



Full wwPDB EM Validation Report ⓘ

Aug 12, 2026 – 09:58 PM JST

PDB ID : 8IB7 / pdb_00008ib7
EMDB ID : EMD-35334
Title : Respiratory complex CIII2, focus-refined of type IA, Wild type mouse under cold 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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

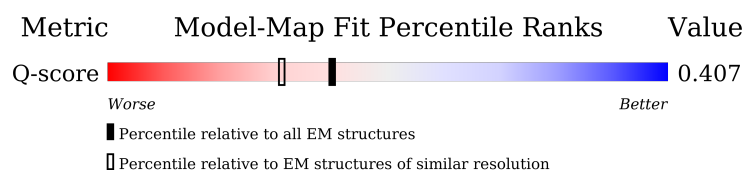
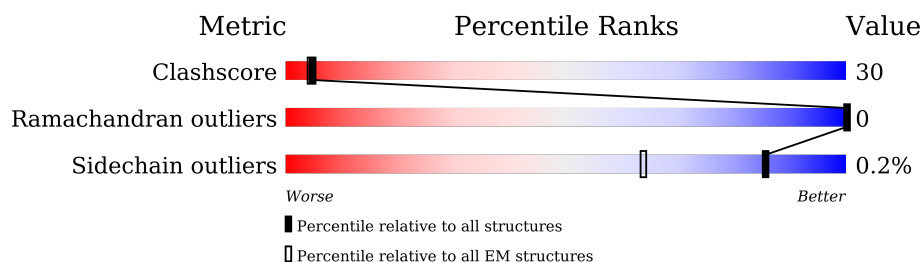
1 Overall quality at a glance

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.



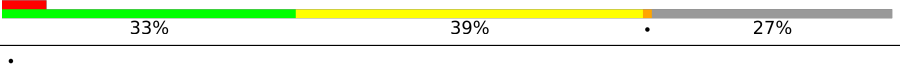
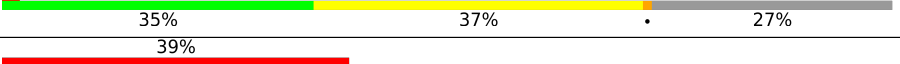
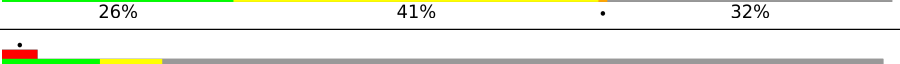
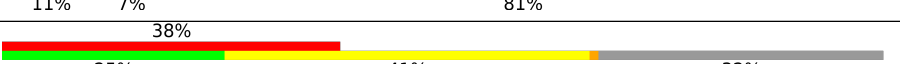
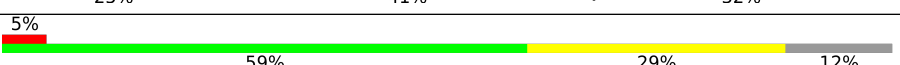
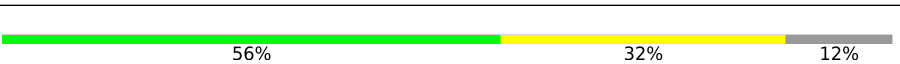
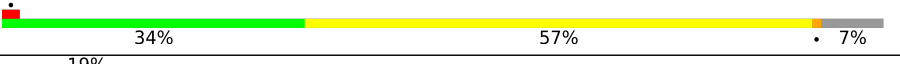
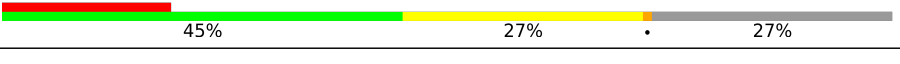
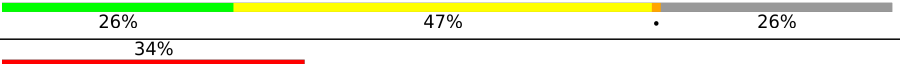
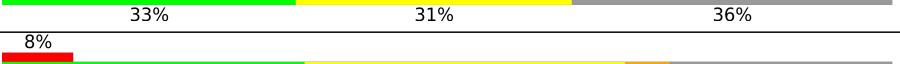
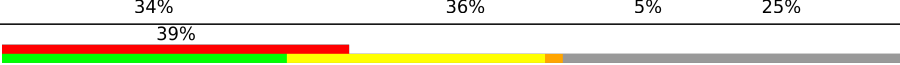
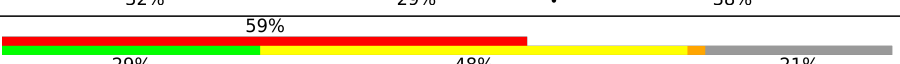
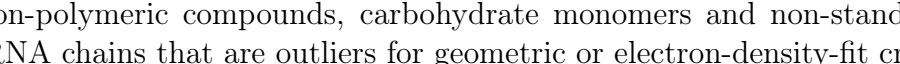
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 $\leq 5\%$. 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	
1	Aa	480	
2	AB	453	
2	Ab	453	

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Mol	Chain	Length	Quality of chain
3	AC	381	
3	Ac	381	
4	AD	325	
4	Ad	325	
5	AE	274	
5	AI	274	
5	Ae	274	
6	AF	111	
6	Af	111	
7	AG	82	
7	Ag	82	
8	AH	89	
8	Ah	89	
9	AJ	64	
9	Aj	64	
10	AK	56	
10	Ak	56	

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
16	HEC	AD	401	X	-	X	-
16	HEC	Ad	401	X	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31874 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
1	AA	400	Total	C	N	O	S	0	0
			3128	1952	557	603	16		
1	Aa	412	Total	C	N	O	S	0	0
			3225	2016	569	624	16		

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
4	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	185	Total	C	N	O	S	0	0
			1427	902	250	268	7		
5	AI	51	Total	C	N	O		0	0
			345	221	64	60			
5	Ae	185	Total	C	N	O	S	0	0
			1432	905	250	270	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	65	Total	C	N	O	S	0	0
			535	327	99	104	5		
8	Ah	66	Total	C	N	O	S	0	0
			544	333	101	105	5		

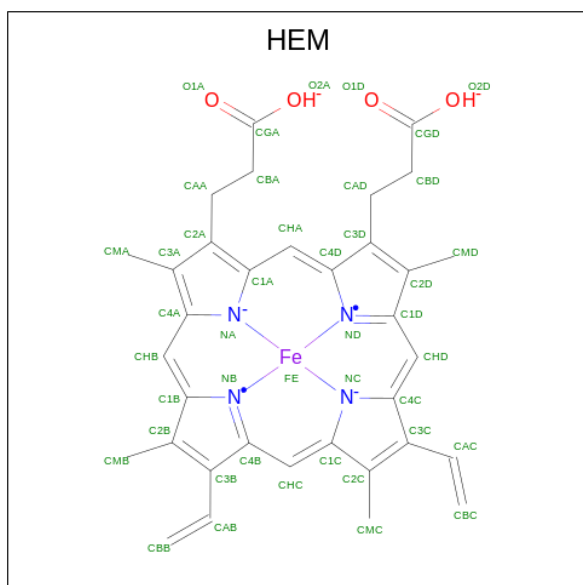
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
9	Aj	48	Total	C	N	O	0	0
			392	257	67	68		

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

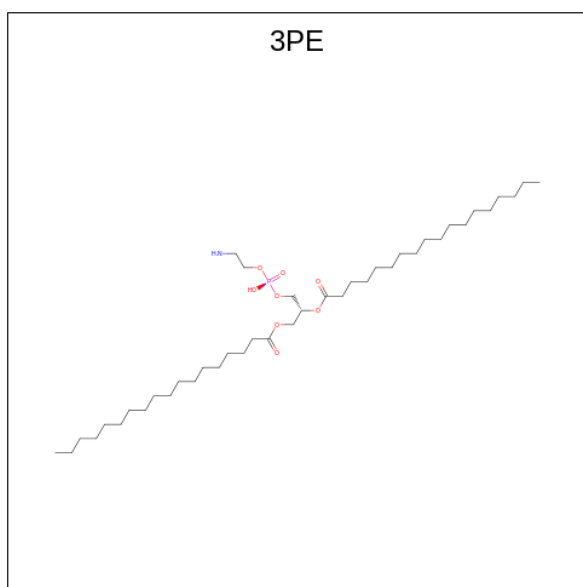
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	35	Total	C	N	O	S	0	0
			281	184	52	44	1		
10	AK	44	Total	C	N	O	S	0	0
			357	236	63	57	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



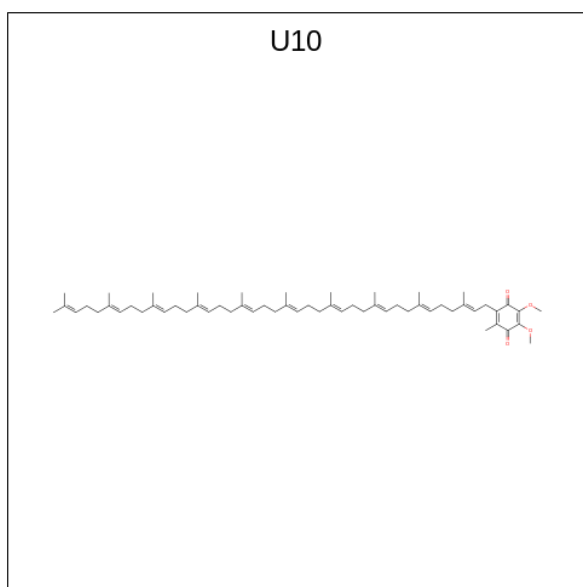
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



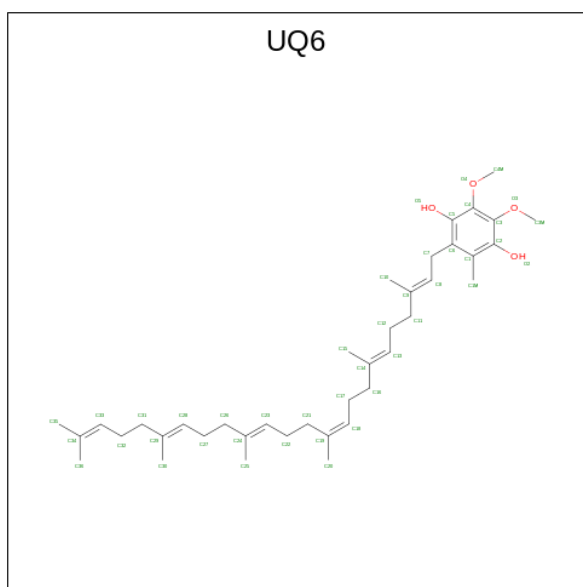
Mol	Chain	Residues	Atoms					AltConf
12	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	AF	1	Total	C	N	O	P	0
			42	32	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	Ag	1	Total	C	N	O	P	0
			39	29	1	8	1	

- 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
13	AC	1	Total	C	O	0
			23	19	4	
13	Ac	1	Total	C	O	0
			38	34	4	

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-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).



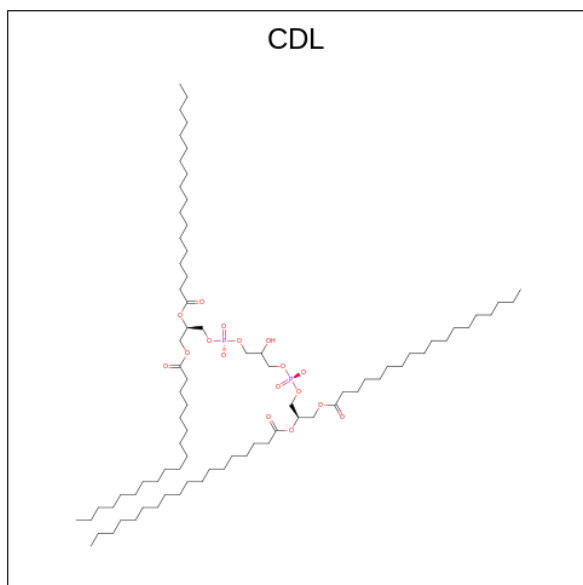
Mol	Chain	Residues	Atoms			AltConf
14	AC	1	Total	C	O	0
			28	24	4	

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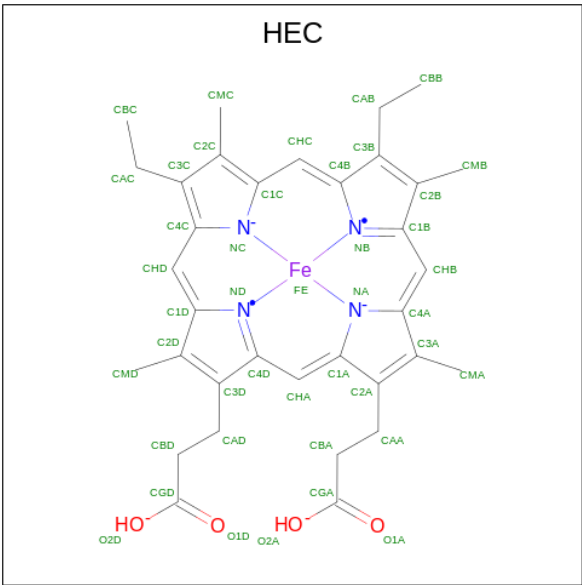
Mol	Chain	Residues	Atoms			AltConf
14	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



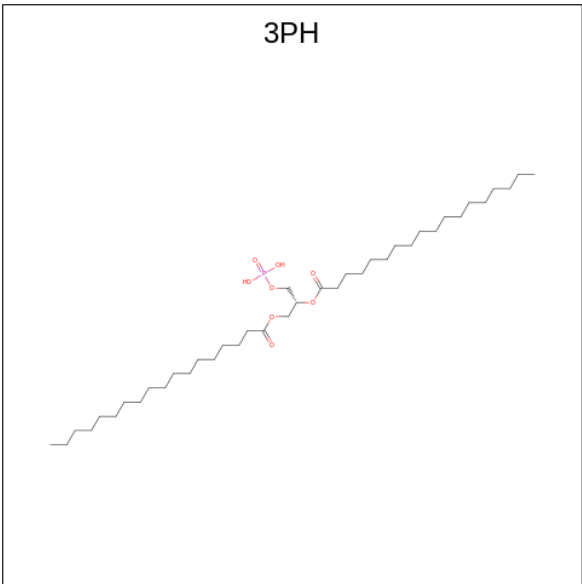
Mol	Chain	Residues	Atoms				AltConf
15	AC	1	Total	C	O	P	0
			56	37	17	2	
15	Aa	1	Total	C	O	P	0
			46	27	17	2	
15	Ac	1	Total	C	O	P	0
			42	23	17	2	
15	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 16 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
16	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
17	AD	1	Total	C	O	P	0
			36	27	8	1	

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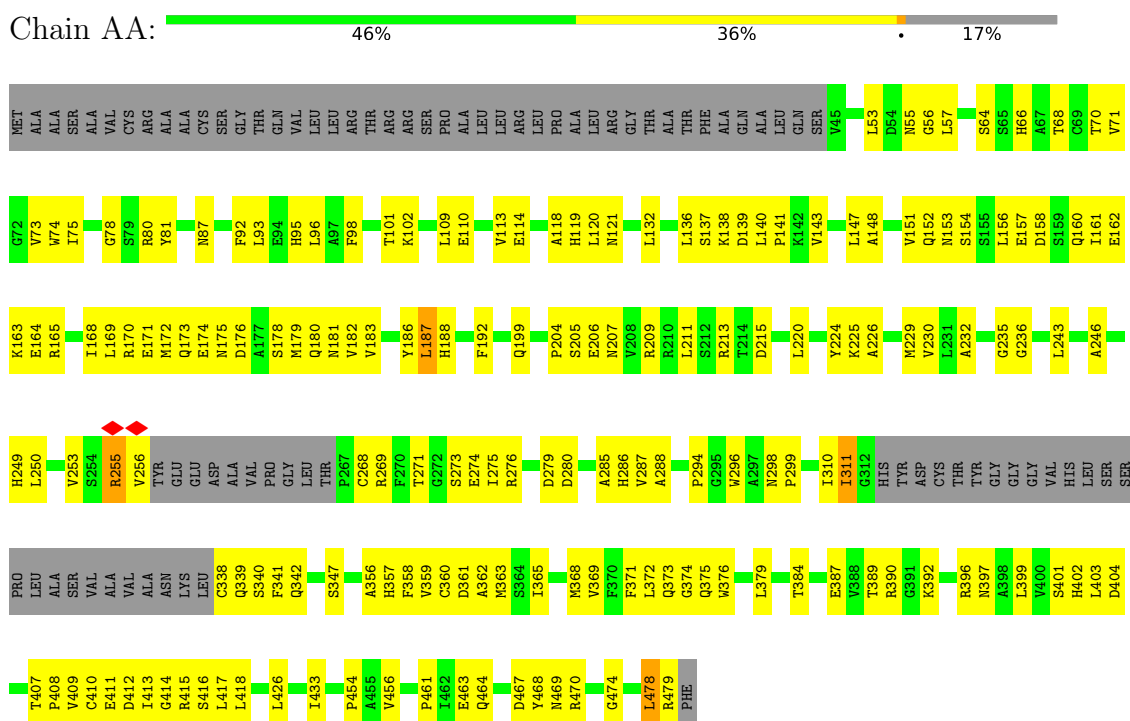
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	Ad	1	36	27	8	1	0

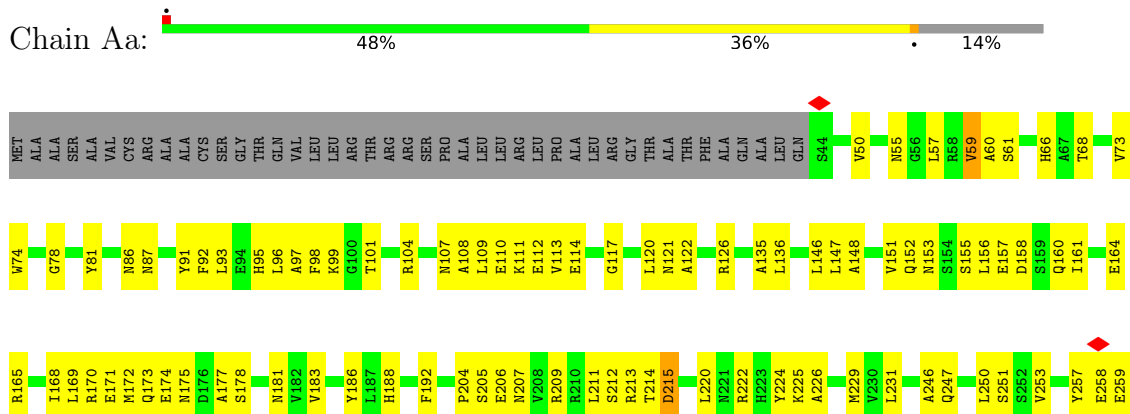
3 Residue-property plots

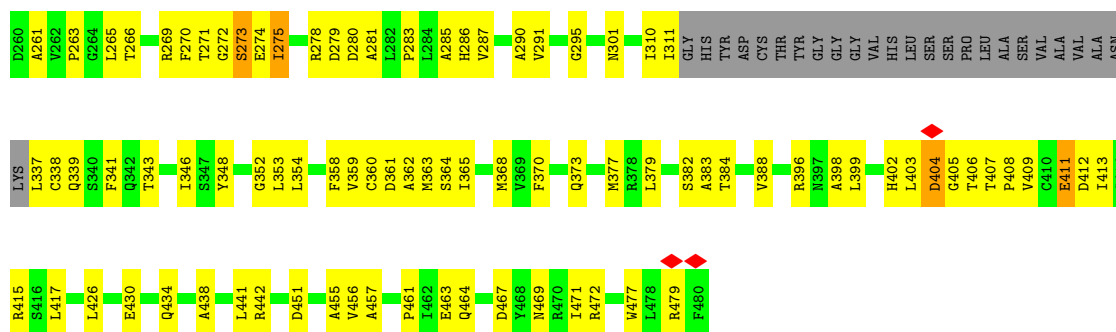
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

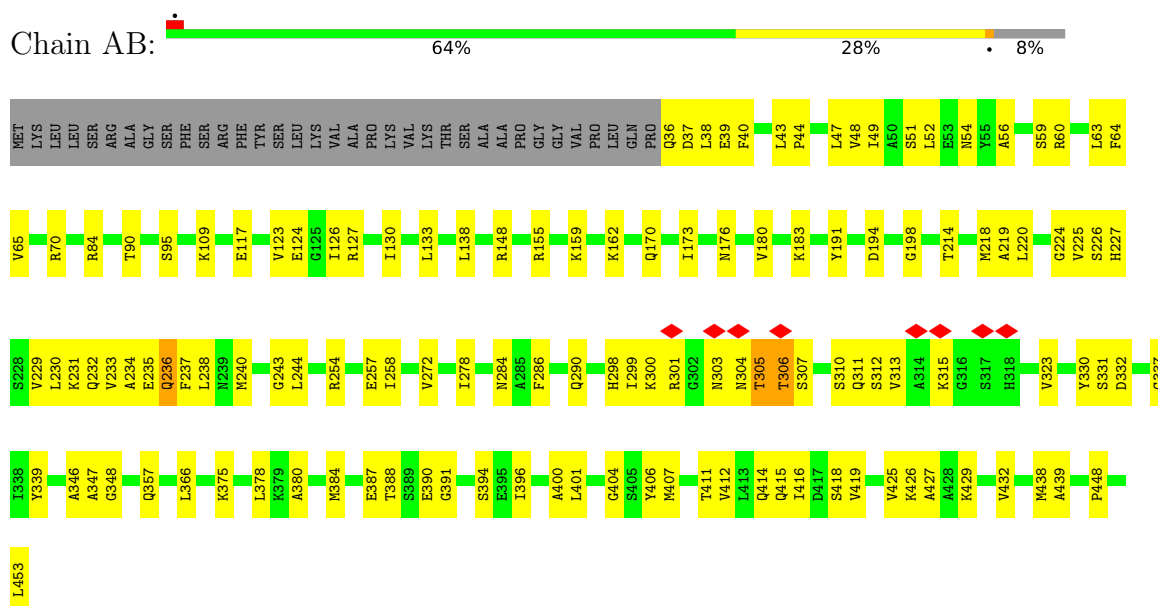


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

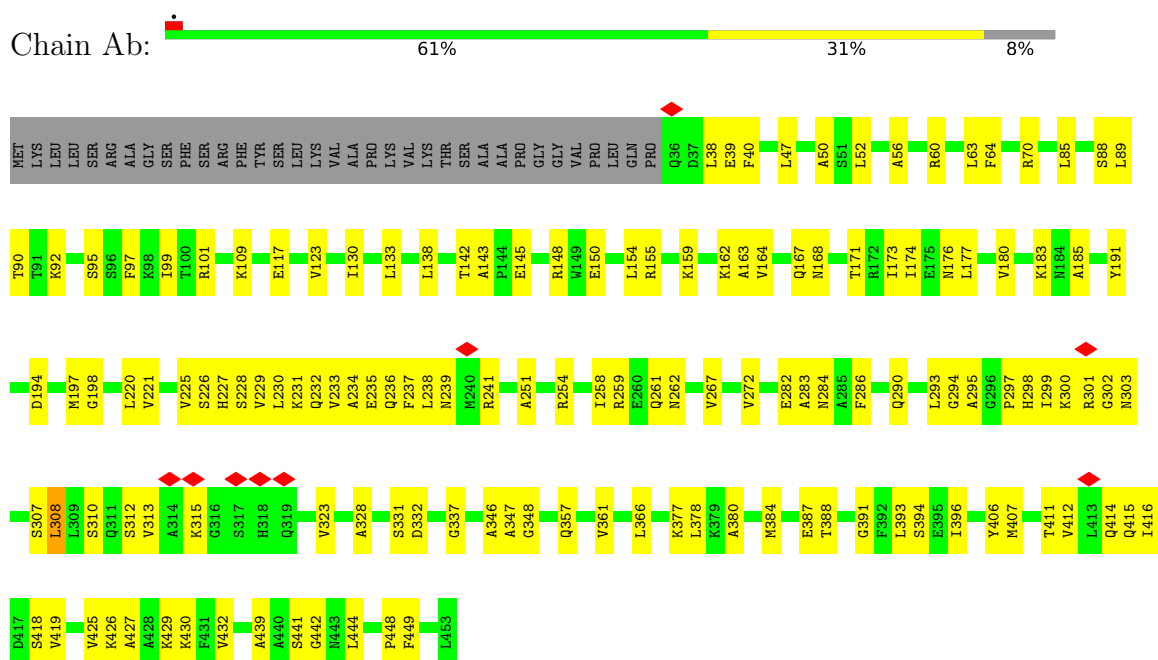




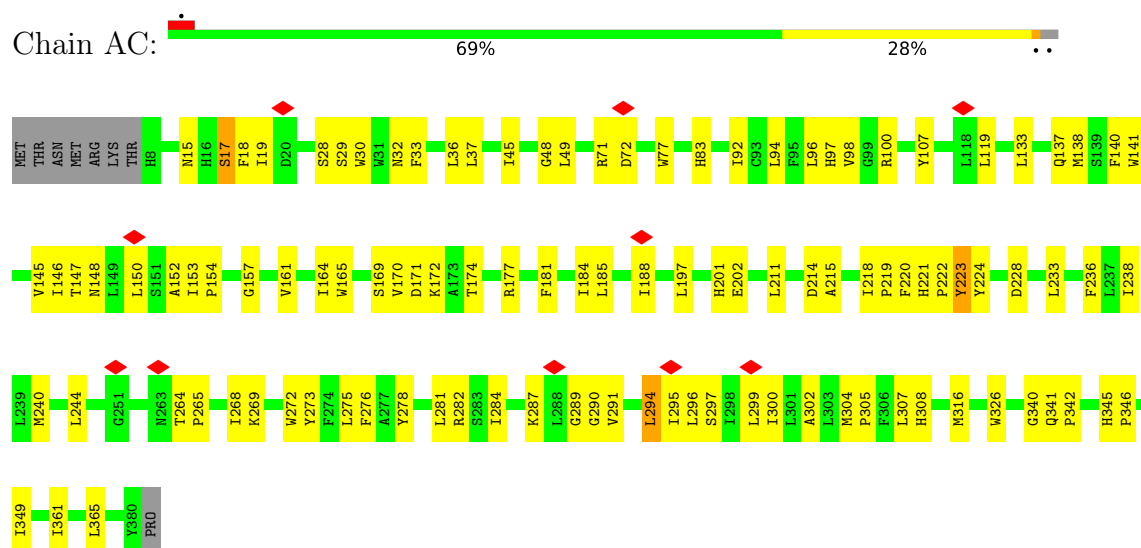
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



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



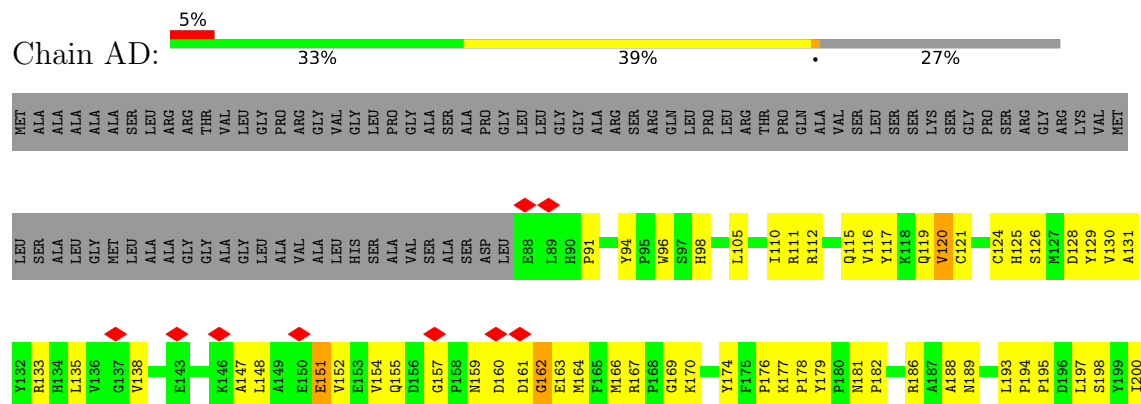
- Molecule 3: Cytochrome b

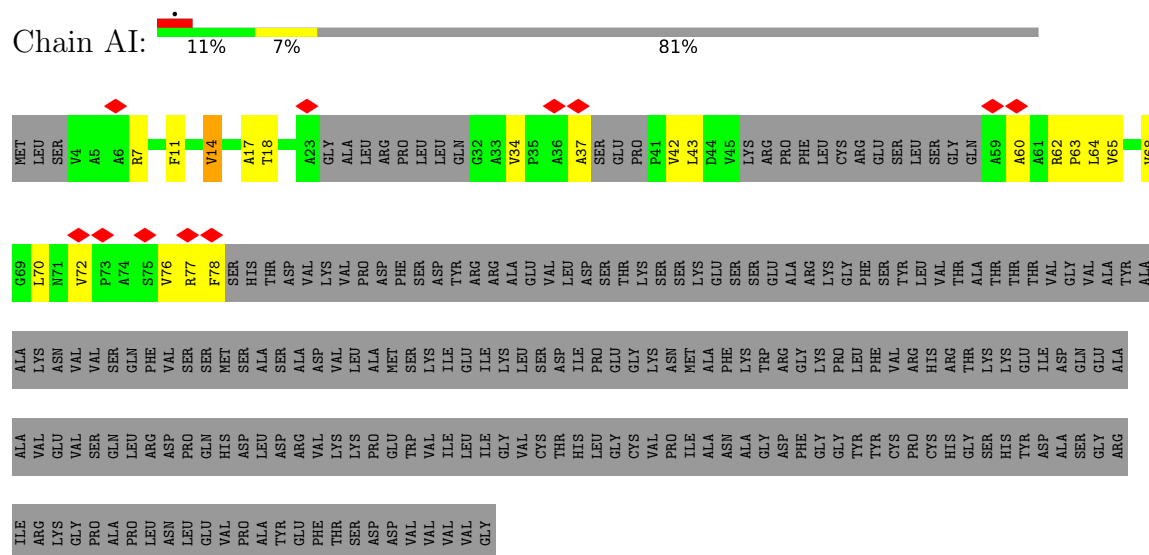


- Molecule 3: Cytochrome b

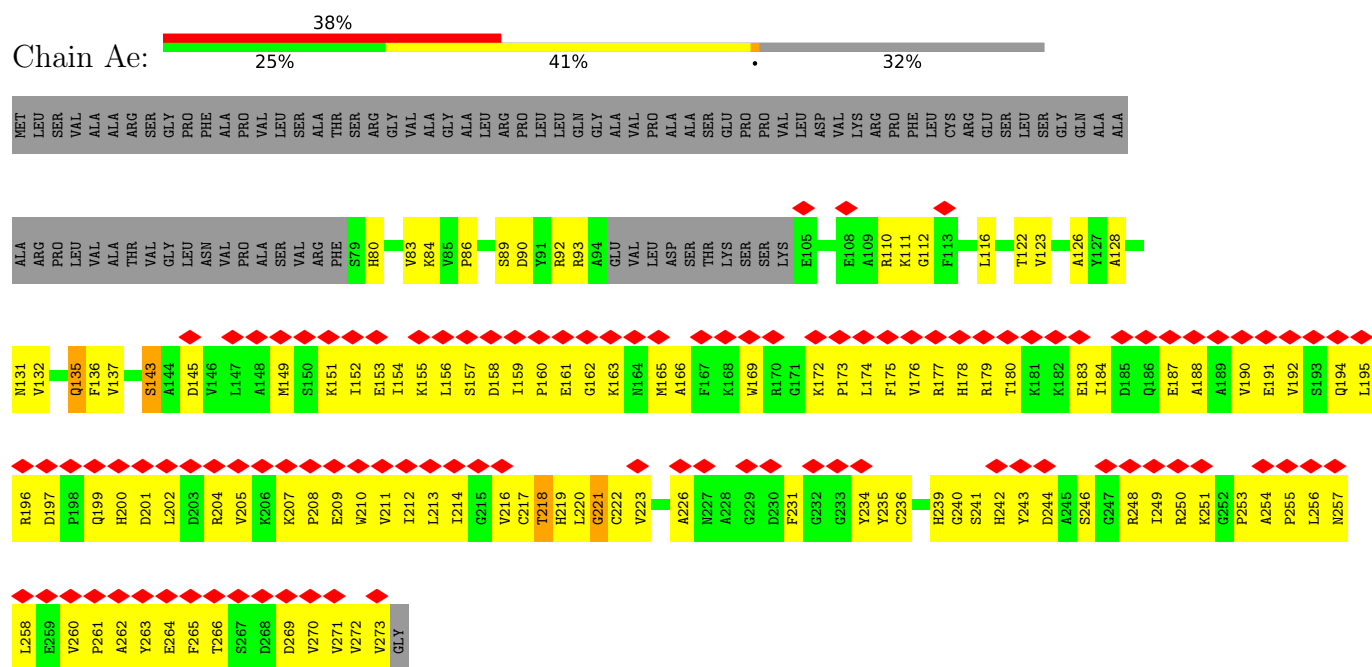


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

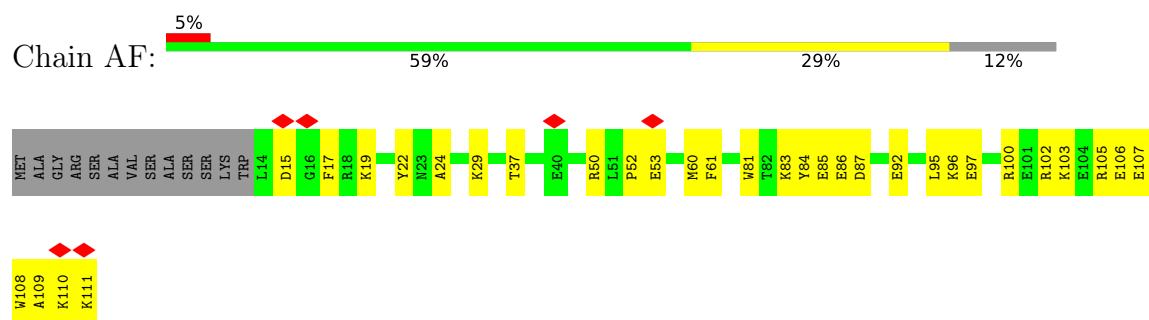




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

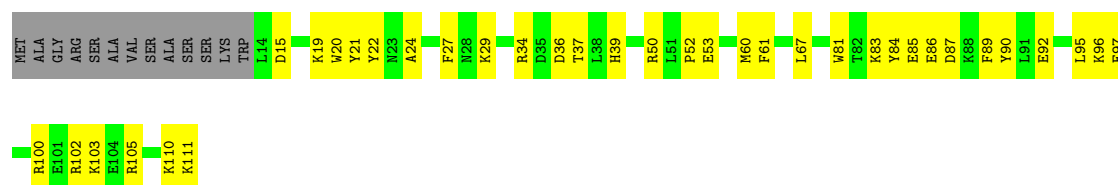


• Molecule 6: Cytochrome b-c1 complex subunit 7



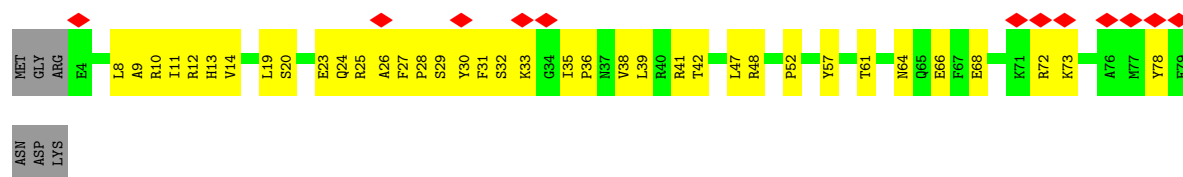
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain Af: 



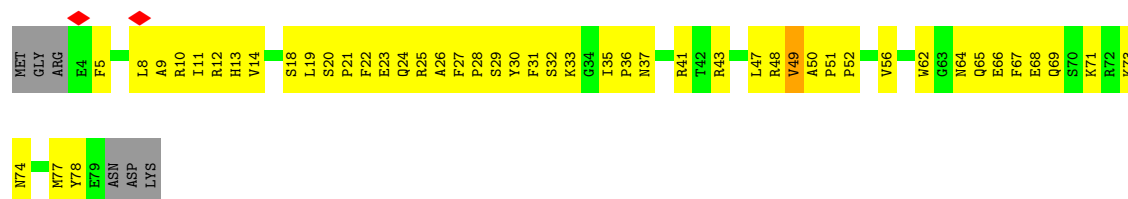
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain AG: 



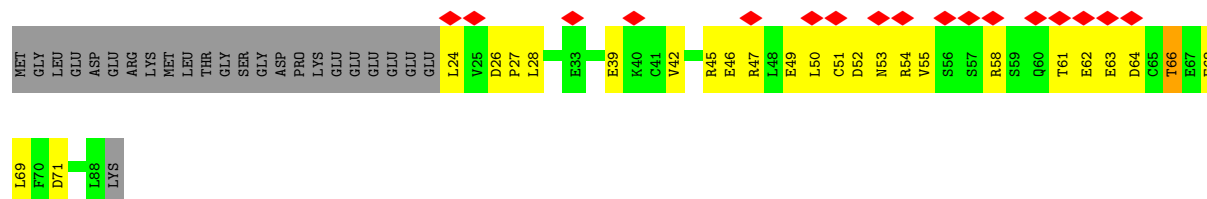
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain Ag: 

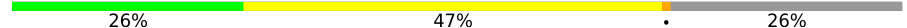


- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH: 

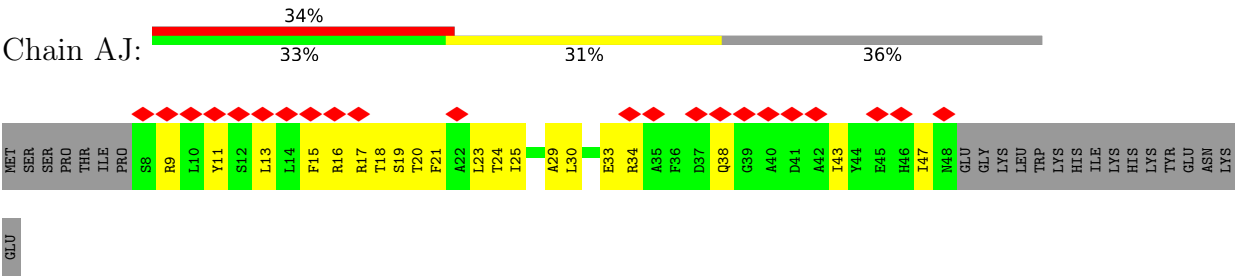


- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

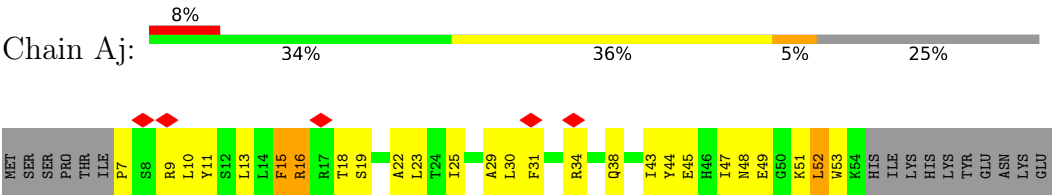
Chain Ah: 



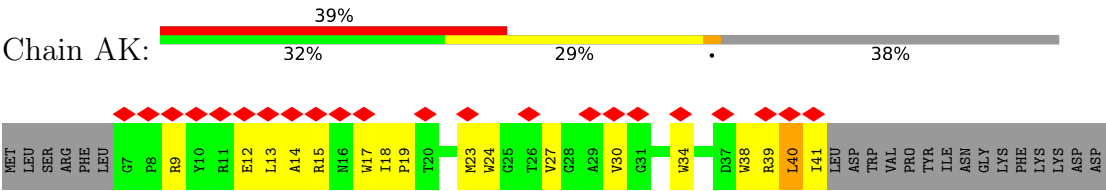
• Molecule 9: Cytochrome b-c1 complex subunit 9



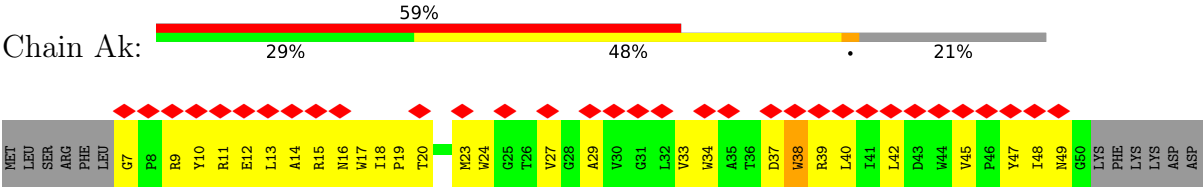
• Molecule 9: Cytochrome b-c1 complex subunit 9



• Molecule 10: Cytochrome b-c1 complex subunit 10



• Molecule 10: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151188	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 ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.856	Depositor
Minimum map value	-1.742	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.58	1/3187 (0.0%)	0.82	5/4320 (0.1%)
1	Aa	0.60	2/3288 (0.1%)	0.84	10/4462 (0.2%)
2	AB	0.44	1/3187 (0.0%)	0.67	5/4308 (0.1%)
2	Ab	0.45	0/3187	0.66	2/4308 (0.0%)
3	AC	0.43	1/3089 (0.0%)	0.69	3/4221 (0.1%)
3	Ac	0.45	0/3089	0.73	4/4221 (0.1%)
4	AD	0.53	0/1955	0.83	4/2655 (0.2%)
4	Ad	0.58	2/1954 (0.1%)	0.81	3/2655 (0.1%)
5	AE	0.66	0/1459	1.05	4/1976 (0.2%)
5	AI	0.75	0/349	1.15	2/476 (0.4%)
5	Ae	0.67	1/1464 (0.1%)	1.04	3/1983 (0.2%)
6	AF	0.38	0/884	0.52	0/1184
6	Af	0.38	0/884	0.53	0/1184
7	AG	0.50	0/662	0.87	1/895 (0.1%)
7	Ag	0.65	0/662	1.00	2/895 (0.2%)
8	AH	0.38	0/542	0.80	2/728 (0.3%)
8	Ah	0.71	0/551	0.99	3/739 (0.4%)
9	AJ	0.53	0/339	0.71	0/457
9	Aj	0.65	0/402	1.01	3/541 (0.6%)
10	AK	0.48	0/291	0.83	1/399 (0.3%)
10	Ak	0.68	1/371 (0.3%)	0.92	1/511 (0.2%)
All	All	0.53	9/31796 (0.0%)	0.80	58/43118 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	240	MET	C-N	8.63	1.45	1.33
4	Ad	180	PRO	N-CD	-8.17	1.36	1.47
10	Ak	38	TRP	CA-C	-7.83	1.41	1.52
5	Ae	143	SER	C-N	7.66	1.44	1.33
4	Ad	217	GLY	C-O	-5.66	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	273	SER	CA-C	-5.43	1.46	1.52
1	AA	311	ILE	C-N	5.20	1.40	1.33
3	AC	223	TYR	C-O	-5.09	1.17	1.23
1	Aa	59	VAL	CA-C	-5.01	1.48	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AI	60	ALA	N-CA-C	11.50	125.51	109.18
9	Aj	16	ARG	N-CA-C	10.41	123.72	111.02
1	Aa	261	ALA	N-CA-C	-10.29	95.20	109.71
2	AB	306	THR	N-CA-C	9.94	123.35	111.33
2	AB	303	ASN	N-CA-C	-9.86	100.16	112.88
9	Aj	15	PHE	N-CA-C	9.81	122.06	111.36
1	AA	187	LEU	N-CA-C	-9.80	100.42	112.38
3	Ac	157	GLY	N-CA-C	9.12	123.08	112.50
8	Ah	83	LYS	N-CA-C	8.66	121.97	110.88
1	AA	360	CYS	N-CA-C	8.08	121.44	109.24
8	AH	68	GLU	N-CA-C	-7.67	102.86	111.07
1	Aa	404	ASP	N-CA-C	-7.54	103.53	112.89
3	AC	202	GLU	N-CA-C	-7.45	103.18	111.82
4	Ad	164	MET	N-CA-C	7.41	120.50	107.61
3	Ac	202	GLU	N-CA-C	-7.38	103.26	111.82
5	Ae	221	GLY	N-CA-C	7.28	126.87	113.76
5	AE	221	GLY	N-CA-C	7.27	126.85	113.76
3	Ac	17	SER	N-CA-C	7.11	121.96	113.28
4	AD	120	VAL	N-CA-C	7.09	118.05	111.45
5	Ae	218	THR	N-CA-C	-7.00	102.80	111.75
5	AE	218	THR	N-CA-C	-6.94	102.87	111.75
5	AE	272	VAL	N-CA-C	-6.88	99.85	109.21
10	Ak	38	TRP	CA-C-O	-6.86	113.39	120.80
4	Ad	165	PHE	N-CA-C	-6.58	99.26	108.54
2	AB	305	THR	N-CA-CB	-6.54	100.36	109.91
4	AD	162	GLY	N-CA-C	-6.49	102.08	113.76
1	AA	215	ASP	N-CA-C	-6.43	103.96	110.97
1	Aa	215	ASP	N-CA-C	-6.42	103.98	110.97
3	AC	17	SER	N-CA-C	6.37	122.00	113.72
8	Ah	53	ASN	N-CA-C	6.25	118.09	111.28
1	Aa	398	ALA	N-CA-C	-6.23	104.84	112.88
4	AD	151	GLU	N-CA-C	-6.12	104.16	111.69
7	AG	31	PHE	N-CA-C	-6.01	105.99	113.38
7	Ag	31	PHE	N-CA-C	-6.00	105.96	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	244	LEU	N-CA-C	-5.94	106.03	113.28
5	AI	60	ALA	N-CA-CB	-5.87	101.94	111.22
1	Aa	59	VAL	CB-CA-C	-5.83	106.04	112.68
3	AC	17	SER	N-CA-CB	-5.82	102.09	110.65
2	Ab	308	LEU	N-CA-C	-5.72	104.41	111.33
1	Aa	275	ILE	N-CA-C	-5.68	100.49	108.27
7	Ag	49	VAL	CB-CA-C	-5.68	106.05	111.44
1	Aa	265	LEU	N-CA-C	5.67	118.46	109.50
1	Aa	409	VAL	N-CA-C	-5.57	105.10	110.72
1	AA	255	ARG	N-CA-C	5.48	118.21	107.57
9	Aj	52	LEU	N-CA-C	-5.41	100.09	108.42
3	Ac	17	SER	N-CA-CB	-5.38	102.01	110.46
2	AB	236	GLN	N-CA-C	-5.36	106.00	112.54
5	Ae	89	SER	N-CA-C	5.35	118.60	111.75
1	Aa	411	GLU	N-CA-C	5.32	117.77	111.33
5	AE	89	SER	N-CA-C	5.31	118.55	111.75
4	AD	227	LEU	N-CA-CB	-5.29	102.17	110.69
8	AH	66	THR	N-CA-C	5.29	116.73	110.97
1	AA	56	GLY	N-CA-C	-5.25	107.28	114.64
2	Ab	295	ALA	N-CA-C	-5.19	105.63	112.94
1	Aa	354	LEU	N-CA-C	-5.12	102.18	110.32
4	Ad	88	GLU	N-CA-C	5.12	117.76	109.06
10	AK	40	LEU	N-CA-C	-5.03	105.24	111.33
8	Ah	51	CYS	N-CA-C	-5.02	105.72	111.14

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	3128	0	3052	191	0
1	Aa	3225	0	3141	194	0
2	AB	3137	0	3143	138	0
2	Ab	3137	0	3143	154	0
3	AC	2988	0	3045	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ac	2988	0	3045	162	0
4	AD	1896	0	1846	155	0
4	Ad	1895	0	1844	175	0
5	AE	1427	0	1409	180	0
5	AI	345	0	364	44	0
5	Ae	1432	0	1412	239	0
6	AF	864	0	854	31	0
6	Af	864	0	854	34	0
7	AG	643	0	643	57	0
7	Ag	643	0	643	73	0
8	AH	535	0	518	27	0
8	Ah	544	0	529	39	0
9	AJ	332	0	324	29	0
9	Aj	392	0	388	43	0
10	AK	281	0	277	19	0
10	Ak	357	0	347	38	0
11	AC	86	0	60	7	0
11	Ac	86	0	60	9	0
12	AC	35	0	44	12	0
12	AF	42	0	61	7	0
12	Ac	58	0	64	6	0
12	Ag	39	0	52	9	0
13	AC	23	0	23	4	0
13	Ac	38	0	47	5	0
14	AC	28	0	31	14	0
14	Ac	28	0	31	12	0
15	AC	56	0	56	4	0
15	Aa	46	0	36	8	0
15	Ac	42	0	28	3	0
15	Ag	56	0	56	9	0
16	AD	43	0	32	24	0
16	Ad	43	0	32	25	0
17	AD	36	0	45	13	0
17	Ad	36	0	45	19	0
All	All	31874	0	31624	1900	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 30.

All (1900) 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:170:LYS:CD	5:Ae:151:LYS:HD2	1.57	1.33
5:Ae:152:ILE:HG23	5:Ae:272:VAL:CG2	1.64	1.25
5:Ae:152:ILE:CG2	5:Ae:273:VAL:H	1.53	1.22
12:AC:403:3PE:H2C1	7:AG:41:ARG:NH2	1.52	1.22
4:Ad:170:LYS:CD	5:Ae:151:LYS:CD	2.20	1.20
1:Aa:402:HIS:CD2	1:Aa:403:LEU:CD1	2.27	1.18
4:Ad:170:LYS:HD2	5:Ae:151:LYS:CD	1.74	1.17
5:Ae:152:ILE:CG2	5:Ae:272:VAL:CG2	2.22	1.15
1:Aa:402:HIS:CD2	1:Aa:403:LEU:HD12	1.81	1.14
1:Aa:68:THR:HG21	2:Ab:384:MET:CG	1.76	1.13
1:Aa:68:THR:HG21	2:Ab:384:MET:HG2	1.15	1.12
5:AI:78:PHE:CZ	2:Ab:168:ASN:ND2	2.21	1.09
1:AA:402:HIS:CE1	1:AA:403:LEU:CD1	2.36	1.09
5:Ae:152:ILE:HG21	5:Ae:273:VAL:H	0.96	1.08
5:AE:204:ARG:HB3	5:AE:260:VAL:HG21	1.35	1.08
5:Ae:152:ILE:CG2	5:Ae:272:VAL:HG22	1.82	1.07
2:AB:48:VAL:CG2	2:AB:219:ALA:HB2	1.85	1.06
1:AA:402:HIS:CE1	1:AA:403:LEU:HD11	1.91	1.06
7:Ag:11:ILE:HG21	7:Ag:14:VAL:HG21	1.36	1.06
5:Ae:93:ARG:HD2	5:Ae:110:ARG:HD2	1.38	1.06
5:Ae:204:ARG:HB3	5:Ae:260:VAL:HG21	1.35	1.04
7:AG:11:ILE:HG21	7:AG:14:VAL:HG21	1.36	1.04
5:Ae:261:PRO:HB2	5:Ae:273:VAL:HG11	1.40	1.03
3:Ac:98:VAL:HG22	11:Ac:403:HEM:HBC2	1.40	1.02
3:AC:98:VAL:HG22	11:AC:402:HEM:HBC2	1.40	1.02
2:AB:48:VAL:CG2	2:AB:219:ALA:CB	2.39	1.01
9:Aj:52:LEU:HD13	9:Aj:53:TRP:H	1.22	1.00
2:Ab:142:THR:HG21	2:Ab:237:PHE:HB3	1.44	0.99
5:Ae:93:ARG:HD2	5:Ae:110:ARG:CD	1.93	0.99
5:Ae:156:LEU:H	5:Ae:269:ASP:HA	1.27	0.98
12:AC:403:3PE:H2C1	7:AG:41:ARG:CZ	1.91	0.98
5:Ae:152:ILE:CG2	5:Ae:272:VAL:HG23	1.90	0.98
1:Aa:222:ARG:CZ	1:Aa:263:PRO:HG3	1.95	0.97
1:AA:470:ARG:HD3	3:AC:222:PRO:HG3	1.47	0.97
5:AE:123:VAL:HG13	9:AJ:29:ALA:HA	1.42	0.97
5:AI:43:LEU:HD13	2:Ab:164:VAL:HG23	1.45	0.97
5:Ae:152:ILE:C	5:Ae:272:VAL:HG23	1.91	0.96
4:Ad:170:LYS:HD3	5:Ae:151:LYS:CD	1.94	0.96
1:AA:478:LEU:HD22	9:AJ:18:THR:HG21	1.45	0.96
5:Ae:152:ILE:HG21	5:Ae:273:VAL:N	1.81	0.95
4:Ad:249:TYR:CE1	4:Ad:252:VAL:HG23	2.02	0.95
5:AI:78:PHE:HZ	2:Ab:168:ASN:ND2	1.60	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:Al:78:PHE:HE1	2:Ab:171:THR:HG1	1.11	0.94
12:AC:403:3PE:C2C	7:AG:41:ARG:NH2	2.30	0.94
5:Ae:152:ILE:CG2	5:Ae:273:VAL:N	2.30	0.94
7:AG:19:LEU:HD23	7:AG:24:GLN:HB3	1.49	0.94
5:Al:43:LEU:HD13	2:Ab:164:VAL:CG2	1.97	0.94
5:AE:218:THR:HG21	5:AE:256:LEU:O	1.68	0.93
3:Ac:197:LEU:HD12	14:Ac:406:UQ6:H1M2	1.48	0.93
4:AD:249:TYR:CE1	4:AD:252:VAL:HG23	2.02	0.93
5:Ae:152:ILE:HG22	5:Ae:272:VAL:HG22	1.51	0.93
3:Ac:137:GLN:HG3	3:Ac:265:PRO:HG3	1.48	0.92
4:Ad:121:CYS:SG	16:Ad:401:HEC:HBB3	2.09	0.92
17:AD:402:3PH:H221	5:AE:135:GLN:HE22	1.35	0.92
1:Aa:402:HIS:NE2	1:Aa:403:LEU:HD11	1.85	0.92
5:Al:78:PHE:HE1	2:Ab:171:THR:OG1	1.52	0.92
5:Ae:152:ILE:HG23	5:Ae:272:VAL:HG23	1.46	0.91
17:AD:402:3PH:H242	5:AE:132:VAL:HG22	1.50	0.91
5:Al:78:PHE:HZ	2:Ab:168:ASN:HD21	1.05	0.91
9:Aj:52:LEU:HD13	9:Aj:53:TRP:N	1.85	0.91
3:AC:137:GLN:HG3	3:AC:265:PRO:HG3	1.50	0.90
4:Ad:170:LYS:HD3	5:Ae:151:LYS:HE2	1.53	0.90
4:Ad:170:LYS:HD3	5:Ae:151:LYS:CE	2.01	0.90
4:Ad:124:CYS:HA	4:Ad:179:TYR:HE2	1.37	0.90
5:Ae:155:LYS:HG3	5:Ae:269:ASP:HB3	1.53	0.90
2:AB:305:THR:HG23	2:AB:306:THR:H	1.36	0.89
5:Ae:152:ILE:HD11	5:Ae:174:LEU:CD2	2.02	0.89
1:Aa:403:LEU:HD21	2:Ab:56:ALA:HB1	1.53	0.89
2:AB:48:VAL:HG21	2:AB:400:ALA:HB1	1.53	0.89
5:Ae:152:ILE:HG23	5:Ae:272:VAL:CA	2.03	0.89
5:Ae:152:ILE:HD11	5:Ae:174:LEU:HD22	1.54	0.88
3:Ac:236:PHE:HD2	17:Ad:402:3PH:H3B2	1.39	0.88
1:Aa:68:THR:CG2	2:Ab:384:MET:HG2	2.03	0.88
1:AA:402:HIS:CE1	1:AA:403:LEU:HD12	2.07	0.88
1:Aa:87:ASN:H	1:Aa:207:ASN:HD22	1.17	0.88
2:AB:48:VAL:HG23	2:AB:219:ALA:CB	2.03	0.87
7:AG:29:SER:HB2	7:AG:32:SER:HB2	1.57	0.87
1:Aa:402:HIS:NE2	1:Aa:403:LEU:CD1	2.38	0.86
4:AD:292:MET:HA	17:AD:402:3PH:H331	1.57	0.86
7:AG:11:ILE:HG21	7:AG:14:VAL:CG2	2.05	0.86
2:AB:48:VAL:HG23	2:AB:219:ALA:HB1	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:121:CYS:HB3	16:AD:401:HEC:HAB	1.58	0.86
4:AD:117:TYR:HA	4:AD:121:CYS:SG	2.14	0.86
3:Ac:138:MET:HE1	3:Ac:268:ILE:HG12	1.57	0.86
2:AB:48:VAL:HG22	2:AB:219:ALA:HB2	1.57	0.85
7:Ag:29:SER:HB2	7:Ag:32:SER:HB2	1.56	0.85
4:AD:121:CYS:HB3	16:AD:401:HEC:CAB	2.07	0.85
4:Ad:215:LEU:HD11	16:Ad:401:HEC:HMB1	1.57	0.84
5:Ae:152:ILE:O	5:Ae:272:VAL:HG23	1.76	0.84
7:Ag:78:TYR:CE1	8:Ah:62:GLU:HB2	2.12	0.84
1:AA:255:ARG:O	1:AA:255:ARG:HG3	1.75	0.84
7:Ag:11:ILE:HG21	7:Ag:14:VAL:CG2	2.05	0.84
5:Ae:156:LEU:N	5:Ae:269:ASP:HA	1.93	0.84
5:AE:263:TYR:HA	5:AE:273:VAL:O	1.77	0.84
2:AB:305:THR:HG23	2:AB:306:THR:N	1.92	0.84
10:Ak:12:GLU:HA	10:Ak:15:ARG:HD3	1.59	0.84
3:AC:214:ASP:HB3	7:AG:9:ALA:HB2	1.58	0.84
4:AD:204:ARG:HH21	16:AD:401:HEC:HBA2	1.40	0.84
1:Aa:402:HIS:CD2	1:Aa:403:LEU:HD11	2.12	0.84
4:Ad:170:LYS:HD2	5:Ae:151:LYS:HD2	0.85	0.84
3:AC:222:PRO:HG2	3:AC:223:TYR:HD1	1.43	0.83
7:AG:73:LYS:HZ3	8:AH:63:GLU:HG2	1.42	0.83
4:AD:270:VAL:HG21	16:AD:401:HEC:HBB3	1.62	0.82
5:AI:64:LEU:HA	5:AI:78:PHE:HA	1.59	0.82
5:AI:43:LEU:HD11	2:Ab:163:ALA:HB3	1.60	0.82
5:Ae:152:ILE:CA	5:Ae:272:VAL:HG23	2.08	0.82
8:Ah:44:ALA:HA	8:Ah:47:ARG:HD3	1.62	0.82
3:Ac:37:LEU:HB3	11:Ac:403:HEM:HMB1	1.60	0.81
4:Ad:125:HIS:HE1	4:Ad:195:PRO:HD2	1.43	0.81
5:AE:154:ILE:HD13	5:AE:273:VAL:HG23	1.61	0.81
1:Aa:117:GLY:HA2	2:Ab:377:LYS:HG2	1.59	0.81
2:Ab:259:ARG:HB3	2:Ab:444:LEU:HD13	1.60	0.81
1:AA:110:GLU:HB2	2:AB:299:ILE:HD13	1.63	0.81
1:Aa:87:ASN:HD22	1:Aa:204:PRO:HD3	1.46	0.80
12:AC:403:3PE:C29	7:AG:41:ARG:HH21	1.94	0.80
3:AC:326:TRP:HZ2	12:AC:403:3PE:H11	1.44	0.80
8:Ah:39:GLU:HB3	8:Ah:43:LYS:HE2	1.61	0.80
5:AE:221:GLY:HA3	3:Ac:148:ASN:ND2	1.97	0.80
1:AA:74:TRP:CZ2	1:AA:411:GLU:HA	2.16	0.80
8:AH:50:LEU:O	8:AH:54:ARG:HG2	1.82	0.79
4:Ad:296:MET:HE2	17:Ad:402:3PH:H362	1.63	0.79
5:Ae:152:ILE:HG23	5:Ae:272:VAL:HG22	1.49	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:152:ILE:HD12	5:Ae:169:TRP:CG	2.17	0.79
5:Ae:152:ILE:HG22	5:Ae:272:VAL:CG2	2.07	0.79
5:AE:111:LYS:HE3	9:AJ:11:TYR:OH	1.83	0.78
5:Ae:155:LYS:HE2	5:Ae:157:SER:HB3	1.65	0.78
7:AG:19:LEU:HD11	7:AG:23:GLU:HG2	1.65	0.78
1:Aa:87:ASN:HB3	1:Aa:204:PRO:HD2	1.64	0.78
4:AD:155:GLN:HA	4:AD:166:MET:HA	1.66	0.78
6:AF:52:PRO:HD3	2:Ab:148:ARG:NH2	1.98	0.78
1:Aa:59:VAL:HG13	1:Aa:231:LEU:HD23	1.66	0.78
1:AA:478:LEU:C	1:AA:478:LEU:HD13	2.08	0.77
4:Ad:167:ARG:HB2	4:Ad:168:PRO:HD2	1.64	0.77
7:Ag:19:LEU:HD11	7:Ag:23:GLU:HG2	1.65	0.77
5:AE:115:TYR:HB3	9:AJ:21:PHE:HE1	1.47	0.77
4:Ad:155:GLN:HA	4:Ad:166:MET:HA	1.66	0.77
1:AA:397:ASN:HD21	2:AB:126:ILE:HD11	1.50	0.77
7:AG:11:ILE:CG2	7:AG:14:VAL:CG2	2.62	0.77
7:Ag:11:ILE:CG2	7:Ag:14:VAL:CG2	2.63	0.77
4:Ad:120:VAL:HG12	16:Ad:401:HEC:HAB	1.67	0.77
1:AA:68:THR:HG21	2:AB:384:MET:HG3	1.67	0.77
1:Aa:360:CYS:SG	1:Aa:364:SER:HB2	2.24	0.77
3:AC:18:PHE:CE1	14:AC:405:UQ6:H72	2.19	0.76
3:AC:137:GLN:HE21	3:AC:265:PRO:HD3	1.50	0.76
4:Ad:244:MET:HB2	16:Ad:401:HEC:C1D	2.15	0.76
2:AB:63:LEU:HD11	2:AB:238:LEU:HD21	1.65	0.76
3:AC:148:ASN:OD1	5:Ae:221:GLY:HA3	1.85	0.76
1:Aa:99:LYS:HE2	2:Ab:302:GLY:HA3	1.67	0.76
5:Ae:152:ILE:O	5:Ae:272:VAL:CG2	2.32	0.76
3:Ac:214:ASP:HB3	7:Ag:9:ALA:HB2	1.66	0.76
5:Ae:270:VAL:O	5:Ae:271:VAL:HG23	1.86	0.76
5:AE:111:LYS:HE3	9:AJ:11:TYR:CZ	2.20	0.76
5:AE:191:GLU:HB2	5:AE:194:GLN:HB2	1.66	0.76
2:AB:407:MET:HG2	2:AB:411:THR:OG1	1.85	0.76
4:AD:195:PRO:HG3	16:AD:401:HEC:HBA1	1.66	0.76
7:AG:11:ILE:HG22	7:AG:14:VAL:HG22	1.69	0.75
7:AG:73:LYS:NZ	8:AH:63:GLU:HG2	2.01	0.75
2:Ab:407:MET:HG2	2:Ab:411:THR:OG1	1.85	0.75
5:Ae:191:GLU:HB2	5:Ae:194:GLN:HB2	1.66	0.75
1:AA:68:THR:HG22	1:AA:136:LEU:HD23	1.67	0.75
5:Ae:169:TRP:CH2	5:Ae:273:VAL:HB	2.21	0.75
1:AA:55:ASN:HB3	1:AA:226:ALA:CB	2.16	0.75
2:AB:429:LYS:HA	2:AB:432:VAL:HG12	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:72:VAL:HG21	2:Ab:109:LYS:HD2	1.69	0.75
5:Ae:173:PRO:HG2	5:Ae:223:VAL:HG22	1.67	0.75
1:AA:255:ARG:O	1:AA:256:VAL:C	2.29	0.74
4:AD:227:LEU:HD12	4:AD:227:LEU:O	1.87	0.74
5:AE:173:PRO:HG2	5:AE:223:VAL:HG22	1.67	0.74
9:AJ:23:LEU:HD22	10:AK:23:MET:SD	2.27	0.74
3:Ac:18:PHE:HE1	14:Ac:406:UQ6:C8	2.00	0.74
5:Ae:154:ILE:HD13	5:Ae:176:VAL:HG21	1.69	0.74
7:Ag:11:ILE:HG22	7:Ag:14:VAL:HG22	1.68	0.74
7:AG:78:TYR:CE1	8:AH:62:GLU:HB2	2.21	0.74
4:AD:200:ILE:HG21	4:AD:274:LEU:HD13	1.68	0.74
1:AA:478:LEU:HD22	9:AJ:18:THR:CG2	2.18	0.74
5:AI:42:VAL:HG11	1:Aa:283:PRO:HB2	1.69	0.73
5:Ae:112:GLY:HA2	9:Aj:15:PHE:HD2	1.52	0.73
1:AA:55:ASN:HB3	1:AA:226:ALA:HB1	1.68	0.73
4:Ad:217:GLY:O	4:Ad:235:PRO:HD2	1.88	0.73
5:Ae:93:ARG:CD	5:Ae:110:ARG:CD	2.66	0.73
2:AB:305:THR:CG2	2:AB:306:THR:H	2.01	0.73
17:Ad:402:3PH:H241	5:Ae:132:VAL:HG22	1.69	0.73
3:Ac:220:PHE:HE2	14:Ac:406:UQ6:H4M2	1.53	0.73
1:AA:478:LEU:HD13	1:AA:478:LEU:O	1.88	0.73
5:Ae:263:TYR:HB2	5:Ae:271:VAL:CG1	2.18	0.73
3:AC:141:TRP:CD1	3:AC:265:PRO:HD3	2.23	0.73
3:AC:148:ASN:OD1	5:Ae:220:LEU:C	2.32	0.73
3:AC:269:LYS:HE3	3:AC:340:GLY:HA2	1.70	0.73
5:AE:132:VAL:O	5:AE:135:GLN:HG2	1.88	0.73
2:AB:48:VAL:HG23	2:AB:48:VAL:O	1.88	0.73
4:AD:152:VAL:HG11	4:AD:176:PRO:HG3	1.71	0.73
5:AE:187:GLU:HB3	5:AE:201:ASP:HB3	1.71	0.73
5:Ae:187:GLU:HB3	5:Ae:201:ASP:HB3	1.71	0.72
3:Ac:148:ASN:OD1	3:Ac:165:TRP:CH2	2.41	0.72
4:Ad:170:LYS:CD	5:Ae:151:LYS:CE	2.63	0.72
1:AA:74:TRP:HZ2	1:AA:411:GLU:HA	1.54	0.72
3:Ac:141:TRP:CD1	3:Ac:265:PRO:HD3	2.24	0.72
3:AC:223:TYR:HE2	4:AD:314:LEU:HG	1.55	0.72
5:AE:156:LEU:HG	5:AE:271:VAL:HG23	1.70	0.72
5:Ae:199:GLN:O	5:Ae:248:ARG:HD3	1.90	0.72
1:AA:249:HIS:O	1:AA:250:LEU:HB2	1.89	0.72
5:AE:264:GLU:N	5:AE:272:VAL:O	2.21	0.72
3:AC:18:PHE:HE1	14:AC:405:UQ6:H72	1.54	0.72
4:Ad:292:MET:HA	17:Ad:402:3PH:H322	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:171:GLU:O	1:AA:174:GLU:HG2	1.89	0.71
5:AE:123:VAL:CG1	9:AJ:29:ALA:HA	2.20	0.71
5:Ae:152:ILE:HG23	5:Ae:272:VAL:CB	2.20	0.71
1:AA:397:ASN:HD21	2:AB:126:ILE:CD1	2.03	0.71
5:AE:199:GLN:O	5:AE:248:ARG:HD3	1.90	0.71
5:AE:220:LEU:HB3	3:Ac:145:VAL:HG13	1.71	0.71
12:AC:403:3PE:H2C1	7:AG:41:ARG:HH21	1.51	0.71
5:Ae:207:LYS:HB2	5:Ae:210:TRP:HB2	1.73	0.71
8:Ah:42:VAL:HG13	8:Ah:45:ARG:HH21	1.55	0.71
1:AA:310:ILE:HG21	1:AA:379:LEU:HD21	1.73	0.71
4:AD:159:ASN:O	4:AD:162:GLY:N	2.22	0.71
1:Aa:57:LEU:HD12	1:Aa:229:MET:HE2	1.73	0.71
5:Ae:178:HIS:HB2	5:Ae:210:TRP:CZ3	2.26	0.71
5:AE:152:ILE:HB	5:AE:169:TRP:NE1	2.06	0.70
1:Aa:120:LEU:HB3	2:Ab:299:ILE:HG13	1.73	0.70
5:Ae:116:LEU:HA	9:Aj:15:PHE:CZ	2.26	0.70
5:Ae:264:GLU:H	5:Ae:271:VAL:HG13	1.56	0.70
5:AE:178:HIS:HB2	5:AE:210:TRP:CZ3	2.26	0.70
1:Aa:279:ASP:OD1	7:Ag:12:ARG:NE	2.24	0.70
4:Ad:248:ILE:HD11	16:Ad:401:HEC:HBB1	1.72	0.70
5:Ae:154:ILE:HD11	5:Ae:174:LEU:HD21	1.73	0.70
5:AE:192:VAL:HA	5:AE:195:LEU:HD12	1.73	0.70
5:Ae:220:LEU:HD12	5:Ae:239:HIS:CE1	2.27	0.70
1:AA:362:ALA:HB2	1:AA:461:PRO:HB2	1.72	0.70
5:Ae:152:ILE:HG23	5:Ae:272:VAL:HA	1.73	0.70
1:Aa:87:ASN:ND2	1:Aa:204:PRO:HD3	2.06	0.70
3:Ac:269:LYS:HE3	3:Ac:340:GLY:HA2	1.74	0.70
5:Ae:152:ILE:HG23	5:Ae:273:VAL:N	2.07	0.70
3:Ac:147:THR:HG22	3:Ac:161:VAL:HG13	1.74	0.70
4:Ad:218:TYR:CD1	4:Ad:246:PRO:HG3	2.26	0.70
5:AE:220:LEU:HD12	5:AE:239:HIS:CE1	2.26	0.69
5:Ae:192:VAL:HA	5:Ae:195:LEU:HD12	1.73	0.69
5:Ae:202:LEU:HA	5:Ae:205:VAL:HG22	1.74	0.69
5:AE:159:ILE:HG23	5:AE:163:LYS:HE3	1.74	0.69
5:AE:220:LEU:O	3:Ac:145:VAL:HA	1.92	0.69
4:Ad:249:TYR:CZ	4:Ad:252:VAL:HA	2.28	0.69
1:AA:186:TYR:CZ	5:AE:80:HIS:HB2	2.27	0.69
4:AD:244:MET:HB2	16:AD:401:HEC:C1D	2.23	0.69
5:AE:115:TYR:HB3	9:AJ:21:PHE:CE1	2.27	0.69
5:Ae:180:THR:H	5:Ae:183:GLU:HB2	1.58	0.69
5:AE:207:LYS:HB2	5:AE:210:TRP:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:43:LEU:HD11	2:Ab:163:ALA:CB	2.23	0.69
9:AJ:17:ARG:HD2	9:AJ:20:THR:HG23	1.75	0.69
3:AC:146:ILE:HG13	13:AC:404:U10:H4M3	1.73	0.69
4:AD:244:MET:HB2	16:AD:401:HEC:ND	2.08	0.69
1:Aa:171:GLU:HA	1:Aa:174:GLU:HG2	1.74	0.69
1:Aa:403:LEU:HD12	1:Aa:403:LEU:N	2.08	0.69
2:Ab:412:VAL:HG13	2:Ab:415:GLN:HE21	1.58	0.69
4:Ad:214:LEU:HD11	4:Ad:237:PHE:HB2	1.75	0.69
5:AI:43:LEU:HB2	2:Ab:167:GLN:NE2	2.08	0.68
3:Ac:197:LEU:HD12	14:Ac:406:UQ6:C1M	2.22	0.68
4:Ad:186:ARG:HE	4:Ad:193:LEU:HB2	1.58	0.68
2:AB:233:VAL:HA	2:AB:236:GLN:HG2	1.76	0.68
4:AD:121:CYS:HA	16:AD:401:HEC:HMC2	1.74	0.68
4:AD:170:LYS:HD2	5:AE:151:LYS:HE2	1.74	0.68
4:AD:249:TYR:CZ	4:AD:252:VAL:HA	2.28	0.68
1:Aa:188:HIS:HE2	1:Aa:348:TYR:HE2	1.41	0.68
5:Ae:159:ILE:HG23	5:Ae:163:LYS:HE3	1.74	0.68
5:AE:202:LEU:HA	5:AE:205:VAL:HG22	1.74	0.68
1:Aa:68:THR:HG21	2:Ab:384:MET:HG3	1.69	0.68
4:AD:117:TYR:HA	4:AD:121:CYS:HG	1.58	0.68
7:AG:19:LEU:HD11	7:AG:23:GLU:CG	2.24	0.68
1:Aa:68:THR:CG2	2:Ab:384:MET:CG	2.64	0.68
4:Ad:124:CYS:HA	4:Ad:179:TYR:CE2	2.24	0.68
5:Ae:197:ASP:HB3	5:Ae:257:ASN:CG	2.19	0.68
1:Aa:281:ALA:HB2	7:Ag:10:ARG:HH22	1.59	0.68
1:Aa:337:LEU:HB3	1:Aa:368:MET:SD	2.34	0.68
3:Ac:29:SER:OG	15:Ac:407:CDL:HA61	1.93	0.68
2:AB:51:SER:HB2	2:AB:230:LEU:HD12	1.75	0.68
1:Aa:280:ASP:OD2	7:Ag:10:ARG:HA	1.94	0.68
3:AC:147:THR:HG22	3:AC:161:VAL:HG13	1.74	0.67
2:AB:51:SER:HB2	2:AB:230:LEU:CD1	2.24	0.67
4:AD:218:TYR:CD1	4:AD:246:PRO:HG3	2.29	0.67
1:AA:342:GLN:HE21	1:AA:357:HIS:HB3	1.59	0.67
2:AB:159:LYS:HE2	5:AI:37:ALA:O	1.94	0.67
2:AB:305:THR:HG23	2:AB:306:THR:HG23	1.77	0.67
5:AE:180:THR:H	5:AE:183:GLU:HB2	1.58	0.67
3:Ac:197:LEU:CD1	14:Ac:406:UQ6:H1M2	2.23	0.67
5:AE:154:ILE:CD1	5:AE:273:VAL:HG23	2.25	0.67
3:Ac:242:LEU:HD21	3:Ac:250:LEU:HD11	1.75	0.67
8:Ah:39:GLU:HA	8:Ah:42:VAL:HB	1.75	0.67
1:AA:470:ARG:CD	3:AC:222:PRO:HG3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:120:VAL:CG1	16:Ad:401:HEC:HAB	2.24	0.67
5:Ae:270:VAL:O	5:Ae:271:VAL:CG2	2.42	0.67
2:AB:412:VAL:HG13	2:AB:415:GLN:HE21	1.58	0.67
1:Aa:66:HIS:CE1	1:Aa:402:HIS:HB2	2.31	0.67
5:Ae:261:PRO:CB	5:Ae:273:VAL:HG11	2.22	0.67
4:AD:186:ARG:NE	4:AD:193:LEU:HB2	2.09	0.66
5:AE:153:GLU:C	5:AE:154:ILE:HD12	2.19	0.66
5:AE:197:ASP:HB3	5:AE:257:ASN:CG	2.19	0.66
4:Ad:248:ILE:HD11	16:Ad:401:HEC:CBB	2.25	0.66
7:AG:11:ILE:CG2	7:AG:14:VAL:HG21	2.18	0.66
7:Ag:49:VAL:O	7:Ag:52:PRO:HD2	1.96	0.66
9:Aj:31:PHE:CD1	10:Ak:48:ILE:HG23	2.30	0.66
1:AA:186:TYR:CE1	5:AE:80:HIS:HB2	2.30	0.66
2:AB:229:VAL:O	2:AB:232:GLN:HG2	1.95	0.66
7:AG:11:ILE:CG2	7:AG:14:VAL:HG22	2.25	0.66
5:Ae:112:GLY:HA2	9:Aj:15:PHE:CD2	2.30	0.66
7:Ag:19:LEU:HD11	7:Ag:23:GLU:CG	2.24	0.66
5:Ae:169:TRP:CZ3	5:Ae:273:VAL:HB	2.31	0.66
1:Aa:68:THR:HB	2:Ab:387:GLU:OE1	1.96	0.66
1:Aa:74:TRP:CZ2	1:Aa:411:GLU:HA	2.31	0.66
3:Ac:257:MET:HG3	4:Ad:203:ALA:HB1	1.78	0.66
5:Ae:152:ILE:HG23	5:Ae:273:VAL:H	1.56	0.66
3:Ac:240:MET:HE1	17:Ad:402:3PH:H231	1.76	0.66
7:Ag:11:ILE:CG2	7:Ag:14:VAL:HG22	2.25	0.66
3:AC:45:ILE:HA	11:AC:401:HEM:HAB	1.79	0.65
5:Ae:93:ARG:HH11	5:Ae:110:ARG:CG	2.09	0.65
4:Ad:121:CYS:SG	16:Ad:401:HEC:CBB	2.83	0.65
4:Ad:192:ALA:CB	16:Ad:401:HEC:HMD3	2.25	0.65
5:AI:64:LEU:HD13	2:Ab:174:ILE:HG21	1.78	0.65
2:Ab:261:GLN:HA	2:Ab:442:GLY:O	1.97	0.65
3:AC:137:GLN:CG	3:AC:265:PRO:HG3	2.27	0.65
4:AD:138:VAL:HG11	4:AD:276:TRP:NE1	2.11	0.65
5:AI:70:LEU:HD13	2:Ab:88:SER:HB3	1.78	0.65
3:Ac:240:MET:CE	17:Ad:402:3PH:H231	2.27	0.65
3:AC:197:LEU:O	3:AC:201:HIS:CD2	2.50	0.65
4:AD:181:ASN:HB2	4:AD:182:PRO:HD2	1.78	0.65
5:Ae:152:ILE:HD12	5:Ae:169:TRP:CD2	2.31	0.65
3:AC:287:LYS:HZ1	5:Ae:255:PRO:HG2	1.62	0.65
4:AD:202:ARG:HG3	4:AD:278:SER:HB3	1.78	0.65
5:AE:127:TYR:CE1	9:AJ:33:GLU:HG3	2.30	0.65
2:Ab:307:SER:HB2	2:Ab:310:SER:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:403:LEU:HD21	2:AB:56:ALA:HB1	1.79	0.64
3:Ac:141:TRP:HD1	3:Ac:265:PRO:HD3	1.62	0.64
1:AA:403:LEU:HD12	1:AA:403:LEU:N	2.12	0.64
1:Aa:50:VAL:HG11	1:Aa:417:LEU:HD11	1.80	0.64
4:Ad:201:VAL:HG21	4:Ad:275:ARG:HA	1.80	0.64
4:Ad:248:ILE:HG22	4:Ad:263:MET:HG3	1.79	0.64
5:Ae:93:ARG:CD	5:Ae:110:ARG:HD3	2.26	0.64
5:Ae:152:ILE:HD11	5:Ae:174:LEU:HD21	1.78	0.64
3:AC:201:HIS:HE1	14:AC:405:UQ6:C1M	2.09	0.64
4:AD:214:LEU:HG	4:AD:234:ASN:ND2	2.12	0.64
1:Aa:87:ASN:H	1:Aa:207:ASN:ND2	1.94	0.64
5:Ae:153:GLU:HA	5:Ae:271:VAL:O	1.98	0.64
5:AE:218:THR:CG2	5:AE:256:LEU:O	2.45	0.64
5:AI:77:ARG:O	5:AI:78:PHE:C	2.40	0.64
3:Ac:220:PHE:CE2	14:Ac:406:UQ6:H4M2	2.33	0.64
5:Ae:93:ARG:HD2	5:Ae:110:ARG:HD3	1.76	0.64
1:AA:274:GLU:HG3	1:AA:456:VAL:HB	1.80	0.64
5:Ae:156:LEU:HB2	5:Ae:269:ASP:HA	1.80	0.64
5:Ae:234:TYR:HB2	5:Ae:243:TYR:HB2	1.79	0.64
4:AD:248:ILE:HG22	4:AD:263:MET:HG3	1.79	0.64
1:Aa:171:GLU:O	1:Aa:175:ASN:N	2.28	0.64
2:Ab:426:LYS:O	2:Ab:429:LYS:HG2	1.97	0.64
3:Ac:137:GLN:HE21	3:Ac:265:PRO:HD3	1.62	0.64
5:Ae:152:ILE:CD1	5:Ae:174:LEU:HD22	2.28	0.64
2:AB:48:VAL:CG2	2:AB:400:ALA:HB1	2.27	0.63
10:Ak:13:LEU:HB3	10:Ak:17:TRP:CH2	2.33	0.63
1:AA:92:PHE:CZ	1:AA:161:ILE:HG23	2.33	0.63
1:AA:182:VAL:HG12	1:AA:186:TYR:CE2	2.33	0.63
4:AD:323:PRO:HG2	4:AD:325:LYS:HD2	1.80	0.63
3:Ac:253:PRO:O	4:Ad:203:ALA:HA	1.98	0.63
5:Ae:188:ALA:HA	5:Ae:200:HIS:NE2	2.13	0.63
5:Ae:218:THR:CG2	5:Ae:256:LEU:O	2.45	0.63
5:AE:188:ALA:HA	5:AE:200:HIS:NE2	2.13	0.63
4:AD:91:PRO:HB3	4:AD:213:SER:OG	1.99	0.63
4:AD:255:TYR:OH	4:AD:266:VAL:HA	1.98	0.63
1:AA:204:PRO:HB2	1:AA:206:GLU:OE1	1.98	0.63
2:Ab:60:ARG:HD2	2:Ab:393:LEU:HD13	1.81	0.63
2:Ab:230:LEU:HA	2:Ab:233:VAL:HG22	1.80	0.63
3:Ac:37:LEU:HD13	11:Ac:403:HEM:C3B	2.34	0.63
1:AA:96:LEU:HD11	1:AA:161:ILE:HG12	1.79	0.63
2:AB:40:PHE:CZ	2:AB:48:VAL:HB	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:426:LYS:O	2:AB:429:LYS:HG2	1.97	0.63
3:AC:141:TRP:HD1	3:AC:265:PRO:HD3	1.61	0.63
3:AC:326:TRP:CZ2	12:AC:403:3PE:H11	2.31	0.63
4:AD:195:PRO:CG	16:AD:401:HEC:HBA1	2.29	0.63
1:Aa:266:THR:HG23	1:Aa:266:THR:O	1.99	0.63
1:Aa:403:LEU:HD21	2:Ab:56:ALA:CB	2.29	0.63
5:Ae:93:ARG:HH11	5:Ae:110:ARG:HG2	1.63	0.63
1:Aa:110:GLU:O	1:Aa:114:GLU:HG2	1.99	0.63
1:AA:469:ASN:ND2	3:AC:223:TYR:CZ	2.67	0.63
2:AB:48:VAL:HG22	2:AB:219:ALA:CB	2.21	0.63
3:AC:287:LYS:NZ	5:Ae:255:PRO:HG2	2.14	0.63
5:Ae:161:GLU:HA	5:Ae:178:HIS:CG	2.34	0.63
12:AC:403:3PE:H291	7:AG:41:ARG:HE	1.62	0.63
8:AH:49:GLU:HA	8:AH:52:ASP:OD2	1.99	0.63
3:AC:218:ILE:HD11	3:AC:224:TYR:CE2	2.34	0.62
1:Aa:274:GLU:HG3	1:Aa:456:VAL:HB	1.80	0.62
2:Ab:92:LYS:HG2	2:Ab:145:GLU:HG3	1.81	0.62
3:Ac:223:TYR:O	4:Ad:311:TRP:NE1	2.27	0.62
4:Ad:186:ARG:NE	4:Ad:193:LEU:HB2	2.14	0.62
4:AD:129:TYR:HD2	4:AD:198:SER:CB	2.12	0.62
5:AE:161:GLU:HA	5:AE:178:HIS:CG	2.34	0.62
5:AE:174:LEU:HD21	5:AE:273:VAL:HG21	1.81	0.62
3:Ac:138:MET:CE	3:Ac:268:ILE:HG23	2.28	0.62
4:Ad:255:TYR:OH	4:Ad:266:VAL:HA	1.98	0.62
5:Ae:179:ARG:HH12	5:Ae:201:ASP:HB2	1.64	0.62
5:Ae:213:LEU:HD23	5:Ae:260:VAL:HG22	1.81	0.62
1:AA:169:LEU:HD11	1:AA:209:ARG:HG2	1.82	0.62
12:AC:403:3PE:H292	7:AG:41:ARG:HH21	1.62	0.62
7:Ag:74:ASN:HB3	7:Ag:77:MET:HB2	1.81	0.62
7:Ag:43:ARG:HD3	12:Ag:102:3PE:H3B2	1.81	0.62
5:AE:234:TYR:HB2	5:AE:243:TYR:HB2	1.79	0.62
1:AA:119:HIS:ND1	2:AB:298:HIS:HA	2.15	0.62
1:Aa:222:ARG:NH2	1:Aa:263:PRO:HB3	2.15	0.62
9:Aj:30:LEU:HD23	10:Ak:48:ILE:HG21	1.82	0.62
1:AA:399:LEU:HB3	1:AA:426:LEU:CD2	2.30	0.62
2:Ab:117:GLU:OE2	2:Ab:331:SER:N	2.24	0.62
10:Ak:45:VAL:HB	10:Ak:48:ILE:HD11	1.82	0.62
4:AD:235:PRO:HA	4:AD:240:GLN:HG3	1.82	0.62
4:AD:244:MET:HB2	16:AD:401:HEC:C4D	2.30	0.62
16:AD:401:HEC:CGA	16:AD:401:HEC:HHA	2.30	0.62
5:AE:152:ILE:HB	5:AE:169:TRP:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:388:VAL:HG22	1:Aa:441:LEU:HD13	1.81	0.62
6:Af:110:LYS:O	6:Af:111:LYS:C	2.43	0.62
2:AB:412:VAL:O	2:AB:415:GLN:HG2	2.00	0.61
1:Aa:92:PHE:CZ	1:Aa:161:ILE:HG23	2.35	0.61
2:Ab:412:VAL:O	2:Ab:415:GLN:HG2	2.00	0.61
5:Ae:261:PRO:HB2	5:Ae:273:VAL:CG1	2.25	0.61
1:AA:182:VAL:CG1	1:AA:186:TYR:CE2	2.83	0.61
6:Af:92:GLU:HG2	6:Af:96:LYS:HE2	1.82	0.61
1:AA:80:ARG:NH2	1:AA:268:CYS:SG	2.72	0.61
1:AA:384:THR:O	1:AA:387:GLU:HG2	2.00	0.61
5:AE:213:LEU:HD23	5:AE:260:VAL:HG22	1.82	0.61
10:Ak:42:LEU:HD22	10:Ak:48:ILE:HD13	1.82	0.61
6:AF:92:GLU:HG2	6:AF:96:LYS:HE2	1.82	0.61
2:Ab:183:LYS:HG3	2:Ab:254:ARG:HB3	1.82	0.61
5:AE:221:GLY:HA3	3:Ac:148:ASN:HD22	1.63	0.61
2:AB:176:ASN:O	2:AB:258:ILE:HD11	2.00	0.61
6:AF:108:TRP:CZ2	2:Ab:101:ARG:HB3	2.35	0.61
3:AC:138:MET:CE	3:AC:268:ILE:HG23	2.31	0.61
3:Ac:107:TYR:HB2	3:Ac:305:PRO:HG3	1.80	0.61
3:Ac:311:LYS:O	6:Af:39:HIS:N	2.27	0.61
2:AB:307:SER:HB2	2:AB:310:SER:HB2	1.82	0.61
4:AD:262:THR:HG22	8:AH:24:LEU:HG	1.83	0.61
5:AE:244:ASP:HB3	5:AE:250:ARG:HH11	1.65	0.61
1:Aa:186:TYR:CE1	5:Ae:80:HIS:HB2	2.36	0.61
2:Ab:313:VAL:HG21	2:Ab:323:VAL:HG21	1.83	0.61
4:AD:131:ALA:HB2	4:AD:174:TYR:CD2	2.36	0.61
4:AD:197:LEU:O	4:AD:198:SER:C	2.44	0.61
5:AE:179:ARG:HH12	5:AE:201:ASP:HB2	1.64	0.61
5:AE:263:TYR:HA	5:AE:273:VAL:C	2.26	0.61
2:Ab:300:LYS:HG2	2:Ab:301:ARG:HG3	1.83	0.61
4:Ad:244:MET:HB2	16:Ad:401:HEC:ND	2.15	0.61
5:Ae:244:ASP:HB3	5:Ae:250:ARG:HH11	1.65	0.61
1:AA:341:PHE:HE1	1:AA:356:ALA:HB1	1.66	0.61
3:AC:265:PRO:HD2	3:AC:268:ILE:HD11	1.81	0.61
5:AI:62:ARG:CD	5:AI:63:PRO:HD2	2.31	0.61
1:AA:168:ILE:O	1:AA:171:GLU:HG2	2.01	0.60
3:AC:222:PRO:HG2	3:AC:223:TYR:CD1	2.31	0.60
2:Ab:262:ASN:OD1	2:Ab:442:GLY:HA2	2.01	0.60
3:Ac:8:HIS:CE1	3:Ac:10:LEU:HB3	2.35	0.60
4:Ad:121:CYS:SG	16:Ad:401:HEC:CAB	2.89	0.60
3:AC:219:PRO:HG2	3:AC:223:TYR:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:403:LEU:CD1	1:Aa:403:LEU:N	2.65	0.60
2:Ab:97:PHE:CZ	2:Ab:101:ARG:HG3	2.36	0.60
8:Ah:39:GLU:O	8:Ah:40:LYS:C	2.41	0.60
4:AD:195:PRO:HG3	16:AD:401:HEC:CBA	2.31	0.60
4:Ad:232:TYR:CZ	4:Ad:245:ALA:HB2	2.35	0.60
5:Ae:207:LYS:HD2	5:Ae:210:TRP:HD1	1.66	0.60
1:AA:363:MET:HA	1:AA:464:GLN:OE1	2.01	0.60
7:AG:64:ASN:O	7:AG:68:GLU:HG2	2.01	0.60
5:AI:64:LEU:HD21	2:Ab:171:THR:HA	1.82	0.60
1:AA:478:LEU:C	1:AA:478:LEU:CD1	2.74	0.60
3:AC:240:MET:SD	17:AD:402:3PH:H251	2.42	0.60
6:AF:108:TRP:HA	6:AF:111:LYS:NZ	2.17	0.60
10:Ak:48:ILE:HD12	10:Ak:49:ASN:N	2.17	0.60
5:AE:207:LYS:HD2	5:AE:210:TRP:HD1	1.67	0.60
1:AA:101:THR:HG22	1:AA:154:SER:HA	1.83	0.60
3:AC:302:ALA:O	3:AC:305:PRO:HD2	2.02	0.60
4:AD:121:CYS:HB3	16:AD:401:HEC:HHC	1.84	0.60
1:Aa:295:GLY:O	1:Aa:301:ASN:ND2	2.35	0.60
4:Ad:95:PRO:HG2	8:Ah:85:PHE:HB2	1.84	0.60
4:Ad:138:VAL:HG12	4:Ad:139:CYS:SG	2.42	0.60
4:Ad:146:LYS:O	4:Ad:150:GLU:HG2	2.00	0.60
2:AB:138:LEU:CD2	2:AB:238:LEU:HG	2.32	0.59
5:AE:111:LYS:CE	9:AJ:11:TYR:CZ	2.84	0.59
1:Aa:338:CYS:SG	1:Aa:368:MET:HB2	2.41	0.59
1:AA:186:TYR:OH	5:AE:80:HIS:CB	2.50	0.59
1:AA:225:LYS:HE3	1:AA:256:VAL:HA	1.83	0.59
2:Ab:138:LEU:HB3	2:Ab:237:PHE:CD2	2.36	0.59
5:Ae:262:ALA:C	5:Ae:273:VAL:HG13	2.26	0.59
7:Ag:19:LEU:CD2	7:Ag:24:GLN:HB3	2.29	0.59
5:AE:146:VAL:HA	5:AE:149:MET:HE3	1.84	0.59
10:AK:38:TRP:CD1	3:Ac:155:TYR:HH	2.21	0.59
3:Ac:28:SER:HB2	15:Ac:407:CDL:HA21	1.84	0.59
1:AA:98:PHE:CE1	1:AA:120:LEU:HD21	2.37	0.59
1:AA:402:HIS:NE2	1:AA:403:LEU:HD12	2.17	0.59
1:AA:402:HIS:CD2	1:AA:403:LEU:HD12	2.38	0.59
2:AB:313:VAL:HG21	2:AB:323:VAL:HG21	1.83	0.59
3:Ac:138:MET:HE1	3:Ac:268:ILE:CG1	2.32	0.59
1:AA:64:SER:OG	1:AA:235:GLY:HA2	2.02	0.59
3:Ac:302:ALA:O	3:Ac:305:PRO:HD2	2.02	0.59
3:Ac:320:ILE:HG23	12:Ag:102:3PE:H121	1.85	0.59
5:Ae:132:VAL:HA	5:Ae:135:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:286:PHE:CE1	2:AB:427:ALA:HB1	2.38	0.59
3:AC:345:HIS:CE1	3:AC:346:PRO:HB3	2.37	0.59
4:Ad:157:GLY:HA2	4:Ad:163:GLU:O	2.03	0.59
5:AE:123:VAL:HG13	9:AJ:29:ALA:CA	2.26	0.59
2:Ab:90:THR:HG23	2:Ab:95:SER:HA	1.83	0.59
5:Ae:163:LYS:O	5:Ae:177:ARG:HG3	2.02	0.59
8:Ah:28:LEU:HD13	8:Ah:84:LEU:HD22	1.84	0.59
10:AK:18:ILE:N	10:AK:19:PRO:HD2	2.18	0.59
1:Aa:225:LYS:HG3	1:Aa:257:TYR:CZ	2.37	0.59
1:AA:66:HIS:HE1	1:AA:402:HIS:HB2	1.68	0.59
1:AA:92:PHE:CE2	1:AA:161:ILE:HG23	2.38	0.59
1:AA:186:TYR:HB3	1:AA:275:ILE:HG21	1.84	0.59
2:AB:39:GLU:O	2:AB:227:HIS:CE1	2.56	0.59
4:AD:233:PHE:HA	4:AD:240:GLN:O	2.02	0.59
5:AE:163:LYS:O	5:AE:177:ARG:HG3	2.02	0.59
1:Aa:111:LYS:O	1:Aa:114:GLU:N	2.35	0.59
3:Ac:240:MET:CE	17:Ad:402:3PH:H251	2.33	0.59
7:Ag:47:LEU:HD12	12:Ag:102:3PE:H342	1.85	0.59
1:AA:70:THR:HG21	1:AA:407:THR:HA	1.85	0.59
3:Ac:236:PHE:CD2	17:Ad:402:3PH:H3B2	2.30	0.59
3:Ac:345:HIS:CE1	3:Ac:346:PRO:HB3	2.37	0.59
2:AB:170:GLN:HG3	2:AB:339:TYR:OH	2.03	0.58
3:AC:197:LEU:HD12	14:AC:405:UQ6:H1M2	1.84	0.58
6:AF:24:ALA:O	7:AG:48:ARG:NH2	2.35	0.58
1:Aa:111:LYS:O	1:Aa:112:GLU:C	2.44	0.58
1:Aa:222:ARG:NH2	1:Aa:263:PRO:CB	2.66	0.58
2:Ab:60:ARG:CG	2:Ab:393:LEU:HD13	2.33	0.58
7:Ag:30:TYR:OH	15:Ag:101:CDL:H132	2.04	0.58
5:AE:122:THR:HG21	9:AJ:25:ILE:HG21	1.85	0.58
7:AG:11:ILE:HG22	7:AG:12:ARG:N	2.18	0.58
1:Aa:222:ARG:NH2	1:Aa:263:PRO:HG3	2.17	0.58
2:Ab:286:PHE:CE1	2:Ab:427:ALA:HB1	2.38	0.58
4:Ad:193:LEU:O	4:Ad:194:PRO:C	2.46	0.58
4:Ad:215:LEU:CD1	16:Ad:401:HEC:HMB1	2.29	0.58
3:AC:29:SER:HB3	15:AC:406:CDL:HB61	1.85	0.58
1:Aa:66:HIS:HE1	1:Aa:402:HIS:HB2	1.66	0.58
3:Ac:162:GLU:O	3:Ac:166:GLY:N	2.36	0.58
7:Ag:50:ALA:O	7:Ag:51:PRO:C	2.46	0.58
7:AG:19:LEU:CD2	7:AG:24:GLN:HB3	2.29	0.58
4:AD:197:LEU:HA	4:AD:200:ILE:HB	1.84	0.58
5:AE:156:LEU:HD13	5:AE:210:TRP:NE1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:18:THR:HG22	5:AI:18:THR:O	2.02	0.58
1:Aa:96:LEU:HG	1:Aa:164:GLU:HG3	1.84	0.58
3:Ac:163:TRP:O	3:Ac:177:ARG:NH1	2.36	0.58
5:Ae:159:ILE:O	5:Ae:210:TRP:HH2	1.86	0.58
3:AC:233:LEU:HD23	4:AD:300:LEU:HA	1.85	0.58
1:AA:403:LEU:CD1	1:AA:403:LEU:H	2.16	0.58
5:AE:160:PRO:O	5:AE:178:HIS:HB3	2.03	0.58
4:Ad:284:HIS:NE2	4:Ad:288:MET:HE3	2.19	0.58
5:Ae:160:PRO:O	5:Ae:178:HIS:HB3	2.03	0.58
4:AD:126:SER:HB3	4:AD:178:PRO:CD	2.34	0.58
1:Aa:104:ARG:HB3	1:Aa:108:ALA:HB3	1.85	0.58
1:Aa:220:LEU:O	1:Aa:224:TYR:HB2	2.04	0.58
7:Ag:11:ILE:HG22	7:Ag:12:ARG:N	2.18	0.58
1:AA:220:LEU:O	1:AA:224:TYR:HB2	2.03	0.58
5:AE:159:ILE:O	5:AE:210:TRP:HH2	1.86	0.58
2:Ab:177:LEU:HD11	2:Ab:272:VAL:HG22	1.85	0.58
5:Ae:116:LEU:CA	9:Aj:15:PHE:CZ	2.86	0.58
8:Ah:33:GLU:O	8:Ah:37:GLN:HG3	2.04	0.58
2:AB:47:LEU:HA	2:AB:218:MET:O	2.03	0.58
5:Ae:156:LEU:H	5:Ae:269:ASP:CA	2.11	0.58
1:AA:57:LEU:HD13	1:AA:229:MET:HB3	1.85	0.57
3:AC:215:ALA:HA	7:AG:11:ILE:HD11	1.86	0.57
6:AF:106:GLU:O	6:AF:110:LYS:HG3	2.03	0.57
1:Aa:104:ARG:NH1	1:Aa:146:LEU:HD23	2.19	0.57
1:Aa:107:ASN:O	1:Aa:110:GLU:HG2	2.03	0.57
1:AA:87:ASN:HD21	1:AA:199:GLN:HB2	1.69	0.57
4:AD:249:TYR:CE2	4:AD:252:VAL:HA	2.39	0.57
4:AD:284:HIS:NE2	4:AD:288:MET:HE3	2.18	0.57
7:AG:35:ILE:HB	7:AG:36:PRO:HD3	1.86	0.57
2:Ab:293:LEU:HD21	2:Ab:361:VAL:HG21	1.86	0.57
7:Ag:27:PHE:HB3	7:Ag:30:TYR:HB2	1.87	0.57
1:AA:158:ASP:HA	1:AA:161:ILE:HD12	1.86	0.57
10:AK:38:TRP:CZ2	10:AK:40:LEU:HD12	2.40	0.57
1:Aa:57:LEU:HA	1:Aa:226:ALA:O	2.05	0.57
3:Ac:45:ILE:HG12	11:Ac:402:HEM:HAB	1.85	0.57
3:AC:141:TRP:NE1	3:AC:264:THR:HA	2.19	0.57
3:AC:150:LEU:HD13	3:AC:164:ILE:HD12	1.86	0.57
6:AF:107:GLU:OE2	6:AF:111:LYS:HD3	2.05	0.57
3:Ac:138:MET:HE1	3:Ac:268:ILE:HG23	1.86	0.57
3:Ac:185:LEU:HD11	13:Ac:405:U10:H221	1.86	0.57
4:Ad:195:PRO:HD2	16:Ad:401:HEC:CHA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:402:HIS:ND1	1:AA:403:LEU:CD1	2.67	0.57
3:AC:137:GLN:HG3	3:AC:265:PRO:CG	2.31	0.57
4:AD:223:THR:HG21	8:AH:55:VAL:HG21	1.86	0.57
5:AI:68:VAL:HG11	2:Ab:85:LEU:HD21	1.86	0.57
1:Aa:269:ARG:HD2	5:Ae:92:ARG:NH2	2.20	0.57
4:Ad:249:TYR:CE2	4:Ad:252:VAL:HA	2.40	0.57
8:Ah:84:LEU:O	8:Ah:88:LEU:HG	2.05	0.57
2:AB:162:LYS:NZ	2:AB:194:ASP:OD1	2.38	0.57
3:AC:147:THR:HG21	3:AC:165:TRP:CD1	2.40	0.57
3:AC:201:HIS:HE1	14:AC:405:UQ6:H1M1	1.68	0.57
5:AE:168:LYS:HE2	3:Ac:261:PRO:HG2	1.86	0.57
5:AE:207:LYS:HB3	5:AE:209:GLU:OE1	2.05	0.57
5:AE:272:VAL:HG12	5:AE:274:GLY:H	1.69	0.57
5:Ae:218:THR:HG21	5:Ae:256:LEU:C	2.30	0.57
1:AA:158:ASP:O	1:AA:162:GLU:HG2	2.05	0.57
4:Ad:222:PRO:O	4:Ad:225:VAL:HG12	2.05	0.57
8:Ah:45:ARG:O	8:Ah:49:GLU:HG2	2.04	0.57
4:AD:222:PRO:O	4:AD:225:VAL:HG12	2.05	0.57
4:AD:296:MET:CE	17:AD:402:3PH:H362	2.34	0.57
1:Aa:55:ASN:HB3	1:Aa:226:ALA:CB	2.35	0.57
1:Aa:92:PHE:HD1	1:Aa:168:ILE:HD12	1.68	0.57
2:Ab:142:THR:HG21	2:Ab:237:PHE:CB	2.28	0.57
4:Ad:136:VAL:HA	4:Ad:140:TYR:O	2.05	0.57
1:AA:402:HIS:CG	1:AA:403:LEU:HD12	2.40	0.56
2:AB:40:PHE:CE1	2:AB:48:VAL:HB	2.40	0.56
2:AB:117:GLU:OE2	2:AB:330:TYR:HB3	2.05	0.56
4:Ad:185:ALA:O	4:Ad:186:ARG:C	2.46	0.56
5:Ae:156:LEU:HD13	5:Ae:210:TRP:NE1	2.19	0.56
1:AA:74:TRP:CH2	1:AA:410:CYS:SG	2.97	0.56
3:AC:92:ILE:HG13	3:AC:272:TRP:HH2	1.69	0.56
3:AC:107:TYR:HB2	3:AC:305:PRO:HG3	1.87	0.56
7:AG:33:LYS:C	7:AG:36:PRO:HD2	2.30	0.56
2:Ab:425:VAL:HG12	2:Ab:429:LYS:HZ1	1.70	0.56
3:Ac:164:ILE:O	3:Ac:177:ARG:HD2	2.05	0.56
5:Ae:112:GLY:O	9:Aj:15:PHE:CE2	2.59	0.56
1:AA:120:LEU:N	2:AB:298:HIS:O	2.38	0.56
5:AE:219:HIS:HB2	5:AE:254:ALA:HA	1.88	0.56
1:Aa:222:ARG:NH1	1:Aa:263:PRO:HG3	2.20	0.56
4:Ad:170:LYS:HZ3	5:Ae:151:LYS:HD3	1.70	0.56
7:Ag:51:PRO:HB2	7:Ag:52:PRO:HD3	1.87	0.56
3:AC:171:ASP:CG	3:AC:172:LYS:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:147:ALA:O	4:AD:151:GLU:HG3	2.05	0.56
5:AE:221:GLY:O	3:Ac:141:TRP:HZ3	1.88	0.56
5:AI:62:ARG:HB3	5:AI:78:PHE:O	2.06	0.56
1:Aa:363:MET:HA	1:Aa:464:GLN:OE1	2.04	0.56
1:AA:402:HIS:ND1	1:AA:403:LEU:HD12	2.20	0.56
3:AC:138:MET:HE1	3:AC:268:ILE:HA	1.87	0.56
6:AF:22:TYR:CD2	6:AF:84:TYR:HB2	2.41	0.56
3:Ac:171:ASP:CG	3:Ac:172:LYS:H	2.13	0.56
5:Ae:270:VAL:C	5:Ae:271:VAL:HG23	2.31	0.56
6:Af:15:ASP:OD2	6:Af:19:LYS:NZ	2.39	0.56
1:AA:74:TRP:HH2	1:AA:410:CYS:HG	1.51	0.56
5:AE:197:ASP:HB3	5:AE:257:ASN:OD1	2.06	0.56
5:Ae:207:LYS:HB3	5:Ae:209:GLU:OE1	2.05	0.56
7:Ag:35:ILE:HB	7:Ag:36:PRO:HD3	1.86	0.56
1:AA:403:LEU:CD1	1:AA:403:LEU:N	2.69	0.56
2:AB:236:GLN:HG3	2:AB:237:PHE:CD2	2.41	0.56
3:AC:119:LEU:HD22	11:AC:402:HEM:HBB2	1.86	0.56
4:AD:321:TYR:HB2	6:AF:61:PHE:CZ	2.41	0.56
6:AF:15:ASP:OD2	6:AF:19:LYS:NZ	2.39	0.56
4:Ad:116:VAL:HA	4:Ad:253:LEU:HD21	1.88	0.56
5:Ae:219:HIS:HB2	5:Ae:254:ALA:HA	1.88	0.56
1:AA:120:LEU:HD12	1:AA:121:ASN:H	1.71	0.56
2:AB:43:LEU:HB3	2:AB:44:PRO:HD2	1.88	0.56
3:Ac:97:HIS:CE1	3:Ac:100:ARG:HH21	2.24	0.56
17:Ad:402:3PH:H341	5:Ae:128:ALA:HB1	1.88	0.56
7:Ag:33:LYS:C	7:Ag:36:PRO:HD2	2.30	0.56
3:AC:201:HIS:CE1	14:AC:405:UQ6:H1M1	2.41	0.56
4:AD:124:CYS:SG	16:AD:401:HEC:CAC	2.94	0.56
4:AD:321:TYR:HB2	6:AF:61:PHE:CE1	2.40	0.56
5:AE:218:THR:HG21	5:AE:256:LEU:C	2.30	0.56
8:AH:47:ARG:HA	8:AH:50:LEU:HB2	1.86	0.56
9:AJ:30:LEU:HD12	10:AK:34:TRP:HB2	1.87	0.56
2:Ab:162:LYS:NZ	2:Ab:194:ASP:OD1	2.38	0.56
6:Af:22:TYR:CD2	6:Af:84:TYR:HB2	2.41	0.56
2:AB:117:GLU:OE2	2:AB:331:SER:N	2.25	0.56
2:AB:300:LYS:HG2	2:AB:301:ARG:HG3	1.86	0.56
16:AD:401:HEC:HHA	16:AD:401:HEC:O2A	2.06	0.56
1:Aa:274:GLU:HG2	1:Aa:275:ILE:N	2.21	0.56
5:Ae:177:ARG:HB3	5:Ae:211:VAL:HG13	1.88	0.56
5:AE:156:LEU:HD22	5:AE:210:TRP:CE2	2.42	0.55
2:Ab:366:LEU:HD21	2:Ab:425:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:77:ASP:O	8:Ah:78:HIS:C	2.48	0.55
3:AC:272:TRP:HA	3:AC:275:LEU:HG	1.87	0.55
17:AD:402:3PH:H261	17:AD:402:3PH:H371	1.88	0.55
5:AE:177:ARG:HB3	5:AE:211:VAL:HG13	1.88	0.55
7:AG:27:PHE:HB3	7:AG:30:TYR:HB2	1.87	0.55
9:Aj:30:LEU:HA	10:Ak:34:TRP:CD1	2.41	0.55
2:AB:366:LEU:HD21	2:AB:425:VAL:HG22	1.87	0.55
3:AC:153:ILE:HB	3:AC:157:GLY:CA	2.36	0.55
5:AE:248:ARG:HA	5:AE:257:ASN:CG	2.32	0.55
7:AG:78:TYR:HB3	8:AH:63:GLU:HB2	1.88	0.55
2:Ab:290:GLN:O	2:Ab:294:GLY:O	2.24	0.55
2:AB:36:GLN:O	2:AB:52:LEU:HD13	2.07	0.55
5:AI:11:PHE:O	5:AI:14:VAL:HG22	2.05	0.55
5:AI:65:VAL:HG11	5:AI:77:ARG:HH22	1.71	0.55
4:Ad:179:TYR:O	4:Ad:180:PRO:C	2.49	0.55
3:AC:148:ASN:OD1	5:Ae:221:GLY:CA	2.54	0.55
5:Ae:191:GLU:H	5:Ae:191:GLU:CD	2.14	0.55
3:AC:97:HIS:CE1	3:AC:100:ARG:HH21	2.23	0.55
3:AC:238:ILE:HD12	15:AC:406:CDL:H762	1.86	0.55
4:AD:253:LEU:HD12	4:AD:253:LEU:C	2.32	0.55
1:Aa:362:ALA:HB2	1:Aa:461:PRO:HB2	1.88	0.55
1:Aa:477:TRP:HA	15:Aa:501:CDL:OB4	2.07	0.55
4:Ad:253:LEU:C	4:Ad:253:LEU:HD12	2.32	0.55
5:Ae:156:LEU:HD22	5:Ae:210:TRP:CE2	2.42	0.55
1:AA:74:TRP:CD2	1:AA:414:GLY:HA3	2.42	0.55
3:AC:49:LEU:HD22	3:Ac:184:ILE:HD13	1.88	0.55
3:AC:233:LEU:CD2	4:AD:300:LEU:HA	2.37	0.55
3:AC:272:TRP:CE2	3:AC:273:TYR:HD2	2.25	0.55
4:AD:223:THR:CG2	8:AH:55:VAL:HG21	2.36	0.55
4:AD:135:LEU:HD23	4:AD:276:TRP:CH2	2.41	0.55
4:AD:318:LYS:CD	5:AE:86:PRO:HB2	2.37	0.55
6:AF:102:ARG:HH21	6:AF:103:LYS:HE3	1.72	0.55
5:Ae:155:LYS:HA	5:Ae:269:ASP:O	2.07	0.55
5:Ae:192:VAL:HA	5:Ae:195:LEU:CD1	2.37	0.55
1:AA:139:ASP:O	1:AA:143:VAL:HG23	2.07	0.55
1:AA:296:TRP:HH2	1:AA:415:ARG:HH11	1.55	0.55
12:AC:403:3PE:H291	7:AG:41:ARG:HH21	1.68	0.55
8:Ah:42:VAL:O	8:Ah:46:GLU:HG3	2.07	0.55
1:AA:74:TRP:HB3	1:AA:418:LEU:HD11	1.89	0.55
4:AD:124:CYS:SG	16:AD:401:HEC:CBC	2.95	0.55
5:Ae:132:VAL:O	5:Ae:135:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:248:ARG:HA	5:Ae:257:ASN:CG	2.32	0.55
9:Aj:11:TYR:HE2	9:Aj:16:ARG:HH21	1.55	0.55
3:AC:138:MET:HE1	3:AC:268:ILE:HG23	1.89	0.54
3:AC:201:HIS:CE1	14:AC:405:UQ6:C1M	2.89	0.54
5:AE:127:TYR:HE1	9:AJ:33:GLU:HG3	1.71	0.54
1:Aa:101:THR:HA	1:Aa:155:SER:H	1.72	0.54
2:Ab:89:LEU:HD11	2:Ab:154:LEU:HD12	1.89	0.54
8:Ah:29:THR:O	8:Ah:33:GLU:HG3	2.07	0.54
8:Ah:46:GLU:O	8:Ah:50:LEU:HG	2.07	0.54
1:AA:87:ASN:H	1:AA:207:ASN:HD22	1.53	0.54
5:AE:207:LYS:CD	5:AE:210:TRP:HD1	2.20	0.54
5:Ae:112:GLY:O	9:Aj:15:PHE:HE2	1.88	0.54
5:Ae:195:LEU:HD11	5:Ae:248:ARG:HH11	1.72	0.54
1:AA:187:LEU:HD22	1:AA:288:ALA:HB1	1.89	0.54
2:AB:60:ARG:CZ	2:AB:390:GLU:HB3	2.37	0.54
3:AC:30:TRP:HB3	3:AC:100:ARG:HD3	1.90	0.54
5:AE:161:GLU:HA	5:AE:178:HIS:CD2	2.43	0.54
1:Aa:411:GLU:CD	1:Aa:415:ARG:HE	2.15	0.54
3:Ac:312:GLN:HE21	6:Af:37:THR:CB	2.21	0.54
4:Ad:155:GLN:HE21	4:Ad:164:MET:HB3	1.72	0.54
4:Ad:214:LEU:CD1	4:Ad:237:PHE:HB2	2.38	0.54
4:Ad:309:HIS:CE1	7:Ag:21:PRO:HB2	2.41	0.54
14:AC:405:UQ6:C18	14:AC:405:UQ6:H151	2.37	0.54
4:AD:126:SER:HB2	4:AD:128:ASP:OD1	2.07	0.54
2:Ab:159:LYS:HB2	2:Ab:197:MET:SD	2.47	0.54
3:Ac:146:ILE:HG13	13:Ac:405:U10:O4	2.08	0.54
5:Ae:197:ASP:HB3	5:Ae:257:ASN:OD1	2.06	0.54
5:AE:272:VAL:HG12	5:AE:274:GLY:N	2.22	0.54
7:AG:39:LEU:O	7:AG:42:THR:HG22	2.08	0.54
5:Ae:263:TYR:HB2	5:Ae:271:VAL:HG13	1.89	0.54
2:AB:60:ARG:HG3	2:AB:124:GLU:HB3	1.89	0.54
2:AB:290:GLN:NE2	5:Al:7:ARG:O	2.37	0.54
2:AB:300:LYS:HG2	2:AB:301:ARG:CG	2.37	0.54
4:AD:160:ASP:O	4:Ad:183:GLU:HB3	2.08	0.54
5:AE:195:LEU:HD11	5:AE:248:ARG:HH11	1.72	0.54
1:Aa:273:SER:O	1:Aa:455:ALA:HA	2.08	0.54
3:Ac:215:ALA:HA	7:Ag:11:ILE:HD11	1.90	0.54
4:Ad:155:GLN:HB3	4:Ad:166:MET:HG2	1.90	0.54
17:Ad:402:3PH:H222	5:Ae:135:GLN:HE22	1.73	0.54
2:AB:148:ARG:NH2	6:Af:50:ARG:O	2.40	0.54
5:AE:190:VAL:HG11	5:AE:195:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:183:VAL:HG21	1:Aa:286:HIS:HB2	1.88	0.54
3:AC:223:TYR:CE2	4:AD:314:LEU:HG	2.40	0.54
5:AE:143:SER:O	5:AE:146:VAL:HG22	2.08	0.54
7:AG:78:TYR:HE1	8:AH:62:GLU:HB2	1.70	0.54
5:AI:43:LEU:HD13	2:Ab:164:VAL:HG22	1.86	0.54
1:Aa:273:SER:HB3	7:Ag:18:SER:O	2.07	0.54
2:Ab:293:LEU:HD23	2:Ab:308:LEU:HD12	1.89	0.54
4:Ad:116:VAL:HG22	4:Ad:253:LEU:HD21	1.89	0.54
15:Ag:101:CDL:H532	15:Ag:101:CDL:H121	1.88	0.54
2:AB:237:PHE:O	2:AB:238:LEU:HB2	2.07	0.54
1:Aa:186:TYR:HB3	1:Aa:275:ILE:HG21	1.90	0.54
2:Ab:50:ALA:HB3	2:Ab:221:VAL:HG22	1.90	0.54
3:Ac:222:PRO:HG2	3:Ac:223:TYR:CD2	2.43	0.54
5:Ae:136:PHE:O	5:Ae:137:VAL:C	2.51	0.54
6:Af:102:ARG:HH21	6:Af:103:LYS:HE3	1.73	0.54
2:AB:59:SER:OG	2:AB:130:ILE:HG21	2.08	0.53
3:AC:233:LEU:HD23	4:AD:300:LEU:HD23	1.90	0.53
5:AE:123:VAL:HG22	9:AJ:29:ALA:HB2	1.90	0.53
1:Aa:55:ASN:HB3	1:Aa:226:ALA:HB1	1.90	0.53
4:Ad:170:LYS:NZ	5:Ae:151:LYS:HD3	2.23	0.53
4:Ad:255:TYR:HB3	4:Ad:257:ASP:OD1	2.08	0.53
1:AA:170:ARG:HG3	1:AA:171:GLU:N	2.22	0.53
3:AC:164:ILE:O	3:AC:177:ARG:HD2	2.08	0.53
13:AC:404:U10:H111	13:AC:404:U10:C1M	2.39	0.53
8:AH:45:ARG:O	8:AH:49:GLU:HG2	2.09	0.53
15:Aa:501:CDL:HB31	15:Aa:501:CDL:H111	1.90	0.53
3:Ac:18:PHE:CE1	14:Ac:406:UQ6:C8	2.89	0.53
4:Ad:125:HIS:CE1	4:Ad:194:PRO:HB3	2.43	0.53
5:Ae:161:GLU:HA	5:Ae:178:HIS:CD2	2.43	0.53
7:Ag:74:ASN:O	7:Ag:77:MET:HB3	2.08	0.53
1:AA:119:HIS:HA	2:AB:298:HIS:O	2.09	0.53
4:AD:121:CYS:HA	16:AD:401:HEC:CMC	2.38	0.53
5:AE:191:GLU:CD	5:AE:191:GLU:H	2.14	0.53
5:AE:192:VAL:HA	5:AE:195:LEU:CD1	2.37	0.53
12:AF:201:3PE:H392	12:AF:201:3PE:H241	1.89	0.53
1:Aa:99:LYS:HE2	2:Ab:302:GLY:CA	2.39	0.53
1:Aa:403:LEU:CD1	1:Aa:403:LEU:H	2.22	0.53
4:Ad:165:PHE:O	4:Ad:166:MET:C	2.52	0.53
5:Ae:207:LYS:CD	5:Ae:210:TRP:HD1	2.20	0.53
9:Aj:31:PHE:HA	10:Ak:48:ILE:CG2	2.39	0.53
4:AD:255:TYR:HB3	4:AD:257:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:264:GLU:HB3	5:AE:272:VAL:HB	1.89	0.53
1:Aa:338:CYS:HB2	1:Aa:368:MET:SD	2.48	0.53
3:Ac:294:LEU:HD21	13:Ac:405:U10:H1M2	1.90	0.53
4:Ad:139:CYS:C	9:Aj:53:TRP:CZ3	2.87	0.53
1:AA:478:LEU:HA	9:AJ:18:THR:HG21	1.90	0.53
2:AB:47:LEU:HD11	2:AB:238:LEU:HD13	1.91	0.53
4:AD:222:PRO:HD2	4:AD:225:VAL:HG11	1.89	0.53
2:Ab:229:VAL:HA	2:Ab:232:GLN:HG2	1.89	0.53
5:Ae:180:THR:N	5:Ae:183:GLU:HB2	2.23	0.53
9:Aj:7:PRO:HB2	9:Aj:10:LEU:HG	1.91	0.53
9:Aj:45:GLU:O	9:Aj:49:GLU:N	2.42	0.53
4:Ad:170:LYS:CD	5:Ae:151:LYS:HD3	2.32	0.53
5:Ae:263:TYR:HA	5:Ae:273:VAL:HG22	1.89	0.53
1:AA:136:LEU:HD21	2:AB:380:ALA:HA	1.91	0.53
3:AC:77:TRP:CD2	4:AD:281:GLU:HG3	2.44	0.53
5:AE:132:VAL:HA	5:AE:135:GLN:NE2	2.23	0.53
5:AE:204:ARG:HB3	5:AE:260:VAL:CG2	2.25	0.53
1:Aa:136:LEU:HD21	2:Ab:380:ALA:HA	1.90	0.53
1:Aa:270:PHE:HE1	1:Aa:353:LEU:HD22	1.72	0.53
4:AD:111:ARG:O	4:AD:115:GLN:HG3	2.09	0.53
9:AJ:43:ILE:O	9:AJ:47:ILE:HG13	2.09	0.53
1:AA:255:ARG:O	1:AA:255:ARG:CG	2.51	0.53
2:AB:257:GLU:HA	2:AB:438:MET:O	2.09	0.53
5:AE:262:ALA:O	5:AE:273:VAL:O	2.27	0.53
5:AI:76:VAL:HG22	5:AI:78:PHE:H	1.73	0.53
3:Ac:30:TRP:HB3	3:Ac:100:ARG:HD3	1.90	0.53
3:Ac:275:LEU:O	3:Ac:276:PHE:C	2.51	0.53
4:Ad:213:SER:O	4:Ad:217:GLY:N	2.42	0.53
1:AA:74:TRP:HH2	1:AA:410:CYS:SG	2.31	0.53
2:AB:348:GLY:HA2	2:AB:448:PRO:HD3	1.91	0.53
3:AC:141:TRP:CD1	3:AC:265:PRO:CD	2.90	0.53
3:AC:148:ASN:OD1	5:Ae:220:LEU:O	2.26	0.53
3:AC:170:VAL:HG23	3:AC:174:THR:CB	2.39	0.53
4:AD:206:GLY:HA3	4:AD:210:TYR:HB2	1.91	0.53
4:AD:227:LEU:HD12	4:AD:227:LEU:C	2.34	0.53
1:Aa:311:ILE:HB	1:Aa:343:THR:HG21	1.91	0.53
2:Ab:226:SER:O	2:Ab:229:VAL:HG22	2.09	0.53
3:Ac:170:VAL:HG23	3:Ac:174:THR:CB	2.39	0.53
7:Ag:43:ARG:HD3	12:Ag:102:3PE:C3B	2.39	0.53
7:Ag:48:ARG:HE	12:Ag:102:3PE:H332	1.74	0.53
5:AE:207:LYS:HD2	5:AE:210:TRP:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:43:LEU:HB2	2:Ab:167:GLN:HE21	1.73	0.52
2:Ab:60:ARG:HG2	2:Ab:393:LEU:HD13	1.90	0.52
3:Ac:312:GLN:HE21	6:Af:37:THR:HB	1.74	0.52
5:Ae:116:LEU:HB2	9:Aj:15:PHE:CE2	2.44	0.52
17:AD:402:3PH:H371	17:AD:402:3PH:C26	2.40	0.52
5:AE:180:THR:N	5:AE:183:GLU:HB2	2.23	0.52
3:Ac:223:TYR:C	4:Ad:311:TRP:HE1	2.14	0.52
17:Ad:402:3PH:H12	5:Ae:131:ASN:HD21	1.73	0.52
8:Ah:27:PRO:HB3	8:Ah:87:ASN:CG	2.34	0.52
4:AD:284:HIS:CE1	4:AD:288:MET:HE3	2.43	0.52
6:AF:108:TRP:HA	6:AF:111:LYS:HZ2	1.74	0.52
1:Aa:57:LEU:CA	1:Aa:226:ALA:O	2.57	0.52
4:Ad:192:ALA:HB3	16:Ad:401:HEC:HMD3	1.92	0.52
4:Ad:214:LEU:HA	4:Ad:234:ASN:HD21	1.73	0.52
4:Ad:321:TYR:CD2	4:Ad:323:PRO:HD3	2.44	0.52
5:Ae:190:VAL:HG11	5:Ae:195:LEU:HD21	1.90	0.52
5:Ae:207:LYS:HD2	5:Ae:210:TRP:CD1	2.43	0.52
5:Ae:241:SER:OG	5:Ae:253:PRO:HD2	2.10	0.52
1:AA:339:GLN:HB2	1:AA:359:VAL:O	2.10	0.52
3:AC:28:SER:HB2	15:AC:406:CDL:OA3	2.09	0.52
5:AI:62:ARG:HD2	5:AI:63:PRO:HD2	1.90	0.52
3:Ac:37:LEU:CB	11:Ac:403:HEM:HMB1	2.35	0.52
5:Ae:204:ARG:HB3	5:Ae:260:VAL:CG2	2.25	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
4:AD:248:ILE:CG2	4:AD:263:MET:HG3	2.40	0.52
4:Ad:147:ALA:O	4:Ad:151:GLU:HG3	2.09	0.52
7:Ag:77:MET:HG3	7:Ag:78:TYR:CD2	2.45	0.52
3:AC:145:VAL:HG13	5:Ae:220:LEU:HD13	1.92	0.52
4:AD:112:ARG:HD3	4:AD:257:ASP:OD2	2.10	0.52
4:AD:296:MET:HE2	17:AD:402:3PH:H362	1.90	0.52
7:Ag:68:GLU:HA	7:Ag:71:LYS:HE2	1.92	0.52
2:AB:226:SER:O	2:AB:229:VAL:HG22	2.09	0.52
3:AC:146:ILE:CG1	13:AC:404:U10:H4M3	2.39	0.52
3:AC:169:SER:HB3	5:Ae:172:LYS:HD2	1.91	0.52
1:Aa:169:LEU:HA	1:Aa:172:MET:HE2	1.92	0.52
2:Ab:60:ARG:CD	2:Ab:393:LEU:HD13	2.40	0.52
2:AB:432:VAL:HG22	2:AB:432:VAL:O	2.09	0.52
4:AD:125:HIS:HB3	4:AD:197:LEU:HG	1.91	0.52
1:Aa:479:ARG:NH1	15:Aa:501:CDL:OB2	2.42	0.52
3:Ac:148:ASN:OD1	3:Ac:165:TRP:HH2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:125:HIS:CE1	4:Ad:195:PRO:HD2	2.34	0.52
10:Ak:14:ALA:O	10:Ak:18:ILE:HG12	2.10	0.52
1:AA:170:ARG:HA	1:AA:173:GLN:CD	2.34	0.52
3:AC:141:TRP:CD1	3:AC:264:THR:HA	2.45	0.52
5:AI:43:LEU:CD1	2:Ab:164:VAL:HG23	2.29	0.52
1:Aa:212:SER:O	1:Aa:213:ARG:C	2.50	0.52
2:Ab:70:ARG:NH2	2:Ab:332:ASP:OD2	2.43	0.52
5:Ae:90:ASP:O	7:Ag:25:ARG:NH1	2.43	0.52
1:AA:118:ALA:O	2:AB:298:HIS:HB3	2.09	0.52
5:AE:241:SER:OG	5:AE:253:PRO:HD2	2.10	0.52
5:AE:242:HIS:CD2	5:AE:251:LYS:HB3	2.45	0.52
1:Aa:107:ASN:HB2	1:Aa:110:GLU:CD	2.35	0.52
1:AA:207:ASN:O	1:AA:211:LEU:HG	2.09	0.51
1:AA:407:THR:O	1:AA:408:PRO:C	2.49	0.51
3:AC:140:PHE:CE1	3:AC:170:VAL:HG13	2.45	0.51
4:AD:304:TYR:CZ	4:AD:308:ARG:HD2	2.45	0.51
1:Aa:186:TYR:HE1	5:Ae:80:HIS:HB2	1.75	0.51
1:AA:338:CYS:SG	1:AA:339:GLN:N	2.84	0.51
4:AD:321:TYR:CD2	4:AD:323:PRO:HD3	2.44	0.51
6:AF:97:GLU:HA	6:AF:100:ARG:HH11	1.75	0.51
1:Aa:399:LEU:HD22	1:Aa:426:LEU:CD2	2.40	0.51
2:Ab:95:SER:O	2:Ab:99:ILE:HG13	2.10	0.51
4:Ad:167:ARG:HB2	4:Ad:168:PRO:CD	2.39	0.51
7:Ag:62:TRP:O	7:Ag:65:GLN:HG3	2.11	0.51
1:AA:225:LYS:HD2	1:AA:256:VAL:H	1.74	0.51
5:AE:155:LYS:O	5:AE:158:ASP:HB2	2.09	0.51
5:AE:248:ARG:HG2	5:AE:257:ASN:ND2	2.25	0.51
10:AK:14:ALA:O	10:AK:18:ILE:HG12	2.09	0.51
2:Ab:142:THR:HG21	2:Ab:238:LEU:H	1.74	0.51
4:Ad:112:ARG:HD3	4:Ad:257:ASP:OD2	2.09	0.51
9:Aj:19:SER:HB2	10:Ak:23:MET:CB	2.41	0.51
10:Ak:18:ILE:N	10:Ak:19:PRO:HD2	2.25	0.51
2:AB:56:ALA:O	2:AB:127:ARG:HD2	2.10	0.51
6:AF:50:ARG:O	2:Ab:148:ARG:NH2	2.44	0.51
3:Ac:110:MET:HE1	3:Ac:306:PHE:CE1	2.45	0.51
4:Ad:228:ARG:HG2	4:Ad:231:LEU:CD1	2.40	0.51
4:Ad:248:ILE:CG2	4:Ad:263:MET:HG3	2.40	0.51
3:AC:150:LEU:HB2	3:AC:161:VAL:HG22	1.93	0.51
3:Ac:346:PRO:O	3:Ac:349:ILE:HG22	2.10	0.51
4:Ad:218:TYR:CG	4:Ad:246:PRO:HG3	2.45	0.51
5:Ae:242:HIS:CD2	5:Ae:251:LYS:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:248:ARG:HG2	5:Ae:257:ASN:ND2	2.25	0.51
1:AA:169:LEU:O	1:AA:173:GLN:HG3	2.11	0.51
9:AJ:30:LEU:CD1	10:AK:30:VAL:HG13	2.40	0.51
2:Ab:185:ALA:HB3	2:Ab:251:ALA:HB2	1.93	0.51
3:Ac:140:PHE:CE1	3:Ac:170:VAL:HG13	2.45	0.51
3:Ac:373:GLU:HG2	6:Af:21:TYR:OH	2.11	0.51
1:AA:73:VAL:HG23	1:AA:147:LEU:HD13	1.93	0.51
1:AA:148:ALA:HA	1:AA:250:LEU:HD21	1.92	0.51
4:AD:94:TYR:HB2	4:AD:96:TRP:NE1	2.26	0.51
4:AD:237:PHE:CG	4:AD:242:ILE:HB	2.46	0.51
5:AE:196:ARG:HD2	5:AE:249:ILE:CG2	2.41	0.51
5:Ae:184:ILE:HG21	5:Ae:208:PRO:HB3	1.93	0.51
6:Af:97:GLU:HA	6:Af:100:ARG:HH11	1.75	0.51
1:AA:392:LYS:HE3	1:AA:433:ILE:O	2.11	0.51
10:AK:12:GLU:HA	10:AK:15:ARG:HH11	1.74	0.51
3:Ac:221:HIS:O	3:Ac:225:THR:HB	2.10	0.51
3:Ac:291:VAL:O	3:Ac:295:ILE:HG12	2.11	0.51
4:Ad:124:CYS:SG	16:Ad:401:HEC:CAC	2.99	0.51
4:Ad:237:PHE:CG	4:Ad:242:ILE:HB	2.46	0.51
3:AC:77:TRP:HZ2	4:AD:284:HIS:CD2	2.28	0.51
3:AC:147:THR:HG21	3:AC:165:TRP:NE1	2.26	0.51
5:AI:64:LEU:HD12	5:AI:78:PHE:HB3	1.93	0.51
1:Aa:96:LEU:HD11	1:Aa:161:ILE:HA	1.92	0.51
1:Aa:104:ARG:HH12	1:Aa:146:LEU:HD23	1.75	0.51
2:Ab:89:LEU:HD22	2:Ab:150:GLU:HB3	1.93	0.51
3:Ac:92:ILE:HG13	3:Ac:272:TRP:CH2	2.45	0.51
4:Ad:201:VAL:HG22	4:Ad:278:SER:CB	2.41	0.51
17:Ad:402:3PH:C23	5:Ae:135:GLN:HE22	2.23	0.51
5:Ae:242:HIS:HD2	5:Ae:251:LYS:HB3	1.76	0.51
1:AA:226:ALA:HB2	1:AA:253:VAL:HB	1.93	0.51
2:AB:425:VAL:HG12	2:AB:429:LYS:HZ1	1.75	0.51
5:AI:62:ARG:NH1	2:Ab:290:GLN:HE22	2.09	0.51
17:Ad:402:3PH:H371	5:Ae:128:ALA:HB1	1.93	0.51
7:Ag:77:MET:HE3	7:Ag:78:TYR:CZ	2.46	0.51
8:Ah:79:CYS:O	8:Ah:82:HIS:HB3	2.10	0.51
3:AC:269:LYS:CE	3:AC:340:GLY:HA2	2.39	0.50
4:AD:201:VAL:HG21	4:AD:275:ARG:HA	1.92	0.50
4:AD:215:LEU:HD21	16:AD:401:HEC:CMB	2.41	0.50
2:Ab:348:GLY:HA2	2:Ab:448:PRO:HD3	1.91	0.50
3:Ac:140:PHE:HE1	3:Ac:170:VAL:HG13	1.76	0.50
4:Ad:146:LYS:CD	4:Ad:171:LEU:HG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:155:LYS:O	5:Ae:158:ASP:HB2	2.09	0.50
5:Ae:196:ARG:HD2	5:Ae:249:ILE:CG2	2.40	0.50
1:AA:109:LEU:O	1:AA:113:VAL:HG12	2.11	0.50
4:AD:242:ILE:CD1	4:AD:244:MET:HE2	2.41	0.50
5:AE:242:HIS:HD2	5:AE:251:LYS:HB3	1.76	0.50
1:Aa:57:LEU:C	1:Aa:57:LEU:HD23	2.35	0.50
9:Aj:9:ARG:NH2	9:Aj:13:LEU:HD21	2.26	0.50
1:AA:274:GLU:OE2	1:AA:276:ARG:NH1	2.44	0.50
2:AB:38:LEU:H	2:AB:38:LEU:HD22	1.76	0.50
2:Ab:229:VAL:O	2:Ab:232:GLN:HG2	2.10	0.50
2:Ab:429:LYS:HA	2:Ab:432:VAL:HG12	1.93	0.50
5:Ae:152:ILE:HG23	5:Ae:272:VAL:C	2.36	0.50
3:AC:291:VAL:O	3:AC:295:ILE:HG12	2.11	0.50
8:AH:52:ASP:O	8:AH:55:VAL:HB	2.11	0.50
1:Aa:109:LEU:HD23	1:Aa:113:VAL:HG23	1.94	0.50
4:Ad:192:ALA:HB1	16:Ad:401:HEC:HMD3	1.92	0.50
10:Ak:38:TRP:HE1	10:Ak:40:LEU:HD12	1.76	0.50
1:AA:158:ASP:OD1	1:AA:213:ARG:HD2	2.11	0.50
2:AB:148:ARG:NH2	6:Af:52:PRO:HD3	2.26	0.50
2:AB:384:MET:O	2:AB:387:GLU:HG2	2.12	0.50
4:AD:126:SER:HB3	4:AD:178:PRO:HD2	1.94	0.50
4:AD:232:TYR:HD1	4:AD:242:ILE:O	1.93	0.50
5:AE:195:LEU:HD11	5:AE:248:ARG:NH1	2.26	0.50
1:Aa:188:HIS:HE2	1:Aa:348:TYR:HH	1.57	0.50
15:Aa:501:CDL:H312	3:Ac:221:HIS:CE1	2.46	0.50
5:Ae:123:VAL:HG13	9:Aj:29:ALA:HA	1.94	0.50
1:AA:180:GLN:HG3	1:AA:181:ASN:N	2.25	0.50
4:Ad:242:ILE:HG12	4:Ad:244:MET:H	1.77	0.50
5:Ae:165:MET:O	5:Ae:176:VAL:N	2.44	0.50
8:Ah:51:CYS:O	8:Ah:55:VAL:HG23	2.11	0.50
1:AA:285:ALA:O	1:AA:359:VAL:HA	2.11	0.50
2:AB:176:ASN:CA	2:AB:258:ILE:HD11	2.42	0.50
2:AB:227:HIS:HD2	2:AB:231:LYS:HE2	1.76	0.50
4:AD:148:LEU:HA	4:AD:151:GLU:CD	2.36	0.50
1:Aa:73:VAL:HG23	1:Aa:147:LEU:HD13	1.93	0.50
1:Aa:399:LEU:HD22	1:Aa:426:LEU:HD22	1.93	0.50
2:Ab:180:VAL:O	2:Ab:254:ARG:HG3	2.12	0.50
1:AA:397:ASN:ND2	2:AB:126:ILE:HD11	2.24	0.50
2:AB:48:VAL:HG21	2:AB:219:ALA:HB2	1.87	0.50
2:AB:173:ILE:HD11	2:AB:439:ALA:C	2.37	0.50
2:AB:232:GLN:O	2:AB:235:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:184:ILE:HG21	5:AE:208:PRO:HB3	1.93	0.50
3:AC:211:LEU:HD21	6:AF:37:THR:HA	1.94	0.50
5:AE:154:ILE:HG22	5:AE:155:LYS:N	2.27	0.50
9:AJ:30:LEU:HD13	10:AK:30:VAL:HG13	1.94	0.50
1:Aa:404:ASP:O	1:Aa:408:PRO:HG2	2.12	0.50
4:Ad:154:VAL:HG21	4:Ad:173:ASP:OD2	2.12	0.50
4:Ad:249:TYR:O	4:Ad:250:THR:C	2.55	0.50
3:AC:218:ILE:HB	3:AC:219:PRO:HD2	1.94	0.49
4:AD:249:TYR:O	4:AD:250:THR:C	2.55	0.49
1:Aa:91:TYR:CZ	1:Aa:95:HIS:HE1	2.30	0.49
4:Ad:116:VAL:HA	4:Ad:253:LEU:CD2	2.41	0.49
4:Ad:133:ARG:HB3	4:Ad:171:LEU:O	2.12	0.49
5:Ae:179:ARG:HA	5:Ae:183:GLU:OE1	2.12	0.49
2:AB:48:VAL:CG2	2:AB:48:VAL:O	2.60	0.49
4:AD:323:PRO:HG2	4:AD:325:LYS:CD	2.41	0.49
3:Ac:346:PRO:HG3	7:Ag:66:GLU:HG2	1.94	0.49
4:Ad:255:TYR:HH	4:Ad:266:VAL:HA	1.76	0.49
1:AA:296:TRP:NE1	1:AA:347:SER:O	2.45	0.49
1:AA:341:PHE:HE1	1:AA:356:ALA:CB	2.26	0.49
3:Ac:37:LEU:HB3	11:Ac:403:HEM:CMB	2.38	0.49
4:Ad:213:SER:HB3	4:Ad:236:TYR:CE1	2.47	0.49
4:Ad:308:ARG:HD3	7:Ag:27:PHE:CE2	2.47	0.49
5:Ae:195:LEU:HD11	5:Ae:248:ARG:NH1	2.26	0.49
2:AB:70:ARG:NH2	2:AB:332:ASP:OD2	2.45	0.49
3:AC:140:PHE:HE1	3:AC:170:VAL:HG13	1.77	0.49
4:AD:318:LYS:HD2	5:AE:86:PRO:HB2	1.95	0.49
8:AH:66:THR:O	8:AH:69:LEU:HB3	2.13	0.49
4:Ad:242:ILE:CD1	4:Ad:244:MET:HE2	2.42	0.49
5:Ae:184:ILE:CG2	5:Ae:208:PRO:HB3	2.42	0.49
1:AA:186:TYR:OH	5:AE:80:HIS:HB3	2.12	0.49
2:AB:375:LYS:NZ	2:AB:419:VAL:O	2.36	0.49
4:AD:128:ASP:OD1	4:AD:177:LYS:HD2	2.11	0.49
3:Ac:107:TYR:HE1	3:Ac:308:HIS:HB2	1.77	0.49
5:Ae:152:ILE:CB	5:Ae:272:VAL:HG23	2.40	0.49
5:Ae:197:ASP:HB3	5:Ae:257:ASN:ND2	2.27	0.49
1:AA:171:GLU:O	1:AA:175:ASN:N	2.45	0.49
1:AA:373:GLN:O	1:AA:374:GLY:C	2.53	0.49
2:AB:304:ASN:ND2	2:AB:307:SER:OG	2.45	0.49
2:AB:305:THR:CG2	2:AB:306:THR:N	2.60	0.49
2:Ab:261:GLN:NE2	2:Ab:444:LEU:HB2	2.28	0.49
3:Ac:221:HIS:CE1	12:Ac:401:3PE:H31	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:278:TYR:CZ	3:Ac:282:ARG:HD2	2.48	0.49
11:Ac:402:HEM:O1A	11:Ac:402:HEM:HHA	2.12	0.49
5:Ae:204:ARG:O	5:Ae:260:VAL:HG11	2.12	0.49
1:AA:279:ASP:OD1	7:AG:12:ARG:NE	2.45	0.49
4:AD:105:LEU:HB3	4:AD:110:ILE:HD11	1.95	0.49
2:Ab:298:HIS:C	2:Ab:299:ILE:HD12	2.38	0.49
10:Ak:15:ARG:NH1	10:Ak:15:ARG:HB2	2.28	0.49
1:AA:186:TYR:C	1:AA:188:HIS:N	2.68	0.49
1:AA:280:ASP:OD2	7:AG:10:ARG:HA	2.13	0.49
3:AC:48:GLY:HA3	11:AC:401:HEM:C2B	2.47	0.49
5:AE:179:ARG:HA	5:AE:183:GLU:OE1	2.12	0.49
5:AE:192:VAL:O	5:AE:195:LEU:HB2	2.13	0.49
1:Aa:92:PHE:HZ	1:Aa:161:ILE:HG23	1.76	0.49
2:Ab:307:SER:O	2:Ab:308:LEU:C	2.54	0.49
3:Ac:361:ILE:HA	3:Ac:365:LEU:HB2	1.95	0.49
4:Ad:222:PRO:HD3	4:Ad:233:PHE:CZ	2.48	0.49
7:Ag:77:MET:HE3	7:Ag:78:TYR:CE2	2.48	0.49
1:AA:387:GLU:HB2	1:AA:390:ARG:HH22	1.78	0.49
1:AA:467:ASP:OD2	3:AC:223:TYR:CE1	2.66	0.49
4:AD:115:GLN:O	4:AD:119:GLN:HG3	2.13	0.49
3:Ac:281:LEU:HD12	3:Ac:290:GLY:HA3	1.95	0.49
7:Ag:78:TYR:CZ	8:Ah:62:GLU:HB2	2.48	0.49
9:Aj:43:ILE:O	9:Aj:47:ILE:HG12	2.13	0.49
1:Aa:207:ASN:O	1:Aa:211:LEU:HG	2.13	0.49
1:Aa:346:ILE:O	1:Aa:353:LEU:N	2.40	0.49
3:Ac:242:LEU:HD21	3:Ac:250:LEU:CD1	2.40	0.49
1:AA:96:LEU:HD23	1:AA:164:GLU:HG3	1.94	0.48
3:AC:244:LEU:HD13	4:AD:289:GLY:HA2	1.94	0.48
3:AC:278:TYR:CZ	3:AC:282:ARG:HD2	2.48	0.48
5:AE:155:LYS:HZ3	5:AE:157:SER:HB3	1.77	0.48
5:AE:156:LEU:HB2	5:AE:269:ASP:CA	2.43	0.48
5:AI:64:LEU:HA	5:AI:78:PHE:CA	2.38	0.48
1:Aa:226:ALA:HB2	1:Aa:253:VAL:HB	1.94	0.48
2:Ab:38:LEU:HD11	2:Ab:396:ILE:HD13	1.95	0.48
4:Ad:179:TYR:CD2	4:Ad:185:ALA:HB2	2.48	0.48
5:Ae:192:VAL:O	5:Ae:195:LEU:HB2	2.13	0.48
9:Aj:19:SER:HB2	10:Ak:23:MET:HB2	1.94	0.48
1:AA:409:VAL:O	1:AA:410:CYS:C	2.55	0.48
3:AC:185:LEU:HD23	3:AC:188:ILE:HD12	1.95	0.48
17:AD:402:3PH:H221	5:AE:135:GLN:NE2	2.16	0.48
5:AE:142:ALA:HB1	5:AE:146:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:184:ILE:CG2	5:AE:208:PRO:HB3	2.42	0.48
2:Ab:388:THR:HG23	2:Ab:391:GLY:H	1.78	0.48
5:Ae:217:CYS:O	5:Ae:218:THR:C	2.56	0.48
7:Ag:78:TYR:CB	8:Ah:63:GLU:HB2	2.43	0.48
9:Aj:43:ILE:O	9:Aj:44:TYR:C	2.54	0.48
9:Aj:52:LEU:CD1	9:Aj:53:TRP:N	2.68	0.48
2:AB:388:THR:HG23	2:AB:391:GLY:H	1.78	0.48
2:AB:429:LYS:HA	2:AB:432:VAL:CG1	2.39	0.48
4:Ad:195:PRO:HG3	16:Ad:401:HEC:HAA1	1.94	0.48
8:Ah:38:LEU:O	8:Ah:42:VAL:HG23	2.13	0.48
3:AC:148:ASN:CB	5:Ae:220:LEU:HA	2.43	0.48
3:AC:316:MET:HG3	12:AC:403:3PE:H232	1.95	0.48
4:AD:116:VAL:HA	4:AD:253:LEU:CD2	2.43	0.48
5:AE:197:ASP:HB3	5:AE:257:ASN:ND2	2.27	0.48
6:AF:110:LYS:HA	10:Ak:10:TYR:HE2	1.77	0.48
1:Aa:469:ASN:ND2	3:Ac:223:TYR:CZ	2.80	0.48
2:Ab:109:LYS:O	2:Ab:123:VAL:HA	2.13	0.48
3:Ac:218:ILE:HB	3:Ac:219:PRO:HD2	1.94	0.48
2:AB:286:PHE:CZ	2:AB:427:ALA:HB1	2.49	0.48
3:AC:32:ASN:ND2	3:AC:228:ASP:OD1	2.46	0.48
3:AC:361:ILE:HA	3:AC:365:LEU:HB2	1.95	0.48
4:AD:98:HIS:HB3	4:AD:105:LEU:HD23	1.95	0.48
4:AD:307:LYS:O	4:AD:311:TRP:HB2	2.13	0.48
5:AE:218:THR:OG1	5:AE:254:ALA:HB1	2.13	0.48
1:Aa:338:CYS:HB3	1:Aa:359:VAL:O	2.13	0.48
3:Ac:185:LEU:HD23	3:Ac:188:ILE:HD12	1.95	0.48
3:Ac:304:MET:HA	3:Ac:307:LEU:HD12	1.95	0.48
4:Ad:296:MET:CE	17:Ad:402:3PH:H362	2.41	0.48
5:Ae:218:THR:OG1	5:Ae:254:ALA:HB1	2.13	0.48
9:Aj:10:LEU:O	9:Aj:11:TYR:C	2.56	0.48
4:AD:282:HIS:O	4:AD:286:LYS:HG2	2.13	0.48
5:AE:204:ARG:O	5:AE:260:VAL:HG11	2.13	0.48
1:Aa:405:GLY:C	1:Aa:408:PRO:HD2	2.38	0.48
15:Aa:501:CDL:OB5	12:Ac:401:3PE:N	2.47	0.48
2:Ab:63:LEU:HD11	2:Ab:238:LEU:HD21	1.95	0.48
5:Ae:231:PHE:HD2	5:Ae:250:ARG:NH1	2.12	0.48
2:AB:109:LYS:O	2:AB:123:VAL:HA	2.14	0.48
3:AC:304:MET:HA	3:AC:307:LEU:HD12	1.96	0.48
2:Ab:286:PHE:CZ	2:Ab:427:ALA:HB1	2.49	0.48
3:Ac:197:LEU:HD21	14:Ac:406:UQ6:H13	1.95	0.48
3:Ac:378:LYS:HE3	6:Af:89:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:178:HIS:HD2	5:Ae:179:ARG:N	2.11	0.48
2:AB:49:ILE:CD1	2:AB:220:LEU:HB3	2.43	0.48
2:AB:90:THR:HG23	2:AB:95:SER:HA	1.95	0.48
2:AB:176:ASN:C	2:AB:258:ILE:HD11	2.39	0.48
3:AC:220:PHE:HE2	14:AC:405:UQ6:H4M3	1.77	0.48
4:AD:242:ILE:HD11	4:AD:244:MET:HE2	1.95	0.48
5:AE:217:CYS:O	5:AE:218:THR:C	2.56	0.48
1:Aa:373:GLN:NE2	1:Aa:471:ILE:HG23	2.29	0.48
1:Aa:479:ARG:O	10:Ak:20:THR:HG21	2.13	0.48
2:Ab:92:LYS:HE2	2:Ab:143:ALA:HB1	1.96	0.48
2:Ab:142:THR:CG2	2:Ab:237:PHE:HB3	2.30	0.48
3:Ac:32:ASN:ND2	3:Ac:228:ASP:OD1	2.47	0.48
4:Ad:121:CYS:HG	16:Ad:401:HEC:HBB3	1.77	0.48
5:Ae:176:VAL:HG13	5:Ae:212:ILE:HG12	1.95	0.48
7:Ag:65:GLN:O	7:Ag:69:GLN:HG2	2.13	0.48
9:Aj:22:ALA:O	9:Aj:23:LEU:C	2.57	0.48
5:AE:231:PHE:HD2	5:AE:250:ARG:NH1	2.12	0.48
8:AH:47:ARG:O	8:AH:51:CYS:N	2.41	0.48
1:Aa:104:ARG:N	1:Aa:104:ARG:HD2	2.29	0.48
4:Ad:146:LYS:HD3	4:Ad:171:LEU:HG	1.95	0.48
4:Ad:154:VAL:HG21	4:Ad:173:ASP:CG	2.39	0.48
7:Ag:78:TYR:HB3	8:Ah:63:GLU:HB2	1.95	0.48
1:AA:338:CYS:N	1:AA:368:MET:SD	2.87	0.48
5:AE:178:HIS:HD2	5:AE:179:ARG:N	2.11	0.48
1:Aa:287:VAL:HB	1:Aa:358:PHE:CE1	2.49	0.48
1:AA:113:VAL:HG13	2:AB:299:ILE:HD11	1.95	0.47
5:AE:156:LEU:HB2	5:AE:269:ASP:HA	1.96	0.47
5:AE:172:LYS:HD2	3:Ac:169:SER:HB3	1.96	0.47
1:Aa:463:GLU:OE1	7:Ag:8:LEU:HB2	2.14	0.47
2:Ab:227:HIS:CD2	2:Ab:231:LYS:HG3	2.49	0.47
3:Ac:10:LEU:O	3:Ac:14:ILE:HG12	2.14	0.47
3:Ac:297:SER:O	3:Ac:300:ILE:HG22	2.13	0.47
5:Ae:273:VAL:O	5:Ae:273:VAL:HG12	2.14	0.47
1:AA:172:MET:HA	1:AA:175:ASN:ND2	2.30	0.47
1:AA:407:THR:HB	1:AA:408:PRO:HD3	1.96	0.47
5:AE:176:VAL:HG13	5:AE:212:ILE:HG12	1.95	0.47
3:Ac:243:VAL:O	3:Ac:247:PRO:HB3	2.13	0.47
3:Ac:265:PRO:HD2	3:Ac:268:ILE:HD11	1.95	0.47
1:AA:341:PHE:CZ	1:AA:372:LEU:HD13	2.49	0.47
3:AC:94:LEU:HD13	11:AC:402:HEM:HAB	1.96	0.47
3:AC:281:LEU:HD12	3:AC:290:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:297:SER:O	3:AC:300:ILE:HG22	2.13	0.47
3:Ac:71:ARG:NH2	4:Ad:277:ALA:O	2.47	0.47
3:Ac:96:LEU:HD23	12:Ac:404:3PE:H292	1.95	0.47
4:Ad:170:LYS:HD3	5:Ae:151:LYS:HD3	1.92	0.47
4:Ad:183:GLU:CD	4:Ad:183:GLU:H	2.21	0.47
1:AA:137:SER:HB3	1:AA:236:GLY:O	2.15	0.47
1:Aa:274:GLU:HA	1:Aa:456:VAL:O	2.14	0.47
3:Ac:296:LEU:O	3:Ac:300:ILE:N	2.45	0.47
1:AA:101:THR:O	1:AA:102:LYS:C	2.55	0.47
1:AA:160:GLN:HA	1:AA:163:LYS:NZ	2.29	0.47
1:AA:478:LEU:O	10:AK:24:TRP:HZ2	1.98	0.47
3:AC:148:ASN:OD1	5:Ae:221:GLY:N	2.47	0.47
3:Ac:275:LEU:O	3:Ac:278:TYR:N	2.48	0.47
5:Ae:152:ILE:N	5:Ae:272:VAL:HG23	2.29	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
2:AB:306:THR:O	2:AB:307:SER:C	2.58	0.47
4:AD:242:ILE:HG12	4:AD:244:MET:H	1.80	0.47
5:AI:68:VAL:HG11	2:Ab:85:LEU:CD2	2.45	0.47
1:Aa:266:THR:O	1:Aa:266:THR:CG2	2.62	0.47
4:Ad:207:GLY:O	4:Ad:208:GLU:C	2.58	0.47
5:Ae:166:ALA:HA	5:Ae:174:LEU:O	2.15	0.47
8:Ah:44:ALA:HA	8:Ah:47:ARG:HH11	1.79	0.47
1:AA:74:TRP:C	1:AA:75:ILE:HG13	2.40	0.47
1:AA:138:LYS:O	1:AA:141:PRO:HD2	2.14	0.47
3:AC:153:ILE:HG23	3:AC:154:PRO:HD2	1.96	0.47
4:AD:318:LYS:HE3	5:AE:87:ASP:O	2.15	0.47
8:AH:26:ASP:O	8:AH:27:PRO:C	2.58	0.47
1:Aa:107:ASN:HB2	1:Aa:110:GLU:OE2	2.15	0.47
1:Aa:152:GLN:O	1:Aa:153:ASN:HB2	2.15	0.47
1:Aa:396:ARG:NH2	1:Aa:434:GLN:HB3	2.30	0.47
2:Ab:142:THR:HA	2:Ab:241:ARG:HH22	1.80	0.47
3:Ac:162:GLU:HA	3:Ac:165:TRP:HB2	1.97	0.47
4:Ad:124:CYS:HB3	4:Ad:194:PRO:HG2	1.96	0.47
4:Ad:227:LEU:HD13	4:Ad:231:LEU:HB2	1.97	0.47
8:Ah:28:LEU:HA	8:Ah:84:LEU:HD13	1.95	0.47
5:AE:143:SER:HB2	5:AE:145:ASP:OD1	2.15	0.47
7:AG:11:ILE:CG2	7:AG:12:ARG:N	2.77	0.47
2:Ab:228:SER:HA	2:Ab:231:LYS:HE2	1.97	0.47
3:Ac:140:PHE:CE1	3:Ac:170:VAL:CG1	2.98	0.47
1:AA:375:GLN:O	1:AA:376:TRP:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:284:ASN:HB3	2:AB:419:VAL:CG2	2.45	0.47
2:AB:312:SER:OG	2:AB:357:GLN:NE2	2.40	0.47
4:AD:242:ILE:HG13	16:AD:401:HEC:HBD1	1.97	0.47
6:AF:29:LYS:HA	6:AF:81:TRP:CD1	2.49	0.47
6:AF:29:LYS:HA	6:AF:81:TRP:CD1	2.50	0.47
3:AC:140:PHE:CE1	3:AC:170:VAL:CG1	2.98	0.47
3:AC:218:ILE:HG21	4:AD:314:LEU:HD11	1.97	0.47
4:AD:130:VAL:HG21	4:AD:277:ALA:HB1	1.97	0.47
4:AD:215:LEU:HD21	16:AD:401:HEC:HMB1	1.96	0.47
5:AE:231:PHE:CD2	5:AE:250:ARG:HG3	2.50	0.47
5:AE:246:SER:HB3	5:AE:248:ARG:HE	1.79	0.47
1:Aa:222:ARG:HH22	1:Aa:263:PRO:HA	1.80	0.47
1:Aa:310:ILE:HG21	1:Aa:379:LEU:HD21	1.96	0.47
1:Aa:352:GLY:O	1:Aa:353:LEU:HD23	2.15	0.47
3:Ac:294:LEU:O	3:Ac:297:SER:HB3	2.15	0.47
3:Ac:323:ILE:HD11	12:Ag:102:3PE:H12	1.97	0.47
13:Ac:405:U10:H272	13:Ac:405:U10:H251	1.56	0.47
4:Ad:167:ARG:CB	4:Ad:168:PRO:HD2	2.38	0.47
6:Af:85:GLU:CD	6:Af:85:GLU:H	2.23	0.47
7:Ag:29:SER:CB	7:Ag:32:SER:HB2	2.38	0.47
1:AA:160:GLN:HA	1:AA:163:LYS:HZ3	1.80	0.46
5:Ae:156:LEU:HD11	5:Ae:265:PHE:CE2	2.50	0.46
2:AB:38:LEU:HD13	2:AB:52:LEU:HB2	1.96	0.46
3:AC:220:PHE:HE2	14:AC:405:UQ6:C4M	2.29	0.46
3:AC:294:LEU:O	3:AC:297:SER:HB3	2.15	0.46
5:AE:156:LEU:HD11	5:AE:265:PHE:CE1	2.50	0.46
5:AE:205:VAL:HG12	5:AE:211:VAL:HG23	1.98	0.46
5:AE:265:PHE:CD1	5:AE:271:VAL:HG22	2.50	0.46
5:Ae:226:ALA:HB2	5:Ae:234:TYR:HE1	1.80	0.46
3:AC:296:LEU:O	3:AC:300:ILE:N	2.45	0.46
5:AE:223:VAL:HG23	3:Ac:141:TRP:CH2	2.51	0.46
5:AE:267:SER:C	5:AE:269:ASP:H	2.23	0.46
1:Aa:192:PHE:CZ	1:Aa:353:LEU:HD21	2.50	0.46
2:Ab:225:VAL:HG22	2:Ab:229:VAL:CG2	2.46	0.46
4:Ad:192:ALA:HB1	16:Ad:401:HEC:HBD2	1.97	0.46
4:Ad:309:HIS:NE2	7:Ag:21:PRO:HB2	2.30	0.46
17:Ad:402:3PH:C24	5:Ae:132:VAL:HG22	2.41	0.46
5:Ae:231:PHE:CD2	5:Ae:250:ARG:HG3	2.50	0.46
7:Ag:47:LEU:O	7:Ag:51:PRO:HG2	2.14	0.46
10:Ak:37:ASP:O	10:Ak:38:TRP:C	2.58	0.46
2:AB:183:LYS:HG3	2:AB:254:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:201:HIS:CE1	14:AC:405:UQ6:O2	2.68	0.46
5:AE:166:ALA:HA	5:AE:174:LEU:O	2.15	0.46
15:Ag:101:CDL:H121	15:Ag:101:CDL:H512	1.97	0.46
8:Ah:68:GLU:HA	8:Ah:71:ASP:OD2	2.15	0.46
5:AE:165:MET:O	5:AE:176:VAL:N	2.44	0.46
5:AE:214:ILE:HG12	5:AE:261:PRO:HD3	1.98	0.46
6:AF:17:PHE:HA	12:AF:201:3PE:H111	1.98	0.46
5:AI:63:PRO:HB3	2:Ab:328:ALA:HB1	1.97	0.46
9:AJ:19:SER:HA	10:AK:24:TRP:CH2	2.51	0.46
1:Aa:279:ASP:HA	7:Ag:12:ARG:HA	1.97	0.46
1:Aa:384:THR:HA	10:Ak:12:GLU:CD	2.40	0.46
2:Ab:47:LEU:CD2	2:Ab:234:ALA:HB1	2.45	0.46
3:Ac:37:LEU:CB	11:Ac:403:HEM:CMB	2.93	0.46
1:AA:174:GLU:C	1:AA:176:ASP:N	2.73	0.46
3:AC:92:ILE:HG13	3:AC:272:TRP:CH2	2.48	0.46
5:AE:220:LEU:HD13	3:Ac:145:VAL:HG13	1.97	0.46
6:AF:53:GLU:OE2	7:AG:12:ARG:NH1	2.47	0.46
6:AF:83:LYS:HB3	6:AF:85:GLU:OE2	2.15	0.46
1:Aa:114:GLU:OE2	2:Ab:298:HIS:HB2	2.16	0.46
1:Aa:285:ALA:HB3	1:Aa:365:ILE:HD11	1.97	0.46
1:Aa:338:CYS:O	1:Aa:339:GLN:C	2.57	0.46
1:Aa:407:THR:HB	1:Aa:408:PRO:HD3	1.96	0.46
2:Ab:228:SER:HA	2:Ab:231:LYS:CE	2.45	0.46
6:Af:83:LYS:HB3	6:Af:85:GLU:OE2	2.15	0.46
7:Ag:37:ASN:ND2	15:Ag:101:CDL:OA3	2.49	0.46
1:AA:339:GLN:O	1:AA:340:SER:C	2.56	0.46
1:Aa:383:ALA:O	1:Aa:442:ARG:NH1	2.48	0.46
3:Ac:160:LEU:O	3:Ac:163:TRP:HB3	2.15	0.46
4:Ad:146:LYS:N	4:Ad:171:LEU:HD21	2.31	0.46
5:Ae:246:SER:HB3	5:Ae:248:ARG:HE	1.79	0.46
10:Ak:23:MET:O	10:Ak:27:VAL:HG23	2.15	0.46
2:AB:278:ILE:HB	2:AB:331:SER:HA	1.98	0.46
12:AF:201:3PE:H3B2	7:AG:47:LEU:O	2.16	0.46
9:AJ:11:TYR:HA	9:AJ:15:PHE:HB2	1.97	0.46
10:AK:41:ILE:HD12	10:AK:41:ILE:N	2.31	0.46
1:Aa:109:LEU:HG	1:Aa:146:LEU:HD22	1.97	0.46
1:Aa:157:GLU:HB2	1:Aa:160:GLN:HB2	1.97	0.46
2:Ab:177:LEU:HD21	2:Ab:272:VAL:CG1	2.46	0.46
3:Ac:245:PHE:CE1	4:Ad:102:LEU:HD23	2.51	0.46
1:AA:183:VAL:HG21	1:AA:286:HIS:HB2	1.96	0.46
3:AC:150:LEU:CD1	3:AC:164:ILE:HD12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:62:ARG:CG	5:AI:63:PRO:HD2	2.46	0.46
1:Aa:59:VAL:HG21	1:Aa:246:ALA:HB1	1.97	0.46
1:Aa:117:GLY:HA3	2:Ab:377:LYS:HA	1.98	0.46
1:Aa:222:ARG:NH2	1:Aa:263:PRO:CG	2.79	0.46
1:Aa:250:LEU:O	1:Aa:253:VAL:HG23	2.16	0.46
1:Aa:338:CYS:HB3	1:Aa:360:CYS:HB2	1.55	0.46
4:Ad:131:ALA:HB2	4:Ad:174:TYR:CD2	2.51	0.46
4:Ad:214:LEU:O	4:Ad:234:ASN:ND2	2.49	0.46
7:Ag:64:ASN:O	7:Ag:68:GLU:HG2	2.16	0.46
4:AD:237:PHE:CD1	4:AD:238:PRO:HD2	2.51	0.46
4:AD:321:TYR:HB2	6:AF:61:PHE:CD1	2.51	0.46
8:AH:46:GLU:O	8:AH:50:LEU:HG	2.16	0.46
1:Aa:412:ASP:O	1:Aa:413:ILE:C	2.58	0.46
3:Ac:246:PHE:HB3	3:Ac:249:MET:HE3	1.98	0.46
4:Ad:236:TYR:O	4:Ad:237:PHE:C	2.59	0.46
4:Ad:237:PHE:CD1	4:Ad:238:PRO:HD2	2.51	0.46
4:Ad:242:ILE:HD13	4:Ad:244:MET:HE2	1.98	0.46
5:AE:143:SER:O	5:AE:144:ALA:C	2.59	0.45
9:AJ:9:ARG:O	9:AJ:13:LEU:HD23	2.16	0.45
1:Aa:270:PHE:CE1	1:Aa:353:LEU:HD22	2.51	0.45
5:Ae:188:ALA:HA	5:Ae:200:HIS:HE2	1.79	0.45
2:AB:225:VAL:HG22	2:AB:229:VAL:CG2	2.46	0.45
3:AC:30:TRP:HZ3	3:AC:96:LEU:HD22	1.81	0.45
3:AC:223:TYR:O	4:AD:311:TRP:NE1	2.49	0.45
4:AD:116:VAL:HA	4:AD:253:LEU:HD21	1.99	0.45
4:AD:121:CYS:CB	16:AD:401:HEC:CAB	2.89	0.45
5:AE:156:LEU:HD23	5:AE:156:LEU:HA	1.62	0.45
6:AF:85:GLU:H	6:AF:85:GLU:CD	2.24	0.45
1:Aa:269:ARG:HG3	1:Aa:271:THR:HG23	1.98	0.45
3:Ac:30:TRP:HZ3	3:Ac:96:LEU:HD22	1.81	0.45
1:AA:341:PHE:CE1	1:AA:356:ALA:HB1	2.48	0.45
5:AE:226:ALA:HB2	5:AE:234:TYR:HE1	1.80	0.45
5:AE:231:PHE:CE2	5:AE:250:ARG:HB3	2.51	0.45
1:Aa:98:PHE:CZ	1:Aa:122:ALA:HB2	2.51	0.45
1:Aa:169:LEU:HD23	1:Aa:172:MET:CE	2.46	0.45
17:Ad:402:3PH:C22	5:Ae:135:GLN:HE22	2.29	0.45
5:Ae:205:VAL:HG12	5:Ae:211:VAL:HG23	1.98	0.45
5:Ae:231:PHE:CE2	5:Ae:250:ARG:HB3	2.51	0.45
2:Ab:267:VAL:HA	2:Ab:441:SER:O	2.17	0.45
4:Ad:311:TRP:O	4:Ad:315:LYS:HG3	2.16	0.45
5:Ae:156:LEU:HD11	5:Ae:265:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:214:ILE:HG12	5:Ae:261:PRO:HD3	1.98	0.45
5:Ae:241:SER:OG	5:Ae:254:ALA:HB2	2.17	0.45
1:AA:74:TRP:HB3	1:AA:418:LEU:CD1	2.46	0.45
1:AA:287:VAL:HB	1:AA:358:PHE:CZ	2.50	0.45
1:AA:387:GLU:HB2	1:AA:390:ARG:NH2	2.30	0.45
2:AB:49:ILE:HD13	2:AB:220:LEU:HB3	1.98	0.45
5:AE:155:LYS:HB3	5:AE:158:ASP:OD2	2.17	0.45
9:AJ:34:ARG:NH1	9:AJ:38:GLN:HB2	2.31	0.45
1:Aa:278:ARG:NH2	7:Ag:9:ALA:O	2.50	0.45
4:Ad:139:CYS:HA	9:AJ:53:TRP:CZ3	2.51	0.45
4:Ad:159:ASN:O	4:Ad:160:ASP:C	2.59	0.45
5:Ae:126:ALA:C	10:Ak:34:TRP:HH2	2.24	0.45
7:Ag:67:PHE:CE2	7:Ag:71:LYS:HD3	2.52	0.45
1:AA:114:GLU:HG2	2:AB:299:ILE:CD1	2.47	0.45
3:AC:37:LEU:HB3	11:AC:402:HEM:HMB1	1.98	0.45
5:AE:168:LYS:HZ3	5:AE:171:GLY:HA2	1.82	0.45
5:AE:188:ALA:HA	5:AE:200:HIS:HE2	1.80	0.45
1:Aa:285:ALA:CB	1:Aa:365:ILE:HD11	2.47	0.45
1:Aa:467:ASP:OD2	3:Ac:223:TYR:CE2	2.69	0.45
2:Ab:267:VAL:HG13	2:Ab:444:LEU:CD2	2.46	0.45
4:Ad:167:ARG:NH1	4:Ad:169:GLY:HA2	2.31	0.45
9:AJ:34:ARG:NH1	9:AJ:38:GLN:HB2	2.31	0.45
1:AA:92:PHE:HZ	1:AA:161:ILE:HG23	1.81	0.45
1:AA:294:PRO:HB2	1:AA:298:ASN:HB3	1.98	0.45
1:AA:463:GLU:OE1	7:AG:8:LEU:HB2	2.17	0.45
2:AB:37:ASP:O	2:AB:38:LEU:C	2.60	0.45
4:AD:121:CYS:HB3	16:AD:401:HEC:CHC	2.46	0.45
5:AE:178:HIS:CD2	5:AE:209:GLU:O	2.70	0.45
5:AE:255:PRO:HG2	3:Ac:287:LYS:HZ1	1.82	0.45
7:AG:38:VAL:HA	7:AG:41:ARG:HD3	1.98	0.45
1:Aa:399:LEU:HB3	1:Aa:426:LEU:HD22	1.98	0.45
2:Ab:429:LYS:O	2:Ab:432:VAL:HG12	2.16	0.45
4:Ad:218:TYR:CE2	4:Ad:246:PRO:HA	2.51	0.45
5:Ae:116:LEU:CB	9:AJ:15:PHE:CZ	3.00	0.45
5:Ae:178:HIS:CD2	5:Ae:209:GLU:O	2.70	0.45
5:Ae:261:PRO:HB2	5:Ae:273:VAL:HG21	1.98	0.45
6:Af:20:TRP:CH2	12:Ag:102:3PE:H32	2.52	0.45
7:Ag:12:ARG:HB3	7:Ag:13:HIS:CD2	2.52	0.45
3:AC:138:MET:HE1	3:AC:268:ILE:CD1	2.47	0.45
5:AE:155:LYS:HZ3	5:AE:157:SER:CB	2.28	0.45
5:AE:156:LEU:HG	5:AE:271:VAL:CG2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:241:SER:OG	5:AE:254:ALA:HB2	2.17	0.45
1:Aa:170:ARG:HG3	1:Aa:171:GLU:N	2.32	0.45
5:Ae:201:ASP:OD1	5:Ae:202:LEU:N	2.50	0.45
10:Ak:29:ALA:O	10:Ak:33:VAL:HG23	2.17	0.45
3:AC:138:MET:HE1	3:AC:268:ILE:HD13	1.98	0.45
5:AE:207:LYS:HE3	5:AE:265:PHE:CG	2.51	0.45
5:AE:263:TYR:HA	5:AE:273:VAL:HA	1.98	0.45
7:AG:12:ARG:HB3	7:AG:13:HIS:CD2	2.52	0.45
5:AI:34:VAL:O	5:AI:34:VAL:HG13	2.17	0.45
2:Ab:229:VAL:O	2:Ab:233:VAL:HG13	2.16	0.45
2:Ab:300:LYS:C	2:Ab:302:GLY:H	2.24	0.45
3:AC:170:VAL:HG13	3:AC:170:VAL:O	2.16	0.45
3:AC:346:PRO:HG3	7:AG:66:GLU:HG2	1.99	0.45
4:AD:234:ASN:O	4:AD:235:PRO:C	2.59	0.45
8:AH:58:ARG:HD3	8:AH:61:THR:HB	1.99	0.45
2:Ab:259:ARG:HB3	2:Ab:444:LEU:CD1	2.41	0.45
3:Ac:245:PHE:CZ	4:Ad:289:GLY:C	2.95	0.45
4:Ad:141:THR:CG2	9:Aj:53:TRP:CZ2	3.00	0.45
6:Af:86:GLU:O	6:Af:87:ASP:C	2.60	0.45
8:Ah:47:ARG:NH1	8:Ah:47:ARG:HB2	2.32	0.45
1:AA:139:ASP:O	1:AA:140:LEU:C	2.59	0.44
1:AA:162:GLU:HA	1:AA:165:ARG:NH1	2.32	0.44
1:AA:246:ALA:O	1:AA:249:HIS:O	2.34	0.44
2:AB:39:GLU:O	2:AB:227:HIS:HE1	2.00	0.44
2:AB:418:SER:O	2:AB:419:VAL:C	2.59	0.44
3:AC:107:TYR:HE1	3:AC:308:HIS:HB2	1.82	0.44
3:AC:141:TRP:CH2	5:Ae:223:VAL:HG23	2.52	0.44
4:AD:259:THR:O	4:AD:260:PRO:C	2.60	0.44
17:AD:402:3PH:H352	5:AE:128:ALA:HB1	1.99	0.44
12:AF:201:3PE:H371	7:AG:47:LEU:HD13	2.00	0.44
5:AI:43:LEU:CD1	2:Ab:164:VAL:N	2.80	0.44
1:Aa:68:THR:CG2	2:Ab:384:MET:HG3	2.42	0.44
2:Ab:39:GLU:HG3	2:Ab:227:HIS:ND1	2.32	0.44
2:Ab:173:ILE:HD11	2:Ab:439:ALA:C	2.43	0.44
2:Ab:312:SER:HA	2:Ab:315:LYS:HE3	1.99	0.44
2:Ab:418:SER:O	2:Ab:419:VAL:C	2.59	0.44
3:Ac:211:LEU:HD21	6:Af:37:THR:HA	1.97	0.44
3:Ac:218:ILE:HD11	3:Ac:224:TYR:CE2	2.52	0.44
3:Ac:256:TYR:OH	4:Ad:202:ARG:NH1	2.50	0.44
4:Ad:104:SER:H	9:Aj:48:ASN:ND2	2.15	0.44
4:Ad:167:ARG:HH11	4:Ad:169:GLY:HA2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:92:PHE:HE1	1:AA:165:ARG:N	2.14	0.44
1:AA:140:LEU:O	1:AA:141:PRO:C	2.59	0.44
2:AB:84:ARG:NE	5:AI:17:ALA:CB	2.81	0.44
2:AB:305:THR:O	2:AB:311:GLN:HG3	2.17	0.44
3:AC:341:GLN:HE21	3:AC:342:PRO:HD2	1.82	0.44
1:Aa:121:ASN:OD1	2:Ab:300:LYS:HD2	2.17	0.44
1:Aa:275:ILE:HG23	1:Aa:457:ALA:HA	1.99	0.44
3:Ac:213:SER:HA	6:Af:67:LEU:HD11	1.99	0.44
3:Ac:341:GLN:HE21	3:Ac:342:PRO:HD2	1.82	0.44
4:Ad:131:ALA:HB2	4:Ad:174:TYR:CG	2.52	0.44
4:Ad:138:VAL:HG11	4:Ad:276:TRP:NE1	2.33	0.44
4:Ad:259:THR:O	4:Ad:260:PRO:C	2.61	0.44
1:AA:286:HIS:CG	1:AA:359:VAL:HG22	2.51	0.44
1:AA:311:ILE:CG2	1:AA:341:PHE:CZ	3.01	0.44
2:AB:426:LYS:HA	2:AB:429:LYS:HZ3	1.82	0.44
5:AE:178:HIS:NE2	5:AE:209:GLU:HB2	2.33	0.44
5:AE:217:CYS:C	5:AE:219:HIS:N	2.72	0.44
1:Aa:442:ARG:NH1	10:Ak:16:ASN:HD21	2.15	0.44
3:Ac:165:TRP:CE3	3:Ac:169:SER:HA	2.52	0.44
3:Ac:312:GLN:HG2	6:Af:37:THR:O	2.18	0.44
4:Ad:195:PRO:O	4:Ad:196:ASP:C	2.58	0.44
4:Ad:321:TYR:HB2	6:Af:61:PHE:CD1	2.53	0.44
10:Ak:42:LEU:HD22	10:Ak:48:ILE:CD1	2.47	0.44
10:Ak:45:VAL:HB	10:Ak:48:ILE:CD1	2.48	0.44
1:AA:410:CYS:O	1:AA:411:GLU:C	2.59	0.44
2:AB:64:PHE:HZ	2:AB:394:SER:HA	1.83	0.44
3:AC:19:ILE:HG23	3:AC:221:HIS:CB	2.48	0.44
4:AD:219:CYS:SG	4:AD:220:GLU:N	2.90	0.44
5:AE:161:GLU:HA	5:AE:178:HIS:CB	2.48	0.44
5:AE:243:TYR:CD2	5:AE:258:LEU:HG	2.52	0.44
7:AG:72:ARG:NH1	8:AH:71:ASP:OD2	2.50	0.44
1:Aa:377:MET:HG3	1:Aa:477:TRP:NE1	2.32	0.44
1:Aa:406:THR:O	1:Aa:407:THR:C	2.58	0.44
4:Ad:201:VAL:HG22	4:Ad:278:SER:OG	2.18	0.44
4:Ad:248:ILE:HD12	4:Ad:266:VAL:HG11	2.00	0.44
1:AA:389:THR:O	1:AA:390:ARG:C	2.59	0.44
4:AD:161:ASP:HB3	4:AD:163:GLU:HB2	2.00	0.44
6:AF:86:GLU:O	6:AF:87:ASP:C	2.60	0.44
5:AI:63:PRO:HB3	2:Ab:328:ALA:CB	2.48	0.44
1:Aa:247:GLN:O	1:Aa:251:SER:HB2	2.18	0.44
4:Ad:322:ARG:O	7:Ag:13:HIS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:243:TYR:CD2	5:Ae:258:LEU:HG	2.52	0.44
8:Ah:32:ARG:O	8:Ah:33:GLU:C	2.61	0.44
2:AB:214:THR:OG1	2:AB:243:GLY:O	2.35	0.44
4:AD:312:SER:O	4:AD:313:VAL:C	2.59	0.44
17:AD:402:3PH:H252	17:AD:402:3PH:H281	1.52	0.44
5:AE:161:GLU:HA	5:AE:178:HIS:HB3	1.99	0.44
5:AE:178:HIS:HA	5:AE:209:GLU:O	2.18	0.44
1:Aa:169:LEU:O	1:Aa:173:GLN:HG3	2.18	0.44
3:Ac:33:PHE:HE1	15:Ag:101:CDL:H782	1.82	0.44
3:Ac:317:PHE:HB3	6:Af:27:PHE:HD2	1.83	0.44
5:Ae:161:GLU:HA	5:Ae:178:HIS:HB3	2.00	0.44
10:Ak:15:ARG:HB2	10:Ak:15:ARG:CZ	2.48	0.44
2:AB:312:SER:HA	2:AB:315:LYS:HE3	1.99	0.44
3:AC:72:ASP:OD1	4:AD:133:ARG:NH1	2.51	0.44
3:AC:152:ALA:O	3:AC:153:ILE:C	2.58	0.44
5:AE:91:TYR:CD1	7:AG:28:PRO:HG2	2.52	0.44
1:Aa:78:GLY:H	1:Aa:81:TYR:HD2	1.65	0.44
1:Aa:212:SER:O	1:Aa:215:ASP:N	2.50	0.44
14:Ac:406:UQ6:H172	14:Ac:406:UQ6:H151	1.54	0.44
4:Ad:170:LYS:NZ	5:Ae:151:LYS:CD	2.80	0.44
5:Ae:178:HIS:HA	5:Ae:209:GLU:O	2.18	0.44
1:AA:93:LEU:HD21	1:AA:156:LEU:HD11	1.99	0.44
2:AB:138:LEU:CD1	2:AB:233:VAL:HB	2.47	0.44
2:AB:180:VAL:O	2:AB:254:ARG:HG3	2.18	0.44
2:AB:233:VAL:HA	2:AB:236:GLN:CG	2.47	0.44
3:AC:15:ASN:OD1	3:AC:19:ILE:HB	2.18	0.44
4:AD:321:TYR:HB2	6:AF:61:PHE:CE2	2.53	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:CB	2.48	0.44
5:Ae:263:TYR:HB2	5:Ae:271:VAL:HG11	1.97	0.44
1:AA:172:MET:HE1	1:AA:205:SER:HA	2.00	0.44
4:AD:112:ARG:HB3	4:AD:255:TYR:CE1	2.53	0.44
4:AD:167:ARG:NH1	4:AD:169:GLY:HA2	2.32	0.44
4:AD:189:ASN:ND2	4:AD:194:PRO:HG3	2.33	0.44
7:AG:25:ARG:NH2	7:AG:29:SER:H	2.16	0.44
2:Ab:63:LEU:HD12	2:Ab:220:LEU:HD13	2.00	0.44
2:Ab:297:PRO:HB3	2:Ab:303:ASN:HD22	1.83	0.44
5:Ae:217:CYS:C	5:Ae:219:HIS:N	2.72	0.44
6:Af:97:GLU:HA	6:Af:100:ARG:NH1	2.33	0.44
1:AA:71:VAL:HG21	1:AA:140:LEU:CD1	2.48	0.43
1:AA:78:GLY:H	1:AA:81:TYR:HD2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:225:LYS:HG3	1:AA:256:VAL:HG12	2.00	0.43
2:AB:54:ASN:OD1	2:AB:224:GLY:HA2	2.18	0.43
2:AB:411:THR:O	2:AB:414:GLN:HG2	2.18	0.43
4:AD:186:ARG:HE	4:AD:193:LEU:HB2	1.80	0.43
4:AD:262:THR:O	4:AD:263:MET:C	2.61	0.43
4:AD:288:MET:HE2	17:AD:402:3PH:H11	2.00	0.43
5:AE:173:PRO:HG2	5:AE:223:VAL:CG2	2.45	0.43
2:Ab:282:GLU:OE2	2:Ab:430:LYS:HD2	2.18	0.43
3:Ac:170:VAL:HG13	3:Ac:170:VAL:O	2.16	0.43
5:Ae:145:ASP:O	5:Ae:149:MET:HG3	2.17	0.43
5:Ae:195:LEU:HD13	5:Ae:248:ARG:HD2	1.99	0.43
3:AC:71:ARG:NH2	4:AD:277:ALA:O	2.51	0.43
3:AC:287:LYS:NZ	5:Ae:255:PRO:CG	2.81	0.43
5:AE:235:TYR:CE1	5:AE:240:GLY:HA2	2.53	0.43
1:Aa:157:GLU:O	1:Aa:160:GLN:N	2.51	0.43
3:Ac:77:TRP:CD2	4:Ad:281:GLU:HG3	2.52	0.43
4:Ad:112:ARG:HB3	4:Ad:255:TYR:CE1	2.53	0.43
7:Ag:19:LEU:HG	7:Ag:20:SER:N	2.33	0.43
9:Aj:18:THR:HG22	10:Ak:24:TRP:HH2	1.83	0.43
1:AA:178:SER:O	1:AA:179:MET:C	2.60	0.43
1:AA:371:PHE:CZ	1:AA:375:GLN:NE2	2.74	0.43
1:AA:392:LYS:O	1:AA:396:ARG:HG3	2.18	0.43
1:AA:401:SER:O	1:AA:404:ASP:N	2.51	0.43
3:AC:171:ASP:CG	3:AC:172:LYS:N	2.76	0.43
3:AC:181:PHE:HA	3:AC:184:ILE:HG22	2.00	0.43
4:AD:270:VAL:HG21	16:AD:401:HEC:CBB	2.39	0.43
6:AF:97:GLU:HA	6:AF:100:ARG:NH1	2.33	0.43
2:Ab:97:PHE:CE2	2:Ab:101:ARG:HG3	2.53	0.43
2:Ab:297:PRO:CB	2:Ab:303:ASN:HD22	2.30	0.43
4:Ad:307:LYS:O	4:Ad:311:TRP:HB2	2.19	0.43
2:AB:63:LEU:HD12	2:AB:220:LEU:HD13	2.00	0.43
2:AB:155:ARG:HD2	2:AB:198:GLY:H	1.82	0.43
2:AB:378:LEU:HD23	2:AB:416:ILE:CG2	2.49	0.43
14:AC:405:UQ6:H72	14:AC:405:UQ6:H1M3	1.83	0.43
5:AI:62:ARG:HH12	2:Ab:290:GLN:HE22	1.66	0.43
1:Aa:151:VAL:HG21	1:Aa:250:LEU:HD21	2.00	0.43
2:Ab:130:ILE:HA	2:Ab:133:LEU:HB2	2.00	0.43
4:Ad:321:TYR:HB2	6:Af:61:PHE:CG	2.53	0.43
5:Ae:155:LYS:HB3	5:Ae:158:ASP:OD2	2.19	0.43
5:Ae:178:HIS:NE2	5:Ae:209:GLU:HB2	2.33	0.43
7:Ag:25:ARG:NH2	7:Ag:29:SER:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:54:ARG:O	8:Ah:58:ARG:N	2.46	0.43
4:AD:157:GLY:O	4:AD:164:MET:HA	2.18	0.43
5:AE:195:LEU:HD13	5:AE:248:ARG:HD2	1.99	0.43
2:Ab:236:GLN:HG3	2:Ab:237:PHE:CD2	2.53	0.43
2:Ab:411:THR:O	2:Ab:414:GLN:HG2	2.18	0.43
4:Ad:247:PRO:HB3	16:Ad:401:HEC:CHC	2.48	0.43
5:Ae:222:CYS:HB2	5:Ae:236:CYS:SG	2.59	0.43
5:Ae:263:TYR:CA	5:Ae:273:VAL:HG22	2.47	0.43
10:Ak:7:GLY:O	10:Ak:11:ARG:HD3	2.18	0.43
1:AA:183:VAL:HG21	1:AA:286:HIS:CB	2.48	0.43
12:AF:201:3PE:H381	12:AF:201:3PE:H351	1.70	0.43
1:Aa:57:LEU:N	1:Aa:226:ALA:O	2.52	0.43
1:Aa:339:GLN:OE1	1:Aa:339:GLN:N	2.51	0.43
15:Aa:501:CDL:H121	12:Ac:401:3PE:H221	2.00	0.43
2:Ab:378:LEU:HD23	2:Ab:416:ILE:CG2	2.49	0.43
3:Ac:377:LEU:HB3	6:Af:34:ARG:HD2	1.99	0.43
5:Ae:93:ARG:CD	5:Ae:110:ARG:HD2	2.28	0.43
5:Ae:143:SER:HB2	5:Ae:145:ASP:OD1	2.19	0.43
1:AA:271:THR:HG22	1:AA:273:SER:OG	2.18	0.43
5:AE:155:LYS:HE2	5:AE:157:SER:HB3	1.99	0.43
5:AE:220:LEU:C	3:Ac:148:ASN:HD22	2.26	0.43
5:AE:222:CYS:HB2	5:AE:236:CYS:SG	2.59	0.43
6:AF:109:ALA:HB1	10:Ak:9:ARG:HH21	1.84	0.43
1:Aa:175:ASN:C	1:Aa:177:ALA:N	2.76	0.43
2:Ab:92:LYS:HA	2:Ab:145:GLU:OE1	2.18	0.43
8:Ah:27:PRO:HB3	8:Ah:87:ASN:ND2	2.34	0.43
2:AB:47:LEU:HD12	2:AB:218:MET:O	2.18	0.43
5:AE:166:ALA:HB2	5:AE:175:PHE:HD1	1.84	0.43
6:AF:95:LEU:O	6:AF:96:LYS:C	2.62	0.43
1:Aa:98:PHE:CE1	1:Aa:120:LEU:HD11	2.53	0.43
3:Ac:33:PHE:CE1	15:Ag:101:CDL:H782	2.52	0.43
4:Ad:179:TYR:CG	4:Ad:185:ALA:HB2	2.54	0.43
9:Aj:34:ARG:HG3	10:Ak:47:TYR:CZ	2.54	0.43
1:AA:402:HIS:NE2	1:AA:403:LEU:CD1	2.75	0.43
2:AB:230:LEU:O	2:AB:233:VAL:HG22	2.18	0.43
4:AD:167:ARG:NH1	4:AD:170:LYS:HE2	2.34	0.43
5:AE:83:VAL:HG22	5:AE:84:LYS:N	2.34	0.43
5:AE:143:SER:HB2	5:AE:146:VAL:HG13	2.00	0.43
5:AE:221:GLY:CA	3:Ac:148:ASN:HD22	2.32	0.43
12:AF:201:3PE:H3H1	7:AG:52:PRO:HG3	2.00	0.43
2:Ab:283:ALA:O	2:Ab:284:ASN:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:153:GLU:C	5:Ae:154:ILE:HG13	2.44	0.43
5:Ae:156:LEU:HD23	5:Ae:156:LEU:HA	1.62	0.43
5:Ae:235:TYR:CE1	5:Ae:240:GLY:HA2	2.53	0.43
6:Af:53:GLU:OE2	7:Ag:12:ARG:NH1	2.52	0.43
9:Aj:9:ARG:O	9:Aj:13:LEU:HD23	2.19	0.43
3:Ac:148:ASN:HB3	5:Ae:220:LEU:HA	1.99	0.43
5:Al:78:PHE:CE1	2:Ab:171:THR:OG1	2.42	0.43
9:AJ:23:LEU:HA	10:AK:27:VAL:HG22	2.00	0.43
1:Aa:157:GLU:O	1:Aa:158:ASP:C	2.62	0.43
3:Ac:215:ALA:HB2	6:Af:60:MET:HE3	2.01	0.43
4:Ad:318:LYS:CD	5:Ae:86:PRO:HB2	2.49	0.43
8:Ah:32:ARG:O	8:Ah:36:GLU:HG3	2.19	0.43
2:AB:64:PHE:HB3	2:AB:401:LEU:HD11	2.01	0.42
2:AB:300:LYS:HE2	2:AB:301:ARG:HH11	1.83	0.42
5:AE:205:VAL:CG1	5:AE:211:VAL:HG23	2.49	0.42
5:AE:221:GLY:HA3	3:Ac:148:ASN:HD21	1.82	0.42
10:AK:9:ARG:O	10:AK:13:LEU:HG	2.18	0.42
1:Aa:291:VAL:O	1:Aa:353:LEU:HA	2.19	0.42
2:Ab:307:SER:HB2	2:Ab:310:SER:HB2	2.01	0.42
3:Ac:256:TYR:CD2	4:Ad:202:ARG:HB3	2.54	0.42
4:Ad:97:SER:O	9:Aj:51:LYS:NZ	2.52	0.42
8:Ah:55:VAL:O	8:Ah:59:SER:HA	2.19	0.42
8:Ah:56:SER:O	8:Ah:59:SER:HB3	2.19	0.42
1:AA:71:VAL:HG21	1:AA:140:LEU:HD12	2.01	0.42
1:AA:410:CYS:O	1:AA:413:ILE:N	2.52	0.42
2:AB:286:PHE:CD1	2:AB:427:ALA:HB1	2.54	0.42
4:AD:120:VAL:HG23	4:AD:253:LEU:HD23	2.00	0.42
5:AE:196:ARG:HD2	5:AE:249:ILE:HG23	2.01	0.42
5:AE:201:ASP:OD1	5:AE:202:LEU:N	2.50	0.42
5:AE:249:ILE:HG12	5:AE:254:ALA:HB3	2.01	0.42
5:AE:263:TYR:CB	5:AE:273:VAL:HA	2.49	0.42
2:Ab:40:PHE:CZ	2:Ab:406:TYR:HB2	2.54	0.42
2:Ab:176:ASN:HB3	2:Ab:258:ILE:HD11	2.00	0.42
3:Ac:169:SER:O	3:Ac:170:VAL:C	2.62	0.42
4:Ad:312:SER:O	4:Ad:313:VAL:C	2.59	0.42
1:AA:157:GLU:O	1:AA:161:ILE:HG13	2.19	0.42
2:AB:162:LYS:HG3	2:AB:191:TYR:HB3	2.00	0.42
3:AC:29:SER:CB	15:AC:406:CDL:HB61	2.49	0.42
3:AC:153:ILE:HB	3:AC:157:GLY:HA2	2.01	0.42
4:AD:284:HIS:HE2	4:AD:288:MET:HE3	1.83	0.42
2:Ab:39:GLU:OE2	2:Ab:227:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:83:VAL:HG22	5:Ae:84:LYS:N	2.34	0.42
5:Ae:93:ARG:CZ	7:Ag:22:PHE:O	2.67	0.42
9:Aj:30:LEU:HD12	10:Ak:34:TRP:HB2	2.00	0.42
3:AC:278:TYR:CE2	3:AC:282:ARG:HD2	2.54	0.42
4:AD:252:VAL:HG13	4:AD:253:LEU:N	2.34	0.42
5:AE:152:ILE:HD12	5:AE:153:GLU:H	1.84	0.42
8:AH:39:GLU:HA	8:AH:42:VAL:HG12	2.02	0.42
1:Aa:451:ASP:HA	1:Aa:472:ARG:HH12	1.84	0.42
3:Ac:99:GLY:HA3	12:Ac:404:3PE:H2A1	2.01	0.42
4:Ad:252:VAL:HG13	4:Ad:253:LEU:N	2.33	0.42
4:Ad:262:THR:O	4:Ad:263:MET:C	2.61	0.42
5:Ae:112:GLY:O	5:Ae:116:LEU:HB2	2.19	0.42
5:Ae:196:ARG:HD2	5:Ae:249:ILE:HG23	2.01	0.42
1:AA:74:TRP:CZ3	1:AA:232:ALA:HB3	2.54	0.42
1:AA:174:GLU:C	1:AA:176:ASP:H	2.27	0.42
1:AA:372:LEU:HD21	1:AA:376:TRP:CH2	2.55	0.42
2:AB:130:ILE:HA	2:AB:133:LEU:HB2	2.01	0.42
4:AD:248:ILE:HD12	4:AD:266:VAL:HG11	2.00	0.42
5:AE:263:TYR:HA	5:AE:273:VAL:CA	2.50	0.42
8:AH:58:ARG:HB3	8:AH:61:THR:HB	2.01	0.42
1:Aa:95:HIS:CE1	2:Ab:301:ARG:HD3	2.54	0.42
1:Aa:170:ARG:O	1:Aa:173:GLN:HB2	2.20	0.42
2:Ab:225:VAL:HG22	2:Ab:229:VAL:HG21	2.01	0.42
3:Ac:141:TRP:CD1	3:Ac:265:PRO:CD	2.97	0.42
4:Ad:318:LYS:HD2	5:Ae:86:PRO:HB2	2.01	0.42
5:Ae:122:THR:HG21	9:Aj:25:ILE:HD13	2.01	0.42
8:Ah:31:VAL:HG21	8:Ah:84:LEU:HA	2.01	0.42
1:AA:172:MET:HA	1:AA:175:ASN:CG	2.44	0.42
1:AA:230:VAL:HG21	1:AA:417:LEU:HB3	2.00	0.42
3:AC:17:SER:O	14:AC:405:UQ6:H1M1	2.19	0.42
1:Aa:156:LEU:O	1:Aa:213:ARG:NE	2.52	0.42
1:Aa:212:SER:C	1:Aa:214:THR:N	2.74	0.42
1:Aa:272:GLY:O	7:Ag:19:LEU:HD12	2.19	0.42
1:Aa:370:PHE:HE1	15:Aa:501:CDL:H1O1	1.66	0.42
1:Aa:396:ARG:HE	1:Aa:430:GLU:HG2	1.85	0.42
2:Ab:284:ASN:HB3	2:Ab:419:VAL:CG2	2.48	0.42
2:Ab:332:ASP:OD1	2:Ab:332:ASP:N	2.52	0.42
2:Ab:396:ILE:HG12	2:Ab:406:TYR:HE1	1.85	0.42
4:Ad:231:LEU:HD13	4:Ad:241:ALA:HB1	2.01	0.42
5:Ae:155:LYS:HD3	5:Ae:158:ASP:OD1	2.20	0.42
5:Ae:177:ARG:HB3	5:Ae:211:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:47:LEU:HD12	12:Ag:102:3PE:C34	2.48	0.42
1:AA:120:LEU:HD23	2:AB:299:ILE:HG23	2.00	0.42
2:AB:407:MET:HE1	2:AB:415:GLN:CD	2.45	0.42
4:AD:155:GLN:HA	4:AD:166:MET:CA	2.44	0.42
4:AD:189:ASN:HB3	16:AD:401:HEC:HMD2	2.01	0.42
4:AD:221:PRO:HB2	4:AD:225:VAL:HG13	2.01	0.42
5:AE:178:HIS:CD2	5:AE:179:ARG:N	2.88	0.42
8:AH:42:VAL:HG23	8:AH:45:ARG:HH21	1.84	0.42
10:AK:38:TRP:HB3	10:AK:41:ILE:HD13	2.00	0.42
1:Aa:359:VAL:O	1:Aa:360:CYS:HB2	2.19	0.42
1:Aa:463:GLU:CD	7:Ag:8:LEU:HB2	2.44	0.42
3:Ac:278:TYR:CE2	3:Ac:282:ARG:HD2	2.54	0.42
14:Ac:406:UQ6:H111	14:Ac:406:UQ6:H72	1.80	0.42
4:Ad:201:VAL:HG22	4:Ad:278:SER:HB2	2.00	0.42
5:Ae:173:PRO:HG2	5:Ae:223:VAL:CG2	2.45	0.42
5:Ae:266:THR:HB	5:Ae:270:VAL:HG11	2.01	0.42
6:Af:95:LEU:O	6:Af:96:LYS:C	2.61	0.42
8:Ah:54:ARG:HH21	8:Ah:55:VAL:CG2	2.32	0.42
1:AA:397:ASN:N	1:AA:397:ASN:HD22	2.18	0.42
3:AC:33:PHE:O	3:AC:36:LEU:HB2	2.19	0.42
8:AH:49:GLU:O	8:AH:53:ASN:N	2.50	0.42
2:Ab:162:LYS:HG3	2:Ab:191:TYR:HB3	2.00	0.42
3:Ac:150:LEU:HD23	3:Ac:150:LEU:HA	1.92	0.42
5:Ae:153:GLU:CA	5:Ae:271:VAL:O	2.66	0.42
5:Ae:160:PRO:C	5:Ae:178:HIS:HB3	2.45	0.42
5:Ae:249:ILE:HG12	5:Ae:254:ALA:HB3	2.01	0.42
1:AA:342:GLN:HE21	1:AA:357:HIS:CB	2.31	0.42
5:AE:112:GLY:O	5:AE:116:LEU:HB2	2.19	0.42
5:AE:177:ARG:HB3	5:AE:211:VAL:CG1	2.49	0.42
7:AG:19:LEU:HG	7:AG:20:SER:N	2.33	0.42
1:Aa:178:SER:OG	1:Aa:181:ASN:ND2	2.53	0.42
4:Ad:247:PRO:CB	16:Ad:401:HEC:CHC	2.98	0.42
5:Ae:111:LYS:HE3	9:Aj:11:TYR:CZ	2.55	0.42
5:Ae:122:THR:O	5:Ae:123:VAL:C	2.61	0.42
5:Ae:195:LEU:CD1	5:Ae:248:ARG:HD2	2.50	0.42
8:Ah:58:ARG:CZ	8:Ah:61:THR:HB	2.50	0.42
2:AB:272:VAL:HA	2:AB:337:GLY:HA3	2.02	0.42
3:AC:83:HIS:CD2	11:AC:401:HEM:ND	2.88	0.42
12:AC:403:3PE:C2B	7:AG:41:ARG:NH2	2.82	0.42
5:AE:195:LEU:CD1	5:AE:248:ARG:HD2	2.50	0.42
1:Aa:164:GLU:O	1:Aa:165:ARG:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:330:ALA:HB1	7:Ag:56:VAL:CG2	2.50	0.42
17:Ad:402:3PH:H371	5:Ae:128:ALA:CB	2.50	0.42
5:Ae:166:ALA:HB2	5:Ae:175:PHE:HD1	1.84	0.42
1:AA:53:LEU:HD21	1:AA:243:LEU:CD1	2.50	0.41
1:AA:361:ASP:OD1	1:AA:361:ASP:N	2.52	0.41
1:AA:479:ARG:HG3	10:AK:17:TRP:HZ2	1.85	0.41
3:AC:18:PHE:CE1	14:AC:405:UQ6:H103	2.54	0.41
3:AC:184:ILE:HD13	3:Ac:49:LEU:HD22	2.02	0.41
4:AD:167:ARG:NH1	4:AD:170:LYS:HG3	2.35	0.41
4:AD:300:LEU:O	4:AD:301:PRO:C	2.61	0.41
4:AD:323:PRO:HB2	4:AD:325:LYS:HG3	2.02	0.41
5:AE:172:LYS:HE2	5:AE:172:LYS:HA	2.02	0.41
5:AE:231:PHE:CD2	5:AE:250:ARG:NH1	2.88	0.41
8:AH:26:ASP:C	8:AH:28:LEU:N	2.77	0.41
1:Aa:117:GLY:HA2	2:Ab:377:LYS:CG	2.41	0.41
1:Aa:382:SER:HA	10:Ak:16:ASN:HD22	1.85	0.41
2:Ab:155:ARG:HD2	2:Ab:198:GLY:H	1.84	0.41
2:Ab:307:SER:HB2	2:Ab:310:SER:CB	2.50	0.41
3:Ac:33:PHE:O	3:Ac:36:LEU:HB2	2.19	0.41
4:Ad:199:TYR:HA	4:Ad:278:SER:OG	2.20	0.41
4:Ad:317:ARG:HD2	4:Ad:319:LEU:HD21	2.02	0.41
1:AA:120:LEU:HD12	1:AA:132:LEU:O	2.20	0.41
1:AA:148:ALA:O	1:AA:152:GLN:HG2	2.20	0.41
1:AA:152:GLN:NE2	1:AA:250:LEU:HA	2.36	0.41
1:AA:271:THR:HG23	7:AG:23:GLU:HG2	2.02	0.41
1:AA:467:ASP:OD2	3:AC:223:TYR:CZ	2.73	0.41
13:AC:404:U10:H1M3	13:AC:404:U10:H72	1.93	0.41
4:AD:201:VAL:HG23	4:AD:202:ARG:N	2.35	0.41
6:AF:102:ARG:HA	6:AF:105:ARG:CZ	2.49	0.41
1:Aa:205:SER:O	1:Aa:209:ARG:HG3	2.19	0.41
1:Aa:359:VAL:HG12	1:Aa:360:CYS:N	2.33	0.41
2:Ab:38:LEU:HD13	2:Ab:52:LEU:HB2	2.02	0.41
2:Ab:346:ALA:O	2:Ab:347:ALA:C	2.62	0.41
3:Ac:237:LEU:HD22	4:Ad:300:LEU:HD11	2.02	0.41
3:Ac:284:ILE:HG21	3:Ac:289:GLY:HA3	2.02	0.41
3:Ac:317:PHE:CD1	6:Af:27:PHE:HB3	2.55	0.41
4:Ad:248:ILE:HD11	16:Ad:401:HEC:HBB2	2.01	0.41
1:AA:373:GLN:OE1	1:AA:474:GLY:HA3	2.20	0.41
1:AA:454:PRO:O	1:AA:468:TYR:OH	2.34	0.41
3:AC:233:LEU:HD21	4:AD:300:LEU:N	2.35	0.41
4:AD:98:HIS:CE1	4:AD:208:GLU:OE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:119:GLN:OE1	4:AD:253:LEU:HB2	2.20	0.41
9:AJ:19:SER:HA	10:AK:24:TRP:CZ2	2.55	0.41
1:Aa:278:ARG:CZ	1:Aa:463:GLU:HB2	2.50	0.41
2:Ab:239:ASN:OD1	2:Ab:239:ASN:N	2.53	0.41
3:Ac:171:ASP:CG	3:Ac:172:LYS:N	2.76	0.41
3:Ac:240:MET:SD	17:Ad:402:3PH:H272	2.60	0.41
4:Ad:210:TYR:O	4:Ad:211:VAL:C	2.63	0.41
4:Ad:244:MET:HB2	16:Ad:401:HEC:C4D	2.50	0.41
5:Ae:205:VAL:CG1	5:Ae:211:VAL:HG23	2.49	0.41
8:Ah:67:GLU:HG3	8:Ah:68:GLU:N	2.35	0.41
8:Ah:71:ASP:OD1	8:Ah:72:PHE:N	2.53	0.41
2:AB:138:LEU:HD22	2:AB:238:LEU:HG	2.01	0.41
2:AB:346:ALA:O	2:AB:347:ALA:C	2.62	0.41
2:AB:396:ILE:HG12	2:AB:406:TYR:HE1	1.85	0.41
5:AE:160:PRO:C	5:AE:178:HIS:HB3	2.45	0.41
3:Ac:186:PRO:HG2	11:Ac:402:HEM:CHC	2.50	0.41
5:Ae:244:ASP:OD2	5:Ae:248:ARG:NE	2.54	0.41
8:Ah:45:ARG:O	8:Ah:48:LEU:HB3	2.20	0.41
1:AA:356:ALA:HB3	1:AA:372:LEU:HD21	2.03	0.41
2:AB:37:ASP:N	2:AB:37:ASP:OD1	2.52	0.41
4:AD:167:ARG:HH12	4:AD:170:LYS:HG3	1.86	0.41
4:AD:317:ARG:HD2	4:AD:319:LEU:HD21	2.02	0.41
7:AG:28:PRO:O	7:AG:29:SER:C	2.63	0.41
7:AG:35:ILE:O	7:AG:36:PRO:C	2.63	0.41
3:Ac:197:LEU:HD11	14:Ac:406:UQ6:C7	2.51	0.41
4:Ad:185:ALA:O	4:Ad:188:ALA:N	2.54	0.41
5:Ae:196:ARG:HD2	5:Ae:249:ILE:HG21	2.03	0.41
5:Ae:231:PHE:CD2	5:Ae:250:ARG:NH1	2.88	0.41
10:Ak:48:ILE:O	10:Ak:49:ASN:C	2.62	0.41
1:AA:92:PHE:HD1	1:AA:168:ILE:HD12	1.85	0.41
2:AB:64:PHE:CZ	2:AB:394:SER:HA	2.56	0.41
2:AB:225:VAL:HG22	2:AB:229:VAL:HG21	2.01	0.41
3:AC:133:LEU:HD23	3:AC:133:LEU:HA	1.85	0.41
3:AC:215:ALA:HB2	6:AF:60:MET:HE3	2.02	0.41
3:AC:264:THR:O	3:AC:265:PRO:C	2.59	0.41
4:AD:306:MET:C	4:AD:308:ARG:N	2.78	0.41
5:AI:42:VAL:CG1	1:Aa:283:PRO:HB2	2.42	0.41
2:Ab:284:ASN:HB3	2:Ab:419:VAL:HG21	2.01	0.41
2:Ab:286:PHE:CD1	2:Ab:427:ALA:HB1	2.54	0.41
2:Ab:407:MET:HE1	2:Ab:415:GLN:CD	2.45	0.41
12:Ac:404:3PE:H12	15:Ac:407:CDL:OB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:117:TYR:CE1	4:Ad:127:MET:HG2	2.55	0.41
4:Ad:202:ARG:HG3	4:Ad:278:SER:HB3	2.02	0.41
7:Ag:41:ARG:NH1	15:Ag:101:CDL:OA3	2.51	0.41
9:Aj:52:LEU:HD22	9:Aj:52:LEU:HA	1.86	0.41
1:AA:192:PHE:HD1	1:AA:269:ARG:O	2.04	0.41
3:AC:236:PHE:CE1	17:AD:402:3PH:H291	2.56	0.41
3:AC:284:ILE:HG21	3:AC:289:GLY:HA3	2.02	0.41
4:AD:221:PRO:HB3	4:AD:233:PHE:HB2	2.03	0.41
7:AG:26:ALA:C	7:AG:28:PRO:HD3	2.46	0.41
8:AH:49:GLU:HA	8:AH:52:ASP:CG	2.45	0.41
1:Aa:464:GLN:HA	7:Ag:5:PHE:HB3	2.03	0.41
2:Ab:426:LYS:HA	2:Ab:429:LYS:NZ	2.36	0.41
3:Ac:235:MET:HB2	15:Ag:101:CDL:H762	2.02	0.41
4:Ad:141:THR:HG23	9:Aj:53:TRP:CZ2	2.56	0.41
4:Ad:195:PRO:CG	16:Ad:401:HEC:HAA1	2.50	0.41
5:AE:152:ILE:HD13	5:AE:169:TRP:CD1	2.56	0.41
5:AE:159:ILE:HG23	5:AE:163:LYS:HB3	2.03	0.41
5:AE:255:PRO:HG2	3:Ac:287:LYS:NZ	2.35	0.41
1:Aa:171:GLU:O	1:Aa:174:GLU:HG2	2.21	0.41
1:Aa:206:GLU:H	1:Aa:206:GLU:CD	2.27	0.41
1:Aa:361:ASP:OD1	1:Aa:361:ASP:N	2.54	0.41
3:Ac:8:HIS:HB3	3:Ac:11:PHE:HD2	1.85	0.41
3:Ac:133:LEU:HD23	3:Ac:133:LEU:HA	1.85	0.41
3:Ac:264:THR:O	3:Ac:265:PRO:C	2.63	0.41
4:Ad:124:CYS:HB3	4:Ad:194:PRO:CG	2.51	0.41
4:Ad:131:ALA:O	4:Ad:132:TYR:C	2.64	0.41
4:Ad:148:LEU:HA	4:Ad:151:GLU:CD	2.46	0.41
4:Ad:154:VAL:HG11	4:Ad:173:ASP:OD1	2.21	0.41
1:AA:365:ILE:O	1:AA:369:VAL:HG23	2.21	0.41
1:AA:412:ASP:O	1:AA:416:SER:OG	2.32	0.41
2:AB:176:ASN:CB	2:AB:258:ILE:HD11	2.51	0.41
3:AC:49:LEU:HD13	3:Ac:184:ILE:HD12	2.03	0.41
3:AC:295:ILE:HG22	3:AC:299:LEU:HD12	2.03	0.41
4:AD:235:PRO:HA	4:AD:240:GLN:CG	2.50	0.41
4:AD:281:GLU:O	4:AD:282:HIS:C	2.64	0.41
5:AE:244:ASP:OD2	5:AE:248:ARG:NE	2.54	0.41
12:AF:201:3PE:H381	12:AF:201:3PE:H222	2.03	0.41
7:AG:29:SER:CB	7:AG:32:SER:HB2	2.38	0.41
7:AG:57:TYR:O	7:AG:61:THR:HG23	2.21	0.41
1:Aa:92:PHE:CE2	1:Aa:161:ILE:HG23	2.56	0.41
1:Aa:93:LEU:O	1:Aa:97:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:341:PHE:O	1:Aa:341:PHE:CG	2.70	0.41
15:Aa:501:CDL:HB32	15:Aa:501:CDL:H1	2.02	0.41
2:Ab:64:PHE:HZ	2:Ab:394:SER:HA	1.86	0.41
2:Ab:272:VAL:HA	2:Ab:337:GLY:HA3	2.02	0.41
3:Ac:8:HIS:CG	3:Ac:11:PHE:HD2	2.38	0.41
5:Ae:162:GLY:N	5:Ae:178:HIS:O	2.53	0.41
5:Ae:172:LYS:HA	5:Ae:172:LYS:HE2	2.02	0.41
5:Ae:178:HIS:CD2	5:Ae:179:ARG:N	2.88	0.41
7:Ag:26:ALA:C	7:Ag:28:PRO:HD3	2.46	0.41
9:Aj:48:ASN:HB3	9:Aj:51:LYS:HG3	2.03	0.41
1:AA:95:HIS:HB3	1:AA:164:GLU:OE1	2.21	0.41
2:AB:40:PHE:CE1	2:AB:404:GLY:O	2.73	0.41
2:AB:258:ILE:HD13	2:AB:258:ILE:HG21	1.79	0.41
3:AC:275:LEU:O	3:AC:276:PHE:C	2.64	0.41
3:AC:294:LEU:C	3:AC:294:LEU:HD23	2.46	0.41
4:AD:306:MET:HE2	4:AD:306:MET:HB3	1.92	0.41
9:AJ:21:PHE:O	9:AJ:24:THR:HG22	2.20	0.41
1:Aa:290:ALA:HB1	1:Aa:353:LEU:HB3	2.03	0.41
1:Aa:388:VAL:HG21	1:Aa:438:ALA:HA	2.02	0.41
3:Ac:38:GLY:HA3	14:Ac:406:UQ6:H161	2.01	0.41
3:Ac:103:TYR:HD1	3:Ac:325:TYR:CD2	2.38	0.41
3:Ac:295:ILE:HG22	3:Ac:299:LEU:HD12	2.03	0.41
4:Ad:250:THR:HG23	4:Ad:262:THR:HA	2.03	0.41
5:Ae:116:LEU:HB2	9:Aj:15:PHE:CZ	2.56	0.41
5:Ae:154:ILE:N	5:Ae:271:VAL:O	2.54	0.41
7:Ag:28:PRO:O	7:Ag:29:SER:C	2.64	0.41
7:Ag:73:LYS:HD3	8:Ah:63:GLU:OE2	2.21	0.41
10:Ak:10:TYR:HA	10:Ak:13:LEU:HD12	2.03	0.41
1:AA:298:ASN:OD1	1:AA:299:PRO:HD2	2.20	0.40
4:AD:207:GLY:O	4:AD:208:GLU:C	2.63	0.40
5:AI:64:LEU:HD12	5:AI:78:PHE:HA	2.03	0.40
1:Aa:258:GLU:C	1:Aa:259:GLU:HG2	2.47	0.40
1:Aa:341:PHE:HB2	1:Aa:368:MET:HE2	2.03	0.40
2:Ab:312:SER:OG	2:Ab:357:GLN:NE2	2.40	0.40
4:Ad:129:TYR:HD2	4:Ad:198:SER:CB	2.34	0.40
5:Ae:152:ILE:O	5:Ae:272:VAL:CB	2.68	0.40
6:Af:36:ASP:OD1	6:Af:90:TYR:OH	2.38	0.40
10:Ak:39:ARG:HA	10:Ak:42:LEU:HB2	2.02	0.40
10:Ak:45:VAL:O	10:Ak:49:ASN:HB2	2.21	0.40
1:AA:341:PHE:O	1:AA:341:PHE:CG	2.74	0.40
2:AB:65:VAL:HG22	2:AB:218:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:183:LYS:HE2	2:Ab:449:PHE:CG	2.57	0.40
4:AD:218:TYR:CE1	4:AD:246:PRO:HG3	2.57	0.40
4:AD:324:PRO:O	4:AD:325:LYS:C	2.63	0.40
5:AE:196:ARG:HD2	5:AE:249:ILE:HG21	2.03	0.40
7:AG:10:ARG:NH2	7:AG:12:ARG:HD2	2.36	0.40
1:Aa:68:THR:HG23	1:Aa:135:ALA:O	2.21	0.40
1:Aa:148:ALA:O	1:Aa:152:GLN:HG2	2.20	0.40
4:Ad:321:TYR:HB2	6:Af:61:PHE:CD2	2.57	0.40
5:Ae:159:ILE:HG23	5:Ae:163:LYS:HB3	2.03	0.40
5:Ae:249:ILE:HG23	5:Ae:249:ILE:O	2.22	0.40
1:AA:404:ASP:O	1:AA:408:PRO:HG2	2.21	0.40
3:AC:30:TRP:CB	3:AC:100:ARG:HD3	2.52	0.40
4:AD:179:TYR:CE1	4:AD:188:ALA:HB3	2.56	0.40
10:AK:23:MET:O	10:AK:27:VAL:HG23	2.21	0.40
1:Aa:60:ALA:O	1:Aa:61:SER:HB3	2.21	0.40
1:Aa:278:ARG:NH1	7:Ag:11:ILE:HD13	2.36	0.40
2:Ab:227:HIS:HD2	2:Ab:231:LYS:HE2	1.85	0.40
2:Ab:232:GLN:O	2:Ab:235:GLU:HG3	2.20	0.40
3:Ac:238:ILE:HD12	15:Ag:101:CDL:H772	2.03	0.40
4:Ad:192:ALA:HB3	16:Ad:401:HEC:CMD	2.51	0.40
6:Af:24:ALA:O	7:Ag:48:ARG:NH2	2.53	0.40
9:Aj:48:ASN:O	9:Aj:49:GLU:C	2.64	0.40
10:Ak:11:ARG:HD3	10:Ak:11:ARG:N	2.37	0.40
1:AA:73:VAL:HG11	1:AA:151:VAL:HG11	2.03	0.40
4:AD:110:ILE:HG23	4:AD:273:PHE:HA	2.04	0.40
4:AD:154:VAL:N	4:AD:167:ARG:O	2.52	0.40
4:AD:262:THR:HG22	8:AH:24:LEU:CG	2.49	0.40
6:AF:109:ALA:HB1	10:Ak:9:ARG:NH2	2.36	0.40
1:Aa:86:ASN:OD1	1:Aa:86:ASN:N	2.54	0.40
3:Ac:296:LEU:O	3:Ac:297:SER:C	2.64	0.40
17:Ad:402:3PH:H232	5:Ae:135:GLN:NE2	2.36	0.40
5:Ae:156:LEU:HB2	5:Ae:269:ASP:CA	2.50	0.40
5:Ae:216:VAL:HG13	5:Ae:221:GLY:HA2	2.03	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:NH2	2.37	0.40
7:Ag:10:ARG:NH2	7:Ag:12:ARG:HD2	2.37	0.40
7:Ag:43:ARG:HD3	12:Ag:102:3PE:C39	2.51	0.40
1:AA:57:LEU:HD12	1:AA:229:MET:O	2.22	0.40
1:AA:98:PHE:CD1	1:AA:120:LEU:HD21	2.57	0.40
2:AB:234:ALA:C	2:AB:237:PHE:O	2.65	0.40
2:AB:426:LYS:HA	2:AB:429:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:453:LEU:O	2:AB:453:LEU:HD23	2.21	0.40
5:AE:168:LYS:NZ	5:AE:171:GLY:HA2	2.36	0.40
5:AE:172:LYS:HD2	3:Ac:169:SER:CB	2.51	0.40
7:AG:73:LYS:NZ	8:AH:64:ASP:O	2.55	0.40
9:AJ:11:TYR:CZ	9:AJ:16:ARG:HB2	2.56	0.40
10:AK:39:ARG:O	10:AK:40:LEU:C	2.62	0.40
1:Aa:126:ARG:HD2	1:Aa:348:TYR:OH	2.21	0.40
3:Ac:218:ILE:HG21	4:Ad:314:LEU:HD11	2.03	0.40
3:Ac:244:LEU:HA	4:Ad:285:ARG:HD2	2.02	0.40
3:Ac:294:LEU:C	3:Ac:294:LEU:HD23	2.46	0.40
13:Ac:405:U10:H121	13:Ac:405:U10:H8	1.48	0.40
4:Ad:111:ARG:HG3	4:Ad:140:TYR:CZ	2.57	0.40
4:Ad:155:GLN:HB3	4:Ad:166:MET:HE2	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	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
1	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
2	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
2	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
4	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
4	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100
5	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100
5	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ae	181/274 (66%)	166 (92%)	15 (8%)	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%)	73 (99%)	1 (1%)	0	100	100
8	AH	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
8	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
9	AJ	39/64 (61%)	39 (100%)	0	0	100	100
9	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
10	AK	33/56 (59%)	33 (100%)	0	0	100	100
10	Ak	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	3880/4904 (79%)	3755 (97%)	125 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	338/398 (85%)	337 (100%)	1 (0%)	86	84
1	Aa	349/398 (88%)	349 (100%)	0	100	100
2	AB	328/356 (92%)	328 (100%)	0	100	100
2	Ab	328/356 (92%)	328 (100%)	0	100	100
3	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
3	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
4	AD	203/260 (78%)	203 (100%)	0	100	100
4	Ad	203/260 (78%)	203 (100%)	0	100	100
5	AE	155/224 (69%)	154 (99%)	1 (1%)	78	80
5	AI	34/224 (15%)	33 (97%)	1 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Ae	156/224 (70%)	155 (99%)	1 (1%)	78	80
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	62/83 (75%)	62 (100%)	0	100	100
8	Ah	63/83 (76%)	63 (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	26/46 (56%)	26 (100%)	0	100	100
10	Ak	34/46 (74%)	34 (100%)	0	100	100
All	All	3319/4080 (81%)	3313 (100%)	6 (0%)	85	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	478	LEU
3	AC	294	LEU
5	AE	146	VAL
5	AI	14	VAL
3	Ac	294	LEU
5	Ae	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	87	ASN
1	AA	103	ASN
1	AA	173	GLN
1	AA	207	ASN
1	AA	240	GLN
1	AA	277	HIS
1	AA	301	ASN
1	AA	305	GLN
1	AA	342	GLN
1	AA	345	ASN
1	AA	397	ASN

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Mol	Chain	Res	Type
1	AA	402	HIS
2	AB	284	ASN
2	AB	304	ASN
2	AB	357	GLN
2	AB	365	ASN
2	AB	415	GLN
3	AC	32	ASN
3	AC	201	HIS
3	AC	260	ASN
3	AC	312	GLN
4	AD	98	HIS
4	AD	115	GLN
4	AD	189	ASN
4	AD	190	ASN
5	AE	131	ASN
5	AE	135	GLN
5	AE	227	ASN
5	AE	242	HIS
6	AF	80	GLN
10	AK	16	ASN
1	Aa	49	GLN
1	Aa	87	ASN
1	Aa	103	ASN
1	Aa	119	HIS
1	Aa	173	GLN
1	Aa	181	ASN
1	Aa	207	ASN
1	Aa	240	GLN
2	Ab	227	HIS
2	Ab	284	ASN
2	Ab	290	GLN
2	Ab	291	HIS
2	Ab	303	ASN
2	Ab	304	ASN
2	Ab	357	GLN
2	Ab	415	GLN
2	Ab	443	ASN
3	Ac	32	ASN
3	Ac	148	ASN
3	Ac	260	ASN
3	Ac	312	GLN
4	Ad	115	GLN

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Mol	Chain	Res	Type
4	Ad	155	GLN
4	Ad	190	ASN
5	Ae	131	ASN
5	Ae	135	GLN
5	Ae	227	ASN
5	Ae	242	HIS
6	Af	80	GLN
7	Ag	69	GLN
8	Ah	60	GLN
8	Ah	82	HIS
9	Aj	48	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](#)

21 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	$\# Z > 2$
11	HEM	AC	401	3	50,50,50	1.58	8 (16%)	66,82,82	1.76	14 (21%)
16	HEC	AD	401	4	50,50,50	2.80	26 (52%)	68,82,82	2.48	30 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
17	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)
12	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
11	HEM	Ac	402	3	50,50,50	1.63	9 (18%)	66,82,82	1.98	16 (24%)
15	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
13	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
12	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
17	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
12	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
11	HEM	AC	402	3	50,50,50	1.69	11 (22%)	66,82,82	2.17	23 (34%)
15	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)
15	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
11	HEM	Ac	403	3	50,50,50	1.65	10 (20%)	66,82,82	1.70	13 (19%)
16	HEC	Ad	401	4	50,50,50	2.80	25 (50%)	68,82,82	2.44	26 (38%)
12	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
13	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
14	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
14	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
12	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	AC	401	3	-	8/14/54/54	-
16	HEC	AD	401	4	1/1/3/7	7/14/54/54	-
15	CDL	AC	406	-	-	18/66/66/110	-
17	3PH	AD	402	-	-	8/37/37/49	-
12	3PE	AC	403	-	-	12/38/38/54	-
11	HEM	Ac	402	3	-	5/14/54/54	-
15	CDL	Ac	407	-	-	11/52/52/110	-
13	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
12	3PE	Ag	102	-	-	5/42/42/54	-
17	3PH	Ad	402	-	-	8/37/37/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	3PE	AF	201	-	-	9/45/45/54	-
11	HEM	AC	402	3	-	6/14/54/54	-
15	CDL	Ag	101	-	-	12/66/66/110	-
15	CDL	Aa	501	-	-	16/56/56/110	-
11	HEM	Ac	403	3	-	10/14/54/54	-
16	HEC	Ad	401	4	1/1/3/7	7/14/54/54	-
12	3PE	Ac	404	-	-	8/38/38/54	-
13	U10	AC	404	-	-	0/15/39/87	0/1/1/1
14	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
14	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1
12	3PE	Ac	401	-	-	10/26/26/54	-

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AC	404	U10	C6-C1	7.59	1.49	1.35
13	Ac	405	U10	C6-C1	7.42	1.48	1.35
14	AC	405	UQ6	C2-C3	5.95	1.49	1.39
14	Ac	406	UQ6	C2-C3	5.90	1.49	1.39
14	Ac	406	UQ6	C5-C4	5.87	1.48	1.39
14	Ac	406	UQ6	C5-C6	5.87	1.49	1.40
14	AC	405	UQ6	C5-C4	5.67	1.48	1.39
11	Ac	402	HEM	FE-NB	5.66	2.12	1.94
14	AC	405	UQ6	C5-C6	5.60	1.48	1.40
14	AC	405	UQ6	C6-C1	5.57	1.49	1.40
14	Ac	406	UQ6	C6-C1	5.46	1.49	1.40
16	AD	401	HEC	FE-NB	5.28	2.11	1.94
11	AC	401	HEM	FE-NB	5.17	2.10	1.94
11	Ac	403	HEM	FE-NB	5.08	2.10	1.94
16	AD	401	HEC	C2A-C3A	4.99	1.47	1.36
16	Ad	401	HEC	C2A-C3A	4.94	1.47	1.36
16	AD	401	HEC	C3D-C2D	4.94	1.47	1.36
16	Ad	401	HEC	FE-NB	4.93	2.10	1.94
16	AD	401	HEC	FE-ND	4.93	2.10	1.94
16	Ad	401	HEC	CHB-C4A	4.89	1.47	1.38
16	AD	401	HEC	CHB-C4A	4.87	1.47	1.38
16	Ad	401	HEC	FE-ND	4.86	2.09	1.94
16	AD	401	HEC	CHA-C1A	4.84	1.47	1.38
16	Ad	401	HEC	C3D-C2D	4.83	1.47	1.36
16	Ad	401	HEC	CHA-C1A	4.79	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	AD	401	HEC	C3B-C2B	4.72	1.46	1.36
14	Ac	406	UQ6	C4-C3	4.68	1.49	1.39
16	AD	401	HEC	CHD-C1D	4.68	1.48	1.38
16	Ad	401	HEC	C3B-C2B	4.67	1.46	1.36
16	Ad	401	HEC	FE-NC	4.63	2.10	1.95
11	AC	402	HEM	FE-NB	4.58	2.09	1.94
14	AC	405	UQ6	C4-C3	4.53	1.48	1.39
16	Ad	401	HEC	FE-NA	4.47	2.10	1.95
16	AD	401	HEC	FE-NA	4.42	2.10	1.95
14	AC	405	UQ6	C2-C1	4.40	1.49	1.40
15	AC	406	CDL	OB8-CB7	4.34	1.46	1.33
15	Ag	101	CDL	OB8-CB7	4.27	1.45	1.33
15	Ac	407	CDL	OA8-CA7	4.26	1.45	1.33
15	Ac	407	CDL	OB8-CB7	4.26	1.45	1.33
16	Ad	401	HEC	CHC-C4B	4.25	1.47	1.38
14	Ac	406	UQ6	C2-C1	4.25	1.48	1.40
17	AD	402	3PH	O31-C31	4.24	1.45	1.33
17	Ad	402	3PH	O31-C31	4.23	1.45	1.33
12	Ag	102	3PE	O31-C31	4.22	1.45	1.33
12	Ac	404	3PE	O31-C31	4.20	1.45	1.33
12	AF	201	3PE	O31-C31	4.18	1.45	1.33
12	AC	403	3PE	O31-C31	4.15	1.45	1.33
15	AC	406	CDL	OA8-CA7	4.09	1.45	1.33
11	AC	401	HEM	FE-NC	4.08	2.09	1.95
12	AF	201	3PE	O21-C21	4.05	1.45	1.34
16	AD	401	HEC	FE-NC	4.05	2.08	1.95
15	AC	406	CDL	OB6-CB5	4.04	1.45	1.34
15	Ag	101	CDL	OA8-CA7	4.04	1.45	1.33
15	Ag	101	CDL	OB6-CB5	4.04	1.45	1.34
15	Ac	407	CDL	OA6-CA5	4.03	1.45	1.34
12	AC	403	3PE	O21-C21	4.01	1.45	1.34
12	Ag	102	3PE	O21-C21	4.00	1.45	1.34
11	Ac	403	HEM	C1B-NB	-3.95	1.33	1.40
15	Ag	101	CDL	OA6-CA5	3.95	1.45	1.34
15	Ac	407	CDL	OB6-CB5	3.93	1.45	1.34
11	AC	402	HEM	FE-NC	3.91	2.08	1.95
17	AD	402	3PH	O21-C21	3.91	1.45	1.34
11	Ac	403	HEM	FE-NC	3.91	2.08	1.95
11	AC	402	HEM	C1B-NB	-3.91	1.33	1.40
17	Ad	402	3PH	O21-C21	3.91	1.45	1.34
12	Ac	404	3PE	O21-C21	3.89	1.45	1.34
15	AC	406	CDL	OA6-CA5	3.89	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Ad	401	HEC	CHD-C1D	3.88	1.46	1.38
11	Ac	402	HEM	FE-NC	3.80	2.08	1.95
11	Ac	402	HEM	C1B-NB	-3.80	1.33	1.40
16	Ad	401	HEC	CHB-C1B	3.76	1.47	1.39
16	AD	401	HEC	CHC-C4B	3.75	1.46	1.38
11	Ac	403	HEM	C4D-ND	-3.66	1.34	1.40
16	AD	401	HEC	CHD-C4C	3.65	1.47	1.39
16	AD	401	HEC	CHA-C4D	3.64	1.47	1.39
16	Ad	401	HEC	CHD-C4C	3.57	1.47	1.39
11	AC	402	HEM	C4D-ND	-3.55	1.34	1.40
16	Ad	401	HEC	CHA-C4D	3.53	1.47	1.39
16	Ad	401	HEC	C1D-ND	-3.51	1.34	1.40
11	AC	401	HEM	C4D-ND	-3.44	1.34	1.40
11	AC	401	HEM	C1B-NB	-3.43	1.34	1.40
11	Ac	402	HEM	C4D-ND	-3.39	1.34	1.40
16	AD	401	HEC	C4B-NB	-3.35	1.34	1.40
16	Ad	401	HEC	C4B-NB	-3.34	1.34	1.40
16	Ad	401	HEC	CHC-C1C	3.29	1.46	1.39
16	AD	401	HEC	CHC-C1C	3.18	1.46	1.39
16	Ad	401	HEC	C3C-C2C	3.15	1.47	1.38
16	AD	401	HEC	CHB-C1B	3.10	1.46	1.39
13	AC	404	U10	C4-C3	3.08	1.48	1.36
11	Ac	402	HEM	C1C-C2C	-3.08	1.39	1.45
13	Ac	405	U10	C4-C3	3.04	1.48	1.36
11	AC	402	HEM	C4B-NB	-2.98	1.32	1.38
16	AD	401	HEC	C1C-NC	-2.96	1.34	1.39
11	AC	402	HEM	C1B-C2B	-2.94	1.38	1.44
16	AD	401	HEC	C3C-C2C	2.83	1.46	1.38
11	AC	402	HEM	FE-ND	-2.74	1.86	1.94
16	AD	401	HEC	C1D-ND	-2.74	1.35	1.40
11	Ac	403	HEM	C1C-C2C	-2.68	1.40	1.45
11	AC	401	HEM	C1C-C2C	-2.60	1.40	1.45
11	Ac	403	HEM	FE-ND	-2.58	1.86	1.94
11	AC	402	HEM	C1C-C2C	-2.57	1.40	1.45
11	Ac	402	HEM	C3C-C4C	-2.48	1.41	1.46
11	AC	401	HEM	FE-ND	-2.45	1.87	1.94
16	Ad	401	HEC	C4A-NA	-2.44	1.35	1.39
16	AD	401	HEC	C1A-NA	-2.42	1.35	1.39
16	AD	401	HEC	C4A-NA	-2.41	1.35	1.39
16	Ad	401	HEC	C1A-NA	-2.41	1.35	1.39
16	Ad	401	HEC	C4C-NC	-2.41	1.35	1.39
16	Ad	401	HEC	C1B-C2B	2.39	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	AD	401	HEC	C1B-C2B	2.38	1.49	1.44
16	Ad	401	HEC	C1C-NC	-2.37	1.35	1.39
11	Ac	403	HEM	C4B-NB	-2.36	1.33	1.38
16	AD	401	HEC	C4C-NC	-2.36	1.35	1.39
16	Ad	401	HEC	C1C-C2C	2.35	1.48	1.43
16	AD	401	HEC	C1A-C2A	2.34	1.49	1.45
11	AC	402	HEM	C3C-C4C	-2.33	1.41	1.46
11	AC	402	HEM	C1D-ND	-2.29	1.34	1.38
11	Ac	403	HEM	C3C-C4C	-2.26	1.42	1.46
16	Ad	401	HEC	C4D-C3D	2.23	1.48	1.45
11	Ac	402	HEM	C1D-ND	-2.22	1.34	1.38
11	Ac	403	HEM	C1D-ND	-2.20	1.34	1.38
11	Ac	402	HEM	FE-ND	-2.19	1.88	1.94
16	AD	401	HEC	C1D-C2D	2.16	1.48	1.44
11	Ac	402	HEM	C3B-C4B	2.14	1.49	1.44
11	AC	401	HEM	C4B-NB	-2.13	1.34	1.38
11	AC	402	HEM	C3B-C2B	-2.11	1.33	1.37
16	AD	401	HEC	C4D-C3D	2.08	1.48	1.45
11	AC	401	HEM	C1D-ND	-2.06	1.34	1.38
11	Ac	403	HEM	C1A-C2A	-2.02	1.40	1.44

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
11	AC	402	HEM	CHC-C4B-NB	6.28	131.24	124.42
16	AD	401	HEC	C1B-C2B-C3B	-6.23	100.41	106.96
16	AD	401	HEC	C2B-C1B-NB	6.06	117.14	109.88
16	Ad	401	HEC	C1B-C2B-C3B	-5.58	101.09	106.96
14	AC	405	UQ6	C7-C8-C9	-5.55	118.63	127.24
11	AC	401	HEM	CHC-C4B-NB	5.48	130.37	124.42
16	Ad	401	HEC	C2D-C1D-ND	5.42	116.26	109.84
16	Ad	401	HEC	C1C-C2C-C3C	-5.24	100.70	106.83
16	Ad	401	HEC	C2A-C1A-NA	5.03	115.22	110.32
16	AD	401	HEC	C2A-C1A-NA	4.92	115.11	110.32
16	AD	401	HEC	C3D-C4D-ND	4.92	115.12	110.36
11	Ac	402	HEM	C3B-C2B-C1B	4.83	110.07	106.49
11	AC	402	HEM	CHD-C1D-ND	4.80	129.63	124.42
11	AC	402	HEM	C3B-C2B-C1B	-4.70	103.00	106.49
11	AC	402	HEM	CHB-C1B-NB	4.67	130.13	124.37
16	Ad	401	HEC	C3D-C4D-ND	4.60	114.81	110.36
11	AC	401	HEM	CHD-C1D-ND	4.55	129.36	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Ad	401	HEC	C2B-C1B-NB	4.54	115.32	109.88
11	Ac	403	HEM	CHC-C4B-NB	4.43	129.23	124.42
11	Ac	402	HEM	CHD-C1D-ND	4.43	129.23	124.42
11	AC	402	HEM	C4B-C3B-C2B	4.35	110.57	107.11
16	AD	401	HEC	C3B-C4B-NB	4.34	115.00	110.17
11	Ac	403	HEM	CHD-C1D-ND	4.32	129.11	124.42
16	AD	401	HEC	C2D-C1D-ND	4.27	114.90	109.84
16	Ad	401	HEC	C2C-C1C-NC	4.25	116.55	110.08
12	Ac	404	3PE	O21-C21-C22	4.22	120.61	111.50
16	Ad	401	HEC	C1D-C2D-C3D	-4.20	102.54	106.96
12	Ag	102	3PE	O21-C21-C22	4.11	120.36	111.50
11	Ac	403	HEM	CHA-C4D-ND	4.07	129.39	124.37
11	Ac	402	HEM	CHC-C4B-NB	4.06	128.83	124.42
16	AD	401	HEC	C1C-C2C-C3C	-4.05	102.09	106.83
13	AC	404	U10	C7-C8-C9	-4.04	120.07	126.79
15	Ag	101	CDL	OA6-CA5-C11	4.02	120.17	111.50
16	AD	401	HEC	CMC-C2C-C3C	4.02	134.30	125.61
15	Ac	407	CDL	OB6-CB5-C51	4.00	120.12	111.50
16	AD	401	HEC	C1D-C2D-C3D	-3.95	102.80	106.96
15	Ag	101	CDL	OB6-CB5-C51	3.95	120.01	111.50
11	AC	402	HEM	CHA-C4D-ND	3.93	129.23	124.37
16	Ad	401	HEC	CBB-CAB-C3B	3.89	123.16	112.43
16	AD	401	HEC	C2C-C1C-NC	3.86	115.96	110.08
11	AC	401	HEM	CHA-C4D-ND	3.85	129.12	124.37
12	AC	403	3PE	O21-C21-C22	3.84	119.77	111.50
16	AD	401	HEC	CBB-CAB-C3B	3.82	122.95	112.43
15	AC	406	CDL	OA6-CA5-C11	3.76	119.61	111.50
13	Ac	405	U10	C22-C23-C24	-3.74	118.65	127.66
11	AC	401	HEM	C1B-NB-C4B	3.72	108.92	105.07
15	AC	406	CDL	OB6-CB5-C51	3.72	119.52	111.50
13	Ac	405	U10	C12-C13-C14	-3.71	118.72	127.66
11	AC	401	HEM	CHB-C1B-NB	3.68	128.91	124.37
11	AC	402	HEM	CHB-C1B-C2B	-3.64	116.61	126.73
14	AC	405	UQ6	C15-C14-C16	3.60	121.33	115.27
11	Ac	403	HEM	CHB-C1B-NB	3.57	128.77	124.37
11	Ac	402	HEM	CHA-C4D-ND	3.55	128.76	124.37
17	AD	402	3PH	O21-C21-C22	3.54	119.13	111.50
16	AD	401	HEC	C1A-C2A-C3A	-3.52	102.54	107.13
16	Ad	401	HEC	C3C-C4C-NC	3.49	114.05	110.15
16	Ad	401	HEC	CBC-CAC-C3C	3.48	122.04	112.43
17	Ad	402	3PH	O21-C21-C22	3.44	118.91	111.50
15	Ac	407	CDL	OA6-CA5-C11	3.41	120.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Ac	406	UQ6	C7-C8-C9	-3.40	121.97	127.24
15	Ac	407	CDL	OB8-CB7-C71	3.38	120.24	111.38
16	Ad	401	HEC	C1A-C2A-C3A	-3.36	102.74	107.13
11	Ac	403	HEM	C1B-NB-C4B	3.34	108.53	105.07
12	AF	201	3PE	O21-C21-C22	3.33	118.67	111.50
16	Ad	401	HEC	C3B-C4B-NB	3.32	113.86	110.17
11	AC	401	HEM	C4C-NC-C1C	3.25	108.53	105.35
11	Ac	402	HEM	CHD-C4C-NC	3.22	127.92	124.44
16	AD	401	HEC	CHC-C1C-C2C	-3.20	118.20	127.24
11	AC	402	HEM	C4C-NC-C1C	3.19	108.47	105.35
11	AC	402	HEM	C1B-NB-C4B	3.17	108.35	105.07
16	Ad	401	HEC	CBD-CAD-C3D	-3.13	103.93	112.63
13	Ac	405	U10	C15-C14-C16	3.11	120.51	115.27
13	AC	404	U10	C10-C9-C11	3.11	120.50	115.27
11	Ac	403	HEM	C4C-NC-C1C	3.05	108.33	105.35
11	Ac	402	HEM	C1B-NB-C4B	3.05	108.22	105.07
13	Ac	405	U10	C10-C9-C11	3.04	120.39	115.27
11	Ac	402	HEM	CHD-C1D-C2D	-3.04	120.23	124.98
11	AC	402	HEM	C4D-ND-C1D	3.03	108.20	105.07
15	Ag	101	CDL	CA4-OA6-CA5	-3.02	110.37	117.79
12	Ac	404	3PE	C2-O21-C21	-3.00	110.40	117.79
16	Ad	401	HEC	CAD-C3D-C4D	2.97	129.85	124.66
16	AD	401	HEC	C3A-C4A-NA	2.96	115.16	109.69
13	Ac	405	U10	C20-C19-C21	2.96	120.25	115.27
16	Ad	401	HEC	C3A-C4A-NA	2.96	115.14	109.69
13	Ac	405	U10	C1M-C1-C6	-2.92	119.63	124.40
11	Ac	402	HEM	C4C-NC-C1C	2.92	108.21	105.35
16	Ad	401	HEC	C4D-C3D-C2D	-2.91	102.66	106.90
11	AC	402	HEM	CHD-C4C-NC	2.89	127.57	124.44
11	AC	402	HEM	C2B-C1B-NB	2.89	113.26	109.84
12	Ag	102	3PE	O31-C31-C32	2.86	120.89	111.91
13	Ac	405	U10	C17-C18-C19	-2.85	120.80	127.66
16	Ad	401	HEC	C4A-C3A-C2A	-2.85	102.78	106.94
14	AC	405	UQ6	C10-C9-C11	2.85	120.06	115.27
16	AD	401	HEC	CAA-C2A-C1A	2.82	130.21	124.89
12	AC	403	3PE	C2-O21-C21	-2.82	110.85	117.79
17	AD	402	3PH	O31-C31-C32	2.81	120.74	111.91
16	Ad	401	HEC	CMB-C2B-C1B	2.81	129.32	125.04
11	AC	402	HEM	C4A-CHB-C1B	-2.80	119.69	126.34
15	Ac	407	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
16	Ad	401	HEC	CHD-C1D-C2D	-2.77	119.04	126.73
14	Ac	406	UQ6	C10-C9-C11	2.77	119.92	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Ac	406	UQ6	C4M-O4-C4	2.76	122.35	114.78
15	Ac	407	CDL	CB4-OB6-CB5	-2.75	111.01	117.79
14	AC	405	UQ6	C12-C13-C14	-2.75	121.03	127.66
11	AC	402	HEM	CHD-C1D-C2D	-2.74	120.69	124.98
16	AD	401	HEC	C4D-C3D-C2D	-2.73	102.92	106.90
16	Ad	401	HEC	CAA-CBA-CGA	-2.72	107.76	113.60
16	AD	401	HEC	C4A-C3A-C2A	-2.72	102.97	106.94
11	AC	401	HEM	CHD-C4C-NC	2.70	127.36	124.44
11	AC	402	HEM	CBD-CAD-C3D	-2.69	105.15	112.63
17	Ad	402	3PH	C2-O21-C21	-2.68	111.19	117.79
16	AD	401	HEC	CAC-C3C-C4C	2.67	128.62	124.92
14	Ac	406	UQ6	C6-C7-C8	-2.65	107.97	112.17
16	AD	401	HEC	CHB-C1B-C2B	-2.63	120.87	124.98
15	AC	406	CDL	OB8-CB7-C71	2.62	120.13	111.91
11	Ac	403	HEM	CBD-CAD-C3D	-2.60	105.41	112.63
11	Ac	403	HEM	CHD-C4C-NC	2.59	127.24	124.44
12	AC	403	3PE	O31-C31-C32	2.58	119.99	111.91
11	AC	401	HEM	C4D-ND-C1D	2.57	107.73	105.07
11	AC	401	HEM	CAA-CBA-CGA	-2.57	108.07	113.60
16	AD	401	HEC	CAD-C3D-C4D	2.57	129.15	124.66
11	Ac	403	HEM	CHA-C4D-C3D	-2.56	120.52	125.33
16	AD	401	HEC	CBC-CAC-C3C	2.56	119.48	112.43
11	Ac	403	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
14	Ac	406	UQ6	C17-C18-C19	-2.55	119.05	127.75
11	Ac	402	HEM	C4A-NA-C1A	2.55	107.84	105.35
12	Ac	404	3PE	O31-C31-C32	2.54	119.88	111.91
14	Ac	406	UQ6	C21-C19-C20	2.54	120.22	114.60
15	Ag	101	CDL	OA8-CA7-C31	2.54	119.87	111.91
16	AD	401	HEC	CMD-C2D-C1D	2.53	128.89	125.04
16	Ad	401	HEC	CMC-C2C-C3C	2.53	131.08	125.61
16	AD	401	HEC	CMB-C2B-C1B	2.53	128.89	125.04
15	Ag	101	CDL	CB4-OB6-CB5	-2.52	111.59	117.79
17	Ad	402	3PH	O31-C31-C32	2.52	119.81	111.91
12	AF	201	3PE	O31-C31-C32	2.49	119.73	111.91
11	Ac	402	HEM	C1A-CHA-C4D	-2.49	120.44	126.34
13	Ac	405	U10	C27-C28-C29	-2.48	119.27	127.75
11	AC	402	HEM	CHB-C4A-NA	2.47	128.40	123.85
14	AC	405	UQ6	C21-C19-C20	2.47	120.06	114.60
11	AC	401	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
13	AC	404	U10	C16-C14-C15	2.45	120.02	114.60
11	AC	402	HEM	C4A-NA-C1A	2.45	107.75	105.35
15	Ag	101	CDL	OB8-CB7-C71	2.45	119.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Ac	407	CDL	OA8-CA7-C31	2.45	119.59	111.91
13	AC	404	U10	C1M-C1-C6	-2.38	120.52	124.40
11	Ac	402	HEM	CHC-C1C-NC	2.38	127.01	124.44
17	AD	402	3PH	C2-O21-C21	-2.37	111.94	117.79
15	AC	406	CDL	OA8-CA7-C31	2.37	119.34	111.91
11	AC	401	HEM	CHA-C4D-C3D	-2.37	120.88	125.33
14	AC	405	UQ6	C4M-O4-C4	2.36	121.25	114.78
11	Ac	402	HEM	CHC-C4B-C3B	-2.35	120.07	125.13
15	AC	406	CDL	CB4-OB6-CB5	-2.32	112.07	117.79
11	Ac	402	HEM	CHA-C4D-C3D	-2.32	120.97	125.33
11	Ac	403	HEM	CHB-C1B-C2B	-2.32	120.29	126.73
11	Ac	402	HEM	CHB-C1B-NB	2.31	127.23	124.37
16	Ad	401	HEC	CMA-C3A-C4A	2.31	128.78	124.71
14	AC	405	UQ6	C7-C6-C5	-2.30	117.80	120.82
13	Ac	405	U10	C31-C29-C30	2.30	119.68	114.60
11	Ac	403	HEM	C4D-ND-C1D	2.28	107.43	105.07
16	AD	401	HEC	C3C-C4C-NC	2.27	112.68	110.15
11	Ac	402	HEM	CHA-C1A-NA	2.27	128.02	123.85
11	Ac	403	HEM	C1A-CHA-C4D	-2.25	120.99	126.34
16	AD	401	HEC	CHB-C1B-NB	-2.24	121.98	124.42
13	AC	404	U10	C12-C13-C14	-2.23	120.11	127.75
14	AC	405	UQ6	C17-C18-C19	-2.23	120.11	127.75
16	AD	401	HEC	CMA-C3A-C4A	2.19	128.57	124.71
11	AC	402	HEM	C4C-CHD-C1D	-2.17	121.38	126.06
16	Ad	401	HEC	CHC-C1C-C2C	-2.17	121.11	127.24
11	AC	401	HEM	CHB-C1B-C2B	-2.17	120.71	126.73
16	Ad	401	HEC	CMD-C2D-C3D	2.16	131.99	126.12
16	AD	401	HEC	CBD-CAD-C3D	-2.15	106.65	112.63
15	AC	406	CDL	CA4-OA6-CA5	-2.14	112.52	117.79
14	AC	405	UQ6	C1M-C1-C6	-2.11	117.37	120.42
15	Ac	407	CDL	OB6-CB5-OB7	-2.10	118.62	123.70
12	Ag	102	3PE	C2-O21-C21	-2.09	112.63	117.79
11	AC	402	HEM	C1C-CHC-C4B	-2.09	121.54	126.06
13	Ac	405	U10	C7-C6-C5	2.09	121.00	118.48
13	Ac	405	U10	C25-C24-C26	2.09	118.78	115.27
16	Ad	401	HEC	CHA-C1A-C2A	-2.09	121.56	124.94
14	AC	405	UQ6	C1M-C1-C2	2.08	124.03	120.50
11	AC	402	HEM	C1A-CHA-C4D	-2.08	121.41	126.34
14	Ac	406	UQ6	C7-C6-C5	-2.08	118.09	120.82
11	AC	402	HEM	CMB-C2B-C1B	2.08	128.20	125.04
11	AC	402	HEM	CAA-CBA-CGA	-2.07	109.15	113.60
16	AD	401	HEC	C4B-NB-C1B	-2.07	102.94	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AD	401	HEC	CHA-C1A-NA	-2.06	122.21	124.44
12	Ac	404	3PE	O21-C21-O22	-2.06	118.73	123.70
11	AC	401	HEM	C4C-CHD-C1D	-2.05	121.63	126.06
14	Ac	406	UQ6	C3M-O3-C3	2.04	120.38	114.78
14	Ac	406	UQ6	C17-C16-C14	-2.04	106.26	112.98
13	Ac	405	U10	C7-C8-C9	-2.04	123.40	126.79
11	AC	402	HEM	C2A-C1A-NA	-2.03	107.87	110.15
16	AD	401	HEC	CHA-C4D-C3D	-2.03	121.85	124.84
12	Ag	102	3PE	O31-C31-O32	-2.01	118.52	123.59
11	AC	401	HEM	C4A-CHB-C1B	-2.01	121.58	126.34

All (2) chirality outliers are listed below:

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

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	401	HEM	C2C-C3C-CAC-CBC
11	AC	402	HEM	C2B-C3B-CAB-CBB
11	AC	402	HEM	C4B-C3B-CAB-CBB
11	Ac	402	HEM	C2C-C3C-CAC-CBC
11	Ac	403	HEM	C2B-C3B-CAB-CBB
11	Ac	403	HEM	C4B-C3B-CAB-CBB
12	AC	403	3PE	C1-O11-P-O12
12	AC	403	3PE	C1-O11-P-O13
12	AC	403	3PE	C1-O11-P-O14
12	AC	403	3PE	C11-O13-P-O12
12	AC	403	3PE	C11-O13-P-O14
12	Ac	401	3PE	C1-O11-P-O12
12	Ac	401	3PE	C22-C21-O21-C2
12	Ag	102	3PE	C11-O13-P-O11
12	Ag	102	3PE	C11-O13-P-O12
12	Ag	102	3PE	C11-O13-P-O14
13	Ac	405	U10	C5-C6-C7-C8
14	AC	405	UQ6	C13-C14-C16-C17
14	AC	405	UQ6	C15-C14-C16-C17
14	Ac	406	UQ6	C1-C6-C7-C8
14	Ac	406	UQ6	C13-C14-C16-C17
14	Ac	406	UQ6	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
15	AC	406	CDL	CA2-OA2-PA1-OA4
15	AC	406	CDL	CA3-OA5-PA1-OA3
15	AC	406	CDL	CA3-OA5-PA1-OA4
15	AC	406	CDL	C31-CA7-OA8-CA6
15	Aa	501	CDL	CA3-OA5-PA1-OA2
15	Aa	501	CDL	CB4-CB3-OB5-PB2
15	Ac	407	CDL	CB2-OB2-PB2-OB3
15	Ac	407	CDL	CB2-OB2-PB2-OB4
15	Ac	407	CDL	CB2-OB2-PB2-OB5
15	Ac	407	CDL	CB3-OB5-PB2-OB3
15	Ag	101	CDL	C1-CB2-OB2-PB2
15	Ag	101	CDL	CB2-OB2-PB2-OB5
15	Ag	101	CDL	CB3-OB5-PB2-OB2
15	Ag	101	CDL	CB3-OB5-PB2-OB3
15	Ag	101	CDL	CB3-OB5-PB2-OB4
17	Ad	402	3PH	C22-C21-O21-C2
15	AC	406	CDL	OA9-CA7-OA8-CA6
16	AD	401	HEC	C2B-C3B-CAB-CBB
16	AD	401	HEC	C4B-C3B-CAB-CBB
16	Ad	401	HEC	C2B-C3B-CAB-CBB
16	Ad	401	HEC	C4B-C3B-CAB-CBB
12	AF	201	3PE	O32-C31-O31-C3
16	AD	401	HEC	C4C-C3C-CAC-CBC
16	Ad	401	HEC	C4C-C3C-CAC-CBC
16	AD	401	HEC	C2C-C3C-CAC-CBC
16	Ad	401	HEC	C2C-C3C-CAC-CBC
12	Ac	401	3PE	O22-C21-O21-C2
15	AC	406	CDL	OA7-CA5-OA6-CA4
17	Ad	402	3PH	O22-C21-O21-C2
13	Ac	405	U10	C25-C24-C26-C27
12	AF	201	3PE	C32-C31-O31-C3
12	AC	403	3PE	O32-C31-O31-C3
12	AC	403	3PE	C32-C31-O31-C3
15	AC	406	CDL	C11-CA5-OA6-CA4
15	Ag	101	CDL	CB4-CB3-OB5-PB2
15	AC	406	CDL	OB9-CB7-OB8-CB6
15	AC	406	CDL	C71-CB7-OB8-CB6
15	Aa	501	CDL	CA2-C1-CB2-OB2
15	Aa	501	CDL	O1-C1-CB2-OB2
17	AD	402	3PH	O21-C2-C3-O31
15	Ag	101	CDL	C31-CA7-OA8-CA6
11	Ac	403	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
14	Ac	406	UQ6	C9-C11-C12-C13
15	Ag	101	CDL	OA9-CA7-OA8-CA6
12	AC	403	3PE	C11-O13-P-O11
12	AF	201	3PE	C1-O11-P-O13
12	AF	201	3PE	C11-O13-P-O11
15	AC	406	CDL	CA2-OA2-PA1-OA5
15	AC	406	CDL	CA3-OA5-PA1-OA2
15	AC	406	CDL	CB2-OB2-PB2-OB5
15	Ac	407	CDL	CB3-OB5-PB2-OB2
13	Ac	405	U10	C23-C24-C26-C27
15	Aa	501	CDL	C11-CA5-OA6-CA4
12	AF	201	3PE	C34-C35-C36-C37
15	Aa	501	CDL	OA7-CA5-OA6-CA4
13	Ac	405	U10	C12-C11-C9-C10
13	Ac	405	U10	C20-C19-C21-C22
13	Ac	405	U10	C12-C11-C9-C8
15	Ag	101	CDL	C74-C75-C76-C77
11	Ac	402	HEM	C2A-CAA-CBA-CGA
11	Ac	403	HEM	C2A-CAA-CBA-CGA
13	Ac	405	U10	C18-C19-C21-C22
12	Ac	401	3PE	O21-C21-C22-C23
15	Aa	501	CDL	C72-C71-CB7-OB8
12	Ac	404	3PE	C32-C31-O31-C3
11	AC	402	HEM	C2C-C3C-CAC-CBC
11	AC	401	HEM	C4C-C3C-CAC-CBC
11	Ac	402	HEM	C4C-C3C-CAC-CBC
15	AC	406	CDL	OB6-CB4-CB6-OB8
17	Ad	402	3PH	C25-C26-C27-C28
12	AC	403	3PE	C22-C21-O21-C2
12	Ac	404	3PE	C22-C21-O21-C2
12	AC	403	3PE	C22-C23-C24-C25
16	AD	401	HEC	C2A-CAA-CBA-CGA
17	AD	402	3PH	C1-C2-C3-O31
17	Ad	402	3PH	C1-C2-C3-O31
16	AD	401	HEC	C1A-C2A-CAA-CBA
13	Ac	405	U10	C1-C6-C7-C8
12	Ac	404	3PE	O32-C31-O31-C3
15	AC	406	CDL	CA6-CA4-OA6-CA5
12	AC	403	3PE	O22-C21-O21-C2
17	AD	402	3PH	C32-C31-O31-C3
15	AC	406	CDL	CB3-CB4-CB6-OB8
12	Ag	102	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
17	Ad	402	3PH	O21-C2-C3-O31
12	Ac	404	3PE	O22-C21-O21-C2
15	Aa	501	CDL	C1-CB2-OB2-PB2
16	AD	401	HEC	C3A-C2A-CAA-CBA
14	Ac	406	UQ6	C5-C6-C7-C8
15	Ac	407	CDL	C51-CB5-OB6-CB4
11	AC	401	HEM	C2B-C3B-CAB-CBB
11	Ac	403	HEM	C2C-C3C-CAC-CBC
11	AC	402	HEM	C4C-C3C-CAC-CBC
17	AD	402	3PH	O32-C31-O31-C3
12	Ag	102	3PE	O32-C31-O31-C3
15	Ac	407	CDL	OB7-CB5-OB6-CB4
12	Ac	404	3PE	C23-C24-C25-C26
17	Ad	402	3PH	C2-C3-O31-C31
12	Ac	401	3PE	C1-O11-P-O13
15	AC	406	CDL	CA4-CA3-OA5-PA1
12	AF	201	3PE	C1-O11-P-O14
12	AF	201	3PE	C11-O13-P-O12
12	AF	201	3PE	C11-O13-P-O14
12	Ac	401	3PE	C1-O11-P-O14
15	AC	406	CDL	CB2-OB2-PB2-OB3
15	Aa	501	CDL	CA3-OA5-PA1-OA4
15	Ac	407	CDL	CB3-OB5-PB2-OB4
15	Ag	101	CDL	CB2-OB2-PB2-OB4
15	Ag	101	CDL	C54-C55-C56-C57
12	AF	201	3PE	C35-C36-C37-C38
12	Ac	401	3PE	C2-C1-O11-P
14	Ac	406	UQ6	C3-C4-O4-C4M
17	AD	402	3PH	C2-C3-O31-C31
15	AC	406	CDL	CB4-CB3-OB5-PB2
15	Ac	407	CDL	C1-CA2-OA2-PA1
16	Ad	401	HEC	C3D-CAD-CBD-CGD
11	Ac	403	HEM	CAD-CBD-CGD-O1D
17	AD	402	3PH	C25-C26-C27-C28
11	Ac	403	HEM	C4C-C3C-CAC-CBC
15	Aa	501	CDL	CA4-CA6-OA8-CA7
11	AC	401	HEM	CAD-CBD-CGD-O2D
11	AC	401	HEM	CAD-CBD-CGD-O1D
15	Aa	501	CDL	C33-C34-C35-C36
12	AC	403	3PE	C24-C25-C26-C27
11	AC	402	HEM	CAD-CBD-CGD-O2D
11	Ac	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	Aa	501	CDL	CA6-CA4-OA6-CA5
11	AC	401	HEM	CAA-CBA-CGA-O1A
11	AC	402	HEM	CAD-CBD-CGD-O1D
11	AC	401	HEM	CAA-CBA-CGA-O2A
11	Ac	403	HEM	CAD-CBD-CGD-O2D
17	Ad	402	3PH	C37-C38-C39-C3A
11	Ac	402	HEM	CAD-CBD-CGD-O2D
15	Ag	101	CDL	C11-C12-C13-C14
17	AD	402	3PH	C1-O11-P-O13
12	Ac	401	3PE	C1-C2-O21-C21
13	Ac	405	U10	C5-C4-O4-C4M
14	AC	405	UQ6	C14-C16-C17-C18
17	AD	402	3PH	O22-C21-O21-C2
12	Ac	404	3PE	O21-C21-C22-C23
11	AC	401	HEM	C4B-C3B-CAB-CBB
11	Ac	403	HEM	CAA-CBA-CGA-O1A
15	Aa	501	CDL	C72-C71-CB7-OB9
11	Ac	403	HEM	CAA-CBA-CGA-O2A
14	Ac	406	UQ6	C5-C4-O4-C4M
12	Ac	404	3PE	O22-C21-C22-C23
12	Ac	401	3PE	O22-C21-C22-C23
15	Ac	407	CDL	C71-CB7-OB8-CB6
15	Aa	501	CDL	O1-C1-CA2-OA2
12	Ac	404	3PE	C2-C3-O31-C31
15	Aa	501	CDL	CB3-OB5-PB2-OB3
12	Ac	401	3PE	C3-C2-O21-C21
17	Ad	402	3PH	C23-C24-C25-C26
16	Ad	401	HEC	C2D-C3D-CAD-CBD
15	Ac	407	CDL	OB9-CB7-OB8-CB6
16	Ad	401	HEC	CAA-CBA-CGA-O2A
15	Aa	501	CDL	C12-C11-CA5-OA6

There are no ring outliers.

21 monomers are involved in 187 short contacts:

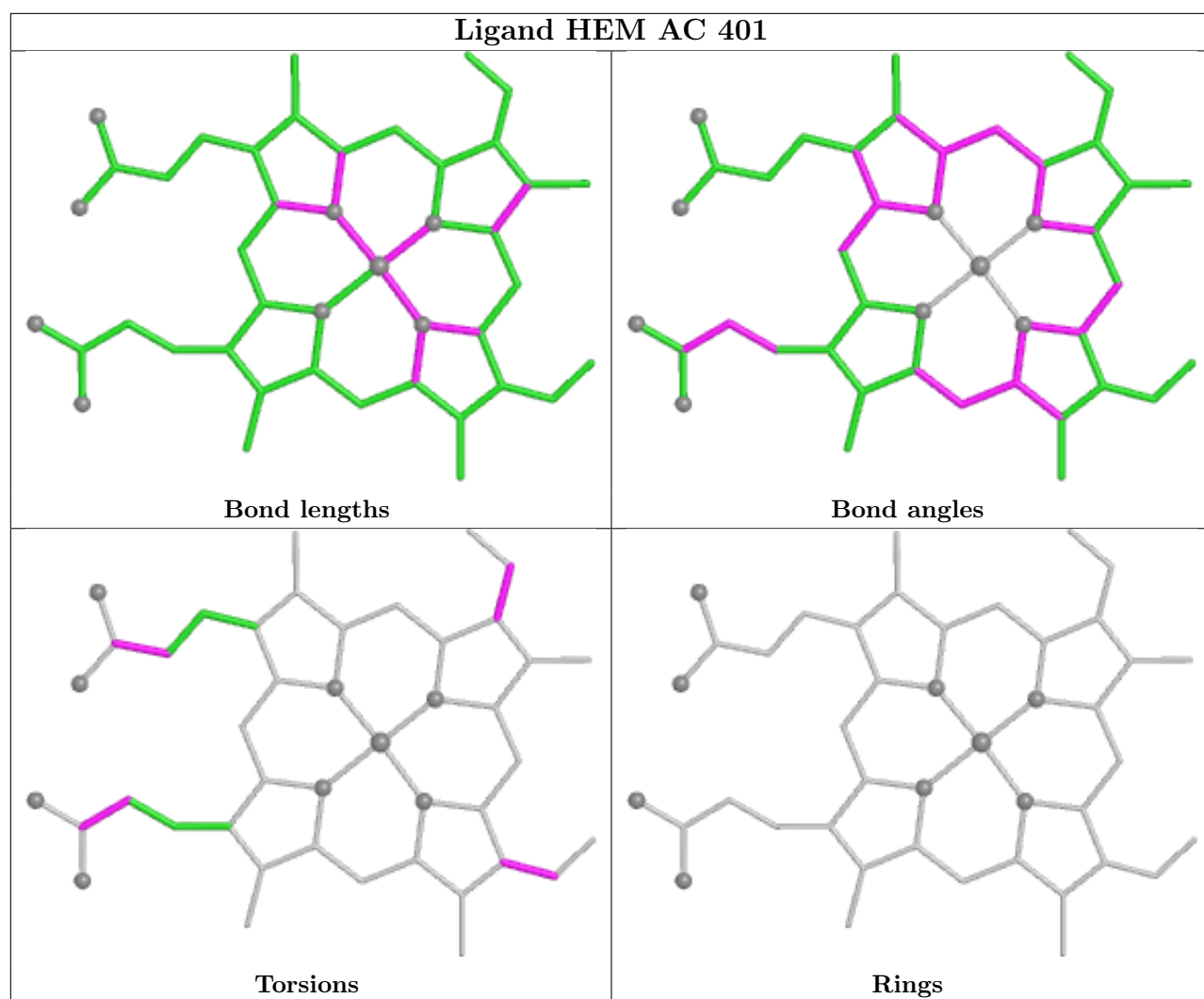
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AC	401	HEM	3	0
16	AD	401	HEC	24	0
15	AC	406	CDL	4	0
17	AD	402	3PH	13	0
12	AC	403	3PE	12	0
11	Ac	402	HEM	3	0

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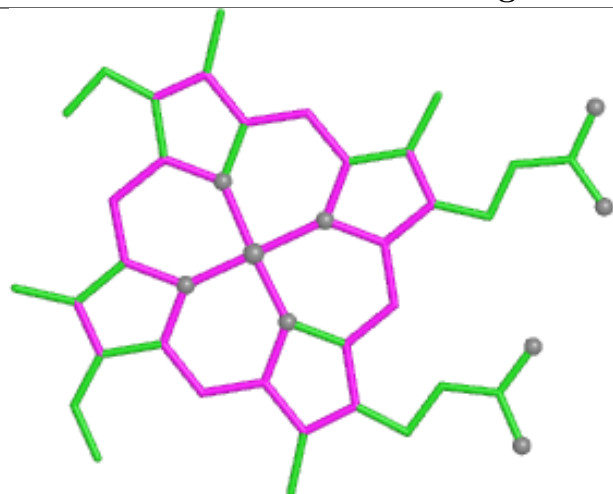
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Ac	407	CDL	3	0
13	Ac	405	U10	5	0
12	Ag	102	3PE	9	0
17	Ad	402	3PH	19	0
12	AF	201	3PE	7	0
11	AC	402	HEM	4	0
15	Ag	101	CDL	9	0
15	Aa	501	CDL	8	0
11	Ac	403	HEM	6	0
16	Ad	401	HEC	25	0
12	Ac	404	3PE	3	0
13	AC	404	U10	4	0
14	AC	405	UQ6	14	0
14	Ac	406	UQ6	12	0
12	Ac	401	3PE	3	0

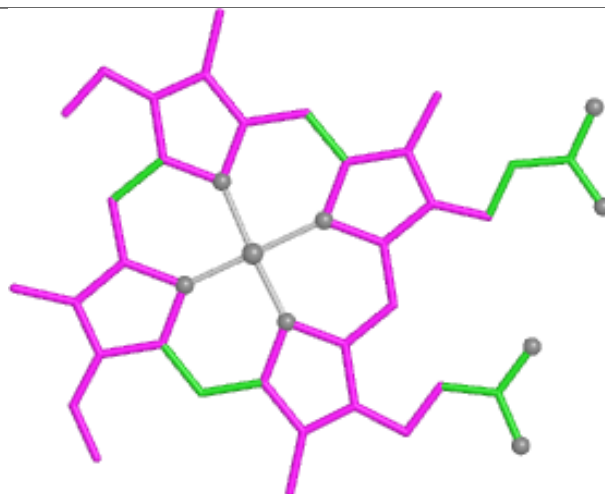
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



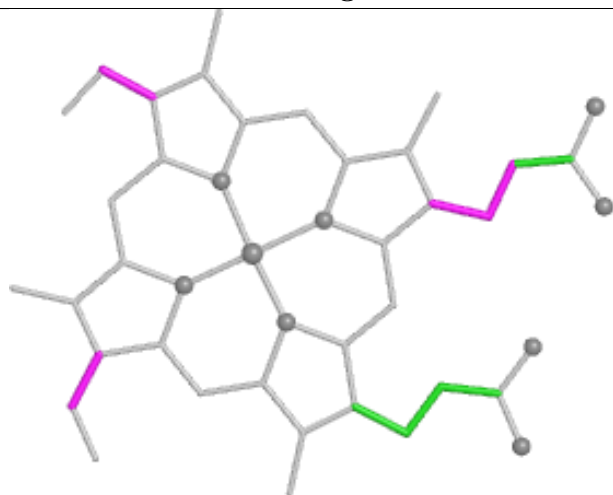
Ligand HEC AD 401



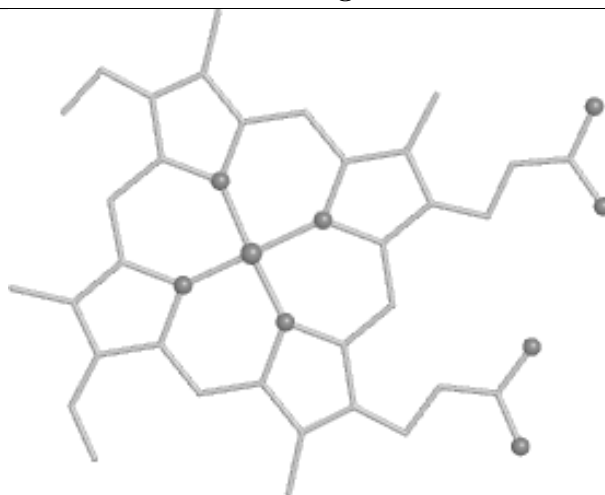
Bond lengths



Bond angles

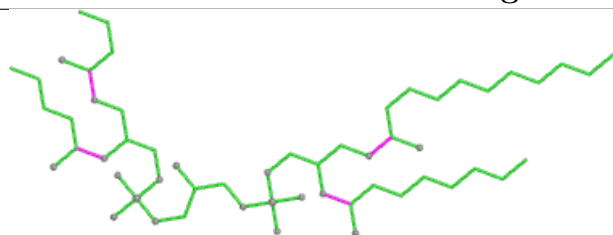


Torsions

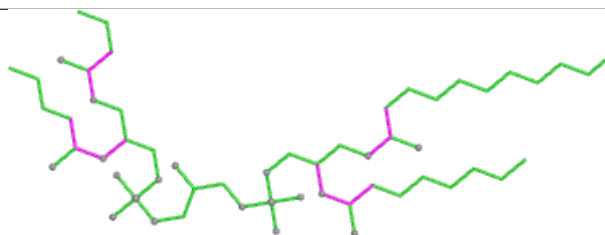


Rings

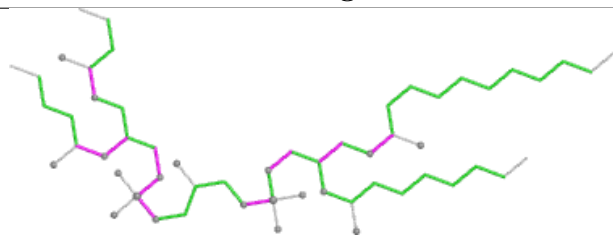
Ligand CDL AC 406



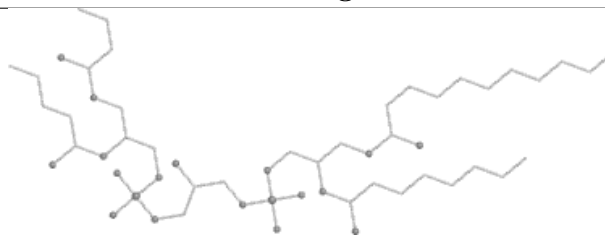
Bond lengths



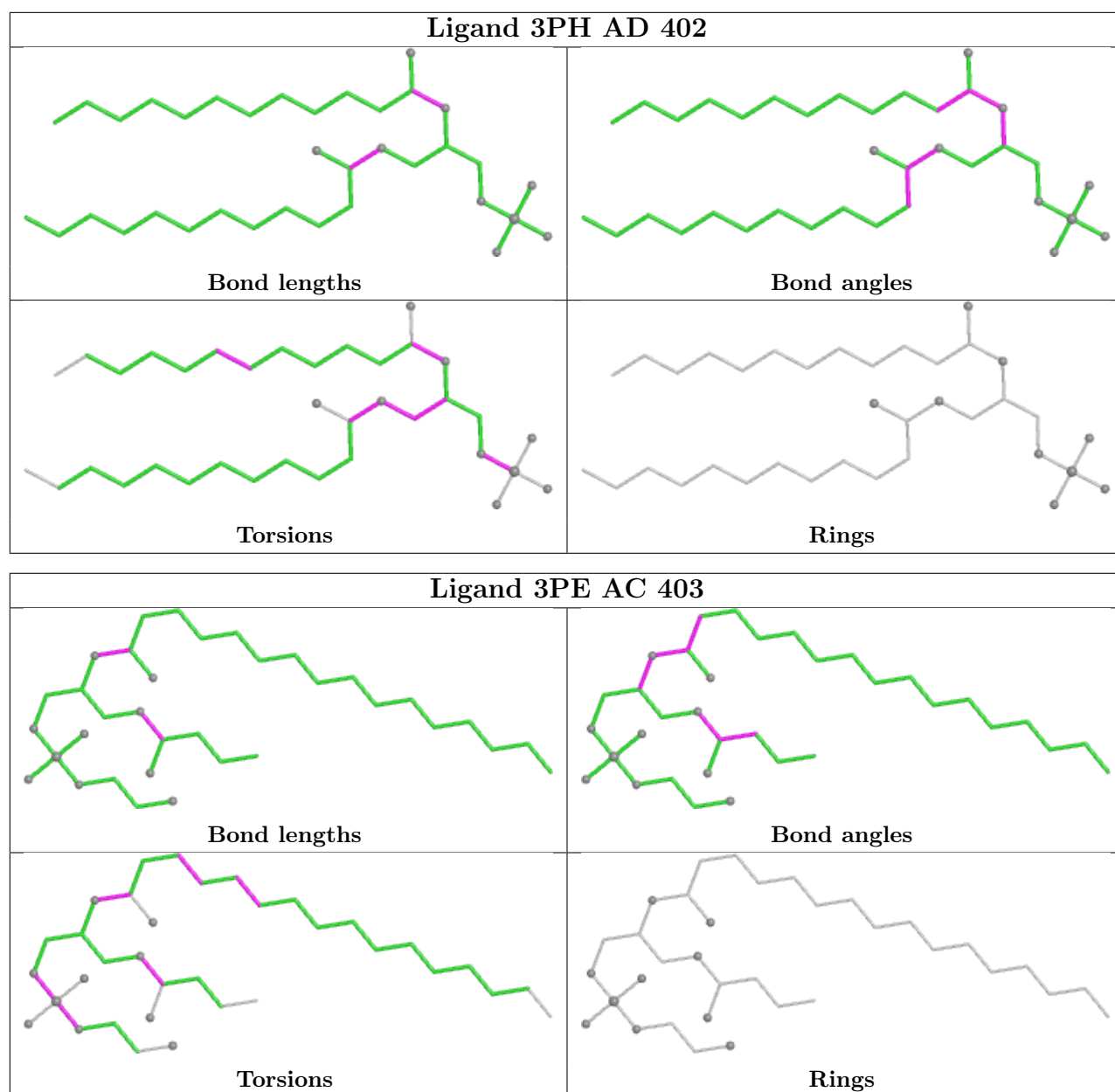
Bond angles

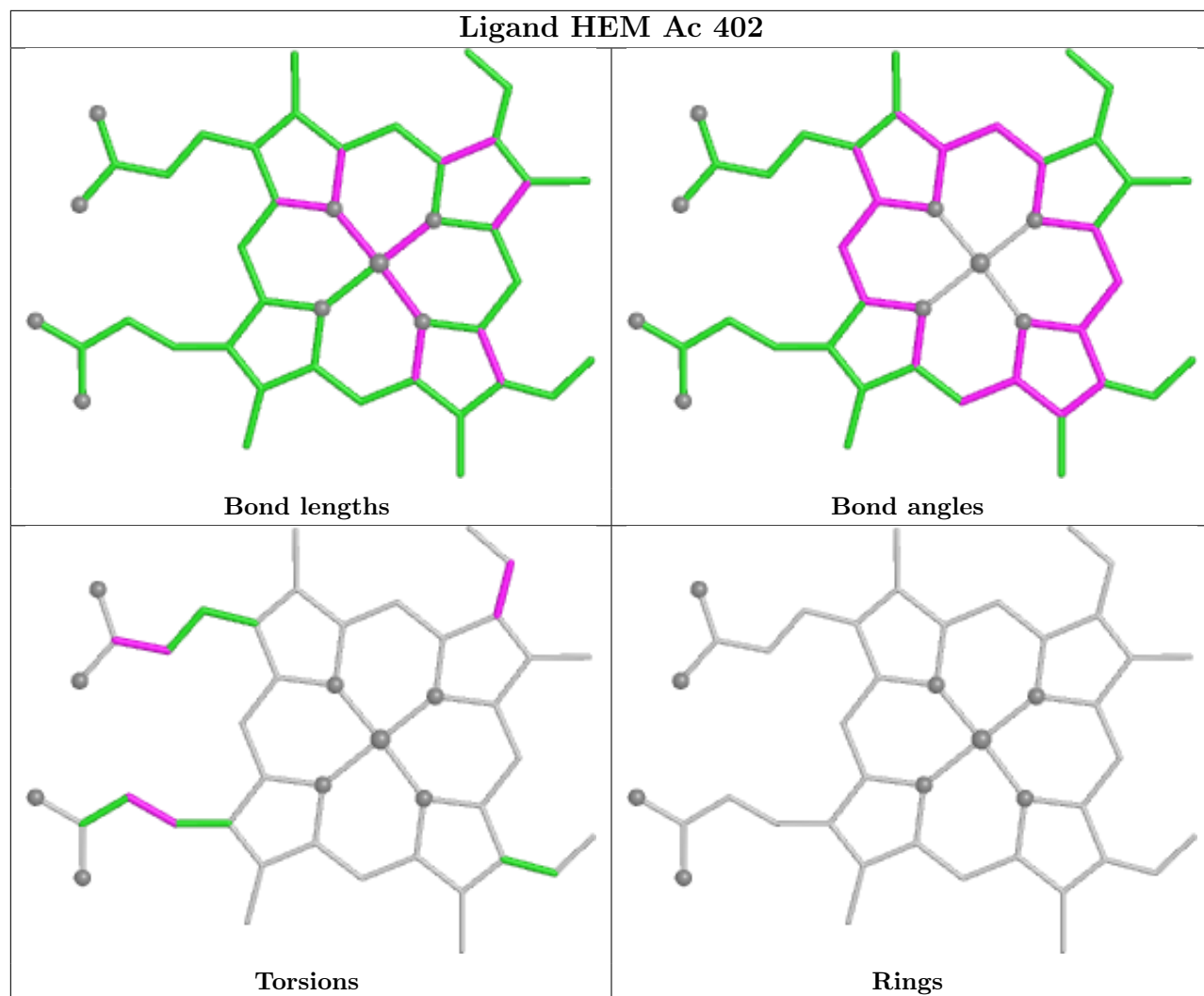


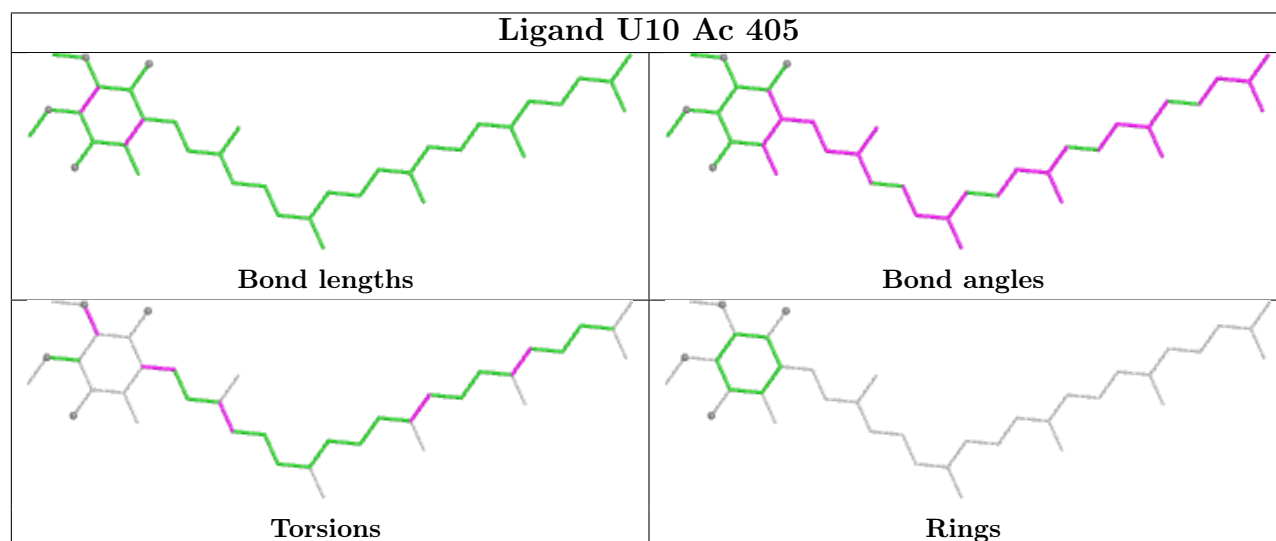
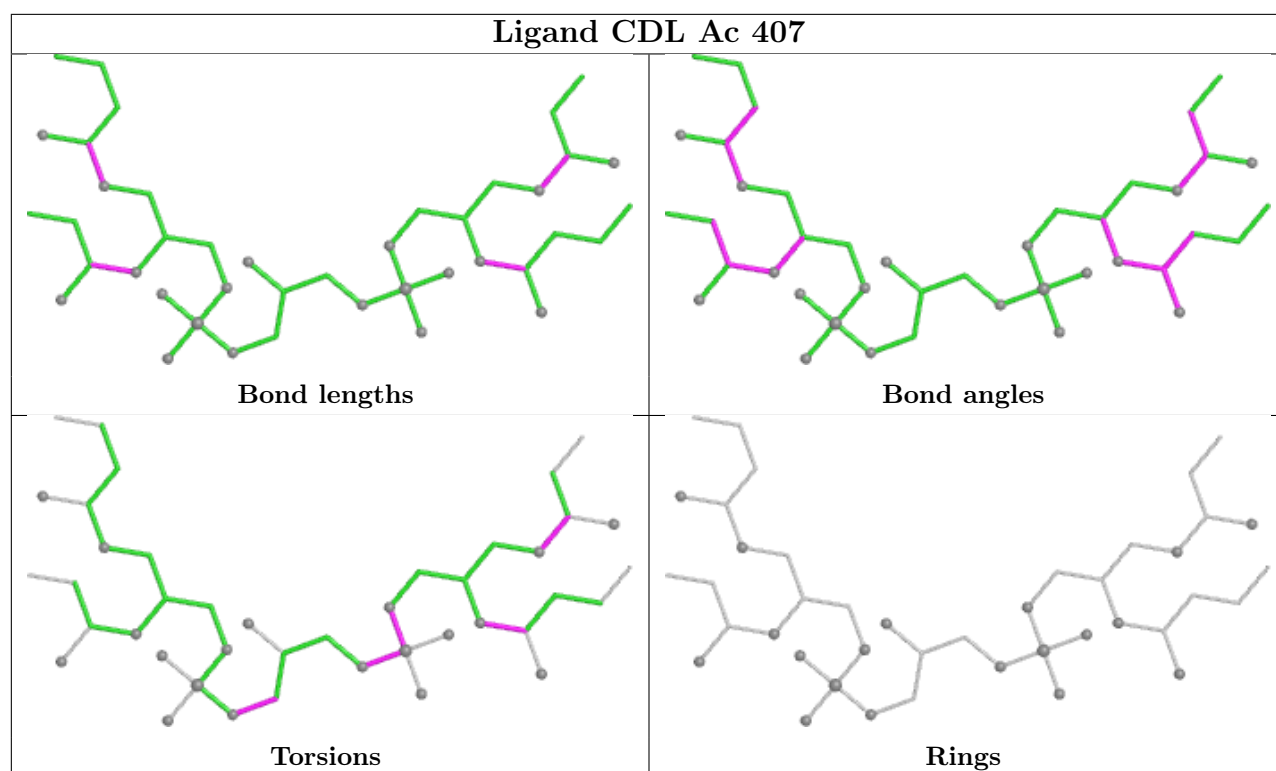
Torsions

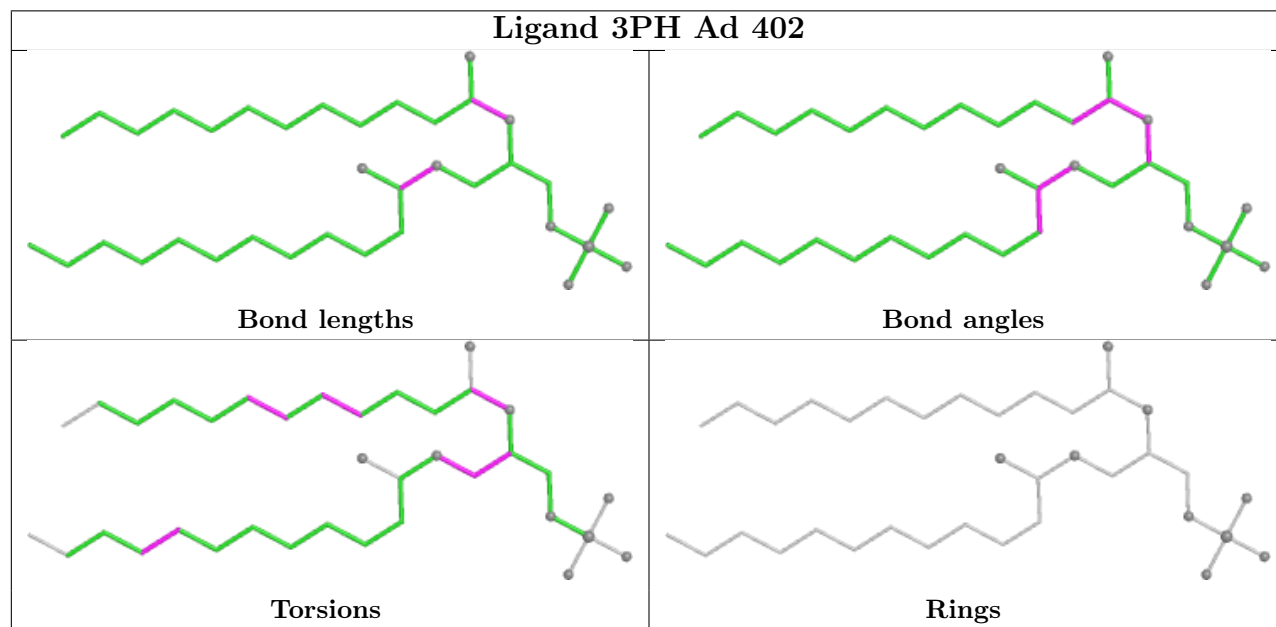
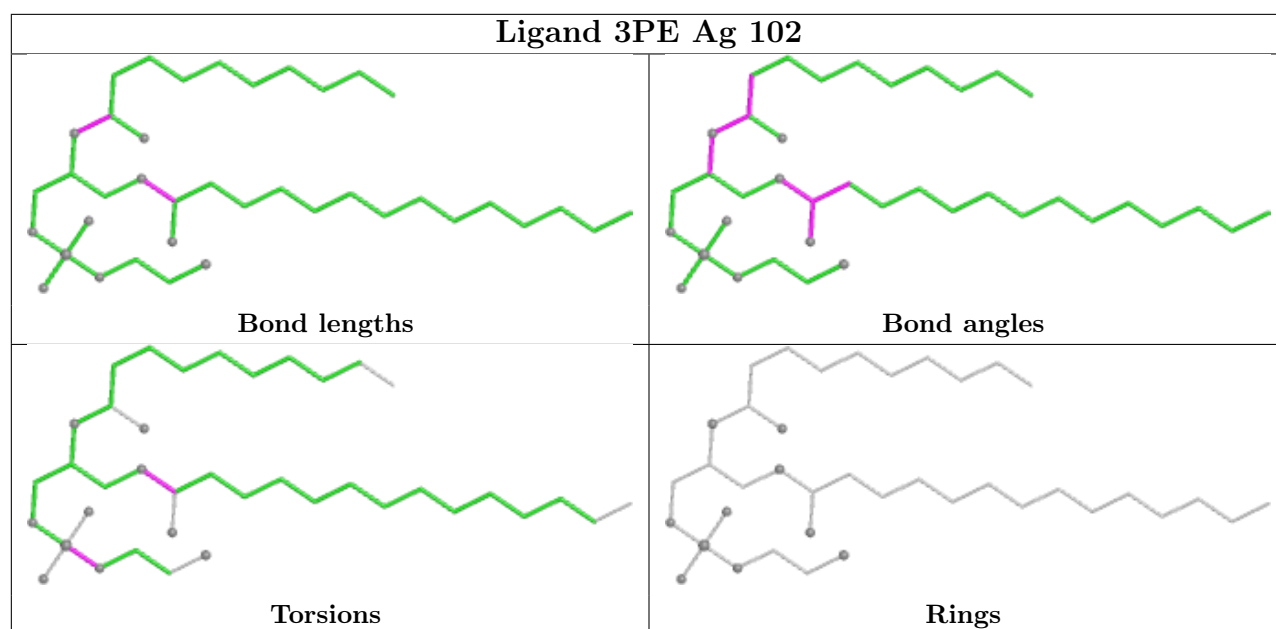


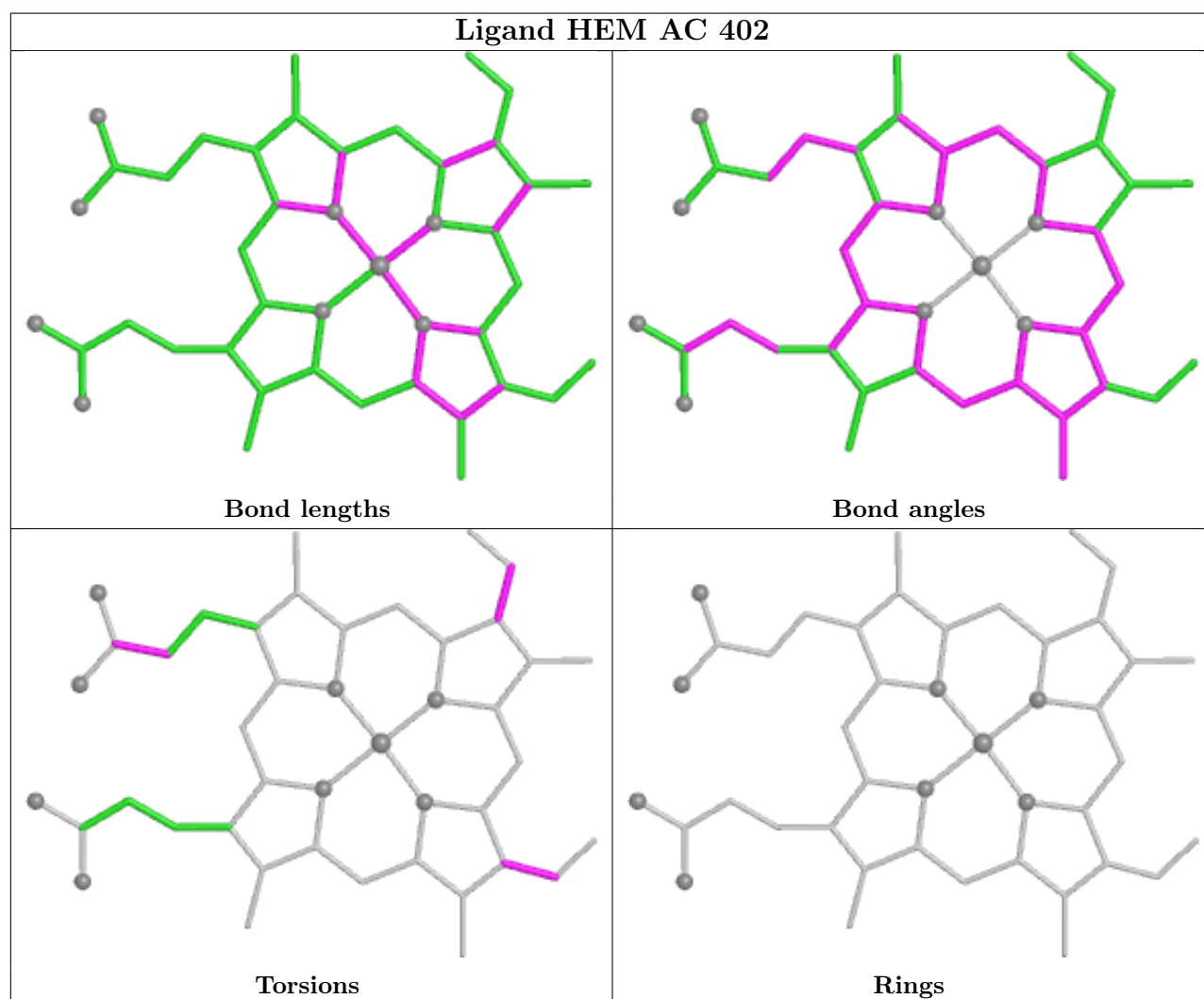
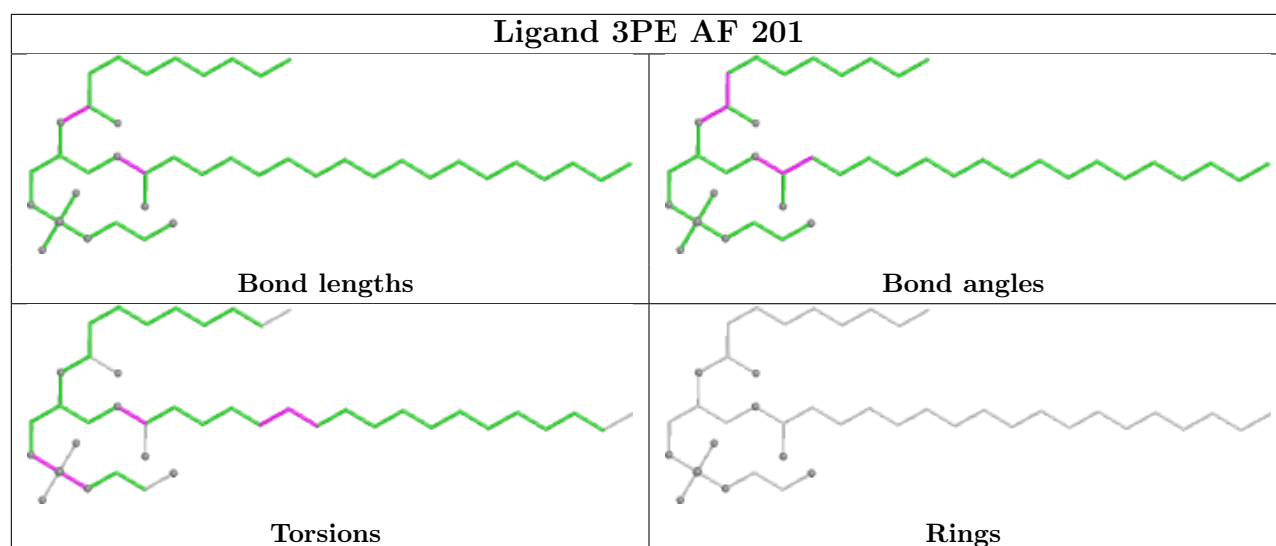
Rings

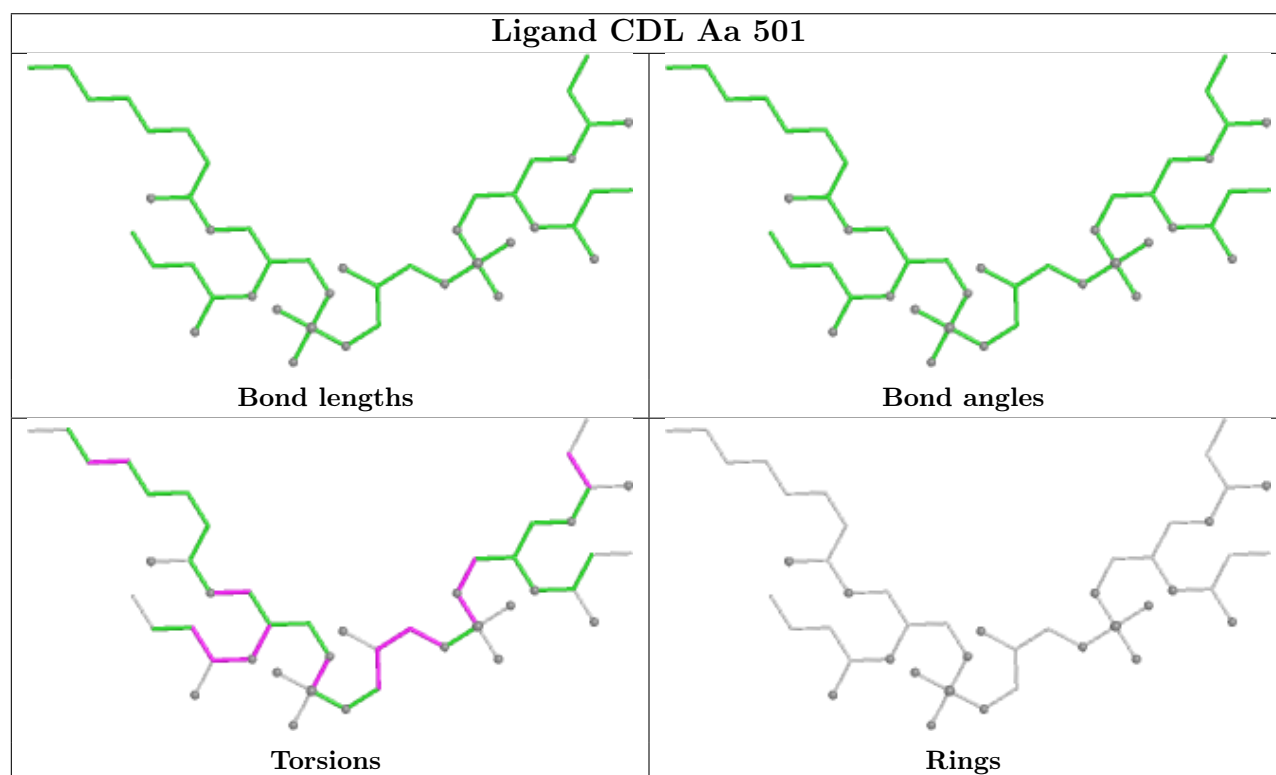
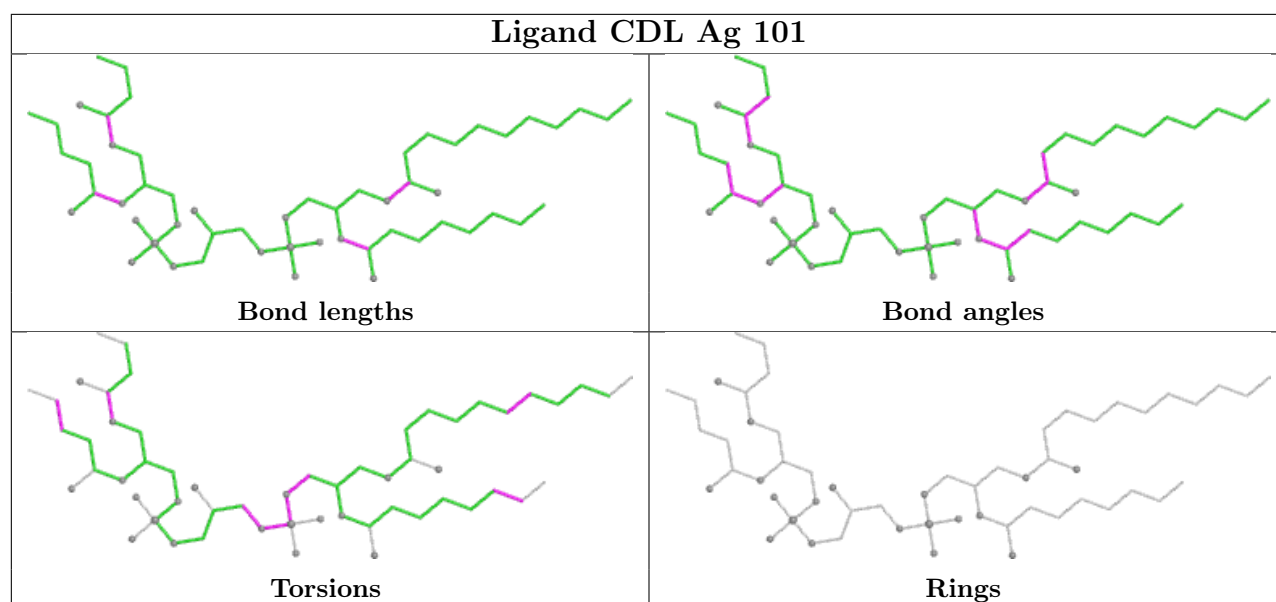


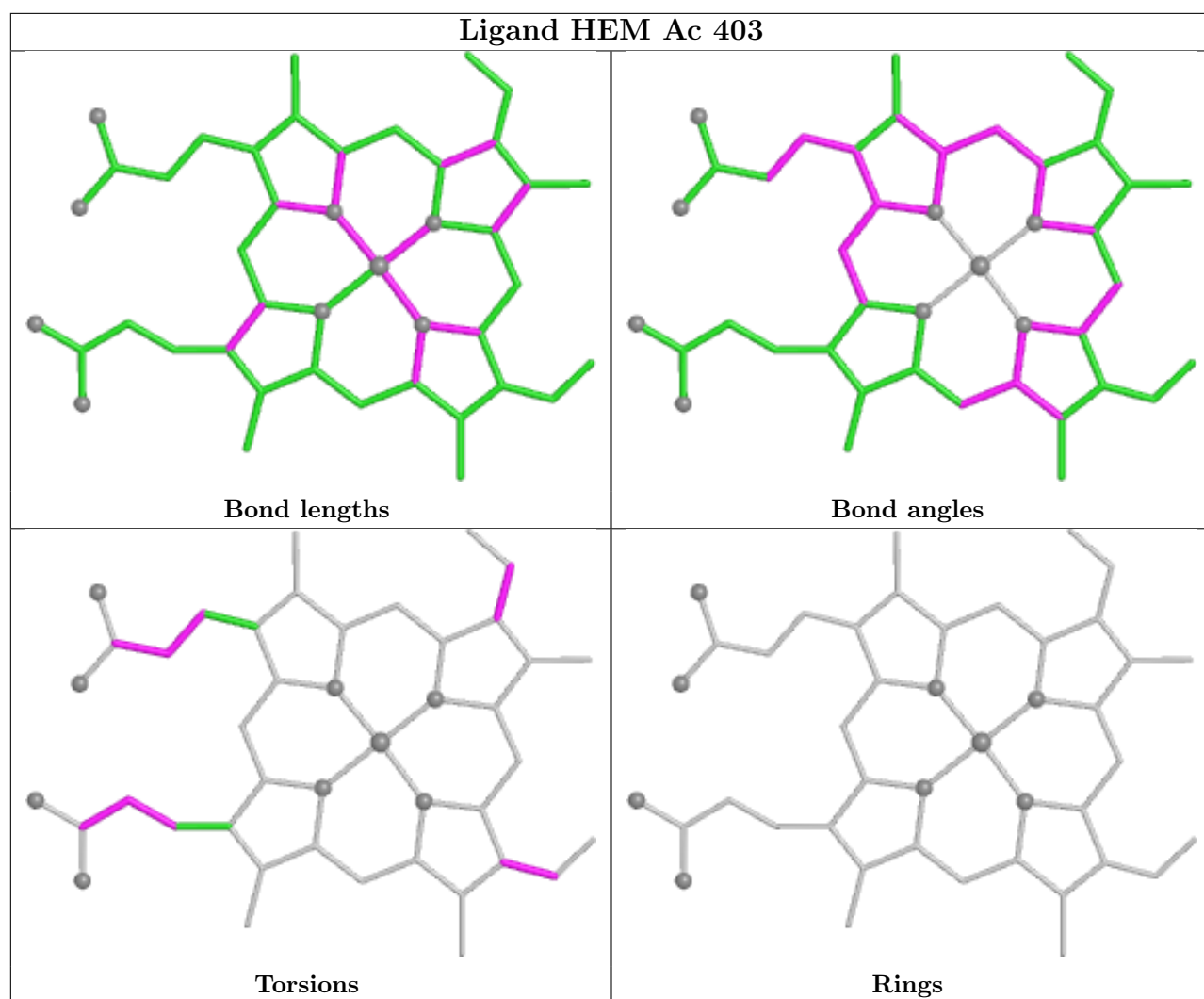




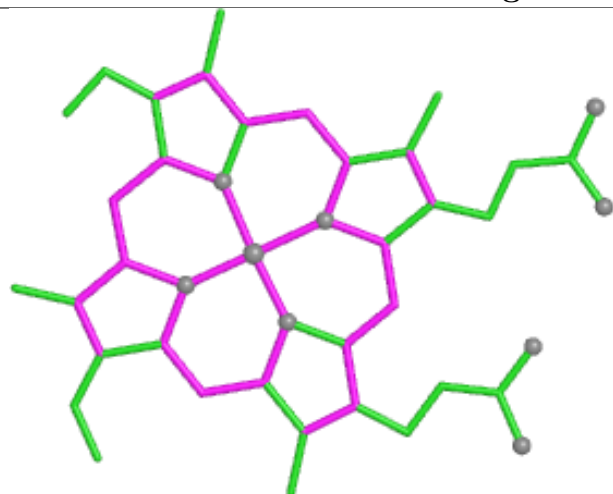




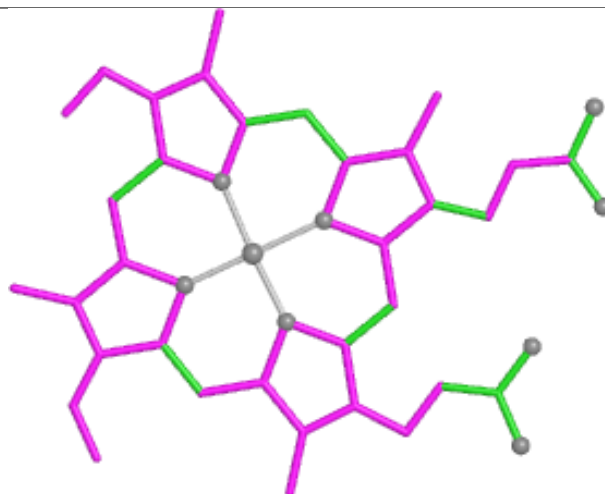




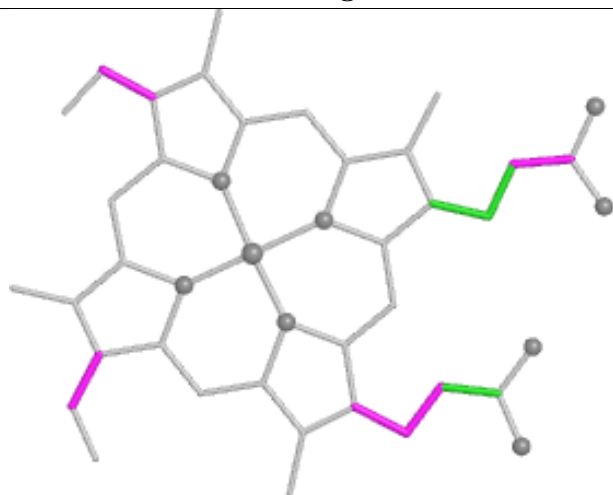
Ligand HEC Ad 401



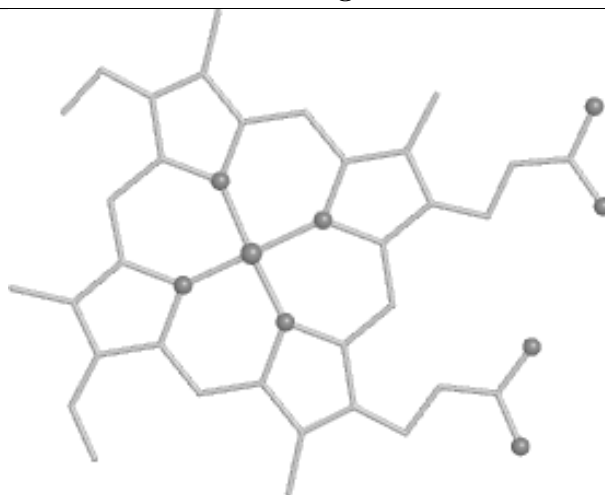
Bond lengths



Bond angles

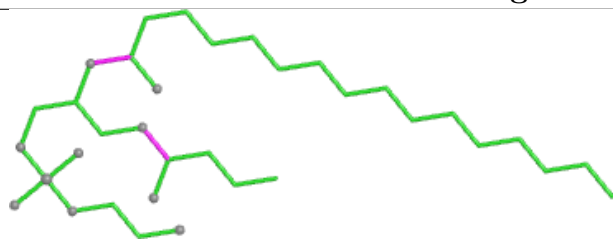


Torsions

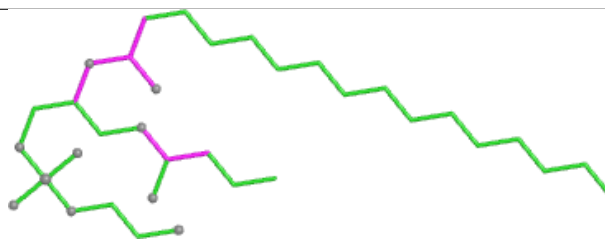


Rings

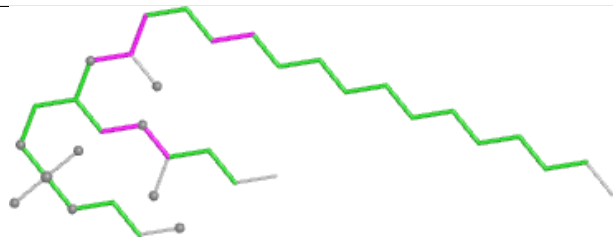
Ligand 3PE Ac 404



Bond lengths



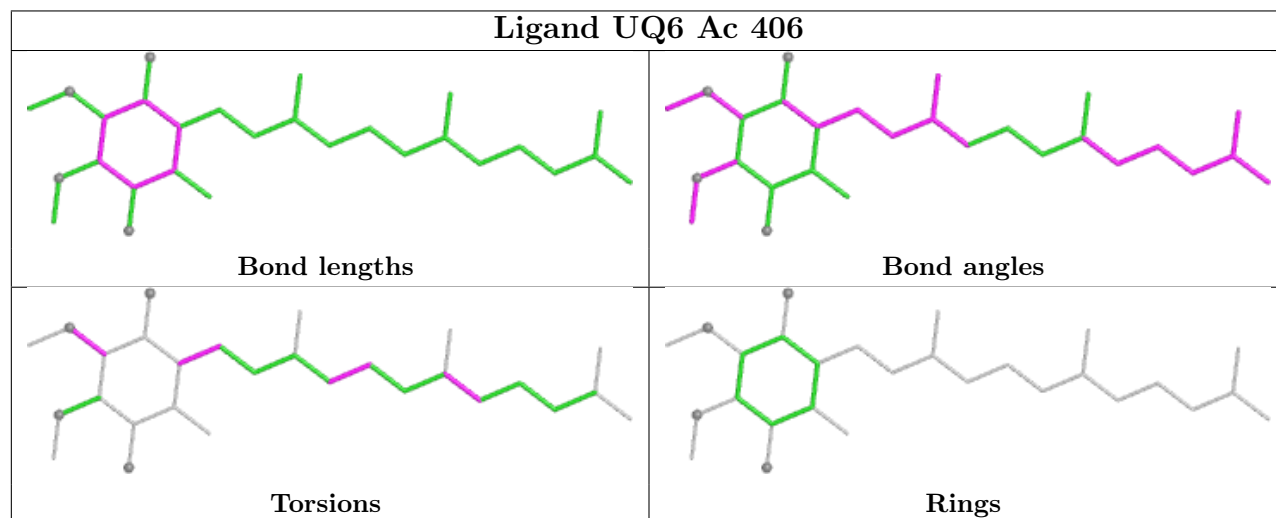
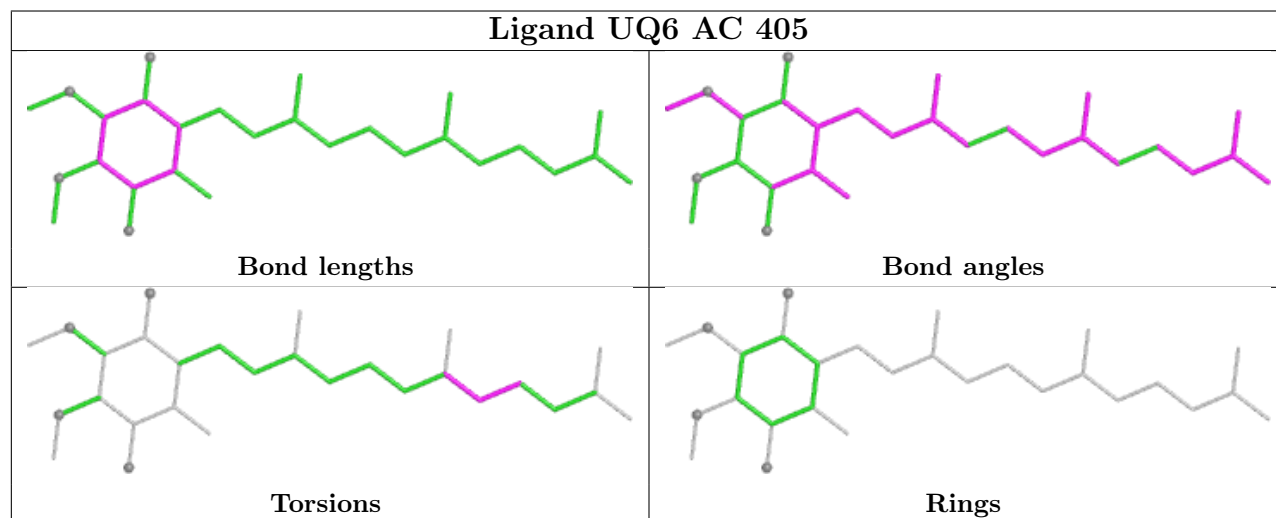
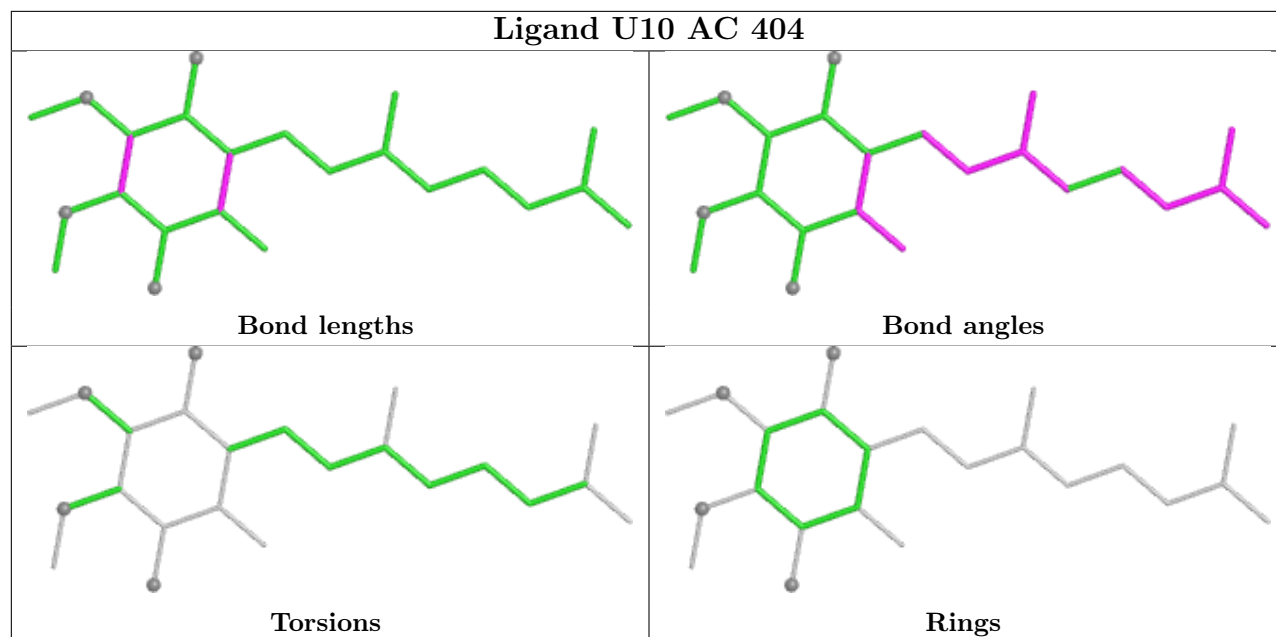
Bond angles

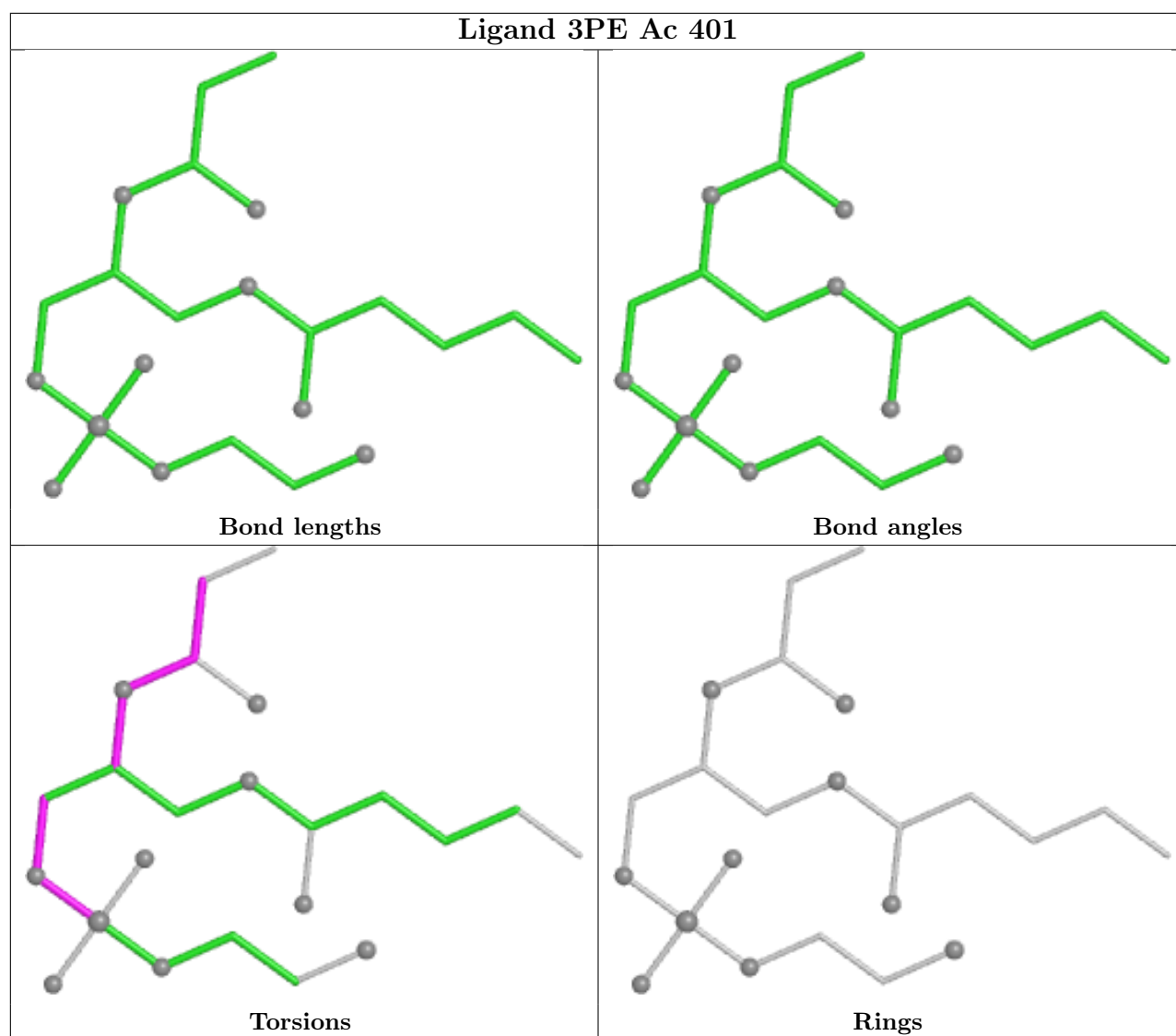


Torsions



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.

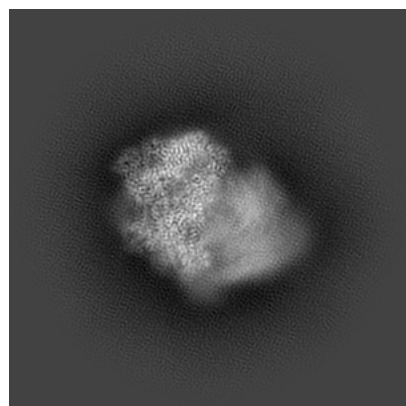
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35334. These allow visual inspection of the internal detail of the map and identification of artifacts.

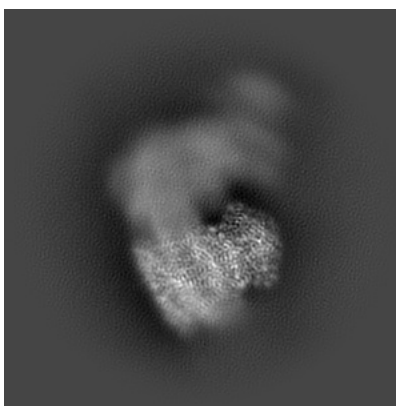
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

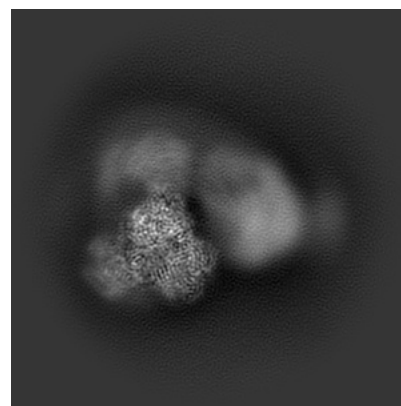
6.1.1 Primary map



X

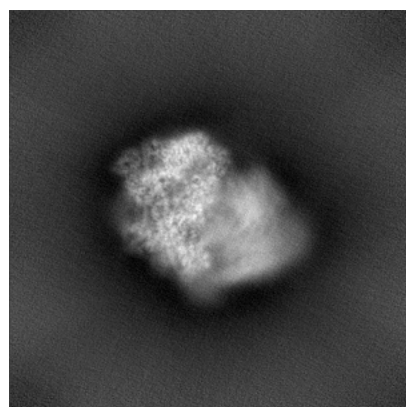


Y

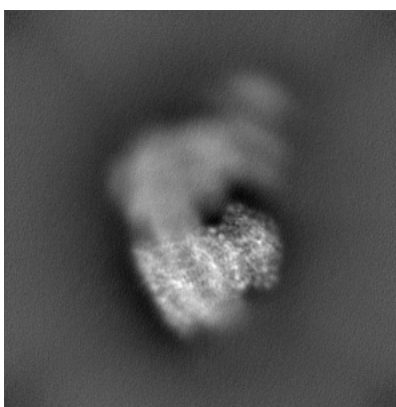


Z

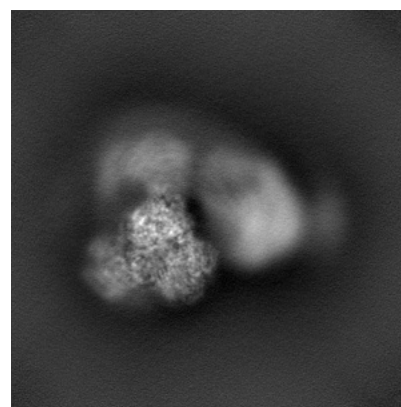
6.1.2 Raw map



X



Y

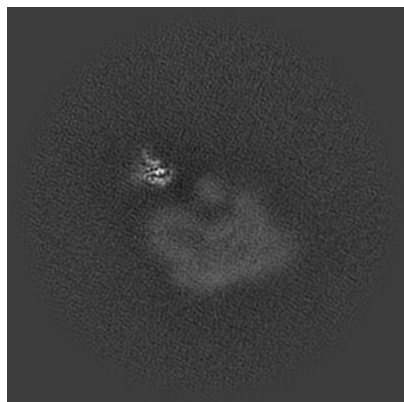


Z

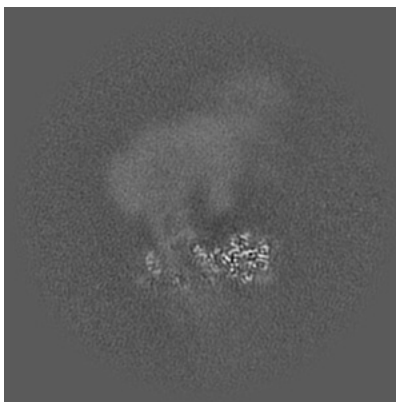
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

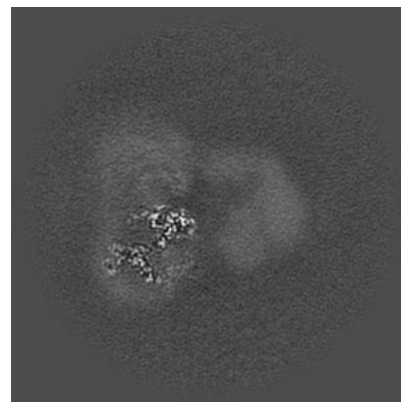
6.2.1 Primary map



X Index: 192

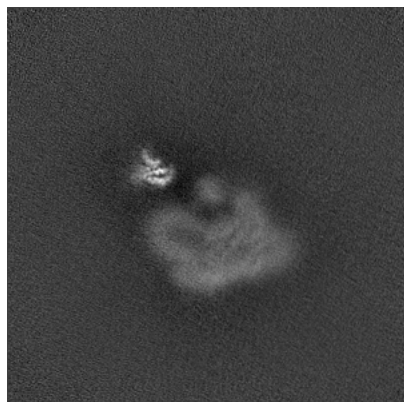


Y Index: 192

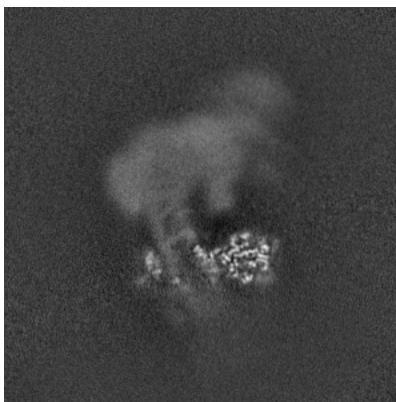


Z Index: 192

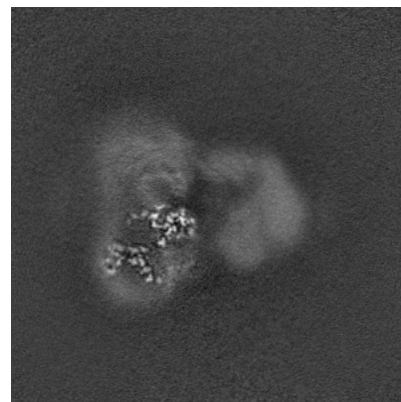
6.2.2 Raw map



X Index: 192



Y Index: 192

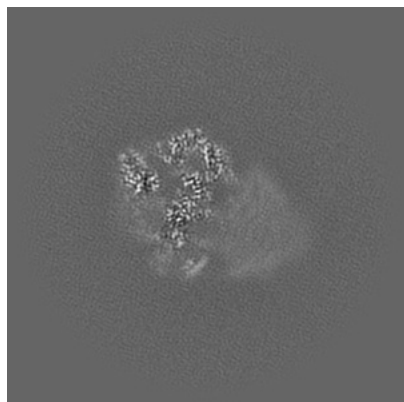


Z Index: 192

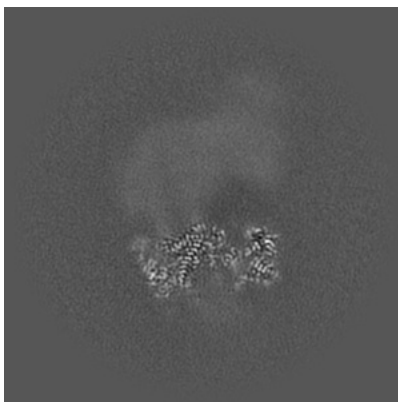
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

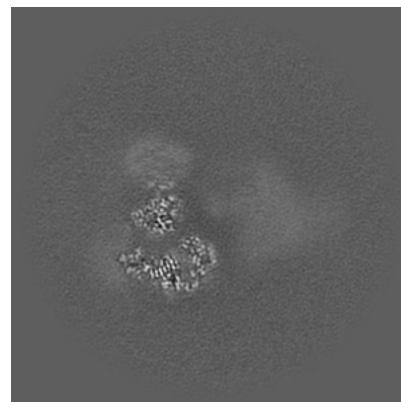
6.3.1 Primary map



X Index: 149

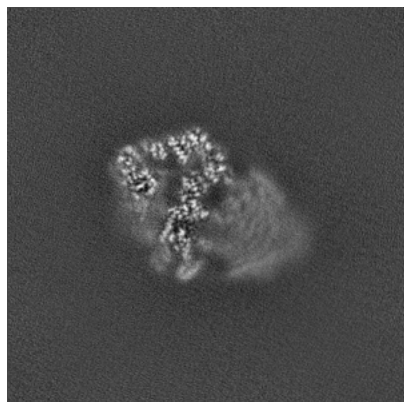


Y Index: 168

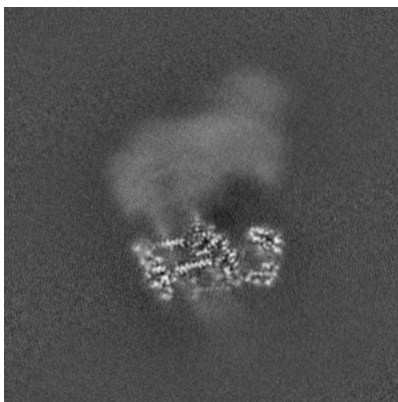


Z Index: 217

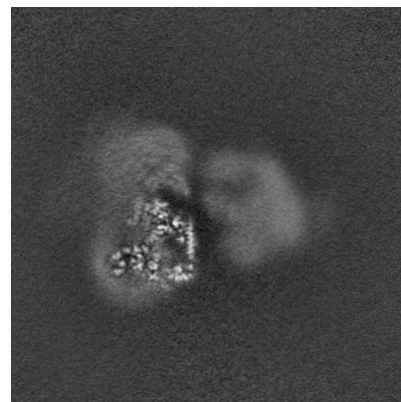
6.3.2 Raw map



X Index: 153



Y Index: 175

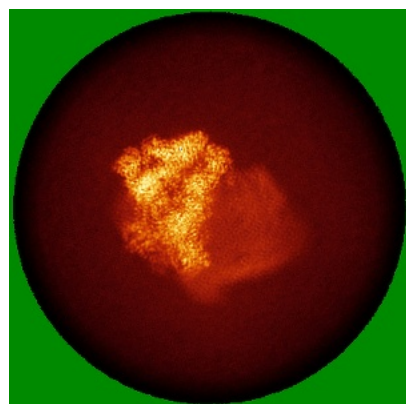


Z Index: 200

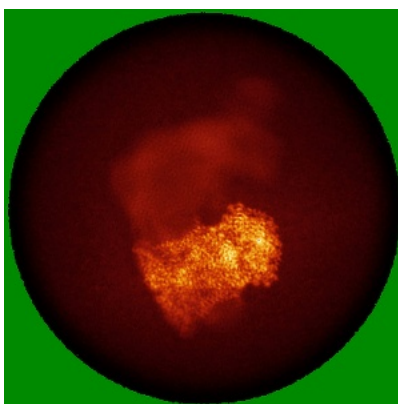
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

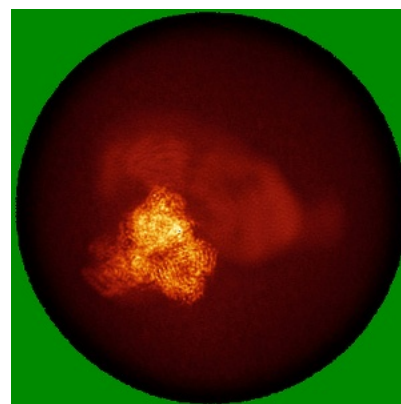
6.4.1 Primary map



X

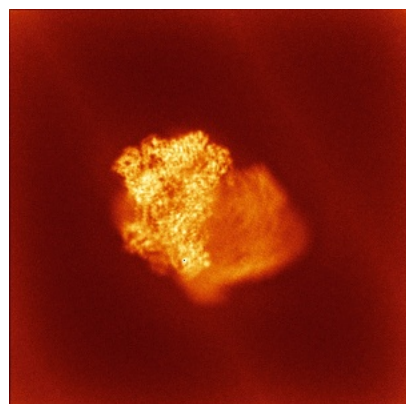


Y

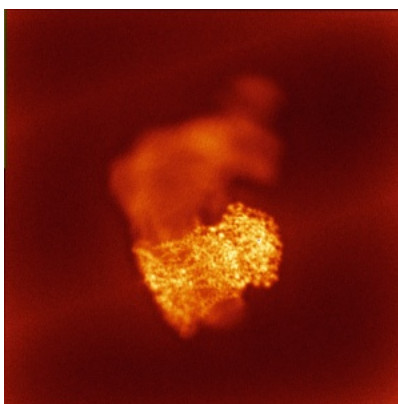


Z

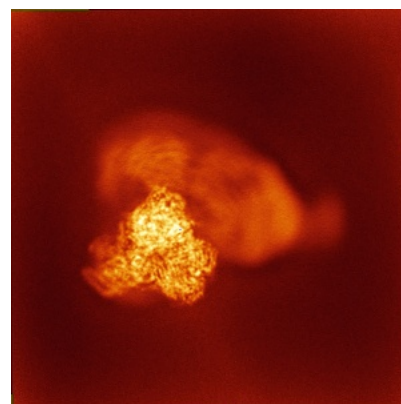
6.4.2 Raw map



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.

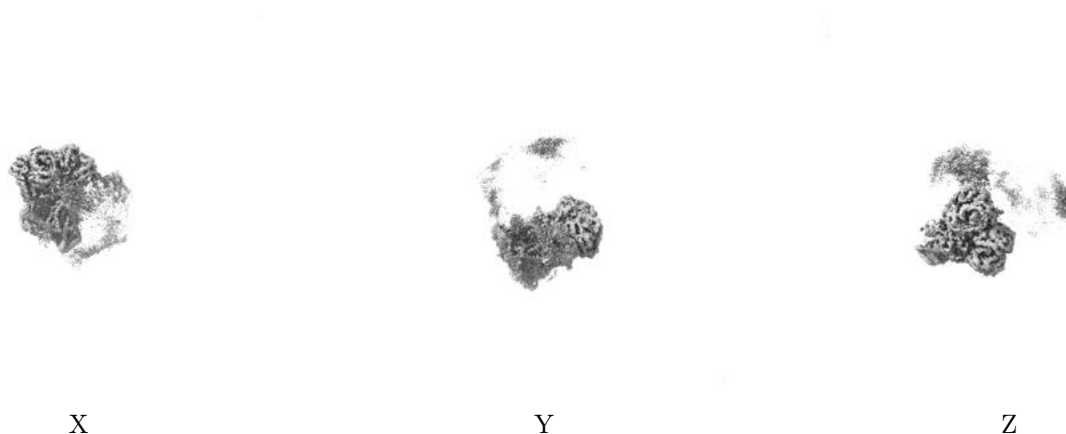
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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



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.

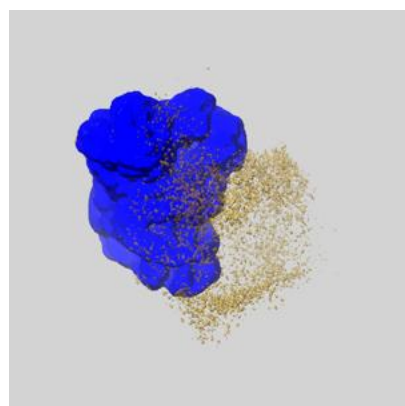
6.6 Mask visualisation [i](#)

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

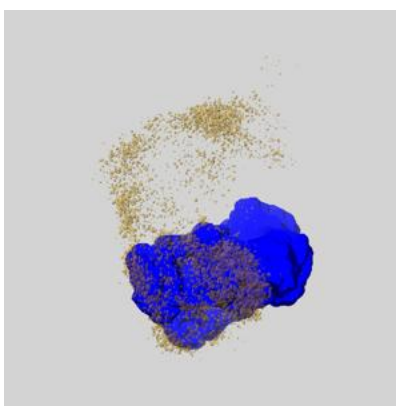
A mask typically either:

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

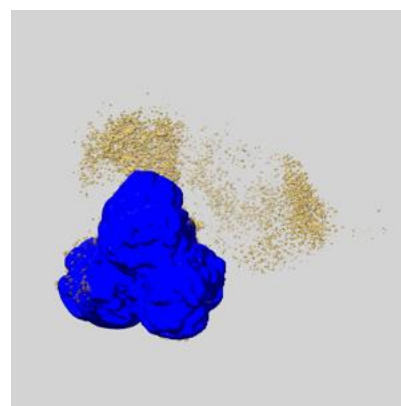
6.6.1 emd_35334_msk_1.map [i](#)



X



Y

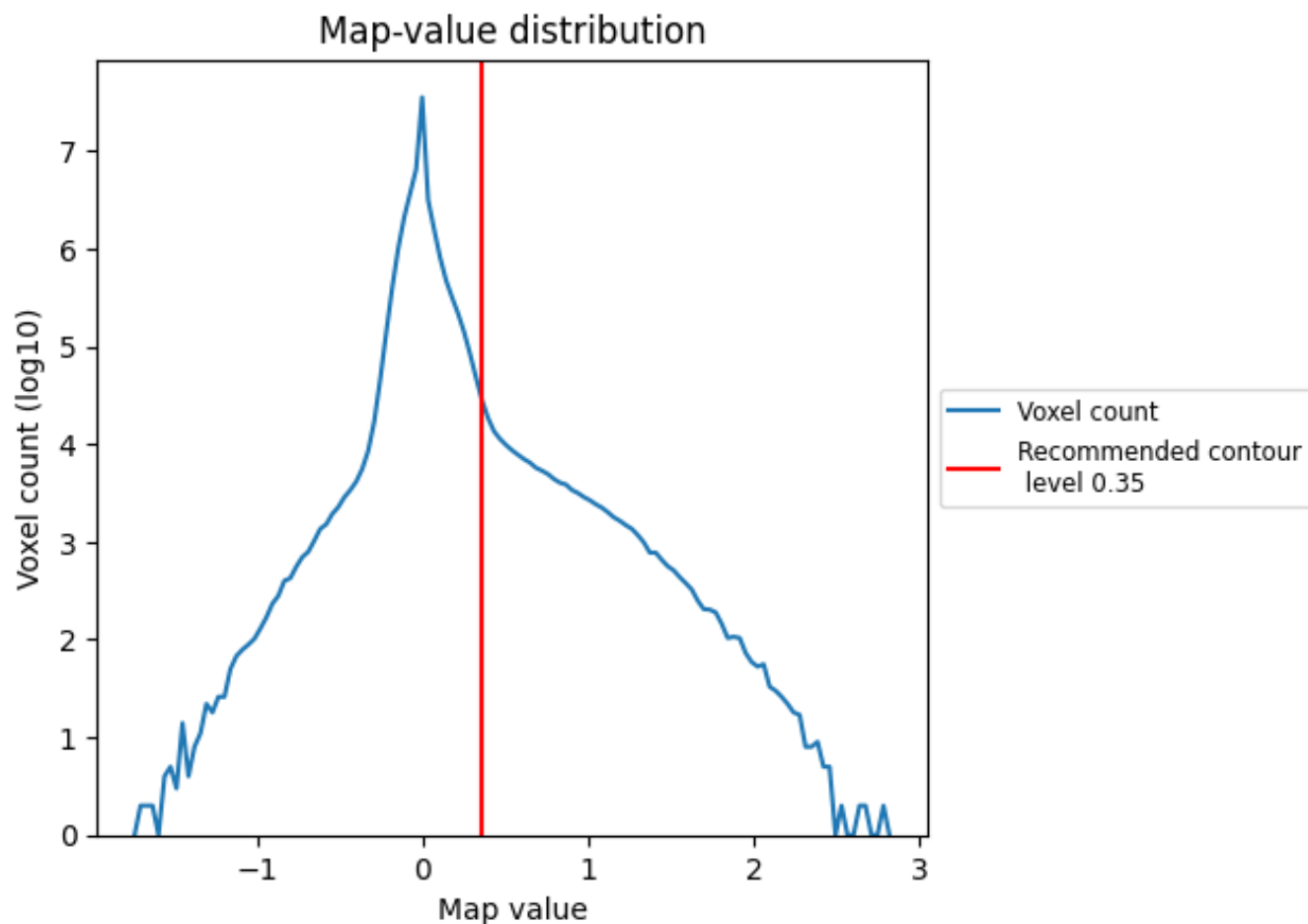


Z

7 Map analysis [i](#)

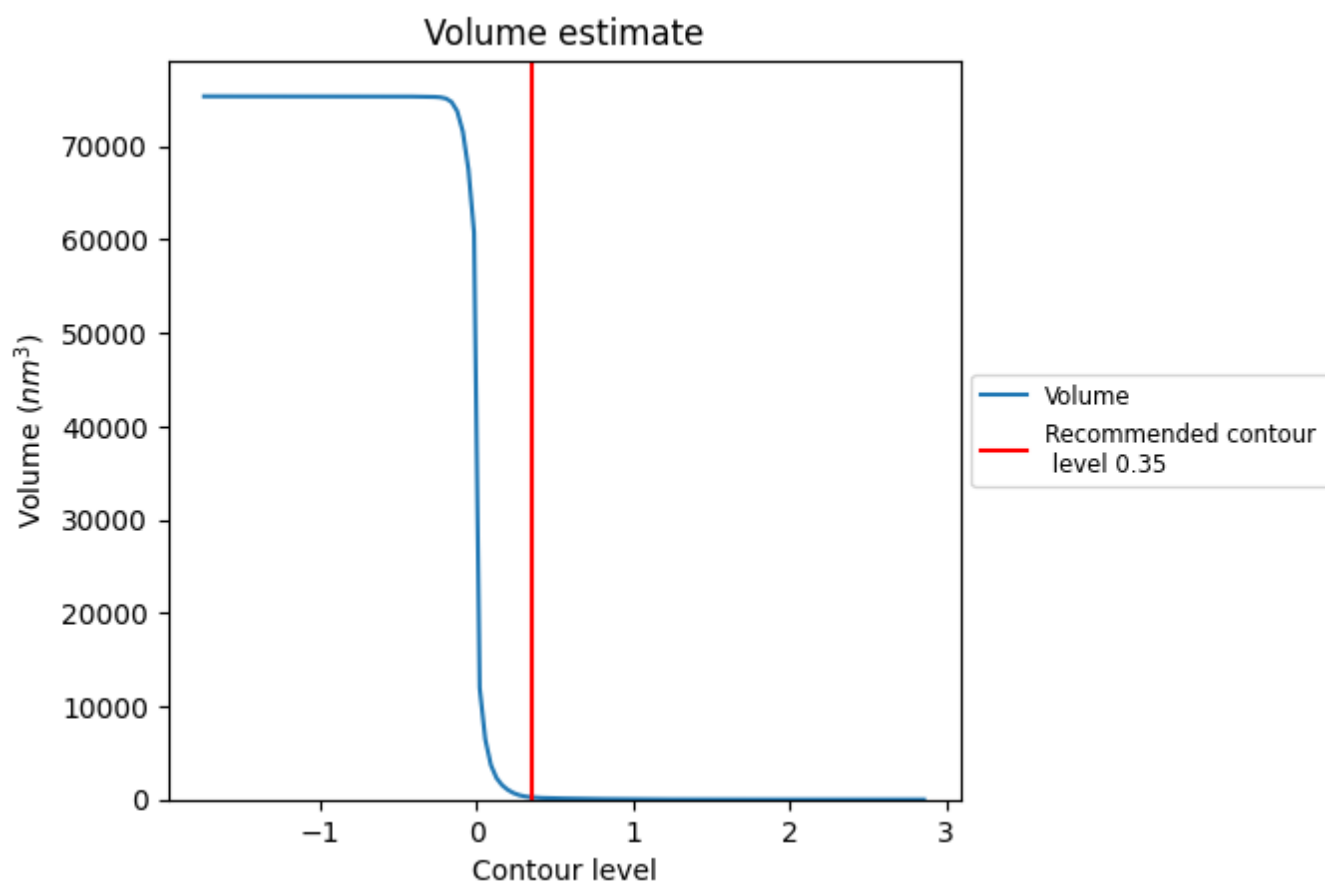
This section contains the results of statistical analysis of the map.

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.

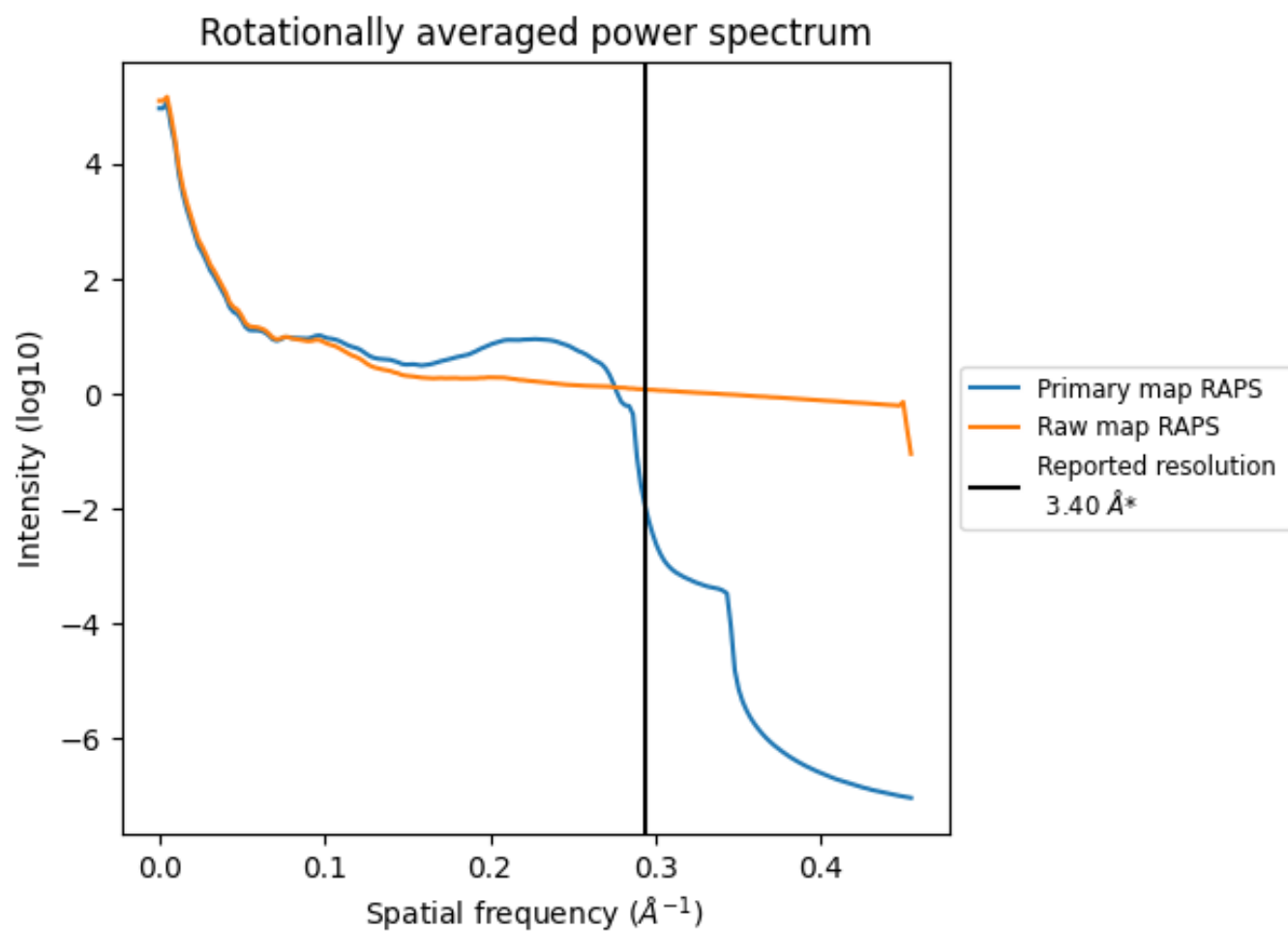
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 244 nm³; this corresponds to an approximate mass of 220 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 ⓘ

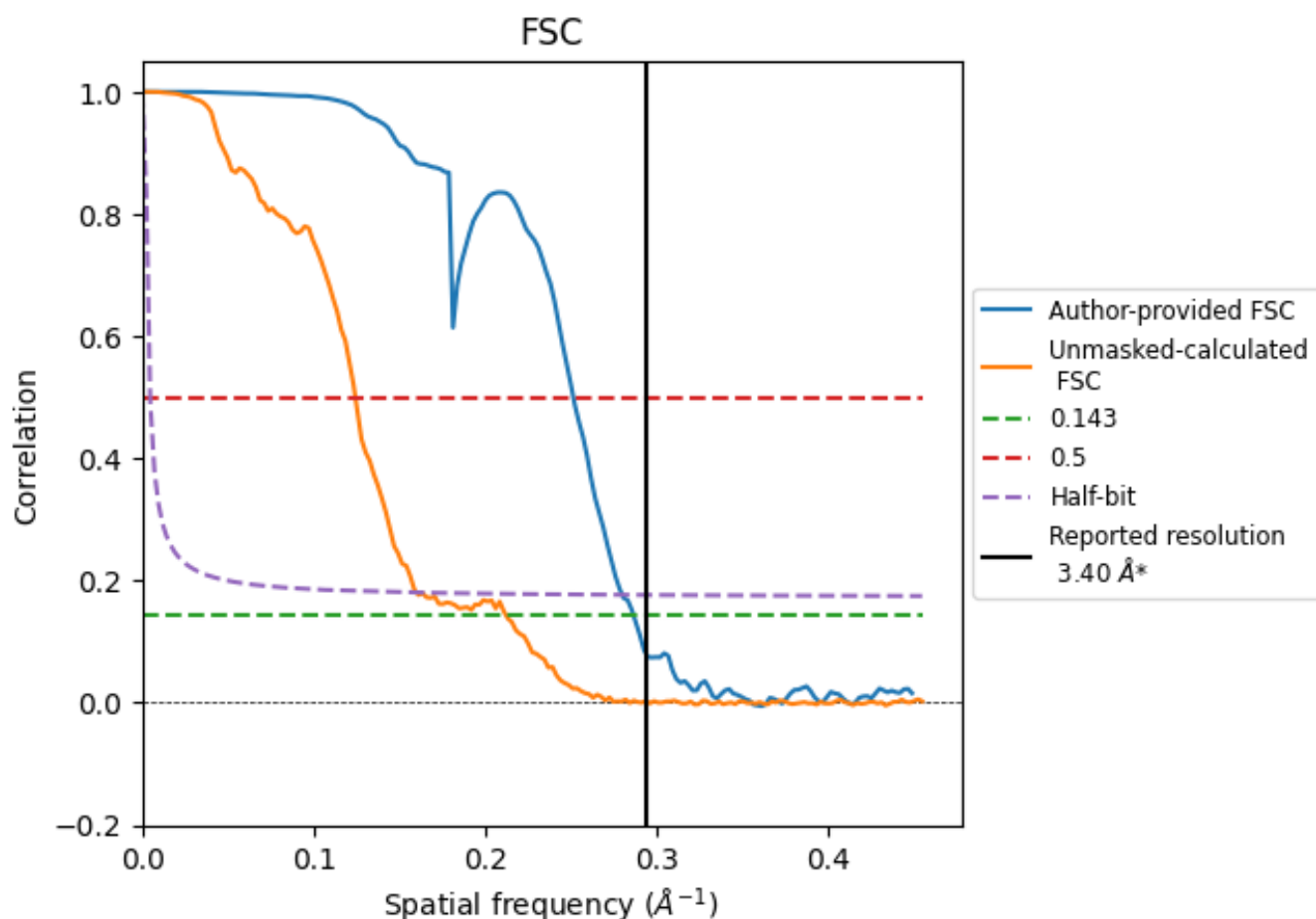


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

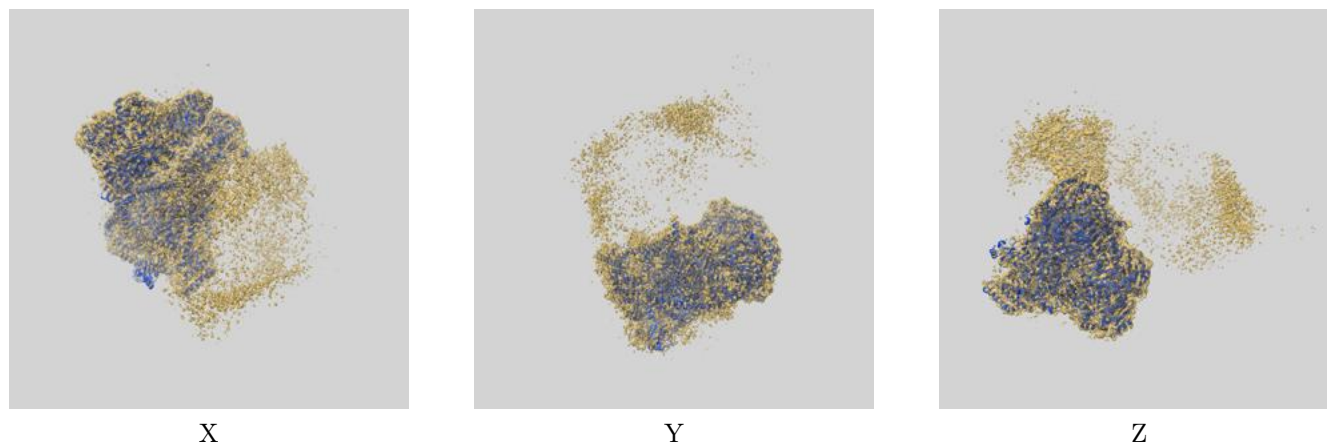
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.49	3.98	3.58
Unmasked-calculated*	4.72	8.05	6.25

*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 4.72 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

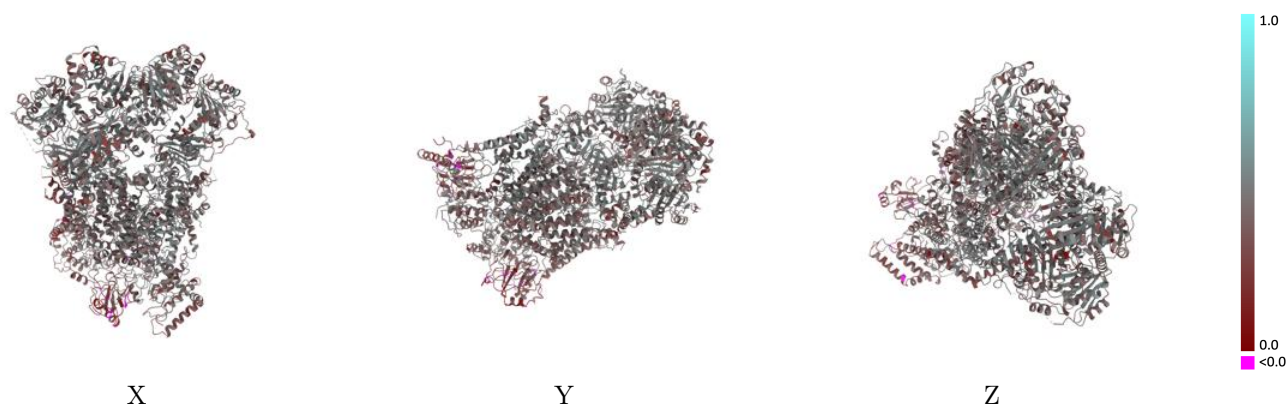
This section contains information regarding the fit between EMDB map EMD-35334 and PDB model 8IB7. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



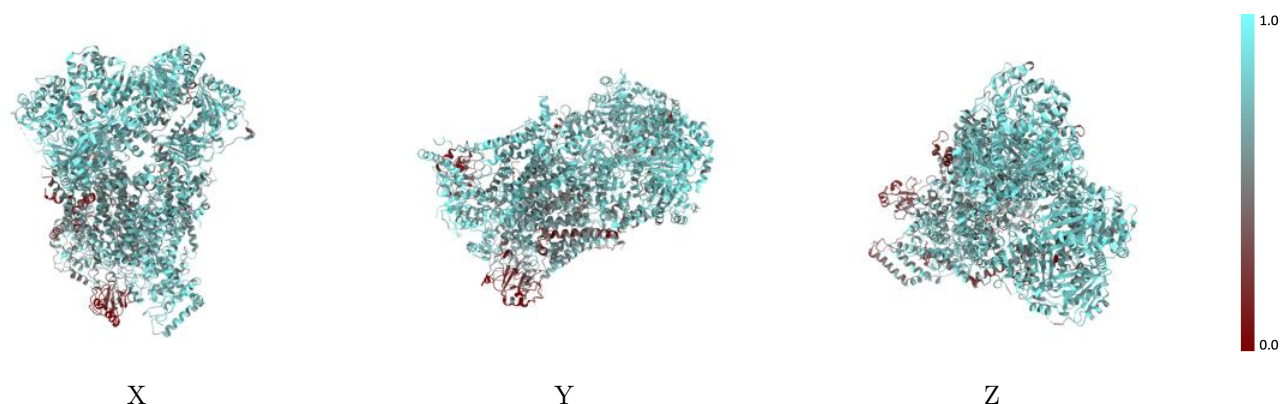
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



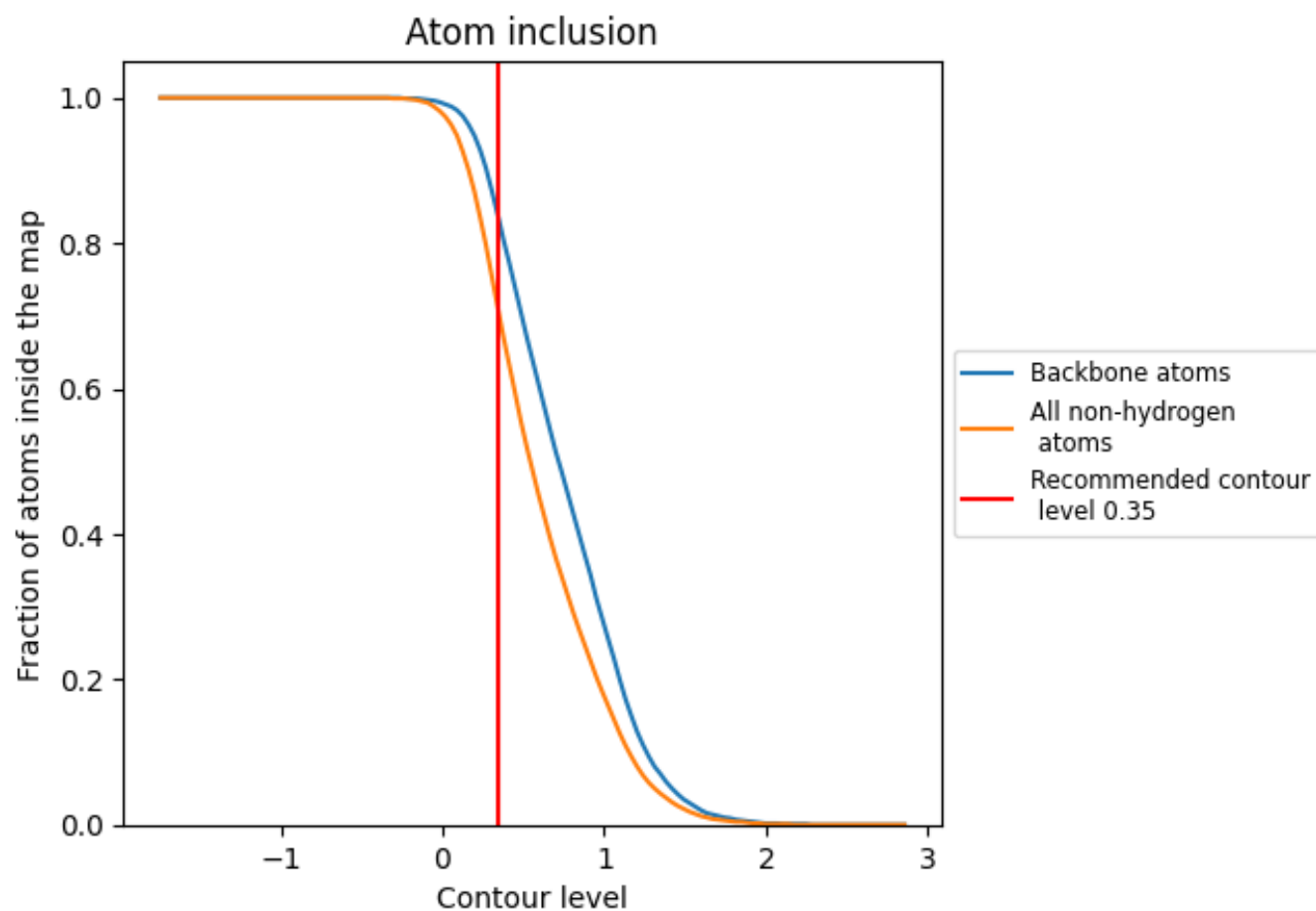
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.4070
AA	 0.7960	 0.4360
AB	 0.7840	 0.4260
AC	 0.7000	 0.4210
AD	 0.7040	 0.3820
AE	 0.3450	 0.2790
AF	 0.7160	 0.4100
AG	 0.6480	 0.3710
AH	 0.5430	 0.2770
AI	 0.5790	 0.4280
AJ	 0.3540	 0.2930
AK	 0.3360	 0.3550
Aa	 0.7780	 0.4360
Ab	 0.7910	 0.4330
Ac	 0.7620	 0.4450
Ad	 0.7940	 0.4150
Ae	 0.3540	 0.2940
Af	 0.7660	 0.4520
Ag	 0.7480	 0.4470
Ah	 0.7740	 0.3640
Aj	 0.6120	 0.3990
Ak	 0.2570	 0.3700

