Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 09:17 AM EDT

PDB ID	:	3H1K
Title	:	Chicken cytochrome BC1 complex with ZN++ and an iodinated derivative of kresoxim-methyl bound
Authors	:	Berry, E.A.; Zhang, Z.; Bellamy, H.D.; Huang, L.S.
Deposited on	:	2009-04-12
Resolution	:	3.48 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 (i) 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 (i)) were used in the production of this report:

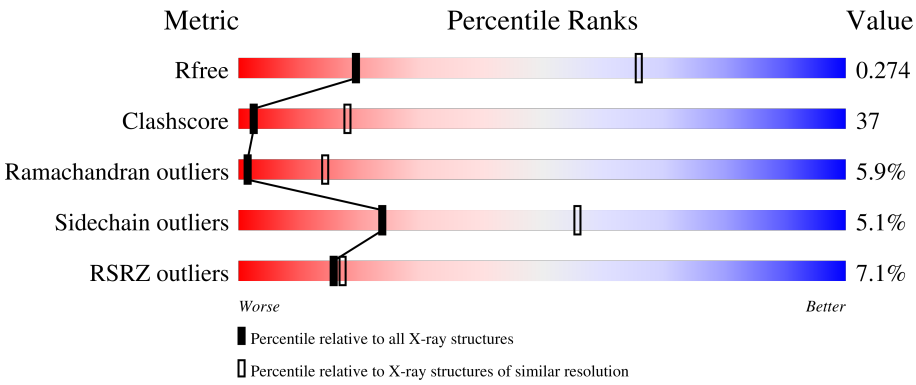
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.48 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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 <=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	2%, 44%, 50%, 5% ••
1	N	446	3%, 40%, 54%, 5% ••
2	B	441	5%, 36%, 51%, 10% •
2	O	441	2%, 34%, 52%, 9% •
3	C	380	2%, 44%, 50%, 5% •

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Mol	Chain	Length	Quality of chain
3	P	380	3% 44% 50% 5%
4	D	241	2% 40% 54% 5%
4	Q	241	3% 41% 55%
5	E	196	48% 44% 48% 8%
5	R	196	27% 41% 51% 8%
6	F	110	50% 34% 8% 8%
6	S	110	2% 51% 35% 6% 8%
7	G	81	5% 53% 38% 7%
7	T	81	19% 49% 41% 7%
8	H	77	43% 45% 10%
8	U	77	3% 39% 47% 13%
9	I	47	34% 43% 49% 6%
9	V	47	23% 40% 38% 15% 6%
10	J	61	3% 57% 34% 8%
10	W	61	3% 61% 28% 10%

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	A	2008	-	-	-	X
11	PEE	E	2005	-	-	-	X
11	PEE	P	3008	-	X	-	-
11	PEE	R	3005	-	-	-	X
12	UNL	A	3231	-	-	-	X
12	UNL	C	4234	-	-	-	X
12	UNL	N	4231	-	-	-	X
12	UNL	P	4236	-	-	-	X
16	CDL	Q	3003	-	-	-	X
20	BOG	D	2091	-	-	-	X
20	BOG	P	2010	-	-	-	X
20	BOG	P	3091	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	FES	E	501	-	-	X	-
21	FES	R	501	-	-	X	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 32673 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
			Total	C	N	O	S			
1	A	443	3442	2157	606	658	21	0	0	0
1	N	442	3437	2154	605	657	21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3164	1987	551	616	10	0	0	0
2	O	422	3147	1977	546	614	10	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	380	3020	2024	478	505	13	0	0	0
3	P	379	3012	2019	477	504	12	0	0	0

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

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

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

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

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

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

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

- 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
			Total	C	N	O	S			
8	H	69	571	348	105	113	5	0	0	0
8	U	67	553	338	103	107	5	0	0	0

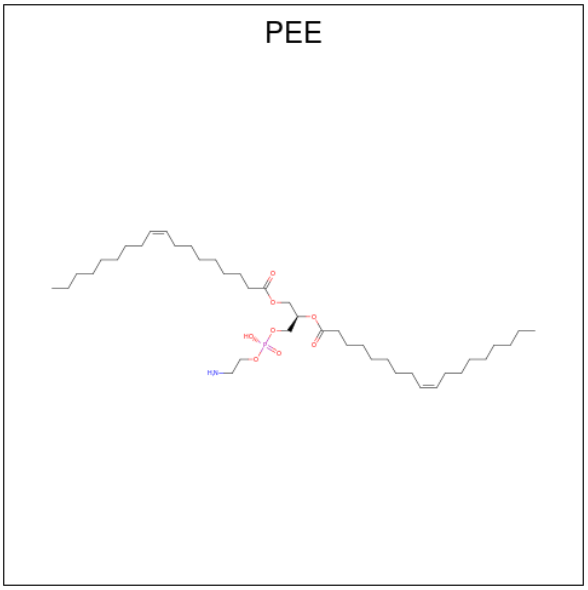
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	46	285	169	58	56	2	0	0	0
9	V	44	275	164	56	53	2	0	0	1

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O	P			
11	A	1	18	9	8	1		0	0
			Total	C	N	O	P		
11	C	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
11	E	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
11	P	1	49	39	1	8	1	0	0
			Total	O	P				
11	P	1	5	4	1			0	0
			Total	C	N	O	P		
11	R	1	50	40	1	8	1	0	0

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	2	2	2	0	0

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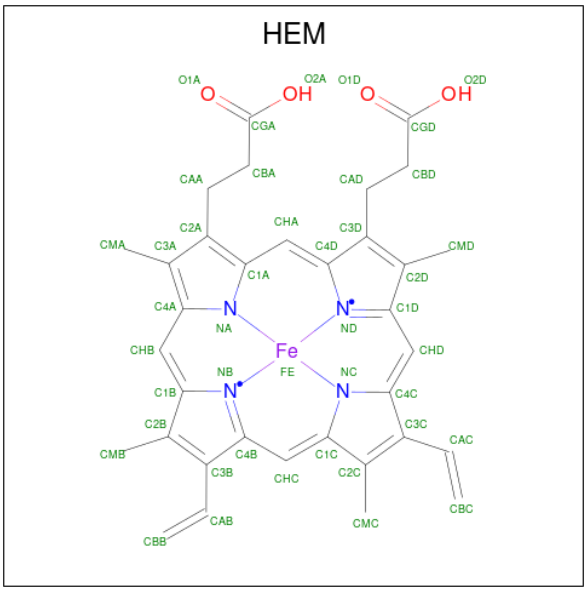
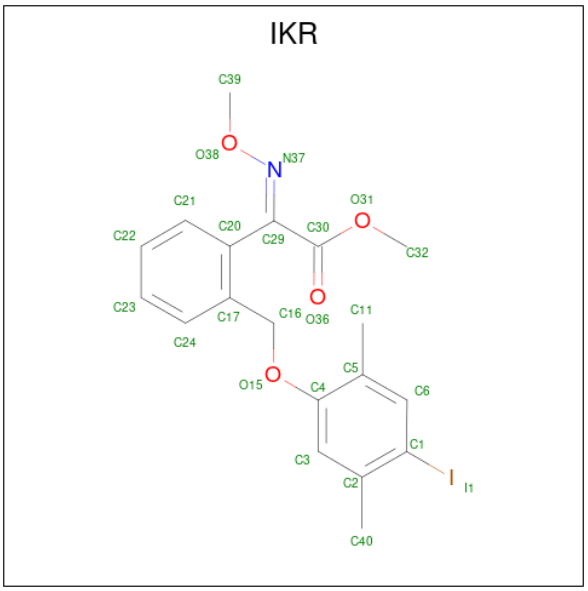
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total O 1 1	0	0
12	N	1	Total O 1 1	0	0
12	P	1	Total O 1 1	0	0

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



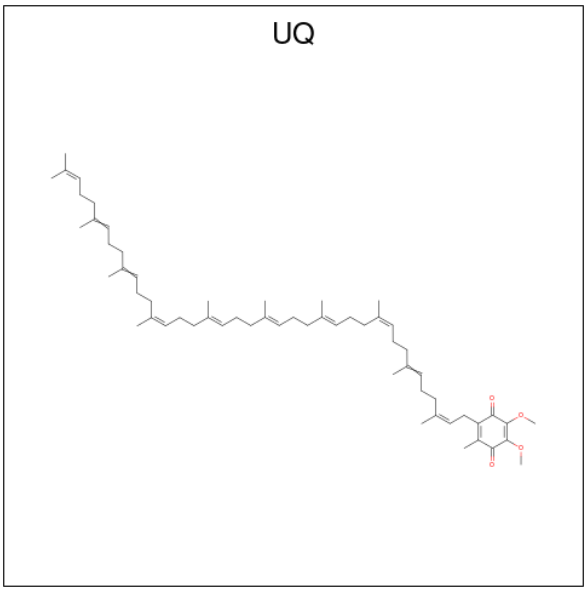
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 14 is methyl (2E)-{2-[(4-iodo-2,5-dimethylphenoxy)methyl]phenyl}(methoxyimino)ethanoate (three-letter code: IKR) (formula: $C_{19}H_{20}INO_4$).



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

- Molecule 15 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



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

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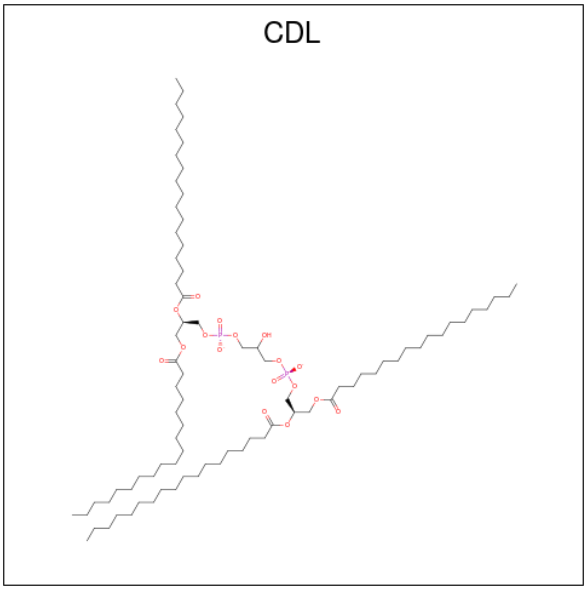
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	P	1	19	15	4	0	0

- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

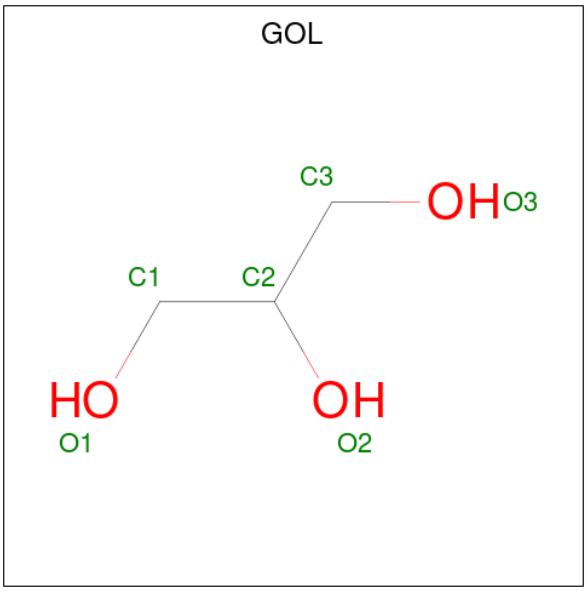


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
16	C	1	40	21	17	2	0	0
			Total	C	O	P		
16	D	1	42	23	17	2	0	0
			Total	C	O	P		
16	P	1	40	21	17	2	0	0
			Total	C	O	P		
16	Q	1	42	23	17	2	0	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

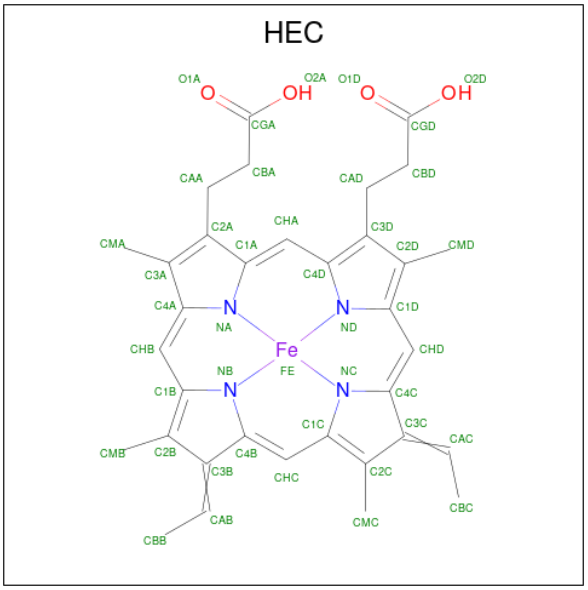
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
17	C	1	1	1	0	0
			Total	Zn		
17	P	1	1	1	0	0

- Molecule 18 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



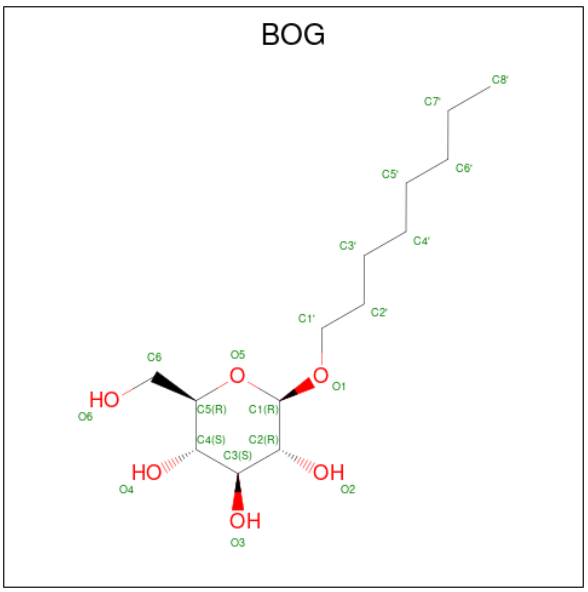
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	C	1	6	3	3	0	0
			Total	C	O		
18	P	1	6	3	3	0	0

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



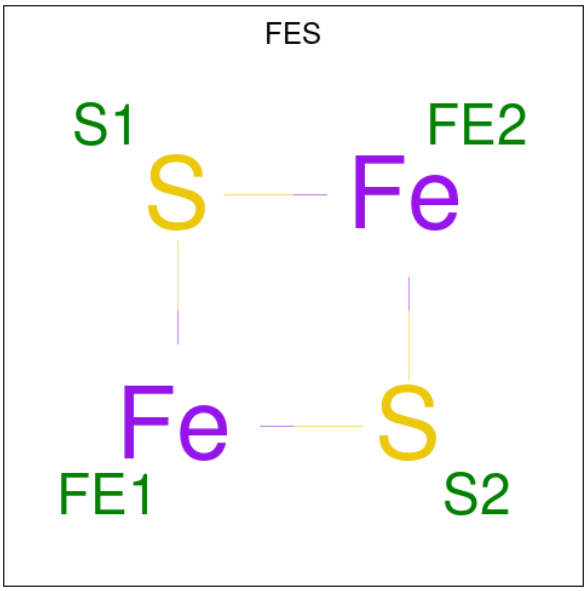
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
19	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
19	Q	1	43	34	1	4	4	0	0

- Molecule 20 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 22 is water.

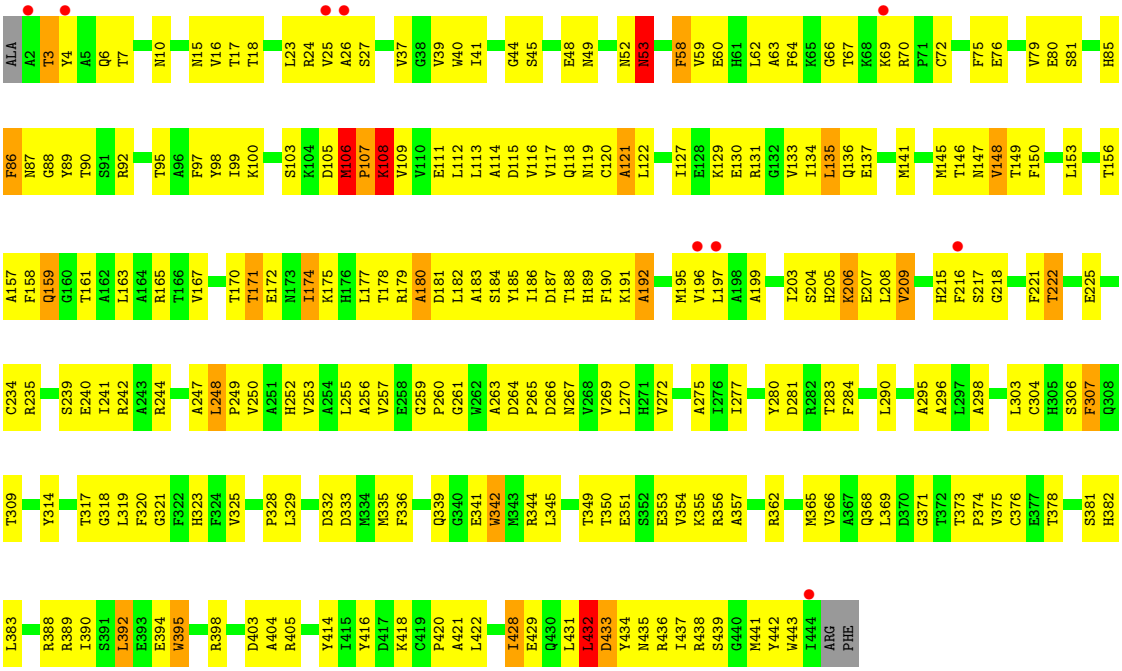
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
22	A	1	1	1	0	0
			Total	O		
22	C	7	7	7	0	0
			Total	O		
22	E	1	1	1	0	0
			Total	O		
22	P	7	7	7	0	0
			Total	O		
22	R	1	1	1	0	0

3 Residue-property plots (i)

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

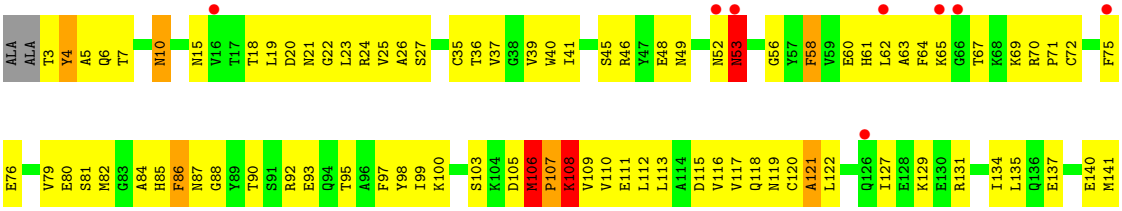
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

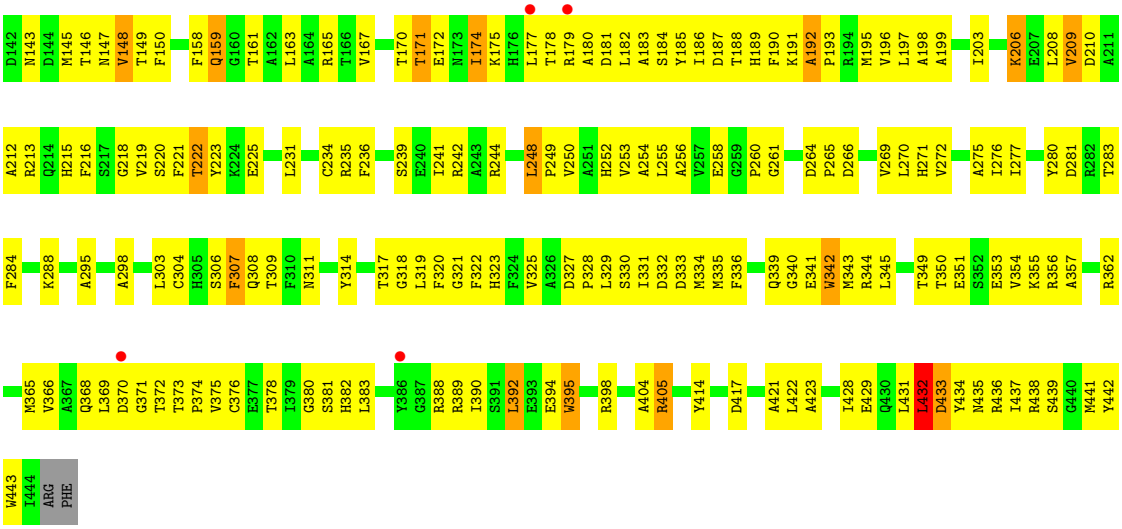
Chain A:



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

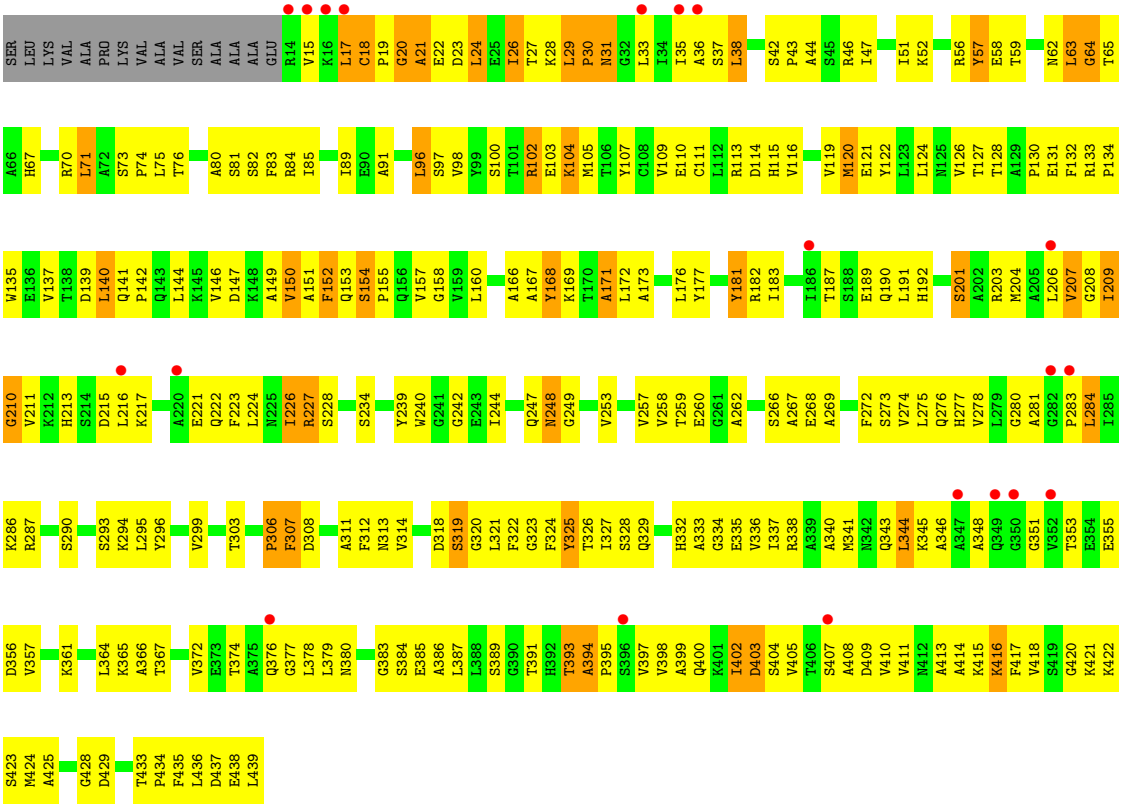
Chain N:





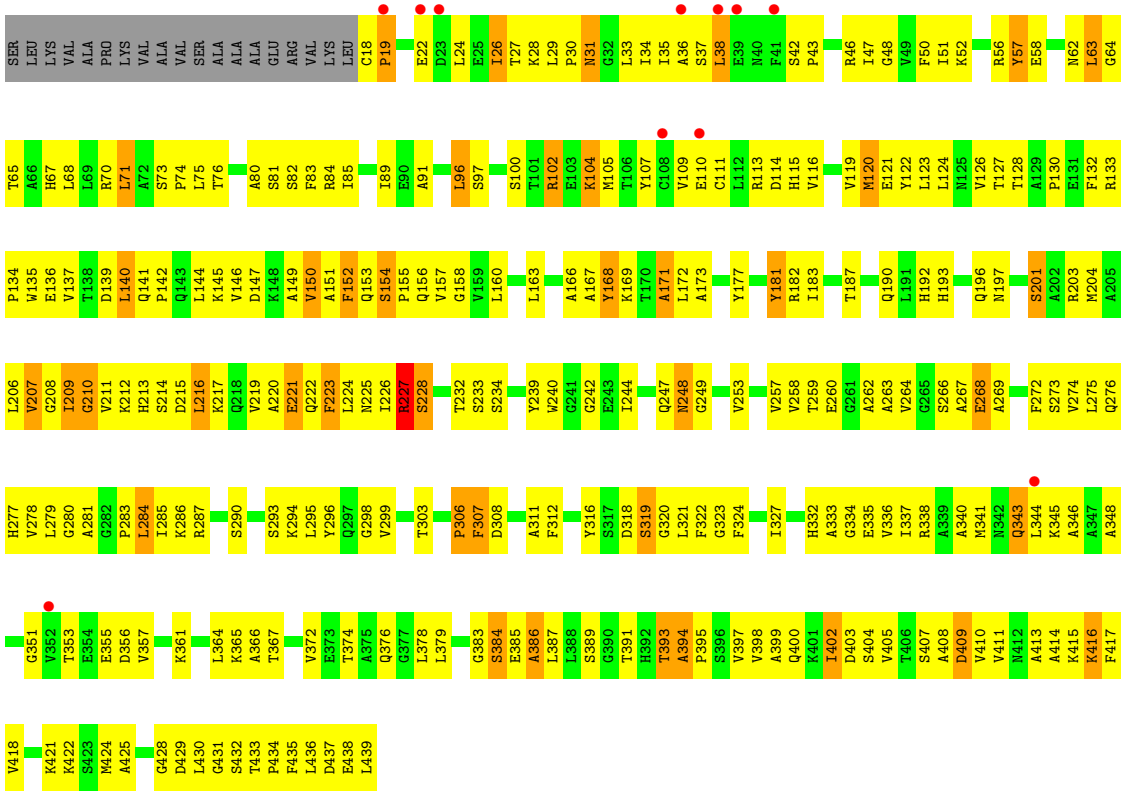
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



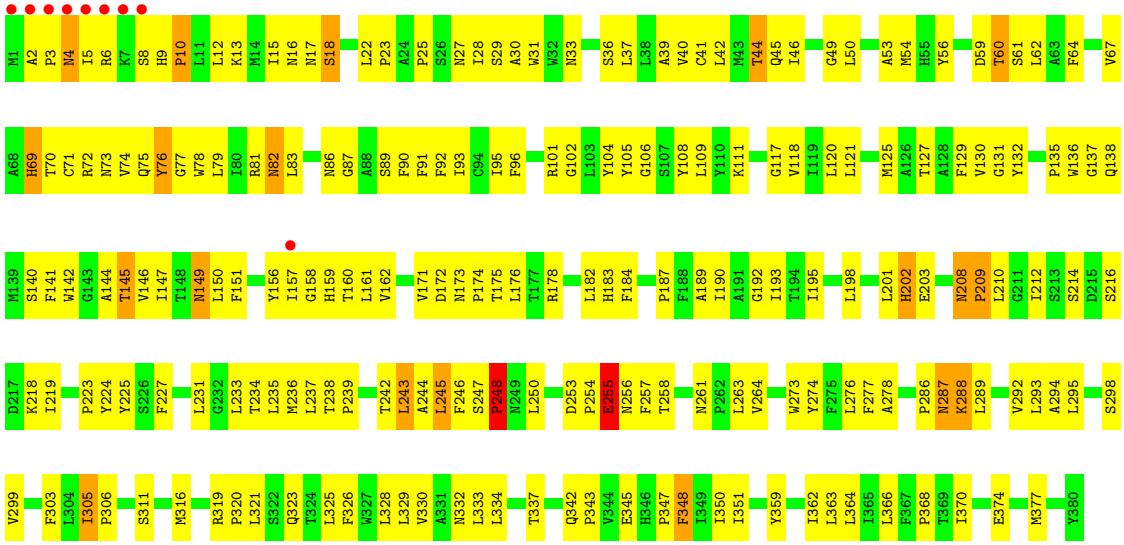
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain O:



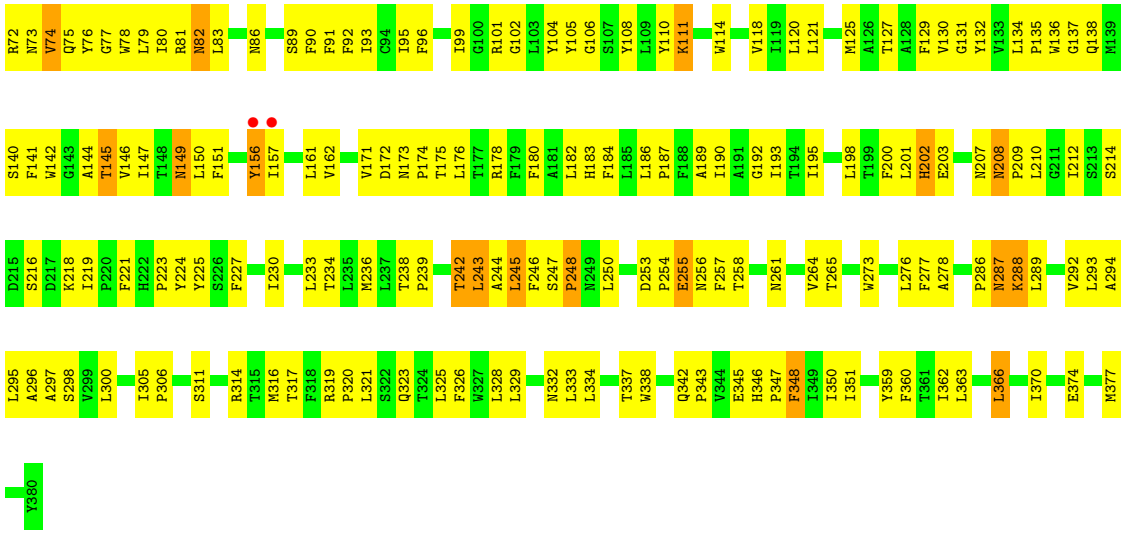
• Molecule 3: Cytochrome b

Chain C:



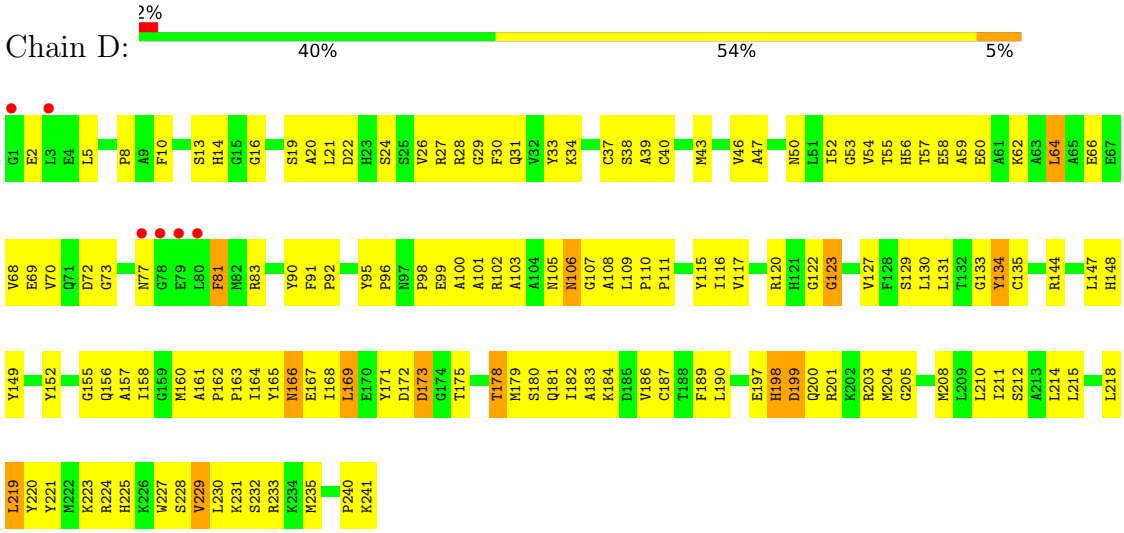
• Molecule 3: Cytochrome b

Chain P:



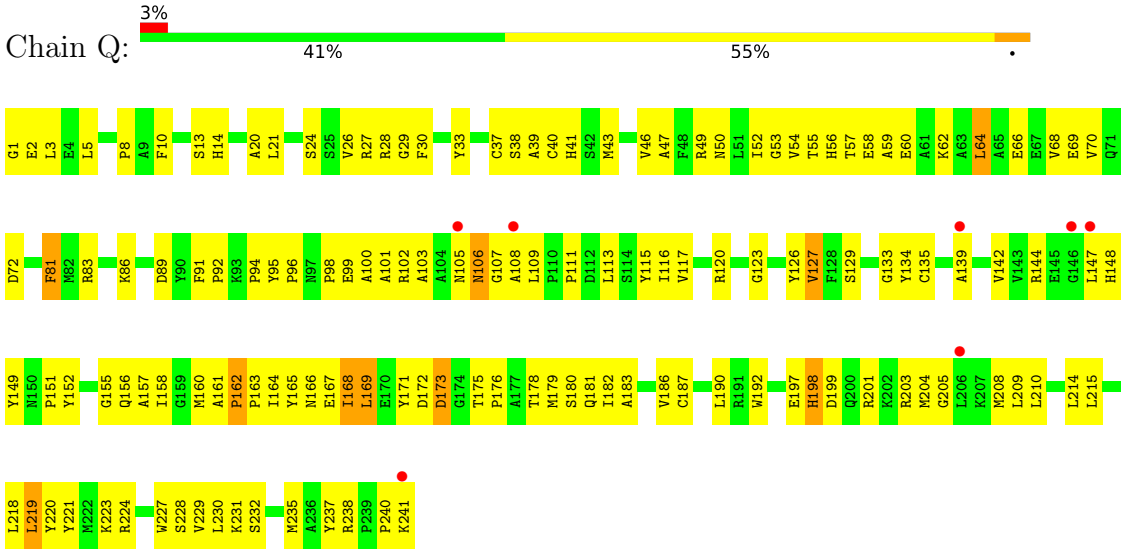
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:



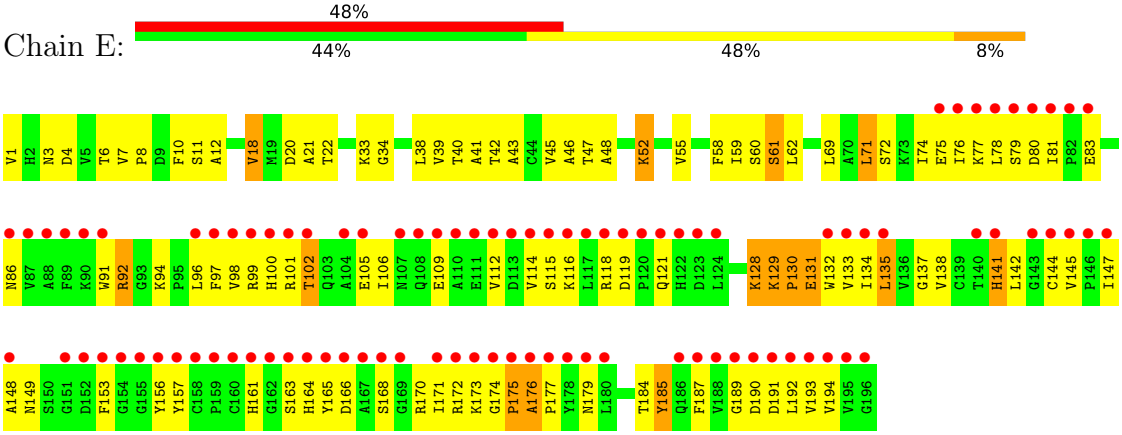
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:



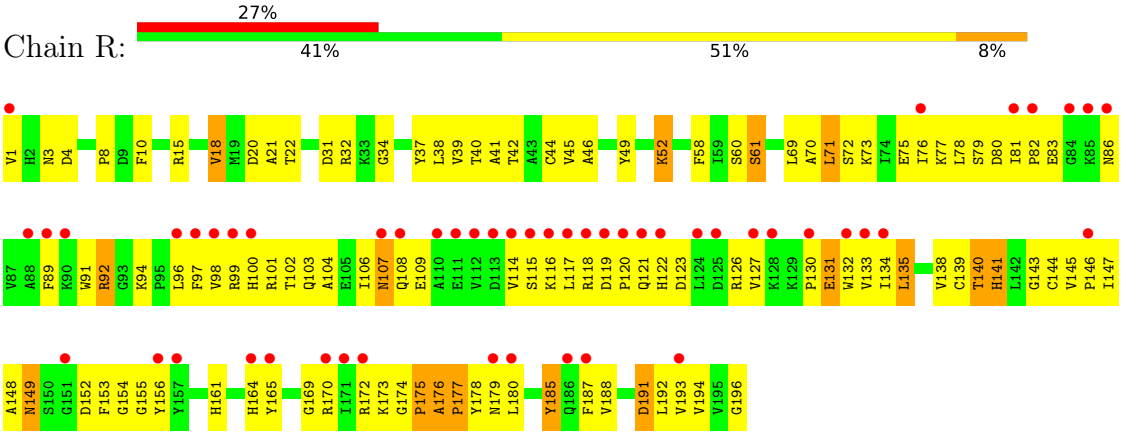
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



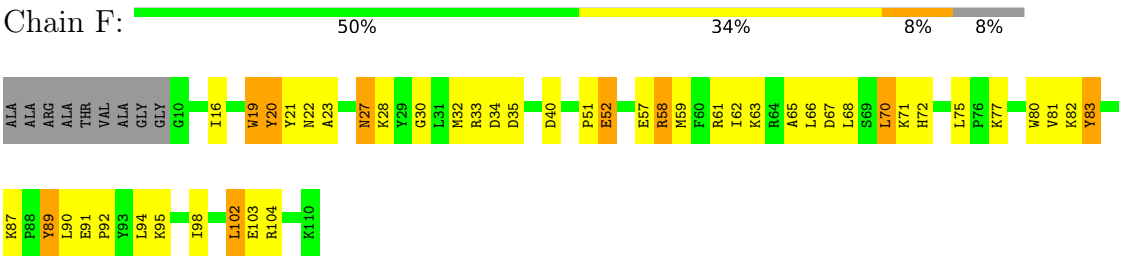
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:



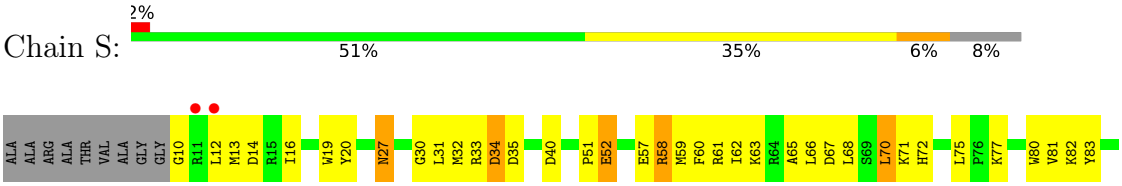
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

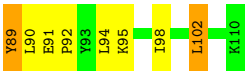
Chain F:



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

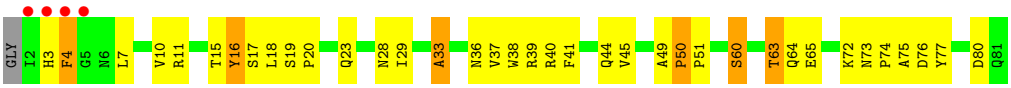
Chain S:





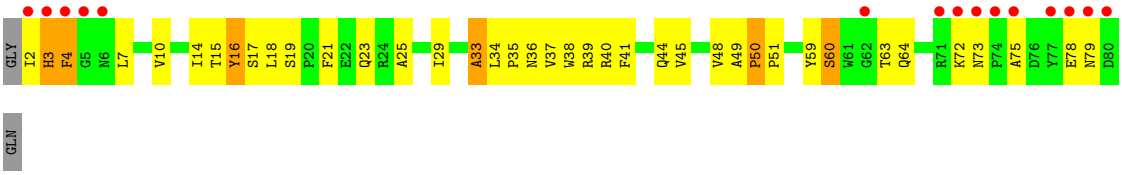
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:



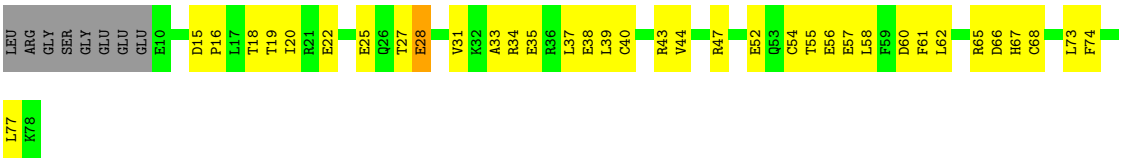
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:



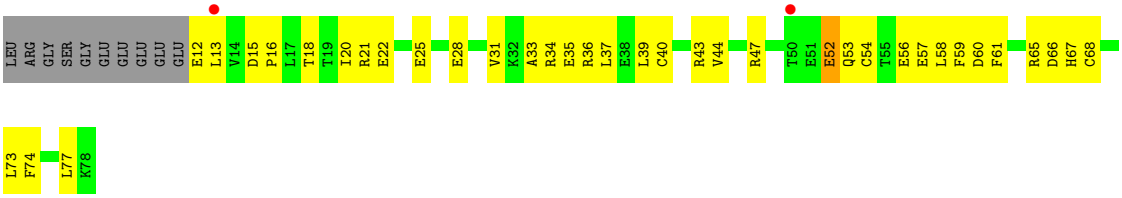
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:



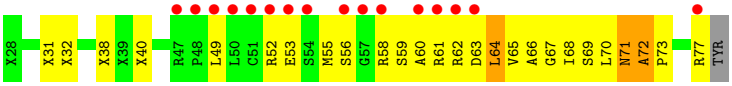
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



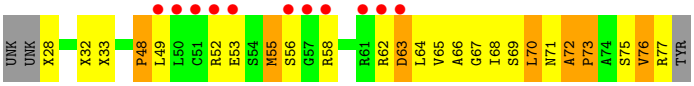
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



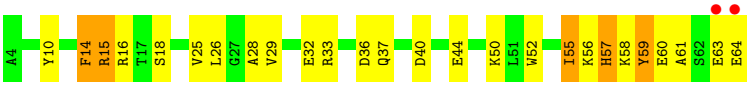
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



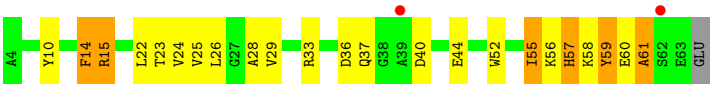
• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:



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

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	171.72Å 181.30Å 241.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.48 42.60 – 3.48	Depositor EDS
% Data completeness (in resolution range)	89.7 (18.00-3.48) 89.7 (42.60-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.284 0.230 , 0.274	Depositor DCC
R_{free} test set	2570 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å^2)	101.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 83.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32673	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.48	0/3513	0.70	1/4760 (0.0%)
1	N	0.50	0/3508	0.70	1/4753 (0.0%)
2	B	0.41	0/3219	0.64	0/4364
2	O	0.46	0/3202	0.67	0/4343
3	C	0.54	0/3122	0.70	0/4273
3	P	0.48	0/3114	0.67	0/4263
4	D	0.52	0/1956	0.68	0/2658
4	Q	0.44	0/1956	0.65	0/2658
5	E	0.37	0/1547	0.56	0/2103
5	R	0.39	0/1547	0.59	0/2103
6	F	0.52	0/911	0.67	0/1219
6	S	0.45	0/911	0.61	0/1219
7	G	0.54	0/694	0.72	0/941
7	T	0.49	0/684	0.71	0/929
8	H	0.50	0/579	0.68	0/775
8	U	0.40	0/561	0.60	0/751
9	I	0.37	0/218	0.64	0/293
9	V	0.40	0/218	0.66	0/293
10	J	0.50	0/508	0.60	0/682
10	W	0.43	0/490	0.61	0/660
All	All	0.47	0/32458	0.66	2/44040 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
4	D	0	1
6	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	LEU	N-CA-C	5.68	126.33	111.00
1	N	432	LEU	N-CA-C	5.29	125.30	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	56	TYR	Sidechain
3	C	76	TYR	Sidechain
4	D	134	TYR	Sidechain
6	F	20	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3354	261	0
1	N	3437	0	3349	280	0
2	B	3164	0	3158	303	0
2	O	3147	0	3146	336	0
3	C	3020	0	3070	240	0
3	P	3012	0	3058	231	0
4	D	1898	0	1846	167	0
4	Q	1898	0	1846	169	0
5	E	1513	0	1478	111	0
5	R	1513	0	1478	118	0
6	F	891	0	893	50	0
6	S	891	0	893	50	0
7	G	672	0	653	38	0
7	T	662	0	645	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	571	0	547	33	0
8	U	553	0	535	41	0
9	I	285	0	238	37	0
9	V	275	0	238	39	0
10	J	497	0	490	28	0
10	W	479	0	478	32	0
11	A	18	0	11	0	0
11	C	49	0	72	3	0
11	E	50	0	77	0	0
11	P	54	0	72	4	0
11	R	50	0	77	0	0
12	A	2	0	0	0	0
12	C	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
13	C	86	0	60	19	0
13	P	86	0	60	20	0
14	C	25	0	20	5	0
14	P	25	0	20	4	0
15	C	19	0	17	6	0
15	P	19	0	17	6	0
16	C	40	0	24	2	0
16	D	42	0	28	1	0
16	P	40	0	24	2	0
16	Q	42	0	28	3	0
17	C	1	0	0	0	0
17	P	1	0	0	0	0
18	C	6	0	8	1	0
18	P	6	0	8	1	0
19	D	43	0	30	2	0
19	Q	43	0	30	2	0
20	D	33	0	39	1	0
20	P	25	0	22	0	0
20	Q	20	0	28	0	0
21	E	4	0	0	3	0
21	R	4	0	0	2	0
22	A	1	0	0	0	0
22	C	7	0	0	1	0
22	E	1	0	0	0	0
22	P	7	0	0	3	0
22	R	1	0	0	1	0
All	All	32673	0	32165	2414	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 37.

All (2414) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:HG22	2:B:210:GLY:H	1.08	1.09
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.28	1.07
2:O:209:ILE:HG22	2:O:210:GLY:H	1.09	1.07
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.38	1.06
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.26	0.99
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.45	0.98
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.43	0.98
3:C:120:LEU:HD13	13:C:502:HEM:HBB2	1.44	0.97
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.47	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	0.97
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.45	0.96
4:D:158:ILE:HG12	4:D:160:MET:H	1.31	0.94
5:R:148:ALA:HA	5:R:156:TYR:HA	1.49	0.94
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.48	0.94
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.48	0.94
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.50	0.93
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.51	0.93
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.50	0.91
2:B:207:VAL:HG12	2:B:208:GLY:H	1.35	0.91
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.51	0.91
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.50	0.91
2:O:71:LEU:O	2:O:74:PRO:HD2	1.71	0.91
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.49	0.91
2:O:76:THR:HG22	2:O:82:SER:H	1.35	0.91
5:E:147:ILE:HG22	5:E:148:ALA:H	1.33	0.90
4:Q:43:MET:HE2	4:Q:46:VAL:HG21	1.52	0.90
1:A:206:LYS:O	1:A:209:VAL:HG12	1.71	0.90
2:B:327:ILE:HD11	9:I:58:ARG:O	1.71	0.90
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.52	0.90
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.52	0.89
4:D:57:THR:HG22	4:D:59:ALA:H	1.36	0.89
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.35	0.89
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.37	0.89
2:O:96:LEU:HB2	2:O:109:VAL:HG12	1.55	0.88
1:A:248:LEU:HD13	1:A:249:PRO:HD2	1.54	0.88
2:B:209:ILE:HG22	2:B:210:GLY:N	1.87	0.88
9:V:49:LEU:HB3	9:V:55:MET:HG2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.88
2:O:209:ILE:HG22	2:O:210:GLY:N	1.87	0.88
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.56	0.88
1:N:328:PRO:HG2	1:N:329:LEU:HD12	1.55	0.88
4:D:47:ALA:H	4:D:50:ASN:HD22	1.19	0.87
7:T:29:ILE:O	7:T:33:ALA:HB3	1.73	0.87
2:O:207:VAL:HG12	2:O:208:GLY:H	1.37	0.87
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.37	0.87
9:I:32:UNK:N	9:I:73:PRO:HG2	1.89	0.87
5:R:58:PHE:O	5:R:61:SER:HB3	1.75	0.86
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.40	0.86
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.38	0.86
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.55	0.86
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.38	0.86
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.38	0.86
1:N:248:LEU:HD13	1:N:249:PRO:HD2	1.56	0.85
2:B:71:LEU:O	2:B:74:PRO:HD2	1.75	0.85
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.40	0.85
2:O:201:SER:HB3	2:O:227:ARG:HB2	1.56	0.85
2:B:96:LEU:HB2	2:B:109:VAL:HG12	1.57	0.85
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.59	0.84
3:C:125:MET:HE2	14:C:2001:IKR:I1	2.48	0.84
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.60	0.83
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.13	0.83
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.60	0.83
1:N:206:LYS:O	1:N:209:VAL:HG12	1.77	0.83
3:C:125:MET:CE	14:C:2001:IKR:I1	2.96	0.82
3:C:253:ASP:OD1	3:C:255:GLU:HG2	1.79	0.82
2:O:201:SER:H	2:O:227:ARG:HB3	1.41	0.82
2:O:353:THR:HG22	2:O:355:GLU:H	1.43	0.82
2:O:209:ILE:CG2	2:O:210:GLY:H	1.91	0.81
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.63	0.81
2:O:353:THR:HB	2:O:356:ASP:OD1	1.81	0.81
2:B:209:ILE:CG2	2:B:210:GLY:H	1.91	0.81
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.77	0.81
2:O:100:SER:HB3	2:O:105:MET:HG2	1.61	0.81
6:S:89:TYR:HD1	6:S:90:LEU:N	1.79	0.81
3:C:118:VAL:N	13:C:502:HEM:HBC2	1.96	0.81
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.46	0.81
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.62	0.81
2:B:353:THR:HG22	2:B:355:GLU:H	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.22	0.80
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.46	0.80
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.63	0.80
2:B:71:LEU:HD11	2:B:144:LEU:HD23	1.62	0.80
1:A:161:THR:HB	1:A:234:CYS:SG	2.22	0.80
1:N:105:ASP:O	1:N:109:VAL:HG23	1.82	0.80
9:V:49:LEU:HD22	9:V:55:MET:HB3	1.62	0.80
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.62	0.80
5:E:116:LYS:H	5:E:116:LYS:HD2	1.46	0.80
1:N:161:THR:HB	1:N:234:CYS:SG	2.21	0.80
1:N:382:HIS:ND1	1:N:389:ARG:HD2	1.98	0.79
3:P:120:LEU:HD13	13:P:502:HEM:HBB2	1.65	0.79
2:B:100:SER:HB3	2:B:105:MET:HG2	1.63	0.79
7:G:29:ILE:O	7:G:33:ALA:HB3	1.81	0.79
3:P:138:GLN:HB2	3:P:255:GLU:O	1.83	0.79
1:N:134:ILE:HG21	1:N:174:ILE:HG12	1.65	0.78
2:B:122:TYR:O	2:B:126:VAL:HG23	1.83	0.78
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.23	0.78
3:P:253:ASP:OD1	3:P:255:GLU:HG2	1.83	0.78
1:A:328:PRO:HG2	1:A:329:LEU:HD12	1.64	0.78
2:O:221:GLU:HG3	2:O:222:GLN:H	1.48	0.78
4:Q:127:VAL:HG12	4:Q:187:CYS:SG	2.23	0.78
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.13	0.78
5:E:114:VAL:HG21	5:E:172:ARG:NH1	1.97	0.78
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.66	0.78
6:F:89:TYR:HD1	6:F:90:LEU:N	1.81	0.78
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.66	0.78
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.66	0.78
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.49	0.78
5:R:188:VAL:O	5:R:192:LEU:HB2	1.83	0.78
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.67	0.77
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.67	0.77
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.66	0.77
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.66	0.77
3:C:61:SER:O	3:C:62:LEU:HG	1.84	0.77
2:O:102:ARG:HG2	2:O:102:ARG:NH1	1.98	0.77
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.67	0.77
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.19	0.77
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.48	0.77
2:O:160:LEU:HB3	9:V:64:LEU:HD22	1.68	0.77
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.67	0.76
1:N:277:ILE:HD11	1:N:345:LEU:HD11	1.66	0.76
3:P:12:LEU:HD23	3:P:15:ILE:HD12	1.67	0.76
3:C:120:LEU:CD1	13:C:502:HEM:HBB2	2.15	0.76
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.47	0.76
3:P:145:THR:O	3:P:149:ASN:HB2	1.85	0.76
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.50	0.76
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.50	0.76
2:O:37:SER:HB2	2:O:213:HIS:ND1	2.01	0.76
2:O:156:GLN:HE22	9:V:77:ARG:C	1.88	0.76
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.01	0.75
2:O:341:MET:HE2	2:O:341:MET:HA	1.66	0.75
3:C:120:LEU:HB3	13:C:502:HEM:CBB	2.16	0.75
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.01	0.75
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.51	0.75
4:D:43:MET:CE	4:D:46:VAL:HG21	2.16	0.75
1:N:170:THR:HG22	1:N:171:THR:H	1.51	0.75
3:P:118:VAL:N	13:P:502:HEM:HBC2	2.02	0.75
2:B:353:THR:HB	2:B:356:ASP:OD1	1.87	0.74
1:A:362:ARG:O	1:A:365:MET:HG2	1.87	0.74
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.04	0.74
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.52	0.74
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.03	0.74
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.69	0.74
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.52	0.74
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.17	0.74
3:C:59:ASP:O	3:C:61:SER:N	2.20	0.74
1:N:80:GLU:HA	2:O:284:LEU:HD12	1.68	0.74
2:B:89:ILE:CD1	2:B:96:LEU:HD23	2.17	0.74
4:D:116:ILE:HG23	4:D:117:VAL:N	2.02	0.74
5:E:58:PHE:O	5:E:61:SER:HB3	1.88	0.74
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.70	0.74
3:P:173:ASN:N	3:P:174:PRO:HD2	2.03	0.74
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.21	0.74
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.70	0.74
1:N:106:MET:HG2	1:N:203:ILE:HD13	1.70	0.74
5:R:1:VAL:HG23	5:R:3:ASN:H	1.50	0.74
6:S:91:GLU:HB3	6:S:92:PRO:HD3	1.70	0.74
9:I:49:LEU:HD11	9:I:58:ARG:NH1	2.03	0.73
2:O:225:ASN:O	2:O:227:ARG:HG3	1.87	0.73
1:A:422:LEU:HD21	1:A:431:LEU:HD21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.68	0.73
9:V:49:LEU:HB3	9:V:55:MET:CG	2.17	0.73
2:O:113:ARG:O	2:O:116:VAL:HG23	1.88	0.73
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.53	0.73
2:O:374:THR:HG22	2:O:376:GLN:H	1.53	0.73
1:A:106:MET:HG2	1:A:203:ILE:HD13	1.69	0.73
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.52	0.73
2:B:100:SER:CB	2:B:105:MET:HG2	2.19	0.73
4:Q:43:MET:CE	4:Q:46:VAL:HG21	2.19	0.73
19:Q:501:HEC:HMB1	19:Q:501:HEC:HBB3	1.71	0.73
10:W:56:LYS:HG2	10:W:60:GLU:OE1	1.89	0.73
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.71	0.72
2:O:150:VAL:O	2:O:153:GLN:HB2	1.88	0.72
2:O:295:LEU:O	2:O:299:VAL:HG23	1.89	0.72
3:P:214:SER:HB2	3:P:218:LYS:NZ	2.03	0.72
1:A:134:ILE:HG21	1:A:174:ILE:HG12	1.71	0.72
1:N:58:PHE:HB3	1:N:182:LEU:HD21	1.69	0.72
2:O:71:LEU:N	2:O:71:LEU:HD23	2.04	0.72
3:C:245:LEU:O	4:D:201:ARG:HD3	1.88	0.72
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.53	0.72
2:B:96:LEU:HG	9:I:70:LEU:HD13	1.71	0.72
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.23	0.72
2:O:100:SER:CB	2:O:105:MET:HG2	2.20	0.72
2:O:122:TYR:O	2:O:126:VAL:HG23	1.90	0.72
3:P:127:THR:O	3:P:130:VAL:HG22	1.90	0.72
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.24	0.72
9:I:49:LEU:HD22	9:I:55:MET:HG2	1.72	0.72
2:B:113:ARG:O	2:B:116:VAL:HG23	1.88	0.72
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.25	0.72
3:P:120:LEU:HB3	13:P:502:HEM:CBB	2.20	0.72
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.25	0.72
5:E:147:ILE:HG22	5:E:148:ALA:N	2.05	0.72
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.71	0.72
2:B:209:ILE:O	2:B:211:VAL:HG22	1.90	0.71
2:B:402:ILE:HG23	2:B:403:ASP:H	1.55	0.71
3:C:214:SER:HB2	3:C:218:LYS:NZ	2.05	0.71
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.53	0.71
2:O:274:VAL:O	2:O:278:VAL:HG23	1.90	0.71
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.24	0.71
5:E:1:VAL:HG23	5:E:3:ASN:H	1.54	0.71
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.30	0.71
3:C:92:PHE:O	3:C:95:ILE:HG22	1.90	0.71
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.26	0.71
2:B:226:ILE:HG23	2:B:227:ARG:HD3	1.71	0.71
2:B:374:THR:HG22	2:B:376:GLN:H	1.56	0.71
3:C:236:MET:O	3:C:239:PRO:HD2	1.90	0.71
2:B:18:CYS:HB3	2:B:19:PRO:HD3	1.70	0.71
3:C:173:ASN:N	3:C:174:PRO:HD2	2.05	0.71
1:N:37:VAL:HG12	1:N:199:ALA:HB2	1.73	0.71
2:B:295:LEU:O	2:B:299:VAL:HG23	1.91	0.71
2:B:280:GLY:HA3	2:B:293:SER:OG	1.91	0.70
2:O:361:LYS:O	2:O:365:LYS:HG3	1.90	0.70
2:O:154:SER:O	2:O:157:VAL:HG12	1.90	0.70
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.26	0.70
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.27	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.70
1:N:422:LEU:HD21	1:N:431:LEU:HD21	1.73	0.70
1:N:365:MET:HG3	1:N:366:VAL:N	2.07	0.70
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.71	0.70
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.91	0.70
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.73	0.70
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.74	0.70
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.06	0.70
5:R:148:ALA:HB2	5:R:156:TYR:CD2	2.27	0.70
3:C:138:GLN:HB2	3:C:255:GLU:O	1.92	0.70
4:D:57:THR:HB	4:D:60:GLU:HG3	1.74	0.70
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.73	0.70
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.73	0.70
1:A:342:TRP:O	1:A:345:LEU:HB2	1.92	0.69
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.07	0.69
2:B:76:THR:CG2	2:B:82:SER:H	2.04	0.69
2:B:341:MET:HE2	2:B:341:MET:HA	1.72	0.69
3:P:125:MET:HE2	14:P:3001:IKR:I1	2.61	0.69
3:P:247:SER:OG	3:P:250:LEU:HB2	1.92	0.69
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.07	0.69
3:C:238:THR:HB	3:C:239:PRO:HD3	1.74	0.69
2:O:287:ARG:HA	9:V:53:GLU:HG3	1.72	0.69
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.07	0.69
5:R:71:LEU:N	5:R:71:LEU:HD23	2.08	0.69
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.74	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.74	0.69
3:P:101:ARG:HD2	3:P:101:ARG:C	2.13	0.69
3:P:92:PHE:O	3:P:95:ILE:HG22	1.92	0.69
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.23	0.69
3:C:70:THR:HA	3:C:74:VAL:HG23	1.75	0.69
2:O:89:ILE:CD1	2:O:96:LEU:HD23	2.22	0.69
1:N:239:SER:HB2	7:T:17:SER:O	1.93	0.69
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.26	0.69
2:O:76:THR:CG2	2:O:82:SER:H	2.04	0.69
3:P:61:SER:O	3:P:62:LEU:HG	1.92	0.69
2:O:402:ILE:HG23	2:O:403:ASP:H	1.58	0.68
1:N:170:THR:HG22	1:N:171:THR:N	2.07	0.68
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.74	0.68
5:E:98:VAL:HG22	5:E:134:ILE:HG12	1.75	0.68
3:C:145:THR:O	3:C:149:ASN:HB2	1.94	0.68
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.07	0.68
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.75	0.68
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.75	0.68
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.27	0.68
10:W:40:ASP:O	10:W:44:GLU:HG3	1.94	0.68
1:A:106:MET:HE2	1:A:106:MET:O	1.94	0.68
1:N:369:LEU:HD12	1:N:392:LEU:HD21	1.74	0.68
1:A:433:ASP:OD2	1:A:435:ASN:HB2	1.94	0.68
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.75	0.68
3:C:12:LEU:HD23	3:C:15:ILE:HD12	1.76	0.68
2:O:201:SER:HB3	2:O:227:ARG:CB	2.24	0.68
5:R:98:VAL:HG22	5:R:134:ILE:HG12	1.73	0.68
1:A:45:SER:OG	1:A:92:ARG:HA	1.94	0.68
1:A:170:THR:HG22	1:A:171:THR:H	1.59	0.68
2:O:27:THR:HG22	2:O:28:LYS:N	2.08	0.68
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.59	0.68
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.76	0.68
1:A:117:VAL:HG23	1:A:118:GLN:N	2.09	0.67
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.76	0.67
4:D:20:ALA:HB1	4:D:199:ASP:OD2	1.94	0.67
1:N:106:MET:O	1:N:106:MET:HE2	1.94	0.67
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.24	0.67
1:N:439:SER:HA	1:N:442:TYR:CE2	2.28	0.67
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.28	0.67
2:O:35:ILE:O	2:O:213:HIS:HE1	1.77	0.67
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.88	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.30	0.67
9:I:38:UNK:C	9:I:40:UNK:H	2.06	0.67
1:N:161:THR:HG21	1:N:235:ARG:H	1.58	0.67
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.75	0.67
3:P:31:TRP:O	3:P:101:ARG:HG3	1.94	0.67
4:Q:52:ILE:O	4:Q:54:VAL:HG23	1.94	0.67
2:O:62:ASN:O	2:O:65:THR:HG22	1.94	0.67
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.25	0.67
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.77	0.67
2:B:274:VAL:O	2:B:278:VAL:HG23	1.95	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.10	0.67
2:B:97:SER:HB3	9:I:69:SER:HA	1.76	0.67
1:N:342:TRP:O	1:N:345:LEU:HB2	1.94	0.66
2:B:154:SER:O	2:B:157:VAL:HG12	1.95	0.66
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.31	0.66
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.13	0.66
1:A:80:GLU:HA	2:B:284:LEU:HD12	1.76	0.66
1:N:253:VAL:HG11	1:N:335:MET:HE1	1.77	0.66
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.25	0.66
2:B:306:PRO:HB3	9:I:52:ARG:HG3	1.77	0.66
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.24	0.66
3:C:125:MET:HE1	14:C:2001:IKR:I1	2.66	0.66
1:A:249:PRO:HG2	1:A:250:VAL:H	1.60	0.66
3:P:82:ASN:HD22	3:P:82:ASN:N	1.93	0.66
3:P:70:THR:HA	3:P:74:VAL:HG23	1.76	0.66
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.78	0.66
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.09	0.66
4:D:52:ILE:O	4:D:54:VAL:HG23	1.96	0.66
19:D:501:HEC:HMB1	19:D:501:HEC:HBB3	1.78	0.66
3:C:137:GLY:H	3:C:140:SER:HB2	1.61	0.66
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.26	0.66
1:A:187:ASP:O	1:A:191:LYS:HE3	1.96	0.66
3:C:36:SER:O	3:C:40:VAL:HG23	1.96	0.66
3:P:236:MET:O	3:P:239:PRO:HD2	1.95	0.66
5:R:69:LEU:O	5:R:72:SER:HB3	1.95	0.66
1:N:10:ASN:OD1	2:O:19:PRO:HD2	1.96	0.65
1:N:317:THR:HG23	1:N:318:GLY:N	2.10	0.65
2:O:262:ALA:O	2:O:320:GLY:HA3	1.96	0.65
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	1.78	0.65
1:A:365:MET:HG3	1:A:366:VAL:N	2.10	0.65
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.11	0.65
2:O:152:PHE:HE1	2:O:177:TYR:HD1	1.44	0.65
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.35	0.65
1:A:23:LEU:HD23	1:A:24:ARG:N	2.10	0.65
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.25	0.65
1:N:23:LEU:HD23	1:N:24:ARG:N	2.11	0.65
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.62	0.65
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.77	0.65
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.11	0.65
6:S:13:MET:HA	6:S:16:ILE:HD12	1.76	0.65
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.32	0.65
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.79	0.65
3:C:247:SER:OG	3:C:250:LEU:HB2	1.97	0.65
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.32	0.65
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.60	0.65
2:B:19:PRO:O	2:B:22:GLU:N	2.28	0.65
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.77	0.65
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.27	0.65
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.79	0.65
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.32	0.65
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.31	0.65
5:E:161:HIS:HB2	21:E:501:FES:S1	2.37	0.65
2:O:141:GLN:N	2:O:142:PRO:HD2	2.12	0.65
6:F:89:TYR:CD1	6:F:90:LEU:N	2.65	0.65
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.32	0.65
1:A:27:SER:HA	1:A:199:ALA:O	1.97	0.64
6:F:89:TYR:HD1	6:F:90:LEU:H	1.45	0.64
2:O:96:LEU:HG	9:V:70:LEU:HD13	1.78	0.64
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.79	0.64
2:B:150:VAL:O	2:B:153:GLN:HB2	1.96	0.64
4:D:47:ALA:H	4:D:50:ASN:ND2	1.91	0.64
10:J:14:PHE:CD2	10:J:14:PHE:N	2.64	0.64
2:O:209:ILE:O	2:O:211:VAL:HG22	1.97	0.64
3:C:198:LEU:HD13	15:C:2002:UQ:HM53	1.79	0.64
5:E:18:VAL:HG23	5:E:18:VAL:O	1.95	0.64
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.97	0.64
10:W:26:LEU:O	10:W:29:VAL:HB	1.97	0.64
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.32	0.64
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.27	0.64
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.79	0.64
5:R:161:HIS:HB2	21:R:501:FES:S1	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.78	0.64
5:R:78:LEU:HB2	5:R:191:ASP:HA	1.78	0.64
3:C:239:PRO:HA	3:C:242:THR:HB	1.79	0.64
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.26	0.64
2:O:438:GLU:O	2:O:439:LEU:HD23	1.97	0.64
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.80	0.64
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.27	0.64
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	1.79	0.64
3:P:238:THR:HB	3:P:239:PRO:HD3	1.77	0.64
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.80	0.64
5:E:71:LEU:N	5:E:71:LEU:HD23	2.13	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.31	0.64
7:T:41:PHE:O	7:T:45:VAL:HG23	1.96	0.64
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.80	0.64
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.80	0.64
4:D:186:VAL:O	4:D:190:LEU:HG	1.97	0.64
7:G:77:TYR:HA	7:G:80:ASP:OD2	1.98	0.64
2:O:219:VAL:O	2:O:223:PHE:HB2	1.98	0.64
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.24	0.63
5:E:77:LYS:HE2	5:E:79:SER:OG	1.98	0.63
5:E:78:LEU:HD12	5:E:190:ASP:O	1.97	0.63
1:N:362:ARG:O	1:N:365:MET:HG2	1.97	0.63
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.99	0.63
2:B:160:LEU:HB3	9:I:64:LEU:HD22	1.80	0.63
1:N:199:ALA:HA	1:N:376:CYS:SG	2.38	0.63
2:B:144:LEU:HB2	2:B:183:ILE:CD1	2.28	0.63
3:C:101:ARG:HD2	3:C:101:ARG:C	2.17	0.63
3:C:120:LEU:HD22	13:C:502:HEM:HBB2	1.79	0.63
3:C:323:GLN:O	3:C:326:PHE:HB3	1.98	0.63
1:N:342:TRP:HA	1:N:345:LEU:HD12	1.79	0.63
3:P:70:THR:HA	3:P:74:VAL:CG2	2.27	0.63
3:P:239:PRO:HA	3:P:242:THR:HB	1.78	0.63
10:W:14:PHE:N	10:W:14:PHE:CD2	2.63	0.63
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.29	0.63
4:D:33:TYR:HD1	4:D:37:CYS:HB2	1.63	0.63
4:D:102:ARG:NH1	4:D:107:GLY:O	2.32	0.63
1:N:103:SER:O	1:N:106:MET:HB2	1.99	0.63
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.33	0.63
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.78	0.63
5:R:148:ALA:O	5:R:149:ASN:HB2	1.96	0.63
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.97	0.63
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.63
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.78	0.63
3:C:127:THR:O	3:C:130:VAL:HG22	1.99	0.63
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.28	0.63
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.81	0.63
1:N:433:ASP:OD2	1:N:435:ASN:HB2	1.97	0.63
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.80	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.32	0.63
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.80	0.63
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.34	0.63
1:N:45:SER:OG	1:N:92:ARG:HA	1.98	0.63
9:V:49:LEU:HD22	9:V:55:MET:CB	2.27	0.63
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.81	0.62
5:E:69:LEU:O	5:E:72:SER:HB3	1.99	0.62
6:S:89:TYR:CD1	6:S:90:LEU:N	2.65	0.62
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.82	0.62
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.81	0.62
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.34	0.62
1:N:368:GLN:O	1:N:374:PRO:HB2	1.99	0.62
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.98	0.62
7:G:36:ASN:O	7:G:40:ARG:HG3	2.00	0.62
3:P:323:GLN:O	3:P:326:PHE:HB3	1.99	0.62
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.82	0.62
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.26	0.62
2:O:168:TYR:HB2	2:O:173:ALA:CB	2.27	0.62
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.15	0.62
5:R:126:ARG:HH21	5:R:170:ARG:HG2	1.65	0.62
2:O:31:ASN:HD22	2:O:31:ASN:N	1.98	0.62
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.34	0.62
3:C:82:ASN:HD22	3:C:82:ASN:N	1.97	0.62
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.82	0.62
1:A:163:LEU:HD22	1:A:314:TYR:CE1	2.35	0.62
2:B:402:ILE:HG23	2:B:403:ASP:N	2.14	0.62
1:N:112:LEU:O	1:N:116:VAL:HG23	2.00	0.62
4:Q:147:LEU:HD13	4:Q:157:ALA:HB1	1.81	0.62
4:D:232:SER:HB3	7:G:23:GLN:NE2	2.13	0.62
1:N:178:THR:HG22	1:N:179:ARG:N	2.15	0.62
3:P:125:MET:CE	14:P:3001:IKR:I1	3.17	0.62
1:A:383:LEU:HD23	1:A:388:ARG:O	2.00	0.61
3:C:59:ASP:C	3:C:61:SER:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:PRO:O	3:C:256:ASN:N	2.32	0.61
1:N:270:LEU:HB3	1:N:320:PHE:HE1	1.64	0.61
3:P:234:THR:HG21	4:Q:219:LEU:HD13	1.82	0.61
4:Q:30:PHE:HE2	4:Q:64:LEU:HD11	1.65	0.61
9:V:65:VAL:HG12	9:V:66:ALA:N	2.15	0.61
3:C:286:PRO:O	3:C:287:ASN:HB2	2.00	0.61
4:D:62:LYS:O	4:D:66:GLU:HG3	1.99	0.61
9:I:65:VAL:HG12	9:I:66:ALA:N	2.15	0.61
3:P:242:THR:N	4:Q:208:MET:HE1	2.14	0.61
2:B:385:GLU:C	2:B:387:LEU:H	2.03	0.61
5:E:141:HIS:HB3	21:E:501:FES:S2	2.40	0.61
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.33	0.61
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.61
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.82	0.61
2:O:402:ILE:HG23	2:O:403:ASP:N	2.16	0.61
6:S:89:TYR:HD1	6:S:90:LEU:H	1.46	0.61
5:E:78:LEU:HD13	5:E:129:LYS:HE3	1.82	0.61
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.36	0.61
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.16	0.61
4:D:197:GLU:O	4:D:198:HIS:C	2.39	0.61
1:N:27:SER:HA	1:N:199:ALA:O	2.00	0.61
1:N:106:MET:HB3	1:N:107:PRO:CD	2.30	0.61
5:R:18:VAL:HG23	5:R:18:VAL:O	1.99	0.61
1:A:103:SER:O	1:A:106:MET:HB2	2.01	0.61
2:B:226:ILE:HD13	2:B:227:ARG:NH1	2.16	0.61
2:B:361:LYS:O	2:B:365:LYS:HG3	2.01	0.61
4:D:60:GLU:O	4:D:64:LEU:HB2	2.01	0.61
3:P:370:ILE:O	3:P:374:GLU:HB2	2.01	0.61
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.65	0.61
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.35	0.61
3:C:70:THR:HA	3:C:74:VAL:CG2	2.31	0.61
2:O:156:GLN:NE2	9:V:77:ARG:C	2.53	0.61
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.36	0.61
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.47	0.61
1:A:106:MET:HB3	1:A:107:PRO:CD	2.31	0.61
4:D:37:CYS:C	4:D:39:ALA:H	2.04	0.61
4:D:221:TYR:CD2	5:E:39:VAL:HG21	2.36	0.61
1:A:112:LEU:O	1:A:116:VAL:HG23	2.01	0.60
2:B:24:LEU:O	2:B:24:LEU:HD23	2.01	0.60
5:E:129:LYS:HE2	5:E:187:PHE:HE2	1.65	0.60
8:H:40:CYS:O	8:H:44:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:45:SER:HA	1:N:48:GLU:HG3	1.82	0.60
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.83	0.60
3:P:82:ASN:HD22	3:P:82:ASN:H	1.47	0.60
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.33	0.60
8:U:40:CYS:O	8:U:44:VAL:HG23	2.00	0.60
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.01	0.60
2:B:385:GLU:O	2:B:387:LEU:N	2.34	0.60
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.24	0.60
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.82	0.60
2:O:385:GLU:C	2:O:387:LEU:H	2.03	0.60
2:O:402:ILE:HD13	2:O:402:ILE:C	2.21	0.60
1:A:161:THR:HG21	1:A:235:ARG:H	1.66	0.60
2:B:141:GLN:N	2:B:142:PRO:HD2	2.16	0.60
2:B:187:THR:OG1	2:B:190:GLN:HG3	2.02	0.60
1:N:63:ALA:O	1:N:116:VAL:HG13	2.00	0.60
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.36	0.60
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.37	0.60
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.37	0.60
1:A:67:THR:HA	1:A:121:ALA:H	1.66	0.60
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.84	0.60
4:D:197:GLU:HG2	4:D:198:HIS:N	2.15	0.60
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.01	0.60
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.34	0.60
13:P:502:HEM:HBD1	22:P:384:HOH:O	2.02	0.60
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.16	0.60
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.84	0.60
7:G:41:PHE:O	7:G:45:VAL:HG23	2.01	0.60
2:O:402:ILE:O	2:O:405:VAL:HG23	2.00	0.60
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.01	0.60
2:B:67:HIS:O	2:B:70:ARG:HB3	2.02	0.60
2:B:76:THR:HG22	2:B:82:SER:N	2.14	0.60
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.84	0.60
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.67	0.60
2:O:67:HIS:O	2:O:70:ARG:HB3	2.00	0.60
2:O:76:THR:HG22	2:O:82:SER:N	2.13	0.60
4:Q:95:TYR:CE2	4:Q:101:ALA:HA	2.36	0.60
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.22	0.60
9:V:52:ARG:O	9:V:56:SER:HB3	2.02	0.60
4:D:158:ILE:CD1	4:D:160:MET:HB3	2.32	0.60
4:Q:37:CYS:C	4:Q:39:ALA:H	2.06	0.60
10:W:56:LYS:HE3	10:W:60:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG22	1:A:179:ARG:N	2.17	0.60
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.66	0.60
3:C:120:LEU:CG	13:C:502:HEM:HBB2	2.31	0.60
5:E:114:VAL:CG2	5:E:172:ARG:HH12	2.13	0.60
2:O:96:LEU:O	9:V:70:LEU:HD22	2.01	0.60
2:O:144:LEU:HB2	2:O:183:ILE:CD1	2.32	0.60
2:O:385:GLU:O	2:O:387:LEU:N	2.35	0.60
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.66	0.59
5:E:94:LYS:HD3	5:E:138:VAL:HG21	1.82	0.59
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.66	0.59
2:O:187:THR:OG1	2:O:190:GLN:HG3	2.01	0.59
4:Q:197:GLU:O	4:Q:198:HIS:C	2.40	0.59
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.32	0.59
8:U:35:GLU:O	8:U:39:LEU:HG	2.02	0.59
1:A:7:THR:HG21	2:B:113:ARG:NE	2.17	0.59
2:B:17:LEU:O	2:B:18:CYS:HB3	2.01	0.59
15:C:2002:UQ:HM51	15:C:2002:UQ:C8	2.31	0.59
15:P:3002:UQ:HM51	15:P:3002:UQ:C8	2.32	0.59
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.34	0.59
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.84	0.59
3:P:129:PHE:HB2	14:P:3001:IKR:H40	1.83	0.59
1:A:317:THR:HG23	1:A:318:GLY:N	2.18	0.59
6:F:27:ASN:O	6:F:30:GLY:N	2.30	0.59
6:F:71:LYS:O	6:F:72:HIS:HB2	2.01	0.59
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.83	0.59
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.32	0.59
2:B:71:LEU:N	2:B:71:LEU:HD23	2.16	0.59
2:B:152:PHE:HE1	2:B:177:TYR:HD1	1.50	0.59
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.37	0.59
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.33	0.59
1:N:187:ASP:O	1:N:191:LYS:HE3	2.03	0.59
3:P:101:ARG:NH2	13:P:502:HEM:HBD2	2.18	0.59
1:A:48:GLU:HB3	1:A:52:ASN:OD1	2.03	0.59
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.37	0.59
3:C:347:PRO:O	3:C:350:ILE:HG22	2.02	0.59
4:D:220:TYR:OH	4:D:224:ARG:HD3	2.02	0.59
9:I:31:UNK:C	9:I:73:PRO:HG2	2.32	0.59
1:N:90:THR:O	1:N:90:THR:HG23	2.02	0.59
2:O:132:PHE:HB2	2:O:192:HIS:CE1	2.38	0.59
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.16	0.59
5:R:169:GLY:O	5:R:179:ASN:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:HG23	1:A:24:ARG:HG2	1.85	0.59
1:A:105:ASP:O	1:A:109:VAL:HG23	2.02	0.59
3:C:184:PHE:CD2	3:P:184:PHE:CD2	2.91	0.59
1:N:261:GLY:HA2	1:N:317:THR:O	2.03	0.59
3:P:294:ALA:O	3:P:298:SER:HB3	2.03	0.59
2:B:402:ILE:HD13	2:B:402:ILE:C	2.23	0.58
2:B:438:GLU:O	2:B:439:LEU:HD23	2.03	0.58
5:E:52:LYS:C	5:E:52:LYS:HD3	2.23	0.58
5:E:144:CYS:HB2	21:E:501:FES:S2	2.43	0.58
1:N:163:LEU:HD22	1:N:314:TYR:CE1	2.38	0.58
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.68	0.58
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.03	0.58
2:B:57:TYR:CD1	2:B:57:TYR:N	2.70	0.58
2:B:306:PRO:CB	9:I:52:ARG:HG3	2.33	0.58
3:C:294:ALA:O	3:C:298:SER:HB3	2.03	0.58
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.19	0.58
4:D:223:LYS:C	4:D:223:LYS:HD3	2.24	0.58
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.18	0.58
2:O:75:LEU:HD11	2:O:140:LEU:CD2	2.32	0.58
3:P:316:MET:HG2	3:P:319:ARG:HH21	1.68	0.58
9:I:63:ASP:CG	9:I:64:LEU:H	2.05	0.58
2:O:156:GLN:NE2	9:V:77:ARG:O	2.36	0.58
2:B:20:GLY:O	2:B:21:ALA:HB3	2.03	0.58
1:N:249:PRO:HG2	1:N:250:VAL:H	1.67	0.58
1:N:307:PHE:CD1	1:N:307:PHE:C	2.77	0.58
3:P:286:PRO:O	3:P:287:ASN:HB2	2.03	0.58
3:P:347:PRO:O	3:P:350:ILE:HG22	2.04	0.58
2:B:96:LEU:O	9:I:70:LEU:HD22	2.03	0.58
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.69	0.58
4:D:231:LYS:O	6:F:71:LYS:HE3	2.03	0.58
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.38	0.58
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.33	0.58
1:N:86:PHE:CD2	1:N:99:ILE:HD11	2.37	0.58
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.86	0.58
3:P:137:GLY:H	3:P:140:SER:HB2	1.68	0.58
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.21	0.58
2:B:281:ALA:HB2	2:B:311:ALA:HB3	1.86	0.58
4:Q:43:MET:HE2	4:Q:46:VAL:CG2	2.28	0.58
1:A:90:THR:O	1:A:90:THR:HG23	2.04	0.58
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.18	0.58
1:A:239:SER:HB2	7:G:17:SER:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:PHE:CD1	2:B:308:ASP:N	2.72	0.58
2:B:402:ILE:O	2:B:405:VAL:HG23	2.03	0.58
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.34	0.58
5:R:52:LYS:C	5:R:52:LYS:HD3	2.23	0.58
1:A:368:GLN:O	1:A:374:PRO:HB2	2.02	0.58
2:B:394:ALA:HB1	2:B:395:PRO:HD2	1.85	0.58
3:C:320:PRO:HG2	3:C:321:LEU:H	1.67	0.58
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.38	0.58
4:Q:180:SER:OG	8:U:77:LEU:HD21	2.03	0.58
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.39	0.58
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.18	0.58
2:O:318:ASP:O	2:O:319:SER:HB2	2.04	0.58
3:P:214:SER:HB2	3:P:218:LYS:HZ1	1.69	0.58
6:S:65:ALA:O	6:S:68:LEU:HB2	2.04	0.58
1:A:261:GLY:HA2	1:A:317:THR:O	2.04	0.58
3:C:82:ASN:HD22	3:C:82:ASN:H	1.52	0.58
1:N:354:VAL:HG23	1:N:355:LYS:N	2.19	0.58
2:O:247:GLN:HE21	2:O:249:GLY:H	1.50	0.58
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.19	0.58
1:A:137:GLU:O	1:A:141:MET:HG3	2.04	0.57
2:B:37:SER:HB2	2:B:213:HIS:ND1	2.19	0.57
3:C:362:ILE:HG22	3:C:363:LEU:N	2.19	0.57
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.85	0.57
3:P:2:ALA:CB	3:P:8:SER:HB3	2.33	0.57
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.03	0.57
9:V:49:LEU:HD13	9:V:55:MET:HB3	1.85	0.57
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.39	0.57
3:C:370:ILE:O	3:C:374:GLU:HB2	2.03	0.57
4:D:235:MET:HB3	7:G:15:THR:HG22	1.85	0.57
1:N:439:SER:C	1:N:441:MET:H	2.06	0.57
3:P:101:ARG:HD2	3:P:102:GLY:N	2.18	0.57
6:S:71:LYS:O	6:S:72:HIS:HB2	2.04	0.57
3:C:187:PRO:HG2	13:C:501:HEM:HMC3	1.85	0.57
4:D:57:THR:CB	4:D:60:GLU:HG3	2.35	0.57
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.84	0.57
2:O:57:TYR:CE2	2:O:234:SER:HB2	2.38	0.57
2:O:96:LEU:C	2:O:96:LEU:HD12	2.25	0.57
2:O:294:LYS:HE3	2:O:356:ASP:OD2	2.05	0.57
4:Q:181:GLN:CA	8:U:77:LEU:HD22	2.34	0.57
8:U:73:LEU:HD12	8:U:73:LEU:O	2.03	0.57
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.86	0.57
2:O:399:ALA:O	2:O:402:ILE:HG22	2.05	0.57
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.34	0.57
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.40	0.57
6:S:75:LEU:O	6:S:80:TRP:NE1	2.31	0.57
9:V:72:ALA:HB1	9:V:73:PRO:HD3	1.87	0.57
1:A:439:SER:HA	1:A:442:TYR:CE2	2.39	0.57
1:N:307:PHE:HA	1:N:323:HIS:O	2.04	0.57
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.87	0.57
2:O:407:SER:O	2:O:411:VAL:HG23	2.04	0.57
4:Q:5:LEU:HG	4:Q:152:TYR:HE1	1.69	0.57
2:B:262:ALA:O	2:B:320:GLY:HA3	2.05	0.57
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.86	0.57
1:N:117:VAL:HG23	1:N:118:GLN:N	2.19	0.57
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.86	0.57
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.04	0.57
1:A:90:THR:O	1:A:167:VAL:HG11	2.04	0.57
2:B:207:VAL:HG12	2:B:208:GLY:N	2.12	0.57
3:C:64:PHE:CE1	18:C:2011:GOL:H2	2.39	0.57
3:C:147:ILE:HG13	14:C:2001:IKR:H16A	1.87	0.57
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.87	0.57
3:P:59:ASP:C	3:P:61:SER:H	2.08	0.57
5:R:116:LYS:O	5:R:117:LEU:HG	2.05	0.57
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.39	0.57
5:E:12:ALA:HB1	7:G:28:ASN:HD21	1.70	0.57
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.86	0.57
2:B:150:VAL:CG2	2:B:151:ALA:N	2.68	0.57
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.87	0.57
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.85	0.57
2:O:96:LEU:CB	2:O:109:VAL:HG12	2.32	0.57
3:C:261:ASN:ND2	3:C:264:VAL:H	2.03	0.56
1:N:280:TYR:O	1:N:306:SER:HA	2.04	0.56
2:O:57:TYR:N	2:O:57:TYR:CD1	2.73	0.56
2:O:394:ALA:HB1	2:O:395:PRO:HD2	1.87	0.56
3:P:59:ASP:O	3:P:61:SER:N	2.38	0.56
3:P:198:LEU:HD13	15:P:3002:UQ:HM53	1.87	0.56
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	2.88	0.56
1:A:75:PHE:O	1:A:79:VAL:HG23	2.05	0.56
2:B:393:THR:HG22	2:B:397:VAL:HB	1.86	0.56
5:E:94:LYS:HB3	5:E:138:VAL:CG2	2.36	0.56
4:Q:221:TYR:HE1	7:T:25:ALA:CB	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:94:LYS:HD3	5:R:138:VAL:HG21	1.85	0.56
1:A:7:THR:HG21	2:B:113:ARG:CD	2.35	0.56
1:A:63:ALA:O	1:A:116:VAL:HG13	2.06	0.56
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.39	0.56
1:A:280:TYR:O	1:A:306:SER:HA	2.04	0.56
1:A:307:PHE:CD1	1:A:307:PHE:C	2.78	0.56
1:A:365:MET:CG	1:A:366:VAL:N	2.68	0.56
2:B:306:PRO:HA	9:I:52:ARG:HE	1.71	0.56
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.41	0.56
2:O:268:GLU:HG2	2:O:268:GLU:O	2.05	0.56
2:O:281:ALA:HB2	2:O:311:ALA:HB3	1.87	0.56
3:P:120:LEU:HD22	13:P:502:HEM:HBB2	1.87	0.56
4:Q:33:TYR:HD1	4:Q:37:CYS:HB2	1.70	0.56
4:Q:43:MET:HG2	4:Q:46:VAL:HG23	1.87	0.56
2:O:424:MET:HG2	2:O:425:ALA:N	2.20	0.56
4:Q:60:GLU:O	4:Q:64:LEU:HB2	2.05	0.56
1:A:266:ASP:HA	1:A:269:VAL:HG23	1.87	0.56
1:A:344:ARG:NH2	1:A:353:GLU:OE2	2.38	0.56
2:B:168:TYR:N	2:B:168:TYR:CD1	2.72	0.56
3:C:33:ASN:HB3	22:C:1008:HOH:O	2.05	0.56
3:C:129:PHE:HB2	14:C:2001:IKR:H40	1.87	0.56
2:O:403:ASP:C	2:O:405:VAL:H	2.08	0.56
2:O:437:ASP:OD1	2:O:438:GLU:HG3	2.06	0.56
1:A:270:LEU:HD13	1:A:320:PHE:CD1	2.41	0.56
2:B:168:TYR:N	2:B:168:TYR:HD1	2.04	0.56
2:B:294:LYS:HE3	2:B:356:ASP:OD2	2.05	0.56
10:J:26:LEU:O	10:J:29:VAL:HB	2.06	0.56
2:O:146:VAL:O	2:O:149:ALA:N	2.33	0.56
3:P:95:ILE:CD1	3:P:121:LEU:HD13	2.30	0.56
4:Q:30:PHE:CE2	4:Q:64:LEU:HD11	2.40	0.56
5:R:99:ARG:NH2	5:R:149:ASN:HD22	2.04	0.56
8:U:44:VAL:HG22	8:U:52:GLU:OE1	2.06	0.56
2:B:247:GLN:HE21	2:B:249:GLY:H	1.53	0.56
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.87	0.56
1:N:365:MET:CG	1:N:366:VAL:N	2.67	0.56
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.72	0.56
2:O:75:LEU:HD11	2:O:140:LEU:HD23	1.88	0.56
2:O:207:VAL:HG12	2:O:208:GLY:N	2.15	0.56
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.88	0.56
1:A:242:ARG:NH2	1:A:432:LEU:HA	2.21	0.56
1:A:350:THR:OG1	1:A:353:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:LEU:HD13	9:I:55:MET:CE	2.35	0.56
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.36	0.56
10:W:57:HIS:HA	10:W:60:GLU:CG	2.36	0.56
1:N:277:ILE:HB	1:N:309:THR:HG21	1.88	0.56
1:A:16:VAL:O	1:A:17:THR:HG23	2.06	0.56
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.88	0.56
1:A:277:ILE:HB	1:A:309:THR:HG21	1.88	0.56
2:B:345:LYS:O	2:B:348:ALA:N	2.39	0.56
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.88	0.56
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.06	0.56
2:O:37:SER:CB	2:O:213:HIS:ND1	2.69	0.56
5:R:76:ILE:HG23	5:R:89:PHE:CZ	2.41	0.56
9:V:65:VAL:CG1	9:V:66:ALA:N	2.69	0.56
5:E:101:ARG:HB3	5:E:105:GLU:OE1	2.07	0.55
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.21	0.55
10:J:59:TYR:N	10:J:59:TYR:CD1	2.73	0.55
4:Q:40:CYS:HA	4:Q:95:TYR:HE1	1.70	0.55
5:R:100:HIS:CD2	5:R:131:GLU:HB2	2.41	0.55
1:A:180:ALA:O	1:A:183:ALA:HB3	2.06	0.55
4:D:100:ALA:O	4:D:103:ALA:HB3	2.06	0.55
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.41	0.55
6:F:75:LEU:O	6:F:80:TRP:NE1	2.32	0.55
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.42	0.55
2:O:280:GLY:HA3	2:O:293:SER:OG	2.06	0.55
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.88	0.55
1:A:199:ALA:HA	1:A:376:CYS:SG	2.46	0.55
1:A:270:LEU:HB3	1:A:320:PHE:HE1	1.71	0.55
1:A:354:VAL:HG23	1:A:355:LYS:N	2.22	0.55
6:F:61:ARG:HH11	6:F:61:ARG:HG3	1.72	0.55
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.89	0.55
2:O:259:THR:HG22	2:O:260:GLU:N	2.22	0.55
5:R:82:PRO:O	5:R:100:HIS:HB3	2.05	0.55
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.87	0.55
9:I:65:VAL:CG1	9:I:66:ALA:N	2.69	0.55
1:N:143:ASN:HA	1:N:145:MET:HE1	1.88	0.55
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.06	0.55
3:P:36:SER:O	3:P:40:VAL:HG23	2.06	0.55
4:Q:20:ALA:HB1	4:Q:199:ASP:OD2	2.05	0.55
4:Q:167:GLU:C	4:Q:169:LEU:H	2.10	0.55
4:Q:231:LYS:HA	6:S:71:LYS:HG2	1.88	0.55
1:A:433:ASP:O	1:A:437:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.89	0.55
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.42	0.55
4:D:24:SER:OG	10:J:55:ILE:HG21	2.07	0.55
2:O:307:PHE:H	9:V:52:ARG:HG2	1.72	0.55
3:P:172:ASP:C	3:P:174:PRO:HD2	2.26	0.55
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.86	0.55
9:V:70:LEU:HD23	9:V:71:ASN:N	2.21	0.55
5:E:55:VAL:O	5:E:59:ILE:HG12	2.06	0.55
1:N:253:VAL:HG11	1:N:335:MET:CE	2.35	0.55
2:O:27:THR:HG22	2:O:28:LYS:H	1.72	0.55
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.42	0.55
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.89	0.55
8:H:43:ARG:HD2	8:H:47:ARG:CZ	2.37	0.55
8:H:65:ARG:O	8:H:68:CYS:HB3	2.07	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.42	0.55
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.42	0.55
3:C:120:LEU:HB3	13:C:502:HEM:HBB2	1.87	0.55
3:C:377:MET:CE	6:F:20:TYR:HB2	2.37	0.55
1:N:67:THR:HA	1:N:121:ALA:H	1.70	0.55
1:N:134:ILE:HG21	1:N:174:ILE:CG1	2.35	0.55
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.35	0.55
2:O:166:ALA:HA	2:O:240:TRP:CZ3	2.42	0.55
1:A:87:ASN:HB3	1:A:98:TYR:CZ	2.42	0.55
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.42	0.55
2:B:424:MET:HG2	2:B:425:ALA:N	2.21	0.55
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.71	0.55
3:C:350:ILE:HG23	3:C:351:ILE:N	2.22	0.55
4:D:171:TYR:HD1	4:D:175:THR:HB	1.72	0.55
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.55
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.42	0.55
9:V:65:VAL:H	9:V:77:ARG:HB2	1.72	0.55
2:B:58:GLU:OE1	2:B:64:GLY:N	2.39	0.55
3:P:95:ILE:O	3:P:99:ILE:HG13	2.07	0.55
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.71	0.55
4:Q:100:ALA:O	4:Q:103:ALA:HB3	2.06	0.55
9:V:32:UNK:O	9:V:33:UNK:C	2.54	0.55
3:C:31:TRP:O	3:C:101:ARG:HG3	2.07	0.54
3:C:137:GLY:N	3:C:140:SER:HB2	2.22	0.54
3:C:214:SER:HB2	3:C:218:LYS:HZ1	1.72	0.54
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.36	0.54
1:N:107:PRO:O	1:N:109:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:148:HIS:N	4:Q:148:HIS:CD2	2.75	0.54
10:W:59:TYR:N	10:W:59:TYR:CD1	2.74	0.54
1:A:45:SER:HA	1:A:48:GLU:HG3	1.87	0.54
4:D:116:ILE:CG2	4:D:117:VAL:N	2.70	0.54
1:N:212:ALA:O	1:N:216:PHE:HB2	2.07	0.54
1:N:266:ASP:HA	1:N:269:VAL:HG23	1.89	0.54
1:N:333:ASP:O	1:N:336:PHE:HB3	2.07	0.54
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.72	0.54
2:O:97:SER:HB3	9:V:69:SER:HA	1.88	0.54
3:P:244:ALA:O	3:P:245:LEU:HD23	2.08	0.54
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.42	0.54
6:F:32:MET:CE	6:F:87:LYS:HG2	2.37	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.89	0.54
1:N:19:LEU:O	1:N:21:ASN:N	2.40	0.54
1:N:22:GLY:O	1:N:193:PRO:HA	2.08	0.54
1:N:90:THR:O	1:N:167:VAL:HG11	2.07	0.54
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.07	0.54
5:R:118:ARG:NH2	5:R:174:GLY:O	2.41	0.54
2:B:115:HIS:O	2:B:119:VAL:HG23	2.07	0.54
2:B:146:VAL:O	2:B:149:ALA:N	2.35	0.54
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.07	0.54
3:C:141:PHE:O	3:C:144:ALA:HB3	2.07	0.54
1:N:90:THR:HA	1:N:95:THR:HA	1.88	0.54
4:Q:10:PHE:HD2	8:U:74:PHE:CE2	2.26	0.54
1:N:62:LEU:CD1	1:N:127:ILE:HG12	2.37	0.54
1:N:107:PRO:HG2	1:N:108:LYS:H	1.73	0.54
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.28	0.54
2:O:107:TYR:CG	2:O:127:THR:HG22	2.43	0.54
2:O:374:THR:HG22	2:O:376:GLN:N	2.22	0.54
1:A:304:CYS:HB2	1:A:325:VAL:O	2.08	0.54
2:B:318:ASP:O	2:B:319:SER:HB2	2.08	0.54
2:B:399:ALA:O	2:B:402:ILE:HG22	2.07	0.54
2:B:403:ASP:C	2:B:405:VAL:H	2.10	0.54
5:E:142:LEU:O	3:P:265:THR:N	2.39	0.54
8:H:20:ILE:HD12	8:H:73:LEU:HA	1.88	0.54
1:N:75:PHE:O	1:N:79:VAL:HG23	2.08	0.54
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.89	0.54
5:R:99:ARG:NH2	5:R:149:ASN:ND2	2.55	0.54
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.37	0.54
2:B:333:ALA:O	2:B:337:ILE:HG13	2.08	0.54
4:D:147:LEU:HD13	4:D:157:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:O	5:E:193:VAL:HG12	2.08	0.54
8:U:25:GLU:HG2	8:U:61:PHE:HZ	1.71	0.54
5:E:116:LYS:HD2	5:E:116:LYS:N	2.19	0.54
6:F:51:PRO:O	6:F:52:GLU:C	2.45	0.54
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.42	0.54
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.43	0.54
6:S:13:MET:HA	6:S:16:ILE:CD1	2.37	0.54
4:D:56:HIS:HB3	4:D:60:GLU:HB2	1.90	0.54
8:H:35:GLU:O	8:H:39:LEU:HG	2.08	0.54
3:P:189:ALA:O	3:P:193:ILE:HG13	2.08	0.54
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.38	0.54
2:B:259:THR:HG22	2:B:260:GLU:N	2.22	0.54
9:I:49:LEU:HB3	9:I:55:MET:SD	2.48	0.54
1:N:25:VAL:HG22	1:N:197:LEU:HB3	1.90	0.54
1:A:3:THR:HG23	1:A:6:GLN:OE1	2.08	0.53
1:A:307:PHE:HA	1:A:323:HIS:O	2.09	0.53
2:B:201:SER:OG	2:B:228:SER:HA	2.08	0.53
3:C:9:HIS:HD2	3:C:12:LEU:H	1.56	0.53
3:C:244:ALA:O	3:C:245:LEU:HD23	2.09	0.53
1:N:48:GLU:HB3	1:N:52:ASN:OD1	2.08	0.53
2:O:115:HIS:O	2:O:119:VAL:HG23	2.08	0.53
2:O:393:THR:HG22	2:O:397:VAL:HB	1.89	0.53
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.89	0.53
3:P:147:ILE:HG13	14:P:3001:IKR:H16A	1.89	0.53
4:Q:5:LEU:HG	4:Q:152:TYR:CE1	2.43	0.53
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.43	0.53
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.90	0.53
4:D:27:ARG:O	4:D:30:PHE:HB3	2.08	0.53
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.89	0.53
2:O:306:PRO:HB3	9:V:52:ARG:N	2.23	0.53
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.35	0.53
5:R:109:GLU:OE1	5:R:123:ASP:HB2	2.08	0.53
2:B:31:ASN:HD22	2:B:31:ASN:N	2.05	0.53
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.39	0.53
2:B:227:ARG:HD3	2:B:227:ARG:N	2.23	0.53
3:C:254:PRO:C	3:C:256:ASN:N	2.61	0.53
1:N:147:ASN:O	1:N:148:VAL:C	2.47	0.53
1:N:383:LEU:HD23	1:N:388:ARG:O	2.09	0.53
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.53
3:C:254:PRO:C	3:C:256:ASN:H	2.12	0.53
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:78:TRP:CD2	3:P:79:LEU:N	2.77	0.53
5:R:170:ARG:HG2	5:R:179:ASN:ND2	2.24	0.53
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.90	0.53
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.44	0.53
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.39	0.53
1:N:158:PHE:O	1:N:159:GLN:O	2.27	0.53
1:N:318:GLY:O	1:N:319:LEU:HD23	2.08	0.53
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.44	0.53
2:O:26:ILE:HG23	2:O:26:ILE:O	2.08	0.53
2:O:201:SER:CB	2:O:227:ARG:HB2	2.32	0.53
2:O:287:ARG:CA	9:V:53:GLU:HG3	2.39	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.44	0.53
1:A:145:MET:HB2	1:A:252:HIS:NE2	2.24	0.53
2:B:19:PRO:O	2:B:20:GLY:C	2.45	0.53
3:C:130:VAL:HG23	3:C:131:GLY:N	2.23	0.53
4:D:28:ARG:O	4:D:31:GLN:N	2.42	0.53
4:D:148:HIS:CE1	4:D:161:ALA:HA	2.42	0.53
8:H:73:LEU:HD12	8:H:73:LEU:O	2.09	0.53
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.43	0.53
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.53
3:P:142:TRP:HA	3:P:145:THR:OG1	2.08	0.53
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.90	0.53
3:P:243:LEU:C	3:P:243:LEU:HD12	2.27	0.53
3:P:273:TRP:HA	3:P:276:LEU:HG	1.91	0.53
4:Q:52:ILE:O	4:Q:54:VAL:N	2.41	0.53
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.09	0.53
1:N:433:ASP:O	1:N:437:ILE:HG13	2.07	0.53
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.91	0.53
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.44	0.53
6:S:70:LEU:HG	6:S:71:LYS:N	2.23	0.53
3:C:4:ASN:O	3:C:5:ILE:HD13	2.09	0.53
1:N:277:ILE:CD1	1:N:345:LEU:HD11	2.39	0.53
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.44	0.53
16:P:3004:CDL:HA31	7:T:40:ARG:HB3	1.90	0.53
8:U:20:ILE:HD12	8:U:73:LEU:HA	1.91	0.53
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.44	0.53
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.44	0.53
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.91	0.53
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.44	0.53
7:G:63:THR:HG22	7:G:64:GLN:N	2.23	0.53
1:N:52:ASN:O	1:N:53:ASN:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:134:ILE:CG2	1:N:174:ILE:HG12	2.36	0.53
3:P:9:HIS:HD2	3:P:12:LEU:H	1.57	0.53
4:Q:27:ARG:CZ	10:W:59:TYR:HE2	2.21	0.53
5:R:15:ARG:HD2	7:T:21:PHE:O	2.09	0.53
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.90	0.53
3:C:101:ARG:HD2	3:C:102:GLY:N	2.23	0.53
3:C:350:ILE:CG2	3:C:351:ILE:N	2.72	0.53
4:D:180:SER:OG	8:H:77:LEU:HD21	2.08	0.53
3:P:120:LEU:CD1	13:P:502:HEM:HBB2	2.38	0.53
3:P:261:ASN:HD22	3:P:264:VAL:HB	1.74	0.53
4:Q:24:SER:OG	10:W:55:ILE:HG21	2.09	0.53
6:S:16:ILE:O	6:S:19:TRP:HB3	2.09	0.53
1:A:117:VAL:CG2	1:A:118:GLN:N	2.72	0.52
2:B:107:TYR:CG	2:B:127:THR:HG22	2.44	0.52
2:B:226:ILE:HD13	2:B:227:ARG:HH12	1.73	0.52
3:C:13:LYS:O	3:C:13:LYS:HG2	2.09	0.52
4:D:27:ARG:CZ	10:J:59:TYR:CE2	2.91	0.52
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.74	0.52
5:R:107:ASN:O	5:R:109:GLU:N	2.39	0.52
1:A:253:VAL:HG11	1:A:335:MET:CE	2.39	0.52
1:A:277:ILE:HD11	1:A:345:LEU:HD11	1.90	0.52
2:B:437:ASP:OD1	2:B:438:GLU:HG3	2.08	0.52
4:D:43:MET:HG2	4:D:46:VAL:CG2	2.39	0.52
1:N:19:LEU:C	1:N:21:ASN:H	2.12	0.52
2:O:258:VAL:HG11	2:O:312:PHE:CD2	2.41	0.52
1:A:255:LEU:HD13	1:A:422:LEU:CD1	2.39	0.52
2:B:20:GLY:O	2:B:21:ALA:CB	2.57	0.52
2:B:26:ILE:HG23	2:B:26:ILE:O	2.09	0.52
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.40	0.52
2:O:152:PHE:CE1	2:O:177:TYR:HD1	2.26	0.52
4:Q:165:TYR:O	4:Q:168:ILE:HB	2.09	0.52
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.08	0.52
4:Q:215:LEU:HD13	5:R:46:ALA:CB	2.40	0.52
5:R:141:HIS:HB3	21:R:501:FES:S2	2.49	0.52
1:A:373:THR:N	1:A:374:PRO:HD2	2.25	0.52
4:D:165:TYR:O	4:D:168:ILE:HB	2.08	0.52
10:J:40:ASP:O	10:J:44:GLU:HG3	2.08	0.52
1:N:15:ASN:O	1:N:26:ALA:HA	2.09	0.52
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.39	0.52
2:O:124:LEU:HD23	2:O:124:LEU:C	2.29	0.52
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:186:VAL:CG1	4:Q:187:CYS:N	2.72	0.52
6:S:61:ARG:HH11	6:S:61:ARG:HG3	1.74	0.52
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.45	0.52
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.45	0.52
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.90	0.52
3:C:120:LEU:CD2	13:C:502:HEM:HBB2	2.39	0.52
1:N:147:ASN:O	1:N:149:THR:N	2.43	0.52
2:O:168:TYR:N	2:O:168:TYR:CD1	2.75	0.52
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.25	0.52
3:P:326:PHE:O	3:P:329:LEU:HB3	2.09	0.52
1:A:332:ASP:O	1:A:333:ASP:C	2.48	0.52
5:R:107:ASN:C	5:R:109:GLU:H	2.13	0.52
5:R:140:THR:O	5:R:141:HIS:C	2.48	0.52
2:B:43:PRO:O	2:B:113:ARG:HG3	2.09	0.52
2:B:166:ALA:HA	2:B:240:TRP:CE3	2.45	0.52
4:D:57:THR:HG22	4:D:58:GLU:N	2.23	0.52
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.45	0.52
1:N:255:LEU:HD13	1:N:422:LEU:CD1	2.39	0.52
2:O:73:SER:N	2:O:74:PRO:HD2	2.25	0.52
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.45	0.52
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.45	0.52
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.52
7:T:36:ASN:O	7:T:40:ARG:HG3	2.10	0.52
1:A:284:PHE:CD2	9:I:71:ASN:HA	2.45	0.52
4:D:43:MET:HE2	4:D:46:VAL:CG2	2.38	0.52
4:D:81:PHE:H	4:D:81:PHE:HD2	1.57	0.52
3:P:13:LYS:HG2	3:P:13:LYS:O	2.09	0.52
3:P:120:LEU:HB3	13:P:502:HEM:HBB2	1.90	0.52
3:P:329:LEU:O	3:P:332:ASN:HB3	2.09	0.52
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.44	0.52
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.25	0.52
2:B:110:GLU:O	2:B:111:CYS:HB3	2.09	0.52
2:B:155:PRO:O	2:B:158:GLY:N	2.40	0.52
4:D:168:ILE:O	4:D:168:ILE:HG12	2.10	0.52
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.10	0.52
6:F:70:LEU:HG	6:F:71:LYS:N	2.25	0.52
2:O:119:VAL:HG12	2:O:119:VAL:O	2.10	0.52
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.92	0.52
4:Q:235:MET:HE1	6:S:63:LYS:HG2	1.91	0.52
4:D:167:GLU:C	4:D:169:LEU:H	2.13	0.52
2:O:264:VAL:HG23	2:O:316:TYR:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:267:ALA:C	2:O:269:ALA:H	2.13	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.52
2:B:96:LEU:C	2:B:96:LEU:HD12	2.30	0.51
2:B:168:TYR:CE2	2:B:172:LEU:HB2	2.46	0.51
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.45	0.51
4:D:40:CYS:HA	4:D:95:TYR:HE1	1.75	0.51
2:O:290:SER:CB	2:O:293:SER:HB3	2.40	0.51
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.46	0.51
1:N:171:THR:HB	5:R:4:ASP:OD2	2.11	0.51
2:O:73:SER:OG	2:O:74:PRO:HD3	2.09	0.51
2:O:168:TYR:N	2:O:168:TYR:HD1	2.08	0.51
2:O:333:ALA:O	2:O:337:ILE:HG13	2.10	0.51
1:A:242:ARG:HH22	1:A:432:LEU:HA	1.76	0.51
3:C:86:ASN:ND2	3:C:243:LEU:HD11	2.26	0.51
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.91	0.51
5:E:142:LEU:HD12	5:E:161:HIS:HE1	1.74	0.51
9:I:59:SER:O	9:I:60:ALA:HB3	2.11	0.51
3:P:137:GLY:N	3:P:140:SER:HB2	2.25	0.51
7:T:78:GLU:C	7:T:79:ASN:HD22	2.13	0.51
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.75	0.51
2:B:374:THR:HG22	2:B:376:GLN:N	2.25	0.51
4:D:148:HIS:ND1	4:D:161:ALA:HA	2.25	0.51
8:H:57:GLU:O	8:H:60:ASP:HB2	2.10	0.51
2:O:341:MET:HE3	2:O:417:PHE:CZ	2.46	0.51
3:P:142:TRP:O	3:P:146:VAL:HG23	2.09	0.51
1:A:158:PHE:O	1:A:159:GLN:O	2.28	0.51
1:A:255:LEU:HD12	1:A:421:ALA:O	2.10	0.51
1:A:333:ASP:O	1:A:336:PHE:HB3	2.10	0.51
2:B:259:THR:HG23	2:B:421:LYS:O	2.11	0.51
2:B:341:MET:O	2:B:344:LEU:HB2	2.11	0.51
4:D:171:TYR:OH	4:D:182:ILE:HA	2.11	0.51
2:O:201:SER:H	2:O:227:ARG:CB	2.17	0.51
3:P:130:VAL:HG23	3:P:131:GLY:N	2.26	0.51
3:P:132:TYR:O	3:P:135:PRO:HD2	2.11	0.51
5:R:76:ILE:O	5:R:193:VAL:HG12	2.10	0.51
9:V:28:UNK:HA	9:V:72:ALA:HB2	1.93	0.51
1:A:163:LEU:HD22	1:A:314:TYR:HE1	1.74	0.51
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.40	0.51
6:F:81:VAL:HG12	6:F:82:LYS:N	2.26	0.51
2:O:341:MET:CE	2:O:417:PHE:CE2	2.93	0.51
3:P:187:PRO:HG2	13:P:501:HEM:HMC3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.41	0.51
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.45	0.51
1:A:106:MET:HB3	1:A:107:PRO:HD3	1.93	0.51
1:A:381:SER:O	1:A:382:HIS:C	2.49	0.51
3:C:78:TRP:CD2	3:C:79:LEU:N	2.79	0.51
4:D:52:ILE:C	4:D:54:VAL:H	2.13	0.51
4:D:134:TYR:CD2	4:D:162:PRO:HG3	2.45	0.51
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.91	0.51
1:N:221:PHE:O	1:N:222:THR:O	2.28	0.51
2:O:415:LYS:O	2:O:417:PHE:N	2.44	0.51
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.31	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
6:F:61:ARG:HG3	6:F:61:ARG:NH1	2.26	0.51
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.25	0.51
1:N:106:MET:HB3	1:N:107:PRO:HD3	1.93	0.51
1:N:373:THR:N	1:N:374:PRO:HD2	2.24	0.51
2:O:42:SER:O	2:O:113:ARG:HD2	2.10	0.51
5:R:101:ARG:NH2	5:R:127:VAL:HG11	2.26	0.51
5:R:101:ARG:HH21	5:R:127:VAL:HG21	1.74	0.51
5:R:133:VAL:O	5:R:133:VAL:HG13	2.11	0.51
1:A:206:LYS:O	1:A:207:GLU:C	2.49	0.51
1:A:221:PHE:O	1:A:222:THR:O	2.29	0.51
3:C:216:SER:HB3	6:F:59:MET:CE	2.41	0.51
3:C:243:LEU:C	3:C:243:LEU:HD12	2.31	0.51
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.26	0.51
1:N:255:LEU:O	1:N:321:GLY:HA3	2.11	0.51
6:S:58:ARG:HG3	6:S:89:TYR:OH	2.11	0.51
8:U:52:GLU:HG2	8:U:53:GLN:N	2.26	0.51
2:B:424:MET:HG2	2:B:425:ALA:H	1.75	0.51
2:O:102:ARG:NH1	2:O:102:ARG:CG	2.66	0.51
2:O:203:ARG:O	2:O:387:LEU:HD11	2.11	0.51
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.94	0.50
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.92	0.50
3:C:89:SER:O	3:C:90:PHE:C	2.49	0.50
3:C:95:ILE:CG2	3:C:96:PHE:N	2.74	0.50
3:C:198:LEU:HD21	13:C:502:HEM:CMA	2.41	0.50
5:E:129:LYS:HD2	5:E:132:TRP:CD1	2.46	0.50
1:N:180:ALA:O	1:N:183:ALA:HB3	2.10	0.50
2:O:58:GLU:OE1	2:O:64:GLY:N	2.43	0.50
2:O:168:TYR:CE2	2:O:172:LEU:HB2	2.45	0.50
3:P:75:GLN:O	3:P:77:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:52:ILE:C	4:Q:54:VAL:H	2.15	0.50
8:U:65:ARG:O	8:U:68:CYS:HB3	2.10	0.50
1:A:64:PHE:HA	1:A:75:PHE:HE2	1.76	0.50
3:C:175:THR:O	3:C:178:ARG:HG2	2.11	0.50
4:D:57:THR:H	4:D:60:GLU:HG3	1.75	0.50
5:E:81:ILE:HD12	5:E:132:TRP:CZ3	2.46	0.50
10:J:60:GLU:O	10:J:61:ALA:HB3	2.11	0.50
2:O:221:GLU:HG3	2:O:222:GLN:N	2.23	0.50
2:O:341:MET:O	2:O:344:LEU:HB2	2.11	0.50
3:P:320:PRO:HG2	3:P:321:LEU:H	1.76	0.50
4:Q:10:PHE:HD2	8:U:74:PHE:HE2	1.59	0.50
1:A:105:ASP:O	1:A:106:MET:C	2.49	0.50
1:A:261:GLY:O	1:A:267:ASN:ND2	2.45	0.50
2:B:81:SER:C	2:B:83:PHE:N	2.64	0.50
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.75	0.50
2:B:378:LEU:HD12	2:B:378:LEU:O	2.11	0.50
4:D:37:CYS:O	4:D:39:ALA:N	2.45	0.50
2:O:109:VAL:HG23	2:O:109:VAL:O	2.11	0.50
2:O:225:ASN:C	2:O:227:ARG:H	2.14	0.50
2:O:395:PRO:O	2:O:398:VAL:HG12	2.11	0.50
3:P:4:ASN:O	3:P:5:ILE:HD13	2.11	0.50
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.73	0.50
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.92	0.50
1:A:90:THR:HA	1:A:95:THR:HA	1.93	0.50
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.92	0.50
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.42	0.50
4:D:208:MET:O	4:D:212:SER:HB2	2.12	0.50
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.40	0.50
4:Q:186:VAL:HG13	4:Q:187:CYS:N	2.25	0.50
6:S:10:GLY:O	6:S:14:ASP:HB2	2.10	0.50
2:B:150:VAL:HG22	2:B:151:ALA:N	2.26	0.50
3:C:29:SER:HB2	16:C:2004:CDL:OB4	2.12	0.50
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.46	0.50
1:N:253:VAL:CG1	1:N:335:MET:HE1	2.41	0.50
2:O:152:PHE:HE1	2:O:177:TYR:CD1	2.28	0.50
2:O:341:MET:CE	2:O:417:PHE:HE2	2.23	0.50
2:O:378:LEU:HD12	2:O:378:LEU:O	2.12	0.50
4:Q:221:TYR:HE1	7:T:25:ALA:HB2	1.75	0.50
5:R:126:ARG:HH21	5:R:179:ASN:ND2	2.10	0.50
1:A:418:LYS:O	1:A:420:PRO:HD3	2.12	0.50
2:B:96:LEU:CB	2:B:109:VAL:HG12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.18	0.50
2:O:209:ILE:HD11	2:O:378:LEU:HG	1.93	0.50
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.41	0.50
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.94	0.50
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.11	0.50
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.94	0.50
8:U:18:THR:O	8:U:22:GLU:HG3	2.12	0.50
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.47	0.50
1:A:344:ARG:HB3	1:A:344:ARG:CZ	2.42	0.50
3:C:247:SER:N	3:C:248:PRO:HD3	2.27	0.50
3:C:316:MET:HG2	3:C:319:ARG:NH2	2.26	0.50
3:C:345:GLU:O	3:C:348:PHE:HB2	2.10	0.50
1:N:87:ASN:OD1	1:N:88:GLY:N	2.37	0.50
1:N:107:PRO:O	1:N:108:LYS:C	2.49	0.50
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.94	0.50
16:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.11	0.50
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.92	0.50
6:S:57:GLU:HB3	6:S:61:ARG:HH12	1.76	0.50
8:U:57:GLU:O	8:U:60:ASP:HB2	2.12	0.50
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.94	0.50
3:C:158:GLY:C	3:C:160:THR:N	2.65	0.50
3:C:329:LEU:O	3:C:332:ASN:HB3	2.11	0.50
4:D:52:ILE:O	4:D:54:VAL:N	2.45	0.50
2:O:259:THR:HG23	2:O:421:LYS:O	2.11	0.50
2:O:345:LYS:O	2:O:348:ALA:N	2.45	0.50
4:Q:148:HIS:CE1	4:Q:161:ALA:HA	2.46	0.50
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.12	0.50
1:A:429:GLU:O	1:A:429:GLU:HG2	2.11	0.50
3:C:210:LEU:HD12	6:F:66:LEU:HD23	1.92	0.50
3:C:287:ASN:O	3:C:288:LYS:C	2.50	0.50
5:E:130:PRO:HG2	5:E:131:GLU:H	1.77	0.50
9:I:63:ASP:O	9:I:64:LEU:HB2	2.12	0.50
1:N:105:ASP:O	1:N:106:MET:C	2.50	0.50
2:O:85:ILE:HA	2:O:122:TYR:CD2	2.47	0.50
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.93	0.50
4:Q:235:MET:HE1	6:S:63:LYS:C	2.31	0.50
1:A:365:MET:CG	1:A:366:VAL:H	2.25	0.49
2:B:124:LEU:HD23	2:B:124:LEU:C	2.31	0.49
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.42	0.49
2:O:263:ALA:O	2:O:266:SER:HB3	2.12	0.49
4:Q:81:PHE:H	4:Q:81:PHE:HD2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:79:ASN:HD22	7:T:79:ASN:N	2.10	0.49
8:U:37:LEU:O	8:U:40:CYS:N	2.44	0.49
9:V:49:LEU:CD2	9:V:55:MET:HB3	2.39	0.49
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.77	0.49
4:D:109:LEU:O	4:D:111:PRO:HD3	2.12	0.49
2:O:268:GLU:HG2	2:O:272:PHE:HE1	1.77	0.49
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.43	0.49
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.11	0.49
1:A:67:THR:HA	1:A:121:ALA:N	2.27	0.49
5:E:20:ASP:C	5:E:22:THR:H	2.16	0.49
8:H:43:ARG:HD2	8:H:47:ARG:NH2	2.26	0.49
1:N:147:ASN:C	1:N:149:THR:N	2.66	0.49
1:N:365:MET:CG	1:N:366:VAL:H	2.23	0.49
2:O:100:SER:HA	2:O:104:LYS:O	2.12	0.49
2:O:124:LEU:O	2:O:128:THR:HG23	2.12	0.49
2:O:290:SER:HB3	2:O:293:SER:HB3	1.94	0.49
3:P:70:THR:O	3:P:74:VAL:HG23	2.12	0.49
4:Q:57:THR:H	4:Q:60:GLU:HG3	1.76	0.49
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.48	0.49
8:H:18:THR:O	8:H:22:GLU:HG3	2.12	0.49
1:N:253:VAL:O	1:N:323:HIS:HA	2.11	0.49
2:O:283:PRO:C	2:O:284:LEU:HD23	2.32	0.49
6:S:61:ARG:HG3	6:S:61:ARG:NH1	2.28	0.49
1:A:171:THR:HB	5:E:4:ASP:OD2	2.12	0.49
2:B:313:ASN:O	9:I:62:ARG:O	2.31	0.49
3:C:245:LEU:O	4:D:201:ARG:CD	2.60	0.49
9:I:32:UNK:N	9:I:73:PRO:CG	2.70	0.49
3:P:86:ASN:ND2	3:P:243:LEU:HD11	2.27	0.49
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.77	0.49
3:C:277:PHE:CG	3:C:278:ALA:N	2.80	0.49
1:N:4:TYR:O	1:N:6:GLN:N	2.46	0.49
2:O:27:THR:CG2	2:O:28:LYS:N	2.74	0.49
6:S:68:LEU:O	6:S:71:LYS:N	2.46	0.49
2:B:283:PRO:C	2:B:284:LEU:HD23	2.33	0.49
2:B:385:GLU:C	2:B:387:LEU:N	2.66	0.49
3:C:137:GLY:H	3:C:140:SER:CB	2.26	0.49
4:D:10:PHE:CD1	4:D:10:PHE:N	2.81	0.49
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.49
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.48	0.49
2:O:120:MET:O	2:O:121:GLU:C	2.50	0.49
4:Q:158:ILE:CD1	4:Q:160:MET:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:ILE:HB	5:R:132:TRP:HH2	1.77	0.49
1:A:40:TRP:CH2	1:A:376:CYS:HB3	2.48	0.49
1:A:107:PRO:O	1:A:108:LYS:C	2.50	0.49
1:A:122:LEU:HD11	1:A:186:ILE:CD1	2.43	0.49
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.95	0.49
2:B:306:PRO:HB3	9:I:52:ARG:N	2.28	0.49
2:B:395:PRO:O	2:B:398:VAL:HG12	2.12	0.49
4:D:27:ARG:CZ	10:J:59:TYR:HE2	2.25	0.49
8:H:25:GLU:HG2	8:H:61:PHE:HZ	1.78	0.49
1:N:343:MET:O	1:N:344:ARG:C	2.50	0.49
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.94	0.49
5:R:1:VAL:HG23	5:R:3:ASN:N	2.24	0.49
5:R:15:ARG:HH11	5:R:32:ARG:HB3	1.76	0.49
1:A:147:ASN:O	1:A:148:VAL:C	2.51	0.49
1:A:244:ARG:NE	7:G:10:VAL:HB	2.27	0.49
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.78	0.49
6:F:68:LEU:O	6:F:71:LYS:N	2.46	0.49
7:G:60:SER:O	7:G:64:GLN:HB2	2.13	0.49
7:G:77:TYR:CD1	8:H:52:GLU:HB2	2.48	0.49
1:N:170:THR:HG22	1:N:172:GLU:H	1.78	0.49
1:N:178:THR:CG2	1:N:179:ARG:N	2.76	0.49
1:N:281:ASP:OD1	1:N:281:ASP:O	2.31	0.49
2:O:150:VAL:CG2	2:O:151:ALA:N	2.75	0.49
3:P:287:ASN:O	3:P:288:LYS:C	2.52	0.49
1:A:134:ILE:CG2	1:A:174:ILE:HG12	2.42	0.49
1:A:434:TYR:CE2	7:G:19:SER:HB2	2.48	0.49
2:B:372:VAL:O	2:B:372:VAL:HG12	2.12	0.49
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.94	0.49
3:C:189:ALA:O	3:C:193:ILE:HG13	2.12	0.49
4:D:116:ILE:HG23	4:D:117:VAL:H	1.75	0.49
4:D:117:VAL:HG13	4:D:190:LEU:HB3	1.95	0.49
4:D:235:MET:HE1	6:F:63:LYS:HG2	1.94	0.49
1:N:371:GLY:O	1:N:375:VAL:HG23	2.13	0.49
2:O:424:MET:HG2	2:O:425:ALA:H	1.77	0.49
3:P:82:ASN:H	3:P:82:ASN:ND2	2.11	0.49
4:Q:10:PHE:N	4:Q:10:PHE:CD1	2.80	0.49
5:R:141:HIS:HB2	5:R:176:ALA:CB	2.43	0.49
1:A:52:ASN:O	1:A:53:ASN:C	2.51	0.48
3:C:172:ASP:C	3:C:174:PRO:HD2	2.33	0.48
3:P:104:TYR:HD2	3:P:105:TYR:CE1	2.30	0.48
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:117:VAL:HG13	4:Q:190:LEU:HB3	1.95	0.48
6:S:51:PRO:O	6:S:52:GLU:C	2.51	0.48
2:B:415:LYS:O	2:B:417:PHE:N	2.45	0.48
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.49	0.48
3:C:273:TRP:HA	3:C:276:LEU:HG	1.94	0.48
4:D:240:PRO:O	4:D:241:LYS:C	2.51	0.48
5:E:129:LYS:HG2	5:E:187:PHE:CZ	2.48	0.48
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.48
2:O:415:LYS:C	2:O:417:PHE:N	2.66	0.48
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.95	0.48
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	3.01	0.48
1:A:53:ASN:OD1	1:A:165:ARG:HD3	2.14	0.48
1:A:342:TRP:HA	1:A:345:LEU:HD12	1.94	0.48
1:A:433:ASP:OD2	1:A:435:ASN:N	2.47	0.48
2:B:157:VAL:HG22	2:B:157:VAL:O	2.14	0.48
4:D:47:ALA:N	4:D:50:ASN:HD22	2.00	0.48
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.91	0.48
1:N:271:HIS:NE2	1:N:311:ASN:HB3	2.28	0.48
3:P:150:LEU:HB3	3:P:292:VAL:CG2	2.43	0.48
3:P:175:THR:O	3:P:178:ARG:HG2	2.12	0.48
3:P:253:ASP:OD1	3:P:254:PRO:N	2.46	0.48
4:Q:98:PRO:HG2	4:Q:99:GLU:OE1	2.13	0.48
1:A:87:ASN:HB3	1:A:98:TYR:CE1	2.48	0.48
2:B:203:ARG:O	2:B:387:LEU:HD11	2.14	0.48
3:C:41:CYS:SG	3:C:91:PHE:HA	2.54	0.48
3:C:242:THR:N	4:D:208:MET:HE1	2.27	0.48
4:D:187:CYS:O	4:D:190:LEU:HB2	2.14	0.48
4:D:218:LEU:HD13	5:E:43:ALA:HA	1.94	0.48
5:E:163:SER:HA	5:E:174:GLY:HA3	1.96	0.48
1:N:349:THR:HA	1:N:353:GLU:OE1	2.13	0.48
2:O:385:GLU:C	2:O:387:LEU:N	2.66	0.48
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.93	0.48
3:P:175:THR:O	3:P:176:LEU:C	2.51	0.48
3:P:297:ALA:HA	3:P:300:LEU:HB2	1.96	0.48
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.47	0.48
4:Q:135:CYS:O	4:Q:149:TYR:HB3	2.12	0.48
5:R:83:GLU:HA	5:R:100:HIS:O	2.14	0.48
1:A:53:ASN:CG	1:A:165:ARG:HD3	2.33	0.48
1:A:191:LYS:C	1:A:195:MET:HE2	2.33	0.48
2:B:415:LYS:C	2:B:417:PHE:N	2.66	0.48
4:D:164:ILE:HG21	4:D:182:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:LYS:HG2	5:E:187:PHE:CE2	2.48	0.48
1:N:178:THR:C	1:N:180:ALA:N	2.64	0.48
1:N:281:ASP:OD1	1:N:281:ASP:C	2.52	0.48
2:O:166:ALA:O	2:O:242:GLY:N	2.46	0.48
2:O:220:ALA:O	2:O:224:LEU:HB2	2.14	0.48
5:R:118:ARG:O	5:R:120:PRO:HD3	2.13	0.48
1:A:4:TYR:OH	1:A:362:ARG:HD3	2.12	0.48
1:A:356:ARG:HG3	2:B:91:ALA:HA	1.95	0.48
3:C:132:TYR:O	3:C:135:PRO:HD2	2.13	0.48
4:D:135:CYS:O	4:D:149:TYR:HB3	2.14	0.48
1:N:64:PHE:HA	1:N:75:PHE:HE2	1.79	0.48
1:N:106:MET:HE1	1:N:208:LEU:HD13	1.96	0.48
1:N:158:PHE:HB3	1:N:161:THR:OG1	2.13	0.48
1:N:242:ARG:NH2	1:N:432:LEU:HA	2.28	0.48
3:P:78:TRP:CG	3:P:79:LEU:N	2.82	0.48
4:Q:43:MET:HG2	4:Q:46:VAL:CG2	2.44	0.48
2:B:57:TYR:CE2	2:B:234:SER:HB2	2.49	0.48
2:B:76:THR:HG22	2:B:81:SER:HA	1.95	0.48
3:C:60:THR:HG23	3:C:173:ASN:HA	1.96	0.48
3:C:61:SER:C	3:C:62:LEU:HG	2.34	0.48
3:C:72:ARG:HG2	3:C:72:ARG:NH1	2.29	0.48
4:D:171:TYR:C	4:D:173:ASP:H	2.17	0.48
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.96	0.48
1:N:270:LEU:HD13	1:N:320:PHE:HD1	1.79	0.48
1:N:317:THR:HG23	1:N:318:GLY:H	1.78	0.48
2:O:43:PRO:O	2:O:113:ARG:HG3	2.13	0.48
2:O:81:SER:C	2:O:83:PHE:N	2.65	0.48
2:O:258:VAL:HG21	2:O:321:LEU:HD22	1.95	0.48
3:P:60:THR:HG23	3:P:173:ASN:HA	1.95	0.48
3:P:277:PHE:CG	3:P:278:ALA:N	2.82	0.48
5:R:175:PRO:HG2	5:R:176:ALA:H	1.79	0.48
10:W:10:TYR:CD2	10:W:10:TYR:O	2.67	0.48
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.71	0.48
4:D:218:LEU:CD1	5:E:43:ALA:HA	2.44	0.48
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.35	0.48
10:J:15:ARG:HG2	10:J:15:ARG:HH11	1.77	0.48
1:N:40:TRP:CH2	1:N:376:CYS:HB3	2.49	0.48
1:N:87:ASN:HB3	1:N:98:TYR:CZ	2.48	0.48
1:N:122:LEU:HD11	1:N:186:ILE:CD1	2.44	0.48
1:N:184:SER:O	1:N:187:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:312:PHE:O	2:O:322:PHE:HA	2.14	0.48
3:P:201:LEU:C	3:P:203:GLU:H	2.17	0.48
5:R:20:ASP:C	5:R:22:THR:H	2.17	0.48
8:U:43:ARG:O	8:U:47:ARG:HG3	2.14	0.48
1:A:134:ILE:HG21	1:A:174:ILE:CG1	2.43	0.48
1:A:178:THR:HG22	1:A:180:ALA:H	1.79	0.48
2:B:47:ILE:HD13	2:B:120:MET:CE	2.43	0.48
2:B:56:ARG:HG2	2:B:234:SER:OG	2.13	0.48
2:B:248:ASN:C	2:B:248:ASN:HD22	2.16	0.48
3:C:147:ILE:HA	3:C:150:LEU:HD12	1.96	0.48
5:E:133:VAL:O	5:E:133:VAL:HG13	2.13	0.48
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.18	0.48
6:F:67:ASP:HA	6:F:70:LEU:CD2	2.32	0.48
2:O:137:VAL:O	2:O:140:LEU:HB3	2.14	0.48
5:R:15:ARG:NH1	5:R:32:ARG:HB3	2.29	0.48
10:W:23:THR:O	10:W:24:VAL:C	2.53	0.48
5:E:40:THR:O	5:E:41:ALA:C	2.53	0.48
5:E:116:LYS:H	5:E:116:LYS:CD	2.20	0.48
5:E:147:ILE:CG2	5:E:148:ALA:H	2.15	0.48
8:H:37:LEU:O	8:H:40:CYS:N	2.47	0.48
1:N:277:ILE:O	1:N:277:ILE:HG22	2.12	0.48
2:O:24:LEU:O	2:O:24:LEU:HD23	2.14	0.48
2:O:422:LYS:O	2:O:436:LEU:HD21	2.14	0.48
3:P:141:PHE:O	3:P:144:ALA:HB3	2.13	0.48
3:P:184:PHE:CE2	13:P:501:HEM:HBC1	2.49	0.48
4:Q:220:TYR:OH	4:Q:224:ARG:HD3	2.14	0.48
10:W:52:TRP:O	10:W:56:LYS:HB2	2.13	0.48
2:B:109:VAL:HG23	2:B:109:VAL:O	2.14	0.47
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.49	0.47
3:C:67:VAL:CG2	13:C:501:HEM:HBD2	2.44	0.47
3:C:95:ILE:HG23	3:C:96:PHE:N	2.29	0.47
2:O:383:GLY:O	2:O:384:SER:C	2.52	0.47
4:Q:56:HIS:HB3	4:Q:60:GLU:HB2	1.96	0.47
5:R:73:LYS:HB3	5:R:196:GLY:HA3	1.95	0.47
5:R:76:ILE:HD13	5:R:89:PHE:CE1	2.49	0.47
5:R:99:ARG:NH2	5:R:148:ALA:HB1	2.28	0.47
5:R:139:CYS:O	5:R:141:HIS:N	2.47	0.47
1:A:182:LEU:O	1:A:186:ILE:HG13	2.14	0.47
1:A:378:THR:O	1:A:382:HIS:N	2.43	0.47
2:B:132:PHE:HB2	2:B:192:HIS:CE1	2.49	0.47
3:C:142:TRP:O	3:C:146:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:THR:O	3:C:176:LEU:C	2.50	0.47
3:C:316:MET:HG2	3:C:319:ARG:HH21	1.78	0.47
4:D:72:ASP:HB3	4:D:81:PHE:CE2	2.50	0.47
4:D:186:VAL:HG13	4:D:187:CYS:N	2.27	0.47
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.49	0.47
2:O:222:GLN:O	2:O:223:PHE:CG	2.67	0.47
2:O:247:GLN:NE2	2:O:249:GLY:H	2.12	0.47
3:P:75:GLN:C	3:P:77:GLY:H	2.18	0.47
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.14	0.47
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.79	0.47
7:T:63:THR:HG22	7:T:64:GLN:N	2.28	0.47
1:A:270:LEU:HD13	1:A:320:PHE:HD1	1.77	0.47
3:C:45:GLN:O	3:C:49:GLY:N	2.38	0.47
1:N:439:SER:C	1:N:441:MET:N	2.68	0.47
2:O:209:ILE:CG2	2:O:210:GLY:N	2.60	0.47
4:Q:106:ASN:C	4:Q:108:ALA:H	2.18	0.47
8:U:52:GLU:CG	8:U:53:GLN:N	2.77	0.47
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.27	0.47
2:B:253:VAL:HG11	2:B:433:THR:OG1	2.13	0.47
2:B:407:SER:O	2:B:411:VAL:HG23	2.14	0.47
4:D:122:GLY:O	4:D:123:GLY:C	2.52	0.47
5:E:96:LEU:HD12	5:E:135:LEU:O	2.14	0.47
2:O:248:ASN:C	2:O:248:ASN:HD22	2.17	0.47
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.47
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.49	0.47
3:C:120:LEU:CB	13:C:502:HEM:HBB2	2.43	0.47
3:C:208:ASN:C	3:C:208:ASN:OD1	2.53	0.47
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.79	0.47
2:O:215:ASP:C	2:O:217:LYS:N	2.67	0.47
2:O:306:PRO:HB3	9:V:52:ARG:H	1.80	0.47
2:O:385:GLU:HB3	2:O:391:THR:O	2.15	0.47
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.78	0.47
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.97	0.47
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.96	0.47
10:W:60:GLU:O	10:W:61:ALA:HB2	2.15	0.47
1:A:15:ASN:HB2	1:A:205:HIS:ND1	2.30	0.47
2:B:266:SER:OG	2:B:267:ALA:N	2.47	0.47
2:B:332:HIS:O	2:B:336:VAL:HG23	2.14	0.47
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.96	0.47
4:D:186:VAL:CG1	4:D:187:CYS:N	2.77	0.47
5:E:81:ILE:HD12	5:E:132:TRP:CH2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:O	2:O:74:PRO:CD	2.55	0.47
2:O:257:VAL:CG2	2:O:424:MET:HG3	2.42	0.47
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.54	0.47
4:Q:108:ALA:HB1	19:Q:501:HEC:HMD1	1.97	0.47
4:Q:221:TYR:CD2	5:R:39:VAL:HG21	2.50	0.47
1:A:23:LEU:HA	1:A:192:ALA:O	2.15	0.47
2:B:152:PHE:CE1	2:B:177:TYR:HD1	2.31	0.47
2:B:209:ILE:O	2:B:211:VAL:N	2.48	0.47
2:B:383:GLY:O	2:B:384:SER:C	2.52	0.47
3:C:30:ALA:HB1	16:D:2003:CDL:H111	1.95	0.47
4:D:106:ASN:C	4:D:108:ALA:H	2.17	0.47
5:E:175:PRO:O	5:E:176:ALA:C	2.53	0.47
1:N:106:MET:HE2	1:N:106:MET:C	2.35	0.47
1:N:121:ALA:O	1:N:122:LEU:HB2	2.13	0.47
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.15	0.47
1:N:254:ALA:HB3	1:N:423:ALA:HB3	1.96	0.47
1:N:365:MET:HG3	1:N:366:VAL:H	1.80	0.47
1:N:378:THR:O	1:N:382:HIS:N	2.42	0.47
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.96	0.47
2:O:151:ALA:C	2:O:153:GLN:H	2.18	0.47
2:O:215:ASP:O	2:O:217:LYS:N	2.47	0.47
2:O:272:PHE:O	2:O:276:GLN:N	2.39	0.47
3:P:30:ALA:HB1	16:Q:3003:CDL:H111	1.96	0.47
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.50	0.47
5:R:79:SER:C	5:R:81:ILE:H	2.18	0.47
5:R:170:ARG:HA	5:R:179:ASN:CG	2.35	0.47
1:A:44:GLY:HA3	1:A:92:ARG:O	2.15	0.47
3:C:254:PRO:O	3:C:257:PHE:N	2.47	0.47
5:E:101:ARG:HD2	5:E:105:GLU:HB3	1.96	0.47
1:N:58:PHE:HA	1:N:134:ILE:HD11	1.96	0.47
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.50	0.47
1:N:256:ALA:HA	1:N:320:PHE:O	2.15	0.47
1:N:344:ARG:HG3	1:N:344:ARG:NH1	2.30	0.47
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.50	0.47
1:A:15:ASN:O	1:A:26:ALA:HA	2.15	0.47
2:B:73:SER:N	2:B:74:PRO:HD2	2.29	0.47
2:B:73:SER:OG	2:B:74:PRO:HD3	2.15	0.47
2:B:119:VAL:HG12	2:B:119:VAL:O	2.15	0.47
3:C:187:PRO:O	3:C:190:ILE:HB	2.14	0.47
4:D:73:GLY:N	4:D:81:PHE:HE2	2.13	0.47
4:D:98:PRO:HG2	4:D:99:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:16:ILE:O	6:F:19:TRP:HB3	2.15	0.47
1:N:332:ASP:O	1:N:333:ASP:C	2.51	0.47
2:O:109:VAL:CG2	2:O:119:VAL:HG12	2.45	0.47
3:P:254:PRO:O	3:P:256:ASN:N	2.48	0.47
5:R:185:TYR:CD2	5:R:185:TYR:N	2.82	0.47
1:A:52:ASN:OD1	1:A:52:ASN:C	2.52	0.47
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.79	0.47
3:C:72:ARG:HG2	3:C:72:ARG:HH11	1.78	0.47
4:D:28:ARG:O	4:D:29:GLY:C	2.53	0.47
4:D:70:VAL:HG23	4:D:83:ARG:HG2	1.97	0.47
6:F:32:MET:O	6:F:33:ARG:C	2.52	0.47
6:F:90:LEU:O	6:F:91:GLU:C	2.51	0.47
1:N:191:LYS:N	1:N:195:MET:HE2	2.30	0.47
1:N:394:GLU:O	1:N:395:TRP:C	2.53	0.47
3:P:184:PHE:HA	13:P:501:HEM:HBC2	1.97	0.47
2:B:85:ILE:HA	2:B:122:TYR:CD2	2.51	0.46
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.80	0.46
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.45	0.46
1:N:65:LYS:NZ	2:O:287:ARG:O	2.41	0.46
1:N:67:THR:HA	1:N:121:ALA:N	2.30	0.46
1:N:178:THR:HG22	1:N:180:ALA:H	1.80	0.46
1:N:295:ALA:O	1:N:298:ALA:HB3	2.15	0.46
2:O:34:ILE:HG21	2:O:386:ALA:O	2.15	0.46
2:O:140:LEU:C	2:O:142:PRO:HD2	2.36	0.46
2:O:272:PHE:HA	2:O:275:LEU:HB3	1.96	0.46
4:Q:148:HIS:ND1	4:Q:162:PRO:HD3	2.30	0.46
9:V:32:UNK:N	9:V:73:PRO:HG2	2.31	0.46
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.46
1:A:107:PRO:O	1:A:109:VAL:N	2.48	0.46
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.15	0.46
1:A:260:PRO:HB3	1:A:414:TYR:CE2	2.51	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.15	0.46
3:C:120:LEU:HD21	3:C:193:ILE:HB	1.96	0.46
5:E:79:SER:OG	5:E:191:ASP:HB2	2.14	0.46
8:H:31:VAL:C	8:H:33:ALA:H	2.17	0.46
1:N:341:GLU:O	1:N:342:TRP:C	2.53	0.46
2:O:258:VAL:HG12	2:O:323:GLY:HA3	1.98	0.46
16:Q:3003:CDL:HA21	6:S:72:HIS:CD2	2.50	0.46
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.45	0.46
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.80	0.46
1:N:170:THR:CG2	1:N:171:THR:H	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:219:VAL:HG12	1:N:220:SER:N	2.30	0.46
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.45	0.46
5:R:44:CYS:HB3	10:W:24:VAL:HG11	1.97	0.46
6:S:67:ASP:O	6:S:71:LYS:HG3	2.15	0.46
2:B:215:ASP:C	2:B:217:LYS:N	2.69	0.46
2:B:341:MET:HE3	2:B:417:PHE:CZ	2.51	0.46
4:D:127:VAL:O	4:D:131:LEU:HG	2.14	0.46
4:D:200:GLN:NE2	20:D:2091:BOG:H3	2.30	0.46
9:I:77:ARG:HE	9:I:77:ARG:HB2	1.56	0.46
1:N:76:GLU:HA	2:O:285:ILE:HD11	1.96	0.46
1:N:163:LEU:HD22	1:N:314:TYR:HE1	1.81	0.46
2:O:337:ILE:O	2:O:340:ALA:HB3	2.16	0.46
3:P:82:ASN:N	3:P:82:ASN:ND2	2.63	0.46
3:P:253:ASP:OD1	3:P:254:PRO:CD	2.63	0.46
1:A:58:PHE:HA	1:A:134:ILE:HD11	1.97	0.46
2:B:18:CYS:CB	2:B:19:PRO:HD3	2.42	0.46
3:C:72:ARG:NE	4:D:115:TYR:OH	2.48	0.46
3:C:92:PHE:O	3:C:93:ILE:C	2.51	0.46
3:C:158:GLY:C	3:C:160:THR:H	2.18	0.46
4:D:155:GLY:C	4:D:157:ALA:H	2.19	0.46
4:D:218:LEU:HD13	5:E:43:ALA:N	2.31	0.46
4:D:218:LEU:HB3	5:E:43:ALA:HB2	1.96	0.46
7:G:72:LYS:NZ	8:H:52:GLU:HG3	2.30	0.46
1:N:161:THR:HG21	1:N:234:CYS:HA	1.97	0.46
1:N:161:THR:HG21	1:N:235:ARG:N	2.29	0.46
1:N:270:LEU:HB3	1:N:320:PHE:CE1	2.48	0.46
1:N:382:HIS:HB3	1:N:389:ARG:HA	1.97	0.46
2:O:81:SER:O	2:O:83:PHE:N	2.48	0.46
2:O:160:LEU:CB	9:V:64:LEU:HD22	2.42	0.46
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.31	0.46
2:O:430:LEU:O	2:O:432:SER:N	2.49	0.46
3:P:40:VAL:O	3:P:44:THR:OG1	2.32	0.46
3:P:261:ASN:ND2	3:P:264:VAL:H	2.14	0.46
4:Q:120:ARG:HG2	4:Q:120:ARG:HH11	1.80	0.46
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.98	0.46
2:B:81:SER:O	2:B:83:PHE:N	2.48	0.46
2:B:400:GLN:O	2:B:404:SER:HB3	2.16	0.46
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.50	0.46
4:D:158:ILE:HD11	4:D:160:MET:HB3	1.96	0.46
4:D:184:LYS:HG2	8:H:74:PHE:CE1	2.51	0.46
4:D:218:LEU:HD13	5:E:42:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.79	0.46
1:N:272:VAL:O	1:N:275:ALA:HB3	2.16	0.46
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.45	0.46
3:P:147:ILE:HA	3:P:150:LEU:HD12	1.98	0.46
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.98	0.46
5:R:20:ASP:O	5:R:22:THR:N	2.40	0.46
10:W:55:ILE:O	10:W:55:ILE:HG13	2.15	0.46
1:A:178:THR:CG2	1:A:179:ARG:N	2.79	0.46
1:A:249:PRO:HG2	1:A:250:VAL:N	2.28	0.46
2:B:341:MET:CE	2:B:417:PHE:HE2	2.28	0.46
2:B:410:VAL:O	2:B:413:ALA:N	2.48	0.46
2:B:422:LYS:O	2:B:436:LEU:HD21	2.16	0.46
3:C:5:ILE:O	3:C:5:ILE:HG22	2.16	0.46
3:C:234:THR:HG21	4:D:219:LEU:HD13	1.98	0.46
3:C:319:ARG:HB3	3:C:374:GLU:OE1	2.16	0.46
5:E:38:LEU:HB2	10:J:14:PHE:HE1	1.81	0.46
1:N:304:CYS:HB2	1:N:325:VAL:O	2.16	0.46
2:O:102:ARG:H	2:O:102:ARG:HD2	1.80	0.46
2:O:155:PRO:O	2:O:158:GLY:N	2.46	0.46
2:O:168:TYR:HE2	2:O:172:LEU:HD12	1.80	0.46
3:P:89:SER:O	3:P:90:PHE:C	2.52	0.46
4:Q:10:PHE:H	4:Q:10:PHE:HD1	1.64	0.46
1:A:272:VAL:O	1:A:275:ALA:HB3	2.16	0.46
1:A:392:LEU:CD2	1:A:392:LEU:N	2.79	0.46
2:B:24:LEU:HD23	2:B:24:LEU:C	2.36	0.46
2:B:124:LEU:O	2:B:128:THR:HG23	2.16	0.46
2:B:152:PHE:HE1	2:B:177:TYR:CD1	2.33	0.46
3:C:289:LEU:O	3:C:293:LEU:HG	2.16	0.46
4:D:184:LYS:CG	8:H:74:PHE:CE1	2.99	0.46
8:H:58:LEU:HD11	8:H:62:LEU:CD1	2.46	0.46
2:O:338:ARG:O	2:O:341:MET:N	2.48	0.46
2:O:415:LYS:O	2:O:418:VAL:N	2.49	0.46
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.46	0.46
5:R:139:CYS:O	5:R:140:THR:C	2.55	0.46
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.27	0.46
1:A:242:ARG:HH12	1:A:432:LEU:N	2.13	0.46
2:B:31:ASN:N	2:B:31:ASN:ND2	2.64	0.46
2:B:287:ARG:C	9:I:53:GLU:HG3	2.35	0.46
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.73	0.46
3:C:142:TRP:HA	3:C:145:THR:OG1	2.15	0.46
3:C:238:THR:CB	3:C:239:PRO:HD3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:SER:HG	3:C:250:LEU:HB2	1.81	0.46
3:C:253:ASP:OD1	3:C:254:PRO:N	2.49	0.46
4:D:227:TRP:O	4:D:228:SER:C	2.54	0.46
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.16	0.46
4:Q:155:GLY:C	4:Q:157:ALA:H	2.19	0.46
8:U:21:ARG:HH11	8:U:21:ARG:HG3	1.81	0.46
1:A:344:ARG:NH1	1:A:344:ARG:CB	2.79	0.46
2:B:341:MET:CE	2:B:417:PHE:CE2	2.98	0.46
4:D:148:HIS:CD2	4:D:148:HIS:N	2.82	0.46
3:P:79:LEU:HD12	3:P:79:LEU:O	2.15	0.46
3:P:216:SER:HB3	6:S:59:MET:CE	2.46	0.46
5:R:139:CYS:HB3	5:R:143:GLY:O	2.16	0.46
6:S:81:VAL:HG12	6:S:82:LYS:N	2.31	0.46
8:U:12:GLU:HG2	8:U:13:LEU:N	2.31	0.46
1:A:178:THR:C	1:A:180:ALA:N	2.67	0.45
2:B:62:ASN:HD22	2:B:65:THR:HG21	1.81	0.45
2:B:290:SER:CB	2:B:293:SER:HB3	2.46	0.45
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.50	0.45
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.51	0.45
5:E:128:LYS:HG3	5:E:129:LYS:N	2.32	0.45
5:E:189:GLY:O	5:E:192:LEU:O	2.35	0.45
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.50	0.45
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.45	0.45
3:P:366:LEU:HD22	3:P:366:LEU:N	2.31	0.45
4:Q:147:LEU:C	4:Q:148:HIS:HD2	2.19	0.45
4:Q:171:TYR:HD1	4:Q:175:THR:HB	1.81	0.45
5:R:114:VAL:O	5:R:114:VAL:HG12	2.17	0.45
1:A:107:PRO:HG2	1:A:108:LYS:H	1.82	0.45
1:A:191:LYS:N	1:A:195:MET:HE2	2.32	0.45
2:B:42:SER:O	2:B:113:ARG:HD2	2.17	0.45
2:B:107:TYR:CD2	2:B:127:THR:HG22	2.51	0.45
2:B:111:CYS:HB3	2:B:119:VAL:HG21	1.97	0.45
2:B:169:LYS:HG2	2:O:435:PHE:CZ	2.51	0.45
3:C:89:SER:O	3:C:92:PHE:N	2.48	0.45
4:D:165:TYR:O	4:D:166:ASN:C	2.55	0.45
10:J:36:ASP:O	10:J:37:GLN:C	2.54	0.45
7:T:79:ASN:N	7:T:79:ASN:ND2	2.64	0.45
1:A:39:VAL:HG13	1:A:39:VAL:O	2.16	0.45
1:A:116:VAL:O	1:A:120:CYS:HB2	2.17	0.45
1:A:439:SER:C	1:A:441:MET:H	2.20	0.45
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:VAL:HG11	2:B:312:PHE:CD2	2.41	0.45
8:H:43:ARG:HG3	8:H:44:VAL:N	2.30	0.45
3:P:5:ILE:O	3:P:5:ILE:HG22	2.16	0.45
3:P:75:GLN:C	3:P:77:GLY:N	2.69	0.45
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.52	0.45
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.45
3:P:334:LEU:O	3:P:337:THR:HB	2.17	0.45
4:Q:72:ASP:HB3	4:Q:81:PHE:CE2	2.52	0.45
6:S:40:ASP:C	6:S:40:ASP:OD1	2.54	0.45
1:A:259:GLY:N	1:A:318:GLY:O	2.47	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.15	0.45
2:B:70:ARG:NH2	2:B:177:TYR:CE2	2.85	0.45
2:B:102:ARG:H	2:B:102:ARG:HD2	1.81	0.45
2:B:146:VAL:HG12	2:B:147:ASP:N	2.31	0.45
2:B:272:PHE:O	2:B:276:GLN:N	2.39	0.45
2:B:338:ARG:O	2:B:341:MET:N	2.49	0.45
4:D:210:LEU:O	4:D:211:ILE:C	2.54	0.45
1:N:429:GLU:O	1:N:429:GLU:HG2	2.16	0.45
2:O:332:HIS:O	2:O:336:VAL:HG23	2.17	0.45
6:S:90:LEU:O	6:S:91:GLU:C	2.55	0.45
1:A:117:VAL:HG23	1:A:118:GLN:H	1.81	0.45
2:B:111:CYS:CB	2:B:119:VAL:HG21	2.46	0.45
3:C:75:GLN:C	3:C:77:GLY:N	2.70	0.45
3:C:75:GLN:C	3:C:77:GLY:H	2.20	0.45
3:C:101:ARG:NH2	13:C:502:HEM:HBD2	2.31	0.45
4:D:215:LEU:O	4:D:219:LEU:HD12	2.16	0.45
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.98	0.45
8:H:37:LEU:O	8:H:38:GLU:C	2.55	0.45
8:H:58:LEU:HD12	8:H:58:LEU:O	2.16	0.45
1:N:53:ASN:CG	1:N:165:ARG:HD3	2.36	0.45
2:O:27:THR:CG2	2:O:28:LYS:H	2.29	0.45
2:O:215:ASP:C	2:O:217:LYS:H	2.20	0.45
2:O:400:GLN:O	2:O:404:SER:HB3	2.16	0.45
3:P:238:THR:CB	3:P:239:PRO:HD3	2.44	0.45
5:R:187:PHE:O	5:R:188:VAL:HG13	2.16	0.45
6:S:12:LEU:C	6:S:14:ASP:H	2.19	0.45
6:S:58:ARG:HG3	6:S:58:ARG:HH11	1.82	0.45
8:U:66:ASP:O	8:U:67:HIS:C	2.53	0.45
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.81	0.45
1:A:156:THR:HA	5:E:7:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HG22	2:B:52:LYS:N	2.30	0.45
3:C:104:TYR:O	3:C:104:TYR:CD2	2.69	0.45
1:N:76:GLU:HA	2:O:285:ILE:CD1	2.46	0.45
1:N:88:GLY:O	2:O:286:LYS:NZ	2.42	0.45
3:P:120:LEU:HD21	3:P:193:ILE:HB	1.98	0.45
3:P:208:ASN:OD1	3:P:210:LEU:N	2.42	0.45
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.46	0.45
4:Q:171:TYR:C	4:Q:173:ASP:H	2.20	0.45
5:R:73:LYS:HG3	22:R:1240:HOH:O	2.17	0.45
10:W:57:HIS:HA	10:W:60:GLU:HG2	1.99	0.45
1:A:67:THR:HB	1:A:119:ASN:O	2.16	0.45
1:A:106:MET:HE2	1:A:106:MET:C	2.37	0.45
2:B:303:THR:HB	2:B:336:VAL:HG22	1.97	0.45
6:F:94:LEU:HG	6:F:98:ILE:HD11	1.98	0.45
7:G:4:PHE:HD2	7:G:4:PHE:HA	1.69	0.45
1:N:177:LEU:HD23	1:N:177:LEU:HA	1.80	0.45
2:O:253:VAL:HG11	2:O:433:THR:OG1	2.17	0.45
3:P:86:ASN:HD21	3:P:243:LEU:HD11	1.82	0.45
3:P:92:PHE:O	3:P:93:ILE:C	2.53	0.45
3:P:127:THR:O	3:P:130:VAL:CG2	2.64	0.45
3:P:223:PRO:O	3:P:227:PHE:HB2	2.17	0.45
3:P:247:SER:HG	3:P:250:LEU:HB2	1.82	0.45
3:P:253:ASP:OD1	3:P:254:PRO:HD2	2.17	0.45
3:P:254:PRO:C	3:P:256:ASN:N	2.70	0.45
4:Q:37:CYS:O	4:Q:39:ALA:N	2.48	0.45
10:W:15:ARG:HG2	10:W:15:ARG:HH11	1.82	0.45
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.83	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.31	0.45
2:B:242:GLY:O	2:B:423:SER:HB2	2.17	0.45
3:C:158:GLY:O	3:C:160:THR:N	2.50	0.45
3:C:247:SER:N	3:C:248:PRO:CD	2.79	0.45
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.64	0.45
10:J:52:TRP:O	10:J:56:LYS:HB2	2.16	0.45
2:O:181:TYR:CE1	2:O:182:ARG:CG	2.99	0.45
3:P:28:ILE:CG1	3:P:225:TYR:CE2	3.00	0.45
4:Q:57:THR:CB	4:Q:60:GLU:HG3	2.47	0.45
1:A:170:THR:CG2	1:A:171:THR:N	2.80	0.45
1:A:208:LEU:O	1:A:209:VAL:C	2.55	0.45
1:A:257:VAL:HG23	1:A:320:PHE:HB3	1.99	0.45
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.98	0.45
3:C:39:ALA:O	3:C:42:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:16:TYR:CD1	7:G:16:TYR:N	2.84	0.45
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.52	0.45
2:O:227:ARG:HB2	2:O:228:SER:H	1.48	0.45
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.25	0.45
2:O:272:PHE:O	2:O:273:SER:C	2.54	0.45
4:Q:1:GLY:C	4:Q:3:LEU:H	2.20	0.45
8:U:31:VAL:C	8:U:33:ALA:H	2.20	0.45
1:A:86:PHE:HE2	1:A:116:VAL:HG21	1.82	0.45
1:A:284:PHE:HD2	9:I:71:ASN:HA	1.80	0.45
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.37	0.45
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.98	0.45
2:B:286:LYS:HE2	2:B:287:ARG:NH2	2.32	0.45
3:C:117:GLY:O	3:C:120:LEU:HB2	2.17	0.45
6:F:27:ASN:O	6:F:28:LYS:C	2.54	0.45
2:O:35:ILE:O	2:O:213:HIS:CE1	2.66	0.45
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.99	0.45
3:P:221:PHE:HE1	15:P:3002:UQ:O1	2.00	0.45
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.47	0.45
4:Q:83:ARG:HH12	4:Q:86:LYS:HG2	1.82	0.45
6:S:32:MET:O	6:S:33:ARG:C	2.55	0.45
6:S:98:ILE:O	6:S:102:LEU:HB2	2.17	0.45
8:U:43:ARG:HG3	8:U:44:VAL:N	2.31	0.45
2:B:326:THR:C	2:B:327:ILE:HG13	2.38	0.44
2:B:415:LYS:O	2:B:418:VAL:N	2.50	0.44
1:N:109:VAL:O	1:N:112:LEU:N	2.50	0.44
1:N:137:GLU:O	1:N:141:MET:HG3	2.17	0.44
1:N:356:ARG:HG3	2:O:91:ALA:HA	1.99	0.44
1:N:382:HIS:CG	1:N:389:ARG:HD2	2.51	0.44
3:P:67:VAL:CG2	13:P:501:HEM:HBD2	2.47	0.44
3:P:137:GLY:H	3:P:140:SER:CB	2.29	0.44
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.35	0.44
5:R:70:ALA:C	5:R:72:SER:H	2.20	0.44
6:S:94:LEU:O	6:S:95:LYS:C	2.55	0.44
1:A:147:ASN:C	1:A:149:THR:N	2.70	0.44
2:B:37:SER:O	2:B:38:LEU:CB	2.65	0.44
2:B:385:GLU:HB3	2:B:391:THR:O	2.17	0.44
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.82	0.44
1:N:206:LYS:H	1:N:206:LYS:HD2	1.82	0.44
2:O:408:ALA:O	2:O:410:VAL:N	2.50	0.44
5:R:175:PRO:O	5:R:176:ALA:C	2.56	0.44
9:V:28:UNK:HA	9:V:72:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:VAL:O	9:I:67:GLY:HA2	2.18	0.44
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.46	0.44
3:C:83:LEU:O	3:C:87:GLY:N	2.46	0.44
3:C:104:TYR:HA	3:C:316:MET:SD	2.57	0.44
3:C:150:LEU:HB3	3:C:292:VAL:HG22	2.00	0.44
4:D:47:ALA:N	4:D:50:ASN:ND2	2.62	0.44
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.48	0.44
7:G:72:LYS:HZ3	8:H:52:GLU:HG3	1.83	0.44
10:J:58:LYS:C	10:J:59:TYR:CD1	2.91	0.44
2:O:97:SER:HB3	9:V:69:SER:CB	2.47	0.44
2:O:135:TRP:O	2:O:136:GLU:C	2.55	0.44
3:P:114:TRP:HE3	13:P:502:HEM:HMD1	1.83	0.44
1:A:255:LEU:O	1:A:321:GLY:HA3	2.18	0.44
2:B:23:ASP:O	2:B:24:LEU:HB3	2.16	0.44
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.46	0.44
3:C:82:ASN:O	3:C:83:LEU:C	2.54	0.44
3:C:201:LEU:C	3:C:203:GLU:H	2.21	0.44
3:C:202:HIS:NE2	15:C:2002:UQ:O4	2.49	0.44
4:D:8:PRO:HG2	4:D:10:PHE:HE1	1.81	0.44
4:D:37:CYS:C	4:D:39:ALA:N	2.70	0.44
8:H:34:ARG:HB2	8:H:61:PHE:CE1	2.52	0.44
1:N:7:THR:HG21	2:O:113:ARG:CD	2.47	0.44
1:N:438:ARG:O	1:N:441:MET:HG2	2.17	0.44
3:P:157:ILE:O	3:P:161:LEU:HB3	2.17	0.44
4:Q:126:TYR:CD2	4:Q:126:TYR:C	2.91	0.44
1:A:242:ARG:CZ	1:A:432:LEU:HA	2.48	0.44
2:B:259:THR:HG22	2:B:260:GLU:H	1.82	0.44
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.53	0.44
4:D:2:GLU:OE1	4:D:2:GLU:HA	2.17	0.44
4:D:68:VAL:HG12	4:D:69:GLU:N	2.32	0.44
5:E:109:GLU:HA	5:E:112:VAL:HG13	1.98	0.44
9:I:67:GLY:O	9:I:68:ILE:HD13	2.18	0.44
1:N:35:CYS:HA	1:N:372:THR:HG21	2.00	0.44
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.82	0.44
1:N:249:PRO:HG2	1:N:250:VAL:N	2.32	0.44
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.86	0.44
2:O:303:THR:HB	2:O:336:VAL:HG22	1.98	0.44
2:O:374:THR:HG22	2:O:376:GLN:HB3	1.99	0.44
3:P:70:THR:CA	3:P:74:VAL:HG23	2.45	0.44
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.33	0.44
5:R:126:ARG:HH22	5:R:179:ASN:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:33:ALA:O	7:T:37:VAL:HG23	2.18	0.44
1:A:127:ILE:C	1:A:129:LYS:N	2.70	0.44
1:A:295:ALA:O	1:A:298:ALA:N	2.51	0.44
1:N:39:VAL:HG13	1:N:39:VAL:O	2.16	0.44
1:N:52:ASN:OD1	1:N:52:ASN:C	2.56	0.44
1:N:56:GLY:HA2	1:N:185:TYR:CE2	2.52	0.44
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.99	0.44
2:O:43:PRO:HA	2:O:113:ARG:HD2	2.00	0.44
2:O:393:THR:O	2:O:394:ALA:O	2.35	0.44
2:O:415:LYS:O	2:O:416:LYS:C	2.55	0.44
3:P:41:CYS:SG	3:P:91:PHE:HA	2.57	0.44
3:P:156:TYR:N	3:P:156:TYR:CD2	2.85	0.44
4:Q:151:PRO:HB2	8:U:59:PHE:HE1	1.83	0.44
5:R:127:VAL:HG23	5:R:127:VAL:O	2.18	0.44
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.65	0.44
10:W:57:HIS:HA	10:W:60:GLU:CD	2.38	0.44
1:A:121:ALA:O	1:A:122:LEU:HB2	2.18	0.44
1:A:349:THR:HA	1:A:353:GLU:OE1	2.17	0.44
2:B:137:VAL:O	2:B:140:LEU:HB3	2.17	0.44
2:B:290:SER:HB3	2:B:293:SER:HB3	1.99	0.44
3:C:135:PRO:HG2	3:C:140:SER:OG	2.18	0.44
3:C:261:ASN:ND2	3:C:264:VAL:N	2.65	0.44
3:C:334:LEU:O	3:C:337:THR:HB	2.18	0.44
4:D:34:LYS:O	4:D:34:LYS:HG2	2.18	0.44
5:E:118:ARG:O	5:E:119:ASP:HB2	2.18	0.44
5:E:184:THR:HG22	5:E:185:TYR:N	2.33	0.44
1:N:36:THR:HG21	1:N:373:THR:HA	2.00	0.44
2:O:81:SER:O	2:O:82:SER:C	2.56	0.44
2:O:193:HIS:O	2:O:197:ASN:ND2	2.51	0.44
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.81	0.44
1:A:25:VAL:HG22	1:A:197:LEU:HB3	2.00	0.44
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.44
2:B:29:LEU:CB	2:B:30:PRO:CD	2.96	0.44
3:C:81:ARG:O	3:C:82:ASN:C	2.56	0.44
5:E:10:PHE:O	5:E:11:SER:C	2.56	0.44
6:F:94:LEU:O	6:F:95:LYS:C	2.56	0.44
1:N:79:VAL:O	1:N:82:MET:HG2	2.18	0.44
1:N:182:LEU:O	1:N:186:ILE:HG13	2.16	0.44
1:N:327:ASP:HB3	1:N:328:PRO:HD2	2.00	0.44
1:N:370:ASP:OD2	2:O:374:THR:HG23	2.18	0.44
2:O:287:ARG:HB3	9:V:53:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.53	0.44
3:P:192:GLY:O	3:P:195:ILE:HB	2.18	0.44
7:T:2:ILE:O	7:T:3:HIS:CG	2.71	0.44
2:B:31:ASN:HB2	2:B:228:SER:HB3	2.00	0.44
5:E:33:LYS:HE3	10:J:10:TYR:OH	2.17	0.44
5:E:52:LYS:C	5:E:52:LYS:CD	2.86	0.44
5:E:106:ILE:O	5:E:106:ILE:HG22	2.17	0.44
8:H:27:THR:O	8:H:28:GLU:C	2.56	0.44
1:N:434:TYR:O	1:N:435:ASN:C	2.56	0.44
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.99	0.44
2:O:37:SER:OG	2:O:38:LEU:N	2.49	0.44
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.51	0.44
3:P:254:PRO:C	3:P:256:ASN:H	2.21	0.44
3:P:319:ARG:HA	3:P:320:PRO:HD2	1.84	0.44
3:P:345:GLU:O	3:P:348:PHE:HB2	2.18	0.44
7:T:38:TRP:O	7:T:39:ARG:C	2.56	0.44
1:A:133:VAL:O	1:A:134:ILE:C	2.54	0.43
1:A:253:VAL:O	1:A:323:HIS:HA	2.17	0.43
2:B:169:LYS:HG3	2:B:240:TRP:HB2	2.00	0.43
2:B:312:PHE:N	2:B:323:GLY:O	2.42	0.43
2:B:415:LYS:O	2:B:416:LYS:C	2.55	0.43
3:C:59:ASP:C	3:C:61:SER:N	2.68	0.43
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.83	0.43
6:F:20:TYR:O	6:F:23:ALA:HB3	2.18	0.43
1:N:140:GLU:HG2	9:V:48:PRO:HB2	1.99	0.43
1:N:199:ALA:CA	1:N:376:CYS:SG	3.05	0.43
1:N:208:LEU:O	1:N:209:VAL:C	2.56	0.43
2:O:286:LYS:HZ3	2:O:287:ARG:HH22	1.66	0.43
3:P:214:SER:HB2	3:P:218:LYS:HZ3	1.79	0.43
4:Q:70:VAL:HG23	4:Q:83:ARG:HG2	1.98	0.43
4:Q:204:MET:O	4:Q:205:GLY:C	2.54	0.43
5:R:141:HIS:HA	5:R:177:PRO:HD2	1.99	0.43
8:U:73:LEU:HD11	8:U:77:LEU:HD11	2.00	0.43
2:B:151:ALA:C	2:B:153:GLN:H	2.21	0.43
2:B:299:VAL:O	2:B:303:THR:HG22	2.18	0.43
3:C:40:VAL:O	3:C:44:THR:OG1	2.35	0.43
4:D:165:TYR:O	4:D:166:ASN:O	2.36	0.43
1:N:40:TRP:CG	1:N:380:GLY:HA3	2.53	0.43
1:N:117:VAL:CG2	1:N:118:GLN:N	2.81	0.43
1:N:241:ILE:HG23	1:N:241:ILE:O	2.18	0.43
2:O:337:ILE:HD12	2:O:434:PRO:CD	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:16:TYR:N	7:T:16:TYR:CD1	2.86	0.43
1:A:90:THR:CB	1:A:95:THR:HG23	2.49	0.43
2:B:100:SER:HA	2:B:104:LYS:O	2.17	0.43
2:B:120:MET:O	2:B:121:GLU:C	2.56	0.43
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.83	0.43
6:F:32:MET:HE1	6:F:87:LYS:HG2	2.00	0.43
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.90	0.43
2:O:62:ASN:O	2:O:65:THR:CG2	2.64	0.43
2:O:157:VAL:O	2:O:157:VAL:HG22	2.17	0.43
4:Q:28:ARG:O	4:Q:29:GLY:C	2.56	0.43
8:U:58:LEU:HD12	8:U:58:LEU:O	2.17	0.43
1:A:87:ASN:OD1	1:A:88:GLY:N	2.44	0.43
1:A:106:MET:CG	1:A:203:ILE:HD13	2.46	0.43
1:A:106:MET:HE1	1:A:208:LEU:HD13	2.00	0.43
1:A:117:VAL:CG2	1:A:118:GLN:H	2.32	0.43
1:A:184:SER:HA	1:A:187:ASP:HB2	2.00	0.43
1:A:239:SER:O	1:A:421:ALA:HA	2.17	0.43
1:A:395:TRP:O	1:A:398:ARG:HB2	2.19	0.43
2:B:206:LEU:HG	2:B:206:LEU:O	2.18	0.43
2:B:408:ALA:O	2:B:409:ASP:C	2.57	0.43
4:D:98:PRO:O	4:D:99:GLU:C	2.56	0.43
2:O:47:ILE:HD13	2:O:120:MET:CE	2.48	0.43
3:P:137:GLY:O	3:P:140:SER:HB2	2.18	0.43
3:P:184:PHE:CD2	13:P:501:HEM:HBC1	2.53	0.43
5:R:141:HIS:HB2	5:R:176:ALA:HB2	2.00	0.43
7:T:4:PHE:HD2	7:T:4:PHE:HA	1.71	0.43
2:B:56:ARG:HD3	2:B:103:GLU:HB3	2.01	0.43
2:B:341:MET:HA	2:B:341:MET:CE	2.46	0.43
2:B:346:ALA:O	2:B:351:GLY:HA3	2.18	0.43
3:C:316:MET:HA	3:C:319:ARG:HE	1.84	0.43
2:O:34:ILE:HD13	2:O:386:ALA:O	2.19	0.43
2:O:167:ALA:HB3	2:O:168:TYR:HD1	1.83	0.43
3:P:34:PHE:HB2	22:P:381:HOH:O	2.18	0.43
4:Q:167:GLU:C	4:Q:169:LEU:N	2.72	0.43
1:A:256:ALA:HA	1:A:320:PHE:O	2.18	0.43
3:C:78:TRP:CG	3:C:79:LEU:N	2.86	0.43
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.53	0.43
6:F:98:ILE:O	6:F:102:LEU:HB2	2.17	0.43
8:H:55:THR:O	8:H:56:GLU:C	2.57	0.43
1:N:381:SER:O	1:N:382:HIS:C	2.57	0.43
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.54	0.43
2:O:430:LEU:H	2:O:430:LEU:HG	1.61	0.43
3:P:101:ARG:CZ	13:P:502:HEM:HBD2	2.49	0.43
9:V:67:GLY:O	9:V:68:ILE:HD13	2.18	0.43
1:A:247:ALA:HB2	7:G:11:ARG:HD2	2.00	0.43
1:A:318:GLY:O	1:A:319:LEU:HD23	2.19	0.43
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.81	0.43
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.52	0.43
2:B:244:ILE:O	2:B:425:ALA:HA	2.19	0.43
3:C:86:ASN:HD21	3:C:243:LEU:HD11	1.83	0.43
3:C:192:GLY:O	3:C:195:ILE:HB	2.19	0.43
3:C:263:LEU:O	5:R:143:GLY:HA3	2.19	0.43
5:E:147:ILE:HG13	5:E:157:TYR:O	2.18	0.43
6:F:21:TYR:C	6:F:21:TYR:CD2	2.92	0.43
1:N:159:GLN:O	1:N:159:GLN:HG3	2.18	0.43
1:N:185:TYR:HA	1:N:189:HIS:HD2	1.83	0.43
1:N:206:LYS:HD2	1:N:206:LYS:N	2.32	0.43
2:O:142:PRO:O	2:O:145:LYS:HB2	2.18	0.43
2:O:372:VAL:O	2:O:372:VAL:HG12	2.19	0.43
3:P:319:ARG:HB3	3:P:374:GLU:CD	2.39	0.43
4:Q:26:VAL:CG1	4:Q:55:THR:HG21	2.45	0.43
4:Q:47:ALA:HB1	4:Q:89:ASP:O	2.18	0.43
4:Q:175:THR:HA	4:Q:176:PRO:HD3	1.84	0.43
6:S:27:ASN:O	6:S:30:GLY:N	2.41	0.43
1:A:76:GLU:O	1:A:80:GLU:HG3	2.19	0.43
1:A:147:ASN:O	1:A:149:THR:N	2.51	0.43
1:A:241:ILE:HG23	1:A:241:ILE:O	2.18	0.43
1:A:242:ARG:NH1	1:A:432:LEU:HA	2.33	0.43
3:C:75:GLN:O	3:C:77:GLY:N	2.52	0.43
10:J:63:GLU:O	10:J:64:GLU:HB3	2.19	0.43
1:N:23:LEU:HA	1:N:192:ALA:O	2.18	0.43
1:N:76:GLU:HG2	2:O:285:ILE:HD13	2.00	0.43
1:N:112:LEU:H	1:N:112:LEU:HG	1.53	0.43
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.82	0.43
2:O:37:SER:O	2:O:38:LEU:CB	2.67	0.43
2:O:258:VAL:HG12	2:O:323:GLY:CA	2.49	0.43
2:O:374:THR:CG2	2:O:376:GLN:HB3	2.48	0.43
3:P:33:ASN:HB3	22:P:385:HOH:O	2.18	0.43
4:Q:41:HIS:HB3	4:Q:113:LEU:HD12	2.00	0.43
1:A:114:ALA:O	1:A:117:VAL:HG22	2.19	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:163:LEU:HD23	1:N:163:LEU:HA	1.86	0.43
2:O:275:LEU:O	2:O:279:LEU:HD12	2.19	0.43
3:P:289:LEU:O	3:P:293:LEU:HG	2.17	0.43
6:S:34:ASP:N	6:S:34:ASP:OD1	2.51	0.43
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.99	0.43
1:A:242:ARG:HH12	1:A:432:LEU:H	1.65	0.43
2:B:166:ALA:O	2:B:242:GLY:N	2.51	0.43
3:C:305:ILE:HA	3:C:305:ILE:HD13	1.83	0.43
4:D:167:GLU:C	4:D:169:LEU:N	2.73	0.43
5:E:20:ASP:O	5:E:22:THR:N	2.45	0.43
5:E:98:VAL:HG22	5:E:134:ILE:HG23	2.01	0.43
6:F:103:GLU:O	6:F:104:ARG:C	2.57	0.43
1:N:116:VAL:O	1:N:120:CYS:HB2	2.19	0.43
2:O:70:ARG:NH2	2:O:177:TYR:CE2	2.87	0.43
2:O:268:GLU:OE1	2:O:416:LYS:NZ	2.48	0.43
3:P:79:LEU:HD11	3:P:83:LEU:HD11	2.01	0.43
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.37	0.43
4:Q:37:CYS:C	4:Q:39:ALA:N	2.72	0.43
5:R:138:VAL:O	5:R:180:LEU:HD22	2.19	0.43
1:A:240:GLU:HB3	1:A:422:LEU:HB3	2.01	0.42
1:A:253:VAL:CG1	1:A:335:MET:HE1	2.47	0.42
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.81	0.42
2:B:167:ALA:HB3	2:B:168:TYR:HD1	1.84	0.42
2:B:215:ASP:C	2:B:217:LYS:H	2.23	0.42
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.34	0.42
3:C:216:SER:HB3	6:F:59:MET:HE2	2.00	0.42
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.18	0.42
5:E:91:TRP:O	5:E:92:ARG:C	2.57	0.42
6:F:82:LYS:O	6:F:83:TYR:C	2.55	0.42
1:N:67:THR:HB	1:N:119:ASN:O	2.19	0.42
1:N:404:ALA:O	1:N:405:ARG:C	2.57	0.42
2:O:51:ILE:N	2:O:105:MET:O	2.51	0.42
2:O:146:VAL:HG12	2:O:147:ASP:N	2.33	0.42
2:O:150:VAL:HG22	2:O:151:ALA:N	2.34	0.42
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.48	0.42
2:O:298:GLY:HA3	2:O:343:GLN:HG3	2.00	0.42
2:O:346:ALA:O	2:O:351:GLY:HA3	2.18	0.42
3:P:255:GLU:HG2	3:P:255:GLU:H	1.60	0.42
6:S:13:MET:HB2	6:S:16:ILE:HD12	2.01	0.42
7:T:60:SER:O	7:T:64:GLN:HB2	2.19	0.42
2:B:324:PHE:HE2	2:B:341:MET:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:ILE:C	4:D:54:VAL:N	2.72	0.42
4:D:197:GLU:HG2	4:D:198:HIS:H	1.84	0.42
2:O:56:ARG:HG2	2:O:234:SER:OG	2.18	0.42
2:O:111:CYS:HB3	2:O:119:VAL:HG21	2.01	0.42
3:P:22:LEU:HA	3:P:23:PRO:HD3	1.88	0.42
3:P:82:ASN:O	3:P:83:LEU:C	2.58	0.42
3:P:186:LEU:HD23	3:P:186:LEU:HA	1.76	0.42
3:P:346:HIS:CG	3:P:347:PRO:HA	2.54	0.42
4:Q:221:TYR:CE2	5:R:39:VAL:HG21	2.54	0.42
5:R:145:VAL:HA	5:R:146:PRO:HD3	1.85	0.42
6:S:12:LEU:C	6:S:14:ASP:N	2.73	0.42
2:B:176:LEU:HD12	2:B:176:LEU:O	2.19	0.42
3:C:82:ASN:H	3:C:82:ASN:ND2	2.14	0.42
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.54	0.42
1:N:127:ILE:C	1:N:129:LYS:N	2.73	0.42
1:N:219:VAL:CG1	1:N:220:SER:N	2.82	0.42
1:N:308:GLN:O	1:N:322:PHE:HA	2.19	0.42
2:O:24:LEU:HD23	2:O:24:LEU:C	2.40	0.42
3:P:4:ASN:HD22	3:P:6:ARG:H	1.68	0.42
3:P:68:ALA:HA	18:P:3011:GOL:O3	2.20	0.42
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.54	0.42
1:A:156:THR:CG2	1:A:157:ALA:N	2.83	0.42
2:B:181:TYR:CE1	2:B:182:ARG:CG	3.00	0.42
2:B:215:ASP:O	2:B:217:LYS:N	2.52	0.42
2:B:248:ASN:C	2:B:248:ASN:ND2	2.73	0.42
5:E:1:VAL:HG23	5:E:3:ASN:N	2.27	0.42
6:F:58:ARG:HG3	6:F:89:TYR:OH	2.20	0.42
9:I:49:LEU:HD13	9:I:55:MET:HE2	2.01	0.42
1:N:109:VAL:HA	1:N:112:LEU:CD1	2.47	0.42
1:N:242:ARG:O	7:T:14:ILE:HA	2.19	0.42
3:P:207:ASN:ND2	3:P:314:ARG:NH1	2.67	0.42
3:P:230:ILE:O	3:P:233:LEU:HB3	2.19	0.42
4:Q:148:HIS:ND1	4:Q:161:ALA:HA	2.35	0.42
16:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.34	0.42
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.50	0.42
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.48	0.42
2:B:337:ILE:O	2:B:340:ALA:HB3	2.20	0.42
3:C:81:ARG:NH2	13:C:501:HEM:O1A	2.53	0.42
3:C:214:SER:HB2	3:C:218:LYS:HZ3	1.81	0.42
1:N:260:PRO:HB3	1:N:414:TYR:CE2	2.54	0.42
1:N:340:GLY:O	1:N:343:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:HA	2:O:144:LEU:HD21	2.00	0.42
2:O:209:ILE:O	2:O:211:VAL:N	2.53	0.42
2:O:272:PHE:HB3	2:O:322:PHE:CE1	2.55	0.42
3:P:175:THR:HA	3:P:178:ARG:HG2	2.01	0.42
5:R:146:PRO:C	5:R:147:ILE:HG13	2.38	0.42
1:A:170:THR:HG22	1:A:172:GLU:H	1.85	0.42
1:A:204:SER:O	1:A:205:HIS:C	2.58	0.42
1:A:295:ALA:O	1:A:298:ALA:HB3	2.20	0.42
2:B:42:SER:C	2:B:44:ALA:H	2.23	0.42
2:B:268:GLU:O	2:B:269:ALA:C	2.58	0.42
3:C:231:LEU:O	3:C:235:LEU:HG	2.19	0.42
16:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.20	0.42
5:E:71:LEU:N	5:E:71:LEU:CD2	2.83	0.42
6:F:89:TYR:CD1	6:F:89:TYR:C	2.93	0.42
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.55	0.42
2:O:327:ILE:HD11	9:V:58:ARG:O	2.19	0.42
3:P:173:ASN:N	3:P:174:PRO:CD	2.80	0.42
3:P:183:HIS:CE1	13:P:501:HEM:NB	2.87	0.42
5:R:69:LEU:HD23	5:R:69:LEU:HA	1.92	0.42
5:R:156:TYR:HB2	5:R:165:TYR:HB2	2.00	0.42
8:U:34:ARG:HB2	8:U:61:PHE:CE1	2.54	0.42
1:A:109:VAL:O	1:A:112:LEU:N	2.52	0.42
3:C:59:ASP:O	3:C:62:LEU:N	2.47	0.42
3:C:273:TRP:CD2	3:C:274:TYR:N	2.88	0.42
5:E:175:PRO:HG2	5:E:176:ALA:H	1.84	0.42
7:G:73:ASN:HB3	7:G:76:ASP:OD2	2.20	0.42
1:N:41:ILE:HG12	1:N:195:MET:HG2	2.01	0.42
1:N:242:ARG:HH12	1:N:432:LEU:N	2.18	0.42
2:O:80:ALA:HA	2:O:84:ARG:NH2	2.35	0.42
2:O:201:SER:N	2:O:227:ARG:HB3	2.22	0.42
2:O:267:ALA:O	2:O:269:ALA:N	2.52	0.42
3:P:350:ILE:HG23	3:P:351:ILE:N	2.34	0.42
10:W:22:LEU:C	10:W:22:LEU:HD23	2.40	0.42
1:A:59:VAL:HG23	1:A:182:LEU:HD23	2.02	0.42
1:A:60:GLU:OE2	1:A:89:TYR:C	2.58	0.42
2:B:306:PRO:HA	9:I:52:ARG:CG	2.50	0.42
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.54	0.42
3:C:160:THR:O	3:C:161:LEU:C	2.58	0.42
4:D:102:ARG:HG2	4:D:107:GLY:O	2.18	0.42
5:E:137:GLY:O	5:E:145:VAL:HG13	2.20	0.42
1:N:7:THR:HG21	2:O:113:ARG:NE	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.44	0.42
1:N:244:ARG:NE	7:T:10:VAL:HB	2.34	0.42
2:O:212:LYS:HG2	2:O:214:SER:OG	2.20	0.42
2:O:272:PHE:HB3	2:O:322:PHE:CD1	2.55	0.42
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.19	0.42
3:P:52:LEU:HD21	3:P:80:ILE:HG22	2.01	0.42
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.54	0.42
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.50	0.42
9:V:75:SER:O	9:V:76:VAL:HB	2.20	0.42
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.31	0.42
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.42
3:C:28:ILE:CG1	3:C:225:TYR:CE2	3.03	0.42
3:C:236:MET:O	3:C:238:THR:N	2.53	0.42
5:E:33:LYS:HE3	10:J:10:TYR:CZ	2.55	0.42
5:E:119:ASP:CG	5:E:179:ASN:ND2	2.74	0.42
5:E:156:TYR:HB2	5:E:165:TYR:HB2	2.01	0.42
1:N:86:PHE:HE2	1:N:116:VAL:HG21	1.85	0.42
1:N:433:ASP:OD2	1:N:435:ASN:N	2.53	0.42
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.19	0.42
2:O:71:LEU:N	2:O:71:LEU:CD2	2.75	0.42
2:O:232:THR:HG22	2:O:233:SER:N	2.35	0.42
3:P:362:ILE:HG22	3:P:363:LEU:N	2.35	0.42
4:Q:2:GLU:H	4:Q:2:GLU:CD	2.23	0.42
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	2.01	0.42
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.55	0.42
10:W:36:ASP:O	10:W:37:GLN:C	2.57	0.42
2:B:43:PRO:HA	2:B:113:ARG:HD2	2.02	0.42
2:B:100:SER:HB2	2:B:105:MET:HG2	1.99	0.42
2:B:402:ILE:CG2	2:B:403:ASP:H	2.29	0.42
4:D:16:GLY:N	4:D:19:SER:OG	2.52	0.42
4:D:204:MET:O	4:D:205:GLY:C	2.56	0.42
1:N:280:TYR:HA	1:N:284:PHE:CE1	2.55	0.42
1:N:354:VAL:O	1:N:355:LYS:C	2.58	0.42
2:O:56:ARG:HH22	2:O:318:ASP:CG	2.24	0.42
2:O:366:ALA:O	2:O:367:THR:C	2.58	0.42
3:P:134:LEU:HD21	3:P:180:PHE:HA	2.01	0.42
5:R:77:LYS:HE3	5:R:191:ASP:OD2	2.20	0.42
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.68	0.42
1:A:134:ILE:O	1:A:136:GLN:N	2.53	0.41
2:B:19:PRO:O	2:B:22:GLU:CB	2.68	0.41
2:B:306:PRO:O	2:B:307:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:PHE:O	3:C:330:VAL:HG23	2.20	0.41
4:D:81:PHE:N	4:D:81:PHE:CD2	2.87	0.41
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.20	0.41
1:N:23:LEU:HD23	1:N:23:LEU:C	2.41	0.41
1:N:220:SER:HA	1:N:225:GLU:OE1	2.19	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:18:CYS:HA	2:O:19:PRO:HD3	1.84	0.41
2:O:51:ILE:HG22	2:O:52:LYS:N	2.35	0.41
2:O:287:ARG:HA	9:V:53:GLU:CG	2.46	0.41
3:P:9:HIS:HD2	3:P:12:LEU:HG	1.80	0.41
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.49	0.41
1:A:172:GLU:O	1:A:175:LYS:HB2	2.20	0.41
2:B:402:ILE:CG2	2:B:403:ASP:N	2.83	0.41
3:C:39:ALA:O	3:C:40:VAL:C	2.57	0.41
3:C:130:VAL:HG23	3:C:183:HIS:HD1	1.85	0.41
3:C:216:SER:O	6:F:63:LYS:HD2	2.19	0.41
4:D:161:ALA:O	4:D:163:PRO:HD3	2.19	0.41
5:E:100:HIS:NE2	5:E:131:GLU:HG3	2.35	0.41
6:F:20:TYR:HA	6:F:23:ALA:HB3	2.02	0.41
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.20	0.41
3:P:81:ARG:O	3:P:82:ASN:C	2.57	0.41
3:P:202:HIS:NE2	15:P:3002:UQ:O4	2.52	0.41
4:Q:81:PHE:N	4:Q:81:PHE:CD2	2.88	0.41
4:Q:198:HIS:O	4:Q:201:ARG:HB3	2.20	0.41
1:A:86:PHE:CD2	1:A:99:ILE:HD11	2.55	0.41
1:A:127:ILE:C	1:A:129:LYS:H	2.22	0.41
1:A:341:GLU:O	1:A:342:TRP:C	2.59	0.41
2:B:372:VAL:CG1	2:B:378:LEU:HD13	2.50	0.41
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.02	0.41
2:B:393:THR:O	2:B:394:ALA:O	2.37	0.41
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.89	0.41
3:C:333:LEU:HB3	11:C:2007:PEE:H75	2.02	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.73	0.41
4:D:178:THR:O	4:D:181:GLN:HB3	2.20	0.41
1:N:106:MET:HE1	1:N:208:LEU:CD1	2.50	0.41
2:O:163:LEU:HD12	2:O:425:ALA:CB	2.50	0.41
2:O:290:SER:HB2	2:O:293:SER:HB3	2.02	0.41
2:O:408:ALA:O	2:O:409:ASP:C	2.58	0.41
3:P:316:MET:HA	3:P:319:ARG:HE	1.85	0.41
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.35	0.41
4:Q:161:ALA:O	4:Q:163:PRO:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:103:GLN:HA	5:R:106:ILE:HD12	2.01	0.41
1:A:23:LEU:HD23	1:A:23:LEU:C	2.41	0.41
1:A:99:ILE:HG13	1:A:113:LEU:HD21	2.02	0.41
1:A:240:GLU:CB	1:A:422:LEU:HB3	2.50	0.41
2:B:35:ILE:HG23	2:B:216:LEU:HG	2.02	0.41
2:B:51:ILE:CG2	2:B:52:LYS:N	2.83	0.41
2:B:247:GLN:NE2	2:B:249:GLY:H	2.19	0.41
3:C:127:THR:O	3:C:130:VAL:CG2	2.68	0.41
3:C:276:LEU:O	3:C:277:PHE:C	2.56	0.41
3:C:311:SER:CB	3:C:319:ARG:NH1	2.82	0.41
4:D:10:PHE:CD2	8:H:74:PHE:HE2	2.38	0.41
4:D:160:MET:HB2	19:D:501:HEC:C4D	2.50	0.41
4:D:183:ALA:O	4:D:186:VAL:HG12	2.20	0.41
4:D:230:LEU:HD23	4:D:230:LEU:HA	1.87	0.41
1:N:39:VAL:HG11	1:N:117:VAL:HG11	2.03	0.41
1:N:210:ASP:O	1:N:213:ARG:N	2.54	0.41
1:N:239:SER:O	1:N:421:ALA:HA	2.21	0.41
1:N:417:ASP:OD2	1:N:438:ARG:NH2	2.46	0.41
2:O:299:VAL:O	2:O:303:THR:HG22	2.19	0.41
3:P:95:ILE:CG2	3:P:96:PHE:N	2.82	0.41
3:P:104:TYR:CD2	11:P:3007:PEE:H14	2.55	0.41
3:P:311:SER:CB	3:P:319:ARG:NH1	2.84	0.41
4:Q:228:SER:OG	4:Q:229:VAL:N	2.54	0.41
4:Q:232:SER:CB	7:T:23:GLN:HE22	2.20	0.41
5:R:37:TYR:HB3	10:W:14:PHE:HB3	2.02	0.41
5:R:102:THR:C	5:R:104:ALA:N	2.73	0.41
1:A:23:LEU:HB2	1:A:192:ALA:HB1	2.02	0.41
1:A:86:PHE:HD1	1:A:87:ASN:N	2.19	0.41
2:B:312:PHE:O	2:B:322:PHE:HA	2.21	0.41
3:C:246:PHE:CZ	4:D:205:GLY:HA3	2.55	0.41
4:D:33:TYR:HA	4:D:37:CYS:SG	2.60	0.41
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.55	0.41
1:N:335:MET:O	1:N:336:PHE:C	2.59	0.41
2:O:157:VAL:HG23	9:V:64:LEU:HD21	2.03	0.41
4:Q:94:PRO:HB2	4:Q:95:TYR:CD1	2.54	0.41
4:Q:161:ALA:O	4:Q:163:PRO:HD3	2.20	0.41
6:S:58:ARG:HA	6:S:61:ARG:NH2	2.35	0.41
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.34	0.41
1:A:295:ALA:O	1:A:296:ALA:C	2.59	0.41
1:A:428:ILE:H	1:A:428:ILE:HG12	1.57	0.41
2:B:272:PHE:HB3	2:B:322:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:GLY:O	2:B:380:ASN:HB3	2.21	0.41
3:C:50:LEU:O	3:C:53:ALA:N	2.54	0.41
3:C:247:SER:O	3:C:248:PRO:C	2.59	0.41
4:D:26:VAL:CG1	4:D:55:THR:HG21	2.47	0.41
8:H:66:ASP:O	8:H:67:HIS:C	2.56	0.41
10:J:57:HIS:ND1	10:J:58:LYS:HG3	2.36	0.41
1:N:86:PHE:CE2	1:N:116:VAL:HG21	2.55	0.41
1:N:339:GLN:HE22	1:N:437:ILE:HG23	1.86	0.41
2:O:239:TYR:CD2	2:O:240:TRP:N	2.89	0.41
2:O:324:PHE:HD2	2:O:344:LEU:HD12	1.85	0.41
3:P:36:SER:O	3:P:39:ALA:HB3	2.21	0.41
3:P:79:LEU:HD12	3:P:79:LEU:C	2.41	0.41
3:P:366:LEU:N	3:P:366:LEU:CD2	2.83	0.41
4:Q:120:ARG:HG2	4:Q:120:ARG:NH1	2.35	0.41
4:Q:210:LEU:HD23	4:Q:210:LEU:HA	1.88	0.41
5:R:40:THR:O	5:R:41:ALA:C	2.56	0.41
8:U:15:ASP:HA	8:U:16:PRO:HD2	1.87	0.41
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.55	0.41
2:B:81:SER:O	2:B:82:SER:C	2.58	0.41
2:B:131:GLU:O	2:B:132:PHE:C	2.59	0.41
2:B:366:ALA:O	2:B:367:THR:C	2.58	0.41
3:C:137:GLY:O	3:C:140:SER:HB2	2.21	0.41
3:C:320:PRO:HG2	3:C:321:LEU:N	2.33	0.41
4:D:22:ASP:HA	10:J:50:LYS:HB3	2.02	0.41
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.84	0.41
1:N:85:HIS:CD2	2:O:284:LEU:HB3	2.55	0.41
1:N:184:SER:HA	1:N:187:ASP:HB2	2.02	0.41
1:N:242:ARG:CZ	1:N:432:LEU:HA	2.51	0.41
1:N:354:VAL:CG2	1:N:355:LYS:N	2.82	0.41
1:N:365:MET:SD	1:N:392:LEU:HD13	2.60	0.41
2:O:222:GLN:O	2:O:223:PHE:CB	2.69	0.41
1:A:90:THR:HB	1:A:95:THR:HG23	2.03	0.41
1:A:127:ILE:O	1:A:130:GLU:N	2.54	0.41
1:A:178:THR:O	1:A:179:ARG:C	2.59	0.41
1:A:281:ASP:OD1	1:A:281:ASP:C	2.59	0.41
2:B:70:ARG:NH2	2:B:177:TYR:HE2	2.18	0.41
3:C:54:MET:SD	5:E:62:LEU:HD21	2.61	0.41
5:E:112:VAL:HG23	5:E:112:VAL:O	2.20	0.41
7:G:44:GLN:O	7:G:45:VAL:C	2.59	0.41
1:N:19:LEU:C	1:N:21:ASN:N	2.74	0.41
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:86:PHE:CE1	1:N:97:PHE:HB3	2.55	0.41
1:N:269:VAL:O	1:N:272:VAL:N	2.54	0.41
1:N:398:ARG:NH1	1:N:398:ARG:HG2	2.35	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.41	0.41
2:O:111:CYS:CB	2:O:119:VAL:HG21	2.50	0.41
3:P:317:THR:HG23	11:P:3007:PEE:H9	2.03	0.41
4:Q:164:ILE:HG21	4:Q:182:ILE:CG2	2.48	0.41
1:A:86:PHE:CE1	1:A:97:PHE:HB3	2.56	0.41
1:A:90:THR:O	1:A:90:THR:CG2	2.69	0.41
1:A:150:PHE:O	1:A:153:LEU:HB3	2.21	0.41
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.41
1:A:339:GLN:NE2	1:A:437:ILE:HG23	2.36	0.41
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.02	0.41
1:A:416:TYR:CE1	1:A:442:TYR:HA	2.56	0.41
2:B:33:LEU:HD21	2:B:224:LEU:HD12	2.02	0.41
2:B:80:ALA:HA	2:B:84:ARG:NH2	2.36	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.90	0.41
3:C:184:PHE:CZ	3:P:184:PHE:HB3	2.56	0.41
3:C:253:ASP:OD1	3:C:254:PRO:CD	2.68	0.41
3:C:326:PHE:CD2	3:C:326:PHE:C	2.94	0.41
13:C:502:HEM:HHA	13:C:502:HEM:HBD1	2.02	0.41
4:D:66:GLU:C	4:D:68:VAL:H	2.23	0.41
4:D:72:ASP:HB2	4:D:83:ARG:HE	1.84	0.41
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.54	0.41
7:G:38:TRP:O	7:G:39:ARG:C	2.57	0.41
1:N:84:ALA:HA	1:N:100:LYS:O	2.21	0.41
1:N:145:MET:O	1:N:146:THR:C	2.60	0.41
1:N:171:THR:O	1:N:175:LYS:HG3	2.20	0.41
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.41
1:N:330:SER:O	1:N:331:ILE:C	2.60	0.41
1:N:435:ASN:O	1:N:438:ARG:HB3	2.20	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.81	0.41
2:O:26:ILE:HA	2:O:35:ILE:O	2.21	0.41
2:O:47:ILE:HG22	2:O:48:GLY:N	2.35	0.41
2:O:70:ARG:NH2	2:O:177:TYR:HE2	2.19	0.41
2:O:206:LEU:HG	2:O:216:LEU:HD11	2.03	0.41
3:P:45:GLN:O	3:P:49:GLY:N	2.44	0.41
3:P:52:LEU:HD13	13:P:501:HEM:O2D	2.20	0.41
3:P:59:ASP:C	3:P:61:SER:N	2.74	0.41
3:P:208:ASN:OD1	3:P:208:ASN:C	2.58	0.41
4:Q:52:ILE:C	4:Q:54:VAL:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.34	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.76	0.41
4:Q:98:PRO:O	4:Q:99:GLU:C	2.59	0.41
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.41
6:S:13:MET:CA	6:S:16:ILE:HD12	2.47	0.41
6:S:13:MET:CB	6:S:16:ILE:HD12	2.51	0.41
1:A:64:PHE:C	1:A:66:GLY:H	2.25	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.75	0.41
1:A:277:ILE:CD1	1:A:345:LEU:HD11	2.51	0.41
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.83	0.41
1:A:403:ASP:O	1:A:404:ALA:C	2.59	0.41
2:B:102:ARG:NH1	2:B:172:LEU:O	2.54	0.41
2:B:307:PHE:CD1	2:B:307:PHE:C	2.91	0.41
2:B:408:ALA:O	2:B:410:VAL:N	2.54	0.41
3:C:70:THR:CA	3:C:74:VAL:HG23	2.49	0.41
1:N:46:ARG:HD3	1:N:231:LEU:HD13	2.02	0.41
1:N:149:THR:HG22	1:N:150:PHE:N	2.35	0.41
1:N:434:TYR:CE2	7:T:19:SER:HB2	2.56	0.41
2:O:206:LEU:HG	2:O:206:LEU:O	2.20	0.41
2:O:225:ASN:C	2:O:227:ARG:HG3	2.40	0.41
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.21	0.41
4:Q:179:MET:O	4:Q:182:ILE:HB	2.21	0.41
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.21	0.41
4:Q:209:LEU:HD23	4:Q:209:LEU:HA	1.77	0.41
5:R:96:LEU:HD12	5:R:135:LEU:O	2.20	0.41
7:T:44:GLN:O	7:T:45:VAL:C	2.60	0.41
2:B:272:PHE:O	2:B:273:SER:C	2.59	0.40
4:D:130:LEU:HD12	4:D:130:LEU:HA	1.92	0.40
4:D:203:ARG:HD3	10:J:40:ASP:OD1	2.21	0.40
6:F:57:GLU:HB3	6:F:61:ARG:HH12	1.85	0.40
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.49	0.40
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.93	0.40
2:O:192:HIS:O	2:O:196:GLN:HG3	2.21	0.40
2:O:402:ILE:CG2	2:O:403:ASP:H	2.30	0.40
2:O:410:VAL:O	2:O:413:ALA:N	2.54	0.40
3:P:110:TYR:O	3:P:111:LYS:C	2.60	0.40
3:P:254:PRO:O	3:P:257:PHE:N	2.52	0.40
3:P:350:ILE:CG2	3:P:351:ILE:N	2.84	0.40
1:A:135:LEU:HG	1:A:174:ILE:HG21	2.01	0.40
3:C:4:ASN:C	3:C:5:ILE:HD13	2.41	0.40
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:VAL:HG22	13:C:501:HEM:HBD2	2.02	0.40
3:C:364:LEU:O	3:C:368:PRO:HG3	2.21	0.40
4:D:10:PHE:H	4:D:10:PHE:HD1	1.67	0.40
4:D:30:PHE:HE2	4:D:64:LEU:HD11	1.86	0.40
4:D:81:PHE:HD2	4:D:81:PHE:N	2.19	0.40
4:D:164:ILE:O	4:D:179:MET:CE	2.69	0.40
10:J:14:PHE:N	10:J:14:PHE:HD2	2.17	0.40
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.56	0.40
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.77	0.40
2:O:107:TYR:CD2	2:O:127:THR:HG22	2.56	0.40
2:O:163:LEU:CD1	2:O:425:ALA:HB3	2.51	0.40
2:O:403:ASP:C	2:O:405:VAL:N	2.74	0.40
3:P:201:LEU:O	3:P:203:GLU:N	2.54	0.40
3:P:377:MET:HE2	6:S:20:TYR:HB2	2.04	0.40
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.39	0.40
5:R:38:LEU:O	5:R:39:VAL:C	2.59	0.40
5:R:52:LYS:C	5:R:52:LYS:CD	2.88	0.40
5:R:80:ASP:OD1	5:R:80:ASP:O	2.38	0.40
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.53	0.40
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.36	0.40
2:B:280:GLY:HA3	2:B:293:SER:CB	2.52	0.40
2:B:410:VAL:O	2:B:411:VAL:C	2.59	0.40
3:C:10:PRO:HG2	3:P:200:PHE:CE1	2.56	0.40
3:C:16:ASN:O	3:C:18:SER:N	2.47	0.40
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.52	0.40
3:C:28:ILE:HG12	3:C:225:TYR:CZ	2.56	0.40
3:C:303:PHE:O	3:C:306:PRO:HD2	2.21	0.40
4:D:90:TYR:O	4:D:91:PHE:C	2.60	0.40
4:D:233:ARG:HG3	7:G:17:SER:OG	2.21	0.40
6:F:65:ALA:O	6:F:68:LEU:HB2	2.21	0.40
7:G:33:ALA:O	7:G:37:VAL:HG23	2.21	0.40
1:N:37:VAL:HA	1:N:198:ALA:O	2.22	0.40
1:N:276:ILE:HG13	1:N:357:ALA:HB2	2.02	0.40
2:O:166:ALA:HB1	2:O:242:GLY:C	2.42	0.40
2:O:169:LYS:HE3	2:O:240:TRP:HA	2.02	0.40
4:Q:227:TRP:O	4:Q:228:SER:C	2.60	0.40
4:Q:238:ARG:HB3	4:Q:238:ARG:NH1	2.37	0.40
5:R:38:LEU:CA	10:W:14:PHE:CE1	3.04	0.40
5:R:153:PHE:C	5:R:155:GLY:H	2.24	0.40
8:U:25:GLU:HG2	8:U:61:PHE:CZ	2.55	0.40
1:A:86:PHE:CE2	1:A:116:VAL:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:CE	1:A:208:LEU:HD13	2.52	0.40
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.56	0.40
1:A:127:ILE:O	1:A:129:LYS:N	2.54	0.40
2:B:325:TYR:C	2:B:325:TYR:CD2	2.94	0.40
3:C:4:ASN:HD22	3:C:6:ARG:H	1.69	0.40
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.61	0.40
6:F:19:TRP:O	6:F:22:ASN:N	2.52	0.40
6:F:40:ASP:OD1	6:F:40:ASP:C	2.58	0.40
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.86	0.40
1:N:223:TYR:CD1	1:N:223:TYR:C	2.94	0.40
1:N:331:ILE:O	1:N:334:MET:HB3	2.21	0.40
2:O:122:TYR:O	2:O:123:LEU:C	2.58	0.40
2:O:341:MET:HE3	2:O:417:PHE:CE2	2.57	0.40
3:P:42:LEU:CD2	3:P:190:ILE:HG22	2.52	0.40
15:P:3002:UQ:HM51	15:P:3002:UQ:H8	2.02	0.40
4:Q:49:ARG:O	4:Q:52:ILE:HG13	2.22	0.40
5:R:126:ARG:HH22	5:R:179:ASN:CB	2.35	0.40
7:T:34:LEU:HB2	7:T:35:PRO:HD3	2.03	0.40
1:A:185:TYR:HA	1:A:189:HIS:HD2	1.86	0.40
1:A:248:LEU:HA	1:A:248:LEU:HD22	1.89	0.40
2:B:280:GLY:HA3	2:B:293:SER:HG	1.85	0.40
2:B:324:PHE:HD2	2:B:344:LEU:HD12	1.84	0.40
2:B:328:SER:O	2:B:329:GLN:C	2.59	0.40
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.50	0.40
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.45	0.40
3:C:70:THR:O	3:C:74:VAL:HG23	2.22	0.40
3:C:236:MET:O	3:C:237:LEU:C	2.60	0.40
5:E:47:THR:O	5:E:48:ALA:C	2.59	0.40
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.68	0.40
10:J:16:ARG:C	10:J:18:SER:H	2.25	0.40
10:J:16:ARG:C	10:J:18:SER:N	2.75	0.40
1:N:295:ALA:O	1:N:298:ALA:N	2.54	0.40
2:O:110:GLU:O	2:O:111:CYS:HB3	2.21	0.40
2:O:286:LYS:NZ	2:O:287:ARG:HH22	2.19	0.40
3:P:39:ALA:O	3:P:40:VAL:C	2.59	0.40
3:P:362:ILE:HA	3:P:366:LEU:HB2	2.04	0.40
4:Q:28:ARG:HH21	4:Q:181:GLN:NE2	2.19	0.40
4:Q:162:PRO:HA	4:Q:163:PRO:HD2	1.91	0.40
4:Q:168:ILE:HG23	4:Q:169:LEU:HD22	2.04	0.40
4:Q:221:TYR:CE1	7:T:25:ALA:CB	3.02	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%)	335 (76%)	84 (19%)	22 (5%)	2	18
1	N	440/446 (99%)	330 (75%)	87 (20%)	23 (5%)	2	16
2	B	424/441 (96%)	315 (74%)	78 (18%)	31 (7%)	1	10
2	O	420/441 (95%)	313 (74%)	78 (19%)	29 (7%)	1	11
3	C	378/380 (100%)	298 (79%)	61 (16%)	19 (5%)	2	18
3	P	377/380 (99%)	294 (78%)	67 (18%)	16 (4%)	3	22
4	D	239/241 (99%)	177 (74%)	51 (21%)	11 (5%)	2	19
4	Q	239/241 (99%)	181 (76%)	47 (20%)	11 (5%)	2	19
5	E	194/196 (99%)	119 (61%)	60 (31%)	15 (8%)	1	9
5	R	194/196 (99%)	122 (63%)	50 (26%)	22 (11%)	0	5
6	F	99/110 (90%)	74 (75%)	21 (21%)	4 (4%)	3	22
6	S	99/110 (90%)	77 (78%)	19 (19%)	3 (3%)	4	28
7	G	78/81 (96%)	59 (76%)	16 (20%)	3 (4%)	3	24
7	T	77/81 (95%)	57 (74%)	15 (20%)	5 (6%)	1	12
8	H	67/77 (87%)	44 (66%)	22 (33%)	1 (2%)	10	42
8	U	65/77 (84%)	43 (66%)	20 (31%)	2 (3%)	4	28
9	I	29/47 (62%)	15 (52%)	10 (34%)	4 (14%)	0	3
9	V	29/47 (62%)	15 (52%)	9 (31%)	5 (17%)	0	1
10	J	59/61 (97%)	38 (64%)	16 (27%)	5 (8%)	1	8
10	W	58/61 (95%)	39 (67%)	14 (24%)	5 (9%)	1	8
All	All	4006/4160 (96%)	2945 (74%)	825 (21%)	236 (6%)	1	14

All (236) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	222	THR
1	A	432	LEU
2	B	15	VAL
2	B	17	LEU
2	B	18	CYS
2	B	29	LEU
2	B	38	LEU
2	B	201	SER
2	B	210	GLY
2	B	221	GLU
2	B	386	ALA
3	C	18	SER
3	C	60	THR
3	C	111	LYS
3	C	248	PRO
3	C	287	ASN
4	D	166	ASN
4	D	198	HIS
5	E	102	THR
5	E	115	SER
5	E	130	PRO
5	E	177	PRO
7	G	7	LEU
7	G	33	ALA
9	I	56	SER
9	I	61	ARG
1	N	20	ASP
1	N	159	GLN
1	N	222	THR
1	N	432	LEU
2	O	19	PRO
2	O	38	LEU
2	O	201	SER
2	O	223	PHE
2	O	226	ILE
2	O	227	ARG
3	P	18	SER
3	P	60	THR
3	P	111	LYS
3	P	287	ASN
4	Q	166	ASN
4	Q	198	HIS

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Mol	Chain	Res	Type
5	R	8	PRO
5	R	107	ASN
5	R	130	PRO
5	R	140	THR
5	R	141	HIS
5	R	178	TYR
5	R	191	ASP
7	T	3	HIS
7	T	7	LEU
7	T	33	ALA
10	W	61	ALA
1	A	206	LYS
2	B	171	ALA
2	B	226	ILE
3	C	157	ILE
4	D	53	GLY
4	D	77	ASN
5	E	8	PRO
5	E	21	ALA
8	H	28	GLU
1	N	4	TYR
1	N	5	ALA
1	N	81	SER
1	N	108	LYS
1	N	433	ASP
2	O	171	ALA
2	O	210	GLY
2	O	268	GLU
2	O	386	ALA
3	P	76	TYR
3	P	202	HIS
4	Q	53	GLY
4	Q	172	ASP
5	R	21	ALA
5	R	108	GLN
5	R	115	SER
5	R	122	HIS
5	R	131	GLU
5	R	144	CYS
5	R	177	PRO
8	U	52	GLU
9	V	63	ASP

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Mol	Chain	Res	Type
9	V	72	ALA
9	V	76	VAL
10	W	25	VAL
1	A	72	CYS
1	A	81	SER
1	A	107	PRO
1	A	108	LYS
1	A	135	LEU
1	A	290	LEU
2	B	20	GLY
2	B	26	ILE
2	B	63	LEU
2	B	152	PHE
2	B	207	VAL
2	B	389	SER
3	C	3	PRO
3	C	156	TYR
3	C	202	HIS
3	C	255	GLU
4	D	38	SER
4	D	133	GLY
6	F	52	GLU
6	F	77	LYS
6	F	83	TYR
9	I	64	LEU
10	J	25	VAL
10	J	33	ARG
10	J	55	ILE
1	N	72	CYS
1	N	107	PRO
1	N	121	ALA
1	N	135	LEU
1	N	206	LYS
1	N	218	GLY
1	N	288	LYS
2	O	140	LEU
2	O	389	SER
2	O	431	GLY
3	P	248	PRO
4	Q	38	SER
4	Q	133	GLY
8	U	28	GLU

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Mol	Chain	Res	Type
10	W	15	ARG
10	W	33	ARG
10	W	55	ILE
1	A	121	ALA
1	A	180	ALA
1	A	217	SER
1	A	218	GLY
1	A	433	ASP
2	B	24	LEU
2	B	140	LEU
2	B	222	GLN
2	B	306	PRO
2	B	393	THR
3	C	288	LYS
3	C	348	PHE
4	D	172	ASP
5	E	92	ARG
5	E	128	LYS
5	E	176	ALA
10	J	15	ARG
2	O	63	LEU
2	O	152	PHE
2	O	221	GLU
2	O	393	THR
2	O	409	ASP
2	O	416	LYS
3	P	3	PRO
3	P	156	TYR
3	P	255	GLU
3	P	288	LYS
3	P	348	PHE
5	R	49	TYR
5	R	149	ASN
5	R	175	PRO
6	S	52	GLU
7	T	50	PRO
9	V	73	PRO
1	A	53	ASN
1	A	106	MET
1	A	192	ALA
2	B	21	ALA
2	B	30	PRO

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Mol	Chain	Res	Type
2	B	307	PHE
2	B	319	SER
2	B	394	ALA
2	B	416	LYS
3	C	4	ASN
3	C	17	ASN
3	C	76	TYR
3	C	159	HIS
4	D	96	PRO
4	D	123	GLY
5	E	80	ASP
5	E	141	HIS
5	E	149	ASN
6	F	19	TRP
7	G	50	PRO
10	J	32	GLU
1	N	192	ALA
2	O	26	ILE
2	O	207	VAL
2	O	216	LEU
2	O	228	SER
2	O	306	PRO
2	O	307	PHE
2	O	319	SER
2	O	394	ALA
3	P	17	ASN
3	P	296	ALA
3	P	366	LEU
4	Q	106	ASN
5	R	92	ARG
5	R	121	GLN
6	S	77	LYS
6	S	83	TYR
9	V	48	PRO
1	A	263	ALA
4	D	106	ASN
5	E	129	LYS
1	N	53	ASN
1	N	106	MET
1	N	148	VAL
2	O	384	SER
3	P	10	PRO

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Mol	Chain	Res	Type
3	C	10	PRO
5	E	175	PRO
1	N	209	VAL
4	Q	96	PRO
4	Q	162	PRO
5	R	176	ALA
1	A	209	VAL
2	B	209	ILE
2	B	420	GLY
9	I	72	ALA
2	O	209	ILE
5	R	18	VAL
7	T	48	VAL
1	A	148	VAL
2	B	64	GLY
3	C	209	PRO
4	D	229	VAL
1	N	428	ILE
5	E	18	VAL
4	Q	123	GLY
4	Q	168	ILE
5	R	154	GLY
1	A	428	ILE
3	C	305	ILE
1	N	110	VAL

5.3.2 Protein sidechains (i)

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%)	346 (95%)	19 (5%)	23	55
1	N	365/368 (99%)	346 (95%)	19 (5%)	23	55
2	B	333/347 (96%)	308 (92%)	25 (8%)	13	43
2	O	333/347 (96%)	312 (94%)	21 (6%)	18	50
3	C	329/329 (100%)	317 (96%)	12 (4%)	35	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	328/329 (100%)	318 (97%)	10 (3%)	41	70
4	D	200/200 (100%)	191 (96%)	9 (4%)	27	60
4	Q	200/200 (100%)	191 (96%)	9 (4%)	27	60
5	E	166/166 (100%)	158 (95%)	8 (5%)	25	58
5	R	166/166 (100%)	158 (95%)	8 (5%)	25	58
6	F	93/96 (97%)	87 (94%)	6 (6%)	17	49
6	S	93/96 (97%)	87 (94%)	6 (6%)	17	49
7	G	71/71 (100%)	66 (93%)	5 (7%)	15	46
7	T	70/71 (99%)	67 (96%)	3 (4%)	29	61
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	84
8	U	63/71 (89%)	63 (100%)	0	100	100
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	61
9	V	23/26 (88%)	19 (83%)	4 (17%)	2	10
10	J	49/49 (100%)	46 (94%)	3 (6%)	18	50
10	W	47/49 (96%)	44 (94%)	3 (6%)	17	49
All	All	3382/3446 (98%)	3210 (95%)	172 (5%)	24	56

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	10	ASN
1	A	49	ASN
1	A	53	ASN
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	108	LYS
1	A	171	THR
1	A	174	ILE
1	A	181	ASP
1	A	188	THR
1	A	248	LEU
1	A	283	THR
1	A	307	PHE
1	A	342	TRP
1	A	392	LEU

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Mol	Chain	Res	Type
1	A	395	TRP
1	A	405	ARG
2	B	31	ASN
2	B	57	TYR
2	B	59	THR
2	B	71	LEU
2	B	96	LEU
2	B	102	ARG
2	B	104	LYS
2	B	114	ASP
2	B	120	MET
2	B	139	ASP
2	B	150	VAL
2	B	154	SER
2	B	168	TYR
2	B	181	TYR
2	B	189	GLU
2	B	227	ARG
2	B	248	ASN
2	B	284	LEU
2	B	296	TYR
2	B	325	TYR
2	B	335	GLU
2	B	343	GLN
2	B	344	LEU
2	B	402	ILE
2	B	403	ASP
3	C	44	THR
3	C	69	HIS
3	C	82	ASN
3	C	145	THR
3	C	149	ASN
3	C	182	LEU
3	C	208	ASN
3	C	243	LEU
3	C	245	LEU
3	C	248	PRO
3	C	255	GLU
3	C	299	VAL
4	D	13	SER
4	D	64	LEU
4	D	81	PHE

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Mol	Chain	Res	Type
4	D	169	LEU
4	D	173	ASP
4	D	178	THR
4	D	199	ASP
4	D	214	LEU
4	D	219	LEU
5	E	6	THR
5	E	52	LYS
5	E	60	SER
5	E	61	SER
5	E	71	LEU
5	E	131	GLU
5	E	135	LEU
5	E	185	TYR
6	F	27	ASN
6	F	34	ASP
6	F	58	ARG
6	F	70	LEU
6	F	89	TYR
6	F	102	LEU
7	G	4	PHE
7	G	16	TYR
7	G	60	SER
7	G	63	THR
7	G	65	GLU
8	H	19	THR
9	I	71	ASN
10	J	14	PHE
10	J	57	HIS
10	J	59	TYR
1	N	3	THR
1	N	10	ASN
1	N	49	ASN
1	N	53	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	108	LYS
1	N	171	THR
1	N	174	ILE
1	N	181	ASP
1	N	188	THR

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Mol	Chain	Res	Type
1	N	248	LEU
1	N	283	THR
1	N	307	PHE
1	N	342	TRP
1	N	392	LEU
1	N	395	TRP
1	N	405	ARG
2	O	22	GLU
2	O	31	ASN
2	O	57	TYR
2	O	71	LEU
2	O	96	LEU
2	O	102	ARG
2	O	104	LYS
2	O	114	ASP
2	O	120	MET
2	O	139	ASP
2	O	150	VAL
2	O	154	SER
2	O	168	TYR
2	O	181	TYR
2	O	227	ARG
2	O	248	ASN
2	O	284	LEU
2	O	296	TYR
2	O	335	GLU
2	O	343	GLN
2	O	402	ILE
3	P	44	THR
3	P	74	VAL
3	P	82	ASN
3	P	145	THR
3	P	149	ASN
3	P	182	LEU
3	P	208	ASN
3	P	242	THR
3	P	243	LEU
3	P	245	LEU
4	Q	13	SER
4	Q	64	LEU
4	Q	81	PHE
4	Q	127	VAL

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Mol	Chain	Res	Type
4	Q	169	LEU
4	Q	173	ASP
4	Q	178	THR
4	Q	214	LEU
4	Q	219	LEU
5	R	31	ASP
5	R	52	LYS
5	R	60	SER
5	R	61	SER
5	R	71	LEU
5	R	135	LEU
5	R	152	ASP
5	R	185	TYR
6	S	27	ASN
6	S	34	ASP
6	S	58	ARG
6	S	70	LEU
6	S	89	TYR
6	S	102	LEU
7	T	4	PHE
7	T	16	TYR
7	T	60	SER
9	V	55	MET
9	V	62	ARG
9	V	63	ASP
9	V	70	LEU
10	W	14	PHE
10	W	57	HIS
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	173	ASN
1	A	271	HIS
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
1	A	435	ASN
2	B	31	ASN
2	B	156	GLN

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Mol	Chain	Res	Type
2	B	192	HIS
2	B	197	ASN
2	B	247	GLN
2	B	248	ASN
2	B	250	HIS
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	376	GLN
3	C	9	HIS
3	C	16	ASN
3	C	69	HIS
3	C	82	ASN
3	C	86	ASN
3	C	207	ASN
3	C	261	ASN
3	C	309	HIS
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	97	ASN
4	D	105	ASN
4	D	200	GLN
5	E	57	GLN
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	28	ASN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	21	ASN
1	N	32	GLN
1	N	118	GLN
1	N	126	GLN
1	N	173	ASN
1	N	274	ASN
1	N	305	HIS
1	N	308	GLN
1	N	339	GLN
1	N	435	ASN

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Mol	Chain	Res	Type
2	O	31	ASN
2	O	156	GLN
2	O	192	HIS
2	O	197	ASN
2	O	247	GLN
2	O	248	ASN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	376	GLN
3	P	9	HIS
3	P	16	ASN
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	261	ASN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	97	ASN
4	Q	105	ASN
5	R	57	GLN
5	R	107	ASN
5	R	149	ASN
5	R	164	HIS
5	R	186	GLN
7	T	23	GLN
7	T	28	ASN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	75	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 5 are unknown and 2 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
13	HEM	C	501	3	41,50,50	1.73	7 (17%)	45,82,82	2.32	17 (37%)
19	HEC	Q	501	4	32,50,50	2.27	5 (15%)	24,82,82	2.20	6 (25%)
13	HEM	C	502	3	41,50,50	1.98	11 (26%)	45,82,82	2.27	13 (28%)
13	HEM	P	501	3	41,50,50	1.81	7 (17%)	45,82,82	2.13	15 (33%)
15	UQ	C	2002	-	19,19,63	2.54	10 (52%)	23,26,79	1.36	4 (17%)
18	GOL	P	3011	-	5,5,5	1.32	0	5,5,5	0.59	0
20	BOG	D	2009	-	20,20,20	1.10	2 (10%)	25,25,25	0.90	2 (8%)
16	CDL	P	3004	-	39,39,99	1.27	5 (12%)	45,51,111	1.13	5 (11%)
16	CDL	C	2004	-	39,39,99	1.30	5 (12%)	45,51,111	1.14	5 (11%)
16	CDL	Q	3003	-	41,41,99	1.16	1 (2%)	47,53,111	1.05	4 (8%)
13	HEM	P	502	3	41,50,50	1.74	6 (14%)	45,82,82	1.58	10 (22%)
14	IKR	C	2001	-	25,26,26	1.40	4 (16%)	31,35,35	1.42	6 (19%)
11	PEE	C	2007	-	48,48,50	1.33	5 (10%)	51,53,55	0.81	2 (3%)
20	BOG	P	2010	-	12,12,20	1.44	2 (16%)	17,17,25	0.64	0
11	PEE	P	3007	-	48,48,50	1.31	5 (10%)	51,53,55	0.78	2 (3%)
21	FES	R	501	5	0,4,4	-	-	-		
15	UQ	P	3002	-	19,19,63	2.70	10 (52%)	23,26,79	1.37	4 (17%)
21	FES	E	501	5	0,4,4	-	-	-		
20	BOG	Q	3009	-	20,20,20	1.04	2 (10%)	25,25,25	1.01	1 (4%)
20	BOG	P	3091	-	13,13,20	1.35	2 (15%)	18,18,25	1.11	2 (11%)
11	PEE	E	2005	-	49,49,50	1.52	10 (20%)	52,54,55	0.90	3 (5%)
16	CDL	D	2003	-	41,41,99	1.16	1 (2%)	47,53,111	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	IKR	P	3001	-	25,26,26	1.39	5 (20%)	31,35,35	1.43	6 (19%)
20	BOG	D	2091	-	13,13,20	1.48	3 (23%)	18,18,25	1.17	2 (11%)
18	GOL	C	2011	-	5,5,5	1.31	0	5,5,5	0.53	0
19	HEC	D	501	4	32,50,50	2.19	7 (21%)	24,82,82	2.44	7 (29%)
11	PEE	P	3008	-	4,4,50	3.51	4 (100%)	6,6,55	0.63	0
11	PEE	R	3005	-	49,49,50	1.56	10 (20%)	52,54,55	0.89	3 (5%)
11	PEE	A	2008	-	16,16,50	1.74	5 (31%)	18,20,55	0.51	0

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
13	HEM	C	501	3	-	6/12/54/54	-
19	HEC	Q	501	4	-	2/10/54/54	-
13	HEM	C	502	3	-	9/12/54/54	-
13	HEM	P	501	3	-	6/12/54/54	-
15	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
18	GOL	P	3011	-	-	2/4/4/4	-
20	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
16	CDL	P	3004	-	-	21/49/49/110	-
16	CDL	C	2004	-	-	21/49/49/110	-
16	CDL	Q	3003	-	-	20/51/51/110	-
13	HEM	P	502	3	-	8/12/54/54	-
14	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
11	PEE	C	2007	-	-	19/52/52/54	-
20	BOG	P	2010	-	-	1/2/22/31	0/1/1/1
11	PEE	P	3007	-	-	19/52/52/54	-
21	FES	R	501	5	-	-	0/1/1/1
15	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
21	FES	E	501	5	-	-	0/1/1/1
20	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
20	BOG	P	3091	-	-	4/4/24/31	0/1/1/1
11	PEE	E	2005	-	-	25/53/53/54	-
16	CDL	D	2003	-	-	21/51/51/110	-
14	IKR	P	3001	-	-	1/18/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BOG	D	2091	-	-	1/4/24/31	0/1/1/1
18	GOL	C	2011	-	-	4/4/4/4	-
19	HEC	D	501	4	-	2/10/54/54	-
11	PEE	R	3005	-	-	27/53/53/54	-
11	PEE	A	2008	-	-	2/19/19/54	-

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	501	HEC	C2B-C3B	-9.35	1.31	1.40
19	D	501	HEC	C3C-C2C	-6.87	1.33	1.40
19	D	501	HEC	C2B-C3B	-6.77	1.33	1.40
15	P	3002	UQ	C7-C6	5.98	1.61	1.51
19	Q	501	HEC	C3C-C2C	-5.63	1.34	1.40
15	P	3002	UQ	C6-C5	5.05	1.44	1.35
15	C	2002	UQ	C7-C6	4.97	1.59	1.51
13	C	501	HEM	CBC-CAC	4.76	1.60	1.29
15	C	2002	UQ	C6-C5	4.68	1.43	1.35
11	P	3008	PEE	P-O1P	4.67	1.61	1.50
13	P	501	HEM	CBB-CAB	4.66	1.53	1.30
13	C	501	HEM	CBB-CAB	4.65	1.53	1.30
13	P	501	HEM	C3C-CAC	-4.57	1.38	1.47
13	P	502	HEM	C3C-CAC	-4.47	1.38	1.47
13	C	502	HEM	C3C-C2C	-4.47	1.34	1.40
13	C	502	HEM	CBB-CAB	4.26	1.51	1.30
11	E	2005	PEE	C39-C38	4.02	1.55	1.31
11	P	3007	PEE	C39-C38	4.01	1.55	1.31
11	R	3005	PEE	C39-C38	3.99	1.54	1.31
11	C	2007	PEE	C39-C38	3.98	1.54	1.31
13	P	502	HEM	CBB-CAB	3.97	1.49	1.30
15	C	2002	UQ	C6-C1	3.95	1.57	1.46
13	P	501	HEM	CBC-CAC	3.93	1.55	1.29
13	P	502	HEM	CBC-CAC	3.83	1.54	1.29
13	C	502	HEM	CBC-CAC	3.80	1.54	1.29
13	P	502	HEM	CAB-C3B	-3.78	1.37	1.47
11	R	3005	PEE	O2-C10	3.78	1.45	1.34
15	P	3002	UQ	C6-C1	3.77	1.57	1.46
13	P	501	HEM	C3C-C2C	-3.63	1.35	1.40
13	C	502	HEM	C3C-CAC	-3.57	1.40	1.47
13	C	501	HEM	C3C-C2C	-3.55	1.35	1.40
11	R	3005	PEE	O3-C30	3.52	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2002	UQ	O3-C3	3.51	1.45	1.36
11	E	2005	PEE	O2-C10	3.47	1.44	1.34
13	P	502	HEM	C3C-C2C	-3.46	1.35	1.40
13	P	501	HEM	CAB-C3B	-3.45	1.38	1.47
13	C	501	HEM	CAB-C3B	-3.43	1.38	1.47
11	R	3005	PEE	P-O1P	3.38	1.62	1.50
11	P	3008	PEE	P-O4P	3.36	1.64	1.54
13	C	502	HEM	C1B-C2B	3.30	1.51	1.44
13	C	502	HEM	C4A-CHB	-3.26	1.31	1.41
11	E	2005	PEE	O3-C30	3.24	1.42	1.33
14	C	2001	IKR	C40-C2	3.23	1.57	1.51
15	P	3002	UQ	C7-C8	3.23	1.55	1.50
13	C	501	HEM	C3C-CAC	-3.22	1.41	1.47
11	P	3008	PEE	P-O3P	3.17	1.64	1.54
11	A	2008	PEE	P-O1P	3.13	1.62	1.50
11	E	2005	PEE	P-O1P	3.07	1.61	1.50
11	P	3007	PEE	C21-C22	-3.04	1.34	1.51
15	P	3002	UQ	O3-C3	3.03	1.44	1.36
13	C	502	HEM	CAB-C3B	-3.01	1.39	1.47
11	C	2007	PEE	P-O1P	3.00	1.61	1.50
13	C	502	HEM	CMB-C2B	3.00	1.57	1.50
14	P	3001	IKR	C40-C2	2.98	1.57	1.51
11	P	3007	PEE	O3-C30	2.98	1.42	1.33
11	A	2008	PEE	O2-C10	2.96	1.42	1.34
20	D	2091	BOG	C4-C5	2.94	1.59	1.53
11	C	2007	PEE	O2-C10	2.93	1.42	1.34
11	E	2005	PEE	C21-C22	-2.89	1.35	1.51
11	C	2007	PEE	C21-C22	-2.89	1.35	1.51
16	C	2004	CDL	O1-C1	2.88	1.52	1.43
19	D	501	HEC	C3C-C4C	2.86	1.48	1.43
11	R	3005	PEE	C21-C22	-2.86	1.35	1.51
19	Q	501	HEC	C4D-CHA	-2.86	1.33	1.41
11	C	2007	PEE	O3-C30	2.85	1.41	1.33
11	P	3007	PEE	O2-C10	2.80	1.42	1.34
13	P	502	HEM	C4A-CHB	-2.76	1.33	1.41
11	P	3007	PEE	P-O1P	2.75	1.60	1.50
20	P	2010	BOG	C4-C5	2.75	1.58	1.53
15	P	3002	UQ	C5-C4	2.70	1.56	1.47
14	C	2001	IKR	C20-C17	2.68	1.44	1.40
15	P	3002	UQ	C2-C1	2.67	1.56	1.48
13	P	501	HEM	C3B-C2B	-2.64	1.31	1.37
20	P	2010	BOG	C1-C2	2.64	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2002	UQ	C5-C4	2.64	1.56	1.47
15	P	3002	UQ	CM5-C5	2.64	1.56	1.50
15	C	2002	UQ	C3-C4	2.63	1.56	1.48
11	E	2005	PEE	C11-C10	2.61	1.58	1.50
15	C	2002	UQ	CM5-C5	2.58	1.56	1.50
14	P	3001	IKR	C3-C4	2.57	1.43	1.38
19	D	501	HEC	C4D-CHA	-2.53	1.34	1.41
14	C	2001	IKR	C3-C4	2.50	1.43	1.38
11	E	2005	PEE	C3-C2	2.47	1.58	1.50
14	P	3001	IKR	C20-C17	2.47	1.43	1.40
20	D	2009	BOG	O5-C1	2.47	1.48	1.41
15	C	2002	UQ	C7-C8	2.46	1.54	1.50
15	C	2002	UQ	C2-C1	2.46	1.56	1.48
11	P	3008	PEE	P-O2P	2.46	1.62	1.54
20	P	3091	BOG	O5-C1	2.45	1.48	1.41
11	R	3005	PEE	C11-C10	2.44	1.57	1.50
14	C	2001	IKR	C24-C17	2.43	1.43	1.39
16	C	2004	CDL	CB3-CB4	2.41	1.58	1.50
14	P	3001	IKR	C24-C17	2.39	1.43	1.39
11	R	3005	PEE	C1-C2	2.38	1.58	1.50
16	P	3004	CDL	O1-C1	2.38	1.50	1.43
11	R	3005	PEE	C31-C30	2.37	1.57	1.50
20	D	2091	BOG	O5-C1	2.37	1.47	1.41
11	A	2008	PEE	C3-C2	2.36	1.57	1.51
11	E	2005	PEE	O2-C2	2.35	1.52	1.46
11	R	3005	PEE	O2-C2	2.35	1.52	1.46
15	P	3002	UQ	C3-C4	2.34	1.55	1.48
16	P	3004	CDL	OA8-CA6	-2.34	1.39	1.45
11	A	2008	PEE	C1-C2	2.33	1.57	1.50
13	C	502	HEM	C4B-NB	-2.33	1.34	1.38
13	C	501	HEM	C1B-C2B	2.32	1.49	1.44
20	P	3091	BOG	C4-C5	2.31	1.57	1.53
11	R	3005	PEE	C3-C2	2.30	1.57	1.50
20	Q	3009	BOG	O5-C1	2.29	1.47	1.41
13	C	501	HEM	CHC-C4B	-2.28	1.34	1.41
15	P	3002	UQ	O2-C2	2.28	1.42	1.36
11	E	2005	PEE	C31-C30	2.27	1.57	1.50
11	E	2005	PEE	C1-C2	2.26	1.57	1.50
19	D	501	HEC	C3A-C4A	2.24	1.47	1.42
15	C	2002	UQ	O2-C2	2.23	1.42	1.36
13	P	501	HEM	C4A-CHB	-2.20	1.34	1.41
19	D	501	HEC	C1D-CHD	-2.20	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	2004	CDL	OA8-CA6	-2.19	1.40	1.45
19	Q	501	HEC	CAD-C3D	2.17	1.55	1.52
16	C	2004	CDL	OA5-CA3	-2.16	1.36	1.44
16	P	3004	CDL	OB8-CB7	2.16	1.39	1.33
20	D	2009	BOG	C1-C2	2.15	1.58	1.52
16	P	3004	CDL	CB3-CB4	2.14	1.57	1.50
19	Q	501	HEC	C3C-C4C	2.13	1.46	1.43
16	D	2003	CDL	O1-C1	2.12	1.49	1.43
20	D	2091	BOG	C1-C2	2.12	1.58	1.52
14	P	3001	IKR	C21-C20	2.11	1.43	1.39
13	C	502	HEM	FE-ND	-2.10	1.86	1.96
11	A	2008	PEE	C11-C10	2.08	1.56	1.50
13	C	502	HEM	CHC-C4B	-2.07	1.35	1.41
20	Q	3009	BOG	C4-C5	2.07	1.57	1.53
16	Q	3003	CDL	O1-C1	2.04	1.49	1.43
19	D	501	HEC	C1B-CHB	-2.04	1.35	1.41
16	C	2004	CDL	OA6-CA5	2.03	1.40	1.34
16	P	3004	CDL	OB6-CB5	2.01	1.40	1.34

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Q	501	HEC	CBA-CAA-C2A	7.60	125.41	112.60
13	C	501	HEM	CBA-CAA-C2A	-7.57	99.70	112.62
19	D	501	HEC	CBA-CAA-C2A	7.47	125.19	112.60
13	C	502	HEM	C3B-C2B-C1B	-7.12	101.20	106.49
13	C	502	HEM	CMB-C2B-C1B	5.82	133.91	125.04
13	C	501	HEM	CMA-C3A-C4A	-5.77	119.59	128.46
13	P	501	HEM	CBA-CAA-C2A	-5.54	103.16	112.62
13	P	501	HEM	CMB-C2B-C1B	4.90	132.50	125.04
13	C	501	HEM	C4A-C3A-C2A	4.51	110.13	107.00
19	D	501	HEC	CBD-CAD-C3D	4.14	119.69	112.62
19	D	501	HEC	C1D-C2D-C3D	4.14	109.88	107.00
20	Q	3009	BOG	C1'-O1-C1	4.14	120.70	113.84
13	C	502	HEM	C4A-C3A-C2A	-4.11	104.14	107.00
13	C	502	HEM	CAD-C3D-C4D	4.08	131.78	124.66
15	P	3002	UQ	C8-C7-C6	4.07	123.02	112.05
13	C	502	HEM	C2B-C1B-NB	4.05	114.64	109.84
15	C	2002	UQ	C8-C7-C6	4.05	122.96	112.05
13	C	501	HEM	CMB-C2B-C1B	3.95	131.05	125.04
19	D	501	HEC	CMC-C2C-C3C	-3.88	121.26	125.82
13	P	502	HEM	C4A-C3A-C2A	-3.75	104.39	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Q	501	HEC	CBD-CAD-C3D	3.68	118.91	112.62
13	P	501	HEM	CMA-C3A-C4A	-3.58	122.96	128.46
13	P	501	HEM	C3B-C2B-C1B	-3.57	103.84	106.49
19	Q	501	HEC	CMC-C2C-C3C	-3.57	121.62	125.82
20	P	3091	BOG	C1'-O1-C1	3.52	118.70	113.27
13	P	502	HEM	CMB-C2B-C1B	3.50	130.37	125.04
20	D	2091	BOG	C1'-O1-C1	3.50	118.67	113.27
13	C	501	HEM	C3B-C2B-C1B	-3.49	103.90	106.49
13	C	502	HEM	C4B-CHC-C1C	3.47	127.13	122.56
14	P	3001	IKR	C40-C2-C3	-3.34	113.31	119.49
13	P	501	HEM	CMD-C2D-C1D	3.31	130.07	125.04
20	D	2009	BOG	C1'-O1-C1	3.29	119.30	113.84
13	P	502	HEM	CBA-CAA-C2A	3.28	118.22	112.62
13	P	501	HEM	C1B-NB-C4B	-3.24	101.73	105.07
15	C	2002	UQ	C7-C6-C1	-3.20	114.63	118.48
15	P	3002	UQ	C7-C6-C1	-3.20	114.63	118.48
13	C	501	HEM	C1B-NB-C4B	-3.19	101.77	105.07
13	P	501	HEM	C2B-C1B-NB	3.18	113.61	109.84
14	C	2001	IKR	C40-C2-C3	-3.17	113.64	119.49
11	R	3005	PEE	C22-C21-C20	3.11	127.34	113.79
19	D	501	HEC	CMC-C2C-C1C	3.10	133.23	128.46
13	P	501	HEM	C2C-C3C-C4C	-3.07	104.75	106.90
11	E	2005	PEE	C22-C21-C20	3.06	127.12	113.79
13	P	501	HEM	C4B-CHC-C1C	3.03	126.56	122.56
14	P	3001	IKR	O31-C30-O36	3.00	129.30	123.53
13	C	502	HEM	C1B-NB-C4B	-2.99	101.98	105.07
14	C	2001	IKR	O31-C30-O36	2.96	129.23	123.53
13	C	502	HEM	C4C-CHD-C1D	2.90	126.39	122.56
11	P	3007	PEE	C22-C21-C20	2.87	126.31	113.79
11	C	2007	PEE	C22-C21-C20	2.87	126.28	113.79
16	P	3004	CDL	CB4-OB6-CB5	-2.85	110.77	117.79
13	C	502	HEM	CAD-C3D-C2D	-2.84	122.59	127.88
13	C	501	HEM	C2B-C1B-NB	2.80	113.16	109.84
19	Q	501	HEC	C1D-C2D-C3D	2.80	108.94	107.00
14	C	2001	IKR	O31-C30-C29	-2.76	108.66	111.83
13	C	501	HEM	CMD-C2D-C1D	2.74	129.21	125.04
13	C	501	HEM	C4D-ND-C1D	-2.74	102.25	105.07
13	P	501	HEM	C4D-ND-C1D	-2.74	102.25	105.07
14	P	3001	IKR	C3-C2-C1	2.72	119.40	117.21
20	D	2091	BOG	O1-C1-C2	2.71	111.33	108.15
14	C	2001	IKR	C17-C20-C29	2.71	123.57	121.22
13	P	501	HEM	CMA-C3A-C2A	2.69	130.02	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501	HEM	CMA-C3A-C2A	2.69	130.01	124.94
16	C	2004	CDL	CB4-OB6-CB5	-2.68	111.20	117.79
16	P	3004	CDL	CA6-CA4-CA3	-2.64	105.55	111.79
14	P	3001	IKR	C17-C20-C29	2.61	123.48	121.22
19	D	501	HEC	CAA-C2A-C3A	-2.58	119.83	127.25
13	P	502	HEM	C3B-C2B-C1B	-2.58	104.57	106.49
14	C	2001	IKR	C3-C2-C1	2.58	119.28	117.21
14	P	3001	IKR	O31-C30-C29	-2.57	108.87	111.83
16	D	2003	CDL	CB4-OB6-CB5	-2.56	111.49	117.79
16	C	2004	CDL	CA6-CA4-CA3	-2.55	105.76	111.79
13	P	502	HEM	CAD-C3D-C2D	-2.49	123.24	127.88
13	C	502	HEM	C2D-C1D-ND	2.49	112.86	109.88
13	P	501	HEM	CMC-C2C-C3C	2.47	129.30	124.68
11	C	2007	PEE	C21-C22-C23	2.47	126.94	114.42
20	P	3091	BOG	O1-C1-C2	2.44	111.01	108.15
11	P	3007	PEE	C21-C22-C23	2.43	126.78	114.42
11	E	2005	PEE	C21-C22-C23	2.42	126.71	114.42
13	P	502	HEM	C2B-C1B-NB	2.42	112.70	109.84
13	P	501	HEM	CHC-C4B-NB	-2.39	121.83	124.43
11	R	3005	PEE	C21-C22-C23	2.38	126.51	114.42
13	P	502	HEM	C4B-CHC-C1C	2.35	125.66	122.56
16	Q	3003	CDL	CB4-OB6-CB5	-2.32	112.07	117.79
16	P	3004	CDL	OB6-CB4-CB3	2.31	116.77	108.40
13	C	502	HEM	CAB-C3B-C2B	-2.30	121.01	128.60
13	P	502	HEM	CAD-C3D-C4D	2.29	128.66	124.66
15	C	2002	UQ	C10-C9-C8	-2.28	117.83	123.68
13	C	501	HEM	CMC-C2C-C3C	2.28	128.94	124.68
19	Q	501	HEC	CMC-C2C-C1C	2.27	131.95	128.46
16	C	2004	CDL	OB6-CB4-CB3	2.25	116.56	108.40
16	D	2003	CDL	CA6-CA4-CA3	-2.22	106.54	111.79
13	P	501	HEM	CHB-C1B-NB	-2.22	121.64	124.38
15	P	3002	UQ	C10-C9-C8	-2.22	117.99	123.68
11	E	2005	PEE	O3-C3-C2	2.19	114.80	108.43
13	C	501	HEM	CAD-C3D-C2D	-2.17	123.84	127.88
14	P	3001	IKR	O15-C4-C5	2.16	119.19	115.10
13	C	501	HEM	C2C-C3C-C4C	-2.14	105.40	106.90
16	Q	3003	CDL	CA4-OA6-CA5	-2.12	112.58	117.79
14	C	2001	IKR	O15-C4-C5	2.11	119.11	115.10
16	Q	3003	CDL	CA6-CA4-CA3	-2.11	106.79	111.79
16	C	2004	CDL	CA4-OA6-CA5	-2.11	112.60	117.79
13	P	502	HEM	CMA-C3A-C2A	2.09	128.89	124.94
13	P	501	HEM	C4C-CHD-C1D	2.09	125.31	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	502	HEM	C1B-NB-C4B	-2.08	102.92	105.07
11	R	3005	PEE	O3-C3-C2	2.08	114.50	108.43
13	C	501	HEM	CBB-CAB-C3B	-2.08	117.26	127.62
13	C	501	HEM	CAD-C3D-C4D	2.07	128.28	124.66
13	C	501	HEM	CHD-C1D-ND	-2.07	122.18	124.43
13	C	502	HEM	C4B-C3B-C2B	2.07	108.75	107.11
16	P	3004	CDL	CA6-OA8-CA7	-2.07	111.91	117.10
16	Q	3003	CDL	CA6-OA8-CA7	-2.07	111.91	117.10
19	D	501	HEC	C2B-C3B-C4B	-2.05	104.14	106.35
15	C	2002	UQ	C11-C9-C8	2.04	125.55	120.50
19	Q	501	HEC	CAA-C2A-C3A	-2.04	121.38	127.25
13	C	501	HEM	CHC-C4B-NB	-2.03	122.23	124.43
16	P	3004	CDL	CA4-OA6-CA5	-2.02	112.81	117.79
13	C	502	HEM	C2C-C3C-C4C	-2.02	105.49	106.90
20	D	2009	BOG	O1-C1-C2	2.00	111.43	108.30
15	P	3002	UQ	C11-C9-C8	2.00	125.45	120.50
16	C	2004	CDL	CA6-OA8-CA7	-2.00	112.07	117.10

There are no chirality outliers.

All (238) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	O4P-C4-C5-N
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C4-O4P-P-O1P
11	R	3005	PEE	O4P-C4-C5-N
13	C	501	HEM	C2B-C3B-CAB-CBB
13	C	501	HEM	C4B-C3B-CAB-CBB
13	C	502	HEM	C2B-C3B-CAB-CBB
13	C	502	HEM	C4B-C3B-CAB-CBB
13	P	501	HEM	C2B-C3B-CAB-CBB
13	P	501	HEM	C4B-C3B-CAB-CBB
13	P	502	HEM	C2B-C3B-CAB-CBB
13	P	502	HEM	C4B-C3B-CAB-CBB
15	C	2002	UQ	C1-C6-C7-C8
15	C	2002	UQ	C5-C6-C7-C8
15	C	2002	UQ	C12-C11-C9-C8
15	C	2002	UQ	C12-C11-C9-C10
15	P	3002	UQ	C1-C6-C7-C8
15	P	3002	UQ	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	P	3002	UQ	C12-C11-C9-C8
15	P	3002	UQ	C12-C11-C9-C10
16	C	2004	CDL	CB2-OB2-PB2-OB3
16	C	2004	CDL	CB2-OB2-PB2-OB4
16	C	2004	CDL	C51-CB5-OB6-CB4
16	P	3004	CDL	CB2-OB2-PB2-OB3
16	P	3004	CDL	CB2-OB2-PB2-OB4
16	P	3004	CDL	C51-CB5-OB6-CB4
18	C	2011	GOL	O1-C1-C2-C3
18	P	3011	GOL	C1-C2-C3-O3
19	D	501	HEC	C1A-C2A-CAA-CBA
19	D	501	HEC	C3A-C2A-CAA-CBA
19	Q	501	HEC	C1A-C2A-CAA-CBA
19	Q	501	HEC	C3A-C2A-CAA-CBA
20	D	2009	BOG	C2-C1-O1-C1'
20	D	2009	BOG	O5-C1-O1-C1'
20	P	3091	BOG	C2-C1-O1-C1'
20	P	3091	BOG	O5-C1-O1-C1'
20	Q	3009	BOG	C2-C1-O1-C1'
20	Q	3009	BOG	O5-C1-O1-C1'
16	C	2004	CDL	C31-CA7-OA8-CA6
16	P	3004	CDL	C31-CA7-OA8-CA6
16	C	2004	CDL	OA9-CA7-OA8-CA6
16	P	3004	CDL	OA9-CA7-OA8-CA6
16	D	2003	CDL	C31-CA7-OA8-CA6
11	E	2005	PEE	O5-C30-O3-C3
11	R	3005	PEE	O5-C30-O3-C3
16	C	2004	CDL	OB9-CB7-OB8-CB6
16	P	3004	CDL	OB9-CB7-OB8-CB6
16	Q	3003	CDL	C31-CA7-OA8-CA6
11	A	2008	PEE	O4-C10-O2-C2
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	O4-C10-O2-C2
16	C	2004	CDL	OB7-CB5-OB6-CB4
16	P	3004	CDL	OB7-CB5-OB6-CB4
11	E	2005	PEE	C31-C30-O3-C3
11	R	3005	PEE	C31-C30-O3-C3
11	A	2008	PEE	C11-C10-O2-C2
20	P	3091	BOG	O5-C5-C6-O6
16	C	2004	CDL	C71-CB7-OB8-CB6
16	P	3004	CDL	C71-CB7-OB8-CB6
16	D	2003	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
20	P	3091	BOG	C4-C5-C6-O6
16	Q	3003	CDL	OA9-CA7-OA8-CA6
16	D	2003	CDL	C71-CB7-OB8-CB6
16	Q	3003	CDL	C71-CB7-OB8-CB6
16	D	2003	CDL	OB9-CB7-OB8-CB6
16	Q	3003	CDL	OB9-CB7-OB8-CB6
11	E	2005	PEE	C30-C31-C32-C33
11	R	3005	PEE	C30-C31-C32-C33
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
20	D	2009	BOG	O1-C1'-C2'-C3'
11	P	3007	PEE	C10-C11-C12-C13
20	Q	3009	BOG	O1-C1'-C2'-C3'
16	C	2004	CDL	CB2-OB2-PB2-OB5
16	D	2003	CDL	CB2-OB2-PB2-OB5
16	P	3004	CDL	CA2-OA2-PA1-OA5
16	P	3004	CDL	CB2-OB2-PB2-OB5
16	Q	3003	CDL	CB2-OB2-PB2-OB5
11	C	2007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C15-C16-C17-C18
11	R	3005	PEE	C42-C43-C44-C45
11	P	3007	PEE	C12-C13-C14-C15
11	E	2005	PEE	C42-C43-C44-C45
11	C	2007	PEE	C12-C13-C14-C15
18	C	2011	GOL	C1-C2-C3-O3
11	R	3005	PEE	C34-C35-C36-C37
11	P	3007	PEE	C15-C16-C17-C18
11	E	2005	PEE	C34-C35-C36-C37
11	R	3005	PEE	C21-C22-C23-C24
11	E	2005	PEE	C21-C22-C23-C24
11	R	3005	PEE	C10-C11-C12-C13
18	C	2011	GOL	O1-C1-C2-O2
16	D	2003	CDL	CB5-C51-C52-C53
16	Q	3003	CDL	CB5-C51-C52-C53
11	E	2005	PEE	C10-C11-C12-C13
16	D	2003	CDL	CB7-C71-C72-C73
11	C	2007	PEE	C20-C21-C22-C23
11	P	3007	PEE	C20-C21-C22-C23
11	C	2007	PEE	C11-C10-O2-C2
16	C	2004	CDL	OB5-CB3-CB4-OB6
16	Q	3003	CDL	CB7-C71-C72-C73
11	E	2005	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C35-C36-C37-C38
13	C	502	HEM	C4D-C3D-CAD-CBD
11	E	2005	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C4-O4P-P-O3P
16	C	2004	CDL	CA2-OA2-PA1-OA5
11	P	3007	PEE	C14-C15-C16-C17
16	C	2004	CDL	OA5-CA3-CA4-CA6
16	P	3004	CDL	OA5-CA3-CA4-CA6
11	C	2007	PEE	C11-C12-C13-C14
11	R	3005	PEE	C19-C20-C21-C22
11	R	3005	PEE	C35-C36-C37-C38
16	C	2004	CDL	CA3-CA4-CA6-OA8
16	P	3004	CDL	CA3-CA4-CA6-OA8
11	P	3007	PEE	C11-C12-C13-C14
18	C	2011	GOL	O2-C2-C3-O3
18	P	3011	GOL	O2-C2-C3-O3
11	C	2007	PEE	C14-C15-C16-C17
16	P	3004	CDL	OB5-CB3-CB4-OB6
11	C	2007	PEE	O2-C2-C3-O3
11	P	3007	PEE	O2-C2-C3-O3
16	Q	3003	CDL	C71-C72-C73-C74
11	C	2007	PEE	C41-C42-C43-C44
16	D	2003	CDL	C71-C72-C73-C74
11	E	2005	PEE	O3P-C1-C2-C3
11	R	3005	PEE	O3P-C1-C2-C3
16	C	2004	CDL	OB5-CB3-CB4-CB6
16	D	2003	CDL	OA5-CA3-CA4-CA6
16	P	3004	CDL	OB5-CB3-CB4-CB6
16	Q	3003	CDL	OA5-CA3-CA4-CA6
11	C	2007	PEE	O4-C10-O2-C2
11	P	3007	PEE	C41-C42-C43-C44
11	E	2005	PEE	O3P-C1-C2-O2
11	R	3005	PEE	O3P-C1-C2-O2
11	E	2005	PEE	C43-C44-C45-C46
16	C	2004	CDL	C1-CB2-OB2-PB2
16	P	3004	CDL	C1-CB2-OB2-PB2
13	C	502	HEM	C2D-C3D-CAD-CBD
11	P	3007	PEE	C11-C10-O2-C2
11	R	3005	PEE	C43-C44-C45-C46
20	D	2009	BOG	C2'-C3'-C4'-C5'
20	D	2091	BOG	O5-C5-C6-O6
11	C	2007	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
16	Q	3003	CDL	OA5-CA3-CA4-OA6
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C35-C36-C37-C38
11	R	3005	PEE	C14-C15-C16-C17
11	P	3007	PEE	O4-C10-O2-C2
11	P	3007	PEE	C40-C41-C42-C43
11	C	2007	PEE	C4-O4P-P-O3P
16	C	2004	CDL	CA3-OA5-PA1-OA2
16	P	3004	CDL	CA3-OA5-PA1-OA2
11	P	3007	PEE	C32-C33-C34-C35
11	E	2005	PEE	C4-O4P-P-O2P
11	R	3005	PEE	C4-O4P-P-O2P
16	C	2004	CDL	CA2-OA2-PA1-OA4
16	D	2003	CDL	CB2-OB2-PB2-OB4
16	P	3004	CDL	CA2-OA2-PA1-OA4
16	Q	3003	CDL	CB2-OB2-PB2-OB4
11	E	2005	PEE	C11-C12-C13-C14
11	E	2005	PEE	C14-C15-C16-C17
11	E	2005	PEE	C39-C40-C41-C42
16	D	2003	CDL	OA5-CA3-CA4-OA6
16	P	3004	CDL	OA5-CA3-CA4-OA6
11	C	2007	PEE	C40-C41-C42-C43
16	C	2004	CDL	OA6-CA4-CA6-OA8
16	P	3004	CDL	OA6-CA4-CA6-OA8
20	Q	3009	BOG	C2'-C3'-C4'-C5'
16	D	2003	CDL	O1-C1-CB2-OB2
11	C	2007	PEE	C32-C33-C34-C35
16	C	2004	CDL	OA5-CA3-CA4-OA6
11	P	3007	PEE	C4-O4P-P-O3P
16	D	2003	CDL	CA2-OA2-PA1-OA5
16	Q	3003	CDL	CA2-OA2-PA1-OA5
11	R	3005	PEE	C11-C12-C13-C14
11	P	3007	PEE	C1-C2-C3-O3
11	P	3007	PEE	C42-C43-C44-C45
11	R	3005	PEE	C39-C40-C41-C42
16	D	2003	CDL	C1-CA2-OA2-PA1
16	Q	3003	CDL	C1-CA2-OA2-PA1
13	P	501	HEM	CAA-CBA-CGA-O2A
16	Q	3003	CDL	O1-C1-CB2-OB2
13	C	501	HEM	CAA-CBA-CGA-O1A
11	C	2007	PEE	C42-C43-C44-C45
13	P	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C1-C2-O2-C10
11	R	3005	PEE	C1-C2-O2-C10
11	P	3007	PEE	C34-C35-C36-C37
13	P	502	HEM	CAD-CBD-CGD-O2D
20	P	2010	BOG	C4-C5-C6-O6
13	P	502	HEM	CAD-CBD-CGD-O1D
13	C	502	HEM	C2A-CAA-CBA-CGA
13	C	501	HEM	CAA-CBA-CGA-O2A
14	P	3001	IKR	O15-C16-C17-C20
11	R	3005	PEE	C17-C18-C19-C20
13	P	501	HEM	CAD-CBD-CGD-O2D
13	C	502	HEM	CAD-CBD-CGD-O2D
13	C	502	HEM	CAA-CBA-CGA-O2A
13	C	501	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAA-CBA-CGA-O1A
13	C	502	HEM	CAD-CBD-CGD-O1D
13	P	502	HEM	CAA-CBA-CGA-O2A
11	R	3005	PEE	C38-C39-C40-C41
13	C	502	HEM	CAA-CBA-CGA-O1A
16	D	2003	CDL	C72-C71-CB7-OB8
20	Q	3009	BOG	C1'-C2'-C3'-C4'
13	P	502	HEM	C2A-CAA-CBA-CGA
16	Q	3003	CDL	C72-C71-CB7-OB8
11	E	2005	PEE	C38-C39-C40-C41
16	P	3004	CDL	OA7-CA5-OA6-CA4
13	P	501	HEM	CAD-CBD-CGD-O1D
11	E	2005	PEE	C17-C18-C19-C20
11	R	3005	PEE	C23-C24-C25-C26
16	D	2003	CDL	CA2-C1-CB2-OB2
13	C	501	HEM	CAD-CBD-CGD-O1D
13	P	502	HEM	C4D-C3D-CAD-CBD
16	Q	3003	CDL	C72-C71-CB7-OB9
16	C	2004	CDL	OA7-CA5-OA6-CA4
16	D	2003	CDL	C72-C71-CB7-OB9
16	Q	3003	CDL	C52-C51-CB5-OB6
11	C	2007	PEE	C31-C32-C33-C34
11	E	2005	PEE	C1-O3P-P-O1P
11	R	3005	PEE	C1-O3P-P-O1P
16	C	2004	CDL	CA2-OA2-PA1-OA3
16	D	2003	CDL	CA3-OA5-PA1-OA3
16	P	3004	CDL	CA2-OA2-PA1-OA3
16	Q	3003	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O3-C30-C31-C32
11	R	3005	PEE	C33-C34-C35-C36
11	C	2007	PEE	C34-C35-C36-C37
16	D	2003	CDL	C52-C51-CB5-OB6
16	D	2003	CDL	CA4-CA3-OA5-PA1
16	Q	3003	CDL	C12-C11-CA5-OA6
16	Q	3003	CDL	C52-C51-CB5-OB7
16	D	2003	CDL	C52-C51-CB5-OB7

There are no ring outliers.

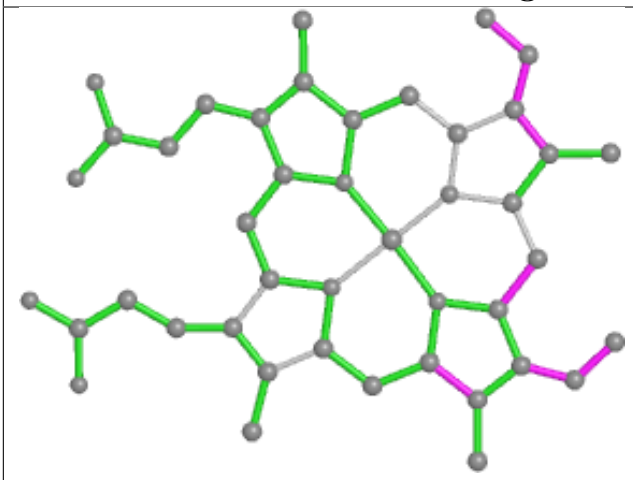
21 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	501	HEM	6	0
19	Q	501	HEC	2	0
13	C	502	HEM	13	0
13	P	501	HEM	9	0
15	C	2002	UQ	6	0
18	P	3011	GOL	1	0
16	P	3004	CDL	2	0
16	C	2004	CDL	2	0
16	Q	3003	CDL	3	0
13	P	502	HEM	11	0
14	C	2001	IKR	5	0
11	C	2007	PEE	3	0
11	P	3007	PEE	4	0
21	R	501	FES	2	0
15	P	3002	UQ	6	0
21	E	501	FES	3	0
16	D	2003	CDL	1	0
14	P	3001	IKR	4	0
20	D	2091	BOG	1	0
18	C	2011	GOL	1	0
19	D	501	HEC	2	0

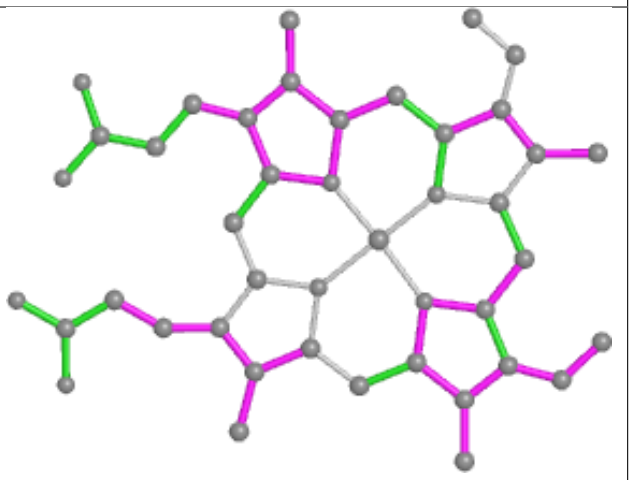
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

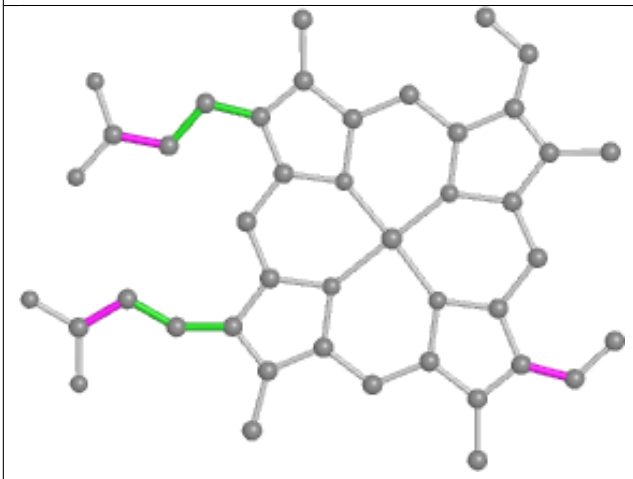
Ligand HEM C 501



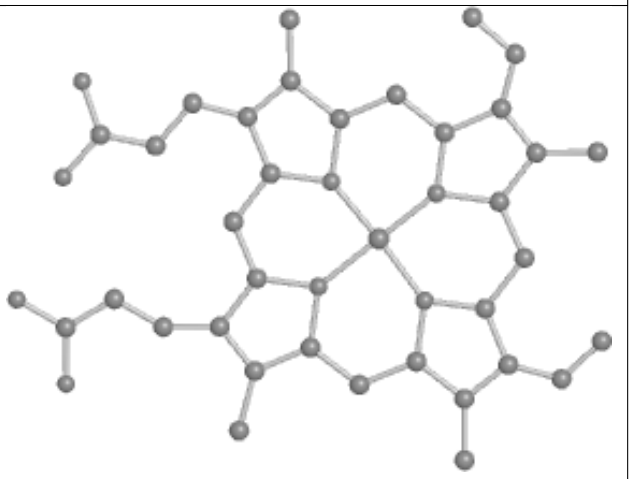
Bond lengths



Bond angles

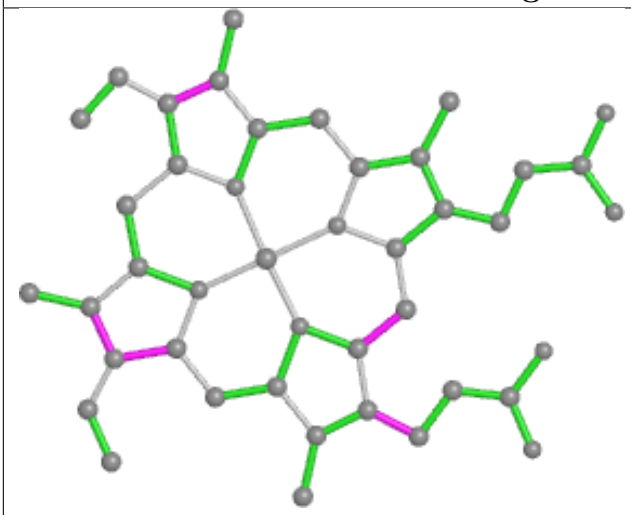


Torsions

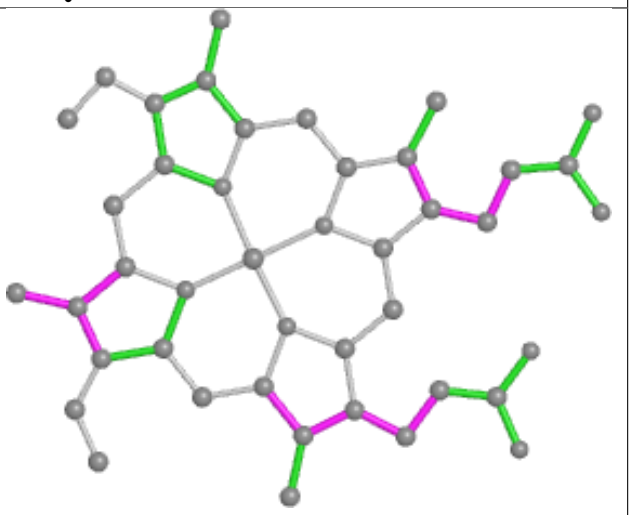


Rings

Ligand HEC Q 501



Bond lengths



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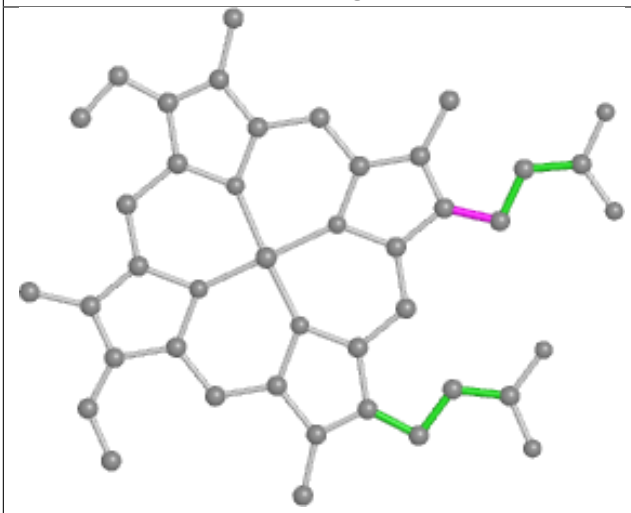

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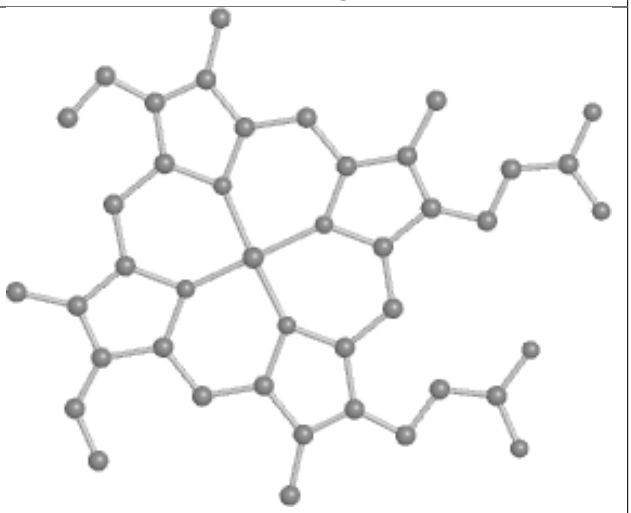

Rings

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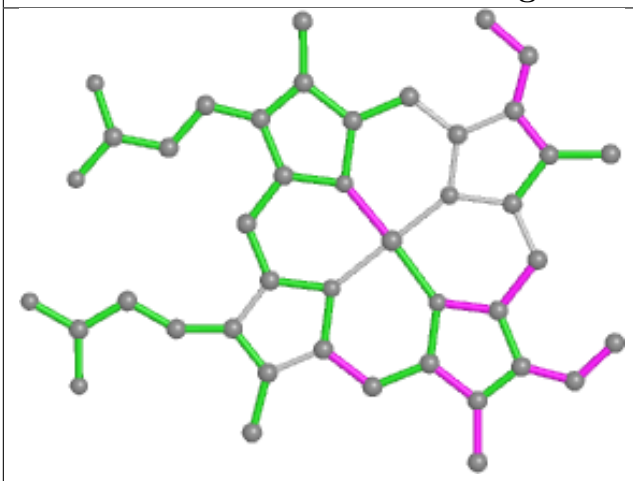

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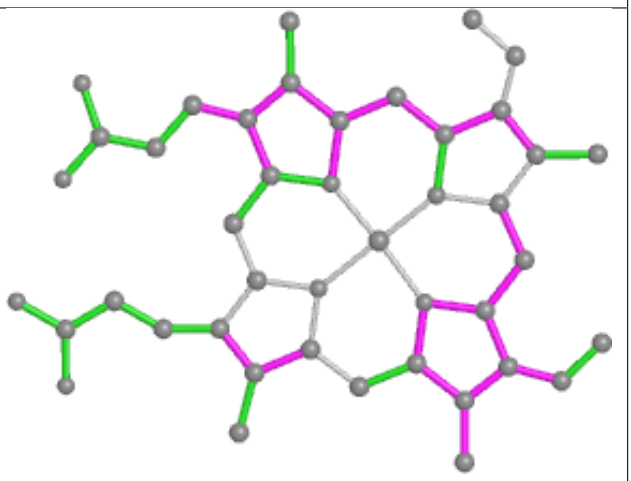

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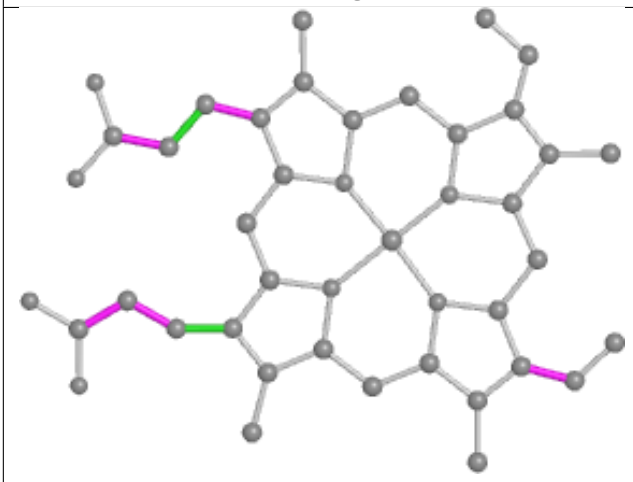

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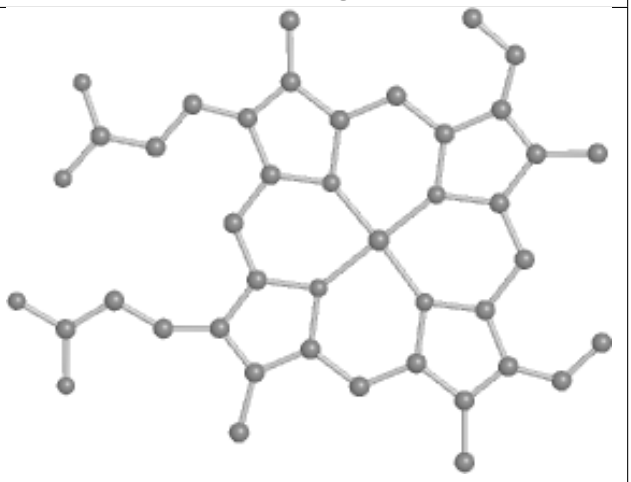
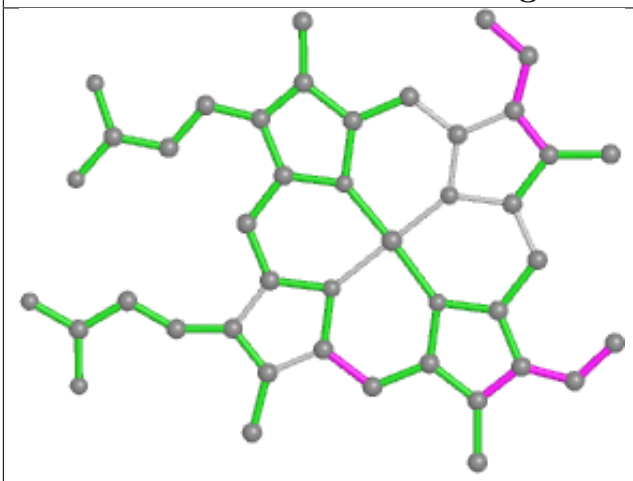


Rings

Ligand HEM P 501



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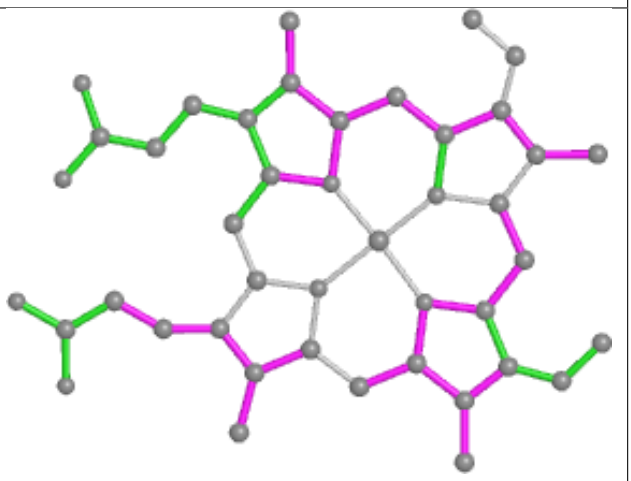

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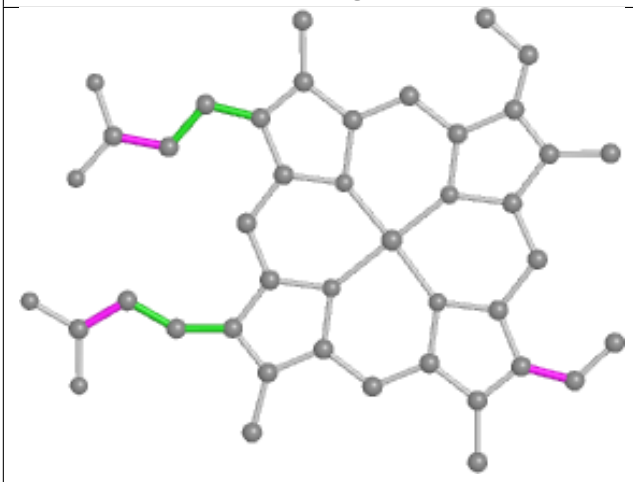

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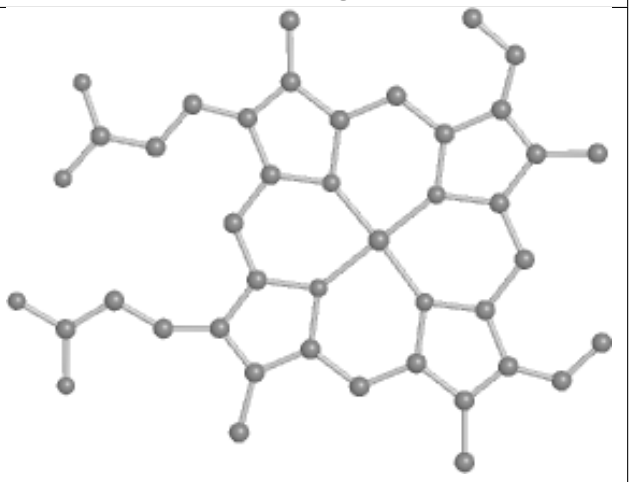
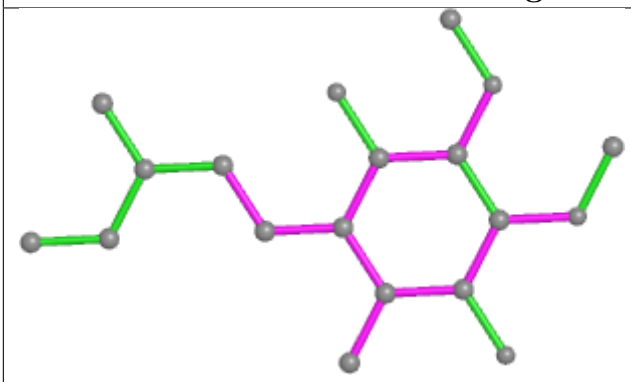


Rings

Ligand UQ C 2002



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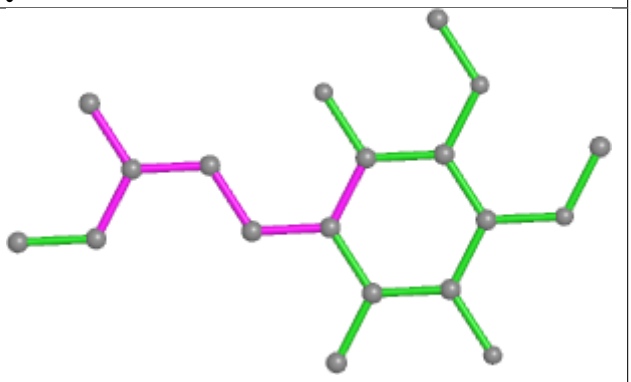

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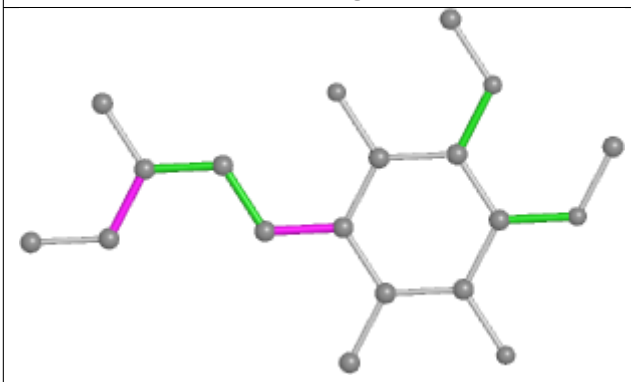

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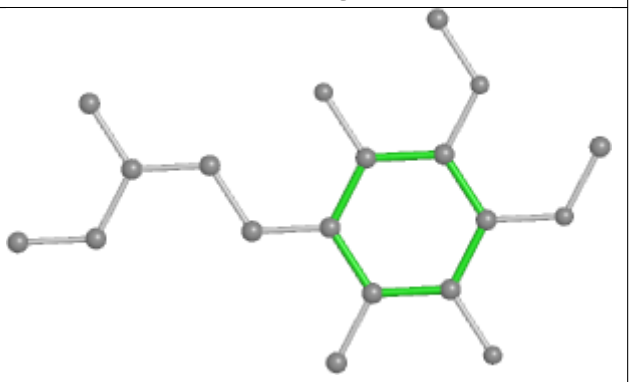

Rings

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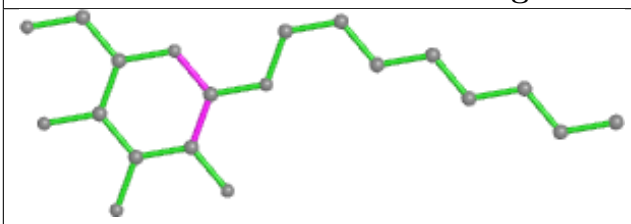

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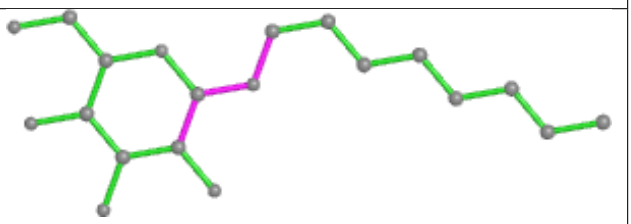

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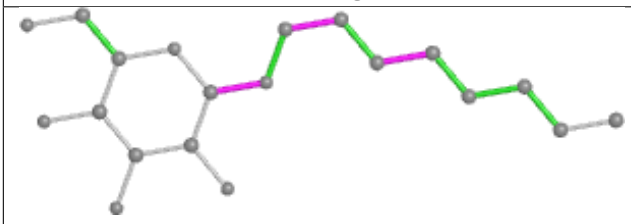

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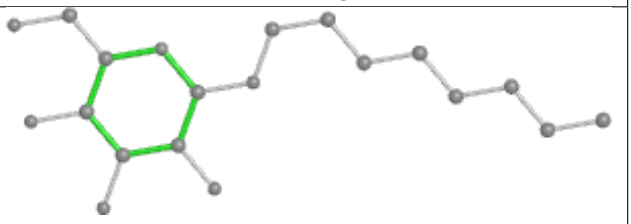
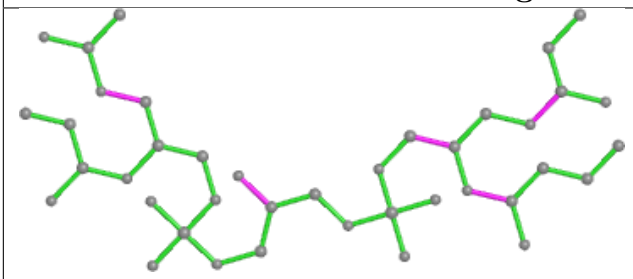


Rings

Ligand CDL P 3004



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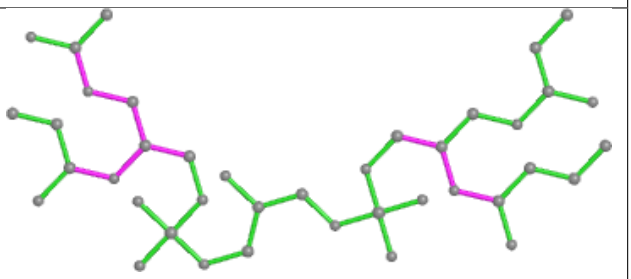

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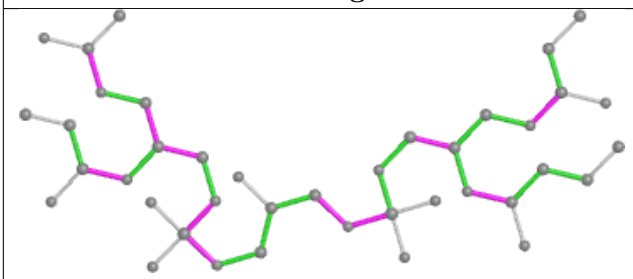

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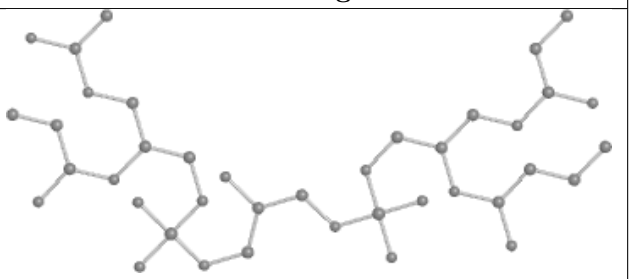
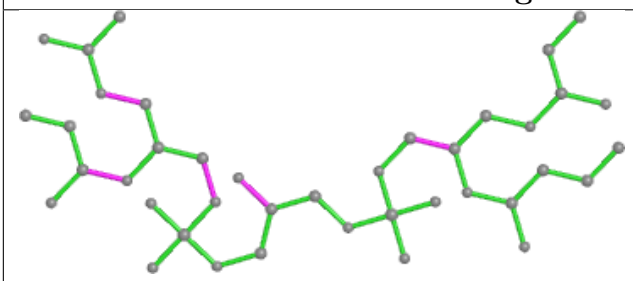


Rings

Ligand CDL C 2004



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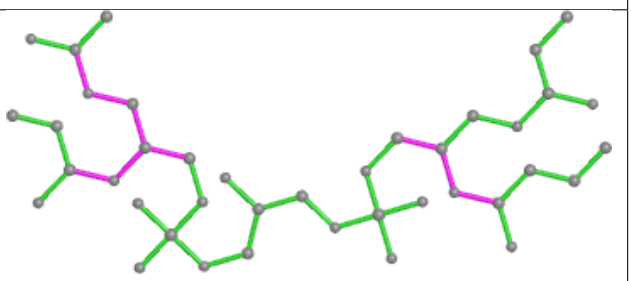

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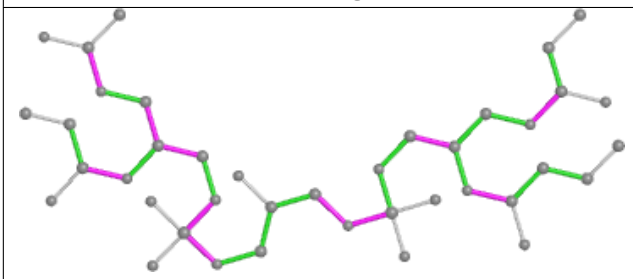

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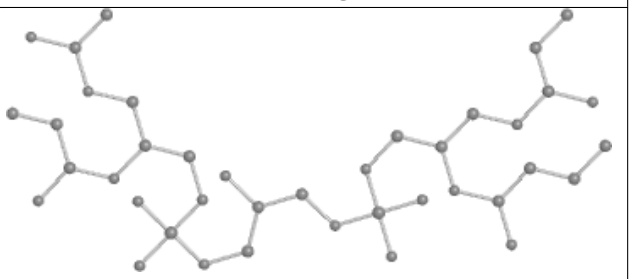
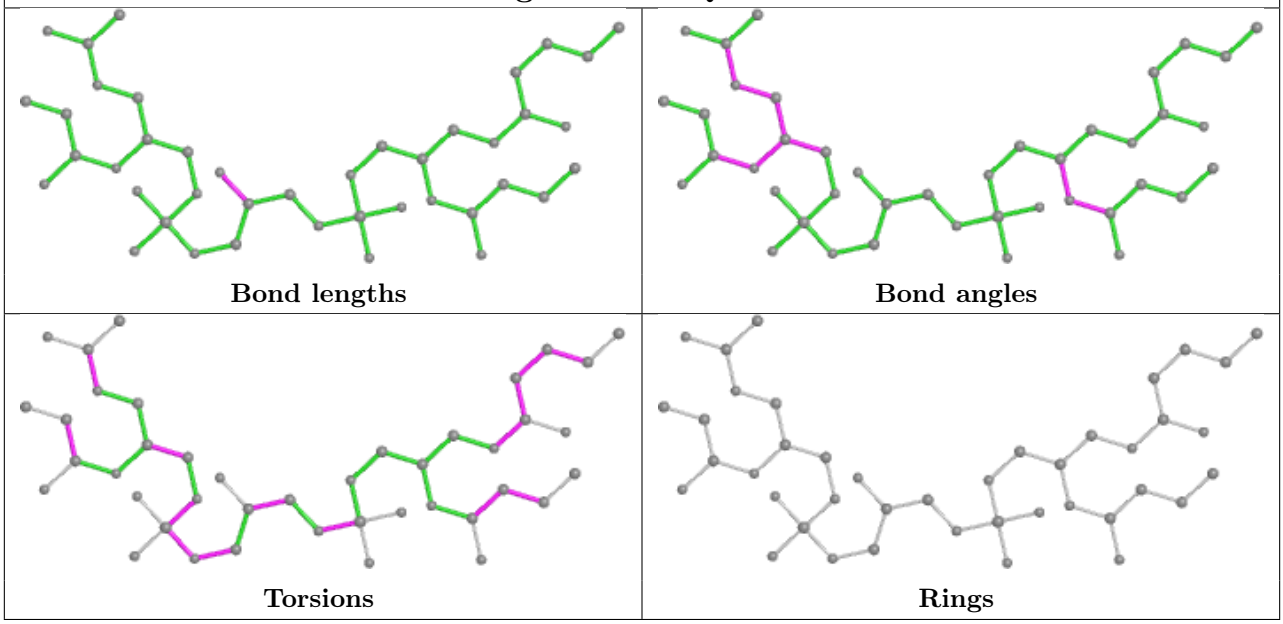
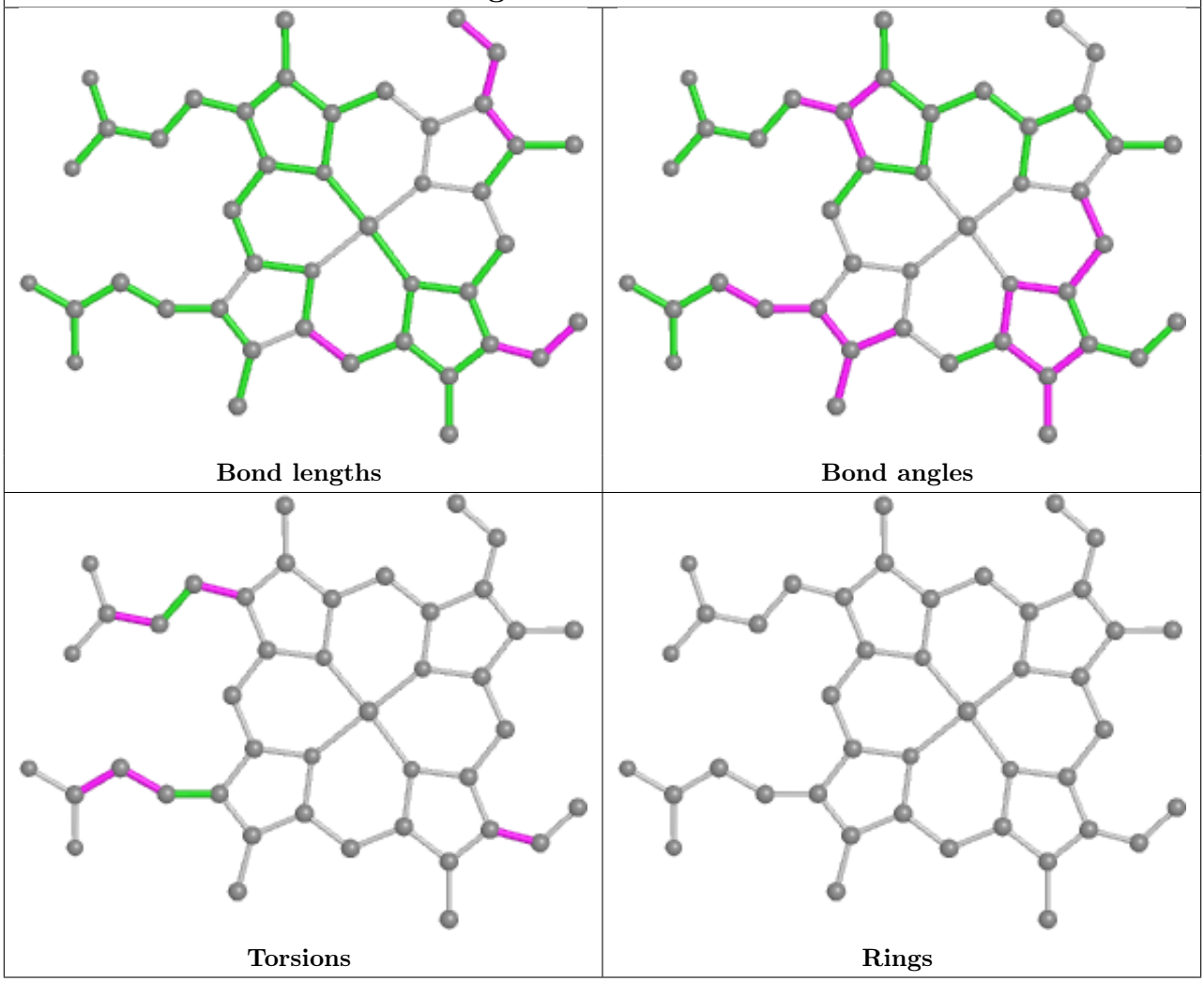


Rings

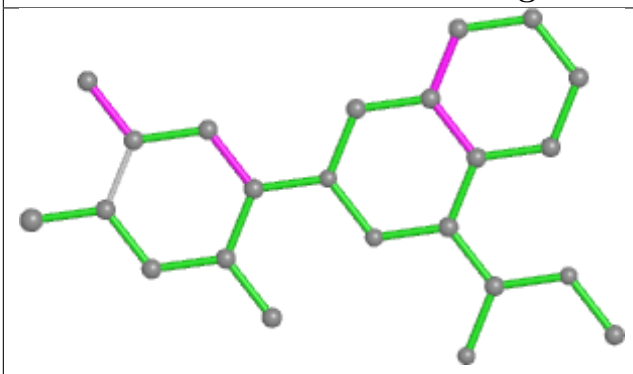
Ligand CDL Q 3003



Ligand HEM P 502



Ligand IKR C 2001



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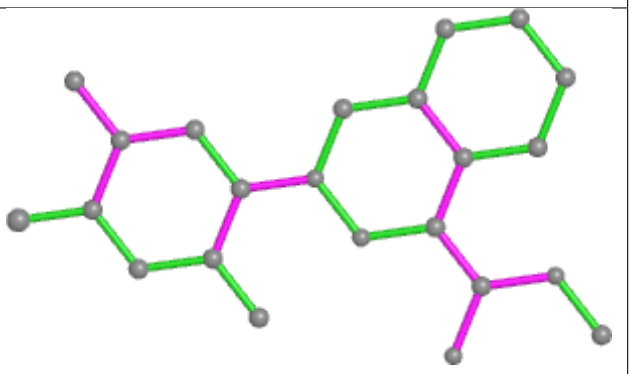
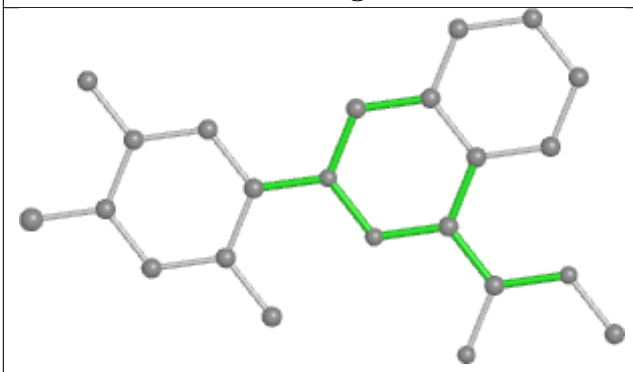


Bond angles



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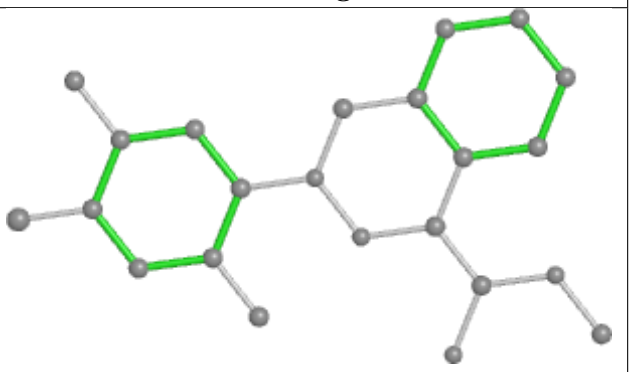
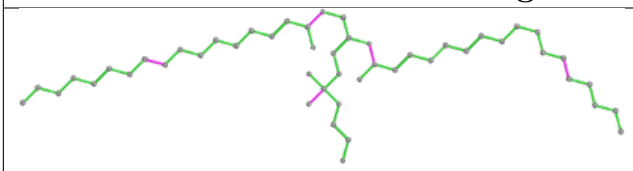


Rings

Ligand PEE C 2007



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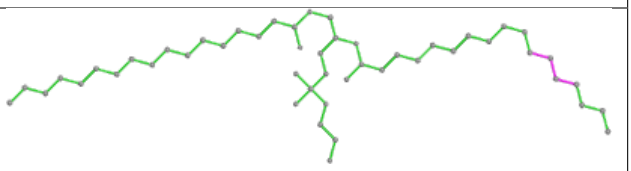

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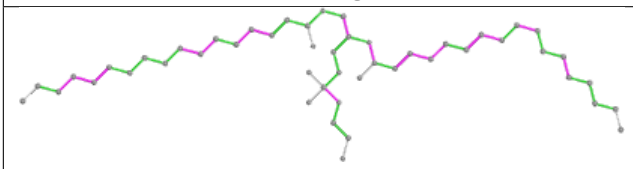

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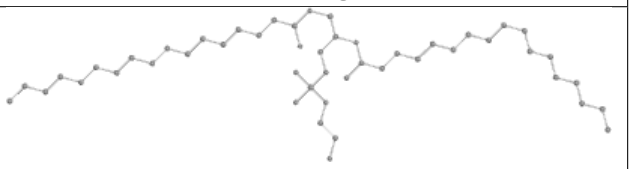
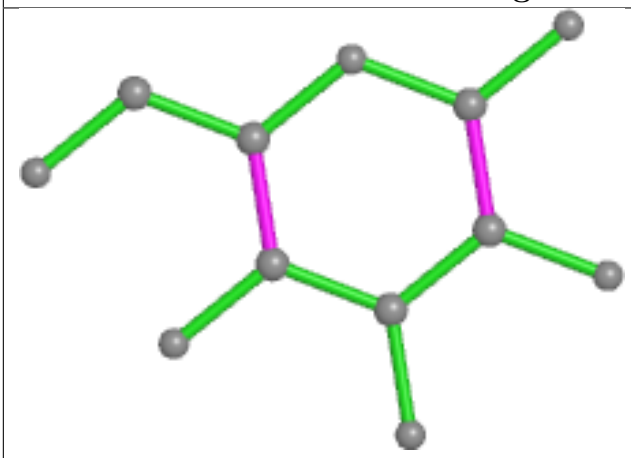


Rings

Ligand BOG P 2010



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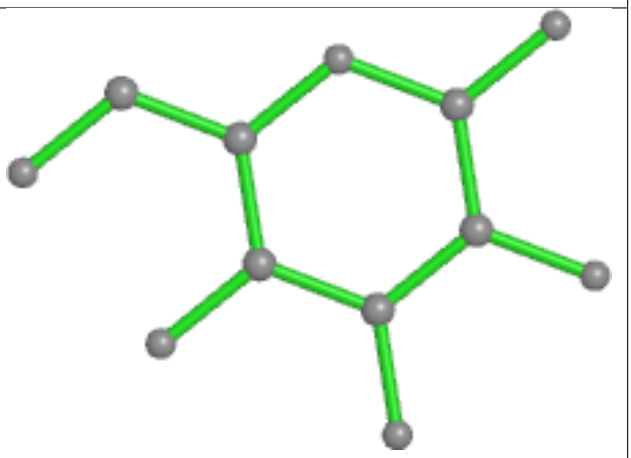
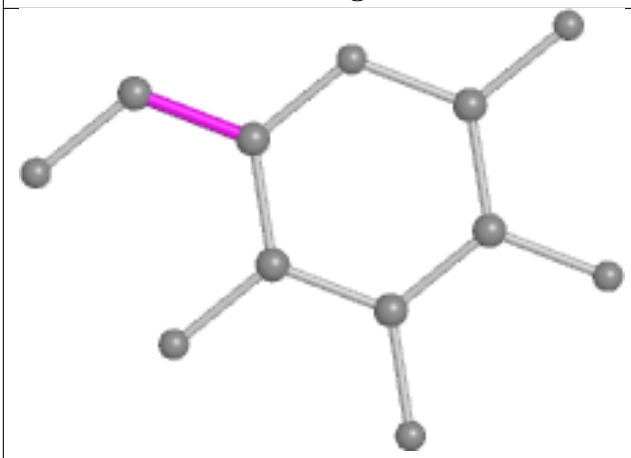
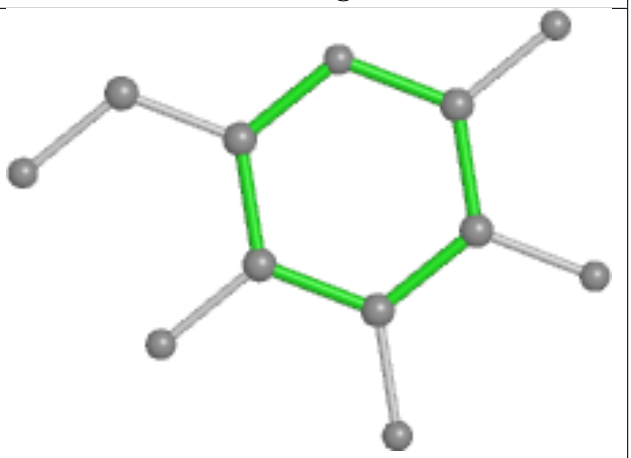


Bond angles

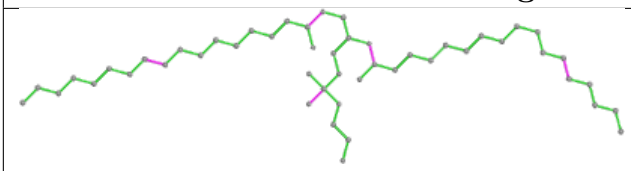


Torsions

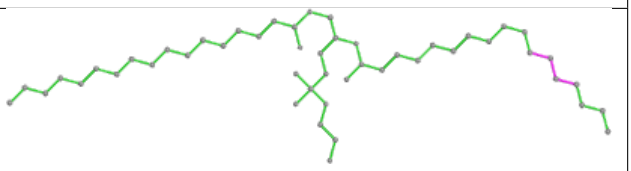


Rings

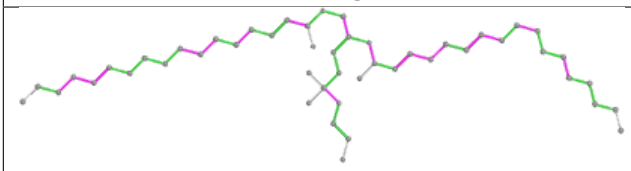
Ligand PEE P 3007



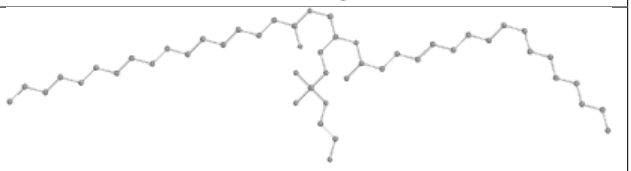
Bond lengths



Bond angles

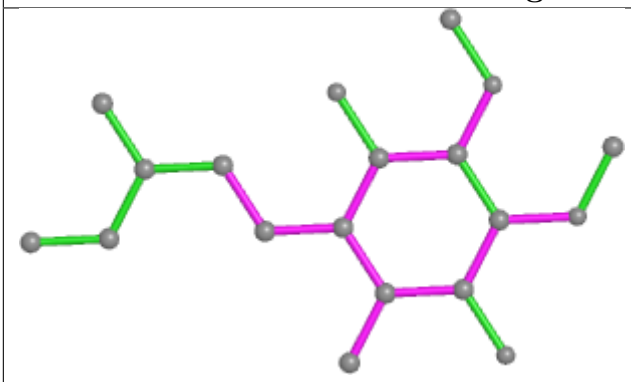


Torsions

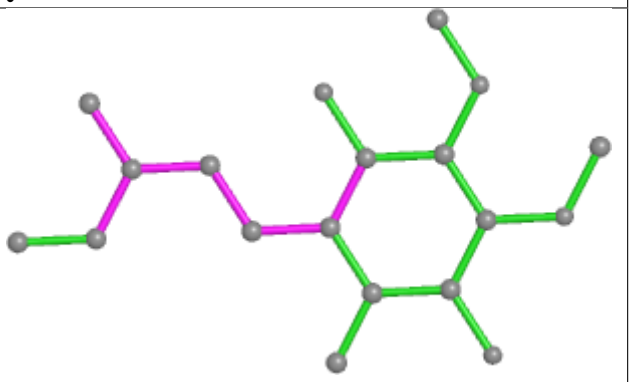


Rings

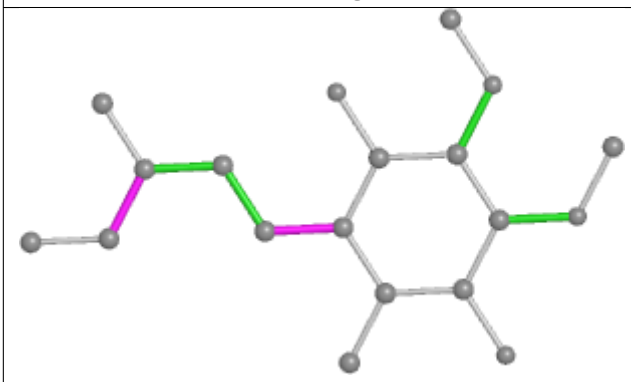
Ligand UQ P 3002



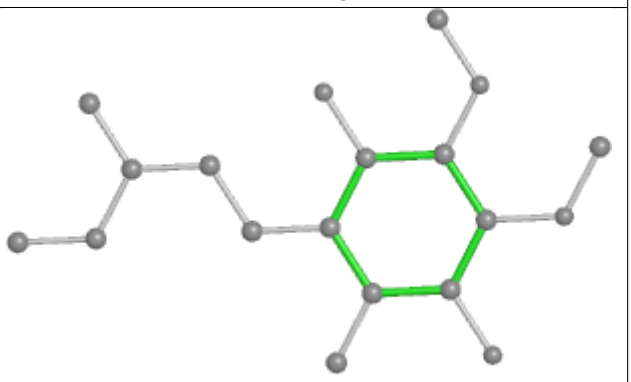
Bond lengths



Bond angles

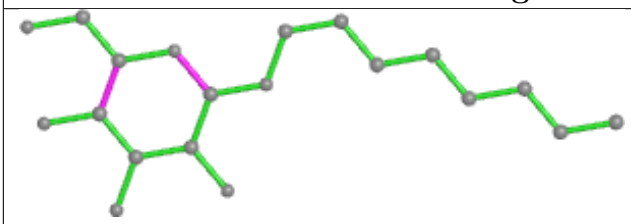


Torsions



Rings

Ligand BOG Q 3009



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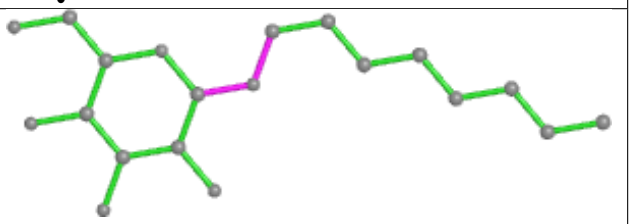
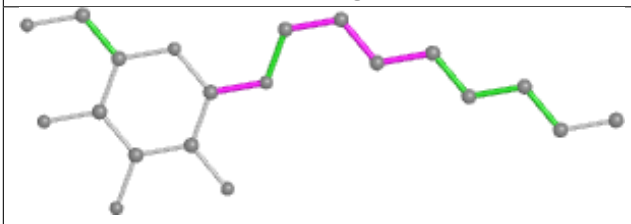
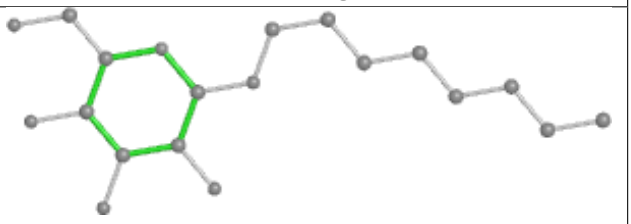


Bond angles

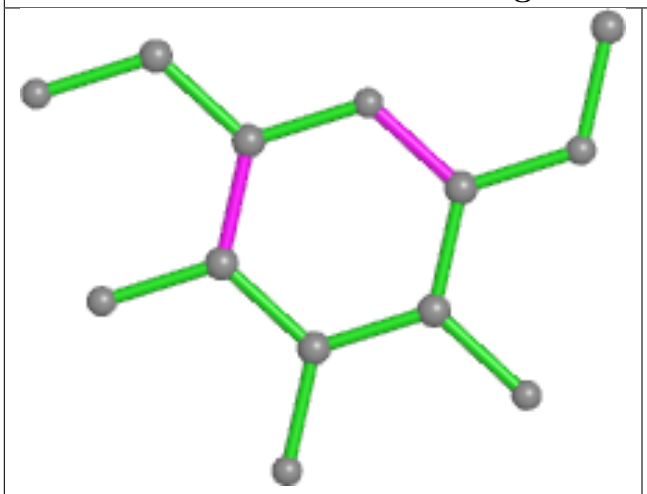


Torsions

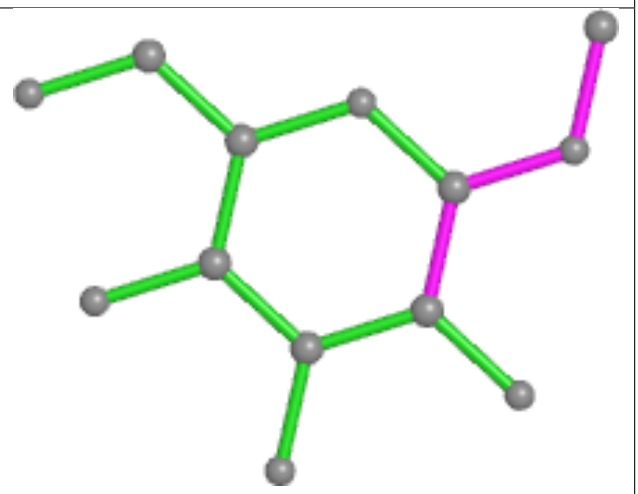


Rings

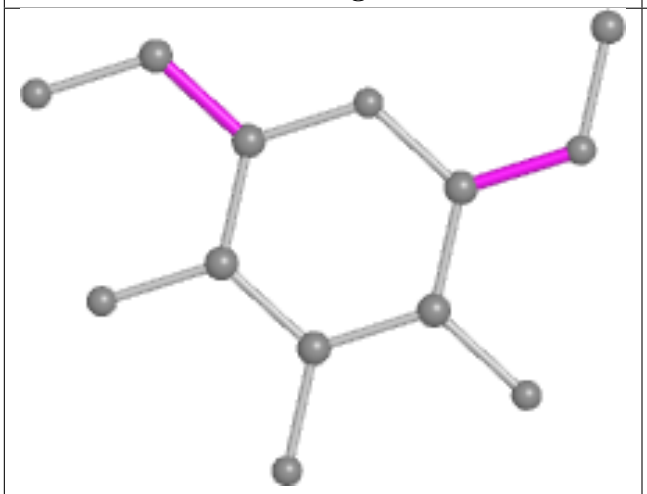
Ligand BOG P 3091



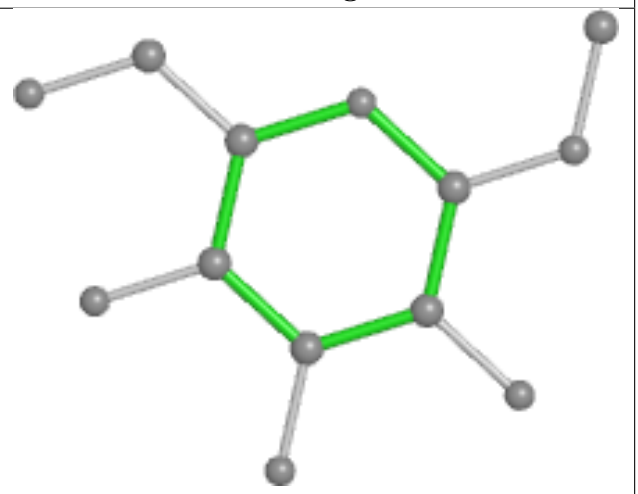
Bond lengths



Bond angles

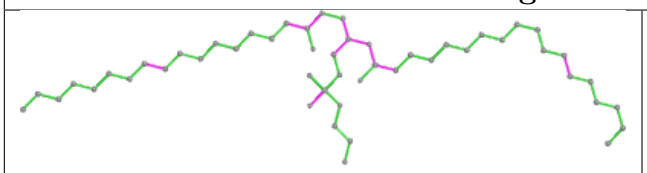


Torsions

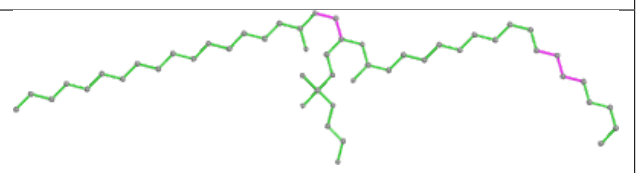


Rings

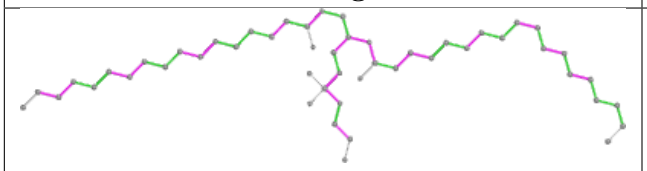
Ligand PEE E 2005



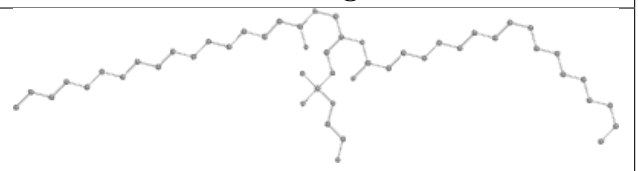
Bond lengths



Bond angles

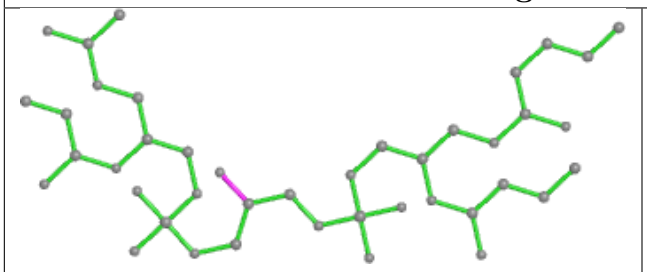


Torsions

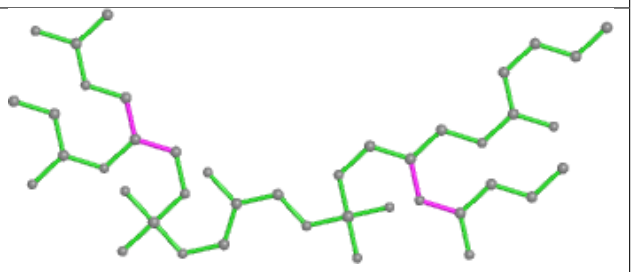


Rings

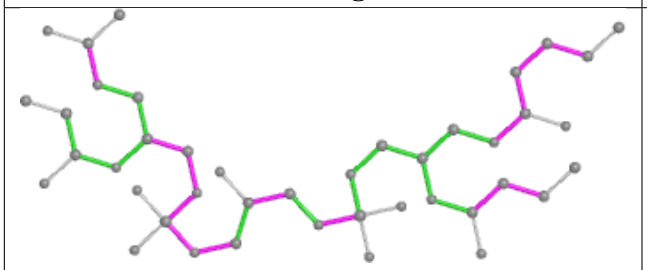
Ligand CDL D 2003



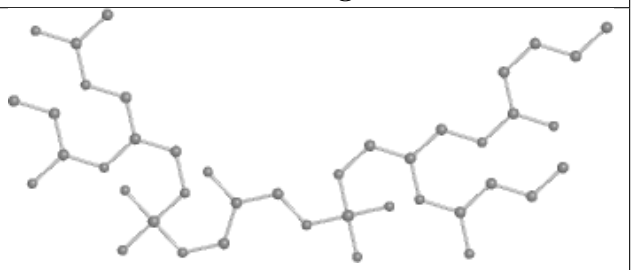
Bond lengths



Bond angles

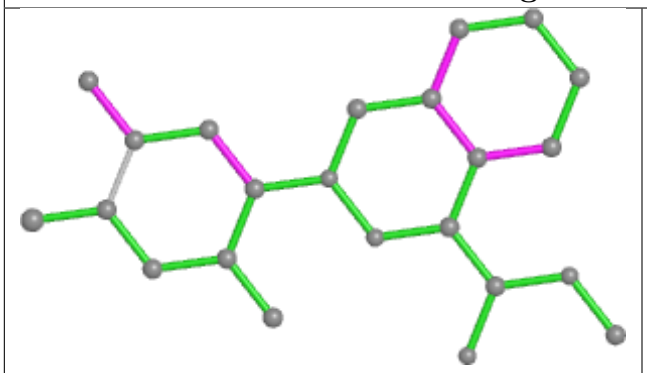


Torsions

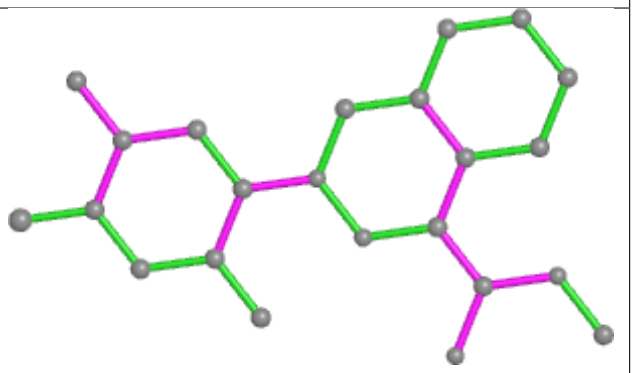


Rings

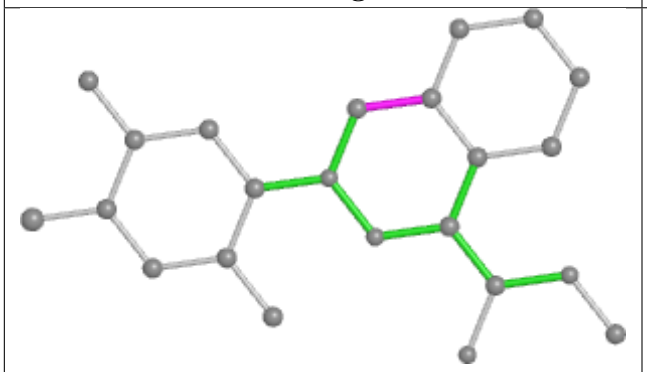
Ligand IKR P 3001



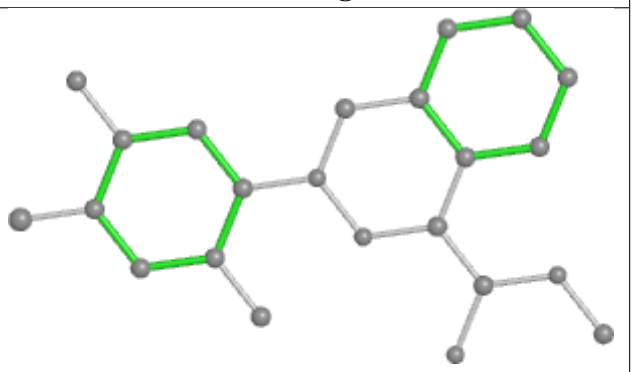
Bond lengths



Bond angles

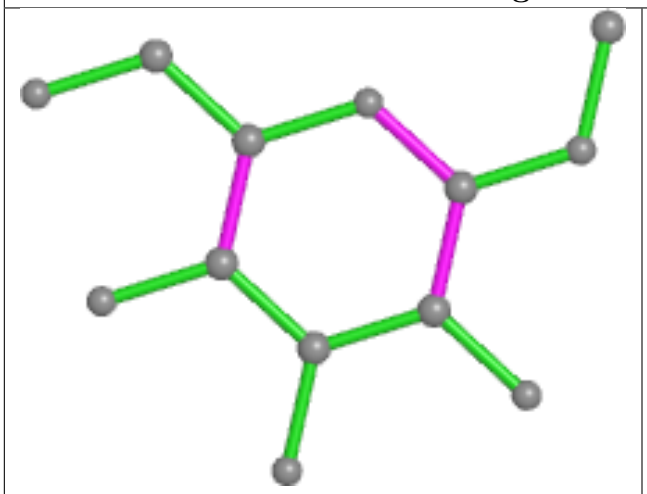


Torsions

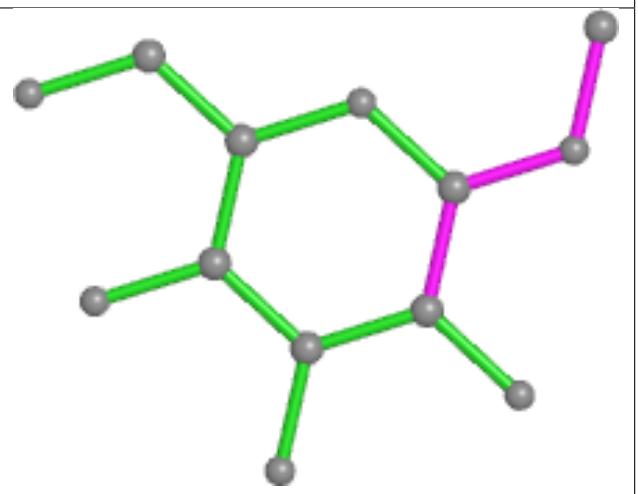


Rings

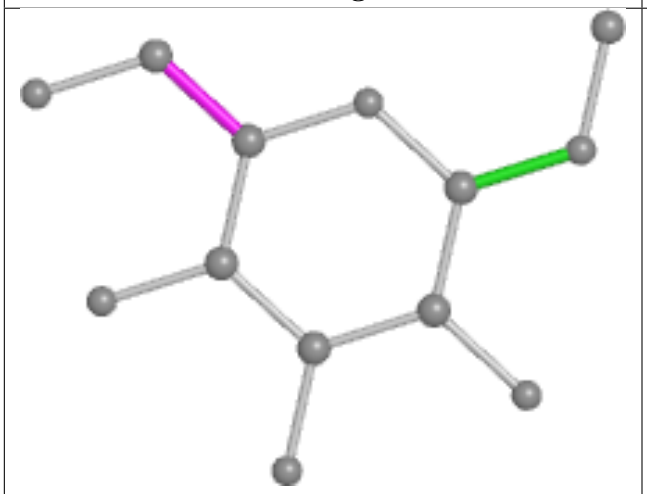
Ligand BOG D 2091



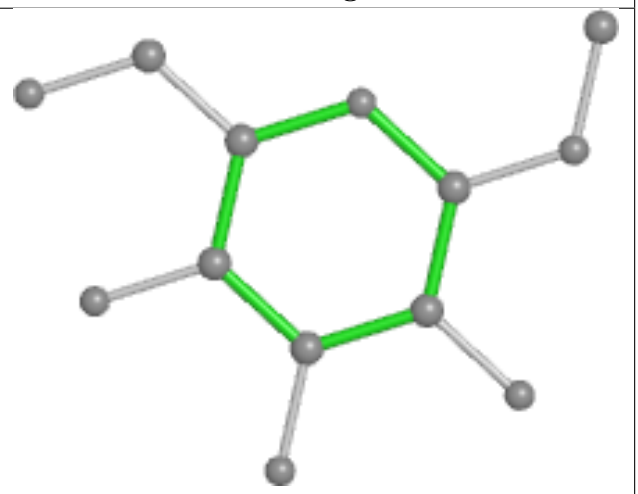
Bond lengths



Bond angles

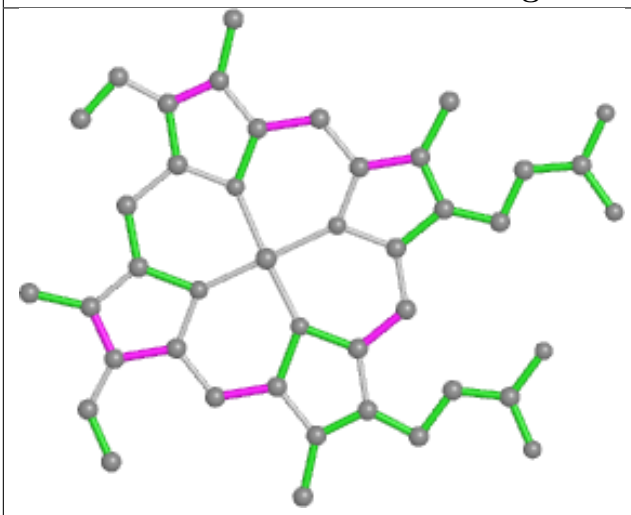


Torsions

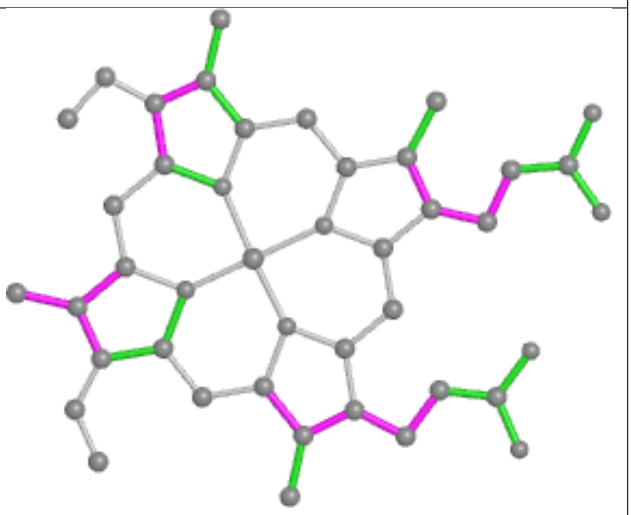


Rings

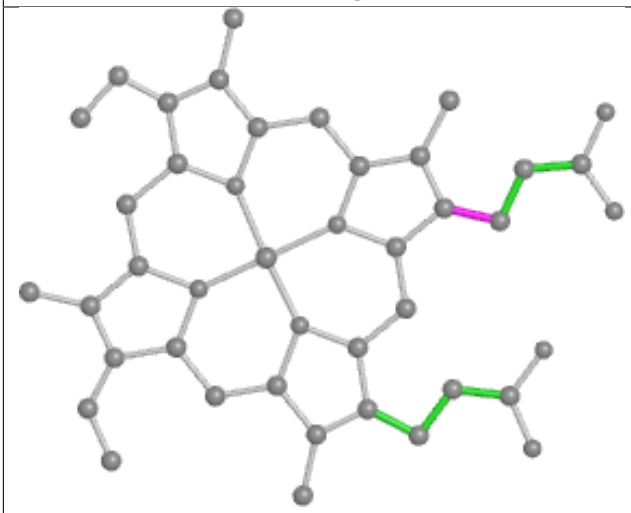
Ligand HEC D 501



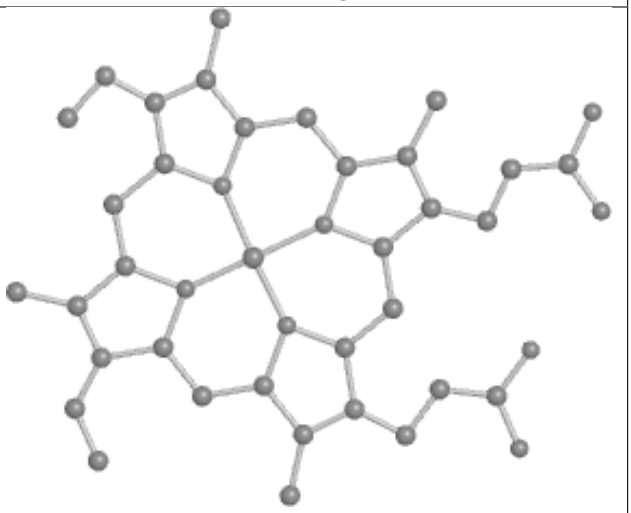
Bond lengths



Bond angles

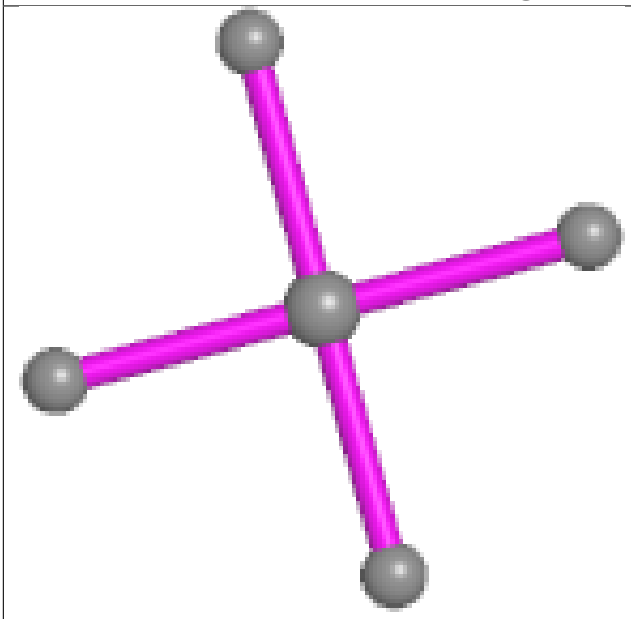


Torsions

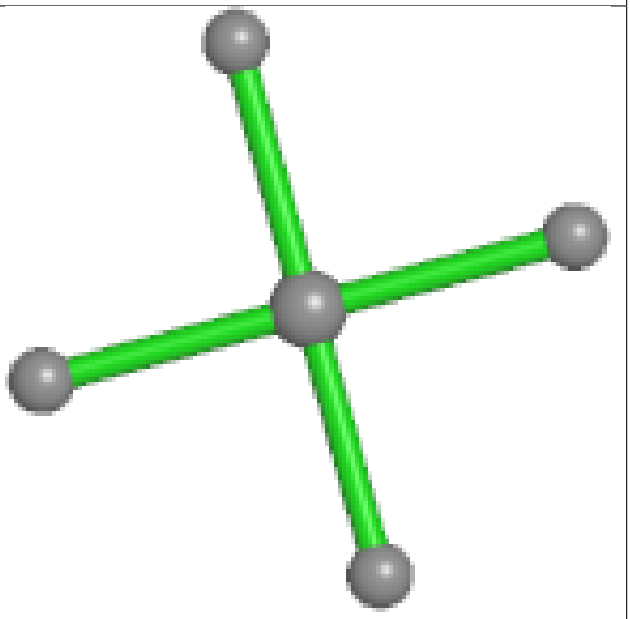


Rings

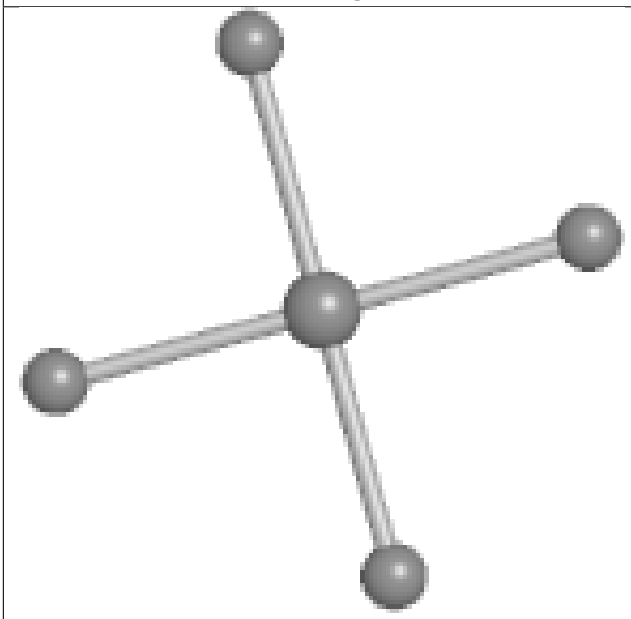
Ligand PEE P 3008



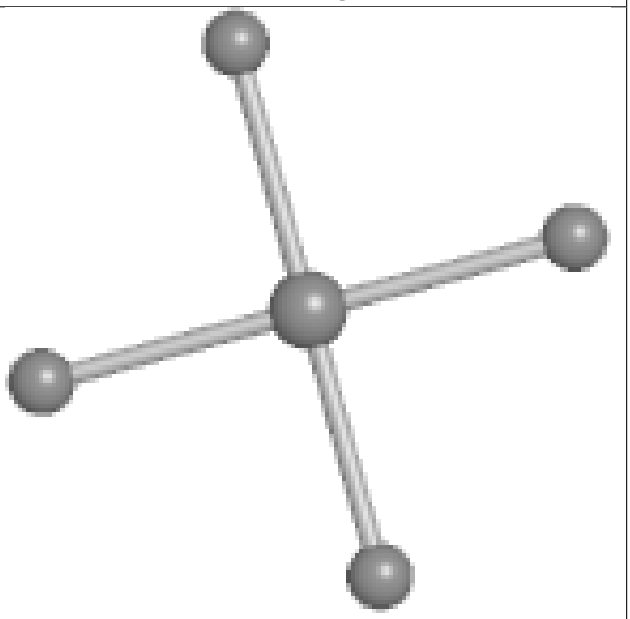
Bond lengths



Bond angles

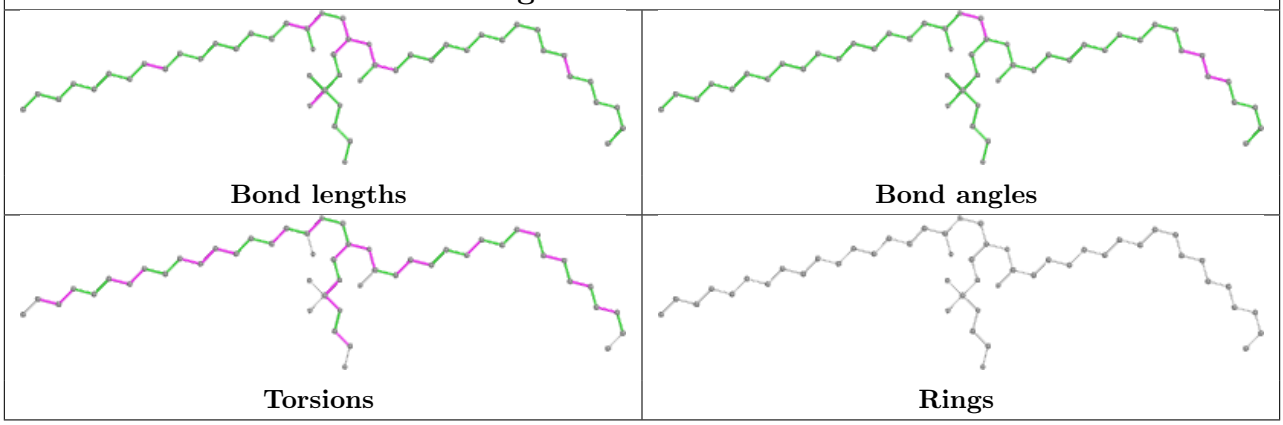


Torsions

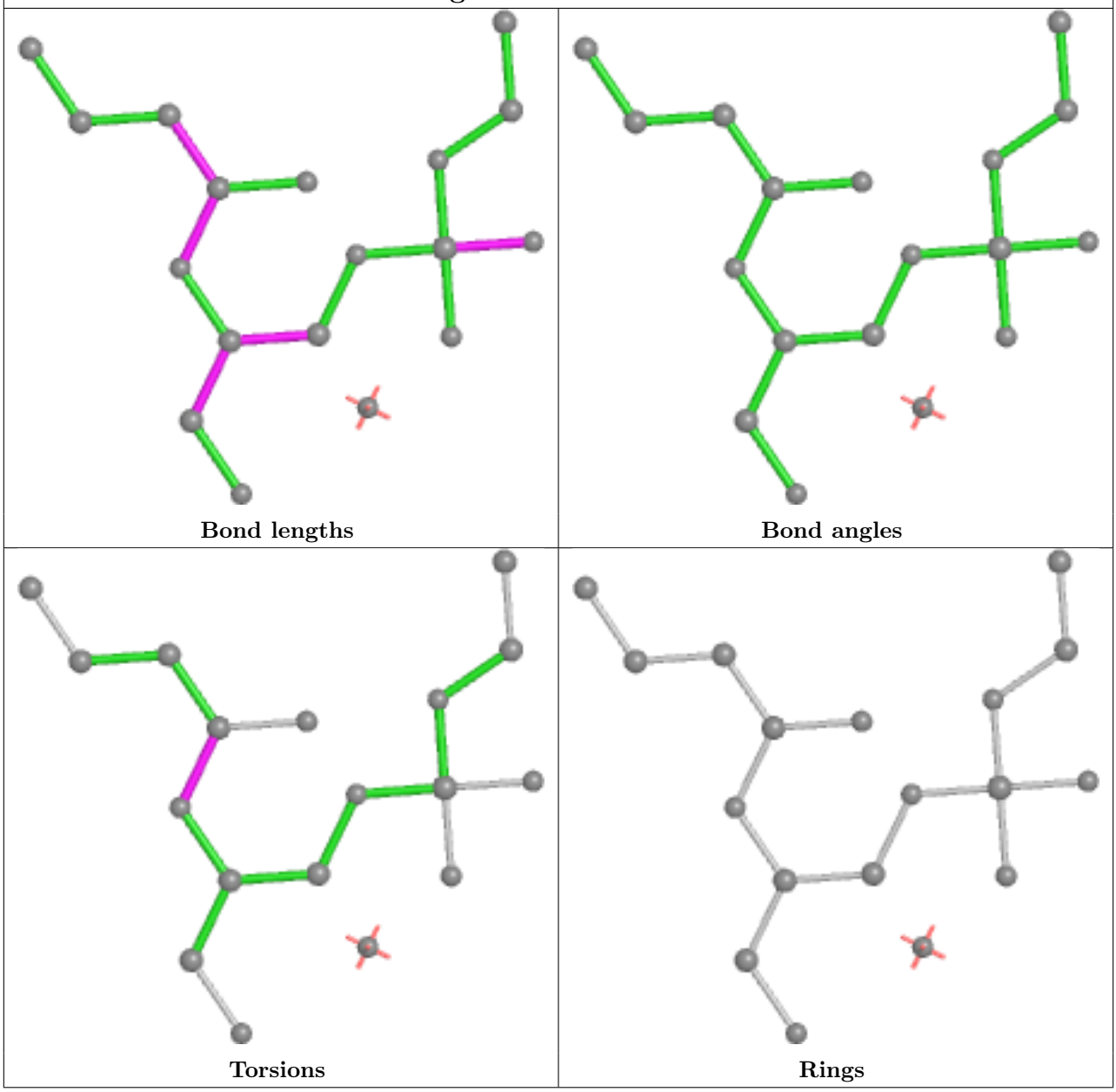


Rings

Ligand PEE R 3005



Ligand PEE A 2008



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.10	9 (2%)	65	61	56, 103, 147, 160	0
1	N	442/446 (99%)	-0.07	12 (2%)	54	51	65, 100, 132, 147	0
2	B	426/441 (96%)	0.20	20 (4%)	31	30	85, 126, 182, 218	0
2	O	422/441 (95%)	-0.05	11 (2%)	56	52	70, 108, 147, 161	0
3	C	380/380 (100%)	-0.30	9 (2%)	59	55	40, 64, 131, 204	0
3	P	379/380 (99%)	-0.12	13 (3%)	45	42	52, 97, 148, 187	0
4	D	241/241 (100%)	-0.23	6 (2%)	57	53	48, 72, 121, 138	0
4	Q	241/241 (100%)	-0.00	7 (2%)	51	48	74, 108, 149, 167	0
5	E	196/196 (100%)	2.70	94 (47%)	0	0	57, 214, 260, 262	125 (63%)
5	R	196/196 (100%)	1.20	52 (26%)	0	0	64, 183, 229, 234	1 (0%)
6	F	101/110 (91%)	-0.35	0	100	100	56, 75, 97, 116	0
6	S	101/110 (91%)	0.03	2 (1%)	65	61	87, 124, 174, 190	0
7	G	80/81 (98%)	0.07	4 (5%)	28	27	58, 86, 158, 166	0
7	T	79/81 (97%)	0.60	15 (18%)	1	1	81, 126, 222, 227	0
8	H	69/77 (89%)	-0.25	0	100	100	70, 98, 119, 154	0
8	U	67/77 (87%)	0.17	2 (2%)	50	47	133, 165, 209, 211	0
9	I	31/47 (65%)	3.40	16 (51%)	0	0	147, 185, 257, 259	0
9	V	31/47 (65%)	1.84	11 (35%)	0	0	121, 163, 242, 244	0
10	J	61/61 (100%)	0.10	2 (3%)	46	43	75, 93, 139, 177	0
10	W	60/61 (98%)	0.39	2 (3%)	46	43	84, 108, 157, 165	0
All	All	4046/4160 (97%)	0.18	287 (7%)	16	17	40, 104, 204, 262	126 (3%)

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	51	CYS	25.6
5	E	162	GLY	15.2
5	E	172	ARG	13.7
5	E	117	LEU	12.8
5	E	173	LYS	12.7
2	B	14	ARG	12.4
5	E	171	ILE	12.3
5	E	98	VAL	12.0
2	B	15	VAL	11.7
5	E	114	VAL	11.6
5	E	163	SER	11.6
5	E	115	SER	11.4
5	E	174	GLY	11.2
5	E	120	PRO	10.6
5	E	119	ASP	10.2
5	E	133	VAL	9.9
5	E	113	ASP	9.8
5	E	159	PRO	9.7
5	E	116	LYS	9.2
5	E	144	CYS	9.1
5	E	152	ASP	8.8
5	E	157	TYR	8.7
5	R	113	ASP	8.6
3	C	4	ASN	8.6
9	I	50	LEU	8.4
5	R	117	LEU	8.4
5	E	118	ARG	8.3
5	E	145	VAL	8.1
2	B	16	LYS	8.1
5	E	188	VAL	8.1
9	I	62	ARG	7.8
5	R	120	PRO	7.7
5	E	107	ASN	7.7
5	R	98	VAL	7.6
5	E	76	ILE	7.6
5	E	134	ILE	7.2
9	I	61	ARG	7.2
5	E	89	PHE	7.1
5	R	121	GLN	7.0
3	C	7	LYS	7.0
5	E	78	LEU	6.9
5	E	146	PRO	6.6
3	C	5	ILE	6.6

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
5	E	154	GLY	6.5
5	E	87	VAL	6.5
9	I	52	ARG	6.2
5	E	175	PRO	6.2
3	C	8	SER	6.1
3	P	8	SER	6.0
5	R	111	GLU	6.0
5	R	172	ARG	6.0
5	E	75	GLU	5.9
5	R	119	ASP	5.9
9	V	51	CYS	5.8
5	E	164	HIS	5.8
5	E	88	ALA	5.7
5	E	193	VAL	5.7
5	E	96	LEU	5.6
5	E	121	GLN	5.6
5	R	116	LYS	5.6
5	E	105	GLU	5.6
5	R	112	VAL	5.6
5	E	190	ASP	5.5
8	U	50	THR	5.5
5	E	168	SER	5.5
5	R	133	VAL	5.5
5	R	186	GLN	5.5
3	C	6	ARG	5.3
9	I	53	GLU	5.3
5	E	108	GLN	5.2
5	E	112	VAL	5.2
3	P	7	LYS	5.2
7	T	74	PRO	5.2
5	R	81	ILE	5.2
5	E	81	ILE	5.2
5	R	157	TYR	5.1
5	E	180	LEU	5.0
5	R	114	VAL	5.0
5	E	109	GLU	5.0
5	E	195	VAL	5.0
5	E	178	TYR	5.0
5	E	165	TYR	4.9
3	P	6	ARG	4.9
5	R	171	ILE	4.8
9	I	58	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
5	E	147	ILE	4.8
5	R	118	ARG	4.8
5	R	115	SER	4.7
5	R	122	HIS	4.7
5	E	158	CYS	4.6
5	E	132	TRP	4.6
5	E	160	CYS	4.6
4	D	1	GLY	4.6
9	I	54	SER	4.5
5	E	140	THR	4.4
5	E	156	TYR	4.4
3	C	2	ALA	4.3
3	P	4	ASN	4.3
5	R	97	PHE	4.3
5	R	193	VAL	4.3
2	B	216	LEU	4.2
7	T	75	ALA	4.2
5	E	100	HIS	4.2
9	V	50	LEU	4.2
9	V	53	GLU	4.1
7	T	73	ASN	4.1
7	T	3	HIS	4.1
5	R	146	PRO	4.1
5	E	99	ARG	4.1
7	T	2	ILE	4.1
5	E	97	PHE	4.0
5	E	151	GLY	4.0
5	E	176	ALA	4.0
5	E	77	LYS	3.9
5	E	153	PHE	3.9
5	R	76	ILE	3.9
9	V	49	LEU	3.9
5	R	132	TRP	3.9
10	J	64	GLU	3.9
5	E	79	SER	3.8
5	E	123	ASP	3.8
1	N	66	GLY	3.8
2	B	350	GLY	3.8
6	S	11	ARG	3.8
7	T	4	PHE	3.8
5	E	187	PHE	3.8
5	R	164	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	LYS	3.7
3	C	3	PRO	3.6
5	R	110	ALA	3.6
7	T	77	TYR	3.6
1	A	444	ILE	3.6
5	E	167	ALA	3.6
5	E	179	ASN	3.5
7	T	78	GLU	3.5
5	E	135	LEU	3.5
5	E	169	GLY	3.5
9	I	77	ARG	3.5
5	R	82	PRO	3.5
3	P	5	ILE	3.5
5	R	134	ILE	3.5
5	R	88	ALA	3.5
5	R	156	TYR	3.5
7	T	5	GLY	3.4
9	V	56	SER	3.4
5	R	165	TYR	3.4
7	T	6	ASN	3.4
1	A	197	LEU	3.3
5	E	122	HIS	3.3
5	R	96	LEU	3.3
10	J	63	GLU	3.3
3	P	156	TYR	3.3
5	R	127	VAL	3.3
5	E	82	PRO	3.3
5	E	196	GLY	3.3
9	V	63	ASP	3.2
2	O	19	PRO	3.2
5	R	85	LYS	3.2
2	O	38	LEU	3.2
5	R	108	GLN	3.2
5	E	192	LEU	3.2
5	E	189	GLY	3.1
3	P	29	SER	3.1
9	I	49	LEU	3.1
9	V	61	ARG	3.1
5	E	143	GLY	3.0
5	R	128	LYS	3.0
5	R	180	LEU	3.0
1	A	4	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	36	ALA	3.0
5	E	161	HIS	3.0
9	V	58	ARG	3.0
1	N	65	LYS	3.0
2	B	347	ALA	3.0
2	B	352	VAL	3.0
1	N	75	PHE	3.0
3	P	157	ILE	2.9
9	I	56	SER	2.9
9	V	52	ARG	2.9
7	T	71	ARG	2.9
9	I	47	ARG	2.9
7	T	72	LYS	2.9
2	B	396	SER	2.9
5	E	101	ARG	2.9
10	W	39	ALA	2.8
9	I	60	ALA	2.8
5	E	194	VAL	2.8
5	R	124	LEU	2.8
2	O	23	ASP	2.8
5	E	148	ALA	2.8
4	D	78	GLY	2.8
2	B	220	ALA	2.8
9	I	57	GLY	2.7
9	I	48	PRO	2.7
3	P	3	PRO	2.7
5	E	91	TRP	2.7
3	P	17	ASN	2.7
4	Q	105	ASN	2.7
3	P	21	ASP	2.7
5	E	102	THR	2.7
5	R	99	ARG	2.6
1	A	2	ALA	2.6
5	R	151	GLY	2.6
10	W	62	SER	2.6
5	E	111	GLU	2.6
5	E	141	HIS	2.6
2	B	282	GLY	2.6
5	R	125	ASP	2.6
2	B	17	LEU	2.6
2	B	35	ILE	2.6
5	R	84	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
9	V	62	ARG	2.6
4	D	3	LEU	2.6
1	A	25	VAL	2.5
2	O	108	CYS	2.5
5	E	186	GLN	2.5
5	R	90	LYS	2.5
4	D	77	ASN	2.5
5	E	80	ASP	2.5
7	T	62	GLY	2.5
2	B	206	LEU	2.5
7	G	3	HIS	2.5
3	C	1	MET	2.5
5	E	104	ALA	2.5
5	R	187	PHE	2.5
6	S	12	LEU	2.5
5	E	166	ASP	2.5
2	B	186	ILE	2.5
5	R	170	ARG	2.5
1	N	126	GLN	2.4
2	O	344	LEU	2.4
4	Q	139	ALA	2.4
1	N	62	LEU	2.4
5	E	90	LYS	2.4
7	G	4	PHE	2.4
5	E	177	PRO	2.4
5	R	86	ASN	2.4
1	A	196	VAL	2.4
2	B	349	GLN	2.3
5	E	86	ASN	2.3
5	R	130	PRO	2.3
3	P	13	LYS	2.3
4	Q	206	LEU	2.3
1	N	386	TYR	2.3
4	Q	108	ALA	2.3
4	D	79	GLU	2.3
1	A	26	ALA	2.3
5	E	110	ALA	2.3
7	T	79	ASN	2.3
5	R	1	VAL	2.3
5	E	83	GLU	2.2
5	R	179	ASN	2.2
1	N	179	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	283	PRO	2.2
5	R	107	ASN	2.2
4	Q	241	LYS	2.2
1	N	52	ASN	2.2
5	R	89	PHE	2.2
1	A	216	PHE	2.2
2	O	352	VAL	2.2
5	E	124	LEU	2.2
7	T	80	ASP	2.2
1	N	53	ASN	2.2
7	G	2	ILE	2.2
2	B	376	GLN	2.2
9	I	63	ASP	2.2
2	O	110	GLU	2.1
9	V	57	GLY	2.1
3	P	16	ASN	2.1
2	O	36	ALA	2.1
7	G	5	GLY	2.1
1	N	370	ASP	2.1
2	O	39	GLU	2.1
5	R	100	HIS	2.1
2	B	407	SER	2.1
5	E	155	GLY	2.1
3	C	157	ILE	2.1
5	E	191	ASP	2.1
2	B	33	LEU	2.1
2	O	22	GLU	2.0
4	Q	147	LEU	2.0
4	Q	146	GLY	2.0
4	D	80	LEU	2.0
8	U	13	LEU	2.0
2	O	41	PHE	2.0
1	N	177	LEU	2.0
1	N	16	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	BOG	P	3091	13/20	0.28	0.82	298,299,299,300	0
12	UNL	N	4231	1/-	0.34	0.59	90,90,90,90	0
20	BOG	P	2010	12/20	0.44	0.53	248,249,250,250	0
12	UNL	C	4234	1/-	0.53	0.99	58,58,58,58	0
20	BOG	D	2091	13/20	0.63	0.47	191,192,193,193	0
12	UNL	P	4236	1/-	0.67	0.71	94,94,94,94	0
11	PEE	A	2008	18/51	0.68	0.58	89,197,198,199	0
11	PEE	R	3005	50/51	0.69	0.47	114,131,139,141	0
16	CDL	Q	3003	42/100	0.72	0.43	183,193,208,208	0
16	CDL	P	3004	40/100	0.76	0.38	147,157,162,162	0
12	UNL	A	3231	1/-	0.78	0.77	45,45,45,45	0
11	PEE	E	2005	50/51	0.79	0.52	113,127,137,139	0
20	BOG	Q	3009	20/20	0.82	0.51	103,118,120,121	0
11	PEE	P	3008	5/51	0.84	0.38	184,184,184,185	0
12	UNL	A	3284	1/-	0.84	0.50	31,31,31,31	0
15	UQ	P	3002	19/63	0.86	0.35	134,146,148,149	0
16	CDL	D	2003	42/100	0.87	0.34	134,141,153,153	0
18	GOL	P	3011	6/6	0.88	0.30	103,108,109,110	0
11	PEE	P	3007	49/51	0.89	0.32	102,116,140,141	0
16	CDL	C	2004	40/100	0.90	0.28	103,110,126,128	0
20	BOG	D	2009	20/20	0.90	0.40	93,104,108,108	0
21	FES	R	501	4/4	0.90	0.06	201,201,201,202	0
15	UQ	C	2002	19/63	0.91	0.27	107,111,115,115	0
21	FES	E	501	4/4	0.93	0.36	257,257,257,257	4
18	GOL	C	2011	6/6	0.94	0.34	69,72,75,78	0
11	PEE	C	2007	49/51	0.94	0.24	68,80,102,104	0
17	ZN	C	2012	1/1	0.94	0.05	104,104,104,104	0
19	HEC	Q	501	43/43	0.96	0.21	87,91,97,99	0
14	IKR	P	3001	25/25	0.97	0.23	86,89,108,116	0
13	HEM	C	501	43/43	0.98	0.23	48,52,62,66	0
19	HEC	D	501	43/43	0.98	0.20	57,60,68,70	0
13	HEM	P	501	43/43	0.98	0.24	65,72,79,81	0

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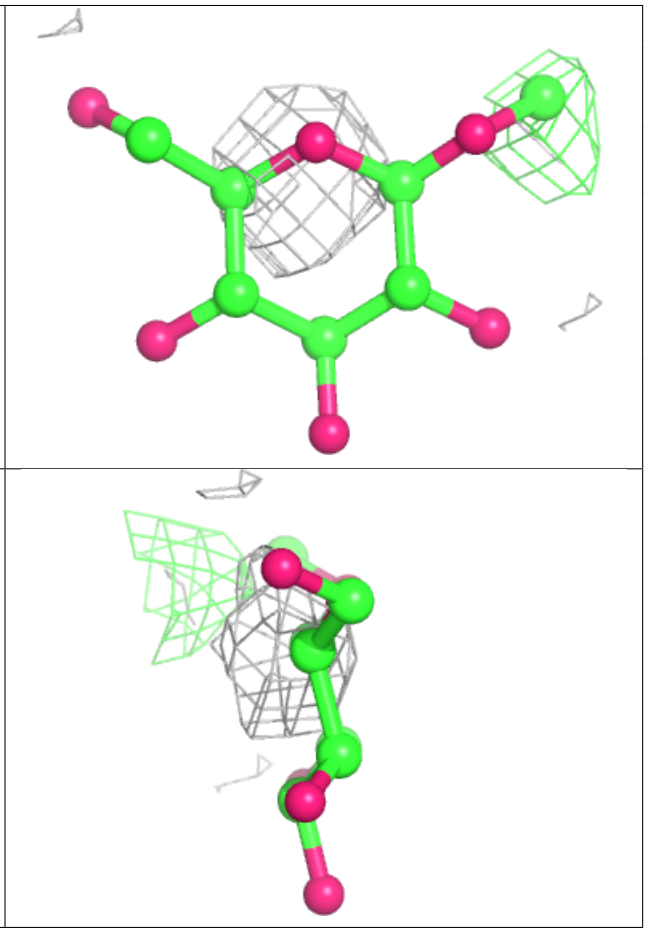
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	ZN	P	3012	1/1	0.98	0.04	121,121,121,121	0
13	HEM	P	502	43/43	0.98	0.20	68,73,82,82	0
13	HEM	C	502	43/43	0.99	0.21	41,46,56,61	0
14	IKR	C	2001	25/25	0.99	0.17	65,67,75,79	0

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.

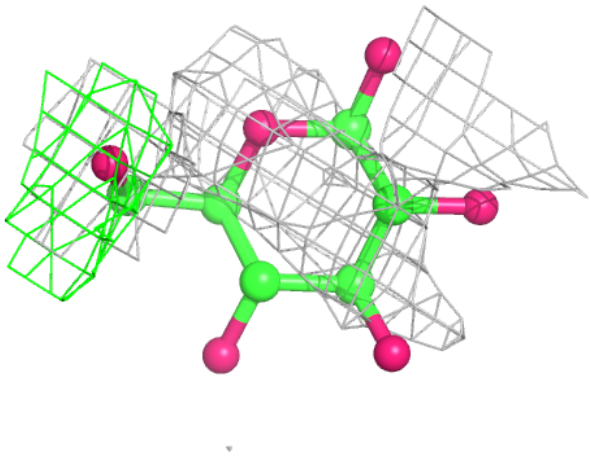
Electron density around BOG P 3091:

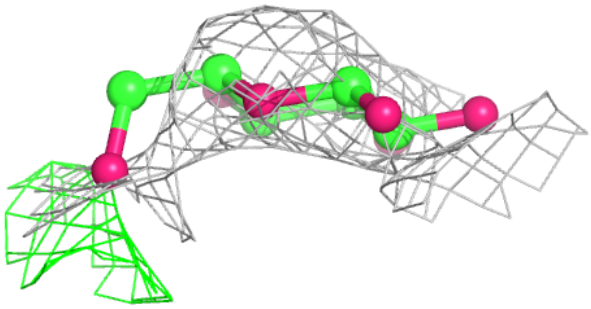
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

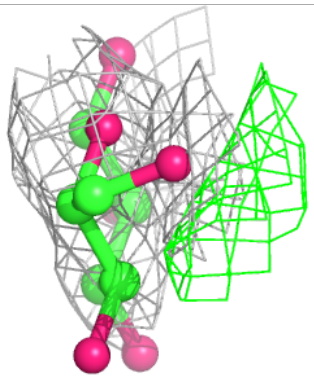


Electron density around BOG P 2010:

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

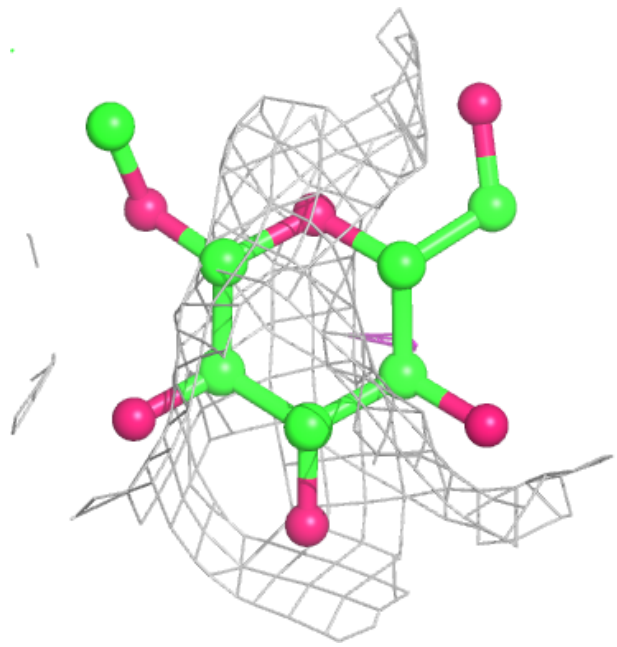


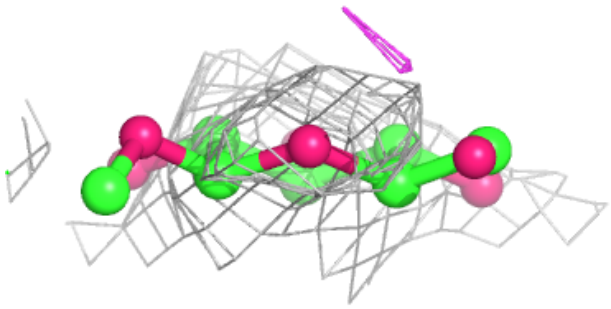


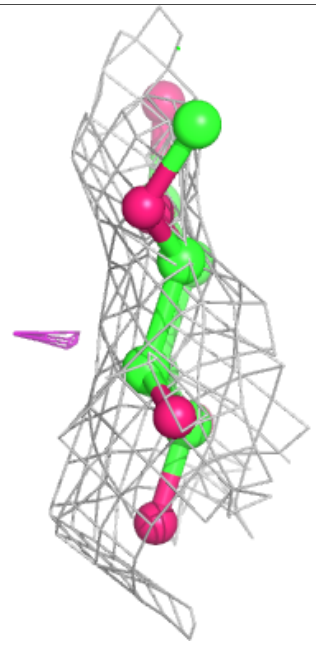


Electron density around BOG D 2091:

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

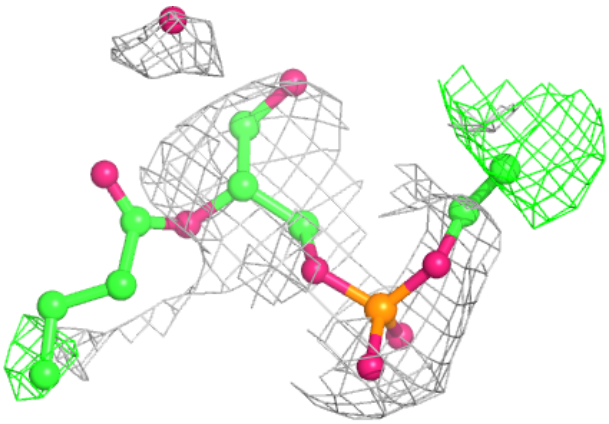


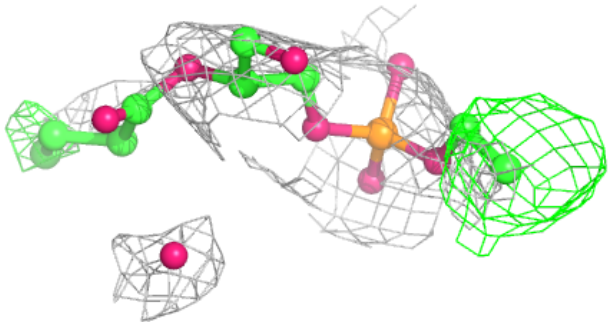


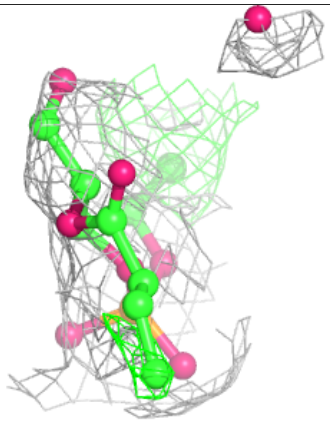


Electron density around PEE A 2008:

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

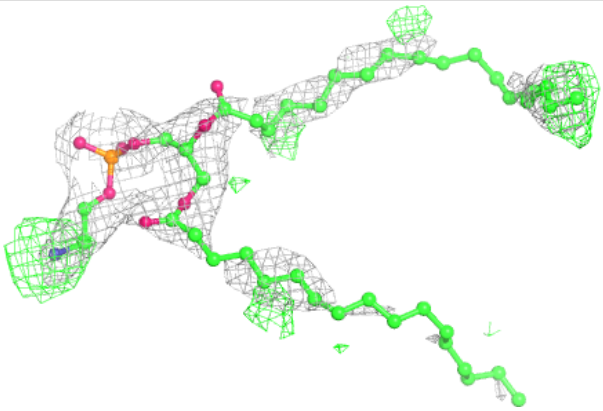


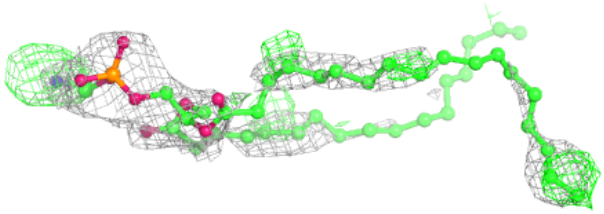


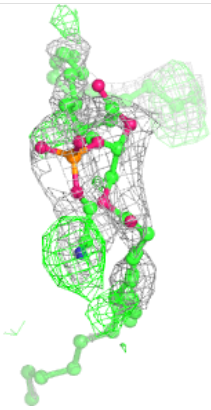


Electron density around PEE R 3005:

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

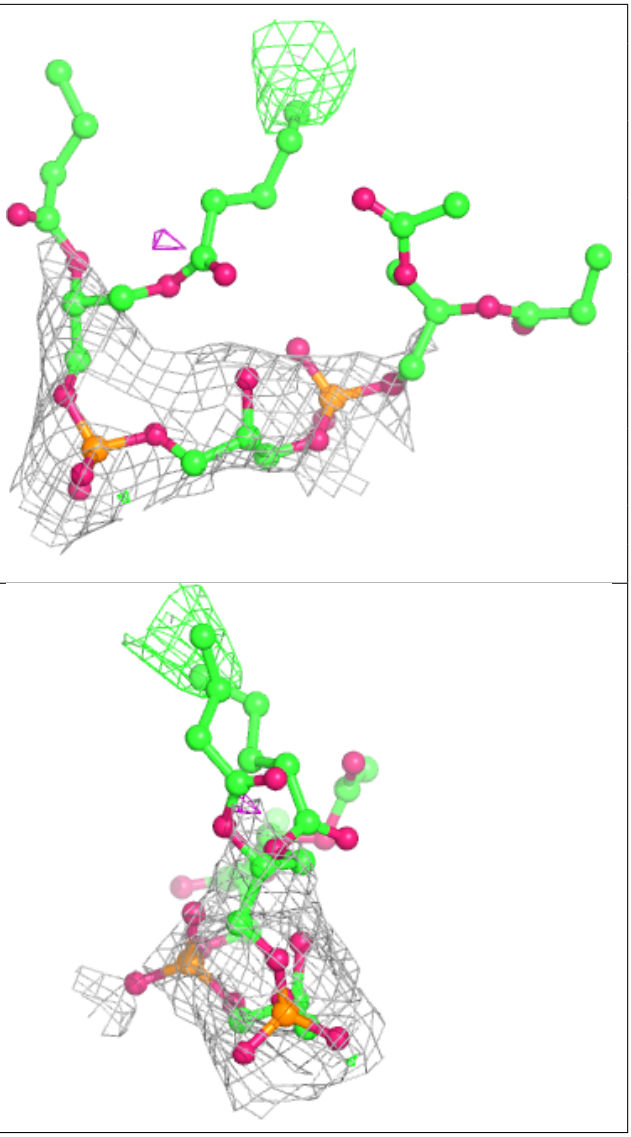






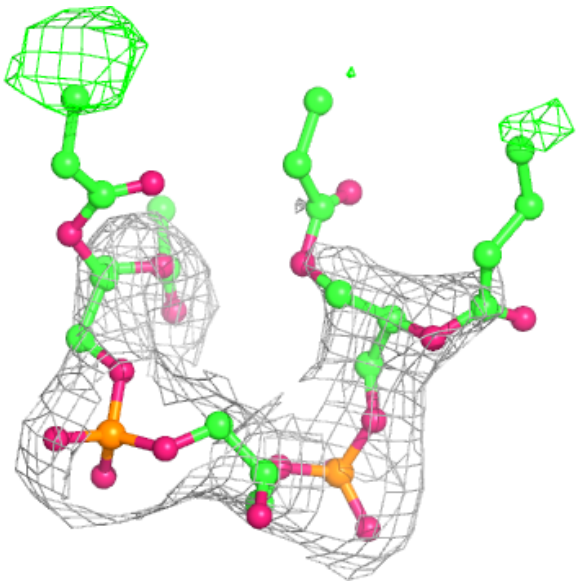
Electron density around CDL Q 3003:

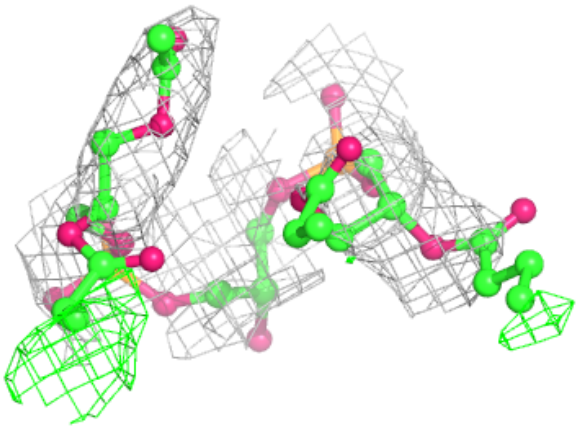
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

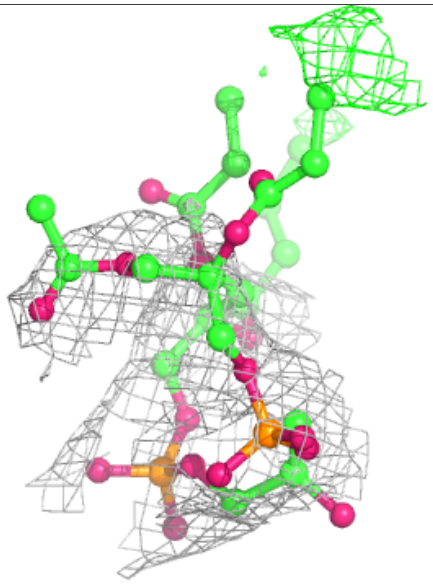


Electron density around CDL P 3004:

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

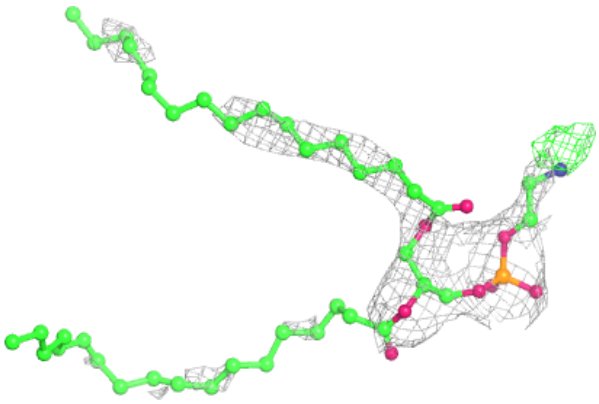


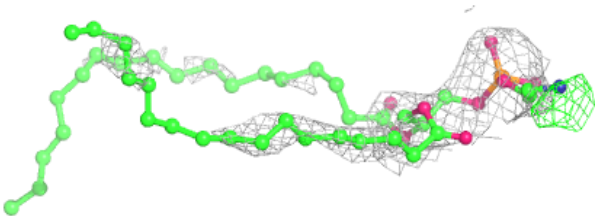


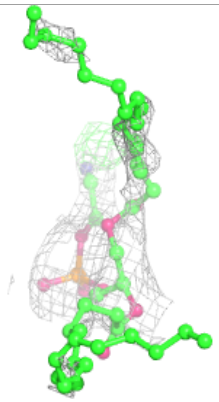


Electron density around PEE E 2005:

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

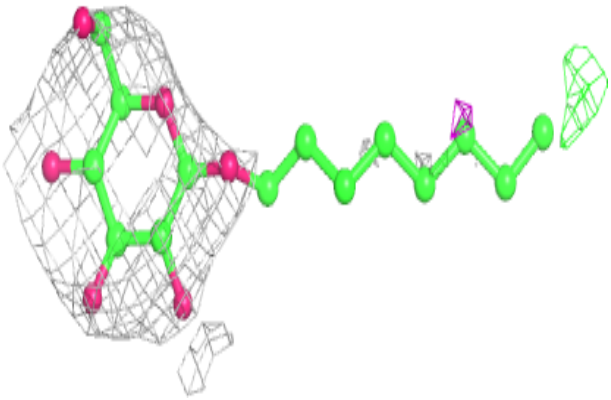


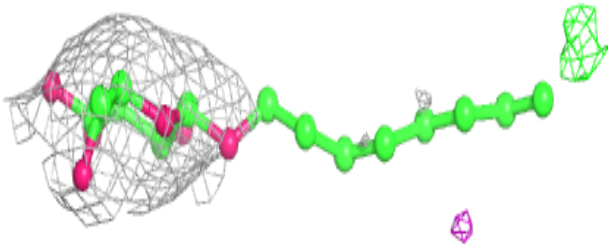


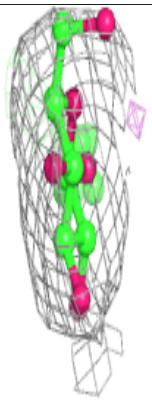


Electron density around BOG Q 3009:

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

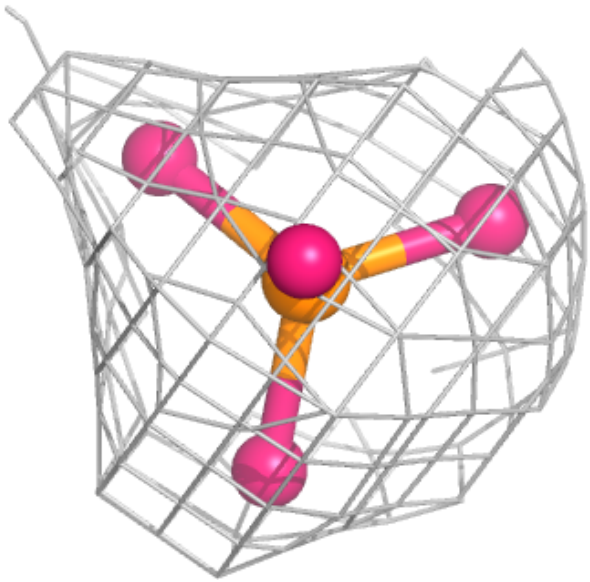


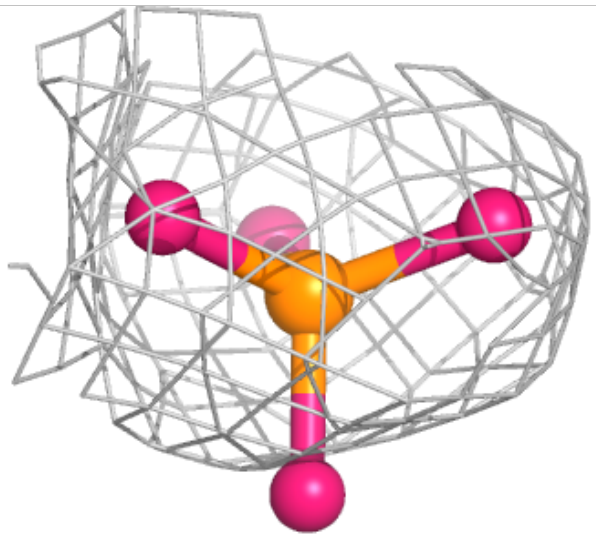


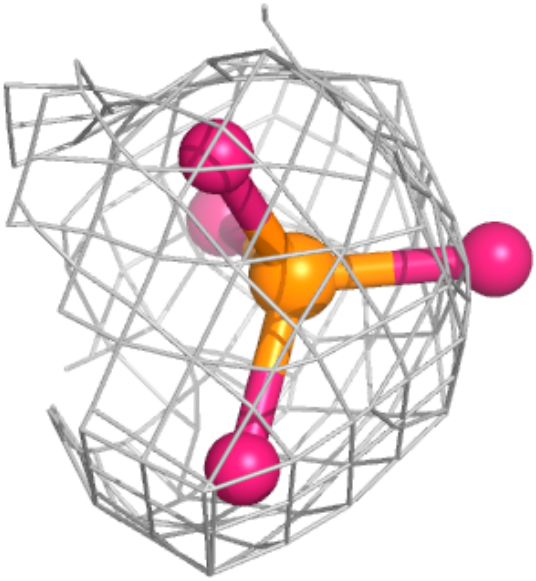


Electron density around PEE P 3008:

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

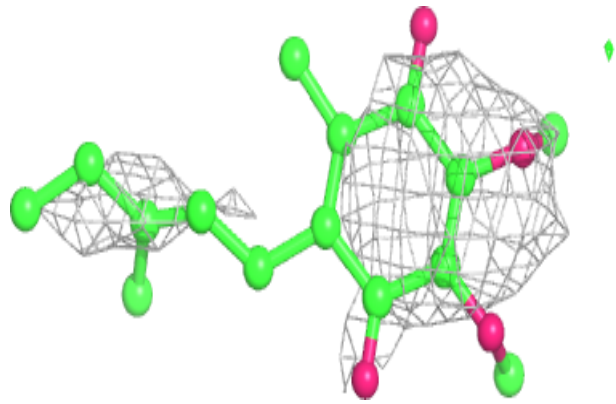


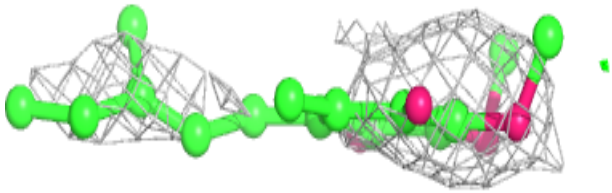


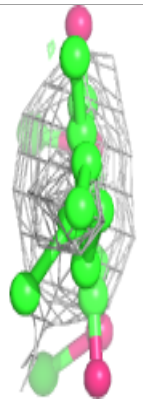


Electron density around UQ P 3002:

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

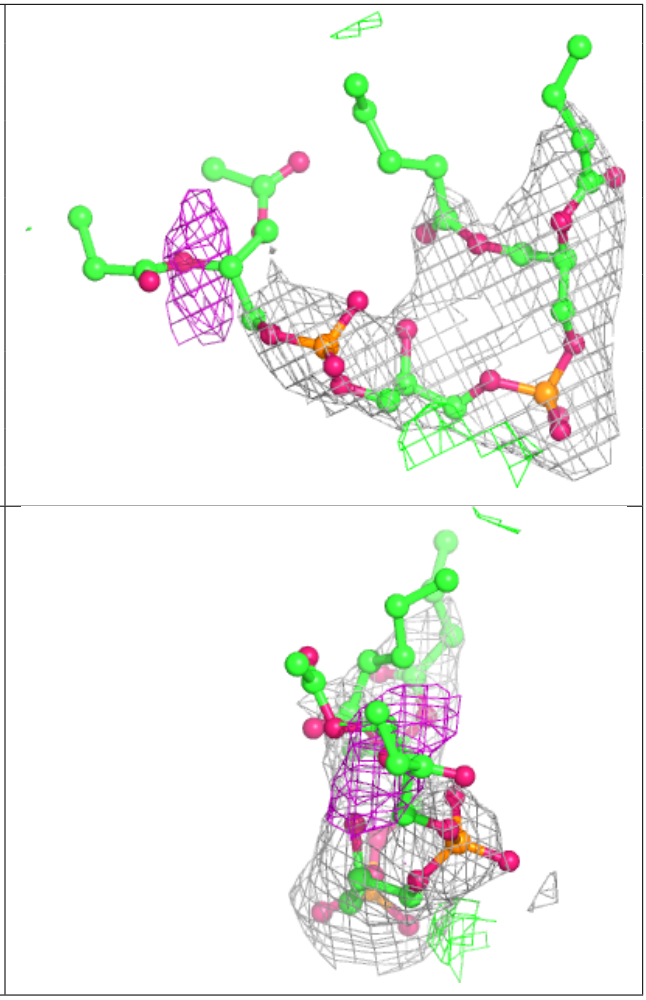






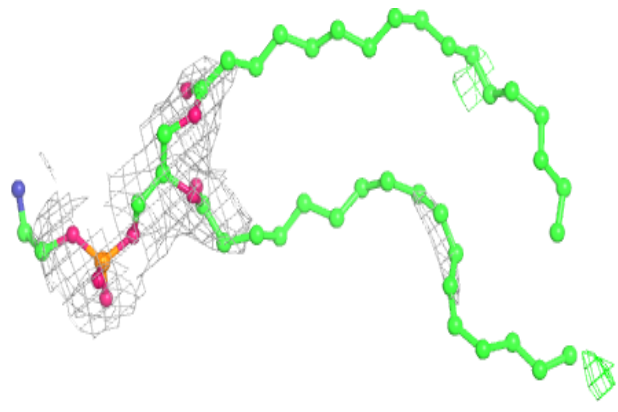
Electron density around CDL D 2003:

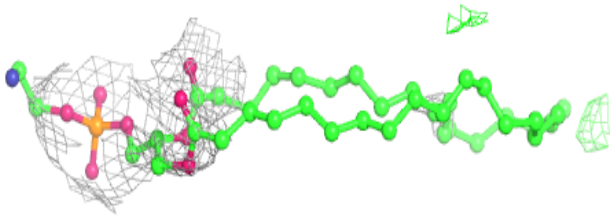
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

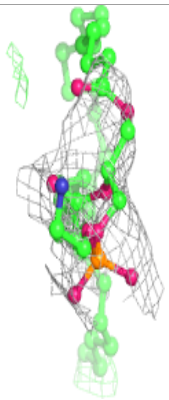


Electron density around PEE P 3007:

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

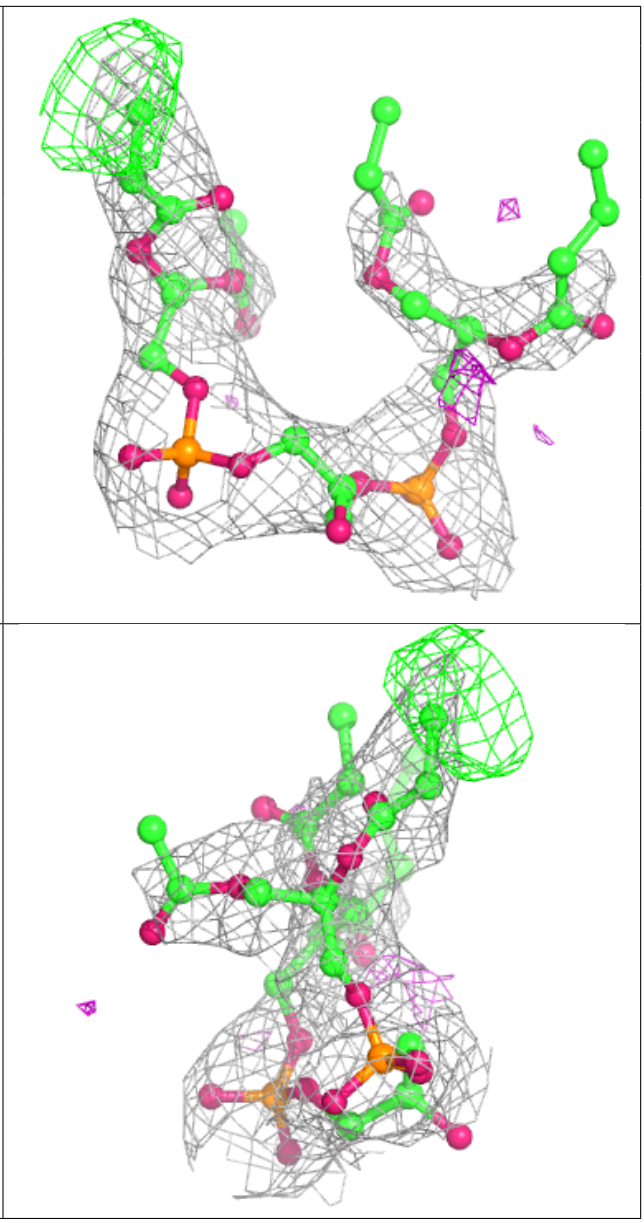






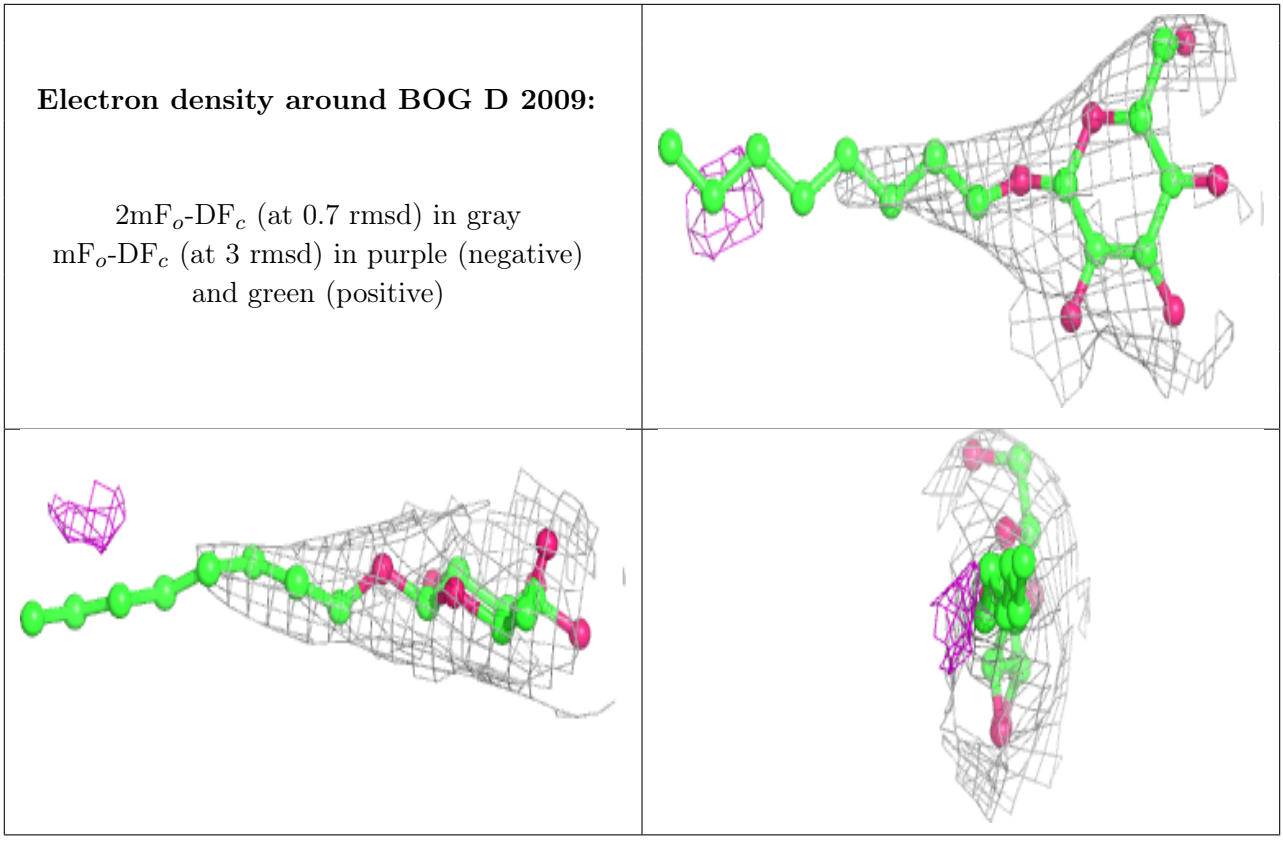
Electron density around CDL C 2004:

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



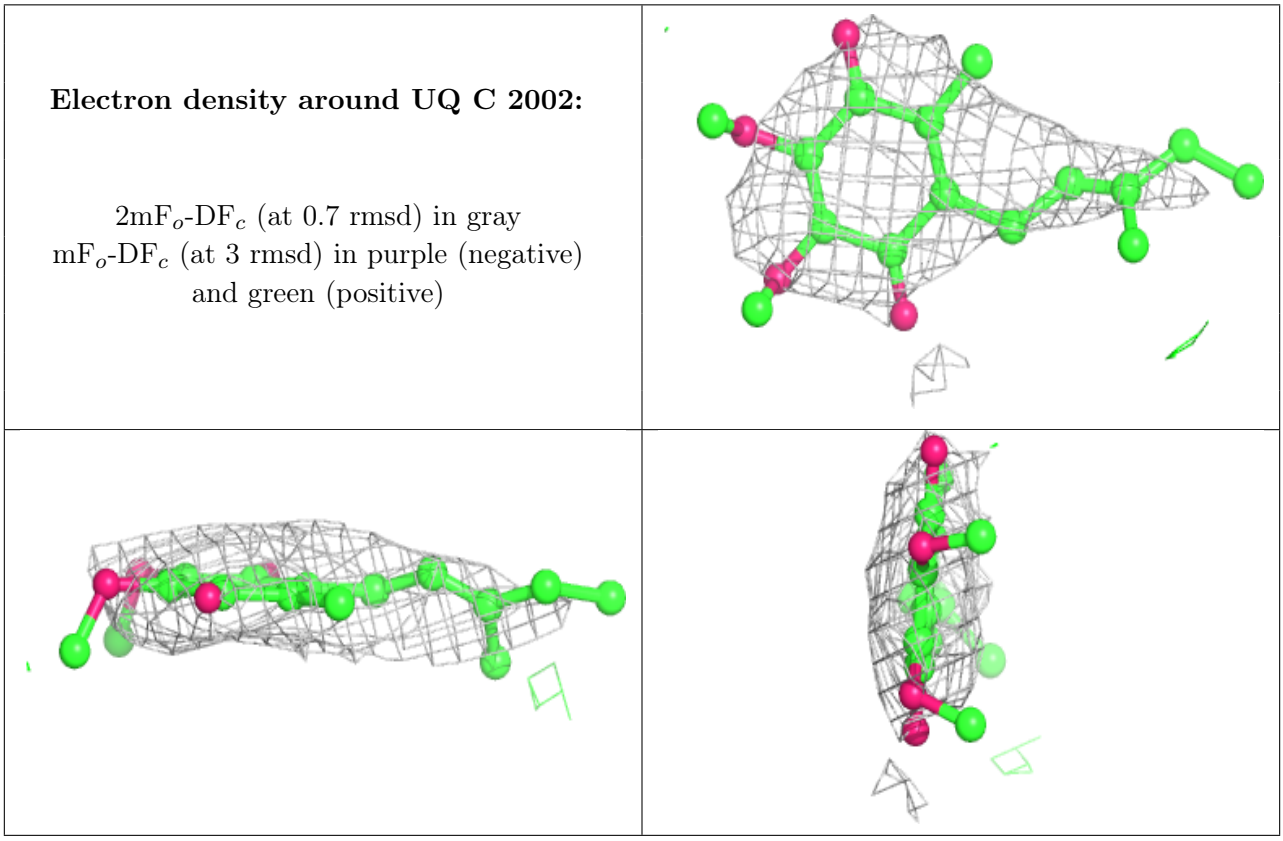
Electron density around BOG D 2009:

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



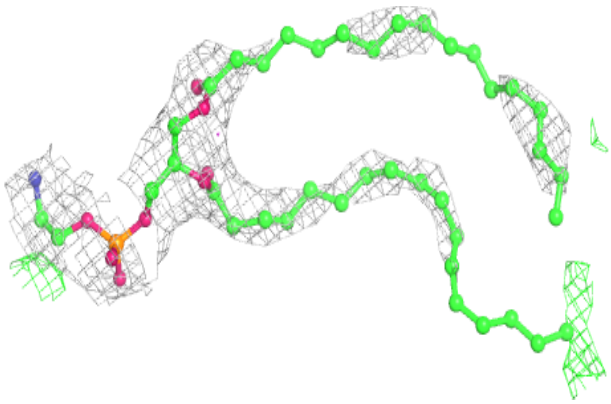
Electron density around UQ C 2002:

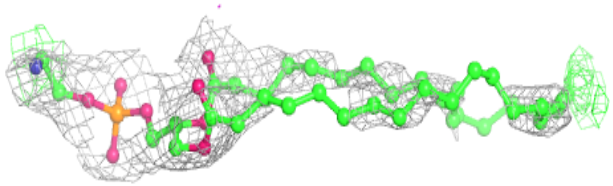
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

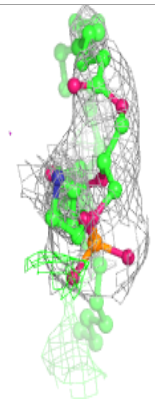


Electron density around PEE C 2007:

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

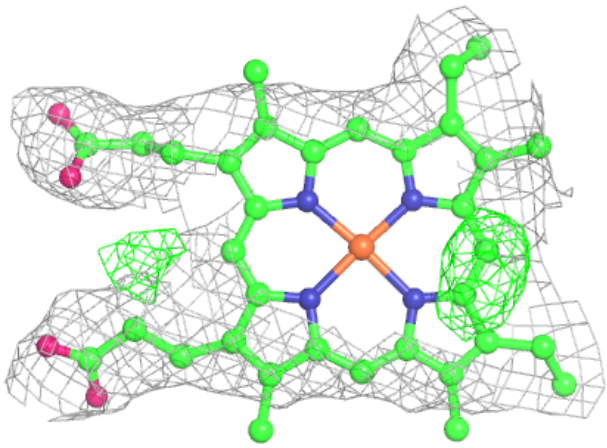


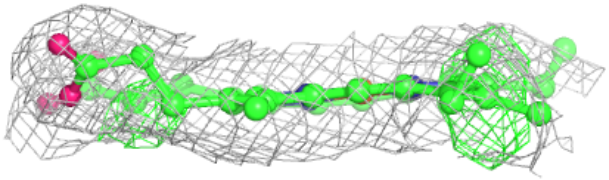


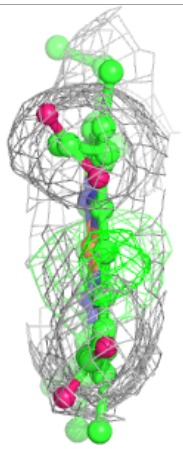


Electron density around HEC Q 501:

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

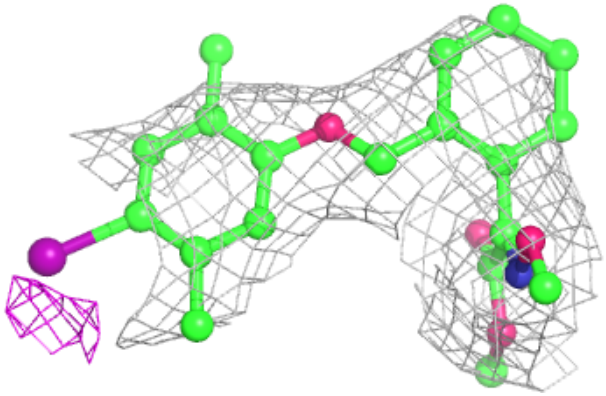


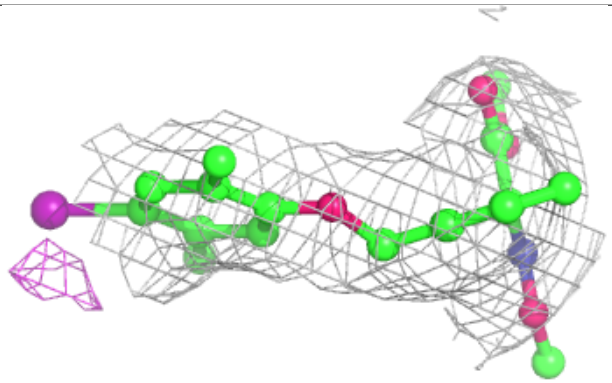


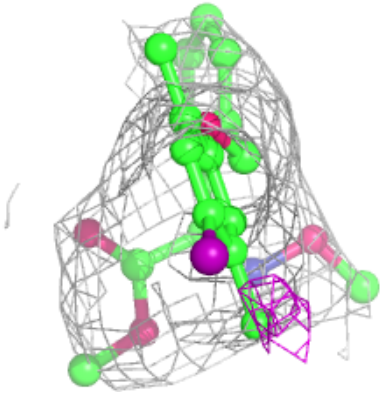


Electron density around IKR P 3001:

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

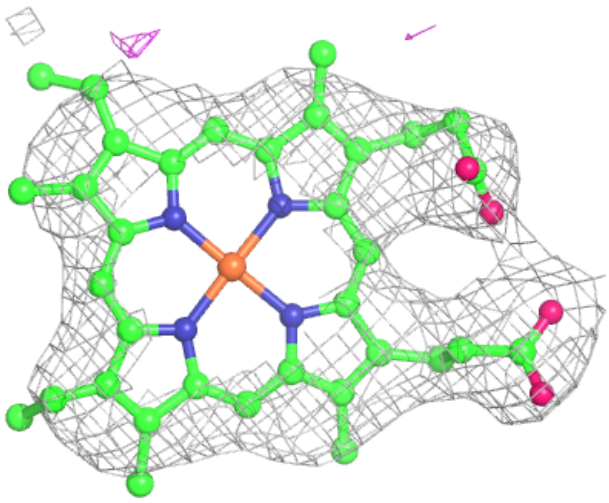


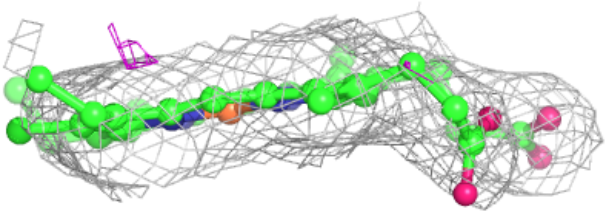


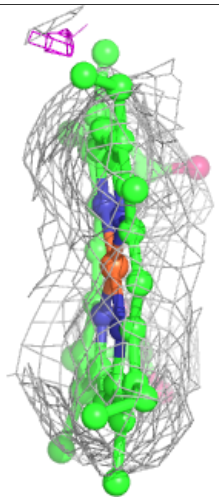


Electron density around HEM C 501:

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

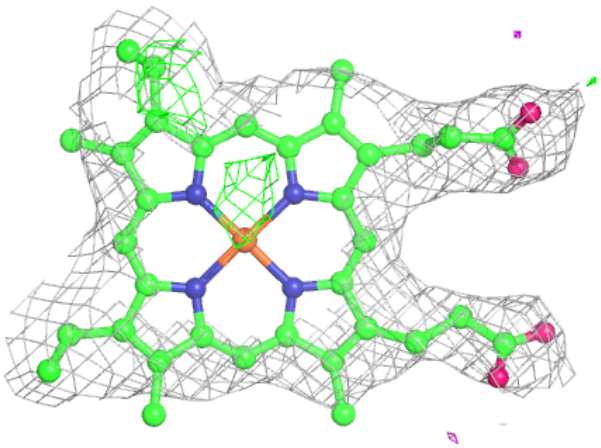


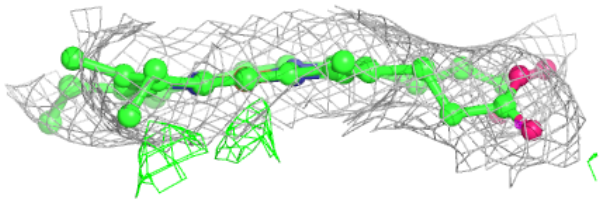


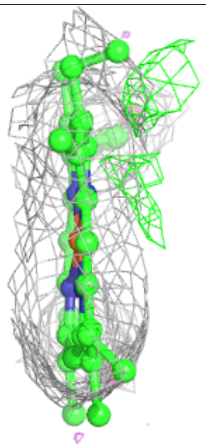


Electron density around HEC D 501:

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

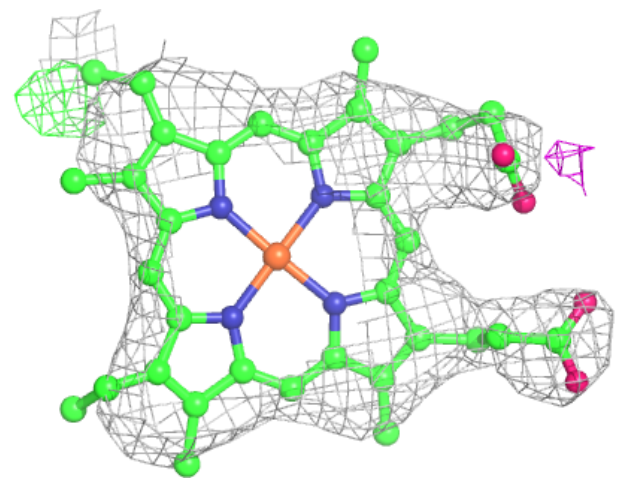


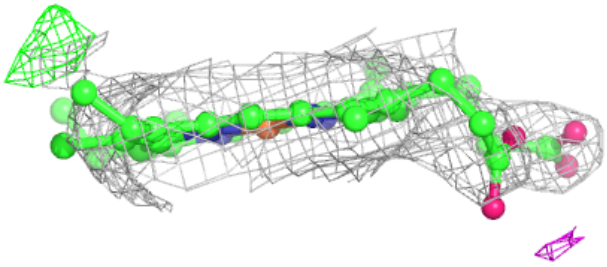


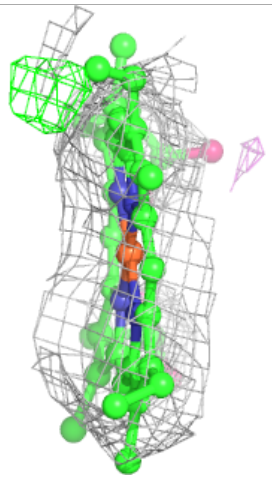


Electron density around HEM P 501:

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

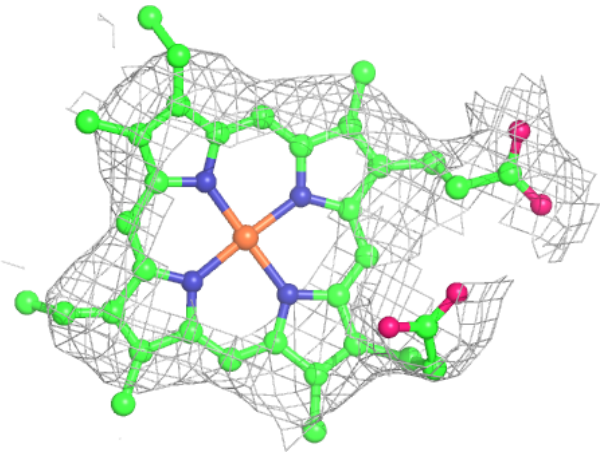


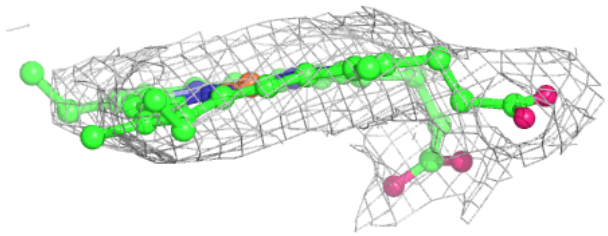


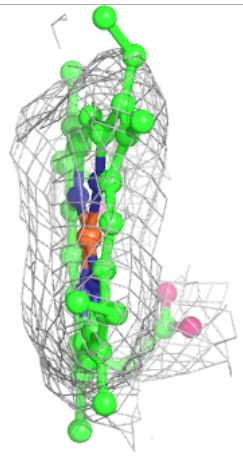


Electron density around HEM P 502:

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

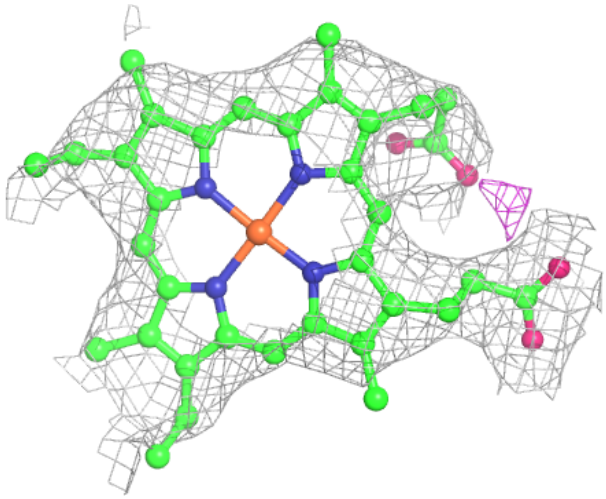


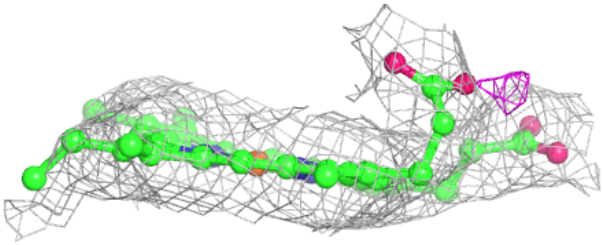


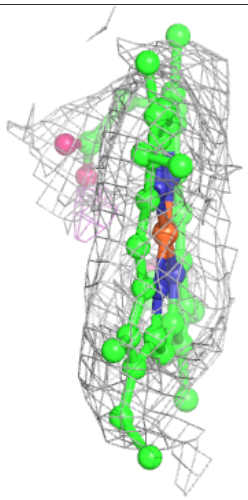


Electron density around HEM C 502:

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

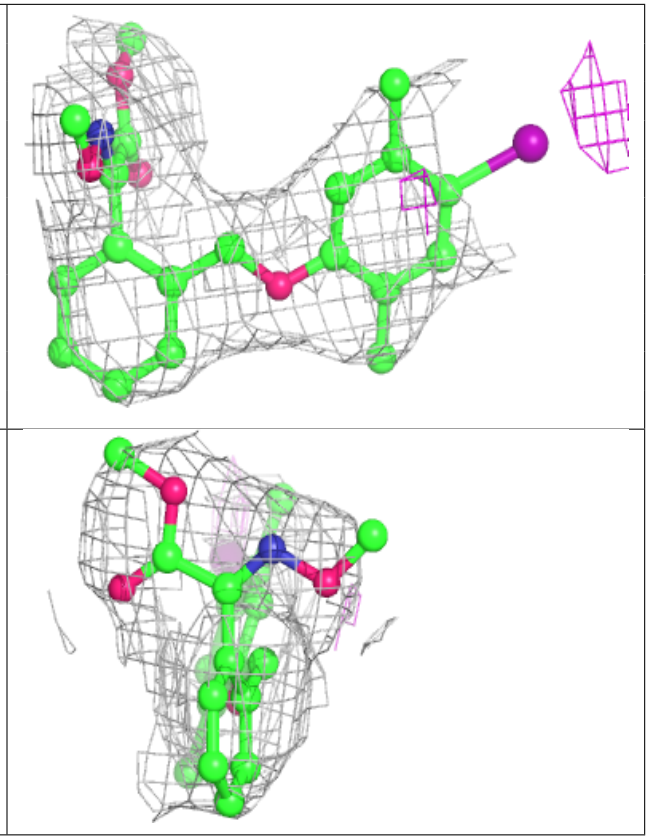






Electron density around IKR C 2001:

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



6.5 Other polymers (i)

There are no such residues in this entry.