Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 09:36 PM JST

PDB ID	:	5XTE / pdb_00005xte
EMDB ID	:	EMD-6774
Title	:	Cryo-EM structure of human respiratory complex III (cytochrome bc1 complex)
Authors	:	Gu, J.; Wu, M.; Yang, M.
Deposited on	:	2017-06-19
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

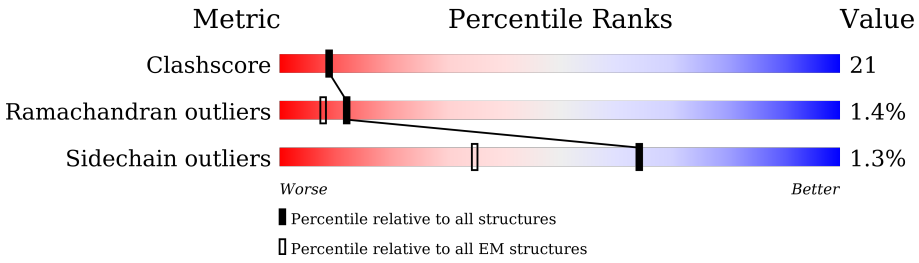
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	81	26% 65% 27% 7%
1	N	81	27% 75% 23% .
2	B	57	95% 49% 46% 5%
2	O	57	98% 51% 40% 9%
3	C	196	60% 69% 29% .
3	P	196	53% 64% 35% .
4	D	62	29% 76% 24%
4	Q	62	32% 61% 39%

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Mol	Chain	Length	Quality of chain
5	E	75	45% 68% 28%
5	R	75	36% 73% 24%
6	F	106	12% 56% 34% 10%
6	S	106	10% 63% 37%
7	G	51	24% 73% 27%
7	T	51	43% 65% 31%
8	H	241	12% 72% 27%
8	U	241	10% 70% 29%
9	J	378	67% 33%
9	V	378	61% 37%
10	K	419	12% 61% 37%
10	W	419	13% 65% 33%
11	L	446	16% 63% 36%
11	Y	446	18% 64% 34%

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
12	CDL	G	101	-	-	X	-
12	CDL	L	502	-	-	X	-
13	FES	C	301	-	-	X	-
13	FES	P	301	-	-	X	-
14	PEE	H	401	-	-	X	-
14	PEE	L	503	-	-	X	-
14	PEE	U	401	-	-	X	-
14	PEE	V	403	-	-	X	-
14	PEE	Y	502	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 34492 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
1	N	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
2	O	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
3	P	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
4	Q	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
5	R	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
6	S	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	51	Total	C	N	O	0	0
			425	287	72	66		
7	T	51	Total	C	N	O	0	0
			425	287	72	66		

- Molecule 8 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		
8	U	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 9 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
9	V	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		

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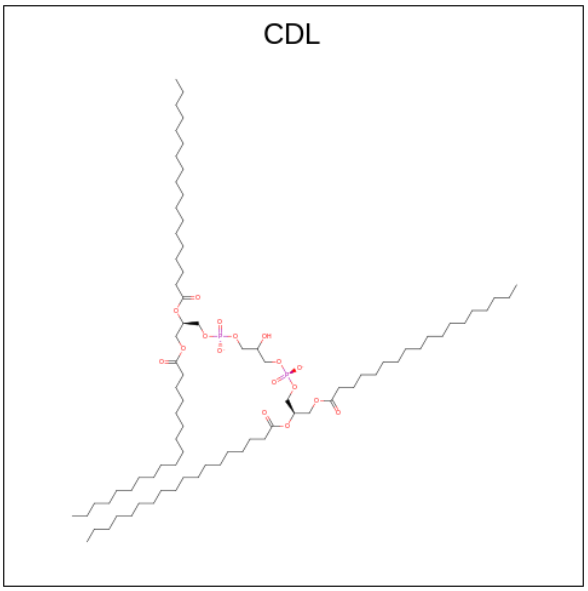
Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
11	Y	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			64	45	17	2	
12	G	1	Total	C	O	P	0
			64	45	17	2	
12	H	1	Total	C	O	P	0
			64	45	17	2	
12	J	1	Total	C	O	P	0
			64	45	17	2	
12	J	1	Total	C	O	P	0
			64	45	17	2	
12	L	1	Total	C	O	P	0
			64	45	17	2	

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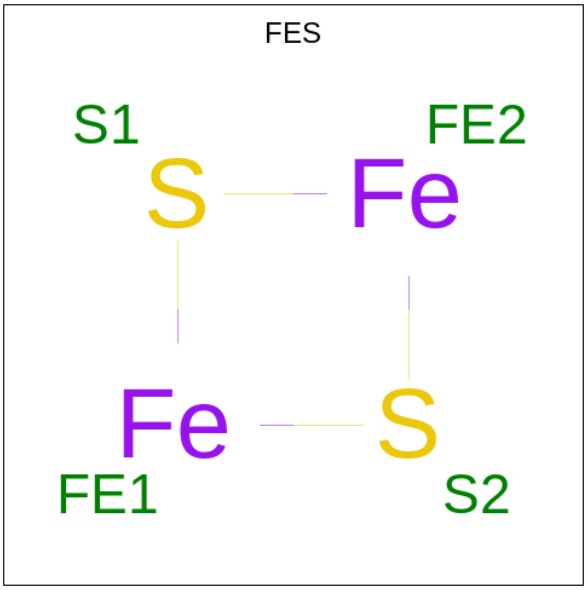
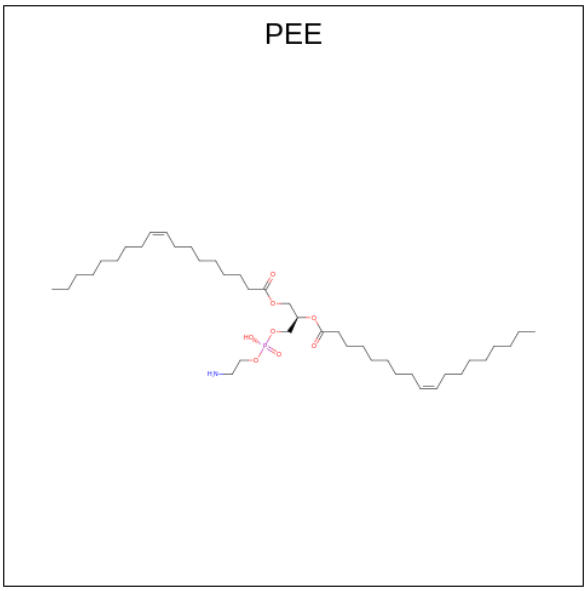
Mol	Chain	Residues	Atoms				AltConf
12	N	1	Total	C	O	P	0
			64	45	17	2	
12	U	1	Total	C	O	P	0
			64	45	17	2	
12	Y	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



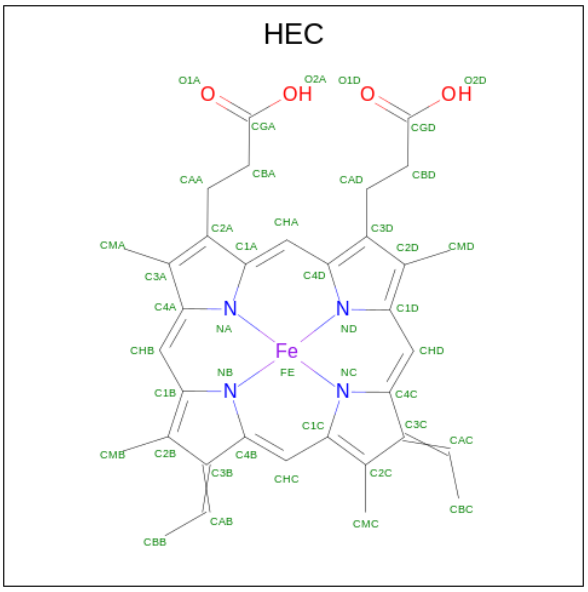
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	Fe	S	0
			4	2	2	
13	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



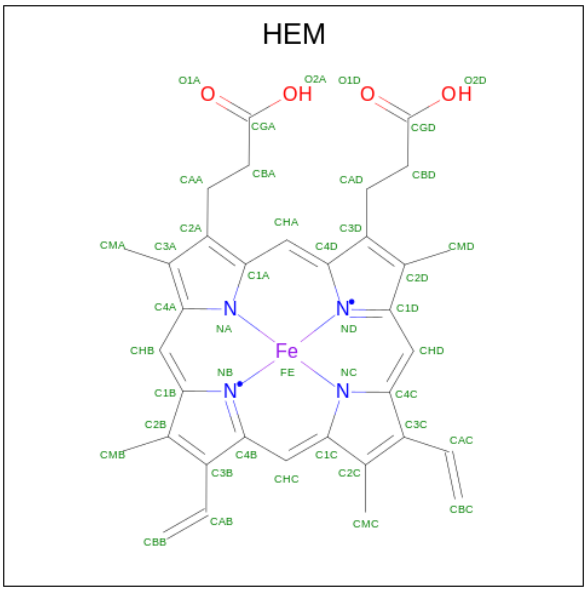
Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	U	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	V	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	Y	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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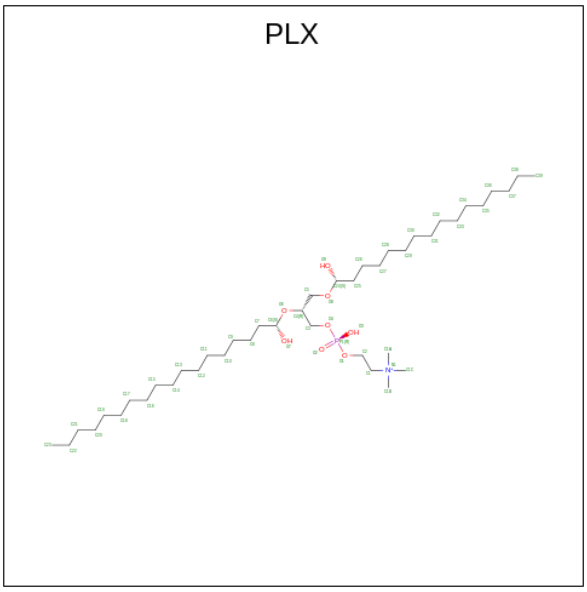
Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



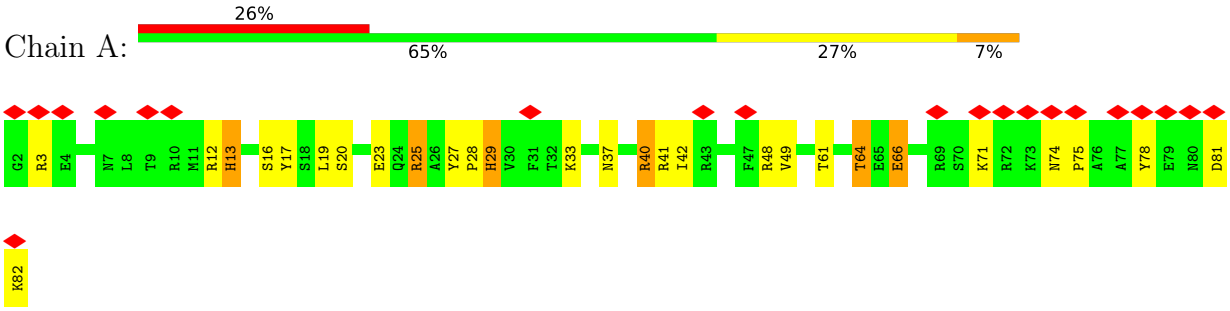
Mol	Chain	Residues	Atoms					AltConf
17	L	1	Total	C	N	O	P	0
			52	42	1	8	1	
17	Q	1	Total	C	N	O	P	0
			52	42	1	8	1	
17	T	1	Total	C	N	O	P	0
			52	42	1	8	1	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

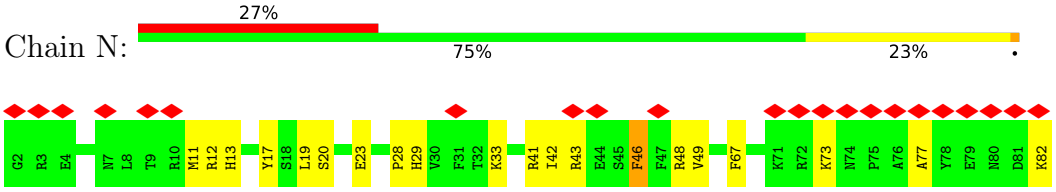
• Molecule 1: Cytochrome b-c1 complex subunit 8

Chain A:



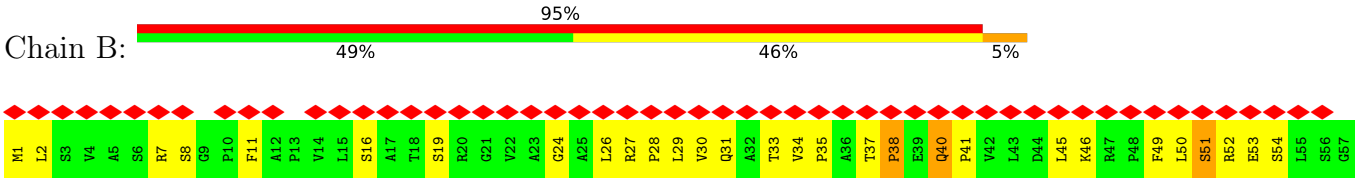
• Molecule 1: Cytochrome b-c1 complex subunit 8

Chain N:



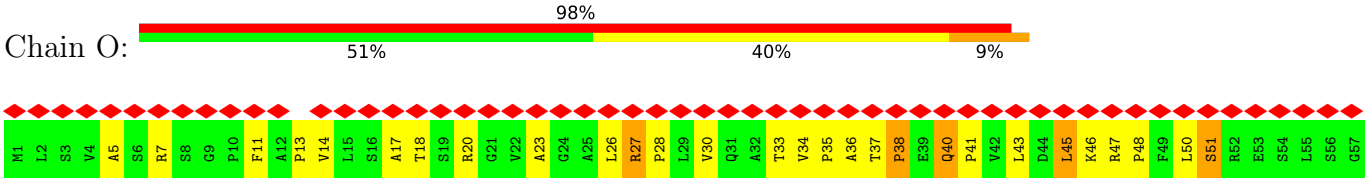
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain B:



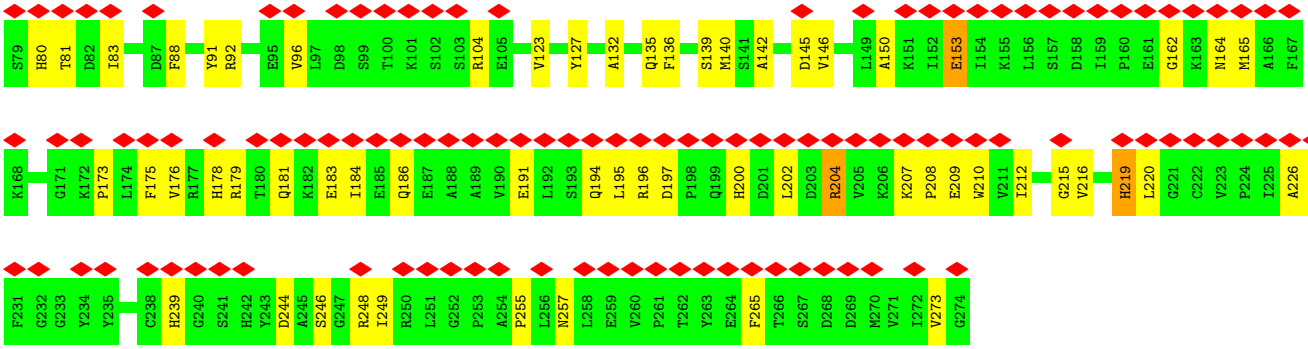
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain O:



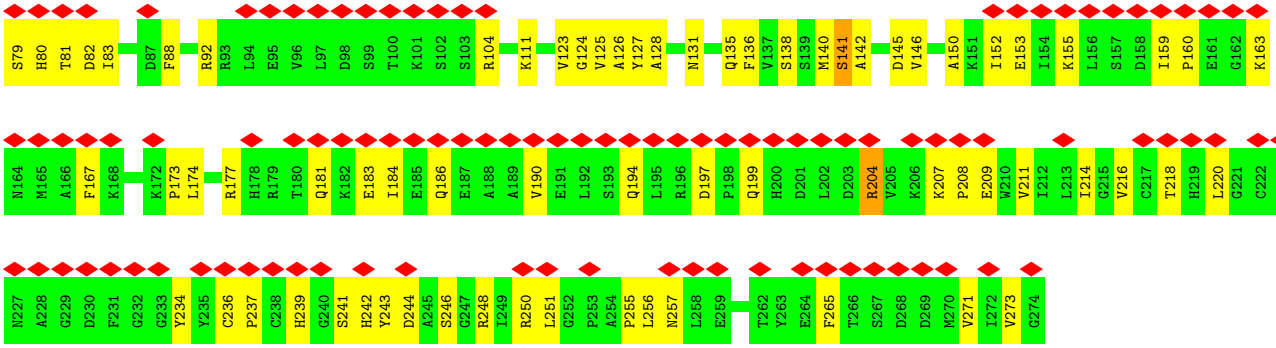
• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C:



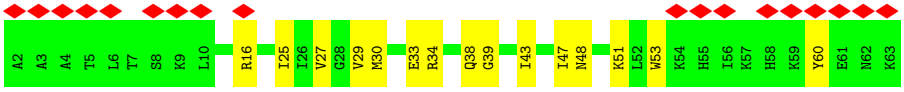
• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



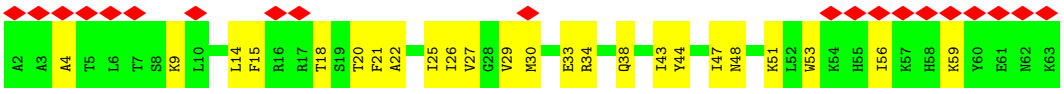
• Molecule 4: Cytochrome b-c1 complex subunit 9

Chain D:



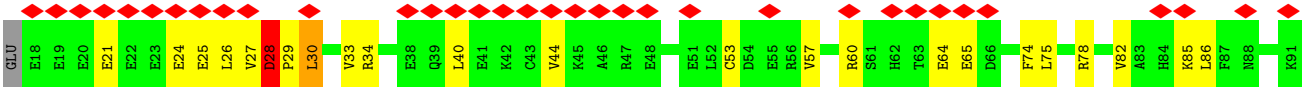
• Molecule 4: Cytochrome b-c1 complex subunit 9

Chain Q:



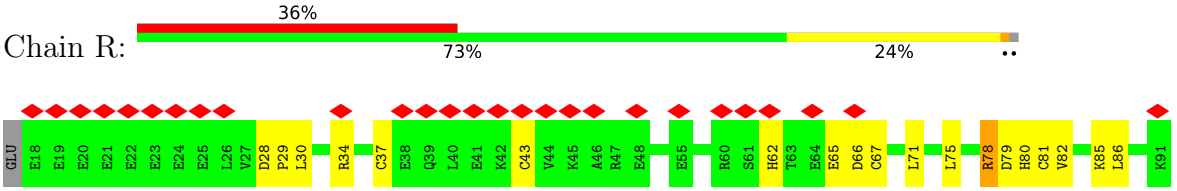
• Molecule 5: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain E:



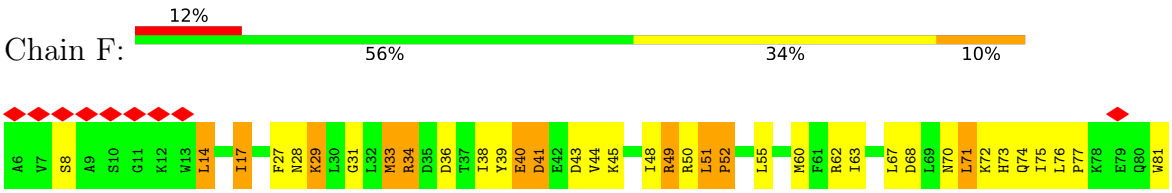
• Molecule 5: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain R:



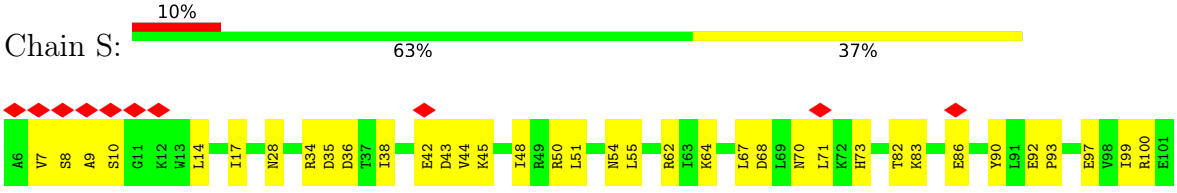
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



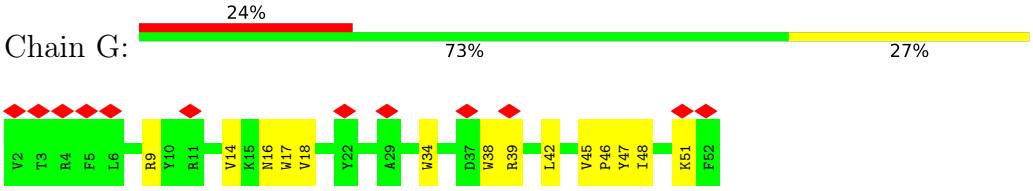
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain S:



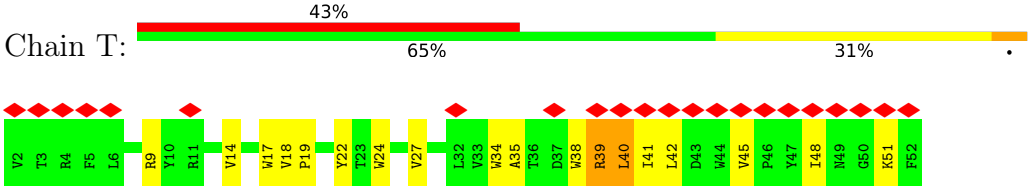
• Molecule 7: Cytochrome b-c1 complex subunit 10

Chain G:



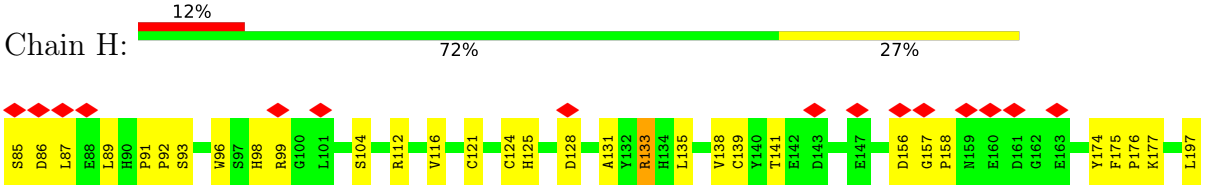
• Molecule 7: Cytochrome b-c1 complex subunit 10

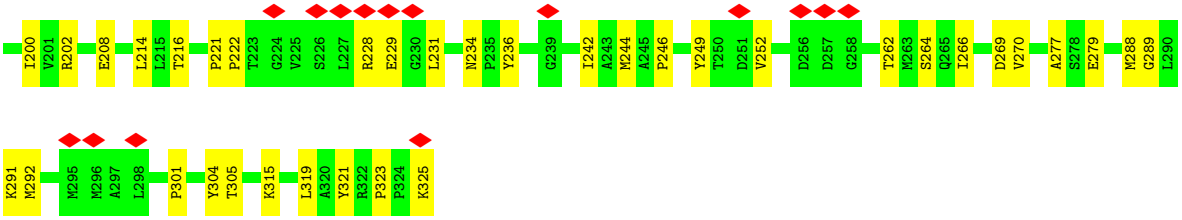
Chain T:



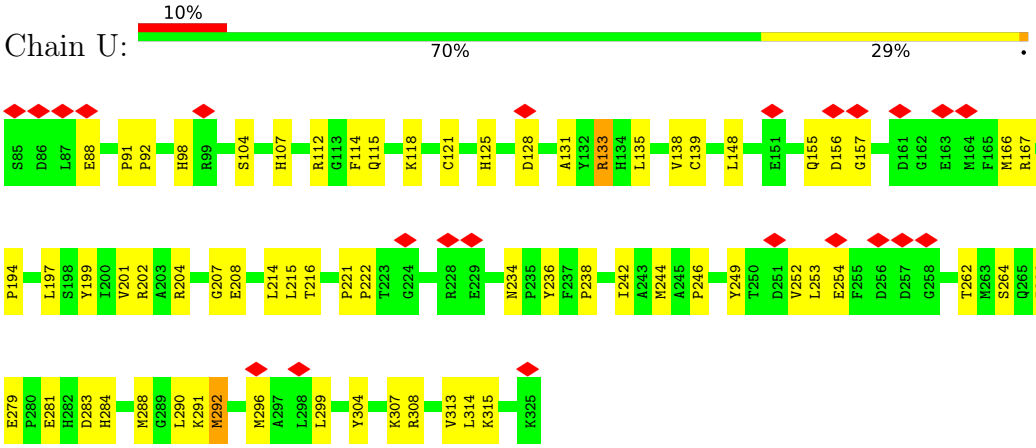
• Molecule 8: Cytochrome c1, heme protein, mitochondrial

Chain H:

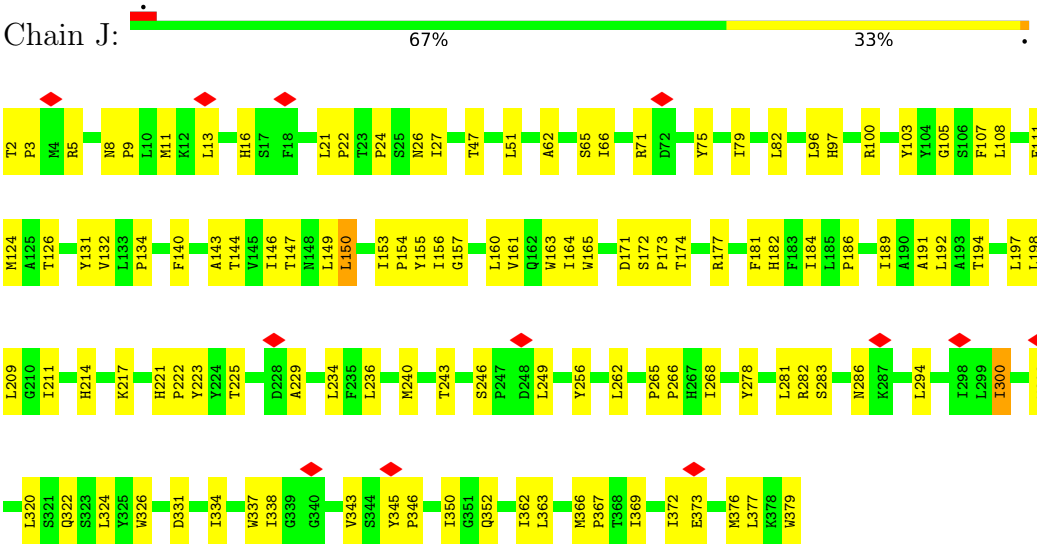




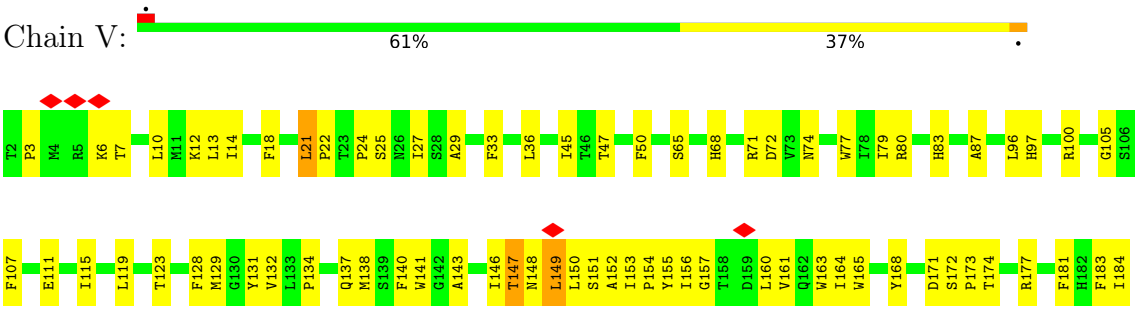
• Molecule 8: Cytochrome c1, heme protein, mitochondrial

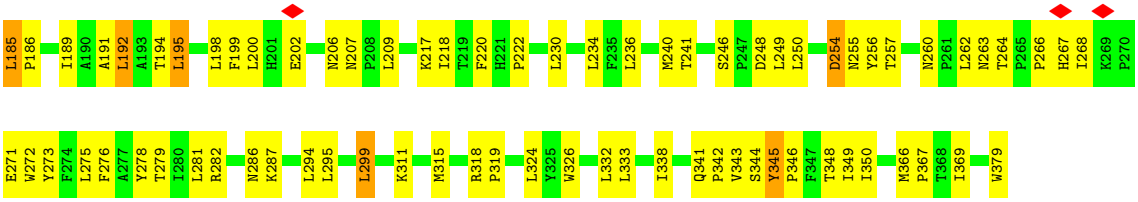


• Molecule 9: Cytochrome b



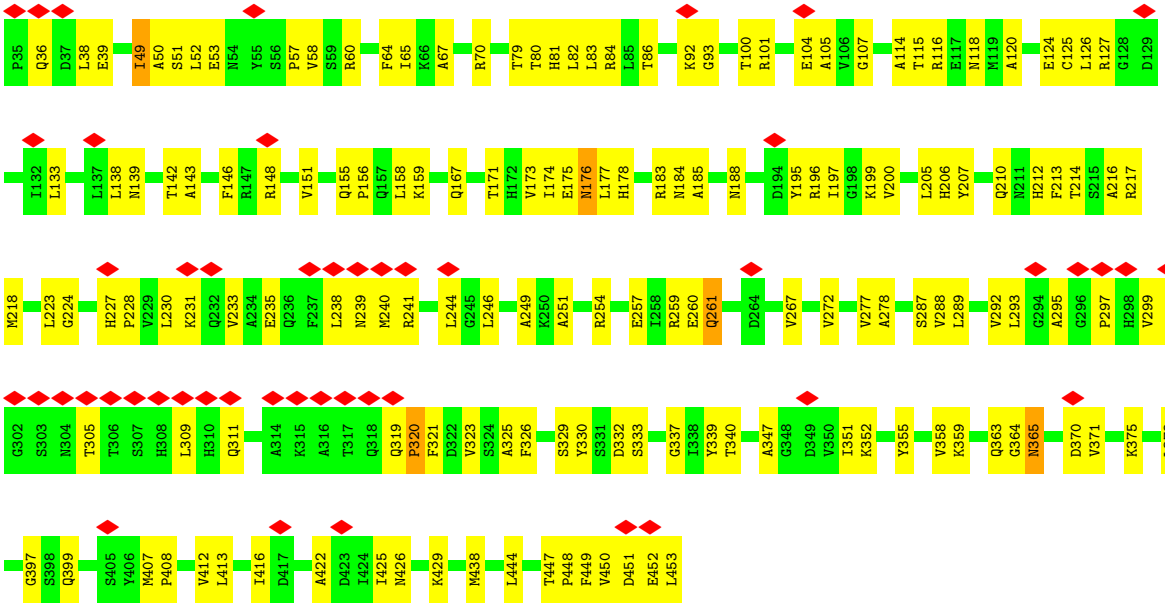
• Molecule 9: Cytochrome b





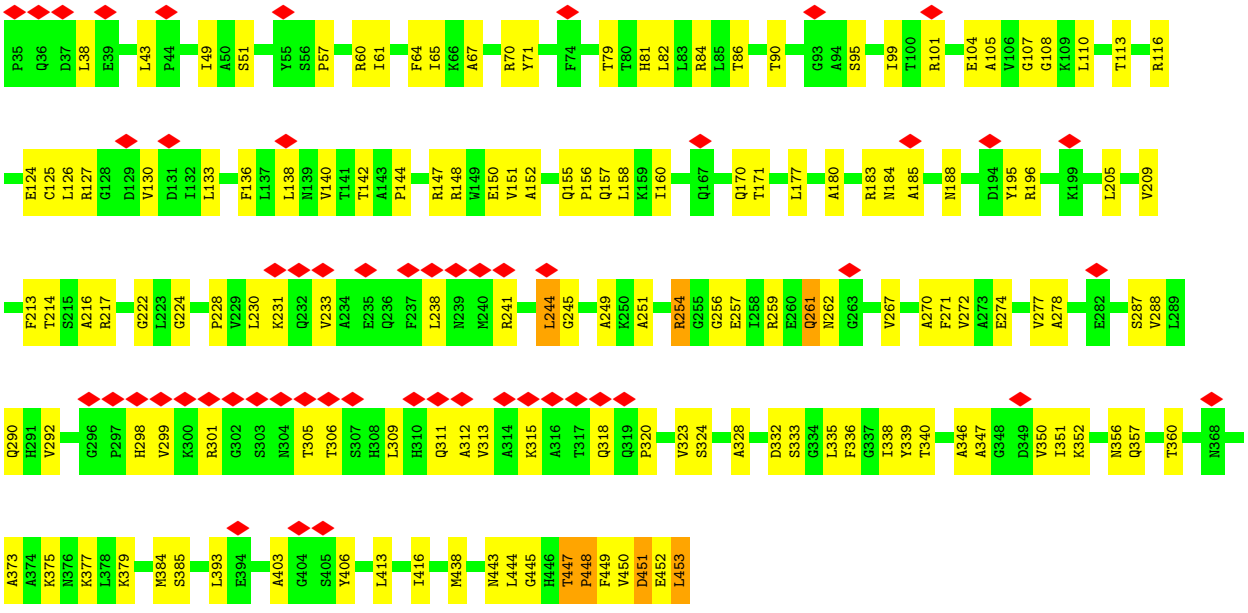
• Molecule 10: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain K:



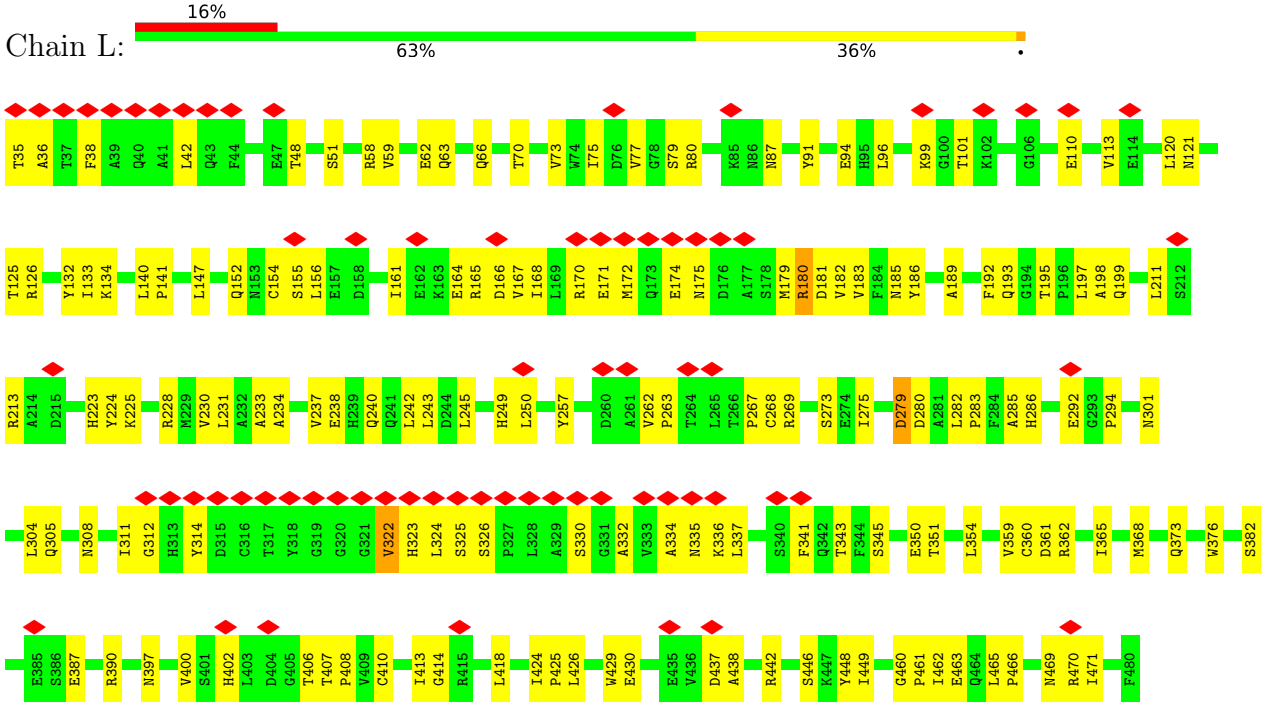
• Molecule 10: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain W:



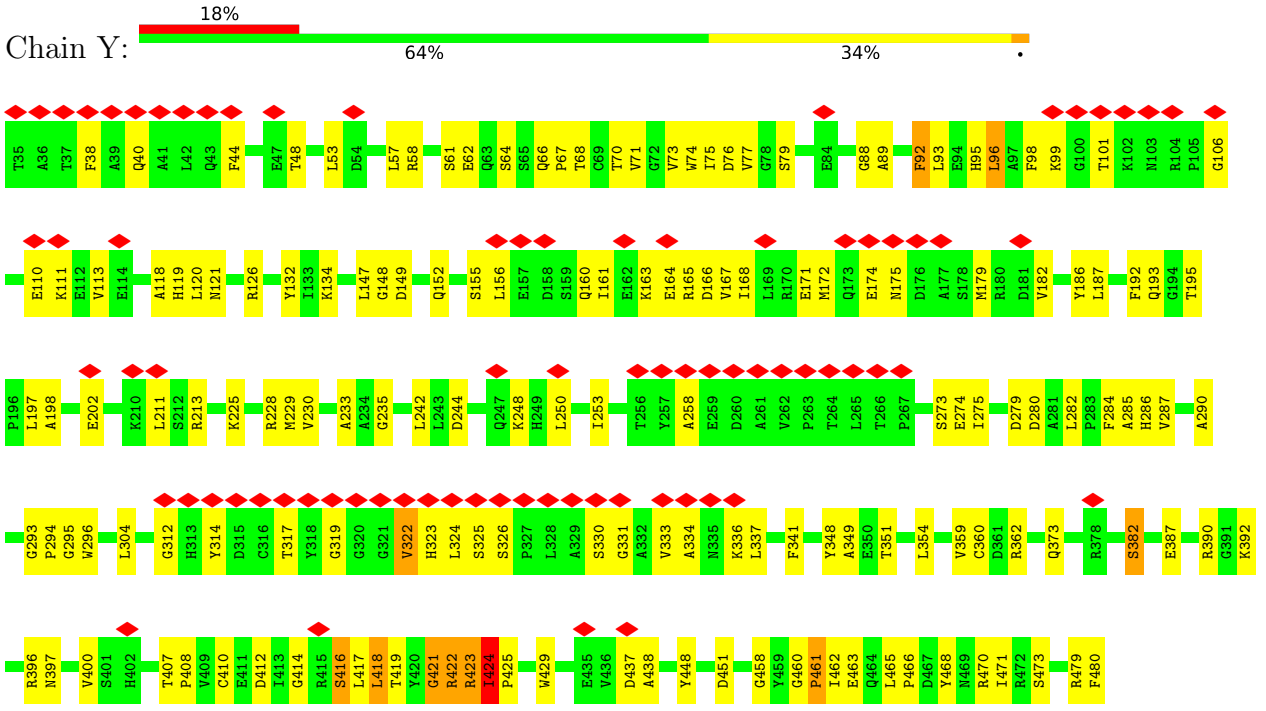
• Molecule 11: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



• Molecule 11: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.339	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0783	Depositor
Map size (Å)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/715	0.48	0/964
1	N	0.27	0/707	0.49	0/953
2	B	0.23	0/421	0.60	1/574 (0.2%)
2	O	0.25	0/417	0.61	1/569 (0.2%)
3	C	0.24	0/1554	0.43	0/2104
3	P	0.23	0/1554	0.42	0/2104
4	D	0.26	0/521	0.42	0/699
4	Q	0.27	0/521	0.43	0/699
5	E	0.35	0/587	0.54	1/789 (0.1%)
5	R	0.27	0/587	0.46	0/789
6	F	0.42	1/942 (0.1%)	0.52	1/1263 (0.1%)
6	S	0.27	0/942	0.44	0/1263
7	G	0.27	0/442	0.48	0/608
7	T	0.28	0/442	0.49	0/608
8	H	0.26	0/1983	0.46	0/2691
8	U	0.27	0/1983	0.45	0/2691
9	J	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)
9	V	0.34	1/3108 (0.0%)	0.54	3/4254 (0.1%)
10	K	0.27	0/3217	0.49	0/4361
10	W	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)
11	L	0.27	0/3527	0.47	0/4788
11	Y	0.29	1/3527 (0.0%)	0.50	2/4788 (0.0%)
All	All	0.29	5/34025 (0.0%)	0.49	11/46178 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	W	448	PRO	N-CD	5.33	1.55	1.47
9	J	154	PRO	N-CD	5.18	1.55	1.47
9	V	154	PRO	N-CD	5.18	1.55	1.47
11	Y	425	PRO	N-CD	5.12	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	52	PRO	N-CD	5.04	1.54	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	28	ASP	C-N-CD	6.17	141.36	128.40
9	V	345	TYR	C-N-CD	5.81	140.59	128.40
9	V	153	ILE	C-N-CD	5.76	140.50	128.40
9	J	153	ILE	C-N-CD	5.75	140.48	128.40
6	F	51	LEU	C-N-CD	5.68	140.34	128.40
11	Y	424	ILE	C-N-CD	5.65	140.26	128.40
10	W	447	THR	C-N-CD	5.64	140.25	128.40
2	B	45	LEU	CA-CB-CG	5.47	127.88	115.30
11	Y	421	GLY	N-CA-C	-5.39	99.63	113.10
2	O	45	LEU	CA-CB-CG	5.28	127.45	115.30
9	V	21	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	694	0	683	47	0
1	N	687	0	676	25	0
2	B	413	0	438	26	0
2	O	409	0	432	27	0
3	C	1521	0	1505	55	0
3	P	1521	0	1505	61	0
4	D	509	0	511	15	0
4	Q	509	0	511	24	0
5	E	580	0	526	51	0
5	R	580	0	526	34	0
6	F	921	0	909	70	0
6	S	921	0	910	29	0
7	G	425	0	422	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	425	0	422	30	0
8	H	1924	0	1874	59	0
8	U	1924	0	1874	80	0
9	J	3009	0	3065	108	0
9	V	3009	0	3065	167	0
10	K	3159	0	3130	154	0
10	W	3162	0	3139	125	0
11	L	3453	0	3370	142	0
11	Y	3453	0	3368	160	0
12	A	64	0	72	3	0
12	G	64	0	72	28	0
12	H	64	0	72	6	0
12	J	128	0	144	23	0
12	L	64	0	72	22	0
12	N	64	0	72	8	0
12	U	64	0	72	12	0
12	Y	64	0	72	4	0
13	C	4	0	0	3	0
13	P	4	0	0	2	0
14	H	49	0	75	32	0
14	J	49	0	75	8	0
14	L	49	0	75	37	0
14	U	41	0	56	25	0
14	V	49	0	75	23	0
14	Y	49	0	75	21	0
15	H	43	0	32	5	0
15	U	43	0	32	8	0
16	J	86	0	60	7	0
16	V	86	0	60	13	0
17	L	52	0	88	4	0
17	Q	52	0	88	7	0
17	T	52	0	88	3	0
All	All	34492	0	34388	1416	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 21.

All (1416) 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)
11:Y:296:TRP:CD1	11:Y:419:THR:CG2	1.74	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:29:LYS:CD	6:F:75:ILE:HD11	1.30	1.58
12:J:405:CDL:H112	14:Y:502:PEE:C45	1.18	1.58
6:F:29:LYS:CG	6:F:75:ILE:HD11	1.16	1.54
11:Y:296:TRP:CD1	11:Y:419:THR:HG23	0.99	1.51
6:F:29:LYS:HG2	6:F:75:ILE:CD1	1.40	1.49
3:C:150:ALA:CB	9:V:168:TYR:HE2	1.29	1.44
11:Y:296:TRP:NE1	11:Y:419:THR:CG2	1.73	1.43
1:A:78:TYR:CB	5:E:65:GLU:HG2	1.48	1.41
6:F:29:LYS:CD	6:F:75:ILE:CD1	1.97	1.41
1:A:78:TYR:HB3	5:E:65:GLU:CG	1.50	1.40
6:F:29:LYS:CG	6:F:75:ILE:CD1	1.96	1.39
3:C:150:ALA:CB	9:V:168:TYR:CE2	2.05	1.38
9:V:14:ILE:CD1	14:Y:502:PEE:H41	1.58	1.33
10:K:259:ARG:CG	10:K:444:LEU:HD13	1.60	1.31
11:Y:296:TRP:HE1	11:Y:419:THR:CB	1.42	1.31
3:C:150:ALA:HB3	9:V:168:TYR:CE2	1.61	1.30
9:V:10:LEU:HD21	14:Y:502:PEE:C27	1.60	1.29
12:J:405:CDL:C11	14:Y:502:PEE:C45	2.08	1.29
12:L:502:CDL:C57	14:L:503:PEE:H63	1.61	1.29
1:A:78:TYR:CD1	5:E:65:GLU:HA	1.70	1.26
8:U:308:ARG:NH1	12:U:403:CDL:O1	1.70	1.24
14:U:401:PEE:H17	9:V:240:MET:CE	1.68	1.22
14:H:401:PEE:H18	9:J:240:MET:CE	1.70	1.21
6:F:29:LYS:HD3	6:F:75:ILE:CD1	1.64	1.20
12:L:502:CDL:H572	14:L:503:PEE:C40	1.73	1.17
11:Y:98:PHE:CE2	11:Y:120:LEU:CD1	2.29	1.16
11:Y:296:TRP:NE1	11:Y:419:THR:HG21	1.57	1.15
7:T:42:LEU:O	7:T:45:VAL:HG22	1.41	1.14
11:Y:296:TRP:NE1	11:Y:419:THR:CB	2.03	1.12
9:V:10:LEU:CD2	14:Y:502:PEE:H46	1.78	1.12
10:K:259:ARG:HG3	10:K:444:LEU:HD13	1.27	1.12
1:A:37:ASN:OD1	1:A:40:ARG:NH2	1.83	1.11
3:C:150:ALA:HB1	9:V:168:TYR:CE2	1.80	1.11
14:U:401:PEE:H17	9:V:240:MET:HE1	1.25	1.11
12:G:101:CDL:H332	12:G:101:CDL:HA62	1.25	1.11
7:T:40:LEU:HD12	7:T:41:ILE:N	1.63	1.11
12:L:502:CDL:C57	14:L:503:PEE:H66	1.80	1.10
14:L:503:PEE:H19	14:L:503:PEE:H49	1.11	1.10
11:Y:98:PHE:CE2	11:Y:120:LEU:HD13	1.87	1.10
12:L:502:CDL:H571	14:L:503:PEE:H63	1.12	1.09
12:G:101:CDL:H531	12:G:101:CDL:H712	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:HE1	5:E:64:GLU:O	1.36	1.05
8:U:296:MET:HE1	14:U:401:PEE:H53	1.32	1.04
1:A:78:TYR:CE1	5:E:64:GLU:O	2.09	1.04
6:F:29:LYS:HG2	6:F:75:ILE:CG1	1.87	1.04
8:U:296:MET:CE	14:U:401:PEE:H53	1.86	1.04
5:R:34:ARG:HG3	5:R:78:ARG:NH1	1.72	1.04
5:E:34:ARG:HD3	5:E:78:ARG:NH2	1.71	1.04
10:K:259:ARG:HB2	10:K:259:ARG:HH21	1.22	1.03
8:U:288:MET:HB3	14:U:401:PEE:O4	1.57	1.03
9:V:10:LEU:CD2	14:Y:502:PEE:C27	2.36	1.03
9:V:14:ILE:HD12	14:Y:502:PEE:H41	1.41	1.03
7:G:38:TRP:CD1	12:G:101:CDL:H511	1.94	1.02
12:G:101:CDL:H712	12:G:101:CDL:C53	1.90	1.02
10:K:438:MET:HE2	10:K:450:VAL:HG13	1.40	1.01
5:R:34:ARG:NH1	5:R:78:ARG:HH12	1.59	1.01
5:R:79:ASP:OD2	8:U:236:TYR:OH	1.79	1.00
8:H:121:CYS:SG	15:H:402:HEC:HBB2	2.01	1.00
10:K:257:GLU:OE2	10:K:450:VAL:N	1.92	1.00
7:T:39:ARG:HA	7:T:51:LYS:HE3	1.45	0.99
14:L:503:PEE:H50	14:L:503:PEE:H16	1.45	0.99
14:H:401:PEE:H64	14:H:401:PEE:H73	1.42	0.99
9:J:156:ILE:HG22	9:J:160:LEU:HB2	1.42	0.98
5:E:30:LEU:HD11	5:E:34:ARG:HH21	1.26	0.98
10:W:351:ILE:HD11	10:W:448:PRO:HD2	1.44	0.98
12:G:101:CDL:HA62	12:G:101:CDL:C33	1.94	0.97
14:H:401:PEE:C13	9:J:240:MET:CE	2.42	0.97
12:L:502:CDL:C57	14:L:503:PEE:C38	2.43	0.97
14:H:401:PEE:H18	9:J:240:MET:HE1	1.47	0.97
10:K:259:ARG:CG	10:K:444:LEU:CD1	2.42	0.97
9:V:14:ILE:HD13	14:Y:502:PEE:H41	1.45	0.96
14:L:503:PEE:H16	14:L:503:PEE:C32	1.95	0.96
6:F:67:LEU:HD23	9:J:209:LEU:HD12	1.47	0.95
14:L:503:PEE:H49	14:L:503:PEE:C14	1.95	0.95
10:K:259:ARG:HB2	10:K:259:ARG:NH2	1.82	0.95
14:L:503:PEE:H19	14:L:503:PEE:C31	1.96	0.95
10:K:259:ARG:HG3	10:K:444:LEU:CD1	1.97	0.94
11:Y:424:ILE:HG23	11:Y:429:TRP:HE1	1.31	0.94
3:C:150:ALA:HB1	9:V:168:TYR:CD2	2.02	0.94
11:Y:98:PHE:CD2	11:Y:120:LEU:HD11	2.01	0.94
14:L:503:PEE:C31	14:L:503:PEE:H26	1.97	0.94
1:A:78:TYR:CD1	5:E:65:GLU:CA	2.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:257:GLU:CG	10:K:450:VAL:HG22	1.99	0.93
9:V:137:GLN:HE21	9:V:141:TRP:HE1	1.10	0.93
11:Y:98:PHE:CD2	11:Y:120:LEU:CD1	2.52	0.93
3:C:150:ALA:HB3	9:V:168:TYR:HE2	0.77	0.93
14:H:401:PEE:H66	14:H:401:PEE:H28	1.50	0.92
10:K:259:ARG:HG2	10:K:444:LEU:HD13	1.49	0.92
5:E:29:PRO:HD3	8:H:262:THR:HG21	1.52	0.92
5:E:34:ARG:HD3	5:E:78:ARG:HH22	1.30	0.91
9:V:143:ALA:O	9:V:147:THR:OG1	1.86	0.91
11:Y:99:LYS:O	11:Y:106:GLY:HA3	1.71	0.90
10:K:257:GLU:OE2	10:K:450:VAL:HG22	1.70	0.89
10:W:450:VAL:HA	10:W:453:LEU:CD1	2.03	0.89
6:F:29:LYS:HD2	6:F:75:ILE:HD11	1.52	0.89
9:V:149:LEU:HD21	9:V:281:LEU:HD21	1.52	0.89
9:V:14:ILE:CD1	14:Y:502:PEE:C25	2.49	0.89
14:H:401:PEE:H18	9:J:240:MET:SD	2.12	0.88
14:U:401:PEE:H17	9:V:240:MET:HE2	1.56	0.88
3:C:150:ALA:CB	9:V:168:TYR:CD2	2.55	0.88
12:G:101:CDL:H712	12:G:101:CDL:C52	2.03	0.87
11:Y:296:TRP:CE2	11:Y:419:THR:HG21	2.08	0.87
1:A:78:TYR:CE1	5:E:65:GLU:HA	2.08	0.87
10:K:183:ARG:NH1	10:W:451:ASP:OD2	2.08	0.86
9:V:137:GLN:NE2	9:V:141:TRP:HE1	1.73	0.86
10:K:438:MET:HB3	10:K:450:VAL:CG1	2.05	0.86
10:K:438:MET:CB	10:K:450:VAL:CG1	2.54	0.86
9:V:10:LEU:HD21	14:Y:502:PEE:H46	0.88	0.85
9:V:295:LEU:O	9:V:299:LEU:HD22	1.77	0.85
5:E:21:GLU:O	5:E:25:GLU:N	2.09	0.85
5:E:30:LEU:HD21	8:H:216:THR:CG2	2.07	0.85
11:L:70:THR:HG1	11:L:410:CYS:HG	1.25	0.85
9:V:344:SER:O	9:V:348:THR:HG23	1.76	0.84
10:W:259:ARG:NH1	10:W:449:PHE:CE1	2.44	0.84
11:Y:412:ASP:O	11:Y:416:SER:HB2	1.76	0.84
6:F:52:PRO:HG2	6:F:55:LEU:HB2	1.57	0.84
6:F:71:LEU:HD23	6:F:71:LEU:H	1.40	0.84
11:Y:296:TRP:CD1	11:Y:419:THR:HG21	1.91	0.84
5:E:30:LEU:HD21	8:H:216:THR:HG23	1.59	0.84
6:F:50:ARG:O	10:W:148:ARG:NH2	2.11	0.83
5:R:34:ARG:NH1	5:R:78:ARG:NH1	2.25	0.83
12:G:101:CDL:H542	12:G:101:CDL:H731	1.60	0.83
12:G:101:CDL:H332	12:G:101:CDL:CA6	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:503:PEE:H16	14:L:503:PEE:C31	2.08	0.83
1:A:25:ARG:HG2	3:C:91:TYR:O	1.79	0.83
14:H:401:PEE:H64	14:H:401:PEE:C43	2.08	0.82
2:B:27:ARG:HE	10:K:174:ILE:HD12	1.43	0.82
10:W:449:PHE:N	10:W:452:GLU:OE2	2.10	0.82
5:R:86:LEU:HD23	5:R:86:LEU:O	1.79	0.82
8:H:291:LYS:HD2	14:H:401:PEE:H8	1.62	0.82
17:L:501:PLX:H71	14:L:503:PEE:H17	1.60	0.81
5:R:79:ASP:HB3	8:U:92:PRO:HG2	1.60	0.81
8:U:307:LYS:NZ	12:U:403:CDL:OA3	2.12	0.81
5:E:29:PRO:CD	8:H:262:THR:HG21	2.09	0.81
5:E:34:ARG:CD	5:E:78:ARG:NH2	2.42	0.81
6:F:34:ARG:HG2	6:F:34:ARG:HH11	1.46	0.81
10:K:259:ARG:HG2	10:K:444:LEU:CD1	2.08	0.81
3:C:220:LEU:HB2	13:C:301:FES:S2	2.21	0.81
10:K:257:GLU:CD	10:K:450:VAL:HG22	1.99	0.81
10:W:257:GLU:OE2	10:W:450:VAL:N	2.09	0.81
7:T:39:ARG:HG2	7:T:39:ARG:HH21	1.45	0.80
8:U:121:CYS:SG	15:U:402:HEC:HBB2	2.21	0.80
17:Q:101:PLX:H322	14:Y:502:PEE:H59	1.63	0.80
5:E:28:ASP:OD1	5:E:30:LEU:N	2.15	0.80
9:V:326:TRP:CZ2	14:V:403:PEE:H13	2.16	0.80
1:A:78:TYR:CG	5:E:65:GLU:HG2	2.15	0.80
9:J:262:LEU:HD22	3:P:216:VAL:HG21	1.64	0.80
9:V:195:LEU:CD2	9:V:199:PHE:HE2	1.94	0.79
11:Y:74:TRP:O	11:Y:418:LEU:HD21	1.82	0.79
16:V:401:HEM:HBC2	16:V:401:HEM:HHD	1.64	0.79
12:J:405:CDL:H351	12:J:405:CDL:H732	1.65	0.79
7:T:35:ALA:HB1	14:Y:502:PEE:H75	1.63	0.78
1:A:82:LYS:HE2	5:E:60:ARG:HD3	1.66	0.78
12:G:101:CDL:H351	12:G:101:CDL:H742	1.64	0.78
10:K:363:GLN:HB2	10:K:365:ASN:OD1	1.83	0.78
8:U:315:LYS:HE3	12:U:403:CDL:H1	1.65	0.78
6:F:34:ARG:NH1	9:J:379:TRP:HE1	1.82	0.78
9:V:148:ASN:O	9:V:151:SER:HB3	1.84	0.78
10:K:438:MET:HB3	10:K:450:VAL:HG11	1.66	0.78
9:V:165:TRP:CZ3	9:V:168:TYR:O	2.37	0.78
9:J:149:LEU:HD21	9:J:281:LEU:HD21	1.65	0.77
12:G:101:CDL:H531	12:G:101:CDL:H731	1.66	0.77
14:L:503:PEE:H26	14:L:503:PEE:H48	1.66	0.77
6:F:29:LYS:HD3	6:F:75:ILE:HD13	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:34:ARG:HH11	5:R:78:ARG:HH22	1.33	0.77
11:Y:230:VAL:HG21	11:Y:418:LEU:CD1	2.15	0.77
14:H:401:PEE:H49	14:H:401:PEE:H14	1.65	0.77
9:J:324:LEU:HD11	9:J:369:ILE:HD12	1.65	0.77
10:W:375:LYS:NZ	10:W:416:ILE:O	2.18	0.77
5:R:78:ARG:O	5:R:82:VAL:HG23	1.84	0.76
10:W:277:VAL:HG13	10:W:278:ALA:HB2	1.66	0.76
6:F:68:ASP:HA	6:F:71:LEU:HD21	1.66	0.76
1:N:41:ARG:NE	12:N:101:CDL:OA4	2.19	0.76
6:S:36:ASP:OD2	6:S:62:ARG:NH1	2.19	0.75
10:W:450:VAL:HA	10:W:453:LEU:HD12	1.67	0.75
5:E:30:LEU:CD1	5:E:34:ARG:HH21	2.00	0.75
11:L:73:VAL:HG23	11:L:147:LEU:HD23	1.66	0.75
8:U:125:HIS:NE2	15:U:402:HEC:NC	2.33	0.75
12:L:502:CDL:H572	14:L:503:PEE:H66	0.84	0.75
2:B:2:LEU:HD22	10:K:278:ALA:HB1	1.68	0.75
2:B:52:ARG:NH1	11:L:343:THR:O	2.18	0.75
10:K:300:LYS:HG2	10:K:301:ARG:HG2	1.69	0.75
3:P:234:TYR:HB2	3:P:243:TYR:HB2	1.69	0.75
6:F:29:LYS:CG	6:F:75:ILE:HD13	2.16	0.74
2:O:33:THR:HA	2:O:38:PRO:HG3	1.69	0.74
10:W:270:ALA:HB2	10:W:339:TYR:HD1	1.52	0.74
1:N:67:PHE:HB2	9:V:346:PRO:HG3	1.69	0.74
9:V:195:LEU:CD2	9:V:199:PHE:CE2	2.70	0.74
12:G:101:CDL:OB8	12:G:101:CDL:H521	1.86	0.74
12:N:101:CDL:OA3	14:V:403:PEE:H12	1.86	0.74
11:Y:192:PHE:HB3	11:Y:195:THR:HB	1.70	0.74
9:J:8:ASN:HD22	9:J:11:MET:HG2	1.50	0.74
11:Y:421:GLY:C	11:Y:422:ARG:HG3	2.06	0.74
10:K:127:ARG:HB3	11:L:36:ALA:HB1	1.68	0.74
9:V:165:TRP:CE3	9:V:168:TYR:O	2.41	0.74
14:L:503:PEE:H50	14:L:503:PEE:C12	2.18	0.74
6:F:34:ARG:HG2	6:F:34:ARG:NH1	2.00	0.74
11:Y:171:GLU:OE2	11:Y:175:ASN:ND2	2.21	0.74
14:H:401:PEE:C13	9:J:240:MET:HE2	2.18	0.73
4:Q:30:MET:SD	7:T:34:TRP:HB2	2.29	0.73
10:K:438:MET:CE	10:K:450:VAL:HG13	2.16	0.73
10:W:65:ILE:HG22	10:W:67:ALA:H	1.53	0.73
1:A:78:TYR:CE1	5:E:64:GLU:C	2.62	0.73
14:H:401:PEE:C13	9:J:240:MET:HE1	2.09	0.73
10:K:125:CYS:HB3	10:K:133:LEU:HD22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:438:MET:CB	10:K:450:VAL:HG11	2.16	0.73
6:F:29:LYS:HG2	6:F:75:ILE:HG12	1.70	0.72
14:U:401:PEE:H27	14:U:401:PEE:H61	1.69	0.72
6:F:29:LYS:HG2	6:F:75:ILE:HD11	1.02	0.72
11:L:280:ASP:HA	11:L:461:PRO:HB3	1.71	0.72
9:V:96:LEU:HD23	14:V:403:PEE:H26	1.69	0.72
11:L:195:THR:HG22	11:L:197:LEU:H	1.53	0.72
12:J:405:CDL:H742	12:J:405:CDL:C78	2.20	0.72
6:F:29:LYS:HZ3	6:F:29:LYS:HB2	1.54	0.72
8:U:288:MET:CB	14:U:401:PEE:O4	2.35	0.72
10:K:65:ILE:HG22	10:K:67:ALA:H	1.54	0.72
11:Y:322:VAL:HG12	11:Y:323:HIS:H	1.53	0.72
4:Q:22:ALA:HB2	17:Q:101:PLX:H272	1.72	0.72
5:R:34:ARG:HH11	5:R:78:ARG:NH2	1.87	0.72
10:W:184:ASN:HB3	10:W:251:ALA:HA	1.72	0.72
12:G:101:CDL:H731	12:G:101:CDL:C54	2.18	0.71
11:Y:296:TRP:HD1	11:Y:419:THR:HG23	0.90	0.71
6:F:29:LYS:HD3	6:F:75:ILE:HD12	1.65	0.71
11:L:470:ARG:NH2	12:L:502:CDL:OA4	2.22	0.71
14:U:401:PEE:C13	9:V:240:MET:HE1	2.14	0.71
12:G:101:CDL:H712	12:G:101:CDL:H521	1.72	0.71
8:U:296:MET:HE2	14:U:401:PEE:H53	1.73	0.71
8:U:296:MET:HE1	14:U:401:PEE:C33	2.18	0.71
5:E:21:GLU:O	5:E:24:GLU:N	2.24	0.70
11:L:192:PHE:HB3	11:L:195:THR:HB	1.72	0.70
10:W:351:ILE:HD11	10:W:448:PRO:CD	2.20	0.70
6:F:29:LYS:HB2	6:F:29:LYS:NZ	2.06	0.70
9:V:324:LEU:HD11	9:V:369:ILE:HD12	1.72	0.70
9:V:344:SER:OG	9:V:346:PRO:HD2	1.91	0.70
11:Y:48:THR:HG22	11:Y:62:GLU:HB2	1.73	0.70
4:D:48:ASN:HB2	4:D:51:LYS:HD2	1.74	0.70
14:H:401:PEE:H28	14:H:401:PEE:C40	2.21	0.70
11:Y:417:LEU:HD23	11:Y:422:ARG:O	1.91	0.70
6:F:29:LYS:CD	6:F:75:ILE:HD12	2.17	0.70
14:H:401:PEE:C12	9:J:240:MET:HE1	2.22	0.70
11:Y:195:THR:HG22	11:Y:197:LEU:H	1.55	0.70
14:H:401:PEE:H15	9:J:240:MET:HE1	1.74	0.70
12:L:502:CDL:H772	14:L:503:PEE:H70	1.73	0.70
5:R:34:ARG:HH11	5:R:78:ARG:HH12	1.34	0.70
9:J:156:ILE:CG2	9:J:160:LEU:HB2	2.18	0.69
9:J:300:ILE:O	9:J:303:MET:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:57:PRO:HG2	11:Y:400:VAL:HG11	1.74	0.69
10:K:257:GLU:CG	10:K:450:VAL:CG2	2.70	0.69
2:B:8:SER:OG	2:B:26:LEU:O	2.09	0.69
6:F:14:LEU:O	6:F:17:ILE:HG13	1.92	0.69
10:W:261:GLN:NE2	10:W:443:ASN:O	2.25	0.69
8:U:202:ARG:NH1	8:U:279:GLU:OE2	2.25	0.69
9:V:332:LEU:CD1	14:V:403:PEE:H37	2.22	0.69
7:G:38:TRP:CD1	12:G:101:CDL:C51	2.74	0.69
11:L:171:GLU:OE2	11:L:175:ASN:ND2	2.26	0.69
3:C:216:VAL:HG21	9:V:262:LEU:HD22	1.74	0.69
9:V:80:ARG:NH1	16:V:401:HEM:O1A	2.25	0.69
5:E:34:ARG:CD	5:E:78:ARG:HH22	2.03	0.69
12:G:101:CDL:H542	12:G:101:CDL:C73	2.22	0.69
2:O:35:PRO:HB3	10:W:320:PRO:HA	1.75	0.69
6:F:39:TYR:CD1	6:F:40:GLU:N	2.61	0.69
12:G:101:CDL:HA62	12:G:101:CDL:C34	2.22	0.69
8:H:124:CYS:SG	15:H:402:HEC:HBC2	2.33	0.69
9:V:295:LEU:O	9:V:299:LEU:CD2	2.40	0.69
10:K:399:GLN:HE22	10:K:407:MET:HB3	1.56	0.68
6:S:67:LEU:HD23	9:V:209:LEU:HD12	1.75	0.68
5:E:30:LEU:HD12	5:E:30:LEU:O	1.93	0.68
10:K:257:GLU:HG3	10:K:450:VAL:CG2	2.23	0.68
9:V:150:LEU:HD23	9:V:164:ILE:HD13	1.75	0.68
10:K:100:THR:HG21	11:L:324:LEU:HB3	1.75	0.68
10:K:183:ARG:HH21	10:K:183:ARG:HG3	1.57	0.68
10:K:438:MET:HB2	10:K:450:VAL:CG1	2.22	0.68
7:T:24:TRP:CZ3	12:Y:501:CDL:H551	2.28	0.68
8:U:290:LEU:HD23	8:U:290:LEU:C	2.14	0.68
11:Y:285:ALA:HB3	11:Y:360:CYS:HB2	1.76	0.68
8:U:112:ARG:NH1	8:U:269:ASP:OD2	2.26	0.68
9:J:338:ILE:HD11	9:J:350:ILE:HG22	1.76	0.67
11:Y:165:ARG:NH2	11:Y:211:LEU:O	2.24	0.67
3:P:236:CYS:HB3	3:P:241:SER:HB2	1.74	0.67
9:J:66:ILE:HD11	9:J:134:PRO:HA	1.77	0.67
2:O:18:THR:OG1	10:W:110:LEU:O	2.11	0.67
5:R:79:ASP:HB3	8:U:92:PRO:CG	2.23	0.67
6:F:29:LYS:HD2	6:F:75:ILE:CD1	2.17	0.67
1:A:12:ARG:HG2	1:A:13:HIS:ND1	2.10	0.67
14:J:403:PEE:H25	14:J:403:PEE:H61	1.77	0.67
11:Y:101:THR:HA	11:Y:155:SER:H	1.60	0.67
2:B:16:SER:OG	2:B:19:SER:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:PHE:O	11:L:180:ARG:NH1	2.26	0.67
12:G:101:CDL:C53	12:G:101:CDL:H731	2.24	0.67
9:V:111:GLU:HG2	9:V:199:PHE:CE1	2.29	0.67
11:L:80:ARG:NH1	11:L:268:CYS:SG	2.67	0.67
11:Y:387:GLU:OE2	11:Y:390:ARG:NH2	2.23	0.67
6:F:33:MET:HG3	6:F:62:ARG:NH1	2.09	0.66
10:K:107:GLY:O	11:L:397:ASN:ND2	2.28	0.66
11:L:257:TYR:HD2	11:L:262:VAL:HG22	1.59	0.66
12:G:101:CDL:H531	12:G:101:CDL:C71	2.19	0.66
8:H:277:ALA:O	9:J:71:ARG:NH2	2.29	0.66
10:K:176:ASN:ND2	10:K:260:GLU:OE2	2.29	0.66
7:T:45:VAL:HG21	7:T:48:ILE:HB	1.77	0.66
2:O:17:ALA:HA	11:Y:319:GLY:H	1.61	0.66
9:V:195:LEU:HD21	9:V:199:PHE:HE2	1.60	0.66
5:E:27:VAL:O	5:E:28:ASP:HB3	1.96	0.66
5:E:34:ARG:HH22	8:H:216:THR:HG22	1.61	0.66
10:K:183:ARG:NH2	10:K:254:ARG:HB3	2.11	0.66
12:G:101:CDL:H521	12:G:101:CDL:CB7	2.25	0.66
9:V:326:TRP:HZ2	14:V:403:PEE:H13	1.60	0.66
10:W:60:ARG:HG3	10:W:124:GLU:HG2	1.78	0.66
11:Y:121:ASN:ND2	11:Y:132:TYR:OH	2.29	0.66
5:R:34:ARG:HH11	5:R:78:ARG:NH1	1.87	0.65
10:K:351:ILE:HD11	10:K:448:PRO:CG	2.27	0.65
9:J:165:TRP:O	9:J:174:THR:OG1	2.14	0.65
10:W:299:VAL:HG13	11:Y:120:LEU:HD11	1.79	0.65
3:C:162:GLY:O	3:C:227:ASN:ND2	2.30	0.65
11:L:280:ASP:O	11:L:362:ARG:NH2	2.30	0.65
10:W:449:PHE:HB2	10:W:452:GLU:OE1	1.97	0.65
6:F:36:ASP:OD2	6:F:62:ARG:NH1	2.28	0.65
4:Q:22:ALA:CB	17:Q:101:PLX:H272	2.26	0.65
7:T:42:LEU:O	7:T:45:VAL:CG2	2.34	0.65
14:U:401:PEE:C19	14:U:401:PEE:H64	2.27	0.65
10:K:36:GLN:NE2	10:K:39:GLU:OE2	2.29	0.65
1:N:12:ARG:HG2	1:N:13:HIS:ND1	2.12	0.65
10:K:230:LEU:HA	10:K:233:VAL:HG22	1.78	0.65
8:U:202:ARG:NH2	9:V:256:TYR:OH	2.28	0.65
11:L:48:THR:HG22	11:L:62:GLU:HB2	1.78	0.64
1:N:12:ARG:HG2	1:N:13:HIS:HD1	1.62	0.64
14:H:401:PEE:H49	14:H:401:PEE:C11	2.27	0.64
10:K:183:ARG:HH21	10:K:254:ARG:HB3	1.62	0.64
10:K:351:ILE:HD11	10:K:448:PRO:CD	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:401:HEM:HMC1	16:J:401:HEM:HBC2	1.80	0.64
12:J:405:CDL:HB61	12:J:405:CDL:C31	2.27	0.64
5:R:29:PRO:HD2	8:U:262:THR:HG21	1.79	0.64
12:L:502:CDL:C58	14:L:503:PEE:C38	2.76	0.64
11:Y:75:ILE:HG22	11:Y:77:VAL:H	1.62	0.64
10:K:60:ARG:HG3	10:K:124:GLU:HG2	1.78	0.64
10:K:365:ASN:OD1	10:K:365:ASN:N	2.31	0.64
10:K:422:ALA:O	10:K:426:ASN:ND2	2.31	0.64
10:W:444:LEU:HD23	10:W:447:THR:HG21	1.79	0.64
11:Y:424:ILE:CG2	11:Y:429:TRP:HE1	2.09	0.64
10:K:257:GLU:HG3	10:K:450:VAL:HG22	1.74	0.64
11:L:75:ILE:HG22	11:L:77:VAL:H	1.61	0.64
9:V:22:PRO:HB3	9:V:217:LYS:HB3	1.78	0.64
8:H:202:ARG:NH2	9:J:256:TYR:OH	2.31	0.64
6:F:40:GLU:HG2	6:F:45:LYS:HG3	1.77	0.63
5:R:34:ARG:CZ	5:R:78:ARG:HH12	2.11	0.63
10:W:313:VAL:HG21	10:W:323:VAL:HG21	1.80	0.63
11:Y:460:GLY:HA2	11:Y:462:ILE:HD12	1.78	0.63
1:A:49:VAL:HG21	14:J:403:PEE:O5	1.98	0.63
14:J:403:PEE:H61	14:J:403:PEE:H28	1.81	0.63
8:U:288:MET:SD	14:U:401:PEE:O4	2.55	0.63
10:K:413:LEU:HA	10:K:416:ILE:HG22	1.80	0.63
6:F:28:ASN:OD1	6:F:29:LYS:N	2.31	0.63
8:H:262:THR:HG22	8:H:264:SER:H	1.63	0.63
11:L:322:VAL:HG12	11:L:323:HIS:H	1.64	0.63
9:V:332:LEU:HD11	14:V:403:PEE:H37	1.79	0.63
2:O:7:ARG:NH1	10:W:287:SER:OG	2.32	0.63
9:V:333:LEU:HD21	14:V:403:PEE:C39	2.29	0.63
10:W:151:VAL:HG12	10:W:155:GLN:HE21	1.64	0.63
11:Y:280:ASP:HA	11:Y:461:PRO:HB3	1.79	0.63
10:K:70:ARG:NH2	10:K:332:ASP:OD2	2.31	0.63
6:S:97:GLU:OE1	6:S:100:ARG:NH2	2.31	0.63
9:V:200:LEU:HD13	16:V:402:HEM:HAD2	1.79	0.63
10:W:450:VAL:O	10:W:453:LEU:HD13	1.98	0.63
1:A:19:LEU:HD23	11:L:273:SER:HB3	1.81	0.62
10:K:185:ALA:HB3	10:K:251:ALA:HB2	1.81	0.62
8:U:296:MET:CE	14:U:401:PEE:C33	2.71	0.62
9:V:138:MET:HB2	9:V:255:ASN:HD21	1.62	0.62
4:D:53:TRP:NE1	8:H:139:CYS:O	2.32	0.62
10:K:184:ASN:HB3	10:K:251:ALA:HA	1.81	0.62
11:L:228:ARG:HH22	11:L:263:PRO:HG2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:34:ARG:HG3	5:R:78:ARG:HH12	1.61	0.62
12:G:101:CDL:H551	12:G:101:CDL:H512	1.81	0.62
8:H:112:ARG:NH1	8:H:269:ASP:OD2	2.31	0.62
8:H:202:ARG:HD2	8:H:279:GLU:HG3	1.81	0.62
8:H:231:LEU:HD21	3:P:239:HIS:HA	1.81	0.62
11:Y:424:ILE:HG23	11:Y:424:ILE:O	2.00	0.62
10:K:295:ALA:HB2	10:K:325:ALA:HB3	1.82	0.62
10:W:443:ASN:O	10:W:444:LEU:HB2	2.00	0.62
10:W:127:ARG:NH1	10:W:224:GLY:O	2.31	0.62
5:E:26:LEU:O	5:E:28:ASP:N	2.27	0.62
11:L:70:THR:OG1	11:L:410:CYS:SG	2.50	0.62
5:R:30:LEU:HD13	5:R:86:LEU:HD11	1.82	0.62
9:V:119:LEU:HD12	9:V:192:LEU:HB3	1.81	0.62
9:V:141:TRP:HB3	9:V:268:ILE:HD11	1.82	0.61
12:L:502:CDL:C58	14:L:503:PEE:H63	2.29	0.61
10:W:299:VAL:HG21	11:Y:110:GLU:HG3	1.81	0.61
6:F:34:ARG:HH11	6:F:34:ARG:CG	2.13	0.61
11:L:96:LEU:HD23	11:L:164:GLU:HG3	1.80	0.61
7:T:38:TRP:CE3	7:T:41:ILE:HD13	2.35	0.61
10:W:125:CYS:HB3	10:W:133:LEU:HD22	1.81	0.61
12:L:502:CDL:H572	14:L:503:PEE:C38	2.24	0.61
10:K:51:SER:HB2	10:K:230:LEU:HD12	1.82	0.61
9:J:96:LEU:HD23	14:J:403:PEE:H26	1.82	0.61
11:L:165:ARG:NH2	11:L:211:LEU:O	2.32	0.61
5:R:34:ARG:HH11	5:R:78:ARG:CZ	2.13	0.61
8:U:135:LEU:HA	8:U:138:VAL:HG12	1.82	0.61
8:U:242:ILE:HG12	8:U:244:MET:H	1.64	0.61
3:C:104:ARG:HH21	11:L:292:GLU:HG3	1.64	0.61
4:Q:34:ARG:HH12	4:Q:38:GLN:HB3	1.64	0.61
8:U:308:ARG:HH11	12:U:403:CDL:H1O1	1.47	0.61
10:W:116:ARG:NH1	10:W:188:ASN:O	2.33	0.61
10:W:318:GLN:HB3	10:W:320:PRO:HD2	1.83	0.61
4:D:48:ASN:HD22	8:H:104:SER:HB3	1.66	0.61
12:L:502:CDL:OA9	14:L:503:PEE:O5	2.19	0.61
14:L:503:PEE:H49	14:L:503:PEE:H26	1.78	0.61
6:F:29:LYS:CB	6:F:75:ILE:HD11	2.22	0.61
10:K:183:ARG:HH21	10:K:183:ARG:CG	2.14	0.61
5:R:86:LEU:HD23	5:R:86:LEU:C	2.21	0.61
9:V:83:HIS:NE2	16:V:401:HEM:C4D	2.67	0.61
8:U:133:ARG:O	8:U:135:LEU:N	2.29	0.60
5:E:30:LEU:HD21	8:H:216:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:CYS:CB	15:H:402:HEC:HBC2	2.31	0.60
9:V:272:TRP:HA	9:V:275:LEU:HG	1.84	0.60
12:J:404:CDL:HB62	9:V:13:LEU:HD22	1.83	0.60
10:K:363:GLN:CB	10:K:365:ASN:OD1	2.49	0.60
11:Y:460:GLY:HA2	11:Y:462:ILE:H	1.65	0.60
1:A:78:TYR:HB3	5:E:65:GLU:HG2	0.68	0.60
1:N:73:LYS:O	1:N:77:ALA:N	2.35	0.60
9:V:200:LEU:CD1	16:V:402:HEM:HAD2	2.32	0.60
6:S:71:LEU:O	8:U:315:LYS:NZ	2.35	0.60
9:V:206:ASN:OD1	9:V:207:ASN:N	2.34	0.60
7:T:14:VAL:O	7:T:18:VAL:HG23	2.02	0.60
11:Y:98:PHE:CZ	11:Y:120:LEU:HD13	2.36	0.60
2:O:34:VAL:HB	2:O:35:PRO:HD3	1.83	0.60
7:T:39:ARG:HH21	7:T:39:ARG:CG	2.15	0.60
11:Y:89:ALA:O	11:Y:93:LEU:HG	2.02	0.60
11:Y:96:LEU:HA	11:Y:99:LYS:HG2	1.83	0.60
2:B:7:ARG:NH1	10:K:287:SER:OG	2.25	0.60
7:G:38:TRP:O	7:G:42:LEU:HD12	2.02	0.60
9:J:282:ARG:HD2	9:J:343:VAL:HG22	1.83	0.60
11:Y:96:LEU:CD2	11:Y:161:ILE:CD1	2.80	0.60
8:H:315:LYS:NZ	12:H:403:CDL:OB3	2.21	0.59
10:K:101:ARG:NH1	11:L:325:SER:O	2.33	0.59
1:A:71:LYS:HE2	8:H:87:LEU:HD12	1.84	0.59
11:L:79:SER:HB3	11:L:126:ARG:HA	1.84	0.59
3:P:131:ASN:HD22	14:U:401:PEE:H7	1.66	0.59
11:Y:73:VAL:HG23	11:Y:147:LEU:HD23	1.83	0.59
12:L:502:CDL:H761	14:L:503:PEE:H74	1.82	0.59
6:S:43:ASP:OD2	6:S:102:ARG:NH1	2.35	0.59
9:V:181:PHE:HA	9:V:184:ILE:HG22	1.83	0.59
9:V:311:LYS:HG3	9:V:379:TRP:HE1	1.67	0.59
12:G:101:CDL:H521	12:G:101:CDL:C71	2.32	0.59
4:Q:48:ASN:HB2	4:Q:51:LYS:HD2	1.85	0.59
2:B:33:THR:HA	2:B:38:PRO:HG3	1.82	0.59
4:D:34:ARG:NH1	4:D:38:GLN:OE1	2.35	0.59
1:A:40:ARG:HG3	1:A:41:ARG:N	2.17	0.59
5:R:30:LEU:HD21	8:U:216:THR:HG23	1.84	0.59
7:T:40:LEU:HD12	7:T:40:LEU:C	2.21	0.59
11:Y:326:SER:O	11:Y:330:SER:N	2.30	0.59
5:E:33:VAL:HG11	5:E:85:LYS:O	2.03	0.59
3:P:79:SER:N	3:P:82:ASP:OD2	2.35	0.59
9:V:338:ILE:HD11	9:V:350:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:CG	5:E:65:GLU:HA	2.33	0.59
2:B:37:THR:HA	11:L:174:GLU:HG2	1.85	0.59
10:W:70:ARG:NH2	10:W:332:ASP:OD2	2.21	0.59
3:P:244:ASP:OD1	3:P:248:ARG:N	2.36	0.58
3:C:96:VAL:O	11:L:269:ARG:NH1	2.36	0.58
3:C:132:ALA:HB2	14:H:401:PEE:H24	1.84	0.58
3:P:81:THR:HG21	11:Y:202:GLU:HB2	1.84	0.58
6:S:7:VAL:HB	6:S:10:SER:HB2	1.84	0.58
11:L:387:GLU:OE2	11:L:390:ARG:NH2	2.27	0.58
9:V:333:LEU:HD21	14:V:403:PEE:H62	1.85	0.58
16:V:402:HEM:HMB1	16:V:402:HEM:HBB2	1.85	0.58
11:Y:98:PHE:CD2	11:Y:120:LEU:HD13	2.29	0.58
1:A:29:HIS:HD2	1:A:33:LYS:HB2	1.69	0.58
10:K:57:PRO:O	10:K:127:ARG:HG3	2.04	0.58
10:K:323:VAL:HG13	10:K:340:THR:HG22	1.85	0.58
10:K:438:MET:HB3	10:K:450:VAL:HG13	1.86	0.58
5:R:37:CYS:SG	5:R:85:LYS:NZ	2.73	0.58
16:V:402:HEM:HBA1	16:V:402:HEM:HHA	1.86	0.58
10:W:357:GLN:O	10:W:360:THR:OG1	2.17	0.58
6:F:41:ASP:OD1	6:F:41:ASP:N	2.36	0.58
9:J:100:ARG:NH2	16:J:402:HEM:O2A	2.37	0.58
8:U:296:MET:HE2	14:U:401:PEE:H51	1.86	0.58
11:Y:423:ARG:O	11:Y:424:ILE:HG22	2.03	0.58
3:C:204:ARG:NH1	3:C:248:ARG:HG3	2.19	0.57
11:L:282:LEU:HB2	11:L:461:PRO:HD3	1.86	0.57
6:F:36:ASP:OD1	6:F:90:TYR:OH	2.18	0.57
3:P:183:GLU:HA	3:P:186:GLN:HG2	1.86	0.57
9:V:343:VAL:HG13	9:V:348:THR:HG22	1.84	0.57
2:B:27:ARG:NH1	10:K:171:THR:HG22	2.19	0.57
10:K:177:LEU:HD21	10:K:272:VAL:HG21	1.85	0.57
17:L:501:PLX:H71	14:L:503:PEE:C13	2.33	0.57
9:J:283:SER:O	9:J:352:GLN:NE2	2.33	0.57
1:A:78:TYR:CD1	5:E:65:GLU:N	2.73	0.57
9:J:163:TRP:CD2	12:J:405:CDL:H331	2.39	0.57
3:P:104:ARG:NH2	11:Y:293:GLY:O	2.37	0.57
9:V:14:ILE:HD13	14:Y:502:PEE:C25	2.22	0.57
9:V:333:LEU:CD2	14:V:403:PEE:H66	2.35	0.57
14:Y:502:PEE:H19	14:Y:502:PEE:O4	2.04	0.57
6:F:97:GLU:OE2	10:W:147:ARG:NH1	2.38	0.57
9:J:206:ASN:OD1	9:J:207:ASN:N	2.37	0.57
11:Y:113:VAL:HG21	11:Y:120:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:98:PHE:CE2	11:Y:120:LEU:HD12	2.36	0.57
11:L:134:LYS:NZ	11:L:407:THR:OG1	2.38	0.57
3:P:197:ASP:O	3:P:257:ASN:ND2	2.37	0.57
6:S:70:ASN:HD22	9:V:209:LEU:HG	1.69	0.57
7:T:40:LEU:HD12	7:T:41:ILE:H	1.64	0.57
10:W:274:GLU:OE2	10:W:333:SER:OG	2.16	0.57
10:W:217:ARG:HE	10:W:245:GLY:HA3	1.69	0.57
10:W:449:PHE:HB2	10:W:452:GLU:OE2	2.04	0.57
9:V:333:LEU:HD22	14:V:403:PEE:H66	1.87	0.56
14:H:401:PEE:H66	14:H:401:PEE:C18	2.30	0.56
6:F:67:LEU:O	6:F:71:LEU:HD23	2.05	0.56
8:H:156:ASP:OD1	8:H:157:GLY:N	2.37	0.56
10:K:378:LEU:HB3	10:K:416:ILE:HD11	1.87	0.56
1:N:19:LEU:HD23	11:Y:273:SER:HB3	1.86	0.56
1:N:19:LEU:HD11	3:P:88:PHE:HB3	1.88	0.56
11:Y:96:LEU:HD23	11:Y:161:ILE:HD13	1.87	0.56
11:Y:280:ASP:O	11:Y:362:ARG:NH2	2.37	0.56
9:J:24:PRO:HD2	9:J:27:ILE:HD11	1.87	0.56
9:J:51:LEU:HD13	16:J:401:HEM:HBD1	1.88	0.56
10:K:351:ILE:HD11	10:K:448:PRO:HD2	1.86	0.56
1:N:41:ARG:HE	12:N:101:CDL:PA1	2.28	0.56
11:Y:74:TRP:CD2	11:Y:414:GLY:HA3	2.40	0.56
8:H:242:ILE:HG12	8:H:244:MET:H	1.70	0.56
3:P:204:ARG:NH1	3:P:246:SER:O	2.38	0.56
8:U:315:LYS:HZ2	12:U:403:CDL:HB22	1.71	0.56
15:U:402:HEC:HHC	15:U:402:HEC:HBB3	1.88	0.56
10:W:272:VAL:HG11	10:W:335:LEU:HB3	1.87	0.56
9:J:100:ARG:HH22	16:J:402:HEM:HBD1	1.71	0.56
11:L:470:ARG:HH22	12:L:502:CDL:PA1	2.28	0.56
10:W:185:ALA:HB3	10:W:251:ALA:HB2	1.88	0.56
10:K:259:ARG:CD	10:K:444:LEU:HD13	2.30	0.56
10:K:375:LYS:NZ	10:K:416:ILE:O	2.30	0.56
2:O:20:ARG:HD2	2:O:51:SER:HB3	1.88	0.56
8:U:133:ARG:NH1	9:V:72:ASP:OD1	2.32	0.56
10:W:259:ARG:NH2	10:W:447:THR:OG1	2.39	0.56
10:K:195:TYR:O	10:K:199:LYS:NZ	2.30	0.56
10:K:387:GLU:OE2	11:L:406:THR:OG1	2.15	0.56
9:V:111:GLU:HG2	9:V:199:PHE:CD1	2.41	0.56
11:Y:230:VAL:CG2	11:Y:418:LEU:HD11	2.36	0.56
7:G:17:TRP:NE1	11:L:382:SER:OG	2.39	0.56
9:V:165:TRP:O	9:V:174:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:181:PHE:HA	9:J:184:ILE:HG22	1.88	0.55
16:J:401:HEM:HBB2	16:J:401:HEM:HMB2	1.88	0.55
11:L:337:LEU:HB3	11:L:368:MET:HG2	1.87	0.55
3:P:131:ASN:O	3:P:135:GLN:HG2	2.05	0.55
3:C:83:ILE:HD12	11:L:189:ALA:HB2	1.87	0.55
6:F:29:LYS:HG2	6:F:75:ILE:HD13	1.67	0.55
12:J:405:CDL:HB62	12:J:405:CDL:OB7	2.05	0.55
10:K:399:GLN:NE2	10:K:407:MET:HB3	2.20	0.55
5:E:30:LEU:CD2	8:H:216:THR:HG23	2.33	0.55
10:K:235:GLU:HA	10:K:238:LEU:HD13	1.88	0.55
3:P:123:VAL:HG13	4:Q:29:VAL:HG22	1.87	0.55
3:P:220:LEU:HB2	13:P:301:FES:S2	2.46	0.55
11:Y:424:ILE:HG23	11:Y:429:TRP:NE1	2.12	0.55
9:J:316:MET:HA	9:J:322:GLN:NE2	2.21	0.55
8:H:304:TYR:HE1	12:H:403:CDL:OA3	1.90	0.55
3:P:155:LYS:HZ3	3:P:273:VAL:HG21	1.70	0.55
11:Y:152:GLN:HE21	11:Y:253:ILE:HG13	1.72	0.55
2:O:27:ARG:NH1	10:W:171:THR:HG22	2.21	0.55
11:Y:160:GLN:NE2	11:Y:164:GLU:OE2	2.39	0.55
6:F:49:ARG:HE	6:F:49:ARG:HA	1.71	0.55
15:H:402:HEC:HBC3	15:H:402:HEC:HHD	1.87	0.55
9:J:119:LEU:HD11	9:J:192:LEU:HB3	1.89	0.55
10:K:93:GLY:HA3	10:K:139:ASN:HD21	1.72	0.55
1:N:43:ARG:HA	1:N:46:PHE:HD2	1.72	0.55
3:P:204:ARG:NH1	3:P:248:ARG:HG3	2.21	0.55
6:S:68:ASP:HA	6:S:71:LEU:HD12	1.89	0.55
11:Y:161:ILE:O	11:Y:165:ARG:HG3	2.07	0.55
6:F:27:PHE:CD1	6:F:28:ASN:N	2.75	0.55
9:V:138:MET:HB2	9:V:255:ASN:ND2	2.22	0.55
11:L:470:ARG:HH12	12:L:502:CDL:HA31	1.72	0.54
3:P:207:LYS:HD3	3:P:265:PHE:HE2	1.71	0.54
10:K:364:GLY:HA2	10:K:425:ILE:HD12	1.89	0.54
11:L:465:LEU:HD12	11:L:466:PRO:HD2	1.89	0.54
14:U:401:PEE:C19	14:U:401:PEE:C39	2.86	0.54
10:W:449:PHE:HB2	10:W:452:GLU:CD	2.27	0.54
1:A:78:TYR:O	1:A:81:ASP:HB2	2.07	0.54
3:C:153:GLU:HB3	3:C:273:VAL:HB	1.88	0.54
12:G:101:CDL:H331	9:V:163:TRP:CD1	2.43	0.54
4:Q:48:ASN:HD22	8:U:104:SER:HB3	1.72	0.54
9:V:10:LEU:CD2	14:Y:502:PEE:H45	2.34	0.54
9:V:326:TRP:CH2	14:V:403:PEE:H51	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HA	11:L:279:ASP:HA	1.89	0.54
11:L:311:ILE:O	11:L:326:SER:OG	2.26	0.54
11:Y:76:ASP:HB3	11:Y:228:ARG:HG3	1.89	0.54
11:Y:156:LEU:HB2	11:Y:213:ARG:HE	1.73	0.54
1:A:19:LEU:HD11	3:C:88:PHE:HB3	1.88	0.54
3:C:173:PRO:HB2	3:C:215:GLY:HA3	1.90	0.54
12:J:405:CDL:C78	12:J:405:CDL:C74	2.85	0.54
11:L:77:VAL:HG21	11:L:223:HIS:HB3	1.89	0.54
10:W:185:ALA:HB2	10:W:249:ALA:HB1	1.89	0.54
11:Y:79:SER:HB3	11:Y:126:ARG:HA	1.90	0.54
1:A:78:TYR:CE1	5:E:65:GLU:CA	2.87	0.54
3:C:164:ASN:OD1	3:C:165:MET:N	2.41	0.54
9:V:150:LEU:CD2	9:V:164:ILE:HD13	2.37	0.54
2:B:29:LEU:O	2:B:31:GLN:N	2.38	0.54
16:J:402:HEM:HBC2	16:J:402:HEM:HMC2	1.89	0.54
2:O:45:LEU:HA	11:Y:284:PHE:HE2	1.71	0.54
4:D:60:TYR:HD2	8:H:141:THR:HG21	1.72	0.54
11:L:294:PRO:HG3	11:L:448:TYR:CZ	2.43	0.54
10:K:36:GLN:HG2	10:K:53:GLU:HB3	1.90	0.53
10:K:217:ARG:HH21	10:K:246:LEU:H	1.56	0.53
2:O:5:ALA:HB1	10:W:385:SER:HB2	1.90	0.53
11:L:66:GLN:NE2	11:L:406:THR:OG1	2.41	0.53
12:L:502:CDL:C58	14:L:503:PEE:H62	2.37	0.53
2:B:31:GLN:NE2	10:K:297:PRO:HA	2.24	0.53
5:E:21:GLU:O	5:E:24:GLU:CA	2.57	0.53
6:S:28:ASN:HD22	6:S:82:THR:HB	1.73	0.53
16:V:401:HEM:HBB2	16:V:401:HEM:HMB1	1.91	0.53
16:V:402:HEM:HMC2	16:V:402:HEM:HBC2	1.90	0.53
10:W:267:VAL:HG11	10:W:347:ALA:HB2	1.90	0.53
1:A:12:ARG:HG2	1:A:13:HIS:CE1	2.43	0.53
1:N:12:ARG:HG3	11:Y:279:ASP:HA	1.91	0.53
12:N:101:CDL:OB9	9:V:29:ALA:HB3	2.08	0.53
9:V:149:LEU:HD21	9:V:281:LEU:CD2	2.31	0.53
2:B:54:SER:HA	11:L:402:HIS:CE1	2.43	0.53
6:F:70:ASN:HB3	9:J:26:ASN:HB2	1.91	0.53
2:O:45:LEU:HD13	10:W:160:ILE:HG23	1.91	0.53
6:S:55:LEU:HD21	6:S:90:TYR:CD2	2.43	0.53
9:V:341:GLN:HB3	9:V:342:PRO:HD2	1.91	0.53
9:J:173:PRO:O	9:J:177:ARG:HG2	2.09	0.53
9:J:229:ALA:HB1	17:L:501:PLX:H131	1.90	0.53
10:K:116:ARG:HH21	10:K:175:GLU:HG3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:57:PRO:HG2	11:L:400:VAL:HG11	1.91	0.53
6:F:36:ASP:OD1	6:F:62:ARG:NH1	2.42	0.53
6:F:72:LYS:O	6:F:73:HIS:HB2	2.09	0.53
10:K:254:ARG:NH2	10:W:257:GLU:OE1	2.41	0.53
10:K:289:LEU:O	10:K:293:LEU:HD13	2.09	0.53
10:K:319:GLN:O	10:K:321:PHE:N	2.41	0.53
1:N:20:SER:HB3	1:N:23:GLU:HG2	1.91	0.53
3:P:194:GLN:O	3:P:250:ARG:NH1	2.40	0.53
2:B:30:VAL:O	2:B:33:THR:OG1	2.22	0.53
5:E:34:ARG:HD3	5:E:78:ARG:CZ	2.35	0.53
6:F:67:LEU:CD2	9:J:209:LEU:HD12	2.28	0.53
12:L:502:CDL:C76	14:L:503:PEE:H74	2.38	0.53
3:P:131:ASN:ND2	14:U:401:PEE:H7	2.24	0.53
7:T:19:PRO:HA	7:T:22:TYR:HD2	1.74	0.53
11:Y:70:THR:HG1	11:Y:410:CYS:HG	1.57	0.53
12:J:405:CDL:HB61	12:J:405:CDL:H312	1.90	0.52
9:J:281:LEU:HD11	9:J:294:LEU:HD22	1.90	0.52
11:L:121:ASN:ND2	11:L:132:TYR:OH	2.36	0.52
8:U:98:HIS:NE2	8:U:208:GLU:OE2	2.38	0.52
12:G:101:CDL:H741	9:V:156:ILE:HG23	1.91	0.52
5:R:37:CYS:SG	5:R:85:LYS:CE	2.97	0.52
11:Y:473:SER:HB3	14:Y:502:PEE:H10	1.91	0.52
11:L:285:ALA:HB3	11:L:360:CYS:SG	2.50	0.52
11:L:361:ASP:OD1	11:L:362:ARG:N	2.42	0.52
3:C:80:HIS:CE1	11:L:185:ASN:HD22	2.27	0.52
8:H:291:LYS:HD2	14:H:401:PEE:C3	2.37	0.52
14:H:401:PEE:C40	14:H:401:PEE:C18	2.86	0.52
10:K:299:VAL:HG21	11:L:110:GLU:HG3	1.91	0.52
9:V:333:LEU:HD21	14:V:403:PEE:C38	2.39	0.52
10:K:352:LYS:HE2	10:K:453:LEU:CB	2.40	0.52
1:A:78:TYR:HE1	5:E:64:GLU:C	1.99	0.52
12:J:405:CDL:H312	12:J:405:CDL:OB4	2.10	0.52
4:Q:51:LYS:O	8:U:107:HIS:ND1	2.32	0.52
8:H:135:LEU:HA	8:H:138:VAL:HG12	1.91	0.52
11:Y:96:LEU:CD2	11:Y:161:ILE:HD13	2.40	0.52
11:Y:160:GLN:O	11:Y:164:GLU:HG2	2.09	0.52
11:Y:462:ILE:HG23	11:Y:465:LEU:HB3	1.91	0.52
3:C:219:HIS:ND1	13:C:301:FES:S1	2.74	0.52
3:P:128:ALA:HB1	14:U:401:PEE:H55	1.90	0.52
3:P:239:HIS:HB2	13:P:301:FES:S1	2.50	0.52
9:V:173:PRO:HB2	9:V:177:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:134:LYS:NZ	11:Y:407:THR:OG1	2.42	0.52
11:L:334:ALA:H	11:L:336:LYS:H	1.58	0.52
11:L:470:ARG:NH1	12:L:502:CDL:HA31	2.25	0.52
9:V:97:HIS:CE1	9:V:100:ARG:HH21	2.27	0.52
12:J:405:CDL:OA9	12:J:405:CDL:H332	2.10	0.51
12:J:405:CDL:H111	14:Y:502:PEE:C45	2.30	0.51
10:K:116:ARG:NH2	10:K:175:GLU:HG3	2.24	0.51
10:K:146:PHE:HD2	10:K:206:HIS:CE1	2.28	0.51
11:L:460:GLY:HA2	11:L:462:ILE:HG13	1.92	0.51
3:P:153:GLU:HB3	3:P:273:VAL:HB	1.91	0.51
1:A:41:ARG:NE	12:A:101:CDL:OA4	2.34	0.51
3:C:244:ASP:OD1	3:C:248:ARG:N	2.44	0.51
7:G:9:ARG:HD3	6:S:109:ALA:O	2.10	0.51
14:U:401:PEE:H57	9:V:236:LEU:HD13	1.92	0.51
11:Y:230:VAL:HG21	11:Y:418:LEU:HD11	1.92	0.51
11:Y:437:ASP:OD1	11:Y:438:ALA:N	2.43	0.51
6:F:109:ALA:O	7:T:9:ARG:HD3	2.11	0.51
9:J:191:ALA:O	9:J:194:THR:OG1	2.20	0.51
12:L:502:CDL:H772	14:L:503:PEE:C43	2.41	0.51
8:U:125:HIS:HB3	8:U:197:LEU:HD13	1.91	0.51
10:W:309:LEU:HD23	10:W:323:VAL:HG12	1.93	0.51
4:D:43:ILE:O	4:D:47:ILE:HD12	2.10	0.51
10:K:65:ILE:HG13	10:K:218:MET:HG2	1.92	0.51
10:K:159:LYS:HG3	10:K:197:ILE:HG21	1.92	0.51
8:U:270:VAL:HG11	15:U:402:HEC:HMB1	1.93	0.51
10:W:57:PRO:O	10:W:127:ARG:HG3	2.11	0.51
11:Y:296:TRP:CD1	11:Y:419:THR:CB	2.67	0.51
3:C:183:GLU:HA	3:C:186:GLN:HG2	1.93	0.51
6:F:43:ASP:OD2	6:F:102:ARG:NH1	2.44	0.51
9:J:103:TYR:O	9:J:315:MET:HB2	2.10	0.51
9:V:47:THR:HG23	9:V:79:ILE:HG23	1.93	0.51
10:W:101:ARG:NH1	11:Y:325:SER:O	2.44	0.51
11:Y:230:VAL:HG21	11:Y:418:LEU:HD13	1.92	0.51
11:Y:304:LEU:HD13	11:Y:354:LEU:HD11	1.92	0.51
5:E:75:LEU:HD23	5:E:78:ARG:HD3	1.92	0.51
9:V:96:LEU:CD2	14:V:403:PEE:H26	2.40	0.51
9:V:263:ASN:OD1	9:V:264:THR:N	2.44	0.51
10:W:107:GLY:O	11:Y:397:ASN:ND2	2.41	0.51
10:W:180:ALA:HA	10:W:254:ARG:NH1	2.26	0.51
5:E:21:GLU:O	5:E:24:GLU:CB	2.59	0.51
6:F:63:ILE:HD13	9:J:211:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:438:MET:HB2	10:K:450:VAL:HG11	1.89	0.51
6:S:71:LEU:HD21	9:V:25:SER:HB2	1.92	0.51
9:V:326:TRP:CH2	14:V:403:PEE:H13	2.46	0.51
7:G:39:ARG:HB2	12:G:101:CDL:HB31	1.93	0.51
10:W:95:SER:O	10:W:99:ILE:HD12	2.11	0.51
10:W:214:THR:HG22	10:W:216:ALA:H	1.75	0.51
11:Y:182:VAL:HG12	11:Y:186:TYR:CE2	2.46	0.51
12:G:101:CDL:C54	12:G:101:CDL:C73	2.85	0.51
10:W:288:VAL:O	10:W:292:VAL:HG23	2.11	0.51
3:C:132:ALA:CB	14:H:401:PEE:H24	2.41	0.50
5:E:29:PRO:HD2	8:H:262:THR:HG21	1.91	0.50
10:K:92:LYS:HD2	10:K:143:ALA:HB1	1.93	0.50
10:K:309:LEU:HD23	10:K:323:VAL:HG12	1.92	0.50
1:N:29:HIS:ND1	1:N:33:LYS:HB2	2.27	0.50
8:U:104:SER:OG	8:U:283:ASP:OD1	2.27	0.50
9:V:282:ARG:NH1	9:V:343:VAL:HG22	2.26	0.50
1:A:74:ASN:N	1:A:75:PRO:HD2	2.27	0.50
3:C:197:ASP:O	3:C:257:ASN:ND2	2.45	0.50
7:G:16:ASN:ND2	11:L:442:ARG:HH12	2.09	0.50
9:J:326:TRP:CH2	14:J:403:PEE:H50	2.46	0.50
12:L:502:CDL:H772	14:L:503:PEE:C42	2.38	0.50
1:N:42:ILE:HG22	1:N:46:PHE:CE2	2.47	0.50
3:P:242:HIS:HB2	3:P:251:LEU:HB2	1.92	0.50
9:V:141:TRP:HZ2	9:V:260:ASN:O	1.93	0.50
9:V:173:PRO:HB2	9:V:177:ARG:NH1	2.27	0.50
11:Y:412:ASP:O	11:Y:416:SER:CB	2.56	0.50
15:H:402:HEC:HBB3	15:H:402:HEC:HHC	1.92	0.50
11:L:285:ALA:HB2	11:L:461:PRO:O	2.11	0.50
9:V:87:ALA:HB2	16:V:401:HEM:HHB	1.92	0.50
3:C:123:VAL:HG13	4:D:29:VAL:HG22	1.94	0.50
6:F:39:TYR:HD1	6:F:40:GLU:H	1.59	0.50
16:J:402:HEM:HMB1	16:J:402:HEM:HBB2	1.92	0.50
11:L:161:ILE:O	11:L:165:ARG:HG3	2.12	0.50
11:Y:168:ILE:O	11:Y:172:MET:HG2	2.11	0.50
10:K:185:ALA:HB2	10:K:249:ALA:HB1	1.92	0.50
8:U:193:LEU:HD12	8:U:194:PRO:HD2	1.93	0.50
9:V:151:SER:HB2	9:V:161:VAL:HG21	1.92	0.50
10:W:254:ARG:HG2	10:W:256:GLY:H	1.76	0.50
11:L:308:ASN:HD21	11:L:345:SER:HB3	1.77	0.50
3:P:160:PRO:HD2	3:P:163:LYS:HD3	1.94	0.50
4:D:16:ARG:NH1	11:L:446:SER:OG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:125:HIS:HB3	8:H:197:LEU:HD13	1.94	0.50
10:K:49:ILE:HG12	10:K:50:ALA:N	2.26	0.50
2:O:28:PRO:HG3	10:W:324:SER:OG	2.10	0.50
7:T:38:TRP:CD2	7:T:41:ILE:HD13	2.47	0.50
7:T:40:LEU:CD1	7:T:41:ILE:N	2.56	0.50
10:K:183:ARG:NH2	10:K:183:ARG:CG	2.73	0.50
10:K:299:VAL:HG13	11:L:120:LEU:HD11	1.94	0.50
1:A:20:SER:HB3	1:A:23:GLU:HG2	1.94	0.50
1:A:28:PRO:HB2	1:A:29:HIS:CE1	2.46	0.50
4:Q:34:ARG:NH1	4:Q:38:GLN:HB3	2.26	0.50
6:S:54:ASN:OD1	6:S:55:LEU:N	2.45	0.50
8:U:155:GLN:HA	8:U:166:MET:HA	1.94	0.50
9:V:186:PRO:HA	9:V:189:ILE:HD12	1.94	0.50
11:Y:96:LEU:HD12	11:Y:96:LEU:C	2.32	0.50
6:F:71:LEU:HD23	6:F:71:LEU:N	2.20	0.49
3:P:126:ALA:HA	14:Y:502:PEE:H61	1.94	0.49
11:Y:164:GLU:O	11:Y:168:ILE:HG12	2.12	0.49
10:K:299:VAL:HG22	11:L:120:LEU:HG	1.94	0.49
12:L:502:CDL:H572	14:L:503:PEE:C39	2.38	0.49
8:H:289:GLY:HA2	8:H:292:MET:HG2	1.93	0.49
8:H:323:PRO:HB2	8:H:325:LYS:HG2	1.93	0.49
10:K:173:VAL:HG11	10:K:339:TYR:HE1	1.77	0.49
10:K:239:ASN:OD1	10:K:240:MET:N	2.45	0.49
8:U:296:MET:HE2	14:U:401:PEE:C33	2.40	0.49
9:V:150:LEU:HD23	9:V:164:ILE:CD1	2.42	0.49
9:V:281:LEU:HD11	9:V:294:LEU:HD22	1.94	0.49
8:H:93:SER:HB2	8:H:99:ARG:HH12	1.77	0.49
9:J:131:TYR:O	9:J:134:PRO:HD2	2.11	0.49
11:L:75:ILE:HG21	11:L:224:TYR:CD1	2.48	0.49
11:L:168:ILE:O	11:L:172:MET:HG2	2.13	0.49
9:V:140:PHE:CD1	9:V:140:PHE:C	2.85	0.49
10:K:64:PHE:CE2	10:K:397:GLY:HA3	2.48	0.49
5:R:80:HIS:C	5:R:80:HIS:CD2	2.86	0.49
7:T:39:ARG:HG2	7:T:39:ARG:NH2	2.19	0.49
9:J:186:PRO:HA	9:J:189:ILE:HD12	1.94	0.49
10:K:116:ARG:NH1	10:K:188:ASN:O	2.45	0.49
10:K:305:THR:HA	10:K:311:GLN:HE21	1.78	0.49
8:U:288:MET:CG	14:U:401:PEE:O4	2.61	0.49
9:V:10:LEU:CD2	14:Y:502:PEE:C26	2.91	0.49
10:W:105:ALA:HA	11:Y:390:ARG:HG3	1.94	0.49
10:W:230:LEU:HA	10:W:233:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:101:CDL:H741	9:V:156:ILE:CG2	2.43	0.49
4:Q:53:TRP:NE1	8:U:139:CYS:O	2.45	0.49
5:R:66:ASP:OD1	5:R:67:CYS:N	2.44	0.49
9:V:254:ASP:OD2	9:V:267:HIS:NE2	2.46	0.49
9:V:286:ASN:OD1	9:V:287:LYS:N	2.46	0.49
11:Y:119:HIS:HB2	11:Y:134:LYS:HB3	1.93	0.49
9:J:97:HIS:HE1	9:J:100:ARG:HH21	1.58	0.49
9:J:126:THR:O	9:J:182:HIS:ND1	2.45	0.49
11:L:75:ILE:HG21	11:L:224:TYR:HD1	1.77	0.49
6:S:34:ARG:NH2	6:S:92:GLU:OE2	2.45	0.49
11:L:304:LEU:HD13	11:L:354:LEU:HD11	1.95	0.49
11:L:426:LEU:HA	11:L:429:TRP:HD1	1.78	0.49
4:Q:43:ILE:O	4:Q:47:ILE:HD12	2.13	0.49
11:Y:75:ILE:HG12	11:Y:229:MET:SD	2.52	0.49
6:F:29:LYS:NZ	6:F:29:LYS:CB	2.73	0.49
12:J:405:CDL:H132	12:J:405:CDL:H762	1.95	0.49
10:K:259:ARG:HH12	10:K:438:MET:CE	2.26	0.49
10:K:378:LEU:HD13	10:K:416:ILE:HD11	1.94	0.49
11:L:192:PHE:HB2	11:L:198:ALA:HB2	1.95	0.49
12:N:101:CDL:C58	14:V:403:PEE:H52	2.42	0.49
8:U:307:LYS:HE2	12:U:403:CDL:CA3	2.43	0.49
9:V:246:SER:HB3	9:V:249:LEU:HD23	1.95	0.49
9:V:366:MET:HB3	9:V:367:PRO:HD3	1.95	0.49
11:Y:98:PHE:N	11:Y:98:PHE:CD1	2.79	0.49
11:Y:187:LEU:HD11	11:Y:290:ALA:HB3	1.94	0.49
11:Y:294:PRO:HG3	11:Y:448:TYR:CE1	2.48	0.49
6:F:83:LYS:HB2	6:F:86:GLU:HB2	1.95	0.48
9:V:131:TYR:O	9:V:134:PRO:HD2	2.13	0.48
11:Y:101:THR:OG1	11:Y:149:ASP:OD1	2.31	0.48
11:Y:119:HIS:HB2	11:Y:134:LYS:HD2	1.94	0.48
11:Y:424:ILE:HG13	11:Y:429:TRP:NE1	2.27	0.48
3:C:136:PHE:CE2	14:H:401:PEE:H34	2.48	0.48
5:R:34:ARG:CG	5:R:78:ARG:NH1	2.61	0.48
7:T:39:ARG:CG	7:T:39:ARG:NH2	2.73	0.48
9:V:195:LEU:HD22	9:V:199:PHE:CE2	2.48	0.48
8:U:284:HIS:O	8:U:288:MET:HG3	2.13	0.48
9:J:22:PRO:HB3	9:J:217:LYS:HB3	1.94	0.48
9:J:177:ARG:NH2	3:P:140:MET:O	2.47	0.48
10:K:207:TYR:HA	10:K:210:GLN:NE2	2.28	0.48
11:L:179:MET:O	11:L:181:ASP:N	2.45	0.48
3:P:111:LYS:NZ	11:Y:451:ASP:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:27:VAL:O	4:Q:30:MET:HB2	2.13	0.48
9:V:254:ASP:O	9:V:257:THR:OG1	2.28	0.48
8:U:115:GLN:HA	8:U:118:LYS:HE2	1.96	0.48
9:V:96:LEU:HD23	14:V:403:PEE:C17	2.39	0.48
6:F:51:LEU:HD22	6:F:55:LEU:HB3	1.96	0.48
14:H:401:PEE:H17	9:J:240:MET:HE2	1.95	0.48
10:K:438:MET:HB2	10:K:450:VAL:HG12	1.94	0.48
11:L:326:SER:O	11:L:330:SER:N	2.43	0.48
4:Q:56:ILE:O	4:Q:59:LYS:HG2	2.14	0.48
11:Y:286:HIS:ND1	11:Y:359:VAL:HG22	2.29	0.48
6:F:45:LYS:HB3	6:F:45:LYS:HZ2	1.79	0.48
10:K:38:LEU:HB3	10:K:52:LEU:HB2	1.94	0.48
11:L:101:THR:HA	11:L:154:CYS:HA	1.95	0.48
11:L:186:TYR:CD1	11:L:275:ILE:HG21	2.48	0.48
9:V:45:ILE:HA	16:V:401:HEM:CMC	2.44	0.48
10:W:384:MET:SD	11:Y:68:THR:HG21	2.54	0.48
10:W:413:LEU:HA	10:W:416:ILE:HG22	1.94	0.48
6:F:36:ASP:CG	6:F:62:ARG:NH1	2.67	0.48
7:T:17:TRP:NE1	11:Y:382:SER:OG	2.41	0.48
8:U:214:LEU:O	8:U:234:ASN:ND2	2.44	0.48
1:A:66:GLU:HG2	9:J:346:PRO:HB3	1.96	0.48
14:L:503:PEE:H26	14:L:503:PEE:C33	2.44	0.48
3:P:124:GLY:HA3	8:U:299:LEU:HD21	1.94	0.48
11:Y:296:TRP:NE1	11:Y:419:THR:OG1	1.64	0.48
8:H:96:TRP:CZ3	8:H:208:GLU:HG3	2.49	0.48
8:H:249:TYR:O	8:H:252:VAL:HG23	2.14	0.48
9:J:82:LEU:HD23	9:J:243:THR:HG21	1.96	0.48
10:K:82:LEU:HD21	10:K:151:VAL:HG13	1.94	0.48
2:O:26:LEU:HA	2:O:27:ARG:O	2.14	0.48
3:P:88:PHE:O	3:P:92:ARG:HG3	2.14	0.48
10:W:136:PHE:O	10:W:140:VAL:HG23	2.13	0.48
10:W:157:GLN:NE2	11:Y:317:THR:O	2.45	0.48
9:J:13:LEU:HD11	9:V:198:LEU:HD11	1.95	0.47
10:K:425:ILE:HG22	10:K:429:LYS:HE2	1.95	0.47
11:L:113:VAL:HG11	11:L:120:LEU:HD23	1.95	0.47
11:L:183:VAL:HG21	11:L:286:HIS:HD2	1.79	0.47
14:L:503:PEE:H16	14:L:503:PEE:C30	2.44	0.47
10:K:115:THR:HG23	10:K:118:ASN:H	1.80	0.47
10:K:267:VAL:HG21	10:K:447:THR:HG21	1.95	0.47
1:N:28:PRO:HB2	1:N:29:HIS:CD2	2.50	0.47
5:R:34:ARG:NH1	5:R:78:ARG:CZ	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:14:LEU:HA	6:S:17:ILE:HG12	1.96	0.47
9:V:65:SER:O	9:V:68:HIS:HB3	2.14	0.47
11:Y:322:VAL:HG12	11:Y:323:HIS:N	2.27	0.47
12:J:405:CDL:OB9	12:J:405:CDL:HA4	2.13	0.47
11:L:133:ILE:HG22	11:L:134:LYS:H	1.79	0.47
9:V:278:TYR:CE2	9:V:282:ARG:HD2	2.49	0.47
11:Y:294:PRO:HG3	11:Y:448:TYR:CZ	2.50	0.47
11:Y:296:TRP:HB3	11:Y:349:ALA:HA	1.96	0.47
9:J:140:PHE:O	9:J:144:THR:OG1	2.26	0.47
10:K:183:ARG:NH2	10:K:254:ARG:CB	2.78	0.47
10:K:277:VAL:HG22	10:K:278:ALA:HA	1.96	0.47
3:P:138:SER:O	9:V:74:ASN:ND2	2.44	0.47
4:Q:56:ILE:HG23	4:Q:59:LYS:HE3	1.97	0.47
5:R:71:LEU:HD22	8:U:222:PRO:HG3	1.97	0.47
14:H:401:PEE:C11	14:H:401:PEE:C30	2.92	0.47
9:J:47:THR:HG23	9:J:79:ILE:HG23	1.96	0.47
10:K:64:PHE:CE1	10:K:120:ALA:HB1	2.49	0.47
8:U:128:ASP:OD1	8:U:177:LYS:NZ	2.47	0.47
10:W:301:ARG:HD2	11:Y:95:HIS:CD2	2.48	0.47
10:W:443:ASN:OD1	10:W:445:GLY:N	2.43	0.47
10:W:444:LEU:HD23	10:W:447:THR:CG2	2.42	0.47
2:B:26:LEU:HA	2:B:27:ARG:C	2.35	0.47
4:D:38:GLN:NE2	7:G:47:TYR:OH	2.48	0.47
6:F:70:ASN:HD22	9:J:209:LEU:HG	1.80	0.47
10:K:84:ARG:HH11	10:K:114:ALA:HB3	1.79	0.47
3:P:136:PHE:HB3	9:V:50:PHE:CE2	2.49	0.47
9:V:141:TRP:CZ2	9:V:260:ASN:O	2.67	0.47
1:A:27:TYR:HE2	8:H:305:THR:HG22	1.80	0.47
5:E:30:LEU:HD12	5:E:30:LEU:C	2.35	0.47
7:G:14:VAL:O	7:G:18:VAL:HG23	2.14	0.47
11:L:376:TRP:HB3	11:L:449:ILE:HG21	1.96	0.47
11:L:437:ASP:OD1	11:L:438:ALA:N	2.44	0.47
5:R:30:LEU:HD13	5:R:86:LEU:CD1	2.44	0.47
7:T:40:LEU:HD12	7:T:41:ILE:CA	2.36	0.47
10:W:138:LEU:O	10:W:142:THR:OG1	2.25	0.47
3:C:164:ASN:HD21	3:C:175:PHE:HB3	1.80	0.47
3:C:207:LYS:HD3	3:C:265:PHE:CE2	2.50	0.47
12:U:403:CDL:H732	12:U:403:CDL:HB62	1.96	0.47
9:V:111:GLU:O	9:V:115:ILE:HG12	2.15	0.47
2:B:34:VAL:HB	2:B:35:PRO:HD3	1.96	0.47
2:B:35:PRO:HB3	10:K:320:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:97:HIS:CE1	9:J:100:ARG:HH21	2.32	0.47
9:J:221:HIS:HB3	9:J:222:PRO:HD3	1.97	0.47
11:L:96:LEU:HA	11:L:99:LYS:HG2	1.97	0.47
3:P:177:ARG:HB3	3:P:211:VAL:HG13	1.97	0.47
8:U:262:THR:HG22	8:U:264:SER:H	1.78	0.47
9:J:62:ALA:O	9:J:65:SER:OG	2.22	0.47
11:L:373:GLN:HE22	11:L:471:ILE:HG23	1.80	0.47
2:O:43:LEU:HD11	11:Y:179:MET:HG3	1.97	0.47
3:P:199:GLN:NE2	3:P:204:ARG:HG2	2.29	0.47
8:U:215:LEU:HD11	15:U:402:HEC:HMB1	1.97	0.47
9:V:343:VAL:CG1	9:V:348:THR:HG22	2.45	0.47
2:B:11:PHE:CD1	2:B:24:GLY:HA3	2.50	0.46
6:F:28:ASN:O	6:F:31:GLY:N	2.42	0.46
8:H:133:ARG:O	8:H:135:LEU:N	2.37	0.46
12:J:405:CDL:H341	12:J:405:CDL:H371	1.67	0.46
3:P:136:PHE:HD1	9:V:50:PHE:HD2	1.62	0.46
6:S:44:VAL:O	6:S:48:ILE:HG12	2.14	0.46
7:T:24:TRP:CH2	12:Y:501:CDL:H551	2.50	0.46
12:G:101:CDL:H341	12:G:101:CDL:H371	1.78	0.46
14:H:401:PEE:C11	14:H:401:PEE:C31	2.93	0.46
14:J:403:PEE:H61	14:J:403:PEE:C17	2.42	0.46
11:L:164:GLU:O	11:L:168:ILE:HG12	2.14	0.46
2:O:11:PHE:H	2:O:27:ARG:CZ	2.27	0.46
5:R:62:HIS:O	5:R:62:HIS:ND1	2.48	0.46
6:S:55:LEU:HD11	6:S:90:TYR:HB2	1.97	0.46
7:T:9:ARG:HH22	17:T:101:PLX:H1A1	1.79	0.46
8:U:131:ALA:HA	8:U:174:TYR:HA	1.97	0.46
8:H:321:TYR:CD2	8:H:323:PRO:HD3	2.51	0.46
10:K:214:THR:HG22	10:K:216:ALA:H	1.80	0.46
11:L:101:THR:HA	11:L:155:SER:H	1.81	0.46
14:L:503:PEE:H49	14:L:503:PEE:C17	2.44	0.46
10:K:305:THR:HA	10:K:311:GLN:NE2	2.30	0.46
10:K:370:ASP:OD1	10:K:371:VAL:N	2.49	0.46
3:P:159:ILE:HA	3:P:160:PRO:HD3	1.76	0.46
1:A:16:SER:HA	8:H:319:LEU:HA	1.98	0.46
5:R:75:LEU:HD23	5:R:75:LEU:HA	1.80	0.46
6:S:93:PRO:O	6:S:97:GLU:HG2	2.15	0.46
10:W:450:VAL:HA	10:W:453:LEU:HD13	1.94	0.46
10:K:277:VAL:HG11	10:K:329:SER:HA	1.97	0.46
11:L:125:THR:HG22	11:L:126:ARG:H	1.81	0.46
11:L:166:ASP:OD1	11:L:167:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:PHE:CB	9:V:346:PRO:HG3	2.42	0.46
3:P:181:GLN:HA	3:P:184:ILE:HD12	1.98	0.46
1:A:74:ASN:OD1	1:A:78:TYR:HE2	1.99	0.46
11:L:332:ALA:O	11:L:337:LEU:N	2.44	0.46
2:O:11:PHE:CD1	2:O:27:ARG:HD2	2.51	0.46
6:S:35:ASP:O	6:S:38:ILE:HG22	2.15	0.46
10:W:152:ALA:HA	10:W:155:GLN:HG2	1.98	0.46
11:Y:148:GLY:O	11:Y:152:GLN:N	2.43	0.46
5:E:74:PHE:CZ	5:E:78:ARG:HD2	2.51	0.46
9:J:246:SER:HB3	9:J:249:LEU:HD23	1.98	0.46
10:K:178:HIS:HE1	10:K:330:TYR:CE2	2.34	0.46
10:K:259:ARG:HH21	10:K:259:ARG:CB	2.10	0.46
9:V:24:PRO:HD2	9:V:27:ILE:HD11	1.97	0.46
10:W:259:ARG:NH1	10:W:449:PHE:CZ	2.83	0.46
10:W:277:VAL:HA	10:W:278:ALA:HA	1.73	0.46
10:W:298:HIS:HE1	10:W:377:LYS:HG2	1.81	0.46
3:C:164:ASN:HB3	3:C:226:ALA:HB1	1.98	0.46
3:C:178:HIS:HD2	3:C:209:GLU:O	1.99	0.46
14:H:401:PEE:C30	14:H:401:PEE:C10	2.93	0.46
11:L:286:HIS:ND1	11:L:359:VAL:HG22	2.31	0.46
1:N:67:PHE:HD1	9:V:344:SER:HG	1.61	0.46
1:A:12:ARG:NH1	11:L:279:ASP:OD1	2.49	0.45
6:F:34:ARG:HH11	9:J:379:TRP:HE1	1.60	0.45
1:N:41:ARG:HH21	12:N:101:CDL:H1	1.81	0.45
3:P:136:PHE:HB3	9:V:50:PHE:HE2	1.81	0.45
8:U:204:ARG:HE	15:U:402:HEC:CGA	2.29	0.45
10:W:38:LEU:HD21	10:W:406:TYR:CD1	2.51	0.45
10:W:49:ILE:HD11	10:W:230:LEU:HB3	1.98	0.45
10:W:306:THR:OG1	11:Y:111:LYS:NZ	2.46	0.45
3:C:135:GLN:HG3	9:J:75:TYR:CD2	2.51	0.45
6:F:38:ILE:HG12	6:F:39:TYR:N	2.30	0.45
9:J:362:ILE:HG13	9:J:363:LEU:HD12	1.98	0.45
9:J:366:MET:HB3	9:J:367:PRO:HD3	1.98	0.45
10:K:57:PRO:HG2	11:L:400:VAL:CG1	2.47	0.45
3:P:167:PHE:HB2	3:P:174:LEU:HB3	1.97	0.45
4:Q:14:LEU:O	4:Q:20:THR:OG1	2.33	0.45
9:V:333:LEU:CD2	14:V:403:PEE:C40	2.94	0.45
11:Y:192:PHE:HB2	11:Y:198:ALA:HB2	1.98	0.45
11:Y:465:LEU:HD12	11:Y:466:PRO:HD2	1.97	0.45
11:L:294:PRO:HB2	11:L:301:ASN:HD21	1.82	0.45
8:U:88:GLU:HB3	8:U:238:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:313:VAL:HG13	8:U:314:LEU:HD12	1.98	0.45
5:E:53:CYS:O	5:E:57:VAL:HG23	2.17	0.45
9:J:265:PRO:HA	9:J:266:PRO:HD3	1.82	0.45
6:S:83:LYS:HB2	6:S:86:GLU:HB2	1.98	0.45
8:U:201:VAL:O	8:U:207:GLY:HA2	2.17	0.45
9:V:25:SER:HB3	9:V:218:ILE:HD12	1.98	0.45
7:G:39:ARG:HE	7:G:51:LYS:HD2	1.80	0.45
8:H:291:LYS:CD	14:H:401:PEE:H8	2.42	0.45
9:J:223:TYR:OH	11:L:469:ASN:ND2	2.44	0.45
11:L:140:LEU:HD21	11:L:237:VAL:HG13	1.99	0.45
11:L:332:ALA:HA	11:L:337:LEU:HB2	1.97	0.45
2:O:36:ALA:HB3	10:W:320:PRO:HB3	1.97	0.45
10:W:312:ALA:HA	10:W:315:LYS:HE3	1.98	0.45
8:H:288:MET:SD	14:H:401:PEE:O4	2.75	0.45
12:J:404:CDL:O1	12:J:404:CDL:OB9	2.33	0.45
10:K:148:ARG:NH1	6:S:50:ARG:O	2.50	0.45
11:L:63:GLN:HE22	11:L:238:GLU:HA	1.81	0.45
9:V:276:PHE:O	9:V:279:THR:OG1	2.24	0.45
11:Y:66:GLN:OE1	11:Y:67:PRO:HD2	2.16	0.45
11:Y:424:ILE:HD12	11:Y:424:ILE:HA	1.85	0.45
2:B:46:LYS:HD2	2:B:49:PHE:CZ	2.52	0.45
8:H:158:PRO:HG3	8:U:181:ASN:HD22	1.82	0.45
9:J:16:HIS:O	9:J:21:LEU:HB3	2.16	0.45
9:J:372:ILE:O	9:J:376:MET:HG2	2.17	0.45
9:V:18:PHE:O	9:V:220:PHE:HB3	2.17	0.45
4:D:34:ARG:NH1	4:D:38:GLN:HB3	2.32	0.45
9:J:278:TYR:O	9:J:281:LEU:HB2	2.17	0.45
11:L:42:LEU:HD11	11:L:430:GLU:OE1	2.17	0.45
11:L:126:ARG:NH1	11:L:199:GLN:O	2.50	0.45
4:Q:26:ILE:HD12	7:T:27:VAL:HG13	1.98	0.45
4:Q:53:TRP:HA	4:Q:56:ILE:HB	1.99	0.45
3:C:80:HIS:CE1	11:L:182:VAL:HG22	2.52	0.45
3:C:195:LEU:HD13	3:C:248:ARG:HD2	1.99	0.45
9:V:7:THR:O	9:V:12:LYS:HE3	2.16	0.45
10:W:444:LEU:HA	10:W:447:THR:HG23	1.99	0.45
11:Y:96:LEU:HD23	11:Y:161:ILE:CD1	2.47	0.45
11:Y:96:LEU:C	11:Y:96:LEU:CD1	2.86	0.45
11:Y:166:ASP:OD1	11:Y:167:VAL:N	2.49	0.45
2:B:26:LEU:HG	2:B:28:PRO:HA	1.99	0.45
3:C:140:MET:HA	9:V:177:ARG:HH21	1.81	0.45
4:D:27:VAL:O	4:D:30:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:304:TYR:CE1	12:H:403:CDL:OA3	2.70	0.45
11:L:113:VAL:HG21	11:L:120:LEU:HD23	1.99	0.45
11:L:373:GLN:NE2	11:L:471:ILE:HG23	2.31	0.45
6:S:51:LEU:HD22	6:S:55:LEU:HD22	1.99	0.45
7:T:40:LEU:C	7:T:40:LEU:CD1	2.85	0.45
8:U:292:MET:HE1	9:V:241:THR:HG23	1.99	0.45
10:W:328:ALA:HB3	10:W:335:LEU:HB2	1.99	0.45
11:Y:421:GLY:O	11:Y:422:ARG:HG3	2.16	0.45
3:C:81:THR:O	3:C:83:ILE:N	2.48	0.44
6:F:34:ARG:NH1	9:J:379:TRP:NE1	2.60	0.44
14:H:401:PEE:C12	9:J:240:MET:CE	2.91	0.44
9:J:300:ILE:H	9:J:300:ILE:HG13	1.57	0.44
10:K:155:GLN:NE2	10:K:200:VAL:O	2.50	0.44
11:L:75:ILE:HD13	11:L:224:TYR:CD1	2.51	0.44
11:Y:479:ARG:HH11	12:Y:501:CDL:HB62	1.82	0.44
6:F:44:VAL:O	6:F:48:ILE:HG12	2.17	0.44
11:L:125:THR:HG22	11:L:126:ARG:N	2.31	0.44
9:V:155:TYR:O	9:V:155:TYR:CD1	2.70	0.44
10:W:108:GLY:HA2	11:Y:397:ASN:ND2	2.33	0.44
11:Y:92:PHE:HD1	11:Y:92:PHE:O	2.00	0.44
11:Y:101:THR:HA	11:Y:155:SER:N	2.30	0.44
11:Y:225:LYS:NZ	11:Y:258:ALA:H	2.14	0.44
8:H:301:PRO:O	8:H:305:THR:HG23	2.17	0.44
9:J:8:ASN:HB3	9:J:11:MET:HB2	2.00	0.44
11:L:279:ASP:OD2	11:L:282:LEU:HG	2.17	0.44
11:L:286:HIS:CE1	11:L:359:VAL:HG22	2.52	0.44
6:S:71:LEU:HD21	9:V:25:SER:CB	2.48	0.44
2:B:41:PRO:HB2	10:K:167:GLN:NE2	2.31	0.44
4:D:25:ILE:O	4:D:29:VAL:HG23	2.18	0.44
10:K:126:LEU:HB3	11:L:38:PHE:CZ	2.52	0.44
11:L:225:LYS:HD2	11:L:257:TYR:CE1	2.52	0.44
9:V:10:LEU:HD21	14:Y:502:PEE:H45	1.78	0.44
9:V:315:MET:SD	9:V:318:ARG:NH2	2.90	0.44
10:W:323:VAL:HG13	10:W:340:THR:HG22	1.99	0.44
9:J:105:GLY:HA2	9:J:107:PHE:CE2	2.53	0.44
9:J:156:ILE:HG21	9:J:160:LEU:HD13	2.00	0.44
8:U:197:LEU:HD23	8:U:274:LEU:HD21	1.99	0.44
8:U:249:TYR:O	8:U:252:VAL:HG23	2.17	0.44
8:U:253:LEU:HD23	8:U:254:GLU:N	2.32	0.44
9:V:160:LEU:O	9:V:164:ILE:HD12	2.17	0.44
11:Y:64:SER:HB3	11:Y:235:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TYR:CE2	8:H:305:THR:HG22	2.53	0.44
9:J:198:LEU:CD1	12:J:404:CDL:H332	2.48	0.44
14:J:403:PEE:H61	14:J:403:PEE:C18	2.45	0.44
1:N:17:TYR:HD1	11:Y:275:ILE:HG12	1.83	0.44
12:N:101:CDL:C58	14:V:403:PEE:C33	2.96	0.44
8:U:114:PHE:CE2	8:U:148:LEU:HD21	2.52	0.44
9:V:191:ALA:O	9:V:194:THR:OG1	2.24	0.44
11:Y:324:LEU:O	11:Y:325:SER:OG	2.33	0.44
11:Y:333:VAL:HG13	11:Y:336:LYS:HD2	1.99	0.44
12:H:403:CDL:O1	12:H:403:CDL:OB8	2.35	0.44
12:L:502:CDL:H511	14:L:503:PEE:H67	1.98	0.44
10:W:104:GLU:OE1	11:Y:325:SER:HA	2.17	0.44
10:W:452:GLU:HG2	10:W:453:LEU:N	2.31	0.44
2:B:50:LEU:O	2:B:51:SER:OG	2.32	0.44
6:F:34:ARG:HD2	9:J:377:LEU:HB3	2.00	0.44
10:K:158:LEU:HB2	10:K:197:ILE:HG23	1.99	0.44
2:O:37:THR:N	11:Y:174:GLU:OE2	2.41	0.44
9:V:129:MET:CE	9:V:185:LEU:CD1	2.95	0.44
3:C:145:ASP:OD1	3:C:146:VAL:N	2.51	0.44
6:S:99:ILE:O	6:S:103:LYS:HG2	2.17	0.44
8:U:202:ARG:NH2	9:V:248:ASP:OD1	2.51	0.44
12:U:403:CDL:H112	9:V:234:LEU:HD12	2.00	0.44
10:W:81:HIS:CD2	10:W:158:LEU:HD22	2.53	0.44
10:W:228:PRO:O	10:W:231:LYS:HB2	2.18	0.44
8:H:221:PRO:HA	8:H:222:PRO:HD3	1.77	0.43
10:K:257:GLU:HG3	10:K:450:VAL:HG21	1.98	0.43
11:L:231:LEU:HD22	11:L:250:LEU:HD12	2.00	0.43
11:L:414:GLY:O	11:L:418:LEU:HD13	2.18	0.43
1:A:78:TYR:HB3	5:E:65:GLU:CD	2.30	0.43
10:K:60:ARG:HB3	10:K:223:LEU:HD12	2.00	0.43
11:L:152:GLN:NE2	11:L:249:HIS:O	2.51	0.43
5:R:43:CYS:SG	5:R:78:ARG:HA	2.57	0.43
5:R:86:LEU:C	5:R:86:LEU:CD2	2.86	0.43
1:A:12:ARG:HG2	1:A:13:HIS:HD1	1.78	0.43
2:B:1:MET:SD	10:K:412:VAL:HG13	2.58	0.43
5:E:40:LEU:O	5:E:44:VAL:HG23	2.18	0.43
8:H:131:ALA:HA	8:H:174:TYR:HA	2.00	0.43
10:K:155:GLN:N	10:K:156:PRO:HD2	2.33	0.43
11:L:360:CYS:HB3	11:L:368:MET:SD	2.59	0.43
11:Y:57:LEU:HD13	11:Y:250:LEU:HB3	1.99	0.43
5:E:34:ARG:HE	5:E:34:ARG:HB2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:70:ASN:ND2	9:J:209:LEU:HG	2.33	0.43
10:K:227:HIS:N	10:K:228:PRO:HD2	2.33	0.43
14:L:503:PEE:H1	14:L:503:PEE:H13	1.74	0.43
3:P:214:ILE:HG22	3:P:216:VAL:H	1.83	0.43
6:S:36:ASP:OD1	6:S:90:TYR:OH	2.37	0.43
8:U:291:LYS:HE3	14:U:401:PEE:O1P	2.18	0.43
9:V:171:ASP:OD1	9:V:172:SER:N	2.50	0.43
10:W:79:THR:HG23	10:W:205:LEU:HD23	2.00	0.43
10:W:379:LYS:HG2	10:W:413:LEU:HG	2.01	0.43
3:C:200:HIS:O	3:C:204:ARG:HG3	2.18	0.43
9:J:155:TYR:HE2	7:T:38:TRP:CZ2	2.35	0.43
10:K:105:ALA:HA	11:L:390:ARG:HG3	2.00	0.43
10:K:326:PHE:HB3	10:K:337:GLY:O	2.19	0.43
11:L:58:ARG:HB2	11:L:230:VAL:HG22	2.01	0.43
3:P:125:VAL:CG2	17:Q:101:PLX:H141	2.49	0.43
3:P:127:TYR:HE1	4:Q:33:GLU:HG2	1.83	0.43
6:F:99:ILE:O	6:F:103:LYS:HG2	2.19	0.43
9:J:331:ASP:HA	9:J:334:ILE:HD12	2.01	0.43
11:L:133:ILE:HG22	11:L:134:LYS:N	2.33	0.43
11:L:350:GLU:HG2	11:L:351:THR:HG23	2.00	0.43
3:P:82:ASP:OD1	3:P:83:ILE:N	2.51	0.43
4:Q:44:TYR:HB2	8:U:290:LEU:HD13	2.00	0.43
8:U:296:MET:HE2	14:U:401:PEE:C32	2.49	0.43
12:U:403:CDL:OA6	9:V:230:LEU:HD23	2.19	0.43
10:W:346:ALA:O	10:W:350:VAL:HG23	2.19	0.43
1:A:78:TYR:CD1	5:E:64:GLU:C	2.91	0.43
3:C:179:ARG:NE	3:C:208:PRO:O	2.43	0.43
8:H:131:ALA:HB3	8:H:133:ARG:HG2	2.00	0.43
7:T:17:TRP:HE1	11:Y:382:SER:HG	1.60	0.43
10:W:323:VAL:HG22	10:W:340:THR:HG22	1.99	0.43
11:Y:287:VAL:HG12	11:Y:458:GLY:HA2	2.01	0.43
5:E:21:GLU:HA	5:E:24:GLU:CB	2.49	0.43
7:G:45:VAL:HA	7:G:46:PRO:HD3	1.80	0.43
11:L:267:PRO:HA	11:L:350:GLU:OE1	2.18	0.43
3:P:80:HIS:CD2	3:P:81:THR:HG23	2.53	0.43
9:V:206:ASN:H	16:V:402:HEM:CGD	2.31	0.43
10:W:61:ILE:HG22	10:W:222:GLY:HA2	1.99	0.43
11:Y:295:GLY:HA2	11:Y:351:THR:O	2.19	0.43
6:F:51:LEU:CD2	6:F:55:LEU:HD13	2.49	0.43
9:J:8:ASN:OD1	9:J:9:PRO:HD2	2.19	0.43
9:J:197:LEU:HD22	12:J:404:CDL:H162	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:257:TYR:CD2	11:L:262:VAL:HG22	2.45	0.43
8:U:221:PRO:HA	8:U:222:PRO:HD3	1.85	0.43
9:V:333:LEU:HD21	14:V:403:PEE:C40	2.48	0.43
1:A:74:ASN:OD1	1:A:78:TYR:CE2	2.72	0.43
3:C:132:ALA:HB1	14:H:401:PEE:H27	2.00	0.43
6:F:27:PHE:HD1	6:F:28:ASN:N	2.17	0.43
12:J:404:CDL:H121	12:J:404:CDL:H152	1.70	0.43
10:K:127:ARG:NH1	10:K:224:GLY:O	2.49	0.43
2:O:28:PRO:O	10:W:170:GLN:NE2	2.52	0.43
2:O:46:LYS:HG2	2:O:47:ARG:O	2.18	0.43
8:U:292:MET:CE	9:V:241:THR:CG2	2.96	0.43
10:W:262:ASN:O	10:W:443:ASN:HA	2.18	0.43
11:Y:74:TRP:CG	11:Y:414:GLY:HA3	2.54	0.43
10:K:82:LEU:O	10:K:86:THR:HG23	2.19	0.42
10:K:138:LEU:O	10:K:142:THR:N	2.53	0.42
10:K:293:LEU:HD21	10:K:358:VAL:HG22	2.00	0.42
10:K:355:TYR:CE2	10:K:359:LYS:HD2	2.54	0.42
11:L:121:ASN:HB3	11:L:132:TYR:CZ	2.54	0.42
12:H:403:CDL:H122	9:J:234:LEU:HD12	2.01	0.42
9:J:312:GLN:HG3	9:J:379:TRP:HH2	1.84	0.42
11:L:156:LEU:HB3	11:L:161:ILE:HD11	2.01	0.42
11:L:294:PRO:HB2	11:L:301:ASN:ND2	2.34	0.42
11:L:324:LEU:O	11:L:325:SER:OG	2.32	0.42
14:L:503:PEE:C33	14:L:503:PEE:C17	2.97	0.42
9:V:326:TRP:CZ2	14:V:403:PEE:O5	2.72	0.42
10:W:373:ALA:O	10:W:377:LYS:HG3	2.19	0.42
11:Y:64:SER:N	11:Y:235:GLY:O	2.49	0.42
11:Y:88:GLY:O	11:Y:92:PHE:HB2	2.19	0.42
1:A:3:ARG:HH12	9:J:217:LYS:CE	2.32	0.42
2:B:50:LEU:HD23	2:B:51:SER:O	2.19	0.42
5:E:29:PRO:HD3	8:H:262:THR:CG2	2.37	0.42
5:E:78:ARG:O	5:E:82:VAL:HG23	2.19	0.42
14:H:401:PEE:H61	9:J:236:LEU:HD13	2.01	0.42
9:J:214:HIS:ND1	9:J:217:LYS:NZ	2.68	0.42
10:K:178:HIS:HE1	10:K:330:TYR:HE2	1.66	0.42
10:K:449:PHE:CE2	10:W:183:ARG:HB3	2.54	0.42
2:O:14:VAL:HA	10:W:113:THR:HA	2.01	0.42
8:U:91:PRO:HA	8:U:92:PRO:HD3	1.84	0.42
10:W:90:THR:HG22	10:W:150:GLU:OE1	2.19	0.42
10:W:444:LEU:HD23	10:W:444:LEU:HA	1.78	0.42
6:F:110:LYS:HG3	6:F:111:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:87:ASN:HD21	11:L:199:GLN:HB2	1.85	0.42
3:P:244:ASP:OD2	3:P:248:ARG:HB2	2.18	0.42
6:S:8:SER:OG	6:S:9:ALA:N	2.51	0.42
8:U:156:ASP:OD1	8:U:157:GLY:N	2.43	0.42
10:W:82:LEU:O	10:W:86:THR:HG23	2.19	0.42
3:C:246:SER:OG	3:C:248:ARG:NE	2.47	0.42
10:K:195:TYR:CE2	10:K:196:ARG:HG2	2.54	0.42
10:K:330:TYR:HB2	10:K:333:SER:O	2.20	0.42
1:N:82:LYS:HE2	5:R:65:GLU:HB2	2.01	0.42
5:R:34:ARG:NH1	5:R:78:ARG:HH22	2.10	0.42
8:U:114:PHE:HE2	8:U:148:LEU:HD21	1.83	0.42
8:U:290:LEU:HD23	8:U:290:LEU:O	2.19	0.42
8:U:292:MET:CE	9:V:241:THR:HG22	2.49	0.42
2:B:53:GLU:O	11:L:402:HIS:ND1	2.47	0.42
6:F:39:TYR:CE2	9:J:108:LEU:HD13	2.55	0.42
10:K:347:ALA:O	10:K:351:ILE:HG12	2.20	0.42
3:C:200:HIS:HE1	3:C:202:LEU:HB3	1.84	0.42
3:C:239:HIS:HB2	13:C:301:FES:S1	2.59	0.42
8:H:214:LEU:O	8:H:234:ASN:ND2	2.41	0.42
9:J:163:TRP:CG	12:J:405:CDL:H331	2.55	0.42
11:L:51:SER:HB2	11:L:59:VAL:HB	2.01	0.42
11:L:233:ALA:HB1	11:L:237:VAL:HG21	2.01	0.42
4:Q:18:THR:HG22	11:Y:480:PHE:OXT	2.19	0.42
12:U:403:CDL:O1	12:U:403:CDL:HB61	2.20	0.42
9:V:123:THR:HG22	9:V:189:ILE:HD13	2.00	0.42
11:Y:98:PHE:HE2	11:Y:120:LEU:CD1	2.19	0.42
1:N:11:MET:SD	6:S:64:LYS:HD2	2.60	0.42
1:N:49:VAL:HG21	14:V:403:PEE:H7	2.02	0.42
15:U:402:HEC:HBC3	15:U:402:HEC:HHD	2.02	0.42
12:U:403:CDL:H742	12:U:403:CDL:H711	1.77	0.42
9:V:10:LEU:HD22	14:Y:502:PEE:C27	2.41	0.42
9:V:346:PRO:O	9:V:349:ILE:HG22	2.19	0.42
10:W:271:PHE:CZ	10:W:338:ILE:HB	2.55	0.42
3:C:136:PHE:O	3:C:139:SER:OG	2.28	0.42
12:H:403:CDL:H311	12:H:403:CDL:H341	1.79	0.42
10:K:65:ILE:HG21	10:K:213:PHE:HD1	1.83	0.42
11:L:233:ALA:HB3	11:L:242:LEU:HD22	2.01	0.42
1:N:19:LEU:HD11	3:P:88:PHE:CB	2.50	0.42
1:N:48:ARG:HE	9:V:319:PRO:HB3	1.84	0.42
9:V:149:LEU:O	9:V:152:ALA:HB3	2.19	0.42
11:Y:58:ARG:HH11	11:Y:230:VAL:HG22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:HIS:CE1	3:C:202:LEU:HB3	2.55	0.42
7:G:16:ASN:CG	11:L:442:ARG:HH12	2.24	0.42
2:O:50:LEU:O	2:O:51:SER:OG	2.33	0.42
3:P:145:ASP:OD1	3:P:146:VAL:N	2.53	0.42
10:W:257:GLU:HG2	10:W:450:VAL:HB	2.02	0.42
10:W:450:VAL:CA	10:W:453:LEU:CD1	2.89	0.42
11:Y:392:LYS:O	11:Y:396:ARG:HG3	2.20	0.42
4:D:39:GLY:O	4:D:43:ILE:HG12	2.19	0.41
6:F:63:ILE:HD13	9:J:211:ILE:CG2	2.50	0.41
9:J:9:PRO:HB3	9:V:202:GLU:OE1	2.20	0.41
9:J:171:ASP:CG	9:J:172:SER:H	2.23	0.41
9:J:316:MET:HB3	14:J:403:PEE:O2P	2.20	0.41
9:J:320:LEU:HB2	9:J:373:GLU:OE2	2.20	0.41
12:J:405:CDL:H711	12:J:405:CDL:H741	1.59	0.41
11:L:407:THR:HB	11:L:408:PRO:HD3	2.02	0.41
1:N:13:HIS:H	11:Y:279:ASP:H	1.67	0.41
10:W:43:LEU:HD13	10:W:238:LEU:HD11	2.01	0.41
10:W:125:CYS:SG	10:W:130:VAL:HG22	2.60	0.41
11:Y:40:GLN:HB3	11:Y:44:PHE:HE2	1.84	0.41
6:F:76:LEU:HD12	6:F:77:PRO:HD2	2.02	0.41
9:J:160:LEU:O	9:J:164:ILE:HD12	2.20	0.41
10:K:79:THR:HG23	10:K:205:LEU:HD23	2.02	0.41
10:K:80:THR:HA	10:K:83:LEU:HB3	2.03	0.41
11:L:156:LEU:HB2	11:L:213:ARG:HE	1.85	0.41
11:L:240:GLN:HE22	11:L:243:LEU:HD23	1.84	0.41
11:L:360:CYS:SG	11:L:365:ILE:HG12	2.60	0.41
5:R:34:ARG:NH1	5:R:78:ARG:NH2	2.63	0.41
7:T:24:TRP:HZ3	12:Y:501:CDL:H551	1.79	0.41
9:V:271:GLU:HG3	9:V:273:TYR:CZ	2.55	0.41
14:V:403:PEE:H65	14:V:403:PEE:H71	1.48	0.41
11:Y:373:GLN:NE2	11:Y:471:ILE:HG23	2.35	0.41
6:F:76:LEU:O	6:F:81:TRP:NE1	2.37	0.41
7:G:45:VAL:HG21	7:G:48:ILE:HB	2.02	0.41
14:L:503:PEE:H19	14:L:503:PEE:C30	2.47	0.41
3:P:207:LYS:HE3	3:P:209:GLU:OE2	2.20	0.41
17:Q:101:PLX:H1C3	17:Q:101:PLX:H21	1.84	0.41
14:U:401:PEE:H55	14:U:401:PEE:H49	1.81	0.41
9:V:33:PHE:HA	9:V:36:LEU:HD12	2.01	0.41
10:W:195:TYR:CE2	10:W:196:ARG:HG2	2.55	0.41
10:W:214:THR:HG21	10:W:244:LEU:N	2.34	0.41
11:Y:407:THR:HB	11:Y:408:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:266:ILE:O	8:H:270:VAL:HG23	2.20	0.41
9:J:147:THR:HG22	9:J:161:VAL:HG13	2.02	0.41
10:K:261:GLN:H	10:K:444:LEU:HD12	1.86	0.41
1:N:17:TYR:CD1	11:Y:275:ILE:HG12	2.55	0.41
12:N:101:CDL:OB4	6:S:73:HIS:CE1	2.73	0.41
2:O:40:GLN:HA	2:O:41:PRO:HD3	1.90	0.41
3:P:155:LYS:NZ	3:P:273:VAL:HG21	2.36	0.41
3:P:218:THR:HG21	3:P:256:LEU:HD12	2.02	0.41
4:Q:4:ALA:HB3	4:Q:9:LYS:HE3	2.02	0.41
6:S:42:GLU:HA	6:S:45:LYS:HD3	2.03	0.41
10:W:209:VAL:HG13	10:W:213:PHE:CD2	2.55	0.41
11:Y:314:TYR:HB3	11:Y:341:PHE:CE1	2.56	0.41
3:C:181:GLN:HA	3:C:184:ILE:HD12	2.01	0.41
4:D:30:MET:SD	7:G:34:TRP:HB2	2.60	0.41
8:H:91:PRO:HA	8:H:92:PRO:HD3	1.91	0.41
8:H:197:LEU:HA	8:H:200:ILE:HB	2.03	0.41
9:J:9:PRO:HG2	9:V:199:PHE:CE1	2.55	0.41
10:K:67:ALA:HB2	10:K:212:HIS:HB3	2.02	0.41
11:L:35:THR:OG1	11:L:36:ALA:N	2.52	0.41
9:V:87:ALA:HB2	16:V:401:HEM:CHB	2.50	0.41
3:C:88:PHE:O	3:C:92:ARG:HG3	2.20	0.41
3:C:127:TYR:HE1	4:D:33:GLU:HG2	1.85	0.41
9:J:132:VAL:HG22	9:J:143:ALA:HB2	2.03	0.41
10:K:81:HIS:CD2	10:K:158:LEU:HD22	2.55	0.41
10:K:452:GLU:O	10:K:452:GLU:HG3	2.20	0.41
8:U:288:MET:HE1	9:V:77:TRP:CH2	2.56	0.41
9:V:105:GLY:HA2	9:V:107:PHE:CE2	2.56	0.41
10:W:64:PHE:HZ	10:W:393:LEU:HD23	1.86	0.41
10:W:155:GLN:N	10:W:156:PRO:HD2	2.35	0.41
10:W:290:GLN:HB3	10:W:336:PHE:HE1	1.85	0.41
11:Y:274:GLU:OE2	11:Y:468:TYR:HB2	2.20	0.41
11:Y:282:LEU:HB2	11:Y:461:PRO:HD3	2.03	0.41
1:A:64:THR:HG23	9:J:337:TRP:HZ2	1.86	0.41
3:C:248:ARG:HG2	3:C:257:ASN:ND2	2.36	0.41
7:G:17:TRP:HE1	11:L:382:SER:HG	1.68	0.41
8:H:112:ARG:O	8:H:116:VAL:HG23	2.21	0.41
9:J:146:ILE:HA	9:J:149:LEU:HD13	2.02	0.41
9:V:156:ILE:HG22	9:V:160:LEU:HB2	2.01	0.41
10:W:299:VAL:HG22	11:Y:120:LEU:HG	2.02	0.41
10:W:384:MET:HE2	11:Y:134:LYS:HD3	2.02	0.41
11:Y:244:ASP:O	11:Y:248:LYS:NZ	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:CD1	5:E:65:GLU:CG	3.04	0.41
3:C:196:ARG:HB3	3:C:249:ILE:HG23	2.01	0.41
8:H:128:ASP:OD1	8:H:177:LYS:HE2	2.20	0.41
9:J:2:THR:HG21	11:L:335:ASN:HD22	1.86	0.41
11:L:141:PRO:HA	11:L:245:LEU:HD13	2.03	0.41
2:O:13:PRO:HB2	10:W:84:ARG:HH12	1.86	0.41
3:P:207:LYS:HA	3:P:208:PRO:HD3	1.84	0.41
7:T:9:ARG:HH22	17:T:101:PLX:C1A	2.33	0.41
8:U:156:ASP:HB2	8:U:167:ARG:HB2	2.03	0.41
10:W:352:LYS:O	10:W:356:ASN:ND2	2.54	0.41
8:H:85:SER:OG	8:H:86:ASP:N	2.52	0.41
14:H:401:PEE:C30	14:H:401:PEE:H13	2.50	0.41
9:J:103:TYR:OH	9:J:322:GLN:NE2	2.54	0.41
11:L:91:TYR:O	11:L:94:GLU:HB3	2.21	0.41
11:L:424:ILE:HA	11:L:425:PRO:HD2	1.91	0.41
11:L:462:ILE:HG23	11:L:465:LEU:HB3	2.03	0.41
2:O:20:ARG:NH2	2:O:48:PRO:HG2	2.36	0.41
3:P:141:SER:OG	3:P:142:ALA:N	2.51	0.41
3:P:236:CYS:HA	3:P:237:PRO:HD2	1.75	0.41
4:Q:15:PHE:O	17:Q:101:PLX:H1A1	2.21	0.41
4:Q:21:PHE:CE2	4:Q:25:ILE:HD11	2.56	0.41
4:Q:25:ILE:O	4:Q:29:VAL:HG23	2.21	0.41
8:U:201:VAL:HG13	8:U:208:GLU:N	2.36	0.41
9:V:146:ILE:O	9:V:149:LEU:HB2	2.21	0.41
10:W:205:LEU:O	10:W:209:VAL:HG23	2.21	0.41
10:W:261:GLN:H	10:W:444:LEU:HD12	1.85	0.41
11:Y:61:SER:HB2	11:Y:242:LEU:HD23	2.03	0.41
11:Y:225:LYS:O	11:Y:228:ARG:HB3	2.20	0.41
11:Y:331:GLY:O	11:Y:337:LEU:HD12	2.21	0.41
3:C:176:VAL:HG22	3:C:212:ILE:HG12	2.02	0.41
9:J:111:GLU:O	9:J:115:ILE:HG12	2.20	0.41
9:J:221:HIS:HA	9:J:225:THR:HG23	2.02	0.41
10:K:58:VAL:HG23	11:L:400:VAL:HG11	2.03	0.41
10:K:288:VAL:O	10:K:292:VAL:HG23	2.21	0.41
10:K:449:PHE:HE2	10:W:183:ARG:HB3	1.86	0.41
11:L:170:ARG:O	11:L:174:GLU:HG3	2.20	0.41
11:L:314:TYR:HB3	11:L:341:PHE:CZ	2.55	0.41
14:L:503:PEE:H53	14:L:503:PEE:H25	2.01	0.41
3:P:150:ALA:C	3:P:152:ILE:H	2.24	0.41
3:P:186:GLN:O	3:P:190:VAL:HG23	2.20	0.41
17:T:101:PLX:H1A2	17:T:101:PLX:H21	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:266:ILE:O	8:U:270:VAL:HG23	2.20	0.41
9:V:3:PRO:HG2	9:V:6:LYS:HG2	2.03	0.41
9:V:249:LEU:CD1	9:V:250:LEU:HD12	2.50	0.41
10:W:51:SER:HB2	10:W:230:LEU:HD12	2.02	0.41
10:W:67:ALA:HA	10:W:71:TYR:CD2	2.56	0.41
10:W:305:THR:HA	10:W:311:GLN:NE2	2.36	0.41
11:Y:71:VAL:HG22	11:Y:233:ALA:HB2	2.02	0.41
3:C:209:GLU:HG2	3:C:210:TRP:CD1	2.56	0.40
12:G:101:CDL:C52	12:G:101:CDL:C71	2.86	0.40
10:K:227:HIS:HD1	10:K:231:LYS:HE2	1.86	0.40
10:K:239:ASN:OD1	10:K:240:MET:HG2	2.21	0.40
11:L:234:ALA:HB2	11:L:413:ILE:HD12	2.03	0.40
11:L:282:LEU:HA	11:L:283:PRO:HD3	1.89	0.40
3:P:248:ARG:HG2	3:P:257:ASN:ND2	2.36	0.40
8:U:199:TYR:OH	9:V:71:ARG:NH1	2.53	0.40
10:W:177:LEU:HD21	10:W:272:VAL:HG21	2.02	0.40
10:W:449:PHE:N	10:W:452:GLU:CD	2.73	0.40
11:Y:61:SER:HA	11:Y:233:ALA:O	2.21	0.40
11:Y:113:VAL:HG13	11:Y:118:ALA:HB3	2.03	0.40
11:Y:334:ALA:H	11:Y:336:LYS:H	1.68	0.40
3:C:191:GLU:HB2	3:C:194:GLN:HG2	2.03	0.40
8:H:89:LEU:HD23	8:H:236:TYR:CZ	2.56	0.40
8:H:175:PHE:HA	8:H:176:PRO:HD3	1.84	0.40
9:J:3:PRO:HB2	9:J:5:ARG:HG2	2.03	0.40
9:J:198:LEU:HD12	12:J:404:CDL:H311	2.02	0.40
2:O:35:PRO:CB	10:W:320:PRO:HA	2.48	0.40
3:P:173:PRO:HD2	3:P:216:VAL:HG23	2.03	0.40
9:V:21:LEU:O	9:V:21:LEU:HD12	2.22	0.40
9:V:128:PHE:O	9:V:132:VAL:HG23	2.22	0.40
9:V:129:MET:HE3	9:V:185:LEU:HD12	2.03	0.40
10:W:126:LEU:HB3	11:Y:38:PHE:HZ	1.86	0.40
8:H:98:HIS:NE2	8:H:208:GLU:OE2	2.42	0.40
9:J:345:TYR:N	9:J:346:PRO:HD2	2.36	0.40
10:K:159:LYS:HG2	10:K:197:ILE:HD13	2.03	0.40
11:L:322:VAL:HG12	11:L:323:HIS:N	2.31	0.40
9:V:222:PRO:HG3	11:Y:470:ARG:HD3	2.04	0.40
11:Y:53:LEU:HD12	11:Y:57:LEU:HB3	2.04	0.40
11:Y:296:TRP:HB2	11:Y:348:TYR:C	2.42	0.40
1:A:17:TYR:CD1	11:L:275:ILE:HG12	2.56	0.40
2:B:40:GLN:HA	2:B:41:PRO:HD3	1.87	0.40
11:L:294:PRO:HG3	11:L:448:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:301:ASN:O	11:L:305:GLN:HG2	2.21	0.40
3:P:155:LYS:HB2	3:P:271:VAL:HG13	2.04	0.40
3:P:184:ILE:HD13	3:P:208:PRO:HB2	2.04	0.40
8:U:281:GLU:HG3	9:V:77:TRP:CD2	2.56	0.40
9:V:186:PRO:O	9:V:189:ILE:HB	2.21	0.40
9:V:333:LEU:HD11	14:V:403:PEE:H62	2.02	0.40
1:A:41:ARG:HH21	12:A:101:CDL:HA21	1.86	0.40
1:A:42:ILE:HG23	12:A:101:CDL:H121	2.03	0.40
3:C:207:LYS:HA	3:C:208:PRO:HD3	1.86	0.40
8:H:228:ARG:NH1	8:H:229:GLU:HB3	2.36	0.40
14:H:401:PEE:H70	17:L:501:PLX:H212	2.03	0.40
9:J:150:LEU:HA	9:J:150:LEU:HD12	1.87	0.40
10:K:104:GLU:OE1	11:L:325:SER:HA	2.21	0.40
10:K:407:MET:HA	10:K:408:PRO:HD2	1.99	0.40
2:O:14:VAL:O	2:O:14:VAL:HG12	2.22	0.40
3:P:125:VAL:HG21	17:Q:101:PLX:H141	2.03	0.40
8:U:125:HIS:NE2	15:U:402:HEC:C4C	2.84	0.40
8:U:304:TYR:OH	12:U:403:CDL:H732	2.22	0.40
10:W:438:MET:HB2	10:W:450:VAL:HG23	2.03	0.40
11:Y:163:LYS:O	11:Y:167:VAL:HG23	2.22	0.40
11:Y:423:ARG:O	11:Y:424:ILE:CB	2.70	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 PDB entries followed by that with respect to all EM entries.

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	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4 22
1	N	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	10 33
2	B	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1 10
2	O	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4 22
3	P	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8 30
4	D	60/62 (97%)	57 (95%)	3 (5%)	0	100 100
4	Q	60/62 (97%)	55 (92%)	5 (8%)	0	100 100
5	E	72/75 (96%)	65 (90%)	5 (7%)	2 (3%)	4 20
5	R	72/75 (96%)	69 (96%)	2 (3%)	1 (1%)	9 31
6	F	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	13 39
6	S	104/106 (98%)	102 (98%)	2 (2%)	0	100 100
7	G	49/51 (96%)	48 (98%)	1 (2%)	0	100 100
7	T	49/51 (96%)	47 (96%)	2 (4%)	0	100 100
8	H	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16 44
8	U	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16 44
9	J	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16 44
9	V	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16 44
10	K	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	11 35
10	W	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	11 35
11	L	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	9 31
11	Y	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	8 29
All	All	4178/4224 (99%)	3911 (94%)	210 (5%)	57 (1%)	12 31

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	268	ILE
10	K	241	ARG
2	O	23	ALA
3	P	141	SER
11	Y	424	ILE
3	C	153	GLU
3	C	255	PRO
9	J	157	GLY
10	K	176	ASN
2	O	38	PRO
3	P	255	PRO
9	V	157	GLY
9	V	254	ASP

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Mol	Chain	Res	Type
9	V	266	PRO
10	W	244	LEU
11	Y	312	GLY
11	Y	322	VAL
1	A	13	HIS
1	A	29	HIS
2	B	38	PRO
6	F	8	SER
8	H	133	ARG
10	K	244	LEU
11	L	180	ARG
11	L	312	GLY
11	L	322	VAL
1	N	46	PHE
2	O	51	SER
10	W	241	ARG
10	W	261	GLN
11	Y	382	SER
2	B	51	SER
3	C	142	ALA
3	C	204	ARG
3	C	219	HIS
5	E	86	LEU
10	K	261	GLN
11	L	193	GLN
5	R	28	ASP
8	U	133	ARG
10	W	144	PRO
10	W	403	ALA
11	Y	193	GLN
11	Y	461	PRO
2	B	40	GLN
5	E	28	ASP
11	L	463	GLU
2	O	27	ARG
2	O	40	GLN
3	P	204	ARG
8	U	246	PRO
11	Y	463	GLU
8	H	246	PRO
9	J	286	ASN
11	L	279	ASP

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Mol	Chain	Res	Type
2	O	30	VAL
10	K	320	PRO

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 PDB entries followed by that with respect to all EM entries.

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	74/74 (100%)	68 (92%)	6 (8%)	9 31
1	N	73/74 (99%)	73 (100%)	0	100 100
2	B	46/46 (100%)	46 (100%)	0	100 100
2	O	45/46 (98%)	45 (100%)	0	100 100
3	C	166/166 (100%)	166 (100%)	0	100 100
3	P	166/166 (100%)	166 (100%)	0	100 100
4	D	52/52 (100%)	52 (100%)	0	100 100
4	Q	52/52 (100%)	52 (100%)	0	100 100
5	E	61/72 (85%)	59 (97%)	2 (3%)	33 58
5	R	61/72 (85%)	59 (97%)	2 (3%)	33 58
6	F	95/95 (100%)	84 (88%)	11 (12%)	4 17
6	S	95/95 (100%)	95 (100%)	0	100 100
7	G	42/42 (100%)	42 (100%)	0	100 100
7	T	42/42 (100%)	40 (95%)	2 (5%)	21 48
8	H	207/207 (100%)	207 (100%)	0	100 100
8	U	207/207 (100%)	206 (100%)	1 (0%)	86 91
9	J	330/330 (100%)	327 (99%)	3 (1%)	75 86
9	V	330/330 (100%)	322 (98%)	8 (2%)	44 66
10	K	334/335 (100%)	331 (99%)	3 (1%)	75 86
10	W	335/335 (100%)	332 (99%)	3 (1%)	75 86
11	L	367/367 (100%)	367 (100%)	0	100 100
11	Y	367/367 (100%)	361 (98%)	6 (2%)	58 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3547/3572 (99%)	3500 (99%)	47 (1%)	64 78

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	40	ARG
1	A	48	ARG
1	A	61	THR
1	A	64	THR
1	A	66	GLU
5	E	28	ASP
5	E	30	LEU
6	F	14	LEU
6	F	17	ILE
6	F	29	LYS
6	F	33	MET
6	F	34	ARG
6	F	40	GLU
6	F	41	ASP
6	F	49	ARG
6	F	60	MET
6	F	71	LEU
6	F	74	GLN
9	J	124	MET
9	J	150	LEU
9	J	300	ILE
10	K	49	ILE
10	K	365	ASN
10	K	451	ASP
5	R	78	ARG
5	R	81	CYS
7	T	39	ARG
7	T	40	LEU
8	U	292	MET
9	V	147	THR
9	V	149	LEU
9	V	183	PHE
9	V	185	LEU
9	V	192	LEU
9	V	195	LEU
9	V	299	LEU

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Mol	Chain	Res	Type
9	V	345	TYR
10	W	254	ARG
10	W	451	ASP
10	W	453	LEU
11	Y	92	PHE
11	Y	96	LEU
11	Y	416	SER
11	Y	418	LEU
11	Y	422	ARG
11	Y	423	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
2	B	31	GLN
3	C	80	HIS
3	C	135	GLN
3	C	178	HIS
6	F	23	ASN
6	F	70	ASN
6	F	73	HIS
7	G	16	ASN
8	H	107	HIS
8	H	205	HIS
9	J	8	ASN
9	J	97	HIS
9	J	322	GLN
10	K	167	GLN
10	K	178	HIS
10	K	184	ASN
10	K	206	HIS
10	K	212	HIS
10	K	310	HIS
10	K	311	GLN
10	K	343	GLN
10	K	399	GLN
11	L	87	ASN
11	L	188	HIS
11	L	239	HIS
11	L	240	GLN
11	L	301	ASN

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Mol	Chain	Res	Type
11	L	308	ASN
3	P	135	GLN
3	P	178	HIS
4	Q	38	GLN
5	R	80	HIS
5	R	84	HIS
6	S	70	ASN
6	S	73	HIS
8	U	284	HIS
9	V	97	HIS
9	V	137	GLN
9	V	255	ASN
9	V	260	ASN
10	W	81	HIS
10	W	139	ASN
10	W	155	GLN
10	W	206	HIS
10	W	212	HIS
10	W	227	HIS
10	W	291	HIS
10	W	298	HIS
10	W	310	HIS
10	W	421	ASN
10	W	446	HIS
11	Y	87	ASN
11	Y	121	ASN
11	Y	152	GLN
11	Y	223	HIS
11	Y	301	ASN
11	Y	342	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	PLX	T	101	-	51,51,51	0.76	1 (1%)	55,59,59	0.60	1 (1%)
12	CDL	L	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
15	HEC	H	402	8	32,50,50	2.23	3 (9%)	24,82,82	1.35	1 (4%)
16	HEM	J	402	9	41,50,50	1.90	6 (14%)	45,82,82	1.58	9 (20%)
17	PLX	Q	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
14	PEE	V	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
17	PLX	L	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
12	CDL	Y	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)
16	HEM	J	401	9	41,50,50	1.92	6 (14%)	45,82,82	1.60	5 (11%)
12	CDL	U	403	-	63,63,99	1.25	6 (9%)	69,75,111	1.04	4 (5%)
15	HEC	U	402	8	32,50,50	2.27	3 (9%)	24,82,82	1.39	2 (8%)
12	CDL	H	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)
14	PEE	U	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
14	PEE	Y	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
14	PEE	J	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.99	2 (3%)
14	PEE	H	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
14	PEE	L	503	-	48,48,50	1.38	4 (8%)	51,53,55	0.92	2 (3%)
13	FES	C	301	3	0,4,4	-	-	-		
16	HEM	V	402	9	41,50,50	1.90	6 (14%)	45,82,82	1.60	8 (17%)
12	CDL	N	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
12	CDL	J	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
12	CDL	G	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.16	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CDL	J	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
16	HEM	V	401	9	41,50,50	1.97	5 (12%)	45,82,82	1.54	5 (11%)
13	FES	P	301	3	0,4,4	-	-	-		
12	CDL	A	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PLX	T	101	-	-	23/55/55/55	-
12	CDL	L	502	-	-	43/74/74/110	-
15	HEC	H	402	8	-	2/10/54/54	-
16	HEM	J	402	9	-	2/12/54/54	-
17	PLX	Q	101	-	-	25/55/55/55	-
14	PEE	V	403	-	-	30/52/52/54	-
17	PLX	L	501	-	-	23/55/55/55	-
12	CDL	Y	501	-	-	36/74/74/110	-
16	HEM	J	401	9	-	1/12/54/54	-
12	CDL	U	403	-	-	48/74/74/110	-
15	HEC	U	402	8	-	0/10/54/54	-
12	CDL	H	403	-	-	42/74/74/110	-
14	PEE	U	401	-	-	17/44/44/54	-
14	PEE	Y	502	-	-	20/52/52/54	-
14	PEE	J	403	-	-	20/52/52/54	-
14	PEE	H	401	-	-	27/52/52/54	-
14	PEE	L	503	-	-	22/52/52/54	-
13	FES	C	301	3	-	-	0/1/1/1
16	HEM	V	402	9	-	4/12/54/54	-
12	CDL	N	101	-	-	40/74/74/110	-
12	CDL	J	404	-	-	33/74/74/110	-
12	CDL	G	101	-	-	38/74/74/110	-
12	CDL	J	405	-	-	28/74/74/110	-
16	HEM	V	401	9	-	3/12/54/54	-
13	FES	P	301	3	-	-	0/1/1/1
12	CDL	A	101	-	-	35/74/74/110	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	402	HEM	C3D-C2D	7.86	1.53	1.36
16	J	401	HEM	C3D-C2D	7.85	1.53	1.36
16	J	402	HEM	C3D-C2D	7.83	1.53	1.36
16	V	401	HEM	C3D-C2D	7.75	1.53	1.36
15	U	402	HEC	C3C-C2C	-6.96	1.33	1.40
15	U	402	HEC	C2B-C3B	-6.63	1.33	1.40
15	H	402	HEC	C2B-C3B	-6.62	1.33	1.40
15	H	402	HEC	C3C-C2C	-6.50	1.34	1.40
16	V	401	HEM	C3C-C2C	-5.44	1.32	1.40
15	U	402	HEC	C3D-C2D	5.41	1.53	1.37
15	H	402	HEC	C3D-C2D	5.40	1.53	1.37
12	H	403	CDL	OA6-CA5	4.35	1.46	1.34
12	L	502	CDL	OA6-CA5	4.32	1.46	1.34
14	Y	502	PEE	C39-C38	4.31	1.56	1.31
12	H	403	CDL	OB8-CB7	4.30	1.45	1.33
12	G	101	CDL	OB8-CB7	4.30	1.45	1.33
12	J	405	CDL	OA8-CA7	4.29	1.45	1.33
12	U	403	CDL	OA6-CA5	4.29	1.46	1.34
12	Y	501	CDL	OA6-CA5	4.29	1.46	1.34
12	J	404	CDL	OA6-CA5	4.27	1.46	1.34
14	U	401	PEE	C39-C38	4.27	1.56	1.31
14	L	503	PEE	O3-C30	4.25	1.45	1.33
14	V	403	PEE	C39-C38	4.25	1.56	1.31
14	L	503	PEE	C39-C38	4.24	1.56	1.31
12	U	403	CDL	OB8-CB7	4.24	1.45	1.33
12	G	101	CDL	OA6-CA5	4.24	1.46	1.34
14	J	403	PEE	C39-C38	4.24	1.56	1.31
14	H	401	PEE	C39-C38	4.24	1.56	1.31
14	Y	502	PEE	O3-C30	4.23	1.45	1.33
12	Y	501	CDL	OB8-CB7	4.22	1.45	1.33
12	L	502	CDL	OB8-CB7	4.22	1.45	1.33
12	G	101	CDL	OA8-CA7	4.22	1.45	1.33
12	A	101	CDL	OB8-CB7	4.21	1.45	1.33
14	Y	502	PEE	C18-C19	4.20	1.56	1.31
14	H	401	PEE	O3-C30	4.20	1.45	1.33
12	J	404	CDL	OB8-CB7	4.19	1.45	1.33
14	L	503	PEE	C18-C19	4.19	1.56	1.31
12	A	101	CDL	OA6-CA5	4.19	1.46	1.34
14	H	401	PEE	C18-C19	4.19	1.56	1.31
16	J	401	HEM	C3C-C2C	-4.17	1.34	1.40
12	N	101	CDL	OB8-CB7	4.16	1.45	1.33
12	J	405	CDL	OB8-CB7	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	101	CDL	OA6-CA5	4.14	1.46	1.34
14	J	403	PEE	C18-C19	4.14	1.55	1.31
14	V	403	PEE	O3-C30	4.12	1.45	1.33
14	V	403	PEE	C18-C19	4.12	1.55	1.31
12	J	405	CDL	OB6-CB5	4.10	1.45	1.34
14	U	401	PEE	O3-C30	4.10	1.45	1.33
14	U	401	PEE	C19-C18	4.06	1.56	1.28
16	V	402	HEM	C3C-C2C	-4.00	1.34	1.40
12	G	101	CDL	OB6-CB5	4.00	1.45	1.34
14	J	403	PEE	O3-C30	3.98	1.45	1.33
12	J	405	CDL	OA6-CA5	3.98	1.45	1.34
12	J	404	CDL	OA8-CA7	3.97	1.44	1.33
12	Y	501	CDL	OA8-CA7	3.96	1.44	1.33
12	H	403	CDL	OA8-CA7	3.95	1.44	1.33
12	U	403	CDL	OA8-CA7	3.95	1.44	1.33
16	J	402	HEM	C3C-C2C	-3.95	1.34	1.40
12	N	101	CDL	OA8-CA7	3.93	1.44	1.33
12	A	101	CDL	OA8-CA7	3.91	1.44	1.33
12	L	502	CDL	OA8-CA7	3.89	1.44	1.33
16	V	402	HEM	C3C-CAC	3.78	1.55	1.47
16	J	401	HEM	C3C-CAC	3.71	1.55	1.47
16	J	402	HEM	C3C-CAC	3.65	1.55	1.47
14	L	503	PEE	O2-C10	3.46	1.44	1.34
14	Y	502	PEE	O2-C10	3.45	1.44	1.34
16	V	401	HEM	C3C-CAC	3.41	1.54	1.47
12	Y	501	CDL	OB6-CB5	3.29	1.43	1.34
14	J	403	PEE	O2-C10	3.24	1.43	1.34
12	J	404	CDL	OB6-CB5	3.22	1.43	1.34
12	N	101	CDL	OB6-CB5	3.21	1.43	1.34
14	U	401	PEE	O2-C10	3.20	1.43	1.34
12	H	403	CDL	OB6-CB5	3.19	1.43	1.34
12	U	403	CDL	OB6-CB5	3.17	1.43	1.34
14	V	403	PEE	O2-C10	3.15	1.43	1.34
12	A	101	CDL	OB6-CB5	3.14	1.43	1.34
12	L	502	CDL	OB6-CB5	3.11	1.43	1.34
14	H	401	PEE	O2-C10	3.10	1.43	1.34
16	J	402	HEM	CAB-C3B	2.98	1.55	1.47
16	V	401	HEM	CAB-C3B	2.96	1.55	1.47
16	J	401	HEM	CAB-C3B	2.93	1.55	1.47
16	V	402	HEM	CAB-C3B	2.90	1.55	1.47
12	L	502	CDL	OB6-CB4	-2.65	1.40	1.46
17	L	501	PLX	O6-C4	-2.63	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	401	HEM	FE-ND	2.61	2.09	1.96
17	Q	101	PLX	O6-C4	-2.59	1.41	1.44
12	H	403	CDL	OB6-CB4	-2.59	1.40	1.46
12	A	101	CDL	OB6-CB4	-2.58	1.40	1.46
12	J	404	CDL	OB6-CB4	-2.56	1.40	1.46
12	N	101	CDL	OB6-CB4	-2.54	1.40	1.46
12	U	403	CDL	OB6-CB4	-2.52	1.40	1.46
17	T	101	PLX	O6-C4	-2.52	1.41	1.44
12	Y	501	CDL	OB6-CB4	-2.44	1.40	1.46
16	J	402	HEM	FE-ND	2.17	2.07	1.96
16	J	401	HEM	FE-NB	2.16	2.07	1.96
16	J	402	HEM	CAA-C2A	2.12	1.55	1.52
16	V	402	HEM	CAA-C2A	2.12	1.55	1.52
16	J	401	HEM	FE-ND	2.04	2.06	1.96
12	U	403	CDL	C11-CA5	2.02	1.56	1.50
16	V	402	HEM	FE-ND	2.01	2.06	1.96

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	402	HEM	C4D-ND-C1D	6.17	111.44	105.07
16	J	401	HEM	C4D-ND-C1D	6.12	111.40	105.07
16	J	402	HEM	C4D-ND-C1D	6.04	111.31	105.07
16	V	401	HEM	C4D-ND-C1D	5.31	110.56	105.07
14	Y	502	PEE	O2-C10-C11	4.31	120.78	111.50
12	J	405	CDL	OB6-CB5-C51	4.28	120.72	111.50
12	L	502	CDL	OA6-CA5-C11	4.25	120.67	111.50
12	G	101	CDL	OB6-CB5-C51	4.20	120.56	111.50
12	Y	501	CDL	OA6-CA5-C11	4.19	120.53	111.50
12	H	403	CDL	OA6-CA5-C11	4.17	120.49	111.50
12	U	403	CDL	OA6-CA5-C11	4.17	120.49	111.50
12	J	404	CDL	OA6-CA5-C11	4.13	120.41	111.50
12	A	101	CDL	OA6-CA5-C11	4.08	120.29	111.50
12	J	404	CDL	OB6-CB5-C51	4.04	120.20	111.50
14	J	403	PEE	O2-C10-C11	4.03	120.18	111.50
12	U	403	CDL	OB6-CB5-C51	4.03	120.18	111.50
12	A	101	CDL	OB6-CB5-C51	4.00	120.12	111.50
12	N	101	CDL	OA6-CA5-C11	3.96	120.03	111.50
14	V	403	PEE	O2-C10-C11	3.93	119.97	111.50
12	H	403	CDL	OB6-CB5-C51	3.91	119.93	111.50
12	Y	501	CDL	OB6-CB5-C51	3.86	119.81	111.50
12	N	101	CDL	OB6-CB5-C51	3.85	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	502	CDL	OB6-CB5-C51	3.83	119.76	111.50
12	G	101	CDL	OA6-CA5-C11	3.57	119.19	111.50
14	H	401	PEE	O2-C10-C11	3.56	119.17	111.50
12	J	405	CDL	OA6-CA5-C11	3.55	119.16	111.50
14	L	503	PEE	O2-C10-C11	3.49	119.03	111.50
12	J	405	CDL	OB8-CB7-C71	3.25	122.12	111.91
14	U	401	PEE	O2-C10-C11	3.23	118.45	111.50
14	V	403	PEE	O3-C30-C31	3.07	121.53	111.91
16	V	401	HEM	C4B-CHC-C1C	3.05	126.58	122.56
12	A	101	CDL	OA8-CA7-C31	2.97	121.23	111.91
16	V	401	HEM	CAD-CBD-CGD	-2.96	107.23	113.60
12	G	101	CDL	CB4-OB6-CB5	-2.90	110.64	117.79
16	J	401	HEM	C4C-CHD-C1D	2.86	126.33	122.56
16	J	401	HEM	C4B-CHC-C1C	2.83	126.29	122.56
16	V	401	HEM	C4C-CHD-C1D	2.76	126.20	122.56
12	G	101	CDL	OB8-CB7-C71	2.74	120.51	111.91
12	L	502	CDL	OA8-CA7-C31	2.72	120.45	111.91
12	J	405	CDL	OA8-CA7-C31	2.70	120.39	111.91
16	V	402	HEM	C4C-CHD-C1D	2.69	126.11	122.56
12	L	502	CDL	OB8-CB7-C71	2.69	120.34	111.91
12	H	403	CDL	OB8-CB7-C71	2.68	120.31	111.91
12	U	403	CDL	OA8-CA7-C31	2.67	120.29	111.91
12	N	101	CDL	OA8-CA7-C31	2.67	120.28	111.91
14	H	401	PEE	O3-C30-C31	2.65	120.22	111.91
12	J	404	CDL	OA8-CA7-C31	2.65	120.21	111.91
16	J	402	HEM	C1B-NB-C4B	2.60	107.76	105.07
12	A	101	CDL	OB8-CB7-C71	2.60	120.06	111.91
12	U	403	CDL	OB8-CB7-C71	2.59	120.03	111.91
12	G	101	CDL	OA8-CA7-C31	2.57	119.98	111.91
12	J	404	CDL	OB8-CB7-C71	2.54	119.88	111.91
12	Y	501	CDL	OA8-CA7-C31	2.53	119.84	111.91
12	N	101	CDL	OB8-CB7-C71	2.52	119.81	111.91
12	Y	501	CDL	OB8-CB7-C71	2.51	119.79	111.91
12	H	403	CDL	OA8-CA7-C31	2.50	119.77	111.91
15	H	402	HEC	CMC-C2C-C1C	-2.50	124.62	128.46
14	L	503	PEE	O3-C30-C31	2.48	119.69	111.91
16	V	402	HEM	C1B-NB-C4B	2.47	107.62	105.07
17	T	101	PLX	C1C-N1-C1	2.44	119.89	109.92
16	V	401	HEM	C1B-NB-C4B	2.43	107.58	105.07
16	J	402	HEM	C4C-CHD-C1D	2.38	125.70	122.56
16	J	401	HEM	CMC-C2C-C3C	2.38	129.13	124.68
14	J	403	PEE	O3-C30-C31	2.38	119.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	402	HEM	CAD-C3D-C4D	2.37	128.79	124.66
17	L	501	PLX	C1C-N1-C1	2.35	119.54	109.92
14	U	401	PEE	O3-C30-C31	2.31	119.15	111.91
14	Y	502	PEE	O3-C30-C31	2.29	119.10	111.91
16	J	402	HEM	CAD-C3D-C4D	2.28	128.64	124.66
16	J	401	HEM	CAD-CBD-CGD	-2.21	108.84	113.60
12	J	405	CDL	OB8-CB7-OB9	-2.21	118.02	123.59
16	J	402	HEM	C4A-C3A-C2A	2.19	108.52	107.00
16	J	402	HEM	CMC-C2C-C3C	2.18	128.76	124.68
15	U	402	HEC	CMB-C2B-C1B	-2.18	125.11	128.46
16	V	402	HEM	C4A-C3A-C2A	2.17	108.51	107.00
16	J	402	HEM	C4B-CHC-C1C	2.17	125.43	122.56
16	V	402	HEM	CAD-CBD-CGD	-2.16	108.96	113.60
14	U	401	PEE	C17-C18-C19	-2.14	112.26	126.84
15	U	402	HEC	C1D-C2D-C3D	-2.11	105.53	107.00
16	V	402	HEM	C4B-CHC-C1C	2.11	125.34	122.56
16	V	402	HEM	CMC-C2C-C3C	2.07	128.54	124.68
16	J	402	HEM	C3B-C2B-C1B	2.06	108.01	106.49
17	Q	101	PLX	C2-C1-N1	-2.05	108.93	115.78
12	G	101	CDL	OB6-CB5-OB7	-2.04	118.77	123.70
17	Q	101	PLX	C1C-N1-C1	2.03	118.23	109.92
16	J	402	HEM	CHD-C1D-ND	2.01	126.61	124.43

There are no chirality outliers.

All (562) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	101	CDL	O1-C1-CB2-OB2
12	A	101	CDL	CB2-OB2-PB2-OB4
12	A	101	CDL	CB2-OB2-PB2-OB5
12	G	101	CDL	OA9-CA7-OA8-CA6
12	G	101	CDL	CB2-OB2-PB2-OB4
12	H	403	CDL	CA2-OA2-PA1-OA3
12	H	403	CDL	CA2-OA2-PA1-OA4
12	H	403	CDL	CA3-OA5-PA1-OA2
12	H	403	CDL	C11-CA5-OA6-CA4
12	H	403	CDL	CB3-OB5-PB2-OB3
12	H	403	CDL	OB7-CB5-OB6-CB4
12	J	404	CDL	CA3-OA5-PA1-OA2
12	J	404	CDL	CA3-OA5-PA1-OA3
12	J	404	CDL	CA3-OA5-PA1-OA4
12	J	404	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
12	J	404	CDL	CB3-OB5-PB2-OB2
12	J	404	CDL	CB3-OB5-PB2-OB3
12	J	404	CDL	CB3-OB5-PB2-OB4
12	J	405	CDL	CA3-OA5-PA1-OA4
12	J	405	CDL	C51-CB5-OB6-CB4
12	L	502	CDL	O1-C1-CA2-OA2
12	L	502	CDL	CA3-OA5-PA1-OA2
12	L	502	CDL	C11-CA5-OA6-CA4
12	L	502	CDL	CB2-OB2-PB2-OB3
12	L	502	CDL	CB2-OB2-PB2-OB4
12	L	502	CDL	C71-CB7-OB8-CB6
12	N	101	CDL	CA3-OA5-PA1-OA3
12	N	101	CDL	OA7-CA5-OA6-CA4
12	N	101	CDL	C11-CA5-OA6-CA4
12	N	101	CDL	CB2-OB2-PB2-OB4
12	N	101	CDL	CB2-OB2-PB2-OB5
12	U	403	CDL	CA3-OA5-PA1-OA2
12	U	403	CDL	CA3-OA5-PA1-OA3
12	U	403	CDL	C11-CA5-OA6-CA4
12	U	403	CDL	CB3-OB5-PB2-OB2
12	U	403	CDL	CB3-OB5-PB2-OB3
12	U	403	CDL	OB7-CB5-OB6-CB4
12	Y	501	CDL	CB2-C1-CA2-OA2
12	Y	501	CDL	C11-CA5-OA6-CA4
14	H	401	PEE	C4-O4P-P-O2P
14	J	403	PEE	C37-C38-C39-C40
14	L	503	PEE	C11-C10-O2-C2
14	L	503	PEE	O4-C10-O2-C2
14	U	401	PEE	C11-C10-O2-C2
14	U	401	PEE	C1-O3P-P-O2P
14	U	401	PEE	C1-O3P-P-O1P
14	U	401	PEE	C4-O4P-P-O2P
14	V	403	PEE	O4P-C4-C5-N
14	V	403	PEE	C39-C40-C41-C42
14	Y	502	PEE	C1-O3P-P-O2P
14	Y	502	PEE	C4-O4P-P-O3P
14	Y	502	PEE	C4-O4P-P-O2P
14	Y	502	PEE	C4-O4P-P-O1P
16	J	402	HEM	C1A-C2A-CAA-CBA
16	V	402	HEM	C1A-C2A-CAA-CBA
16	V	402	HEM	C3A-C2A-CAA-CBA
17	L	501	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	Q	101	PLX	O7-C6-O6-C4
17	Q	101	PLX	O6-C4-C5-O8
17	Q	101	PLX	N1-C1-C2-O1
17	Q	101	PLX	C25-C24-O8-C5
17	Q	101	PLX	O9-C24-C25-C26
17	T	101	PLX	C2-O1-P1-O4
17	T	101	PLX	O9-C24-O8-C5
12	L	502	CDL	OB9-CB7-OB8-CB6
12	A	101	CDL	OB9-CB7-OB8-CB6
12	N	101	CDL	OB9-CB7-OB8-CB6
12	U	403	CDL	OB9-CB7-OB8-CB6
12	J	404	CDL	OA7-CA5-OA6-CA4
12	J	405	CDL	OB7-CB5-OB6-CB4
12	L	502	CDL	OA7-CA5-OA6-CA4
12	U	403	CDL	OA7-CA5-OA6-CA4
12	Y	501	CDL	OA7-CA5-OA6-CA4
12	Y	501	CDL	OB7-CB5-OB6-CB4
14	U	401	PEE	O4-C10-O2-C2
12	G	101	CDL	C31-CA7-OA8-CA6
12	N	101	CDL	C71-CB7-OB8-CB6
12	U	403	CDL	C71-CB7-OB8-CB6
12	H	403	CDL	C51-CB5-OB6-CB4
12	U	403	CDL	C51-CB5-OB6-CB4
12	Y	501	CDL	C51-CB5-OB6-CB4
12	A	101	CDL	C71-CB7-OB8-CB6
12	H	403	CDL	C71-CB7-OB8-CB6
12	L	502	CDL	C31-CA7-OA8-CA6
12	H	403	CDL	OA7-CA5-OA6-CA4
17	L	501	PLX	C2-C1-N1-C1C
12	G	101	CDL	O1-C1-CB2-OB2
12	Y	501	CDL	O1-C1-CA2-OA2
12	Y	501	CDL	O1-C1-CB2-OB2
12	J	405	CDL	C31-CA7-OA8-CA6
12	U	403	CDL	C31-CA7-OA8-CA6
12	H	403	CDL	OB9-CB7-OB8-CB6
12	A	101	CDL	C51-CB5-OB6-CB4
12	U	403	CDL	OA9-CA7-OA8-CA6
14	U	401	PEE	C31-C32-C33-C34
12	H	403	CDL	C31-C32-C33-C34
12	J	405	CDL	OA9-CA7-OA8-CA6
12	L	502	CDL	OA9-CA7-OA8-CA6
12	J	405	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
12	Y	501	CDL	C12-C13-C14-C15
12	Y	501	CDL	C31-CA7-OA8-CA6
12	A	101	CDL	CA2-C1-CB2-OB2
12	J	404	CDL	CB2-C1-CA2-OA2
12	L	502	CDL	CB2-C1-CA2-OA2
12	L	502	CDL	CA2-C1-CB2-OB2
12	H	403	CDL	C31-CA7-OA8-CA6
12	A	101	CDL	O1-C1-CA2-OA2
12	J	404	CDL	O1-C1-CA2-OA2
12	Y	501	CDL	CB5-C51-C52-C53
17	T	101	PLX	O6-C4-C5-O8
12	H	403	CDL	OA9-CA7-OA8-CA6
12	H	403	CDL	CB5-C51-C52-C53
12	N	101	CDL	CA5-C11-C12-C13
12	Y	501	CDL	CA7-C31-C32-C33
14	H	401	PEE	C37-C38-C39-C40
12	N	101	CDL	C71-C72-C73-C74
12	J	404	CDL	CA7-C31-C32-C33
12	L	502	CDL	CA5-C11-C12-C13
12	U	403	CDL	CA5-C11-C12-C13
14	V	403	PEE	C10-C11-C12-C13
12	L	502	CDL	C52-C53-C54-C55
12	A	101	CDL	OB7-CB5-OB6-CB4
12	A	101	CDL	CB7-C71-C72-C73
12	G	101	CDL	CB7-C71-C72-C73
12	J	405	CDL	CB7-C71-C72-C73
16	J	401	HEM	C3D-CAD-CBD-CGD
16	V	401	HEM	C3D-CAD-CBD-CGD
14	L	503	PEE	C30-C31-C32-C33
12	L	502	CDL	O1-C1-CB2-OB2
12	N	101	CDL	C14-C15-C16-C17
12	Y	501	CDL	OA9-CA7-OA8-CA6
12	H	403	CDL	C33-C34-C35-C36
12	G	101	CDL	CA2-OA2-PA1-OA5
12	G	101	CDL	CB2-OB2-PB2-OB5
12	H	403	CDL	CA2-OA2-PA1-OA5
12	H	403	CDL	CB3-OB5-PB2-OB2
12	J	405	CDL	CA3-OA5-PA1-OA2
12	L	502	CDL	CB2-OB2-PB2-OB5
12	L	502	CDL	CB3-OB5-PB2-OB2
12	N	101	CDL	CA3-OA5-PA1-OA2
12	Y	501	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
14	H	401	PEE	C4-O4P-P-O3P
14	U	401	PEE	C1-O3P-P-O4P
14	U	401	PEE	C4-O4P-P-O3P
14	Y	502	PEE	C1-O3P-P-O4P
12	Y	501	CDL	C71-CB7-OB8-CB6
17	L	501	PLX	C12-C13-C14-C15
12	G	101	CDL	CA2-C1-CB2-OB2
12	Y	501	CDL	CA2-C1-CB2-OB2
17	L	501	PLX	C2-C1-N1-C1A
17	Q	101	PLX	O8-C24-C25-C26
12	Y	501	CDL	C32-C33-C34-C35
12	G	101	CDL	C51-CB5-OB6-CB4
12	G	101	CDL	C33-C34-C35-C36
12	J	405	CDL	C12-C13-C14-C15
17	Q	101	PLX	C19-C20-C21-C22
17	T	101	PLX	C7-C8-C9-C10
12	U	403	CDL	C13-C14-C15-C16
14	J	403	PEE	C20-C21-C22-C23
14	Y	502	PEE	C11-C12-C13-C14
17	T	101	PLX	C9-C10-C11-C12
12	L	502	CDL	CA6-CA4-OA6-CA5
12	G	101	CDL	OB7-CB5-OB6-CB4
17	Q	101	PLX	C10-C11-C12-C13
12	J	404	CDL	C1-CB2-OB2-PB2
12	Y	501	CDL	OA5-CA3-CA4-OA6
12	A	101	CDL	C51-C52-C53-C54
12	G	101	CDL	C14-C15-C16-C17
12	L	502	CDL	C51-C52-C53-C54
12	U	403	CDL	C54-C55-C56-C57
17	Q	101	PLX	C12-C13-C14-C15
12	A	101	CDL	CA5-C11-C12-C13
12	A	101	CDL	C31-C32-C33-C34
17	L	501	PLX	C15-C16-C17-C18
17	L	501	PLX	C13-C14-C15-C16
14	H	401	PEE	C21-C22-C23-C24
14	J	403	PEE	C13-C14-C15-C16
14	J	403	PEE	C11-C12-C13-C14
12	N	101	CDL	CB4-CB6-OB8-CB7
14	L	503	PEE	C32-C33-C34-C35
17	Q	101	PLX	C34-C35-C36-C37
12	J	405	CDL	C33-C34-C35-C36
12	L	502	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
12	U	403	CDL	C31-C32-C33-C34
14	H	401	PEE	C11-C12-C13-C14
17	L	501	PLX	C10-C11-C12-C13
12	Y	501	CDL	C14-C15-C16-C17
14	H	401	PEE	C22-C23-C24-C25
14	J	403	PEE	C22-C23-C24-C25
14	U	401	PEE	C11-C12-C13-C14
14	V	403	PEE	C35-C36-C37-C38
14	Y	502	PEE	C19-C20-C21-C22
12	G	101	CDL	CA5-C11-C12-C13
12	L	502	CDL	CA7-C31-C32-C33
12	U	403	CDL	CB7-C71-C72-C73
14	L	503	PEE	C11-C12-C13-C14
17	L	501	PLX	C2-C1-N1-C1B
14	Y	502	PEE	C22-C23-C24-C25
12	G	101	CDL	C73-C74-C75-C76
17	Q	101	PLX	C15-C16-C17-C18
14	J	403	PEE	C32-C33-C34-C35
14	L	503	PEE	C34-C35-C36-C37
12	U	403	CDL	C14-C15-C16-C17
14	V	403	PEE	C32-C33-C34-C35
12	G	101	CDL	C72-C73-C74-C75
12	Y	501	CDL	C33-C34-C35-C36
14	H	401	PEE	C32-C33-C34-C35
12	Y	501	CDL	OB9-CB7-OB8-CB6
12	L	502	CDL	C51-CB5-OB6-CB4
17	T	101	PLX	O9-C24-C25-C26
12	H	403	CDL	C32-C33-C34-C35
12	U	403	CDL	C53-C54-C55-C56
17	T	101	PLX	C11-C12-C13-C14
12	J	404	CDL	C11-C12-C13-C14
12	J	404	CDL	C14-C15-C16-C17
12	J	405	CDL	C52-C53-C54-C55
12	Y	501	CDL	C13-C14-C15-C16
12	G	101	CDL	C31-C32-C33-C34
14	V	403	PEE	C41-C42-C43-C44
14	V	403	PEE	C30-C31-C32-C33
14	H	401	PEE	C11-C10-O2-C2
12	A	101	CDL	C33-C34-C35-C36
14	L	503	PEE	C10-C11-C12-C13
12	G	101	CDL	C52-C53-C54-C55
12	N	101	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
14	V	403	PEE	C12-C13-C14-C15
14	U	401	PEE	C33-C34-C35-C36
14	L	503	PEE	C37-C38-C39-C40
12	L	502	CDL	OB7-CB5-OB6-CB4
14	V	403	PEE	O4-C10-O2-C2
12	J	405	CDL	CB5-C51-C52-C53
17	T	101	PLX	C33-C34-C35-C36
14	Y	502	PEE	C20-C21-C22-C23
14	V	403	PEE	C11-C10-O2-C2
12	L	502	CDL	OA5-CA3-CA4-OA6
12	L	502	CDL	OB5-CB3-CB4-OB6
12	A	101	CDL	C12-C13-C14-C15
17	Q	101	PLX	C13-C14-C15-C16
14	V	403	PEE	C40-C41-C42-C43
14	H	401	PEE	O4-C10-O2-C2
17	L	501	PLX	O6-C4-C5-O8
14	L	503	PEE	C12-C13-C14-C15
17	Q	101	PLX	C18-C19-C20-C21
12	H	403	CDL	C53-C54-C55-C56
14	U	401	PEE	C34-C35-C36-C37
14	V	403	PEE	C19-C20-C21-C22
17	Q	101	PLX	C7-C8-C9-C10
12	L	502	CDL	CA2-OA2-PA1-OA5
14	V	403	PEE	C1-O3P-P-O4P
14	V	403	PEE	C4-O4P-P-O3P
12	U	403	CDL	C73-C74-C75-C76
14	V	403	PEE	C33-C34-C35-C36
14	H	401	PEE	C2-C1-O3P-P
17	L	501	PLX	C7-C8-C9-C10
14	J	403	PEE	O3P-C1-C2-C3
17	L	501	PLX	O4-C3-C4-C5
12	G	101	CDL	C34-C35-C36-C37
17	T	101	PLX	C32-C33-C34-C35
12	G	101	CDL	CA7-C31-C32-C33
12	Y	501	CDL	CB7-C71-C72-C73
17	Q	101	PLX	C26-C27-C28-C29
17	T	101	PLX	C18-C19-C20-C21
14	L	503	PEE	C21-C22-C23-C24
17	T	101	PLX	C34-C35-C36-C37
17	T	101	PLX	C13-C14-C15-C16
12	L	502	CDL	C14-C15-C16-C17
12	H	403	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
12	J	405	CDL	CB3-CB4-CB6-OB8
12	L	502	CDL	CA3-CA4-CA6-OA8
12	L	502	CDL	CB3-CB4-CB6-OB8
12	N	101	CDL	CB3-CB4-CB6-OB8
12	U	403	CDL	CA3-CA4-CA6-OA8
14	V	403	PEE	C1-C2-C3-O3
12	L	502	CDL	C13-C14-C15-C16
14	Y	502	PEE	C33-C34-C35-C36
12	G	101	CDL	C75-C76-C77-C78
12	J	404	CDL	C15-C16-C17-C18
14	J	403	PEE	C41-C42-C43-C44
12	J	404	CDL	CA5-C11-C12-C13
12	Y	501	CDL	C15-C16-C17-C18
12	U	403	CDL	C15-C16-C17-C18
14	J	403	PEE	C35-C36-C37-C38
14	J	403	PEE	C39-C40-C41-C42
14	U	401	PEE	C15-C16-C17-C18
14	V	403	PEE	C15-C16-C17-C18
12	H	403	CDL	C55-C56-C57-C58
12	L	502	CDL	C31-C32-C33-C34
12	J	404	CDL	C74-C75-C76-C77
17	Q	101	PLX	C36-C37-C38-C39
14	Y	502	PEE	C42-C43-C44-C45
12	U	403	CDL	CB5-C51-C52-C53
12	J	405	CDL	C55-C56-C57-C58
12	N	101	CDL	C55-C56-C57-C58
12	J	404	CDL	CA3-CA4-OA6-CA5
12	J	405	CDL	CB6-CB4-OB6-CB5
17	Q	101	PLX	C31-C32-C33-C34
17	Q	101	PLX	C9-C10-C11-C12
12	H	403	CDL	C32-C31-CA7-OA8
12	N	101	CDL	C15-C16-C17-C18
12	J	405	CDL	CA7-C31-C32-C33
14	H	401	PEE	C34-C35-C36-C37
17	L	501	PLX	C34-C35-C36-C37
12	A	101	CDL	C71-C72-C73-C74
14	H	401	PEE	C30-C31-C32-C33
12	G	101	CDL	C71-CB7-OB8-CB6
14	H	401	PEE	C24-C25-C26-C27
14	V	403	PEE	C13-C14-C15-C16
12	H	403	CDL	C15-C16-C17-C18
12	J	405	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
12	J	404	CDL	C73-C74-C75-C76
12	L	502	CDL	OA5-CA3-CA4-CA6
12	U	403	CDL	OA5-CA3-CA4-CA6
12	Y	501	CDL	OA5-CA3-CA4-CA6
12	Y	501	CDL	OB5-CB3-CB4-CB6
14	H	401	PEE	C20-C21-C22-C23
12	J	404	CDL	C12-C13-C14-C15
14	J	403	PEE	C40-C41-C42-C43
12	A	101	CDL	C75-C76-C77-C78
12	A	101	CDL	CB3-CB4-CB6-OB8
17	L	501	PLX	C3-C4-C5-O8
17	Q	101	PLX	C3-C4-C5-O8
17	T	101	PLX	C3-C4-C5-O8
14	V	403	PEE	C22-C23-C24-C25
12	J	404	CDL	C71-C72-C73-C74
17	Q	101	PLX	C14-C15-C16-C17
17	T	101	PLX	C3-O4-P1-O1
12	H	403	CDL	C52-C53-C54-C55
17	L	501	PLX	C32-C33-C34-C35
12	N	101	CDL	OA5-CA3-CA4-OA6
14	J	403	PEE	O3P-C1-C2-O2
12	G	101	CDL	OB9-CB7-OB8-CB6
12	J	404	CDL	C31-C32-C33-C34
12	G	101	CDL	OB6-CB4-CB6-OB8
12	H	403	CDL	OB6-CB4-CB6-OB8
12	L	502	CDL	OA6-CA4-CA6-OA8
12	L	502	CDL	OB6-CB4-CB6-OB8
12	U	403	CDL	OA6-CA4-CA6-OA8
14	L	503	PEE	C14-C15-C16-C17
12	G	101	CDL	C74-C75-C76-C77
12	N	101	CDL	C52-C53-C54-C55
12	A	101	CDL	C1-CA2-OA2-PA1
12	A	101	CDL	C1-CB2-OB2-PB2
12	A	101	CDL	CB4-CB3-OB5-PB2
12	H	403	CDL	C1-CA2-OA2-PA1
12	N	101	CDL	CB4-CB3-OB5-PB2
14	V	403	PEE	C34-C35-C36-C37
12	U	403	CDL	C74-C75-C76-C77
12	L	502	CDL	C53-C54-C55-C56
12	A	101	CDL	OA5-CA3-CA4-CA6
12	J	404	CDL	OB5-CB3-CB4-CB6
12	N	101	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
12	U	403	CDL	OB5-CB3-CB4-CB6
14	V	403	PEE	C20-C21-C22-C23
14	Y	502	PEE	C14-C15-C16-C17
14	V	403	PEE	C16-C17-C18-C19
14	H	401	PEE	C39-C40-C41-C42
14	V	403	PEE	C11-C12-C13-C14
12	A	101	CDL	C35-C36-C37-C38
12	U	403	CDL	C55-C56-C57-C58
12	U	403	CDL	C71-C72-C73-C74
17	T	101	PLX	C26-C27-C28-C29
12	J	405	CDL	CA6-CA4-OA6-CA5
12	U	403	CDL	CA6-CA4-OA6-CA5
12	Y	501	CDL	CA6-CA4-OA6-CA5
12	Y	501	CDL	CB3-CB4-OB6-CB5
14	L	503	PEE	C31-C32-C33-C34
12	G	101	CDL	C11-C12-C13-C14
12	A	101	CDL	CA3-CA4-CA6-OA8
12	N	101	CDL	CA3-CA4-CA6-OA8
12	U	403	CDL	C1-CB2-OB2-PB2
12	Y	501	CDL	CA3-CA4-CA6-OA8
12	J	404	CDL	OB5-CB3-CB4-OB6
12	U	403	CDL	OA5-CA3-CA4-OA6
17	L	501	PLX	O4-C3-C4-O6
17	Q	101	PLX	O4-C3-C4-O6
17	L	501	PLX	C6-C7-C8-C9
12	A	101	CDL	OA6-CA4-CA6-OA8
12	G	101	CDL	OA6-CA4-CA6-OA8
12	J	405	CDL	OA6-CA4-CA6-OA8
12	J	405	CDL	OB6-CB4-CB6-OB8
12	N	101	CDL	OA6-CA4-CA6-OA8
12	A	101	CDL	C32-C31-CA7-OA8
12	H	403	CDL	C12-C13-C14-C15
14	H	401	PEE	C15-C16-C17-C18
14	J	403	PEE	O4-C10-O2-C2
12	J	404	CDL	C33-C34-C35-C36
12	L	502	CDL	C11-C12-C13-C14
12	J	405	CDL	CB2-OB2-PB2-OB5
12	H	403	CDL	CA4-CA3-OA5-PA1
12	H	403	CDL	C1-CB2-OB2-PB2
12	J	404	CDL	CA4-CA3-OA5-PA1
12	N	101	CDL	C1-CA2-OA2-PA1
12	N	101	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
12	A	101	CDL	CB2-OB2-PB2-OB3
12	G	101	CDL	CA2-OA2-PA1-OA3
12	G	101	CDL	CB2-OB2-PB2-OB3
12	L	502	CDL	CA2-OA2-PA1-OA4
12	L	502	CDL	CB3-OB5-PB2-OB3
12	L	502	CDL	CB3-OB5-PB2-OB4
12	N	101	CDL	CA2-OA2-PA1-OA3
12	N	101	CDL	CB2-OB2-PB2-OB3
12	Y	501	CDL	CA3-OA5-PA1-OA4
14	H	401	PEE	C4-O4P-P-O1P
14	U	401	PEE	C4-O4P-P-O1P
14	V	403	PEE	C1-O3P-P-O2P
14	V	403	PEE	C1-O3P-P-O1P
14	Y	502	PEE	C1-O3P-P-O1P
17	Q	101	PLX	C3-O4-P1-O3
17	T	101	PLX	C2-O1-P1-O3
12	L	502	CDL	OB5-CB3-CB4-CB6
17	Q	101	PLX	O4-C3-C4-C5
12	L	502	CDL	C33-C34-C35-C36
14	H	401	PEE	C17-C18-C19-C20
14	V	403	PEE	C17-C18-C19-C20
14	H	401	PEE	C5-C4-O4P-P
17	T	101	PLX	C1-C2-O1-P1
17	T	101	PLX	C25-C24-O8-C5
12	N	101	CDL	CA2-C1-CB2-OB2
12	U	403	CDL	CA2-C1-CB2-OB2
12	U	403	CDL	OB5-CB3-CB4-OB6
12	Y	501	CDL	OB5-CB3-CB4-OB6
16	V	401	HEM	C2A-CAA-CBA-CGA
14	J	403	PEE	C11-C10-O2-C2
14	H	401	PEE	C14-C15-C16-C17
17	L	501	PLX	C19-C20-C21-C22
12	G	101	CDL	CA3-CA4-CA6-OA8
15	H	402	HEC	C1A-C2A-CAA-CBA
15	H	402	HEC	C3A-C2A-CAA-CBA
16	J	402	HEM	C3A-C2A-CAA-CBA
17	L	501	PLX	N1-C1-C2-O1
12	H	403	CDL	OA6-CA4-CA6-OA8
12	Y	501	CDL	OA6-CA4-CA6-OA8
14	V	403	PEE	O2-C2-C3-O3
12	J	404	CDL	C55-C56-C57-C58
12	J	404	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
14	L	503	PEE	C33-C34-C35-C36
12	H	403	CDL	O1-C1-CB2-OB2
12	H	403	CDL	C13-C14-C15-C16
12	H	403	CDL	CA3-CA4-OA6-CA5
12	A	101	CDL	CB2-C1-CA2-OA2
12	H	403	CDL	C54-C55-C56-C57
12	J	404	CDL	CB4-CB3-OB5-PB2
12	A	101	CDL	OA5-CA3-CA4-OA6
14	H	401	PEE	C31-C32-C33-C34
14	Y	502	PEE	C38-C39-C40-C41
12	N	101	CDL	OB6-CB4-CB6-OB8
12	G	101	CDL	CB3-OB5-PB2-OB2
12	J	405	CDL	CA2-OA2-PA1-OA5
12	J	405	CDL	CB3-OB5-PB2-OB2
12	U	403	CDL	CA2-OA2-PA1-OA5
14	H	401	PEE	C1-O3P-P-O4P
14	L	503	PEE	C4-O4P-P-O3P
12	G	101	CDL	CB3-CB4-CB6-OB8
16	V	402	HEM	C4D-C3D-CAD-CBD
14	Y	502	PEE	C40-C41-C42-C43
14	V	403	PEE	C31-C32-C33-C34
12	N	101	CDL	CB5-C51-C52-C53
12	G	101	CDL	C1-CA2-OA2-PA1
12	U	403	CDL	CB4-CB3-OB5-PB2
12	J	405	CDL	C14-C15-C16-C17
12	J	405	CDL	C34-C35-C36-C37
12	G	101	CDL	C51-C52-C53-C54
14	Y	502	PEE	O4P-C4-C5-N
12	L	502	CDL	C54-C55-C56-C57
12	J	405	CDL	C15-C16-C17-C18
12	Y	501	CDL	C52-C53-C54-C55
12	N	101	CDL	C32-C33-C34-C35
12	G	101	CDL	C71-C72-C73-C74
12	U	403	CDL	CB3-CB4-OB6-CB5
12	N	101	CDL	CA2-OA2-PA1-OA5
17	Q	101	PLX	C5-C4-O6-C6
16	V	402	HEM	C2D-C3D-CAD-CBD
12	N	101	CDL	C31-CA7-OA8-CA6
14	J	403	PEE	C15-C16-C17-C18
12	H	403	CDL	C51-C52-C53-C54
14	U	401	PEE	C30-C31-C32-C33
12	A	101	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
14	L	503	PEE	C19-C20-C21-C22
12	H	403	CDL	C14-C15-C16-C17
14	V	403	PEE	C14-C15-C16-C17
14	L	503	PEE	C16-C17-C18-C19
14	L	503	PEE	C40-C41-C42-C43
12	H	403	CDL	C32-C31-CA7-OA9
12	N	101	CDL	OA9-CA7-OA8-CA6
12	U	403	CDL	O1-C1-CA2-OA2
12	N	101	CDL	C53-C54-C55-C56
12	H	403	CDL	CB7-C71-C72-C73
12	N	101	CDL	C35-C36-C37-C38
14	J	403	PEE	C36-C37-C38-C39
12	Y	501	CDL	C72-C71-CB7-OB8
17	L	501	PLX	O6-C6-C7-C8
12	U	403	CDL	C34-C35-C36-C37
14	L	503	PEE	C23-C24-C25-C26
17	T	101	PLX	C30-C31-C32-C33
14	U	401	PEE	C14-C15-C16-C17
14	U	401	PEE	C38-C39-C40-C41
14	Y	502	PEE	C36-C37-C38-C39
14	U	401	PEE	C42-C43-C44-C45
12	H	403	CDL	C73-C74-C75-C76
14	J	403	PEE	C19-C20-C21-C22
12	A	101	CDL	C15-C16-C17-C18
12	J	404	CDL	C52-C51-CB5-OB6
12	G	101	CDL	C32-C31-CA7-OA8
14	H	401	PEE	C40-C41-C42-C43
14	V	403	PEE	C36-C37-C38-C39
12	H	403	CDL	CB3-CB4-CB6-OB8
12	J	405	CDL	CA3-CA4-CA6-OA8
14	H	401	PEE	O3P-C1-C2-O2
12	N	101	CDL	C12-C11-CA5-OA6
17	T	101	PLX	C10-C11-C12-C13
14	H	401	PEE	C36-C37-C38-C39
12	U	403	CDL	O1-C1-CB2-OB2
17	L	501	PLX	C11-C12-C13-C14
17	L	501	PLX	C29-C30-C31-C32
12	A	101	CDL	C32-C33-C34-C35
14	L	503	PEE	O2-C10-C11-C12
12	N	101	CDL	C12-C11-CA5-OA7
12	G	101	CDL	C32-C31-CA7-OA9
12	U	403	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
12	U	403	CDL	C72-C71-CB7-OB8
17	L	501	PLX	C33-C34-C35-C36
12	G	101	CDL	C15-C16-C17-C18
14	L	503	PEE	C41-C42-C43-C44
12	N	101	CDL	C72-C71-CB7-OB8
12	U	403	CDL	C1-CA2-OA2-PA1
12	J	404	CDL	C52-C51-CB5-OB7
14	Y	502	PEE	C21-C22-C23-C24
12	J	405	CDL	CA2-OA2-PA1-OA3
12	L	502	CDL	CA2-OA2-PA1-OA3
12	U	403	CDL	CA2-OA2-PA1-OA3
12	U	403	CDL	CB2-OB2-PB2-OB3
12	Y	501	CDL	CA2-OA2-PA1-OA3
14	H	401	PEE	C1-O3P-P-O1P
14	J	403	PEE	C4-O4P-P-O2P
17	T	101	PLX	C3-O4-P1-O3
12	U	403	CDL	OB6-CB4-CB6-OB8
12	U	403	CDL	C75-C76-C77-C78
16	V	401	HEM	CAA-CBA-CGA-O2A
14	J	403	PEE	O4P-C4-C5-N
17	T	101	PLX	C25-C26-C27-C28
17	L	501	PLX	C1-C2-O1-P1
14	J	403	PEE	C10-C11-C12-C13
12	Y	501	CDL	C51-C52-C53-C54
12	A	101	CDL	C12-C11-CA5-OA6
12	G	101	CDL	C52-C51-CB5-OB6
14	Y	502	PEE	O3-C30-C31-C32
12	J	404	CDL	C12-C11-CA5-OA6
14	H	401	PEE	O2-C10-C11-C12
14	L	503	PEE	O3-C30-C31-C32
12	U	403	CDL	C72-C71-CB7-OB9
14	L	503	PEE	O4-C10-C11-C12
17	Q	101	PLX	C6-C7-C8-C9
12	H	403	CDL	C12-C11-CA5-OA6
12	H	403	CDL	C12-C11-CA5-OA7
14	Y	502	PEE	O5-C30-C31-C32
12	A	101	CDL	C12-C11-CA5-OA7
12	N	101	CDL	O1-C1-CB2-OB2
12	J	404	CDL	C12-C11-CA5-OA7
12	N	101	CDL	C72-C71-CB7-OB9
17	T	101	PLX	C17-C18-C19-C20
12	Y	501	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	A	101	CDL	C52-C51-CB5-OB6

There are no ring outliers.

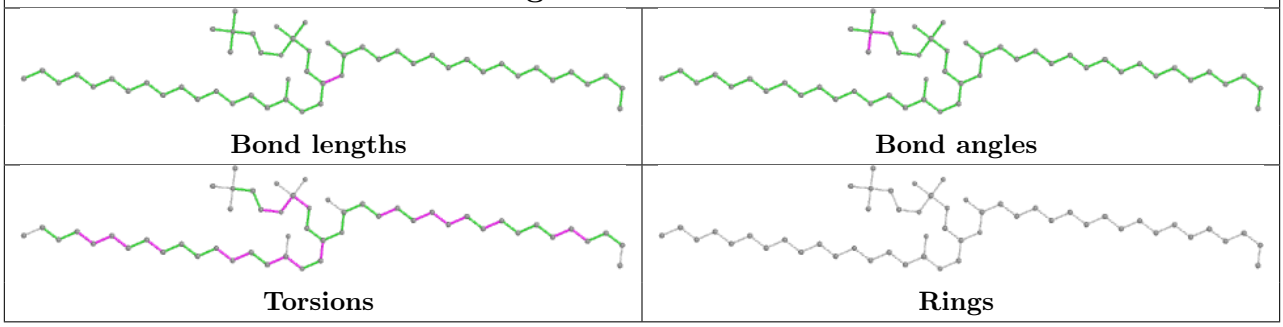
26 monomers are involved in 276 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	101	PLX	3	0
12	L	502	CDL	22	0
15	H	402	HEC	5	0
16	J	402	HEM	4	0
17	Q	101	PLX	7	0
14	V	403	PEE	23	0
17	L	501	PLX	4	0
12	Y	501	CDL	4	0
16	J	401	HEM	3	0
12	U	403	CDL	12	0
15	U	402	HEC	8	0
12	H	403	CDL	6	0
14	U	401	PEE	25	0
14	Y	502	PEE	21	0
14	J	403	PEE	8	0
14	H	401	PEE	32	0
14	L	503	PEE	37	0
13	C	301	FES	3	0
16	V	402	HEM	6	0
12	N	101	CDL	8	0
12	J	404	CDL	6	0
12	G	101	CDL	28	0
12	J	405	CDL	17	0
16	V	401	HEM	7	0
13	P	301	FES	2	0
12	A	101	CDL	3	0

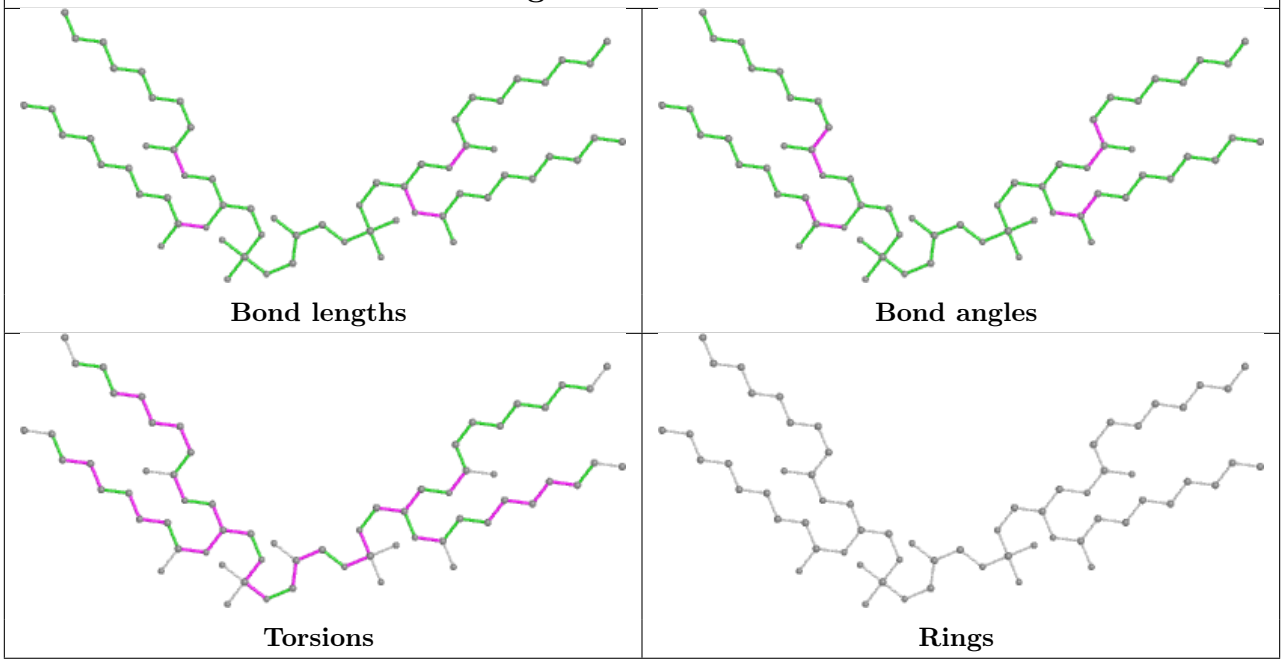
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

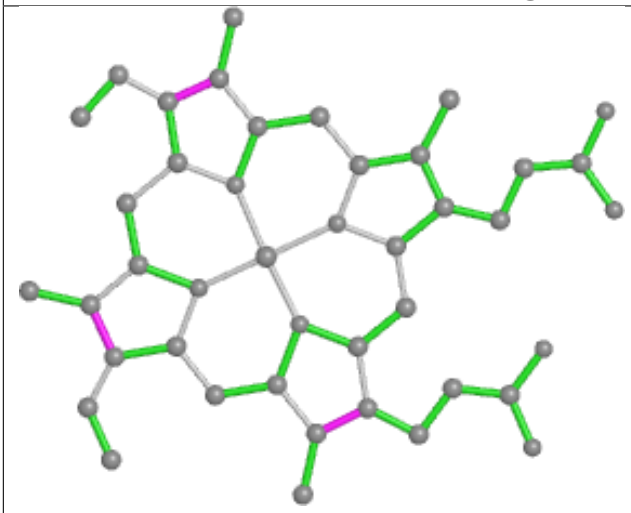
Ligand PLX T 101



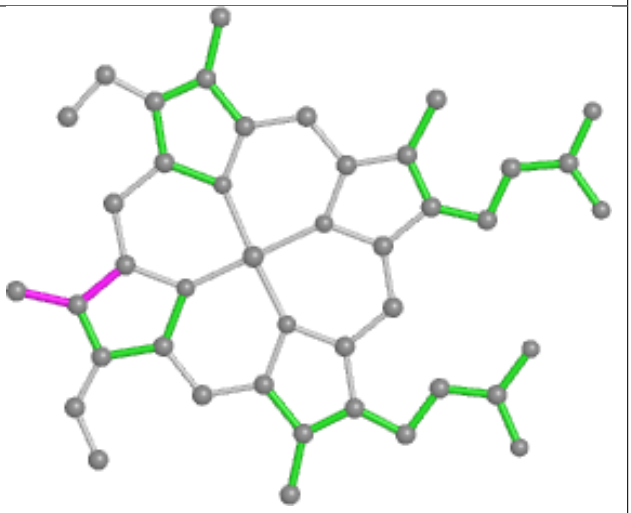
Ligand CDL L 502



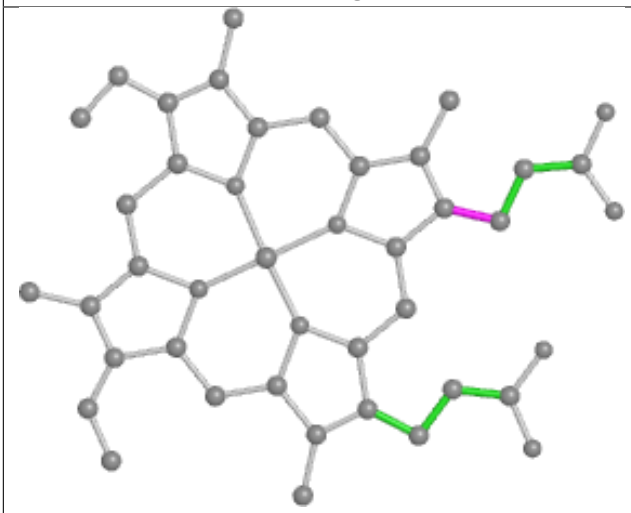
Ligand HEC H 402



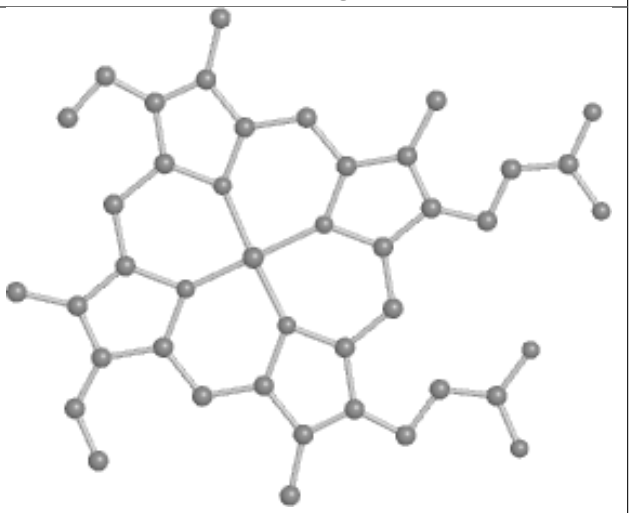
Bond lengths



Bond angles

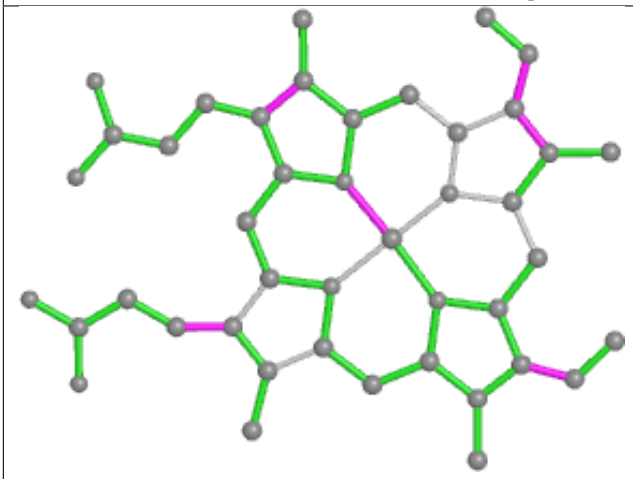


Torsions

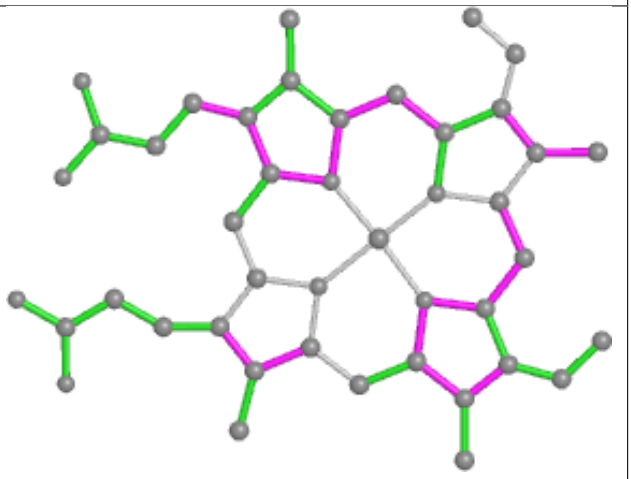


Rings

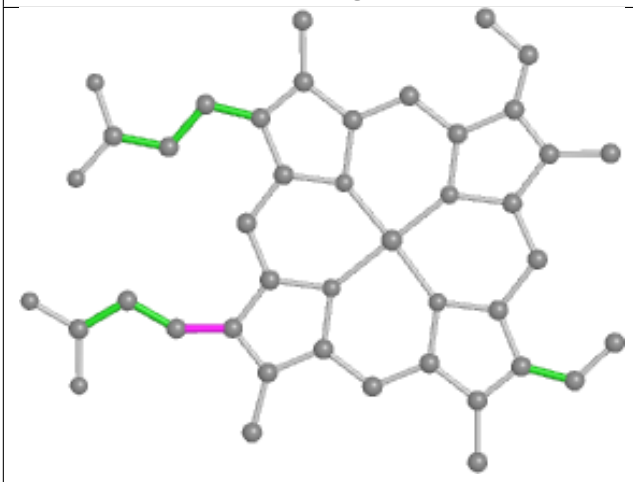
Ligand HEM J 402



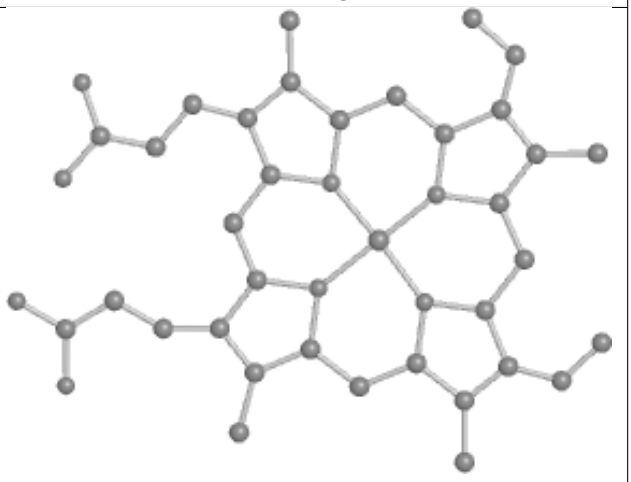
Bond lengths



Bond angles

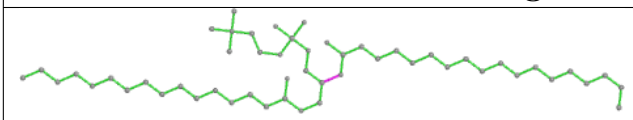


Torsions



Rings

Ligand PLX Q 101



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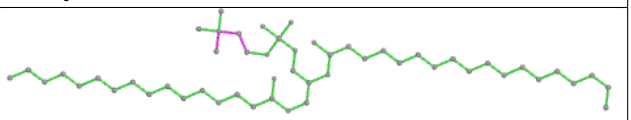
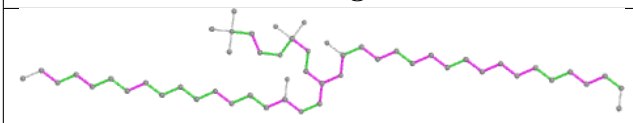
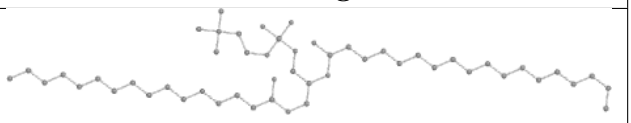


Bond angles

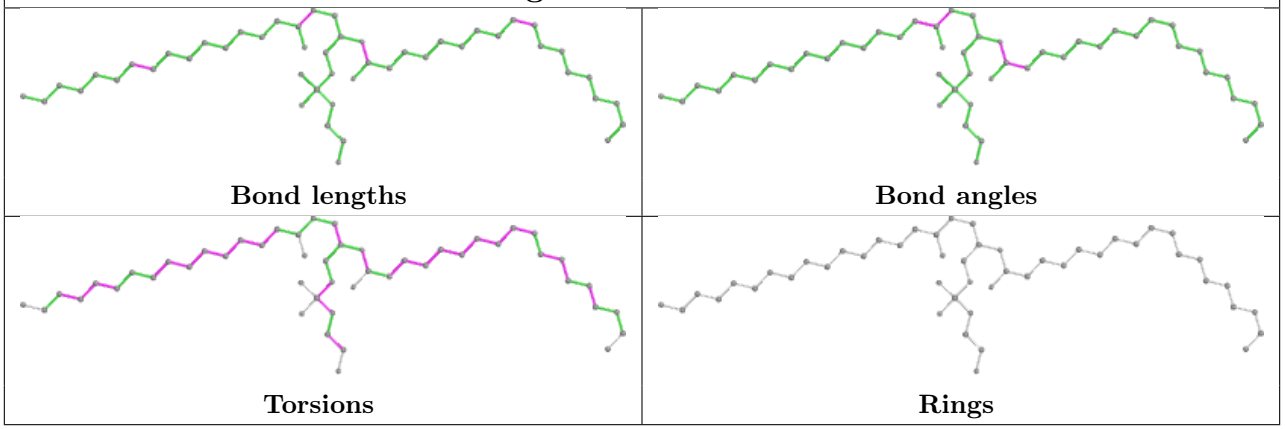


Torsions



Rings

Ligand PEE V 403



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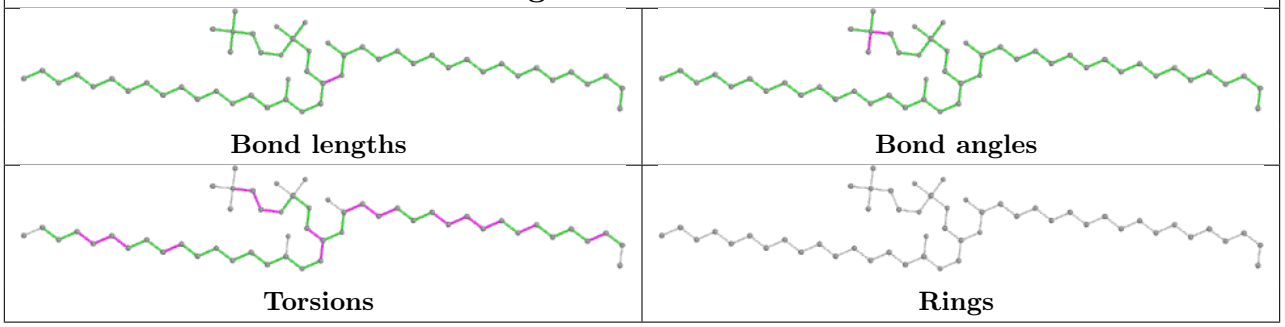
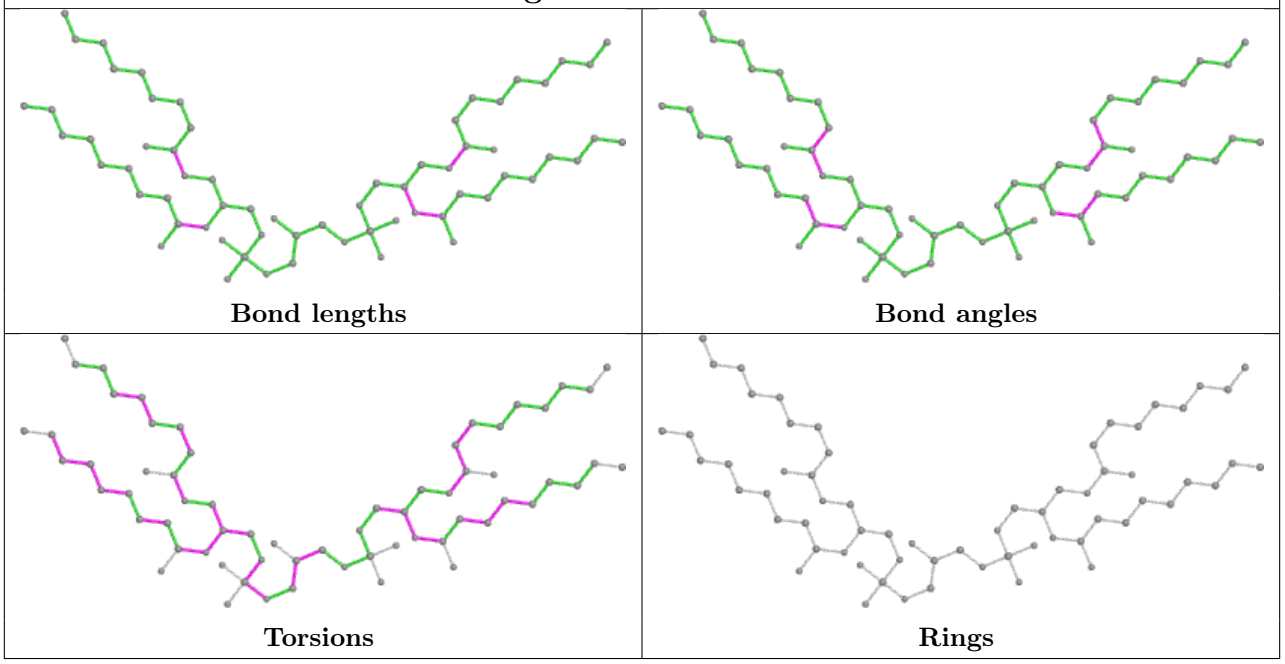
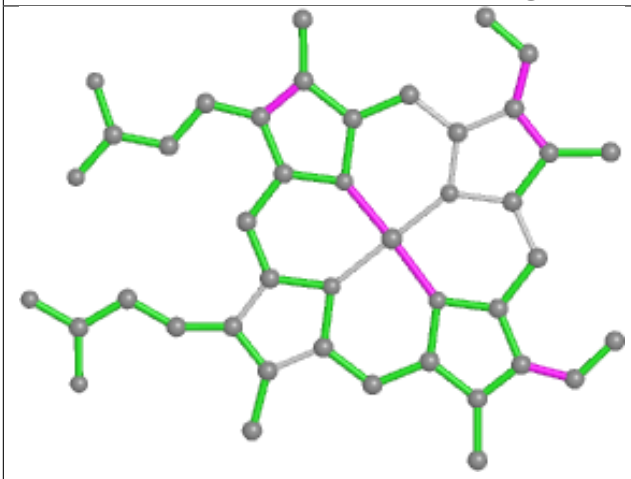


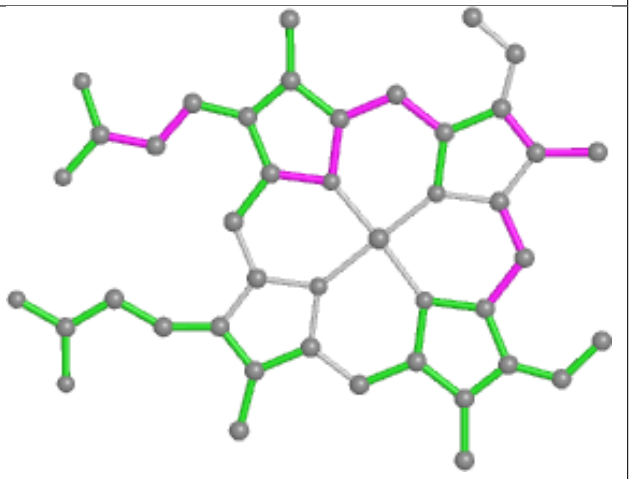
Ligand CDL Y 501



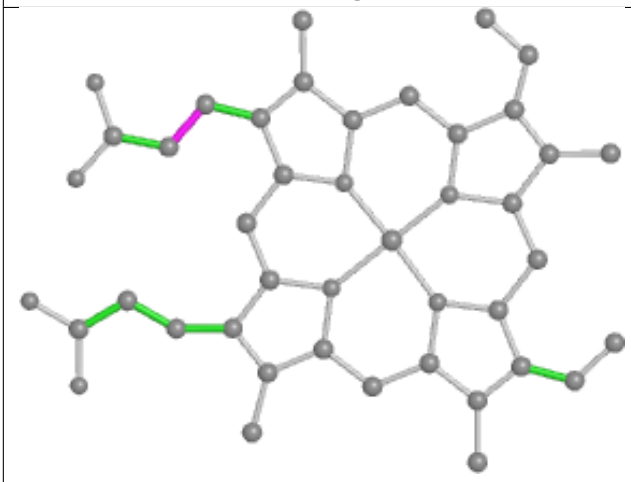
Ligand HEM J 401



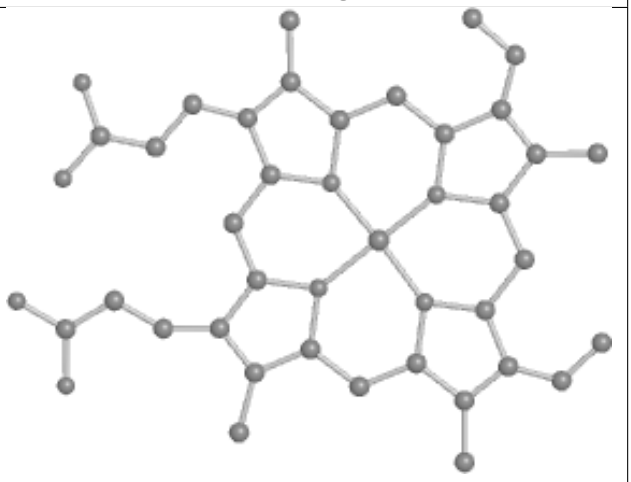
Bond lengths



Bond angles



Torsions



Rings

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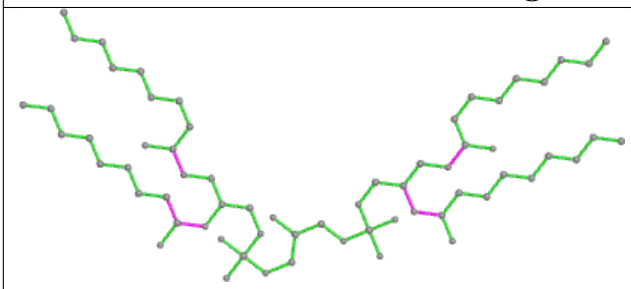

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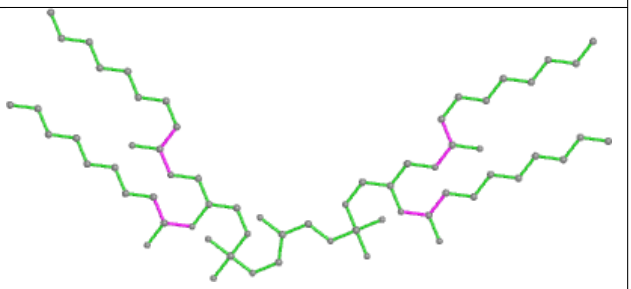
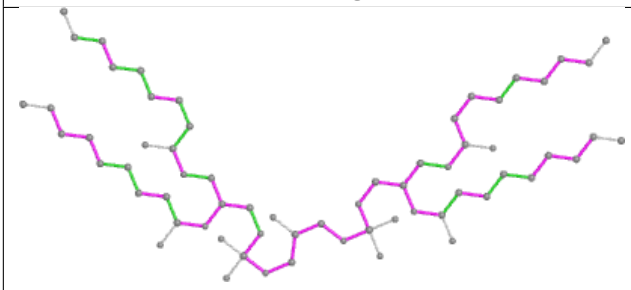


Bond angles



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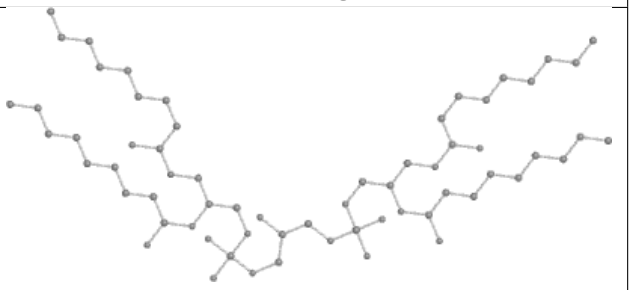
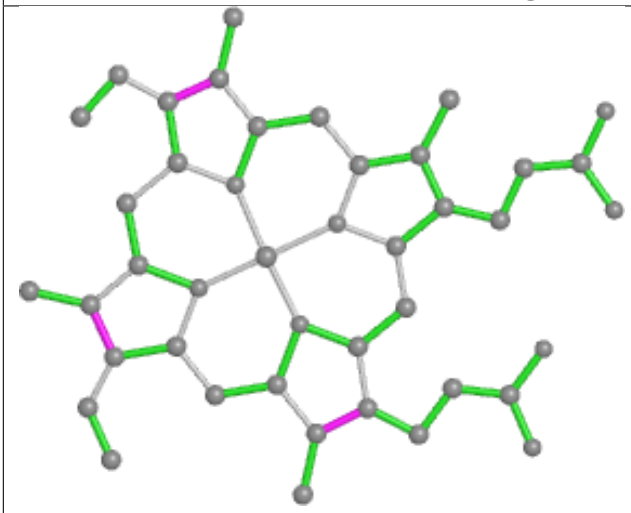


Rings

Ligand HEC U 402



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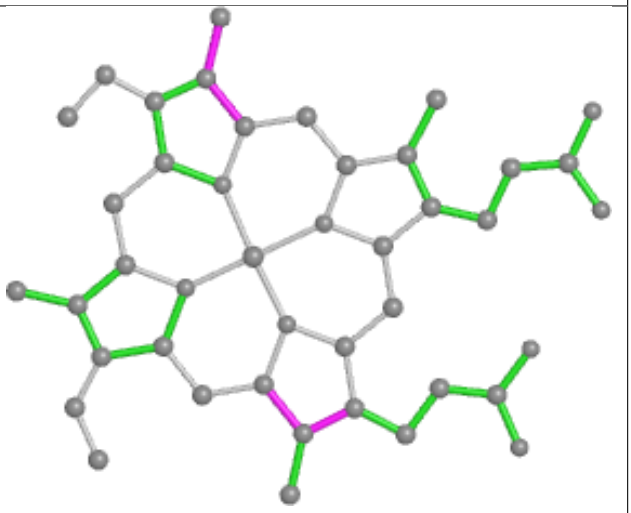
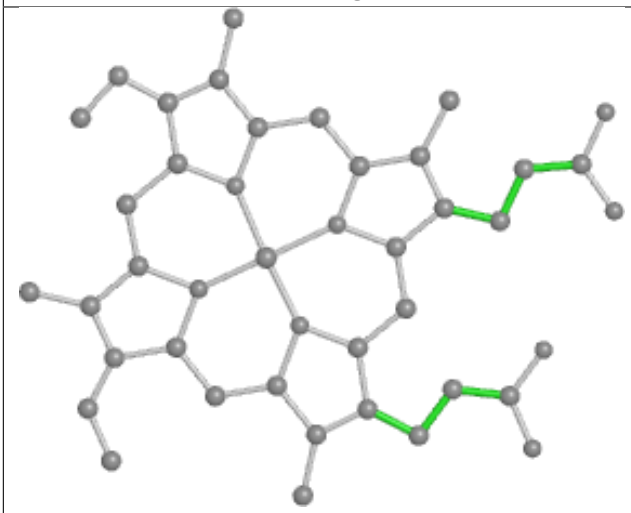


Bond angles



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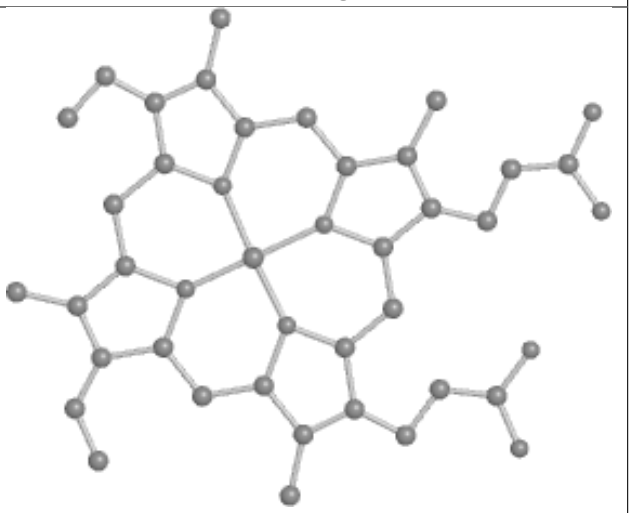
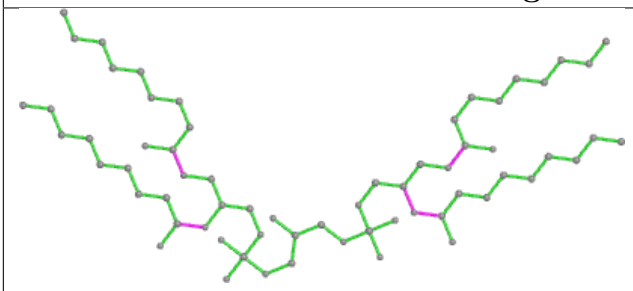


Rings

Ligand CDL H 403



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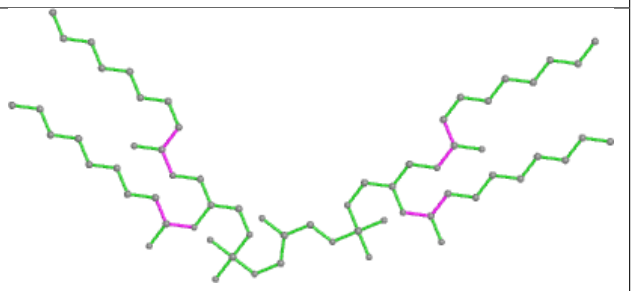
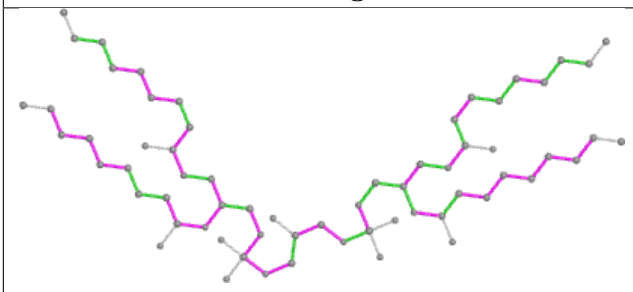


Bond angles



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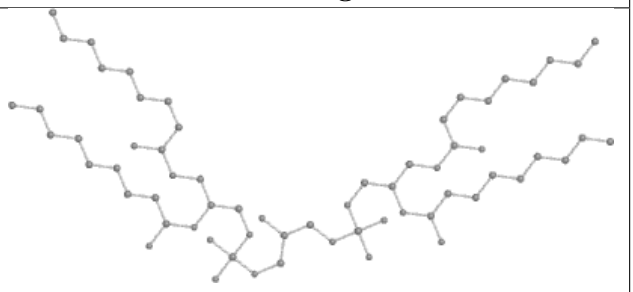
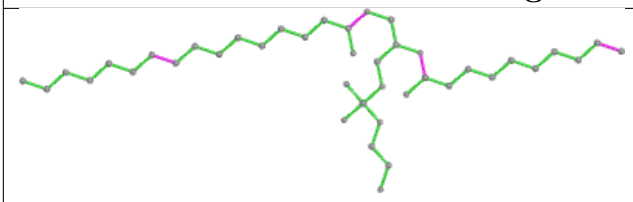


Rings

Ligand PEE U 401



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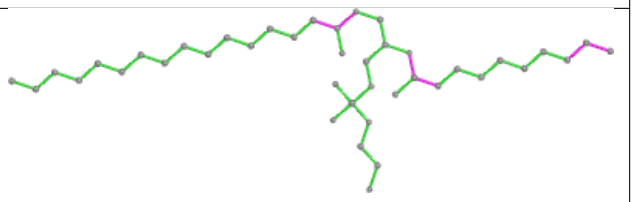
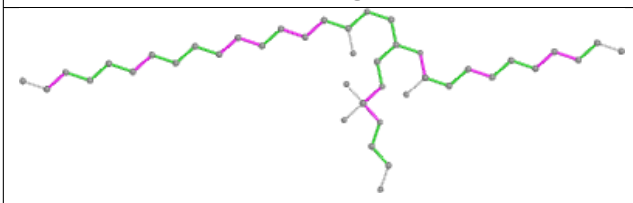
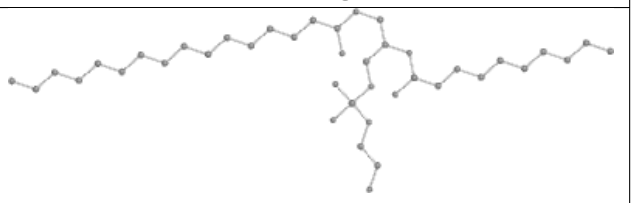


Bond angles

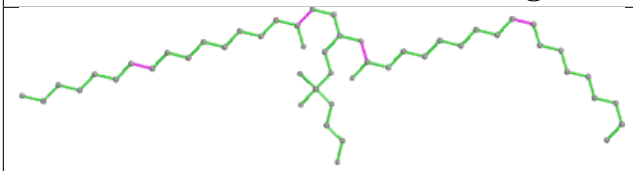


Torsions

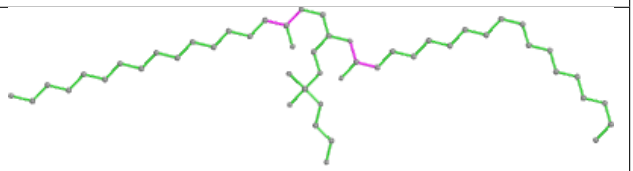


Rings

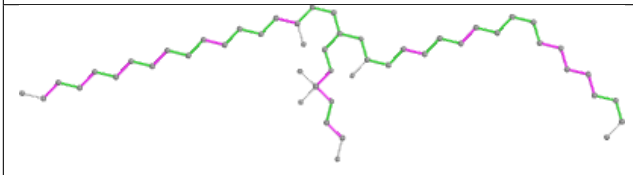
Ligand PEE Y 502



Bond lengths



Bond angles



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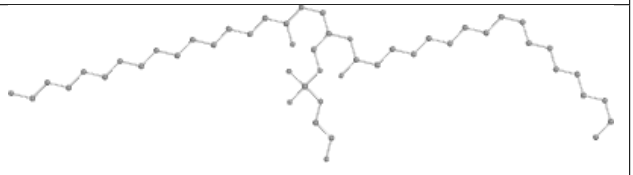
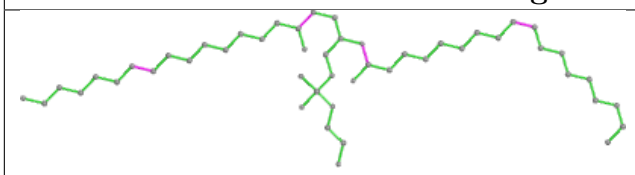
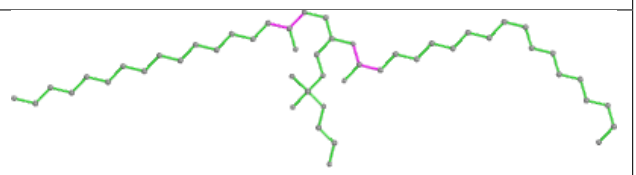


Rings

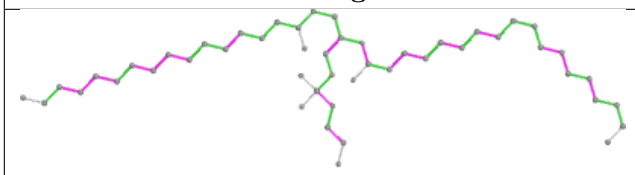
Ligand PEE J 403



Bond lengths



Bond angles



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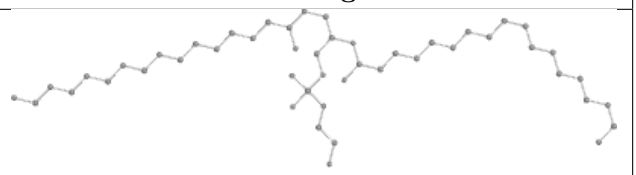
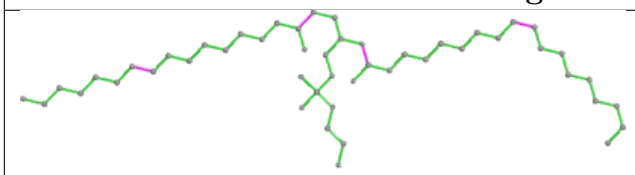
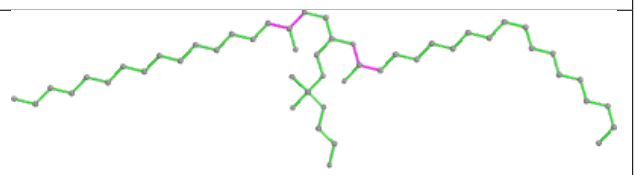


Rings

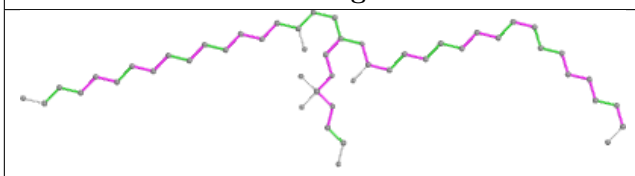
Ligand PEE H 401



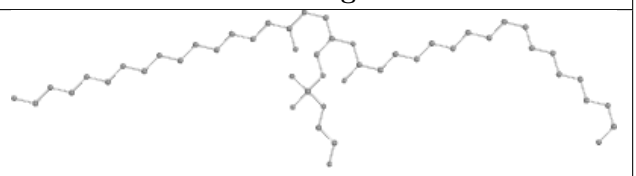
Bond lengths



Bond angles

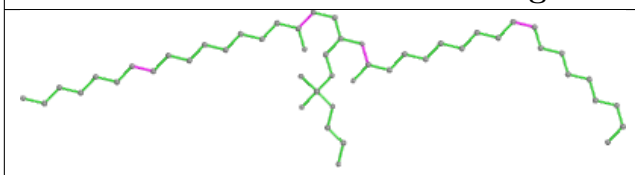


Torsions

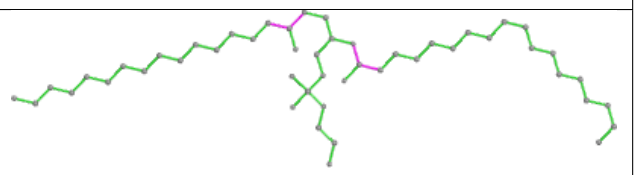


Rings

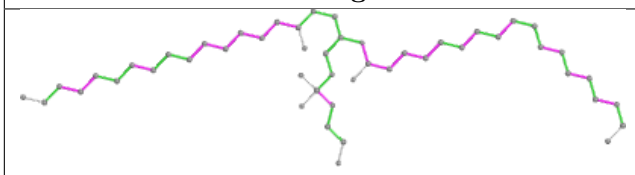
Ligand PEE L 503



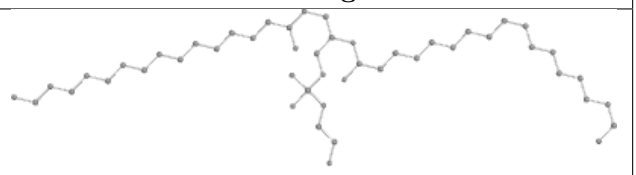
Bond lengths



Bond angles

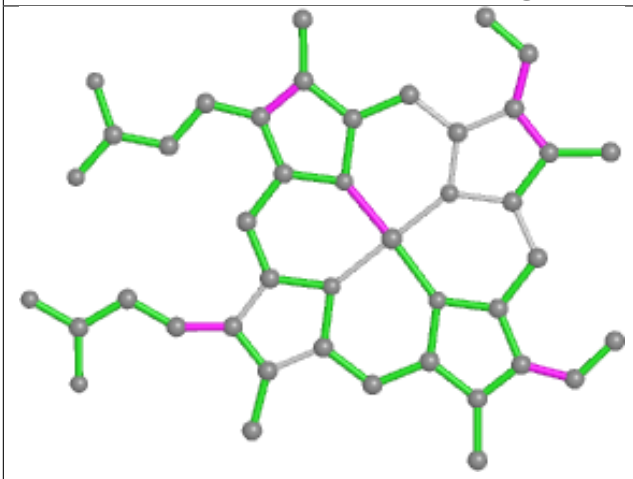


Torsions

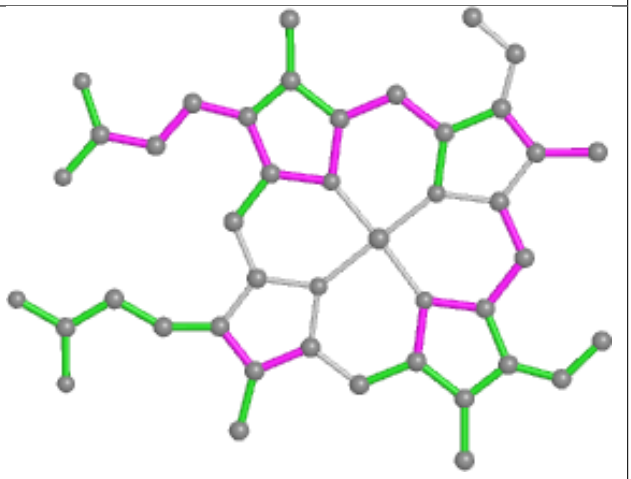


Rings

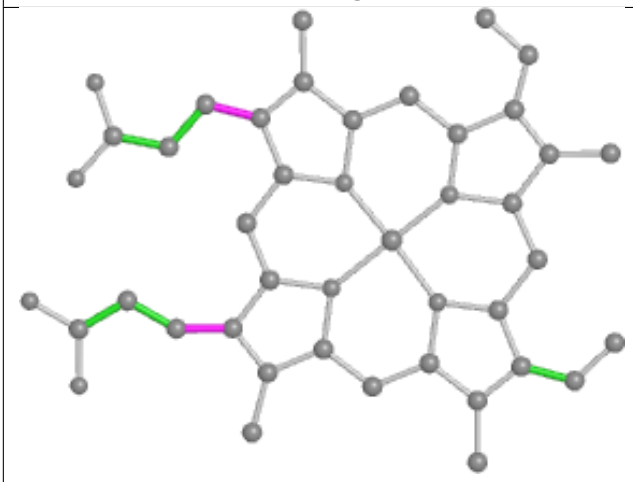
Ligand HEM V 402



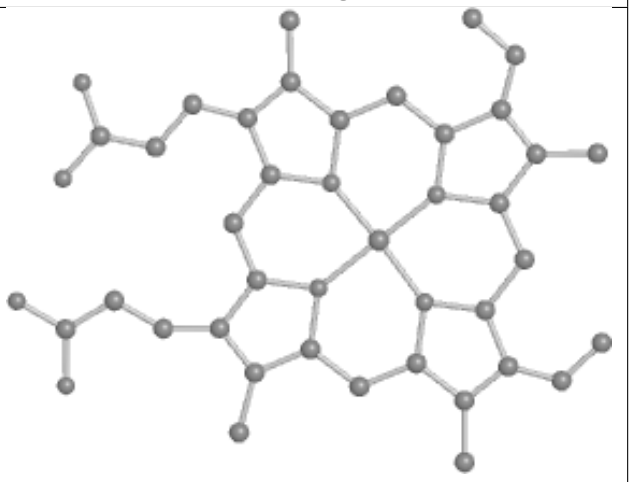
Bond lengths



Bond angles

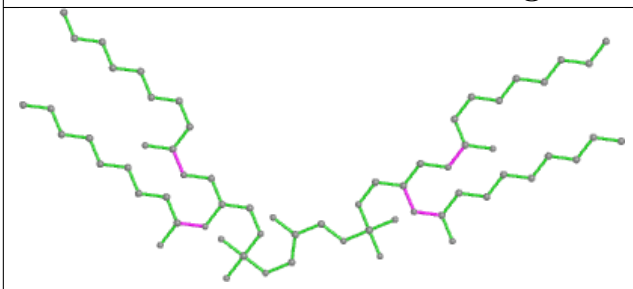


Torsions

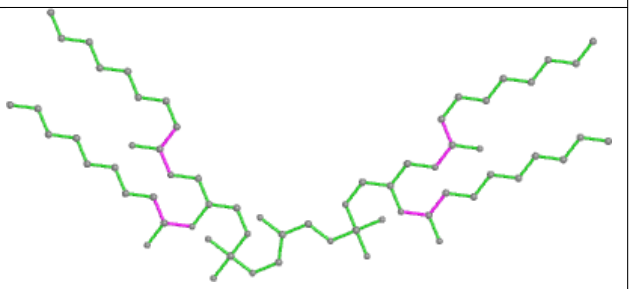


Rings

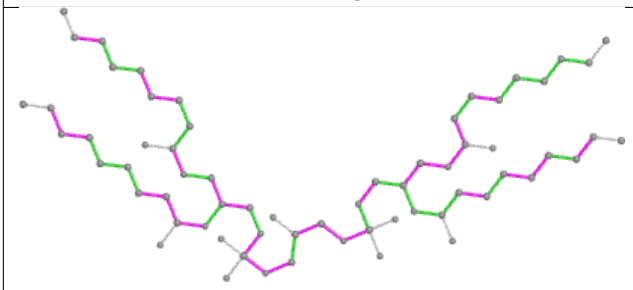
Ligand CDL N 101



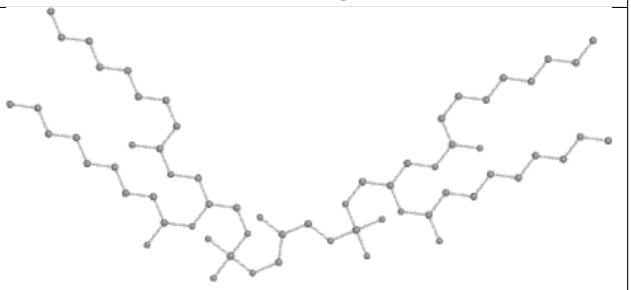
Bond lengths



Bond angles

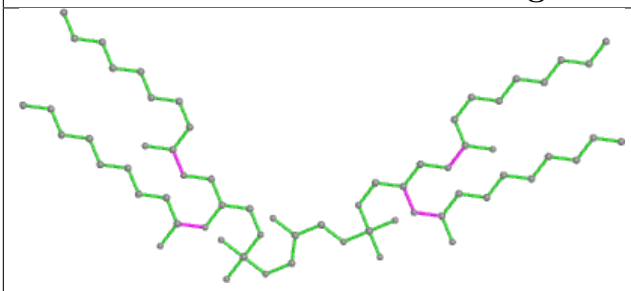


Torsions

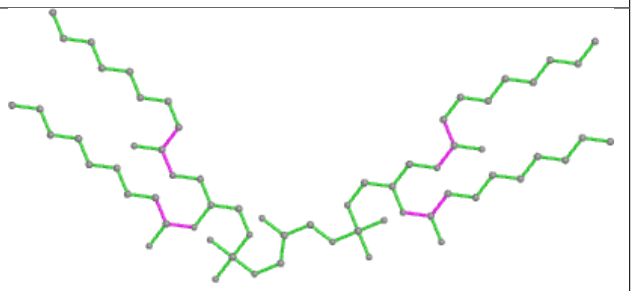


Rings

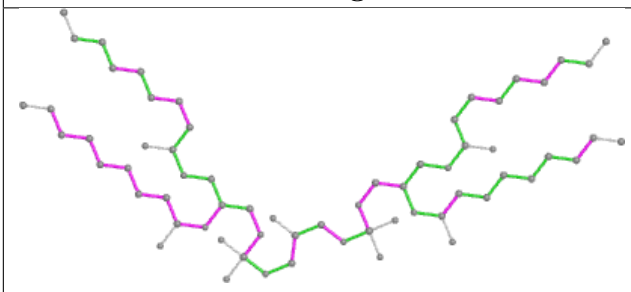
Ligand CDL J 404



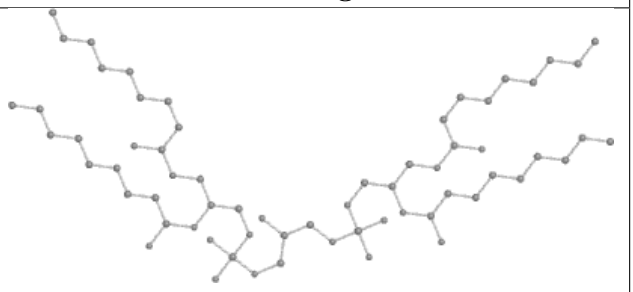
Bond lengths



Bond angles

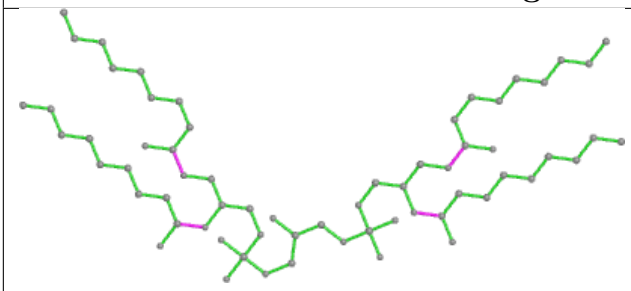


Torsions

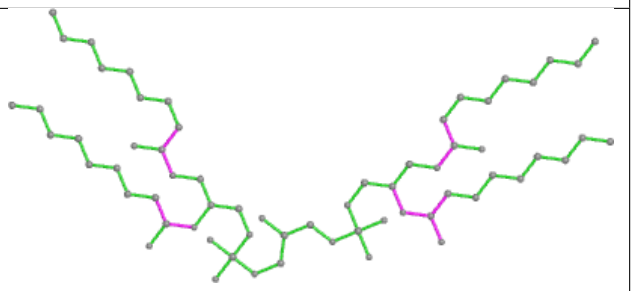


Rings

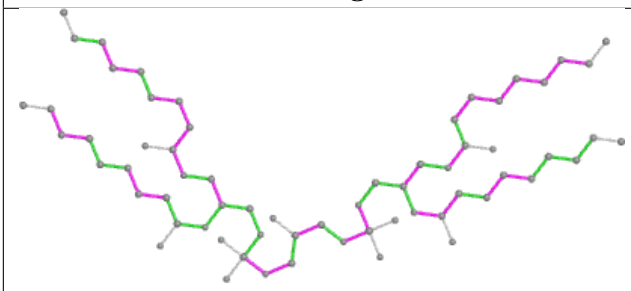
Ligand CDL G 101



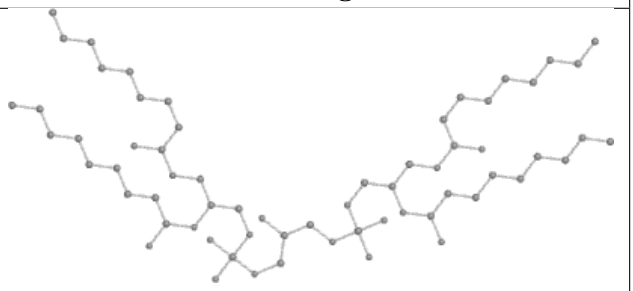
Bond lengths



Bond angles

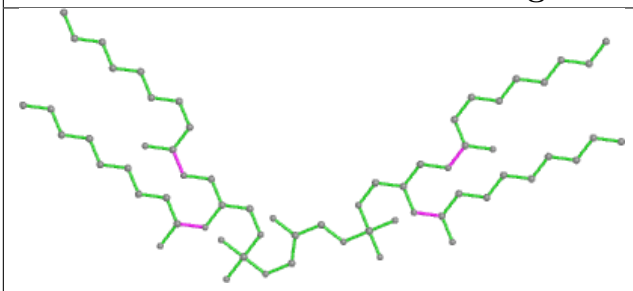


Torsions

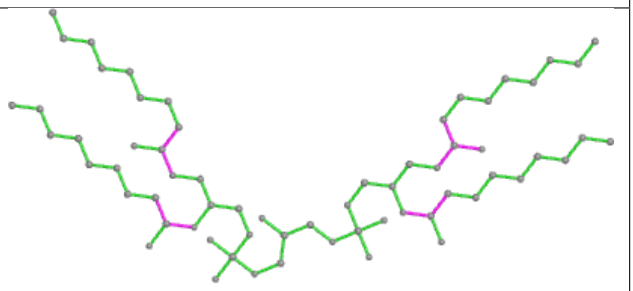


Rings

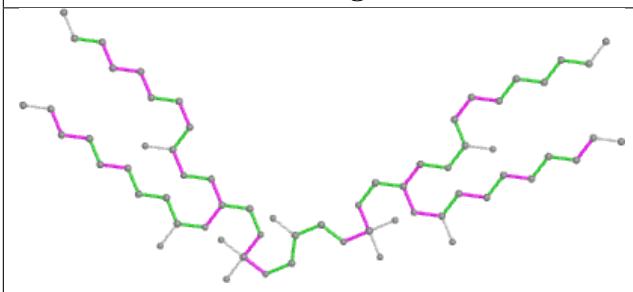
Ligand CDL J 405



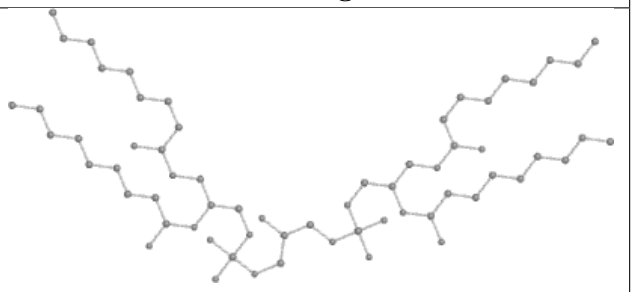
Bond lengths



Bond angles

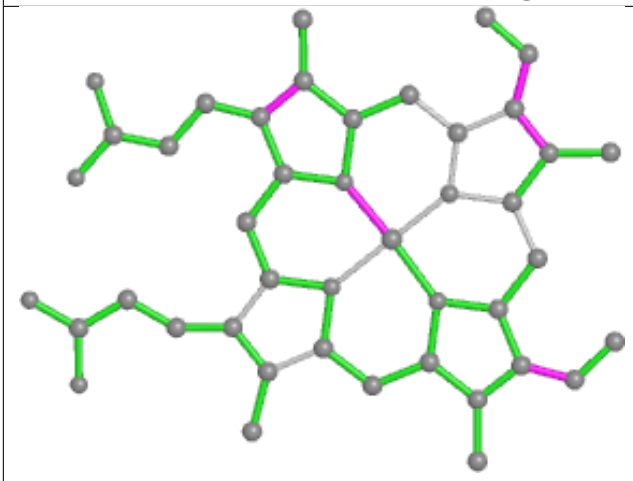


Torsions

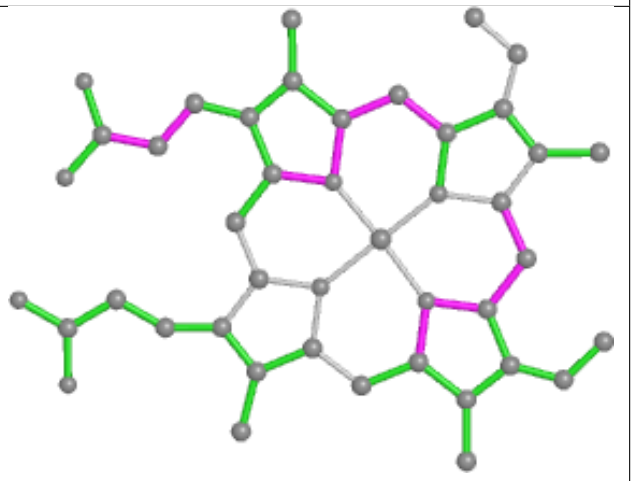


Rings

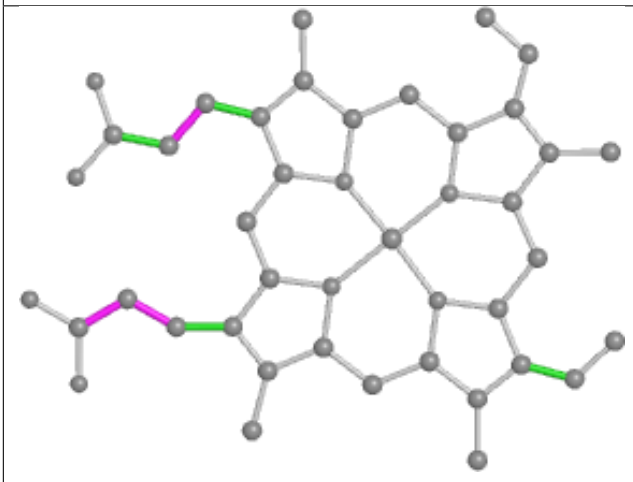
Ligand HEM V 401



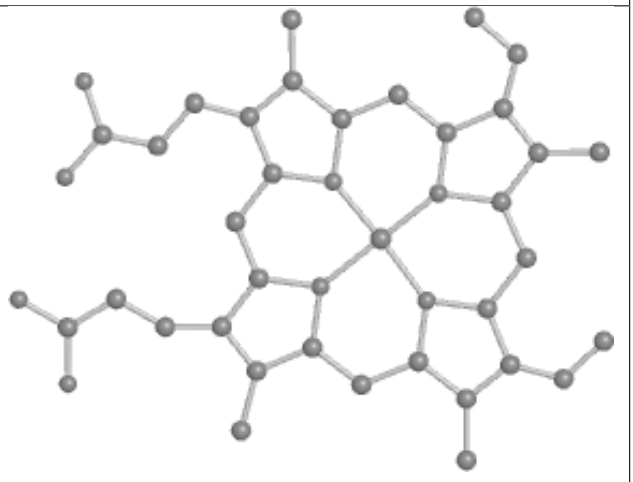
Bond lengths



Bond angles

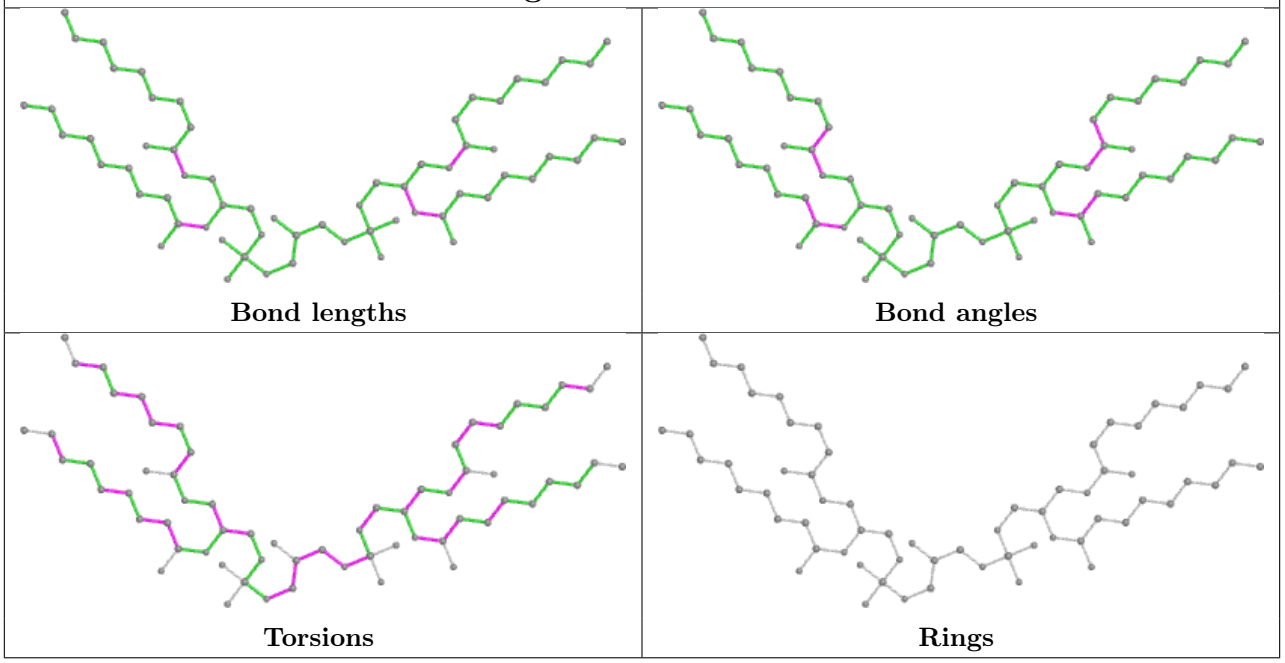


Torsions



Rings

Ligand CDL A 101



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.

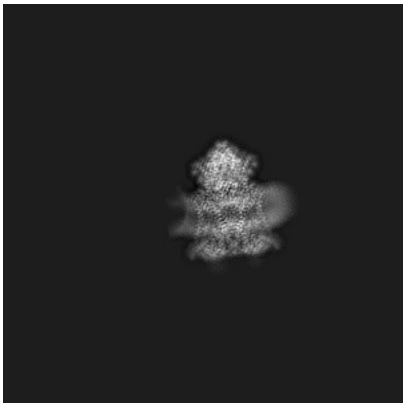
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6774. These allow visual inspection of the internal detail of the map and identification of artifacts.

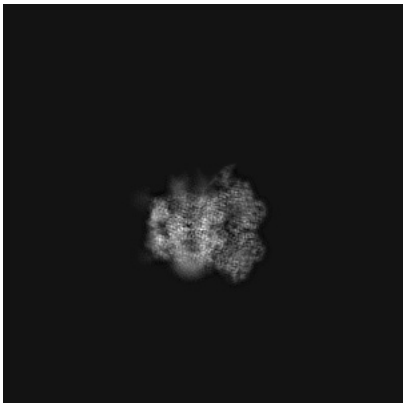
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

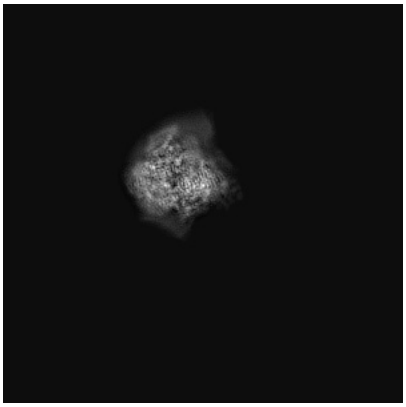
6.1.1 Primary map



X



Y

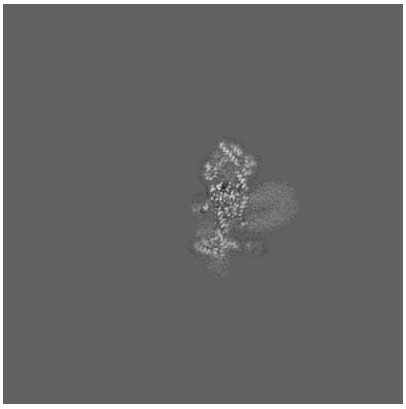


Z

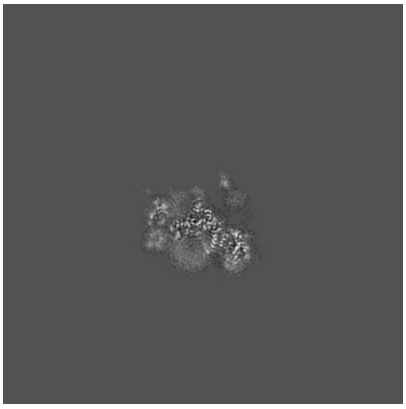
The images above show the map projected in three orthogonal directions.

6.2 Central slices

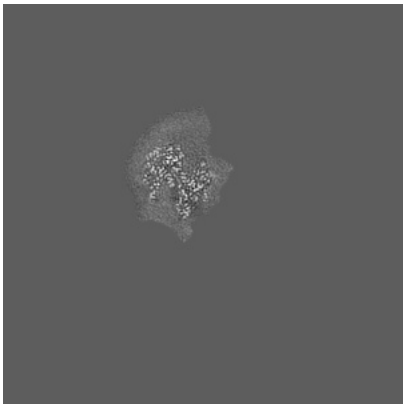
6.2.1 Primary map



X Index: 240



Y Index: 240

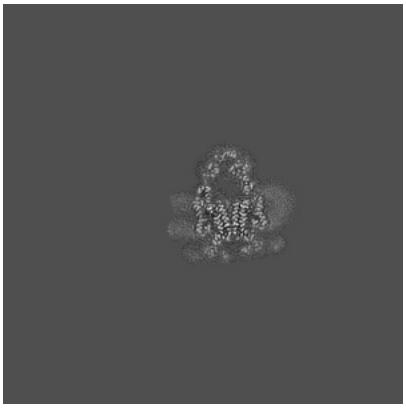


Z Index: 240

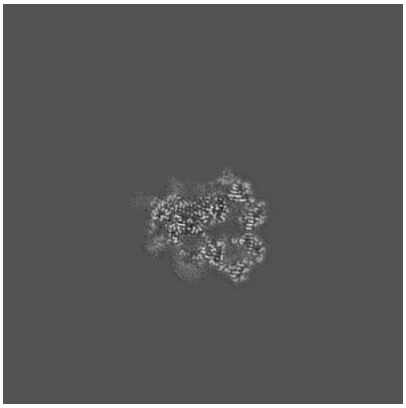
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

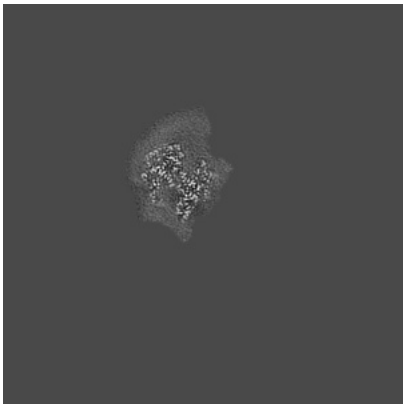
6.3.1 Primary map



X Index: 209



Y Index: 263

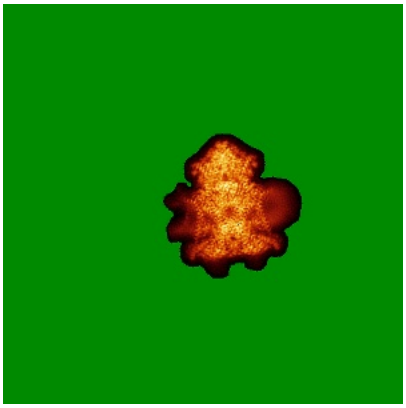


Z Index: 241

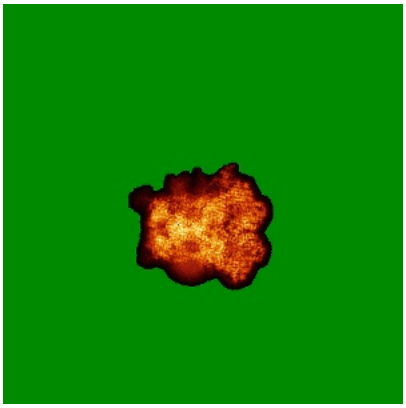
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

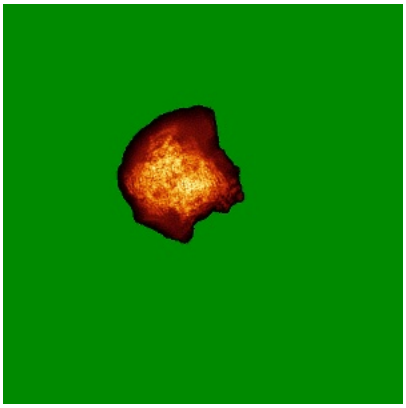
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0783. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

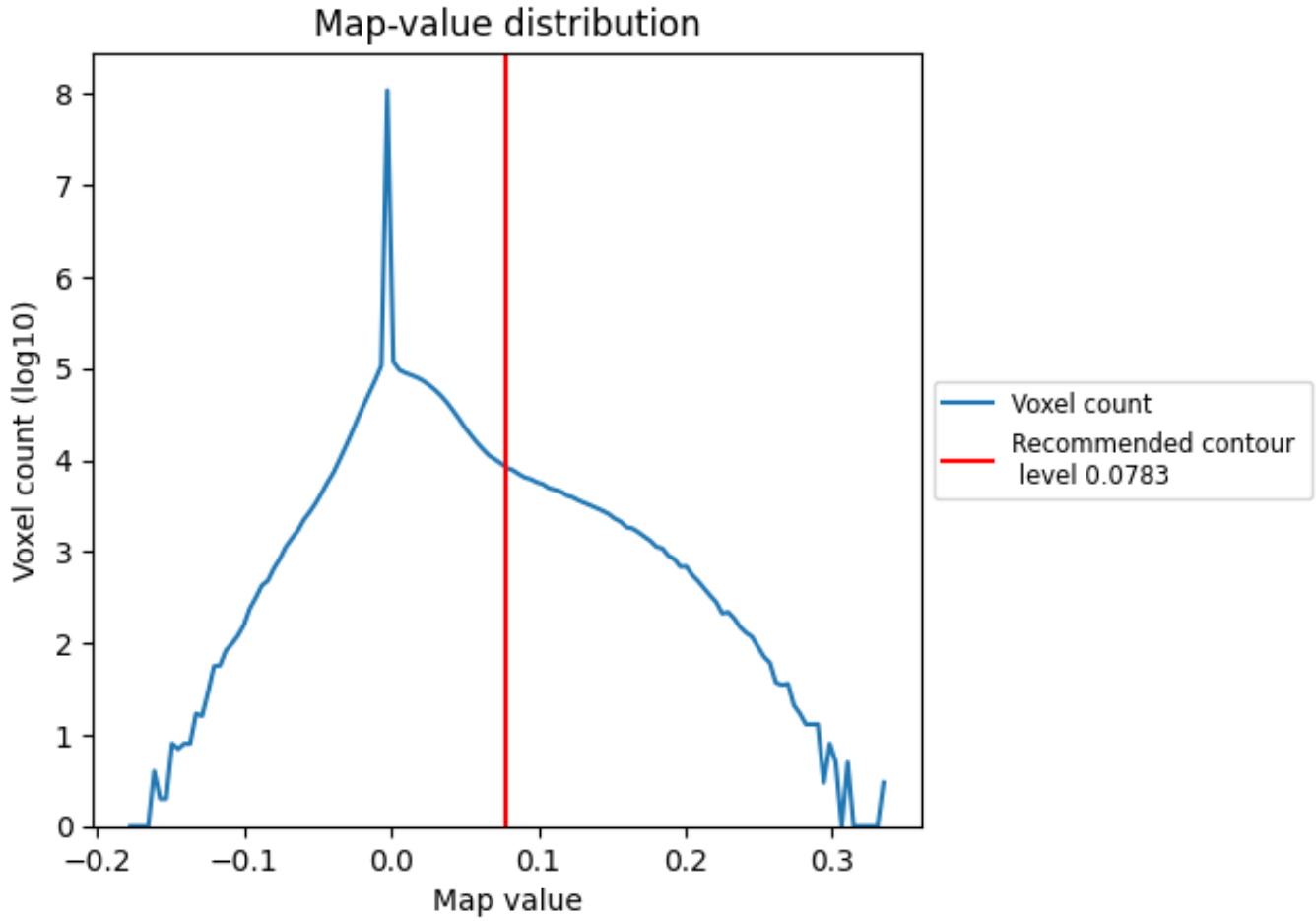
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

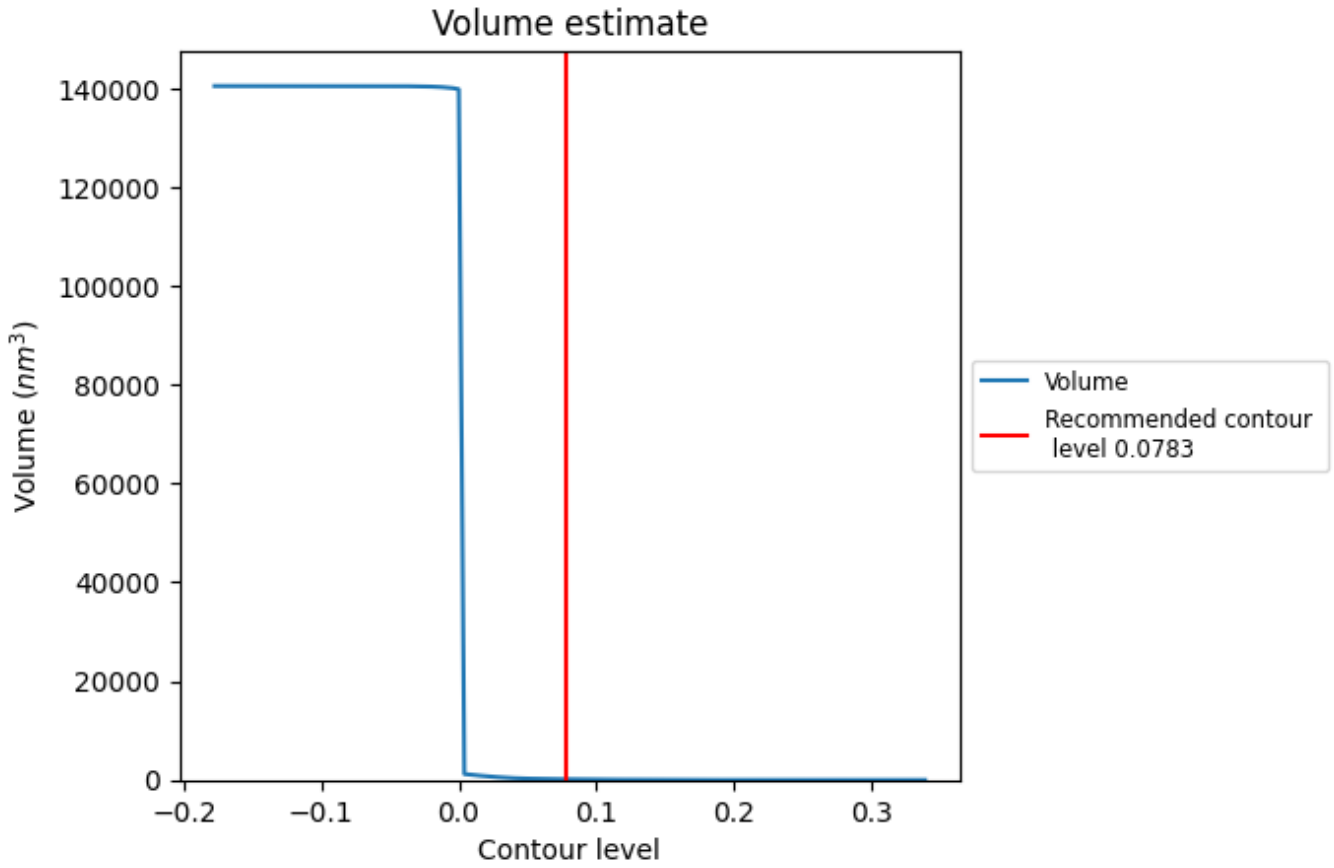
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

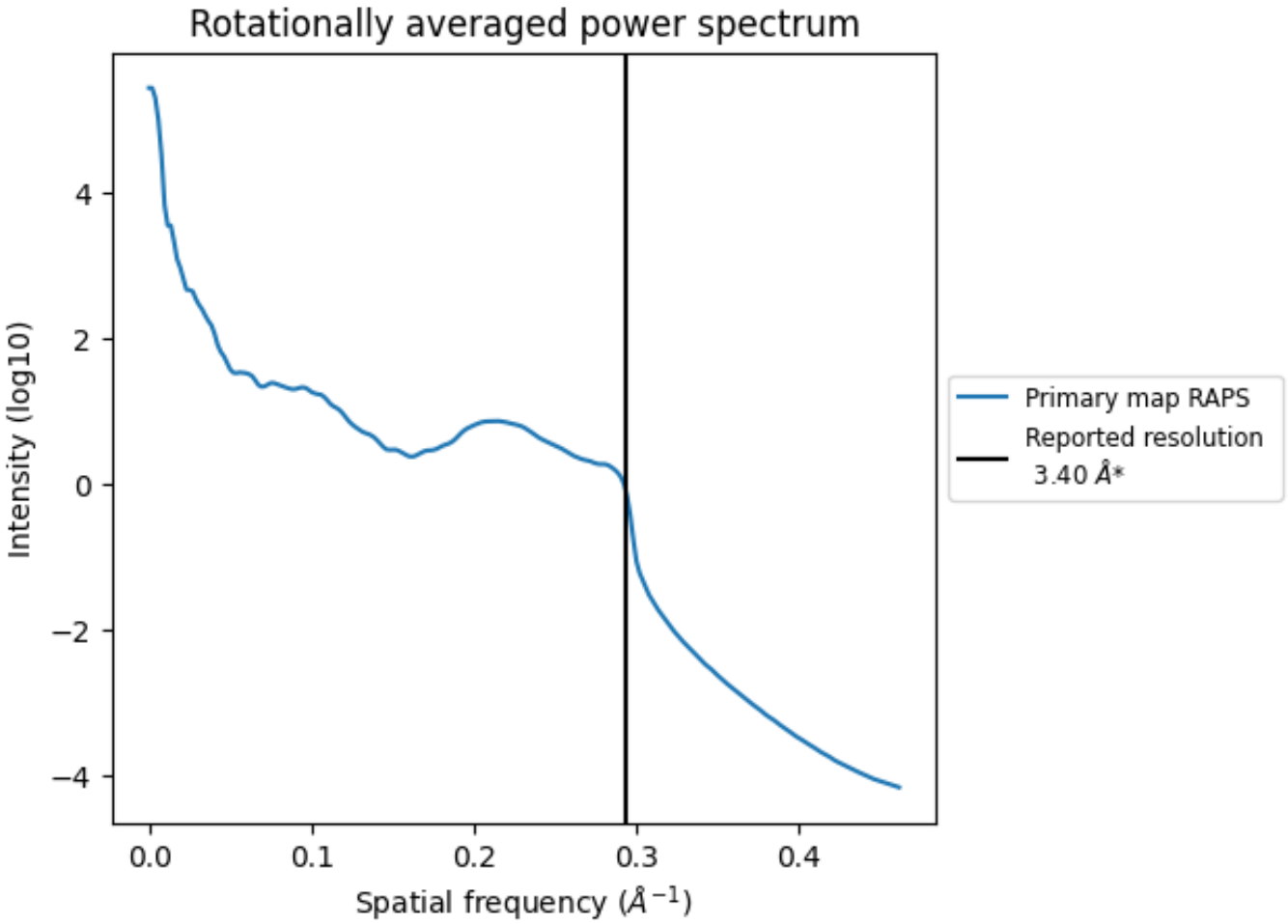
7.2 Volume estimate



The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 126 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

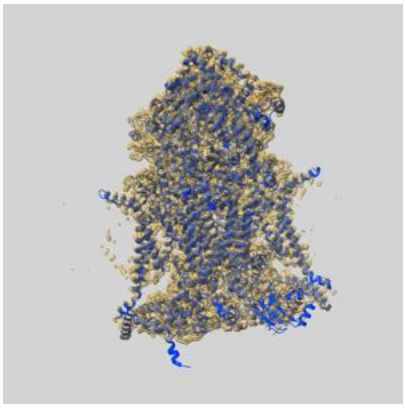
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

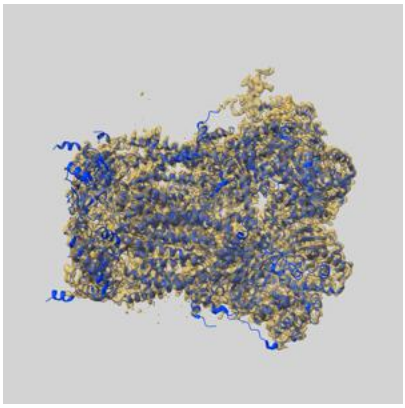
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6774 and PDB model 5XTE. Per-residue inclusion information can be found in section 3 on page 11.

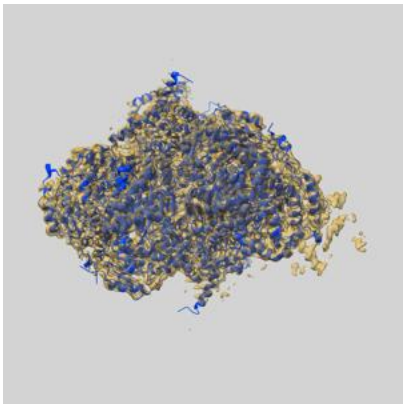
9.1 Map-model overlay



X



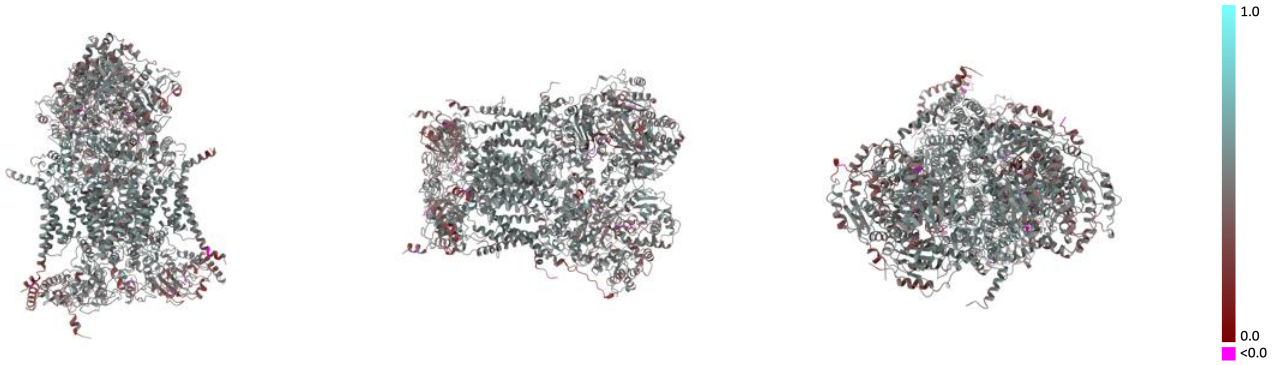
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0783 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

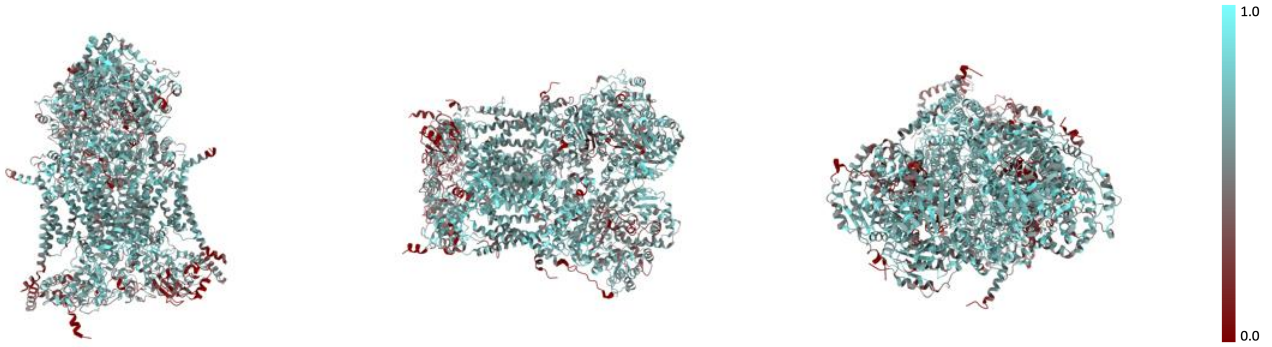
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

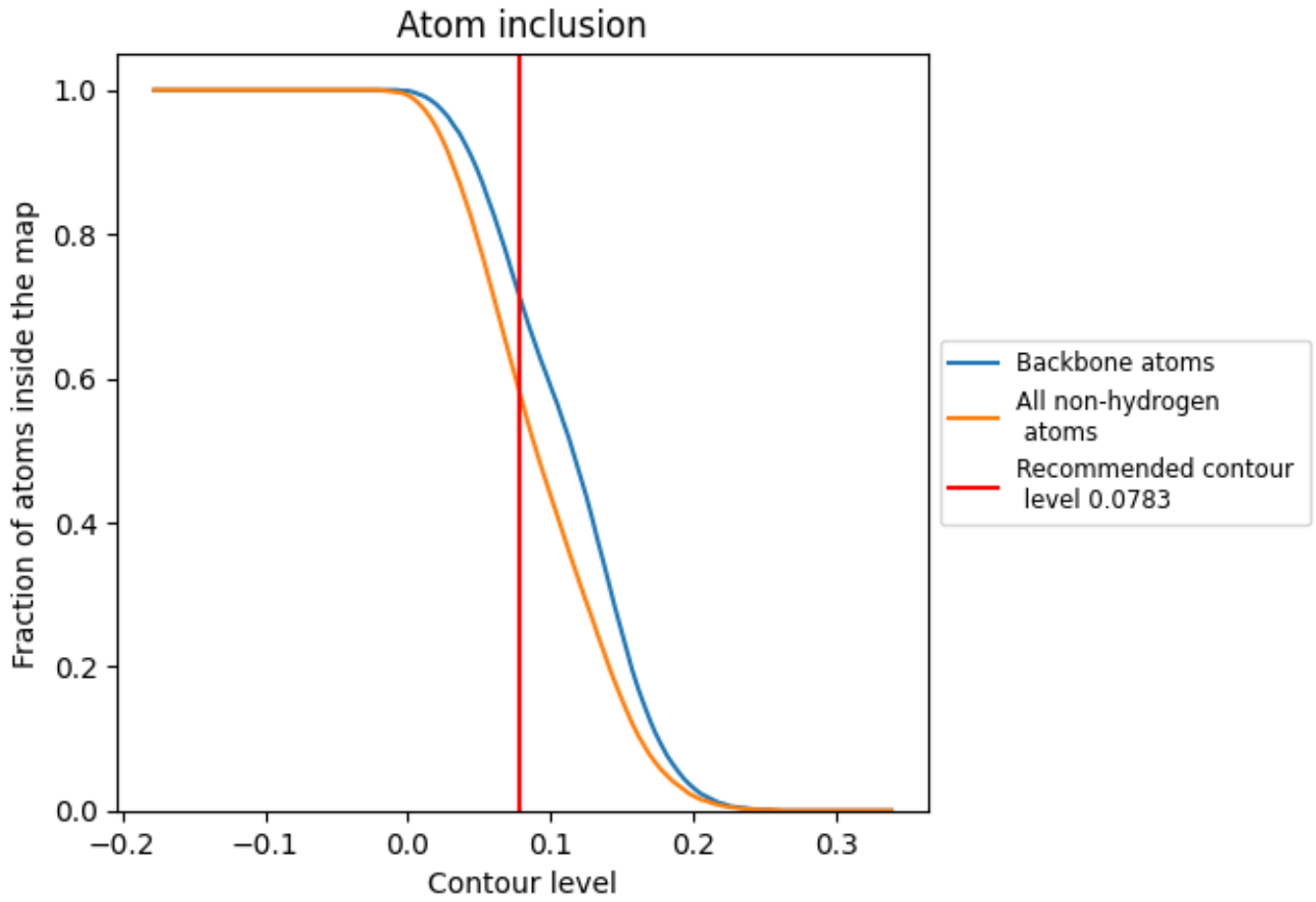
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0783).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0783) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4640
A	0.5490	0.4510
B	0.0270	0.2470
C	0.3410	0.4050
D	0.4730	0.4470
E	0.4310	0.3710
F	0.6540	0.5240
G	0.4860	0.4840
H	0.6230	0.4850
J	0.6690	0.5210
K	0.6410	0.4730
L	0.6080	0.4590
N	0.5500	0.4560
O	0.0150	0.2100
P	0.3710	0.4030
Q	0.4570	0.4190
R	0.5020	0.4050
S	0.6660	0.4810
T	0.3970	0.4610
U	0.6620	0.4890
V	0.7120	0.5160
W	0.6300	0.4750
Y	0.5910	0.4470