.69
1	N	428	ILE	N-CA-C	5.71	121.21	109.34
1	N	301	HIS	N-CA-C	5.69	119.54	112.59
6	S	35	ASP	N-CA-C	-5.68	105.46	112.90
3	C	257	PHE	N-CA-C	-5.67	105.57	112.88
1	A	304	CYS	N-CA-C	5.65	117.11	108.52
5	R	72	SER	N-CA-C	5.64	122.82	110.80
3	C	265	THR	N-CA-C	-5.64	102.67	109.72
8	U	21	ARG	N-CA-C	-5.63	105.28	111.82
2	B	276	GLN	N-CA-C	-5.61	104.81	111.03
1	A	347	THR	N-CA-C	5.61	120.99	114.04
1	N	402	VAL	N-CA-C	5.61	116.94	109.37
2	B	329	GLN	N-CA-C	-5.60	102.61	110.50
1	A	263	ALA	N-CA-C	5.59	117.84	111.02
3	P	110	TYR	N-CA-C	-5.59	101.23	109.62
3	P	278	ALA	N-CA-C	-5.58	104.89	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	265	THR	N-CA-C	-5.57	102.75	109.72
4	Q	91	PHE	CA-C-N	5.57	125.50	119.76
4	Q	91	PHE	C-N-CA	5.57	125.50	119.76
1	N	256	ALA	N-CA-C	5.57	117.31	108.79
6	S	16	ILE	N-CA-C	-5.56	105.68	110.74
2	O	42	SER	N-CA-C	-5.55	102.42	110.08
6	F	97	VAL	N-CA-C	-5.55	104.92	110.30
3	C	146	VAL	CB-CA-C	-5.50	105.01	111.94
7	G	37	VAL	N-CA-C	-5.49	105.02	110.62
4	Q	44	ASP	N-CA-C	5.49	122.48	110.80
1	N	442	TYR	N-CA-C	5.48	117.43	108.55
1	N	231	LEU	N-CA-C	5.48	118.24	110.24
2	B	189	GLU	N-CA-C	-5.47	105.01	110.97
2	B	356	ASP	N-CA-C	-5.47	105.32	111.28
2	B	61	ALA	N-CA-C	5.47	119.05	112.38
1	A	189	HIS	N-CA-C	5.45	120.41	113.55
2	O	113	ARG	N-CA-C	5.44	117.91	111.33
3	P	186	LEU	N-CA-C	5.43	120.94	113.77
2	B	153	GLN	N-CA-C	-5.42	105.92	112.54
2	B	305	GLN	CA-C-N	5.42	125.43	119.90
2	B	305	GLN	C-N-CA	5.42	125.43	119.90
3	C	69	HIS	N-CA-C	-5.42	105.37	111.28
1	A	32	GLN	CA-C-N	5.41	125.11	119.64
1	A	32	GLN	C-N-CA	5.41	125.11	119.64
1	A	428	ILE	N-CA-C	5.40	120.57	109.34
1	A	214	GLN	N-CA-C	5.39	119.02	112.23
3	P	252	GLY	N-CA-C	5.38	120.32	110.95
1	N	134	ILE	N-CA-C	-5.38	104.71	110.36
5	E	16	GLU	N-CA-C	5.38	117.84	111.33
2	O	102	ARG	N-CA-C	-5.36	106.00	112.54
3	C	247	SER	CA-C-N	5.34	126.52	119.84
3	C	247	SER	C-N-CA	5.34	126.52	119.84
4	D	44	ASP	N-CA-C	5.34	122.18	110.80
4	D	114	SER	N-CA-C	-5.31	105.62	112.68
2	O	61	ALA	N-CA-C	5.29	118.84	112.38
4	Q	114	SER	N-CA-C	-5.29	105.64	112.68
1	A	235	ARG	N-CA-C	5.29	117.36	109.59
1	N	170	THR	N-CA-C	5.29	117.35	110.43
4	D	19	SER	N-CA-C	5.26	117.33	108.96
6	F	53	ASP	N-CA-C	5.26	116.70	110.97
1	A	134	ILE	N-CA-C	-5.25	104.85	110.36
2	B	157	VAL	N-CA-C	5.23	117.63	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ALA	N-CA-C	5.23	121.37	109.81
4	Q	41	HIS	N-CA-C	5.23	117.04	108.52
2	O	356	ASP	N-CA-C	-5.23	105.58	111.28
2	B	100	SER	N-CA-C	5.22	117.19	108.99
4	D	191	ARG	N-CA-C	-5.21	105.29	110.97
5	E	39	VAL	N-CA-C	-5.20	104.82	110.23
1	N	329	LEU	N-CA-C	5.20	118.44	112.57
1	N	432	LEU	CA-C-N	-5.19	113.17	121.58
1	N	432	LEU	C-N-CA	-5.19	113.17	121.58
2	O	369	LEU	N-CA-C	5.18	118.39	111.75
9	V	76	VAL	N-CA-C	5.17	114.68	108.06
7	G	79	ASN	N-CA-C	-5.16	107.54	113.88
6	F	105	GLU	N-CA-C	5.16	116.59	111.07
2	O	126	VAL	CB-CA-C	-5.15	105.38	111.97
4	Q	77	ASN	N-CA-C	-5.15	107.05	113.38
3	C	111	LYS	N-CA-C	5.14	119.81	111.37
8	H	44	VAL	N-CA-C	5.14	115.36	110.53
1	A	329	LEU	N-CA-C	5.14	118.58	112.72
3	P	167	GLY	N-CA-C	-5.14	106.99	114.90
5	E	103	GLN	N-CA-C	-5.13	105.87	111.82
1	N	431	LEU	N-CA-C	-5.13	100.95	109.46
8	U	14	VAL	N-CA-C	5.11	115.33	108.17
4	D	133	GLY	N-CA-C	5.11	125.29	113.18
5	E	73	LYS	N-CA-C	-5.11	99.91	110.80
3	C	289	LEU	N-CA-C	5.10	116.53	111.07
2	B	66	ALA	N-CA-C	-5.08	105.20	111.40
4	D	136	ASP	N-CA-C	5.07	116.22	109.93
10	W	57	HIS	N-CA-C	5.06	119.08	113.01
5	E	99	ARG	N-CA-C	5.05	117.29	108.76
2	B	274	VAL	N-CA-C	-5.04	107.47	111.81
5	E	106	ILE	N-CA-C	5.04	116.37	110.62
4	Q	19	SER	N-CA-C	5.03	116.51	108.41
5	R	99	ARG	N-CA-C	5.03	117.26	108.76
10	J	57	HIS	N-CA-C	5.02	119.03	113.01
1	N	304	CYS	N-CA-C	5.01	116.13	108.52
8	H	13	LEU	N-CA-C	5.00	116.43	108.67
3	P	224	TYR	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	260	0
1	N	3437	0	3349	244	0
2	B	3141	0	3142	296	0
2	O	3147	0	3146	280	0
3	C	3020	0	3070	246	0
3	P	3012	0	3058	234	0
4	D	1898	0	1846	131	0
4	Q	1898	0	1846	142	0
5	E	1513	0	1478	138	0
5	R	1508	0	1466	136	0
6	F	881	0	887	50	0
6	S	881	0	887	56	0
7	G	676	0	659	44	0
7	T	658	0	647	50	0
8	H	574	0	548	38	0
8	U	553	0	535	44	0
9	I	302	0	251	38	0
9	V	292	0	251	30	0
10	J	497	0	490	21	0
10	W	478	0	478	32	0
11	A	21	0	13	0	0
11	C	99	0	149	5	0
11	P	54	0	72	2	0
11	W	50	0	77	1	0
12	C	12	0	18	0	0
12	D	20	0	28	5	0
12	E	20	0	28	1	0
12	P	19	0	24	1	0
12	Q	40	0	56	0	0
13	C	3	0	0	0	0
13	P	3	0	0	0	0
14	C	86	0	60	19	0
14	P	86	0	60	20	0
15	C	30	0	25	2	0
15	P	30	0	25	2	0
16	C	19	0	17	4	0
16	P	19	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	43	0	30	3	0
17	Q	43	0	30	3	0
18	D	42	0	28	3	0
18	G	40	0	24	1	0
18	P	82	0	52	5	0
19	E	4	0	0	1	0
19	R	4	0	0	0	0
20	E	2	0	0	0	0
20	P	2	0	0	0	0
20	Q	1	0	0	0	0
21	C	8	0	0	2	0
21	P	7	0	0	2	0
21	U	1	0	0	0	0
All	All	32696	0	32220	2302	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 35.

All (2302) 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)
3:C:17:ASN:HD21	7:G:1:GLY:HA3	1.15	1.08
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.37	1.04
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.42	1.01
5:E:73:LYS:O	5:E:74:ILE:HG13	1.60	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	1.00
2:B:353:THR:HG22	2:B:355:GLU:H	1.26	0.98
5:E:74:ILE:HD12	5:E:195:VAL:HB	1.45	0.97
3:P:17:ASN:HD21	7:T:1:GLY:HA3	1.28	0.96
1:A:233:ARG:HB3	1:A:233:ARG:HH11	1.30	0.95
5:R:72:SER:HB3	5:R:92:ARG:HD3	1.49	0.95
1:A:336:PHE:HE2	3:C:4:ASN:HB3	1.29	0.95
2:B:76:THR:HG22	2:B:81:SER:HA	1.49	0.94
4:Q:224:ARG:HH21	7:T:26:ILE:HG23	1.27	0.94
4:D:224:ARG:HH21	7:G:26:ILE:HG23	1.32	0.94
2:O:353:THR:HG22	2:O:355:GLU:H	1.31	0.94
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.04	0.92
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.52	0.92
2:O:310:SER:HB2	9:V:59:SER:HB2	1.53	0.91
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.53	0.90
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.88
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.09	0.88
2:B:248:ASN:ND2	2:B:428:GLY:HA2	1.89	0.88
2:O:76:THR:HG22	2:O:81:SER:HA	1.54	0.88
2:O:274:VAL:O	2:O:278:VAL:HG23	1.73	0.87
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.56	0.87
2:B:150:VAL:O	2:B:153:GLN:HG3	1.73	0.87
2:B:53:ALA:HB3	2:B:105:MET:HG3	1.54	0.87
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.20	0.86
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.11	0.86
2:O:361:LYS:O	2:O:365:LYS:HG3	1.75	0.85
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.41	0.84
3:P:241:LEU:HB3	4:Q:208:MET:HE2	1.56	0.84
5:R:98:VAL:HA	5:R:134:ILE:HG12	1.58	0.84
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.13	0.83
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.58	0.83
3:P:184:PHE:HA	14:P:501:HEM:HBC2	1.59	0.83
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.58	0.83
6:F:59:MET:HA	6:F:59:MET:HE3	1.61	0.82
5:E:119:ASP:HB3	5:E:179:ASN:ND2	1.95	0.82
2:O:150:VAL:O	2:O:153:GLN:HG3	1.79	0.82
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.14	0.82
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.45	0.82
1:N:336:PHE:HE2	3:P:4:ASN:HB3	1.45	0.82
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.05	0.81
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.44	0.81
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.14	0.81
3:C:241:LEU:HB3	4:D:208:MET:HE2	1.60	0.81
2:B:274:VAL:O	2:B:278:VAL:HG23	1.80	0.81
5:E:98:VAL:HA	5:E:134:ILE:HG12	1.61	0.81
6:S:89:TYR:HD1	6:S:90:LEU:N	1.79	0.81
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.16	0.81
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.63	0.80
6:F:89:TYR:HD1	6:F:90:LEU:N	1.78	0.80
2:O:53:ALA:HB3	2:O:105:MET:HG3	1.63	0.80
6:F:61:ARG:NH2	6:F:89:TYR:HE2	1.80	0.80
2:O:220:ALA:O	2:O:224:LEU:HB2	1.81	0.80
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.47	0.80
2:B:361:LYS:O	2:B:365:LYS:HG3	1.81	0.80
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.64	0.80
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:O	1:A:134:ILE:HG13	1.82	0.79
1:A:339:GLN:HE22	1:A:437:ILE:HG23	1.47	0.79
2:B:160:LEU:HD12	9:I:63:ASP:O	1.82	0.79
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.62	0.79
5:R:98:VAL:HG13	5:R:134:ILE:HD11	1.64	0.79
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.18	0.79
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.65	0.79
4:D:43:MET:HE1	4:D:189:PHE:HE2	1.46	0.79
3:C:129:PHE:CZ	3:C:147:ILE:HB	2.17	0.79
2:B:248:ASN:C	2:B:248:ASN:HD22	1.91	0.79
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.64	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.79	0.79
2:O:248:ASN:C	2:O:248:ASN:HD22	1.86	0.78
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.47	0.78
1:N:105:ASP:O	1:N:109:VAL:HG23	1.82	0.78
5:R:58:PHE:O	5:R:61:SER:HB3	1.82	0.78
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.13	0.78
4:Q:239:PRO:HB2	4:Q:240:PRO:HD2	1.65	0.78
9:I:63:ASP:O	9:I:64:LEU:HB2	1.84	0.78
2:B:327:ILE:HD11	9:I:58:ARG:O	1.84	0.78
1:A:339:GLN:NE2	1:A:437:ILE:HG23	1.99	0.78
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.64	0.78
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.66	0.77
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.77
1:A:277:ILE:HD11	1:A:345:LEU:HD11	1.66	0.77
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.49	0.77
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.66	0.77
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.19	0.77
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.19	0.77
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.48	0.77
2:O:248:ASN:ND2	2:O:428:GLY:HA2	1.98	0.77
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.20	0.77
3:P:347:PRO:O	3:P:350:ILE:HG22	1.85	0.77
5:E:76:ILE:O	5:E:192:LEU:HD12	1.85	0.76
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.50	0.76
3:P:127:THR:HG21	14:P:501:HEM:HBB2	1.66	0.76
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.33	0.76
3:P:40:VAL:HA	3:P:43:MET:HE3	1.68	0.76
5:R:102:THR:HG23	5:R:105:GLU:HG2	1.68	0.76
6:F:32:MET:CE	6:F:87:LYS:HG2	2.15	0.76
4:Q:43:MET:HE1	4:Q:189:PHE:HE2	1.48	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.22	0.75
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.68	0.75
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.68	0.75
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.22	0.75
4:D:223:LYS:C	4:D:223:LYS:HD3	2.11	0.75
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.34	0.75
1:A:106:MET:HE2	1:A:106:MET:O	1.85	0.75
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.69	0.75
5:E:160:CYS:SG	3:P:269:ILE:HD13	2.27	0.75
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.50	0.75
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.87	0.75
1:A:294:LEU:HD11	1:A:334:MET:HE1	1.67	0.75
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.69	0.75
5:R:71:LEU:HD22	5:R:92:ARG:NH1	2.02	0.74
6:S:61:ARG:NH2	6:S:89:TYR:HE2	1.85	0.74
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.69	0.74
2:O:47:ILE:HD12	2:O:47:ILE:N	2.02	0.74
3:C:17:ASN:ND2	7:G:1:GLY:HA3	1.98	0.74
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.22	0.74
1:N:342:TRP:HA	1:N:345:LEU:HD12	1.69	0.74
3:C:33:ASN:ND2	18:D:2003:CDL:H112	2.02	0.74
5:R:38:LEU:HD13	10:W:14:PHE:HZ	1.51	0.74
3:C:347:PRO:O	3:C:350:ILE:HG22	1.87	0.74
3:C:127:THR:HG21	14:C:501:HEM:HBB2	1.68	0.74
8:H:34:ARG:O	8:H:38:GLU:HG2	1.88	0.74
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.69	0.74
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.70	0.74
2:O:76:THR:CG2	2:O:82:SER:H	2.01	0.73
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.70	0.73
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.17	0.73
4:D:200:GLN:NE2	12:D:2091:BOG:H5	2.04	0.73
1:N:433:ASP:OD1	1:N:435:ASN:HB2	1.87	0.73
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.18	0.73
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.71	0.73
2:B:76:THR:CG2	2:B:82:SER:H	2.02	0.73
5:E:71:LEU:HB3	5:E:92:ARG:HD2	1.70	0.73
7:G:77:TYR:HA	7:G:80:ASP:OD1	1.89	0.73
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.04	0.73
2:O:154:SER:O	2:O:157:VAL:HG12	1.89	0.73
3:P:31:TRP:O	3:P:101:ARG:HG3	1.89	0.73
2:B:47:ILE:HD12	2:B:47:ILE:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.71	0.73
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.53	0.73
1:N:339:GLN:NE2	1:N:437:ILE:HG23	2.04	0.73
3:P:129:PHE:CZ	3:P:147:ILE:HB	2.24	0.73
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.03	0.73
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.69	0.72
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.71	0.72
2:O:150:VAL:HG23	2:O:151:ALA:N	2.03	0.72
1:N:339:GLN:HE22	1:N:437:ILE:HG23	1.54	0.72
3:C:184:PHE:HA	14:C:501:HEM:HBC2	1.72	0.72
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.24	0.72
1:A:433:ASP:OD1	1:A:435:ASN:HB2	1.90	0.72
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.25	0.72
1:A:178:THR:HB	1:A:181:ASP:OD1	1.89	0.72
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.25	0.72
3:C:269:ILE:O	3:C:270:LYS:HD3	1.89	0.71
6:S:59:MET:HA	6:S:59:MET:HE3	1.71	0.71
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.72	0.71
1:N:29:GLU:OE2	1:N:204:SER:HA	1.89	0.71
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.71	0.71
4:Q:117:VAL:HG21	4:Q:190:LEU:O	1.91	0.71
2:O:62:ASN:O	2:O:65:THR:HG22	1.91	0.71
2:O:248:ASN:ND2	2:O:250:HIS:H	1.86	0.71
5:E:98:VAL:HG13	5:E:134:ILE:HD11	1.73	0.71
1:N:130:GLU:O	1:N:134:ILE:HG13	1.90	0.71
2:O:327:ILE:HD11	9:V:58:ARG:O	1.88	0.71
1:N:3:THR:HG23	1:N:6:GLN:OE1	1.91	0.71
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.71	0.71
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.19	0.71
4:D:47:ALA:H	4:D:50:ASN:ND2	1.87	0.71
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.30	0.71
6:S:32:MET:HE1	6:S:87:LYS:HG2	1.72	0.71
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.26	0.71
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.73	0.71
2:B:33:LEU:HD21	2:B:224:LEU:HD22	1.73	0.71
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.72	0.71
2:B:248:ASN:ND2	2:B:250:HIS:H	1.88	0.71
3:C:265:THR:HB	5:R:145:VAL:HG12	1.73	0.70
1:N:294:LEU:HD11	1:N:334:MET:CE	2.21	0.70
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.73	0.70
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.72	0.70
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.73	0.70
1:N:371:GLY:O	1:N:375:VAL:HG23	1.92	0.70
4:Q:120:ARG:HG2	4:Q:120:ARG:HH11	1.55	0.70
1:A:251:ALA:HB1	1:A:428:ILE:HG22	1.72	0.70
3:C:316:MET:HE2	3:C:322:SER:HB3	1.74	0.70
17:D:501:HEC:HMB1	17:D:501:HEC:HBB3	1.74	0.70
3:C:269:ILE:HD13	5:R:160:CYS:SG	2.32	0.70
1:N:49:ASN:C	1:N:49:ASN:HD22	1.99	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.70
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.26	0.70
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.74	0.70
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.74	0.70
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.74	0.70
1:N:298:ALA:HA	1:N:303:LEU:HD12	1.74	0.69
1:A:342:TRP:HA	1:A:345:LEU:HD12	1.72	0.69
2:B:241:GLY:HA2	2:B:423:SER:OG	1.92	0.69
3:C:344:VAL:HG21	5:R:162:GLY:HA3	1.73	0.69
5:R:102:THR:O	5:R:106:ILE:HG13	1.92	0.69
3:C:265:THR:H	5:R:145:VAL:CG1	2.05	0.69
3:P:70:THR:HA	3:P:74:VAL:HG23	1.74	0.69
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.07	0.69
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.75	0.69
4:D:138:PRO:O	4:D:141:VAL:HG23	1.92	0.69
5:R:71:LEU:HD22	5:R:92:ARG:HH11	1.55	0.69
1:N:342:TRP:O	1:N:345:LEU:HB2	1.93	0.69
1:N:49:ASN:ND2	1:N:52:ASN:H	1.90	0.69
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.75	0.68
2:O:37:SER:HB3	2:O:213:HIS:ND1	2.08	0.68
2:B:258:VAL:HG11	2:B:312:PHE:CD2	2.28	0.68
9:I:53:GLU:C	9:I:55:MET:H	2.02	0.68
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.68
1:A:140:GLU:OE2	9:I:50:LEU:HB2	1.92	0.68
1:N:277:ILE:HD11	1:N:345:LEU:HD11	1.74	0.68
2:B:150:VAL:HG23	2:B:151:ALA:N	2.07	0.68
1:A:294:LEU:HD11	1:A:334:MET:CE	2.24	0.68
1:N:251:ALA:HB1	1:N:428:ILE:HG22	1.76	0.68
2:O:407:SER:O	2:O:411:VAL:HG23	1.94	0.68
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.28	0.68
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.27	0.68
3:C:238:THR:HB	3:C:239:PRO:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:502:HEM:HBB2	14:C:502:HEM:HMB1	1.74	0.68
5:E:58:PHE:O	5:E:61:SER:HB3	1.94	0.68
3:P:359:TYR:HD2	3:P:360:PHE:HD1	1.41	0.68
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.74	0.68
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.77	0.67
3:C:187:PRO:HG2	14:C:501:HEM:HMC3	1.75	0.67
5:E:1:VAL:HG23	5:E:3:ASN:H	1.57	0.67
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.24	0.67
5:E:72:SER:H	5:E:92:ARG:HD3	1.58	0.67
5:E:73:LYS:O	5:E:74:ILE:CG1	2.40	0.67
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.29	0.67
8:U:34:ARG:O	8:U:38:GLU:HG2	1.93	0.67
1:A:105:ASP:O	1:A:109:VAL:HG23	1.94	0.67
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.28	0.67
1:A:29:GLU:OE2	1:A:204:SER:HA	1.95	0.67
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.76	0.67
10:W:56:LYS:HG2	10:W:60:GLU:HG3	1.77	0.67
3:C:241:LEU:CB	4:D:208:MET:HE2	2.23	0.67
5:R:72:SER:HB2	5:R:91:TRP:HE1	1.59	0.67
4:D:28:ARG:HD2	4:D:171:TYR:CE1	2.30	0.67
1:N:431:LEU:HD12	1:N:432:LEU:N	2.10	0.67
1:N:29:GLU:HG3	1:N:203:ILE:O	1.95	0.67
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.77	0.67
2:B:220:ALA:O	2:B:224:LEU:HB2	1.95	0.67
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.59	0.67
3:C:359:TYR:HD2	3:C:360:PHE:HD1	1.43	0.67
2:B:33:LEU:CD2	2:B:224:LEU:HD22	2.25	0.67
8:H:58:LEU:HG	8:H:62:LEU:HD12	1.76	0.67
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.75	0.67
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.13	0.66
4:D:54:VAL:CG2	12:D:2091:BOG:H7'1	2.25	0.66
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.76	0.66
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.10	0.66
5:R:171:ILE:N	5:R:179:ASN:OD1	2.26	0.66
2:B:259:THR:HG22	2:B:260:GLU:N	2.10	0.66
4:D:43:MET:HG3	4:D:43:MET:O	1.96	0.66
7:G:40:ARG:HD2	18:G:2004:CDL:OA4	1.95	0.66
2:O:33:LEU:HD21	2:O:220:ALA:HB1	1.78	0.66
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.77	0.66
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.78	0.66
3:P:238:THR:HB	3:P:239:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.77	0.66
5:E:117:LEU:HD12	5:E:120:PRO:HA	1.78	0.66
1:N:49:ASN:C	1:N:49:ASN:ND2	2.50	0.66
4:Q:171:TYR:OH	4:Q:182:ILE:HA	1.96	0.66
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.76	0.66
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.76	0.66
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.78	0.66
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.26	0.66
2:O:241:GLY:HA2	2:O:423:SER:OG	1.95	0.66
5:R:168:SER:HB3	5:R:170:ARG:HG3	1.78	0.66
5:E:102:THR:O	5:E:106:ILE:HG13	1.96	0.66
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.77	0.66
3:P:41:CYS:O	3:P:44:THR:HG22	1.96	0.66
5:R:1:VAL:HG23	5:R:3:ASN:H	1.59	0.66
1:A:29:GLU:HG3	1:A:203:ILE:O	1.96	0.65
1:A:371:GLY:O	1:A:375:VAL:HG23	1.95	0.65
3:C:269:ILE:O	3:C:269:ILE:HG23	1.95	0.65
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.79	0.65
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.30	0.65
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.76	0.65
2:B:37:SER:HB2	2:B:213:HIS:HD1	1.60	0.65
5:E:38:LEU:HD13	10:J:14:PHE:HZ	1.60	0.65
5:E:83:GLU:HA	5:E:100:HIS:CG	2.31	0.65
5:R:177:PRO:C	5:R:178:TYR:HD2	2.03	0.65
5:R:185:TYR:H	5:R:185:TYR:HD2	1.43	0.65
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.26	0.65
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.78	0.65
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.61	0.65
5:E:52:LYS:C	5:E:52:LYS:HD3	2.22	0.65
1:N:156:THR:HA	1:N:159:GLN:HB3	1.77	0.65
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.61	0.65
1:A:431:LEU:HD12	1:A:432:LEU:N	2.11	0.65
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.31	0.65
1:N:107:PRO:HG2	1:N:108:LYS:H	1.60	0.65
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.77	0.65
5:E:83:GLU:HA	5:E:100:HIS:ND1	2.11	0.65
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.38	0.65
3:P:92:PHE:O	3:P:95:ILE:HG22	1.96	0.65
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.78	0.65
4:Q:117:VAL:HG23	4:Q:194:ALA:HB2	1.79	0.65
5:R:52:LYS:C	5:R:52:LYS:HD3	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:73:LEU:HD12	8:U:73:LEU:O	1.97	0.65
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.77	0.65
1:N:37:VAL:HG12	1:N:199:ALA:HB2	1.79	0.65
3:C:120:LEU:HD22	14:C:502:HEM:CAB	2.27	0.65
8:H:15:ASP:O	8:H:17:LEU:N	2.30	0.65
1:N:106:MET:O	1:N:106:MET:HE2	1.97	0.65
7:T:41:PHE:HD2	7:T:41:PHE:C	2.05	0.65
2:B:62:ASN:O	2:B:65:THR:HG22	1.97	0.64
2:B:333:ALA:O	2:B:337:ILE:HG13	1.97	0.64
1:A:298:ALA:HA	1:A:303:LEU:HD12	1.79	0.64
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.62	0.64
4:Q:235:MET:HE1	6:S:63:LYS:HG2	1.79	0.64
3:C:70:THR:HA	3:C:74:VAL:HG23	1.79	0.64
4:Q:95:TYR:CE2	4:Q:101:ALA:HA	2.32	0.64
3:C:271:PRO:HG2	3:C:276:LEU:HD23	1.79	0.64
3:C:127:THR:O	3:C:130:VAL:HG22	1.97	0.64
1:N:48:GLU:OE1	1:N:53:ASN:HA	1.98	0.64
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.13	0.64
3:P:316:MET:HE2	3:P:322:SER:HB3	1.79	0.64
1:A:170:THR:HG22	1:A:171:THR:N	2.11	0.64
2:B:212:LYS:HD3	2:B:213:HIS:N	2.13	0.64
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.79	0.64
1:N:35:CYS:HB2	1:N:200:ALA:O	1.97	0.64
2:O:341:MET:HE2	2:O:341:MET:HA	1.79	0.64
3:P:79:LEU:HD11	3:P:83:LEU:HD11	1.80	0.64
4:Q:138:PRO:O	4:Q:141:VAL:HG23	1.98	0.64
3:C:198:LEU:HD21	14:C:502:HEM:CMA	2.27	0.64
4:D:117:VAL:HG23	4:D:194:ALA:HB2	1.80	0.64
5:E:94:LYS:HE2	3:P:170:SER:HB2	1.80	0.64
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.80	0.64
1:A:156:THR:HA	1:A:159:GLN:HB3	1.78	0.64
1:A:67:THR:HG21	1:A:115:ASP:OD2	1.98	0.64
1:A:106:MET:HE3	1:A:208:LEU:HD13	1.80	0.64
4:D:235:MET:HB3	7:G:15:THR:HG22	1.78	0.64
6:F:52:LYS:CE	7:G:11:ARG:HH11	2.11	0.64
3:P:101:ARG:HD2	3:P:101:ARG:C	2.22	0.64
2:O:337:ILE:O	2:O:340:ALA:HB3	1.98	0.63
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.80	0.63
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.34	0.63
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.63	0.63
1:A:245:ASP:OD1	1:A:247:ALA:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:O	2:O:74:PRO:HD2	1.98	0.63
5:R:18:VAL:HG23	5:R:18:VAL:O	1.97	0.63
3:C:13:LYS:O	3:C:17:ASN:HB2	1.97	0.63
3:C:120:LEU:HD22	14:C:502:HEM:CBB	2.28	0.63
1:N:170:THR:HG22	1:N:171:THR:N	2.14	0.63
4:Q:43:MET:HG2	4:Q:91:PHE:CD2	2.34	0.63
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.89	0.63
5:R:15:ARG:HD2	7:T:21:PHE:O	1.99	0.63
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.34	0.63
2:B:154:SER:O	2:B:157:VAL:HG12	1.98	0.63
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.34	0.63
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.39	0.63
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.81	0.63
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.29	0.63
1:A:69:LYS:CE	1:A:70:ARG:HH21	2.12	0.63
1:A:433:ASP:O	1:A:437:ILE:HG13	1.99	0.63
6:F:71:LYS:O	6:F:72:HIS:HB2	1.97	0.63
1:N:69:LYS:CE	1:N:70:ARG:HH21	2.12	0.63
3:P:32:TRP:HA	3:P:101:ARG:NH1	2.14	0.63
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.98	0.63
1:N:46:ARG:HG2	1:N:46:ARG:HH11	1.64	0.62
3:P:241:LEU:CB	4:Q:208:MET:HE2	2.27	0.62
2:B:407:SER:O	2:B:411:VAL:HG23	1.99	0.62
1:N:284:PHE:CE2	9:V:71:ASN:O	2.52	0.62
2:B:110:GLU:O	2:B:111:CYS:HB3	1.99	0.62
2:O:76:THR:HG22	2:O:82:SER:H	1.62	0.62
2:O:150:VAL:CG2	2:O:151:ALA:N	2.61	0.62
7:G:49:ALA:O	7:G:50:PRO:C	2.42	0.62
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.29	0.62
1:A:107:PRO:HG2	1:A:108:LYS:H	1.64	0.62
3:C:32:TRP:HA	3:C:101:ARG:NH1	2.15	0.62
4:D:218:LEU:HD13	5:E:43:ALA:N	2.14	0.62
5:E:77:LYS:HB2	5:E:80:ASP:OD2	2.00	0.62
2:O:166:ALA:HB2	2:O:244:ILE:HD12	1.82	0.62
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	1.82	0.62
1:A:106:MET:HE2	1:A:106:MET:C	2.25	0.62
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.80	0.62
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.80	0.62
4:D:37:CYS:C	4:D:39:ALA:H	2.07	0.62
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.35	0.62
3:P:70:THR:HA	3:P:74:VAL:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.64	0.62
4:Q:238:ARG:HB3	4:Q:238:ARG:NH1	2.15	0.62
1:A:49:ASN:ND2	1:A:49:ASN:C	2.56	0.62
2:B:60:THR:HG23	2:B:61:ALA:N	2.15	0.62
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.17	0.62
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.81	0.62
2:B:424:MET:HG2	2:B:425:ALA:N	2.14	0.62
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.82	0.62
5:R:15:ARG:HG3	7:T:22:GLU:O	2.00	0.62
3:C:202:HIS:NE2	16:C:2002:UQ:O4	2.32	0.62
5:E:52:LYS:HD3	5:E:52:LYS:O	1.99	0.62
6:S:73:ARG:HH11	6:S:73:ARG:HG3	1.65	0.62
1:A:137:GLU:O	1:A:141:MET:HG3	1.99	0.61
3:C:32:TRP:HA	3:C:101:ARG:HH12	1.65	0.61
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.35	0.61
5:E:95:PRO:HG2	5:E:145:VAL:HG21	1.80	0.61
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.30	0.61
3:P:173:ASN:N	3:P:174:PRO:HD2	2.15	0.61
5:R:72:SER:HB3	5:R:92:ARG:CD	2.26	0.61
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.15	0.61
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.30	0.61
7:G:41:PHE:HD2	7:G:41:PHE:C	2.07	0.61
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.34	0.61
2:O:141:GLN:N	2:O:142:PRO:HD2	2.15	0.61
2:B:141:GLN:N	2:B:142:PRO:HD2	2.15	0.61
2:B:403:ASP:C	2:B:405:VAL:H	2.07	0.61
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.35	0.61
7:G:41:PHE:C	7:G:41:PHE:CD2	2.78	0.61
2:O:248:ASN:C	2:O:248:ASN:ND2	2.54	0.61
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.17	0.61
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.82	0.61
5:E:15:ARG:HD2	7:G:21:PHE:O	2.01	0.61
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.64	0.61
3:P:13:LYS:O	3:P:17:ASN:HB2	2.01	0.61
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.31	0.61
7:T:41:PHE:C	7:T:41:PHE:CD2	2.76	0.61
2:B:76:THR:HG22	2:B:82:SER:H	1.66	0.61
2:B:307:PHE:CD1	2:B:308:ASP:N	2.69	0.61
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.82	0.61
5:R:163:SER:OG	5:R:175:PRO:HD2	1.99	0.61
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:THR:OG1	1:N:100:LYS:HG2	2.01	0.61
1:N:136:GLN:C	1:N:138:LEU:H	2.07	0.61
1:A:49:ASN:C	1:A:49:ASN:HD22	2.08	0.61
1:A:178:THR:HG22	1:A:180:ALA:H	1.65	0.61
3:C:1:MET:HG2	3:C:2:ALA:H	1.65	0.61
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.30	0.61
14:C:502:HEM:HBB2	14:C:502:HEM:CMB	2.30	0.61
4:D:158:ILE:HG12	4:D:160:MET:H	1.63	0.61
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.36	0.61
4:Q:43:MET:O	4:Q:43:MET:HG3	2.00	0.61
4:Q:113:LEU:HD22	4:Q:116:ILE:HG21	1.82	0.61
9:V:70:LEU:O	9:V:70:LEU:HG	2.01	0.61
1:A:362:ARG:O	1:A:365:MET:HE2	2.01	0.61
2:B:218:GLN:O	2:B:222:GLN:HG3	2.01	0.61
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.83	0.61
4:D:171:TYR:OH	4:D:182:ILE:HA	2.01	0.61
5:E:117:LEU:HD12	5:E:121:GLN:H	1.65	0.61
6:F:52:LYS:HE2	7:G:11:ARG:HH11	1.64	0.61
2:O:357:VAL:O	2:O:361:LYS:HG3	2.01	0.61
3:P:36:SER:O	3:P:39:ALA:N	2.33	0.61
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.36	0.61
4:D:117:VAL:HG21	4:D:190:LEU:O	2.00	0.61
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.30	0.61
1:A:49:ASN:ND2	1:A:52:ASN:H	1.99	0.60
1:A:369:LEU:HD11	1:A:392:LEU:HD21	1.83	0.60
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.83	0.60
4:D:197:GLU:HG2	4:D:198:HIS:N	2.16	0.60
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.82	0.60
4:D:224:ARG:HH12	4:D:231:LYS:HE2	1.66	0.60
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.60
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.36	0.60
1:A:40:TRP:HZ3	1:A:376:CYS:SG	2.24	0.60
5:R:188:VAL:HG12	5:R:189:GLY:N	2.16	0.60
1:A:233:ARG:HH11	1:A:233:ARG:CB	2.11	0.60
4:Q:117:VAL:HG21	4:Q:190:LEU:C	2.25	0.60
10:W:40:ASP:O	10:W:44:GLU:HG3	2.01	0.60
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.83	0.60
9:I:70:LEU:HD23	9:I:71:ASN:HB2	1.81	0.60
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.66	0.60
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.35	0.60
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:51:PRO:O	6:S:52:LYS:C	2.45	0.60
3:C:173:ASN:N	3:C:174:PRO:HD2	2.17	0.60
3:C:265:THR:H	5:R:145:VAL:HG12	1.64	0.60
1:N:140:GLU:HG2	9:V:48:PRO:O	2.00	0.60
1:N:268:VAL:O	1:N:272:VAL:HG23	2.02	0.60
2:O:140:LEU:HD12	2:O:140:LEU:O	2.02	0.60
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.66	0.60
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.36	0.60
1:A:178:THR:O	1:A:179:ARG:C	2.45	0.60
3:C:101:ARG:HD2	3:C:101:ARG:C	2.27	0.60
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.65	0.60
3:P:198:LEU:HD21	14:P:502:HEM:CMA	2.32	0.60
4:Q:224:ARG:NH2	7:T:26:ILE:HG23	2.08	0.60
5:R:96:LEU:HD12	5:R:135:LEU:O	2.02	0.60
2:B:295:LEU:O	2:B:299:VAL:HG23	2.02	0.60
6:F:89:TYR:HD1	6:F:89:TYR:C	2.10	0.60
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.32	0.60
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.31	0.60
3:C:92:PHE:O	3:C:95:ILE:HG22	2.01	0.60
1:N:178:THR:HG22	1:N:180:ALA:H	1.65	0.60
1:N:433:ASP:O	1:N:437:ILE:HG13	2.02	0.60
3:P:271:PRO:HG2	3:P:276:LEU:HD23	1.84	0.60
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.67	0.59
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.83	0.59
4:D:109:LEU:O	4:D:111:PRO:HD3	2.02	0.59
17:D:501:HEC:HBB3	17:D:501:HEC:CMB	2.33	0.59
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.84	0.59
1:N:80:GLU:OE2	2:O:290:SER:HA	2.02	0.59
1:N:106:MET:HE2	1:N:106:MET:C	2.27	0.59
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.17	0.59
2:O:424:MET:HG2	2:O:425:ALA:N	2.16	0.59
6:S:52:LYS:HE2	7:T:11:ARG:HH11	1.67	0.59
3:P:79:LEU:HD12	3:P:79:LEU:O	2.02	0.59
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.66	0.59
3:C:30:ALA:HB1	18:D:2003:CDL:H111	1.84	0.59
5:E:72:SER:C	5:E:73:LYS:HG3	2.27	0.59
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.84	0.59
3:P:30:ALA:HB1	18:P:3003:CDL:H111	1.84	0.59
3:P:33:ASN:HB3	21:P:3020:HOH:O	2.02	0.59
5:R:52:LYS:HD3	5:R:52:LYS:O	2.03	0.59
6:S:89:TYR:HD1	6:S:89:TYR:C	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:64:LEU:HD12	9:V:77:ARG:C	2.27	0.59
2:B:150:VAL:CG2	2:B:151:ALA:N	2.65	0.59
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.84	0.59
3:C:41:CYS:O	3:C:44:THR:HG22	2.03	0.59
3:C:253:ASP:OD1	3:C:255:GLU:N	2.33	0.59
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.38	0.59
2:B:46:ARG:HG3	2:B:110:GLU:HG2	1.84	0.59
4:D:186:VAL:O	4:D:190:LEU:HG	2.02	0.59
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.33	0.59
4:D:62:LYS:O	4:D:66:GLU:HG3	2.01	0.59
1:N:84:ALA:HB2	1:N:101:ALA:HB2	1.85	0.59
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.85	0.59
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.83	0.59
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.30	0.59
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.37	0.59
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.02	0.59
9:I:33:UNK:HB2	9:I:73:PRO:HB3	1.85	0.59
2:O:29:LEU:HD22	2:O:30:PRO:HD2	1.83	0.59
5:R:114:VAL:O	5:R:114:VAL:HG12	2.02	0.59
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.84	0.59
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.85	0.59
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.18	0.59
8:H:65:ARG:O	8:H:68:CYS:HB3	2.03	0.59
9:I:70:LEU:HD23	9:I:70:LEU:C	2.28	0.59
3:P:32:TRP:HA	3:P:101:ARG:HH12	1.68	0.59
2:B:181:TYR:CE1	2:O:249:GLY:HA3	2.38	0.58
4:D:169:LEU:HD23	4:D:169:LEU:C	2.28	0.58
1:N:90:THR:O	1:N:167:VAL:HG11	2.03	0.58
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.18	0.58
8:U:15:ASP:O	8:U:17:LEU:N	2.36	0.58
1:A:106:MET:O	1:A:110:VAL:HG23	2.04	0.58
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.68	0.58
2:B:140:LEU:HD12	2:B:140:LEU:O	2.04	0.58
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.33	0.58
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.84	0.58
1:A:307:PHE:CD1	1:A:307:PHE:C	2.81	0.58
2:B:280:GLY:HA3	2:B:293:SER:OG	2.02	0.58
2:B:353:THR:HG22	2:B:355:GLU:N	2.09	0.58
5:E:117:LEU:CD1	5:E:121:GLN:H	2.15	0.58
6:S:21:TYR:C	6:S:21:TYR:CD2	2.82	0.58
6:S:89:TYR:C	6:S:89:TYR:CD1	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HG21	1:A:234:CYS:HA	1.85	0.58
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.19	0.58
8:H:24:CYS:C	8:H:26:GLN:H	2.11	0.58
2:B:199:PHE:O	2:B:226:ILE:HD13	2.04	0.58
3:C:195:ILE:O	3:C:199:THR:HB	2.03	0.58
2:O:60:THR:HG23	2:O:61:ALA:N	2.18	0.58
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.58
3:P:282:LEU:HD12	3:P:291:GLY:C	2.29	0.58
8:U:73:LEU:HD12	8:U:73:LEU:C	2.28	0.58
1:N:84:ALA:CB	1:N:101:ALA:HB2	2.34	0.58
2:O:225:ASN:O	2:O:226:ILE:C	2.45	0.58
9:V:30:UNK:HG3	9:V:31:UNK:N	2.19	0.58
2:B:76:THR:HG23	2:B:82:SER:H	1.67	0.58
3:C:139:MET:O	3:C:140:SER:C	2.47	0.58
4:D:43:MET:HG2	4:D:91:PHE:CD2	2.39	0.58
5:E:83:GLU:CG	5:E:102:THR:HG22	2.26	0.58
5:E:144:CYS:HB3	3:P:265:THR:HG21	1.85	0.58
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.33	0.58
4:D:200:GLN:HE21	12:D:2091:BOG:H5	1.69	0.58
5:E:109:GLU:OE2	5:E:166:ASP:HB2	2.03	0.58
6:F:73:ARG:HH11	6:F:73:ARG:HG3	1.68	0.58
2:O:75:LEU:HD11	2:O:140:LEU:HD23	1.86	0.58
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.85	0.58
4:Q:10:PHE:HD2	8:U:74:PHE:CE2	2.21	0.58
8:U:65:ARG:O	8:U:68:CYS:HB3	2.04	0.58
9:V:34:UNK:N	9:V:35:UNK:N	2.51	0.58
2:B:58:GLU:OE1	2:B:64:GLY:N	2.36	0.58
2:O:272:PHE:O	2:O:276:GLN:N	2.34	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.39	0.58
5:R:177:PRO:C	5:R:178:TYR:CD2	2.82	0.58
2:B:31:ASN:HB3	2:B:227:ARG:NH1	2.19	0.58
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.84	0.58
8:H:43:ARG:O	8:H:47:ARG:HG3	2.04	0.58
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.33	0.57
4:Q:10:PHE:HB3	8:U:74:PHE:CE2	2.39	0.57
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.86	0.57
6:F:53:ASP:OD1	6:F:54:LEU:N	2.37	0.57
6:F:89:TYR:C	6:F:89:TYR:CD1	2.80	0.57
2:O:229:GLY:C	2:O:231:GLY:H	2.12	0.57
2:O:307:PHE:CD1	2:O:308:ASP:N	2.71	0.57
3:P:142:TRP:O	3:P:146:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:33:LYS:HG2	7:T:21:PHE:CE1	2.38	0.57
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.38	0.57
1:A:269:VAL:HG11	1:A:410:VAL:HG21	1.86	0.57
6:F:51:PRO:O	6:F:52:LYS:C	2.48	0.57
4:Q:224:ARG:HH12	4:Q:231:LYS:HE2	1.66	0.57
6:S:13:MET:O	6:S:17:ARG:HG3	2.04	0.57
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.69	0.57
4:D:22:ASP:O	4:D:24:SER:N	2.37	0.57
2:O:146:VAL:HG12	2:O:147:ASP:N	2.18	0.57
4:Q:117:VAL:HG22	4:Q:190:LEU:HB3	1.85	0.57
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.69	0.57
2:B:217:LYS:O	2:B:221:GLU:HG2	2.04	0.57
2:B:258:VAL:HG23	2:B:321:LEU:HD22	1.86	0.57
3:C:142:TRP:O	3:C:146:VAL:HG23	2.05	0.57
3:P:292:VAL:O	3:P:295:LEU:HB3	2.05	0.57
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.86	0.57
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.68	0.57
1:N:127:ILE:C	1:N:129:LYS:H	2.10	0.57
2:O:403:ASP:C	2:O:405:VAL:H	2.11	0.57
3:P:101:ARG:NH2	14:P:502:HEM:HBD2	2.20	0.57
4:Q:28:ARG:HD2	4:Q:171:TYR:CE1	2.40	0.57
3:C:33:ASN:HB3	21:C:3017:HOH:O	2.05	0.57
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.20	0.57
5:E:28:SER:O	5:E:32:ARG:HG3	2.04	0.57
2:B:50:PHE:N	2:B:50:PHE:CD1	2.72	0.57
4:D:102:ARG:NH1	4:D:107:GLY:O	2.38	0.57
7:G:38:TRP:O	7:G:39:ARG:C	2.47	0.57
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.87	0.57
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.86	0.57
2:O:259:THR:HG22	2:O:260:GLU:N	2.18	0.57
5:R:33:LYS:O	5:R:34:GLY:C	2.48	0.57
1:A:268:VAL:O	1:A:272:VAL:HG23	2.05	0.57
3:C:292:VAL:O	3:C:295:LEU:HB3	2.05	0.57
1:N:106:MET:HE3	1:N:208:LEU:HD13	1.86	0.57
1:N:182:LEU:O	1:N:186:ILE:HG13	2.05	0.57
1:N:307:PHE:CD1	1:N:307:PHE:C	2.82	0.57
2:O:50:PHE:C	2:O:51:ILE:HG13	2.29	0.57
1:A:114:ALA:HA	1:A:216:PHE:HE2	1.70	0.56
1:A:182:LEU:O	1:A:186:ILE:HG13	2.05	0.56
1:A:433:ASP:HB3	1:A:436:ARG:HB2	1.87	0.56
2:B:71:LEU:O	2:B:74:PRO:HD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ASN:HD21	2:B:250:HIS:CB	2.18	0.56
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.20	0.56
5:E:71:LEU:HB3	5:E:92:ARG:CD	2.35	0.56
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.87	0.56
5:E:145:VAL:O	5:E:145:VAL:HG12	2.04	0.56
10:J:60:GLU:O	10:J:61:ALA:HB3	2.05	0.56
4:Q:126:TYR:C	4:Q:126:TYR:CD2	2.82	0.56
1:A:240:GLU:HA	1:A:422:LEU:O	2.05	0.56
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.38	0.56
2:B:314:VAL:HG11	9:I:63:ASP:HB3	1.86	0.56
2:O:258:VAL:HG11	2:O:312:PHE:CD2	2.40	0.56
3:P:269:ILE:HG23	3:P:269:ILE:O	2.04	0.56
5:R:38:LEU:HD13	10:W:14:PHE:CZ	2.37	0.56
1:A:342:TRP:O	1:A:345:LEU:HB2	2.04	0.56
2:B:229:GLY:C	2:B:231:GLY:H	2.14	0.56
3:C:88:ALA:O	3:C:91:PHE:HB3	2.05	0.56
4:D:54:VAL:HG21	12:D:2091:BOG:H7'1	1.87	0.56
1:N:178:THR:HB	1:N:181:ASP:OD1	2.04	0.56
1:N:429:GLU:OE1	7:T:7:LEU:HB2	2.06	0.56
2:O:37:SER:CB	2:O:213:HIS:ND1	2.68	0.56
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.71	0.56
1:A:170:THR:HG22	1:A:172:GLU:H	1.71	0.56
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.87	0.56
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.35	0.56
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.40	0.56
6:F:52:LYS:HE2	7:G:11:ARG:NH1	2.19	0.56
1:N:255:LEU:CD1	1:N:422:LEU:HD13	2.35	0.56
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.69	0.56
5:R:91:TRP:O	5:R:93:GLY:N	2.38	0.56
5:R:179:ASN:O	5:R:180:LEU:C	2.48	0.56
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.20	0.56
3:C:111:LYS:HE2	3:C:307:PHE:HE1	1.70	0.56
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.40	0.56
4:D:83:ARG:HB2	4:D:84:PRO:HD2	1.88	0.56
5:E:96:LEU:HD12	5:E:135:LEU:O	2.06	0.56
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.87	0.56
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.14	0.56
4:Q:43:MET:HG2	4:Q:91:PHE:HD2	1.69	0.56
8:U:58:LEU:HG	8:U:62:LEU:HD12	1.88	0.56
3:C:187:PRO:HG3	14:C:501:HEM:HBB2	1.87	0.56
6:F:21:TYR:C	6:F:21:TYR:CD2	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:45:SER:HA	1:N:48:GLU:CG	2.36	0.56
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.34	0.56
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.41	0.56
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.88	0.56
4:D:23:HIS:HB2	10:J:50:LYS:O	2.05	0.56
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.88	0.56
1:N:145:MET:HE2	1:N:145:MET:N	2.21	0.56
1:N:191:LYS:C	1:N:193:PRO:HD2	2.31	0.56
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.88	0.56
2:B:205:ALA:HB2	2:B:387:LEU:HD13	1.87	0.55
2:B:318:ASP:O	2:B:319:SER:HB2	2.05	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.86	0.55
3:C:279:TYR:CZ	3:C:283:ARG:HD3	2.41	0.55
2:O:42:SER:OG	2:O:43:PRO:HD2	2.06	0.55
2:O:56:ARG:HH22	2:O:318:ASP:CG	2.14	0.55
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.35	0.55
2:O:333:ALA:O	2:O:337:ILE:HG13	2.05	0.55
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.87	0.55
4:D:117:VAL:HG22	4:D:190:LEU:HB3	1.88	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.07	0.55
5:E:152:ASP:C	5:E:153:PHE:CD1	2.85	0.55
5:E:185:TYR:CB	5:E:195:VAL:HG22	2.37	0.55
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.06	0.55
3:P:182:LEU:HD12	3:P:186:LEU:HD11	1.88	0.55
8:U:50:THR:OG1	8:U:51:GLU:N	2.39	0.55
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.21	0.55
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.41	0.55
1:N:334:MET:O	1:N:335:MET:C	2.49	0.55
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.55	0.55
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.88	0.55
2:B:124:LEU:HD12	2:B:128:THR:HG21	1.87	0.55
2:B:272:PHE:O	2:B:276:GLN:N	2.38	0.55
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.06	0.55
1:N:240:GLU:HA	1:N:422:LEU:O	2.06	0.55
2:O:205:ALA:HB2	2:O:387:LEU:HD13	1.87	0.55
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.40	0.55
2:B:230:ALA:O	2:B:232:THR:N	2.40	0.55
4:D:227:TRP:O	4:D:228:SER:C	2.49	0.55
2:O:280:GLY:HA3	2:O:293:SER:OG	2.07	0.55
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.42	0.55
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ALA:HB2	1:A:427:PRO:HD2	1.89	0.55
3:C:64:PHE:CD1	3:C:259:PRO:HG3	2.42	0.55
3:C:72:ARG:HG2	3:C:72:ARG:HH11	1.72	0.55
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.22	0.55
1:N:178:THR:O	1:N:179:ARG:C	2.49	0.55
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.89	0.55
2:O:215:ASP:C	2:O:217:LYS:N	2.62	0.55
3:P:127:THR:O	3:P:130:VAL:HG22	2.06	0.55
1:A:277:ILE:CD1	1:A:345:LEU:HD11	2.35	0.55
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.22	0.55
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.72	0.55
1:N:49:ASN:HD21	1:N:52:ASN:H	1.53	0.55
2:O:76:THR:HG23	2:O:82:SER:H	1.69	0.55
2:O:248:ASN:HD21	2:O:250:HIS:CB	2.19	0.55
2:B:402:ILE:O	2:B:405:VAL:HG23	2.07	0.55
3:C:34:PHE:HB2	21:C:3011:HOH:O	2.06	0.55
3:C:187:PRO:HG3	14:C:501:HEM:CBB	2.37	0.55
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.36	0.55
6:F:72:HIS:C	6:F:73:ARG:HD3	2.31	0.55
2:O:264:VAL:HG23	2:O:316:TYR:C	2.31	0.55
3:P:139:MET:O	3:P:140:SER:C	2.50	0.55
3:P:158:GLY:O	3:P:159:HIS:C	2.49	0.55
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.89	0.55
4:Q:120:ARG:HG2	4:Q:120:ARG:NH1	2.22	0.55
1:A:106:MET:CE	1:A:110:VAL:HG21	2.36	0.55
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.89	0.55
2:B:248:ASN:ND2	2:B:248:ASN:C	2.57	0.55
3:C:33:ASN:HD22	18:D:2003:CDL:H112	1.71	0.55
8:H:73:LEU:HD12	8:H:73:LEU:O	2.07	0.55
3:P:132:TYR:HA	14:P:501:HEM:HAA2	1.89	0.55
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.88	0.55
6:S:52:LYS:CE	7:T:11:ARG:HH11	2.18	0.55
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.72	0.54
3:C:372:THR:O	3:C:373:LEU:C	2.50	0.54
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.22	0.54
2:O:323:GLY:HA2	2:O:417:PHE:HE1	1.72	0.54
3:P:36:SER:O	3:P:37:LEU:C	2.50	0.54
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.41	0.54
8:U:35:GLU:HA	8:U:38:GLU:HG3	1.89	0.54
1:A:136:GLN:C	1:A:138:LEU:H	2.15	0.54
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:LEU:O	10:J:9:ALA:HB3	2.08	0.54
1:N:136:GLN:C	1:N:138:LEU:N	2.64	0.54
2:B:286:LYS:HG2	2:B:287:ARG:HG3	1.90	0.54
2:O:402:ILE:O	2:O:405:VAL:HG23	2.07	0.54
3:P:56:TYR:OH	3:P:134:LEU:O	2.23	0.54
4:Q:28:ARG:O	4:Q:29:GLY:C	2.51	0.54
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.07	0.54
5:R:29:SER:O	5:R:30:GLU:C	2.50	0.54
2:B:220:ALA:HA	2:B:224:LEU:HD13	1.89	0.54
1:N:106:MET:O	1:N:110:VAL:HG23	2.08	0.54
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.23	0.54
1:A:36:THR:OG1	1:A:100:LYS:HG2	2.06	0.54
1:A:365:MET:O	1:A:368:GLN:HB2	2.08	0.54
2:B:252:LEU:CD1	9:I:49:LEU:HB2	2.37	0.54
3:C:56:TYR:OH	3:C:176:LEU:HD11	2.08	0.54
1:N:45:SER:HA	1:N:48:GLU:HG3	1.88	0.54
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.38	0.54
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.89	0.54
5:R:78:LEU:HD22	5:R:132:TRP:CD2	2.43	0.54
3:C:22:LEU:HD21	16:C:2002:UQ:O4	2.08	0.54
3:C:31:TRP:O	3:C:101:ARG:HG3	2.08	0.54
4:D:117:VAL:HG21	4:D:190:LEU:C	2.32	0.54
5:E:102:THR:OG1	5:E:104:ALA:HB3	2.08	0.54
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.38	0.54
2:O:259:THR:O	2:O:260:GLU:C	2.50	0.54
2:O:353:THR:HG22	2:O:355:GLU:N	2.13	0.54
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.07	0.54
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.38	0.54
1:N:206:LYS:O	1:N:209:VAL:HG12	2.08	0.54
3:P:37:LEU:O	3:P:41:CYS:HB2	2.08	0.54
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.42	0.54
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.08	0.54
5:R:193:VAL:HG22	5:R:194:VAL:N	2.23	0.54
1:A:45:SER:HA	1:A:48:GLU:CD	2.32	0.54
1:N:40:TRP:HZ3	1:N:376:CYS:SG	2.30	0.54
5:R:32:ARG:HH12	7:T:22:GLU:CD	2.16	0.54
2:B:323:GLY:HA2	2:B:417:PHE:HE1	1.73	0.54
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.90	0.54
2:O:266:SER:O	2:O:268:GLU:N	2.41	0.54
3:P:198:LEU:HD21	14:P:502:HEM:HMA1	1.88	0.54
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.43	0.54
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.23	0.53
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.38	0.53
2:B:357:VAL:O	2:B:361:LYS:HG3	2.08	0.53
3:C:198:LEU:HD21	14:C:502:HEM:HMA1	1.89	0.53
2:O:47:ILE:N	2:O:47:ILE:CD1	2.71	0.53
3:P:31:TRP:HE1	18:P:3004:CDL:H1	1.73	0.53
3:P:118:VAL:HG11	3:P:303:PHE:CE1	2.43	0.53
3:P:253:ASP:OD1	3:P:255:GLU:N	2.40	0.53
1:A:48:GLU:OE1	1:A:53:ASN:HA	2.06	0.53
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.71	0.53
3:C:316:MET:O	3:C:317:THR:C	2.50	0.53
4:D:171:TYR:HD1	4:D:175:THR:HB	1.73	0.53
4:D:224:ARG:NH2	7:G:26:ILE:HG23	2.13	0.53
4:Q:235:MET:HE1	6:S:63:LYS:C	2.34	0.53
6:S:32:MET:CE	6:S:87:LYS:HG2	2.36	0.53
1:A:95:THR:HG22	1:A:96:ALA:N	2.23	0.53
1:A:250:VAL:HG21	1:A:325:VAL:CG1	2.39	0.53
2:B:291:VAL:C	2:B:293:SER:H	2.16	0.53
2:B:428:GLY:O	2:B:430:LEU:HG	2.09	0.53
3:C:38:LEU:HB3	14:C:502:HEM:CMB	2.39	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.24	0.53
8:H:73:LEU:HD12	8:H:73:LEU:C	2.34	0.53
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.43	0.53
1:A:45:SER:HA	1:A:48:GLU:CG	2.38	0.53
1:N:271:HIS:NE2	1:N:311:ASN:HB3	2.23	0.53
2:O:150:VAL:CG2	2:O:151:ALA:H	2.21	0.53
2:O:393:THR:CG2	2:O:397:VAL:HB	2.39	0.53
3:P:72:ARG:HG2	3:P:72:ARG:HH11	1.72	0.53
4:D:37:CYS:O	4:D:39:ALA:N	2.40	0.53
5:E:114:VAL:O	5:E:114:VAL:HG12	2.08	0.53
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.73	0.53
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.44	0.53
1:N:137:GLU:O	1:N:141:MET:HG3	2.08	0.53
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.44	0.53
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.43	0.53
4:Q:94:PRO:HB2	4:Q:95:TYR:CE1	2.43	0.53
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.24	0.53
5:E:79:SER:HB3	5:E:191:ASP:HB2	1.90	0.53
2:O:57:TYR:N	2:O:57:TYR:CD1	2.76	0.53
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:79:LEU:HD22	4:Q:204:MET:HE1	1.90	0.53
17:Q:501:HEC:HBB3	17:Q:501:HEC:CMB	2.38	0.53
5:R:147:ILE:N	5:R:157:TYR:O	2.40	0.53
7:T:38:TRP:O	7:T:39:ARG:C	2.51	0.53
1:A:90:THR:O	1:A:167:VAL:HG11	2.09	0.53
3:C:70:THR:HA	3:C:74:VAL:CG2	2.38	0.53
3:C:118:VAL:N	14:C:502:HEM:HBC2	2.24	0.53
3:C:344:VAL:HG21	5:R:162:GLY:CA	2.39	0.53
4:D:10:PHE:CD1	4:D:10:PHE:N	2.76	0.53
5:E:32:ARG:HH12	7:G:22:GLU:CD	2.17	0.53
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	2.94	0.53
6:S:70:LEU:HD12	6:S:70:LEU:O	2.09	0.53
6:F:43:VAL:O	6:F:44:LYS:C	2.52	0.53
2:O:258:VAL:HG23	2:O:321:LEU:HD22	1.91	0.53
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.38	0.53
1:A:247:ALA:HB2	7:G:11:ARG:HD2	1.90	0.53
2:B:398:VAL:HG13	2:B:399:ALA:N	2.22	0.53
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.08	0.53
6:F:20:TYR:O	6:F:23:ALA:HB3	2.09	0.53
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.44	0.53
1:N:156:THR:HG21	1:N:241:ILE:HG22	1.91	0.53
2:O:97:SER:HB3	9:V:69:SER:OG	2.08	0.53
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.16	0.53
1:A:259:GLY:N	1:A:318:GLY:O	2.31	0.53
3:C:56:TYR:OH	3:C:134:LEU:O	2.25	0.53
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.44	0.53
5:E:168:SER:HB3	5:E:170:ARG:HG3	1.90	0.53
8:H:35:GLU:HA	8:H:38:GLU:HG3	1.91	0.53
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.08	0.53
3:P:279:TYR:CZ	3:P:283:ARG:HD3	2.44	0.53
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.91	0.53
8:U:24:CYS:C	8:U:26:GLN:H	2.17	0.53
2:B:306:PRO:CB	9:I:51:CYS:HA	2.40	0.52
3:C:37:LEU:O	3:C:41:CYS:HB2	2.08	0.52
3:C:120:LEU:HB3	14:C:502:HEM:HAB	1.91	0.52
3:C:330:VAL:O	3:C:333:LEU:HB2	2.08	0.52
5:E:162:GLY:HA3	3:P:344:VAL:HG21	1.90	0.52
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.69	0.52
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.90	0.52
1:N:85:HIS:HD2	2:O:284:LEU:HB3	1.74	0.52
3:P:326:PHE:O	3:P:330:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.34	0.52
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.74	0.52
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.44	0.52
2:B:341:MET:HE2	2:B:341:MET:HA	1.89	0.52
3:C:28:ILE:CD1	16:C:2002:UQ:HM21	2.38	0.52
5:E:91:TRP:O	5:E:93:GLY:N	2.42	0.52
7:G:80:ASP:O	7:G:81:GLN:HG3	2.10	0.52
8:H:26:GLN:OE1	8:H:26:GLN:HA	2.09	0.52
3:P:34:PHE:HB2	21:P:3015:HOH:O	2.09	0.52
3:P:215:ASP:C	3:P:217:ASP:H	2.18	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG2	1.91	0.52
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.42	0.52
5:R:38:LEU:HD12	5:R:38:LEU:O	2.10	0.52
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.91	0.52
8:U:37:LEU:O	8:U:38:GLU:C	2.52	0.52
3:C:338:TRP:O	3:C:341:SER:HB3	2.08	0.52
2:O:58:GLU:OE1	2:O:64:GLY:N	2.42	0.52
3:P:270:LYS:HG3	3:P:270:LYS:O	2.08	0.52
4:Q:180:SER:OG	8:U:77:LEU:HD21	2.08	0.52
6:S:67:ASP:OD1	6:S:71:LYS:HD2	2.09	0.52
8:U:31:VAL:HA	8:U:34:ARG:HB3	1.91	0.52
1:A:127:ILE:C	1:A:129:LYS:H	2.17	0.52
2:B:29:LEU:HD22	2:B:30:PRO:HD2	1.91	0.52
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.44	0.52
5:E:3:ASN:C	5:E:5:VAL:H	2.18	0.52
5:E:18:VAL:HG23	5:E:18:VAL:O	2.10	0.52
1:N:22:GLY:O	1:N:193:PRO:HA	2.10	0.52
1:N:45:SER:HA	1:N:48:GLU:CD	2.34	0.52
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.25	0.52
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.25	0.52
1:A:61:HIS:ND1	1:A:134:ILE:HG12	2.25	0.52
2:B:102:ARG:CZ	2:B:164:HIS:CD2	2.92	0.52
2:B:212:LYS:HD2	2:B:214:SER:OG	2.10	0.52
2:B:393:THR:CG2	2:B:397:VAL:HB	2.39	0.52
8:H:37:LEU:O	8:H:38:GLU:C	2.52	0.52
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.40	0.52
2:O:286:LYS:HG2	2:O:287:ARG:HG3	1.92	0.52
3:P:147:ILE:O	3:P:150:LEU:HB2	2.10	0.52
4:Q:29:GLY:O	4:Q:32:VAL:HB	2.08	0.52
1:A:168:GLU:CD	1:A:168:GLU:H	2.18	0.52
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:VAL:O	3:C:165:ALA:HB3	2.09	0.52
6:F:59:MET:HA	6:F:59:MET:CE	2.36	0.52
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.10	0.52
3:P:72:ARG:HG2	3:P:72:ARG:NH1	2.24	0.52
3:P:116:THR:O	3:P:117:GLY:C	2.53	0.52
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.73	0.52
2:B:176:LEU:HD12	2:B:176:LEU:O	2.10	0.52
3:C:216:SER:HB3	6:F:59:MET:HE2	1.92	0.52
4:D:113:LEU:HD22	4:D:116:ILE:HG21	1.92	0.52
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.37	0.52
3:P:372:THR:O	3:P:373:LEU:C	2.53	0.52
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.91	0.52
1:A:280:TYR:CG	1:A:281:ASP:N	2.78	0.52
2:B:187:THR:OG1	2:B:190:GLN:HG3	2.09	0.52
3:C:36:SER:O	3:C:39:ALA:N	2.43	0.52
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.39	0.52
3:C:367:PHE:N	3:C:368:PRO:HD2	2.25	0.52
4:D:32:VAL:HG21	4:D:182:ILE:HG23	1.92	0.52
4:D:134:TYR:OH	4:D:160:MET:O	2.11	0.52
5:E:160:CYS:HA	3:P:269:ILE:HG21	1.92	0.52
6:F:103:GLU:O	6:F:104:ARG:C	2.53	0.52
2:O:110:GLU:O	2:O:111:CYS:HB3	2.10	0.52
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.75	0.52
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.45	0.52
1:A:343:MET:O	1:A:344:ARG:C	2.52	0.52
2:B:37:SER:HB2	2:B:213:HIS:ND1	2.25	0.52
3:C:87:GLY:N	3:C:240:PHE:HE2	2.08	0.52
1:N:161:THR:HG21	1:N:234:CYS:HA	1.92	0.52
3:P:78:TRP:CD2	3:P:79:LEU:N	2.78	0.52
3:P:271:PRO:HB3	15:P:3001:ICX:O32	2.10	0.52
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.75	0.52
4:Q:227:TRP:O	4:Q:228:SER:C	2.53	0.52
5:R:165:TYR:CE2	5:R:180:LEU:HG	2.45	0.52
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.91	0.51
2:B:50:PHE:C	2:B:51:ILE:HG13	2.34	0.51
2:B:55:SER:O	2:B:174:ASN:HB2	2.10	0.51
3:C:93:ILE:O	3:C:94:CYS:C	2.50	0.51
3:C:155:PRO:O	3:C:156:TYR:HB2	2.11	0.51
2:O:345:LYS:C	2:O:347:ALA:H	2.17	0.51
2:O:428:GLY:O	2:O:430:LEU:HG	2.11	0.51
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.53	0.51
10:W:32:GLU:O	10:W:33:ARG:C	2.52	0.51
10:W:59:TYR:N	10:W:59:TYR:CD1	2.77	0.51
1:A:45:SER:HA	1:A:48:GLU:HG3	1.92	0.51
1:A:338:ALA:O	1:A:341:GLU:N	2.43	0.51
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.91	0.51
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.46	0.51
1:N:140:GLU:OE2	9:V:49:LEU:HA	2.09	0.51
2:O:21:ALA:O	2:O:22:GLU:HG2	2.09	0.51
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.93	0.51
2:O:366:ALA:O	2:O:367:THR:C	2.52	0.51
5:R:84:GLY:O	5:R:85:LYS:HD3	2.11	0.51
1:A:206:LYS:O	1:A:207:GLU:C	2.53	0.51
3:P:82:ASN:HD22	3:P:82:ASN:N	2.09	0.51
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.74	0.51
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.91	0.51
4:Q:197:GLU:O	4:Q:199:ASP:N	2.43	0.51
5:R:15:ARG:HH11	5:R:32:ARG:HB3	1.75	0.51
8:U:13:LEU:HD23	8:U:13:LEU:H	1.75	0.51
2:B:47:ILE:N	2:B:47:ILE:CD1	2.70	0.51
2:B:146:VAL:O	2:B:147:ASP:C	2.53	0.51
3:C:91:PHE:CE1	3:C:124:LEU:HD22	2.45	0.51
5:E:74:ILE:HD12	5:E:195:VAL:CB	2.31	0.51
1:N:69:LYS:NZ	1:N:70:ARG:HH21	2.08	0.51
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.40	0.51
2:O:291:VAL:C	2:O:293:SER:H	2.18	0.51
3:P:40:VAL:O	3:P:44:THR:HB	2.11	0.51
3:P:58:ALA:O	3:P:177:THR:HG22	2.11	0.51
1:A:251:ALA:HB1	1:A:428:ILE:CG2	2.40	0.51
3:C:265:THR:H	5:R:145:VAL:HG11	1.75	0.51
4:D:10:PHE:H	4:D:10:PHE:HD1	1.57	0.51
4:D:218:LEU:HD22	5:E:39:VAL:HG12	1.93	0.51
3:P:22:LEU:HD21	16:P:3002:UQ:O4	2.11	0.51
2:B:162:ASN:O	2:B:244:ILE:HD12	2.10	0.51
3:C:127:THR:HG21	14:C:501:HEM:CBB	2.39	0.51
3:C:319:ARG:HB3	3:C:374:GLU:OE1	2.10	0.51
4:D:83:ARG:HG3	4:D:83:ARG:HH11	1.76	0.51
9:I:59:SER:O	9:I:60:ALA:HB3	2.10	0.51
1:N:433:ASP:HB3	1:N:436:ARG:HB2	1.93	0.51
2:O:81:SER:O	2:O:85:ILE:HG13	2.11	0.51
2:O:295:LEU:O	2:O:299:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.78	0.51
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.10	0.51
1:A:363:SER:HB3	2:B:112:LEU:HD21	1.93	0.51
2:B:255:ALA:O	2:B:325:TYR:HA	2.11	0.51
2:B:337:ILE:O	2:B:340:ALA:HB3	2.11	0.51
9:I:38:UNK:C	9:I:40:UNK:N	2.72	0.51
2:O:46:ARG:HG3	2:O:110:GLU:HG2	1.92	0.51
2:O:220:ALA:HA	2:O:224:LEU:HD13	1.91	0.51
2:O:275:LEU:HD12	2:O:275:LEU:O	2.11	0.51
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.36	0.51
4:Q:83:ARG:HH11	4:Q:83:ARG:HG3	1.75	0.51
4:Q:240:PRO:HG2	4:Q:241:LYS:H	1.76	0.51
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.76	0.51
10:W:12:ALA:O	10:W:13:LEU:HD23	2.11	0.51
10:W:49:GLY:N	10:W:54:HIS:ND1	2.59	0.51
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.45	0.51
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.45	0.51
5:E:100:HIS:HA	5:E:131:GLU:O	2.11	0.51
1:N:49:ASN:ND2	1:N:51:LYS:H	2.08	0.51
1:N:127:ILE:O	1:N:129:LYS:N	2.43	0.51
1:N:369:LEU:HD11	1:N:392:LEU:HD21	1.93	0.51
1:N:394:GLU:O	1:N:395:TRP:C	2.53	0.51
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.10	0.51
4:Q:197:GLU:O	4:Q:198:HIS:C	2.54	0.51
5:R:28:SER:O	5:R:32:ARG:HG3	2.10	0.51
1:A:85:HIS:O	1:A:99:ILE:HA	2.11	0.51
2:B:415:LYS:C	2:B:417:PHE:H	2.19	0.51
1:N:171:THR:HB	5:R:4:ASP:OD2	2.10	0.51
1:N:343:MET:O	1:N:344:ARG:C	2.51	0.51
2:O:55:SER:O	2:O:174:ASN:HB2	2.11	0.51
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.11	0.51
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.46	0.51
5:R:109:GLU:CD	5:R:167:ALA:HB3	2.35	0.51
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.74	0.51
2:B:89:ILE:O	2:B:92:VAL:HG22	2.11	0.50
2:B:181:TYR:CZ	2:O:249:GLY:HA3	2.47	0.50
8:H:24:CYS:C	8:H:26:GLN:N	2.68	0.50
8:H:66:ASP:HA	8:H:69:VAL:HG23	1.93	0.50
3:P:95:ILE:O	3:P:99:ILE:HG13	2.11	0.50
3:P:120:LEU:HD22	14:P:502:HEM:CBB	2.41	0.50
14:P:502:HEM:HBB2	14:P:502:HEM:HMB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:14:HIS:HA	4:Q:19:SER:HB3	1.93	0.50
1:A:334:MET:O	1:A:335:MET:C	2.54	0.50
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.11	0.50
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.39	0.50
2:B:259:THR:HG22	2:B:260:GLU:H	1.73	0.50
3:C:158:GLY:O	3:C:159:HIS:C	2.55	0.50
6:F:12:LEU:O	6:F:13:MET:C	2.52	0.50
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.46	0.50
10:J:40:ASP:O	10:J:44:GLU:HG3	2.12	0.50
10:J:49:GLY:N	10:J:54:HIS:ND1	2.59	0.50
1:N:158:PHE:O	1:N:159:GLN:O	2.29	0.50
1:N:161:THR:HG21	1:N:235:ARG:H	1.75	0.50
2:O:398:VAL:O	2:O:402:ILE:HG13	2.12	0.50
3:P:53:ALA:N	14:P:501:HEM:HMD2	2.26	0.50
4:Q:10:PHE:HD2	8:U:74:PHE:HE2	1.54	0.50
4:Q:16:GLY:C	4:Q:18:LEU:H	2.20	0.50
4:Q:37:CYS:C	4:Q:39:ALA:H	2.19	0.50
5:R:134:ILE:C	5:R:135:LEU:HG	2.33	0.50
1:A:236:PHE:HB2	1:A:258:GLU:OE1	2.10	0.50
3:C:215:ASP:C	3:C:217:ASP:H	2.17	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.50
1:N:108:LYS:O	1:N:112:LEU:HG	2.12	0.50
1:N:332:ASP:O	1:N:333:ASP:C	2.54	0.50
2:O:318:ASP:O	2:O:319:SER:HB2	2.10	0.50
3:C:166:TRP:HA	3:C:175:THR:HG23	1.92	0.50
3:C:329:LEU:O	3:C:332:ASN:HB3	2.12	0.50
5:E:38:LEU:HD13	10:J:14:PHE:CZ	2.45	0.50
5:E:103:GLN:C	5:E:105:GLU:H	2.20	0.50
2:O:248:ASN:ND2	2:O:250:HIS:CB	2.74	0.50
3:P:14:MET:HG2	12:P:2010:BOG:O3	2.12	0.50
4:Q:23:HIS:HB2	10:W:50:LYS:O	2.10	0.50
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.76	0.50
2:O:201:SER:OG	2:O:228:SER:HB3	2.12	0.50
3:P:305:ILE:HD11	3:P:363:LEU:HD22	1.94	0.50
8:U:59:PHE:O	8:U:60:ASP:C	2.55	0.50
1:A:35:CYS:HB2	1:A:200:ALA:O	2.11	0.50
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.92	0.50
1:A:233:ARG:HB2	5:E:22:THR:O	2.12	0.50
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.25	0.50
2:B:415:LYS:C	2:B:417:PHE:N	2.66	0.50
4:D:197:GLU:O	4:D:198:HIS:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.46	0.50
5:E:95:PRO:HG2	5:E:145:VAL:CG2	2.41	0.50
5:R:102:THR:HG23	5:R:105:GLU:CG	2.39	0.50
1:A:7:THR:HG21	2:B:113:ARG:CD	2.42	0.50
1:A:69:LYS:NZ	1:A:70:ARG:HH21	2.10	0.50
1:N:121:ALA:O	1:N:122:LEU:HB2	2.12	0.50
1:N:178:THR:HG22	1:N:179:ARG:N	2.25	0.50
2:O:135:TRP:O	2:O:136:GLU:C	2.53	0.50
3:P:37:LEU:CD2	3:P:233:LEU:HA	2.41	0.50
6:S:72:HIS:C	6:S:73:ARG:HD3	2.37	0.50
2:B:56:ARG:HH22	2:B:318:ASP:CG	2.20	0.50
5:E:148:ALA:HB2	5:E:156:TYR:CE2	2.47	0.50
2:O:146:VAL:O	2:O:147:ASP:C	2.54	0.50
2:O:324:PHE:HE2	2:O:341:MET:HE3	1.76	0.50
2:O:353:THR:C	2:O:355:GLU:N	2.69	0.50
5:R:145:VAL:CG1	5:R:145:VAL:O	2.59	0.50
1:A:58:PHE:HB3	1:A:182:LEU:HD11	1.94	0.50
2:B:306:PRO:HB3	9:I:51:CYS:HA	1.93	0.50
3:C:282:LEU:HD12	3:C:291:GLY:C	2.37	0.50
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.47	0.50
5:E:70:ALA:C	5:E:71:LEU:HG	2.37	0.50
1:N:143:ASN:ND2	9:V:48:PRO:HD2	2.26	0.50
1:N:280:TYR:CG	1:N:281:ASP:N	2.80	0.50
2:O:162:ASN:O	2:O:244:ILE:HD12	2.12	0.50
2:O:266:SER:O	2:O:267:ALA:C	2.55	0.50
2:O:385:GLU:HG2	2:O:391:THR:O	2.12	0.50
3:P:92:PHE:O	3:P:96:PHE:CD2	2.65	0.50
3:P:220:PRO:O	3:P:221:PHE:C	2.54	0.50
6:S:71:LYS:O	6:S:72:HIS:HB2	2.11	0.50
9:V:65:VAL:HB	9:V:77:ARG:HD2	1.94	0.50
1:A:279:ARG:HA	1:A:307:PHE:CE1	2.47	0.49
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.90	0.49
3:C:72:ARG:HG2	3:C:72:ARG:NH1	2.25	0.49
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.49
5:E:53:ASN:O	5:E:57:GLN:HG3	2.11	0.49
8:H:66:ASP:O	8:H:67:HIS:C	2.53	0.49
1:N:106:MET:CE	1:N:110:VAL:HG21	2.42	0.49
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.77	0.49
1:N:269:VAL:HG11	1:N:410:VAL:CG2	2.42	0.49
1:N:294:LEU:HG	1:N:307:PHE:CE2	2.46	0.49
3:P:187:PRO:HG2	14:P:501:HEM:HMC3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:22:ASP:O	4:Q:24:SER:N	2.45	0.49
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	2.95	0.49
4:D:165:TYR:O	4:D:166:ASN:C	2.55	0.49
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.40	0.49
5:E:183:PRO:HG2	5:E:185:TYR:HD2	1.76	0.49
8:H:40:CYS:O	8:H:44:VAL:HG23	2.12	0.49
1:N:127:ILE:C	1:N:129:LYS:N	2.70	0.49
1:N:251:ALA:HB1	1:N:428:ILE:CG2	2.41	0.49
1:N:410:VAL:O	1:N:413:LYS:HB3	2.11	0.49
2:O:63:LEU:C	2:O:65:THR:H	2.20	0.49
5:R:42:THR:O	5:R:45:VAL:N	2.44	0.49
1:A:6:GLN:C	1:A:8:LEU:N	2.67	0.49
1:A:136:GLN:C	1:A:138:LEU:N	2.69	0.49
1:A:245:ASP:C	1:A:247:ALA:H	2.20	0.49
3:C:36:SER:O	3:C:37:LEU:C	2.55	0.49
3:C:79:LEU:HD11	3:C:83:LEU:HD11	1.93	0.49
3:C:133:VAL:CG2	3:C:144:ALA:HB2	2.42	0.49
4:D:238:ARG:NH1	4:D:238:ARG:HB3	2.27	0.49
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.42	0.49
1:N:61:HIS:ND1	1:N:134:ILE:HG12	2.26	0.49
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.27	0.49
2:O:398:VAL:HG13	2:O:399:ALA:N	2.27	0.49
18:P:3003:CDL:HB22	6:S:72:HIS:HD2	1.77	0.49
4:Q:223:LYS:C	4:Q:223:LYS:CD	2.83	0.49
5:R:114:VAL:O	5:R:120:PRO:HB3	2.13	0.49
2:B:50:PHE:HD1	2:B:50:PHE:H	1.59	0.49
3:C:82:ASN:HD22	3:C:82:ASN:N	2.10	0.49
4:D:28:ARG:O	4:D:29:GLY:C	2.55	0.49
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.95	0.49
1:N:6:GLN:C	1:N:8:LEU:N	2.67	0.49
3:P:61:SER:C	3:P:62:LEU:HD12	2.37	0.49
3:P:137:GLY:H	3:P:140:SER:CB	2.26	0.49
5:R:42:THR:O	5:R:43:ALA:C	2.55	0.49
5:R:177:PRO:O	5:R:178:TYR:HD2	1.95	0.49
1:A:170:THR:CG2	1:A:171:THR:N	2.75	0.49
2:B:50:PHE:CE1	2:B:207:VAL:HB	2.47	0.49
2:B:53:ALA:CB	2:B:105:MET:HG3	2.36	0.49
2:B:81:SER:O	2:B:85:ILE:HG13	2.12	0.49
2:B:146:VAL:HG12	2:B:147:ASP:N	2.28	0.49
2:B:248:ASN:ND2	2:B:250:HIS:CB	2.75	0.49
3:C:117:GLY:O	3:C:120:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:73:SER:N	2:O:74:PRO:HD2	2.28	0.49
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.49
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.94	0.49
3:P:134:LEU:HD21	3:P:180:PHE:HA	1.95	0.49
4:Q:223:LYS:HD3	4:Q:223:LYS:O	2.11	0.49
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.47	0.49
2:O:147:ASP:O	2:O:150:VAL:HG22	2.11	0.49
3:P:127:THR:HG21	14:P:501:HEM:CBB	2.40	0.49
3:P:166:TRP:HA	3:P:175:THR:HG23	1.94	0.49
1:A:106:MET:N	1:A:107:PRO:HD2	2.28	0.49
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.47	0.49
3:C:164:TRP:O	3:C:165:ALA:C	2.55	0.49
1:N:61:HIS:CD2	2:O:287:ARG:CZ	2.95	0.49
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.48	0.49
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.43	0.49
2:O:50:PHE:CE1	2:O:207:VAL:HB	2.48	0.49
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.47	0.49
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.26	0.49
6:S:43:VAL:O	6:S:44:LYS:C	2.54	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.12	0.49
1:A:362:ARG:HD2	1:A:396:ASP:OD2	2.13	0.49
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.43	0.49
2:B:53:ALA:O	2:B:103:GLU:C	2.55	0.49
5:E:10:PHE:O	5:E:14:ARG:HG3	2.12	0.49
2:O:374:THR:O	2:O:377:GLY:N	2.45	0.49
4:Q:48:PHE:CE2	4:Q:65:ALA:HA	2.47	0.49
1:A:277:ILE:HD11	1:A:345:LEU:CD1	2.39	0.49
1:N:187:ASP:O	1:N:191:LYS:HE3	2.13	0.49
1:N:261:GLY:HA2	1:N:317:THR:O	2.13	0.49
2:O:50:PHE:N	2:O:50:PHE:CD1	2.80	0.49
2:O:325:TYR:HB3	9:V:59:SER:HB3	1.93	0.49
5:R:31:ASP:OD1	10:W:7:ARG:HG3	2.12	0.49
1:A:255:LEU:CD1	1:A:422:LEU:HD13	2.42	0.49
4:D:48:PHE:CE2	4:D:65:ALA:HA	2.47	0.49
4:D:138:PRO:HG2	4:D:141:VAL:HG21	1.93	0.49
5:E:72:SER:C	5:E:73:LYS:CG	2.85	0.49
10:J:32:GLU:O	10:J:33:ARG:C	2.55	0.49
1:N:223:TYR:CD2	1:N:223:TYR:N	2.80	0.49
2:O:66:ALA:O	2:O:69:LEU:HB3	2.12	0.49
2:O:100:SER:HA	2:O:104:LYS:O	2.13	0.49
2:O:345:LYS:C	2:O:347:ALA:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:187:PRO:HG3	14:P:501:HEM:HBB2	1.94	0.49
3:P:325:LEU:HD21	3:P:366:LEU:CB	2.42	0.49
1:A:59:VAL:C	1:A:61:HIS:N	2.71	0.48
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.47	0.48
3:C:304:LEU:O	3:C:305:ILE:C	2.56	0.48
4:D:197:GLU:O	4:D:199:ASP:N	2.45	0.48
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.48	0.48
1:N:365:MET:O	1:N:368:GLN:HB2	2.12	0.48
3:P:89:SER:O	3:P:90:PHE:C	2.56	0.48
3:P:195:ILE:O	3:P:199:THR:HB	2.13	0.48
3:P:261:ASN:ND2	3:P:264:VAL:HG23	2.28	0.48
3:P:345:GLU:O	3:P:348:PHE:HB2	2.13	0.48
5:R:15:ARG:HG3	7:T:22:GLU:C	2.38	0.48
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.95	0.48
2:B:84:ARG:NH1	2:B:122:TYR:HE2	2.10	0.48
4:D:180:SER:OG	8:H:77:LEU:HD21	2.13	0.48
2:B:353:THR:C	2:B:355:GLU:N	2.71	0.48
3:C:247:SER:N	3:C:248:PRO:HD3	2.28	0.48
2:O:143:GLN:O	2:O:146:VAL:N	2.45	0.48
7:T:29:ILE:HA	7:T:33:ALA:HB3	1.95	0.48
10:W:21:ALA:O	10:W:23:THR:N	2.47	0.48
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
3:C:23:PRO:HG2	7:G:3:HIS:CB	2.43	0.48
4:D:54:VAL:HG12	4:D:55:THR:N	2.27	0.48
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.47	0.48
1:A:273:ALA:O	1:A:276:ILE:N	2.45	0.48
1:A:343:MET:HE3	1:A:441:MET:HA	1.94	0.48
1:A:434:TYR:CE2	7:G:19:SER:HA	2.48	0.48
4:D:110:PRO:HB3	17:D:501:HEC:C1D	2.44	0.48
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.76	0.48
18:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.13	0.48
4:Q:127:VAL:O	4:Q:131:LEU:HG	2.13	0.48
5:R:10:PHE:O	5:R:14:ARG:HG3	2.14	0.48
1:A:180:ALA:O	1:A:183:ALA:HB3	2.14	0.48
1:A:404:ALA:O	1:A:405:ARG:C	2.57	0.48
2:B:57:TYR:CD1	2:B:57:TYR:N	2.81	0.48
3:C:111:LYS:HE2	3:C:307:PHE:CE1	2.47	0.48
3:C:147:ILE:O	3:C:150:LEU:HB2	2.13	0.48
3:C:207:ASN:ND2	3:C:208:ASN:H	2.11	0.48
5:E:70:ALA:O	5:E:71:LEU:CB	2.61	0.48
8:H:55:THR:O	8:H:56:GLU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:167:ALA:O	2:O:168:TYR:CD1	2.66	0.48
3:P:79:LEU:HD12	3:P:79:LEU:C	2.36	0.48
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.95	0.48
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.96	0.48
5:R:35:PHE:O	5:R:38:LEU:N	2.47	0.48
1:A:410:VAL:O	1:A:413:LYS:HB3	2.13	0.48
4:D:47:ALA:HB1	4:D:89:ASP:O	2.13	0.48
4:D:158:ILE:O	4:D:158:ILE:HG23	2.13	0.48
5:E:33:LYS:O	5:E:34:GLY:C	2.55	0.48
5:E:35:PHE:O	5:E:38:LEU:N	2.45	0.48
5:E:185:TYR:HB2	5:E:195:VAL:HG22	1.96	0.48
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.95	0.48
3:P:28:ILE:CD1	16:P:3002:UQ:HM21	2.44	0.48
3:P:151:PHE:C	3:P:153:ALA:H	2.22	0.48
3:P:358:SER:O	3:P:362:ILE:HG13	2.13	0.48
4:Q:221:TYR:CE1	7:T:25:ALA:CB	2.97	0.48
7:T:34:LEU:N	7:T:35:PRO:HD2	2.29	0.48
8:U:15:ASP:C	8:U:17:LEU:N	2.72	0.48
2:B:31:ASN:O	2:B:228:SER:HB3	2.14	0.48
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.96	0.48
5:E:185:TYR:HB3	5:E:195:VAL:HG22	1.95	0.48
1:N:3:THR:O	1:N:7:THR:HG23	2.14	0.48
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.44	0.48
2:O:73:SER:OG	2:O:74:PRO:HD3	2.13	0.48
2:O:116:VAL:O	2:O:119:VAL:HG22	2.13	0.48
2:O:248:ASN:ND2	2:O:250:HIS:HB2	2.29	0.48
2:O:353:THR:C	2:O:355:GLU:H	2.21	0.48
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.22	0.48
7:T:49:ALA:O	7:T:50:PRO:C	2.57	0.48
1:A:223:TYR:N	1:A:223:TYR:HD2	2.12	0.48
1:A:338:ALA:O	1:A:340:GLY:N	2.46	0.48
8:H:21:ARG:O	8:H:25:GLU:HG3	2.13	0.48
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.95	0.48
9:V:28:UNK:H	9:V:71:ASN:HD21	1.61	0.48
10:W:27:GLY:O	10:W:28:ALA:C	2.56	0.48
1:A:108:LYS:O	1:A:112:LEU:HG	2.14	0.48
1:A:431:LEU:HD12	1:A:431:LEU:C	2.39	0.48
2:B:76:THR:HG22	2:B:82:SER:N	2.29	0.48
2:B:366:ALA:O	2:B:367:THR:C	2.56	0.48
5:E:112:VAL:HG11	5:E:172:ARG:NH2	2.28	0.48
1:N:158:PHE:O	1:N:159:GLN:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:317:THR:OG1	1:N:318:GLY:N	2.44	0.48
1:N:362:ARG:O	1:N:365:MET:HE2	2.14	0.48
2:O:169:LYS:HD2	2:O:238:THR:HG21	1.96	0.48
2:O:415:LYS:C	2:O:417:PHE:N	2.69	0.48
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.12	0.48
4:Q:94:PRO:HB2	4:Q:95:TYR:CD1	2.49	0.48
4:Q:239:PRO:CB	4:Q:240:PRO:HD2	2.41	0.48
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.96	0.48
9:V:59:SER:O	9:V:60:ALA:HB3	2.12	0.48
1:A:241:ILE:HG23	1:A:241:ILE:O	2.14	0.47
2:B:150:VAL:CG2	2:B:151:ALA:H	2.26	0.47
3:C:212:ILE:O	3:C:213:SER:C	2.57	0.47
4:D:28:ARG:NH1	4:D:173:ASP:OD2	2.47	0.47
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.44	0.47
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.95	0.47
10:J:59:TYR:N	10:J:59:TYR:CD1	2.82	0.47
1:N:56:GLY:HA2	1:N:185:TYR:CE2	2.49	0.47
1:N:404:ALA:O	1:N:405:ARG:C	2.56	0.47
3:P:207:ASN:ND2	3:P:208:ASN:H	2.11	0.47
3:P:346:HIS:CG	3:P:347:PRO:HA	2.49	0.47
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	1.96	0.47
7:T:55:ALA:O	7:T:56:TYR:C	2.56	0.47
1:A:55:ALA:O	1:A:56:GLY:C	2.57	0.47
1:A:223:TYR:HD2	1:A:223:TYR:H	1.63	0.47
2:B:398:VAL:O	2:B:402:ILE:HG13	2.14	0.47
5:E:52:LYS:C	5:E:52:LYS:CD	2.87	0.47
6:F:89:TYR:CD1	6:F:90:LEU:N	2.69	0.47
8:H:15:ASP:C	8:H:17:LEU:N	2.71	0.47
3:P:38:LEU:HB3	14:P:502:HEM:CMB	2.44	0.47
4:Q:1:GLY:O	4:Q:3:LEU:N	2.47	0.47
4:Q:127:VAL:HG12	4:Q:187:CYS:SG	2.54	0.47
5:R:38:LEU:HB2	10:W:14:PHE:CE1	2.48	0.47
1:A:176:HIS:O	1:A:177:LEU:C	2.55	0.47
2:B:206:LEU:HG	2:B:206:LEU:O	2.13	0.47
2:B:248:ASN:ND2	2:B:250:HIS:HB2	2.29	0.47
3:C:78:TRP:CD2	3:C:79:LEU:N	2.82	0.47
4:D:135:CYS:O	4:D:149:TYR:HB3	2.14	0.47
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.96	0.47
12:D:2091:BOG:H3	12:E:2009:BOG:O4	2.14	0.47
1:N:19:LEU:C	1:N:21:ASN:H	2.21	0.47
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.14	0.47
2:O:75:LEU:HD11	2:O:140:LEU:CD2	2.45	0.47
3:P:93:ILE:O	3:P:94:CYS:C	2.56	0.47
3:P:107:SER:C	3:P:109:LEU:H	2.22	0.47
5:R:91:TRP:O	5:R:92:ARG:C	2.57	0.47
5:R:101:ARG:O	5:R:106:ILE:HD11	2.14	0.47
8:U:66:ASP:O	8:U:67:HIS:C	2.57	0.47
1:A:223:TYR:N	1:A:223:TYR:CD2	2.81	0.47
3:C:27:ASN:HD22	3:C:209:PRO:HG2	1.79	0.47
3:C:269:ILE:O	3:C:269:ILE:CG2	2.62	0.47
9:I:53:GLU:C	9:I:55:MET:N	2.70	0.47
9:I:53:GLU:O	9:I:55:MET:N	2.47	0.47
2:O:299:VAL:O	2:O:303:THR:HG22	2.14	0.47
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.97	0.47
5:R:194:VAL:HG12	5:R:195:VAL:N	2.28	0.47
6:S:103:GLU:O	6:S:104:ARG:C	2.58	0.47
1:A:338:ALA:C	1:A:340:GLY:N	2.72	0.47
2:B:84:ARG:NH1	2:B:84:ARG:HG2	2.28	0.47
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.95	0.47
4:D:29:GLY:O	4:D:32:VAL:HB	2.14	0.47
4:D:75:ASP:OD1	4:D:78:GLY:N	2.46	0.47
8:H:24:CYS:O	8:H:26:GLN:N	2.47	0.47
2:O:239:TYR:CD2	2:O:240:TRP:N	2.82	0.47
3:P:238:THR:CB	3:P:239:PRO:HD3	2.45	0.47
3:P:247:SER:N	3:P:248:PRO:HD3	2.29	0.47
4:Q:138:PRO:HG2	4:Q:141:VAL:HG21	1.97	0.47
5:R:145:VAL:O	5:R:145:VAL:HG13	2.14	0.47
2:B:73:SER:OG	2:B:74:PRO:HD3	2.15	0.47
2:B:345:LYS:C	2:B:347:ALA:H	2.20	0.47
3:C:40:VAL:HG11	3:C:233:LEU:HD11	1.96	0.47
3:C:114:TRP:O	3:C:115:ASN:C	2.57	0.47
5:E:32:ARG:NH1	7:G:22:GLU:HA	2.29	0.47
7:G:48:VAL:HG12	7:G:49:ALA:N	2.29	0.47
1:N:40:TRP:CZ3	1:N:376:CYS:SG	3.00	0.47
1:N:274:ASN:CG	1:N:309:THR:HB	2.38	0.47
1:N:443:TRP:O	1:N:444:ILE:CB	2.63	0.47
2:O:46:ARG:HH11	2:O:110:GLU:CD	2.22	0.47
3:P:86:ASN:O	3:P:87:GLY:C	2.58	0.47
4:Q:1:GLY:C	4:Q:3:LEU:H	2.23	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.97	0.47
5:R:153:PHE:CD1	5:R:153:PHE:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:HG13	5:E:2:HIS:CB	2.44	0.47
1:A:191:LYS:C	1:A:193:PRO:HD2	2.39	0.47
2:B:60:THR:HG23	2:B:61:ALA:H	1.79	0.47
2:B:81:SER:C	2:B:83:PHE:N	2.70	0.47
3:C:28:ILE:HD11	16:C:2002:UQ:HM21	1.97	0.47
3:C:87:GLY:HA2	3:C:240:PHE:CE2	2.49	0.47
3:C:238:THR:CB	3:C:239:PRO:HD3	2.44	0.47
3:C:326:PHE:C	3:C:326:PHE:CD2	2.92	0.47
4:D:14:HIS:HA	4:D:19:SER:HB3	1.96	0.47
5:E:144:CYS:O	5:E:146:PRO:HD3	2.15	0.47
8:H:15:ASP:O	8:H:16:PRO:C	2.58	0.47
1:N:63:ALA:O	1:N:116:VAL:CG1	2.63	0.47
1:N:178:THR:CG2	1:N:179:ARG:N	2.77	0.47
2:O:37:SER:OG	2:O:38:LEU:N	2.47	0.47
2:O:47:ILE:HD12	2:O:47:ILE:H	1.78	0.47
2:O:269:ALA:O	2:O:272:PHE:N	2.47	0.47
2:O:415:LYS:C	2:O:417:PHE:H	2.22	0.47
3:P:134:LEU:N	3:P:135:PRO:HD2	2.30	0.47
3:P:162:VAL:O	3:P:165:ALA:HB3	2.14	0.47
4:Q:147:LEU:HD23	4:Q:159:GLY:HA2	1.95	0.47
4:Q:238:ARG:HB3	4:Q:238:ARG:HH11	1.80	0.47
5:R:36:SER:O	5:R:39:VAL:HG23	2.15	0.47
1:A:332:ASP:HB2	1:A:430:GLN:HG2	1.96	0.47
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.30	0.47
3:C:49:GLY:C	14:C:501:HEM:HAC	2.40	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.30	0.47
1:N:41:ILE:HG21	1:N:190:PHE:CD2	2.49	0.47
1:N:180:ALA:O	1:N:183:ALA:HB3	2.14	0.47
1:N:382:HIS:HB3	1:N:388:ARG:O	2.14	0.47
2:O:27:THR:HG22	2:O:28:LYS:N	2.29	0.47
2:O:417:PHE:C	2:O:417:PHE:CD2	2.92	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.96	0.47
5:R:168:SER:CB	5:R:170:ARG:HG3	2.43	0.47
6:S:11:ARG:O	6:S:15:ARG:HG2	2.15	0.47
1:A:84:ALA:HB2	1:A:101:ALA:HB2	1.97	0.47
3:C:186:LEU:HB2	3:C:187:PRO:HD3	1.97	0.47
3:C:356:SER:O	3:C:357:LEU:C	2.57	0.47
5:E:31:ASP:O	5:E:32:ARG:C	2.56	0.47
1:N:223:TYR:N	1:N:223:TYR:HD2	2.11	0.47
1:N:434:TYR:O	1:N:435:ASN:C	2.56	0.47
2:O:176:LEU:HD12	2:O:176:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.29	0.47
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.45	0.47
1:A:142:ASP:OD1	5:E:2:HIS:N	2.38	0.47
1:A:332:ASP:O	1:A:333:ASP:C	2.58	0.47
2:B:76:THR:HG22	2:B:81:SER:CA	2.32	0.47
3:C:133:VAL:HG21	3:C:144:ALA:HB2	1.97	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.50	0.47
11:C:2005:PEE:O2P	5:E:40:THR:HG21	2.15	0.47
6:F:16:ILE:HG22	6:F:17:ARG:N	2.29	0.47
6:F:53:ASP:O	6:F:54:LEU:C	2.57	0.47
8:H:31:VAL:HA	8:H:34:ARG:HB3	1.95	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.50	0.47
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.50	0.47
3:P:311:SER:HB2	3:P:319:ARG:HH11	1.79	0.47
3:P:367:PHE:N	3:P:368:PRO:HD2	2.30	0.47
6:S:73:ARG:HG3	6:S:73:ARG:NH1	2.29	0.47
8:U:58:LEU:O	8:U:61:PHE:HB3	2.15	0.47
1:A:84:ALA:CB	1:A:101:ALA:HB2	2.45	0.46
1:A:138:LEU:C	1:A:140:GLU:N	2.71	0.46
1:A:178:THR:HG22	1:A:179:ARG:N	2.30	0.46
1:A:261:GLY:HA2	1:A:317:THR:O	2.16	0.46
2:B:177:TYR:O	2:B:178:CYS:C	2.58	0.46
2:B:225:ASN:O	2:B:226:ILE:C	2.57	0.46
3:C:265:THR:CB	5:R:145:VAL:HG12	2.41	0.46
2:O:26:ILE:HA	2:O:35:ILE:O	2.15	0.46
2:O:53:ALA:O	2:O:103:GLU:C	2.59	0.46
2:O:76:THR:HG22	2:O:82:SER:N	2.28	0.46
3:P:155:PRO:O	3:P:156:TYR:HB2	2.15	0.46
3:P:316:MET:O	3:P:317:THR:C	2.58	0.46
2:B:246:GLU:O	2:B:427:SER:HA	2.15	0.46
2:B:259:THR:CG2	2:B:260:GLU:N	2.77	0.46
1:N:85:HIS:O	1:N:99:ILE:HA	2.15	0.46
2:O:46:ARG:NH1	2:O:110:GLU:OE2	2.48	0.46
2:O:229:GLY:C	2:O:231:GLY:N	2.73	0.46
3:P:28:ILE:HD11	16:P:3002:UQ:HM21	1.98	0.46
6:S:20:TYR:O	6:S:23:ALA:HB3	2.15	0.46
6:S:70:LEU:HD12	6:S:70:LEU:C	2.40	0.46
1:A:294:LEU:HB2	1:A:341:GLU:HG3	1.98	0.46
2:B:209:ILE:CD1	2:B:378:LEU:HD23	2.42	0.46
3:C:89:SER:O	3:C:90:PHE:C	2.57	0.46
5:E:126:ARG:HG2	5:E:126:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:ALA:O	5:E:149:ASN:HB2	2.14	0.46
5:E:186:GLN:O	5:E:193:VAL:HG23	2.16	0.46
1:N:223:TYR:HD2	1:N:223:TYR:H	1.63	0.46
2:O:169:LYS:HD2	2:O:238:THR:CG2	2.46	0.46
2:O:177:TYR:O	2:O:178:CYS:C	2.58	0.46
3:P:325:LEU:HD11	3:P:362:ILE:HG23	1.96	0.46
5:R:178:TYR:CD2	5:R:178:TYR:N	2.82	0.46
6:S:68:LEU:O	6:S:71:LYS:N	2.48	0.46
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.97	0.46
2:B:198:ASN:OD1	2:B:203:ARG:NH2	2.48	0.46
5:E:29:SER:O	5:E:30:GLU:C	2.59	0.46
8:H:28:GLU:O	8:H:29:LYS:C	2.58	0.46
1:N:349:THR:HA	1:N:353:GLU:OE1	2.16	0.46
2:O:81:SER:C	2:O:83:PHE:N	2.71	0.46
2:O:124:LEU:HD12	2:O:128:THR:HG21	1.97	0.46
2:O:146:VAL:O	2:O:149:ALA:N	2.48	0.46
2:O:217:LYS:O	2:O:219:VAL:N	2.48	0.46
14:P:502:HEM:HBB2	14:P:502:HEM:CMB	2.45	0.46
5:R:152:ASP:C	5:R:153:PHE:CD1	2.93	0.46
1:A:90:THR:HB	1:A:95:THR:HG23	1.96	0.46
2:B:167:ALA:O	2:B:168:TYR:CD1	2.68	0.46
5:E:30:GLU:CB	10:J:7:ARG:HG2	2.43	0.46
5:E:91:TRP:O	5:E:92:ARG:C	2.58	0.46
5:E:103:GLN:C	5:E:105:GLU:N	2.73	0.46
9:I:28:UNK:N	9:I:72:ALA:HB2	2.25	0.46
3:P:86:ASN:O	3:P:89:SER:N	2.49	0.46
3:P:90:PHE:HB2	3:P:240:PHE:CD2	2.50	0.46
4:Q:95:TYR:CD2	4:Q:101:ALA:CA	2.97	0.46
4:Q:134:TYR:OH	4:Q:160:MET:O	2.29	0.46
4:Q:165:TYR:O	4:Q:166:ASN:C	2.57	0.46
1:A:106:MET:HE3	1:A:208:LEU:CD1	2.45	0.46
1:A:317:THR:OG1	1:A:318:GLY:N	2.48	0.46
2:B:42:SER:OG	2:B:43:PRO:HD2	2.15	0.46
2:B:426:ALA:O	2:B:427:SER:HB3	2.14	0.46
4:D:16:GLY:C	4:D:18:LEU:H	2.24	0.46
7:G:16:TYR:N	7:G:16:TYR:CD1	2.83	0.46
1:N:106:MET:HE3	1:N:208:LEU:CD1	2.46	0.46
1:N:122:LEU:HD11	1:N:186:ILE:CD1	2.46	0.46
2:O:29:LEU:CD2	2:O:30:PRO:HD2	2.46	0.46
3:P:117:GLY:O	3:P:120:LEU:HB2	2.16	0.46
3:P:164:TRP:O	3:P:165:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:311:SER:CB	3:P:319:ARG:NH1	2.78	0.46
4:Q:46:VAL:HG12	4:Q:47:ALA:N	2.31	0.46
6:S:89:TYR:CD1	6:S:90:LEU:N	2.70	0.46
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.45	0.46
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.80	0.46
2:B:52:LYS:O	2:B:203:ARG:NH2	2.48	0.46
2:B:73:SER:N	2:B:74:PRO:HD2	2.31	0.46
3:C:64:PHE:CE1	3:C:259:PRO:HG3	2.51	0.46
3:C:82:ASN:HD22	3:C:82:ASN:H	1.64	0.46
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.80	0.46
4:D:221:TYR:CE2	5:E:39:VAL:HG21	2.51	0.46
6:F:19:TRP:O	6:F:20:TYR:C	2.58	0.46
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.45	0.46
3:P:77:GLY:O	3:P:78:TRP:C	2.58	0.46
3:P:115:ASN:HA	3:P:118:VAL:HG23	1.96	0.46
4:Q:54:VAL:HG12	4:Q:55:THR:N	2.30	0.46
4:Q:239:PRO:HB2	4:Q:240:PRO:CD	2.42	0.46
5:R:109:GLU:O	5:R:123:ASP:HB2	2.15	0.46
10:W:10:TYR:CD2	10:W:10:TYR:C	2.94	0.46
2:B:63:LEU:C	2:B:65:THR:H	2.24	0.46
2:B:403:ASP:C	2:B:405:VAL:N	2.74	0.46
4:D:43:MET:CE	4:D:189:PHE:CE2	2.97	0.46
6:F:32:MET:O	6:F:33:ARG:C	2.57	0.46
9:I:65:VAL:O	9:I:76:VAL:HA	2.16	0.46
1:N:136:GLN:O	1:N:138:LEU:N	2.49	0.46
1:N:245:ASP:OD1	1:N:247:ALA:HB3	2.15	0.46
2:O:89:ILE:O	2:O:92:VAL:HG22	2.16	0.46
2:O:341:MET:HA	2:O:341:MET:CE	2.44	0.46
5:R:53:ASN:O	5:R:57:GLN:HG3	2.16	0.46
2:B:374:THR:O	2:B:377:GLY:N	2.49	0.46
1:N:25:VAL:HG22	1:N:197:LEU:HB3	1.98	0.46
1:N:59:VAL:C	1:N:61:HIS:N	2.73	0.46
1:N:145:MET:O	1:N:146:THR:C	2.59	0.46
2:O:239:TYR:HE1	2:O:260:GLU:N	2.13	0.46
3:P:34:PHE:CE1	3:P:97:LEU:HD12	2.51	0.46
3:P:242:THR:O	3:P:246:PHE:HB2	2.16	0.46
3:P:338:TRP:O	3:P:341:SER:HB3	2.16	0.46
3:P:362:ILE:HA	3:P:366:LEU:HB2	1.96	0.46
5:R:32:ARG:NH1	7:T:22:GLU:HA	2.31	0.46
2:B:31:ASN:HD22	2:B:32:GLY:N	2.14	0.46
3:C:79:LEU:O	3:C:79:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:316:MET:O	3:C:318:PHE:N	2.49	0.46
3:C:325:LEU:HD21	3:C:366:LEU:CB	2.44	0.46
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.51	0.46
2:O:221:GLU:HG3	2:O:222:GLN:N	2.27	0.46
3:P:147:ILE:HD11	15:P:3001:ICX:H34	1.97	0.46
3:P:216:SER:O	3:P:217:ASP:HB2	2.15	0.46
3:P:261:ASN:C	3:P:263:LEU:H	2.23	0.46
3:P:350:ILE:HG23	3:P:351:ILE:N	2.31	0.46
8:U:24:CYS:C	8:U:26:GLN:N	2.74	0.46
1:A:109:VAL:O	1:A:110:VAL:C	2.59	0.45
1:A:122:LEU:HD11	1:A:186:ILE:CD1	2.46	0.45
2:B:249:GLY:HA3	2:O:181:TYR:CE1	2.51	0.45
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.97	0.45
3:C:320:PRO:HG2	3:C:321:LEU:H	1.81	0.45
4:D:150:ASN:O	4:D:156:GLN:HA	2.16	0.45
9:I:70:LEU:O	9:I:70:LEU:HG	2.14	0.45
1:N:170:THR:HG22	1:N:172:GLU:H	1.80	0.45
1:N:365:MET:HG2	1:N:366:VAL:N	2.30	0.45
3:P:139:MET:O	3:P:143:GLY:N	2.38	0.45
3:P:245:LEU:O	4:Q:201:ARG:CD	2.64	0.45
4:Q:32:VAL:HG21	4:Q:182:ILE:HG23	1.98	0.45
2:B:418:VAL:O	2:B:418:VAL:HG12	2.16	0.45
5:E:134:ILE:C	5:E:135:LEU:HG	2.39	0.45
5:E:153:PHE:CD1	5:E:153:PHE:N	2.84	0.45
2:O:383:GLY:O	2:O:384:SER:C	2.59	0.45
4:Q:51:LEU:O	4:Q:52:ILE:C	2.60	0.45
1:A:127:ILE:O	1:A:129:LYS:N	2.50	0.45
1:A:240:GLU:CD	1:A:242:ARG:HE	2.24	0.45
2:B:46:ARG:HH11	2:B:110:GLU:CD	2.24	0.45
8:H:58:LEU:HD12	8:H:58:LEU:O	2.17	0.45
3:P:5:ILE:O	3:P:12:LEU:HD23	2.17	0.45
3:P:118:VAL:N	14:P:502:HEM:HBC2	2.31	0.45
4:Q:215:LEU:HD13	5:R:46:ALA:CB	2.46	0.45
5:R:29:SER:O	5:R:31:ASP:N	2.49	0.45
5:R:38:LEU:HA	10:W:14:PHE:CZ	2.51	0.45
4:D:117:VAL:O	4:D:123:GLY:HA2	2.16	0.45
6:F:79:GLN:HE21	6:F:79:GLN:HB3	1.63	0.45
7:G:29:ILE:HA	7:G:33:ALA:HB3	1.97	0.45
8:H:72:LYS:O	8:H:73:LEU:C	2.60	0.45
2:O:353:THR:HB	2:O:356:ASP:OD2	2.16	0.45
3:P:87:GLY:HA2	3:P:240:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:126:ARG:HD3	5:R:168:SER:OG	2.16	0.45
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.82	0.45
8:U:28:GLU:O	8:U:29:LYS:C	2.60	0.45
1:A:53:ASN:OD1	1:A:165:ARG:HD3	2.16	0.45
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.76	0.45
2:B:257:VAL:O	2:B:323:GLY:HA3	2.16	0.45
4:D:43:MET:HG2	4:D:91:PHE:HD2	1.80	0.45
4:D:215:LEU:HD13	5:E:46:ALA:CB	2.45	0.45
5:E:70:ALA:O	5:E:71:LEU:HB2	2.17	0.45
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.56	0.45
1:N:206:LYS:O	1:N:208:LEU:N	2.49	0.45
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.52	0.45
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.51	0.45
3:P:326:PHE:CD2	3:P:326:PHE:C	2.94	0.45
8:U:55:THR:O	8:U:56:GLU:C	2.60	0.45
9:V:63:ASP:OD1	9:V:63:ASP:N	2.49	0.45
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.52	0.45
1:A:80:GLU:OE2	2:B:290:SER:HA	2.17	0.45
2:B:229:GLY:C	2:B:231:GLY:N	2.74	0.45
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.99	0.45
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.32	0.45
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.44	0.45
6:F:40:ASP:OD1	6:F:40:ASP:C	2.59	0.45
7:G:80:ASP:OD2	8:H:50:THR:HA	2.17	0.45
1:N:287:GLY:O	1:N:289:HIS:N	2.49	0.45
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.98	0.45
3:P:246:PHE:CE2	4:Q:205:GLY:HA3	2.52	0.45
6:S:52:LYS:HE2	7:T:11:ARG:NH1	2.29	0.45
1:A:133:VAL:O	1:A:134:ILE:C	2.56	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.69	0.45
2:B:385:GLU:HG2	2:B:391:THR:O	2.17	0.45
4:D:37:CYS:C	4:D:39:ALA:N	2.73	0.45
1:N:39:VAL:HG11	1:N:117:VAL:CG1	2.47	0.45
1:N:106:MET:N	1:N:107:PRO:HD2	2.32	0.45
1:N:279:ARG:NH2	9:V:30:UNK:C	2.80	0.45
1:N:439:SER:HA	1:N:442:TYR:CE2	2.52	0.45
2:O:47:ILE:HG21	2:O:120:MET:CE	2.46	0.45
2:O:167:ALA:C	2:O:168:TYR:CD1	2.95	0.45
2:O:325:TYR:HD2	2:O:326:THR:N	2.15	0.45
3:P:213:SER:HB2	6:S:39:GLU:OE2	2.16	0.45
5:R:14:ARG:HG2	5:R:14:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.47	0.45
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.51	0.45
2:B:167:ALA:C	2:B:168:TYR:CD1	2.95	0.45
2:B:248:ASN:HD22	2:B:249:GLY:N	2.14	0.45
3:C:175:THR:HG22	3:C:179:PHE:CE1	2.51	0.45
6:F:100:GLU:OE1	2:O:133:ARG:NH1	2.50	0.45
7:G:34:LEU:N	7:G:35:PRO:HD2	2.32	0.45
2:O:269:ALA:O	2:O:271:ALA:N	2.50	0.45
2:O:269:ALA:C	2:O:271:ALA:N	2.71	0.45
2:O:341:MET:CE	2:O:344:LEU:HD23	2.47	0.45
7:T:16:TYR:N	7:T:16:TYR:CD1	2.85	0.45
7:T:48:VAL:HG12	7:T:49:ALA:N	2.31	0.45
10:W:6:LEU:O	10:W:9:ALA:HB3	2.16	0.45
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.45
3:C:134:LEU:N	3:C:135:PRO:HD2	2.32	0.45
5:E:112:VAL:O	5:E:113:ASP:C	2.60	0.45
1:N:23:LEU:HA	1:N:192:ALA:O	2.17	0.45
4:Q:158:ILE:HG23	4:Q:158:ILE:O	2.15	0.45
5:R:91:TRP:CD1	5:R:92:ARG:H	2.35	0.45
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.99	0.45
6:S:52:LYS:HE3	6:S:56:ASN:HD21	1.82	0.45
1:A:242:ARG:O	7:G:14:ILE:HA	2.17	0.45
1:A:265:PRO:O	1:A:268:VAL:HG23	2.17	0.45
1:A:418:LYS:O	1:A:420:PRO:HD3	2.17	0.45
1:A:433:ASP:O	1:A:434:TYR:C	2.59	0.45
2:B:207:VAL:HG12	2:B:379:LEU:CD1	2.47	0.45
2:B:258:VAL:HG12	2:B:323:GLY:HA3	1.99	0.45
2:B:397:VAL:O	2:B:400:GLN:HB3	2.17	0.45
3:C:104:TYR:O	3:C:316:MET:HG3	2.17	0.45
5:E:109:GLU:CD	5:E:166:ASP:HB2	2.41	0.45
5:E:185:TYR:CD1	5:E:185:TYR:C	2.95	0.45
9:I:70:LEU:C	9:I:70:LEU:CD2	2.89	0.45
10:J:27:GLY:O	10:J:28:ALA:C	2.60	0.45
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.99	0.45
1:N:332:ASP:HB2	1:N:430:GLN:HG2	1.98	0.45
1:N:379:ILE:O	1:N:380:GLY:C	2.58	0.45
2:O:63:LEU:O	2:O:65:THR:N	2.49	0.45
6:S:78:GLU:H	6:S:78:GLU:CD	2.25	0.45
1:A:238:GLY:O	1:A:239:SER:HB3	2.17	0.44
2:B:26:ILE:O	2:B:26:ILE:HG12	2.17	0.44
1:N:245:ASP:C	1:N:247:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:186:VAL:CG1	4:Q:187:CYS:N	2.79	0.44
2:B:220:ALA:O	2:B:224:LEU:HD13	2.18	0.44
3:C:59:ASP:O	3:C:60:THR:C	2.59	0.44
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.52	0.44
2:O:18:CYS:HA	2:O:19:PRO:HD3	1.78	0.44
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.51	0.44
2:B:157:VAL:O	2:B:157:VAL:HG22	2.17	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.53	0.44
2:B:292:THR:O	2:B:292:THR:HG22	2.17	0.44
3:C:95:ILE:CG2	3:C:96:PHE:N	2.80	0.44
3:C:192:GLY:O	3:C:195:ILE:HB	2.17	0.44
3:C:208:ASN:OD1	3:C:208:ASN:C	2.61	0.44
3:C:335:ILE:O	3:C:336:LEU:C	2.60	0.44
1:N:39:VAL:HG13	1:N:39:VAL:O	2.17	0.44
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.99	0.44
2:O:292:THR:O	2:O:292:THR:HG22	2.18	0.44
3:P:56:TYR:OH	3:P:176:LEU:HD11	2.17	0.44
3:P:245:LEU:HA	3:P:245:LEU:HD23	1.64	0.44
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.47	0.44
18:P:3003:CDL:HB22	6:S:72:HIS:CD2	2.53	0.44
5:R:36:SER:C	5:R:39:VAL:HG23	2.41	0.44
5:R:76:ILE:HG12	5:R:89:PHE:CE2	2.52	0.44
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.17	0.44
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.82	0.44
1:A:19:LEU:C	1:A:21:ASN:H	2.25	0.44
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.17	0.44
1:A:106:MET:CE	1:A:110:VAL:CG2	2.95	0.44
2:B:37:SER:OG	2:B:38:LEU:N	2.48	0.44
2:B:130:PRO:CB	2:B:132:PHE:CE2	2.96	0.44
2:B:155:PRO:O	2:B:156:GLN:C	2.59	0.44
2:B:353:THR:HB	2:B:356:ASP:OD2	2.18	0.44
3:C:245:LEU:O	4:D:201:ARG:HD2	2.17	0.44
6:F:32:MET:HE3	6:F:87:LYS:HE3	2.00	0.44
1:N:270:LEU:HB3	1:N:311:ASN:ND2	2.33	0.44
2:O:19:PRO:HG3	2:O:41:PHE:CE2	2.53	0.44
2:O:99:TYR:O	2:O:106:THR:N	2.50	0.44
2:O:206:LEU:HG	2:O:206:LEU:O	2.17	0.44
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.50	0.44
4:Q:224:ARG:O	4:Q:225:HIS:C	2.60	0.44
2:B:37:SER:O	2:B:38:LEU:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:TYR:O	2:B:106:THR:N	2.49	0.44
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.23	0.44
4:D:235:MET:HE1	6:F:63:LYS:C	2.42	0.44
8:H:58:LEU:HD11	8:H:62:LEU:CD1	2.47	0.44
4:Q:117:VAL:CG2	4:Q:194:ALA:HB2	2.45	0.44
7:T:29:ILE:O	7:T:33:ALA:HB3	2.17	0.44
1:A:64:PHE:HE2	1:A:86:PHE:CE2	2.36	0.44
1:A:292:SER:O	1:A:293:ARG:C	2.59	0.44
1:A:362:ARG:HA	1:A:365:MET:HE2	2.00	0.44
2:B:34:ILE:HG21	2:B:386:ALA:O	2.18	0.44
2:B:84:ARG:NH1	2:B:122:TYR:CE2	2.85	0.44
2:B:226:ILE:HG23	2:B:226:ILE:O	2.18	0.44
3:C:13:LYS:O	3:C:17:ASN:N	2.51	0.44
6:F:73:ARG:HG3	6:F:73:ARG:NH1	2.31	0.44
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.46	0.44
2:O:248:ASN:HD22	2:O:249:GLY:N	2.14	0.44
2:O:394:ALA:HB3	2:O:397:VAL:HG23	2.00	0.44
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.52	0.44
5:R:68:VAL:O	5:R:69:LEU:O	2.35	0.44
1:A:58:PHE:CD2	1:A:134:ILE:HD11	2.53	0.44
1:A:349:THR:HA	1:A:353:GLU:OE1	2.18	0.44
4:D:168:ILE:O	4:D:168:ILE:HG12	2.17	0.44
6:F:32:MET:HE1	6:F:87:LYS:HG2	1.97	0.44
2:O:418:VAL:O	2:O:418:VAL:HG12	2.18	0.44
3:P:359:TYR:CD2	3:P:360:PHE:CD1	3.03	0.44
1:A:63:ALA:O	1:A:116:VAL:CG1	2.66	0.44
1:A:365:MET:HG2	1:A:366:VAL:N	2.33	0.44
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.53	0.44
3:C:79:LEU:HD22	4:D:204:MET:HE1	1.99	0.44
3:C:167:GLY:HA3	3:C:178:ARG:NH2	2.32	0.44
3:C:345:GLU:O	3:C:348:PHE:HB2	2.18	0.44
5:E:10:PHE:CB	7:G:18:LEU:HD11	2.48	0.44
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.53	0.44
8:H:59:PHE:O	8:H:60:ASP:C	2.61	0.44
2:O:115:HIS:O	2:O:116:VAL:C	2.60	0.44
2:O:269:ALA:O	2:O:270:ASN:C	2.59	0.44
3:P:44:THR:CG2	3:P:45:GLN:N	2.81	0.44
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.75	0.44
3:P:329:LEU:O	3:P:332:ASN:HB3	2.18	0.44
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.43	0.44
1:A:159:GLN:HG3	1:A:159:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.48	0.44
3:C:359:TYR:CD2	3:C:360:PHE:CD1	3.03	0.44
1:N:26:ALA:O	1:N:198:ALA:HA	2.18	0.44
1:N:170:THR:CG2	1:N:171:THR:N	2.79	0.44
2:O:143:GLN:O	2:O:144:LEU:C	2.61	0.44
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.52	0.44
2:O:310:SER:HB2	9:V:59:SER:CB	2.35	0.44
3:P:330:VAL:O	3:P:333:LEU:HB2	2.18	0.44
4:Q:178:THR:HG21	8:U:16:PRO:HD2	1.99	0.44
1:A:61:HIS:CD2	2:B:287:ARG:CZ	3.00	0.43
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.59	0.43
2:B:100:SER:HA	2:B:104:LYS:O	2.18	0.43
2:B:193:HIS:O	2:B:197:ASN:HB2	2.18	0.43
3:C:132:TYR:HA	14:C:501:HEM:HAA2	2.00	0.43
3:C:245:LEU:O	4:D:201:ARG:CD	2.66	0.43
4:D:117:VAL:CG2	4:D:194:ALA:HB2	2.47	0.43
4:D:169:LEU:HD23	4:D:169:LEU:O	2.17	0.43
9:I:51:CYS:O	9:I:55:MET:SD	2.76	0.43
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.70	0.43
1:N:279:ARG:HA	1:N:307:PHE:CE1	2.53	0.43
2:O:81:SER:O	2:O:82:SER:C	2.61	0.43
3:P:156:TYR:C	3:P:158:GLY:H	2.26	0.43
5:R:3:ASN:C	5:R:5:VAL:H	2.26	0.43
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.48	0.43
1:A:90:THR:HA	1:A:95:THR:HA	1.99	0.43
2:B:146:VAL:C	2:B:148:LYS:N	2.74	0.43
2:B:306:PRO:HB3	9:I:51:CYS:C	2.43	0.43
3:C:187:PRO:O	3:C:190:ILE:HB	2.18	0.43
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.46	0.43
3:P:63:ALA:HB2	3:P:176:LEU:HD21	2.01	0.43
3:P:78:TRP:CG	3:P:79:LEU:N	2.85	0.43
3:P:192:GLY:O	3:P:195:ILE:HB	2.17	0.43
4:Q:1:GLY:C	4:Q:3:LEU:N	2.76	0.43
5:R:32:ARG:HH11	7:T:22:GLU:HA	1.84	0.43
8:U:50:THR:O	8:U:51:GLU:HB2	2.18	0.43
2:B:383:GLY:O	2:B:384:SER:C	2.62	0.43
3:C:50:LEU:O	3:C:51:LEU:C	2.61	0.43
3:C:77:GLY:O	3:C:78:TRP:C	2.61	0.43
1:N:262:TRP:CD1	1:N:314:TYR:C	2.96	0.43
1:N:303:LEU:HB3	1:N:334:MET:SD	2.58	0.43
2:O:84:ARG:NH1	2:O:84:ARG:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:332:HIS:O	2:O:333:ALA:C	2.60	0.43
3:P:64:PHE:CD2	3:P:64:PHE:C	2.96	0.43
3:P:105:TYR:HD2	3:P:209:PRO:HA	1.78	0.43
4:Q:43:MET:CE	4:Q:189:PHE:CE2	3.00	0.43
9:V:61:ARG:O	9:V:62:ARG:HG3	2.18	0.43
1:A:403:ASP:O	1:A:404:ALA:C	2.61	0.43
2:B:252:LEU:HD12	9:I:49:LEU:HD12	2.01	0.43
2:B:258:VAL:CG1	2:B:312:PHE:HD2	2.24	0.43
4:D:222:MET:HE3	5:E:40:THR:HG23	2.01	0.43
1:N:134:ILE:HG21	1:N:174:ILE:CD1	2.49	0.43
2:O:102:ARG:CZ	2:O:164:HIS:CD2	3.02	0.43
2:O:116:VAL:HA	2:O:119:VAL:HG22	1.99	0.43
3:P:50:LEU:O	3:P:51:LEU:C	2.61	0.43
1:A:158:PHE:CE1	1:A:319:LEU:HD21	2.54	0.43
2:B:239:TYR:CD2	2:B:240:TRP:N	2.86	0.43
3:C:173:ASN:O	3:C:174:PRO:C	2.60	0.43
3:C:221:PHE:CD2	3:C:221:PHE:C	2.97	0.43
3:C:293:LEU:O	3:C:294:ALA:C	2.62	0.43
3:C:346:HIS:CG	3:C:347:PRO:HA	2.53	0.43
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.53	0.43
1:N:197:LEU:HD12	1:N:197:LEU:HA	1.79	0.43
2:O:59:THR:O	2:O:60:THR:C	2.60	0.43
2:O:76:THR:HG22	2:O:81:SER:CA	2.37	0.43
3:P:89:SER:C	3:P:91:PHE:N	2.74	0.43
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.17	0.43
5:R:52:LYS:C	5:R:52:LYS:CD	2.89	0.43
8:U:21:ARG:O	8:U:25:GLU:HG3	2.18	0.43
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.01	0.43
1:A:228:VAL:O	1:A:228:VAL:HG22	2.17	0.43
1:A:310:PHE:CE2	1:A:321:GLY:N	2.87	0.43
2:B:60:THR:CG2	2:B:61:ALA:N	2.82	0.43
2:B:84:ARG:HG2	2:B:84:ARG:HH11	1.83	0.43
2:B:307:PHE:CG	2:B:308:ASP:N	2.86	0.43
3:C:75:GLN:O	3:C:76:TYR:HB2	2.19	0.43
3:C:86:ASN:O	3:C:87:GLY:C	2.60	0.43
3:C:127:THR:O	3:C:130:VAL:CG2	2.66	0.43
3:C:226:SER:O	3:C:230:ILE:HG12	2.19	0.43
3:C:230:ILE:HG23	11:C:2005:PEE:H25	2.01	0.43
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.53	0.43
4:D:147:LEU:HD23	4:D:159:GLY:HA2	2.01	0.43
5:E:192:LEU:HG	5:E:193:VAL:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:58:PHE:HB3	1:N:182:LEU:HD11	1.99	0.43
1:N:176:HIS:O	1:N:177:LEU:C	2.60	0.43
1:N:255:LEU:O	1:N:321:GLY:HA3	2.18	0.43
1:N:429:GLU:O	1:N:432:LEU:HD13	2.19	0.43
2:O:277:HIS:HB2	2:O:360:ALA:HB1	1.99	0.43
2:O:397:VAL:O	2:O:400:GLN:HB3	2.18	0.43
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.18	0.43
4:Q:218:LEU:HD22	5:R:39:VAL:HG12	2.01	0.43
4:Q:221:TYR:CE1	7:T:25:ALA:HB1	2.52	0.43
2:B:50:PHE:HZ	2:B:379:LEU:HG	1.84	0.43
2:B:52:LYS:HD2	2:B:203:ARG:HG2	2.01	0.43
2:B:353:THR:C	2:B:355:GLU:H	2.25	0.43
2:B:379:LEU:HG	2:B:379:LEU:O	2.18	0.43
4:D:101:ALA:O	4:D:102:ARG:C	2.60	0.43
4:D:175:THR:HA	4:D:176:PRO:HD3	1.90	0.43
1:N:62:LEU:CD1	1:N:127:ILE:HG12	2.48	0.43
2:O:75:LEU:CD2	2:O:136:GLU:HB3	2.45	0.43
8:U:40:CYS:O	8:U:44:VAL:HG23	2.19	0.43
1:A:39:VAL:HG11	1:A:117:VAL:HG11	2.01	0.43
1:A:89:TYR:CD1	1:A:89:TYR:C	2.96	0.43
1:A:127:ILE:C	1:A:129:LYS:N	2.76	0.43
1:A:245:ASP:C	1:A:247:ALA:N	2.75	0.43
3:C:89:SER:O	3:C:92:PHE:N	2.52	0.43
5:E:59:ILE:HD13	5:E:59:ILE:HA	1.82	0.43
1:N:133:VAL:O	1:N:134:ILE:C	2.62	0.43
1:N:435:ASN:O	1:N:438:ARG:N	2.52	0.43
3:P:87:GLY:N	3:P:240:PHE:HE2	2.17	0.43
3:P:215:ASP:HB3	7:T:7:LEU:HB3	2.00	0.43
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.83	0.43
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	2.01	0.43
6:S:59:MET:HA	6:S:59:MET:CE	2.44	0.43
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.34	0.43
1:A:171:THR:HB	5:E:4:ASP:OD2	2.19	0.43
1:A:187:ASP:O	1:A:191:LYS:HE3	2.19	0.43
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.34	0.43
2:B:162:ASN:HB3	2:B:244:ILE:HG21	2.01	0.43
2:B:325:TYR:HD2	2:B:326:THR:N	2.15	0.43
3:C:5:ILE:O	3:C:12:LEU:HD23	2.18	0.43
3:C:28:ILE:CG1	3:C:225:TYR:CE2	3.00	0.43
3:C:215:ASP:C	3:C:217:ASP:N	2.77	0.43
3:C:247:SER:OG	3:C:250:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:PHE:HB3	8:H:74:PHE:CE2	2.54	0.43
5:E:106:ILE:HD11	5:E:131:GLU:HA	2.00	0.43
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.99	0.43
1:N:246:ASP:HA	1:N:427:PRO:HB3	2.01	0.43
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.74	0.43
5:R:97:PHE:CE2	5:R:137:GLY:HA3	2.54	0.43
1:A:25:VAL:HG22	1:A:197:LEU:HB3	2.00	0.43
1:A:246:ASP:HA	1:A:427:PRO:HB3	2.00	0.43
1:A:285:GLY:O	1:A:286:GLY:C	2.62	0.43
1:A:392:LEU:N	1:A:392:LEU:HD23	2.33	0.43
2:B:81:SER:O	2:B:82:SER:C	2.62	0.43
2:B:345:LYS:C	2:B:347:ALA:N	2.74	0.43
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.43
4:D:22:ASP:C	4:D:24:SER:H	2.27	0.43
4:D:191:ARG:O	4:D:192:TRP:C	2.62	0.43
1:N:206:LYS:O	1:N:207:GLU:C	2.61	0.43
1:N:431:LEU:HD12	1:N:431:LEU:C	2.43	0.43
2:O:27:THR:HG22	2:O:28:LYS:H	1.83	0.43
3:P:13:LYS:O	3:P:17:ASN:N	2.51	0.43
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	2.00	0.43
6:S:67:ASP:HA	6:S:70:LEU:HD23	2.01	0.43
1:A:394:GLU:O	1:A:395:TRP:C	2.62	0.42
2:B:63:LEU:O	2:B:65:THR:N	2.52	0.42
2:B:121:GLU:HG3	2:B:125:ASN:ND2	2.34	0.42
6:F:68:LEU:O	6:F:71:LYS:N	2.51	0.42
1:N:281:ASP:O	1:N:282:ARG:C	2.62	0.42
2:O:205:ALA:CB	2:O:387:LEU:HD13	2.48	0.42
3:P:216:SER:HB3	6:S:59:MET:HE2	2.01	0.42
4:Q:186:VAL:HG13	4:Q:187:CYS:N	2.33	0.42
5:R:14:ARG:HG2	5:R:14:ARG:NH1	2.34	0.42
5:R:141:HIS:CE1	5:R:142:LEU:HD12	2.54	0.42
6:S:64:ARG:O	6:S:68:LEU:HG	2.18	0.42
1:A:109:VAL:O	1:A:112:LEU:N	2.52	0.42
2:B:417:PHE:CD2	2:B:417:PHE:C	2.97	0.42
5:E:168:SER:CB	5:E:170:ARG:HG3	2.49	0.42
6:F:67:ASP:OD1	6:F:71:LYS:HD2	2.19	0.42
7:G:60:SER:O	7:G:61:TRP:C	2.61	0.42
1:N:22:GLY:C	1:N:193:PRO:HA	2.43	0.42
2:O:84:ARG:HG2	2:O:84:ARG:HH11	1.84	0.42
4:Q:16:GLY:O	4:Q:18:LEU:N	2.52	0.42
4:Q:218:LEU:HD13	5:R:43:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:78:GLU:C	7:T:79:ASN:HD22	2.27	0.42
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.48	0.42
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.83	0.42
1:A:388:ARG:HG3	1:A:388:ARG:NH2	2.34	0.42
3:C:339:ILE:HD13	3:C:339:ILE:HA	1.83	0.42
4:D:127:VAL:O	4:D:131:LEU:HG	2.18	0.42
10:J:14:PHE:CD2	10:J:14:PHE:N	2.85	0.42
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.83	0.42
2:O:67:HIS:C	2:O:67:HIS:CD2	2.97	0.42
3:P:56:TYR:CZ	3:P:134:LEU:HB3	2.54	0.42
3:P:208:ASN:OD1	3:P:208:ASN:C	2.61	0.42
3:P:304:LEU:O	3:P:305:ILE:C	2.62	0.42
5:R:20:ASP:C	5:R:22:THR:H	2.27	0.42
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.20	0.42
1:A:55:ALA:C	1:A:57:TYR:N	2.76	0.42
1:A:138:LEU:O	1:A:139:LYS:C	2.61	0.42
3:C:24:ALA:O	3:C:25:PRO:C	2.62	0.42
3:C:86:ASN:C	3:C:240:PHE:HE2	2.27	0.42
3:C:186:LEU:O	3:C:189:ALA:HB3	2.19	0.42
4:D:54:VAL:CG1	4:D:55:THR:HG23	2.49	0.42
5:E:33:LYS:HG2	7:G:21:PHE:CE1	2.55	0.42
5:E:78:LEU:HD21	5:E:193:VAL:HG11	2.01	0.42
5:E:79:SER:HB3	5:E:191:ASP:CB	2.50	0.42
1:N:42:GLY:HA2	1:N:384:LEU:HD21	2.01	0.42
1:N:140:GLU:C	1:N:142:ASP:N	2.77	0.42
2:O:135:TRP:C	2:O:137:VAL:N	2.77	0.42
2:O:140:LEU:C	2:O:142:PRO:HD2	2.44	0.42
2:O:219:VAL:O	2:O:220:ALA:C	2.62	0.42
3:P:52:LEU:C	3:P:54:MET:N	2.76	0.42
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.20	0.42
6:S:65:ALA:O	6:S:68:LEU:HB2	2.19	0.42
7:T:38:TRP:O	7:T:41:PHE:N	2.52	0.42
1:A:297:LEU:O	1:A:298:ALA:C	2.60	0.42
1:A:379:ILE:O	1:A:380:GLY:C	2.63	0.42
2:B:130:PRO:HB2	2:B:132:PHE:CD2	2.53	0.42
2:B:147:ASP:O	2:B:150:VAL:HG22	2.20	0.42
2:B:217:LYS:O	2:B:218:GLN:C	2.62	0.42
2:B:325:TYR:C	2:B:325:TYR:CD2	2.96	0.42
3:C:106:GLY:C	3:C:108:TYR:N	2.76	0.42
3:C:114:TRP:O	3:C:117:GLY:N	2.53	0.42
3:C:213:SER:HB2	6:F:39:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ASN:C	3:C:263:LEU:H	2.27	0.42
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.77	0.42
1:N:89:TYR:CD1	1:N:89:TYR:C	2.97	0.42
1:N:248:LEU:HB3	1:N:249:PRO:HD2	2.00	0.42
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.50	0.42
2:O:215:ASP:C	2:O:217:LYS:H	2.25	0.42
3:P:114:TRP:O	3:P:115:ASN:C	2.62	0.42
4:Q:54:VAL:CG1	4:Q:55:THR:HG23	2.50	0.42
5:R:135:LEU:HA	5:R:183:PRO:HD3	2.01	0.42
6:S:53:ASP:O	6:S:54:LEU:C	2.60	0.42
1:A:49:ASN:HD21	1:A:52:ASN:H	1.65	0.42
1:A:178:THR:CG2	1:A:179:ARG:N	2.82	0.42
2:B:64:GLY:C	2:B:66:ALA:N	2.75	0.42
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.54	0.42
2:B:200:THR:HB	2:B:227:ARG:O	2.19	0.42
3:C:76:TYR:O	3:C:77:GLY:C	2.62	0.42
3:C:145:THR:O	3:C:149:ASN:HB2	2.20	0.42
3:C:273:TRP:HA	3:C:276:LEU:HG	2.00	0.42
5:E:15:ARG:HG3	7:G:22:GLU:C	2.45	0.42
5:E:113:ASP:HB3	5:E:116:LYS:HG2	2.00	0.42
5:E:135:LEU:HD22	5:E:169:GLY:HA3	2.02	0.42
5:E:136:VAL:O	5:E:138:VAL:N	2.52	0.42
8:H:58:LEU:O	8:H:61:PHE:HB3	2.19	0.42
1:N:163:LEU:HB2	1:N:234:CYS:SG	2.60	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.83	0.42
2:O:348:ALA:HA	2:O:414:ALA:CB	2.49	0.42
2:O:412:ASN:O	2:O:413:ALA:C	2.63	0.42
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	2.01	0.42
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.83	0.42
4:Q:171:TYR:HD1	4:Q:175:THR:HB	1.84	0.42
7:T:29:ILE:HA	7:T:33:ALA:CB	2.50	0.42
8:U:15:ASP:C	8:U:17:LEU:H	2.28	0.42
10:W:35:PHE:O	10:W:36:ASP:C	2.63	0.42
1:A:72:CYS:O	1:A:73:ALA:C	2.61	0.42
1:A:437:ILE:O	1:A:438:ARG:C	2.63	0.42
2:B:325:TYR:HB3	9:I:59:SER:HB3	2.00	0.42
2:B:341:MET:CE	2:B:344:LEU:HD23	2.50	0.42
3:C:278:ALA:O	3:C:279:TYR:C	2.63	0.42
4:D:210:LEU:HD23	4:D:210:LEU:HA	1.81	0.42
5:E:42:THR:O	5:E:43:ALA:C	2.63	0.42
1:N:48:GLU:OE1	1:N:54:GLY:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:LEU:C	1:N:140:GLU:N	2.73	0.42
1:N:142:ASP:O	1:N:148:VAL:HG21	2.19	0.42
2:O:259:THR:CG2	2:O:260:GLU:N	2.83	0.42
2:O:341:MET:HE1	2:O:344:LEU:HD23	2.01	0.42
4:Q:12:TRP:CD1	4:Q:12:TRP:H	2.36	0.42
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.49	0.42
5:R:170:ARG:HA	5:R:179:ASN:HB3	2.02	0.42
2:B:52:LYS:HB2	2:B:203:ARG:HB3	2.01	0.42
3:C:89:SER:C	3:C:91:PHE:N	2.77	0.42
3:C:103:LEU:HD12	3:C:103:LEU:HA	1.65	0.42
3:C:184:PHE:CD2	3:P:184:PHE:CD2	3.08	0.42
3:C:216:SER:O	3:C:217:ASP:HB2	2.19	0.42
4:D:167:GLU:C	4:D:169:LEU:N	2.78	0.42
1:N:63:ALA:O	1:N:116:VAL:HG11	2.20	0.42
1:N:168:GLU:CD	1:N:168:GLU:H	2.27	0.42
1:N:183:ALA:O	1:N:184:SER:C	2.62	0.42
1:N:209:VAL:O	1:N:212:ALA:HB3	2.18	0.42
2:O:47:ILE:CG1	2:O:120:MET:HE1	2.40	0.42
2:O:374:THR:O	2:O:375:ALA:C	2.62	0.42
3:P:89:SER:O	3:P:92:PHE:N	2.53	0.42
3:P:120:LEU:HB3	14:P:502:HEM:HAB	2.02	0.42
3:P:276:LEU:O	3:P:279:TYR:HB3	2.19	0.42
3:P:347:PRO:HG3	7:T:62:GLY:HA2	2.02	0.42
6:S:40:ASP:C	6:S:40:ASP:OD1	2.61	0.42
6:S:59:MET:O	6:S:60:PHE:C	2.61	0.42
6:S:79:GLN:HE21	6:S:79:GLN:HB3	1.65	0.42
8:U:15:ASP:O	8:U:16:PRO:C	2.62	0.42
1:A:86:PHE:CG	1:A:99:ILE:HG12	2.55	0.42
1:A:140:GLU:OE2	9:I:50:LEU:N	2.53	0.42
1:A:429:GLU:OE1	7:G:7:LEU:HB2	2.19	0.42
2:B:163:LEU:O	2:B:166:ALA:N	2.51	0.42
2:B:368:TYR:O	2:B:371:SER:HB2	2.20	0.42
3:C:53:ALA:N	14:C:501:HEM:HMD2	2.35	0.42
3:C:101:ARG:HD2	3:C:101:ARG:O	2.20	0.42
3:C:186:LEU:HD23	3:C:186:LEU:HA	1.77	0.42
3:C:355:ALA:HA	3:C:358:SER:OG	2.20	0.42
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.60	0.42
5:E:31:ASP:OD1	10:J:7:ARG:HG3	2.19	0.42
9:I:31:UNK:C	9:I:73:PRO:HG2	2.50	0.42
1:N:112:LEU:HG	1:N:112:LEU:H	1.59	0.42
1:N:307:PHE:HA	1:N:323:HIS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:31:ASN:HD22	2:O:32:GLY:N	2.18	0.42
2:O:393:THR:HG23	2:O:397:VAL:HB	2.00	0.42
4:Q:191:ARG:O	4:Q:192:TRP:C	2.63	0.42
5:R:121:GLN:O	5:R:122:HIS:C	2.63	0.42
1:A:271:HIS:NE2	1:A:311:ASN:HB3	2.34	0.42
2:B:51:ILE:HD13	2:B:199:PHE:CD2	2.55	0.42
2:B:153:GLN:O	2:B:155:PRO:HD3	2.20	0.42
3:C:60:THR:N	3:C:176:LEU:HD23	2.35	0.42
3:C:151:PHE:C	3:C:153:ALA:H	2.28	0.42
3:C:276:LEU:O	3:C:279:TYR:HB3	2.20	0.42
3:C:285:ILE:CD1	3:C:294:ALA:HB2	2.50	0.42
5:E:72:SER:O	5:E:73:LYS:CG	2.68	0.42
5:E:112:VAL:O	5:E:114:VAL:N	2.53	0.42
2:O:59:THR:HG22	2:O:60:THR:N	2.35	0.42
2:O:141:GLN:N	2:O:142:PRO:CD	2.83	0.42
2:O:239:TYR:HD2	2:O:240:TRP:N	2.18	0.42
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.55	0.42
3:P:88:ALA:O	3:P:91:PHE:HB3	2.20	0.42
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.54	0.42
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	2.01	0.42
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.91	0.42
9:V:70:LEU:HD23	9:V:70:LEU:C	2.45	0.42
1:A:206:LYS:O	1:A:209:VAL:HG12	2.20	0.41
2:B:38:LEU:C	2:B:38:LEU:HD12	2.44	0.41
3:C:130:VAL:HG23	3:C:131:GLY:N	2.34	0.41
3:C:134:LEU:C	3:C:136:TRP:H	2.28	0.41
3:C:378:LEU:O	3:C:379:ASN:HB3	2.20	0.41
4:D:22:ASP:C	4:D:24:SER:N	2.78	0.41
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.55	0.41
1:N:39:VAL:HG11	1:N:117:VAL:HG11	2.01	0.41
1:N:46:ARG:HD3	1:N:231:LEU:HD13	2.02	0.41
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.50	0.41
1:N:205:HIS:O	1:N:206:LYS:C	2.63	0.41
1:N:273:ALA:O	1:N:275:ALA:N	2.53	0.41
1:A:145:MET:O	1:A:146:THR:C	2.62	0.41
1:A:203:ILE:HG22	1:A:204:SER:N	2.34	0.41
3:C:61:SER:C	3:C:62:LEU:HD12	2.45	0.41
3:C:147:ILE:HD11	15:C:2001:ICX:H34	2.01	0.41
3:C:229:ASP:O	3:C:230:ILE:C	2.62	0.41
3:C:285:ILE:HG21	3:C:290:GLY:HA3	2.01	0.41
6:F:82:LYS:O	6:F:83:TYR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:53:ASN:OD1	1:N:165:ARG:HD3	2.19	0.41
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.01	0.41
3:P:120:LEU:HD22	14:P:502:HEM:CAB	2.49	0.41
3:P:212:ILE:O	3:P:213:SER:C	2.63	0.41
4:Q:101:ALA:O	4:Q:102:ARG:C	2.64	0.41
4:Q:221:TYR:CE1	7:T:25:ALA:HB2	2.56	0.41
5:R:185:TYR:HB2	5:R:194:VAL:O	2.20	0.41
8:U:55:THR:O	8:U:58:LEU:HB3	2.19	0.41
10:W:14:PHE:N	10:W:14:PHE:CD2	2.88	0.41
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.51	0.41
2:B:56:ARG:CG	2:B:171:ALA:HB1	2.40	0.41
2:B:318:ASP:OD2	2:B:318:ASP:C	2.63	0.41
4:D:27:ARG:O	4:D:30:PHE:HB3	2.20	0.41
6:F:89:TYR:CD1	6:F:90:LEU:HB2	2.55	0.41
1:N:109:VAL:O	1:N:112:LEU:N	2.52	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.90	0.41
2:O:187:THR:OG1	2:O:190:GLN:HG3	2.19	0.41
2:O:312:PHE:N	2:O:323:GLY:O	2.41	0.41
3:P:12:LEU:HD12	3:P:12:LEU:HA	1.91	0.41
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	2.01	0.41
10:W:21:ALA:C	10:W:23:THR:N	2.75	0.41
1:A:310:PHE:C	1:A:310:PHE:CD2	2.98	0.41
1:A:434:TYR:O	1:A:435:ASN:C	2.61	0.41
2:B:64:GLY:C	2:B:66:ALA:H	2.28	0.41
2:B:189:GLU:O	2:B:190:GLN:C	2.63	0.41
2:B:206:LEU:O	2:B:216:LEU:HD21	2.20	0.41
3:C:34:PHE:CE1	3:C:97:LEU:HD12	2.56	0.41
3:C:143:GLY:HA2	15:C:2001:ICX:H28	2.03	0.41
3:C:287:ASN:O	3:C:288:LYS:C	2.63	0.41
4:D:235:MET:HE2	6:F:64:ARG:HB2	2.02	0.41
5:E:123:ASP:O	5:E:127:VAL:HG22	2.21	0.41
6:F:62:ILE:C	6:F:64:ARG:N	2.77	0.41
1:N:58:PHE:CD2	1:N:134:ILE:HD11	2.55	0.41
2:O:64:GLY:C	2:O:66:ALA:N	2.78	0.41
9:V:28:UNK:O	9:V:71:ASN:ND2	2.53	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.83	0.41
2:B:90:GLU:HG2	9:I:71:ASN:ND2	2.34	0.41
3:C:63:ALA:HB2	3:C:176:LEU:HD21	2.03	0.41
3:C:295:LEU:O	3:C:296:ALA:C	2.64	0.41
3:C:374:GLU:O	3:C:375:ASN:C	2.62	0.41
6:F:102:LEU:HA	6:F:102:LEU:HD23	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:126:GLN:O	1:N:129:LYS:HB3	2.20	0.41
3:P:49:GLY:C	14:P:501:HEM:HAC	2.45	0.41
3:P:107:SER:HB2	14:P:502:HEM:HMD3	2.02	0.41
3:P:198:LEU:HD22	16:P:3002:UQ:HM52	2.01	0.41
3:P:311:SER:OG	3:P:319:ARG:HD3	2.20	0.41
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.35	0.41
4:Q:55:THR:OG1	4:Q:56:HIS:ND1	2.41	0.41
4:Q:70:VAL:HG12	4:Q:71:GLN:H	1.85	0.41
4:Q:195:GLU:N	4:Q:196:PRO:HD3	2.35	0.41
5:R:98:VAL:HG13	5:R:134:ILE:CD1	2.43	0.41
10:W:28:ALA:O	10:W:29:VAL:C	2.63	0.41
1:A:145:MET:HE2	1:A:145:MET:N	2.35	0.41
1:A:274:ASN:CG	1:A:309:THR:HB	2.45	0.41
1:A:324:PHE:CD1	1:A:334:MET:HG2	2.55	0.41
2:B:332:HIS:O	2:B:333:ALA:C	2.62	0.41
3:C:79:LEU:HD12	3:C:79:LEU:C	2.46	0.41
2:O:62:ASN:O	2:O:65:THR:CG2	2.63	0.41
2:O:248:ASN:C	2:O:250:HIS:H	2.28	0.41
2:O:313:ASN:O	9:V:62:ARG:HG2	2.19	0.41
3:P:52:LEU:O	3:P:54:MET:N	2.54	0.41
7:T:41:PHE:HD2	7:T:41:PHE:O	2.03	0.41
1:A:106:MET:HG3	1:A:203:ILE:HD13	2.03	0.41
3:C:31:TRP:CH2	11:C:2007:PEE:H20	2.56	0.41
3:C:172:ASP:C	3:C:174:PRO:HD2	2.46	0.41
3:C:235:LEU:HA	3:C:235:LEU:HD23	1.78	0.41
3:P:107:SER:C	3:P:109:LEU:N	2.78	0.41
4:Q:109:LEU:HA	4:Q:110:PRO:HD2	1.94	0.41
6:S:53:ASP:OD1	6:S:54:LEU:N	2.54	0.41
8:U:66:ASP:HA	8:U:69:VAL:HG23	2.02	0.41
1:A:55:ALA:O	1:A:57:TYR:N	2.53	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.39	0.41
1:A:107:PRO:O	1:A:108:LYS:C	2.64	0.41
2:B:372:VAL:O	2:B:372:VAL:HG12	2.21	0.41
3:C:308:LEU:HD11	3:C:364:LEU:HD23	2.03	0.41
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.91	0.41
5:E:175:PRO:O	5:E:176:ALA:C	2.64	0.41
3:P:59:ASP:O	3:P:60:THR:C	2.63	0.41
3:P:126:ALA:O	3:P:129:PHE:HB3	2.20	0.41
5:R:74:ILE:HG12	5:R:195:VAL:HB	2.02	0.41
6:S:19:TRP:O	6:S:20:TYR:C	2.64	0.41
6:S:89:TYR:CD1	6:S:90:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:32:UNK:O	9:V:33:UNK:C	2.68	0.41
1:A:67:THR:HB	1:A:119:ASN:O	2.21	0.41
1:A:208:LEU:O	1:A:209:VAL:C	2.63	0.41
2:B:66:ALA:O	2:B:69:LEU:HB3	2.21	0.41
2:B:141:GLN:N	2:B:142:PRO:CD	2.84	0.41
2:B:183:ILE:HD13	2:B:183:ILE:HA	1.89	0.41
2:B:209:ILE:HG22	2:B:210:GLY:N	2.36	0.41
2:B:212:LYS:HD3	2:B:212:LYS:C	2.45	0.41
2:B:393:THR:HG23	2:B:397:VAL:HB	2.02	0.41
2:B:395:PRO:O	2:B:398:VAL:HG12	2.20	0.41
3:C:38:LEU:HB3	14:C:502:HEM:HMB1	2.01	0.41
3:C:81:ARG:O	3:C:82:ASN:C	2.63	0.41
3:C:320:PRO:O	3:C:323:GLN:HB2	2.20	0.41
4:D:10:PHE:CD2	8:H:74:PHE:HE2	2.39	0.41
4:D:28:ARG:O	4:D:31:GLN:N	2.54	0.41
4:D:52:ILE:HG22	4:D:53:GLY:N	2.36	0.41
4:D:95:TYR:CD2	4:D:101:ALA:CA	3.00	0.41
4:D:223:LYS:HD3	4:D:223:LYS:O	2.18	0.41
4:D:224:ARG:O	4:D:225:HIS:C	2.62	0.41
5:E:95:PRO:HG3	3:P:263:LEU:CD2	2.50	0.41
5:E:150:SER:OG	5:E:157:TYR:HB3	2.21	0.41
5:E:161:HIS:HB2	19:E:501:FES:S1	2.61	0.41
10:J:6:LEU:HD23	10:J:6:LEU:HA	1.90	0.41
10:J:58:LYS:C	10:J:59:TYR:CD1	2.99	0.41
1:N:107:PRO:O	1:N:108:LYS:C	2.64	0.41
1:N:273:ALA:O	1:N:276:ILE:N	2.52	0.41
1:N:338:ALA:C	1:N:340:GLY:N	2.76	0.41
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.50	0.41
2:O:51:ILE:HD13	2:O:199:PHE:CD2	2.56	0.41
2:O:248:ASN:ND2	2:O:250:HIS:N	2.63	0.41
3:P:28:ILE:CG1	3:P:225:TYR:CE2	3.01	0.41
3:P:76:TYR:O	3:P:77:GLY:C	2.64	0.41
3:P:79:LEU:HD11	3:P:83:LEU:CD1	2.49	0.41
3:P:145:THR:O	3:P:149:ASN:HB2	2.21	0.41
3:P:184:PHE:HA	14:P:501:HEM:CBC	2.42	0.41
3:P:230:ILE:HG23	11:W:3005:PEE:H25	2.03	0.41
3:P:267:PRO:HG2	3:P:268:HIS:H	1.85	0.41
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.03	0.41
3:P:342:GLN:HE21	3:P:343:PRO:CD	2.27	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.51	0.41
6:S:16:ILE:HG22	6:S:17:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:24:CYS:O	8:U:26:GLN:N	2.54	0.41
8:U:32:LYS:O	8:U:36:ARG:HG3	2.21	0.41
9:V:28:UNK:H	9:V:71:ASN:ND2	2.17	0.41
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.56	0.41
1:A:266:ASP:O	1:A:267:ASN:C	2.63	0.41
1:A:293:ARG:HD3	1:A:344:ARG:HD2	2.02	0.41
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.86	0.41
1:A:406:MET:O	1:A:410:VAL:HG23	2.21	0.41
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.41
3:C:87:GLY:O	3:C:88:ALA:C	2.64	0.41
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.56	0.41
5:E:138:VAL:O	5:E:139:CYS:C	2.64	0.41
6:F:16:ILE:O	6:F:17:ARG:C	2.62	0.41
1:N:59:VAL:O	1:N:60:GLU:C	2.64	0.41
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.56	0.41
5:R:37:TYR:HB3	10:W:14:PHE:HB3	2.03	0.41
5:R:53:ASN:HD22	5:R:53:ASN:HA	1.67	0.41
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.51	0.41
9:V:68:ILE:HA	9:V:68:ILE:HD13	1.76	0.41
1:A:382:HIS:HB3	1:A:388:ARG:O	2.20	0.40
2:B:67:HIS:ND1	2:B:178:CYS:N	2.65	0.40
2:B:169:LYS:C	2:B:170:THR:HG23	2.46	0.40
3:C:9:HIS:C	3:C:11:LEU:H	2.29	0.40
3:C:64:PHE:C	3:C:64:PHE:CD2	2.99	0.40
3:C:94:CYS:O	3:C:95:ILE:C	2.64	0.40
3:C:172:ASP:OD1	3:C:173:ASN:N	2.49	0.40
3:C:278:ALA:HB1	3:C:295:LEU:HD11	2.01	0.40
3:C:326:PHE:HA	3:C:367:PHE:HZ	1.85	0.40
5:E:73:LYS:C	5:E:74:ILE:HG13	2.39	0.40
2:O:135:TRP:O	2:O:139:ASP:HB2	2.20	0.40
2:O:262:ALA:O	2:O:320:GLY:HA3	2.21	0.40
2:O:318:ASP:OD2	2:O:318:ASP:C	2.64	0.40
2:O:395:PRO:O	2:O:398:VAL:HG12	2.21	0.40
3:P:151:PHE:C	3:P:153:ALA:N	2.78	0.40
4:Q:86:LYS:N	4:Q:89:ASP:OD2	2.47	0.40
4:Q:169:LEU:HD23	4:Q:169:LEU:O	2.21	0.40
5:R:126:ARG:NE	5:R:168:SER:O	2.45	0.40
1:A:140:GLU:C	1:A:142:ASP:N	2.79	0.40
1:A:142:ASP:O	1:A:148:VAL:HG21	2.21	0.40
1:A:158:PHE:O	1:A:159:GLN:C	2.63	0.40
1:A:338:ALA:O	1:A:339:GLN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:GLU:HG2	9:I:71:ASN:HD21	1.86	0.40
2:B:198:ASN:O	2:B:203:ARG:NE	2.54	0.40
2:B:212:LYS:HD2	2:B:214:SER:H	1.86	0.40
2:B:248:ASN:HD22	2:B:250:HIS:H	1.65	0.40
2:B:296:TYR:O	2:B:297:GLN:C	2.62	0.40
2:B:374:THR:O	2:B:375:ALA:C	2.64	0.40
3:C:101:ARG:C	3:C:101:ARG:CD	2.93	0.40
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.50	0.40
5:E:91:TRP:NE1	5:E:92:ARG:HG3	2.36	0.40
1:N:363:SER:HB3	2:O:112:LEU:HD21	2.04	0.40
1:N:403:ASP:O	1:N:404:ALA:C	2.63	0.40
2:O:183:ILE:HD12	2:O:183:ILE:HG23	1.90	0.40
2:O:426:ALA:O	2:O:427:SER:HB3	2.21	0.40
3:P:60:THR:N	3:P:176:LEU:HD23	2.37	0.40
4:Q:37:CYS:O	4:Q:39:ALA:N	2.54	0.40
4:Q:167:GLU:C	4:Q:169:LEU:N	2.76	0.40
6:S:90:LEU:O	6:S:91:GLU:C	2.63	0.40
8:U:67:HIS:O	8:U:70:ALA:HB3	2.21	0.40
1:A:102:LEU:C	1:A:104:LYS:N	2.78	0.40
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.51	0.40
1:A:257:VAL:HG23	1:A:320:PHE:HB3	2.03	0.40
1:A:269:VAL:HG11	1:A:410:VAL:CG2	2.51	0.40
2:B:248:ASN:ND2	2:B:428:GLY:CA	2.74	0.40
2:B:258:VAL:HG21	2:B:321:LEU:HD22	2.03	0.40
3:C:185:LEU:HD13	3:P:188:PHE:CZ	2.56	0.40
4:D:184:LYS:HG3	8:H:74:PHE:CE1	2.56	0.40
1:N:228:VAL:O	1:N:228:VAL:HG22	2.20	0.40
2:O:148:LYS:HG3	2:O:177:TYR:HB3	2.03	0.40
2:O:248:ASN:HD22	2:O:250:HIS:H	1.61	0.40
3:P:76:TYR:O	3:P:80:ILE:HG13	2.22	0.40
3:P:223:PRO:O	3:P:227:PHE:HB2	2.21	0.40
5:R:112:VAL:HG13	5:R:113:ASP:N	2.37	0.40
1:A:289:HIS:O	1:A:290:LEU:C	2.65	0.40
2:B:67:HIS:CD2	2:B:67:HIS:C	3.00	0.40
2:B:135:TRP:O	2:B:136:GLU:C	2.64	0.40
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.56	0.40
7:G:19:SER:HB3	7:G:22:GLU:HG2	2.04	0.40
1:N:106:MET:CE	1:N:110:VAL:CG2	3.00	0.40
2:O:130:PRO:CB	2:O:132:PHE:CE2	2.93	0.40
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.88	0.40
3:P:172:ASP:C	3:P:174:PRO:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:237:LEU:HD12	3:P:237:LEU:HA	1.89	0.40
5:R:77:LYS:HB2	5:R:80:ASP:OD2	2.22	0.40
8:U:72:LYS:O	8:U:73:LEU:C	2.65	0.40
1:A:273:ALA:C	1:A:275:ALA:N	2.79	0.40
2:B:97:SER:HB2	2:B:99:TYR:CE1	2.56	0.40
2:B:124:LEU:HD12	2:B:128:THR:CG2	2.50	0.40
2:B:181:TYR:CD1	2:B:181:TYR:C	2.99	0.40
2:B:205:ALA:CB	2:B:387:LEU:HD13	2.51	0.40
2:B:398:VAL:CG1	2:B:399:ALA:N	2.84	0.40
3:C:56:TYR:CZ	3:C:134:LEU:HB3	2.57	0.40
3:C:61:SER:OG	3:C:62:LEU:HD12	2.21	0.40
3:C:350:ILE:CG2	3:C:351:ILE:N	2.84	0.40
3:C:352:GLY:O	3:C:353:GLN:C	2.64	0.40
4:D:144:ARG:HB3	4:D:147:LEU:HD12	2.04	0.40
4:D:200:GLN:O	4:D:204:MET:HG3	2.22	0.40
5:E:74:ILE:O	5:E:194:VAL:HG13	2.22	0.40
5:E:126:ARG:HD3	5:E:168:SER:OG	2.22	0.40
1:N:343:MET:HE3	1:N:441:MET:HA	2.03	0.40
2:O:144:LEU:HB3	2:O:183:ILE:CD1	2.51	0.40
3:P:221:PHE:HE1	16:P:3002:UQ:C1	2.35	0.40
3:P:241:LEU:O	3:P:245:LEU:HB2	2.21	0.40
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.94	0.40
4:Q:100:ALA:O	4:Q:101:ALA:C	2.64	0.40
5:R:36:SER:HA	5:R:39:VAL:CG2	2.52	0.40
5:R:126:ARG:HH11	5:R:126:ARG:HG2	1.87	0.40
7:T:28:ASN:HB2	7:T:32:ASP:HB3	2.04	0.40
10:W:34:ALA:O	10:W:35:PHE:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	345 (78%)	75 (17%)	21 (5%)	2	16
1	N	440/446 (99%)	344 (78%)	75 (17%)	21 (5%)	2	16
2	B	419/441 (95%)	342 (82%)	62 (15%)	15 (4%)	2	21
2	O	420/441 (95%)	333 (79%)	67 (16%)	20 (5%)	2	16
3	C	378/380 (100%)	300 (79%)	62 (16%)	16 (4%)	2	18
3	P	377/380 (99%)	302 (80%)	60 (16%)	15 (4%)	2	19
4	D	239/241 (99%)	195 (82%)	35 (15%)	9 (4%)	2	20
4	Q	239/241 (99%)	190 (80%)	36 (15%)	13 (5%)	1	13
5	E	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	11
5	R	194/196 (99%)	146 (75%)	31 (16%)	17 (9%)	0	7
6	F	98/110 (89%)	73 (74%)	22 (22%)	3 (3%)	3	24
6	S	98/110 (89%)	74 (76%)	22 (22%)	2 (2%)	6	32
7	G	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	1	15
7	T	77/81 (95%)	61 (79%)	11 (14%)	5 (6%)	1	11
8	H	68/77 (88%)	49 (72%)	16 (24%)	3 (4%)	2	17
8	U	65/77 (84%)	42 (65%)	17 (26%)	6 (9%)	0	6
9	I	29/52 (56%)	14 (48%)	10 (34%)	5 (17%)	0	2
9	V	29/52 (56%)	18 (62%)	8 (28%)	3 (10%)	0	5
10	J	59/61 (97%)	42 (71%)	15 (25%)	2 (3%)	3	23
10	W	57/61 (93%)	42 (74%)	9 (16%)	6 (10%)	0	5
All	All	4000/4170 (96%)	3120 (78%)	681 (17%)	199 (5%)	1	15

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	159	GLN
2	B	26	ILE
2	B	38	LEU
2	B	171	ALA
2	B	226	ILE
3	C	217	ASP
4	D	38	SER
4	D	198	HIS
5	E	69	LEU
5	E	92	ARG

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Mol	Chain	Res	Type
5	E	177	PRO
7	G	7	LEU
9	I	56	SER
9	I	64	LEU
9	I	73	PRO
1	N	72	CYS
1	N	159	GLN
1	N	262	TRP
1	N	282	ARG
2	O	26	ILE
2	O	38	LEU
2	O	171	ALA
2	O	226	ILE
2	O	267	ALA
4	Q	198	HIS
5	R	69	LEU
5	R	92	ARG
5	R	188	VAL
7	T	7	LEU
8	U	49	HIS
8	U	51	GLU
9	V	56	SER
1	A	71	PRO
1	A	128	GLU
1	A	217	SER
1	A	262	TRP
1	A	282	ARG
2	B	20	GLY
2	B	64	GLY
2	B	231	GLY
2	B	427	SER
3	C	60	THR
3	C	213	SER
3	C	348	PHE
4	D	23	HIS
4	D	44	ASP
4	D	166	ASN
5	E	21	ALA
5	E	72	SER
5	E	113	ASP
5	E	137	GLY
5	E	141	HIS

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Mol	Chain	Res	Type
9	I	54	SER
1	N	20	ASP
1	N	128	GLU
1	N	207	GLU
1	N	217	SER
1	N	288	LYS
1	N	332	ASP
2	O	19	PRO
2	O	64	GLY
2	O	218	GLN
2	O	231	GLY
2	O	427	SER
3	P	60	THR
3	P	217	ASP
4	Q	2	GLU
4	Q	23	HIS
4	Q	38	SER
4	Q	44	ASP
4	Q	166	ASN
5	R	21	ALA
5	R	73	LYS
5	R	109	GLU
5	R	137	GLY
6	S	83	TYR
9	V	63	ASP
10	W	22	LEU
1	A	218	GLY
1	A	274	ASN
1	A	288	LYS
1	A	332	ASP
1	A	339	GLN
1	A	404	ALA
2	B	319	SER
3	C	3	PRO
3	C	29	SER
3	C	58	ALA
3	C	158	GLY
3	C	216	SER
5	E	71	LEU
6	F	52	LYS
7	G	33	ALA
7	G	50	PRO

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Mol	Chain	Res	Type
8	H	25	GLU
8	H	65	ARG
9	I	53	GLU
10	J	32	GLU
10	J	56	LYS
1	N	121	ALA
1	N	274	ASN
1	N	404	ALA
2	O	227	ARG
2	O	290	SER
3	P	108	TYR
3	P	156	TYR
3	P	216	SER
3	P	348	PHE
5	R	63	SER
6	S	52	LYS
10	W	32	GLU
1	A	20	ASP
1	A	121	ALA
1	A	388	ARG
2	B	290	SER
2	B	296	TYR
3	C	156	TYR
3	C	317	THR
5	E	4	ASP
6	F	83	TYR
8	H	16	PRO
1	N	71	PRO
1	N	107	PRO
1	N	388	ARG
1	N	428	ILE
2	O	230	ALA
2	O	270	ASN
2	O	296	TYR
3	P	3	PRO
3	P	29	SER
3	P	58	ALA
3	P	158	GLY
3	P	213	SER
3	P	379	ASN
4	Q	17	PRO
4	Q	75	ASP

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Mol	Chain	Res	Type
5	R	8	PRO
5	R	30	GLU
5	R	123	ASP
5	R	130	PRO
5	R	141	HIS
7	T	25	ALA
7	T	33	ALA
8	U	25	GLU
8	U	65	ARG
1	A	94	GLN
1	A	107	PRO
1	A	164	ALA
1	A	428	ILE
2	B	111	CYS
2	B	230	ALA
2	B	366	ALA
3	C	10	PRO
3	C	379	ASN
4	D	75	ASP
4	D	133	GLY
5	E	74	ILE
6	F	11	ARG
1	N	91	SER
1	N	94	GLN
1	N	122	LEU
2	O	319	SER
2	O	366	ALA
3	P	10	PRO
3	P	53	ALA
4	Q	176	PRO
5	R	90	LYS
7	T	50	PRO
7	T	75	ALA
8	U	16	PRO
8	U	47	ARG
10	W	14	PHE
10	W	33	ARG
1	A	81	SER
7	G	25	ALA
1	N	137	GLU
4	Q	133	GLY
5	R	108	GLN

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Mol	Chain	Res	Type
10	W	56	LYS
2	B	334	GLY
3	C	5	ILE
4	D	176	PRO
2	O	29	LEU
3	P	5	ILE
3	C	248	PRO
5	E	154	GLY
4	Q	52	ILE
4	Q	162	PRO
5	R	114	VAL
9	V	73	PRO
10	W	29	VAL
2	O	334	GLY
4	Q	53	GLY
3	C	93	ILE
4	D	17	PRO
5	E	8	PRO
2	O	249	GLY
5	R	154	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%)	335 (92%)	30 (8%)	10	35
1	N	365/368 (99%)	336 (92%)	29 (8%)	11	37
2	B	332/347 (96%)	310 (93%)	22 (7%)	15	42
2	O	333/347 (96%)	312 (94%)	21 (6%)	16	43
3	C	329/329 (100%)	303 (92%)	26 (8%)	11	37
3	P	328/329 (100%)	302 (92%)	26 (8%)	11	37
4	D	200/200 (100%)	188 (94%)	12 (6%)	17	44
4	Q	200/200 (100%)	188 (94%)	12 (6%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	166/166 (100%)	155 (93%)	11 (7%)	15	42
5	R	165/166 (99%)	154 (93%)	11 (7%)	15	41
6	F	92/96 (96%)	87 (95%)	5 (5%)	20	47
6	S	92/96 (96%)	87 (95%)	5 (5%)	20	47
7	G	71/71 (100%)	64 (90%)	7 (10%)	7	30
7	T	69/71 (97%)	63 (91%)	6 (9%)	9	33
8	H	65/71 (92%)	62 (95%)	3 (5%)	24	50
8	U	63/71 (89%)	59 (94%)	4 (6%)	16	43
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	33
9	V	23/26 (88%)	21 (91%)	2 (9%)	9	33
10	J	49/49 (100%)	46 (94%)	3 (6%)	17	44
10	W	47/49 (96%)	44 (94%)	3 (6%)	16	43
All	All	3377/3446 (98%)	3137 (93%)	240 (7%)	13	39

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	40	TRP
1	A	49	ASN
1	A	50	GLU
1	A	60	GLU
1	A	106	MET
1	A	108	LYS
1	A	163	LEU
1	A	171	THR
1	A	174	ILE
1	A	182	LEU
1	A	188	THR
1	A	223	TYR
1	A	228	VAL
1	A	230	ILE
1	A	233	ARG
1	A	257	VAL
1	A	274	ASN
1	A	281	ASP
1	A	309	THR
1	A	342	TRP

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Mol	Chain	Res	Type
1	A	362	ARG
1	A	365	MET
1	A	366	VAL
1	A	392	LEU
1	A	395	TRP
1	A	405	ARG
1	A	406	MET
1	A	431	LEU
1	A	432	LEU
2	B	22	GLU
2	B	31	ASN
2	B	45	SER
2	B	47	ILE
2	B	50	PHE
2	B	97	SER
2	B	106	THR
2	B	109	VAL
2	B	139	ASP
2	B	154	SER
2	B	160	LEU
2	B	181	TYR
2	B	212	LYS
2	B	248	ASN
2	B	260	GLU
2	B	304	THR
2	B	314	VAL
2	B	328	SER
2	B	341	MET
2	B	367	THR
2	B	403	ASP
2	B	437	ASP
3	C	36	SER
3	C	44	THR
3	C	52	LEU
3	C	82	ASN
3	C	118	VAL
3	C	120	LEU
3	C	138	GLN
3	C	149	ASN
3	C	182	LEU
3	C	194	THR
3	C	199	THR

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Mol	Chain	Res	Type
3	C	208	ASN
3	C	216	SER
3	C	231	LEU
3	C	241	LEU
3	C	258	THR
3	C	272	GLU
3	C	300	LEU
3	C	304	LEU
3	C	317	THR
3	C	324	THR
3	C	334	LEU
3	C	344	VAL
3	C	349	ILE
3	C	357	LEU
3	C	373	LEU
4	D	2	GLU
4	D	3	LEU
4	D	42	SER
4	D	54	VAL
4	D	70	VAL
4	D	76	GLU
4	D	87	ILE
4	D	117	VAL
4	D	141	VAL
4	D	145	GLU
4	D	169	LEU
4	D	188	THR
5	E	23	THR
5	E	39	VAL
5	E	61	SER
5	E	73	LYS
5	E	80	ASP
5	E	125	ASP
5	E	130	PRO
5	E	135	LEU
5	E	136	VAL
5	E	145	VAL
5	E	177	PRO
6	F	27	ASN
6	F	59	MET
6	F	70	LEU
6	F	84	GLU

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Mol	Chain	Res	Type
6	F	89	TYR
7	G	4	PHE
7	G	16	TYR
7	G	17	SER
7	G	27	PRO
7	G	34	LEU
7	G	41	PHE
7	G	63	THR
8	H	19	THR
8	H	71	HIS
8	H	73	LEU
9	I	68	ILE
9	I	70	LEU
10	J	18	SER
10	J	46	LEU
10	J	59	TYR
1	N	3	THR
1	N	32	GLN
1	N	40	TRP
1	N	49	ASN
1	N	50	GLU
1	N	106	MET
1	N	108	LYS
1	N	163	LEU
1	N	171	THR
1	N	174	ILE
1	N	182	LEU
1	N	188	THR
1	N	223	TYR
1	N	228	VAL
1	N	257	VAL
1	N	274	ASN
1	N	281	ASP
1	N	309	THR
1	N	342	TRP
1	N	362	ARG
1	N	365	MET
1	N	366	VAL
1	N	370	ASP
1	N	392	LEU
1	N	395	TRP
1	N	405	ARG

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Mol	Chain	Res	Type
1	N	406	MET
1	N	431	LEU
1	N	432	LEU
2	O	31	ASN
2	O	45	SER
2	O	57	TYR
2	O	97	SER
2	O	105	MET
2	O	106	THR
2	O	109	VAL
2	O	139	ASP
2	O	140	LEU
2	O	154	SER
2	O	160	LEU
2	O	181	TYR
2	O	214	SER
2	O	248	ASN
2	O	304	THR
2	O	314	VAL
2	O	328	SER
2	O	341	MET
2	O	367	THR
2	O	403	ASP
2	O	437	ASP
3	P	36	SER
3	P	44	THR
3	P	52	LEU
3	P	118	VAL
3	P	120	LEU
3	P	138	GLN
3	P	149	ASN
3	P	161	LEU
3	P	173	ASN
3	P	182	LEU
3	P	194	THR
3	P	199	THR
3	P	208	ASN
3	P	216	SER
3	P	231	LEU
3	P	258	THR
3	P	272	GLU
3	P	300	LEU

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Mol	Chain	Res	Type
3	P	304	LEU
3	P	317	THR
3	P	324	THR
3	P	334	LEU
3	P	337	THR
3	P	344	VAL
3	P	357	LEU
3	P	373	LEU
4	Q	3	LEU
4	Q	42	SER
4	Q	54	VAL
4	Q	70	VAL
4	Q	87	ILE
4	Q	117	VAL
4	Q	124	GLU
4	Q	141	VAL
4	Q	145	GLU
4	Q	169	LEU
4	Q	188	THR
4	Q	241	LYS
5	R	23	THR
5	R	39	VAL
5	R	61	SER
5	R	102	THR
5	R	112	VAL
5	R	131	GLU
5	R	135	LEU
5	R	136	VAL
5	R	145	VAL
5	R	184	THR
5	R	185	TYR
6	S	27	ASN
6	S	70	LEU
6	S	79	GLN
6	S	84	GLU
6	S	89	TYR
7	T	4	PHE
7	T	16	TYR
7	T	17	SER
7	T	34	LEU
7	T	41	PHE
7	T	63	THR

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Mol	Chain	Res	Type
8	U	13	LEU
8	U	19	THR
8	U	48	SER
8	U	73	LEU
9	V	68	ILE
9	V	70	LEU
10	W	18	SER
10	W	46	LEU
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	49	ASN
1	A	159	GLN
1	A	274	ASN
1	A	289	HIS
1	A	305	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	125	ASN
2	B	156	GLN
2	B	248	ASN
2	B	270	ASN
2	B	313	ASN
2	B	315	ASN
2	B	329	GLN
2	B	363	GLN
3	C	17	ASN
3	C	55	HIS
3	C	82	ASN
3	C	86	ASN
3	C	115	ASN
3	C	149	ASN
3	C	207	ASN
3	C	342	GLN
3	C	379	ASN
4	D	50	ASN
4	D	105	ASN
4	D	200	GLN

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Mol	Chain	Res	Type
5	E	53	ASN
5	E	57	GLN
5	E	103	GLN
5	E	122	HIS
5	E	164	HIS
6	F	79	GLN
6	F	108	ASN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	136	GLN
1	N	143	ASN
1	N	159	GLN
1	N	176	HIS
1	N	274	ASN
1	N	289	HIS
1	N	305	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	125	ASN
2	O	248	ASN
2	O	276	GLN
2	O	313	ASN
2	O	315	ASN
2	O	329	GLN
2	O	363	GLN
3	P	17	ASN
3	P	55	HIS
3	P	75	GLN
3	P	82	ASN
3	P	86	ASN
3	P	149	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	31	GLN

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Mol	Chain	Res	Type
4	Q	50	ASN
4	Q	105	ASN
5	R	53	ASN
5	R	57	GLN
5	R	164	HIS
6	S	72	HIS
6	S	79	GLN
6	S	108	ASN
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are unknown - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	PEE	P	3007	-	48,48,50	1.43	6 (12%)	51,53,55	0.81	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BOG	E	2009	-	20,20,20	1.14	2 (10%)	25,25,25	0.93	2 (8%)
15	ICX	C	2001	-	31,31,31	1.41	7 (22%)	38,39,39	1.03	2 (5%)
11	PEE	P	3008	-	4,4,50	3.55	4 (100%)	6,6,55	0.60	0
18	CDL	G	2004	-	39,39,99	1.30	4 (10%)	45,51,111	1.10	3 (6%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
19	FES	R	501	5	0,4,4	-	-	-	-	-
13	AZI	P	3011	-	2,2,2	2.42	2 (100%)	0,1,1	-	-
16	UQ	P	3002	-	19,19,63	2.52	10 (52%)	24,26,79	1.28	2 (8%)
12	BOG	Q	3091	-	20,20,20	1.14	2 (10%)	25,25,25	0.96	1 (4%)
14	HEM	P	501	3	50,50,50	1.72	9 (18%)	67,82,82	1.85	19 (28%)
13	AZI	C	2011	-	2,2,2	2.50	2 (100%)	0,1,1	-	-
17	HEC	D	501	4	50,50,50	1.51	9 (18%)	68,82,82	2.11	20 (29%)
12	BOG	D	2091	-	20,20,20	1.11	2 (10%)	25,25,25	0.97	1 (4%)
14	HEM	C	501	3	50,50,50	2.06	14 (28%)	67,82,82	2.13	20 (29%)
17	HEC	Q	501	4	50,50,50	1.40	7 (14%)	68,82,82	1.96	16 (23%)
12	BOG	C	3010	-	11,11,20	1.04	2 (18%)	10,11,25	0.95	1 (10%)
18	CDL	D	2003	-	41,41,99	1.19	1 (2%)	47,53,111	1.08	2 (4%)
18	CDL	P	3003	-	41,41,99	1.18	2 (4%)	47,53,111	1.10	2 (4%)
11	PEE	W	3005	-	49,49,50	1.58	10 (20%)	52,54,55	0.87	3 (5%)
14	HEM	P	502	3	50,50,50	1.64	10 (20%)	67,82,82	1.44	7 (10%)
11	PEE	A	2008	-	20,20,50	1.81	5 (25%)	23,25,55	0.76	1 (4%)
12	BOG	P	2010	-	18,18,20	1.11	3 (16%)	22,22,25	0.56	0
14	HEM	C	502	3	50,50,50	1.83	12 (24%)	67,82,82	1.78	16 (23%)
18	CDL	P	3004	-	39,39,99	1.25	3 (7%)	45,51,111	1.10	3 (6%)
11	PEE	C	2007	-	48,48,50	1.41	7 (14%)	51,53,55	0.81	3 (5%)
12	BOG	Q	3009	-	20,20,20	1.20	3 (15%)	25,25,25	1.14	1 (4%)
15	ICX	P	3001	-	31,31,31	1.48	7 (22%)	38,39,39	0.93	1 (2%)
16	UQ	C	2002	-	19,19,63	2.46	9 (47%)	24,26,79	1.26	2 (8%)
11	PEE	C	2005	-	49,49,50	1.51	10 (20%)	52,54,55	0.86	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEE	P	3007	-	-	25/52/52/54	-
12	BOG	E	2009	-	-	6/11/31/31	0/1/1/1
15	ICX	C	2001	-	-	2/24/24/24	0/2/2/2
18	CDL	G	2004	-	-	21/49/49/110	-
19	FES	E	501	5	-	-	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
16	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
12	BOG	Q	3091	-	-	6/11/31/31	0/1/1/1
14	HEM	P	501	3	-	6/14/54/54	-
17	HEC	D	501	4	1/1/3/7	6/14/54/54	-
12	BOG	D	2091	-	-	4/11/31/31	0/1/1/1
14	HEM	C	501	3	-	8/14/54/54	-
17	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
12	BOG	C	3010	-	-	5/9/9/31	-
18	CDL	D	2003	-	-	21/51/51/110	-
18	CDL	P	3003	-	-	21/51/51/110	-
11	PEE	W	3005	-	-	27/53/53/54	-
14	HEM	P	502	3	-	8/14/54/54	-
11	PEE	A	2008	-	-	12/24/24/54	-
12	BOG	P	2010	-	-	2/6/26/31	0/1/1/1
14	HEM	C	502	3	-	8/14/54/54	-
18	CDL	P	3004	-	-	21/49/49/110	-
11	PEE	C	2007	-	-	24/52/52/54	-
12	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
15	ICX	P	3001	-	-	2/24/24/24	0/2/2/2
16	UQ	C	2002	-	-	2/11/35/87	0/1/1/1
11	PEE	C	2005	-	-	26/53/53/54	-

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	3002	UQ	C7-C6	5.29	1.61	1.51
14	P	502	HEM	CBC-CAC	5.06	1.54	1.30
16	P	3002	UQ	C6-C5	4.92	1.44	1.35
14	C	501	HEM	CBC-CAC	4.92	1.54	1.30
11	P	3008	PEE	P-O1P	4.86	1.61	1.50
14	P	501	HEM	CBC-CAC	4.86	1.53	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	502	HEM	CBC-CAC	4.81	1.53	1.30
14	P	501	HEM	CBB-CAB	4.71	1.53	1.30
16	C	2002	UQ	C7-C6	4.65	1.60	1.51
16	C	2002	UQ	C6-C5	4.58	1.43	1.35
14	C	501	HEM	CAB-C3B	-4.37	1.35	1.47
11	C	2007	PEE	C39-C38	4.31	1.56	1.31
11	C	2005	PEE	C39-C38	4.22	1.55	1.31
14	C	501	HEM	CBB-CAB	4.22	1.50	1.30
14	C	501	HEM	C4C-NC	-4.20	1.31	1.39
14	P	501	HEM	CAB-C3B	-4.19	1.36	1.47
14	C	502	HEM	CAC-C3C	-4.17	1.36	1.47
11	P	3007	PEE	C39-C38	4.14	1.55	1.31
11	W	3005	PEE	C39-C38	4.09	1.54	1.31
14	C	502	HEM	C2A-C3A	-4.03	1.28	1.38
14	C	502	HEM	CAB-C3B	-4.02	1.36	1.47
14	C	501	HEM	CAC-C3C	-3.94	1.36	1.47
14	P	501	HEM	CAC-C3C	-3.82	1.37	1.47
11	W	3005	PEE	O3-C30	3.77	1.44	1.33
14	P	502	HEM	CAB-C3B	-3.76	1.37	1.47
16	C	2002	UQ	C6-C1	3.76	1.57	1.46
16	P	3002	UQ	C6-C1	3.75	1.57	1.46
14	C	502	HEM	C1B-C2B	3.74	1.52	1.44
14	C	501	HEM	C1B-C2B	3.70	1.52	1.44
14	C	501	HEM	CHD-C4C	-3.64	1.31	1.38
11	W	3005	PEE	O2-C10	3.59	1.44	1.34
11	C	2005	PEE	O3-C30	3.53	1.43	1.33
14	P	502	HEM	CBB-CAB	3.52	1.47	1.30
17	Q	501	HEC	C3B-C2B	-3.48	1.29	1.36
11	P	3008	PEE	P-O4P	3.43	1.64	1.54
11	C	2005	PEE	C21-C22	-3.39	1.34	1.51
11	W	3005	PEE	C21-C22	-3.38	1.35	1.51
11	P	3007	PEE	O2-C10	3.32	1.43	1.34
15	P	3001	ICX	C12-C11	3.31	1.44	1.39
11	C	2007	PEE	C21-C22	-3.30	1.35	1.51
17	D	501	HEC	CHC-C4B	-3.28	1.31	1.38
17	Q	501	HEC	C1D-ND	-3.28	1.34	1.40
11	A	2008	PEE	P-O1P	3.27	1.62	1.50
11	C	2005	PEE	O2-C10	3.26	1.43	1.34
17	D	501	HEC	C3B-C2B	-3.24	1.29	1.36
11	P	3007	PEE	C21-C22	-3.24	1.35	1.51
11	A	2008	PEE	O2-C10	3.22	1.43	1.34
11	W	3005	PEE	P-O1P	3.21	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	2002	UQ	O3-C3	3.19	1.44	1.36
14	C	502	HEM	CBB-CAB	3.18	1.45	1.30
17	D	501	HEC	C2A-C3A	-3.18	1.29	1.36
11	C	2005	PEE	P-O1P	3.14	1.61	1.50
11	P	3008	PEE	P-O3P	3.07	1.63	1.54
14	C	501	HEM	C3D-C2D	-3.06	1.30	1.36
11	A	2008	PEE	O3-C30	3.04	1.42	1.33
11	P	3007	PEE	P-O1P	3.00	1.61	1.50
11	P	3007	PEE	O3-C30	2.99	1.42	1.33
15	P	3001	ICX	C13-C12	2.99	1.43	1.38
14	P	501	HEM	C1B-C2B	2.97	1.50	1.44
14	C	501	HEM	C1D-ND	-2.90	1.33	1.38
16	C	2002	UQ	C5-C4	2.89	1.57	1.47
16	P	3002	UQ	CM5-C5	2.87	1.56	1.50
16	C	2002	UQ	CM5-C5	2.87	1.56	1.50
15	P	3001	ICX	C10-C9	2.87	1.43	1.38
13	C	2011	AZI	N1-N2	-2.85	1.17	1.23
11	C	2007	PEE	O2-C10	2.85	1.42	1.34
16	P	3002	UQ	O3-C3	2.83	1.43	1.36
11	C	2007	PEE	P-O1P	2.81	1.60	1.50
14	P	501	HEM	C3B-C2B	-2.79	1.31	1.37
13	P	3011	AZI	N1-N2	-2.78	1.17	1.23
16	C	2002	UQ	O2-C2	2.72	1.43	1.36
14	C	502	HEM	C3C-C2C	-2.68	1.31	1.37
15	C	2001	ICX	C12-C11	2.68	1.43	1.39
15	C	2001	ICX	C13-C12	2.67	1.43	1.38
12	E	2009	BOG	O5-C1	2.67	1.48	1.41
16	P	3002	UQ	C5-C4	2.67	1.56	1.47
16	C	2002	UQ	C2-C1	2.62	1.56	1.48
11	W	3005	PEE	C11-C10	2.61	1.58	1.50
17	D	501	HEC	FE-NB	2.59	2.02	1.94
16	C	2002	UQ	C3-C4	2.59	1.56	1.48
14	C	502	HEM	C4C-NC	-2.58	1.34	1.39
15	C	2001	ICX	C10-C9	2.57	1.43	1.38
14	P	502	HEM	CAC-C3C	-2.56	1.40	1.47
11	C	2007	PEE	O3-C30	2.55	1.40	1.33
12	Q	3091	BOG	O5-C1	2.54	1.48	1.41
12	Q	3009	BOG	O5-C1	2.53	1.48	1.41
12	D	2091	BOG	O5-C1	2.52	1.48	1.41
17	Q	501	HEC	FE-NC	-2.51	1.86	1.95
12	C	3010	BOG	C2-C1	2.49	1.57	1.50
17	D	501	HEC	C4A-NA	-2.49	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2001	ICX	C10-C11	2.49	1.43	1.39
18	D	2003	CDL	O1-C1	2.48	1.50	1.43
14	P	502	HEM	CMC-C2C	2.46	1.55	1.50
15	P	3001	ICX	C9-C8	2.45	1.43	1.38
11	C	2005	PEE	C31-C30	2.43	1.57	1.50
17	Q	501	HEC	CHA-C4D	-2.42	1.33	1.39
16	P	3002	UQ	O2-C2	2.41	1.42	1.36
17	Q	501	HEC	C4C-NC	-2.41	1.35	1.39
11	W	3005	PEE	C3-C2	2.40	1.58	1.50
14	P	502	HEM	C1B-C2B	2.40	1.49	1.44
12	P	2010	BOG	C4-C5	2.39	1.58	1.53
11	W	3005	PEE	C31-C30	2.39	1.57	1.50
18	G	2004	CDL	O1-C1	2.39	1.50	1.43
14	P	501	HEM	C3D-C2D	-2.39	1.31	1.36
14	P	502	HEM	C2A-C3A	-2.38	1.32	1.38
15	P	3001	ICX	C1-C2	2.37	1.42	1.38
18	P	3003	CDL	O1-C1	2.37	1.50	1.43
11	P	3008	PEE	P-O2P	2.35	1.61	1.54
16	P	3002	UQ	C2-C1	2.35	1.55	1.48
11	A	2008	PEE	C3-C2	2.35	1.58	1.50
14	C	501	HEM	CMA-C3A	2.35	1.55	1.50
14	C	502	HEM	C4A-NA	-2.35	1.35	1.39
17	D	501	HEC	C1D-C2D	2.34	1.49	1.44
18	P	3004	CDL	CA3-CA4	2.33	1.58	1.50
11	A	2008	PEE	C1-C2	2.32	1.58	1.50
16	P	3002	UQ	C7-C8	2.32	1.54	1.50
12	D	2091	BOG	C4-C5	2.31	1.58	1.53
18	P	3004	CDL	O1-C1	2.31	1.50	1.43
16	P	3002	UQ	C3-C4	2.29	1.55	1.48
14	C	501	HEM	C2A-C3A	-2.29	1.32	1.38
18	G	2004	CDL	CA3-CA4	2.26	1.57	1.50
14	C	501	HEM	FE-ND	-2.26	1.88	1.94
17	D	501	HEC	C4C-C3C	2.24	1.49	1.44
12	Q	3091	BOG	C4-C5	2.24	1.57	1.53
11	C	2007	PEE	C3-C2	2.24	1.57	1.50
12	Q	3009	BOG	C4-C5	2.23	1.57	1.53
11	C	2005	PEE	P-O4P	2.22	1.68	1.59
12	P	2010	BOG	C1-C2	2.21	1.57	1.52
15	P	3001	ICX	C10-C11	2.20	1.42	1.39
12	E	2009	BOG	O5-C5	2.20	1.49	1.44
11	W	3005	PEE	C1-C2	2.20	1.57	1.50
14	P	501	HEM	C4A-C3A	2.20	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	2005	PEE	C1-C2	2.19	1.57	1.50
14	C	502	HEM	C1C-NC	-2.18	1.35	1.39
11	C	2005	PEE	C11-C10	2.17	1.57	1.50
17	D	501	HEC	C1D-ND	-2.15	1.36	1.40
12	C	3010	BOG	O5-C1	2.15	1.45	1.40
11	W	3005	PEE	O2-C2	2.14	1.51	1.46
14	P	502	HEM	CHC-C1C	-2.14	1.34	1.38
17	D	501	HEC	CHA-C1A	-2.14	1.34	1.38
14	C	501	HEM	FE-NC	-2.13	1.88	1.95
11	C	2007	PEE	C11-C10	2.13	1.56	1.50
17	Q	501	HEC	FE-NA	2.12	2.02	1.95
12	Q	3009	BOG	C1-C2	2.11	1.58	1.52
15	C	2001	ICX	C9-C8	2.11	1.43	1.38
14	P	502	HEM	C1A-NA	-2.11	1.35	1.39
15	P	3001	ICX	C13-C8	2.10	1.43	1.38
14	P	502	HEM	CMB-C2B	2.10	1.55	1.50
13	C	2011	AZI	N3-N2	-2.09	1.18	1.23
11	P	3007	PEE	C31-C30	2.08	1.56	1.50
11	C	2005	PEE	C3-C2	2.08	1.57	1.50
15	C	2001	ICX	C1-C2	2.07	1.42	1.38
18	P	3003	CDL	CA3-CA4	2.07	1.57	1.50
12	P	2010	BOG	O5-C1	2.07	1.47	1.42
17	Q	501	HEC	C4B-NB	-2.07	1.36	1.40
18	G	2004	CDL	OA6-CA5	2.06	1.40	1.34
18	G	2004	CDL	C51-CB5	2.04	1.56	1.50
14	C	501	HEM	CMD-C2D	2.03	1.54	1.50
15	C	2001	ICX	C1-C6	2.03	1.43	1.38
14	P	501	HEM	C4D-C3D	-2.03	1.41	1.45
14	C	502	HEM	FE-NA	2.02	2.01	1.95
18	P	3004	CDL	OB8-CB7	2.02	1.39	1.33
13	P	3011	AZI	N3-N2	-2.01	1.19	1.23
14	C	502	HEM	C3D-C2D	-2.01	1.32	1.36

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	501	HEC	CAC-C3C-C4C	-6.13	116.48	124.91
14	P	501	HEM	CMB-C2B-C1B	5.94	134.31	125.03
17	D	501	HEC	CBC-CAC-C3C	-5.60	97.23	112.42
14	C	501	HEM	CMB-C2B-C1B	5.55	133.71	125.03
14	C	501	HEM	C3B-C4B-NB	5.52	113.44	109.47
17	D	501	HEC	CAC-C3C-C4C	-5.35	117.56	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	502	HEM	C3B-C4B-NB	5.13	113.16	109.47
17	Q	501	HEC	CBC-CAC-C3C	-5.01	98.84	112.42
14	C	502	HEM	C3B-C4B-NB	4.94	113.02	109.47
14	C	501	HEM	CMD-C2D-C1D	4.88	132.65	125.03
12	Q	3009	BOG	C1'-O1-C1	4.85	121.96	113.68
14	C	501	HEM	CAD-C3D-C4D	4.79	133.04	124.70
14	C	502	HEM	CAD-C3D-C4D	4.64	132.78	124.70
14	C	502	HEM	C3B-C2B-C1B	-4.51	103.03	106.41
14	P	501	HEM	CBA-CAA-C2A	-4.34	100.53	112.53
17	D	501	HEC	CAA-C2A-C1A	4.28	133.56	124.85
16	P	3002	UQ	C8-C7-C6	4.26	122.57	112.08
14	P	501	HEM	C3B-C2B-C1B	-4.25	103.22	106.41
17	Q	501	HEC	CAC-C3C-C2C	4.19	133.52	126.89
16	C	2002	UQ	C8-C7-C6	4.16	122.33	112.08
14	C	501	HEM	CBA-CAA-C2A	-4.13	101.11	112.53
14	C	502	HEM	C1D-C2D-C3D	4.13	111.32	106.98
17	D	501	HEC	CAA-C2A-C3A	-4.08	120.22	127.87
12	D	2091	BOG	C1'-O1-C1	4.02	120.54	113.68
15	C	2001	ICX	C30-C31-N33	-3.98	109.09	116.34
14	C	501	HEM	C3C-C2C-C1C	-3.96	103.30	107.05
17	Q	501	HEC	CAA-C2A-C1A	3.90	132.78	124.85
17	D	501	HEC	CMC-C2C-C1C	3.84	131.27	125.42
12	Q	3091	BOG	C1'-O1-C1	3.82	120.20	113.68
17	D	501	HEC	CMA-C3A-C4A	3.79	131.40	124.73
14	C	501	HEM	CAD-C3D-C2D	-3.74	120.86	127.87
17	D	501	HEC	CMD-C2D-C1D	3.73	130.86	125.03
17	D	501	HEC	C3D-C4D-ND	3.71	113.94	110.35
17	Q	501	HEC	C3D-C4D-ND	3.58	113.81	110.35
17	D	501	HEC	CBA-CAA-C2A	3.52	122.28	112.53
14	P	502	HEM	CAD-C3D-C4D	3.47	130.74	124.70
12	E	2009	BOG	C1'-O1-C1	3.45	119.58	113.68
14	C	501	HEM	CBB-CAB-C3B	-3.43	110.39	127.53
14	P	501	HEM	C3B-C4B-NB	3.43	111.93	109.47
14	P	502	HEM	C3B-C2B-C1B	-3.43	103.84	106.41
17	D	501	HEC	CAC-C3C-C2C	3.41	132.29	126.89
15	P	3001	ICX	C30-C31-N33	-3.36	110.21	116.34
14	P	502	HEM	CAD-C3D-C2D	-3.31	121.67	127.87
17	Q	501	HEC	CAA-C2A-C3A	-3.31	121.67	127.87
14	P	501	HEM	CMD-C2D-C1D	3.29	130.18	125.03
14	C	501	HEM	C1B-NB-C4B	-3.29	101.31	105.21
16	P	3002	UQ	C7-C6-C1	-3.29	114.70	118.52
17	Q	501	HEC	CBA-CAA-C2A	3.27	121.58	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	2002	UQ	C7-C6-C1	-3.25	114.74	118.52
18	P	3004	CDL	CB4-OB6-CB5	-3.20	110.13	117.80
17	D	501	HEC	C4B-NB-C1B	-3.20	101.42	105.21
18	G	2004	CDL	CB4-OB6-CB5	-3.13	110.32	117.80
14	C	501	HEM	CMB-C2B-C3B	-3.11	120.90	128.43
17	D	501	HEC	C3B-C4B-NB	3.11	113.58	110.17
17	D	501	HEC	CMB-C2B-C1B	3.08	129.84	125.03
14	C	502	HEM	C4A-NA-C1A	-3.06	100.83	105.82
14	P	501	HEM	CAD-C3D-C4D	3.05	130.00	124.70
17	D	501	HEC	CHC-C4B-NB	-3.04	120.61	124.37
14	P	501	HEM	C1B-NB-C4B	-2.93	101.73	105.21
14	C	501	HEM	C2A-C1A-NA	2.91	113.38	110.15
17	Q	501	HEC	CAD-C3D-C4D	2.87	129.69	124.70
14	C	502	HEM	C4D-C3D-C2D	-2.84	102.76	106.89
17	Q	501	HEC	CMD-C2D-C1D	2.83	129.46	125.03
11	P	3007	PEE	C22-C21-C20	2.81	127.36	113.86
14	P	501	HEM	CBC-CAC-C3C	-2.80	113.55	127.53
14	C	502	HEM	CMB-C2B-C1B	2.77	129.37	125.03
14	C	501	HEM	CBC-CAC-C3C	-2.77	113.69	127.53
14	P	501	HEM	CAD-C3D-C2D	-2.76	122.70	127.87
11	W	3005	PEE	C22-C21-C20	2.75	127.07	113.86
17	Q	501	HEC	CHD-C1D-ND	-2.74	120.97	124.37
17	D	501	HEC	C1C-C2C-C3C	-2.72	103.70	106.82
11	C	2005	PEE	C22-C21-C20	2.71	126.89	113.86
14	C	502	HEM	C3C-C2C-C1C	-2.70	104.49	107.05
11	C	2007	PEE	C22-C21-C20	2.67	126.70	113.86
17	Q	501	HEC	CMC-C2C-C1C	2.67	129.48	125.42
14	P	501	HEM	C2B-C1B-NB	2.65	112.89	109.84
17	Q	501	HEC	CHA-C4D-C3D	-2.64	120.92	124.77
17	Q	501	HEC	CMB-C2B-C1B	2.63	129.14	125.03
17	D	501	HEC	CAD-C3D-C4D	2.62	129.27	124.70
17	Q	501	HEC	CMA-C3A-C4A	2.61	129.33	124.73
14	C	501	HEM	CHD-C4C-NC	-2.60	121.62	124.45
14	C	501	HEM	CHC-C4B-NB	-2.60	121.63	124.42
18	D	2003	CDL	CB4-OB6-CB5	-2.59	111.60	117.80
17	Q	501	HEC	C1C-C2C-C3C	-2.58	103.86	106.82
14	C	502	HEM	CMA-C3A-C4A	2.58	129.34	125.42
14	C	501	HEM	CHC-C1C-C2C	-2.56	120.17	125.49
14	P	501	HEM	CMB-C2B-C3B	-2.51	122.36	128.43
11	P	3007	PEE	C21-C22-C23	2.50	126.99	114.37
17	Q	501	HEC	C1B-C2B-C3B	2.50	109.61	106.98
18	P	3003	CDL	CB4-OB6-CB5	-2.49	111.83	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	502	HEM	CHC-C1C-C2C	-2.49	120.31	125.49
11	C	2007	PEE	C21-C22-C23	2.49	126.95	114.37
14	C	502	HEM	C1B-NB-C4B	-2.43	102.33	105.21
11	W	3005	PEE	O3-C3-C2	2.43	115.39	108.40
14	C	502	HEM	C2C-C1C-NC	2.40	114.08	109.64
11	W	3005	PEE	C21-C22-C23	2.40	126.50	114.37
14	P	502	HEM	CHC-C1C-C2C	-2.39	120.52	125.49
14	C	502	HEM	C2A-C1A-NA	2.39	112.80	110.15
14	P	501	HEM	CBB-CAB-C3B	-2.38	115.61	127.53
11	C	2005	PEE	O3-C3-C2	2.38	115.25	108.40
11	C	2005	PEE	C21-C22-C23	2.37	126.37	114.37
18	D	2003	CDL	CA6-CA4-CA3	-2.35	106.30	111.78
11	C	2007	PEE	O3-C3-C2	2.33	115.10	108.40
14	C	501	HEM	CHB-C1B-NB	-2.33	121.49	124.37
14	C	501	HEM	C2C-C1C-NC	2.30	113.89	109.64
18	G	2004	CDL	CA4-OA6-CA5	-2.28	112.33	117.80
17	D	501	HEC	C4D-C3D-C2D	-2.28	103.58	106.89
18	P	3003	CDL	CA6-CA4-CA3	-2.27	106.48	111.78
14	C	502	HEM	C4C-NC-C1C	-2.25	102.15	105.82
17	D	501	HEC	C2A-C1A-NA	2.25	112.49	110.32
14	P	501	HEM	CHB-C1B-NB	-2.25	121.59	124.37
14	C	502	HEM	C2B-C1B-NB	2.24	112.42	109.84
12	C	3010	BOG	C1'-O1-C1	2.23	118.65	113.81
14	P	502	HEM	C3C-C2C-C1C	-2.23	104.93	107.05
14	P	501	HEM	C4A-C3A-C2A	-2.23	104.26	106.82
17	D	501	HEC	CHA-C4D-C3D	-2.23	121.53	124.77
14	P	501	HEM	C4D-ND-C1D	-2.23	102.57	105.21
14	P	501	HEM	CHC-C4B-NB	-2.18	122.07	124.42
17	D	501	HEC	CHB-C1B-NB	-2.18	122.08	124.42
14	C	501	HEM	C3D-C4D-ND	2.18	112.56	110.17
14	P	502	HEM	C2C-C1C-NC	2.17	113.66	109.64
18	P	3004	CDL	CA4-OA6-CA5	-2.17	112.60	117.80
14	C	502	HEM	CBA-CAA-C2A	2.14	118.45	112.53
11	A	2008	PEE	O3-C3-C2	2.13	114.55	108.40
14	P	501	HEM	CAB-C3B-C2B	-2.13	121.51	128.43
14	C	501	HEM	C4A-NA-C1A	-2.13	102.36	105.82
18	G	2004	CDL	OB6-CB4-CB3	2.12	115.93	108.34
15	C	2001	ICX	O32-C31-C30	2.08	125.78	122.02
18	P	3004	CDL	OB6-CB4-CB3	2.07	115.75	108.34
14	P	501	HEM	CMA-C3A-C4A	2.04	128.53	125.42
14	P	501	HEM	C4B-C3B-C2B	2.02	109.14	107.28
14	C	501	HEM	CMD-C2D-C3D	-2.01	120.71	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	2009	BOG	O1-C1-C2	2.00	111.32	108.27

All (2) chirality outliers are listed below:

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

All (277) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C1-O3P-P-O2P
11	A	2008	PEE	C1-O3P-P-O1P
11	A	2008	PEE	C1-O3P-P-O4P
11	A	2008	PEE	C4-O4P-P-O3P
11	A	2008	PEE	C4-O4P-P-O2P
11	C	2005	PEE	C11-C10-O2-C2
11	C	2005	PEE	C1-O3P-P-O2P
11	C	2005	PEE	C1-O3P-P-O1P
11	C	2005	PEE	C1-O3P-P-O4P
11	C	2005	PEE	C4-O4P-P-O3P
11	C	2005	PEE	C4-O4P-P-O2P
11	C	2005	PEE	C4-O4P-P-O1P
11	C	2007	PEE	C17-C18-C19-C20
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	P	3007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C4-O4P-P-O3P
11	P	3007	PEE	C4-O4P-P-O2P
11	P	3007	PEE	C4-O4P-P-O1P
11	W	3005	PEE	C11-C10-O2-C2
11	W	3005	PEE	C1-O3P-P-O2P
11	W	3005	PEE	C1-O3P-P-O1P
11	W	3005	PEE	C1-O3P-P-O4P
11	W	3005	PEE	C4-O4P-P-O3P
11	W	3005	PEE	C4-O4P-P-O2P
11	W	3005	PEE	C4-O4P-P-O1P
14	C	501	HEM	C2B-C3B-CAB-CBB
14	C	502	HEM	C2C-C3C-CAC-CBC
14	P	501	HEM	C2B-C3B-CAB-CBB
14	P	501	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	C	2002	UQ	C1-C6-C7-C8
16	C	2002	UQ	C5-C6-C7-C8
16	P	3002	UQ	C1-C6-C7-C8
16	P	3002	UQ	C5-C6-C7-C8
17	D	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
18	D	2003	CDL	O1-C1-CB2-OB2
18	D	2003	CDL	CA2-OA2-PA1-OA5
18	D	2003	CDL	CB2-OB2-PB2-OB3
18	D	2003	CDL	CB2-OB2-PB2-OB4
18	D	2003	CDL	CB2-OB2-PB2-OB5
18	G	2004	CDL	O1-C1-CA2-OA2
18	G	2004	CDL	CA3-OA5-PA1-OA2
18	G	2004	CDL	CA3-OA5-PA1-OA3
18	G	2004	CDL	CB3-OB5-PB2-OB3
18	G	2004	CDL	C51-CB5-OB6-CB4
18	P	3003	CDL	O1-C1-CB2-OB2
18	P	3003	CDL	CA2-OA2-PA1-OA5
18	P	3003	CDL	CB2-OB2-PB2-OB3
18	P	3003	CDL	CB2-OB2-PB2-OB4
18	P	3003	CDL	CB2-OB2-PB2-OB5
18	P	3004	CDL	O1-C1-CA2-OA2
18	P	3004	CDL	CA3-OA5-PA1-OA2
18	P	3004	CDL	CA3-OA5-PA1-OA3
18	P	3004	CDL	CB3-OB5-PB2-OB3
18	P	3004	CDL	C51-CB5-OB6-CB4
11	C	2005	PEE	O5-C30-O3-C3
11	W	3005	PEE	O5-C30-O3-C3
17	D	501	HEC	C4B-C3B-CAB-CBB
17	Q	501	HEC	C4B-C3B-CAB-CBB
11	C	2005	PEE	C31-C30-O3-C3
11	W	3005	PEE	C31-C30-O3-C3
18	D	2003	CDL	C31-CA7-OA8-CA6
18	P	3003	CDL	C31-CA7-OA8-CA6
11	C	2005	PEE	O4-C10-O2-C2
11	W	3005	PEE	O4-C10-O2-C2
18	G	2004	CDL	OB7-CB5-OB6-CB4
18	P	3004	CDL	OB7-CB5-OB6-CB4
18	G	2004	CDL	OB9-CB7-OB8-CB6
18	P	3004	CDL	OB9-CB7-OB8-CB6
17	D	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	D	2003	CDL	C71-CB7-OB8-CB6
18	G	2004	CDL	C71-CB7-OB8-CB6
18	P	3003	CDL	C71-CB7-OB8-CB6
18	P	3004	CDL	C71-CB7-OB8-CB6
18	D	2003	CDL	OA9-CA7-OA8-CA6
18	P	3003	CDL	OA9-CA7-OA8-CA6
12	Q	3091	BOG	O5-C5-C6-O6
18	D	2003	CDL	OB9-CB7-OB8-CB6
18	P	3003	CDL	OB9-CB7-OB8-CB6
12	Q	3091	BOG	O5-C1-O1-C1'
12	D	2091	BOG	O5-C5-C6-O6
17	Q	501	HEC	C2B-C3B-CAB-CBB
11	A	2008	PEE	C31-C30-O3-C3
12	D	2091	BOG	C4-C5-C6-O6
12	Q	3091	BOG	C2-C1-O1-C1'
11	A	2008	PEE	C10-C11-C12-C13
11	W	3005	PEE	C30-C31-C32-C33
11	A	2008	PEE	O5-C30-O3-C3
17	D	501	HEC	C2B-C3B-CAB-CBB
12	Q	3009	BOG	O5-C1-O1-C1'
11	C	2005	PEE	C30-C31-C32-C33
12	C	3010	BOG	O1-C1'-C2'-C3'
12	E	2009	BOG	O1-C1'-C2'-C3'
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
12	Q	3009	BOG	O1-C1'-C2'-C3'
18	G	2004	CDL	C11-CA5-OA6-CA4
18	P	3004	CDL	C11-CA5-OA6-CA4
18	P	3004	CDL	C31-CA7-OA8-CA6
18	G	2004	CDL	OA7-CA5-OA6-CA4
18	P	3004	CDL	OA7-CA5-OA6-CA4
18	D	2003	CDL	CA2-C1-CB2-OB2
18	G	2004	CDL	CB2-C1-CA2-OA2
18	P	3003	CDL	CA2-C1-CB2-OB2
18	P	3004	CDL	CB2-C1-CA2-OA2
18	G	2004	CDL	C31-CA7-OA8-CA6
12	Q	3009	BOG	C2-C1-O1-C1'
12	Q	3091	BOG	C4-C5-C6-O6
11	P	3007	PEE	C12-C13-C14-C15
12	C	3010	BOG	C2'-C3'-C4'-C5'
11	C	2005	PEE	C37-C38-C39-C40
11	W	3005	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C35-C36-C37-C38
11	C	2007	PEE	C12-C13-C14-C15
11	C	2007	PEE	C10-C11-C12-C13
12	Q	3091	BOG	O1-C1'-C2'-C3'
11	P	3007	PEE	C34-C35-C36-C37
12	C	3010	BOG	C3'-C4'-C5'-C6'
11	W	3005	PEE	C14-C15-C16-C17
11	C	2005	PEE	C14-C15-C16-C17
11	C	2007	PEE	C34-C35-C36-C37
11	P	3007	PEE	C35-C36-C37-C38
11	W	3005	PEE	C11-C12-C13-C14
11	W	3005	PEE	C40-C41-C42-C43
12	P	2010	BOG	C3'-C4'-C5'-C6'
11	C	2005	PEE	C11-C12-C13-C14
11	C	2005	PEE	C40-C41-C42-C43
11	P	3007	PEE	C14-C15-C16-C17
14	C	502	HEM	C4D-C3D-CAD-CBD
14	P	502	HEM	C4D-C3D-CAD-CBD
11	C	2007	PEE	C15-C16-C17-C18
11	C	2005	PEE	C33-C34-C35-C36
14	C	501	HEM	C2C-C3C-CAC-CBC
14	P	502	HEM	C2C-C3C-CAC-CBC
11	W	3005	PEE	C33-C34-C35-C36
11	C	2007	PEE	C14-C15-C16-C17
12	Q	3091	BOG	C1'-C2'-C3'-C4'
14	C	501	HEM	C4B-C3B-CAB-CBB
14	C	502	HEM	C4C-C3C-CAC-CBC
14	P	501	HEM	C4B-C3B-CAB-CBB
14	P	501	HEM	C4C-C3C-CAC-CBC
14	P	502	HEM	C4C-C3C-CAC-CBC
18	G	2004	CDL	OA9-CA7-OA8-CA6
18	P	3004	CDL	OA9-CA7-OA8-CA6
11	C	2005	PEE	C35-C36-C37-C38
11	W	3005	PEE	C35-C36-C37-C38
18	D	2003	CDL	OA6-CA4-CA6-OA8
18	P	3003	CDL	OA6-CA4-CA6-OA8
11	A	2008	PEE	O3P-C1-C2-C3
14	C	502	HEM	C2D-C3D-CAD-CBD
12	E	2009	BOG	C2-C1-O1-C1'
11	P	3007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
15	P	3001	ICX	N33-C34-C35-O37
11	P	3007	PEE	C40-C41-C42-C43
11	P	3007	PEE	C41-C42-C43-C44
11	P	3007	PEE	C20-C21-C22-C23
11	C	2007	PEE	C40-C41-C42-C43
12	P	2010	BOG	C2'-C3'-C4'-C5'
11	C	2007	PEE	C11-C12-C13-C14
11	C	2005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C20-C21-C22-C23
12	E	2009	BOG	C2'-C3'-C4'-C5'
18	D	2003	CDL	OA5-CA3-CA4-CA6
18	P	3003	CDL	OA5-CA3-CA4-CA6
18	P	3003	CDL	C71-C72-C73-C74
11	C	2005	PEE	C20-C21-C22-C23
18	D	2003	CDL	CA3-CA4-CA6-OA8
18	G	2004	CDL	CA3-CA4-CA6-OA8
18	P	3003	CDL	CA3-CA4-CA6-OA8
18	P	3004	CDL	CA3-CA4-CA6-OA8
18	D	2003	CDL	C71-C72-C73-C74
18	G	2004	CDL	OB5-CB3-CB4-OB6
18	P	3003	CDL	OA5-CA3-CA4-OA6
11	W	3005	PEE	C20-C21-C22-C23
15	C	2001	ICX	N33-C34-C35-O37
15	P	3001	ICX	N33-C34-C35-O36
11	W	3005	PEE	C19-C20-C21-C22
18	D	2003	CDL	OA5-CA3-CA4-OA6
18	P	3004	CDL	OB5-CB3-CB4-OB6
11	C	2007	PEE	C31-C32-C33-C34
12	E	2009	BOG	O5-C1-O1-C1'
11	P	3007	PEE	C32-C33-C34-C35
12	Q	3009	BOG	C2'-C3'-C4'-C5'
11	C	2005	PEE	C15-C16-C17-C18
11	P	3007	PEE	C31-C32-C33-C34
11	A	2008	PEE	O3P-C1-C2-O2
11	C	2005	PEE	O3P-C1-C2-O2
14	P	502	HEM	C2D-C3D-CAD-CBD
18	G	2004	CDL	OA6-CA4-CA6-OA8
18	P	3004	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C32-C33-C34-C35
11	C	2005	PEE	O4P-C4-C5-N
11	W	3005	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
18	G	2004	CDL	CA3-OA5-PA1-OA4
18	G	2004	CDL	CB3-OB5-PB2-OB2
18	G	2004	CDL	CB3-OB5-PB2-OB4
18	P	3004	CDL	CA3-OA5-PA1-OA4
18	P	3004	CDL	CB3-OB5-PB2-OB2
18	P	3004	CDL	CB3-OB5-PB2-OB4
18	G	2004	CDL	C1-CB2-OB2-PB2
18	P	3004	CDL	C1-CB2-OB2-PB2
11	C	2005	PEE	C1-C2-O2-C10
11	W	3005	PEE	C1-C2-O2-C10
12	D	2091	BOG	O5-C1-O1-C1'
15	C	2001	ICX	N33-C34-C35-O36
11	W	3005	PEE	C15-C16-C17-C18
12	C	3010	BOG	C2'-C1'-O1-C1
12	D	2091	BOG	C2'-C1'-O1-C1
18	D	2003	CDL	CB7-C71-C72-C73
18	P	3003	CDL	CB7-C71-C72-C73
14	C	501	HEM	C4C-C3C-CAC-CBC
11	W	3005	PEE	C21-C22-C23-C24
11	P	3007	PEE	C21-C22-C23-C24
11	P	3007	PEE	C43-C44-C45-C46
11	C	2007	PEE	C43-C44-C45-C46
14	P	502	HEM	CAA-CBA-CGA-O2A
14	C	502	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C21-C22-C23-C24
14	C	502	HEM	CAA-CBA-CGA-O1A
14	P	502	HEM	CAA-CBA-CGA-O1A
11	C	2007	PEE	C39-C40-C41-C42
14	P	502	HEM	CAD-CBD-CGD-O2D
14	C	502	HEM	CAD-CBD-CGD-O2D
18	P	3003	CDL	C1-CA2-OA2-PA1
11	W	3005	PEE	O3P-C1-C2-O2
17	Q	501	HEC	CAD-CBD-CGD-O2D
18	G	2004	CDL	OB5-CB3-CB4-CB6
18	P	3004	CDL	OB5-CB3-CB4-CB6
18	D	2003	CDL	OB6-CB4-CB6-OB8
14	C	502	HEM	CAD-CBD-CGD-O1D
18	D	2003	CDL	C1-CA2-OA2-PA1
14	C	501	HEM	CAA-CBA-CGA-O2A
12	E	2009	BOG	C1'-C2'-C3'-C4'
11	W	3005	PEE	C36-C37-C38-C39
14	P	502	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	Q	501	HEC	CAA-CBA-CGA-O2A
11	C	2005	PEE	C21-C22-C23-C24
14	P	501	HEM	CAA-CBA-CGA-O2A
14	P	501	HEM	CAA-CBA-CGA-O1A
17	Q	501	HEC	CAD-CBD-CGD-O1D
11	C	2005	PEE	C2-C1-O3P-P
11	W	3005	PEE	C2-C1-O3P-P
14	C	501	HEM	CAA-CBA-CGA-O1A
11	P	3007	PEE	O2-C10-C11-C12
11	C	2007	PEE	O2-C10-C11-C12
11	C	2005	PEE	C36-C37-C38-C39
11	P	3007	PEE	C39-C40-C41-C42
11	A	2008	PEE	O2-C10-C11-C12
17	D	501	HEC	CAD-CBD-CGD-O2D
17	Q	501	HEC	CAA-CBA-CGA-O1A
18	D	2003	CDL	C72-C71-CB7-OB8
12	E	2009	BOG	C4'-C5'-C6'-C7'
11	P	3007	PEE	O3-C30-C31-C32
18	P	3003	CDL	C72-C71-CB7-OB8
14	C	501	HEM	CAD-CBD-CGD-O2D
11	C	2007	PEE	O3-C30-C31-C32
18	P	3003	CDL	OB6-CB4-CB6-OB8
17	D	501	HEC	CAD-CBD-CGD-O1D
14	C	501	HEM	CAD-CBD-CGD-O1D
11	P	3007	PEE	O5-C30-C31-C32
18	D	2003	CDL	C72-C71-CB7-OB9
11	A	2008	PEE	O4-C10-C11-C12
11	C	2007	PEE	O4-C10-C11-C12
11	W	3005	PEE	C2-C3-O3-C30
12	C	3010	BOG	C2-C1-O1-C1'
11	P	3007	PEE	O4-C10-C11-C12
18	D	2003	CDL	CB3-CB4-CB6-OB8
11	C	2007	PEE	O5-C30-C31-C32
18	P	3003	CDL	C72-C71-CB7-OB9
11	P	3007	PEE	C42-C43-C44-C45
18	P	3003	CDL	C52-C51-CB5-OB6

There are no ring outliers.

22 monomers are involved in 82 short contacts:

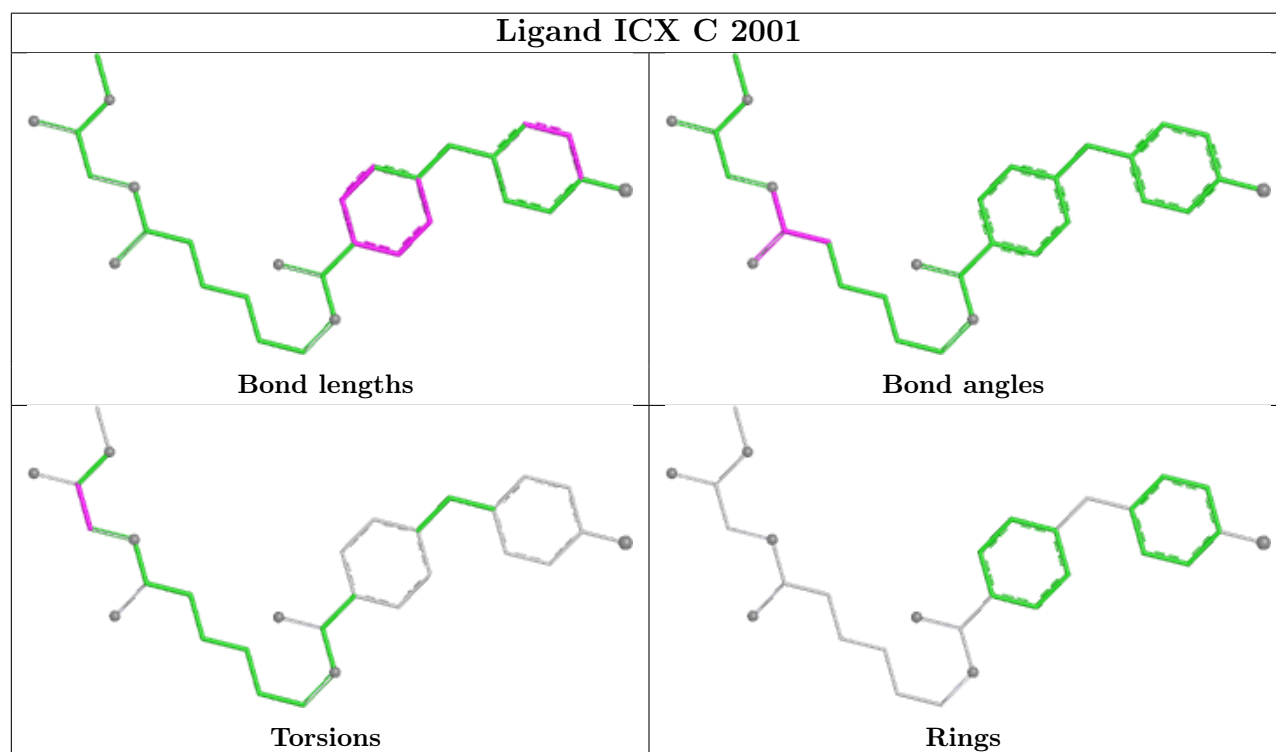
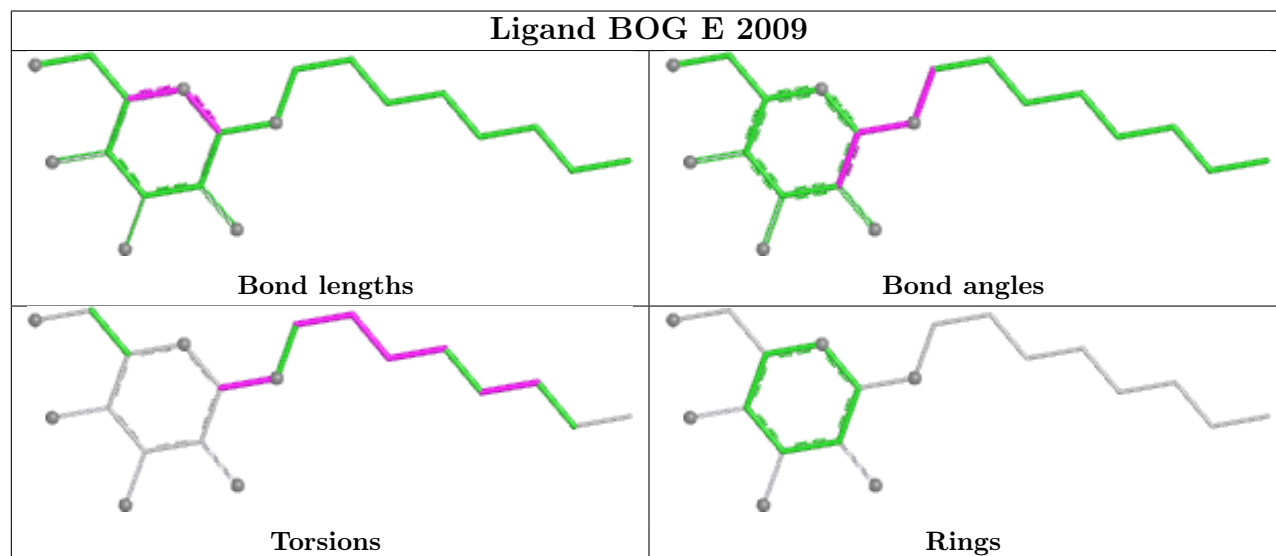
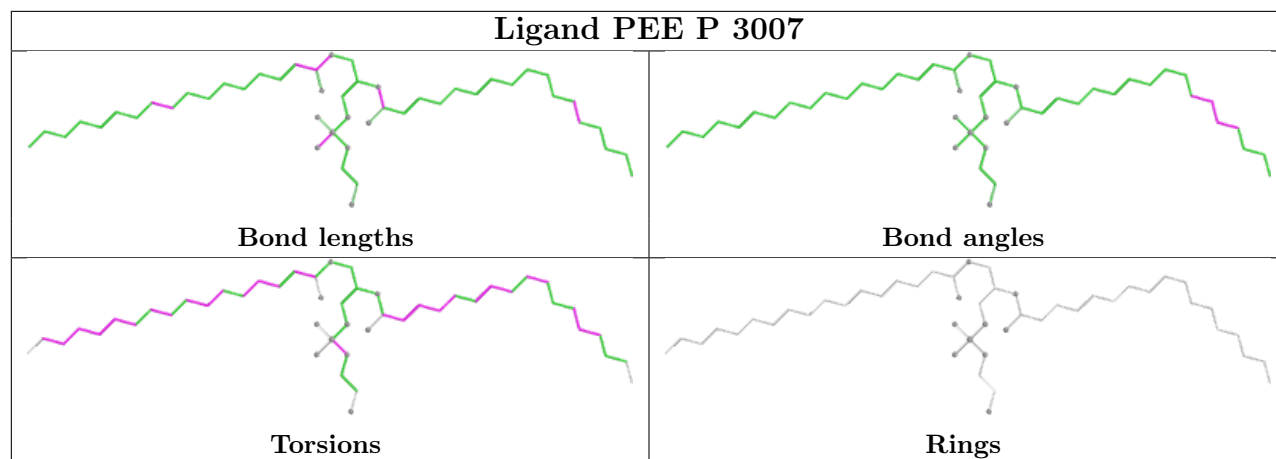
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	3007	PEE	2	0

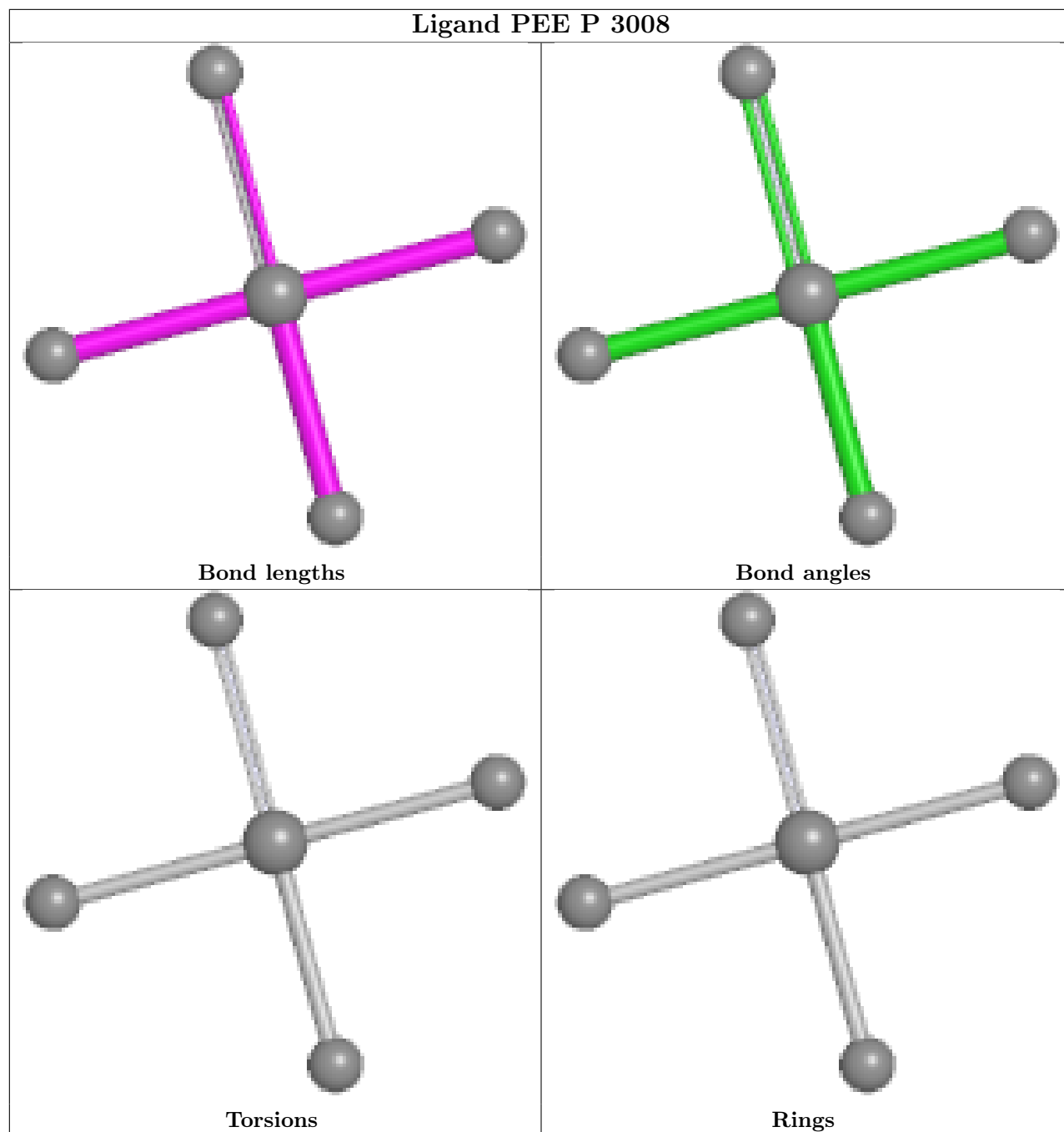
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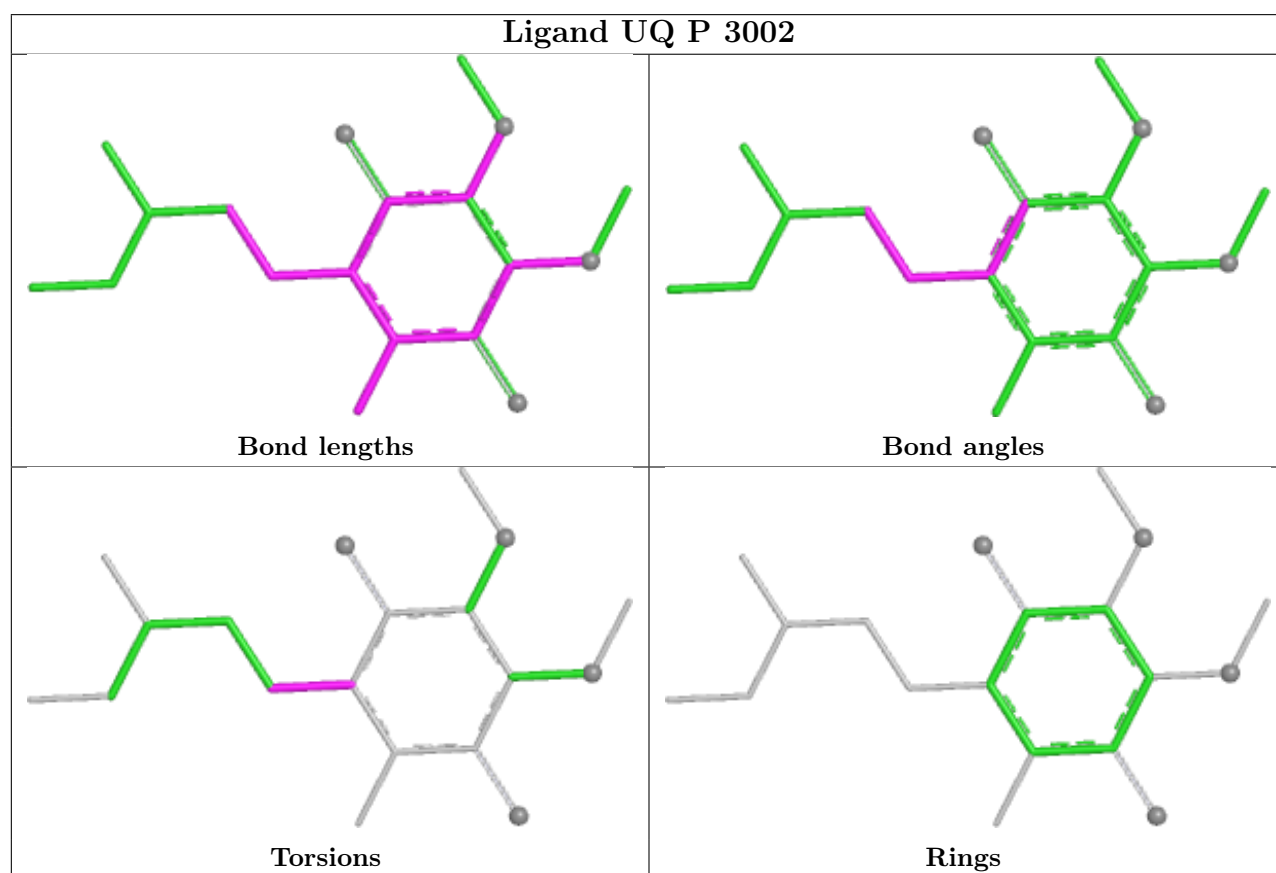
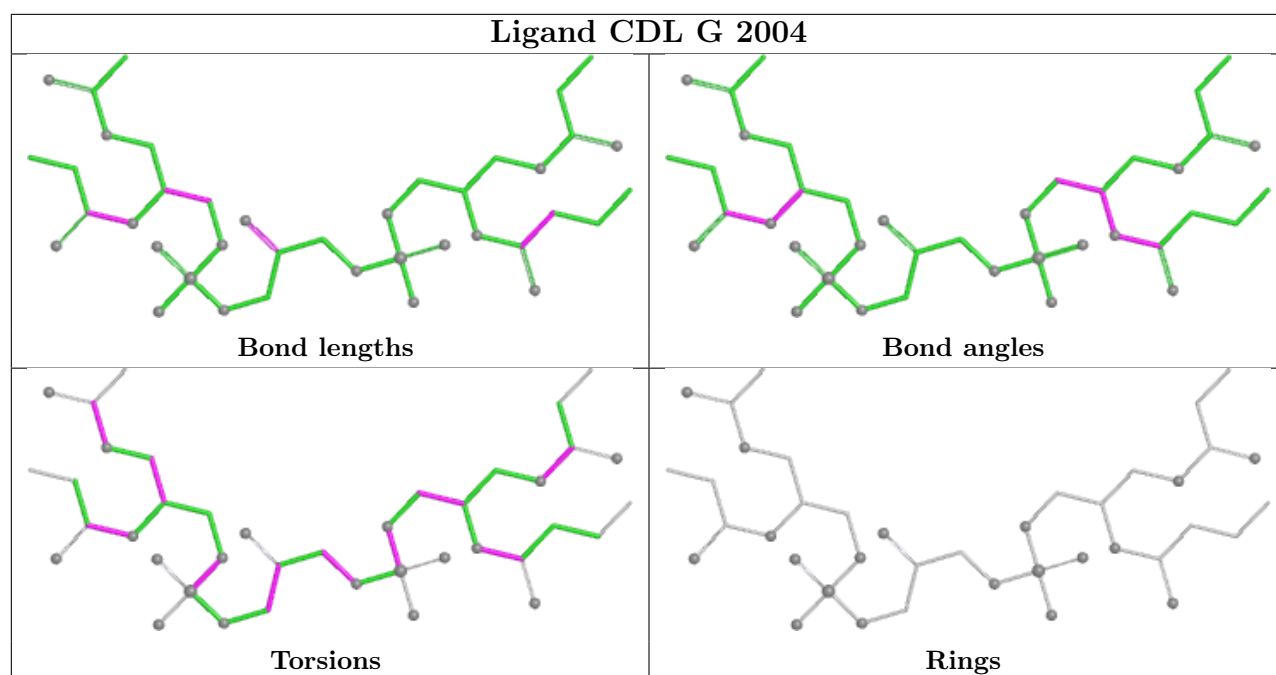
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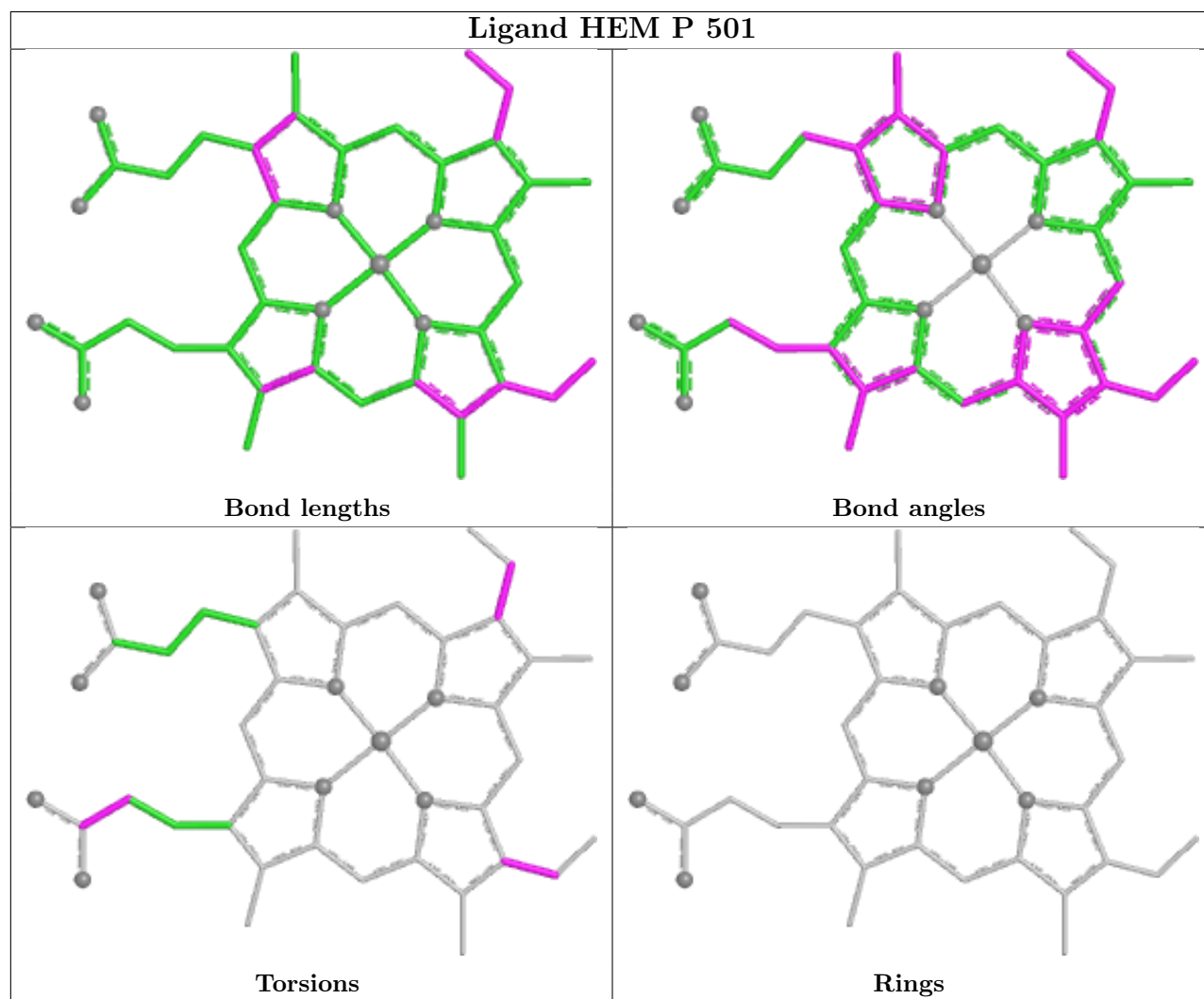
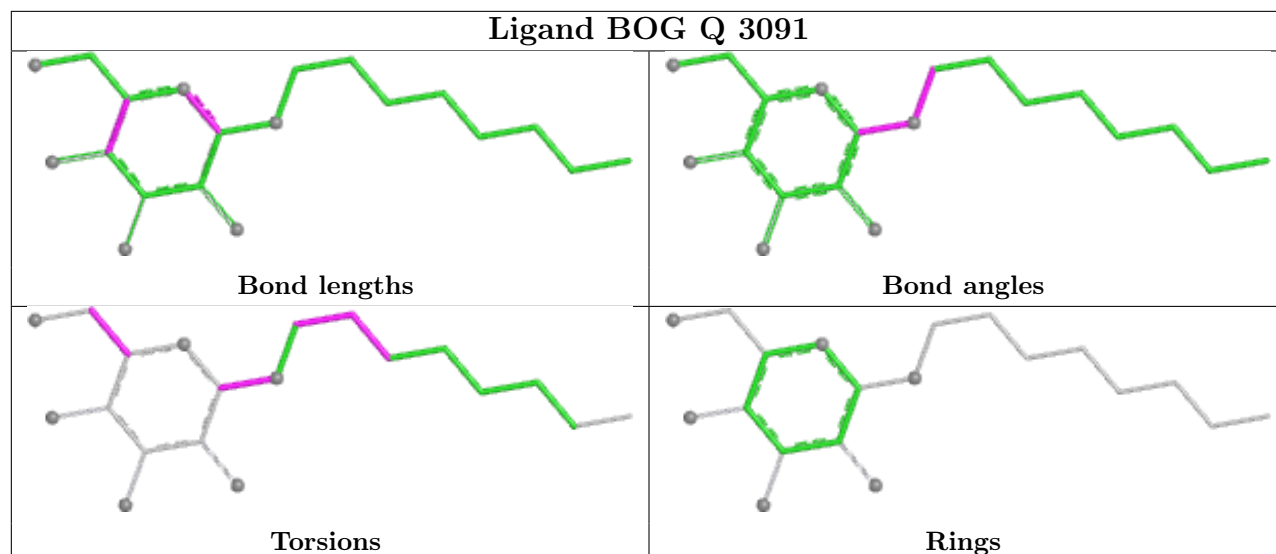
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	2009	BOG	1	0
15	C	2001	ICX	2	0
18	G	2004	CDL	1	0
19	E	501	FES	1	0
16	P	3002	UQ	5	0
14	P	501	HEM	9	0
17	D	501	HEC	3	0
12	D	2091	BOG	5	0
14	C	501	HEM	9	0
17	Q	501	HEC	3	0
18	D	2003	CDL	3	0
18	P	3003	CDL	3	0
11	W	3005	PEE	1	0
14	P	502	HEM	11	0
12	P	2010	BOG	1	0
14	C	502	HEM	10	0
18	P	3004	CDL	2	0
11	C	2007	PEE	3	0
15	P	3001	ICX	2	0
16	C	2002	UQ	4	0
11	C	2005	PEE	2	0

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

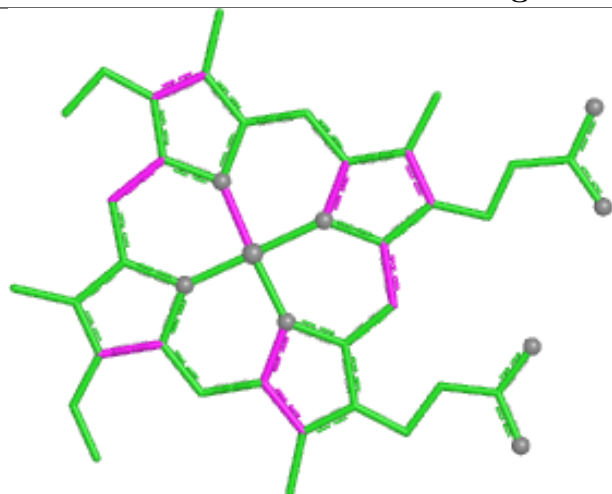




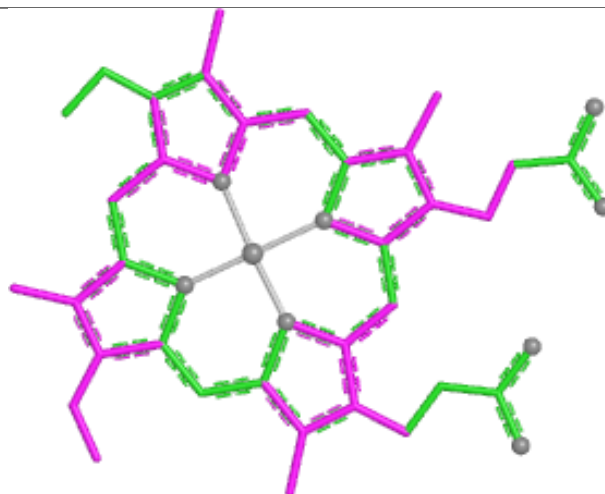




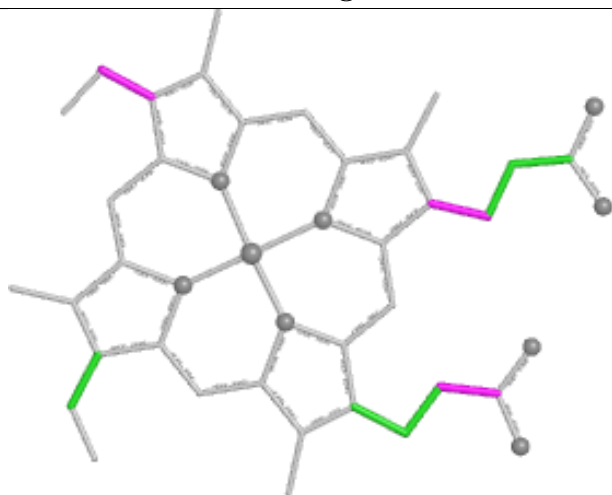
Ligand HEC D 501



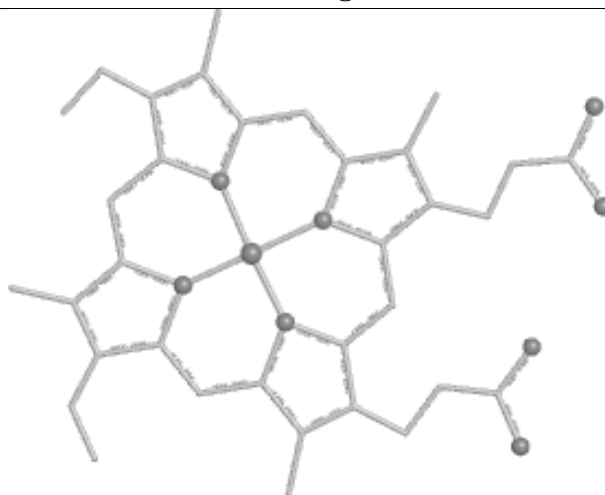
Bond lengths



Bond angles

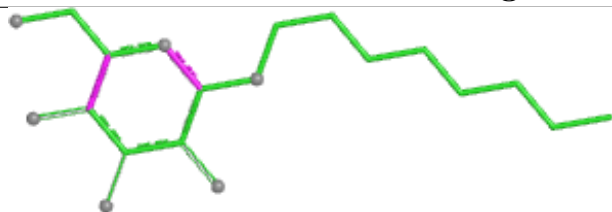


Torsions

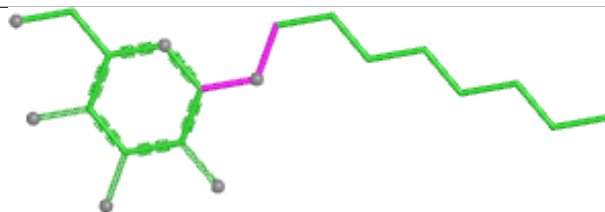


Rings

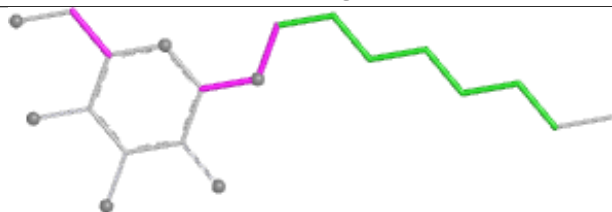
Ligand BOG D 2091



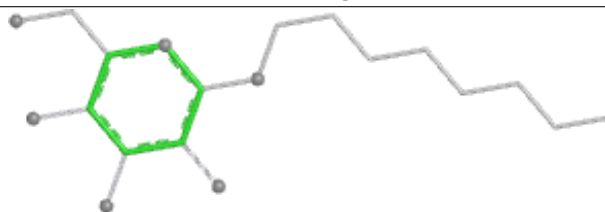
Bond lengths



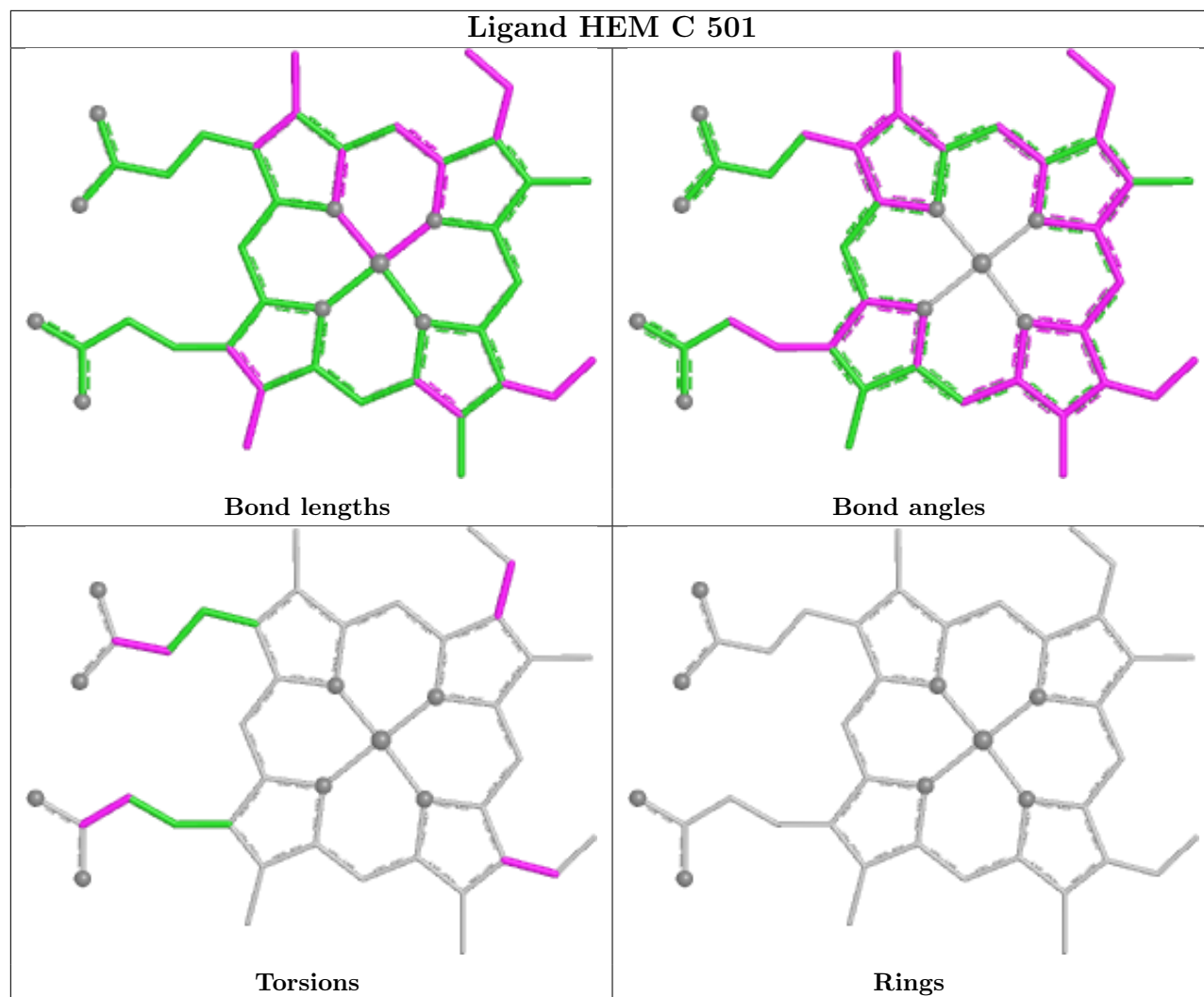
Bond angles



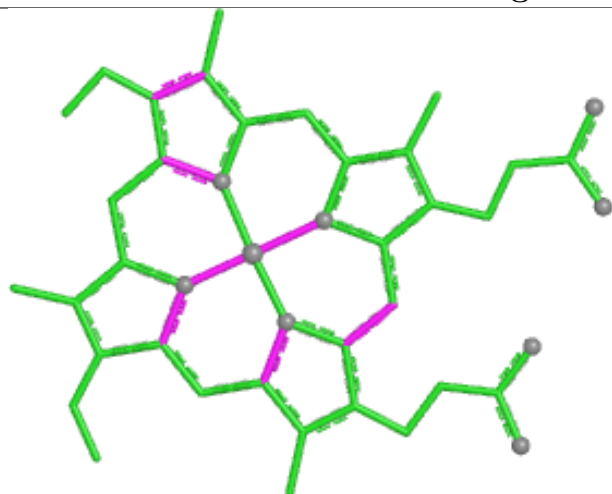
Torsions



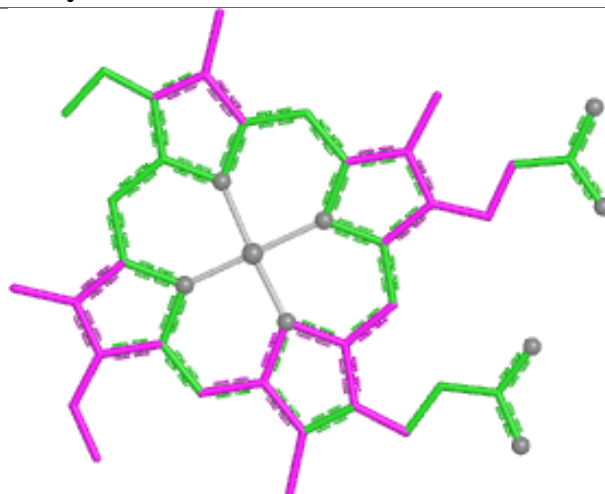
Rings



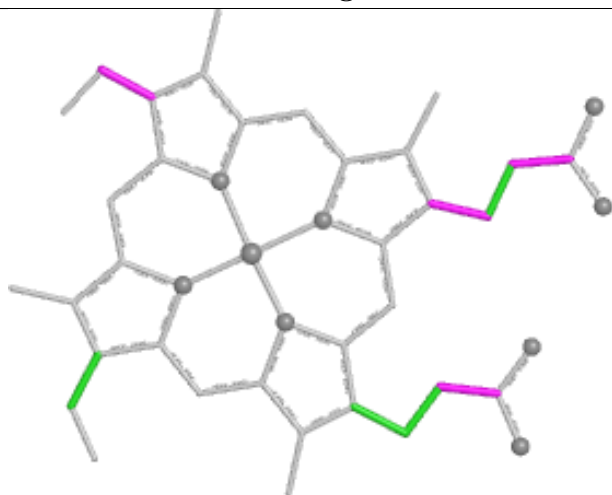
Ligand HEC Q 501



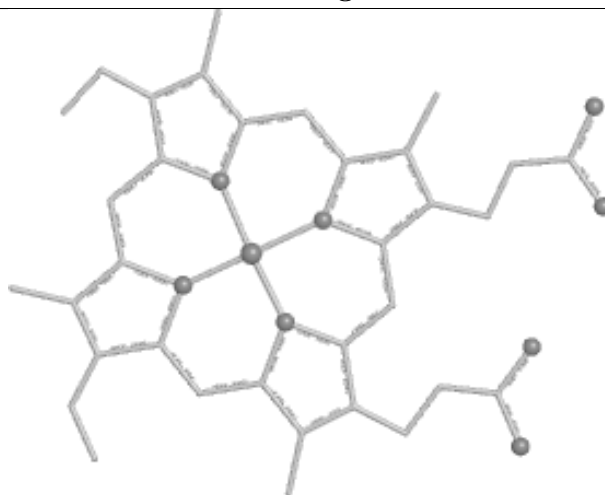
Bond lengths



Bond angles



Torsions

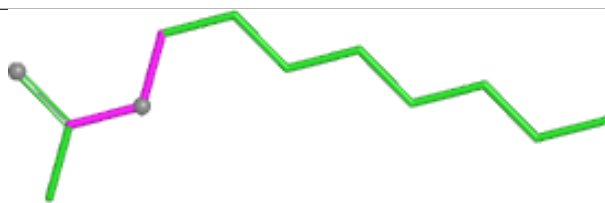


Rings

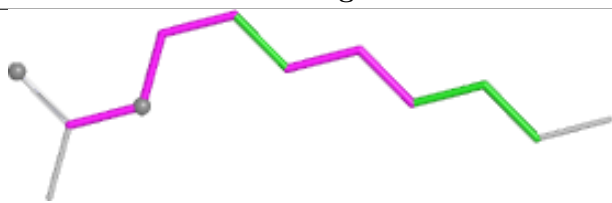
Ligand BOG C 3010



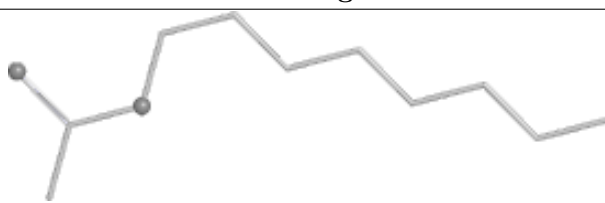
Bond lengths



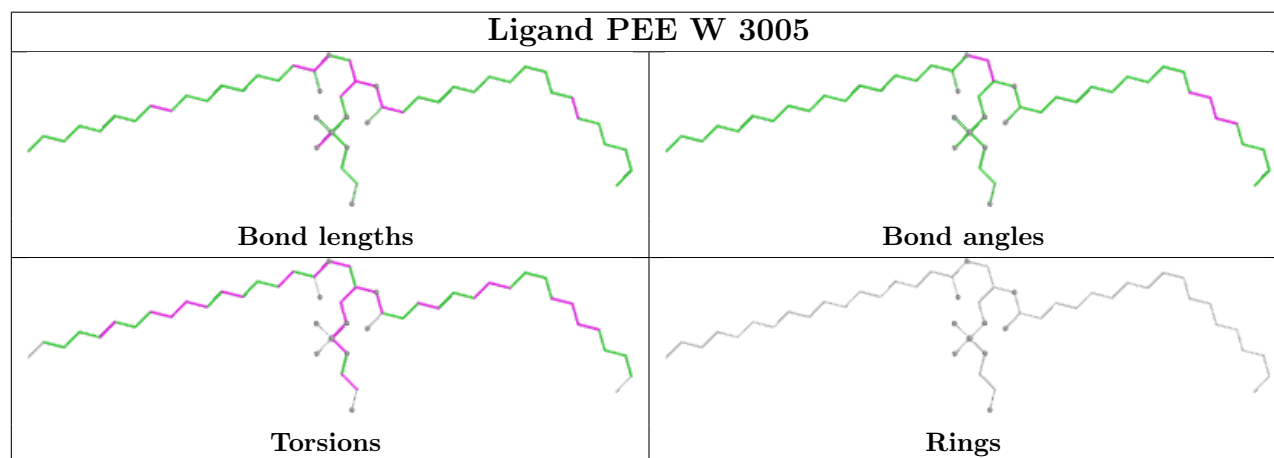
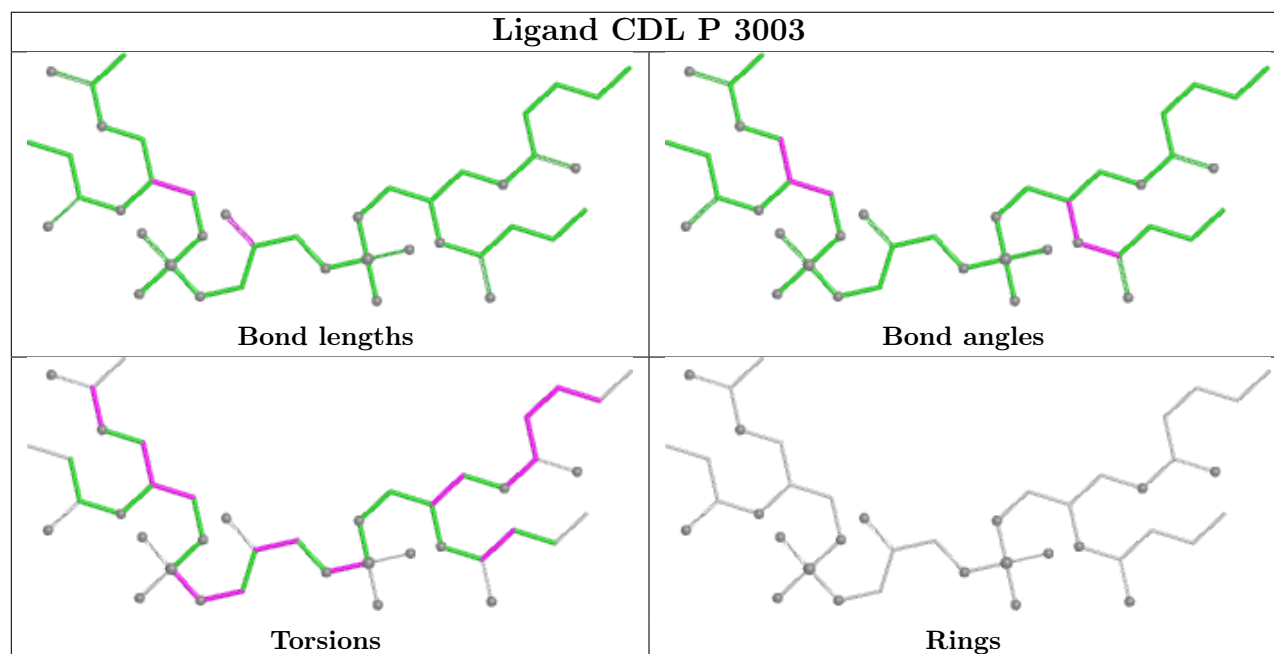
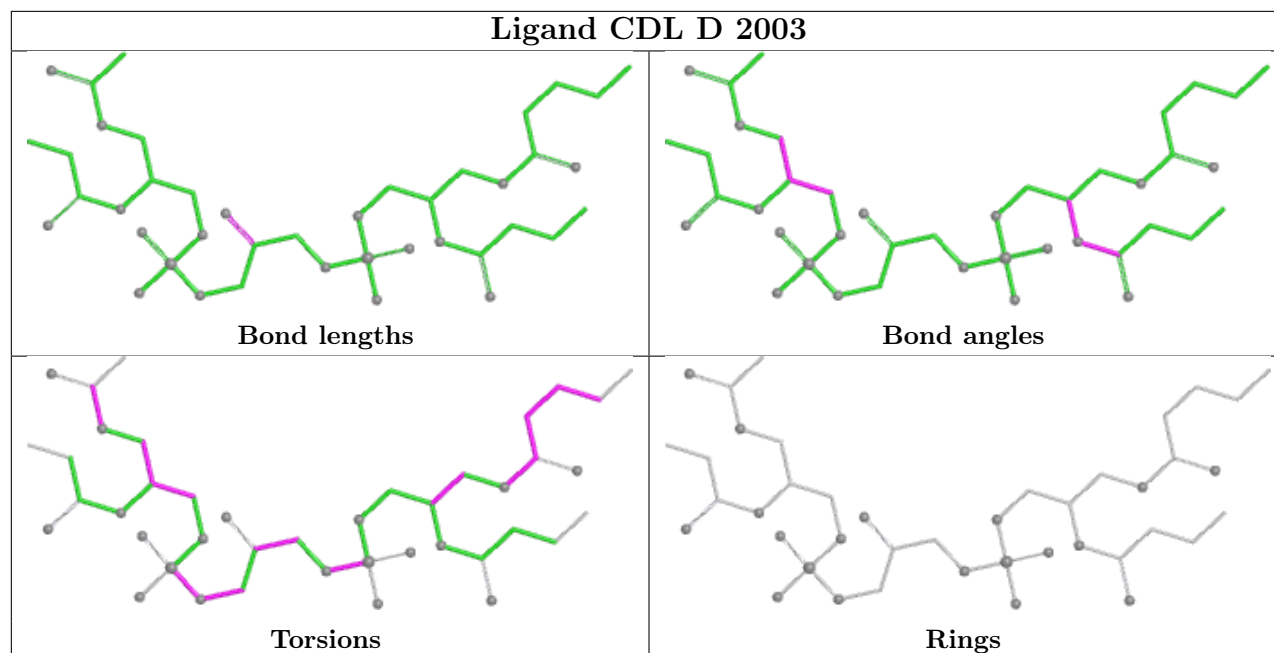
Bond angles

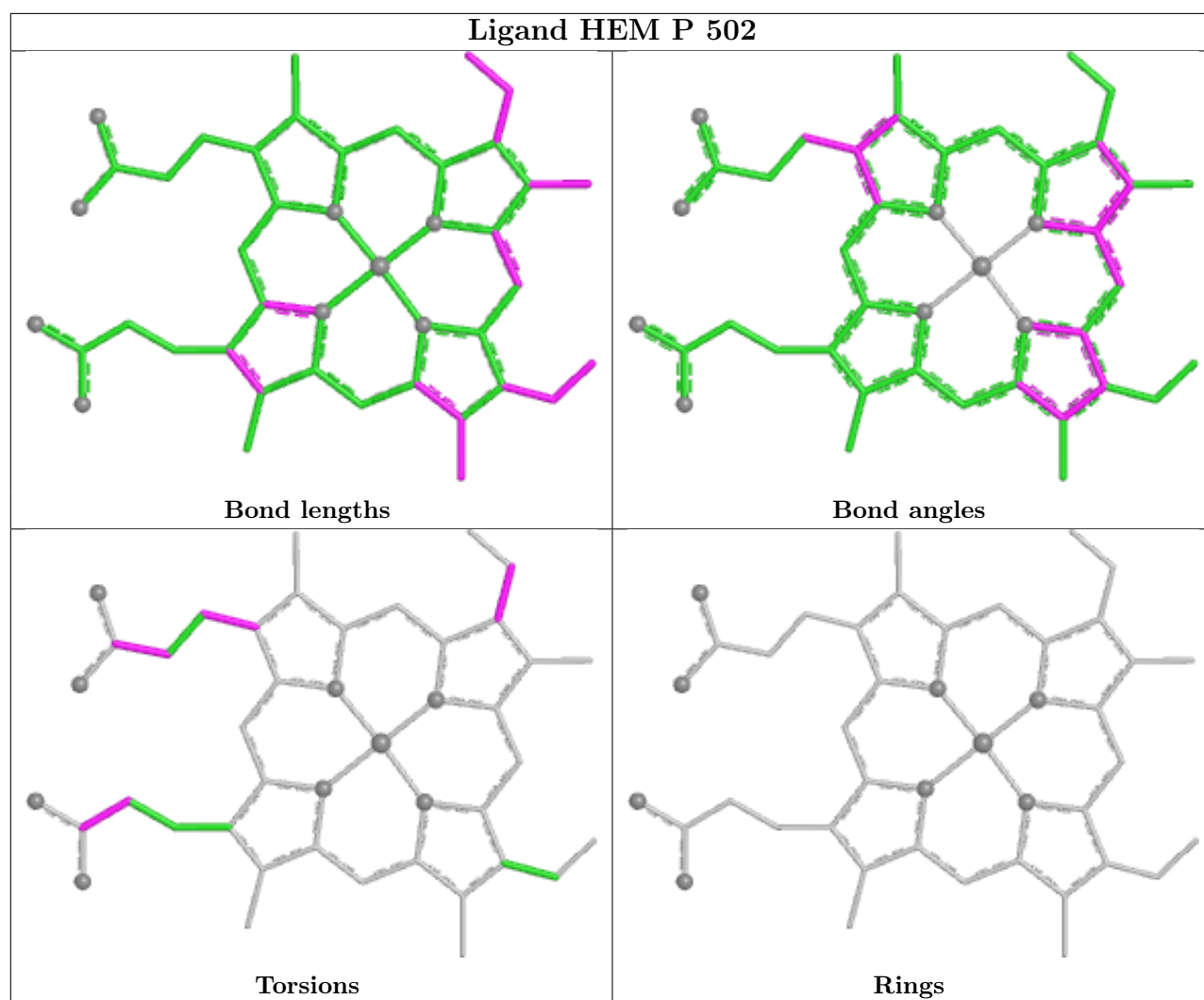


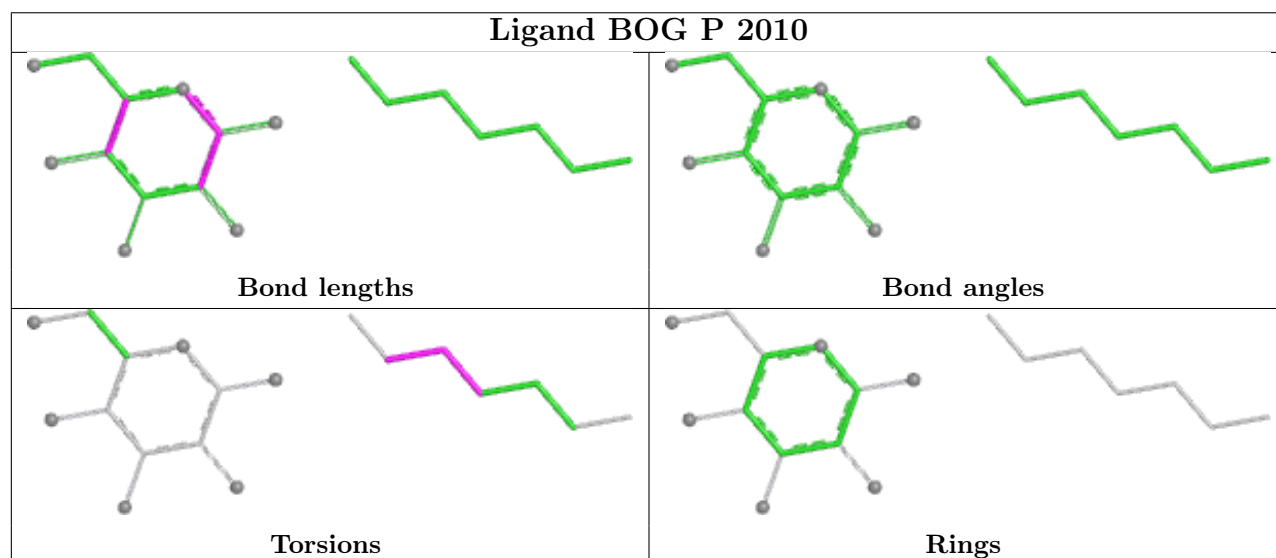
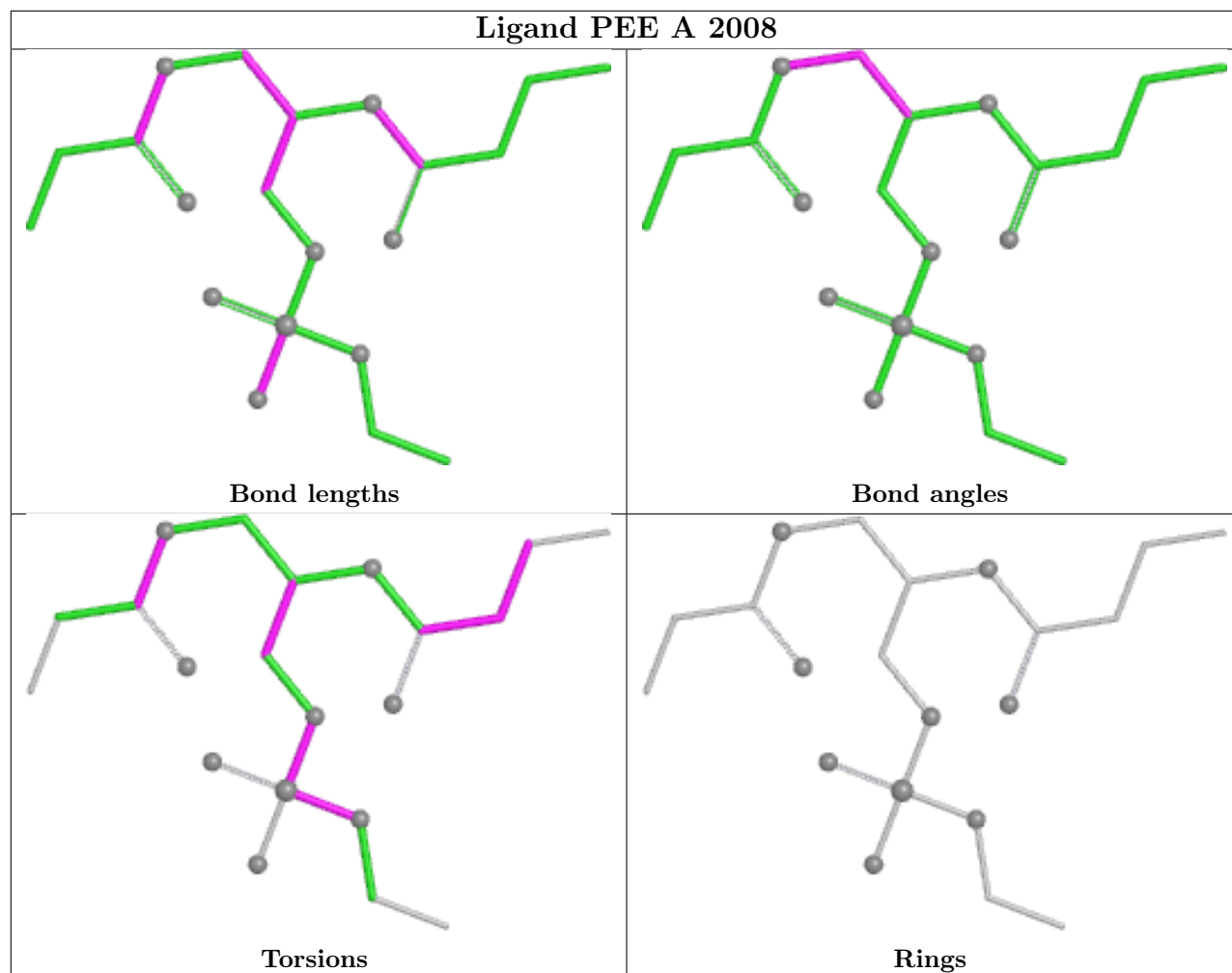
Torsions

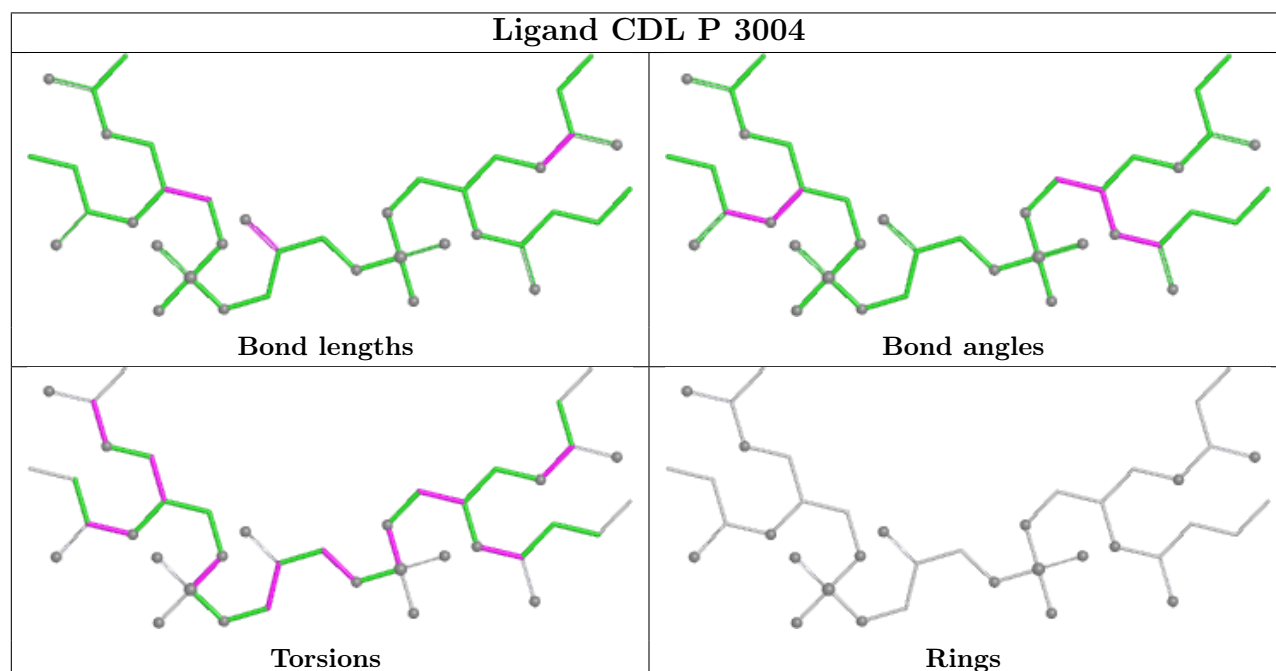
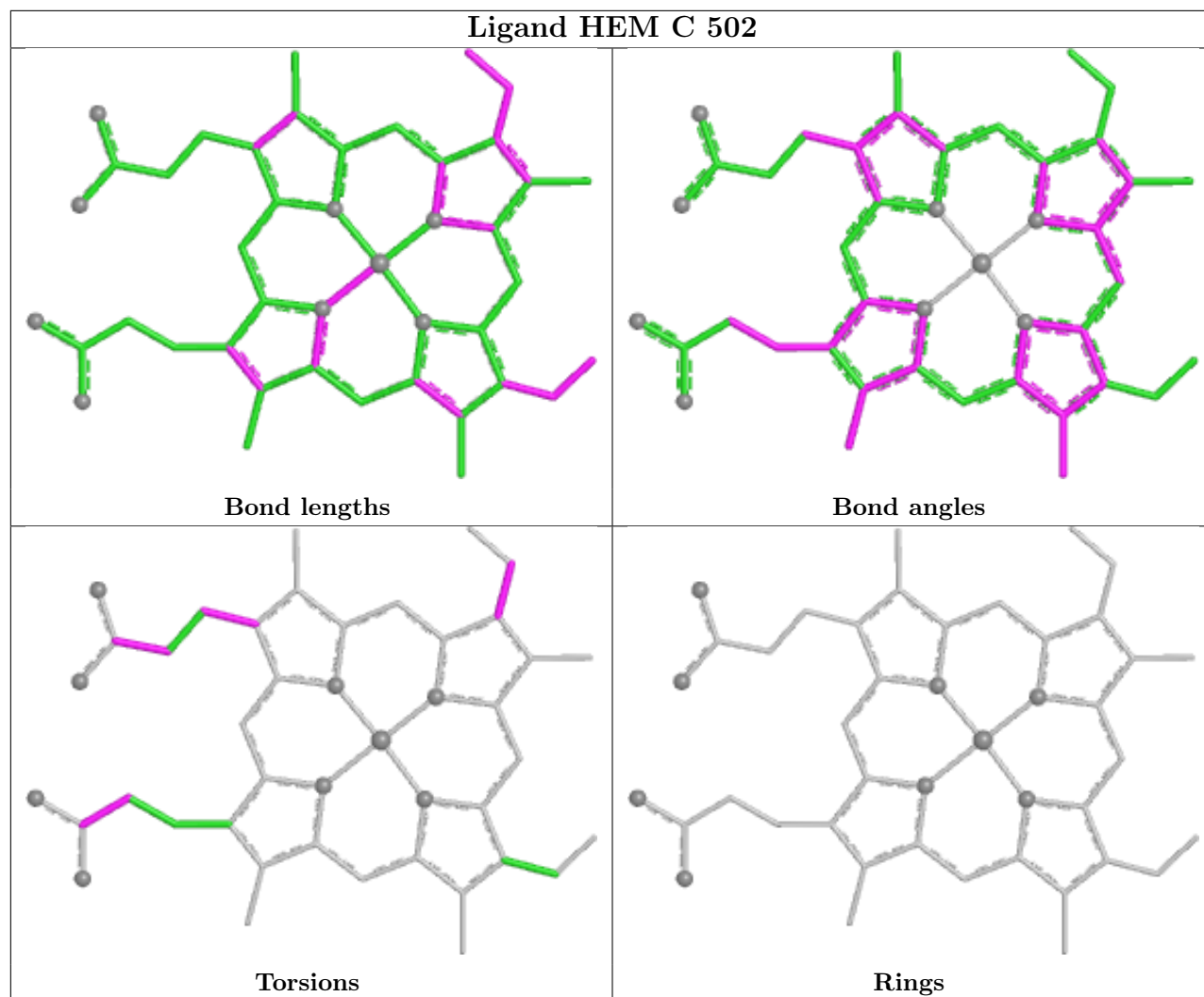


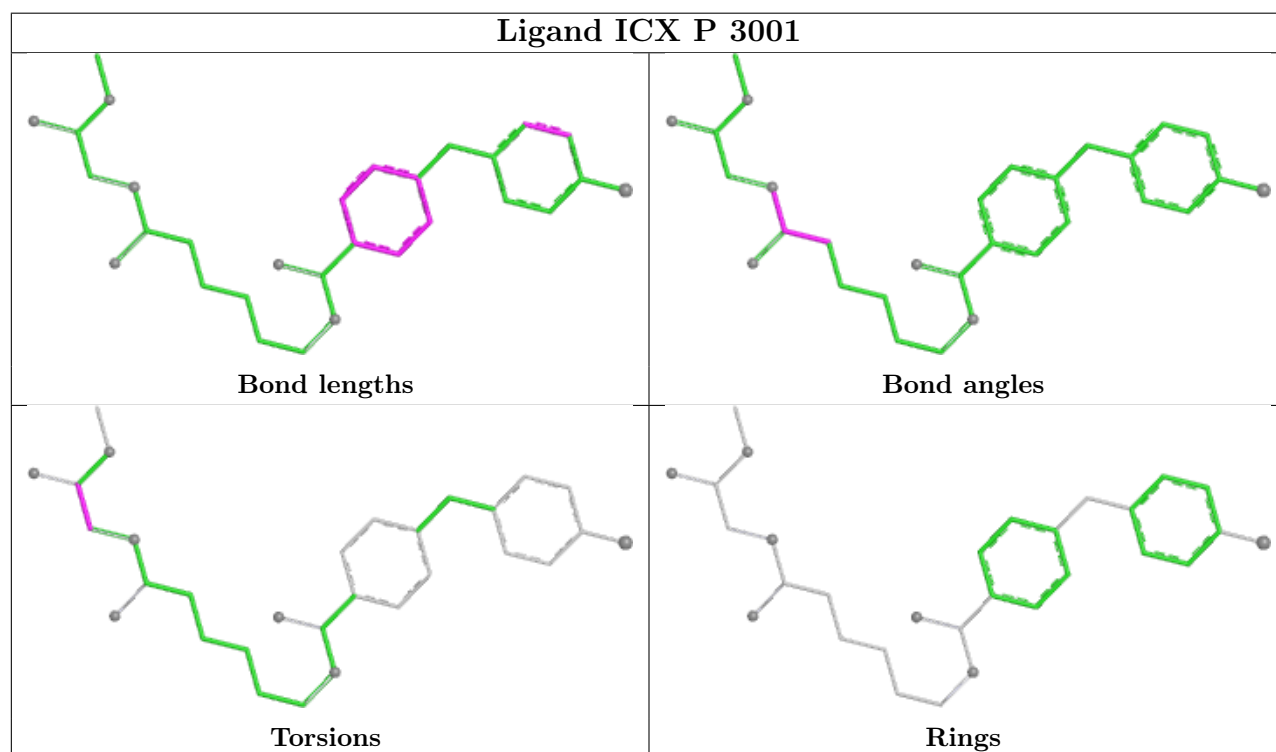
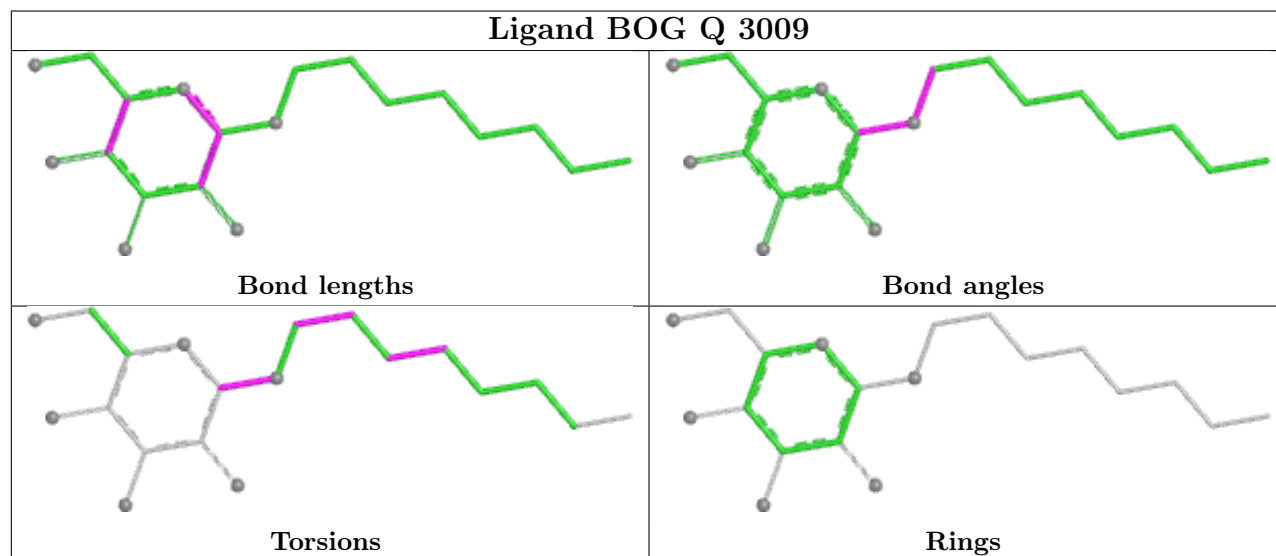
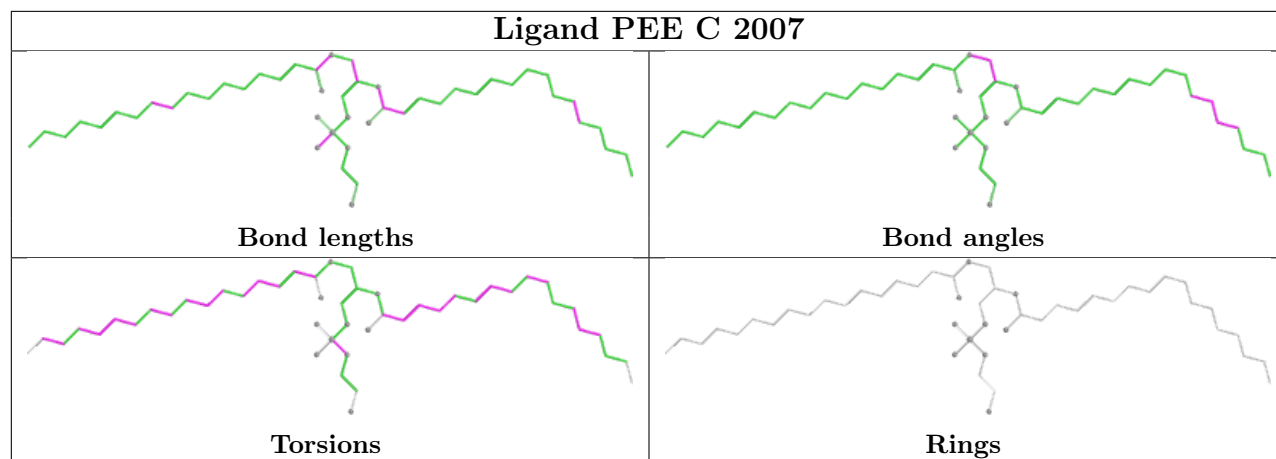
Rings

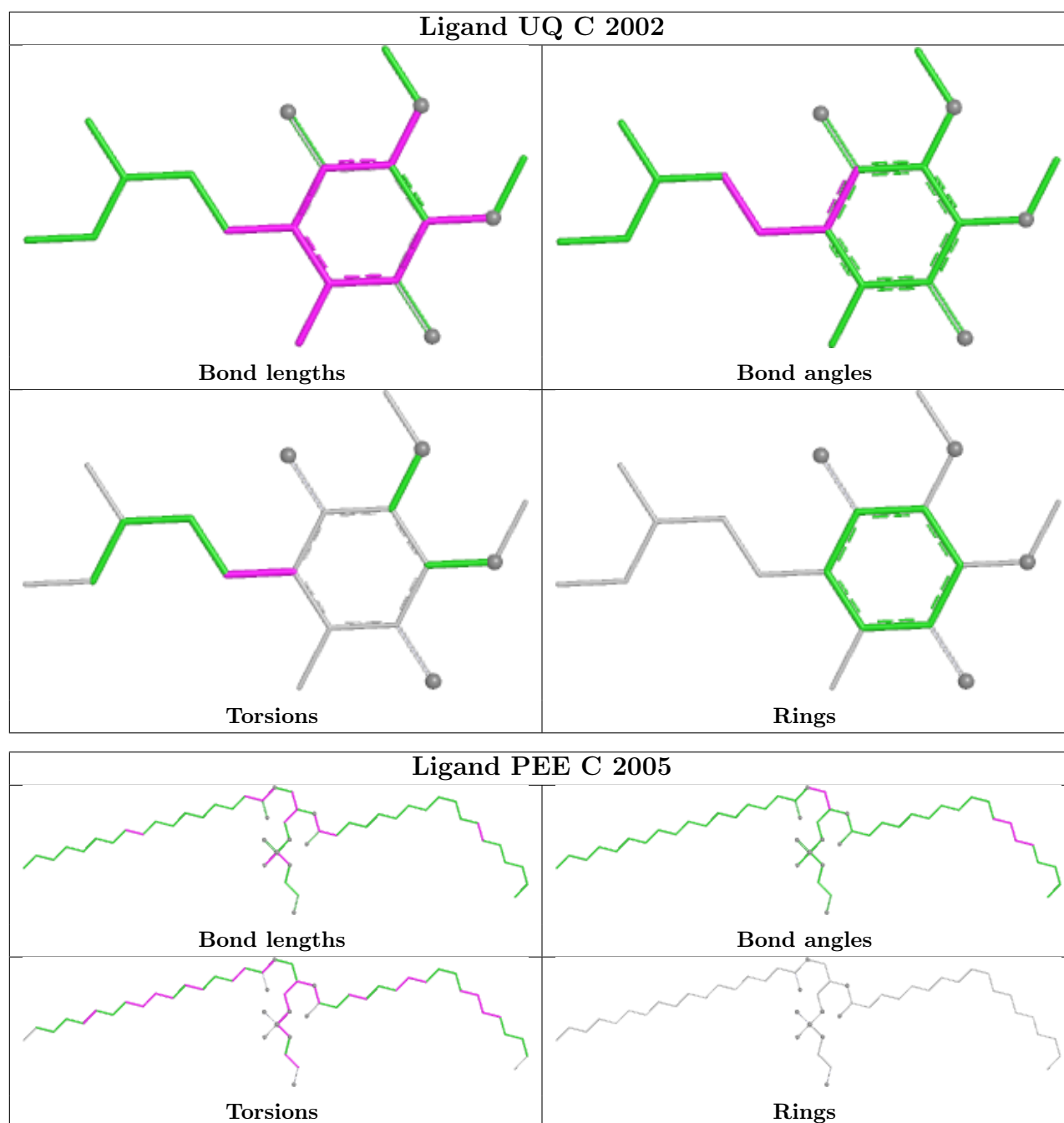












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.02	3 (0%) 84 61	36, 89, 137, 150	0
1	N	442/446 (99%)	0.11	3 (0%) 84 61	54, 91, 136, 153	0
2	B	421/441 (95%)	0.26	2 (0%) 87 67	60, 113, 170, 193	0
2	O	422/441 (95%)	0.11	5 (1%) 76 50	51, 100, 146, 172	0
3	C	380/380 (100%)	-0.45	1 (0%) 90 75	19, 50, 104, 192	0
3	P	379/380 (99%)	-0.02	4 (1%) 78 52	29, 89, 132, 186	0
4	D	241/241 (100%)	-0.33	0 100 100	30, 58, 109, 133	0
4	Q	241/241 (100%)	0.21	1 (0%) 88 70	65, 105, 150, 165	0
5	E	196/196 (100%)	0.74	19 (9%) 13 8	45, 113, 153, 162	127 (64%)
5	R	196/196 (100%)	0.18	0 100 100	53, 101, 166, 184	0
6	F	100/110 (90%)	-0.40	0 100 100	31, 61, 87, 102	0
6	S	100/110 (90%)	0.26	1 (1%) 79 54	77, 117, 167, 188	0
7	G	81/81 (100%)	-0.03	3 (3%) 45 25	43, 77, 128, 156	0
7	T	79/81 (97%)	0.75	6 (7%) 20 13	71, 137, 202, 211	0
8	H	70/77 (90%)	0.02	1 (1%) 73 46	51, 94, 117, 153	0
8	U	67/77 (87%)	0.97	5 (7%) 20 13	141, 175, 213, 219	0
9	I	31/52 (59%)	1.76	11 (35%) 1 1	109, 158, 223, 229	0
9	V	31/52 (59%)	1.53	10 (32%) 1 1	109, 157, 222, 224	0
10	J	61/61 (100%)	-0.08	0 100 100	65, 82, 144, 187	0
10	W	59/61 (96%)	-0.02	0 100 100	75, 107, 139, 154	0
All	All	4040/4170 (96%)	0.10	75 (1%) 66 39	19, 93, 160, 229	127 (3%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	162	GLY	7.3
9	I	63	ASP	5.9
1	A	444	ILE	5.0
9	I	51	CYS	4.6
5	E	163	SER	4.4
7	T	4	PHE	4.2
9	I	50	LEU	4.1
2	O	208	GLY	4.0
5	E	133	VAL	4.0
7	T	2	ILE	4.0
9	I	49	LEU	3.8
8	U	51	GLU	3.6
5	E	132	TRP	3.5
7	T	62	GLY	3.5
9	V	49	LEU	3.4
9	V	54	SER	3.4
5	E	169	GLY	3.3
9	V	53	GLU	3.2
5	E	175	PRO	3.2
5	E	94	LYS	3.1
1	A	192	ALA	3.1
9	I	47	ARG	3.1
9	V	56	SER	3.0
9	I	57	GLY	3.0
9	I	58	ARG	3.0
3	C	7	LYS	2.9
2	O	19	PRO	2.9
8	U	54	CYS	2.8
7	T	22	GLU	2.8
5	E	165	TYR	2.7
9	I	52	ARG	2.7
9	V	61	ARG	2.7
1	N	219	VAL	2.6
8	H	9	GLU	2.6
9	I	56	SER	2.6
9	V	47	ARG	2.6
3	P	7	LYS	2.5
5	E	32	ARG	2.5
9	I	74	ALA	2.5
1	N	444	ILE	2.5
5	E	122	HIS	2.5
7	G	2	ILE	2.5
8	U	24	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	386	TYR	2.5
7	G	5	GLY	2.4
7	T	25	ALA	2.4
9	V	76	VAL	2.4
5	E	156	TYR	2.4
8	U	50	THR	2.3
3	P	3	PRO	2.3
5	E	97	PHE	2.3
3	P	244	ALA	2.3
3	P	17	ASN	2.3
9	I	61	ARG	2.3
2	O	386	ALA	2.2
7	G	4	PHE	2.2
5	E	128	LYS	2.2
2	B	267	ALA	2.2
5	E	121	GLN	2.2
7	T	79	ASN	2.2
5	E	188	VAL	2.2
5	E	127	VAL	2.1
5	E	111	GLU	2.1
5	E	93	GLY	2.1
9	V	58	ARG	2.1
4	Q	9	ALA	2.1
5	E	137	GLY	2.1
8	U	65	ARG	2.1
2	B	226	ILE	2.1
2	O	36	ALA	2.1
1	A	219	VAL	2.1
6	S	10	GLY	2.0
9	V	59	SER	2.0
2	O	362	ASN	2.0
9	V	60	ALA	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 ⓘ

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

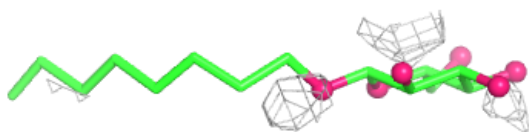
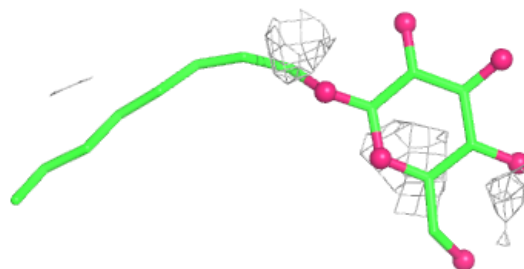
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	BOG	Q	3091	20/20	0.38	0.23	242,249,250,251	0
11	PEE	A	2008	21/51	0.53	0.32	225,229,230,230	0
11	PEE	P	3008	5/51	0.58	0.15	213,213,214,214	0
12	BOG	P	2010	19/20	0.61	0.23	102,248,249,249	0
18	CDL	P	3004	40/100	0.63	0.22	164,168,173,174	0
12	BOG	D	2091	20/20	0.74	0.34	178,180,180,180	0
18	CDL	D	2003	42/100	0.78	0.28	144,158,180,181	0
18	CDL	P	3003	42/100	0.79	0.30	203,214,224,225	0
20	UNL	P	3014	1/-	0.79	0.31	33,33,33,33	0
20	UNL	Q	3012	1/-	0.83	0.15	8,8,8,8	0
11	PEE	W	3005	50/51	0.85	0.28	129,146,150,152	0
18	CDL	G	2004	40/100	0.85	0.14	92,97,116,117	0
11	PEE	P	3007	49/51	0.85	0.25	107,122,143,144	0
11	PEE	C	2005	50/51	0.86	0.28	122,134,139,141	0
13	AZI	C	2011	3/3	0.86	0.14	46,46,47,49	0
20	UNL	E	2012	2/-	0.88	0.14	36,36,36,38	0
11	PEE	C	2007	49/51	0.88	0.20	63,76,100,101	0
12	BOG	C	3010	12/20	0.88	0.28	168,168,170,170	0
20	UNL	P	3013	1/-	0.89	0.26	40,40,40,40	0
12	BOG	Q	3009	20/20	0.91	0.17	87,110,112,112	0
16	UQ	C	2002	19/63	0.92	0.29	123,126,128,129	0
12	BOG	E	2009	20/20	0.92	0.14	71,73,77,77	0
13	AZI	P	3011	3/3	0.92	0.21	54,54,55,56	0
16	UQ	P	3002	19/63	0.93	0.33	163,166,168,168	0
15	ICX	P	3001	30/30	0.94	0.17	101,117,133,136	0
17	HEC	D	501	43/43	0.96	0.09	25,36,45,53	0
19	FES	E	501	4/4	0.96	0.10	105,105,107,107	4
14	HEM	P	501	43/43	0.97	0.11	53,59,72,77	0
14	HEM	P	502	43/43	0.97	0.09	58,62,69,70	0
17	HEC	Q	501	43/43	0.97	0.10	76,84,88,90	0
14	HEM	C	501	43/43	0.98	0.09	30,35,50,57	0
14	HEM	C	502	43/43	0.98	0.07	25,30,40,43	0
15	ICX	C	2001	30/30	0.99	0.09	43,56,65,66	0
19	FES	R	501	4/4	0.99	0.05	60,61,62,63	0

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

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

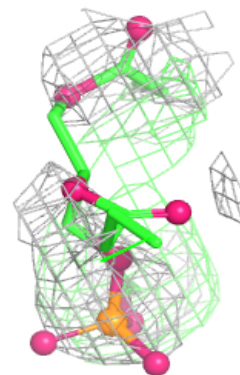
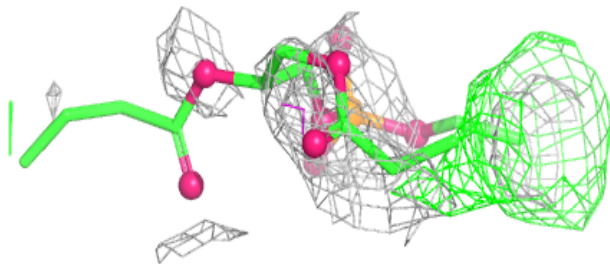
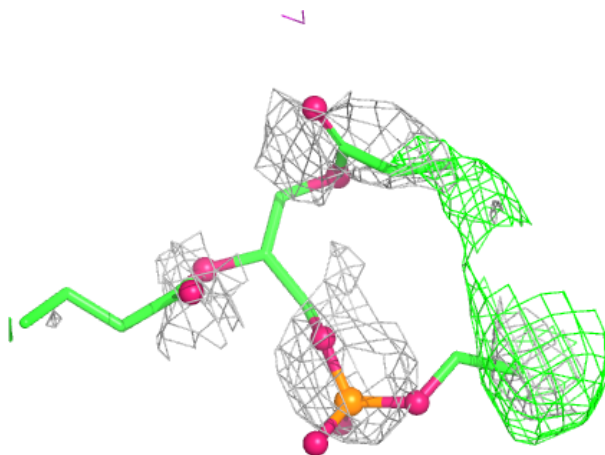
Electron density around BOG Q 3091:

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



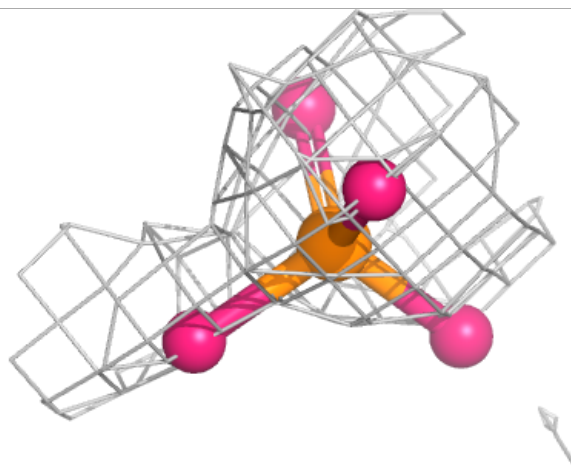
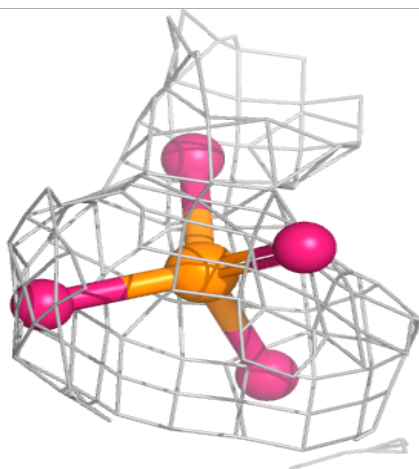
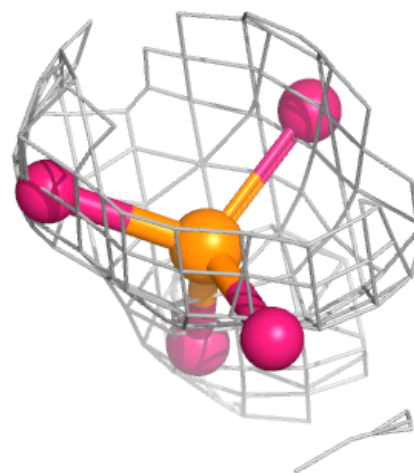
Electron density around PEE A 2008:

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



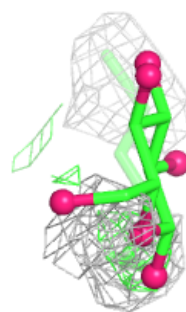
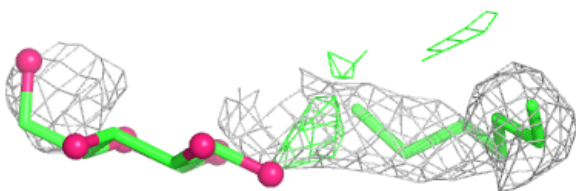
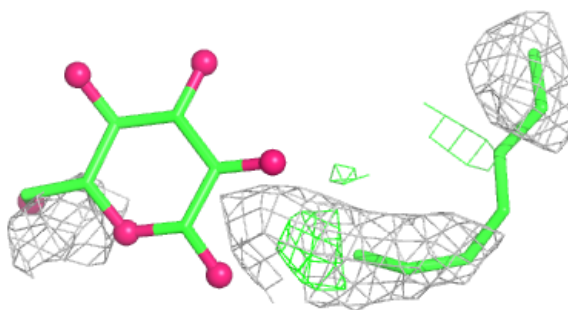
Electron density around PEE P 3008:

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



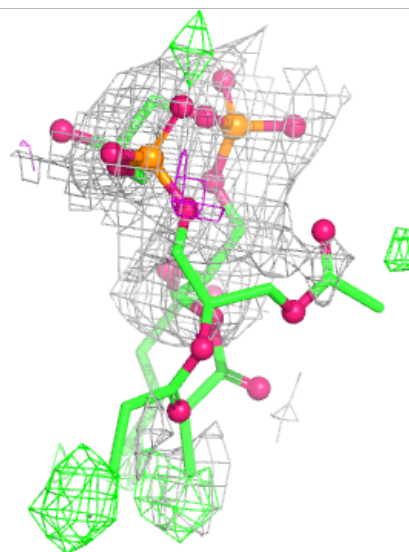
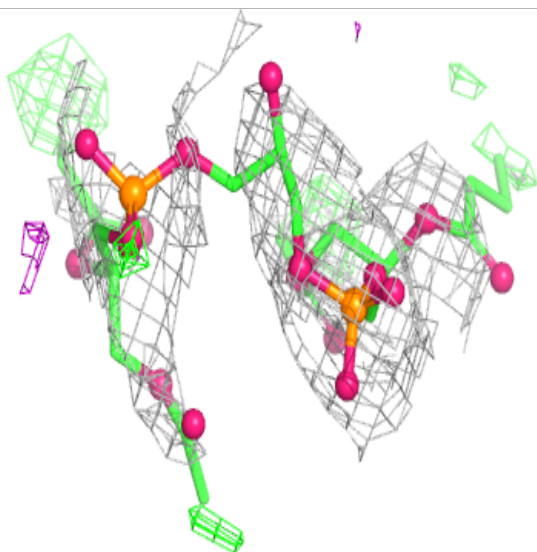
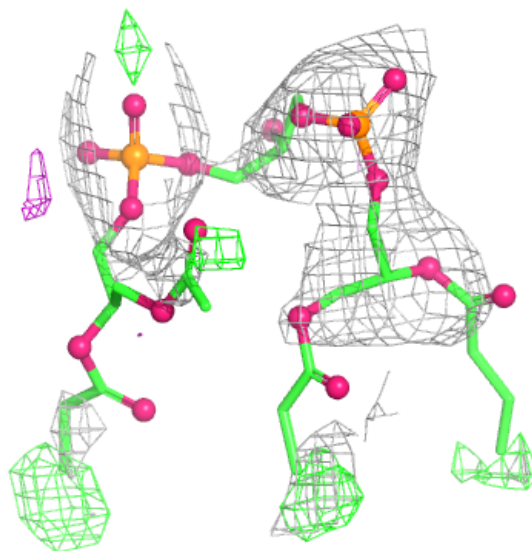
Electron density around BOG P 2010:

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



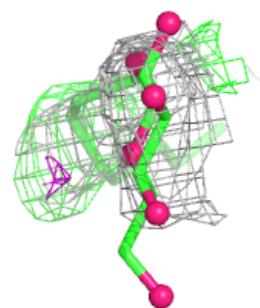
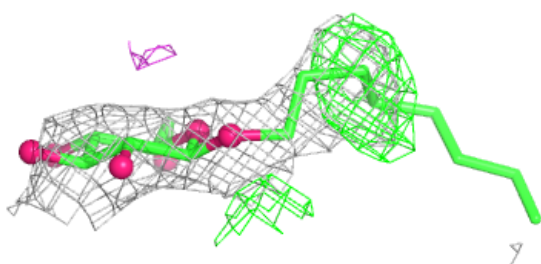
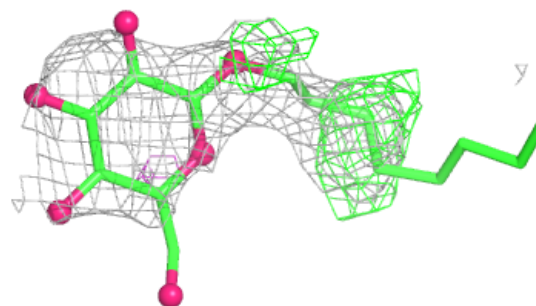
Electron density around CDL P 3004:

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

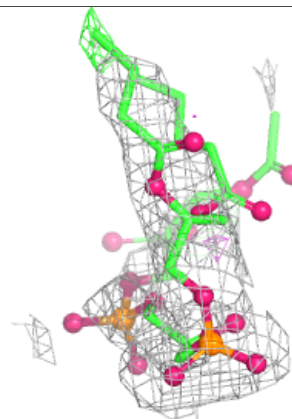
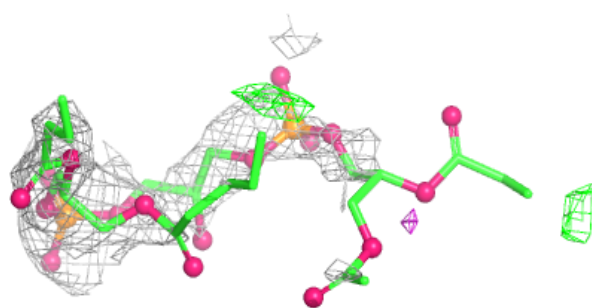
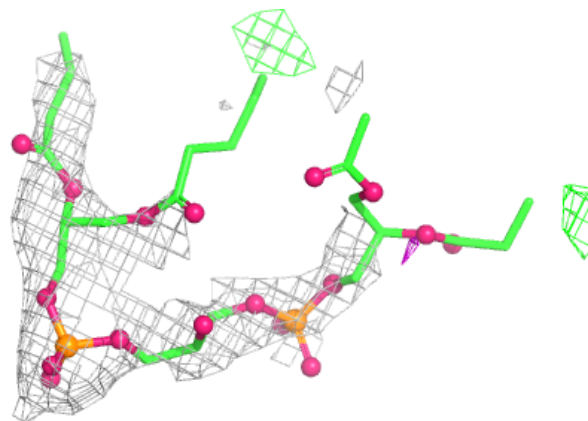


Electron density around BOG D 2091:

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

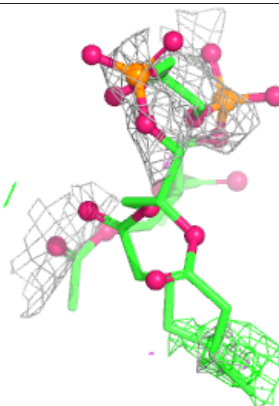
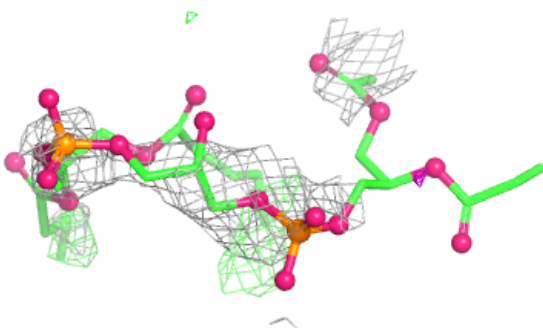
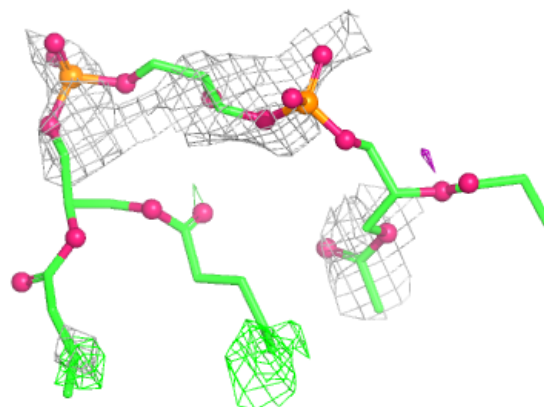
**Electron density around CDL D 2003:**

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

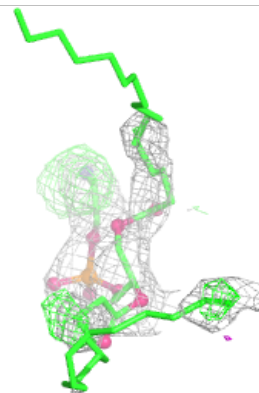
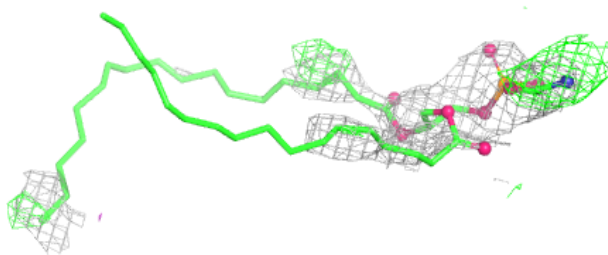
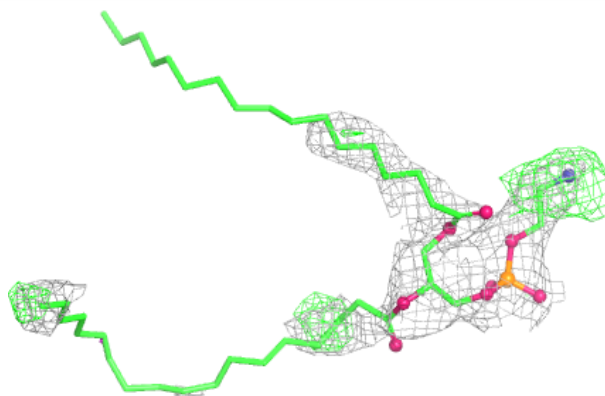


Electron density around CDL P 3003:

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

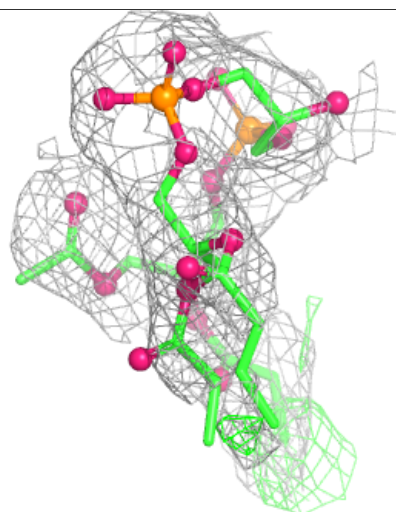
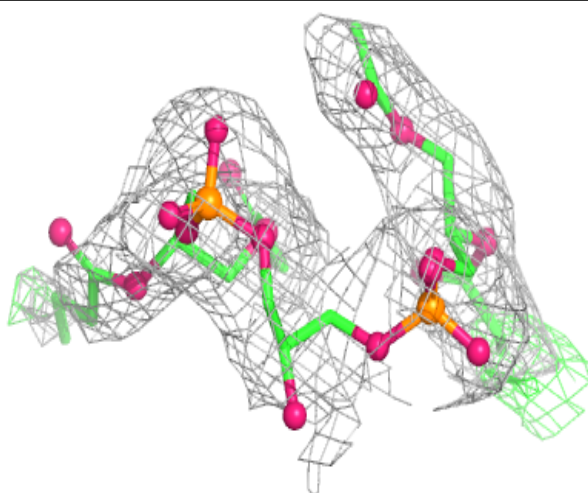
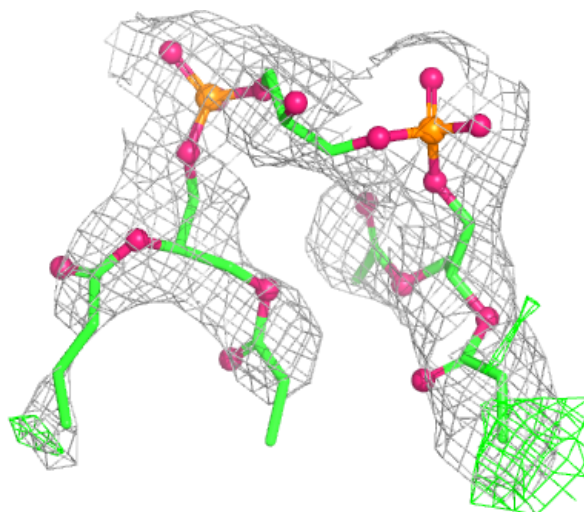
**Electron density around PEE W 3005:**

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



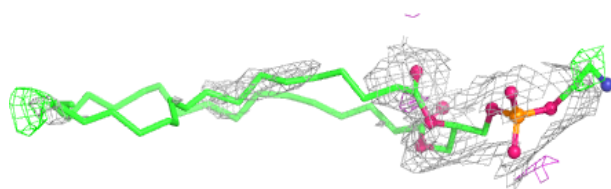
Electron density around CDL G 2004:

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

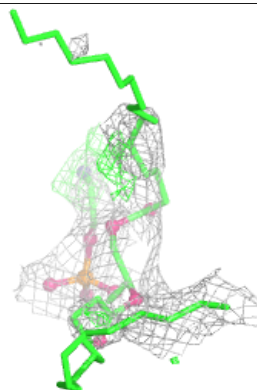
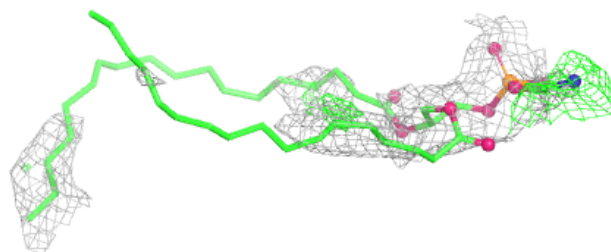
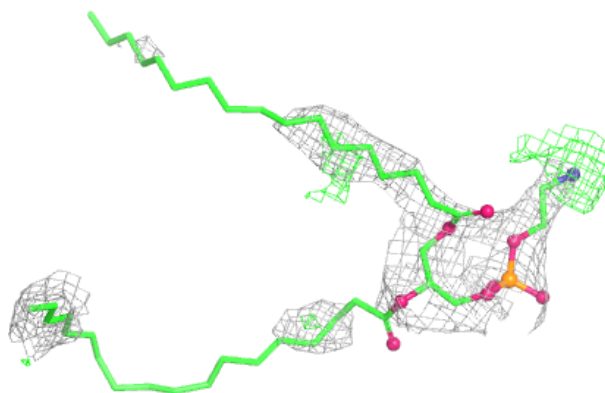


Electron density around PEE P 3007:

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

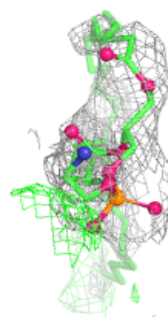
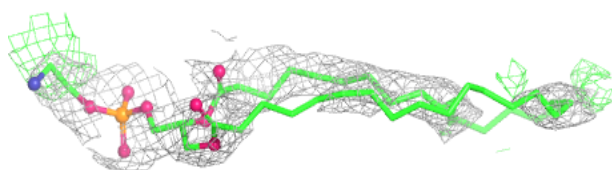
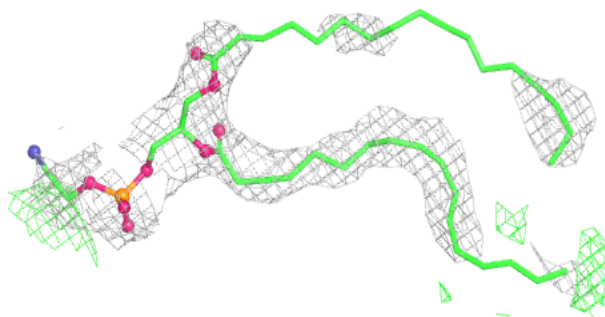
**Electron density around PEE C 2005:**

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

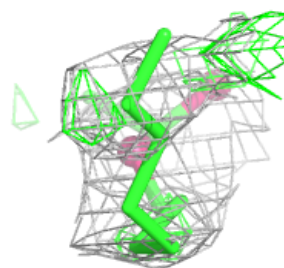
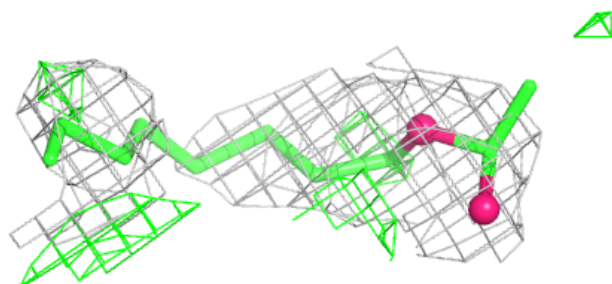
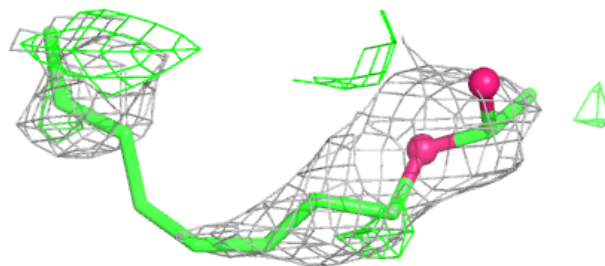


Electron density around PEE C 2007:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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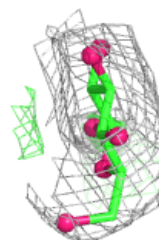
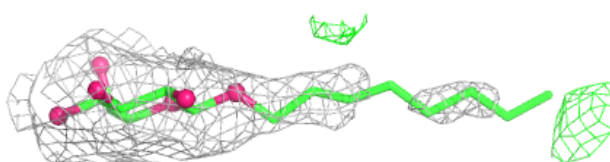
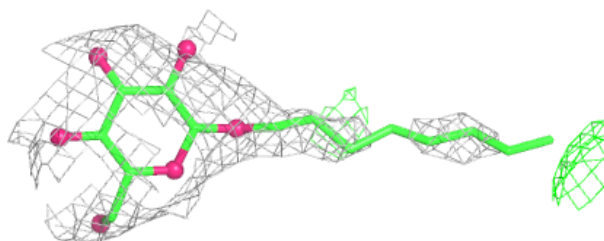
**Electron density around BOG C 3010:**

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

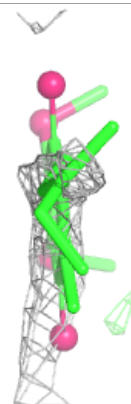
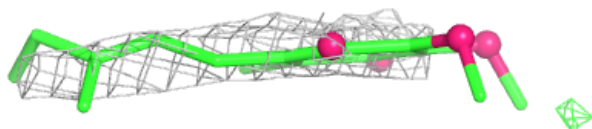


Electron density around BOG Q 3009:

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

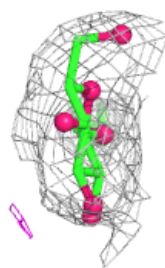
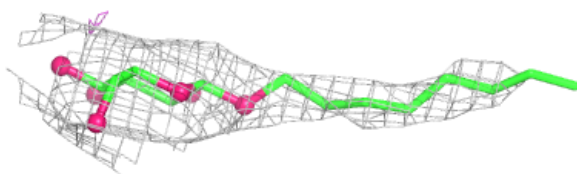
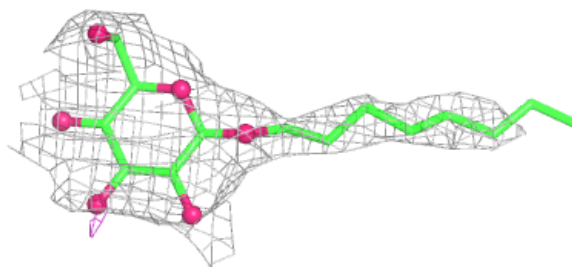
**Electron density around UQ C 2002:**

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

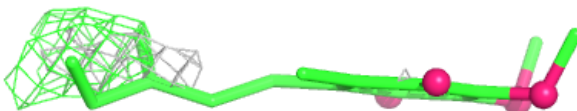
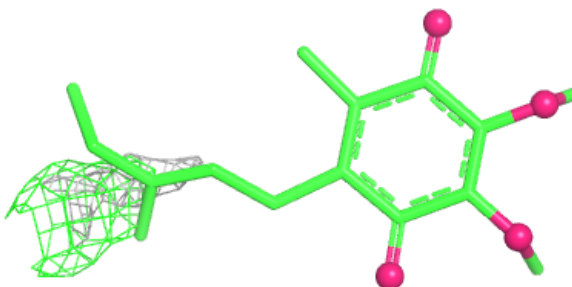


Electron density around BOG E 2009:

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

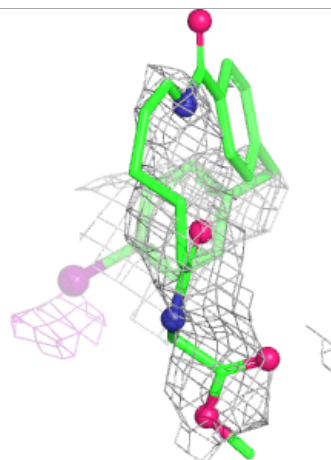
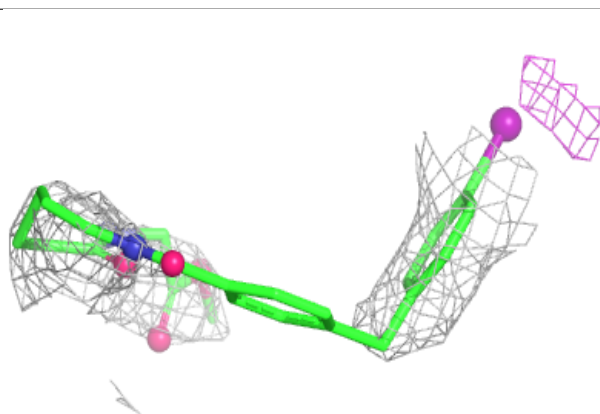
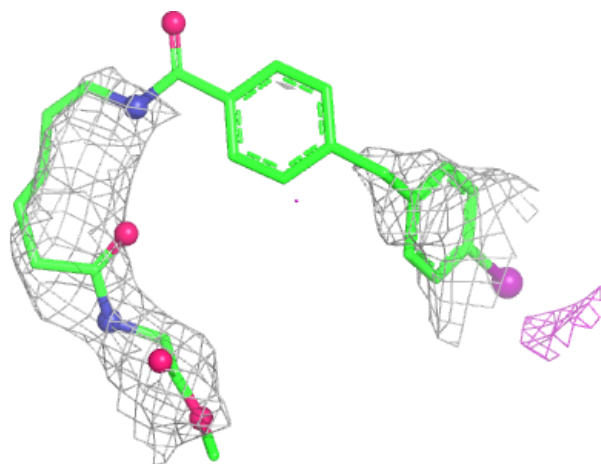
**Electron density around UQ P 3002:**

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



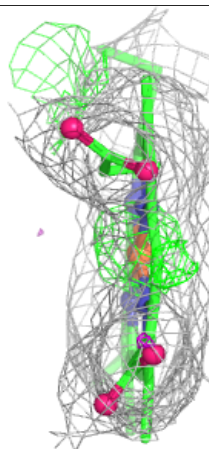
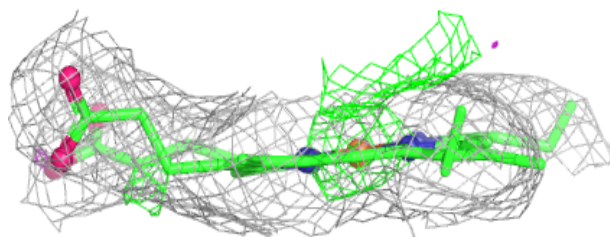
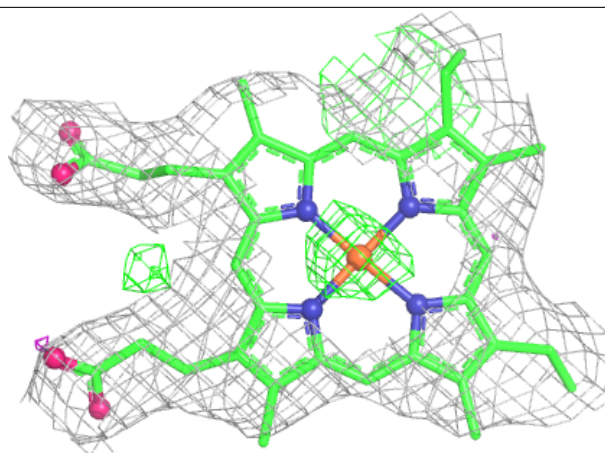
Electron density around ICX P 3001:

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



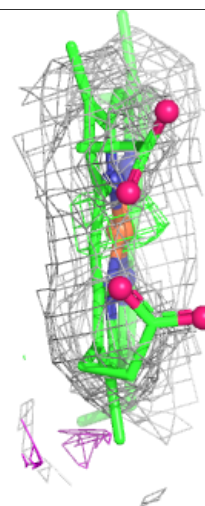
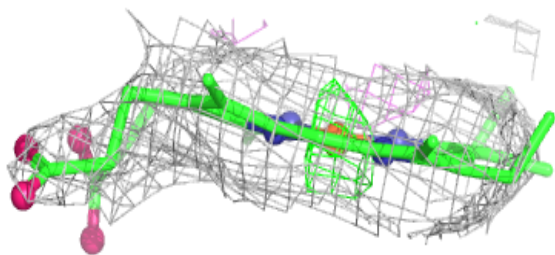
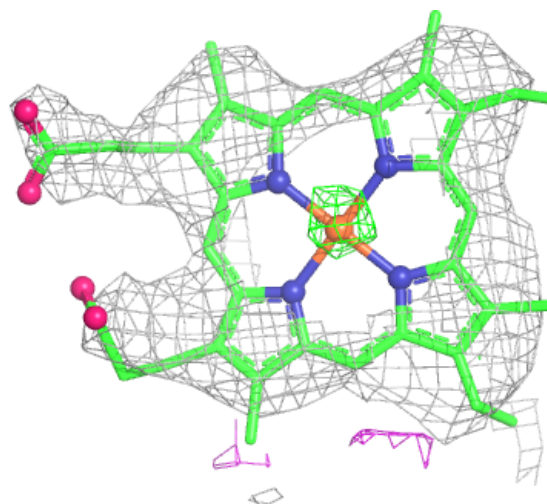
Electron density around HEC D 501:

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



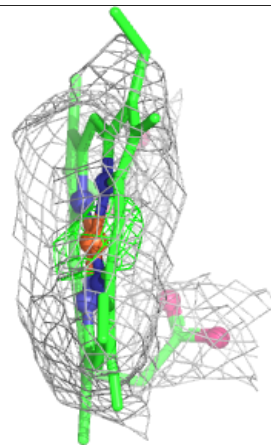
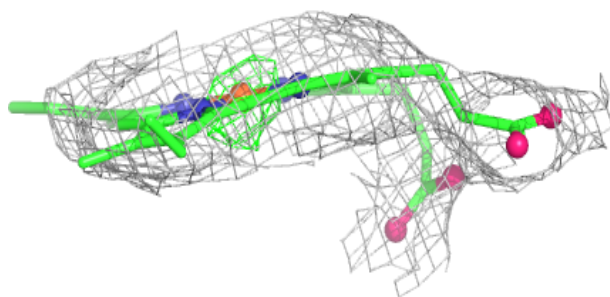
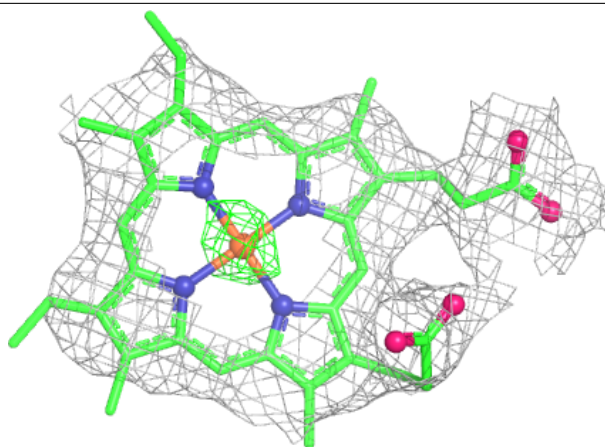
Electron density around HEM P 501:

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



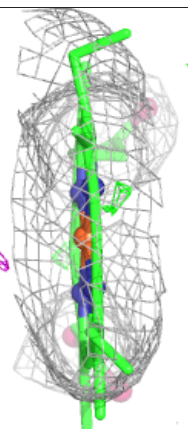
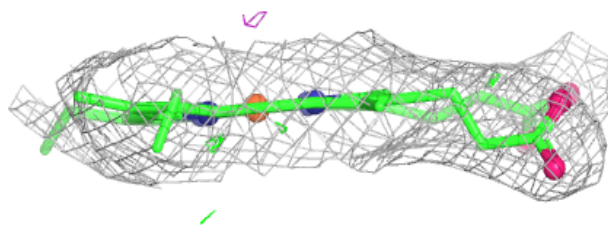
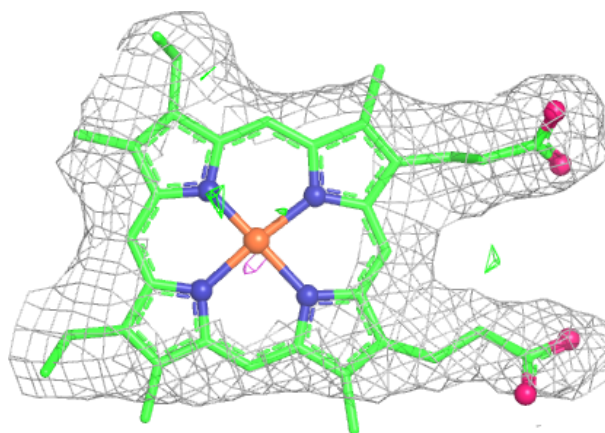
Electron density around HEM P 502:

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



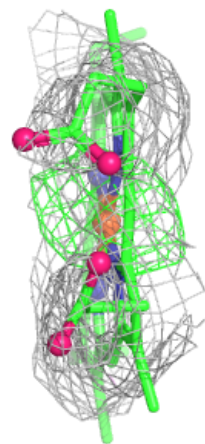
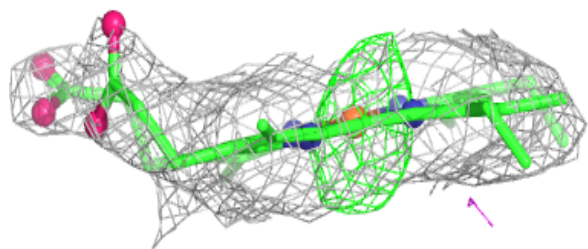
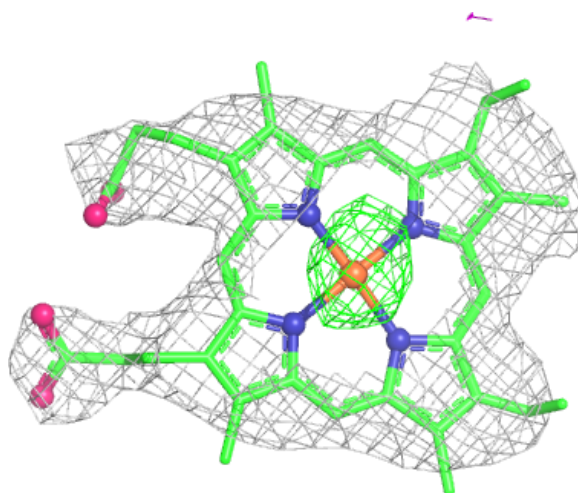
Electron density around HEC Q 501:

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



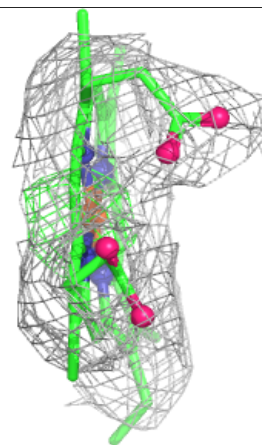
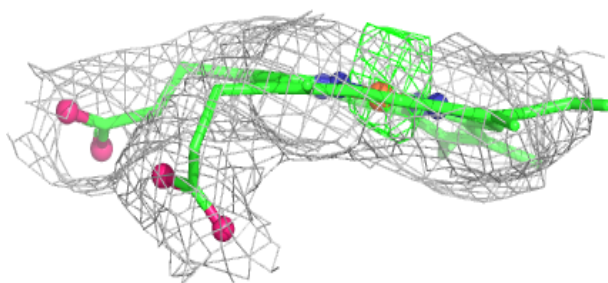
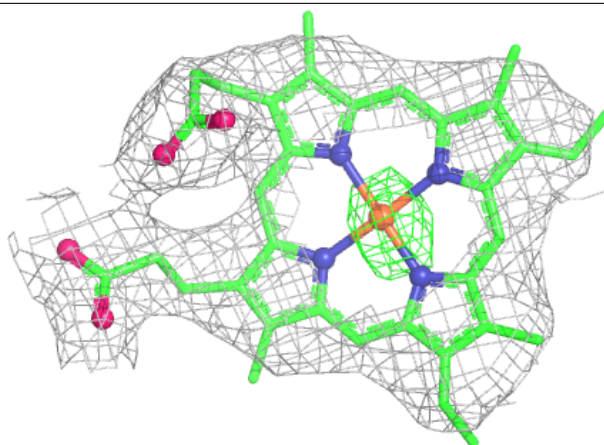
Electron density around HEM C 501:

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



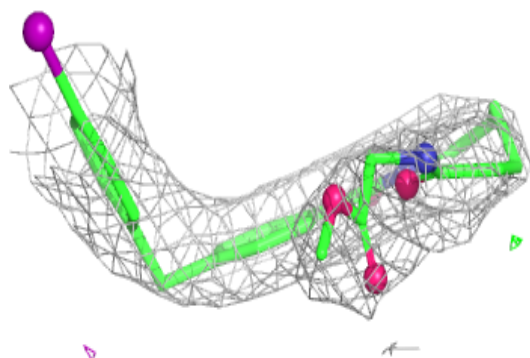
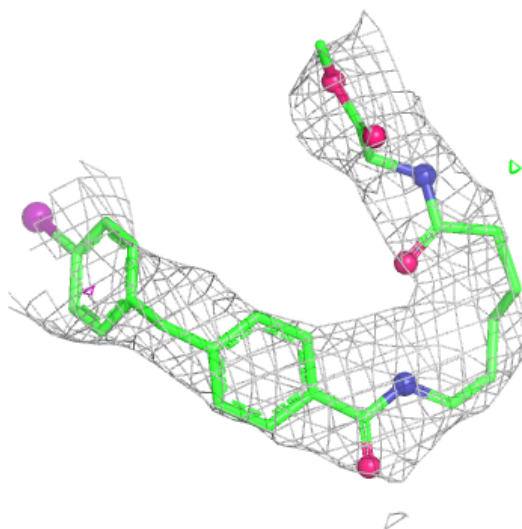
Electron density around HEM C 502:

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



Electron density around ICX 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.