Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 06:03 PM JST

PDB ID	:	8IAR / pdb_00008iar
EMDB ID	:	EMD-35316
Title	:	Respiratory complex CIII2, focus-refined of type I, Wild type mouse under thermoneutral temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
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 (i) symbol.

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

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

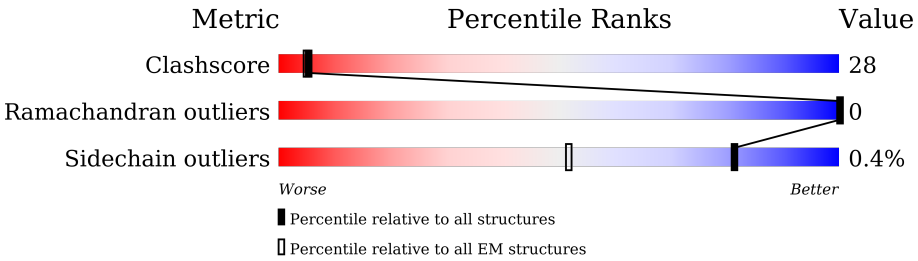
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

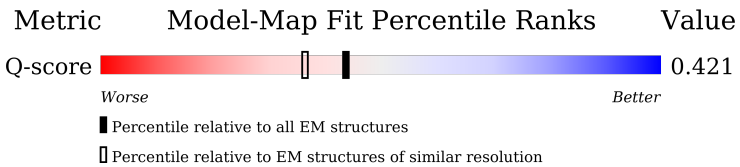
1 Overall quality at a glance (i)

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	AA	480	55% 28% • 16%
1	Aa	480	56% 29% • 14%
2	AB	453	5% 64% 28% • 8%
2	Ab	453	62% 28% • 9%

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Mol	Chain	Length	Quality of chain
3	AC	381	7% 60% 37%
3	Ac	381	5% 60% 37%
4	AD	325	8% 41% 32% 26%
4	Ad	325	6% 32% 42% 26%
5	AE	274	42% 27% 41% 31%
5	AI	274	7% 5% 89%
5	Ae	274	38% 26% 42% 31%
5	Ai	274	7% 5% 90%
6	AF	111	7% 55% 33% 12%
6	Af	111	52% 36% 12%
7	AG	82	17% 49% 44% 7%
7	Ag	82	39% 52% 7%
8	AH	89	28% 54% 22% 24%
8	Ah	89	10% 54% 22% 24%
9	AJ	64	27% 28% 36% 36%
9	Aj	64	23% 38% 38% 25%
10	AK	56	64% 36% 45% 7% 12%
10	Ak	56	45% 43% 41% 12%

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
13	U10	Ac	404	-	-	X	-
14	UQ6	AC	406	-	-	X	-
15	HEC	AD	401	X	-	-	-
15	HEC	Ad	401	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32253 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 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	403	3153	1970	560	607	16	0	0
1	Aa	412	3225	2016	569	624	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	418	3137	1970	552	606	9	0	0
2	Ab	412	3094	1945	542	598	9	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	373	2988	2018	461	489	20	0	0
3	Ac	373	2988	2018	461	489	20	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	240	1912	1221	328	349	14	0	0
4	Ad	240	1912	1221	328	349	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	188	1451	916	254	274	7	0	0
5	AI	30	Total	C	N	O		0	0
			217	138	42	37			
5	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
5	Ai	28	Total	C	N	O		0	0
			207	133	40	34			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	98	864	552	154	155	3	0	0
			Total	C	N	O	S		
6	Af	98	864	552	154	155	3	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	76	643	418	116	108	1	0	0
			Total	C	N	O	S		
7	Ag	76	643	418	116	108	1	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AH	68	562	343	103	111	5	0	0
			Total	C	N	O	S		
8	Ah	68	562	343	103	111	5	0	0

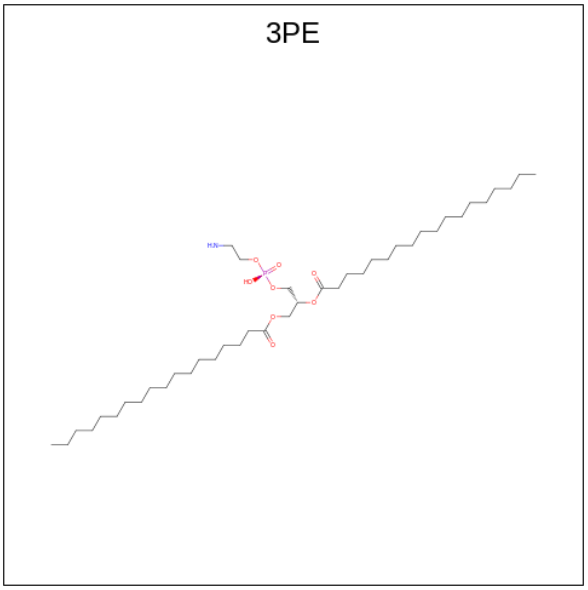
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	AJ	41	332	216	57	59	0	0
			Total	C	N	O		
9	Aj	48	391	257	66	68	0	0

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

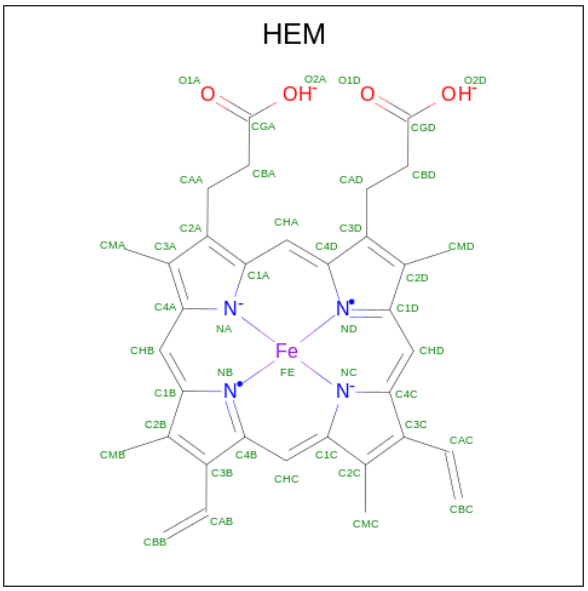
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AK	49	401	266	71	63	1	0	0
			Total	C	N	O	S		
10	Ak	49	401	266	71	63	1	0	0

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



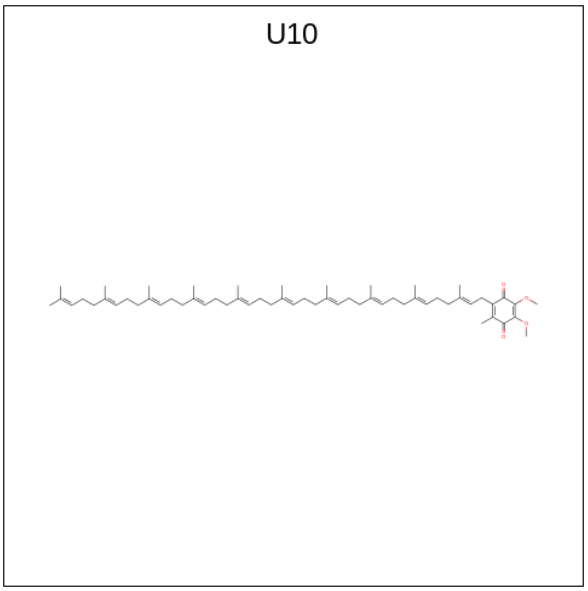
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	AC	1	23	13	1	8	1	0
			Total	C	N	O	P	
11	AC	1	35	25	1	8	1	0
			Total	C	N	O	P	
11	AG	1	51	41	1	8	1	0
			Total	C	N	O	P	
11	Aa	1	23	13	1	8	1	0
			Total	C	N	O	P	
11	Ac	1	35	25	1	8	1	0
			Total	C	N	O	P	
11	Ag	1	51	41	1	8	1	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



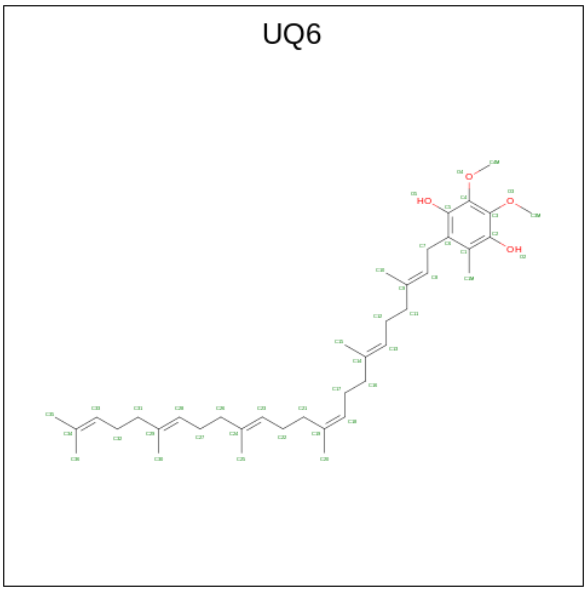
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
12	AC	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
12	AC	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
12	Ac	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
12	Ac	1	43	34	1	4	4	0

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



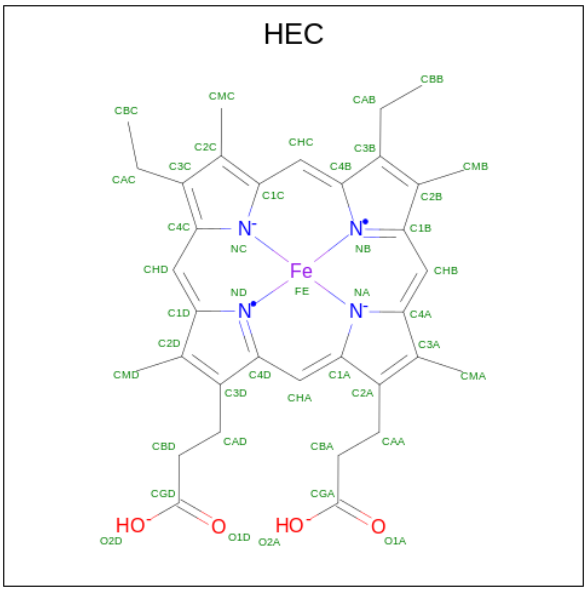
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	AC	1	23	19	4	0
13	Ac	1	23	19	4	0

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



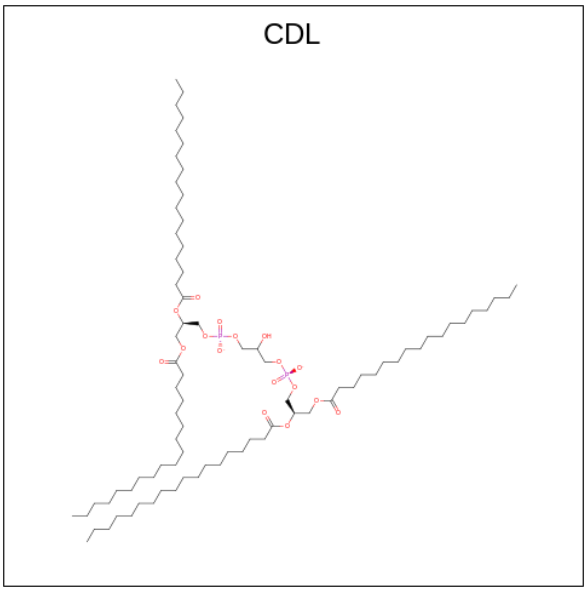
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	AC	1	28	24	4	0
14	Ac	1	28	24	4	0

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	AG	1	42	23	17	2	0

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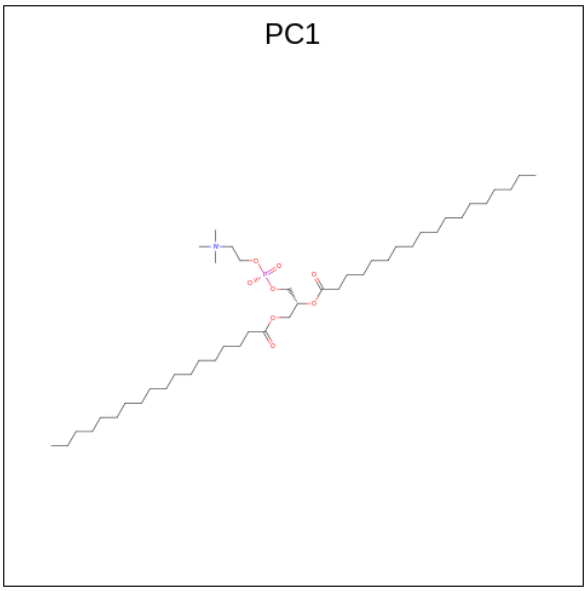
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	AG	1	56	37	17	2	0
16	Aa	1	46	27	17	2	0
16	Ag	1	42	23	17	2	0
16	Ag	1	56	37	17	2	0

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



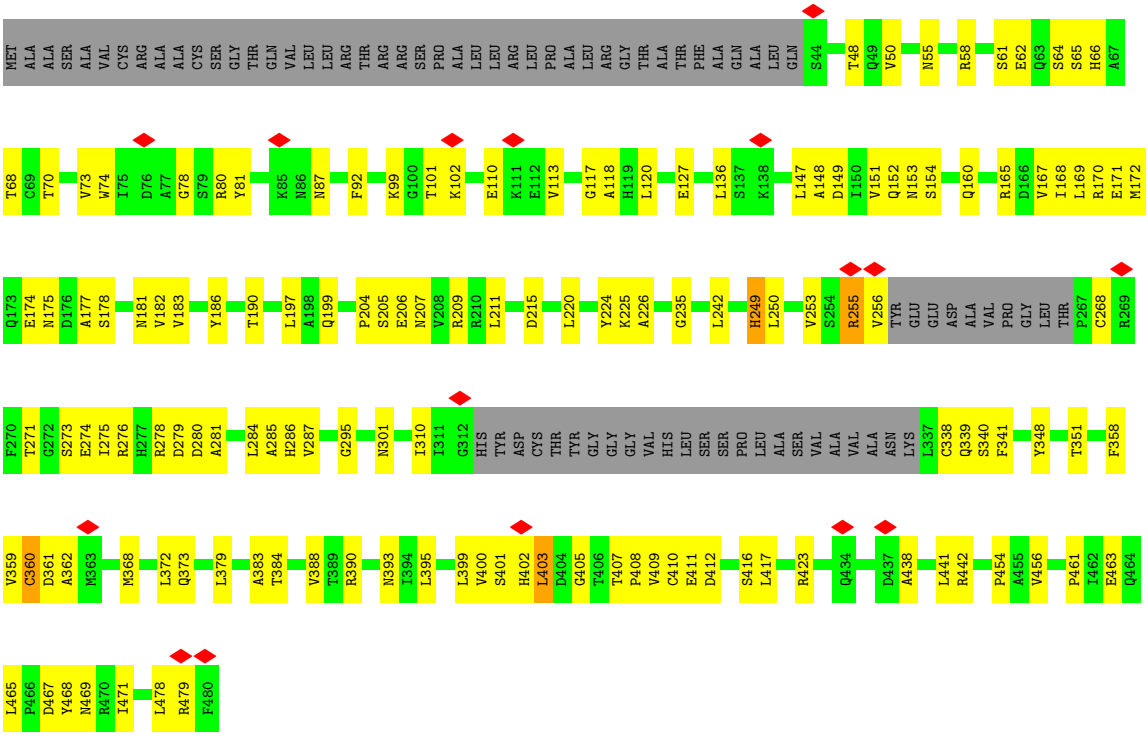
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	Ae	1	35	25	1	8	1	0

3 Residue-property plots (i)

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

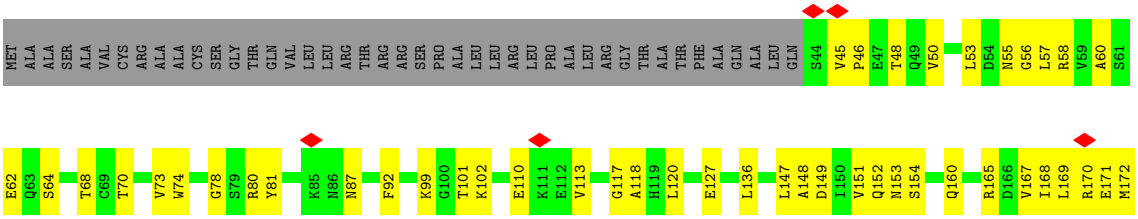
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

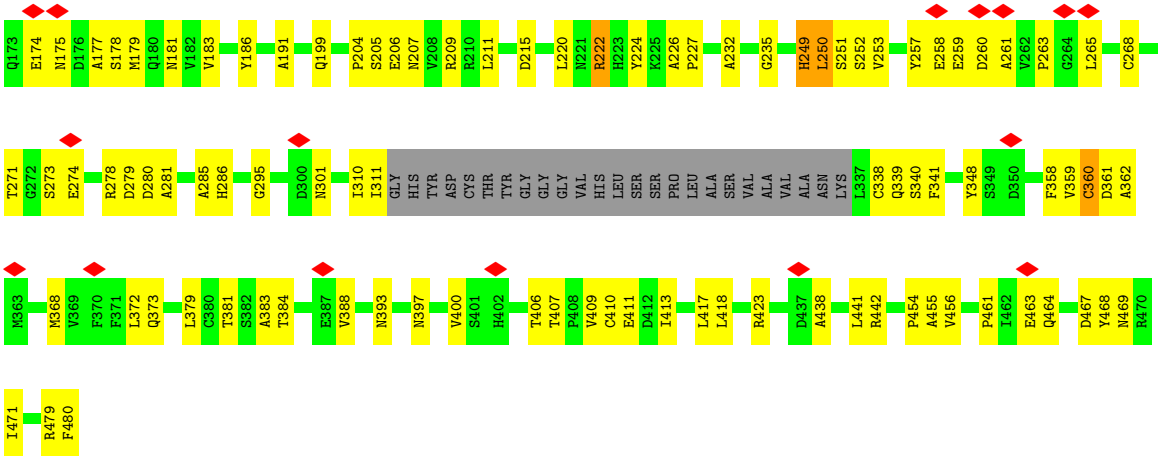
Chain AA:



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

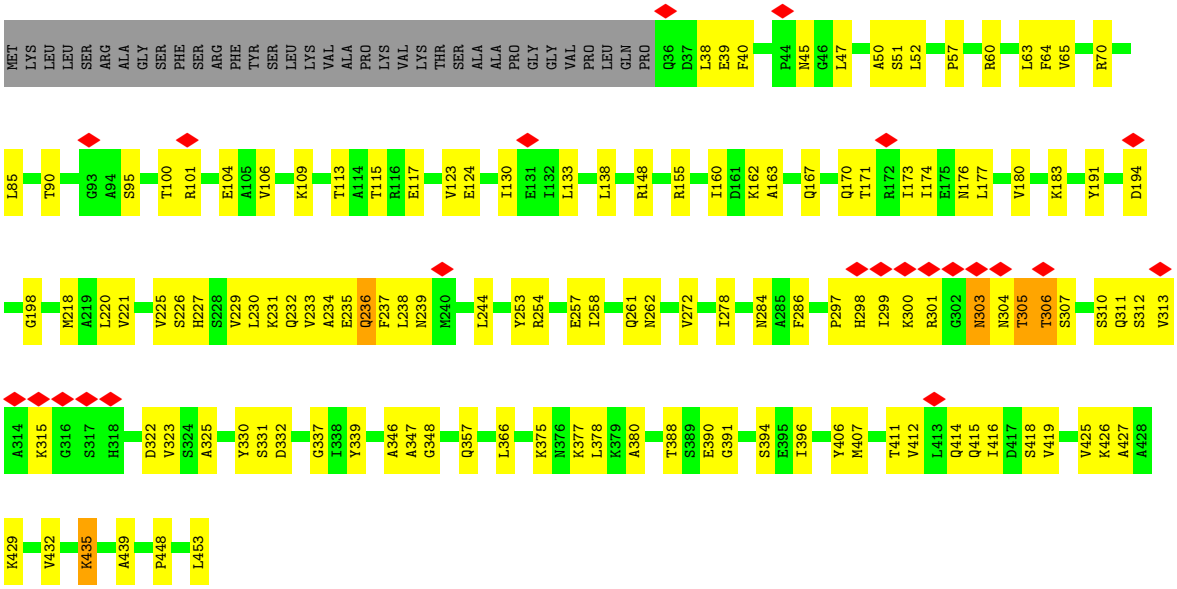
Chain Aa:





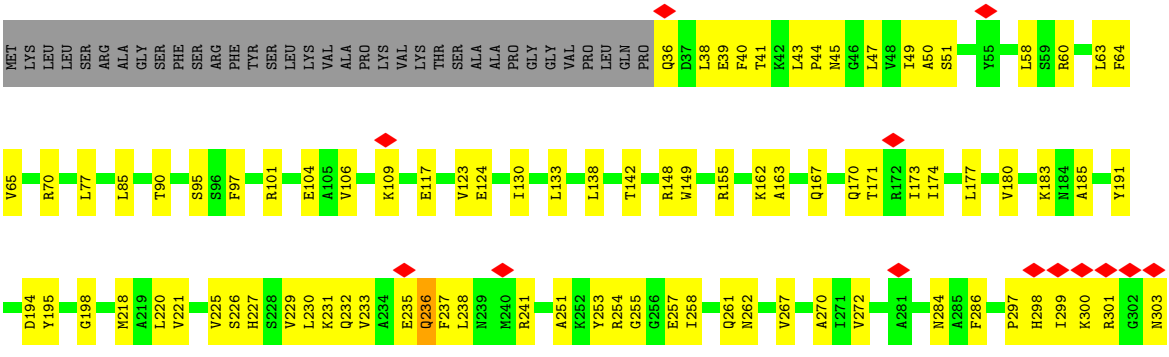
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

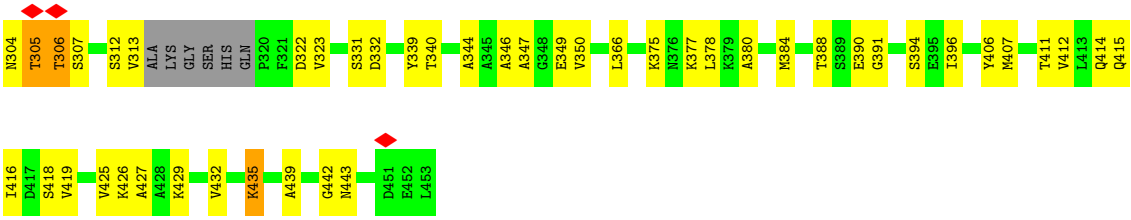
Chain AB:



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

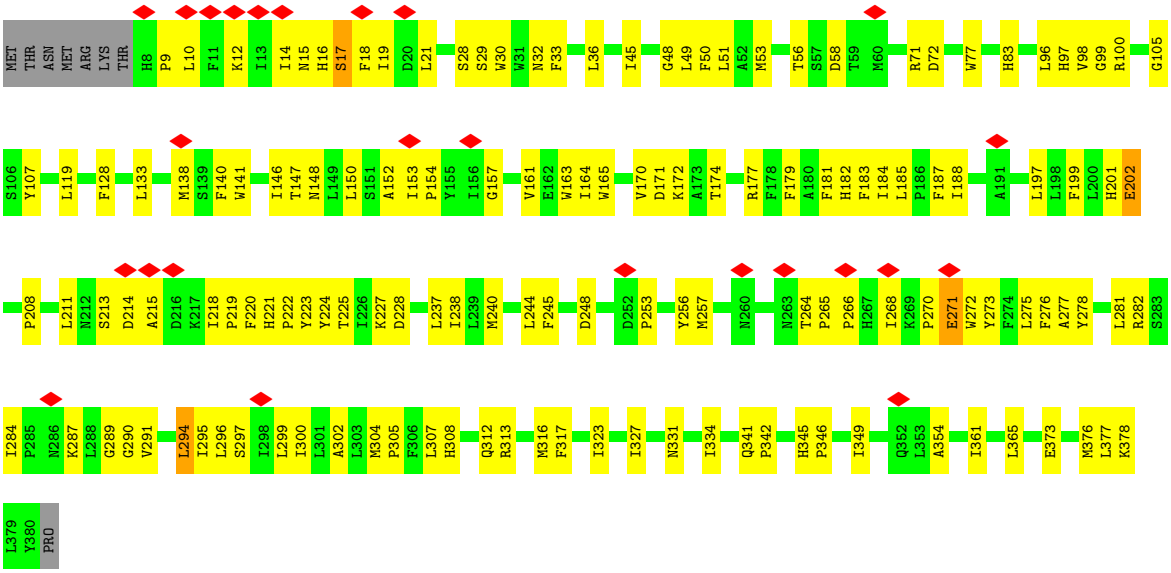
Chain Ab:





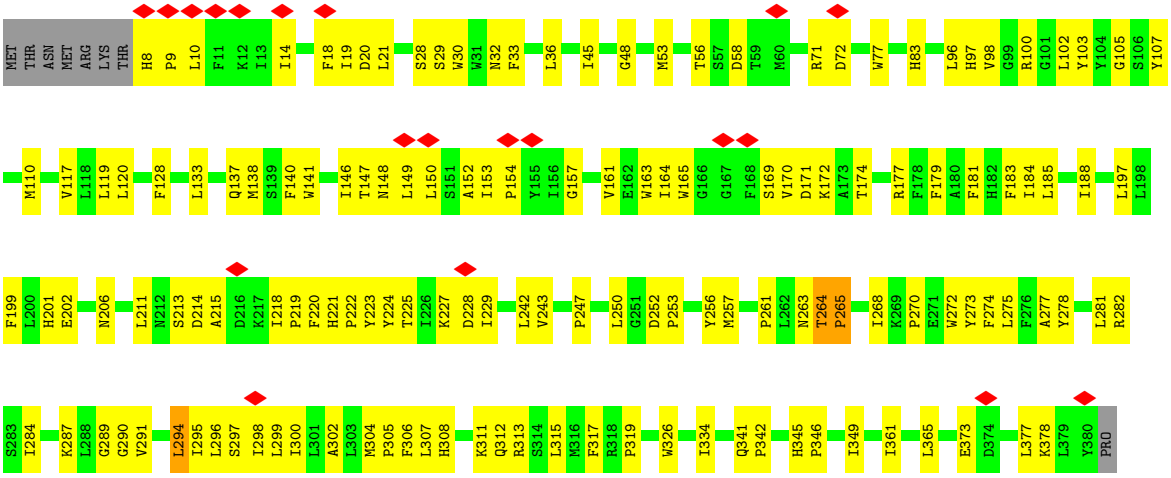
• Molecule 3: Cytochrome b

Chain AC:



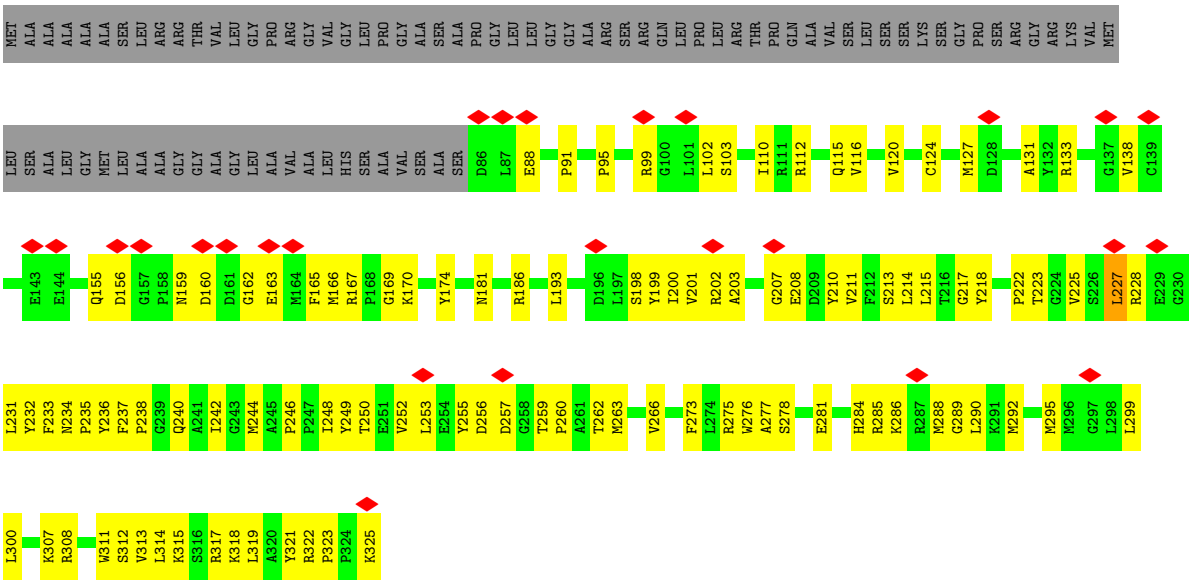
• Molecule 3: Cytochrome b

Chain Ac:



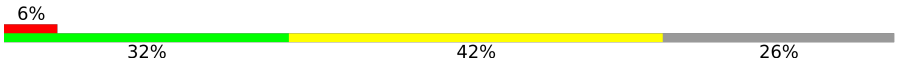
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

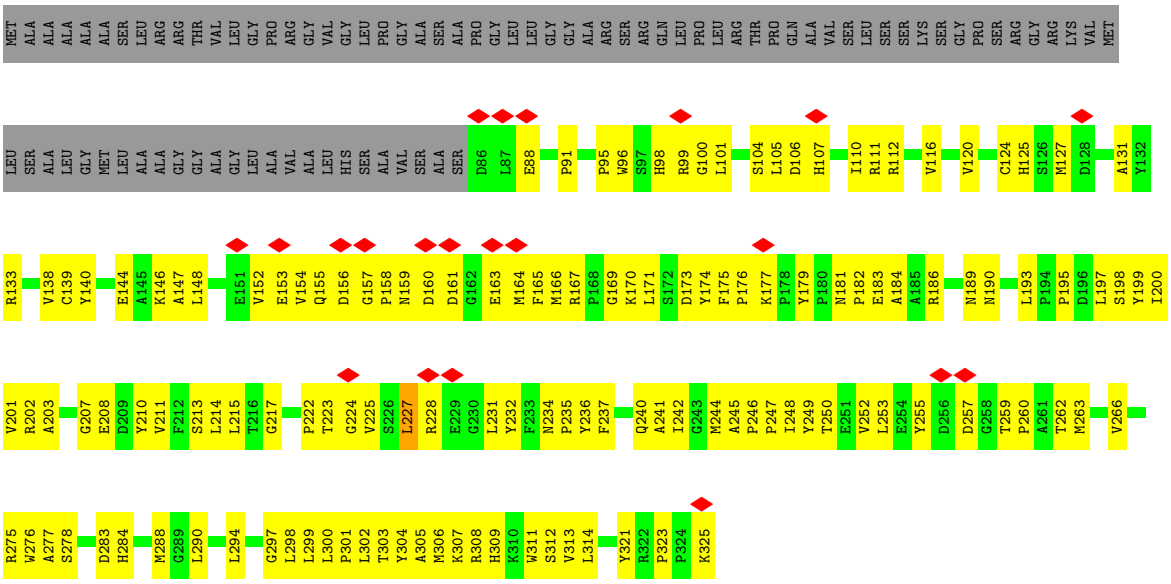
Chain AD:



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

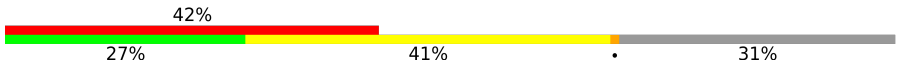
Chain Ad:

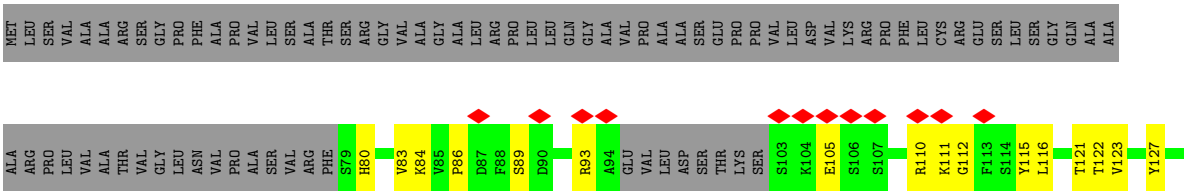


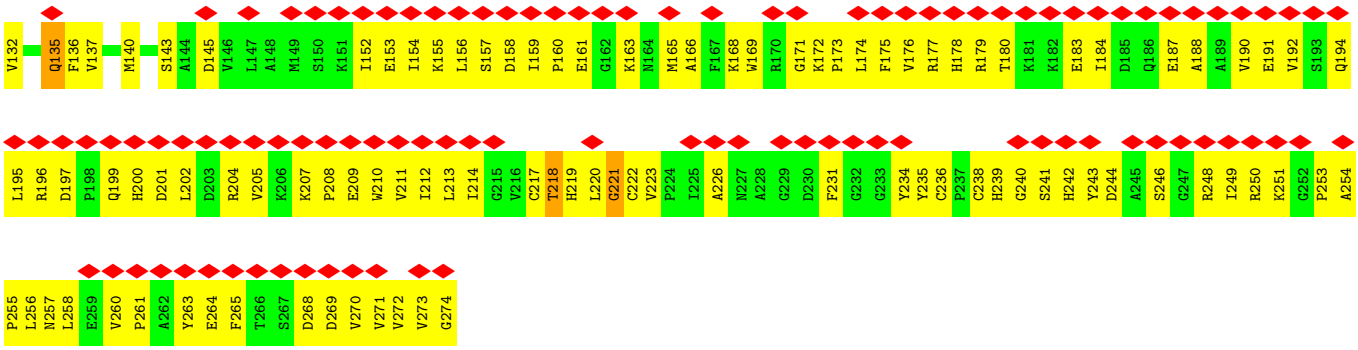


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:

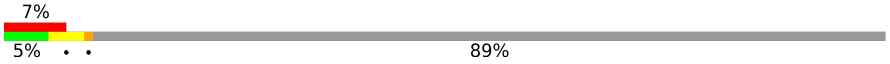


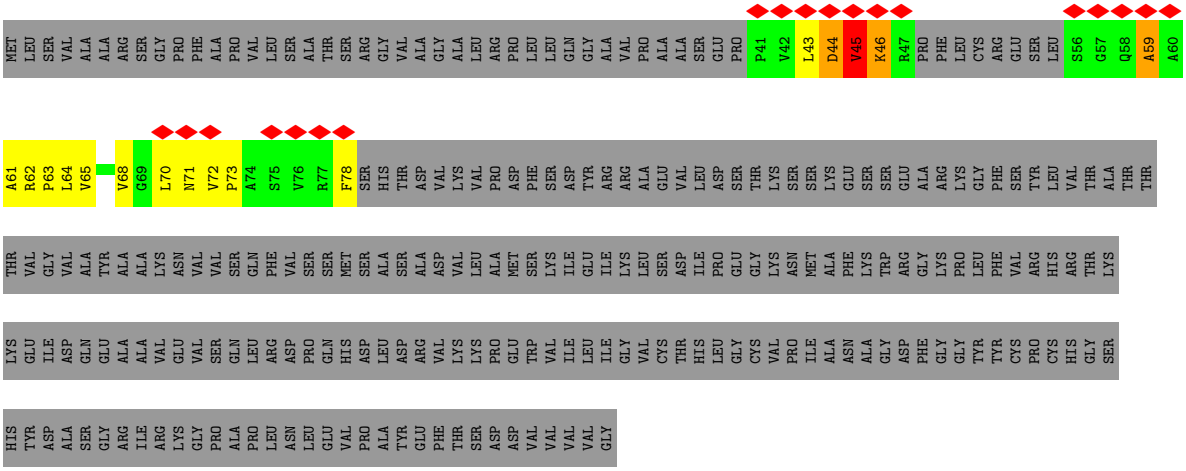




- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

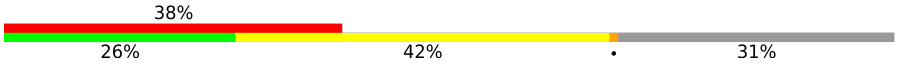
Chain AI:

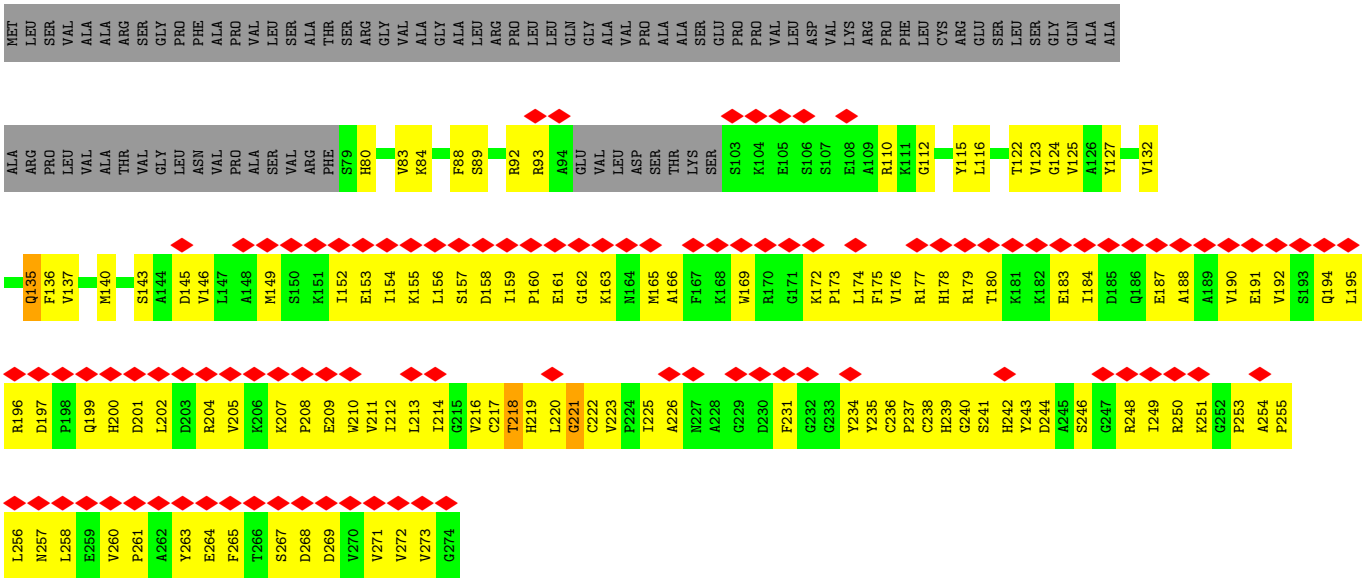




- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

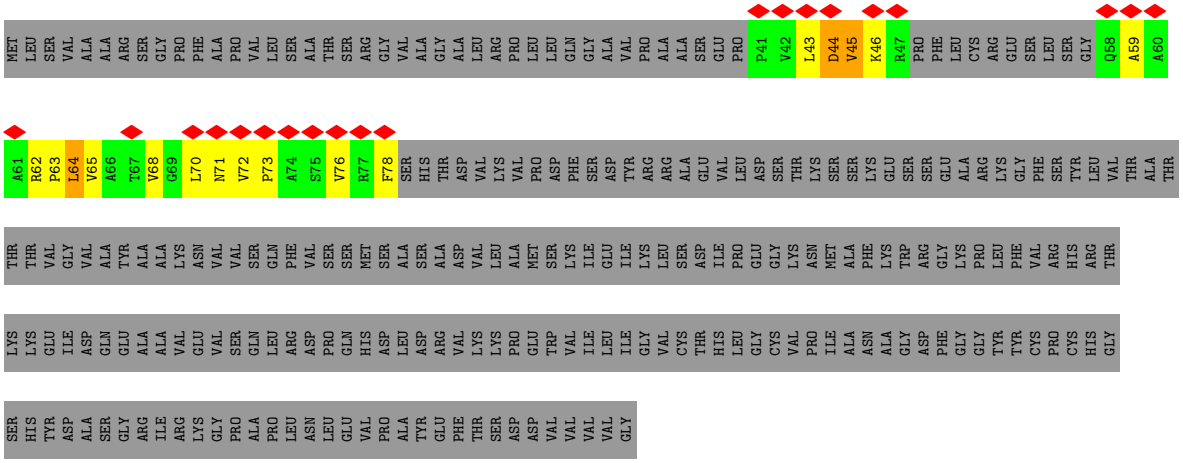
Chain Ae:





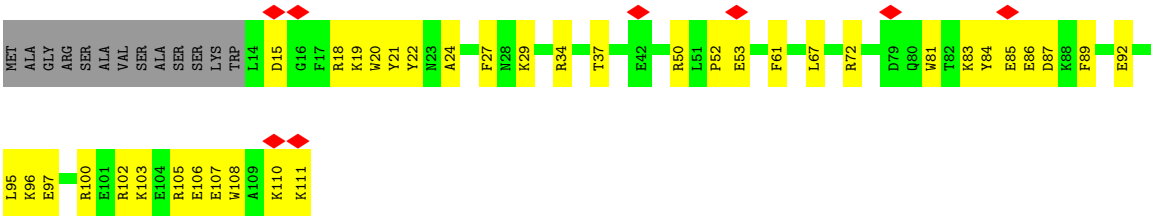
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ai:



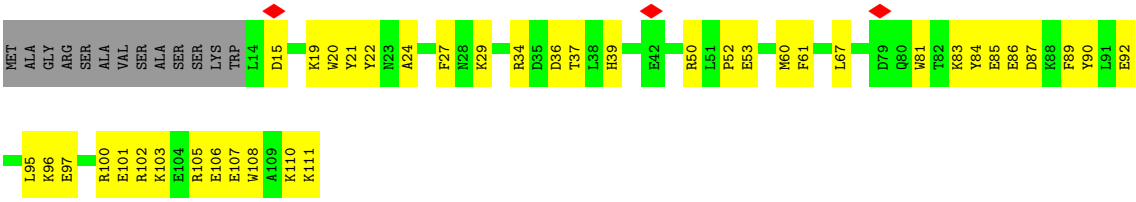
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain AF:



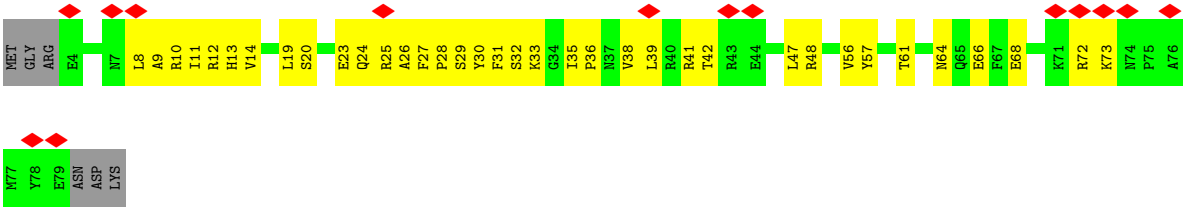
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain Af:



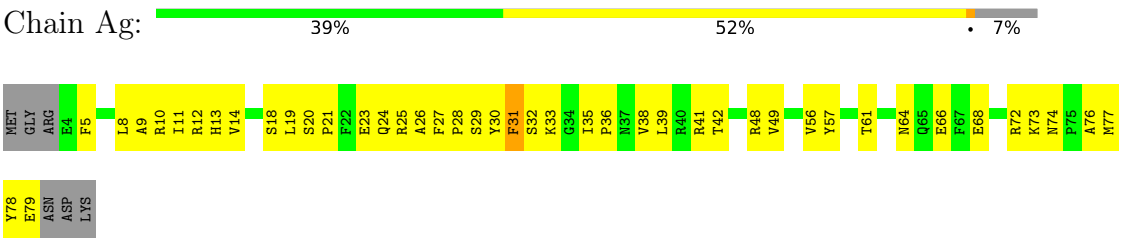
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain AG:



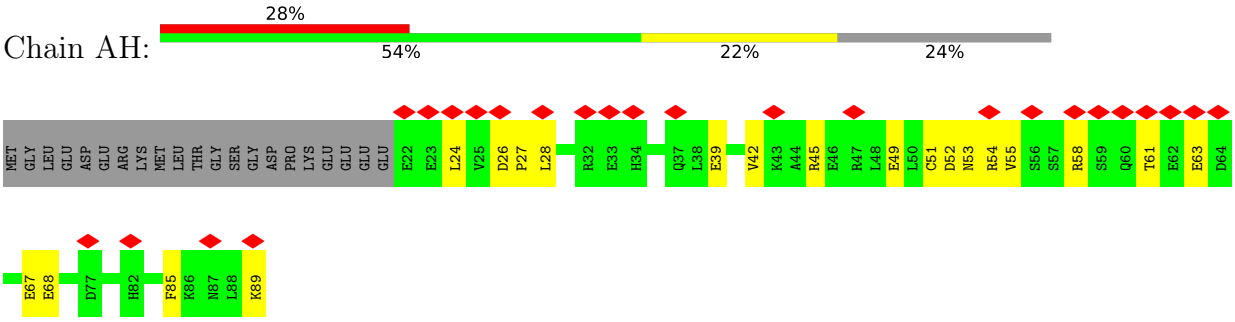
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain Ag:



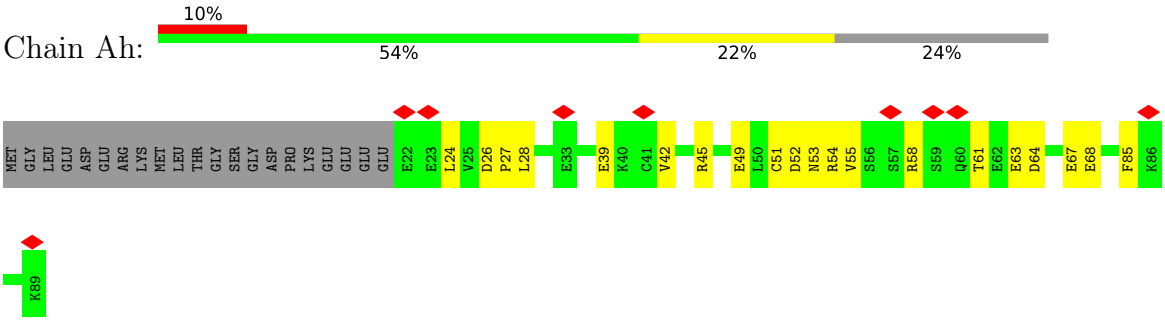
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH:



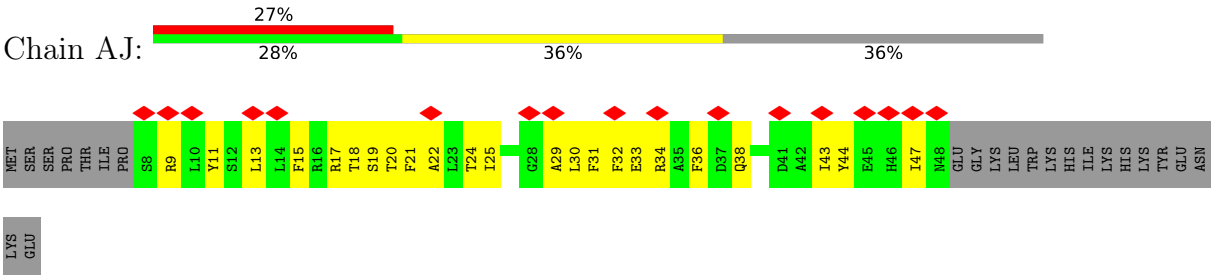
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah:



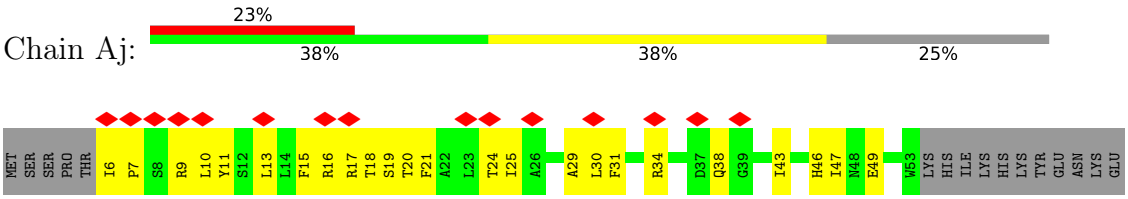
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain AJ:



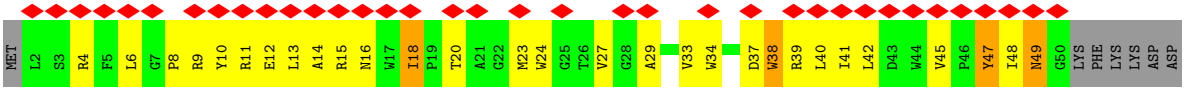
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain Aj:



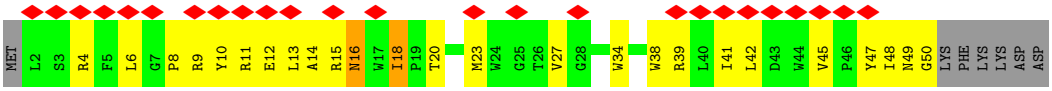
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain AK:



• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.363	Depositor
Minimum map value	-1.370	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, PC1, HEM, CDL, U10, 3PE, UQ6

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	AA	0.38	0/3213	0.69	5/4355 (0.1%)
1	Aa	0.50	1/3288 (0.0%)	0.69	3/4462 (0.1%)
2	AB	0.36	0/3187	0.64	5/4308 (0.1%)
2	Ab	0.43	0/3142	0.68	4/4246 (0.1%)
3	AC	0.48	1/3089 (0.0%)	0.68	3/4221 (0.1%)
3	Ac	0.46	1/3089 (0.0%)	0.73	7/4221 (0.2%)
4	AD	0.41	0/1971	0.70	3/2677 (0.1%)
4	Ad	0.54	0/1971	0.81	5/2677 (0.2%)
5	AE	0.63	0/1483	1.03	3/2007 (0.1%)
5	AI	1.83	2/219 (0.9%)	1.48	5/296 (1.7%)
5	Ae	0.63	0/1483	1.03	3/2007 (0.1%)
5	Ai	1.51	1/209 (0.5%)	1.16	1/283 (0.4%)
6	AF	0.38	0/884	0.52	0/1184
6	Af	0.38	0/884	0.52	0/1184
7	AG	0.49	0/662	0.87	1/895 (0.1%)
7	Ag	0.50	0/662	0.89	1/895 (0.1%)
8	AH	0.38	0/569	0.68	0/763
8	Ah	0.38	0/569	0.68	0/763
9	AJ	0.53	0/339	0.71	0/457
9	Aj	0.55	0/401	0.71	0/542
10	AK	0.53	0/416	0.97	5/571 (0.9%)
10	Ak	0.53	0/416	0.81	2/571 (0.4%)
All	All	0.50	6/32146 (0.0%)	0.75	56/43585 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Ai	44	ASP	C-N	20.05	1.52	1.33
5	AI	44	ASP	C-N	20.05	1.52	1.33
1	Aa	250	LEU	C-N	19.52	1.58	1.33
5	AI	45	VAL	C-N	15.63	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	271	GLU	C-N	13.65	1.52	1.34
3	Ac	265	PRO	N-CD	8.19	1.59	1.47

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AB	306	THR	N-CA-C	9.96	123.38	111.33
2	Ab	306	THR	N-CA-C	9.92	123.33	111.33
2	AB	303	ASN	N-CA-C	-9.88	100.14	112.88
2	Ab	303	ASN	N-CA-C	-9.85	100.17	112.88
1	Aa	250	LEU	O-C-N	-9.83	112.22	121.56
5	AI	46	LYS	N-CA-C	8.81	121.70	110.33
1	AA	360	CYS	N-CA-C	7.91	120.92	109.14
1	Aa	360	CYS	N-CA-C	7.87	120.87	109.14
3	AC	202	GLU	N-CA-C	-7.36	103.28	111.82
3	Ac	8	HIS	CA-C-N	7.29	127.00	119.56
3	Ac	8	HIS	C-N-CA	7.29	127.00	119.56
5	AE	221	GLY	N-CA-C	7.29	126.88	113.76
5	Ae	221	GLY	N-CA-C	7.26	126.83	113.76
10	AK	47	TYR	N-CA-C	7.15	122.19	112.68
3	AC	17	SER	N-CA-C	7.05	122.05	113.38
5	Ae	218	THR	N-CA-C	-6.96	102.84	111.75
5	AE	218	THR	N-CA-C	-6.93	102.88	111.75
5	AI	45	VAL	CA-C-N	-6.92	108.62	120.95
5	AI	45	VAL	C-N-CA	-6.92	108.62	120.95
3	Ac	265	PRO	N-CA-C	-6.54	102.72	110.70
2	AB	305	THR	N-CA-CB	-6.51	100.41	109.91
2	Ab	305	THR	N-CA-CB	-6.49	100.43	109.91
1	Aa	215	ASP	N-CA-C	-6.45	103.94	110.97
1	AA	215	ASP	N-CA-C	-6.43	103.96	110.97
1	AA	402	HIS	N-CA-C	-6.41	102.27	110.53
5	AI	44	ASP	O-C-N	6.37	131.23	121.23
5	Ai	44	ASP	O-C-N	6.36	131.22	121.23
7	AG	31	PHE	N-CA-C	-6.04	105.95	113.38
1	AA	401	SER	N-CA-C	-6.02	104.64	111.14
7	Ag	31	PHE	N-CA-C	-5.97	106.03	113.38
2	AB	244	LEU	N-CA-C	-5.95	106.02	113.28
10	AK	16	ASN	N-CA-C	-5.95	104.92	111.82
10	AK	38	TRP	N-CA-C	-5.95	101.38	110.30
10	Ak	16	ASN	N-CA-C	-5.87	105.01	111.82
4	AD	163	GLU	N-CA-C	5.75	118.16	109.41
3	AC	17	SER	N-CA-CB	-5.68	102.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Ac	252	ASP	CA-C-N	-5.65	112.91	119.47
3	Ac	252	ASP	C-N-CA	-5.65	112.91	119.47
3	Ac	265	PRO	N-CA-CB	5.56	108.47	103.08
5	AI	59	ALA	N-CA-CB	-5.51	101.40	109.95
4	AD	88	GLU	N-CA-C	5.50	117.75	109.23
4	Ad	177	LYS	CA-C-N	-5.50	114.59	120.47
4	Ad	177	LYS	C-N-CA	-5.50	114.59	120.47
1	AA	255	ARG	N-CA-C	5.49	118.23	107.57
2	AB	236	GLN	N-CA-C	-5.43	105.92	112.54
10	Ak	18	ILE	N-CA-C	5.40	120.55	108.88
5	AE	89	SER	N-CA-C	5.37	118.62	111.75
10	AK	18	ILE	N-CA-C	5.37	120.48	108.88
2	Ab	236	GLN	N-CA-C	-5.36	106.00	112.54
4	Ad	227	LEU	N-CA-CB	-5.32	102.12	110.69
5	Ae	89	SER	N-CA-C	5.32	118.56	111.75
4	AD	227	LEU	N-CA-CB	-5.30	102.15	110.69
4	Ad	160	ASP	N-CA-C	-5.28	105.53	111.28
3	Ac	264	THR	N-CA-C	5.21	116.96	109.04
10	AK	49	ASN	N-CA-C	-5.20	103.28	110.35
4	Ad	88	GLU	N-CA-C	5.12	117.77	109.06

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	AA	3153	0	3077	144	0
1	Aa	3225	0	3141	160	0
2	AB	3137	0	3143	170	0
2	Ab	3094	0	3102	176	0
3	AC	2988	0	3045	214	0
3	Ac	2988	0	3045	188	0
4	AD	1912	0	1860	141	0
4	Ad	1912	0	1860	150	0
5	AE	1451	0	1433	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AI	217	0	234	41	0
5	Ae	1451	0	1433	162	0
5	Ai	207	0	226	37	0
6	AF	864	0	854	54	0
6	Af	864	0	854	47	0
7	AG	643	0	643	50	0
7	Ag	643	0	643	64	0
8	AH	562	0	543	24	0
8	Ah	562	0	543	26	0
9	AJ	332	0	324	31	0
9	Aj	391	0	385	25	0
10	AK	401	0	396	46	0
10	Ak	401	0	396	46	0
11	AC	58	0	64	8	0
11	AG	51	0	82	16	0
11	Aa	23	0	20	7	0
11	Ac	35	0	44	4	0
11	Ag	51	0	82	1	0
12	AC	86	0	60	15	0
12	Ac	86	0	60	12	0
13	AC	23	0	23	19	0
13	Ac	23	0	23	21	0
14	AC	28	0	31	27	0
14	Ac	28	0	31	12	0
15	AD	43	0	31	12	0
15	Ad	43	0	31	11	0
16	AG	98	0	84	16	0
16	Aa	46	0	36	4	0
16	Ag	98	0	84	9	0
17	Ae	35	0	44	6	0
All	All	32253	0	32010	1809	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 28.

All (1809) 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)
4:AD:124:CYS:SG	15:AD:401:HEC:HAC	1.40	1.60
2:AB:297:PRO:CG	2:AB:304:ASN:HD21	1.43	1.29
2:Ab:297:PRO:CG	2:Ab:304:ASN:HD21	1.43	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:21:LEU:HD22	14:AC:406:UQ6:C3M	1.66	1.24
4:AD:124:CYS:SG	15:AD:401:HEC:CAC	2.28	1.21
2:AB:297:PRO:HG3	2:AB:304:ASN:ND2	1.57	1.20
2:Ab:297:PRO:HG3	2:Ab:304:ASN:ND2	1.57	1.17
10:AK:4:ARG:HA	6:Af:110:LYS:HE2	1.24	1.14
5:AE:263:TYR:HA	5:AE:273:VAL:HA	1.14	1.13
2:Ab:167:GLN:HE21	5:Ai:43:LEU:CB	1.63	1.11
2:Ab:167:GLN:HG2	5:Ai:43:LEU:HD13	1.32	1.10
3:AC:264:THR:CG2	5:Ae:225:ILE:HD11	1.80	1.10
3:AC:21:LEU:HD22	14:AC:406:UQ6:H3M1	1.10	1.09
6:AF:110:LYS:HE2	10:Ak:4:ARG:HA	1.27	1.09
5:AE:204:ARG:HB3	5:AE:260:VAL:HG21	1.35	1.08
4:Ad:124:CYS:SG	15:Ad:401:HEC:HAC	1.93	1.08
2:Ab:167:GLN:HE21	5:Ai:43:LEU:HB3	1.11	1.08
2:Ab:297:PRO:CB	2:Ab:304:ASN:HD21	1.66	1.08
3:AC:146:ILE:HG13	13:AC:405:U10:C4M	1.83	1.08
2:AB:297:PRO:CB	2:AB:304:ASN:HD21	1.66	1.08
2:Ab:297:PRO:HG3	2:Ab:304:ASN:HD21	1.07	1.07
2:Ab:167:GLN:CG	5:Ai:43:LEU:HD13	1.85	1.05
7:Ag:11:ILE:HG21	7:Ag:14:VAL:HG21	1.36	1.05
4:AD:215:LEU:HD11	15:AD:401:HEC:HMB1	1.35	1.05
3:AC:21:LEU:HD13	14:AC:406:UQ6:O2	1.55	1.05
3:AC:21:LEU:CD2	14:AC:406:UQ6:H3M1	1.87	1.04
3:Ac:146:ILE:HG13	13:Ac:404:U10:C4M	1.86	1.04
4:Ad:215:LEU:HD11	15:Ad:401:HEC:CMB	1.87	1.04
3:AC:146:ILE:HG13	13:AC:405:U10:H4M2	1.38	1.04
4:AD:215:LEU:HD11	15:AD:401:HEC:CMB	1.87	1.04
7:AG:11:ILE:HG21	7:AG:14:VAL:HG21	1.36	1.04
4:Ad:215:LEU:HD11	15:Ad:401:HEC:HMB1	1.34	1.04
5:Ae:204:ARG:HB3	5:Ae:260:VAL:HG21	1.35	1.03
2:AB:167:GLN:CG	5:AI:43:LEU:HD13	1.87	1.03
2:Ab:167:GLN:NE2	5:Ai:43:LEU:HB3	1.73	1.03
1:AA:341:PHE:HD2	1:AA:368:MET:CE	1.74	1.01
2:AB:297:PRO:HG3	2:AB:304:ASN:HD21	1.07	1.00
1:Aa:341:PHE:HD2	1:Aa:368:MET:CE	1.74	0.99
2:AB:167:GLN:HG2	5:AI:43:LEU:HD13	1.45	0.98
1:AA:339:GLN:HB3	5:AI:45:VAL:HG22	1.45	0.97
4:AD:223:THR:HG21	8:AH:52:ASP:HA	1.43	0.97
4:Ad:249:TYR:CE1	4:Ad:252:VAL:HG23	2.02	0.95
2:Ab:297:PRO:CG	2:Ab:304:ASN:ND2	2.22	0.95
7:Ag:19:LEU:HD23	7:Ag:24:GLN:HB3	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:120:LEU:N	2:Ab:298:HIS:O	2.00	0.95
5:Ae:218:THR:HG21	5:Ae:256:LEU:O	1.68	0.94
7:AG:19:LEU:HD23	7:AG:24:GLN:HB3	1.49	0.94
5:AE:218:THR:HG21	5:AE:256:LEU:O	1.68	0.94
1:AA:190:THR:HG21	1:AA:275:ILE:HB	1.49	0.93
1:AA:58:ARG:HE	1:AA:417:LEU:HD12	1.33	0.93
4:AD:249:TYR:CE1	4:AD:252:VAL:HG23	2.02	0.93
3:Ac:146:ILE:HG13	13:Ac:404:U10:H4M2	1.44	0.93
1:Aa:117:GLY:HA2	2:Ab:377:LYS:HG2	1.52	0.92
4:Ad:223:THR:HG21	8:Ah:52:ASP:HA	1.52	0.92
1:Aa:58:ARG:NH2	1:Aa:417:LEU:O	2.03	0.92
9:Aj:6:ILE:HB	9:Aj:7:PRO:HD2	1.52	0.92
11:Aa:501:3PE:H332	17:Ae:301:PC1:H321	1.51	0.91
10:AK:10:TYR:CE1	6:Af:110:LYS:HA	2.06	0.91
3:Ac:214:ASP:HB3	7:Ag:9:ALA:HB2	1.52	0.90
5:AE:263:TYR:CA	5:AE:273:VAL:HA	2.01	0.90
3:AC:223:TYR:O	4:AD:311:TRP:NE1	2.04	0.90
2:AB:305:THR:HG23	2:AB:306:THR:H	1.36	0.89
10:AK:4:ARG:HA	6:Af:110:LYS:CE	2.02	0.88
2:Ab:305:THR:HG23	2:Ab:306:THR:H	1.36	0.88
2:AB:297:PRO:CG	2:AB:304:ASN:ND2	2.23	0.88
1:AA:341:PHE:CD2	1:AA:368:MET:CE	2.56	0.87
1:Aa:341:PHE:CD2	1:Aa:368:MET:CE	2.56	0.87
3:Ac:138:MET:HE1	3:Ac:268:ILE:HA	1.56	0.87
7:AG:29:SER:HB2	7:AG:32:SER:HB2	1.57	0.87
1:AA:120:LEU:N	2:AB:298:HIS:O	2.08	0.87
1:AA:190:THR:HG21	1:AA:275:ILE:CB	2.04	0.87
1:Aa:102:LYS:HZ1	1:Aa:153:ASN:HA	1.38	0.86
7:AG:11:ILE:HG21	7:AG:14:VAL:CG2	2.05	0.86
1:Aa:384:THR:HG21	10:Ak:9:ARG:CG	2.05	0.86
3:AC:98:VAL:HG22	12:AC:403:HEM:HBC2	1.56	0.86
1:AA:190:THR:O	1:AA:273:SER:OG	1.93	0.85
3:AC:294:LEU:HD11	13:AC:405:U10:H1M3	1.58	0.85
5:Ae:174:LEU:HD11	5:Ae:273:VAL:HG11	1.57	0.85
2:AB:45:ASN:ND2	2:AB:239:ASN:HA	1.90	0.85
3:AC:18:PHE:CE1	14:AC:406:UQ6:H1M2	2.10	0.85
1:AA:255:ARG:O	1:AA:255:ARG:HG3	1.75	0.85
3:Ac:294:LEU:HD11	13:Ac:404:U10:H1M3	1.56	0.85
7:Ag:29:SER:HB2	7:Ag:32:SER:HB2	1.56	0.85
5:Ae:155:LYS:HE2	5:Ae:157:SER:HB3	1.57	0.85
3:AC:146:ILE:CG1	13:AC:405:U10:H4M3	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:305:THR:HG23	2:AB:306:THR:N	1.92	0.84
7:Ag:11:ILE:HG21	7:Ag:14:VAL:CG2	2.05	0.84
4:AD:103:SER:O	4:AD:286:LYS:NZ	2.09	0.84
1:AA:58:ARG:NH2	1:AA:417:LEU:O	2.10	0.84
3:Ac:223:TYR:O	4:Ad:311:TRP:NE1	2.09	0.84
1:AA:117:GLY:HA2	2:AB:377:LYS:HG2	1.59	0.84
1:Aa:179:MET:SD	5:Ai:46:LYS:NZ	2.51	0.84
2:Ab:305:THR:HG23	2:Ab:306:THR:N	1.92	0.84
5:AE:123:VAL:HG13	9:AJ:29:ALA:HA	1.59	0.83
2:AB:167:GLN:HE21	5:AI:43:LEU:CB	1.91	0.83
3:Ac:146:ILE:CG1	13:Ac:404:U10:H4M3	2.08	0.83
2:AB:51:SER:HB2	2:AB:230:LEU:HD12	1.61	0.83
9:Aj:31:PHE:HA	10:Ak:48:ILE:HD11	1.60	0.83
10:Ak:42:LEU:HD22	10:Ak:48:ILE:HG21	1.58	0.83
10:AK:10:TYR:HE1	6:Af:110:LYS:HA	1.43	0.82
3:AC:146:ILE:CG1	13:AC:405:U10:C4M	2.57	0.82
2:Ab:51:SER:HB2	2:Ab:230:LEU:HD12	1.61	0.82
3:AC:264:THR:HG23	5:Ae:225:ILE:HD11	1.61	0.82
1:Aa:102:LYS:NZ	1:Aa:153:ASN:HA	1.94	0.82
1:AA:341:PHE:CE2	1:AA:372:LEU:HD13	2.15	0.81
1:Aa:341:PHE:CE2	1:Aa:372:LEU:HD13	2.15	0.81
1:AA:102:LYS:NZ	1:AA:153:ASN:HA	1.94	0.81
2:Ab:297:PRO:CB	2:Ab:304:ASN:ND2	2.41	0.81
1:AA:190:THR:CG2	1:AA:275:ILE:HB	2.10	0.80
3:Ac:270:PRO:HG2	3:Ac:275:LEU:HD23	1.63	0.80
9:Aj:46:HIS:HA	9:Aj:49:GLU:HG3	1.62	0.80
1:AA:102:LYS:HZ1	1:AA:153:ASN:HA	1.46	0.80
1:Aa:341:PHE:CZ	1:Aa:372:LEU:HD13	2.17	0.80
5:AE:263:TYR:HA	5:AE:273:VAL:CA	2.04	0.80
1:AA:190:THR:HG21	1:AA:275:ILE:CG2	2.10	0.80
1:AA:339:GLN:CB	5:AI:45:VAL:HG22	2.12	0.80
3:AC:21:LEU:CD1	14:AC:406:UQ6:O2	2.30	0.79
6:AF:110:LYS:CE	10:Ak:4:ARG:HA	2.11	0.79
3:AC:214:ASP:HB3	7:AG:9:ALA:HB2	1.65	0.79
1:AA:341:PHE:CZ	1:AA:372:LEU:HD13	2.17	0.79
3:AC:45:ILE:HA	12:AC:402:HEM:HAB	1.63	0.79
6:AF:52:PRO:HD3	2:Ab:148:ARG:NH2	1.98	0.79
3:Ac:146:ILE:CG1	13:Ac:404:U10:C4M	2.61	0.79
2:AB:163:ALA:HB1	5:AI:43:LEU:HD23	1.62	0.79
10:AK:4:ARG:CA	6:Af:110:LYS:HE2	2.10	0.78
7:AG:19:LEU:HD11	7:AG:23:GLU:HG2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:297:PRO:HA	2:Ab:304:ASN:OD1	1.84	0.78
6:AF:110:LYS:HA	10:Ak:10:TYR:CE1	2.19	0.78
2:AB:167:GLN:HG3	5:AI:43:LEU:HD13	1.64	0.78
6:AF:108:TRP:CZ2	2:Ab:101:ARG:HB3	2.19	0.78
1:Aa:62:GLU:OE1	1:Aa:409:VAL:HG13	1.83	0.78
7:Ag:19:LEU:HD11	7:Ag:23:GLU:HG2	1.66	0.78
1:Aa:384:THR:CB	10:Ak:9:ARG:HG3	2.14	0.78
2:AB:297:PRO:CB	2:AB:304:ASN:ND2	2.41	0.77
2:AB:167:GLN:HE21	5:AI:43:LEU:HB3	1.49	0.77
3:AC:327:ILE:HG12	11:AG:103:3PE:H2A2	1.67	0.77
7:AG:11:ILE:CG2	7:AG:14:VAL:CG2	2.62	0.77
3:AC:21:LEU:HD22	14:AC:406:UQ6:H3M2	1.63	0.77
1:Aa:62:GLU:HB2	1:Aa:413:ILE:HD11	1.65	0.77
7:Ag:11:ILE:CG2	7:Ag:14:VAL:CG2	2.62	0.77
2:AB:63:LEU:HD11	2:AB:238:LEU:HD21	1.65	0.77
2:AB:297:PRO:HA	2:AB:304:ASN:OD1	1.84	0.77
10:Ak:6:LEU:HA	10:Ak:11:ARG:HH12	1.49	0.76
3:AC:245:PHE:HE1	4:AD:102:LEU:HD23	1.51	0.76
2:Ab:63:LEU:HD11	2:Ab:238:LEU:HD21	1.66	0.76
5:Ae:191:GLU:HB2	5:Ae:194:GLN:HB2	1.66	0.76
5:AE:191:GLU:HB2	5:AE:194:GLN:HB2	1.66	0.76
10:AK:6:LEU:HA	10:AK:11:ARG:HH12	1.49	0.76
3:Ac:146:ILE:HD11	13:Ac:404:U10:C3	2.15	0.76
2:Ab:407:MET:HG2	2:Ab:411:THR:OG1	1.85	0.76
3:Ac:146:ILE:HG13	13:Ac:404:U10:H4M3	1.67	0.76
2:AB:407:MET:HG2	2:AB:411:THR:OG1	1.85	0.75
3:AC:146:ILE:HD11	13:AC:405:U10:C3	2.16	0.75
7:AG:11:ILE:HG22	7:AG:14:VAL:HG22	1.68	0.75
4:Ad:227:LEU:HD12	4:Ad:227:LEU:O	1.87	0.75
1:AA:255:ARG:O	1:AA:256:VAL:C	2.29	0.75
4:Ad:186:ARG:HE	4:Ad:193:LEU:HB2	1.51	0.75
4:AD:227:LEU:HD12	4:AD:227:LEU:O	1.87	0.74
7:Ag:11:ILE:HG22	7:Ag:14:VAL:HG22	1.68	0.74
3:AC:148:ASN:OD1	5:Ae:221:GLY:HA3	1.87	0.74
5:AE:173:PRO:HG2	5:AE:223:VAL:HG22	1.67	0.74
5:Ae:173:PRO:HG2	5:Ae:223:VAL:HG22	1.67	0.74
2:AB:85:LEU:HD23	5:AI:68:VAL:HG21	1.70	0.74
3:AC:17:SER:O	14:AC:406:UQ6:O2	2.06	0.74
2:Ab:323:VAL:HG13	2:Ab:340:THR:HG22	1.68	0.74
5:Ae:123:VAL:HG13	9:Aj:29:ALA:HA	1.70	0.74
3:Ac:137:GLN:HE21	3:Ac:265:PRO:HD3	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:232:TYR:HD1	4:Ad:242:ILE:O	1.71	0.73
6:AF:24:ALA:O	7:AG:48:ARG:NH2	2.21	0.73
1:Aa:80:ARG:HE	1:Aa:265:LEU:HD11	1.53	0.73
2:AB:305:THR:CG2	2:AB:306:THR:H	2.01	0.73
2:Ab:305:THR:CG2	2:Ab:306:THR:H	2.02	0.73
4:Ad:96:TRP:HD1	4:Ad:99:ARG:HH21	1.34	0.73
5:AE:187:GLU:HB3	5:AE:201:ASP:HB3	1.71	0.73
3:Ac:21:LEU:HD22	14:Ac:405:UQ6:H3M1	1.71	0.73
2:Ab:163:ALA:HB1	5:Ai:43:LEU:HD23	1.69	0.73
3:Ac:146:ILE:HD11	13:Ac:404:U10:H3M2	1.69	0.73
5:Ae:187:GLU:HB3	5:Ae:201:ASP:HB3	1.71	0.73
3:AC:21:LEU:CD2	14:AC:406:UQ6:C3M	2.53	0.73
3:AC:29:SER:HB2	16:AG:102:CDL:H712	1.71	0.73
2:AB:297:PRO:CA	2:AB:304:ASN:HD21	2.01	0.72
6:AF:110:LYS:HE2	10:Ak:4:ARG:CA	2.15	0.72
9:AJ:34:ARG:HB2	10:AK:48:ILE:HG13	1.69	0.72
1:Aa:120:LEU:HB3	2:Ab:299:ILE:HA	1.71	0.72
5:AE:221:GLY:HA3	3:Ac:148:ASN:OD1	1.88	0.72
2:Ab:85:LEU:HD21	5:Ai:68:VAL:HG11	1.72	0.72
2:Ab:297:PRO:CA	2:Ab:304:ASN:HD21	2.01	0.72
2:AB:163:ALA:HB1	5:AI:43:LEU:CD2	2.20	0.72
5:Ae:199:GLN:O	5:Ae:248:ARG:HD3	1.90	0.72
9:AJ:30:LEU:HA	10:AK:34:TRP:CD1	2.25	0.72
4:Ad:306:MET:HE1	17:Ae:301:PC1:H331	1.70	0.71
1:AA:58:ARG:NE	1:AA:417:LEU:HD12	2.04	0.71
1:Aa:384:THR:HB	10:Ak:9:ARG:HG3	1.73	0.71
5:AE:199:GLN:O	5:AE:248:ARG:HD3	1.90	0.71
1:AA:190:THR:HG21	1:AA:275:ILE:HG22	1.72	0.71
3:AC:294:LEU:CD1	13:AC:405:U10:H1M3	2.20	0.71
3:AC:245:PHE:CE1	4:AD:102:LEU:HD23	2.26	0.71
3:Ac:294:LEU:CD1	13:Ac:404:U10:H1M3	2.20	0.71
5:Ae:207:LYS:HB2	5:Ae:210:TRP:HB2	1.73	0.71
2:AB:297:PRO:HA	2:AB:304:ASN:CG	2.16	0.71
5:AE:154:ILE:HB	5:AE:271:VAL:O	1.89	0.71
4:Ad:222:PRO:HD2	4:Ad:225:VAL:HG11	1.72	0.71
5:Ae:178:HIS:HB2	5:Ae:210:TRP:CZ3	2.26	0.70
1:Aa:113:VAL:CG1	2:Ab:299:ILE:HD11	2.21	0.70
5:Ae:220:LEU:HD12	5:Ae:239:HIS:CE1	2.27	0.70
4:AD:222:PRO:HD2	4:AD:225:VAL:HG11	1.72	0.70
5:Ae:192:VAL:HA	5:Ae:195:LEU:HD12	1.73	0.70
2:AB:183:LYS:HG3	2:AB:254:ARG:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:93:ARG:HD2	5:AE:110:ARG:HD2	1.72	0.70
3:Ac:45:ILE:HA	12:Ac:401:HEM:HAB	1.71	0.70
5:AE:178:HIS:HB2	5:AE:210:TRP:CZ3	2.26	0.70
5:AE:192:VAL:HA	5:AE:195:LEU:HD12	1.73	0.70
4:AD:215:LEU:HD11	15:AD:401:HEC:HMB3	1.72	0.70
1:Aa:341:PHE:CD2	1:Aa:368:MET:HE1	2.27	0.70
2:Ab:297:PRO:HA	2:Ab:304:ASN:CG	2.16	0.70
1:AA:341:PHE:CD2	1:AA:368:MET:HE1	2.27	0.70
4:Ad:152:VAL:HG21	4:Ad:176:PRO:HG2	1.74	0.70
5:Ae:202:LEU:HA	5:Ae:205:VAL:HG22	1.74	0.70
1:AA:68:THR:HG22	1:AA:136:LEU:HD23	1.73	0.70
5:AE:159:ILE:HG23	5:AE:163:LYS:HE3	1.74	0.70
9:Aj:6:ILE:HB	9:Aj:7:PRO:CD	2.21	0.70
3:AC:265:PRO:HD2	3:AC:268:ILE:HD11	1.74	0.69
1:Aa:62:GLU:OE1	1:Aa:409:VAL:CG1	2.40	0.69
3:Ac:147:THR:HG22	3:Ac:161:VAL:HG13	1.75	0.69
5:Ae:263:TYR:HA	5:Ae:273:VAL:HA	1.74	0.69
3:AC:264:THR:HG22	5:Ae:225:ILE:HD11	1.75	0.69
5:Ae:180:THR:H	5:Ae:183:GLU:HB2	1.58	0.69
4:Ad:249:TYR:CZ	4:Ad:252:VAL:HA	2.28	0.69
5:AE:220:LEU:HD12	5:AE:239:HIS:CE1	2.27	0.69
3:AC:18:PHE:CE1	14:AC:406:UQ6:C1M	2.75	0.69
5:AE:207:LYS:HB2	5:AE:210:TRP:HB2	1.73	0.69
4:AD:214:LEU:HD11	4:AD:237:PHE:HB2	1.75	0.69
9:AJ:17:ARG:HD2	9:AJ:20:THR:HG23	1.75	0.69
2:Ab:412:VAL:HG13	2:Ab:415:GLN:HE21	1.58	0.69
2:AB:101:ARG:HB3	6:Af:108:TRP:CZ2	2.28	0.68
4:Ad:125:HIS:HE1	4:Ad:195:PRO:HD2	1.56	0.68
4:Ad:214:LEU:HD11	4:Ad:237:PHE:HB2	1.75	0.68
2:AB:233:VAL:HA	2:AB:236:GLN:HG2	1.76	0.68
2:AB:297:PRO:CA	2:AB:304:ASN:ND2	2.57	0.68
5:AE:202:LEU:HA	5:AE:205:VAL:HG22	1.74	0.68
1:Aa:384:THR:CG2	10:Ak:9:ARG:HG3	2.22	0.68
11:Aa:501:3PE:H331	3:Ac:229:ILE:HD11	1.76	0.68
2:Ab:297:PRO:CA	2:Ab:304:ASN:ND2	2.57	0.68
5:Ae:159:ILE:HG23	5:Ae:163:LYS:HE3	1.74	0.68
10:AK:33:VAL:HG12	10:AK:42:LEU:HG	1.75	0.68
2:Ab:233:VAL:HA	2:Ab:236:GLN:HG2	1.76	0.68
4:Ad:186:ARG:NE	4:Ad:193:LEU:HB2	2.09	0.68
7:AG:19:LEU:HD11	7:AG:23:GLU:CG	2.24	0.68
5:Ae:197:ASP:HB3	5:Ae:257:ASN:CG	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:16:HIS:CE1	3:AC:201:HIS:NE2	2.62	0.68
4:AD:249:TYR:CZ	4:AD:252:VAL:HA	2.28	0.68
1:Aa:68:THR:HG22	1:Aa:136:LEU:HD23	1.74	0.68
2:AB:148:ARG:NH2	6:Af:52:PRO:HD3	2.09	0.68
1:Aa:80:ARG:NE	1:Aa:265:LEU:HD11	2.09	0.68
1:Aa:101:THR:HG22	1:Aa:154:SER:HA	1.76	0.68
1:Aa:384:THR:HG21	10:Ak:9:ARG:HG3	1.73	0.68
4:Ad:124:CYS:HA	4:Ad:179:TYR:HE2	1.59	0.68
8:AH:45:ARG:O	8:AH:49:GLU:HG2	1.94	0.68
1:Aa:118:ALA:O	2:Ab:298:HIS:HB3	1.94	0.68
4:Ad:215:LEU:HD11	15:Ad:401:HEC:HMB3	1.73	0.68
3:Ac:146:ILE:HD11	13:Ac:404:U10:C3M	2.23	0.68
5:AE:180:THR:H	5:AE:183:GLU:HB2	1.58	0.67
1:AA:101:THR:HG22	1:AA:154:SER:HA	1.76	0.67
1:AA:274:GLU:HG3	1:AA:456:VAL:HB	1.77	0.67
3:AC:146:ILE:HD11	13:AC:405:U10:H3M2	1.76	0.67
6:AF:110:LYS:HA	10:Ak:10:TYR:HE1	1.56	0.67
1:AA:190:THR:CG2	1:AA:275:ILE:CG2	2.72	0.67
3:AC:147:THR:HG22	3:AC:161:VAL:HG13	1.75	0.67
5:Ae:156:LEU:HB2	5:Ae:269:ASP:HA	1.76	0.67
2:AB:305:THR:HG23	2:AB:306:THR:HG23	1.77	0.67
9:AJ:30:LEU:HD12	10:AK:34:TRP:HB2	1.77	0.67
7:Ag:19:LEU:HD11	7:Ag:23:GLU:CG	2.24	0.67
9:Aj:17:ARG:HD2	9:Aj:20:THR:HG23	1.75	0.67
8:Ah:45:ARG:O	8:Ah:49:GLU:HG2	1.94	0.67
3:Ac:20:ASP:O	7:Ag:5:PHE:HE2	1.78	0.67
4:AD:156:ASP:HB2	4:AD:167:ARG:HE	1.58	0.66
5:AE:197:ASP:HB3	5:AE:257:ASN:CG	2.19	0.66
7:AG:11:ILE:CG2	7:AG:14:VAL:HG22	2.25	0.66
1:Aa:400:VAL:HB	2:Ab:58:LEU:HG	1.77	0.66
7:AG:11:ILE:CG2	7:AG:14:VAL:HG21	2.18	0.66
2:AB:412:VAL:HG13	2:AB:415:GLN:HE21	1.58	0.66
2:Ab:270:ALA:HB2	2:Ab:339:TYR:HD1	1.61	0.66
2:AB:229:VAL:O	2:AB:232:GLN:HG2	1.95	0.66
3:Ac:215:ALA:HA	7:Ag:11:ILE:HD11	1.76	0.66
7:Ag:35:ILE:HD11	16:Ag:102:CDL:H322	1.78	0.66
2:Ab:229:VAL:O	2:Ab:232:GLN:HG2	1.95	0.66
3:Ac:257:MET:HG3	4:Ad:203:ALA:HB1	1.78	0.66
2:AB:339:TYR:HD2	5:AI:59:ALA:HB1	1.61	0.66
3:Ac:18:PHE:CZ	14:Ac:405:UQ6:H1M3	2.31	0.66
3:AC:28:SER:HB2	16:AG:101:CDL:HA21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:122:THR:HG21	9:AJ:25:ILE:HD13	1.79	0.65
7:Ag:11:ILE:CG2	7:Ag:14:VAL:HG22	2.25	0.65
4:AD:223:THR:CG2	8:AH:52:ASP:HA	2.23	0.65
2:AB:339:TYR:CD2	5:AI:59:ALA:HB1	2.31	0.65
1:Aa:136:LEU:HD21	2:Ab:380:ALA:HA	1.78	0.65
1:AA:341:PHE:CD2	1:AA:368:MET:HE3	2.32	0.65
3:AC:257:MET:HG3	4:AD:203:ALA:HB1	1.78	0.65
1:Aa:381:THR:O	10:Ak:16:ASN:ND2	2.30	0.65
3:AC:96:LEU:HD23	11:AC:404:3PE:H292	1.78	0.65
1:Aa:110:GLU:HB2	2:Ab:299:ILE:HD13	1.78	0.65
3:Ac:110:MET:HE1	3:Ac:306:PHE:CE1	2.32	0.65
1:AA:339:GLN:HB3	5:AI:45:VAL:CG2	2.22	0.65
3:AC:58:ASP:HB2	3:Ac:56:THR:HG21	1.77	0.65
12:AC:403:HEM:HBA1	14:AC:406:UQ6:C4M	2.27	0.65
2:Ab:167:GLN:NE2	5:Ai:43:LEU:CB	2.40	0.65
2:Ab:305:THR:HG23	2:Ab:306:THR:HG23	1.77	0.65
12:Ac:402:HEM:HBA1	14:Ac:405:UQ6:C4M	2.27	0.64
4:Ad:161:ASP:HB2	4:Ad:163:GLU:HG2	1.79	0.64
4:Ad:201:VAL:HG21	4:Ad:275:ARG:HA	1.79	0.64
1:Aa:249:HIS:O	1:Aa:250:LEU:HB2	1.97	0.64
3:AC:146:ILE:HG12	13:AC:405:U10:H4M3	1.79	0.64
1:Aa:274:GLU:HG3	1:Aa:456:VAL:HB	1.80	0.64
4:Ad:248:ILE:HG22	4:Ad:263:MET:HG3	1.79	0.64
2:Ab:191:TYR:OH	5:Ai:76:VAL:HB	1.98	0.64
3:Ac:311:LYS:O	6:Af:39:HIS:N	2.25	0.64
5:AE:218:THR:CG2	5:AE:256:LEU:O	2.45	0.64
2:Ab:183:LYS:HG3	2:Ab:254:ARG:HB3	1.78	0.64
4:Ad:96:TRP:CD1	4:Ad:99:ARG:HH21	2.16	0.64
2:AB:115:THR:HG22	5:AI:65:VAL:HG22	1.79	0.64
4:AD:248:ILE:HG22	4:AD:263:MET:HG3	1.79	0.64
4:AD:323:PRO:HG2	4:AD:325:LYS:HD2	1.80	0.64
5:Ae:234:TYR:HB2	5:Ae:243:TYR:HB2	1.79	0.64
1:AA:403:LEU:HD23	1:AA:409:VAL:HG22	1.78	0.64
3:Ac:253:PRO:O	4:Ad:203:ALA:HA	1.98	0.64
3:Ac:107:TYR:HB2	3:Ac:305:PRO:HG3	1.79	0.64
4:AD:255:TYR:OH	4:AD:266:VAL:HA	1.98	0.63
10:AK:45:VAL:CG1	10:AK:48:ILE:HG22	2.29	0.63
1:Aa:341:PHE:CD2	1:Aa:368:MET:HE3	2.32	0.63
2:Ab:426:LYS:O	2:Ab:429:LYS:HG2	1.97	0.63
1:AA:74:TRP:CZ2	1:AA:411:GLU:HA	2.33	0.63
2:AB:109:LYS:HD2	5:AI:71:ASN:HD22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:100:ARG:HH12	12:AC:403:HEM:CBD	2.11	0.63
4:AD:186:ARG:HE	4:AD:193:LEU:HB2	1.62	0.63
1:Aa:467:ASP:OD2	3:Ac:223:TYR:CE2	2.51	0.63
1:AA:204:PRO:HB2	1:AA:206:GLU:OE1	1.98	0.63
2:AB:307:SER:HB2	2:AB:310:SER:HB2	1.78	0.63
5:Ae:188:ALA:HA	5:Ae:200:HIS:NE2	2.13	0.63
5:AE:188:ALA:HA	5:AE:200:HIS:NE2	2.13	0.63
3:Ac:107:TYR:HE1	3:Ac:308:HIS:HB2	1.63	0.63
1:AA:388:VAL:HG22	1:AA:441:LEU:HD13	1.81	0.63
9:AJ:30:LEU:O	10:AK:48:ILE:HD12	1.98	0.63
4:Ad:255:TYR:OH	4:Ad:266:VAL:HA	1.98	0.63
2:AB:426:LYS:O	2:AB:429:LYS:HG2	1.97	0.63
3:AC:253:PRO:O	4:AD:203:ALA:HA	1.98	0.63
5:AE:234:TYR:HB2	5:AE:243:TYR:HB2	1.79	0.63
1:Aa:55:ASN:HB3	1:Aa:226:ALA:CB	2.29	0.63
4:Ad:217:GLY:O	4:Ad:235:PRO:HD2	1.99	0.63
5:Ae:161:GLU:HA	5:Ae:178:HIS:CG	2.34	0.63
5:Ae:218:THR:CG2	5:Ae:256:LEU:O	2.45	0.63
2:AB:38:LEU:HD11	2:AB:396:ILE:HD13	1.80	0.63
4:AD:217:GLY:O	4:AD:235:PRO:HD2	1.99	0.63
1:Aa:204:PRO:HB2	1:Aa:206:GLU:OE1	1.98	0.63
5:Ae:179:ARG:HH12	5:Ae:201:ASP:HB2	1.64	0.63
2:AB:45:ASN:HD21	2:AB:239:ASN:HA	1.63	0.62
3:Ac:146:ILE:HG12	13:Ac:404:U10:H4M3	1.81	0.62
7:Ag:31:PHE:CE1	16:Ag:102:CDL:H312	2.34	0.62
4:AD:201:VAL:HG21	4:AD:275:ARG:HA	1.79	0.62
4:Ad:167:ARG:HH12	4:Ad:173:ASP:HB2	1.64	0.62
5:Ae:213:LEU:HD23	5:Ae:260:VAL:HG22	1.81	0.62
1:Aa:53:LEU:CD1	1:Aa:57:LEU:HD23	2.28	0.62
4:AD:290:LEU:HD23	9:AJ:44:TYR:HB2	1.80	0.62
1:AA:478:LEU:HD11	11:AC:401:3PE:H11	1.80	0.62
1:AA:249:HIS:O	1:AA:250:LEU:HB2	1.97	0.62
4:AD:262:THR:HG22	8:AH:24:LEU:HG	1.81	0.62
5:AE:161:GLU:HA	5:AE:178:HIS:CG	2.34	0.62
2:Ab:412:VAL:O	2:Ab:415:GLN:HG2	2.00	0.62
3:Ac:220:PHE:HE2	14:Ac:405:UQ6:H4M2	1.65	0.62
2:AB:412:VAL:O	2:AB:415:GLN:HG2	2.00	0.62
5:AE:152:ILE:HG21	5:AE:274:GLY:H	1.64	0.62
1:Aa:280:ASP:OD2	7:Ag:10:ARG:HA	1.99	0.62
3:AC:202:GLU:OE1	3:Ac:9:PRO:HG3	2.00	0.62
3:Ac:138:MET:HE1	3:Ac:268:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:120:LEU:HB3	2:AB:299:ILE:HA	1.81	0.62
6:AF:20:TRP:HE1	11:AG:103:3PE:H3B2	1.64	0.62
1:Aa:259:GLU:O	1:Aa:260:ASP:C	2.43	0.62
5:AE:213:LEU:HD23	5:AE:260:VAL:HG22	1.81	0.61
4:Ad:223:THR:CG2	8:Ah:52:ASP:HA	2.28	0.61
6:Af:92:GLU:HG2	6:Af:96:LYS:HE2	1.82	0.61
4:AD:235:PRO:HA	4:AD:240:GLN:HG3	1.82	0.61
6:AF:50:ARG:O	2:Ab:148:ARG:NH2	2.34	0.61
2:Ab:262:ASN:OD1	2:Ab:442:GLY:HA2	2.00	0.61
1:AA:268:CYS:SG	1:AA:351:THR:HG21	2.40	0.61
3:AC:29:SER:OG	16:AG:101:CDL:HA61	2.00	0.61
1:Aa:113:VAL:HG13	2:Ab:299:ILE:HD11	1.81	0.61
6:AF:92:GLU:HG2	6:AF:96:LYS:HE2	1.82	0.61
7:AG:47:LEU:HB3	11:AG:103:3PE:O22	2.00	0.61
5:AE:179:ARG:HH12	5:AE:201:ASP:HB2	1.64	0.61
5:AE:244:ASP:HB3	5:AE:250:ARG:HH11	1.66	0.61
1:Aa:388:VAL:HG22	1:Aa:441:LEU:HD13	1.81	0.61
2:Ab:174:ILE:HG21	5:Ai:64:LEU:HD13	1.83	0.61
5:Ae:154:ILE:HB	5:Ae:271:VAL:HG13	1.82	0.61
1:AA:110:GLU:HB2	2:AB:299:ILE:HD13	1.81	0.61
2:AB:167:GLN:NE2	5:AI:43:LEU:HB3	2.16	0.61
4:Ad:124:CYS:HA	4:Ad:179:TYR:CE2	2.35	0.61
7:Ag:64:ASN:O	7:Ag:68:GLU:HG2	2.01	0.61
2:AB:167:GLN:HG2	5:AI:43:LEU:CD1	2.25	0.61
1:Aa:281:ALA:HB2	7:Ag:10:ARG:HH22	1.66	0.61
1:AA:92:PHE:HD1	1:AA:168:ILE:HD12	1.66	0.61
12:AC:403:HEM:HMA1	14:AC:406:UQ6:O5	2.01	0.61
9:Aj:30:LEU:HA	10:Ak:34:TRP:CD1	2.36	0.61
4:Ad:248:ILE:HD11	15:Ad:401:HEC:HBB1	1.83	0.61
4:AD:156:ASP:CB	4:AD:167:ARG:HE	2.14	0.60
7:AG:64:ASN:O	7:AG:68:GLU:HG2	2.01	0.60
2:Ab:305:THR:CG2	2:Ab:306:THR:N	2.60	0.60
4:AD:162:GLY:HA2	4:Ad:183:GLU:HB2	1.82	0.60
3:Ac:128:PHE:CE1	13:Ac:404:U10:H4M2	2.36	0.60
1:AA:407:THR:HB	1:AA:408:PRO:HD3	1.83	0.60
2:AB:45:ASN:HD22	2:AB:239:ASN:HA	1.67	0.60
3:AC:16:HIS:NE2	3:AC:201:HIS:NE2	2.49	0.60
3:AC:119:LEU:HD22	12:AC:403:HEM:HBB2	1.83	0.60
5:AE:152:ILE:CG2	5:AE:274:GLY:H	2.13	0.60
1:Aa:55:ASN:HB3	1:Aa:226:ALA:HB1	1.83	0.60
5:Ae:207:LYS:HD2	5:Ae:210:TRP:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:146:ILE:HD11	13:AC:405:U10:C3M	2.31	0.60
2:Ab:40:PHE:CE1	2:Ab:406:TYR:HB2	2.36	0.60
2:Ab:261:GLN:NE2	2:Ab:443:ASN:HA	2.17	0.60
3:Ac:98:VAL:HG22	12:Ac:402:HEM:HBC2	1.82	0.60
4:Ad:138:VAL:HG12	4:Ad:139:CYS:SG	2.42	0.60
5:Ae:115:TYR:CD1	17:Ae:301:PC1:H122	2.37	0.60
5:Ae:244:ASP:HB3	5:Ae:250:ARG:HH11	1.65	0.60
3:AC:302:ALA:O	3:AC:305:PRO:HD2	2.02	0.60
4:AD:218:TYR:CD1	4:AD:246:PRO:HG3	2.36	0.60
5:AE:223:VAL:HG23	3:Ac:141:TRP:CH2	2.36	0.60
2:Ab:85:LEU:HD23	5:Ai:68:VAL:HG21	1.83	0.60
1:AA:225:LYS:HE3	1:AA:256:VAL:HA	1.83	0.60
5:AE:207:LYS:HD2	5:AE:210:TRP:HD1	1.67	0.60
1:Aa:295:GLY:O	1:Aa:301:ASN:ND2	2.35	0.60
1:AA:341:PHE:HE2	1:AA:372:LEU:HD13	1.67	0.60
1:AA:469:ASN:ND2	3:AC:223:TYR:CZ	2.70	0.60
2:AB:138:LEU:CD2	2:AB:238:LEU:HG	2.32	0.60
2:AB:253:TYR:CE2	2:AB:435:LYS:HG3	2.36	0.60
4:AD:155:GLN:HA	4:AD:166:MET:HA	1.82	0.60
6:AF:108:TRP:HA	6:AF:111:LYS:NZ	2.17	0.60
8:AH:51:CYS:O	8:AH:55:VAL:HG23	2.01	0.59
1:Aa:62:GLU:CB	1:Aa:413:ILE:HD11	2.31	0.59
1:Aa:120:LEU:HD23	2:Ab:299:ILE:HG12	1.83	0.59
2:AB:117:GLU:OE2	2:AB:331:SER:N	2.22	0.59
4:AD:321:TYR:HB2	6:AF:61:PHE:CD1	2.37	0.59
5:AE:132:VAL:HA	5:AE:135:GLN:NE2	2.17	0.59
7:Ag:19:LEU:CD2	7:Ag:24:GLN:HB3	2.29	0.59
2:AB:313:VAL:HG21	2:AB:323:VAL:HG21	1.83	0.59
6:Af:108:TRP:HA	6:Af:111:LYS:NZ	2.17	0.59
3:AC:15:ASN:OD1	3:AC:19:ILE:HB	2.03	0.59
3:Ac:302:ALA:O	3:Ac:305:PRO:HD2	2.02	0.59
1:AA:403:LEU:HD21	1:AA:423:ARG:HH22	1.66	0.59
2:AB:286:PHE:CE1	2:AB:427:ALA:HB1	2.38	0.59
5:AE:163:LYS:O	5:AE:177:ARG:HG3	2.02	0.59
6:Af:106:GLU:O	6:Af:110:LYS:HG3	2.03	0.59
8:Ah:51:CYS:O	8:Ah:55:VAL:HG23	2.02	0.59
4:AD:308:ARG:HD3	7:AG:27:PHE:CE2	2.38	0.59
5:Ae:132:VAL:HA	5:Ae:135:GLN:NE2	2.17	0.59
5:Ai:62:ARG:HB2	5:Ai:78:PHE:C	2.28	0.59
3:AC:179:PHE:HE2	3:Ac:179:PHE:HE2	1.49	0.59
3:Ac:220:PHE:CE2	14:Ac:405:UQ6:H4M2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:215:LEU:CD1	15:Ad:401:HEC:CMB	2.73	0.59
1:AA:55:ASN:HB3	1:AA:226:ALA:HB1	1.84	0.59
1:Aa:279:ASP:OD1	7:Ag:12:ARG:NE	2.35	0.59
2:Ab:322:ASP:OD2	5:Ai:59:ALA:HB2	2.02	0.59
1:AA:120:LEU:HD23	2:AB:299:ILE:HG12	1.85	0.59
1:AA:172:MET:HE1	1:AA:205:SER:HA	1.84	0.59
4:AD:233:PHE:HA	4:AD:240:GLN:O	2.02	0.59
1:AA:113:VAL:CG1	2:AB:299:ILE:HD11	2.33	0.59
4:AD:248:ILE:HD11	15:AD:401:HEC:HBB1	1.85	0.59
7:AG:19:LEU:CD2	7:AG:24:GLN:HB3	2.29	0.59
2:Ab:104:GLU:HG3	5:Ai:70:LEU:HD21	1.84	0.59
4:Ad:106:ASP:O	4:Ad:110:ILE:HG13	2.03	0.59
4:Ad:321:TYR:HB2	6:Af:61:PHE:CD1	2.38	0.59
3:AC:345:HIS:CE1	3:AC:346:PRO:HB3	2.38	0.58
2:Ab:85:LEU:CD2	5:Ai:68:VAL:HG11	2.33	0.58
2:Ab:286:PHE:CE1	2:Ab:427:ALA:HB1	2.38	0.58
5:Ae:264:GLU:HB3	5:Ae:272:VAL:HB	1.85	0.58
7:AG:72:ARG:NH1	8:AH:67:GLU:HB2	2.18	0.58
1:Aa:118:ALA:O	2:Ab:298:HIS:CD2	2.55	0.58
2:Ab:312:SER:O	2:Ab:313:VAL:C	2.46	0.58
1:AA:285:ALA:O	1:AA:360:CYS:N	2.36	0.58
5:AE:152:ILE:HD13	5:AE:169:TRP:CD1	2.38	0.58
6:AF:106:GLU:O	6:AF:110:LYS:HG3	2.03	0.58
10:AK:37:ASP:O	10:AK:39:ARG:HG3	2.03	0.58
10:AK:10:TYR:CD1	6:Af:110:LYS:HA	2.38	0.58
4:Ad:156:ASP:HB2	4:Ad:167:ARG:HG3	1.85	0.58
5:Ae:159:ILE:O	5:Ae:210:TRP:HH2	1.86	0.58
5:AE:156:LEU:HD13	5:AE:210:TRP:NE1	2.19	0.58
5:Ae:146:VAL:HA	5:Ae:149:MET:HE3	1.86	0.58
5:Ae:163:LYS:O	5:Ae:177:ARG:HG3	2.03	0.58
7:Ag:11:ILE:HG22	7:Ag:12:ARG:N	2.18	0.58
5:AE:160:PRO:O	5:AE:178:HIS:HB3	2.03	0.58
1:Aa:92:PHE:HD1	1:Aa:168:ILE:HD12	1.66	0.58
1:Aa:172:MET:HE1	1:Aa:205:SER:HA	1.85	0.58
3:Ac:345:HIS:CE1	3:Ac:346:PRO:HB3	2.38	0.58
5:Ae:156:LEU:HB2	5:Ae:269:ASP:CA	2.34	0.58
4:AD:218:TYR:CG	4:AD:246:PRO:HG3	2.38	0.58
5:AE:156:LEU:HB2	5:AE:269:ASP:C	2.28	0.58
8:AH:58:ARG:HD3	8:AH:61:THR:HB	1.86	0.58
5:Ae:160:PRO:O	5:Ae:178:HIS:HB3	2.03	0.58
1:AA:220:LEU:O	1:AA:224:TYR:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:11:ILE:HG22	7:AG:12:ARG:N	2.18	0.58
1:Aa:220:LEU:O	1:Aa:224:TYR:HB2	2.04	0.58
1:Aa:251:SER:O	1:Aa:252:SER:HB3	2.02	0.58
3:Ac:138:MET:HE1	3:Ac:268:ILE:CA	2.31	0.58
4:Ad:152:VAL:HG21	4:Ad:176:PRO:CG	2.34	0.58
1:AA:286:HIS:CD2	1:AA:359:VAL:HG13	2.38	0.58
1:AA:295:GLY:O	1:AA:301:ASN:ND2	2.35	0.58
5:AE:159:ILE:O	5:AE:210:TRP:HH2	1.86	0.58
10:Ak:39:ARG:HH22	10:Ak:50:GLY:H	1.52	0.58
8:AH:49:GLU:HA	8:AH:52:ASP:OD2	2.04	0.58
1:Aa:70:THR:O	1:Aa:410:CYS:SG	2.60	0.58
1:Aa:171:GLU:O	1:Aa:175:ASN:N	2.37	0.58
2:Ab:170:GLN:HB2	5:Ai:78:PHE:CZ	2.39	0.58
5:Ae:88:PHE:O	5:Ae:92:ARG:HG3	2.04	0.58
7:AG:35:ILE:HB	7:AG:36:PRO:HD3	1.86	0.57
1:Aa:87:ASN:HD21	1:Aa:199:GLN:HB2	1.69	0.57
3:Ac:150:LEU:HD13	3:Ac:164:ILE:HD12	1.86	0.57
1:AA:171:GLU:O	1:AA:175:ASN:N	2.37	0.57
2:Ab:47:LEU:HA	2:Ab:218:MET:O	2.04	0.57
3:AC:150:LEU:HD13	3:AC:164:ILE:HD12	1.86	0.57
4:AD:120:VAL:O	15:AD:401:HEC:HMC3	2.04	0.57
1:Aa:338:CYS:HB2	1:Aa:368:MET:SD	2.45	0.57
4:Ad:104:SER:HB2	4:Ad:283:ASP:CG	2.29	0.57
4:AD:249:TYR:CE2	4:AD:252:VAL:HA	2.39	0.57
6:AF:107:GLU:OE2	6:AF:111:LYS:HD3	2.05	0.57
11:Aa:501:3PE:H32	3:Ac:221:HIS:CE1	2.40	0.57
3:Ac:147:THR:HG21	3:Ac:165:TRP:CD1	2.40	0.57
8:Ah:58:ARG:HD3	8:Ah:61:THR:HB	1.86	0.57
2:AB:162:LYS:NZ	2:AB:194:ASP:OD1	2.38	0.57
4:AD:284:HIS:NE2	4:AD:288:MET:HE3	2.19	0.57
1:Aa:120:LEU:HD23	2:Ab:299:ILE:HG23	1.86	0.57
4:Ad:120:VAL:O	15:Ad:401:HEC:HMC3	2.04	0.57
5:Ae:93:ARG:HD2	5:Ae:110:ARG:HD2	1.85	0.57
7:Ag:27:PHE:HB3	7:Ag:30:TYR:HB2	1.87	0.57
9:Aj:11:TYR:CZ	9:Aj:16:ARG:HB2	2.39	0.57
1:AA:87:ASN:HD21	1:AA:199:GLN:HB2	1.69	0.57
2:AB:322:ASP:OD2	5:AI:59:ALA:CB	2.53	0.57
4:Ad:213:SER:HB3	4:Ad:236:TYR:CD2	2.40	0.57
8:Ah:49:GLU:HA	8:Ah:52:ASP:OD2	2.04	0.57
5:AE:207:LYS:HB3	5:AE:209:GLU:OE1	2.05	0.57
2:Ab:51:SER:HB2	2:Ab:230:LEU:CD1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:297:PRO:CA	2:Ab:304:ASN:OD1	2.52	0.57
4:Ad:249:TYR:CE2	4:Ad:252:VAL:HA	2.40	0.57
3:AC:147:THR:HG21	3:AC:165:TRP:CD1	2.40	0.57
3:AC:378:LYS:HE3	6:AF:89:PHE:HE2	1.69	0.57
3:Ac:21:LEU:HD13	14:Ac:405:UQ6:O2	2.05	0.57
6:Af:107:GLU:OE2	6:Af:111:LYS:HD3	2.05	0.57
1:AA:338:CYS:HB2	1:AA:368:MET:SD	2.45	0.57
4:Ad:98:HIS:HB3	4:Ad:105:LEU:HD23	1.87	0.57
5:Ae:156:LEU:HD13	5:Ae:210:TRP:NE1	2.19	0.57
10:Ak:10:TYR:HA	10:Ak:13:LEU:HD12	1.87	0.57
7:AG:33:LYS:C	7:AG:36:PRO:HD2	2.30	0.56
5:Ae:218:THR:HG21	5:Ae:256:LEU:C	2.30	0.56
1:Aa:222:ARG:CZ	1:Aa:263:PRO:HB3	2.35	0.56
1:AA:68:THR:HG22	1:AA:136:LEU:CD2	2.35	0.56
3:AC:171:ASP:CG	3:AC:172:LYS:H	2.13	0.56
5:AE:219:HIS:HB2	5:AE:254:ALA:HA	1.88	0.56
6:AF:22:TYR:CD2	6:AF:84:TYR:HB2	2.41	0.56
10:AK:10:TYR:HA	10:AK:13:LEU:HD12	1.87	0.56
1:Aa:384:THR:HG21	10:Ak:9:ARG:HG2	1.87	0.56
3:Ac:141:TRP:CD1	3:Ac:265:PRO:HD2	2.41	0.56
3:Ac:171:ASP:CG	3:Ac:172:LYS:H	2.13	0.56
6:Af:22:TYR:CD2	6:Af:84:TYR:HB2	2.41	0.56
10:Ak:6:LEU:HD12	10:Ak:11:ARG:HH12	1.71	0.56
3:AC:18:PHE:CD1	14:AC:406:UQ6:H1M2	2.40	0.56
3:AC:264:THR:CG2	5:Ae:225:ILE:CD1	2.70	0.56
5:AE:152:ILE:HG13	5:AE:154:ILE:CD1	2.35	0.56
5:AE:218:THR:HG21	5:AE:256:LEU:C	2.30	0.56
1:Aa:186:TYR:CE1	5:Ae:80:HIS:HB2	2.40	0.56
2:Ab:300:LYS:HG2	2:Ab:301:ARG:HG3	1.86	0.56
1:AA:190:THR:CG2	1:AA:275:ILE:HG22	2.36	0.56
1:AA:280:ASP:OD2	7:AG:10:ARG:HA	2.05	0.56
2:AB:297:PRO:CA	2:AB:304:ASN:OD1	2.52	0.56
3:AC:9:PRO:O	3:AC:12:LYS:HB3	2.05	0.56
3:AC:56:THR:HG21	3:Ac:58:ASP:HB2	1.86	0.56
2:Ab:162:LYS:NZ	2:Ab:194:ASP:OD1	2.38	0.56
5:AE:197:ASP:HB3	5:AE:257:ASN:OD1	2.06	0.56
6:Af:15:ASP:OD2	6:Af:19:LYS:NZ	2.39	0.56
7:Ag:33:LYS:C	7:Ag:36:PRO:HD2	2.30	0.56
4:AD:213:SER:HB3	4:AD:236:TYR:CD2	2.40	0.56
7:AG:27:PHE:HB3	7:AG:30:TYR:HB2	1.87	0.56
3:Ac:128:PHE:CD1	13:Ac:404:U10:H4M2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:35:ILE:HB	7:Ag:36:PRO:HD3	1.86	0.56
1:AA:407:THR:O	1:AA:408:PRO:C	2.46	0.56
2:AB:51:SER:HB2	2:AB:230:LEU:CD1	2.33	0.56
2:AB:300:LYS:HG2	2:AB:301:ARG:HG3	1.86	0.56
10:AK:45:VAL:HG11	10:AK:48:ILE:HG22	1.88	0.56
1:Aa:58:ARG:HD2	1:Aa:417:LEU:HD12	1.88	0.56
4:Ad:116:VAL:HA	4:Ad:253:LEU:HD21	1.88	0.56
2:AB:236:GLN:HG3	2:AB:237:PHE:CD2	2.41	0.56
3:AC:211:LEU:HD21	6:AF:37:THR:HA	1.87	0.56
7:Ag:78:TYR:CE1	8:Ah:63:GLU:HG3	2.41	0.56
4:AD:215:LEU:CD1	15:AD:401:HEC:CMB	2.73	0.56
4:AD:295:MET:HG2	9:AJ:36:PHE:CZ	2.41	0.56
5:AE:156:LEU:HD22	5:AE:210:TRP:CE2	2.41	0.56
5:AE:177:ARG:HB3	5:AE:211:VAL:HG13	1.88	0.56
10:AK:9:ARG:NH1	10:AK:13:LEU:HD11	2.21	0.56
3:Ac:153:ILE:HB	3:Ac:157:GLY:CA	2.36	0.56
5:Ae:191:GLU:H	5:Ae:191:GLU:CD	2.14	0.56
5:Ae:207:LYS:HB3	5:Ae:209:GLU:OE1	2.05	0.56
5:Ae:219:HIS:HB2	5:Ae:254:ALA:HA	1.88	0.56
10:Ak:9:ARG:NH1	10:Ak:13:LEU:HD11	2.20	0.56
1:AA:183:VAL:HG21	1:AA:286:HIS:HB2	1.88	0.55
2:AB:167:GLN:HE22	5:AI:46:LYS:HA	1.71	0.55
2:AB:366:LEU:HD21	2:AB:425:VAL:HG22	1.87	0.55
3:AC:277:ALA:HB1	13:AC:405:U10:H1M2	1.87	0.55
5:AE:248:ARG:HA	5:AE:257:ASN:CG	2.32	0.55
1:Aa:50:VAL:HG11	1:Aa:417:LEU:HD11	1.89	0.55
3:Ac:97:HIS:CE1	3:Ac:100:ARG:HH21	2.24	0.55
5:AE:132:VAL:O	5:AE:135:GLN:HG2	2.06	0.55
5:Ae:122:THR:HG21	9:Aj:25:ILE:HD13	1.88	0.55
9:Aj:46:HIS:HA	9:Aj:49:GLU:CG	2.35	0.55
4:Ad:245:ALA:O	4:Ad:246:PRO:C	2.49	0.55
4:Ad:284:HIS:NE2	4:Ad:288:MET:HE3	2.20	0.55
5:Ae:156:LEU:HD22	5:Ae:210:TRP:CE2	2.42	0.55
5:Ae:177:ARG:HB3	5:Ae:211:VAL:HG13	1.88	0.55
3:AC:153:ILE:HB	3:AC:157:GLY:CA	2.37	0.55
4:AD:215:LEU:CD1	15:AD:401:HEC:HMB3	2.36	0.55
4:AD:222:PRO:O	4:AD:225:VAL:HG12	2.06	0.55
4:AD:253:LEU:HD12	4:AD:253:LEU:C	2.32	0.55
6:AF:15:ASP:OD2	6:AF:19:LYS:NZ	2.39	0.55
4:AD:321:TYR:HB2	6:AF:61:PHE:CE1	2.42	0.55
11:Ac:403:3PE:H12	16:Ag:101:CDL:OB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:152:ILE:HD13	5:AE:169:TRP:CG	2.42	0.55
8:AH:58:ARG:CD	8:AH:61:THR:HB	2.36	0.55
2:Ab:60:ARG:HG3	2:Ab:124:GLU:HB3	1.89	0.55
2:Ab:366:LEU:HD21	2:Ab:425:VAL:HG22	1.87	0.55
4:Ad:222:PRO:O	4:Ad:225:VAL:HG12	2.06	0.55
4:Ad:253:LEU:C	4:Ad:253:LEU:HD12	2.32	0.55
5:Ae:132:VAL:O	5:Ae:135:GLN:HG2	2.06	0.55
3:AC:97:HIS:CE1	3:AC:100:ARG:HH21	2.23	0.55
3:AC:268:ILE:HG13	5:Ae:238:CYS:SG	2.46	0.55
1:Aa:168:ILE:O	1:Aa:171:GLU:HG2	2.06	0.55
4:Ad:215:LEU:CD1	15:Ad:401:HEC:HMB3	2.36	0.55
2:AB:262:ASN:HA	2:Ab:195:TYR:CD1	2.42	0.55
11:Aa:501:3PE:H32	3:Ac:221:HIS:HE1	1.71	0.55
3:Ac:14:ILE:HG22	3:Ac:19:ILE:HG13	1.88	0.55
3:Ac:197:LEU:HD11	12:Ac:402:HEM:HMA1	1.89	0.55
5:Ae:192:VAL:HA	5:Ae:195:LEU:CD1	2.37	0.55
6:AF:102:ARG:HH21	6:AF:103:LYS:HE3	1.72	0.55
10:AK:6:LEU:HD12	10:AK:11:ARG:HH12	1.71	0.55
2:Ab:300:LYS:HG2	2:Ab:301:ARG:CG	2.37	0.55
8:Ah:58:ARG:CD	8:Ah:61:THR:HB	2.36	0.55
2:Ab:39:GLU:HB2	2:Ab:227:HIS:HD1	1.70	0.55
5:Ae:125:VAL:HG21	17:Ae:301:PC1:C36	2.37	0.55
5:Ae:248:ARG:HA	5:Ae:257:ASN:CG	2.32	0.55
9:Aj:11:TYR:HA	9:Aj:15:PHE:HB2	1.89	0.55
1:AA:87:ASN:H	1:AA:207:ASN:HD22	1.53	0.54
1:AA:118:ALA:O	2:AB:298:HIS:CD2	2.60	0.54
3:AC:183:PHE:CD1	3:Ac:183:PHE:CD1	2.94	0.54
2:Ab:236:GLN:HG3	2:Ab:237:PHE:CD2	2.41	0.54
3:Ac:264:THR:HG23	3:Ac:268:ILE:HD11	1.89	0.54
5:Ae:195:LEU:HD11	5:Ae:248:ARG:HH11	1.72	0.54
5:Ai:72:VAL:HG23	5:Ai:73:PRO:HD3	1.88	0.54
3:AC:30:TRP:HB3	3:AC:100:ARG:HD3	1.90	0.54
5:AI:72:VAL:HG23	5:AI:73:PRO:HD3	1.88	0.54
1:Aa:53:LEU:HD11	1:Aa:57:LEU:HD23	1.89	0.54
4:Ad:235:PRO:HA	4:Ad:240:GLN:HG3	1.89	0.54
1:AA:168:ILE:O	1:AA:171:GLU:HG2	2.06	0.54
1:AA:186:TYR:CE1	5:AE:80:HIS:HB2	2.43	0.54
3:AC:346:PRO:HG3	7:AG:66:GLU:HG2	1.89	0.54
5:AE:161:GLU:HA	5:AE:178:HIS:CD2	2.43	0.54
1:Aa:87:ASN:H	1:Aa:207:ASN:HD22	1.53	0.54
2:Ab:177:LEU:HD11	2:Ab:272:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:312:GLN:HE21	6:Af:37:THR:CB	2.21	0.54
1:AA:281:ALA:HB2	7:AG:10:ARG:HH22	1.71	0.54
3:AC:287:LYS:HZ1	5:Ae:255:PRO:HG2	1.72	0.54
5:AE:195:LEU:HD11	5:AE:248:ARG:HH11	1.72	0.54
5:AE:207:LYS:CD	5:AE:210:TRP:HD1	2.20	0.54
1:Aa:58:ARG:HH21	1:Aa:417:LEU:C	2.15	0.54
3:Ac:119:LEU:HD22	12:Ac:402:HEM:HBB2	1.88	0.54
3:Ac:140:PHE:CE2	3:Ac:261:PRO:HA	2.41	0.54
4:Ad:214:LEU:CD1	4:Ad:237:PHE:HB2	2.38	0.54
5:Ae:197:ASP:HB3	5:Ae:257:ASN:OD1	2.06	0.54
5:Ai:43:LEU:O	5:Ai:44:ASP:C	2.51	0.54
3:AC:222:PRO:HG2	3:AC:223:TYR:CD2	2.43	0.54
5:AE:152:ILE:HG13	5:AE:154:ILE:HD11	1.89	0.54
5:AE:190:VAL:HG11	5:AE:195:LEU:HD21	1.90	0.54
7:AG:39:LEU:O	7:AG:42:THR:HG22	2.08	0.54
4:Ad:308:ARG:HD3	7:Ag:27:PHE:CE2	2.43	0.54
6:Af:102:ARG:HH21	6:Af:103:LYS:HE3	1.72	0.54
5:AE:136:PHE:O	5:AE:137:VAL:C	2.51	0.54
5:AE:153:GLU:C	5:AE:154:ILE:HD12	2.32	0.54
1:Aa:384:THR:HA	10:Ak:12:GLU:CD	2.33	0.54
3:Ac:211:LEU:HD21	6:Af:37:THR:HA	1.89	0.54
7:Ag:39:LEU:O	7:Ag:42:THR:HG22	2.08	0.54
1:AA:136:LEU:HD21	2:AB:380:ALA:HA	1.90	0.54
3:AC:277:ALA:CB	13:AC:405:U10:H1M2	2.37	0.54
4:AD:116:VAL:HG22	4:AD:253:LEU:HD21	1.89	0.54
5:AE:122:THR:HG21	9:AJ:25:ILE:HG21	1.90	0.54
1:Aa:68:THR:HG21	2:Ab:384:MET:HG3	1.89	0.54
4:Ad:300:LEU:HG	16:Ag:102:CDL:H552	1.89	0.54
5:Ae:136:PHE:O	5:Ae:137:VAL:C	2.51	0.54
3:AC:71:ARG:NH2	4:AD:277:ALA:O	2.40	0.54
3:AC:72:ASP:OD1	4:AD:133:ARG:NH2	2.38	0.54
3:AC:163:TRP:HZ2	5:Ae:140:MET:HE1	1.73	0.54
4:AD:214:LEU:CD1	4:AD:237:PHE:HB2	2.38	0.54
1:Aa:183:VAL:HG21	1:Aa:286:HIS:HB2	1.90	0.54
10:Ak:45:VAL:HB	10:Ak:48:ILE:HB	1.88	0.54
1:AA:118:ALA:O	2:AB:298:HIS:HB3	2.08	0.54
2:AB:60:ARG:CZ	2:AB:390:GLU:HB3	2.37	0.54
3:Ac:117:VAL:HG21	3:Ac:302:ALA:HB2	1.89	0.54
3:Ac:222:PRO:HG2	3:Ac:223:TYR:CD2	2.43	0.54
6:Af:24:ALA:O	7:Ag:48:ARG:NH2	2.38	0.54
2:AB:60:ARG:HG3	2:AB:124:GLU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:191:GLU:CD	5:AE:191:GLU:H	2.14	0.54
2:Ab:50:ALA:HB3	2:Ab:221:VAL:HG22	1.90	0.54
1:AA:255:ARG:O	1:AA:255:ARG:CG	2.51	0.53
2:AB:50:ALA:HB3	2:AB:221:VAL:HG22	1.90	0.53
2:AB:300:LYS:HG2	2:AB:301:ARG:CG	2.37	0.53
3:AC:18:PHE:HE1	14:AC:406:UQ6:C8	2.20	0.53
3:AC:377:LEU:HB3	6:AF:34:ARG:HD2	1.90	0.53
4:AD:116:VAL:HA	4:AD:253:LEU:HD21	1.88	0.53
1:Aa:258:GLU:H	1:Aa:258:GLU:CD	2.16	0.53
3:Ac:164:ILE:O	3:Ac:177:ARG:HD2	2.08	0.53
4:Ad:255:TYR:HB3	4:Ad:257:ASP:OD1	2.08	0.53
5:Ae:161:GLU:HA	5:Ae:178:HIS:CD2	2.43	0.53
5:AE:204:ARG:HB3	5:AE:260:VAL:CG2	2.25	0.53
6:AF:110:LYS:O	10:Ak:8:PRO:HD2	2.08	0.53
4:Ad:116:VAL:HG22	4:Ad:253:LEU:HD21	1.89	0.53
2:Ab:167:GLN:HG3	5:Ai:43:LEU:HD13	1.86	0.53
6:Af:108:TRP:HA	6:Af:111:LYS:HZ2	1.72	0.53
3:AC:128:PHE:CE1	13:AC:405:U10:H4M2	2.43	0.53
11:AC:404:3PE:H12	16:AG:101:CDL:OB3	2.08	0.53
4:AD:321:TYR:HB2	6:AF:61:PHE:CG	2.43	0.53
5:AE:192:VAL:HA	5:AE:195:LEU:CD1	2.37	0.53
6:Af:53:GLU:OE2	7:Ag:12:ARG:NH1	2.41	0.53
10:Ak:14:ALA:O	10:Ak:18:ILE:HG12	2.08	0.53
1:AA:393:ASN:HB3	2:AB:106:VAL:O	2.08	0.53
3:Ac:30:TRP:HB3	3:Ac:100:ARG:HD3	1.90	0.53
3:Ac:223:TYR:CE1	4:Ad:314:LEU:HG	2.44	0.53
2:AB:237:PHE:O	2:AB:238:LEU:HB2	2.07	0.53
2:AB:322:ASP:OD2	5:AI:59:ALA:HB3	2.08	0.53
3:AC:218:ILE:HG21	4:AD:314:LEU:HD11	1.91	0.53
3:Ac:141:TRP:NE1	3:Ac:263:ASN:O	2.40	0.53
5:Ae:207:LYS:CD	5:Ae:210:TRP:HD1	2.20	0.53
2:AB:148:ARG:NH2	6:Af:50:ARG:O	2.42	0.53
1:Aa:341:PHE:HE2	1:Aa:372:LEU:HD13	1.67	0.53
5:Ae:190:VAL:HG11	5:Ae:195:LEU:HD21	1.90	0.53
10:Ak:38:TRP:CD2	10:Ak:41:ILE:HD13	2.44	0.53
2:AB:117:GLU:OE2	2:AB:330:TYR:HB3	2.09	0.53
3:AC:164:ILE:O	3:AC:177:ARG:HD2	2.08	0.53
5:AE:207:LYS:HD2	5:AE:210:TRP:CD1	2.44	0.53
2:Ab:117:GLU:OE2	2:Ab:331:SER:N	2.30	0.53
2:Ab:180:VAL:HB	2:Ab:258:ILE:HG13	1.90	0.53
3:Ac:312:GLN:HE21	6:Af:37:THR:HB	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:228:ARG:HG2	4:Ad:231:LEU:HD12	1.91	0.53
5:Ae:115:TYR:HB3	9:Aj:21:PHE:HE1	1.74	0.53
1:AA:55:ASN:HB3	1:AA:226:ALA:CB	2.38	0.53
2:AB:348:GLY:HA2	2:AB:448:PRO:HD3	1.91	0.53
4:AD:255:TYR:HB3	4:AD:257:ASP:OD1	2.08	0.53
5:AI:62:ARG:HB2	5:AI:78:PHE:C	2.33	0.53
9:AJ:43:ILE:O	9:AJ:47:ILE:HG13	2.09	0.53
10:AK:8:PRO:HG2	6:Af:111:LYS:HA	1.91	0.53
2:Ab:226:SER:O	2:Ab:229:VAL:HG22	2.09	0.53
3:Ac:346:PRO:HG3	7:Ag:66:GLU:HG2	1.89	0.53
4:Ad:299:LEU:HD21	5:Ae:124:GLY:HA3	1.90	0.53
1:AA:341:PHE:HZ	1:AA:372:LEU:HD13	1.72	0.53
3:AC:18:PHE:HE1	14:AC:406:UQ6:C7	2.22	0.53
3:AC:170:VAL:HG23	3:AC:174:THR:CB	2.39	0.53
5:AE:180:THR:N	5:AE:183:GLU:HB2	2.23	0.53
6:AF:20:TRP:HZ2	11:AG:103:3PE:H3E1	1.73	0.53
3:Ac:265:PRO:O	3:Ac:268:ILE:HG13	2.08	0.53
4:Ad:152:VAL:HG22	4:Ad:153:GLU:N	2.24	0.53
4:Ad:290:LEU:O	4:Ad:294:LEU:HG	2.09	0.53
5:Ae:180:THR:N	5:Ae:183:GLU:HB2	2.23	0.53
3:AC:202:GLU:CD	3:Ac:9:PRO:HG3	2.34	0.52
4:AD:227:LEU:HD12	4:AD:227:LEU:C	2.34	0.52
4:AD:255:TYR:HH	4:AD:266:VAL:HA	1.74	0.52
11:Aa:501:3PE:H341	11:Aa:501:3PE:H222	1.91	0.52
2:Ab:47:LEU:HD12	2:Ab:218:MET:O	2.09	0.52
2:Ab:170:GLN:CB	5:Ai:78:PHE:CZ	2.92	0.52
3:Ac:28:SER:HB2	16:Ag:101:CDL:HA21	1.90	0.52
3:Ac:71:ARG:NH2	4:Ad:277:ALA:O	2.39	0.52
3:Ac:334:ILE:HD11	7:Ag:56:VAL:HG22	1.90	0.52
4:AD:248:ILE:CG2	4:AD:263:MET:HG3	2.40	0.52
3:Ac:378:LYS:HE3	6:Af:89:PHE:HE2	1.74	0.52
12:Ac:402:HEM:HBA1	14:Ac:405:UQ6:O4	2.10	0.52
4:Ad:262:THR:HG22	8:Ah:24:LEU:HG	1.91	0.52
1:Aa:191:ALA:O	1:Aa:271:THR:N	2.41	0.52
1:Aa:207:ASN:O	1:Aa:211:LEU:HG	2.09	0.52
2:Ab:138:LEU:CD2	2:Ab:238:LEU:HG	2.38	0.52
3:Ac:170:VAL:HG23	3:Ac:174:THR:CB	2.39	0.52
4:Ad:125:HIS:CE1	4:Ad:195:PRO:HD2	2.42	0.52
3:AC:346:PRO:O	3:AC:349:ILE:HG22	2.10	0.52
4:AD:228:ARG:HG2	4:AD:231:LEU:HD12	1.91	0.52
5:AE:127:TYR:HE1	9:AJ:33:GLU:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AK:14:ALA:O	10:AK:18:ILE:HG12	2.08	0.52
1:Aa:80:ARG:CD	1:Aa:265:LEU:HD11	2.39	0.52
4:Ad:155:GLN:HA	4:Ad:166:MET:HG2	1.90	0.52
1:AA:165:ARG:HE	1:AA:209:ARG:HA	1.74	0.52
3:AC:107:TYR:HB2	3:AC:305:PRO:HG3	1.92	0.52
3:AC:287:LYS:NZ	5:Ae:255:PRO:HG2	2.24	0.52
7:AG:73:LYS:NZ	8:AH:63:GLU:HG2	2.24	0.52
1:Aa:171:GLU:O	1:Aa:174:GLU:HG2	2.10	0.52
4:Ad:227:LEU:HD12	4:Ad:227:LEU:C	2.34	0.52
4:AD:112:ARG:HD3	4:AD:257:ASP:OD2	2.09	0.52
5:AI:43:LEU:O	5:AI:44:ASP:C	2.51	0.52
1:Aa:165:ARG:HE	1:Aa:209:ARG:HA	1.74	0.52
3:Ac:110:MET:CE	3:Ac:306:PHE:CE1	2.93	0.52
5:Ae:207:LYS:HD2	5:Ae:210:TRP:CD1	2.44	0.52
5:Ae:241:SER:OG	5:Ae:253:PRO:HD2	2.10	0.52
1:AA:279:ASP:OD1	7:AG:12:ARG:NE	2.42	0.52
2:AB:226:SER:O	2:AB:229:VAL:HG22	2.09	0.52
8:AH:51:CYS:SG	8:AH:54:ARG:NH2	2.83	0.52
1:Aa:70:THR:HG21	1:Aa:407:THR:HA	1.91	0.52
2:AB:325:ALA:O	5:AI:61:ALA:HB1	2.09	0.52
11:AC:404:3PE:H112	16:AG:101:CDL:PB2	2.49	0.52
5:AE:155:LYS:O	5:AE:158:ASP:HB2	2.09	0.52
6:AF:108:TRP:HA	6:AF:111:LYS:HZ2	1.75	0.52
10:AK:38:TRP:HE1	10:AK:40:LEU:HD12	1.74	0.52
3:Ac:20:ASP:O	3:Ac:21:LEU:C	2.52	0.52
2:AB:70:ARG:NH2	2:AB:332:ASP:OD2	2.42	0.52
2:AB:100:THR:HG23	5:AI:70:LEU:CD1	2.40	0.52
2:AB:170:GLN:HG3	2:AB:339:TYR:OH	2.10	0.52
5:AE:242:HIS:CD2	5:AE:251:LYS:HB3	2.45	0.52
4:Ad:215:LEU:HD21	15:Ad:401:HEC:C1B	2.40	0.52
5:AE:241:SER:OG	5:AE:253:PRO:HD2	2.10	0.51
3:AC:36:LEU:HD11	16:AG:102:CDL:H732	1.92	0.51
3:AC:221:HIS:O	3:AC:225:THR:HB	2.10	0.51
4:AD:138:VAL:HG11	4:AD:276:TRP:NE1	2.25	0.51
4:AD:213:SER:HB3	4:AD:236:TYR:CE2	2.46	0.51
5:AE:248:ARG:HG2	5:AE:257:ASN:ND2	2.25	0.51
6:AF:97:GLU:HA	6:AF:100:ARG:HH11	1.75	0.51
10:AK:45:VAL:HB	10:AK:48:ILE:HG22	1.91	0.51
2:Ab:173:ILE:HG21	2:Ab:339:TYR:HE1	1.75	0.51
5:Ae:155:LYS:O	5:Ae:158:ASP:HB2	2.10	0.51
1:AA:171:GLU:O	1:AA:174:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:225:LYS:HD2	1:AA:256:VAL:H	1.75	0.51
3:AC:150:LEU:HB2	3:AC:161:VAL:HG22	1.93	0.51
3:Ac:147:THR:HG21	3:Ac:165:TRP:NE1	2.25	0.51
4:Ad:248:ILE:CG2	4:Ad:263:MET:HG3	2.40	0.51
6:Af:97:GLU:HA	6:Af:100:ARG:HH11	1.75	0.51
1:AA:207:ASN:O	1:AA:211:LEU:HG	2.09	0.51
2:Ab:232:GLN:O	2:Ab:235:GLU:HG3	2.11	0.51
3:Ac:221:HIS:O	3:Ac:225:THR:HB	2.09	0.51
4:Ad:213:SER:HB3	4:Ad:236:TYR:CE2	2.46	0.51
8:Ah:51:CYS:SG	8:Ah:54:ARG:NH2	2.83	0.51
10:Ak:39:ARG:NH2	10:Ak:50:GLY:H	2.09	0.51
3:AC:140:PHE:CE1	3:AC:170:VAL:HG13	2.45	0.51
3:AC:238:ILE:HD12	16:AG:102:CDL:H772	1.92	0.51
4:AD:162:GLY:HA2	4:Ad:183:GLU:CB	2.40	0.51
6:AF:20:TRP:CZ2	11:AG:103:3PE:H3E1	2.45	0.51
1:Aa:148:ALA:HA	1:Aa:250:LEU:HD21	1.92	0.51
1:Aa:257:TYR:CZ	1:Aa:263:PRO:HD2	2.46	0.51
2:Ab:297:PRO:CA	2:Ab:304:ASN:CG	2.83	0.51
3:Ac:140:PHE:CE1	3:Ac:170:VAL:HG13	2.45	0.51
5:Ae:242:HIS:CD2	5:Ae:251:LYS:HB3	2.45	0.51
1:AA:73:VAL:HG23	1:AA:147:LEU:HD13	1.93	0.51
2:AB:167:GLN:HE21	5:AI:43:LEU:HB2	1.69	0.51
3:AC:107:TYR:HE1	3:AC:308:HIS:HB2	1.76	0.51
3:AC:327:ILE:HG23	11:AG:103:3PE:H2B1	1.91	0.51
5:AE:165:MET:O	5:AE:176:VAL:N	2.44	0.51
5:AE:196:ARG:HD2	5:AE:249:ILE:CG2	2.41	0.51
2:Ab:267:VAL:CG2	2:Ab:344:ALA:HA	2.41	0.51
3:Ac:100:ARG:HH12	12:Ac:402:HEM:CBD	2.23	0.51
3:Ac:277:ALA:HB1	13:Ac:404:U10:H1M2	1.93	0.51
3:Ac:346:PRO:O	3:Ac:349:ILE:HG22	2.10	0.51
4:Ad:112:ARG:HD3	4:Ad:257:ASP:OD2	2.09	0.51
4:AD:237:PHE:CG	4:AD:242:ILE:HB	2.46	0.51
4:AD:321:TYR:CD2	4:AD:323:PRO:HD3	2.44	0.51
9:AJ:22:ALA:HB1	10:AK:27:VAL:HG11	1.92	0.51
3:Ac:199:PHE:O	3:Ac:202:GLU:HG2	2.11	0.51
3:Ac:272:TRP:CE2	3:Ac:273:TYR:HD2	2.29	0.51
4:Ad:232:TYR:O	4:Ad:241:ALA:HA	2.10	0.51
5:Ae:184:ILE:HG21	5:Ae:208:PRO:HB3	1.93	0.51
3:AC:197:LEU:HD11	14:AC:406:UQ6:C6	2.41	0.51
4:AD:201:VAL:HG22	4:AD:278:SER:CB	2.41	0.51
5:Ae:248:ARG:HG2	5:Ae:257:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:50:VAL:HG11	1:AA:417:LEU:HD11	1.93	0.51
4:AD:160:ASP:C	4:AD:162:GLY:H	2.18	0.51
5:AE:238:CYS:SG	3:Ac:268:ILE:HD12	2.51	0.51
2:Ab:170:GLN:HG3	2:Ab:339:TYR:OH	2.11	0.51
2:Ab:237:PHE:O	2:Ab:238:LEU:HB2	2.11	0.51
4:Ad:244:MET:HB2	15:Ad:401:HEC:C1D	2.41	0.51
3:AC:147:THR:HG21	3:AC:165:TRP:NE1	2.25	0.51
1:Aa:53:LEU:HD12	1:Aa:57:LEU:HB3	1.92	0.51
1:Aa:259:GLU:C	1:Aa:261:ALA:N	2.65	0.51
3:Ac:28:SER:HB2	16:Ag:101:CDL:OA4	2.10	0.51
3:Ac:150:LEU:HB2	3:Ac:161:VAL:HG22	1.93	0.51
5:Ae:242:HIS:HD2	5:Ae:251:LYS:HB3	1.76	0.51
9:Aj:30:LEU:CD2	10:Ak:48:ILE:HG13	2.41	0.51
1:AA:148:ALA:HA	1:AA:250:LEU:HD21	1.92	0.50
1:AA:226:ALA:HB2	1:AA:253:VAL:HB	1.93	0.50
2:AB:261:GLN:HG3	2:Ab:195:TYR:OH	2.11	0.50
2:AB:429:LYS:HA	2:AB:432:VAL:HG12	1.93	0.50
2:Ab:227:HIS:HD2	2:Ab:231:LYS:HE2	1.76	0.50
3:Ac:291:VAL:O	3:Ac:295:ILE:HG12	2.11	0.50
4:Ad:201:VAL:HG22	4:Ad:278:SER:CB	2.41	0.50
1:AA:70:THR:HG21	1:AA:407:THR:HA	1.93	0.50
2:AB:305:THR:CG2	2:AB:306:THR:N	2.60	0.50
3:AC:334:ILE:HD12	11:AG:103:3PE:H2F2	1.92	0.50
4:AD:215:LEU:HD21	15:AD:401:HEC:C1B	2.40	0.50
1:Aa:117:GLY:CA	2:Ab:377:LYS:HG2	2.32	0.50
1:Aa:310:ILE:HG21	1:Aa:379:LEU:HD21	1.91	0.50
7:Ag:74:ASN:O	7:Ag:77:MET:HB3	2.11	0.50
2:AB:40:PHE:CZ	2:AB:406:TYR:HB2	2.46	0.50
2:AB:113:THR:OG1	5:AI:65:VAL:CG1	2.59	0.50
2:AB:174:ILE:HG21	5:AI:64:LEU:HD13	1.93	0.50
2:AB:425:VAL:HG12	2:AB:429:LYS:HZ1	1.76	0.50
4:AD:116:VAL:HA	4:AD:253:LEU:CD2	2.41	0.50
5:AE:127:TYR:CE1	9:AJ:33:GLU:HG3	2.46	0.50
5:AE:155:LYS:HA	5:AE:270:VAL:HG22	1.93	0.50
5:AE:242:HIS:HD2	5:AE:251:LYS:HB3	1.76	0.50
10:AK:37:ASP:O	10:AK:38:TRP:C	2.51	0.50
1:Aa:68:THR:O	1:Aa:406:THR:HG21	2.11	0.50
4:Ad:146:LYS:N	4:Ad:171:LEU:HD21	2.27	0.50
1:AA:127:GLU:OE2	1:AA:348:TYR:HB3	2.11	0.50
1:AA:478:LEU:HA	9:AJ:18:THR:HG21	1.93	0.50
2:AB:227:HIS:HD2	2:AB:231:LYS:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:214:LEU:HD12	4:AD:234:ASN:CG	2.36	0.50
4:AD:232:TYR:HD1	4:AD:242:ILE:O	1.93	0.50
5:AE:156:LEU:H	5:AE:270:VAL:HA	1.75	0.50
16:AG:101:CDL:HA32	16:AG:101:CDL:H512	1.93	0.50
1:Aa:73:VAL:HG23	1:Aa:147:LEU:HD13	1.93	0.50
1:Aa:101:THR:HG21	1:Aa:149:ASP:HB3	1.94	0.50
2:Ab:425:VAL:HG12	2:Ab:429:LYS:HZ1	1.76	0.50
4:Ad:154:VAL:HG11	4:Ad:173:ASP:OD1	2.11	0.50
5:Ae:196:ARG:HD2	5:Ae:249:ILE:CG2	2.40	0.50
2:AB:297:PRO:HB3	2:AB:304:ASN:ND2	2.25	0.50
3:AC:264:THR:HB	5:Ae:223:VAL:HB	1.92	0.50
3:AC:291:VAL:O	3:AC:295:ILE:HG12	2.11	0.50
4:AD:242:ILE:CD1	4:AD:244:MET:HE2	2.41	0.50
5:AE:93:ARG:HD2	5:AE:110:ARG:CD	2.38	0.50
6:AF:53:GLU:OE2	7:AG:12:ARG:NH1	2.45	0.50
2:Ab:429:LYS:HA	2:Ab:432:VAL:HG12	1.93	0.50
4:Ad:255:TYR:HH	4:Ad:266:VAL:HA	1.76	0.50
2:AB:375:LYS:NZ	2:AB:419:VAL:O	2.36	0.50
4:AD:91:PRO:HG3	4:AD:236:TYR:CD1	2.47	0.50
4:AD:323:PRO:HG2	4:AD:325:LYS:CD	2.41	0.50
1:Aa:393:ASN:O	1:Aa:397:ASN:ND2	2.44	0.50
2:Ab:297:PRO:HB3	2:Ab:304:ASN:ND2	2.26	0.50
3:Ac:72:ASP:OD1	4:Ad:133:ARG:NH1	2.45	0.50
3:Ac:140:PHE:HE1	3:Ac:170:VAL:HG13	1.77	0.50
2:AB:176:ASN:O	2:AB:258:ILE:HD11	2.12	0.50
2:AB:232:GLN:O	2:AB:235:GLU:HG3	2.11	0.50
2:AB:297:PRO:CA	2:AB:304:ASN:CG	2.83	0.50
1:Aa:400:VAL:CB	2:Ab:58:LEU:HG	2.40	0.50
2:Ab:267:VAL:HG23	2:Ab:344:ALA:HA	1.94	0.50
3:Ac:277:ALA:CB	13:Ac:404:U10:H1M2	2.42	0.50
4:Ad:91:PRO:HG3	4:Ad:236:TYR:CD1	2.47	0.50
3:AC:18:PHE:CZ	14:AC:406:UQ6:H1M2	2.45	0.50
3:AC:218:ILE:HB	3:AC:219:PRO:HD2	1.94	0.50
3:AC:294:LEU:CG	13:AC:405:U10:H1M3	2.41	0.50
3:AC:334:ILE:CD1	11:AG:103:3PE:H2F2	2.41	0.50
4:AD:249:TYR:O	4:AD:250:THR:C	2.55	0.50
5:AE:155:LYS:HZ3	5:AE:157:SER:HB3	1.76	0.50
5:AE:195:LEU:HD11	5:AE:248:ARG:NH1	2.26	0.50
1:Aa:55:ASN:O	1:Aa:227:PRO:HG3	2.11	0.50
4:Ad:181:ASN:HB2	4:Ad:182:PRO:HD2	1.94	0.50
5:Ae:165:MET:O	5:Ae:176:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:179:ARG:HA	5:Ae:183:GLU:OE1	2.12	0.50
1:AA:65:SER:O	1:AA:66:HIS:C	2.55	0.50
1:AA:101:THR:HG21	1:AA:149:ASP:HB3	1.94	0.50
4:Ad:167:ARG:CZ	4:Ad:170:LYS:HE2	2.42	0.50
4:Ad:214:LEU:HD12	4:Ad:234:ASN:CG	2.36	0.50
1:AA:405:GLY:C	1:AA:408:PRO:HD2	2.37	0.49
4:AD:155:GLN:HA	4:AD:165:PHE:O	2.12	0.49
5:AE:184:ILE:HG21	5:AE:208:PRO:HB3	1.93	0.49
1:Aa:400:VAL:CG1	2:Ab:58:LEU:HG	2.41	0.49
3:Ac:215:ALA:HB2	6:Af:60:MET:HE3	1.94	0.49
4:Ad:111:ARG:HG3	4:Ad:140:TYR:CE2	2.47	0.49
4:Ad:249:TYR:O	4:Ad:250:THR:C	2.55	0.49
5:Ae:152:ILE:HB	5:Ae:169:TRP:CD1	2.47	0.49
5:Ae:197:ASP:HB3	5:Ae:257:ASN:ND2	2.27	0.49
3:AC:141:TRP:CD1	3:AC:265:PRO:HD3	2.47	0.49
3:AC:199:PHE:CZ	3:Ac:10:LEU:HB2	2.47	0.49
1:AA:271:THR:HG23	7:AG:23:GLU:HG2	1.94	0.49
1:AA:361:ASP:N	1:AA:361:ASP:OD1	2.45	0.49
3:AC:140:PHE:HE1	3:AC:170:VAL:HG13	1.77	0.49
3:AC:220:PHE:HE2	14:AC:406:UQ6:H4M2	1.75	0.49
5:AE:153:GLU:HA	5:AE:272:VAL:HG12	1.93	0.49
1:Aa:53:LEU:HD12	1:Aa:57:LEU:HD23	1.94	0.49
2:AB:64:PHE:HZ	2:AB:394:SER:HA	1.77	0.49
3:AC:197:LEU:HD11	14:AC:406:UQ6:H72	1.93	0.49
6:AF:111:LYS:HA	10:Ak:8:PRO:HG2	1.93	0.49
1:Aa:338:CYS:SG	1:Aa:359:VAL:C	2.96	0.49
2:Ab:167:GLN:HG2	5:Ai:43:LEU:CD1	2.22	0.49
4:Ad:116:VAL:HA	4:Ad:253:LEU:CD2	2.41	0.49
5:Ae:195:LEU:HD11	5:Ae:248:ARG:NH1	2.26	0.49
2:AB:297:PRO:HB3	2:AB:304:ASN:OD1	2.12	0.49
2:AB:176:ASN:CA	2:AB:258:ILE:HD11	2.43	0.49
10:AK:48:ILE:HG12	10:AK:48:ILE:O	2.12	0.49
2:Ab:297:PRO:HB3	2:Ab:304:ASN:OD1	2.12	0.49
3:Ac:278:TYR:CZ	3:Ac:282:ARG:HD2	2.48	0.49
7:Ag:73:LYS:NZ	8:Ah:64:ASP:O	2.45	0.49
1:AA:338:CYS:SG	1:AA:359:VAL:C	2.96	0.49
7:AG:41:ARG:HH21	16:AG:101:CDL:PB2	2.35	0.49
7:AG:48:ARG:HE	11:AG:103:3PE:C31	2.26	0.49
4:Ad:214:LEU:HD21	4:Ad:242:ILE:HD12	1.94	0.49
5:Ae:184:ILE:CG2	5:Ae:208:PRO:HB3	2.42	0.49
3:AC:215:ALA:HA	7:AG:11:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:179:ARG:HA	5:AE:183:GLU:OE1	2.12	0.49
5:AE:184:ILE:CG2	5:AE:208:PRO:HB3	2.42	0.49
3:Ac:281:LEU:HD12	3:Ac:290:GLY:HA3	1.95	0.49
4:Ad:153:GLU:OE2	4:Ad:166:MET:SD	2.70	0.49
2:AB:47:LEU:CD2	2:AB:234:ALA:HB1	2.43	0.49
3:AC:187:PHE:CZ	12:AC:402:HEM:HBB1	2.47	0.49
4:AD:167:ARG:NH1	4:AD:169:GLY:HA2	2.28	0.49
2:Ab:346:ALA:HA	2:Ab:349:GLU:OE2	2.13	0.49
3:Ac:361:ILE:HA	3:Ac:365:LEU:HB2	1.95	0.49
5:Ae:153:GLU:C	5:Ae:154:ILE:HD12	2.38	0.49
7:Ag:73:LYS:HB3	8:Ah:67:GLU:CD	2.37	0.49
4:AD:200:ILE:HG12	15:AD:401:HEC:HMA3	1.95	0.49
1:Aa:339:GLN:HB3	5:Ai:45:VAL:HG22	1.95	0.49
11:Aa:501:3PE:O32	16:Aa:502:CDL:H312	2.13	0.49
5:AE:192:VAL:O	5:AE:195:LEU:HB2	2.13	0.48
3:Ac:141:TRP:HB3	3:Ac:268:ILE:HD11	1.95	0.48
3:Ac:218:ILE:HB	3:Ac:219:PRO:HD2	1.94	0.48
4:Ad:300:LEU:HB3	4:Ad:301:PRO:HD3	1.93	0.48
5:Ae:217:CYS:O	5:Ae:218:THR:C	2.56	0.48
9:Aj:34:ARG:HG3	10:Ak:47:TYR:CZ	2.49	0.48
16:Aa:502:CDL:H342	3:Ac:221:HIS:HD1	1.78	0.48
3:Ac:373:GLU:HG2	6:Af:21:TYR:OH	2.14	0.48
4:Ad:200:ILE:HG12	15:Ad:401:HEC:HMA3	1.95	0.48
4:Ad:302:LEU:O	4:Ad:305:ALA:N	2.44	0.48
5:Ae:204:ARG:O	5:Ae:260:VAL:HG11	2.13	0.48
5:Ae:263:TYR:HB3	5:Ae:273:VAL:HG22	1.94	0.48
3:AC:278:TYR:CZ	3:AC:282:ARG:HD2	2.48	0.48
1:Aa:361:ASP:OD1	1:Aa:361:ASP:N	2.45	0.48
2:Ab:388:THR:HG23	2:Ab:391:GLY:H	1.78	0.48
3:Ac:213:SER:HA	6:Af:67:LEU:HD11	1.94	0.48
4:Ad:131:ALA:HB2	4:Ad:174:TYR:CD2	2.48	0.48
5:Ae:192:VAL:O	5:Ae:195:LEU:HB2	2.13	0.48
2:AB:388:THR:HG23	2:AB:391:GLY:H	1.78	0.48
3:AC:163:TRP:CZ2	5:Ae:140:MET:CE	2.96	0.48
3:AC:266:PRO:O	5:Ae:237:PRO:HB2	2.13	0.48
2:Ab:109:LYS:O	2:Ab:123:VAL:HA	2.13	0.48
5:Ae:263:TYR:CA	5:Ae:273:VAL:HA	2.42	0.48
1:AA:80:ARG:NH2	1:AA:268:CYS:SG	2.87	0.48
1:AA:276:ARG:NH2	1:AA:465:LEU:O	2.38	0.48
3:AC:32:ASN:ND2	3:AC:228:ASP:OD1	2.47	0.48
3:AC:177:ARG:HB3	3:Ac:53:MET:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:185:LEU:HD23	3:AC:188:ILE:HD12	1.95	0.48
3:AC:270:PRO:HG3	13:AC:405:U10:O3	2.12	0.48
3:AC:304:MET:HA	3:AC:307:LEU:HD12	1.96	0.48
3:AC:361:ILE:HA	3:AC:365:LEU:HB2	1.95	0.48
5:AE:197:ASP:HB3	5:AE:257:ASN:ND2	2.27	0.48
1:Aa:80:ARG:HD3	1:Aa:265:LEU:HD11	1.96	0.48
1:Aa:393:ASN:HB3	2:Ab:106:VAL:O	2.14	0.48
2:Ab:43:LEU:HB3	2:Ab:44:PRO:HD2	1.95	0.48
3:Ac:96:LEU:HD23	11:Ac:403:3PE:H292	1.95	0.48
3:Ac:206:ASN:N	12:Ac:402:HEM:O2D	2.40	0.48
1:AA:113:VAL:HG13	2:AB:299:ILE:HD11	1.94	0.48
2:AB:109:LYS:O	2:AB:123:VAL:HA	2.14	0.48
16:AG:101:CDL:H511	16:AG:101:CDL:H112	1.95	0.48
3:Ac:32:ASN:ND2	3:Ac:228:ASP:OD1	2.47	0.48
5:Ae:143:SER:HB2	5:Ae:145:ASP:OD1	2.13	0.48
5:Ae:218:THR:OG1	5:Ae:254:ALA:HB1	2.13	0.48
1:AA:64:SER:OG	1:AA:235:GLY:HA2	2.13	0.48
2:AB:286:PHE:CZ	2:AB:427:ALA:HB1	2.49	0.48
3:AC:58:ASP:HB2	3:Ac:56:THR:CG2	2.44	0.48
3:AC:77:TRP:HZ2	4:AD:284:HIS:CD2	2.32	0.48
3:AC:237:LEU:HD22	4:AD:300:LEU:HD11	1.95	0.48
5:AE:143:SER:HB2	5:AE:145:ASP:OD1	2.13	0.48
5:AE:178:HIS:HD2	5:AE:179:ARG:N	2.11	0.48
5:AE:204:ARG:O	5:AE:260:VAL:HG11	2.13	0.48
5:AE:218:THR:OG1	5:AE:254:ALA:HB1	2.13	0.48
1:Aa:120:LEU:HD23	2:Ab:299:ILE:CG2	2.44	0.48
1:Aa:273:SER:HB2	7:Ag:18:SER:O	2.14	0.48
1:Aa:286:HIS:CD2	1:Aa:359:VAL:HG13	2.48	0.48
3:Ac:304:MET:HA	3:Ac:307:LEU:HD12	1.95	0.48
7:Ag:72:ARG:HD3	7:Ag:73:LYS:H	1.77	0.48
2:AB:177:LEU:HD11	2:AB:272:VAL:HG22	1.94	0.48
3:AC:327:ILE:HD11	11:AG:103:3PE:H272	1.96	0.48
5:AE:231:PHE:HD2	5:AE:250:ARG:NH1	2.11	0.48
5:AI:62:ARG:HB3	5:AI:63:PRO:HD2	1.96	0.48
1:Aa:274:GLU:HB2	1:Aa:468:TYR:HD1	1.79	0.48
2:Ab:90:THR:HG23	2:Ab:95:SER:HA	1.95	0.48
2:Ab:253:TYR:CE2	2:Ab:435:LYS:HG3	2.48	0.48
2:Ab:254:ARG:HG3	2:Ab:255:GLY:N	2.28	0.48
2:Ab:286:PHE:CZ	2:Ab:427:ALA:HB1	2.49	0.48
3:Ac:185:LEU:HD23	3:Ac:188:ILE:HD12	1.95	0.48
4:Ad:95:PRO:HG2	8:Ah:85:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:310:ILE:HG21	1:AA:379:LEU:HD21	1.96	0.48
1:AA:362:ALA:HB2	1:AA:461:PRO:HB2	1.95	0.48
3:AC:244:LEU:HA	4:AD:285:ARG:HD2	1.96	0.48
4:AD:242:ILE:HD11	4:AD:244:MET:HE2	1.95	0.48
3:Ac:153:ILE:HG23	3:Ac:154:PRO:HD2	1.96	0.48
4:Ad:179:TYR:HB3	4:Ad:184:ALA:HB3	1.96	0.48
5:Ae:176:VAL:HG13	5:Ae:212:ILE:HG12	1.95	0.48
7:Ag:78:TYR:CD2	8:Ah:63:GLU:HB2	2.49	0.48
2:AB:90:THR:HG23	2:AB:95:SER:HA	1.95	0.48
2:AB:173:ILE:HD11	2:AB:439:ALA:C	2.39	0.48
2:AB:261:GLN:O	2:Ab:195:TYR:CE1	2.67	0.48
3:AC:323:ILE:HD11	11:AG:103:3PE:H12	1.96	0.48
5:AE:217:CYS:O	5:AE:218:THR:C	2.57	0.48
6:AF:50:ARG:HD3	2:Ab:149:TRP:CE2	2.49	0.48
1:Aa:56:GLY:HA3	1:Aa:227:PRO:HA	1.96	0.48
2:Ab:167:GLN:HE21	5:Ai:43:LEU:CD1	2.27	0.48
7:Ag:11:ILE:CG2	7:Ag:12:ARG:N	2.77	0.48
7:Ag:29:SER:CB	7:Ag:32:SER:HB2	2.38	0.48
3:AC:281:LEU:HD12	3:AC:290:GLY:HA3	1.95	0.47
3:Ac:146:ILE:CD1	13:Ac:404:U10:C3	2.90	0.47
5:Ae:204:ARG:HB3	5:Ae:260:VAL:CG2	2.25	0.47
5:Ae:231:PHE:HD2	5:Ae:250:ARG:NH1	2.12	0.47
2:AB:64:PHE:CZ	2:AB:394:SER:HA	2.48	0.47
3:AC:272:TRP:HA	3:AC:275:LEU:HG	1.96	0.47
5:AE:176:VAL:HG13	5:AE:212:ILE:HG12	1.95	0.47
1:Aa:362:ALA:HB2	1:Aa:461:PRO:HB2	1.95	0.47
5:Ae:178:HIS:HD2	5:Ae:179:ARG:N	2.11	0.47
2:AB:312:SER:OG	2:AB:357:GLN:NE2	2.40	0.47
3:AC:297:SER:O	3:AC:300:ILE:HG22	2.13	0.47
8:AH:67:GLU:HG3	8:AH:68:GLU:N	2.30	0.47
10:AK:41:ILE:HD12	10:AK:41:ILE:N	2.29	0.47
1:AA:383:ALA:O	1:AA:442:ARG:NH1	2.48	0.47
9:AJ:31:PHE:CD1	10:AK:47:TYR:HD2	2.33	0.47
3:Ac:100:ARG:HH12	12:Ac:402:HEM:HBD2	1.79	0.47
3:Ac:297:SER:O	3:Ac:300:ILE:HG22	2.13	0.47
4:Ad:207:GLY:O	4:Ad:208:GLU:C	2.58	0.47
2:AB:306:THR:O	2:AB:307:SER:C	2.58	0.47
4:AD:259:THR:HG23	8:AH:89:LYS:HE2	1.95	0.47
3:Ac:152:ALA:CB	3:Ac:287:LYS:HD2	2.45	0.47
4:Ad:96:TRP:HD1	4:Ad:99:ARG:NH2	2.09	0.47
4:Ad:157:GLY:O	4:Ad:164:MET:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:26:ASP:O	8:Ah:27:PRO:C	2.58	0.47
1:AA:395:LEU:O	1:AA:399:LEU:HG	2.14	0.47
3:AC:18:PHE:CE1	14:AC:406:UQ6:H71	2.49	0.47
5:AE:156:LEU:HD12	5:AE:268:ASP:HA	1.95	0.47
7:AG:11:ILE:CG2	7:AG:12:ARG:N	2.77	0.47
1:Aa:152:GLN:O	1:Aa:153:ASN:HB2	2.15	0.47
1:Aa:341:PHE:HZ	1:Aa:372:LEU:CD1	2.28	0.47
12:Ac:402:HEM:HMA1	14:Ac:405:UQ6:O5	2.14	0.47
4:Ad:156:ASP:HB2	4:Ad:167:ARG:CG	2.43	0.47
1:AA:152:GLN:O	1:AA:153:ASN:HB2	2.15	0.47
4:AD:242:ILE:HG12	4:AD:244:MET:H	1.80	0.47
6:AF:29:LYS:HA	6:AF:81:TRP:CD1	2.50	0.47
10:AK:6:LEU:HD12	10:AK:11:ARG:NH1	2.30	0.47
1:Aa:152:GLN:OE1	1:Aa:253:VAL:HG22	2.14	0.47
3:Ac:294:LEU:O	3:Ac:297:SER:HB3	2.15	0.47
3:Ac:296:LEU:O	3:Ac:300:ILE:N	2.45	0.47
4:Ad:302:LEU:O	4:Ad:303:THR:C	2.56	0.47
5:Ae:88:PHE:C	5:Ae:92:ARG:HG3	2.40	0.47
5:Ae:156:LEU:HD11	5:Ae:265:PHE:CE1	2.50	0.47
5:Ae:166:ALA:HA	5:Ae:174:LEU:O	2.15	0.47
7:Ag:76:ALA:O	7:Ag:79:GLU:HG2	2.13	0.47
1:AA:102:LYS:HZ3	1:AA:153:ASN:HA	1.77	0.47
1:AA:463:GLU:OE1	7:AG:8:LEU:HB2	2.15	0.47
2:AB:100:THR:HG23	5:AI:70:LEU:HD11	1.97	0.47
3:AC:128:PHE:CD1	13:AC:405:U10:H4M2	2.50	0.47
3:AC:220:PHE:CE2	14:AC:406:UQ6:H4M2	2.50	0.47
3:AC:294:LEU:O	3:AC:297:SER:HB3	2.15	0.47
2:Ab:284:ASN:HB3	2:Ab:419:VAL:CG2	2.45	0.47
3:Ac:242:LEU:HD21	3:Ac:250:LEU:CD1	2.44	0.47
1:AA:390:ARG:HG3	2:AB:104:GLU:O	2.15	0.47
3:AC:16:HIS:NE2	3:AC:201:HIS:CD2	2.82	0.47
3:AC:140:PHE:CE1	3:AC:170:VAL:CG1	2.98	0.47
3:AC:245:PHE:CE1	4:AD:102:LEU:CD2	2.97	0.47
4:AD:160:ASP:C	4:AD:162:GLY:N	2.71	0.47
3:Ac:140:PHE:CE1	3:Ac:170:VAL:CG1	2.98	0.47
6:Af:83:LYS:HB3	6:Af:85:GLU:OE2	2.15	0.47
1:AA:120:LEU:HD23	2:AB:299:ILE:HG23	1.96	0.47
1:AA:287:VAL:HB	1:AA:358:PHE:CE2	2.50	0.47
3:AC:227:LYS:HG3	4:AD:307:LYS:HE3	1.97	0.47
4:AD:260:PRO:HD2	8:AH:89:LYS:HE3	1.97	0.47
9:AJ:34:ARG:HG2	10:AK:48:ILE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:31:PHE:CD1	16:Ag:102:CDL:H312	2.50	0.47
2:AB:284:ASN:HB3	2:AB:419:VAL:CG2	2.45	0.46
3:AC:182:HIS:HE1	12:AC:402:HEM:C4C	2.33	0.46
3:AC:221:HIS:NE2	11:AC:401:3PE:O12	2.46	0.46
3:AC:296:LEU:O	3:AC:300:ILE:N	2.45	0.46
5:AE:140:MET:CE	3:Ac:163:TRP:HZ2	2.28	0.46
5:AE:166:ALA:HA	5:AE:174:LEU:O	2.15	0.46
5:AE:231:PHE:CD2	5:AE:250:ARG:HG3	2.50	0.46
10:AK:45:VAL:CB	10:AK:48:ILE:HG22	2.45	0.46
1:Aa:383:ALA:O	1:Aa:442:ARG:NH1	2.48	0.46
3:Ac:128:PHE:CE1	13:Ac:404:U10:C4M	2.98	0.46
4:Ad:156:ASP:N	4:Ad:165:PHE:O	2.43	0.46
5:Ae:226:ALA:HB2	5:Ae:234:TYR:HE1	1.80	0.46
6:Af:85:GLU:CD	6:Af:85:GLU:H	2.24	0.46
1:AA:341:PHE:HZ	1:AA:372:LEU:CD1	2.28	0.46
3:AC:146:ILE:CD1	13:AC:405:U10:C3	2.91	0.46
3:AC:153:ILE:HG23	3:AC:154:PRO:HD2	1.96	0.46
4:AD:244:MET:HB2	15:AD:401:HEC:C4D	2.46	0.46
4:AD:318:LYS:HD2	5:AE:86:PRO:HB2	1.95	0.46
5:AE:156:LEU:HD11	5:AE:265:PHE:CE1	2.50	0.46
1:Aa:99:LYS:HD2	1:Aa:160:GLN:HE21	1.80	0.46
1:Aa:118:ALA:O	2:Ab:298:HIS:HD2	1.97	0.46
3:Ac:141:TRP:HB3	3:Ac:268:ILE:CD1	2.46	0.46
4:Ad:312:SER:O	4:Ad:313:VAL:C	2.59	0.46
5:Ae:93:ARG:HG2	7:Ag:23:GLU:O	2.15	0.46
5:Ae:246:SER:HB3	5:Ae:248:ARG:HE	1.79	0.46
6:Af:29:LYS:HA	6:Af:81:TRP:CD1	2.50	0.46
8:Ah:67:GLU:HG3	8:Ah:68:GLU:N	2.29	0.46
1:AA:118:ALA:O	2:AB:298:HIS:HD2	1.98	0.46
1:AA:169:LEU:HD11	1:AA:209:ARG:HG2	1.97	0.46
3:AC:100:ARG:HH12	12:AC:403:HEM:CGD	2.28	0.46
5:AE:205:VAL:HG12	5:AE:211:VAL:HG23	1.98	0.46
4:Ad:146:LYS:NZ	4:Ad:170:LYS:HA	2.30	0.46
5:Ae:231:PHE:CD2	5:Ae:250:ARG:HG3	2.50	0.46
2:AB:85:LEU:HD21	5:AI:68:VAL:HG11	1.97	0.46
2:AB:278:ILE:HB	2:AB:331:SER:HA	1.98	0.46
4:AD:290:LEU:CD2	9:AJ:44:TYR:HB2	2.46	0.46
9:AJ:31:PHE:HD1	10:AK:47:TYR:HD2	1.63	0.46
2:Ab:49:ILE:HD13	2:Ab:220:LEU:HB3	1.97	0.46
2:Ab:225:VAL:HG22	2:Ab:229:VAL:CG2	2.46	0.46
2:Ab:426:LYS:HA	2:Ab:429:LYS:HZ3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:49:LEU:HD22	3:Ac:184:ILE:HD13	1.97	0.46
3:AC:152:ALA:O	3:AC:153:ILE:C	2.58	0.46
5:AE:214:ILE:HG12	5:AE:261:PRO:HD3	1.98	0.46
5:AE:246:SER:HB3	5:AE:248:ARG:HE	1.79	0.46
3:Ac:326:TRP:CE2	7:Ag:49:VAL:HG22	2.50	0.46
4:Ad:309:HIS:CE1	7:Ag:21:PRO:HB2	2.50	0.46
1:AA:99:LYS:HD2	1:AA:160:GLN:HE21	1.80	0.46
2:AB:426:LYS:HA	2:AB:429:LYS:HZ3	1.79	0.46
2:AB:429:LYS:O	2:AB:432:VAL:HG12	2.16	0.46
3:AC:240:MET:C	4:AD:292:MET:HE2	2.41	0.46
4:AD:213:SER:O	4:AD:217:GLY:N	2.49	0.46
3:Ac:14:ILE:O	3:Ac:18:PHE:N	2.47	0.46
3:Ac:319:PRO:HB3	7:Ag:48:ARG:NH2	2.31	0.46
3:AC:17:SER:HB2	14:AC:406:UQ6:H1M3	1.98	0.46
3:AC:271:GLU:OE1	3:AC:273:TYR:OH	2.32	0.46
3:AC:312:GLN:HE21	6:AF:37:THR:CB	2.28	0.46
3:AC:334:ILE:HD11	7:AG:56:VAL:HG22	1.97	0.46
5:AE:154:ILE:O	5:AE:270:VAL:HG13	2.16	0.46
5:AE:265:PHE:CD1	5:AE:271:VAL:HB	2.51	0.46
6:AF:83:LYS:HB3	6:AF:85:GLU:OE2	2.15	0.46
5:AI:43:LEU:HD12	5:AI:46:LYS:NZ	2.31	0.46
4:Ad:223:THR:HG23	8:Ah:55:VAL:HG21	1.98	0.46
1:AA:168:ILE:HA	1:AA:171:GLU:HG2	1.98	0.46
3:AC:150:LEU:CD1	3:AC:164:ILE:HD12	2.46	0.46
9:AJ:11:TYR:HA	9:AJ:15:PHE:HB2	1.97	0.46
10:Ak:39:ARG:HH22	10:Ak:50:GLY:N	2.13	0.46
3:AC:265:PRO:CD	3:AC:268:ILE:HD11	2.43	0.46
4:AD:237:PHE:CD1	4:AD:238:PRO:HD2	2.51	0.46
5:AE:226:ALA:HB2	5:AE:234:TYR:HE1	1.80	0.46
1:Aa:74:TRP:CZ2	1:Aa:411:GLU:HA	2.51	0.46
1:Aa:340:SER:CB	5:Ai:45:VAL:HG11	2.45	0.46
4:Ad:144:GLU:O	4:Ad:147:ALA:HB3	2.16	0.46
9:Aj:43:ILE:O	9:Aj:47:ILE:HG13	2.16	0.46
3:AC:30:TRP:HZ3	3:AC:96:LEU:HD22	1.81	0.46
3:AC:163:TRP:CZ2	5:Ae:140:MET:HE1	2.51	0.46
4:AD:223:THR:HG21	8:AH:52:ASP:CA	2.30	0.46
9:AJ:30:LEU:CD1	10:AK:34:TRP:HB2	2.45	0.46
3:Ac:18:PHE:CE1	14:Ac:405:UQ6:H1M3	2.51	0.46
3:Ac:152:ALA:O	3:Ac:153:ILE:C	2.58	0.46
4:Ad:146:LYS:O	4:Ad:147:ALA:C	2.58	0.46
10:Ak:6:LEU:HD12	10:Ak:11:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:47:LEU:HD11	2:AB:238:LEU:HD13	1.99	0.45
5:AE:188:ALA:HA	5:AE:200:HIS:HE2	1.80	0.45
9:AJ:9:ARG:O	9:AJ:13:LEU:HD23	2.15	0.45
1:Aa:273:SER:O	1:Aa:455:ALA:HA	2.16	0.45
3:Ac:30:TRP:HZ3	3:Ac:96:LEU:HD22	1.81	0.45
3:Ac:138:MET:CE	3:Ac:268:ILE:HA	2.36	0.45
3:Ac:146:ILE:CD1	13:Ac:404:U10:H3M2	2.42	0.45
3:Ac:150:LEU:CD1	3:Ac:164:ILE:HD12	2.46	0.45
5:Ae:207:LYS:HE3	5:Ae:265:PHE:CG	2.51	0.45
5:Ae:231:PHE:CE2	5:Ae:250:ARG:HB3	2.51	0.45
5:Ai:65:VAL:C	5:Ai:76:VAL:HG23	2.41	0.45
1:AA:409:VAL:O	1:AA:410:CYS:C	2.58	0.45
5:AE:155:LYS:HZ3	5:AE:157:SER:CB	2.28	0.45
5:AE:264:GLU:HB3	5:AE:272:VAL:O	2.16	0.45
1:Aa:311:ILE:HG22	1:Aa:341:PHE:CE1	2.50	0.45
2:Ab:297:PRO:HA	2:Ab:304:ASN:ND2	2.28	0.45
3:Ac:312:GLN:HG2	6:Af:37:THR:O	2.16	0.45
4:Ad:321:TYR:HB2	6:Af:61:PHE:CG	2.51	0.45
1:AA:400:VAL:HG11	2:AB:57:PRO:HB2	1.97	0.45
4:AD:322:ARG:O	7:AG:13:HIS:HB3	2.16	0.45
5:AE:231:PHE:CE2	5:AE:250:ARG:HB3	2.51	0.45
1:Aa:64:SER:OG	1:Aa:235:GLY:HA2	2.16	0.45
1:Aa:168:ILE:HA	1:Aa:171:GLU:HG2	1.98	0.45
4:Ad:213:SER:O	4:Ad:217:GLY:N	2.49	0.45
5:Ae:188:ALA:HA	5:Ae:200:HIS:HE2	1.80	0.45
5:Ae:241:SER:OG	5:Ae:254:ALA:HB2	2.17	0.45
9:Aj:34:ARG:NH1	9:Aj:38:GLN:HB2	2.31	0.45
2:Ab:38:LEU:HA	2:Ab:51:SER:O	2.15	0.45
2:Ab:429:LYS:O	2:Ab:432:VAL:HG12	2.16	0.45
3:Ac:264:THR:O	3:Ac:265:PRO:C	2.58	0.45
3:Ac:377:LEU:HB3	6:Af:34:ARG:HD2	1.97	0.45
5:Ae:123:VAL:HG13	9:Aj:29:ALA:CA	2.43	0.45
5:Ae:155:LYS:HB3	5:Ae:158:ASP:OD2	2.17	0.45
5:Ae:267:SER:C	5:Ae:269:ASP:H	2.24	0.45
2:AB:171:THR:HG23	5:AI:64:LEU:HD23	1.98	0.45
2:AB:322:ASP:OD2	5:AI:59:ALA:HB2	2.17	0.45
10:AK:10:TYR:HE1	6:Af:110:LYS:CA	2.19	0.45
2:Ab:171:THR:HA	5:Ai:64:LEU:HD21	1.97	0.45
4:Ad:214:LEU:O	4:Ad:234:ASN:ND2	2.46	0.45
5:Ae:154:ILE:HD13	5:Ae:273:VAL:HG23	1.99	0.45
2:AB:225:VAL:HG22	2:AB:229:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:213:SER:HA	6:AF:67:LEU:HD11	1.98	0.45
5:AE:207:LYS:HE3	5:AE:265:PHE:CG	2.51	0.45
9:AJ:34:ARG:NH1	9:AJ:38:GLN:HB2	2.31	0.45
2:Ab:418:SER:O	2:Ab:419:VAL:C	2.59	0.45
5:Ae:205:VAL:HG12	5:Ae:211:VAL:HG23	1.97	0.45
5:Ae:214:ILE:HG12	5:Ae:261:PRO:HD3	1.98	0.45
1:AA:274:GLU:OE2	1:AA:276:ARG:NH1	2.45	0.45
2:AB:167:GLN:NE2	5:AI:43:LEU:CB	2.72	0.45
2:AB:180:VAL:HG21	2:AB:257:GLU:CA	2.46	0.45
2:AB:253:TYR:HE2	2:AB:435:LYS:HG3	1.82	0.45
3:AC:33:PHE:HE1	16:AG:102:CDL:H782	1.82	0.45
5:AE:155:LYS:HB3	5:AE:158:ASP:OD2	2.17	0.45
6:AF:85:GLU:H	6:AF:85:GLU:CD	2.24	0.45
1:Aa:393:ASN:HB3	2:Ab:106:VAL:C	2.42	0.45
2:Ab:43:LEU:HB2	2:Ab:45:ASN:OD1	2.17	0.45
3:Ac:137:GLN:HG3	3:Ac:265:PRO:HD3	1.98	0.45
7:Ag:12:ARG:HB3	7:Ag:13:HIS:CD2	2.52	0.45
1:AA:284:LEU:HD11	5:AI:44:ASP:O	2.16	0.45
3:AC:341:GLN:HE21	3:AC:342:PRO:HD2	1.82	0.45
4:AD:234:ASN:O	4:AD:235:PRO:C	2.59	0.45
5:AE:241:SER:OG	5:AE:254:ALA:HB2	2.17	0.45
7:AG:12:ARG:HB3	7:AG:13:HIS:CD2	2.52	0.45
5:AI:71:ASN:HB2	5:AI:73:PRO:HD2	1.97	0.45
1:Aa:74:TRP:HB3	1:Aa:418:LEU:HD11	1.98	0.45
2:Ab:167:GLN:HE21	5:Ai:43:LEU:HB2	1.66	0.45
5:Ai:71:ASN:HB2	5:Ai:73:PRO:HD2	1.97	0.45
3:AC:182:HIS:CE1	12:AC:402:HEM:C4C	3.05	0.45
3:AC:211:LEU:CD2	6:AF:37:THR:HA	2.47	0.45
5:AE:156:LEU:HD23	5:AE:156:LEU:HA	1.62	0.45
5:AE:178:HIS:CD2	5:AE:209:GLU:O	2.70	0.45
1:Aa:285:ALA:O	1:Aa:360:CYS:N	2.46	0.45
3:Ac:141:TRP:CD1	3:Ac:265:PRO:CD	3.00	0.45
3:Ac:341:GLN:HE21	3:Ac:342:PRO:HD2	1.82	0.45
17:Ae:301:PC1:H151	9:Aj:18:THR:OG1	2.17	0.45
10:Ak:23:MET:O	10:Ak:27:VAL:HG23	2.17	0.45
1:AA:373:GLN:NE2	1:AA:471:ILE:O	2.49	0.45
2:AB:39:GLU:HG3	2:AB:227:HIS:ND1	2.32	0.45
2:AB:297:PRO:HA	2:AB:304:ASN:ND2	2.28	0.45
1:Aa:127:GLU:OE2	1:Aa:348:TYR:HB3	2.16	0.45
3:Ac:218:ILE:HD11	3:Ac:224:TYR:CE2	2.52	0.45
4:Ad:259:THR:O	4:Ad:260:PRO:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:217:CYS:C	5:Ae:219:HIS:N	2.72	0.45
1:AA:286:HIS:ND1	1:AA:359:VAL:HG22	2.31	0.44
1:AA:467:ASP:OD2	3:AC:223:TYR:CE2	2.70	0.44
2:AB:418:SER:O	2:AB:419:VAL:C	2.59	0.44
6:AF:86:GLU:O	6:AF:87:ASP:C	2.60	0.44
10:AK:29:ALA:O	10:AK:33:VAL:HG23	2.18	0.44
1:Aa:169:LEU:HD11	1:Aa:209:ARG:HG2	1.97	0.44
2:Ab:155:ARG:HD2	2:Ab:198:GLY:H	1.83	0.44
5:Ae:178:HIS:CD2	5:Ae:209:GLU:O	2.70	0.44
5:Ae:201:ASP:OD1	5:Ae:202:LEU:N	2.50	0.44
6:Af:86:GLU:O	6:Af:87:ASP:C	2.60	0.44
1:AA:197:LEU:HD22	1:AA:268:CYS:SG	2.58	0.44
4:AD:207:GLY:O	4:AD:208:GLU:C	2.58	0.44
10:AK:23:MET:O	10:AK:27:VAL:HG23	2.16	0.44
1:Aa:340:SER:HB2	5:Ai:45:VAL:HG21	1.98	0.44
4:Ad:242:ILE:HG12	4:Ad:244:MET:H	1.82	0.44
3:AC:170:VAL:HG13	3:AC:170:VAL:O	2.16	0.44
3:AC:218:ILE:HD11	3:AC:224:TYR:CE2	2.52	0.44
5:AE:243:TYR:CD2	5:AE:258:LEU:HG	2.52	0.44
8:AH:26:ASP:O	8:AH:27:PRO:C	2.58	0.44
1:Aa:259:GLU:O	1:Aa:261:ALA:N	2.50	0.44
3:Ac:170:VAL:HG13	3:Ac:170:VAL:O	2.16	0.44
4:Ad:201:VAL:HG22	4:Ad:278:SER:OG	2.18	0.44
4:Ad:323:PRO:HG2	4:Ad:325:LYS:CG	2.47	0.44
2:AB:305:THR:O	2:AB:311:GLN:HG3	2.17	0.44
3:AC:256:TYR:OH	4:AD:202:ARG:NH1	2.50	0.44
5:AE:111:LYS:HE3	9:AJ:11:TYR:CZ	2.52	0.44
5:AE:140:MET:CE	3:Ac:163:TRP:CZ2	3.00	0.44
5:AE:154:ILE:HG22	5:AE:155:LYS:N	2.32	0.44
7:AG:38:VAL:HA	7:AG:41:ARG:HD3	1.99	0.44
1:Aa:78:GLY:H	1:Aa:81:TYR:HD2	1.65	0.44
2:Ab:138:LEU:CD1	2:Ab:233:VAL:HB	2.47	0.44
2:Ab:306:THR:O	2:Ab:307:SER:C	2.58	0.44
2:Ab:375:LYS:NZ	2:Ab:419:VAL:O	2.36	0.44
3:Ac:201:HIS:HE1	14:Ac:405:UQ6:C2	2.30	0.44
3:Ac:256:TYR:OH	4:Ad:202:ARG:NH1	2.50	0.44
3:Ac:294:LEU:CG	13:Ac:404:U10:H1M3	2.47	0.44
6:Af:20:TRP:HH2	11:Ag:103:3PE:O11	2.00	0.44
3:AC:223:TYR:CE1	4:AD:314:LEU:HG	2.52	0.44
5:AE:127:TYR:CD2	9:AJ:32:PHE:HE2	2.36	0.44
5:AE:178:HIS:NE2	5:AE:209:GLU:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:178:HIS:HA	5:AE:209:GLU:O	2.18	0.44
4:Ad:248:ILE:HD12	4:Ad:266:VAL:HG11	2.00	0.44
5:Ae:115:TYR:HB3	9:Aj:21:PHE:CE1	2.53	0.44
5:Ae:161:GLU:HA	5:Ae:178:HIS:HB3	2.00	0.44
5:Ae:178:HIS:HA	5:Ae:209:GLU:O	2.18	0.44
2:AB:297:PRO:CB	2:AB:304:ASN:CG	2.91	0.44
2:AB:312:SER:HA	2:AB:315:LYS:HE3	2.00	0.44
3:AC:264:THR:HG21	5:Ae:225:ILE:HD11	1.86	0.44
3:AC:373:GLU:HG2	6:AF:21:TYR:OH	2.17	0.44
4:AD:167:ARG:HH12	4:AD:170:LYS:H	1.65	0.44
5:AE:122:THR:O	5:AE:123:VAL:C	2.61	0.44
5:AE:161:GLU:HA	5:AE:178:HIS:HB3	2.00	0.44
1:Aa:479:ARG:O	10:Ak:20:THR:HG21	2.17	0.44
5:Ae:243:TYR:CD2	5:Ae:258:LEU:HG	2.52	0.44
10:Ak:48:ILE:O	10:Ak:49:ASN:C	2.59	0.44
1:AA:78:GLY:H	1:AA:81:TYR:HD2	1.65	0.44
5:AE:152:ILE:HG21	5:AE:273:VAL:HB	1.98	0.44
5:AE:161:GLU:HA	5:AE:178:HIS:CB	2.48	0.44
5:AE:168:LYS:HZ3	5:AE:171:GLY:HA2	1.83	0.44
5:AE:217:CYS:C	5:AE:219:HIS:N	2.72	0.44
1:Aa:463:GLU:OE1	7:Ag:8:LEU:HB2	2.17	0.44
4:Ad:144:GLU:O	4:Ad:148:LEU:HG	2.16	0.44
4:Ad:234:ASN:O	4:Ad:235:PRO:C	2.59	0.44
4:Ad:298:LEU:C	4:Ad:298:LEU:HD23	2.43	0.44
5:Ae:161:GLU:HA	5:Ae:178:HIS:CB	2.48	0.44
9:Aj:9:ARG:O	9:Aj:13:LEU:HD23	2.18	0.44
9:Aj:30:LEU:HD23	10:Ak:48:ILE:HG13	2.00	0.44
1:AA:110:GLU:HB2	2:AB:299:ILE:CD1	2.45	0.44
1:AA:338:CYS:SG	1:AA:358:PHE:HB2	2.58	0.44
1:AA:393:ASN:HB3	2:AB:106:VAL:C	2.43	0.44
5:AE:140:MET:HE1	3:Ac:163:TRP:HZ2	1.83	0.44
7:AG:25:ARG:NH2	7:AG:29:SER:H	2.16	0.44
11:AG:103:3PE:H372	11:AG:103:3PE:H3C2	2.00	0.44
1:Aa:110:GLU:HB2	2:Ab:299:ILE:CD1	2.47	0.44
1:Aa:373:GLN:NE2	1:Aa:471:ILE:O	2.49	0.44
7:Ag:19:LEU:HG	7:Ag:20:SER:N	2.33	0.44
1:AA:478:LEU:O	10:AK:24:TRP:CZ2	2.70	0.44
2:AB:411:THR:O	2:AB:414:GLN:HG2	2.18	0.44
3:AC:148:ASN:OD1	5:Ae:220:LEU:C	2.61	0.44
3:AC:245:PHE:CZ	4:AD:102:LEU:HD21	2.53	0.44
4:AD:112:ARG:HB3	4:AD:255:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:262:THR:O	4:AD:263:MET:C	2.61	0.44
4:AD:263:MET:HB3	8:AH:26:ASP:OD2	2.17	0.44
4:AD:321:TYR:HB2	6:AF:61:PHE:CZ	2.52	0.44
16:AG:101:CDL:O1	16:AG:101:CDL:HA4	2.18	0.44
1:Aa:222:ARG:NH1	1:Aa:263:PRO:HB3	2.32	0.44
2:Ab:38:LEU:HG	2:Ab:396:ILE:HD13	2.00	0.44
2:Ab:170:GLN:HB3	5:Ai:78:PHE:CE1	2.53	0.44
3:Ac:149:LEU:HG	3:Ac:291:VAL:HG22	2.00	0.44
3:Ac:243:VAL:O	3:Ac:247:PRO:HG3	2.18	0.44
4:Ad:100:GLY:O	4:Ad:101:LEU:C	2.61	0.44
4:Ad:323:PRO:HG2	4:Ad:325:LYS:HD2	2.00	0.44
2:AB:63:LEU:HD12	2:AB:220:LEU:HD13	2.00	0.43
2:AB:233:VAL:HA	2:AB:236:GLN:CG	2.47	0.43
2:AB:254:ARG:NH2	2:Ab:257:GLU:HG3	2.33	0.43
3:AC:99:GLY:HA3	11:AC:404:3PE:H272	2.00	0.43
3:AC:105:GLY:HA3	3:AC:313:ARG:O	2.18	0.43
4:AD:201:VAL:HG22	4:AD:278:SER:HB2	2.00	0.43
11:Aa:501:3PE:O32	16:Aa:502:CDL:H341	2.17	0.43
2:Ab:63:LEU:HD12	2:Ab:220:LEU:HD13	1.99	0.43
2:Ab:297:PRO:HB3	2:Ab:304:ASN:CG	2.43	0.43
3:Ac:120:LEU:HD23	3:Ac:298:ILE:HG23	2.00	0.43
3:Ac:137:GLN:NE2	3:Ac:263:ASN:O	2.50	0.43
6:Af:97:GLU:HA	6:Af:100:ARG:NH1	2.33	0.43
5:Ai:72:VAL:N	5:Ai:73:PRO:HD2	2.34	0.43
1:AA:225:LYS:HG3	1:AA:256:VAL:HG12	2.00	0.43
2:AB:138:LEU:CD1	2:AB:233:VAL:HB	2.47	0.43
3:AC:317:PHE:CD1	6:AF:27:PHE:HB3	2.53	0.43
4:AD:201:VAL:HG22	4:AD:278:SER:OG	2.18	0.43
5:AE:195:LEU:HD13	5:AE:248:ARG:HD2	1.99	0.43
2:Ab:230:LEU:O	2:Ab:233:VAL:HG22	2.19	0.43
3:Ac:317:PHE:HB3	6:Af:27:PHE:HD2	1.83	0.43
11:Ac:403:3PE:H262	11:Ac:403:3PE:H231	1.88	0.43
5:Ae:178:HIS:NE2	5:Ae:209:GLU:HB2	2.33	0.43
5:Ae:195:LEU:HD13	5:Ae:248:ARG:HD2	1.99	0.43
7:Ag:38:VAL:HA	7:Ag:41:ARG:HD3	1.99	0.43
2:AB:297:PRO:HB3	2:AB:304:ASN:CG	2.43	0.43
3:AC:248:ASP:OD2	4:AD:202:ARG:NH1	2.51	0.43
4:AD:214:LEU:O	4:AD:234:ASN:ND2	2.46	0.43
5:AE:155:LYS:HE2	5:AE:157:SER:HB3	1.99	0.43
5:AI:72:VAL:N	5:AI:73:PRO:HD2	2.34	0.43
1:Aa:279:ASP:HA	7:Ag:12:ARG:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:311:ILE:HG22	1:Aa:341:PHE:HE1	1.83	0.43
4:Ad:189:ASN:O	4:Ad:190:ASN:C	2.61	0.43
2:AB:180:VAL:HG21	2:AB:257:GLU:N	2.34	0.43
5:AE:235:TYR:CE1	5:AE:240:GLY:HA2	2.53	0.43
3:Ac:102:LEU:HD12	11:Ac:403:3PE:H2E1	1.99	0.43
3:Ac:120:LEU:CD2	3:Ac:298:ILE:HG23	2.49	0.43
4:Ad:112:ARG:HB3	4:Ad:255:TYR:CE1	2.53	0.43
3:AC:100:ARG:HH12	12:AC:403:HEM:HBD2	1.82	0.43
1:Aa:60:ALA:O	1:Aa:232:ALA:HA	2.18	0.43
2:Ab:130:ILE:HA	2:Ab:133:LEU:HB2	2.01	0.43
2:Ab:173:ILE:CG2	2:Ab:339:TYR:HE1	2.32	0.43
2:Ab:300:LYS:HE2	2:Ab:301:ARG:HH11	1.83	0.43
4:Ad:167:ARG:NH1	4:Ad:169:GLY:HA2	2.33	0.43
1:AA:175:ASN:C	1:AA:177:ALA:N	2.76	0.43
1:AA:182:VAL:HA	5:AE:80:HIS:CD2	2.54	0.43
2:AB:378:LEU:HD23	2:AB:416:ILE:CG2	2.49	0.43
3:AC:48:GLY:HA3	12:AC:402:HEM:C1B	2.54	0.43
3:AC:133:LEU:HD23	3:AC:133:LEU:HA	1.85	0.43
7:AG:29:SER:CB	7:AG:32:SER:HB2	2.38	0.43
10:AK:48:ILE:O	10:AK:49:ASN:C	2.61	0.43
5:Ae:222:CYS:HB2	5:Ae:236:CYS:SG	2.59	0.43
8:Ah:52:ASP:OD1	8:Ah:53:ASN:N	2.52	0.43
2:AB:155:ARG:HD2	2:AB:198:GLY:H	1.83	0.43
3:AC:181:PHE:HA	3:AC:184:ILE:HG22	2.00	0.43
3:AC:218:ILE:HG21	4:AD:314:LEU:CD1	2.48	0.43
3:AC:317:PHE:HB3	6:AF:27:PHE:HD2	1.84	0.43
5:AE:154:ILE:HD12	5:AE:154:ILE:N	2.32	0.43
2:Ab:378:LEU:HD23	2:Ab:416:ILE:CG2	2.49	0.43
2:Ab:411:THR:O	2:Ab:414:GLN:HG2	2.19	0.43
5:Ae:263:TYR:CB	5:Ae:273:VAL:HA	2.49	0.43
7:Ag:25:ARG:NH2	7:Ag:29:SER:H	2.16	0.43
1:AA:61:SER:HB3	1:AA:242:LEU:HD22	2.01	0.43
3:AC:50:PHE:CE2	5:AE:140:MET:HE2	2.54	0.43
4:AD:315:LYS:O	6:AF:72:ARG:NH1	2.48	0.43
5:AE:166:ALA:HB2	5:AE:175:PHE:HD1	1.84	0.43
5:AE:222:CYS:HB2	5:AE:236:CYS:SG	2.59	0.43
1:Aa:175:ASN:C	1:Aa:177:ALA:N	2.76	0.43
1:Aa:338:CYS:SG	1:Aa:358:PHE:HB2	2.58	0.43
2:Ab:36:GLN:OE1	2:Ab:36:GLN:N	2.52	0.43
3:Ac:103:TYR:O	3:Ac:315:LEU:HG	2.19	0.43
13:Ac:404:U10:H1M1	13:Ac:404:U10:H72	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:302:LEU:C	4:Ad:304:TYR:N	2.75	0.43
5:Ai:64:LEU:CD1	5:Ai:78:PHE:HD1	2.32	0.43
2:AB:162:LYS:HG3	2:AB:191:TYR:HB3	2.00	0.43
3:AC:171:ASP:CG	3:AC:172:LYS:N	2.76	0.43
3:AC:208:PRO:HB2	3:AC:316:MET:HE3	2.01	0.43
4:AD:312:SER:O	4:AD:313:VAL:C	2.59	0.43
5:AE:83:VAL:HG22	5:AE:84:LYS:N	2.34	0.43
5:AE:249:ILE:HG12	5:AE:254:ALA:HB3	2.01	0.43
7:AG:73:LYS:HZ3	8:AH:63:GLU:HG2	1.83	0.43
10:AK:33:VAL:CG1	10:AK:42:LEU:HG	2.45	0.43
3:Ac:48:GLY:C	12:Ac:401:HEM:HMB3	2.43	0.43
4:Ad:224:GLY:HA3	8:Ah:64:ASP:HA	1.99	0.43
5:Ae:83:VAL:HG22	5:Ae:84:LYS:N	2.34	0.43
5:Ae:264:GLU:O	5:Ae:272:VAL:N	2.47	0.43
6:AF:95:LEU:O	6:AF:96:LYS:C	2.62	0.43
6:AF:97:GLU:HA	6:AF:100:ARG:NH1	2.32	0.43
8:AH:52:ASP:OD1	8:AH:53:ASN:N	2.52	0.43
2:Ab:64:PHE:HZ	2:Ab:394:SER:HA	1.84	0.43
2:Ab:261:GLN:HE22	2:Ab:443:ASN:HA	1.84	0.43
3:Ac:83:HIS:CD2	12:Ac:401:HEM:ND	2.86	0.43
3:Ac:181:PHE:HA	3:Ac:184:ILE:HG22	2.00	0.43
3:Ac:270:PRO:HG3	3:Ac:278:TYR:HB2	2.00	0.43
5:Ae:156:LEU:HD23	5:Ae:156:LEU:HA	1.62	0.43
1:AA:167:VAL:O	1:AA:170:ARG:HG2	2.19	0.42
2:AB:39:GLU:OE2	2:AB:227:HIS:HB2	2.19	0.42
2:AB:130:ILE:HA	2:AB:133:LEU:HB2	2.00	0.42
2:AB:230:LEU:O	2:AB:233:VAL:HG22	2.18	0.42
3:AC:197:LEU:HD11	14:AC:406:UQ6:C7	2.49	0.42
4:AD:159:ASN:OD1	4:AD:160:ASP:N	2.52	0.42
4:AD:252:VAL:HG13	4:AD:253:LEU:N	2.33	0.42
4:AD:321:TYR:HB2	6:AF:61:PHE:CD2	2.54	0.42
5:AE:196:ARG:HD2	5:AE:249:ILE:HG23	2.01	0.42
16:AG:102:CDL:H742	16:AG:102:CDL:H781	2.01	0.42
2:Ab:60:ARG:CZ	2:Ab:390:GLU:HB3	2.48	0.42
2:Ab:64:PHE:CZ	2:Ab:394:SER:HA	2.54	0.42
2:Ab:173:ILE:HD11	2:Ab:439:ALA:C	2.44	0.42
2:Ab:225:VAL:HG22	2:Ab:229:VAL:HG21	2.01	0.42
2:Ab:297:PRO:CB	2:Ab:304:ASN:CG	2.91	0.42
3:Ac:256:TYR:CD2	4:Ad:202:ARG:HB3	2.54	0.42
3:Ac:263:ASN:OD1	3:Ac:264:THR:N	2.52	0.42
4:Ad:262:THR:O	4:Ad:263:MET:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:235:TYR:CE1	5:Ae:240:GLY:HA2	2.53	0.42
9:Aj:19:SER:HB2	10:Ak:23:MET:HB3	2.01	0.42
10:Ak:48:ILE:HD13	10:Ak:48:ILE:HA	1.87	0.42
4:AD:259:THR:O	4:AD:260:PRO:C	2.60	0.42
5:AE:205:VAL:CG1	5:AE:211:VAL:HG23	2.49	0.42
1:Aa:74:TRP:HB3	1:Aa:418:LEU:CD1	2.49	0.42
1:Aa:117:GLY:HA3	2:Ab:377:LYS:HA	1.99	0.42
1:Aa:120:LEU:HB3	2:Ab:299:ILE:HG13	2.00	0.42
14:Ac:405:UQ6:H171	14:Ac:405:UQ6:H151	1.68	0.42
2:AB:45:ASN:ND2	2:AB:239:ASN:CA	2.74	0.42
2:AB:286:PHE:CD1	2:AB:427:ALA:HB1	2.54	0.42
3:AC:138:MET:HE1	3:AC:268:ILE:HA	2.01	0.42
4:AD:248:ILE:HD12	4:AD:266:VAL:HG11	2.00	0.42
6:AF:111:LYS:HA	10:Ak:8:PRO:CG	2.50	0.42
8:AH:39:GLU:HA	8:AH:42:VAL:HG12	2.01	0.42
1:Aa:464:GLN:HA	7:Ag:5:PHE:HB3	2.02	0.42
2:Ab:162:LYS:HG3	2:Ab:191:TYR:HB3	2.00	0.42
2:Ab:396:ILE:HG12	2:Ab:406:TYR:HE1	1.84	0.42
3:Ac:169:SER:O	3:Ac:170:VAL:C	2.62	0.42
4:Ad:154:VAL:HG21	4:Ad:173:ASP:CG	2.44	0.42
3:AC:331:ASN:HB3	11:AG:103:3PE:H2G1	2.01	0.42
4:AD:318:LYS:CD	5:AE:86:PRO:HB2	2.49	0.42
8:AH:42:VAL:HG23	8:AH:45:ARG:HH21	1.84	0.42
1:Aa:480:PHE:HB3	10:Ak:20:THR:HG21	2.01	0.42
2:Ab:142:THR:HA	2:Ab:241:ARG:NH2	2.35	0.42
5:Ae:112:GLY:O	5:Ae:116:LEU:HB2	2.19	0.42
5:Ae:122:THR:O	5:Ae:123:VAL:C	2.61	0.42
8:Ah:39:GLU:HA	8:Ah:42:VAL:HG12	2.01	0.42
2:AB:177:LEU:HD21	2:AB:272:VAL:CG1	2.49	0.42
4:AD:199:TYR:HA	4:AD:278:SER:OG	2.20	0.42
1:Aa:167:VAL:O	1:Aa:170:ARG:HG2	2.19	0.42
1:Aa:467:ASP:OD2	3:Ac:223:TYR:HE2	1.98	0.42
2:Ab:41:THR:OG1	2:Ab:49:ILE:HB	2.19	0.42
2:Ab:177:LEU:HD21	2:Ab:272:VAL:CG1	2.49	0.42
2:Ab:349:GLU:O	2:Ab:350:VAL:C	2.63	0.42
3:Ac:270:PRO:HB2	3:Ac:274:PHE:HB2	2.01	0.42
1:AA:278:ARG:CZ	1:AA:463:GLU:HB2	2.50	0.42
2:AB:300:LYS:HE2	2:AB:301:ARG:HH11	1.83	0.42
3:AC:33:PHE:O	3:AC:36:LEU:HB2	2.19	0.42
3:AC:51:LEU:HG	12:AC:402:HEM:HBA1	2.00	0.42
3:AC:153:ILE:HB	3:AC:157:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:163:TRP:HZ2	5:Ae:140:MET:CE	2.31	0.42
3:AC:179:PHE:HE2	3:Ac:179:PHE:CE2	2.34	0.42
3:AC:278:TYR:CE2	3:AC:282:ARG:HD2	2.54	0.42
4:AD:131:ALA:HA	4:AD:174:TYR:HA	2.02	0.42
5:AE:195:LEU:CD1	5:AE:248:ARG:HD2	2.50	0.42
7:AG:19:LEU:HG	7:AG:20:SER:N	2.33	0.42
1:Aa:278:ARG:NH1	7:Ag:11:ILE:HD13	2.35	0.42
1:Aa:358:PHE:CD2	1:Aa:368:MET:HG2	2.54	0.42
3:Ac:33:PHE:CE1	16:Ag:102:CDL:H761	2.55	0.42
4:Ad:242:ILE:HD11	4:Ad:244:MET:HE2	2.02	0.42
5:Ae:177:ARG:HB3	5:Ae:211:VAL:CG1	2.49	0.42
6:Af:95:LEU:O	6:Af:96:LYS:C	2.62	0.42
2:AB:407:MET:HE1	2:AB:415:GLN:CD	2.45	0.42
5:AE:122:THR:CG2	9:AJ:25:ILE:HG21	2.49	0.42
5:AE:178:HIS:CD2	5:AE:179:ARG:N	2.88	0.42
9:AJ:19:SER:HA	10:AK:24:TRP:CH2	2.55	0.42
3:Ac:211:LEU:CD2	6:Af:37:THR:HA	2.49	0.42
4:Ad:231:LEU:HD22	4:Ad:241:ALA:O	2.20	0.42
5:Ae:166:ALA:HB2	5:Ae:175:PHE:HD1	1.84	0.42
9:Aj:21:PHE:O	9:Aj:24:THR:HG22	2.20	0.42
4:AD:300:LEU:HB3	16:AG:102:CDL:H552	2.01	0.42
5:AE:112:GLY:O	5:AE:116:LEU:HB2	2.19	0.42
9:AJ:19:SER:HA	10:AK:24:TRP:CZ2	2.55	0.42
1:Aa:58:ARG:CD	1:Aa:417:LEU:HD12	2.50	0.42
2:Ab:163:ALA:HB1	5:Ai:43:LEU:CD2	2.42	0.42
5:Ae:196:ARG:HD2	5:Ae:249:ILE:HG23	2.01	0.42
8:Ah:42:VAL:HG23	8:Ah:45:ARG:HH21	1.84	0.42
5:Ai:62:ARG:HB3	5:Ai:63:PRO:HD2	2.00	0.42
5:Ai:71:ASN:OD1	5:Ai:71:ASN:O	2.38	0.42
10:Ak:6:LEU:HA	10:Ak:11:ARG:NH1	2.27	0.42
2:AB:272:VAL:HA	2:AB:337:GLY:HA3	2.02	0.42
2:AB:346:ALA:O	2:AB:347:ALA:C	2.62	0.42
2:AB:396:ILE:HG12	2:AB:406:TYR:HE1	1.85	0.42
3:AC:244:LEU:C	4:AD:285:ARG:HH11	2.27	0.42
3:AC:312:GLN:HE21	6:AF:37:THR:HB	1.85	0.42
4:AD:308:ARG:HD3	7:AG:27:PHE:CZ	2.55	0.42
4:AD:317:ARG:HD2	4:AD:319:LEU:HD21	2.02	0.42
5:AE:177:ARG:HB3	5:AE:211:VAL:CG1	2.49	0.42
5:AE:201:ASP:OD1	5:AE:202:LEU:N	2.49	0.42
16:AG:102:CDL:H732	16:AG:102:CDL:H761	1.93	0.42
1:Aa:45:VAL:O	1:Aa:46:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:48:THR:HB	1:Aa:423:ARG:HG2	2.02	0.42
1:Aa:178:SER:OG	1:Aa:181:ASN:ND2	2.53	0.42
2:Ab:39:GLU:HB2	2:Ab:227:HIS:ND1	2.33	0.42
3:Ac:33:PHE:O	3:Ac:36:LEU:HB2	2.19	0.42
3:Ac:242:LEU:HD21	3:Ac:250:LEU:HD11	2.01	0.42
4:Ad:199:TYR:HA	4:Ad:278:SER:OG	2.20	0.42
5:Ae:195:LEU:CD1	5:Ae:248:ARG:HD2	2.50	0.42
5:Ae:249:ILE:HG12	5:Ae:254:ALA:HB3	2.01	0.42
1:AA:358:PHE:CD2	1:AA:368:MET:HG2	2.54	0.42
4:AD:202:ARG:HG3	4:AD:278:SER:HB3	2.02	0.42
2:Ab:70:ARG:NH2	2:Ab:332:ASP:OD2	2.53	0.42
2:Ab:346:ALA:O	2:Ab:347:ALA:C	2.61	0.42
3:Ac:133:LEU:HD23	3:Ac:133:LEU:HA	1.85	0.42
5:Ae:160:PRO:C	5:Ae:178:HIS:HB3	2.45	0.42
5:Ae:205:VAL:CG1	5:Ae:211:VAL:HG23	2.49	0.42
1:AA:48:THR:CB	1:AA:423:ARG:HG2	2.50	0.41
1:AA:479:ARG:O	10:AK:20:THR:HG21	2.20	0.41
3:AC:18:PHE:CE1	14:AC:406:UQ6:C7	3.03	0.41
3:AC:141:TRP:CH2	5:Ae:223:VAL:HG23	2.55	0.41
3:AC:148:ASN:OD1	5:Ae:221:GLY:CA	2.65	0.41
4:AD:95:PRO:HG2	8:AH:85:PHE:HB2	2.02	0.41
4:AD:323:PRO:HB2	4:AD:325:LYS:HG3	2.02	0.41
5:AE:156:LEU:N	5:AE:269:ASP:O	2.53	0.41
1:Aa:204:PRO:O	1:Aa:205:SER:C	2.63	0.41
1:Aa:340:SER:O	1:Aa:358:PHE:HA	2.20	0.41
4:Ad:146:LYS:NZ	4:Ad:169:GLY:O	2.48	0.41
6:Af:102:ARG:HA	6:Af:105:ARG:CZ	2.49	0.41
7:Ag:78:TYR:CD1	8:Ah:63:GLU:HG3	2.55	0.41
2:AB:138:LEU:HD22	2:AB:238:LEU:HG	2.01	0.41
5:AE:231:PHE:CD2	5:AE:250:ARG:NH1	2.88	0.41
1:Aa:80:ARG:NH2	1:Aa:268:CYS:SG	2.93	0.41
1:Aa:338:CYS:SG	1:Aa:359:VAL:O	2.79	0.41
2:Ab:185:ALA:HB3	2:Ab:251:ALA:HB2	2.01	0.41
3:Ac:284:ILE:HG21	3:Ac:289:GLY:HA3	2.02	0.41
4:Ad:223:THR:OG1	8:Ah:55:VAL:HB	2.20	0.41
1:AA:148:ALA:O	1:AA:152:GLN:HG2	2.20	0.41
1:AA:338:CYS:SG	1:AA:359:VAL:O	2.78	0.41
3:AC:18:PHE:CZ	14:AC:406:UQ6:C1M	3.03	0.41
3:AC:256:TYR:CD2	4:AD:202:ARG:HB3	2.54	0.41
3:AC:316:MET:HE2	11:AC:404:3PE:H122	2.03	0.41
4:AD:210:TYR:O	4:AD:211:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:299:LEU:HD22	5:AE:121:THR:HG23	2.01	0.41
5:AE:105:GLU:H	5:AE:105:GLU:HG3	1.69	0.41
5:AE:115:TYR:HB3	9:AJ:21:PHE:HE1	1.85	0.41
5:AE:172:LYS:HE2	5:AE:172:LYS:HA	2.02	0.41
6:AF:108:TRP:CE2	2:Ab:101:ARG:HB3	2.55	0.41
7:AG:28:PRO:O	7:AG:29:SER:C	2.63	0.41
8:AH:26:ASP:C	8:AH:28:LEU:N	2.77	0.41
3:Ac:153:ILE:HB	3:Ac:157:GLY:HA2	2.01	0.41
4:Ad:159:ASN:HB2	4:Ad:163:GLU:O	2.20	0.41
4:Ad:201:VAL:HG22	4:Ad:278:SER:HB2	2.00	0.41
4:Ad:210:TYR:O	4:Ad:211:VAL:C	2.63	0.41
4:Ad:252:VAL:HG13	4:Ad:253:LEU:N	2.34	0.41
5:Ae:154:ILE:HD12	5:Ae:154:ILE:N	2.34	0.41
5:Ae:155:LYS:HB3	5:Ae:158:ASP:CG	2.45	0.41
7:Ag:73:LYS:HB3	8:Ah:67:GLU:OE2	2.20	0.41
2:AB:38:LEU:HD13	2:AB:52:LEU:HB2	2.02	0.41
3:AC:77:TRP:CD2	4:AD:281:GLU:HG3	2.55	0.41
14:AC:406:UQ6:H171	14:AC:406:UQ6:H151	1.68	0.41
4:AD:99:ARG:HA	4:AD:99:ARG:HD3	1.94	0.41
3:Ac:171:ASP:CG	3:Ac:172:LYS:N	2.76	0.41
4:Ad:202:ARG:HG3	4:Ad:278:SER:HB3	2.02	0.41
4:Ad:297:GLY:O	4:Ad:301:PRO:HG2	2.20	0.41
3:AC:295:ILE:HG22	3:AC:299:LEU:HD12	2.02	0.41
6:AF:105:ARG:HA	2:Ab:97:PHE:CE2	2.56	0.41
1:Aa:120:LEU:CD2	2:Ab:299:ILE:HG23	2.48	0.41
1:Aa:388:VAL:HG21	1:Aa:438:ALA:HA	2.02	0.41
2:Ab:138:LEU:HD22	2:Ab:238:LEU:HG	2.02	0.41
2:Ab:286:PHE:CD1	2:Ab:427:ALA:HB1	2.54	0.41
3:Ac:295:ILE:HG22	3:Ac:299:LEU:HD12	2.02	0.41
5:Ae:173:PRO:HG2	5:Ae:223:VAL:CG2	2.45	0.41
1:AA:478:LEU:O	10:AK:24:TRP:HZ2	2.04	0.41
3:AC:77:TRP:HZ2	4:AD:284:HIS:HD2	1.68	0.41
3:AC:284:ILE:HG21	3:AC:289:GLY:HA3	2.02	0.41
5:AE:160:PRO:C	5:AE:178:HIS:HB3	2.45	0.41
1:Aa:281:ALA:HA	7:Ag:10:ARG:HH12	1.85	0.41
2:Ab:407:MET:HE1	2:Ab:415:GLN:CD	2.45	0.41
4:Ad:247:PRO:O	4:Ad:248:ILE:HD13	2.21	0.41
5:Ae:172:LYS:HA	5:Ae:172:LYS:HE2	2.02	0.41
5:Ae:196:ARG:HD2	5:Ae:249:ILE:HG21	2.03	0.41
5:Ae:244:ASP:OD2	5:Ae:248:ARG:NE	2.54	0.41
1:AA:340:SER:O	1:AA:358:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:261:GLN:HG2	2:Ab:77:LEU:HD12	2.02	0.41
3:AC:354:ALA:HA	11:AG:103:3PE:H2H2	2.02	0.41
5:AE:159:ILE:HG23	5:AE:163:LYS:HB3	2.03	0.41
10:AK:45:VAL:HB	10:AK:48:ILE:CG2	2.50	0.41
2:Ab:426:LYS:HA	2:Ab:429:LYS:NZ	2.36	0.41
3:Ac:220:PHE:CD2	14:Ac:405:UQ6:H3M3	2.55	0.41
3:Ac:278:TYR:CE2	3:Ac:282:ARG:HD2	2.55	0.41
5:Ae:159:ILE:HG23	5:Ae:163:LYS:HB3	2.03	0.41
7:Ag:28:PRO:O	7:Ag:29:SER:C	2.63	0.41
5:Ai:71:ASN:C	5:Ai:73:PRO:HD2	2.45	0.41
1:AA:178:SER:OG	1:AA:181:ASN:ND2	2.53	0.41
1:AA:388:VAL:HG21	1:AA:438:ALA:HA	2.02	0.41
12:AC:403:HEM:HBA1	14:AC:406:UQ6:O4	2.20	0.41
4:AD:115:GLN:HE22	4:AD:256:ASP:CG	2.29	0.41
4:AD:235:PRO:HA	4:AD:240:GLN:CG	2.50	0.41
6:AF:108:TRP:CH2	2:Ab:101:ARG:HB3	2.55	0.41
7:AG:26:ALA:C	7:AG:28:PRO:HD3	2.46	0.41
5:AI:71:ASN:C	5:AI:73:PRO:HD2	2.45	0.41
1:Aa:384:THR:HA	10:Ak:12:GLU:OE2	2.20	0.41
16:Aa:502:CDL:H362	16:Aa:502:CDL:H332	1.90	0.41
2:Ab:233:VAL:HA	2:Ab:236:GLN:CG	2.47	0.41
2:Ab:297:PRO:CB	2:Ab:304:ASN:OD1	2.69	0.41
3:Ac:105:GLY:HA3	3:Ac:313:ARG:O	2.21	0.41
3:Ac:128:PHE:CD1	13:Ac:404:U10:C4M	3.04	0.41
3:Ac:317:PHE:CD1	6:Af:27:PHE:HB3	2.55	0.41
3:Ac:326:TRP:NE1	7:Ag:49:VAL:HG22	2.36	0.41
5:Ae:231:PHE:CD2	5:Ae:250:ARG:NH1	2.88	0.41
10:Ak:12:GLU:HA	10:Ak:15:ARG:HD3	2.02	0.41
10:Ak:41:ILE:HD12	10:Ak:41:ILE:N	2.36	0.41
1:AA:62:GLU:OE1	1:AA:423:ARG:NH1	2.45	0.41
1:AA:384:THR:HG21	10:AK:9:ARG:CG	2.51	0.41
2:AB:225:VAL:HG22	2:AB:229:VAL:HG21	2.01	0.41
3:AC:275:LEU:O	3:AC:276:PHE:C	2.64	0.41
3:AC:378:LYS:HE3	6:AF:89:PHE:CE2	2.51	0.41
5:AE:244:ASP:OD2	5:AE:248:ARG:NE	2.54	0.41
7:AG:35:ILE:O	7:AG:36:PRO:C	2.63	0.41
5:AI:71:ASN:OD1	5:AI:71:ASN:O	2.38	0.41
10:AK:6:LEU:HA	10:AK:11:ARG:NH1	2.27	0.41
1:Aa:170:ARG:HG3	1:Aa:171:GLU:N	2.36	0.41
3:Ac:227:LYS:HG3	4:Ad:307:LYS:HE3	2.02	0.41
4:Ad:110:ILE:HB	4:Ad:139:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:125:HIS:HB3	4:Ad:197:LEU:HG	2.03	0.41
4:Ad:242:ILE:CD1	4:Ad:244:MET:HE2	2.51	0.41
5:Ae:115:TYR:CE1	17:Ae:301:PC1:H122	2.55	0.41
5:Ae:156:LEU:HD12	5:Ae:268:ASP:HA	2.03	0.41
5:Ae:178:HIS:CD2	5:Ae:179:ARG:N	2.88	0.41
5:Ae:216:VAL:HG13	5:Ae:221:GLY:HA2	2.03	0.41
6:Af:101:GLU:O	6:Af:105:ARG:HG3	2.21	0.41
7:Ag:26:ALA:C	7:Ag:28:PRO:HD3	2.46	0.41
7:Ag:57:TYR:O	7:Ag:61:THR:HG23	2.21	0.41
8:Ah:26:ASP:C	8:Ah:28:LEU:N	2.77	0.41
2:AB:65:VAL:HG22	2:AB:218:MET:HG2	2.03	0.41
3:AC:10:LEU:O	3:AC:14:ILE:HG12	2.20	0.41
3:AC:346:PRO:HG3	7:AG:66:GLU:CG	2.51	0.41
4:AD:181:ASN:ND2	4:Ad:158:PRO:HB3	2.36	0.41
7:AG:57:TYR:O	7:AG:61:THR:HG23	2.21	0.41
1:Aa:469:ASN:ND2	3:Ac:223:TYR:CZ	2.89	0.41
3:Ac:29:SER:OG	16:Ag:101:CDL:HA61	2.21	0.41
3:Ac:334:ILE:CD1	7:Ag:56:VAL:HG22	2.51	0.41
4:Ad:107:HIS:ND1	4:Ad:138:VAL:O	2.54	0.41
4:Ad:250:THR:HG23	4:Ad:262:THR:HA	2.03	0.41
5:Ae:249:ILE:HG23	5:Ae:249:ILE:O	2.22	0.41
1:AA:48:THR:HB	1:AA:423:ARG:HG2	2.02	0.40
1:AA:117:GLY:HA3	2:AB:377:LYS:HA	2.02	0.40
1:AA:120:LEU:HB3	2:AB:299:ILE:HG13	2.01	0.40
1:AA:454:PRO:O	1:AA:468:TYR:OH	2.34	0.40
3:AC:53:MET:HA	3:Ac:177:ARG:HA	2.02	0.40
3:AC:244:LEU:HD13	4:AD:289:GLY:HA2	2.02	0.40
3:AC:323:ILE:HD13	11:AG:103:3PE:H232	2.02	0.40
5:AE:123:VAL:HG13	9:AJ:29:ALA:CA	2.41	0.40
5:AE:254:ALA:HA	5:AE:255:PRO:HD3	1.96	0.40
6:AF:102:ARG:HA	6:AF:105:ARG:CZ	2.49	0.40
10:AK:12:GLU:HA	10:AK:15:ARG:HD3	2.02	0.40
4:Ad:127:MET:HE1	4:Ad:198:SER:HA	2.02	0.40
7:Ag:10:ARG:NH2	7:Ag:12:ARG:HD2	2.36	0.40
10:Ak:23:MET:HE2	10:Ak:23:MET:HB2	1.92	0.40
1:AA:73:VAL:HG11	1:AA:151:VAL:HG11	2.03	0.40
1:AA:170:ARG:HG3	1:AA:171:GLU:N	2.36	0.40
2:AB:297:PRO:CB	2:AB:304:ASN:OD1	2.69	0.40
2:AB:426:LYS:HA	2:AB:429:LYS:NZ	2.36	0.40
2:AB:453:LEU:O	2:AB:453:LEU:HD23	2.21	0.40
3:AC:83:HIS:CD2	12:AC:402:HEM:C4D	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:294:LEU:C	3:AC:294:LEU:HD23	2.46	0.40
4:AD:127:MET:HE1	4:AD:198:SER:HA	2.03	0.40
4:AD:159:ASN:O	4:AD:162:GLY:N	2.47	0.40
5:AE:196:ARG:HD2	5:AE:249:ILE:HG21	2.03	0.40
7:AG:48:ARG:HH21	11:AG:103:3PE:H322	1.86	0.40
9:AJ:21:PHE:O	9:AJ:24:THR:HG22	2.20	0.40
1:Aa:463:GLU:CD	7:Ag:8:LEU:HB2	2.46	0.40
8:Ah:67:GLU:HG3	8:Ah:68:GLU:H	1.86	0.40
2:AB:160:ILE:HG23	5:AI:44:ASP:HB2	2.02	0.40
2:AB:262:ASN:C	2:Ab:195:TYR:CD2	2.99	0.40
3:AC:33:PHE:CE1	16:AG:102:CDL:H782	2.56	0.40
3:AC:268:ILE:CG1	5:Ae:238:CYS:SG	3.09	0.40
8:AH:67:GLU:HG3	8:AH:68:GLU:H	1.87	0.40
3:Ac:77:TRP:HZ2	4:Ad:284:HIS:CD2	2.38	0.40
4:Ad:138:VAL:HG21	4:Ad:276:TRP:CZ2	2.55	0.40
4:Ad:175:PHE:HA	4:Ad:176:PRO:HD3	1.96	0.40
4:Ad:308:ARG:HD3	7:Ag:27:PHE:CZ	2.56	0.40
5:Ae:127:TYR:HA	10:Ak:34:TRP:CH2	2.57	0.40
7:Ag:19:LEU:HD12	7:Ag:20:SER:H	1.86	0.40
9:Aj:10:LEU:O	9:Aj:11:TYR:C	2.64	0.40
1:AA:412:ASP:O	1:AA:416:SER:OG	2.32	0.40
2:AB:303:ASN:O	2:AB:304:ASN:C	2.63	0.40
3:AC:30:TRP:CB	3:AC:100:ARG:HD3	2.52	0.40
3:AC:146:ILE:CD1	13:AC:405:U10:H3M2	2.49	0.40
3:AC:376:MET:CE	6:AF:18:ARG:HG2	2.51	0.40
5:AE:159:ILE:O	5:AE:210:TRP:CH2	2.71	0.40
5:AE:168:LYS:NZ	5:AE:171:GLY:HA2	2.36	0.40
7:AG:10:ARG:NH2	7:AG:12:ARG:HD2	2.36	0.40
1:Aa:73:VAL:HG11	1:Aa:151:VAL:HG11	2.03	0.40
1:Aa:454:PRO:O	1:Aa:468:TYR:OH	2.34	0.40
2:Ab:270:ALA:HB2	2:Ab:339:TYR:CD1	2.50	0.40
3:Ac:294:LEU:HD23	3:Ac:294:LEU:C	2.46	0.40
3:Ac:296:LEU:O	3:Ac:297:SER:C	2.64	0.40
5:Ae:162:GLY:N	5:Ae:178:HIS:O	2.54	0.40
6:Af:36:ASP:OD1	6:Af:90:TYR:OH	2.38	0.40
9:Aj:7:PRO:O	9:Aj:10:LEU:HB2	2.21	0.40
3:AC:99:GLY:HA3	11:AC:404:3PE:H2A1	2.03	0.40
3:AC:128:PHE:CE1	13:AC:405:U10:C4M	3.04	0.40
4:AD:110:ILE:HG23	4:AD:273:PHE:HA	2.04	0.40
1:Aa:148:ALA:HB2	1:Aa:250:LEU:HG	2.04	0.40
1:Aa:384:THR:HG21	10:Ak:9:ARG:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:65:VAL:HG22	2:Ab:218:MET:HG2	2.03	0.40
3:Ac:149:LEU:HD21	3:Ac:294:LEU:HD13	2.04	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	AA	397/480 (83%)	388 (98%)	9 (2%)	0	100	100
1	Aa	408/480 (85%)	395 (97%)	13 (3%)	0	100	100
2	AB	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
2	Ab	408/453 (90%)	396 (97%)	12 (3%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	368 (99%)	3 (1%)	0	100	100
4	AD	238/325 (73%)	230 (97%)	8 (3%)	0	100	100
4	Ad	238/325 (73%)	225 (94%)	13 (6%)	0	100	100
5	AE	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
5	AI	26/274 (10%)	23 (88%)	3 (12%)	0	100	100
5	Ae	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
5	Ai	24/274 (9%)	23 (96%)	1 (4%)	0	100	100
6	AF	96/111 (86%)	96 (100%)	0	0	100	100
6	Af	96/111 (86%)	96 (100%)	0	0	100	100
7	AG	74/82 (90%)	74 (100%)	0	0	100	100
7	Ag	74/82 (90%)	74 (100%)	0	0	100	100
8	AH	66/89 (74%)	66 (100%)	0	0	100	100
8	Ah	66/89 (74%)	66 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	39/64 (61%)	39 (100%)	0	0	100	100
9	Aj	46/64 (72%)	46 (100%)	0	0	100	100
10	AK	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
10	Ak	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
All	All	3916/5178 (76%)	3811 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	341/398 (86%)	339 (99%)	2 (1%)	78	80
1	Aa	349/398 (88%)	347 (99%)	2 (1%)	78	80
2	AB	328/356 (92%)	327 (100%)	1 (0%)	86	84
2	Ab	324/356 (91%)	323 (100%)	1 (0%)	86	84
3	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
3	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
4	AD	205/260 (79%)	205 (100%)	0	100	100
4	Ad	205/260 (79%)	205 (100%)	0	100	100
5	AE	158/224 (70%)	157 (99%)	1 (1%)	78	80
5	AI	23/224 (10%)	22 (96%)	1 (4%)	26	51
5	Ae	158/224 (70%)	157 (99%)	1 (1%)	78	80
5	Ai	22/224 (10%)	20 (91%)	2 (9%)	9	30
6	AF	90/99 (91%)	90 (100%)	0	100	100
6	Af	90/99 (91%)	90 (100%)	0	100	100
7	AG	69/74 (93%)	69 (100%)	0	100	100
7	Ag	69/74 (93%)	69 (100%)	0	100	100
8	AH	65/83 (78%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ah	65/83 (78%)	65 (100%)	0	100	100
9	AJ	33/55 (60%)	33 (100%)	0	100	100
9	Aj	39/55 (71%)	39 (100%)	0	100	100
10	AK	39/46 (85%)	39 (100%)	0	100	100
10	Ak	39/46 (85%)	39 (100%)	0	100	100
All	All	3361/4304 (78%)	3348 (100%)	13 (0%)	81	83

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	249	HIS
1	AA	403	LEU
2	AB	435	LYS
3	AC	294	LEU
5	AE	135	GLN
5	AI	45	VAL
1	Aa	222	ARG
1	Aa	249	HIS
2	Ab	435	LYS
3	Ac	294	LEU
5	Ae	135	GLN
5	Ai	45	VAL
5	Ai	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	87	ASN
1	AA	160	GLN
1	AA	173	GLN
1	AA	181	ASN
1	AA	207	ASN
1	AA	240	GLN
1	AA	342	GLN
1	AA	402	HIS
2	AB	167	GLN
2	AB	284	ASN
2	AB	298	HIS
2	AB	304	ASN

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Mol	Chain	Res	Type
2	AB	357	GLN
2	AB	365	ASN
2	AB	415	GLN
2	AB	443	ASN
3	AC	32	ASN
3	AC	260	ASN
3	AC	312	GLN
4	AD	115	GLN
4	AD	155	GLN
4	AD	181	ASN
4	AD	189	ASN
5	AE	227	ASN
5	AE	242	HIS
6	AF	80	GLN
5	AI	71	ASN
10	AK	16	ASN
1	Aa	55	ASN
1	Aa	87	ASN
1	Aa	128	HIS
1	Aa	160	GLN
1	Aa	173	GLN
1	Aa	181	ASN
1	Aa	207	ASN
1	Aa	240	GLN
1	Aa	342	GLN
1	Aa	397	ASN
2	Ab	167	GLN
2	Ab	284	ASN
2	Ab	298	HIS
2	Ab	304	ASN
2	Ab	357	GLN
2	Ab	415	GLN
2	Ab	443	ASN
3	Ac	32	ASN
3	Ac	201	HIS
3	Ac	312	GLN
4	Ad	115	GLN
4	Ad	190	ASN
5	Ae	227	ASN
5	Ae	242	HIS
6	Af	39	HIS
6	Af	80	GLN

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Mol	Chain	Res	Type
7	Ag	65	GLN
10	Ak	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	UQ6	AC	406	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
11	3PE	Aa	501	-	22,22,50	1.37	2 (9%)	25,27,55	1.20	2 (8%)
16	CDL	AG	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.33	6 (12%)
11	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.21	3 (8%)
12	HEM	AC	403	3	50,50,50	1.34	6 (12%)	66,82,82	1.66	16 (24%)
12	HEM	Ac	402	3	50,50,50	1.32	5 (10%)	66,82,82	1.66	16 (24%)
15	HEC	AD	401	4	50,50,50	1.72	5 (10%)	68,82,82	1.35	7 (10%)
12	HEM	AC	402	3	50,50,50	1.31	7 (14%)	66,82,82	1.68	15 (22%)
16	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.35	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	3PE	AG	103	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
13	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.08	7 (25%)
13	U10	AC	405	-	23,23,63	1.24	3 (13%)	28,31,79	2.10	7 (25%)
15	HEC	Ad	401	4	50,50,50	1.73	5 (10%)	68,82,82	1.36	8 (11%)
17	PC1	Ae	301	-	34,34,53	1.17	2 (5%)	40,42,61	1.18	4 (10%)
11	3PE	AC	401	-	22,22,50	0.47	0	25,27,55	0.73	1 (4%)
16	CDL	Aa	502	-	45,45,99	1.34	4 (8%)	51,57,111	1.36	6 (11%)
11	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.29	0
14	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
11	3PE	AC	404	-	34,34,50	1.10	2 (5%)	37,39,55	1.14	3 (8%)
16	CDL	AG	102	-	55,55,99	1.20	4 (7%)	61,67,111	1.25	6 (9%)
16	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
12	HEM	Ac	401	3	50,50,50	1.30	7 (14%)	66,82,82	1.67	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	UQ6	AC	406	-	-	13/21/21/39	0/1/1/1
11	3PE	Aa	501	-	-	7/26/26/54	-
16	CDL	AG	101	-	-	8/52/52/110	-
11	3PE	Ac	403	-	-	3/38/38/54	-
12	HEM	AC	403	3	-	8/14/54/54	-
15	HEC	AD	401	4	1/1/3/7	0/14/54/54	-
12	HEM	Ac	402	3	-	8/14/54/54	-
12	HEM	AC	402	3	-	9/14/54/54	-
16	CDL	Ag	101	-	-	7/52/52/110	-
11	3PE	AG	103	-	-	9/54/54/54	-
13	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
13	U10	AC	405	-	-	6/15/39/87	0/1/1/1
15	HEC	Ad	401	4	1/1/3/7	0/14/54/54	-
17	PC1	Ae	301	-	-	7/38/38/57	-
11	3PE	AC	401	-	-	7/26/26/54	-
16	CDL	Aa	502	-	-	13/56/56/110	-
11	3PE	Ag	103	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
11	3PE	AC	404	-	-	1/38/38/54	-
16	CDL	AG	102	-	-	15/66/66/110	-
16	CDL	Ag	102	-	-	13/66/66/110	-
12	HEM	Ac	401	3	-	9/14/54/54	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Ad	401	HEC	C3D-C2D	8.07	1.53	1.36
15	AD	401	HEC	C3D-C2D	7.98	1.53	1.36
17	Ae	301	PC1	O31-C31	4.33	1.46	1.33
16	Aa	502	CDL	OA8-CA7	4.24	1.45	1.33
16	Aa	502	CDL	OB8-CB7	4.24	1.45	1.33
16	AG	101	CDL	OA8-CA7	4.24	1.45	1.33
11	AC	404	3PE	O31-C31	4.23	1.45	1.33
11	Aa	501	3PE	O31-C31	4.22	1.45	1.33
11	Ac	403	3PE	O31-C31	4.22	1.45	1.33
11	AG	103	3PE	O31-C31	4.21	1.45	1.33
16	Ag	101	CDL	OB8-CB7	4.20	1.45	1.33
16	Ag	101	CDL	OA8-CA7	4.16	1.45	1.33
16	AG	101	CDL	OB8-CB7	4.16	1.45	1.33
16	AG	102	CDL	OB8-CB7	4.16	1.45	1.33
16	AG	102	CDL	OA8-CA7	4.15	1.45	1.33
11	Aa	501	3PE	O21-C21	4.14	1.46	1.34
11	AG	103	3PE	O21-C21	4.14	1.46	1.34
16	Aa	502	CDL	OB6-CB5	4.11	1.45	1.34
17	Ae	301	PC1	O21-C21	4.10	1.45	1.34
16	AG	101	CDL	OA6-CA5	4.10	1.45	1.34
16	Ag	101	CDL	OA6-CA5	4.05	1.45	1.34
16	AG	101	CDL	OB6-CB5	4.04	1.45	1.34
16	Ag	101	CDL	OB6-CB5	4.03	1.45	1.34
16	AG	102	CDL	OA6-CA5	4.01	1.45	1.34
16	Aa	502	CDL	OA6-CA5	4.01	1.45	1.34
11	AC	404	3PE	O21-C21	3.94	1.45	1.34
11	Ac	403	3PE	O21-C21	3.93	1.45	1.34
16	AG	102	CDL	OB6-CB5	3.92	1.45	1.34
12	AC	403	HEM	C4D-ND	-3.81	1.33	1.40
15	AD	401	HEC	FE-ND	3.76	2.06	1.94
15	Ad	401	HEC	FE-ND	3.75	2.06	1.94
12	Ac	402	HEM	C4D-ND	-3.73	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AC	402	HEM	C4D-ND	-3.67	1.34	1.40
12	Ac	401	HEM	C4D-ND	-3.59	1.34	1.40
15	Ad	401	HEC	FE-NB	3.58	2.05	1.94
15	AD	401	HEC	FE-NB	3.56	2.05	1.94
12	AC	403	HEM	C1B-NB	-3.26	1.34	1.40
12	Ac	402	HEM	C1B-NB	-3.21	1.34	1.40
12	AC	402	HEM	C1B-NB	-3.06	1.35	1.40
12	Ac	401	HEM	C1B-NB	-3.06	1.35	1.40
12	Ac	402	HEM	C1C-C2C	-3.01	1.39	1.45
12	AC	403	HEM	C1C-C2C	-2.98	1.39	1.45
14	Ac	405	UQ6	O2-C2	-2.96	1.30	1.37
14	AC	406	UQ6	O2-C2	-2.95	1.30	1.37
13	AC	405	U10	C6-C5	-2.93	1.38	1.46
13	Ac	404	U10	C6-C5	-2.92	1.38	1.46
15	Ad	401	HEC	FE-NA	2.91	2.05	1.95
13	Ac	404	U10	C4-C3	2.90	1.48	1.36
13	AC	405	U10	C4-C3	2.89	1.48	1.36
15	AD	401	HEC	FE-NA	2.88	2.04	1.95
12	AC	403	HEM	C1D-ND	-2.72	1.33	1.38
12	Ac	402	HEM	C1D-ND	-2.69	1.33	1.38
12	AC	402	HEM	C1C-C2C	-2.67	1.40	1.45
15	AD	401	HEC	FE-NC	2.66	2.04	1.95
12	Ac	401	HEM	C1C-C2C	-2.66	1.40	1.45
15	Ad	401	HEC	FE-NC	2.65	2.04	1.95
12	AC	402	HEM	C1D-ND	-2.55	1.33	1.38
13	Ac	404	U10	C3-C2	-2.50	1.41	1.48
13	AC	405	U10	C3-C2	-2.47	1.41	1.48
12	Ac	401	HEM	C1D-ND	-2.45	1.33	1.38
12	AC	402	HEM	FE-NB	2.32	2.02	1.94
12	Ac	401	HEM	FE-NB	2.32	2.02	1.94
12	AC	403	HEM	FE-NB	2.29	2.01	1.94
12	Ac	402	HEM	FE-NB	2.28	2.01	1.94
12	AC	402	HEM	FE-ND	2.28	2.01	1.94
12	Ac	401	HEM	C3C-C4C	-2.25	1.42	1.46
12	Ac	401	HEM	FE-ND	2.24	2.01	1.94
12	AC	402	HEM	C3C-C4C	-2.22	1.42	1.46
12	AC	403	HEM	C3C-C4C	-2.02	1.42	1.46

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AC	405	U10	C6-C1-C2	7.80	125.35	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Ac	404	U10	C6-C1-C2	7.71	125.28	119.18
15	Ad	401	HEC	C1D-ND-C4D	6.43	111.71	105.07
15	AD	401	HEC	C1D-ND-C4D	6.42	111.70	105.07
12	AC	402	HEM	CHC-C4B-NB	4.75	129.58	124.42
12	Ac	401	HEM	CHC-C4B-NB	4.67	129.49	124.42
12	AC	403	HEM	C4D-ND-C1D	4.47	109.69	105.07
11	AG	103	3PE	O21-C21-C22	4.44	121.07	111.50
12	Ac	401	HEM	CHD-C4C-NC	4.39	129.19	124.44
12	Ac	402	HEM	C4D-ND-C1D	4.38	109.59	105.07
12	AC	402	HEM	CHD-C4C-NC	4.37	129.16	124.44
12	AC	403	HEM	CHC-C4B-NB	4.21	128.99	124.42
12	Ac	402	HEM	CHC-C4B-NB	4.21	128.99	124.42
16	Aa	502	CDL	OA6-CA5-C11	4.17	120.49	111.50
13	AC	405	U10	C1-C6-C5	-4.14	115.69	119.58
13	Ac	404	U10	C1-C6-C5	-4.09	115.73	119.58
11	Ac	403	3PE	O21-C21-C22	4.07	120.27	111.50
17	Ae	301	PC1	O21-C21-C22	4.03	120.19	111.50
12	Ac	402	HEM	CHB-C1B-NB	4.00	129.31	124.37
16	AG	102	CDL	OA6-CA5-C11	3.97	120.06	111.50
16	AG	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
12	AC	403	HEM	CHB-C1B-NB	3.96	129.26	124.37
12	Ac	401	HEM	CHB-C1B-NB	3.95	129.24	124.37
16	AG	101	CDL	OB6-CB5-C51	3.92	119.94	111.50
12	Ac	402	HEM	CHD-C4C-NC	3.90	128.66	124.44
12	AC	402	HEM	CHB-C1B-NB	3.88	129.16	124.37
12	AC	403	HEM	CHD-C4C-NC	3.87	128.63	124.44
16	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
11	AC	404	3PE	O21-C21-C22	3.70	119.48	111.50
16	Ag	101	CDL	OA6-CA5-C11	3.36	120.17	110.80
16	Aa	502	CDL	OB6-CB5-C51	3.34	120.11	110.80
16	Ag	101	CDL	OB8-CB7-C71	3.33	120.12	111.38
12	AC	402	HEM	C4D-ND-C1D	3.29	108.48	105.07
16	Aa	502	CDL	OB8-CB7-C71	3.29	120.00	111.38
13	Ac	404	U10	C4-C3-C2	-3.28	114.23	120.68
11	Aa	501	3PE	O21-C21-C22	3.27	119.92	110.80
13	AC	405	U10	C4-C3-C2	-3.25	114.30	120.68
12	AC	403	HEM	C1B-NB-C4B	3.23	108.41	105.07
12	AC	403	HEM	CHD-C1D-ND	3.23	127.92	124.42
12	Ac	401	HEM	C4D-ND-C1D	3.21	108.39	105.07
12	Ac	402	HEM	C1B-NB-C4B	3.20	108.38	105.07
12	Ac	402	HEM	CHD-C1D-ND	3.18	127.88	124.42
16	AG	101	CDL	OA6-CA5-C11	3.12	119.49	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AG	101	CDL	OB8-CB7-C71	3.11	119.53	111.38
12	Ac	401	HEM	C1B-NB-C4B	3.09	108.27	105.07
12	AC	402	HEM	C1B-NB-C4B	3.07	108.24	105.07
12	AC	402	HEM	CHD-C1D-ND	2.88	127.55	124.42
16	AG	102	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
12	Ac	401	HEM	CHD-C1D-ND	2.83	127.49	124.42
16	AG	102	CDL	CB4-OB6-CB5	-2.79	110.93	117.79
16	Aa	502	CDL	CB4-OB6-CB5	-2.73	111.07	117.79
11	Ac	403	3PE	C2-O21-C21	-2.72	111.08	117.79
12	Ac	402	HEM	C4C-NC-C1C	2.71	108.00	105.35
16	Ag	101	CDL	CA4-OA6-CA5	-2.69	111.16	117.79
11	Ac	403	3PE	O31-C31-C32	2.68	120.31	111.91
12	AC	403	HEM	C4C-NC-C1C	2.66	107.96	105.35
17	Ae	301	PC1	O31-C31-C32	2.66	120.25	111.91
12	AC	402	HEM	CHA-C1A-NA	2.64	128.71	123.85
13	AC	405	U10	C7-C6-C5	2.64	121.66	118.48
11	AC	404	3PE	O31-C31-C32	2.63	120.17	111.91
15	AD	401	HEC	CAA-CBA-CGA	-2.62	107.96	113.60
16	AG	101	CDL	OA8-CA7-C31	2.62	120.11	111.91
16	Aa	502	CDL	CA4-OA6-CA5	-2.61	111.36	117.79
16	AG	101	CDL	CB4-OB6-CB5	-2.60	111.38	117.79
12	AC	402	HEM	CHA-C4D-ND	2.59	127.57	124.37
13	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
17	Ae	301	PC1	C2-O21-C21	-2.59	111.42	117.79
12	Ac	401	HEM	CHA-C1A-NA	2.58	128.60	123.85
15	Ad	401	HEC	CAA-CBA-CGA	-2.58	108.05	113.60
13	Ac	404	U10	O4-C4-C5	-2.55	107.94	116.56
13	AC	405	U10	O4-C4-C5	-2.55	107.95	116.56
11	Aa	501	3PE	O31-C31-C32	2.53	119.85	111.91
16	Ag	101	CDL	OA8-CA7-C31	2.49	119.71	111.91
12	Ac	401	HEM	CHA-C4D-ND	2.47	127.42	124.37
16	AG	102	CDL	OB8-CB7-C71	2.46	119.61	111.91
16	AG	102	CDL	OA8-CA7-C31	2.45	119.59	111.91
12	Ac	402	HEM	C4A-CHB-C1B	-2.45	120.53	126.34
12	AC	403	HEM	C4A-NA-C1A	2.44	107.74	105.35
12	Ac	402	HEM	CHB-C1B-C2B	-2.43	119.98	126.73
11	AG	103	3PE	O31-C31-C32	2.43	119.52	111.91
12	AC	403	HEM	C4A-CHB-C1B	-2.43	120.58	126.34
16	Aa	502	CDL	OA8-CA7-C31	2.42	119.51	111.91
12	AC	403	HEM	CHB-C1B-C2B	-2.42	120.00	126.73
12	Ac	402	HEM	C4A-NA-C1A	2.42	107.71	105.35
17	Ae	301	PC1	C11-C12-N	-2.41	107.73	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Ac	401	HEM	C4B-C3B-C2B	-2.37	105.23	107.11
11	AC	404	3PE	C2-O21-C21	-2.37	111.96	117.79
12	AC	402	HEM	C4B-C3B-C2B	-2.37	105.24	107.11
12	AC	403	HEM	CHA-C4D-ND	2.32	127.24	124.37
12	Ac	401	HEM	C4A-NA-C1A	2.30	107.60	105.35
16	AG	101	CDL	CA4-OA6-CA5	-2.29	112.16	117.79
12	AC	402	HEM	C4A-NA-C1A	2.29	107.59	105.35
16	Ag	101	CDL	CB4-OB6-CB5	-2.27	112.20	117.79
12	Ac	402	HEM	CHA-C4D-ND	2.26	127.16	124.37
12	Ac	401	HEM	CHB-C1B-C2B	-2.24	120.50	126.73
12	Ac	402	HEM	CHA-C1A-NA	2.24	127.97	123.85
12	Ac	402	HEM	C4C-CHD-C1D	-2.23	121.24	126.06
12	AC	402	HEM	CHB-C1B-C2B	-2.23	120.53	126.73
11	AC	401	3PE	C2-O21-C21	2.23	123.29	117.79
12	Ac	402	HEM	C1C-CHC-C4B	-2.23	121.24	126.06
12	AC	403	HEM	CHA-C1A-NA	2.23	127.95	123.85
12	AC	403	HEM	C4C-CHD-C1D	-2.23	121.25	126.06
11	AG	103	3PE	C2-O21-C21	-2.22	112.31	117.79
12	AC	403	HEM	C1C-CHC-C4B	-2.22	121.27	126.06
12	Ac	401	HEM	C4C-NC-C1C	2.21	107.51	105.35
12	AC	402	HEM	C4C-NC-C1C	2.19	107.50	105.35
15	AD	401	HEC	CHA-C4D-ND	2.17	126.78	124.42
15	Ad	401	HEC	CHA-C4D-ND	2.17	126.77	124.42
12	AC	403	HEM	C2A-C1A-NA	-2.16	107.73	110.15
15	Ad	401	HEC	C3C-C4C-NC	-2.13	107.77	110.15
12	Ac	402	HEM	C2A-C1A-NA	-2.13	107.77	110.15
15	AD	401	HEC	C3C-C4C-NC	-2.10	107.80	110.15
12	AC	402	HEM	C1C-CHC-C4B	-2.09	121.54	126.06
12	Ac	401	HEM	C1C-CHC-C4B	-2.09	121.55	126.06
15	AD	401	HEC	C2A-C1A-NA	-2.08	108.30	110.32
15	Ad	401	HEC	C4A-NA-C1A	2.08	107.38	105.35
12	AC	403	HEM	CAD-C3D-C4D	2.07	128.28	124.66
15	Ad	401	HEC	C4C-NC-C1C	2.06	107.37	105.35
15	AD	401	HEC	C4A-NA-C1A	2.05	107.35	105.35
12	Ac	402	HEM	CAD-C3D-C4D	2.04	128.22	124.66
12	Ac	401	HEM	C4A-CHB-C1B	-2.04	121.50	126.34
13	Ac	404	U10	C3M-O3-C3	2.04	123.69	116.47
12	AC	402	HEM	CAA-CBA-CGA	-2.03	109.23	113.60
12	Ac	401	HEM	CAA-CBA-CGA	-2.03	109.23	113.60
13	AC	405	U10	C3M-O3-C3	2.03	123.66	116.47
12	AC	402	HEM	C4A-CHB-C1B	-2.03	121.53	126.34
15	Ad	401	HEC	C4B-NB-C1B	2.03	107.17	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AD	401	HEC	C4C-NC-C1C	2.02	107.33	105.35
13	AC	405	U10	O4-C4-C3	2.02	131.26	123.64
15	Ad	401	HEC	C2A-C1A-NA	-2.01	108.37	110.32
13	Ac	404	U10	O4-C4-C3	2.00	131.20	123.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	AD	401	HEC	NA
15	Ad	401	HEC	NA

All (172) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	401	3PE	C11-O13-P-O12
11	AC	401	3PE	O13-C11-C12-N
11	AG	103	3PE	C1-O11-P-O12
11	AG	103	3PE	C1-O11-P-O13
11	AG	103	3PE	C1-O11-P-O14
11	AG	103	3PE	C11-O13-P-O14
11	Aa	501	3PE	C11-O13-P-O12
11	Ag	103	3PE	C1-O11-P-O12
11	Ag	103	3PE	C1-O11-P-O14
11	Ag	103	3PE	C11-O13-P-O11
11	Ag	103	3PE	O13-C11-C12-N
12	AC	402	HEM	C2B-C3B-CAB-CBB
12	AC	402	HEM	C2C-C3C-CAC-CBC
12	AC	402	HEM	C4C-C3C-CAC-CBC
12	AC	403	HEM	C2B-C3B-CAB-CBB
12	AC	403	HEM	C4B-C3B-CAB-CBB
12	AC	403	HEM	C2C-C3C-CAC-CBC
12	Ac	401	HEM	C2B-C3B-CAB-CBB
12	Ac	401	HEM	C2C-C3C-CAC-CBC
12	Ac	401	HEM	C4C-C3C-CAC-CBC
12	Ac	402	HEM	C2B-C3B-CAB-CBB
12	Ac	402	HEM	C4B-C3B-CAB-CBB
12	Ac	402	HEM	C2C-C3C-CAC-CBC
13	AC	405	U10	C7-C8-C9-C10
13	AC	405	U10	C7-C8-C9-C11
13	Ac	404	U10	C7-C8-C9-C10
13	Ac	404	U10	C7-C8-C9-C11
14	AC	406	UQ6	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	AC	406	UQ6	C7-C8-C9-C10
14	AC	406	UQ6	C7-C8-C9-C11
14	AC	406	UQ6	C12-C13-C14-C15
14	AC	406	UQ6	C12-C13-C14-C16
14	AC	406	UQ6	C13-C14-C16-C17
14	AC	406	UQ6	C15-C14-C16-C17
14	AC	406	UQ6	C17-C18-C19-C20
14	Ac	405	UQ6	C1-C6-C7-C8
14	Ac	405	UQ6	C7-C8-C9-C10
14	Ac	405	UQ6	C7-C8-C9-C11
14	Ac	405	UQ6	C12-C13-C14-C15
14	Ac	405	UQ6	C12-C13-C14-C16
14	Ac	405	UQ6	C13-C14-C16-C17
14	Ac	405	UQ6	C15-C14-C16-C17
14	Ac	405	UQ6	C17-C18-C19-C20
16	AG	101	CDL	CA2-OA2-PA1-OA4
16	AG	101	CDL	CB2-OB2-PB2-OB3
16	AG	102	CDL	C1-CB2-OB2-PB2
16	AG	102	CDL	CB2-OB2-PB2-OB4
16	AG	102	CDL	CB3-OB5-PB2-OB2
16	AG	102	CDL	CB3-OB5-PB2-OB3
16	AG	102	CDL	CB3-OB5-PB2-OB4
16	Aa	502	CDL	CA2-OA2-PA1-OA5
16	Aa	502	CDL	CA3-OA5-PA1-OA3
16	Aa	502	CDL	CB2-OB2-PB2-OB3
16	Aa	502	CDL	CB2-OB2-PB2-OB4
16	Ag	101	CDL	CB2-OB2-PB2-OB3
16	Ag	101	CDL	CB2-OB2-PB2-OB4
16	Ag	101	CDL	CB2-OB2-PB2-OB5
16	Ag	101	CDL	CB3-OB5-PB2-OB2
16	Ag	101	CDL	CB3-OB5-PB2-OB3
16	Ag	101	CDL	CB3-OB5-PB2-OB4
16	Ag	102	CDL	CB2-OB2-PB2-OB5
16	Ag	102	CDL	CB3-OB5-PB2-OB4
17	Ae	301	PC1	C1-O11-P-O12
17	Ae	301	PC1	O13-C11-C12-N
13	AC	405	U10	C12-C13-C14-C15
13	AC	405	U10	C12-C13-C14-C16
13	Ac	404	U10	C12-C13-C14-C15
13	Ac	404	U10	C12-C13-C14-C16
14	AC	406	UQ6	C17-C18-C19-C21
14	Ac	405	UQ6	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
17	Ae	301	PC1	O32-C31-O31-C3
11	Aa	501	3PE	C22-C21-O21-C2
17	Ae	301	PC1	C32-C31-O31-C3
14	AC	406	UQ6	C9-C11-C12-C13
14	AC	406	UQ6	C14-C16-C17-C18
14	Ac	405	UQ6	C9-C11-C12-C13
14	Ac	405	UQ6	C14-C16-C17-C18
11	Aa	501	3PE	O22-C21-O21-C2
11	Ag	103	3PE	C32-C33-C34-C35
11	AC	401	3PE	C11-O13-P-O11
11	AG	103	3PE	C11-O13-P-O11
11	Ag	103	3PE	C1-O11-P-O13
16	AG	101	CDL	CB2-OB2-PB2-OB5
16	AG	102	CDL	CB2-OB2-PB2-OB5
16	Aa	502	CDL	CB2-OB2-PB2-OB5
16	Aa	502	CDL	CB3-OB5-PB2-OB2
16	Ag	102	CDL	CB3-OB5-PB2-OB2
11	AG	103	3PE	C32-C33-C34-C35
11	Ag	103	3PE	C3C-C3D-C3E-C3F
16	AG	101	CDL	C31-CA7-OA8-CA6
16	Aa	502	CDL	C51-CB5-OB6-CB4
11	Ag	103	3PE	C37-C38-C39-C3A
16	Ag	102	CDL	C74-C75-C76-C77
16	Aa	502	CDL	OB7-CB5-OB6-CB4
11	AG	103	3PE	C37-C38-C39-C3A
16	AG	101	CDL	OA9-CA7-OA8-CA6
16	AG	102	CDL	C31-CA7-OA8-CA6
16	AG	102	CDL	C74-C75-C76-C77
12	AC	402	HEM	C4B-C3B-CAB-CBB
12	AC	403	HEM	C4C-C3C-CAC-CBC
12	Ac	401	HEM	C4B-C3B-CAB-CBB
12	Ac	402	HEM	C4C-C3C-CAC-CBC
16	AG	102	CDL	C51-CB5-OB6-CB4
11	Aa	501	3PE	C11-O13-P-O11
16	AG	101	CDL	CA2-OA2-PA1-OA5
16	Ag	102	CDL	C1-CB2-OB2-PB2
16	AG	102	CDL	OA9-CA7-OA8-CA6
17	Ae	301	PC1	C2-C1-O11-P
16	Ag	102	CDL	OB5-CB3-CB4-CB6
16	Aa	502	CDL	C71-CB7-OB8-CB6
12	AC	402	HEM	C2A-CAA-CBA-CGA
12	Ac	401	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	Ae	301	PC1	C1-O11-P-O13
16	Ag	102	CDL	OB5-CB3-CB4-OB6
16	AG	102	CDL	OB7-CB5-OB6-CB4
16	AG	102	CDL	C1-CA2-OA2-PA1
11	Aa	501	3PE	C3-C2-O21-C21
16	Aa	502	CDL	OB9-CB7-OB8-CB6
16	AG	102	CDL	CB4-CB3-OB5-PB2
16	Ag	102	CDL	CB4-CB3-OB5-PB2
11	AC	401	3PE	C11-O13-P-O14
11	AG	103	3PE	C11-O13-P-O12
11	Aa	501	3PE	C11-O13-P-O14
11	Ag	103	3PE	C11-O13-P-O12
16	AG	101	CDL	CA2-OA2-PA1-OA3
16	AG	101	CDL	CB2-OB2-PB2-OB4
16	Aa	502	CDL	CA2-OA2-PA1-OA4
16	Aa	502	CDL	CB3-OB5-PB2-OB3
16	Aa	502	CDL	CB3-OB5-PB2-OB4
16	Ag	102	CDL	CB2-OB2-PB2-OB4
17	Ae	301	PC1	C1-O11-P-O14
16	Ag	102	CDL	C1-CA2-OA2-PA1
16	AG	102	CDL	C71-CB7-OB8-CB6
16	AG	102	CDL	OB9-CB7-OB8-CB6
11	Ag	103	3PE	C35-C36-C37-C38
11	AG	103	3PE	C35-C36-C37-C38
16	Ag	101	CDL	C1-CA2-OA2-PA1
13	AC	405	U10	C12-C11-C9-C10
13	Ac	404	U10	C12-C11-C9-C10
12	AC	403	HEM	CAD-CBD-CGD-O1D
12	Ac	402	HEM	CAD-CBD-CGD-O1D
12	AC	402	HEM	CAD-CBD-CGD-O1D
12	AC	402	HEM	CAD-CBD-CGD-O2D
12	Ac	401	HEM	CAD-CBD-CGD-O2D
12	AC	402	HEM	CAA-CBA-CGA-O2A
12	Ac	401	HEM	CAA-CBA-CGA-O2A
12	Ac	401	HEM	CAD-CBD-CGD-O1D
12	AC	403	HEM	CAD-CBD-CGD-O2D
12	Ac	402	HEM	CAD-CBD-CGD-O2D
12	AC	402	HEM	CAA-CBA-CGA-O1A
12	Ac	401	HEM	CAA-CBA-CGA-O1A
13	AC	405	U10	C12-C11-C9-C8
13	Ac	404	U10	C12-C11-C9-C8
14	AC	406	UQ6	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	Ac	405	UQ6	C5-C6-C7-C8
16	Ag	102	CDL	C72-C73-C74-C75
12	AC	403	HEM	CAA-CBA-CGA-O2A
12	Ac	402	HEM	CAA-CBA-CGA-O2A
16	Ag	102	CDL	C52-C51-CB5-OB6
12	Ac	402	HEM	CAA-CBA-CGA-O1A
12	AC	403	HEM	CAA-CBA-CGA-O1A
11	Ac	403	3PE	C23-C24-C25-C26
11	AC	401	3PE	O31-C31-C32-C33
14	AC	406	UQ6	C6-C7-C8-C9
14	Ac	405	UQ6	C6-C7-C8-C9
11	AC	404	3PE	C11-O13-P-O14
11	Aa	501	3PE	C1-O11-P-O14
11	Ac	403	3PE	C11-O13-P-O14
16	Ag	102	CDL	CB2-C1-CA2-OA2
11	Ac	403	3PE	C22-C23-C24-C25
11	AC	401	3PE	O21-C21-C22-C23
11	AC	401	3PE	O32-C31-C32-C33

There are no ring outliers.

22 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	AC	406	UQ6	27	0
11	Aa	501	3PE	7	0
16	AG	101	CDL	8	0
11	Ac	403	3PE	4	0
12	AC	403	HEM	8	0
12	Ac	402	HEM	9	0
15	AD	401	HEC	12	0
12	AC	402	HEM	7	0
16	Ag	101	CDL	4	0
11	AG	103	3PE	16	0
13	Ac	404	U10	21	0
13	AC	405	U10	19	0
15	Ad	401	HEC	11	0
17	Ae	301	PC1	6	0
11	AC	401	3PE	2	0
16	Aa	502	CDL	4	0
11	Ag	103	3PE	1	0
14	Ac	405	UQ6	12	0
11	AC	404	3PE	6	0

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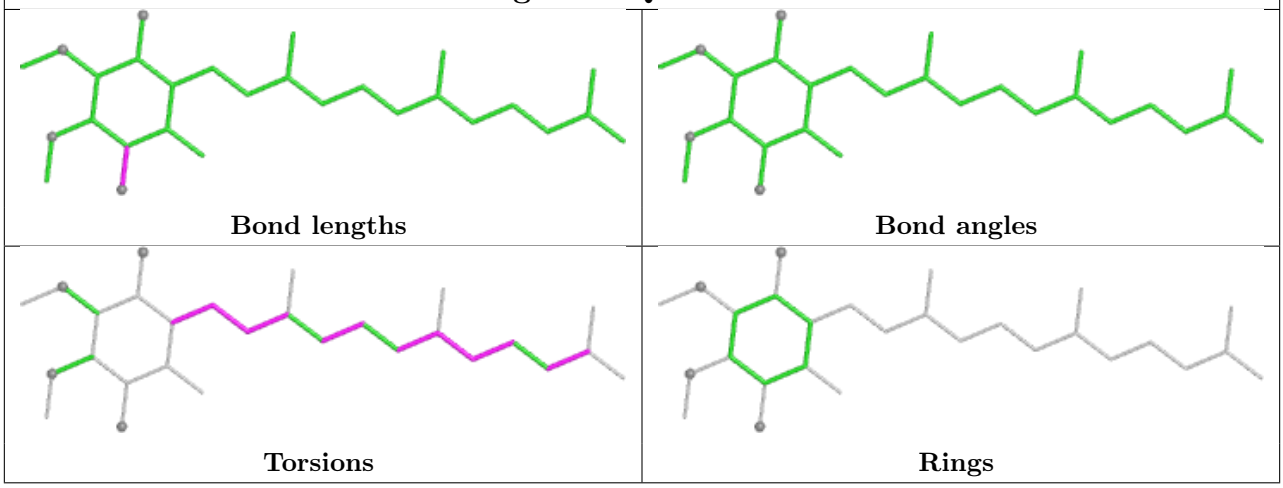
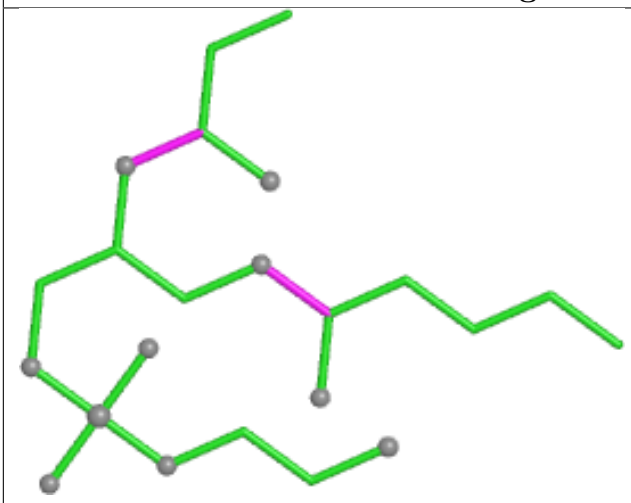
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	AG	102	CDL	8	0
16	Ag	102	CDL	5	0
12	Ac	401	HEM	3	0

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.

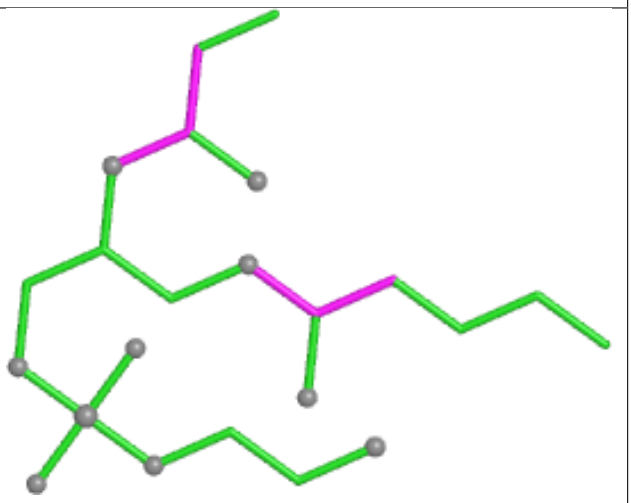
Ligand UQ6 AC 406



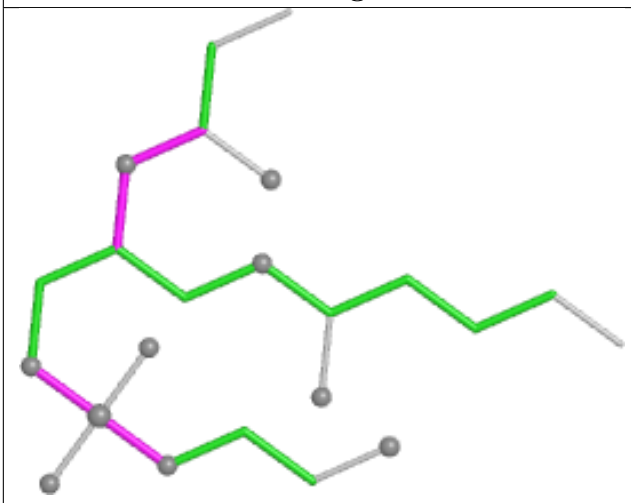
Ligand 3PE Aa 501



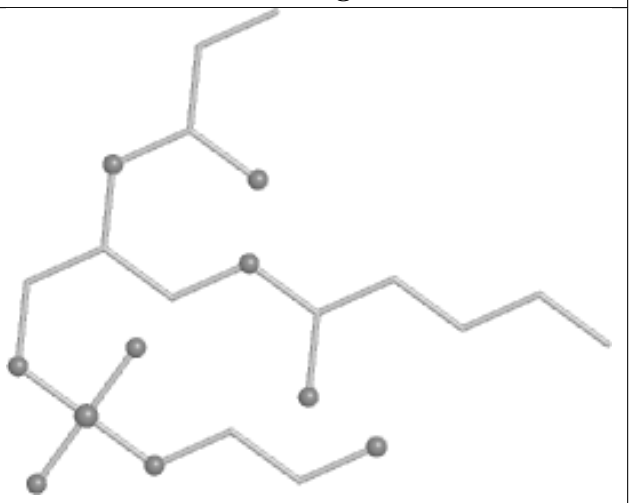
Bond lengths



Bond angles

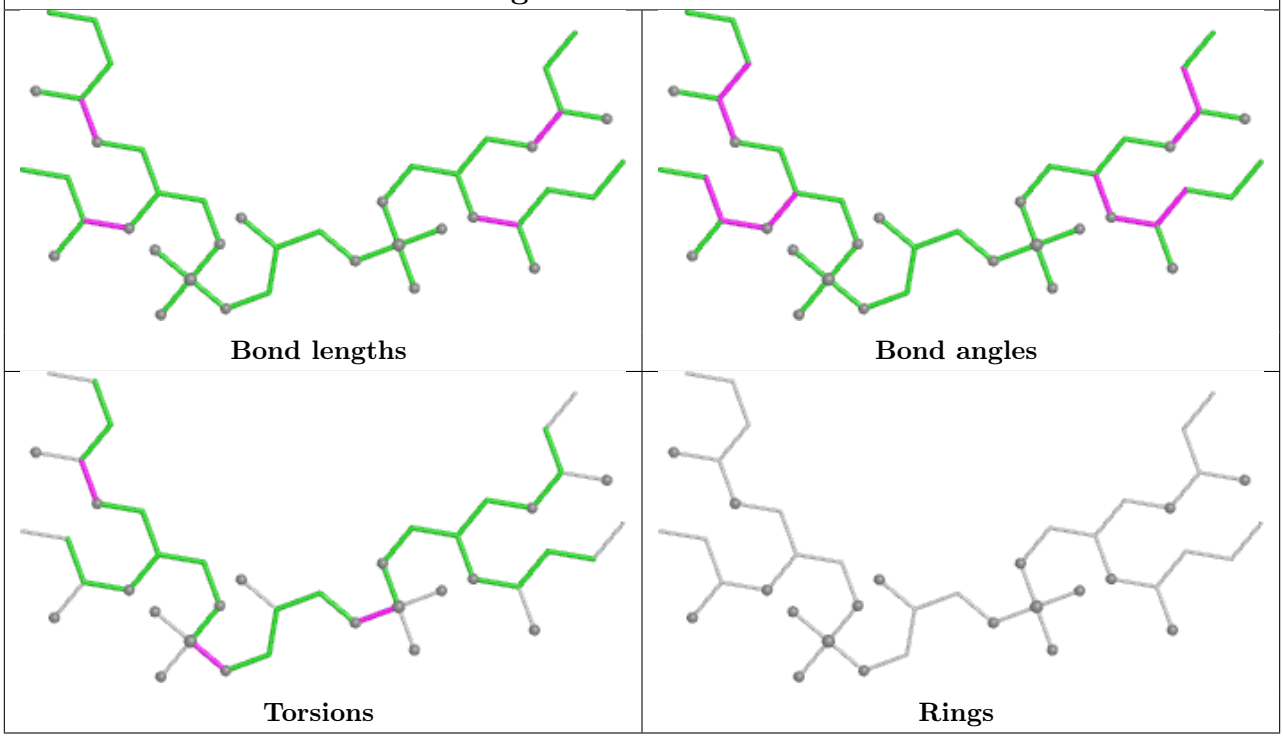


Torsions

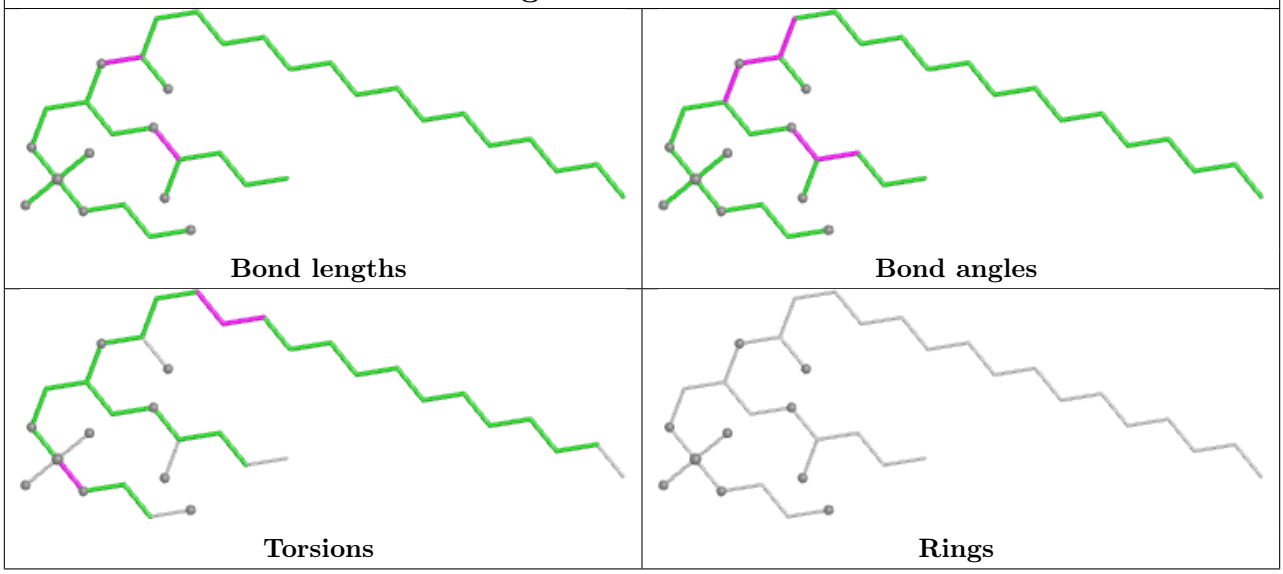


Rings

Ligand CDL AG 101



Ligand 3PE Ac 403



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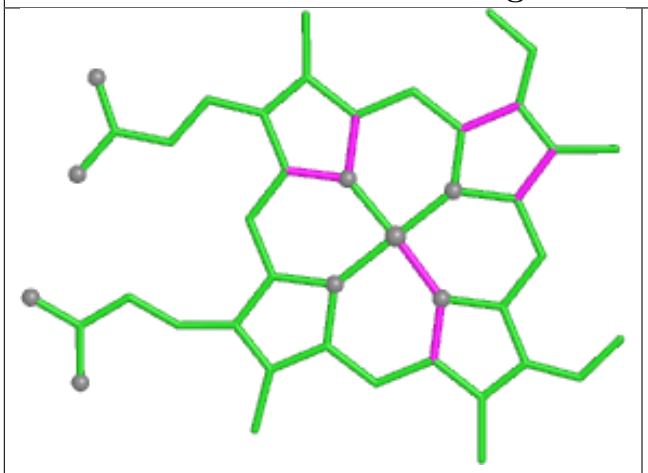

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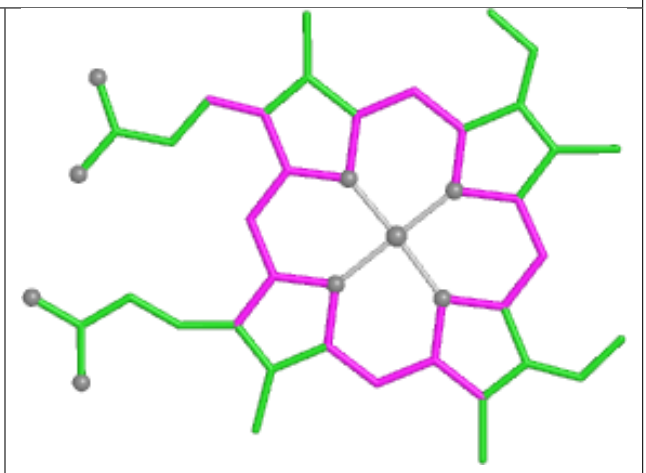
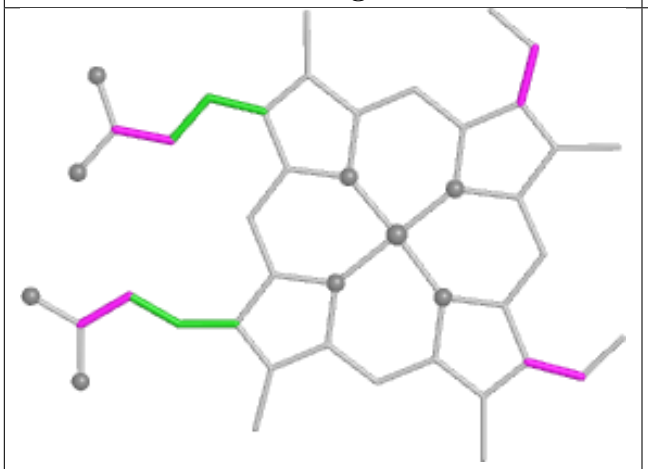


Bond angles



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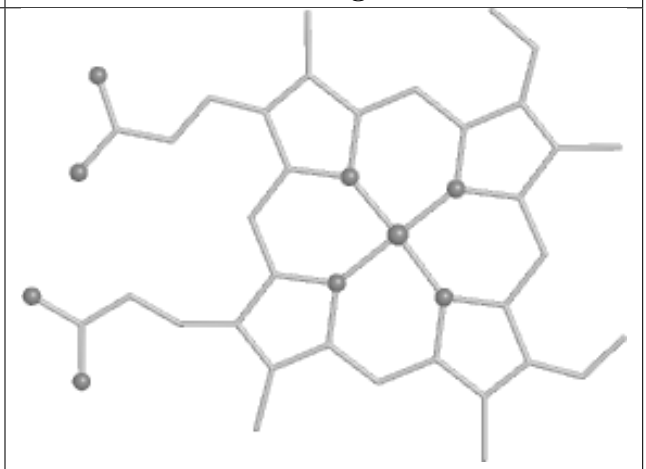
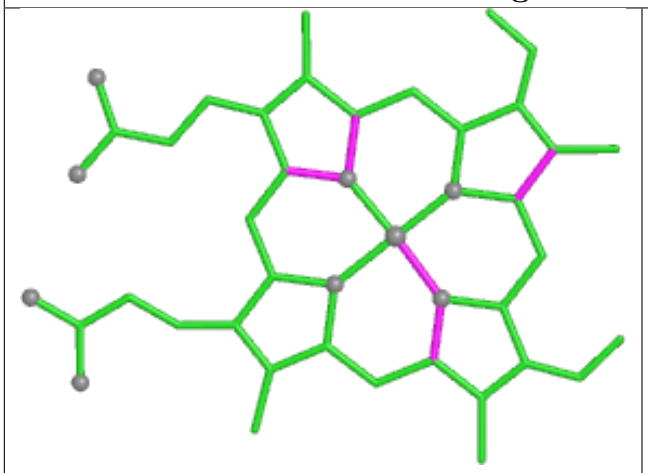


Rings

Ligand HEM Ac 402



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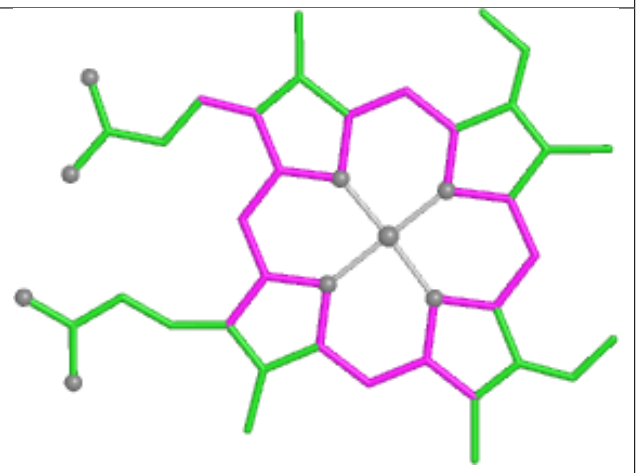
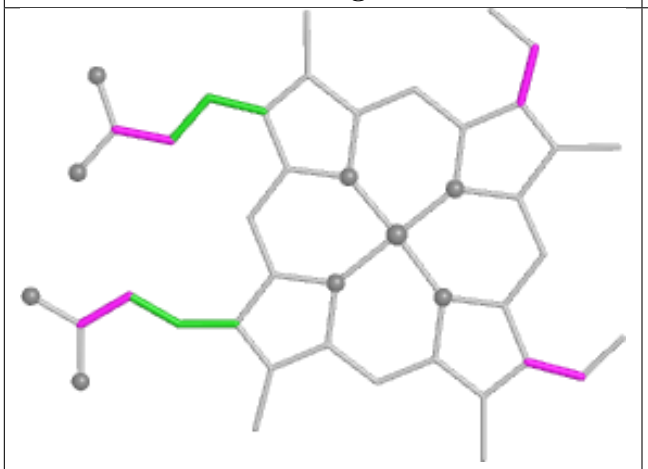
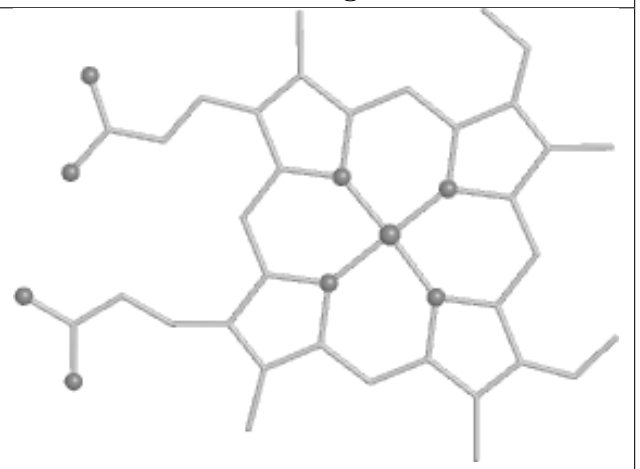


Bond angles

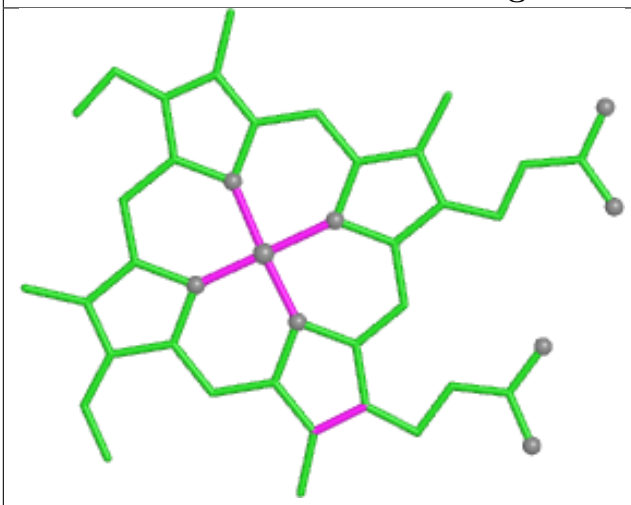


Torsions



Rings

Ligand HEC AD 401



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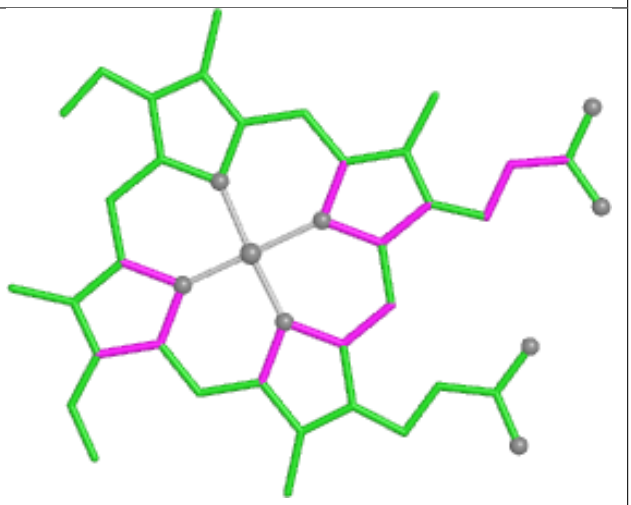
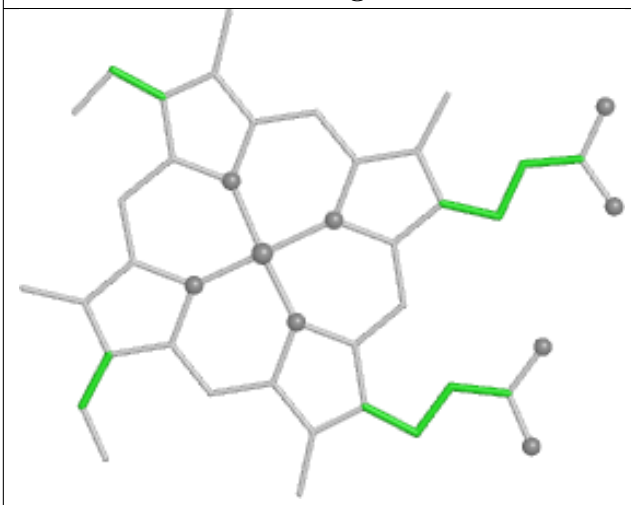


Bond angles



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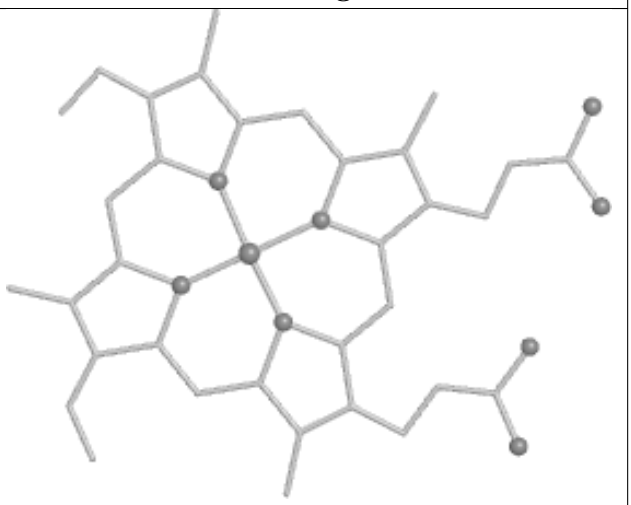
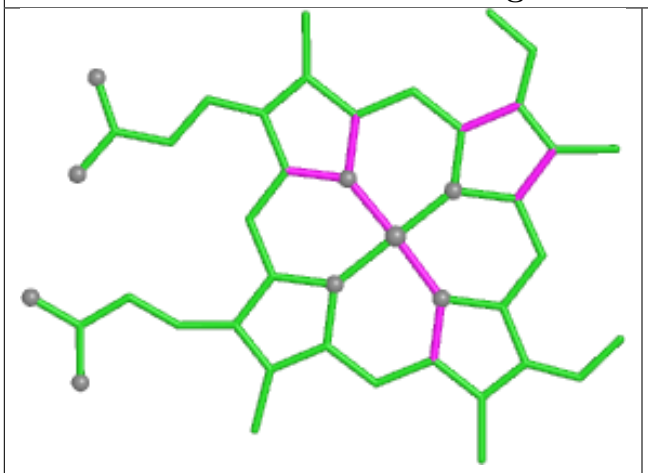


Rings

Ligand HEM AC 402



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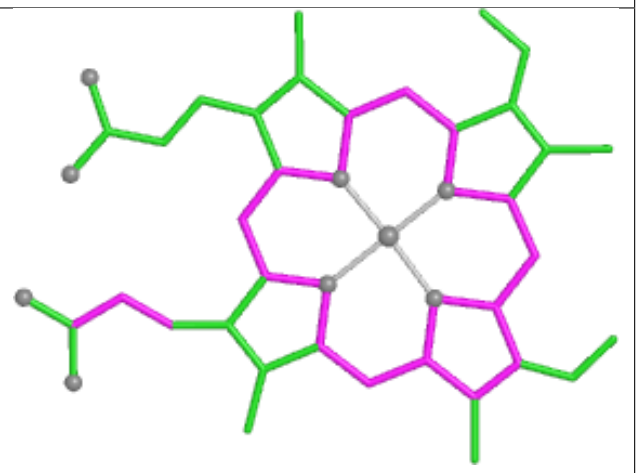
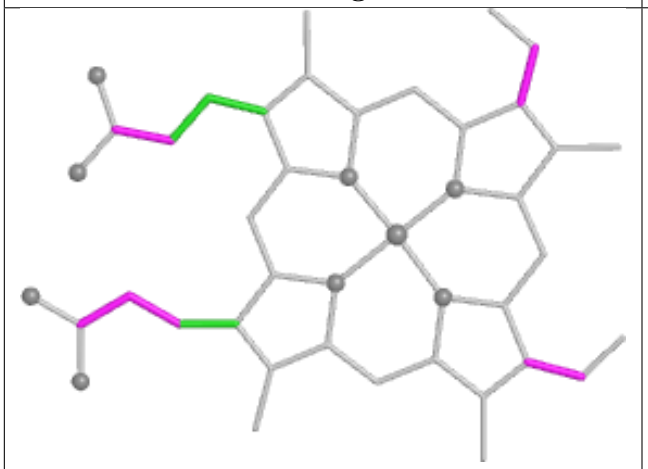


Bond angles



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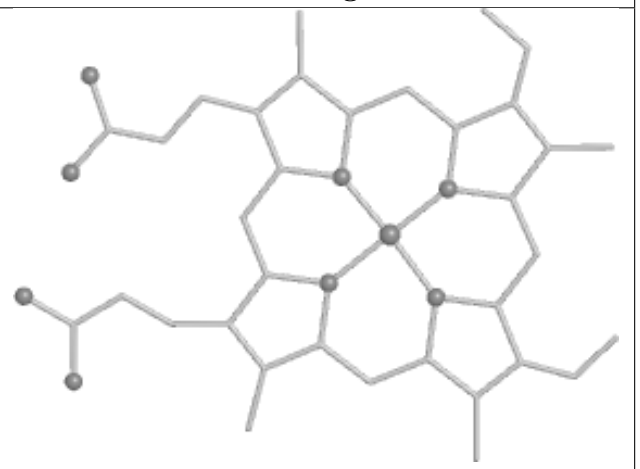
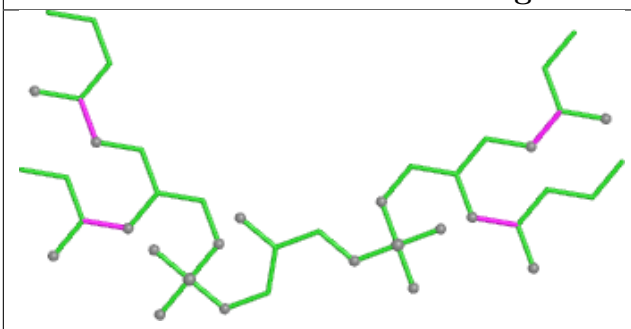


Rings

Ligand CDL Ag 101



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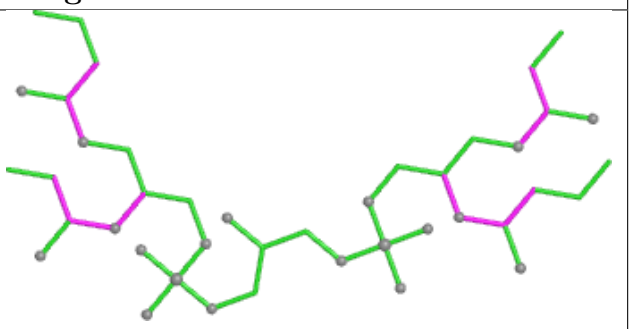
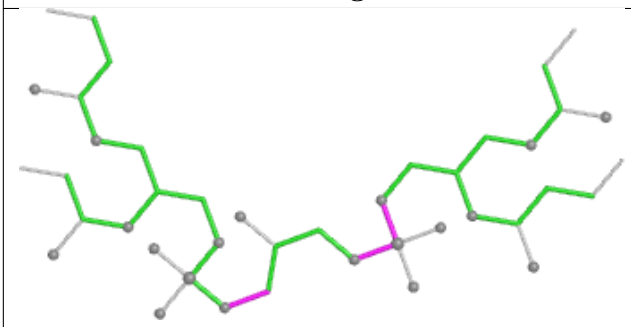


Bond angles



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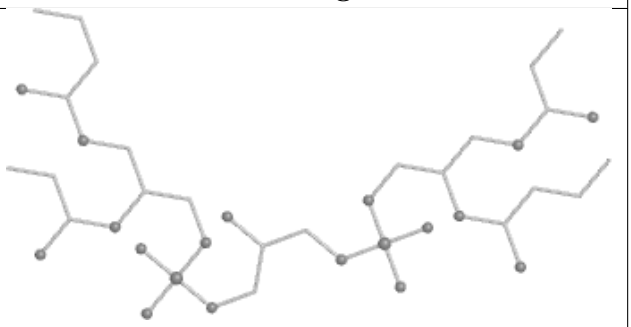
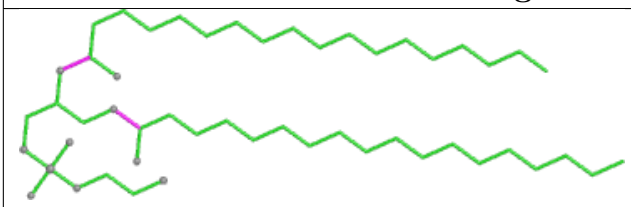
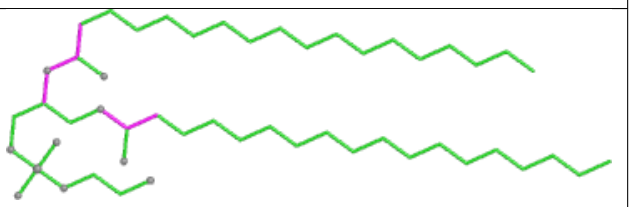


Rings

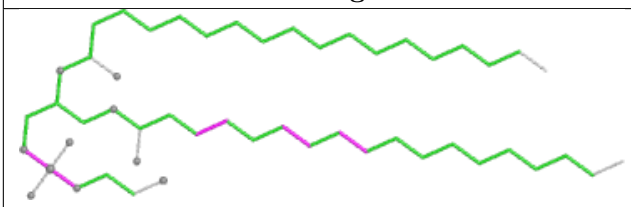
Ligand 3PE AG 103



Bond lengths



Bond angles



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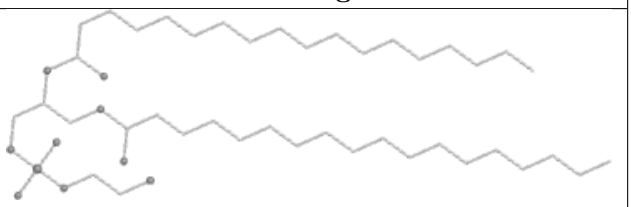
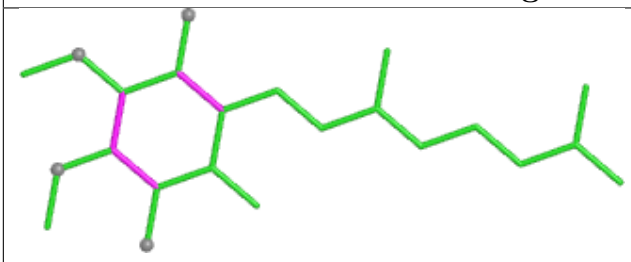
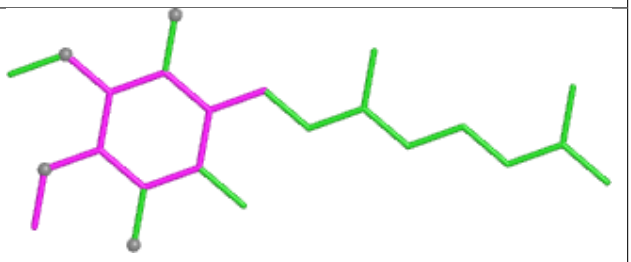
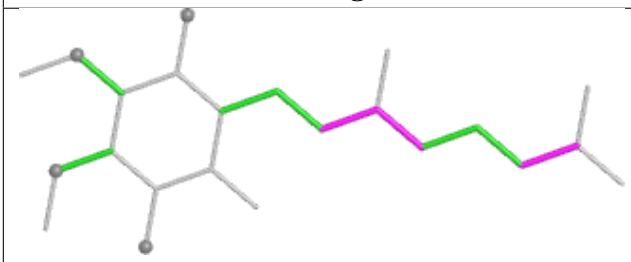
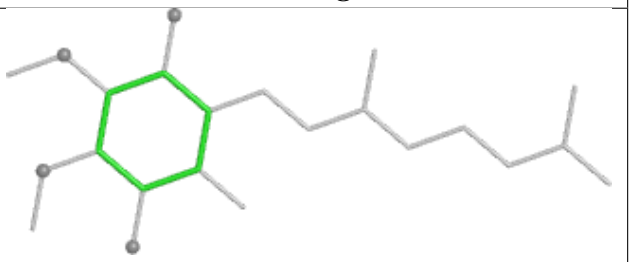
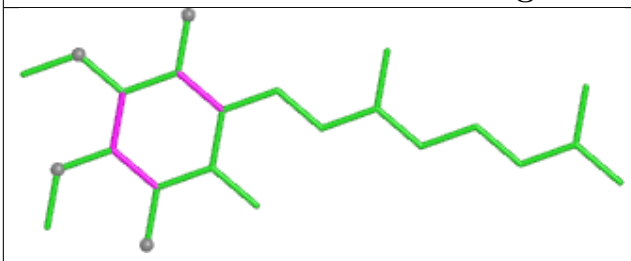
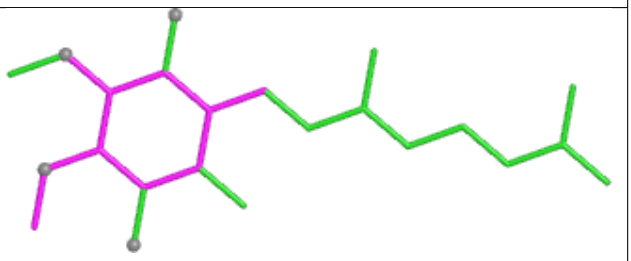
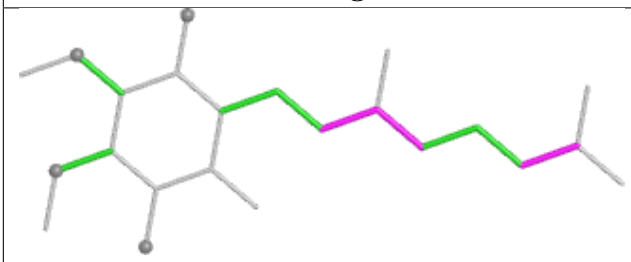
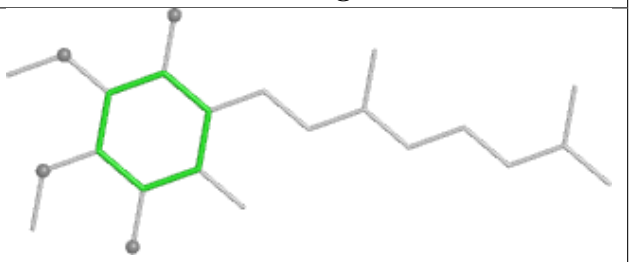
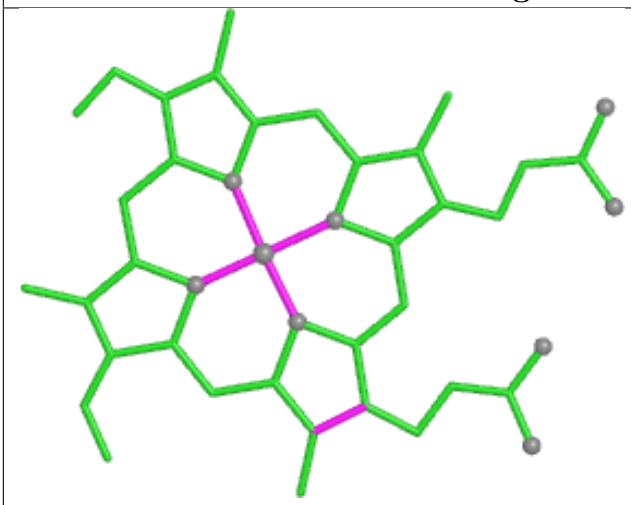


Rings

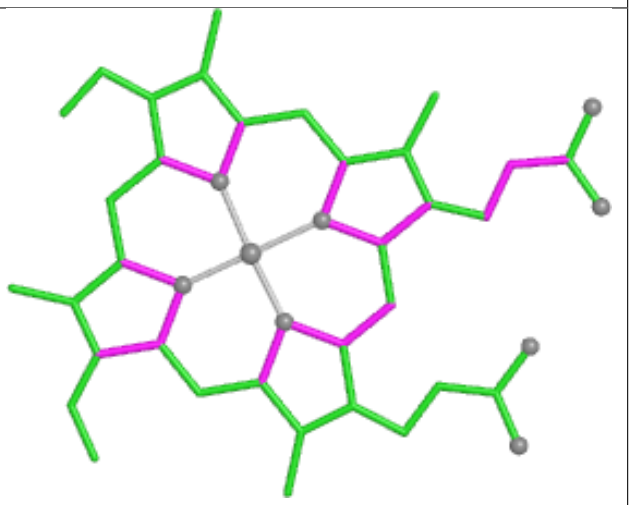
Ligand U10 Ac 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U10 AC 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

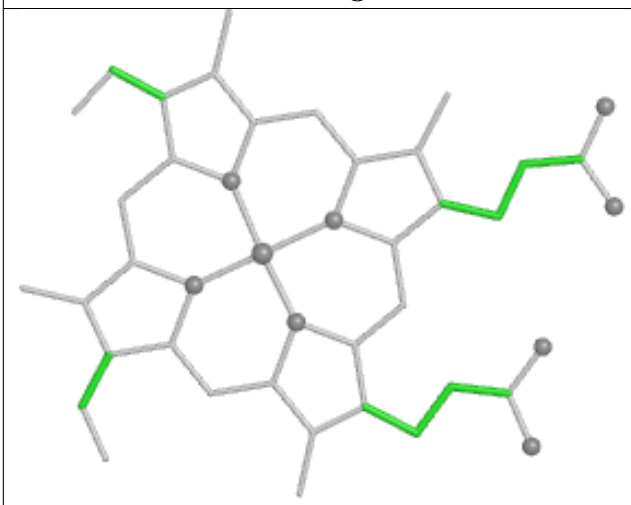
Ligand HEC Ad 401



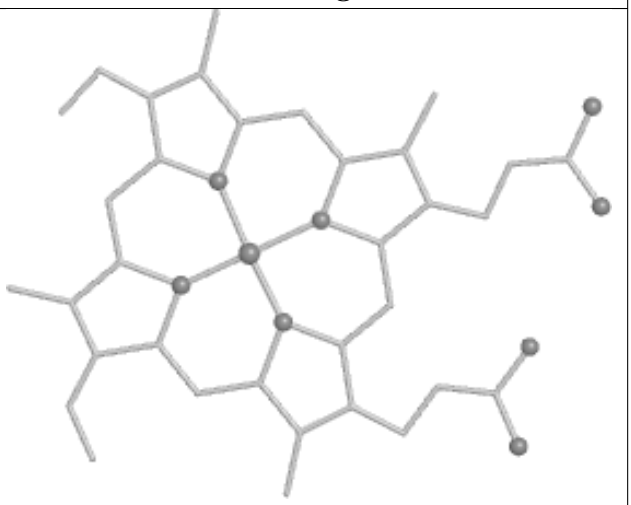
Bond lengths



Bond angles

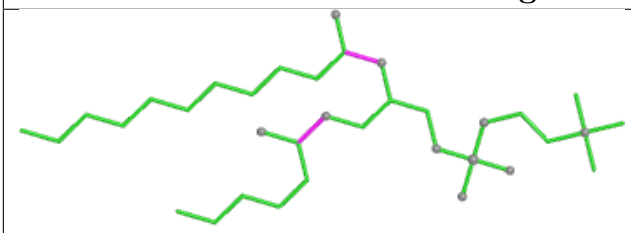


Torsions

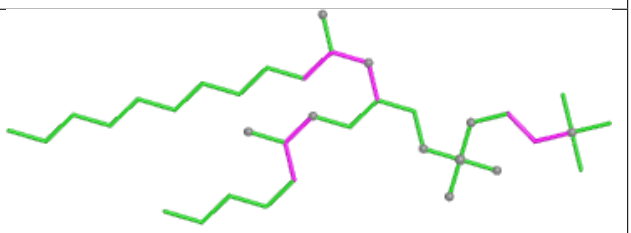


Rings

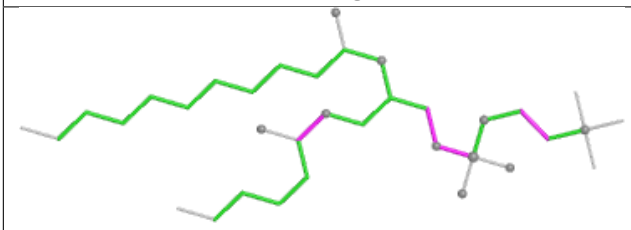
Ligand PC1 Ae 301



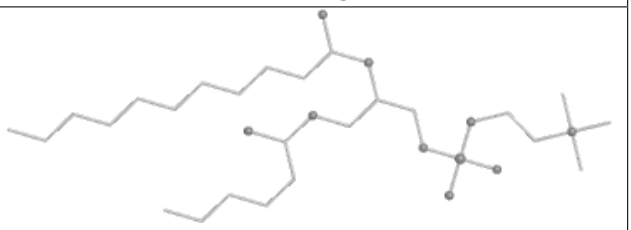
Bond lengths



Bond angles

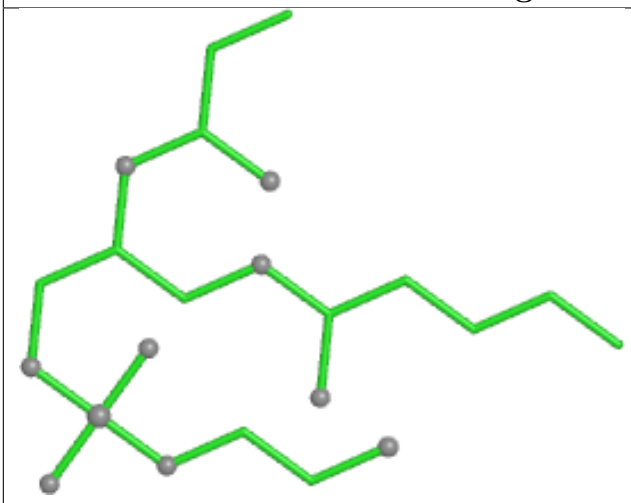


Torsions

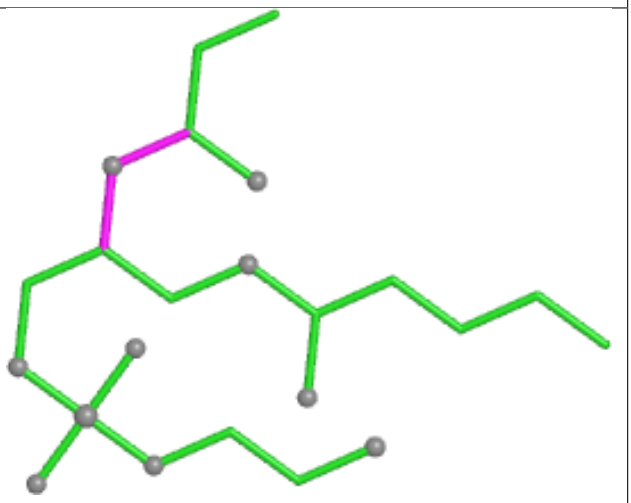


Rings

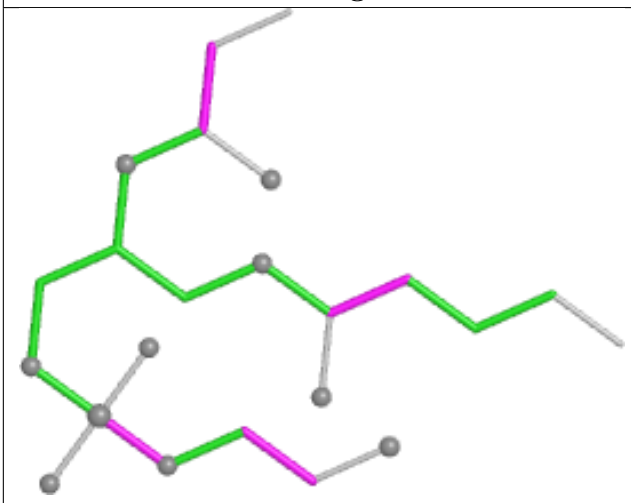
Ligand 3PE AC 401



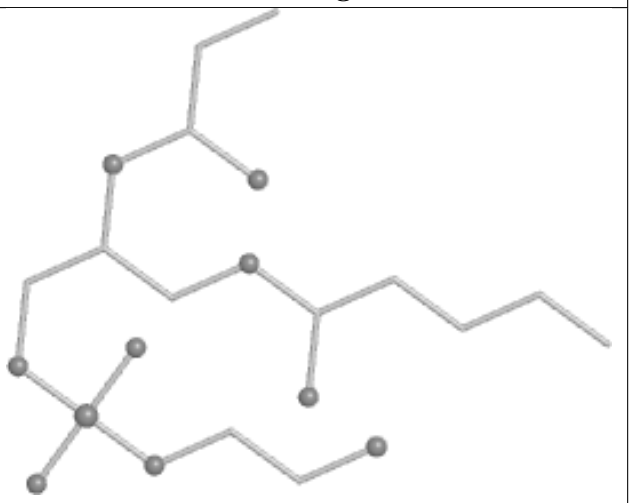
Bond lengths



Bond angles

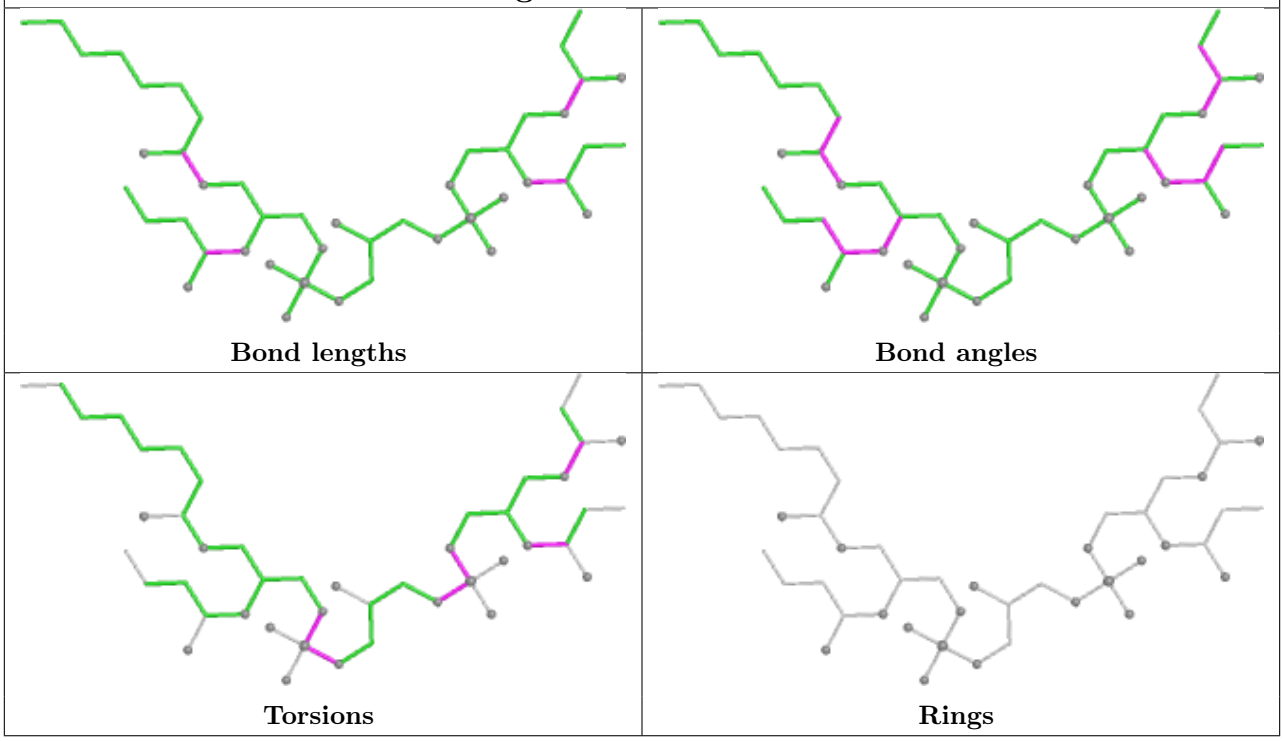


Torsions

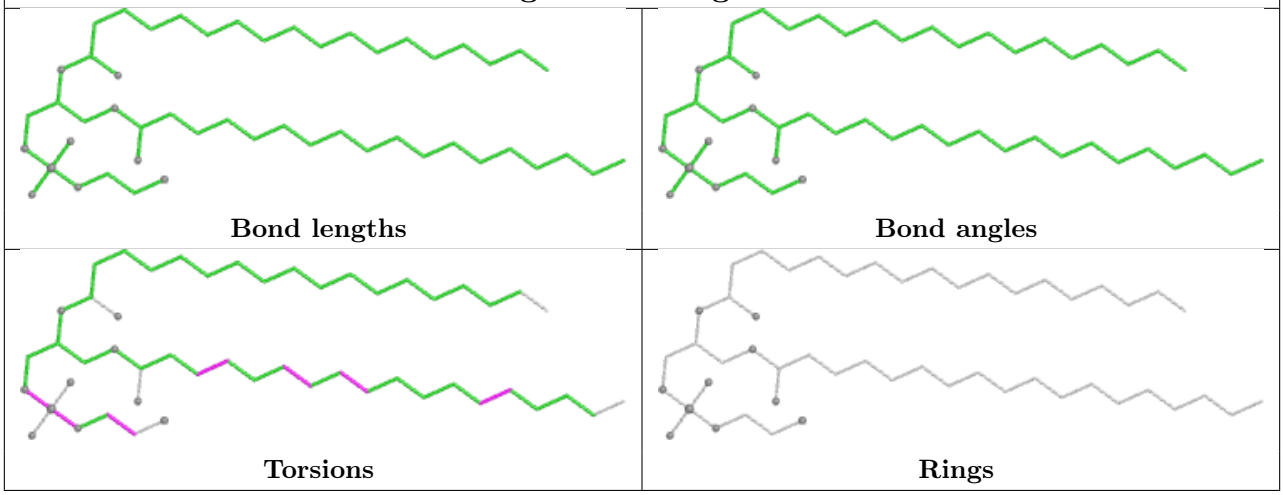


Rings

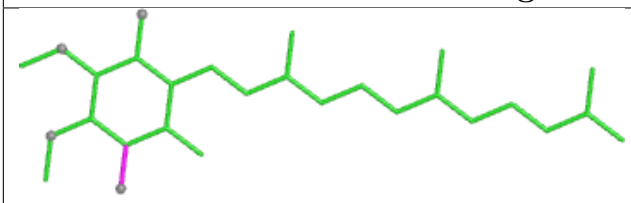
Ligand CDL Aa 502



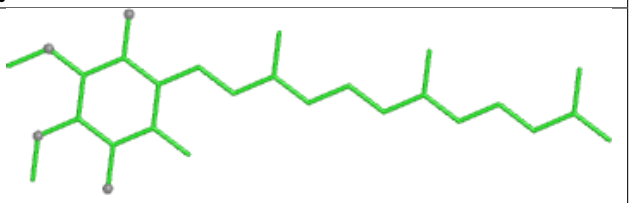
Ligand 3PE Ag 103



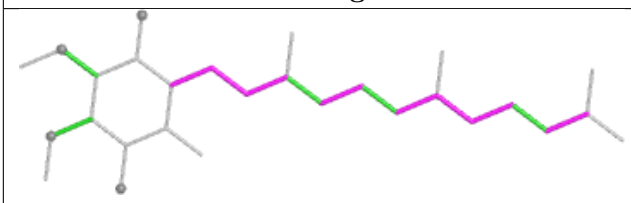
Ligand UQ6 Ac 405



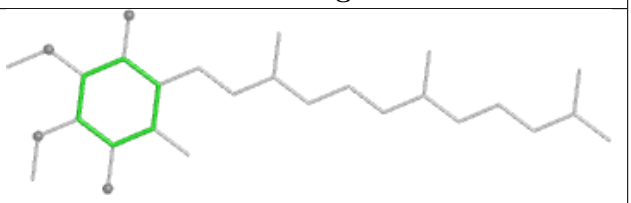
Bond lengths



Bond angles

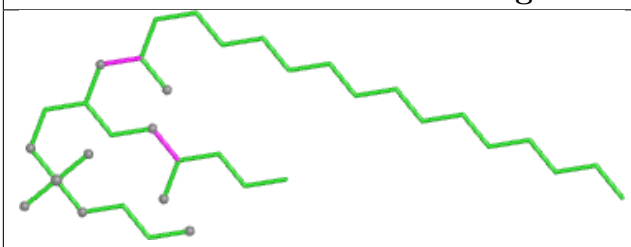


Torsions

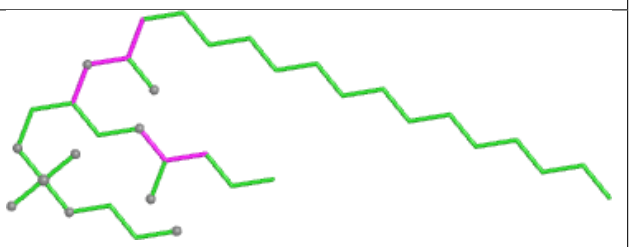


Rings

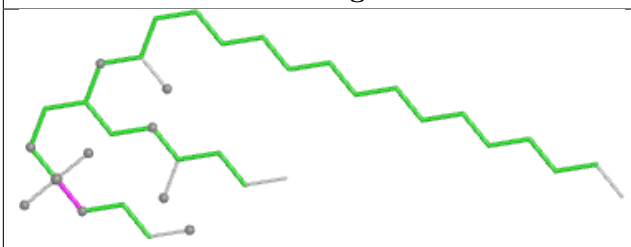
Ligand 3PE AC 404



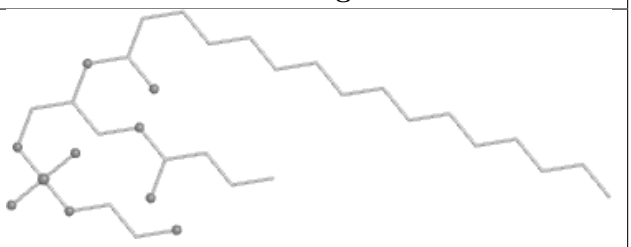
Bond lengths



Bond angles

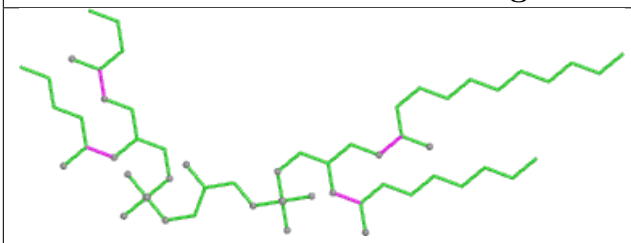


Torsions

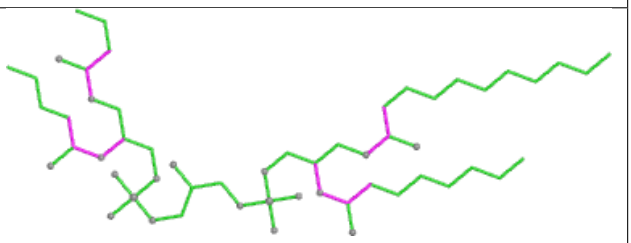


Rings

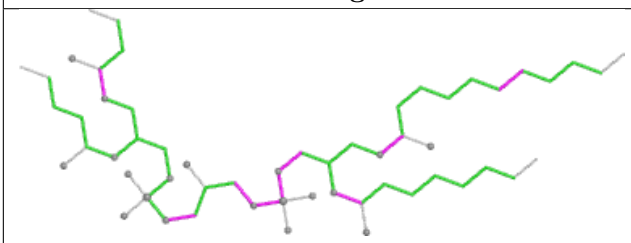
Ligand CDL AG 102



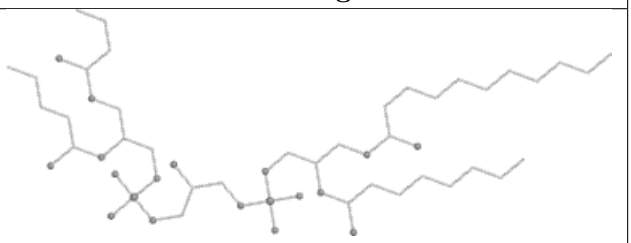
Bond lengths



Bond angles

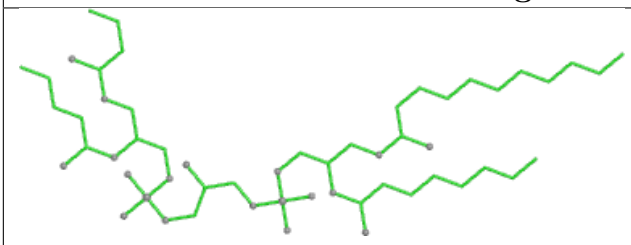


Torsions

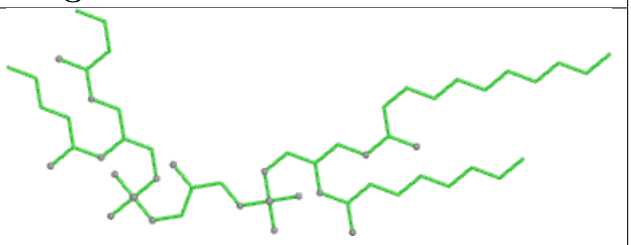


Rings

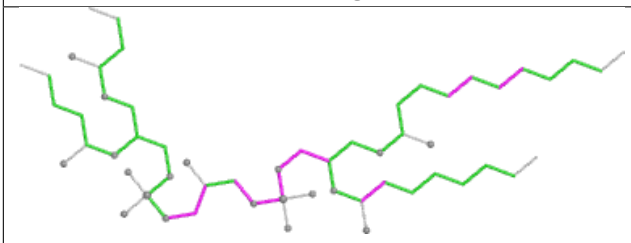
Ligand CDL Ag 102



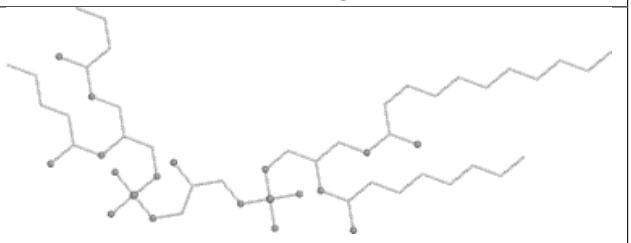
Bond lengths



Bond angles

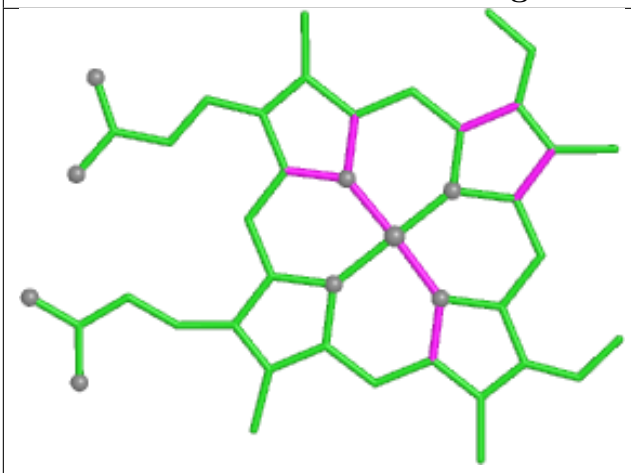


Torsions

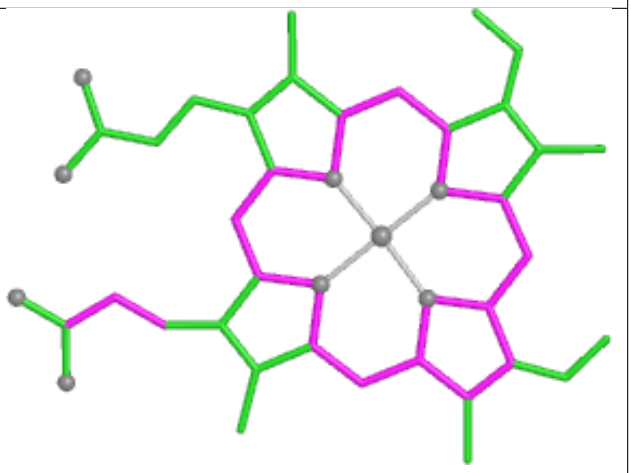


Rings

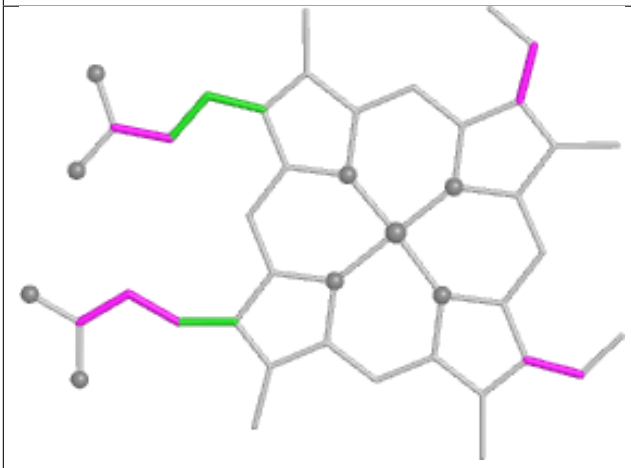
Ligand HEM Ac 401



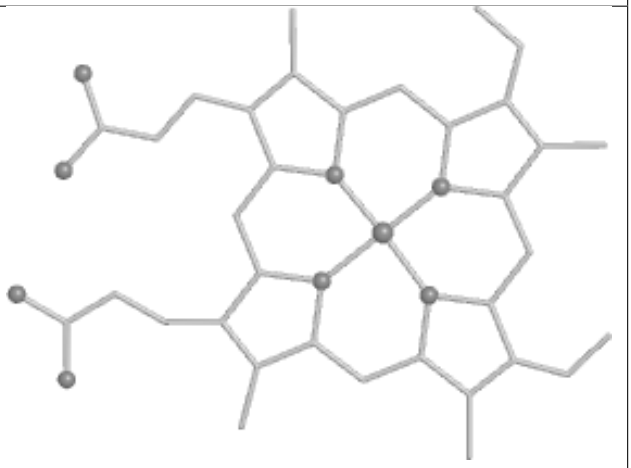
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

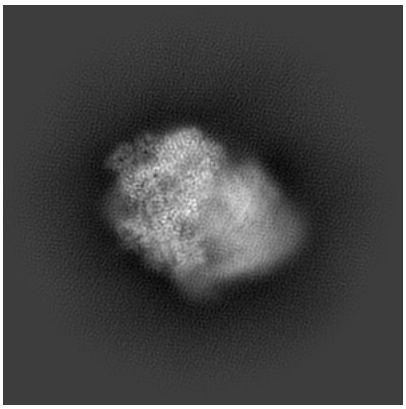
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35316. These allow visual inspection of the internal detail of the map and identification of artifacts.

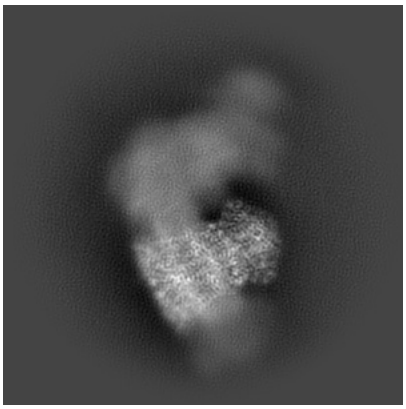
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

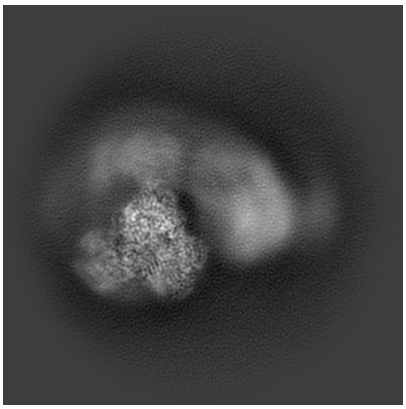
6.1.1 Primary map



X

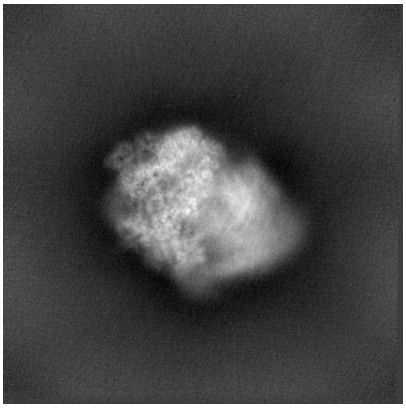


Y

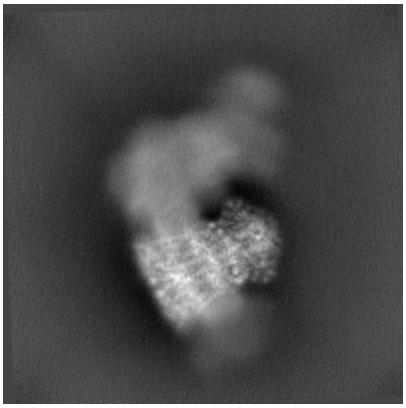


Z

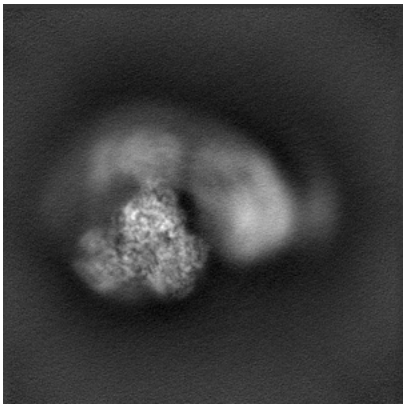
6.1.2 Raw map



X



Y

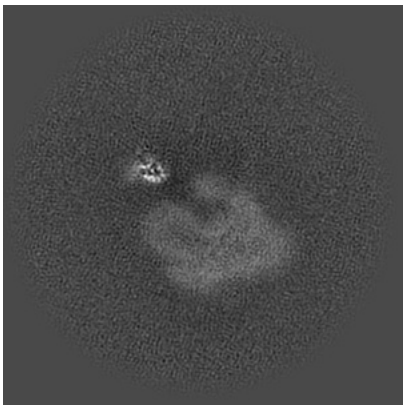


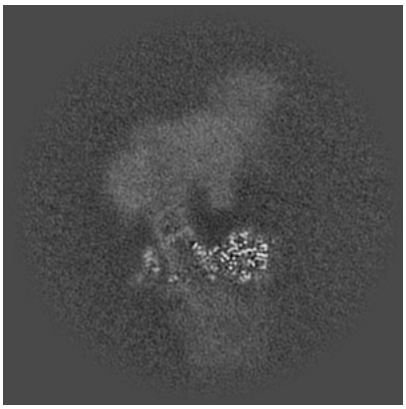
Z

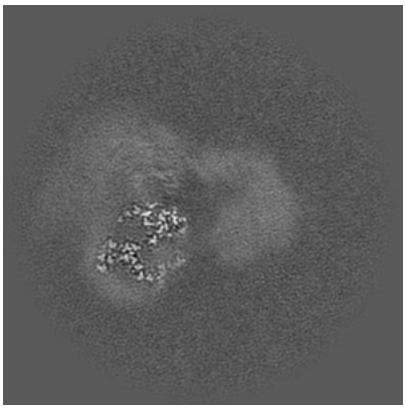
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

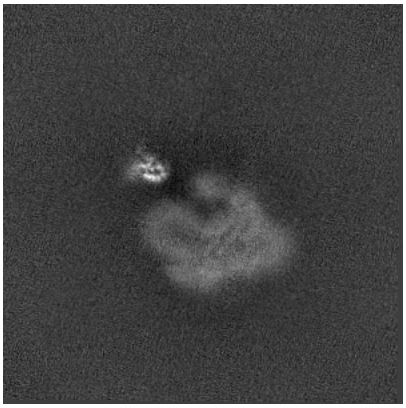
6.2.1 Primary map

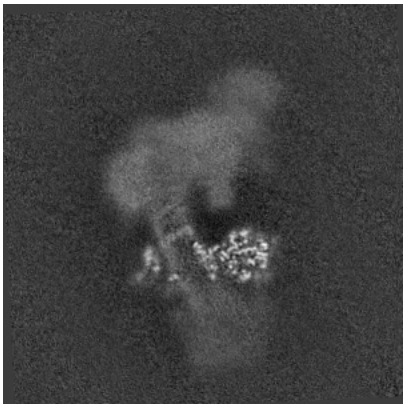

X Index: 192

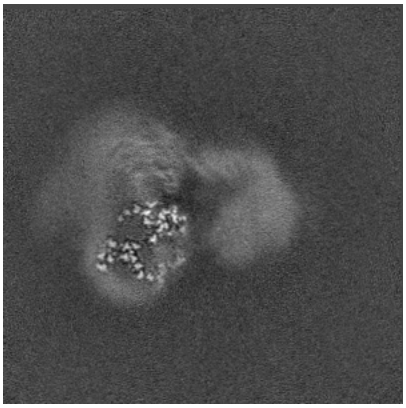

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

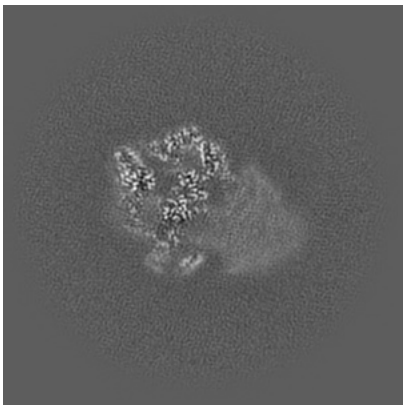

Y Index: 192


Z Index: 192

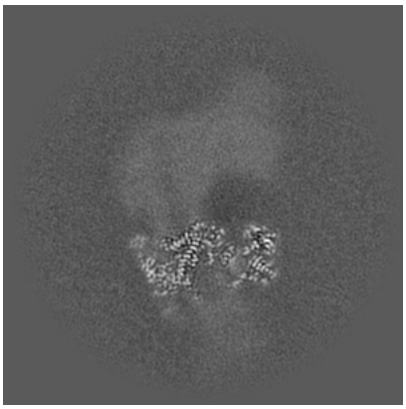
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

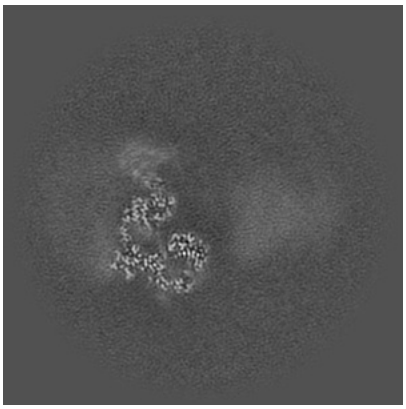
6.3.1 Primary map



X Index: 148

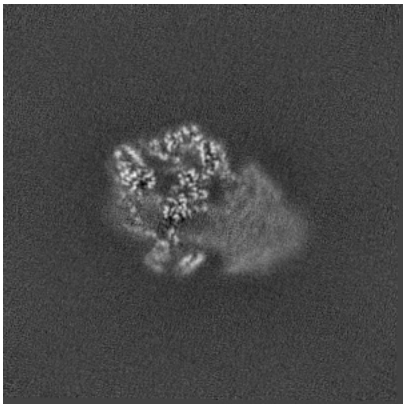


Y Index: 168

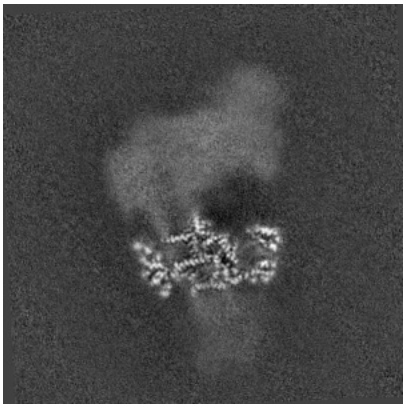


Z Index: 223

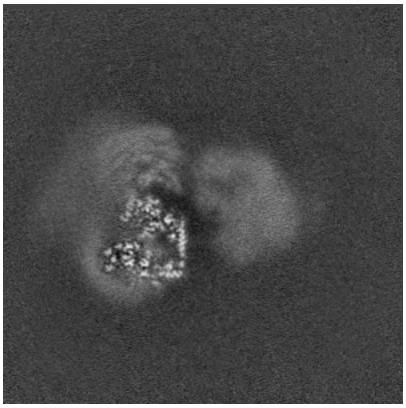
6.3.2 Raw map



X Index: 148



Y Index: 177

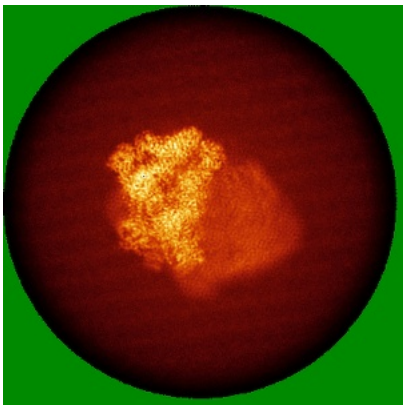


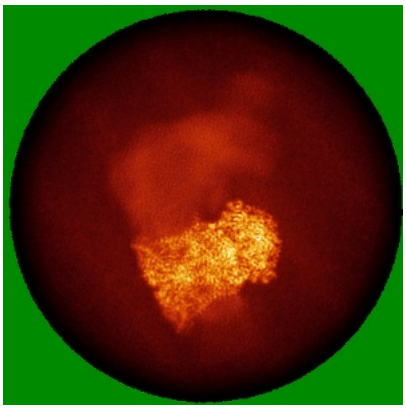
Z Index: 200

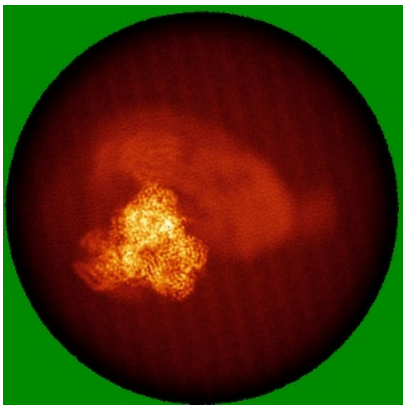
The images above show the largest variance slices of the map in three orthogonal directions.

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

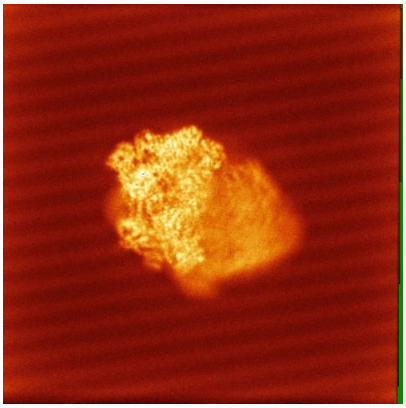
6.4.1 Primary map

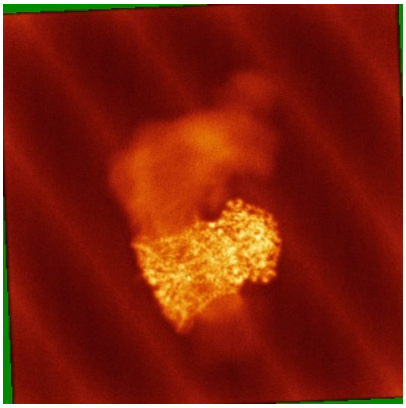

X

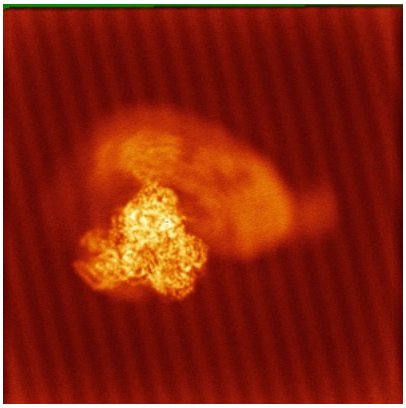

Y


Z

6.4.2 Raw 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 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

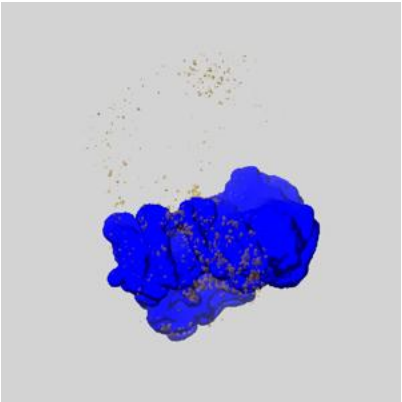
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

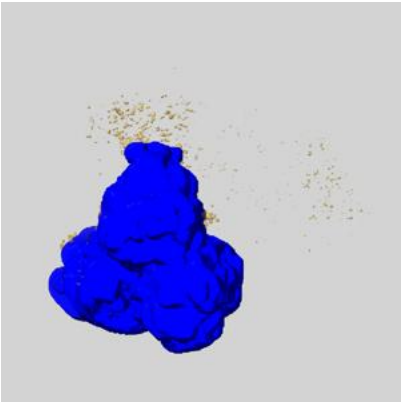
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_35316_msk_1.map (i)

X



Y

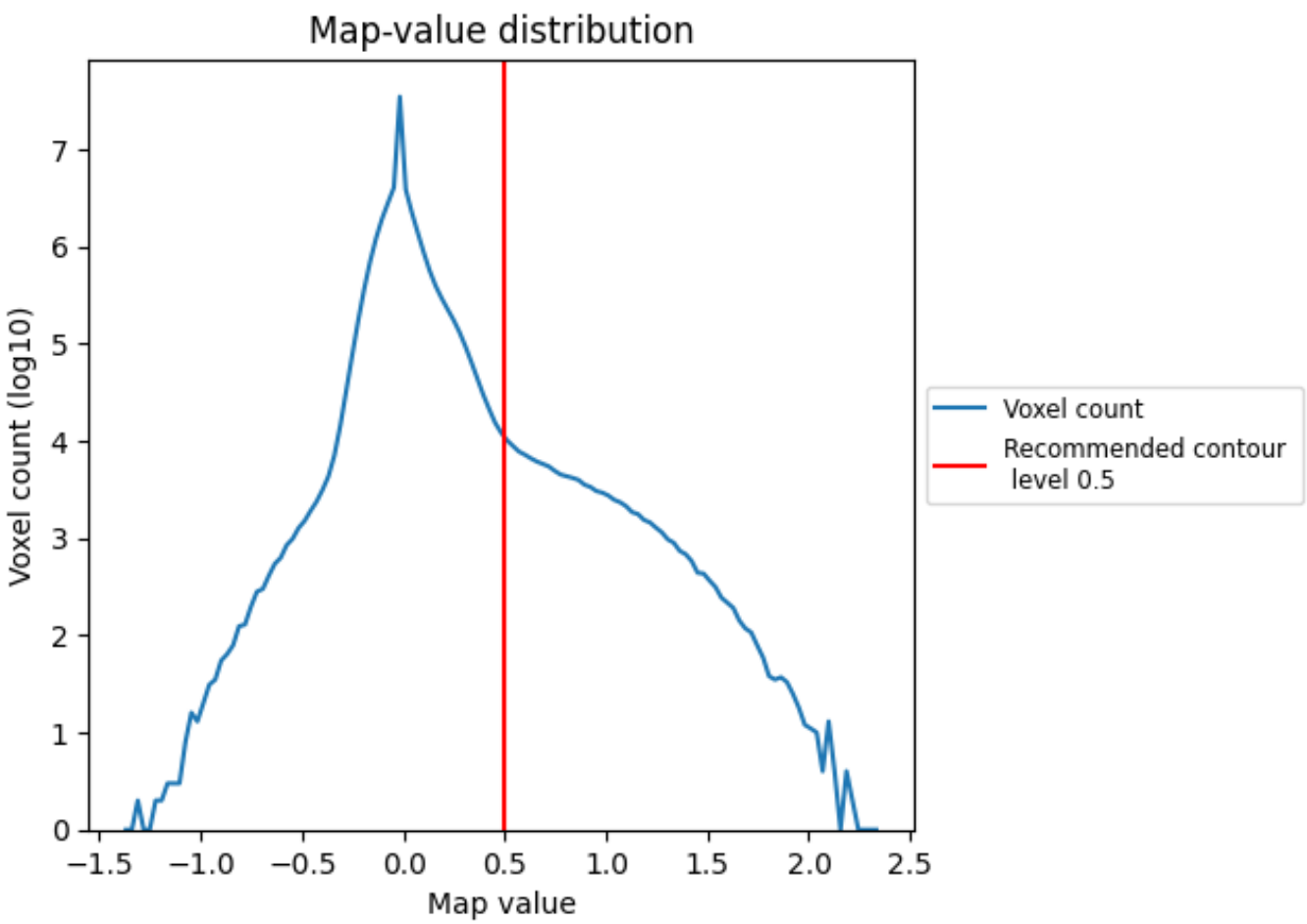


Z

7 Map analysis (i)

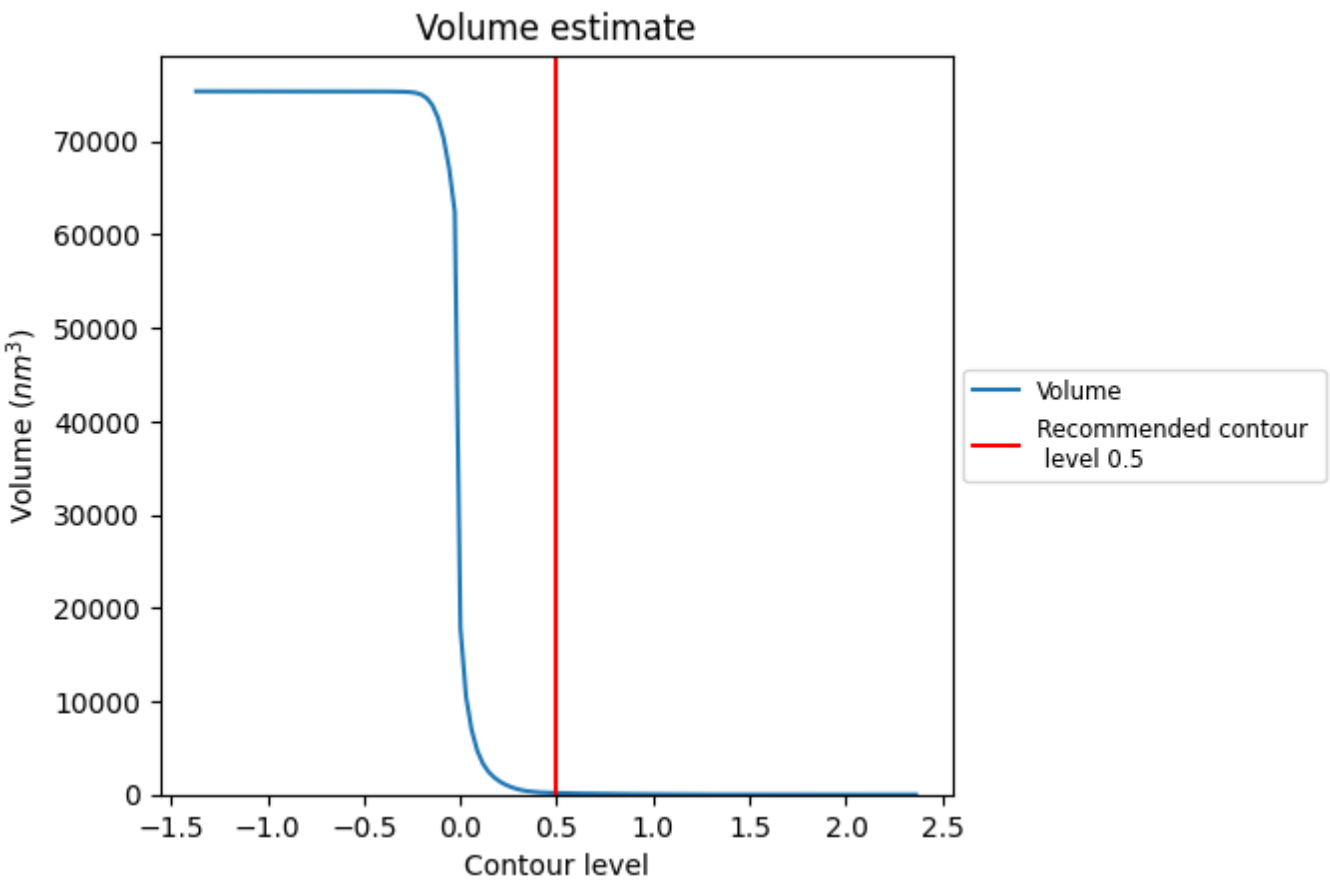
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

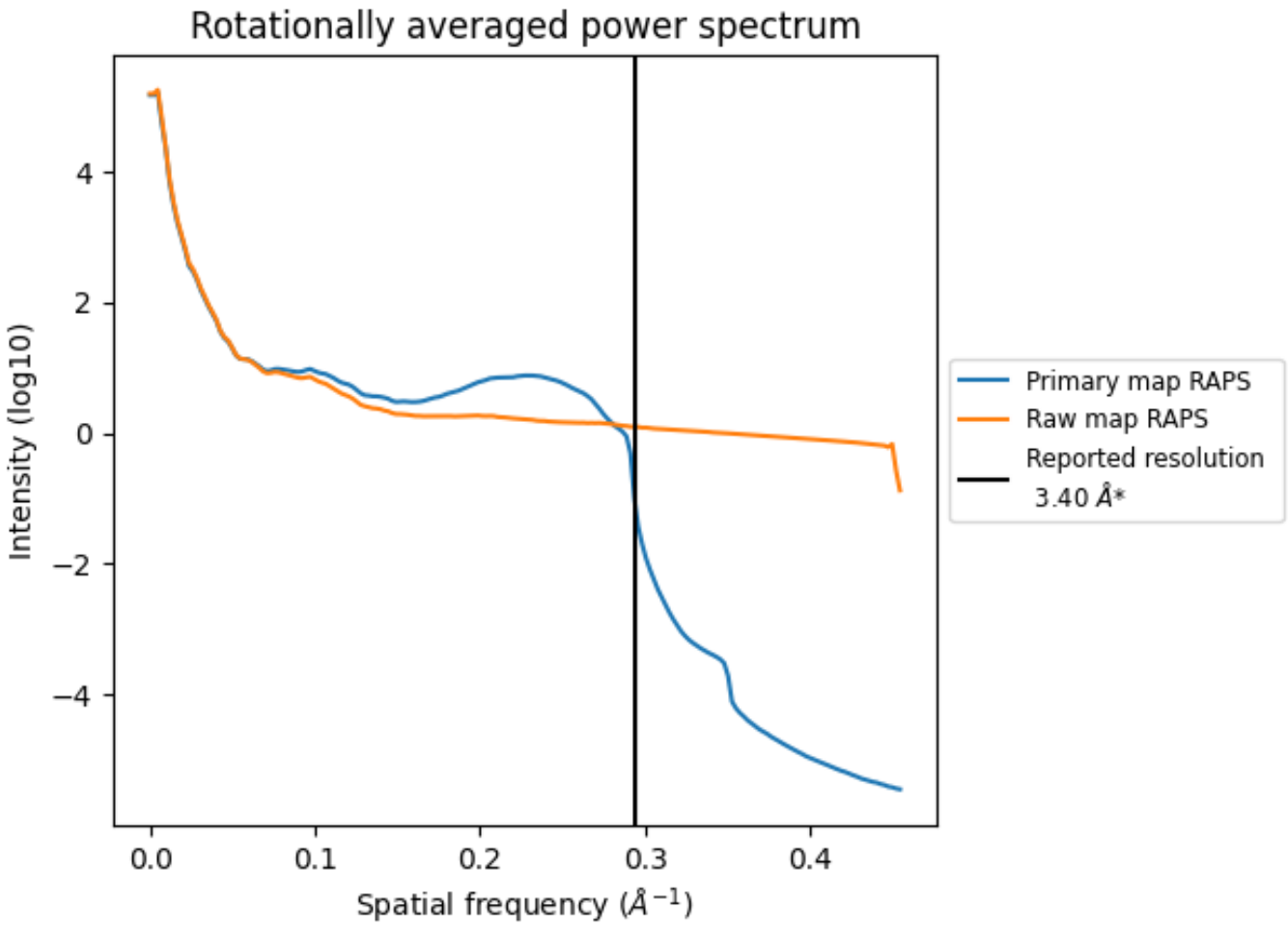
7.2 Volume estimate (i)



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 147 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)

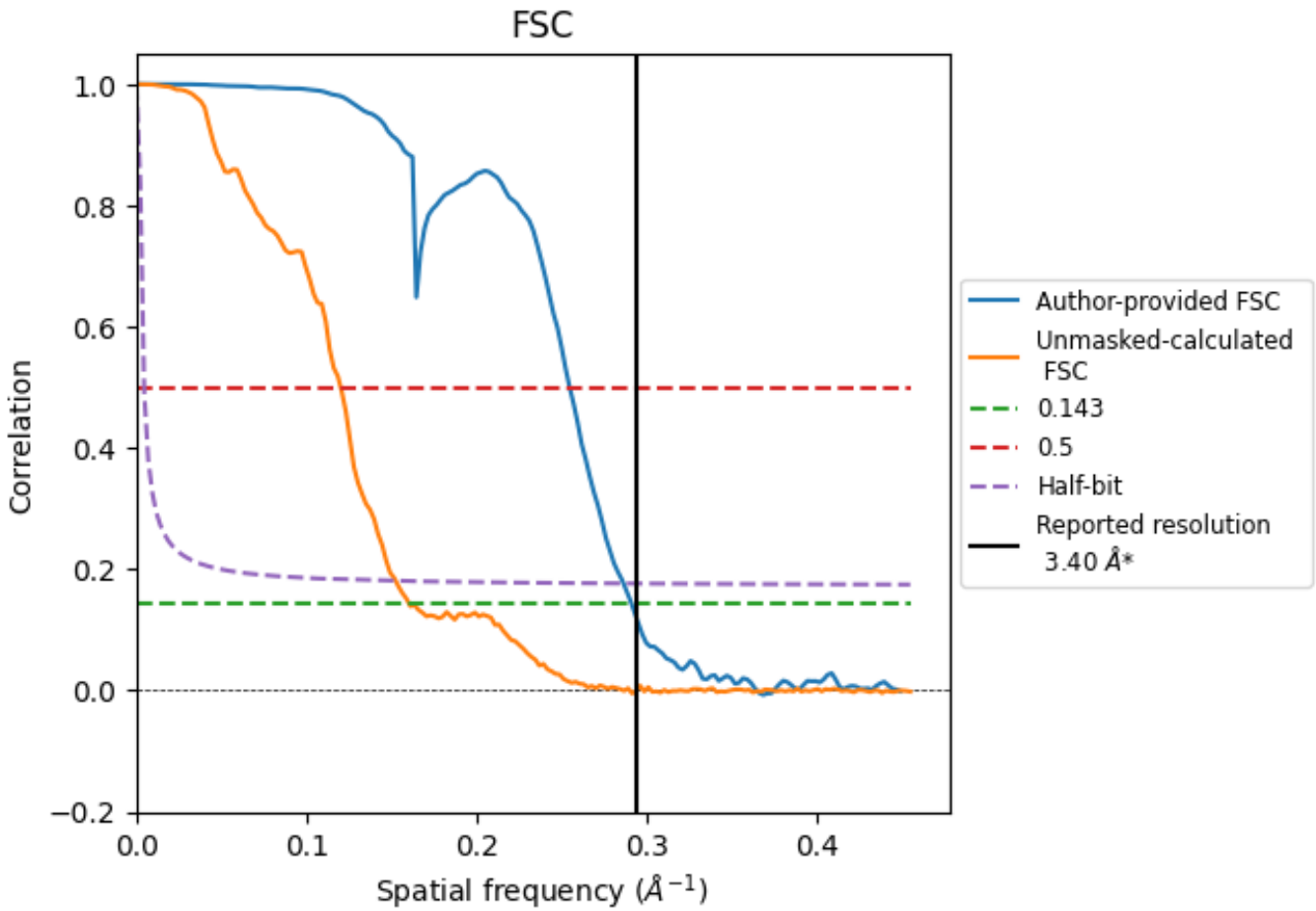


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



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

8.2 Resolution estimates (i)

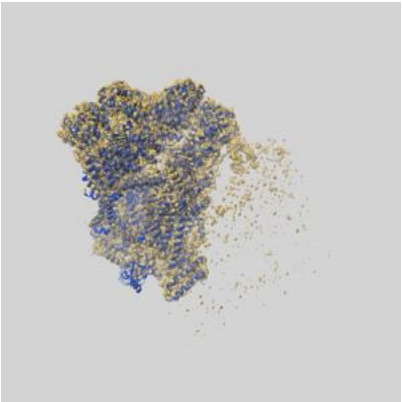
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	3.93	3.50
Unmasked-calculated*	6.24	8.33	6.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.24 differs from the reported value 3.4 by more than 10 %

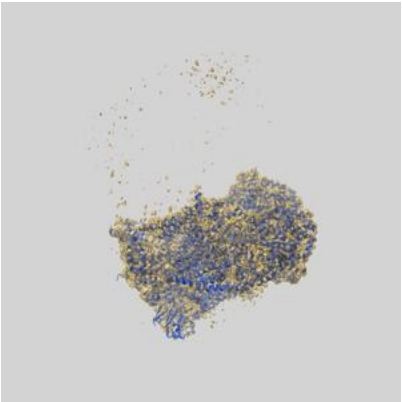
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35316 and PDB model 8IAR. Per-residue inclusion information can be found in section 3 on page 11.

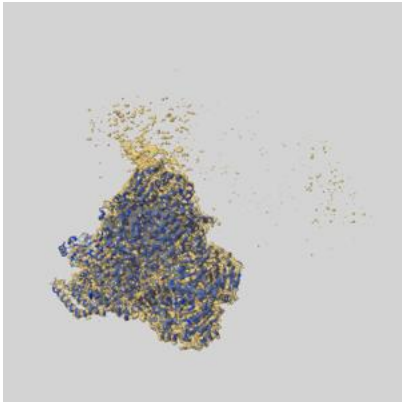
9.1 Map-model overlay (i)



X



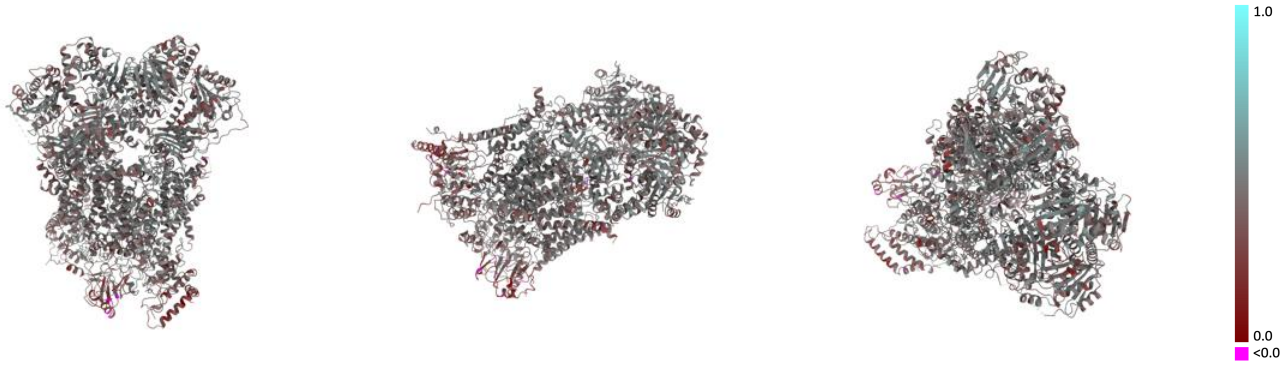
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

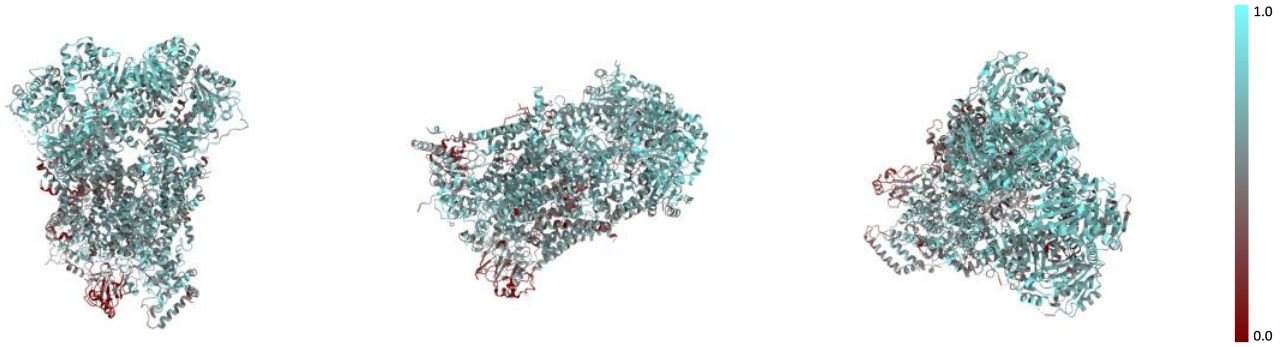
9.2 Q-score mapped to coordinate model (i)



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.

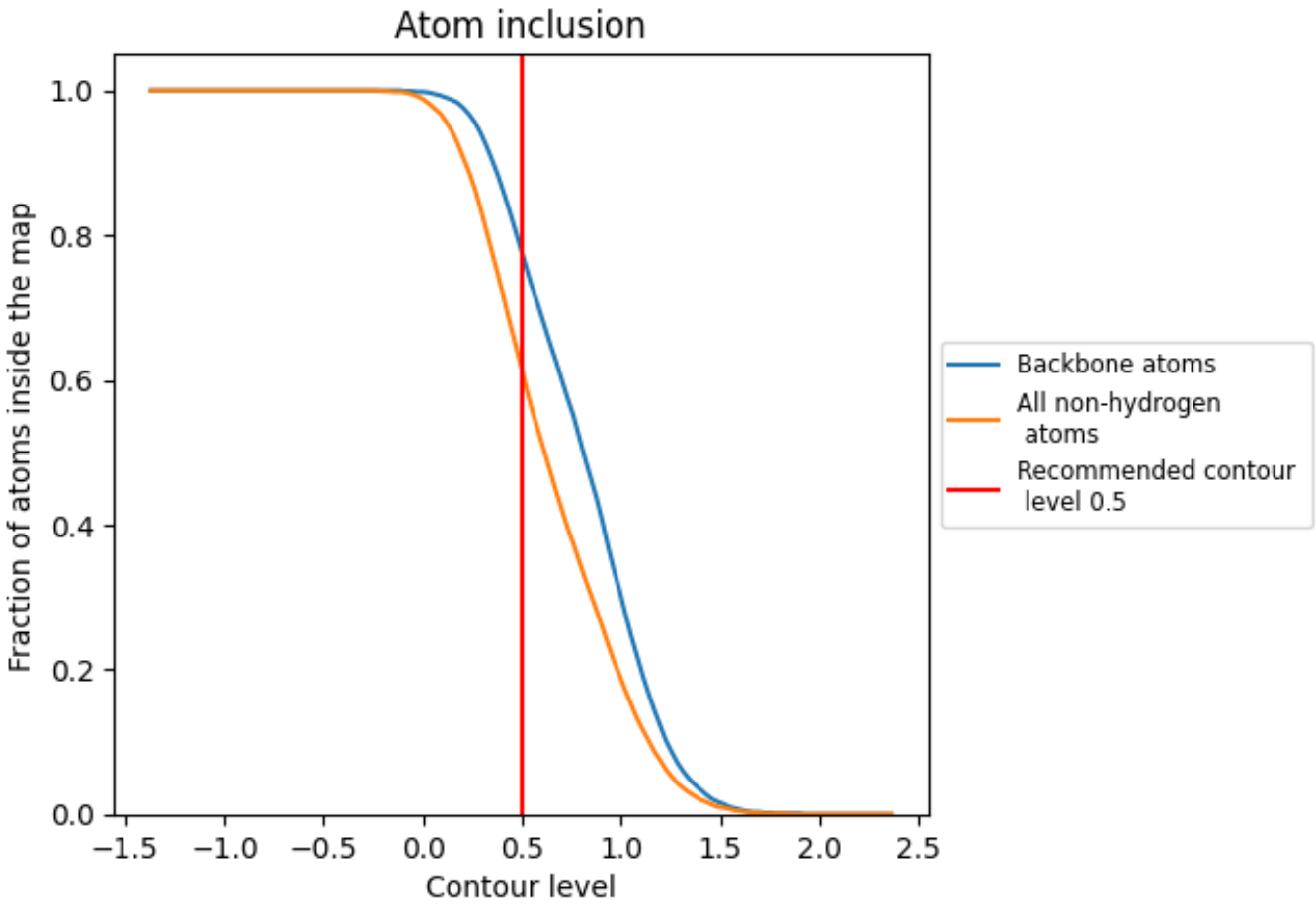
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.4210
AA	0.6930	0.4360
AB	0.6970	0.4430
AC	0.6340	0.4390
AD	0.6420	0.4110
AE	0.3000	0.3300
AF	0.6890	0.4360
AG	0.5460	0.4300
AH	0.4600	0.3000
AI	0.2990	0.4200
AJ	0.4040	0.4060
AK	0.2680	0.4070
Aa	0.6650	0.4410
Ab	0.7140	0.4410
Ac	0.6520	0.4510
Ad	0.6810	0.4290
Ae	0.3660	0.3230
Af	0.6890	0.4560
Ag	0.6160	0.4490
Ah	0.5440	0.3010
Ai	0.2490	0.3150
Aj	0.4970	0.3930
Ak	0.3720	0.3750