



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:07 PM JST

PDB ID : 8IBG / pdb_00008ibg
EMDB ID : EMD-35343
Title : Respiratory complex CIII2, focus-refined of type II, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.80 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:

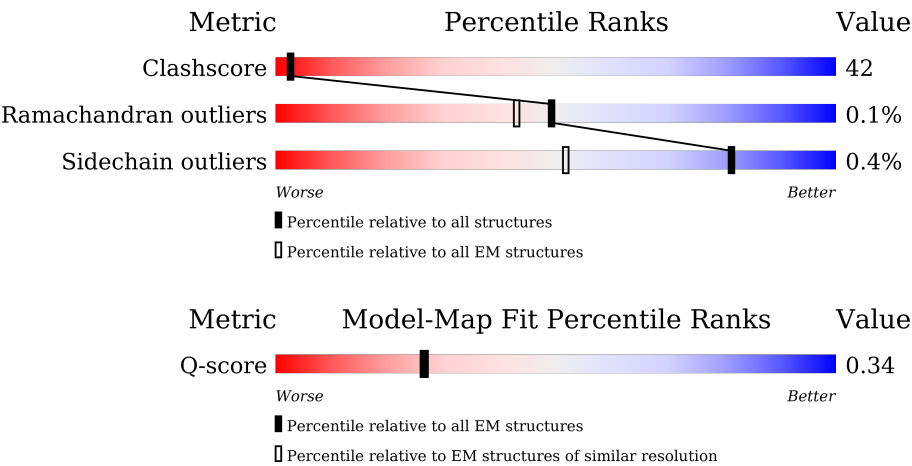
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	5% 45% 36% 18%
1	Aa	480	5% 42% 38% 18%
2	AB	453	5% 62% 29% 8%
2	Ab	453	6% 50% 40% 8%

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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	
5	Ai	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
13	HEC	AD	401	X	-	-	-
13	HEC	Ad	401	X	-	-	-
16	3PH	Ad	402	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 30396 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	395	Total	C	N	O	S	0	0
			3077	1918	545	598	16		
1	Aa	394	Total	C	N	O	S	0	0
			3076	1923	545	592	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	236	Total	C	N	O	S	0	0
			1878	1200	323	341	14		
4	Ad	239	Total	C	N	O	S	0	0
			1903	1215	326	348	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	109	Total	C	N	O	S	0	0
			830	525	152	147	6		
5	AI	28	Total	C	N	O		0	0
			200	129	37	34			
5	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
5	Ai	28	Total	C	N	O		0	0
			204	130	40	34			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	97	Total	C	N	O	S	0	0
			855	546	152	154	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	74	Total	C	N	O	S	0	0
			622	404	114	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	64	Total	C	N	O	S	0	0
			527	321	98	103	5		
8	Ah	62	Total	C	N	O	S	0	0
			512	316	93	98	5		

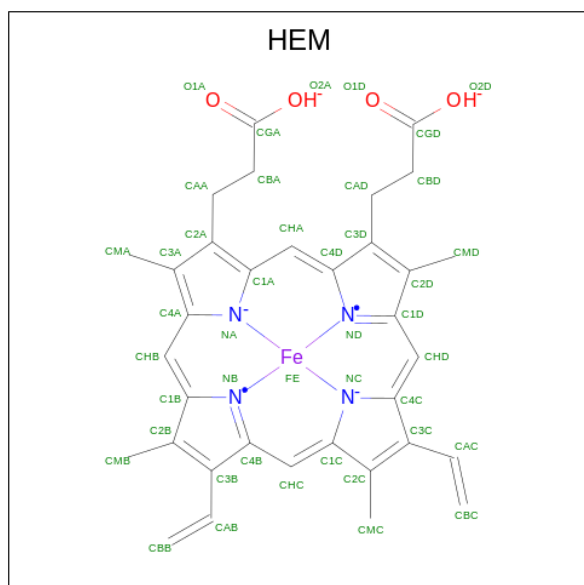
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AJ	21	Total	C	N	O	0	0
			165	109	27	29		
9	Aj	43	Total	C	N	O	0	0
			345	223	59	63		

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

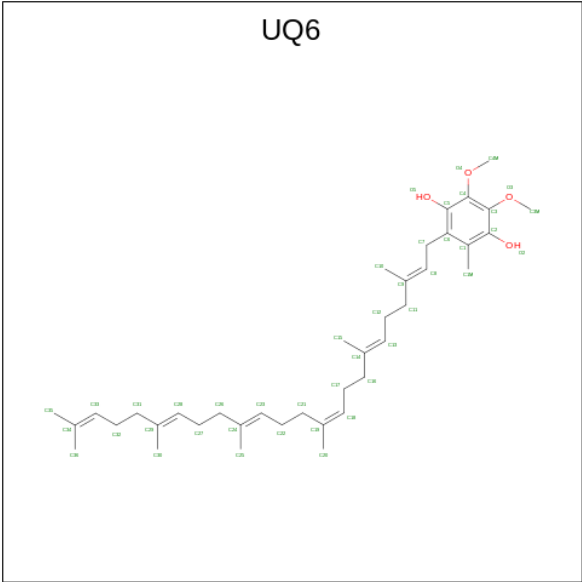
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	17	Total	C	N	O	S	0	0
			118	77	19	21	1		
10	AK	38	Total	C	N	O	S	0	0
			309	202	58	48	1		

- 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).



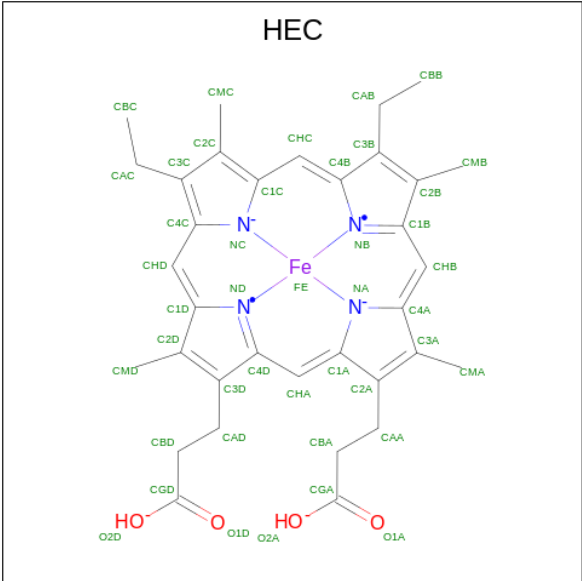
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is 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
12	AC	1	Total	C	O	0
			28	24	4	
12	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 13 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



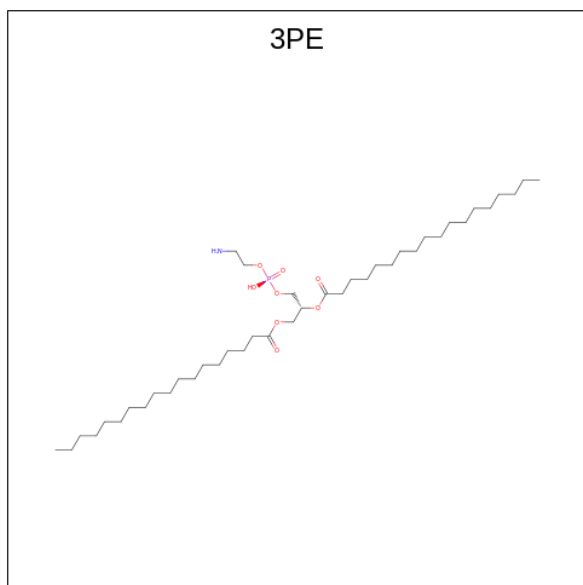
Mol	Chain	Residues	Atoms					AltConf
13	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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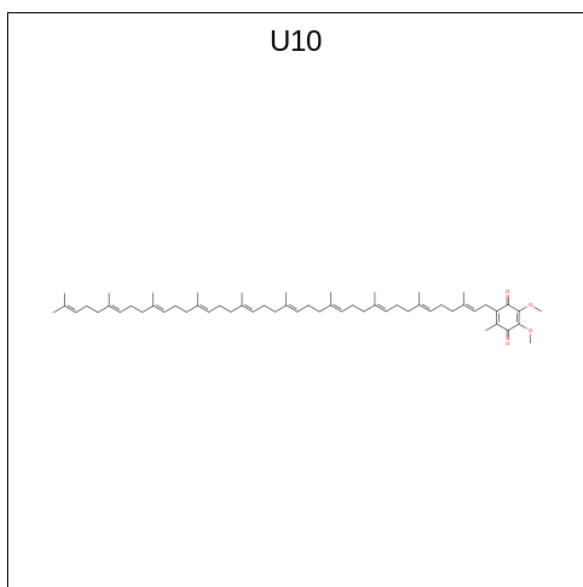
Mol	Chain	Residues	Atoms					AltConf
13	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



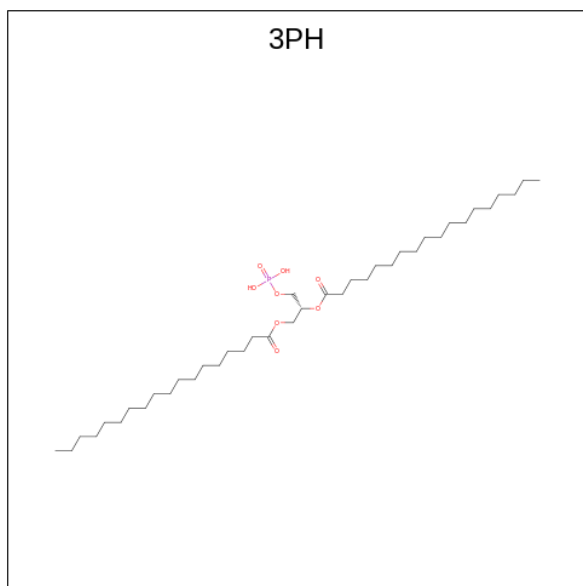
Mol	Chain	Residues	Atoms					AltConf
14	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
14	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
14	Ag	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 15 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



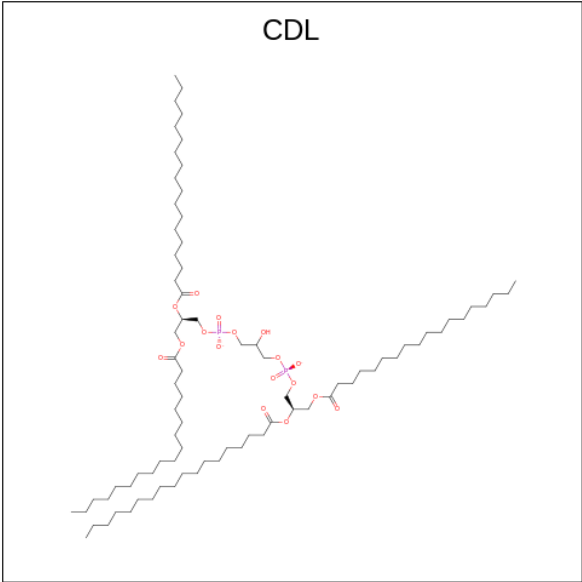
Mol	Chain	Residues	Atoms			AltConf
15	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 16 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



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

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

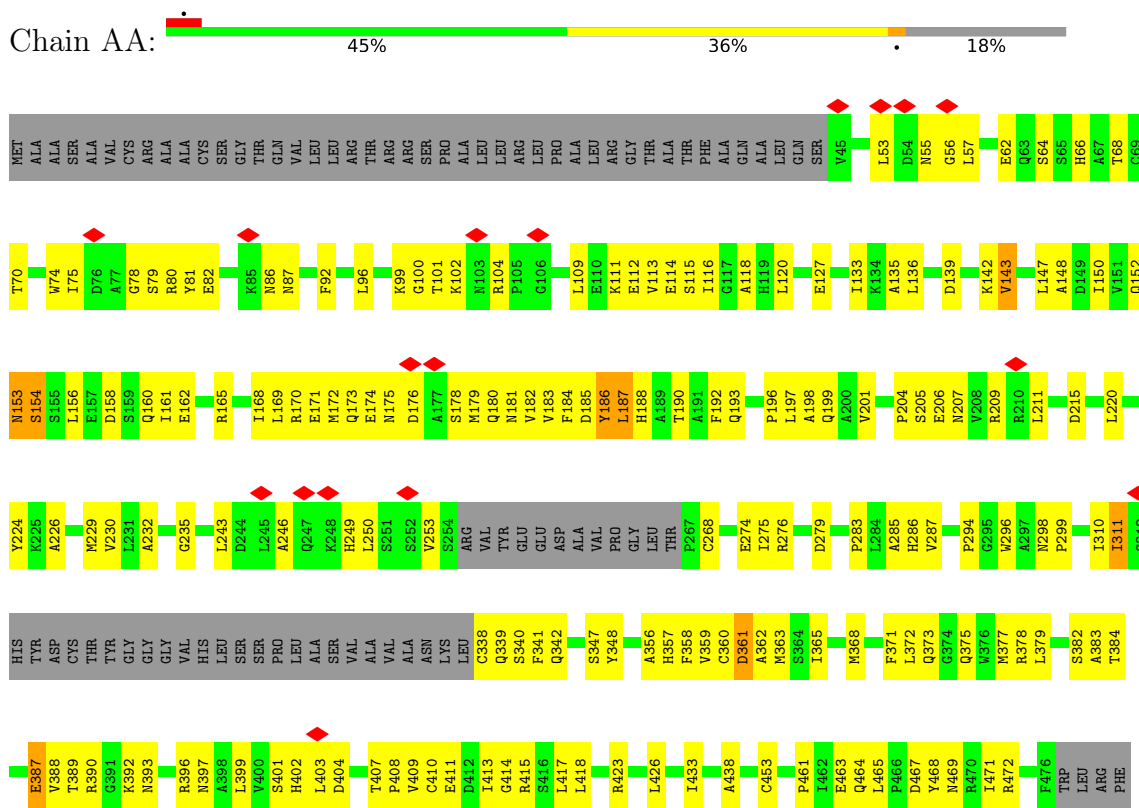


Mol	Chain	Residues	Atoms				AltConf
17	Ag	1	Total	C	O	P	0
			42	23	17	2	
17	Ag	1	Total	C	O	P	0
			56	37	17	2	

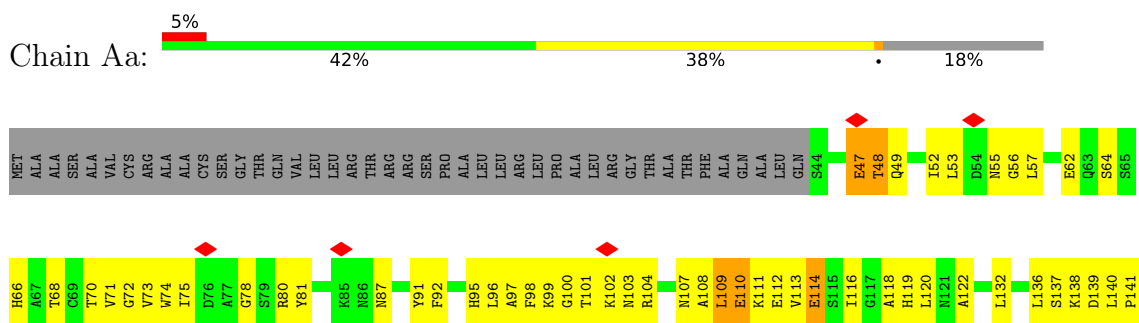
3 Residue-property plots [i](#)

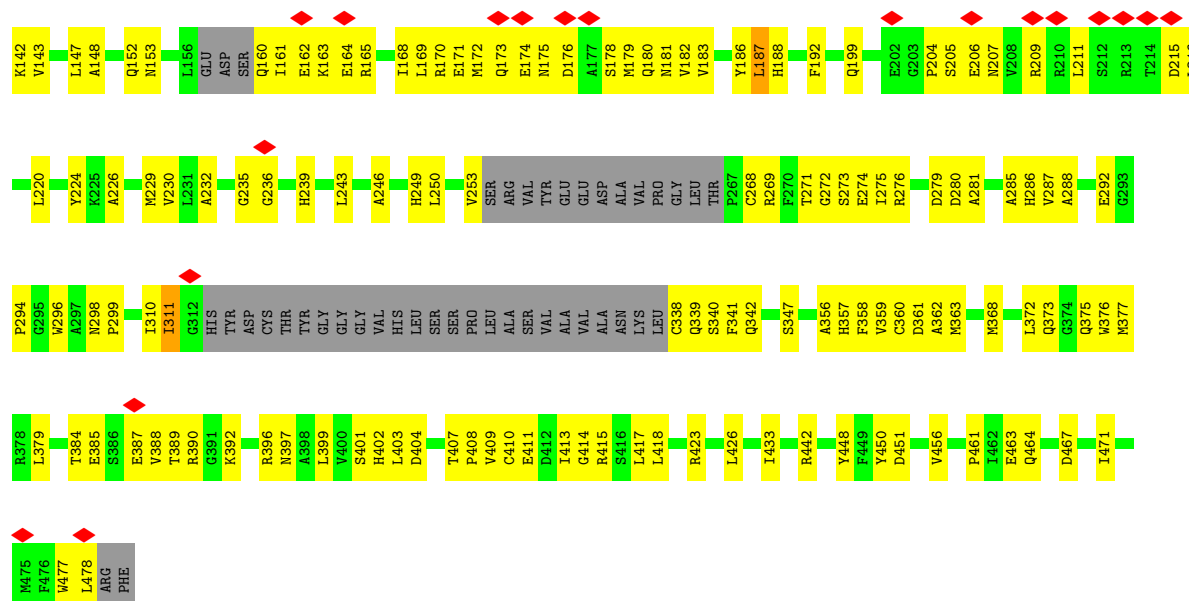
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

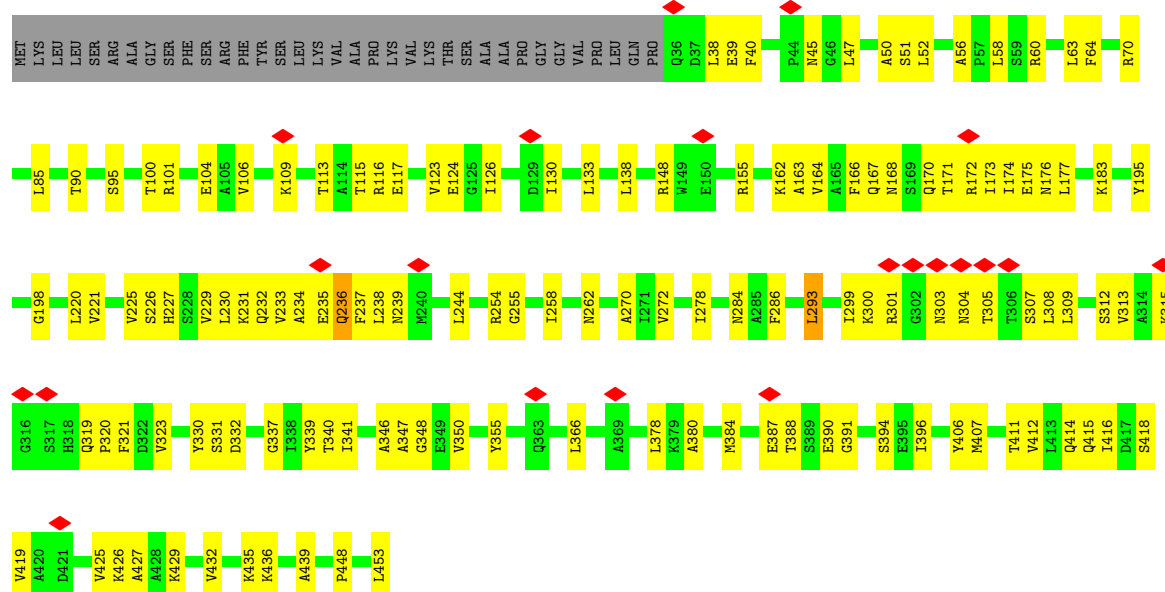


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

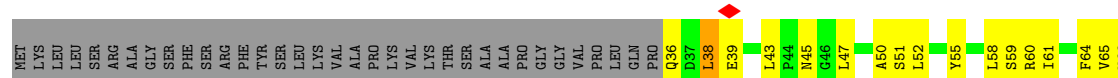


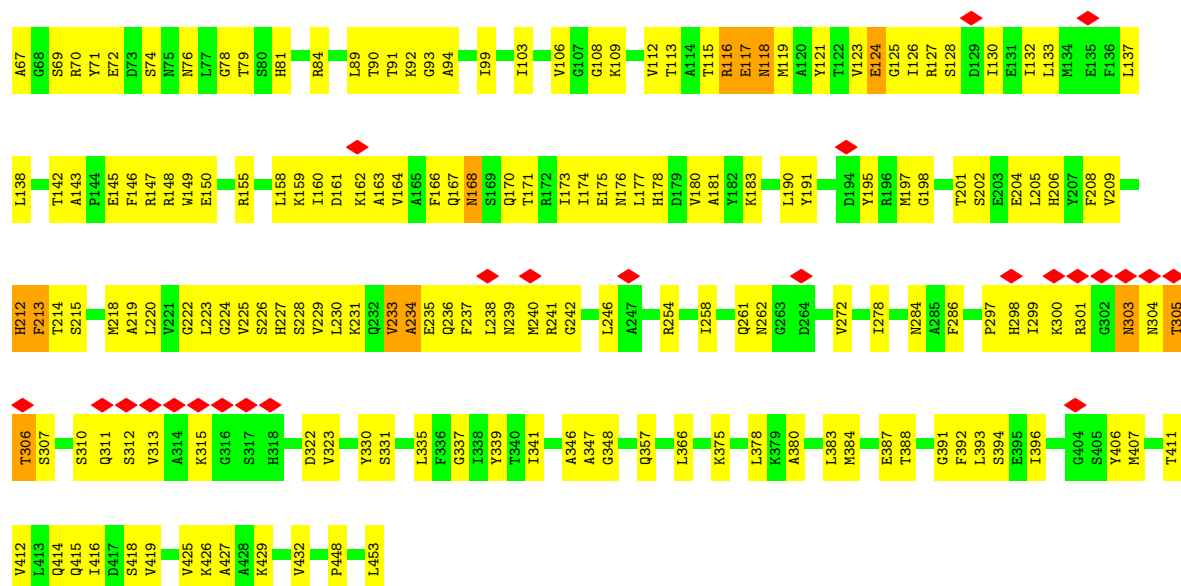


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

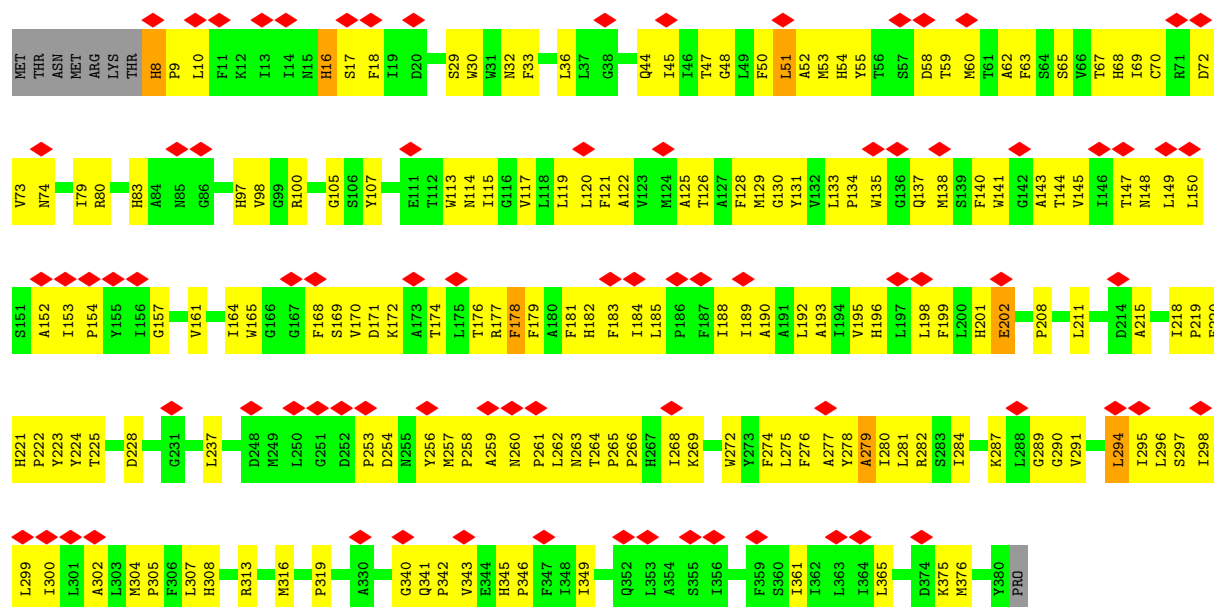


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

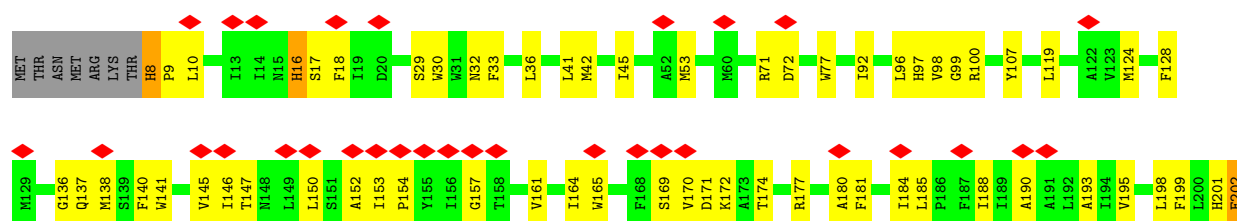




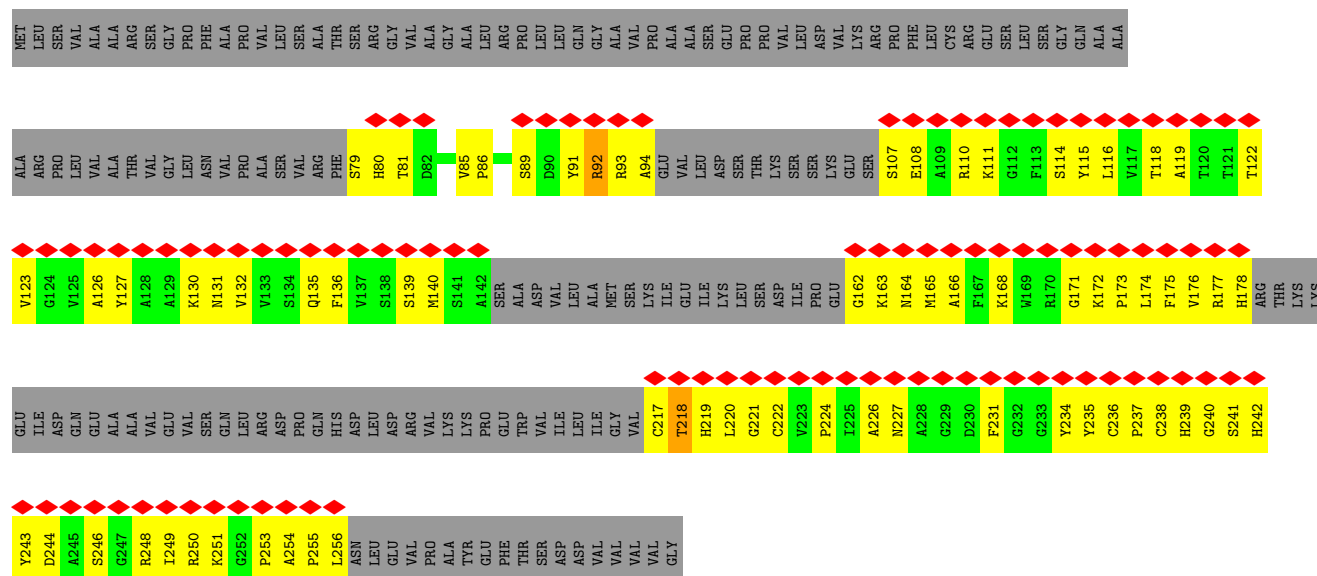
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b



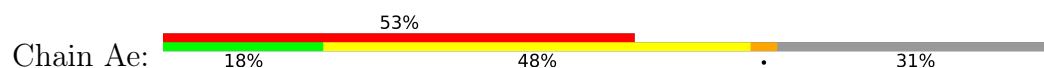
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

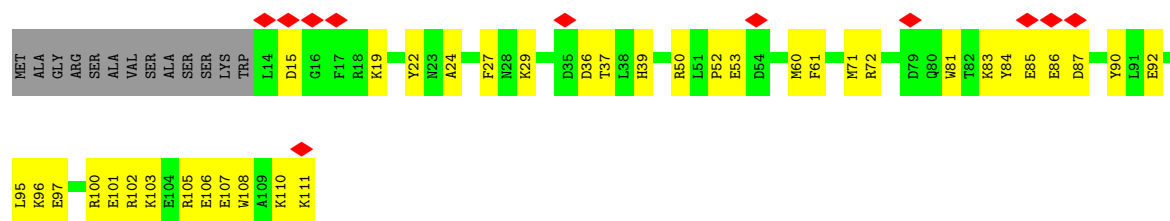


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

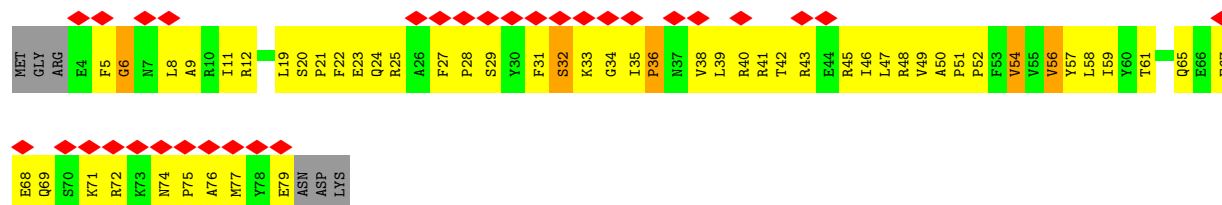


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

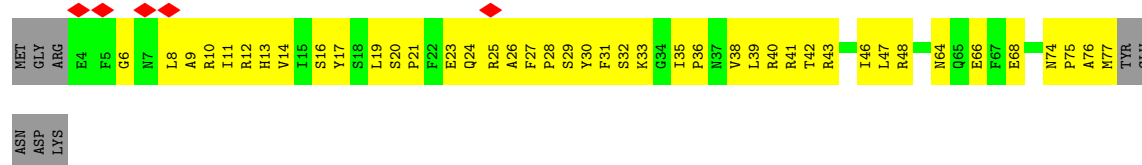
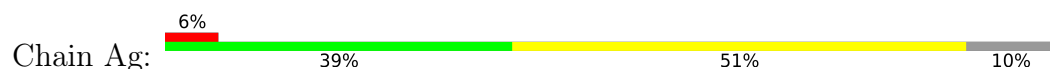




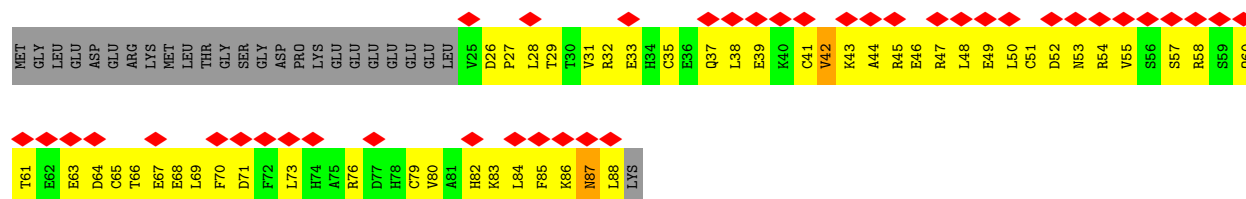
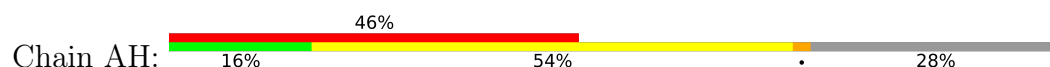
• Molecule 7: Cytochrome b-c1 complex subunit 8



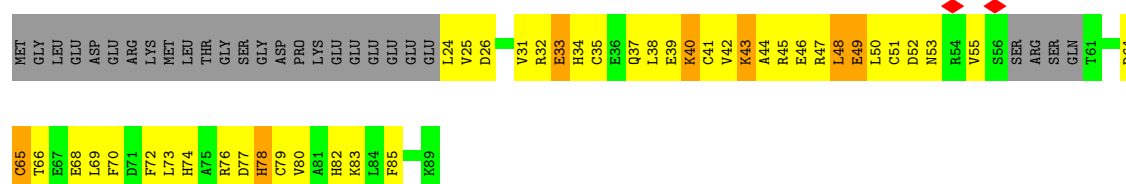
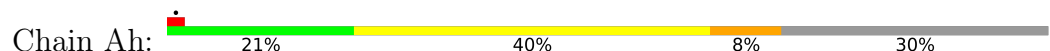
• Molecule 7: Cytochrome b-c1 complex subunit 8



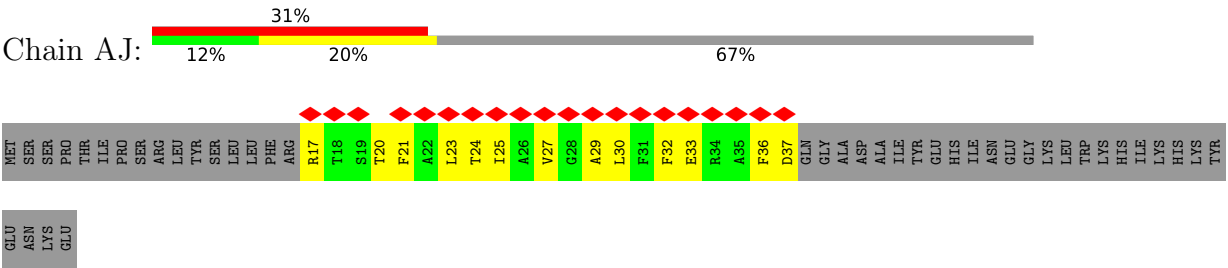
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



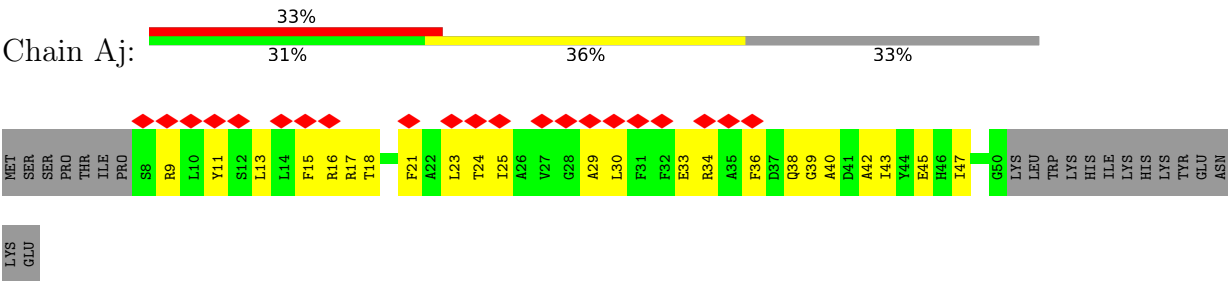
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



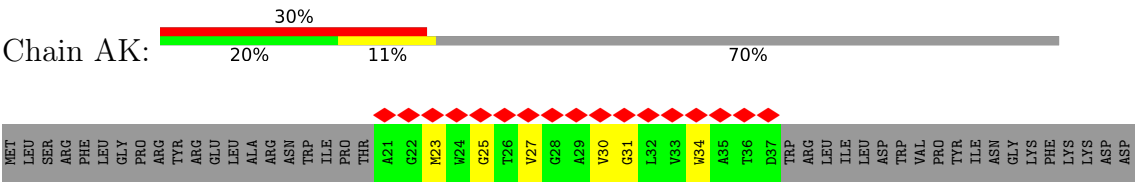
• Molecule 9: Cytochrome b-c1 complex subunit 9



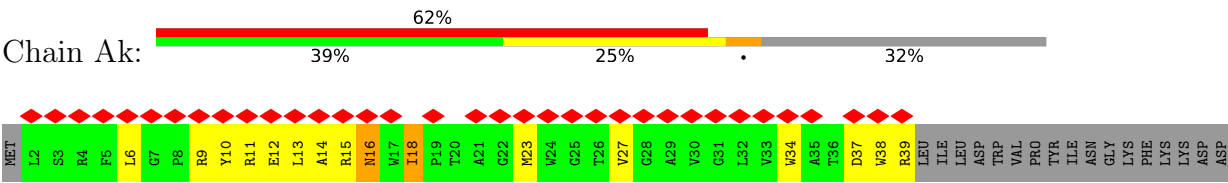
• Molecule 9: Cytochrome b-c1 complex subunit 9



• 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	177076	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	2.293	Depositor
Minimum map value	-1.374	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.053	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: CDL, 3PE, HEC, U10, UQ6, HEM, 3PH

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	0.62	2/3134 (0.1%)	0.89	11/4248 (0.3%)
1	Aa	0.58	1/3134 (0.0%)	0.89	14/4248 (0.3%)
2	AB	0.44	0/3187	0.65	3/4308 (0.1%)
2	Ab	0.58	1/3187 (0.0%)	0.91	18/4308 (0.4%)
3	AC	0.51	0/3089	0.84	10/4221 (0.2%)
3	Ac	0.45	0/3089	0.73	7/4221 (0.2%)
4	AD	0.54	0/1937	0.97	11/2632 (0.4%)
4	Ad	0.85	3/1962 (0.2%)	1.07	17/2666 (0.6%)
5	AE	0.47	0/851	0.94	3/1146 (0.3%)
5	AI	1.86	2/202 (1.0%)	1.43	4/274 (1.5%)
5	Ae	0.63	0/1483	1.10	7/2007 (0.3%)
5	Ai	1.87	2/205 (1.0%)	1.49	5/277 (1.8%)
6	AF	0.64	0/875	0.90	6/1173 (0.5%)
6	Af	0.38	0/884	0.52	0/1184
7	AG	0.57	1/662 (0.2%)	1.10	5/895 (0.6%)
7	Ag	0.55	0/640	0.93	1/865 (0.1%)
8	AH	0.53	0/534	0.84	2/717 (0.3%)
8	Ah	0.76	0/518	1.14	7/694 (1.0%)
9	AJ	0.41	0/168	0.62	0/226
9	Aj	0.59	0/352	0.78	0/474
10	AK	0.47	0/121	0.84	1/166 (0.6%)
10	Ak	0.52	0/320	1.14	6/437 (1.4%)
All	All	0.60	12/30534 (0.0%)	0.89	138/41387 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	44	ASP	C-N	20.17	1.52	1.33
5	Ai	44	ASP	C-N	19.98	1.52	1.33
4	Ad	221	PRO	N-CD	18.51	1.73	1.47
5	Ai	45	VAL	C-N	15.71	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	45	VAL	C-N	14.48	1.53	1.33
4	Ad	180	PRO	N-CD	11.27	1.63	1.47
4	Ad	176	PRO	N-CD	-6.62	1.38	1.47
7	AG	36	PRO	N-CD	6.58	1.56	1.47
2	Ab	117	GLU	CA-C	6.33	1.61	1.52
1	AA	153	ASN	CA-C	5.98	1.61	1.53
1	Aa	311	ILE	C-N	5.19	1.40	1.33
1	AA	311	ILE	C-N	5.02	1.40	1.33

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	115	ILE	N-CA-C	-11.23	99.16	110.62
10	Ak	38	TRP	N-CA-C	10.76	126.05	110.24
2	Ab	303	ASN	N-CA-C	-9.85	100.17	112.88
2	Ab	306	THR	N-CA-C	9.83	123.22	111.33
1	Aa	187	LEU	N-CA-C	-9.79	100.43	112.38
1	Aa	47	GLU	N-CA-C	9.78	125.53	113.50
1	AA	154	SER	N-CA-C	-9.75	94.79	110.20
4	Ad	142	GLU	N-CA-C	9.66	121.40	111.07
6	AF	108	TRP	N-CA-C	-8.84	101.75	112.54
5	Ai	46	LYS	N-CA-C	8.69	121.54	110.33
2	Ab	118	ASN	N-CA-CB	-8.67	97.45	110.97
1	AA	143	VAL	N-CA-C	8.54	119.33	110.36
5	Ae	148	ALA	N-CA-C	-8.40	102.58	112.92
7	AG	6	GLY	N-CA-C	-8.26	102.27	112.68
1	AA	360	CYS	N-CA-C	8.14	121.53	109.24
1	Aa	360	CYS	N-CA-C	8.09	121.45	109.24
2	Ab	118	ASN	N-CA-C	7.64	118.33	108.24
6	AF	106	GLU	N-CA-C	7.62	119.23	111.07
4	AD	226	SER	N-CA-C	7.54	126.87	110.80
4	AD	154	VAL	N-CA-C	7.49	119.30	107.98
3	Ac	202	GLU	N-CA-C	-7.39	103.25	111.82
3	AC	202	GLU	N-CA-C	-7.36	103.29	111.82
10	Ak	39	ARG	N-CA-CB	7.33	122.97	110.50
2	Ab	212	HIS	N-CA-C	7.33	121.98	112.89
5	Ae	221	GLY	N-CA-C	7.30	126.90	113.76
5	AE	221	GLY	N-CA-C	7.30	126.90	113.76
3	Ac	8	HIS	CA-C-N	7.29	127.00	119.56
3	Ac	8	HIS	C-N-CA	7.29	127.00	119.56
5	AI	45	VAL	CA-C-N	-7.27	108.61	121.70
5	AI	45	VAL	C-N-CA	-7.27	108.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	8	HIS	CA-C-N	7.24	126.94	119.56
3	AC	8	HIS	C-N-CA	7.24	126.94	119.56
2	Ab	125	GLY	N-CA-C	7.23	121.20	110.42
1	Aa	47	GLU	CA-C-O	7.12	126.98	119.14
3	Ac	17	SER	N-CA-C	7.08	122.09	113.38
4	Ad	221	PRO	N-CA-C	-7.05	102.10	110.70
7	AG	54	VAL	N-CA-C	-7.01	103.69	110.42
2	Ab	74	SER	N-CA-C	7.00	119.77	111.71
3	AC	17	SER	N-CA-C	7.00	122.00	113.38
8	Ah	33	GLU	N-CA-C	-6.98	103.75	111.36
5	Ai	45	VAL	CA-C-N	-6.96	108.56	120.95
5	Ai	45	VAL	C-N-CA	-6.96	108.56	120.95
5	Ae	218	THR	N-CA-C	-6.95	102.86	111.75
5	AE	218	THR	N-CA-C	-6.94	102.86	111.75
4	AD	244	MET	N-CA-C	-6.91	97.28	108.41
1	Aa	110	GLU	N-CA-CB	6.91	120.28	110.12
2	AB	293	LEU	N-CA-C	-6.83	100.92	110.35
8	Ah	43	LYS	N-CA-C	-6.83	103.84	111.28
2	Ab	234	ALA	N-CA-C	-6.81	105.51	113.88
6	AF	108	TRP	N-CA-CB	6.72	121.54	110.39
1	AA	361	ASP	N-CA-C	-6.70	101.24	110.35
1	Aa	361	ASP	N-CA-C	-6.67	101.28	110.35
1	AA	187	LEU	N-CA-C	-6.65	103.72	110.97
2	Ab	305	THR	N-CA-CB	-6.57	100.32	109.91
1	AA	153	ASN	CA-C-O	6.54	129.26	121.08
5	Ai	44	ASP	O-C-N	6.53	131.27	122.59
1	AA	215	ASP	N-CA-C	-6.50	103.89	110.97
1	Aa	215	ASP	N-CA-C	-6.49	103.89	110.97
4	AD	196	ASP	N-CA-C	-6.43	101.61	110.35
4	Ad	245	ALA	CA-C-N	-6.41	113.78	120.38
4	Ad	245	ALA	C-N-CA	-6.41	113.78	120.38
2	Ab	117	GLU	CA-C-O	6.41	127.24	119.49
8	Ah	78	HIS	N-CA-C	-6.40	103.59	111.33
1	AA	186	TYR	N-CA-C	-6.39	106.02	113.88
1	Aa	48	THR	N-CA-CB	6.38	121.61	111.91
4	Ad	152	VAL	N-CA-C	6.26	117.83	109.37
5	AI	44	ASP	O-C-N	6.25	131.04	121.23
2	Ab	116	ARG	N-CA-C	-6.19	104.08	111.69
8	Ah	49	GLU	N-CA-C	-6.14	104.50	111.07
10	AK	25	GLY	N-CA-C	-6.13	105.39	112.50
7	AG	56	VAL	N-CA-C	6.13	116.61	110.23
4	Ad	180	PRO	N-CA-CB	6.13	109.56	102.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Ah	48	LEU	N-CA-C	-6.13	104.51	111.07
4	AD	153	GLU	N-CA-CB	-6.12	102.14	110.95
7	AG	32	SER	N-CA-C	6.10	117.59	111.07
7	Ag	31	PHE	N-CA-C	-6.05	105.94	113.38
2	Ab	213	PHE	N-CA-CB	-6.04	102.07	110.65
1	Aa	110	GLU	N-CA-C	-6.03	104.71	111.28
6	AF	37	THR	N-CA-C	6.01	120.61	113.28
4	Ad	148	LEU	N-CA-C	-5.97	104.77	111.28
4	AD	227	LEU	N-CA-CB	5.97	118.38	109.19
2	AB	244	LEU	N-CA-C	-5.96	106.01	113.28
4	AD	242	ILE	N-CA-C	5.95	116.61	110.36
2	Ab	213	PHE	N-CA-C	5.93	119.26	112.97
4	AD	191	GLY	N-CA-C	-5.90	108.05	115.08
8	Ah	65	CYS	N-CA-C	-5.89	106.07	113.20
10	Ak	16	ASN	N-CA-C	-5.88	105.00	111.82
8	AH	53	ASN	N-CA-C	-5.81	104.95	111.28
4	AD	243	GLY	N-CA-C	-5.80	107.87	115.47
2	Ab	242	GLY	N-CA-C	5.72	120.74	113.24
3	Ac	17	SER	N-CA-CB	-5.72	102.01	110.53
4	Ad	180	PRO	CA-N-CD	-5.69	104.03	112.00
8	Ah	40	LYS	N-CA-C	5.69	117.93	111.11
3	AC	17	SER	N-CA-CB	-5.68	102.06	110.53
1	AA	185	ASP	N-CA-C	5.67	120.19	113.16
6	AF	25	ALA	N-CA-C	-5.65	105.12	111.28
6	AF	27	PHE	N-CA-C	-5.64	105.50	112.38
3	Ac	368	ILE	N-CA-C	-5.59	105.07	110.72
4	Ad	180	PRO	N-CA-C	-5.59	106.86	114.80
1	AA	153	ASN	CB-CA-C	-5.58	102.89	111.66
2	Ab	233	VAL	CB-CA-C	-5.58	105.17	110.70
4	Ad	297	GLY	N-CA-C	-5.58	107.75	114.66
7	AG	34	GLY	N-CA-C	5.57	118.97	112.50
8	AH	87	ASN	N-CA-C	-5.53	105.16	111.14
5	AI	59	ALA	N-CA-CB	-5.51	101.41	109.95
5	Ae	151	LYS	CA-C-O	-5.50	115.72	121.99
5	Ae	148	ALA	N-CA-CB	5.48	118.56	110.56
5	Ai	59	ALA	N-CA-CB	-5.47	101.47	109.95
2	Ab	124	GLU	N-CA-C	5.44	118.27	109.40
2	AB	236	GLN	N-CA-C	-5.42	105.92	112.54
3	AC	178	PHE	N-CA-C	-5.36	105.55	111.71
1	Aa	48	THR	N-CA-C	-5.36	104.01	111.52
3	AC	279	ALA	N-CA-C	-5.35	105.45	111.28
10	Ak	18	ILE	N-CA-C	5.34	120.42	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Ae	89	SER	N-CA-C	5.34	118.58	111.75
4	Ad	210	TYR	N-CA-C	-5.31	105.39	111.07
4	Ad	230	GLY	N-CA-C	-5.29	108.34	115.21
3	Ac	16	HIS	N-CA-C	5.28	117.78	111.71
1	Aa	56	GLY	N-CA-C	-5.27	107.26	114.64
4	AD	156	ASP	N-CA-C	-5.26	105.62	111.36
4	AD	164	MET	CB-CA-C	-5.26	110.49	116.54
3	AC	183	PHE	N-CA-C	-5.25	107.04	113.50
5	AE	92	ARG	N-CA-C	5.25	117.92	110.10
4	Ad	266	VAL	N-CA-C	-5.23	104.87	110.36
3	AC	16	HIS	N-CA-C	5.22	117.71	111.71
10	Ak	38	TRP	CB-CA-C	-5.22	102.01	109.84
10	Ak	37	ASP	CB-CA-C	5.21	119.72	112.11
1	AA	56	GLY	N-CA-C	-5.21	107.35	114.64
5	Ae	201	ASP	N-CA-C	-5.21	104.86	111.11
4	Ad	220	GLU	CA-C-N	-5.20	115.03	120.38
4	Ad	220	GLU	C-N-CA	-5.20	115.03	120.38
1	Aa	47	GLU	N-CA-CB	-5.16	102.94	110.53
2	Ab	212	HIS	CA-C-O	5.08	125.62	119.31
4	Ad	221	PRO	CA-N-CD	-5.07	104.90	112.00
2	Ab	38	LEU	N-CA-C	-5.06	103.47	110.35
1	Aa	109	LEU	CB-CA-C	-5.05	102.92	110.90
4	Ad	137	GLY	N-CA-C	-5.00	102.97	110.38
1	Aa	114	GLU	N-CA-C	-5.00	105.91	111.36

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	3077	0	2996	199	0
1	Aa	3076	0	3001	230	0
2	AB	3137	0	3143	153	0
2	Ab	3137	0	3143	252	0
3	AC	2988	0	3045	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ac	2988	0	3045	216	0
4	AD	1878	0	1827	294	0
4	Ad	1903	0	1848	279	0
5	AE	830	0	802	136	0
5	AI	200	0	216	32	0
5	Ae	1451	0	1433	264	0
5	Ai	204	0	221	34	0
6	AF	855	0	841	64	0
6	Af	864	0	854	38	0
7	AG	643	0	643	88	0
7	Ag	622	0	628	54	0
8	AH	527	0	507	76	0
8	Ah	512	0	497	84	0
9	AJ	165	0	162	81	0
9	Aj	345	0	333	37	0
10	AK	118	0	111	39	0
10	Ak	309	0	304	27	0
11	AC	86	0	60	27	0
11	Ac	86	0	60	11	0
12	AC	28	0	31	11	0
12	Ac	28	0	31	15	0
13	AD	43	0	32	18	0
13	Ad	43	0	32	12	0
14	Aa	23	0	20	3	0
14	Ac	35	0	44	7	0
14	Ag	38	0	53	9	0
15	Ac	23	0	23	20	0
16	Ad	36	0	45	39	0
17	Ag	98	0	84	9	0
All	All	30396	0	30115	2519	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 42.

All (2519) 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)
5:Ae:239:HIS:ND1	5:Ae:253:PRO:HG3	1.39	1.37
2:Ab:212:HIS:CE1	2:Ab:246:LEU:HD23	1.63	1.32
4:Ad:221:PRO:CD	4:Ad:221:PRO:N	1.73	1.32
3:AC:268:ILE:HD12	5:Ae:238:CYS:SG	1.67	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:297:PRO:CG	2:Ab:304:ASN:HD21	1.43	1.31
3:AC:199:PHE:CZ	3:Ac:8:HIS:CE1	2.23	1.25
3:AC:145:VAL:HA	5:Ae:220:LEU:O	1.35	1.23
1:Aa:109:LEU:HD12	1:Aa:110:GLU:N	1.52	1.22
2:Ab:59:SER:CB	2:Ab:224:GLY:HA3	1.69	1.21
9:AJ:23:LEU:HD22	10:AK:23:MET:SD	1.80	1.20
3:Ac:128:PHE:CD1	15:Ac:404:U10:C4M	2.24	1.19
5:AE:127:TYR:CD1	9:AJ:33:GLU:HA	1.78	1.19
2:Ab:297:PRO:HG3	2:Ab:304:ASN:ND2	1.57	1.18
5:AE:80:HIS:CD2	5:AE:81:THR:HG23	1.78	1.17
3:Ac:128:PHE:CE1	15:Ac:404:U10:C4M	2.28	1.16
5:Ae:164:ASN:HA	5:Ae:177:ARG:HA	1.28	1.15
3:AC:199:PHE:HZ	3:Ac:8:HIS:CE1	1.63	1.14
5:AE:130:LYS:HD3	9:AJ:33:GLU:HG2	1.16	1.14
3:Ac:128:PHE:CE1	15:Ac:404:U10:H4M2	1.83	1.14
8:Ah:32:ARG:HD3	8:Ah:76:ARG:NH1	1.60	1.14
5:Ae:239:HIS:CG	5:Ae:253:PRO:HG3	1.83	1.12
4:AD:157:GLY:HA3	4:AD:167:ARG:HB3	1.32	1.11
7:AG:9:ALA:HB3	7:AG:11:ILE:HD11	1.33	1.11
2:Ab:297:PRO:HG3	2:Ab:304:ASN:HD21	1.07	1.11
5:Ae:263:TYR:HA	5:Ae:273:VAL:HA	1.13	1.10
3:AC:144:THR:HG21	5:Ae:221:GLY:O	1.51	1.10
3:Ac:146:ILE:HG13	15:Ac:404:U10:C4M	1.83	1.09
1:Aa:402:HIS:CE1	1:Aa:403:LEU:CD1	2.36	1.09
4:AD:120:VAL:HG23	4:AD:253:LEU:HD11	1.21	1.09
4:AD:153:GLU:HA	4:AD:168:PRO:HA	1.11	1.09
1:AA:402:HIS:CE1	1:AA:403:LEU:CD1	2.36	1.08
4:AD:215:LEU:HD11	13:AD:401:HEC:HMB3	1.27	1.08
5:AE:220:LEU:HD13	3:Ac:145:VAL:HG13	1.18	1.08
2:Ab:297:PRO:CB	2:Ab:304:ASN:HD21	1.66	1.08
3:AC:266:PRO:O	5:Ae:237:PRO:HB2	1.52	1.08
8:AH:47:ARG:HH22	8:AH:71:ASP:HB2	1.01	1.08
3:Ac:128:PHE:CD1	15:Ac:404:U10:H4M2	1.85	1.08
3:AC:98:VAL:HG22	11:AC:402:HEM:HBC2	1.34	1.07
3:AC:268:ILE:CD1	5:Ae:238:CYS:SG	2.42	1.07
2:Ab:59:SER:HB2	2:Ab:224:GLY:HA3	1.29	1.07
3:Ac:146:ILE:HD11	15:Ac:404:U10:H3M2	1.15	1.07
16:Ad:402:3PH:H12	5:Ae:131:ASN:HD21	1.20	1.07
4:Ad:295:MET:HB2	16:Ad:402:3PH:H341	1.34	1.07
7:Ag:11:ILE:HG21	7:Ag:14:VAL:HG21	1.36	1.07
8:Ah:45:ARG:HH11	8:Ah:48:LEU:HD23	1.00	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:47:ARG:NH2	8:AH:71:ASP:CB	2.17	1.06
4:Ad:223:THR:HG22	8:Ah:65:CYS:HB2	1.36	1.06
3:Ac:146:ILE:HD11	15:Ac:404:U10:C3M	1.84	1.06
4:AD:153:GLU:HG2	4:AD:168:PRO:HB3	1.31	1.05
5:AE:127:TYR:HD1	9:AJ:33:GLU:HA	1.11	1.05
3:Ac:42:MET:HE1	12:Ac:405:UQ6:C21	1.86	1.05
3:Ac:146:ILE:HG13	15:Ac:404:U10:H4M3	1.36	1.05
8:AH:47:ARG:NH2	8:AH:71:ASP:HB2	1.70	1.04
5:Ae:239:HIS:ND1	5:Ae:253:PRO:CG	2.21	1.04
1:Aa:402:HIS:CE1	1:Aa:403:LEU:HD11	1.91	1.04
5:AE:126:ALA:HB3	9:AJ:29:ALA:CB	1.87	1.04
1:AA:402:HIS:CE1	1:AA:403:LEU:HD11	1.91	1.03
3:AC:129:MET:HB3	3:AC:182:HIS:HB2	1.37	1.02
9:AJ:27:VAL:HG22	10:AK:30:VAL:HG11	1.36	1.02
2:Ab:159:LYS:HA	2:Ab:162:LYS:HE2	1.38	1.02
3:Ac:98:VAL:HG22	11:Ac:402:HEM:HBC2	1.41	1.02
3:Ac:128:PHE:CD1	15:Ac:404:U10:H4M1	1.91	1.02
7:AG:31:PHE:HA	7:AG:35:ILE:HD12	1.39	1.02
8:AH:47:ARG:HH22	8:AH:71:ASP:CB	1.72	1.02
9:AJ:23:LEU:CB	10:AK:27:VAL:HG22	1.90	1.02
3:AC:266:PRO:O	5:Ae:237:PRO:CB	2.06	1.01
4:AD:231:LEU:HD13	4:AD:241:ALA:HB1	1.40	1.01
3:AC:199:PHE:CE1	3:Ac:8:HIS:NE2	2.28	1.01
9:AJ:23:LEU:CD2	10:AK:23:MET:SD	2.49	1.00
11:Ac:402:HEM:HMA2	12:Ac:405:UQ6:H152	1.44	1.00
8:Ah:45:ARG:HH11	8:Ah:48:LEU:CD2	1.74	1.00
3:AC:199:PHE:CZ	3:Ac:8:HIS:HE1	1.77	0.99
3:Ac:244:LEU:HD13	4:Ad:289:GLY:HA2	1.41	0.99
5:AE:220:LEU:HD13	3:Ac:145:VAL:CG1	1.92	0.98
3:AC:199:PHE:HZ	3:Ac:8:HIS:HE1	1.07	0.98
5:AE:119:ALA:HA	9:AJ:25:ILE:HD11	1.46	0.98
8:Ah:45:ARG:NH1	8:Ah:48:LEU:HD23	1.79	0.98
4:AD:189:ASN:HB3	13:AD:401:HEC:HMD2	1.44	0.98
5:AE:126:ALA:HB3	9:AJ:29:ALA:HB1	1.47	0.97
1:AA:463:GLU:OE1	7:AG:8:LEU:HB2	1.66	0.96
5:AE:89:SER:HA	5:AE:92:ARG:HB2	1.46	0.96
4:AD:247:PRO:HB3	13:AD:401:HEC:HMC2	1.48	0.96
2:Ab:146:PHE:HD2	2:Ab:202:SER:HB3	1.28	0.95
4:AD:242:ILE:HD11	4:AD:244:MET:HE3	1.44	0.95
9:AJ:23:LEU:HD13	10:AK:27:VAL:HG22	1.45	0.95
2:Ab:215:SER:HA	2:Ab:218:MET:HE2	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:130:LYS:HD3	9:AJ:33:GLU:CG	1.96	0.95
8:Ah:32:ARG:HD3	8:Ah:76:ARG:HH12	1.28	0.95
5:Ae:200:HIS:CD2	5:Ae:201:ASP:OD1	2.19	0.95
5:AE:119:ALA:HA	9:AJ:25:ILE:CD1	1.95	0.95
3:AC:30:TRP:HB3	3:AC:100:ARG:HD3	1.46	0.95
7:Ag:19:LEU:HD23	7:Ag:24:GLN:HB3	1.49	0.95
9:AJ:30:LEU:HG	10:AK:34:TRP:HB2	1.48	0.94
9:AJ:23:LEU:CD1	10:AK:27:VAL:HG22	1.96	0.94
1:Aa:100:GLY:O	1:Aa:101:THR:HG23	1.68	0.94
5:Ae:263:TYR:HA	5:Ae:273:VAL:CA	1.97	0.94
1:Aa:110:GLU:HB2	2:Ab:299:ILE:HD13	1.50	0.93
3:AC:144:THR:CG2	5:Ae:221:GLY:O	2.15	0.93
5:AE:238:CYS:SG	3:Ac:268:ILE:HD12	2.09	0.93
5:Ae:188:ALA:HA	5:Ae:200:HIS:NE2	1.83	0.93
2:AB:85:LEU:HD23	5:AI:68:VAL:HG21	1.50	0.93
3:AC:145:VAL:HG13	5:Ae:220:LEU:HB3	1.51	0.93
10:Ak:6:LEU:HA	10:Ak:11:ARG:HH12	1.32	0.93
5:AE:218:THR:HG21	5:AE:256:LEU:O	1.68	0.93
4:Ad:181:ASN:HB3	4:Ad:183:GLU:HG2	1.49	0.93
1:AA:384:THR:HG23	1:AA:387:GLU:H	1.31	0.92
2:Ab:212:HIS:CE1	2:Ab:246:LEU:CD2	2.52	0.92
2:Ab:297:PRO:CG	2:Ab:304:ASN:ND2	2.23	0.92
2:Ab:212:HIS:HE1	2:Ab:246:LEU:HD23	1.03	0.92
3:AC:74:ASN:HB2	5:AE:139:SER:HA	1.51	0.92
4:AD:264:SER:HB3	8:AH:28:LEU:HB2	1.50	0.92
7:Ag:46:ILE:CG2	14:Ag:103:3PE:H3H1	2.00	0.91
1:Aa:120:LEU:N	2:Ab:298:HIS:O	2.04	0.91
2:Ab:84:ARG:HG2	5:AI:68:VAL:HG22	1.51	0.91
4:Ad:302:LEU:HD13	5:Ae:121:THR:HA	1.49	0.91
3:AC:199:PHE:HE1	3:Ac:8:HIS:NE2	1.68	0.90
5:AE:118:THR:OG1	9:AJ:21:PHE:HZ	1.53	0.90
3:AC:190:ALA:HB1	12:AC:403:UQ6:H203	1.51	0.90
8:Ah:72:PHE:CZ	8:Ah:76:ARG:HD3	2.06	0.90
3:Ac:42:MET:CE	12:Ac:405:UQ6:C21	2.50	0.90
1:Aa:109:LEU:CD1	1:Aa:110:GLU:N	2.35	0.90
7:AG:9:ALA:HB3	7:AG:11:ILE:CD1	2.02	0.89
2:Ab:59:SER:HB3	2:Ab:224:GLY:HA3	1.54	0.89
1:Aa:96:LEU:HD21	1:Aa:161:ILE:HA	1.54	0.89
4:AD:153:GLU:HA	4:AD:168:PRO:CA	2.02	0.89
9:AJ:23:LEU:HB2	10:AK:27:VAL:HG22	1.55	0.89
4:AD:113:GLY:CA	4:AD:270:VAL:HA	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:305:THR:HG23	2:Ab:306:THR:H	1.36	0.89
3:Ac:119:LEU:HD22	11:Ac:402:HEM:HBB2	1.55	0.89
3:Ac:146:ILE:CG1	15:Ac:404:U10:H4M3	2.02	0.88
3:Ac:214:ASP:HB3	7:Ag:9:ALA:HB2	1.54	0.88
4:Ad:302:LEU:HB3	5:Ae:121:THR:OG1	1.74	0.88
5:AE:140:MET:O	3:Ac:177:ARG:NH2	2.07	0.88
9:AJ:23:LEU:HD13	10:AK:27:VAL:CG2	2.03	0.88
1:AA:402:HIS:CE1	1:AA:403:LEU:HD12	2.07	0.87
3:AC:199:PHE:CE1	3:Ac:8:HIS:CE1	2.63	0.87
8:AH:58:ARG:HD3	8:AH:61:THR:HB	1.56	0.87
5:AE:238:CYS:SG	3:Ac:268:ILE:CD1	2.63	0.87
9:AJ:30:LEU:HA	10:AK:34:TRP:CD1	2.10	0.87
7:Ag:11:ILE:HG21	7:Ag:14:VAL:CG2	2.05	0.86
4:AD:135:LEU:HA	4:AD:276:TRP:HH2	1.40	0.86
2:AB:300:LYS:HG2	2:AB:301:ARG:HG3	1.56	0.86
1:Aa:402:HIS:CE1	1:Aa:403:LEU:HD12	2.07	0.86
3:AC:148:ASN:HB2	5:Ae:220:LEU:HA	1.56	0.86
2:Ab:84:ARG:HG2	5:AI:68:VAL:CG2	2.06	0.86
7:Ag:29:SER:HB2	7:Ag:32:SER:HB2	1.57	0.86
2:AB:45:ASN:ND2	2:AB:239:ASN:HA	1.90	0.85
8:AH:47:ARG:NH2	8:AH:71:ASP:HB3	1.89	0.85
1:Aa:109:LEU:HD12	1:Aa:110:GLU:CA	2.05	0.85
5:AE:127:TYR:HH	9:AJ:36:PHE:HD1	0.87	0.85
2:AB:304:ASN:HB3	2:AB:307:SER:CB	2.07	0.85
5:Ae:200:HIS:HD2	5:Ae:201:ASP:H	1.21	0.85
1:AA:384:THR:CG2	1:AA:387:GLU:HB3	2.07	0.85
5:AE:220:LEU:CD1	3:Ac:145:VAL:HG13	2.06	0.85
3:Ac:41:LEU:HD23	12:Ac:405:UQ6:H201	1.56	0.85
5:Ae:163:LYS:H	5:Ae:178:HIS:HB3	1.42	0.84
9:AJ:30:LEU:CG	10:AK:34:TRP:HB2	2.06	0.84
3:AC:45:ILE:HA	11:AC:401:HEM:HAB	1.56	0.84
4:Ad:154:VAL:HG12	4:Ad:155:GLN:HG2	1.57	0.84
5:Ae:123:VAL:HG13	9:AJ:29:ALA:HA	1.59	0.84
4:AD:113:GLY:HA3	4:AD:270:VAL:HA	1.59	0.84
3:AC:145:VAL:CG1	5:Ae:220:LEU:HD13	2.08	0.84
5:AE:130:LYS:CD	9:AJ:33:GLU:HG2	2.04	0.84
4:AD:242:ILE:CD1	4:AD:244:MET:HE3	2.07	0.84
5:AE:127:TYR:CZ	9:AJ:36:PHE:HB3	2.11	0.84
6:AF:99:ILE:HG23	6:AF:102:ARG:HH21	1.39	0.84
9:AJ:23:LEU:HD22	10:AK:23:MET:CG	2.08	0.84
3:Ac:128:PHE:CE1	15:Ac:404:U10:H4M1	2.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:118:THR:HG1	9:AJ:21:PHE:HZ	0.84	0.83
4:Ad:201:VAL:HG21	4:Ad:275:ARG:HA	1.59	0.83
3:AC:145:VAL:HG13	5:Ae:220:LEU:CD1	2.08	0.83
2:Ab:167:GLN:HG2	5:Ai:43:LEU:HD13	1.59	0.83
5:AE:130:LYS:HB3	9:AJ:33:GLU:OE1	1.79	0.83
4:AD:262:THR:HG21	8:AH:27:PRO:HD3	1.58	0.83
9:AJ:23:LEU:HB2	10:AK:27:VAL:CG2	2.07	0.83
3:AC:199:PHE:CZ	3:Ac:8:HIS:NE2	2.46	0.83
4:AD:295:MET:HG2	9:AJ:36:PHE:CZ	2.14	0.83
4:Ad:117:TYR:HA	4:Ad:121:CYS:SG	2.19	0.83
5:AE:127:TYR:CE1	9:AJ:36:PHE:HB3	2.15	0.82
8:AH:44:ALA:HA	8:AH:47:ARG:HD3	1.61	0.82
7:AG:74:ASN:HB3	7:AG:77:MET:HG2	1.61	0.82
5:Ae:234:TYR:HB2	5:Ae:243:TYR:HB2	1.62	0.82
9:AJ:23:LEU:HD13	10:AK:27:VAL:HA	1.59	0.82
2:Ab:341:ILE:HD12	5:Ai:59:ALA:HB2	1.61	0.82
9:AJ:23:LEU:CD1	10:AK:27:VAL:HA	2.09	0.82
5:Ae:142:ALA:CB	5:Ae:147:LEU:HD23	2.08	0.82
3:AC:198:LEU:HD21	3:Ac:9:PRO:C	2.04	0.82
4:AD:227:LEU:HD22	4:AD:231:LEU:HB3	1.62	0.81
8:Ah:32:ARG:CD	8:Ah:76:ARG:HH12	1.92	0.81
5:Ai:46:LYS:HG2	5:Ai:47:ARG:N	1.93	0.81
2:AB:304:ASN:HB3	2:AB:307:SER:OG	1.79	0.81
4:AD:146:LYS:HD3	4:AD:171:LEU:HG	1.63	0.81
4:AD:213:SER:HB3	4:AD:236:TYR:CG	2.15	0.81
5:AE:126:ALA:CB	9:AJ:29:ALA:HB1	2.10	0.81
1:Aa:100:GLY:O	1:Aa:101:THR:CG2	2.28	0.81
2:Ab:163:ALA:C	5:Ai:43:LEU:HD22	2.04	0.81
4:Ad:222:PRO:HB2	8:Ah:65:CYS:HB3	1.59	0.81
4:AD:262:THR:HB	8:AH:26:ASP:HA	1.63	0.81
3:Ac:146:ILE:CD1	15:Ac:404:U10:H3M2	2.07	0.81
3:AC:145:VAL:CA	5:Ae:220:LEU:O	2.25	0.81
5:AE:122:THR:CG2	9:AJ:25:ILE:HG21	2.10	0.81
2:Ab:305:THR:HG23	2:Ab:306:THR:N	1.92	0.81
1:AA:403:LEU:HD21	2:AB:56:ALA:HB1	1.62	0.81
3:Ac:18:PHE:HE1	12:Ac:405:UQ6:H71	1.45	0.81
4:AD:120:VAL:CG2	4:AD:253:LEU:HD11	2.07	0.81
5:Ae:239:HIS:CE1	5:Ae:253:PRO:HB3	2.16	0.81
2:AB:51:SER:HB2	2:AB:230:LEU:HD12	1.61	0.81
4:Ad:223:THR:CG2	8:Ah:65:CYS:HB2	2.11	0.81
4:Ad:202:ARG:HG3	4:Ad:278:SER:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:59:SER:CB	2:Ab:224:GLY:CA	2.56	0.80
2:Ab:59:SER:HB2	2:Ab:224:GLY:CA	2.10	0.80
2:Ab:297:PRO:CB	2:Ab:304:ASN:ND2	2.41	0.80
5:Ae:204:ARG:HB3	5:Ae:260:VAL:HG21	1.64	0.80
8:AH:42:VAL:HG13	8:AH:45:ARG:HH21	1.46	0.80
1:Aa:68:THR:HG21	2:Ab:384:MET:HG3	1.62	0.80
4:AD:255:TYR:OH	4:AD:266:VAL:HA	1.81	0.80
5:AE:126:ALA:CB	9:AJ:29:ALA:CB	2.60	0.80
3:Ac:128:PHE:HD1	15:Ac:404:U10:H4M1	1.43	0.80
4:AD:158:PRO:HB2	4:AD:162:GLY:HA2	1.64	0.80
16:Ad:402:3PH:H12	5:Ae:131:ASN:ND2	1.97	0.80
2:AB:323:VAL:HG22	2:AB:340:THR:HG22	1.64	0.80
7:AG:9:ALA:CB	7:AG:11:ILE:HD11	2.11	0.80
1:AA:74:TRP:CZ2	1:AA:411:GLU:HA	2.16	0.80
3:AC:145:VAL:HG13	5:Ae:220:LEU:HD13	1.64	0.80
4:AD:227:LEU:HD22	4:AD:231:LEU:CB	2.13	0.79
5:Ae:200:HIS:CD2	5:Ae:201:ASP:H	1.99	0.79
4:Ad:153:GLU:HG2	4:Ad:168:PRO:HA	1.64	0.79
2:Ab:109:LYS:HB2	5:AI:71:ASN:OD1	1.82	0.79
1:Aa:338:CYS:HB3	1:Aa:368:MET:SD	2.22	0.79
3:Ac:253:PRO:HG2	4:Ad:205:HIS:CE1	2.17	0.79
3:Ac:138:MET:HE1	3:Ac:268:ILE:HA	1.64	0.79
4:Ad:146:LYS:HD3	4:Ad:171:LEU:HG	1.63	0.79
4:Ad:291:LYS:CB	16:Ad:402:3PH:H32	2.12	0.78
4:AD:215:LEU:HD21	13:AD:401:HEC:C2B	2.14	0.78
1:Aa:74:TRP:CZ2	1:Aa:411:GLU:HA	2.16	0.78
5:Ae:142:ALA:HB3	5:Ae:147:LEU:HD23	1.65	0.78
4:AD:215:LEU:HD23	4:AD:244:MET:CE	2.13	0.78
1:AA:182:VAL:CG1	1:AA:186:TYR:CE2	2.67	0.78
2:AB:113:THR:OG1	5:AI:65:VAL:CG1	2.32	0.78
3:AC:8:HIS:CE1	3:Ac:199:PHE:CZ	2.71	0.78
3:AC:69:ILE:HA	3:AC:73:VAL:HB	1.65	0.78
2:Ab:297:PRO:HA	2:Ab:304:ASN:OD1	1.83	0.78
4:Ad:156:ASP:HB3	4:Ad:167:ARG:HB3	1.64	0.78
2:AB:100:THR:HG23	5:AI:70:LEU:CD1	2.14	0.78
4:AD:249:TYR:H	4:AD:252:VAL:HB	1.49	0.78
2:AB:63:LEU:HD11	2:AB:238:LEU:HD21	1.65	0.77
4:AD:233:PHE:HA	4:AD:240:GLN:O	1.82	0.77
4:Ad:114:PHE:HE1	4:Ad:175:PHE:HE2	1.28	0.77
5:Ae:176:VAL:HG13	5:Ae:212:ILE:HG12	1.64	0.77
3:AC:141:TRP:CD1	3:AC:265:PRO:HD3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:221:PRO:HB2	4:AD:225:VAL:HG11	1.65	0.77
7:AG:45:ARG:HG2	7:AG:48:ARG:NH2	1.98	0.77
1:Aa:104:ARG:HB3	1:Aa:108:ALA:HB3	1.65	0.77
7:Ag:11:ILE:CG2	7:Ag:14:VAL:CG2	2.63	0.77
3:AC:215:ALA:HB2	6:AF:60:MET:HE3	1.67	0.77
7:Ag:19:LEU:HD11	7:Ag:23:GLU:HG2	1.65	0.77
2:AB:407:MET:HG2	2:AB:411:THR:OG1	1.85	0.77
6:AF:110:LYS:HG2	10:Ak:10:TYR:CE1	2.20	0.77
7:AG:25:ARG:HH12	7:AG:28:PRO:HA	1.49	0.77
1:Aa:68:THR:HG22	1:Aa:136:LEU:HD23	1.67	0.77
5:AE:93:ARG:HB3	7:AG:25:ARG:HA	1.65	0.76
5:Ae:200:HIS:NE2	5:Ae:201:ASP:OD1	2.18	0.76
1:AA:190:THR:HB	1:AA:275:ILE:HD12	1.67	0.76
5:AE:126:ALA:HB3	9:AJ:29:ALA:HB2	1.66	0.76
7:Ag:46:ILE:HG23	14:Ag:103:3PE:H3H1	1.66	0.76
4:Ad:193:LEU:HD12	4:Ad:194:PRO:HD2	1.66	0.76
4:Ad:292:MET:HA	16:Ad:402:3PH:H331	1.66	0.76
8:Ah:69:LEU:HD21	8:Ah:73:LEU:HD11	1.67	0.76
2:Ab:407:MET:HG2	2:Ab:411:THR:OG1	1.85	0.76
7:AG:31:PHE:HA	7:AG:35:ILE:CD1	2.16	0.76
5:Ae:167:PHE:HB2	5:Ae:174:LEU:HB3	1.66	0.76
2:Ab:228:SER:HA	2:Ab:231:LYS:HE2	1.68	0.76
4:Ad:291:LYS:HB3	16:Ad:402:3PH:H32	1.66	0.76
4:AD:223:THR:HG21	8:AH:64:ASP:HA	1.66	0.75
4:AD:242:ILE:CD1	4:AD:244:MET:HB3	2.15	0.75
5:AE:127:TYR:CE1	9:AJ:33:GLU:HA	2.21	0.75
5:AE:127:TYR:HD1	9:AJ:33:GLU:CA	1.95	0.75
2:Ab:126:ILE:H	2:Ab:126:ILE:HD12	1.51	0.75
7:Ag:11:ILE:HG22	7:Ag:14:VAL:HG22	1.69	0.75
1:AA:192:PHE:O	1:AA:198:ALA:HB2	1.85	0.75
1:Aa:62:GLU:OE1	1:Aa:423:ARG:NH1	2.19	0.75
5:Ae:191:GLU:HB2	5:Ae:194:GLN:HB2	1.66	0.75
5:AE:175:PHE:CE2	5:AE:224:PRO:HD2	2.22	0.75
1:Aa:68:THR:OG1	2:Ab:387:GLU:OE1	2.04	0.75
3:Ac:128:PHE:HD1	15:Ac:404:U10:C4M	1.93	0.75
5:Ae:142:ALA:HB3	5:Ae:147:LEU:CD2	2.15	0.75
7:Ag:43:ARG:HG3	14:Ag:103:3PE:H382	1.68	0.75
1:Aa:55:ASN:HB3	1:Aa:226:ALA:CB	2.16	0.75
3:AC:145:VAL:HG13	5:Ae:220:LEU:CB	2.17	0.75
5:Ae:218:THR:HG21	5:Ae:256:LEU:O	1.86	0.75
2:Ab:115:THR:HG23	2:Ab:118:ASN:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:32:ARG:CD	8:Ah:76:ARG:NH1	2.44	0.75
1:AA:62:GLU:OE1	1:AA:423:ARG:NH1	2.19	0.74
5:Ae:159:ILE:HB	5:Ae:210:TRP:CH2	2.23	0.74
3:AC:185:LEU:HD23	3:AC:188:ILE:HD12	1.69	0.74
5:AE:123:VAL:HG13	9:AJ:29:ALA:HA	1.69	0.74
1:AA:55:ASN:HB3	1:AA:226:ALA:HB1	1.68	0.74
2:AB:304:ASN:HB3	2:AB:307:SER:HB2	1.68	0.74
11:Ac:402:HEM:HMA2	12:Ac:405:UQ6:C15	2.17	0.74
1:Aa:55:ASN:HB3	1:Aa:226:ALA:HB1	1.68	0.74
2:Ab:429:LYS:HA	2:Ab:432:VAL:HG12	1.67	0.74
5:Ae:218:THR:HG21	5:Ae:256:LEU:C	2.13	0.74
6:AF:42:GLU:HA	6:AF:45:LYS:HD3	1.68	0.74
4:AD:105:LEU:HB3	4:AD:110:ILE:HD11	1.69	0.74
5:AE:220:LEU:HB3	3:Ac:145:VAL:HG22	1.68	0.74
2:Ab:297:PRO:CA	2:Ab:304:ASN:HD21	2.01	0.74
1:AA:55:ASN:HB3	1:AA:226:ALA:CB	2.16	0.74
4:Ad:202:ARG:HH21	4:Ad:279:GLU:HG3	1.53	0.73
2:Ab:146:PHE:CD2	2:Ab:202:SER:HB3	2.18	0.73
16:Ad:402:3PH:C1	5:Ae:131:ASN:HD21	1.99	0.73
1:Aa:171:GLU:O	1:Aa:174:GLU:HG2	1.88	0.73
7:AG:21:PRO:HA	7:AG:24:GLN:HE21	1.54	0.73
9:AJ:23:LEU:HD13	10:AK:27:VAL:CA	2.17	0.73
2:Ab:214:THR:O	2:Ab:218:MET:HG3	1.89	0.73
1:AA:171:GLU:O	1:AA:174:GLU:HG2	1.89	0.73
9:AJ:30:LEU:HA	10:AK:34:TRP:CD1	2.23	0.73
4:Ad:121:CYS:HA	13:Ad:401:HEC:HMC3	1.71	0.73
4:AD:126:SER:HB3	4:AD:178:PRO:HD2	1.70	0.73
5:Ae:239:HIS:CE1	5:Ae:253:PRO:HG3	2.23	0.73
4:AD:252:VAL:HG13	4:AD:253:LEU:N	2.03	0.73
5:AE:80:HIS:HD2	5:AE:81:THR:HG23	1.49	0.73
2:AB:173:ILE:HG21	2:AB:339:TYR:HE1	1.54	0.73
3:AC:141:TRP:CH2	5:Ae:223:VAL:HG23	2.23	0.73
4:AD:215:LEU:CD1	13:AD:401:HEC:HMB3	2.16	0.73
3:Ac:41:LEU:HD23	12:Ac:405:UQ6:C20	2.19	0.73
12:AC:403:UQ6:H13	12:AC:403:UQ6:H101	1.71	0.72
6:AF:106:GLU:O	6:AF:109:ALA:HB3	1.89	0.72
2:Ab:305:THR:CG2	2:Ab:306:THR:H	2.02	0.72
2:AB:173:ILE:HG21	2:AB:339:TYR:CE1	2.24	0.72
8:Ah:72:PHE:HZ	8:Ah:76:ARG:HD3	1.49	0.72
1:Aa:478:LEU:HD23	9:AJ:18:THR:HG21	1.72	0.72
4:Ad:154:VAL:HA	4:Ad:166:MET:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:187:GLU:HB3	5:Ae:201:ASP:HB3	1.71	0.72
1:AA:68:THR:HG21	2:AB:384:MET:HG3	1.71	0.72
1:AA:384:THR:HG22	1:AA:387:GLU:HB3	1.69	0.72
4:AD:110:ILE:HG23	4:AD:273:PHE:HA	1.72	0.72
1:AA:249:HIS:O	1:AA:250:LEU:HB2	1.89	0.72
2:Ab:322:ASP:OD2	5:Ai:59:ALA:HB3	1.88	0.72
4:AD:193:LEU:HD12	4:AD:194:PRO:HD2	1.71	0.72
7:AG:56:VAL:HA	7:AG:59:ILE:HD12	1.72	0.72
4:Ad:124:CYS:SG	13:Ad:401:HEC:HAC	2.29	0.72
4:AD:218:TYR:HE1	4:AD:242:ILE:HG21	1.55	0.72
2:Ab:59:SER:HB3	2:Ab:224:GLY:CA	2.20	0.72
5:Ae:176:VAL:HG22	5:Ae:212:ILE:HG23	1.71	0.72
1:AA:182:VAL:HG12	1:AA:186:TYR:CE2	2.25	0.71
1:Aa:74:TRP:HZ2	1:Aa:411:GLU:HA	1.54	0.71
4:Ad:181:ASN:HB3	4:Ad:183:GLU:CG	2.19	0.71
5:Ae:93:ARG:HD2	5:Ae:110:ARG:HD2	1.72	0.71
2:Ab:109:LYS:HG2	2:Ab:124:GLU:HB3	1.70	0.71
9:AJ:23:LEU:HA	10:AK:27:VAL:HG13	1.73	0.71
1:Aa:340:SER:HB2	5:Ai:45:VAL:HG21	1.72	0.71
5:Ai:46:LYS:CG	5:Ai:47:ARG:N	2.53	0.71
2:Ab:297:PRO:HA	2:Ab:304:ASN:CG	2.16	0.71
4:Ad:249:TYR:CZ	4:Ad:252:VAL:HA	2.25	0.71
3:AC:181:PHE:HA	3:AC:184:ILE:HG22	1.71	0.71
3:AC:266:PRO:O	5:Ae:237:PRO:HB3	1.90	0.71
4:AD:232:TYR:CE1	4:AD:245:ALA:HA	2.24	0.71
5:Ae:207:LYS:HB2	5:Ae:210:TRP:HB2	1.73	0.71
5:Ae:241:SER:HA	5:Ae:252:GLY:HA3	1.70	0.71
4:AD:145:ALA:HA	4:AD:148:LEU:HD12	1.73	0.71
4:Ad:185:ALA:HB1	4:Ad:193:LEU:HA	1.72	0.71
4:AD:313:VAL:HA	7:AG:24:GLN:HE22	1.56	0.71
1:Aa:249:HIS:O	1:Aa:250:LEU:HB2	1.89	0.71
2:Ab:167:GLN:HE22	5:Ai:46:LYS:HA	1.56	0.71
3:AC:141:TRP:NE1	3:AC:263:ASN:O	2.24	0.70
6:Af:24:ALA:O	7:Ag:48:ARG:NH2	2.24	0.70
1:AA:147:LEU:HD23	1:AA:150:ILE:HD12	1.73	0.70
4:AD:215:LEU:HD11	13:AD:401:HEC:CMB	2.16	0.70
5:Ae:164:ASN:HA	5:Ae:177:ARG:CA	2.16	0.70
2:Ab:106:VAL:HG11	2:Ab:132:ILE:HD11	1.72	0.70
2:Ab:167:GLN:HG2	5:Ai:43:LEU:CD1	2.20	0.70
16:Ad:402:3PH:C35	5:Ae:128:ALA:HB1	2.22	0.70
5:AE:80:HIS:CD2	5:AE:81:THR:CG2	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:378:ARG:O	1:AA:382:SER:N	2.23	0.70
11:AC:402:HEM:HMA1	12:AC:403:UQ6:H72	1.72	0.70
2:Ab:60:ARG:N	2:Ab:223:LEU:O	2.24	0.70
4:AD:126:SER:HB3	4:AD:178:PRO:CD	2.21	0.70
2:AB:293:LEU:HB3	2:AB:309:LEU:HG	1.73	0.70
4:AD:227:LEU:HD13	4:AD:231:LEU:C	2.17	0.70
3:Ac:137:GLN:HG3	3:Ac:265:PRO:HD3	1.73	0.70
4:Ad:201:VAL:HG22	4:Ad:278:SER:OG	1.91	0.70
3:Ac:99:GLY:HA3	14:Ac:403:3PE:H272	1.73	0.70
4:AD:121:CYS:SG	13:AD:401:HEC:CAB	2.80	0.70
4:AD:153:GLU:HG2	4:AD:168:PRO:CB	2.17	0.70
4:AD:227:LEU:HB3	4:AD:231:LEU:HB2	1.74	0.70
2:Ab:65:VAL:HG13	2:Ab:218:MET:HG2	1.73	0.70
2:Ab:177:LEU:HD11	2:Ab:272:VAL:HG22	1.72	0.70
5:Ae:235:TYR:CE1	5:Ae:240:GLY:HA2	2.27	0.70
2:Ab:106:VAL:HG23	2:Ab:108:GLY:H	1.56	0.69
5:Ae:202:LEU:HA	5:Ae:205:VAL:HG22	1.74	0.69
8:Ah:76:ARG:O	8:Ah:80:VAL:HG23	1.93	0.69
3:AC:147:THR:HG22	3:AC:161:VAL:HG13	1.75	0.69
9:AJ:23:LEU:CG	10:AK:27:VAL:HG22	2.22	0.69
1:Aa:109:LEU:HD12	1:Aa:109:LEU:C	2.15	0.69
4:Ad:146:LYS:HE3	4:Ad:170:LYS:HA	1.75	0.69
4:Ad:159:ASN:HB2	4:Ad:164:MET:H	1.57	0.69
2:Ab:183:LYS:HG3	2:Ab:254:ARG:HB3	1.74	0.69
3:Ac:128:PHE:HE1	15:Ac:404:U10:C4M	2.01	0.69
5:Ae:192:VAL:HA	5:Ae:195:LEU:HD12	1.73	0.69
1:AA:74:TRP:HZ2	1:AA:411:GLU:HA	1.54	0.69
11:Ac:402:HEM:HBA1	12:Ac:405:UQ6:C4	2.22	0.69
4:Ad:121:CYS:HB3	13:Ad:401:HEC:CAB	2.22	0.69
4:AD:308:ARG:HD3	7:AG:27:PHE:CE2	2.27	0.69
8:Ah:69:LEU:HD21	8:Ah:73:LEU:CD1	2.23	0.69
2:AB:183:LYS:HG3	2:AB:254:ARG:HB3	1.74	0.69
4:Ad:295:MET:CB	16:Ad:402:3PH:H341	2.18	0.69
4:AD:159:ASN:HB3	4:AD:166:MET:HE2	1.75	0.69
4:AD:242:ILE:HG12	4:AD:244:MET:H	1.57	0.69
5:AE:220:LEU:HD12	5:AE:239:HIS:CE1	2.27	0.69
4:Ad:146:LYS:HD2	4:Ad:149:ALA:HB3	1.74	0.69
4:Ad:158:PRO:HG3	4:Ad:167:ARG:HB2	1.73	0.69
5:Ae:127:TYR:HE1	9:Aj:33:GLU:HG3	1.57	0.69
5:AE:93:ARG:HB3	7:AG:25:ARG:CA	2.23	0.69
7:Ag:40:ARG:HA	7:Ag:43:ARG:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:412:VAL:HG13	2:AB:415:GLN:HE21	1.58	0.69
3:AC:48:GLY:HA3	11:AC:401:HEM:C1B	2.28	0.69
4:AD:228:ARG:HG2	4:AD:229:GLU:HG3	1.74	0.69
5:AE:122:THR:HB	9:AJ:25:ILE:HG21	1.75	0.69
3:Ac:41:LEU:CD2	12:Ac:405:UQ6:H201	2.23	0.69
5:Ae:200:HIS:CD2	5:Ae:201:ASP:N	2.59	0.69
9:AJ:30:LEU:HD12	10:AK:34:TRP:HB2	1.73	0.69
4:AD:113:GLY:HA2	4:AD:270:VAL:HA	1.74	0.68
1:Aa:310:ILE:HG21	1:Aa:379:LEU:HD21	1.73	0.68
5:Ae:159:ILE:HB	5:Ae:210:TRP:HH2	1.57	0.68
2:AB:115:THR:HG22	5:AI:65:VAL:HG22	1.76	0.68
5:Ae:162:GLY:H	5:Ae:178:HIS:CD2	2.12	0.68
1:AA:464:GLN:HA	7:AG:5:PHE:HB3	1.75	0.68
4:AD:135:LEU:HA	4:AD:276:TRP:CH2	2.26	0.68
3:Ac:146:ILE:HG13	15:Ac:404:U10:H4M2	1.74	0.68
3:Ac:244:LEU:CD1	4:Ad:289:GLY:HA2	2.21	0.68
8:Ah:38:LEU:HB2	8:Ah:41:CYS:SG	2.32	0.68
3:AC:114:ASN:HA	3:AC:117:VAL:HG22	1.74	0.68
6:AF:33:MET:O	6:AF:36:ASP:HB2	1.93	0.68
2:Ab:412:VAL:HG13	2:Ab:415:GLN:HE21	1.58	0.68
5:Ae:127:TYR:CE1	9:AJ:33:GLU:HG3	2.29	0.68
7:AG:35:ILE:O	7:AG:39:LEU:HG	1.92	0.68
4:Ad:158:PRO:HB2	4:Ad:164:MET:HB3	1.75	0.68
3:Ac:29:SER:HB2	17:Ag:102:CDL:H712	1.74	0.68
3:AC:287:LYS:NZ	5:Ae:255:PRO:HG2	2.07	0.68
3:AC:287:LYS:HZ1	5:Ae:255:PRO:HG2	1.57	0.68
5:AE:164:ASN:HB2	5:AE:234:TYR:OH	1.94	0.68
3:Ac:29:SER:OG	17:Ag:101:CDL:HA61	1.94	0.68
3:Ac:147:THR:HG22	3:Ac:161:VAL:HG13	1.75	0.68
3:AC:256:TYR:CD2	4:AD:202:ARG:HB3	2.28	0.68
4:AD:149:ALA:HB1	4:AD:170:LYS:C	2.18	0.68
1:Aa:338:CYS:N	1:Aa:368:MET:SD	2.67	0.68
2:Ab:123:VAL:HG21	2:Ab:133:LEU:HB3	1.76	0.68
2:Ab:297:PRO:CA	2:Ab:304:ASN:ND2	2.57	0.68
2:AB:233:VAL:HA	2:AB:236:GLN:HG2	1.76	0.67
3:AC:137:GLN:HG3	3:AC:265:PRO:HG3	1.76	0.67
4:AD:111:ARG:HG3	4:AD:140:TYR:CZ	2.29	0.67
8:AH:39:GLU:HA	8:AH:42:VAL:HB	1.75	0.67
3:Ac:16:HIS:CE1	3:Ac:201:HIS:NE2	2.62	0.67
4:Ad:164:MET:HE3	4:Ad:166:MET:HB2	1.76	0.67
1:AA:397:ASN:HD21	2:AB:126:ILE:HD11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:16:HIS:CE1	3:AC:201:HIS:NE2	2.62	0.67
3:AC:137:GLN:HE21	3:AC:264:THR:HA	1.59	0.67
3:Ac:92:ILE:HG13	3:Ac:272:TRP:CH2	2.30	0.67
4:Ad:170:LYS:HD2	5:Ae:151:LYS:HE2	1.77	0.67
4:AD:242:ILE:HD11	4:AD:244:MET:HB3	1.76	0.67
1:Aa:281:ALA:HB2	7:Ag:10:ARG:HH22	1.59	0.67
7:Ag:19:LEU:HD11	7:Ag:23:GLU:CG	2.24	0.67
3:AC:198:LEU:HD21	3:Ac:10:LEU:N	2.09	0.67
9:AJ:23:LEU:CA	10:AK:27:VAL:HG22	2.24	0.67
1:Aa:120:LEU:HB3	2:Ab:299:ILE:HA	1.75	0.67
7:Ag:11:ILE:CG2	7:Ag:14:VAL:HG22	2.25	0.67
7:AG:79:GLU:HG3	8:AH:58:ARG:HD3	1.75	0.67
1:Aa:102:LYS:HB2	1:Aa:153:ASN:O	1.95	0.67
2:Ab:116:ARG:HH22	2:Ab:175:GLU:HA	1.59	0.67
4:Ad:186:ARG:HB3	4:Ad:191:GLY:HA2	1.76	0.67
5:Ae:239:HIS:CE1	5:Ae:253:PRO:CB	2.78	0.67
10:Ak:6:LEU:HA	10:Ak:11:ARG:NH1	2.09	0.67
1:Aa:342:GLN:HE21	1:Aa:357:HIS:HB3	1.59	0.67
4:Ad:232:TYR:CD1	4:Ad:245:ALA:HA	2.30	0.67
5:Ae:273:VAL:O	5:Ae:274:GLY:C	2.38	0.67
4:AD:179:TYR:HB3	4:AD:184:ALA:HB3	1.77	0.67
8:AH:82:HIS:HB3	8:AH:83:LYS:HZ2	1.60	0.67
4:Ad:93:SER:HA	4:Ad:209:ASP:OD2	1.95	0.67
5:AE:177:ARG:HD2	5:AE:234:TYR:OH	1.95	0.67
7:AG:9:ALA:C	7:AG:11:ILE:HD12	2.20	0.67
4:AD:249:TYR:CE1	4:AD:252:VAL:HG23	2.30	0.66
2:Ab:45:ASN:HD22	2:Ab:239:ASN:HA	1.59	0.66
4:Ad:121:CYS:HB3	13:Ad:401:HEC:HAB	1.77	0.66
1:AA:87:ASN:HB3	1:AA:204:PRO:HD2	1.77	0.66
1:AA:116:ILE:HG21	1:AA:142:LYS:HG2	1.77	0.66
1:AA:342:GLN:HE21	1:AA:357:HIS:HB3	1.59	0.66
1:Aa:341:PHE:CZ	1:Aa:372:LEU:HD13	2.31	0.66
3:Ac:346:PRO:HG3	7:Ag:66:GLU:HG2	1.78	0.66
2:AB:109:LYS:HD2	5:AI:71:ASN:HD22	1.60	0.66
3:AC:169:SER:HB3	5:Ae:172:LYS:HD2	1.78	0.66
4:AD:155:GLN:NE2	4:AD:164:MET:O	2.28	0.66
2:Ab:89:LEU:HD22	2:Ab:150:GLU:HB3	1.77	0.66
4:Ad:155:GLN:H	4:Ad:165:PHE:C	2.03	0.66
5:Ae:166:ALA:HA	5:Ae:175:PHE:HA	1.77	0.66
4:AD:110:ILE:HG12	4:AD:272:THR:HG22	1.77	0.66
3:Ac:270:PRO:HG2	3:Ac:275:LEU:HD23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:159:ILE:HG23	5:Ae:163:LYS:HB2	1.78	0.66
1:AA:196:PRO:O	1:AA:199:GLN:HG2	1.95	0.66
2:AB:229:VAL:O	2:AB:232:GLN:HG2	1.95	0.66
4:Ad:177:LYS:HE3	4:Ad:180:PRO:HB3	1.77	0.66
1:AA:397:ASN:HD21	2:AB:126:ILE:CD1	2.08	0.66
3:AC:141:TRP:HD1	3:AC:265:PRO:HD3	1.59	0.66
2:Ab:305:THR:HG23	2:Ab:306:THR:HG23	1.77	0.66
2:Ab:341:ILE:CD1	5:Ai:59:ALA:HB2	2.25	0.66
4:AD:128:ASP:HA	4:AD:177:LYS:HE2	1.78	0.66
4:AD:249:TYR:CZ	4:AD:252:VAL:HA	2.31	0.65
9:Aj:30:LEU:CD1	10:AK:34:TRP:HB2	2.26	0.65
3:AC:8:HIS:CE1	3:Ac:199:PHE:HZ	2.14	0.65
1:AA:388:VAL:HG21	1:AA:438:ALA:HB2	1.78	0.65
4:AD:164:MET:HG3	4:AD:165:PHE:H	1.60	0.65
4:Ad:184:ALA:HA	4:Ad:187:ALA:HB3	1.77	0.65
4:AD:189:ASN:CB	13:AD:401:HEC:HMD2	2.23	0.65
8:AH:58:ARG:CD	8:AH:61:THR:HB	2.26	0.65
1:AA:463:GLU:CD	7:AG:8:LEU:HB2	2.21	0.65
2:Ab:307:SER:HB2	2:Ab:310:SER:HB2	1.78	0.65
1:AA:463:GLU:OE2	7:AG:8:LEU:HG	1.97	0.65
2:AB:117:GLU:OE2	2:AB:331:SER:N	2.22	0.65
2:AB:177:LEU:HD11	2:AB:272:VAL:HG22	1.77	0.65
4:AD:122:SER:HA	4:AD:125:HIS:O	1.97	0.65
4:AD:140:TYR:HA	4:AD:144:GLU:OE1	1.97	0.65
5:AE:118:THR:OG1	9:Aj:21:PHE:CZ	2.35	0.65
5:AE:122:THR:CB	9:Aj:25:ILE:HG21	2.27	0.65
1:Aa:74:TRP:HH2	1:Aa:410:CYS:HG	1.41	0.65
1:Aa:341:PHE:CE1	1:Aa:372:LEU:HD13	2.32	0.65
1:AA:403:LEU:HD12	1:AA:403:LEU:N	2.12	0.65
2:AB:299:ILE:H	2:AB:299:ILE:HD12	1.62	0.65
4:AD:127:MET:HE3	4:AD:198:SER:HA	1.79	0.65
5:Ae:239:HIS:CD2	5:Ae:239:HIS:O	2.49	0.65
1:Aa:403:LEU:HD12	1:Aa:403:LEU:N	2.12	0.65
3:Ac:238:ILE:HD12	17:Ag:102:CDL:H772	1.79	0.65
4:Ad:315:LYS:O	6:Af:72:ARG:NH1	2.26	0.65
5:Ae:166:ALA:HB2	5:Ae:175:PHE:CD1	2.31	0.64
5:Ae:199:GLN:O	5:Ae:248:ARG:HD3	1.96	0.64
3:AC:266:PRO:C	5:Ae:237:PRO:HB2	2.22	0.64
16:Ad:402:3PH:H382	5:Ae:128:ALA:HB1	1.79	0.64
5:Ae:122:THR:HG21	9:Aj:25:ILE:HD13	1.79	0.64
4:Ad:290:LEU:O	4:Ad:294:LEU:HG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:299:LEU:HD12	16:Ad:402:3PH:C37	2.27	0.64
3:AC:145:VAL:CG1	5:Ae:220:LEU:HB3	2.27	0.64
1:Aa:463:GLU:OE1	7:Ag:8:LEU:HB2	1.98	0.64
2:AB:426:LYS:O	2:AB:429:LYS:HG2	1.97	0.64
2:Ab:171:THR:HA	5:Ai:64:LEU:HD21	1.78	0.64
8:Ah:39:GLU:HG2	8:Ah:40:LYS:N	2.12	0.64
8:Ah:45:ARG:NH1	8:Ah:48:LEU:CD2	2.48	0.64
3:AC:144:THR:HG22	5:Ae:221:GLY:HA3	1.80	0.64
4:AD:235:PRO:HA	4:AD:240:GLN:HG3	1.78	0.64
7:AG:9:ALA:CB	7:AG:11:ILE:CD1	2.74	0.64
7:Ag:64:ASN:O	7:Ag:68:GLU:HG2	1.97	0.64
3:AC:211:LEU:CD2	6:AF:37:THR:HA	2.28	0.64
1:Aa:182:VAL:HG12	1:Aa:186:TYR:CE2	2.33	0.64
2:Ab:426:LYS:O	2:Ab:429:LYS:HG2	1.97	0.64
4:Ad:114:PHE:HE1	4:Ad:175:PHE:CE2	2.15	0.64
4:Ad:222:PRO:CB	8:Ah:65:CYS:HB3	2.28	0.64
4:Ad:158:PRO:HG2	4:Ad:164:MET:HG3	1.79	0.64
1:AA:101:THR:HG22	1:AA:154:SER:HA	1.78	0.64
4:AD:148:LEU:HA	4:AD:151:GLU:HB2	1.80	0.64
5:AE:122:THR:HB	9:AJ:25:ILE:CG2	2.28	0.64
5:AE:122:THR:HG21	9:AJ:25:ILE:HG21	1.79	0.64
5:AE:218:THR:CG2	5:AE:256:LEU:O	2.45	0.64
3:Ac:99:GLY:HA3	14:Ac:403:3PE:H2A1	1.80	0.64
3:AC:195:VAL:HG13	3:Ac:10:LEU:HD22	1.80	0.63
4:AD:107:HIS:CG	4:AD:138:VAL:HB	2.32	0.63
4:Ad:232:TYR:O	4:Ad:242:ILE:HG22	1.98	0.63
8:Ah:32:ARG:HG2	8:Ah:80:VAL:HG21	1.78	0.63
3:AC:138:MET:HB2	3:AC:254:ASP:HB2	1.80	0.63
4:AD:221:PRO:HB3	4:AD:233:PHE:CD1	2.34	0.63
3:AC:137:GLN:NE2	3:AC:141:TRP:HE1	1.94	0.63
3:AC:343:VAL:HG21	5:Ae:239:HIS:HD2	1.63	0.63
2:Ab:163:ALA:HB1	5:Ai:43:LEU:CD2	2.28	0.63
4:Ad:133:ARG:HD3	4:Ad:172:SER:HA	1.81	0.63
16:Ad:402:3PH:H262	16:Ad:402:3PH:H332	1.79	0.63
1:AA:468:TYR:HE1	1:AA:472:ARG:HH11	1.46	0.63
4:AD:233:PHE:CE2	4:AD:235:PRO:HD3	2.34	0.63
4:AD:237:PHE:CD1	4:AD:238:PRO:HD2	2.34	0.63
4:AD:263:MET:HE3	8:AH:28:LEU:HD23	1.80	0.63
1:AA:467:ASP:OD2	3:AC:223:TYR:CE2	2.52	0.63
3:AC:128:PHE:CZ	3:AC:143:ALA:HA	2.34	0.63
1:Aa:80:ARG:NH2	1:Aa:268:CYS:SG	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:77:TRP:HZ2	4:Ad:284:HIS:CD2	2.16	0.63
4:Ad:249:TYR:CE1	4:Ad:252:VAL:HA	2.34	0.63
6:AF:78:LYS:HA	6:AF:81:TRP:CE2	2.34	0.63
9:AJ:30:LEU:HA	10:AK:34:TRP:CG	2.33	0.63
4:AD:152:VAL:HG11	4:AD:176:PRO:HG3	1.79	0.62
5:AE:175:PHE:HE2	5:AE:224:PRO:HD2	1.64	0.62
9:Aj:23:LEU:HD13	10:Ak:27:VAL:HG22	1.81	0.62
5:AE:234:TYR:HB2	5:AE:243:TYR:HB2	1.79	0.62
2:Ab:176:ASN:HB3	2:Ab:258:ILE:HD11	1.81	0.62
1:AA:362:ALA:HB2	1:AA:461:PRO:HB2	1.81	0.62
3:AC:223:TYR:O	4:AD:311:TRP:NE1	2.32	0.62
4:AD:215:LEU:HD21	13:AD:401:HEC:CMB	2.29	0.62
5:AE:93:ARG:HB3	7:AG:25:ARG:N	2.14	0.62
8:AH:48:LEU:HD13	8:AH:69:LEU:HA	1.81	0.62
1:AA:74:TRP:HH2	1:AA:410:CYS:HG	1.44	0.62
1:AA:169:LEU:HD11	1:AA:209:ARG:HG2	1.81	0.62
3:AC:69:ILE:HG12	3:AC:73:VAL:HG21	1.82	0.62
4:AD:95:PRO:HA	4:AD:99:ARG:HH21	1.63	0.62
1:Aa:169:LEU:HD11	1:Aa:209:ARG:HG2	1.82	0.62
3:Ac:323:ILE:HD11	14:Ag:103:3PE:H12	1.80	0.62
8:Ah:44:ALA:O	8:Ah:48:LEU:N	2.32	0.62
8:AH:69:LEU:O	8:AH:73:LEU:HG	2.00	0.62
1:Aa:100:GLY:C	1:Aa:101:THR:HG23	2.24	0.62
1:AA:114:GLU:HG2	2:AB:299:ILE:HD11	1.82	0.62
1:Aa:204:PRO:HB2	1:Aa:206:GLU:OE1	1.98	0.62
1:Aa:478:LEU:CD2	9:Aj:18:THR:HG21	2.28	0.62
16:Ad:402:3PH:H352	5:Ae:128:ALA:HB1	1.81	0.62
2:AB:176:ASN:HB3	2:AB:258:ILE:HD11	1.82	0.62
5:AE:130:LYS:HB3	9:AJ:33:GLU:CD	2.25	0.62
1:Aa:274:GLU:HG3	1:Aa:456:VAL:HB	1.80	0.62
2:Ab:65:VAL:HG22	2:Ab:218:MET:HG2	1.82	0.62
5:Ae:239:HIS:ND1	5:Ae:253:PRO:CB	2.62	0.62
1:AA:99:LYS:HG3	1:AA:160:GLN:HG2	1.82	0.62
5:AE:132:VAL:HA	5:AE:135:GLN:HE21	1.65	0.62
8:AH:51:CYS:SG	8:AH:68:GLU:HB2	2.39	0.62
1:Aa:451:ASP:OD2	9:Aj:16:ARG:HG3	2.00	0.62
2:Ab:106:VAL:HG21	2:Ab:133:LEU:HD21	1.81	0.62
7:Ag:11:ILE:CG2	7:Ag:14:VAL:HG21	2.18	0.62
1:AA:399:LEU:HB3	1:AA:426:LEU:CD2	2.30	0.62
3:AC:148:ASN:CB	5:Ae:220:LEU:HA	2.28	0.62
1:Aa:362:ALA:HB2	1:Aa:461:PRO:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:223:TYR:O	4:Ad:311:TRP:NE1	2.33	0.62
5:Ae:229:GLY:HA2	5:Ae:242:HIS:ND1	2.14	0.62
8:Ah:47:ARG:HG2	8:Ah:50:LEU:HD12	1.82	0.62
3:Ac:145:VAL:CG2	5:Ae:222:CYS:SG	2.88	0.62
3:Ac:244:LEU:HD13	4:Ad:289:GLY:CA	2.23	0.62
8:Ah:41:CYS:O	8:Ah:45:ARG:N	2.33	0.62
2:AB:38:LEU:HD11	2:AB:396:ILE:HD13	1.81	0.61
4:AD:215:LEU:HD23	4:AD:244:MET:HE2	1.82	0.61
1:Aa:136:LEU:HD21	2:Ab:380:ALA:HA	1.81	0.61
1:Aa:182:VAL:CG1	1:Aa:186:TYR:CE2	2.83	0.61
1:Aa:399:LEU:HB3	1:Aa:426:LEU:CD2	2.30	0.61
2:Ab:108:GLY:HA2	2:Ab:124:GLU:O	2.00	0.61
16:Ad:402:3PH:H352	5:Ae:128:ALA:CB	2.30	0.61
5:Ae:159:ILE:HG21	5:Ae:178:HIS:HB2	1.81	0.61
3:Ac:254:ASP:HA	3:Ac:257:MET:HE2	1.80	0.61
1:Aa:384:THR:O	1:Aa:387:GLU:HG2	2.00	0.61
2:Ab:163:ALA:HB1	5:Ai:43:LEU:HD23	1.79	0.61
5:Ae:152:ILE:HG13	5:Ae:154:ILE:HD11	1.82	0.61
8:Ah:39:GLU:HG2	8:Ah:40:LYS:H	1.65	0.61
3:Ac:16:HIS:NE2	3:Ac:201:HIS:NE2	2.49	0.61
1:Aa:91:TYR:CZ	1:Aa:95:HIS:HE1	2.17	0.61
3:Ac:45:ILE:HA	11:Ac:401:HEM:HAB	1.81	0.61
5:Ae:181:LYS:HA	5:Ae:184:ILE:HD12	1.81	0.61
4:AD:227:LEU:HD13	4:AD:231:LEU:O	2.00	0.61
5:AE:244:ASP:HB3	5:AE:250:ARG:HH11	1.65	0.61
2:Ab:412:VAL:O	2:Ab:415:GLN:HG2	2.00	0.61
8:Ah:51:CYS:SG	8:Ah:69:LEU:N	2.73	0.61
2:AB:412:VAL:O	2:AB:415:GLN:HG2	2.00	0.61
4:AD:104:SER:HB2	4:AD:283:ASP:CG	2.25	0.61
1:Aa:97:ALA:O	1:Aa:98:PHE:HB2	2.00	0.61
1:Aa:463:GLU:OE2	7:Ag:6:GLY:N	2.34	0.61
6:Af:108:TRP:HA	6:Af:111:LYS:HZ2	1.64	0.61
8:Ah:32:ARG:HD3	8:Ah:76:ARG:HH11	1.59	0.61
9:Aj:23:LEU:HD22	10:Ak:23:MET:SD	2.40	0.61
1:Aa:477:TRP:O	9:Aj:17:ARG:NH2	2.34	0.61
4:AD:223:THR:CG2	8:AH:64:ASP:HA	2.31	0.61
8:AH:26:ASP:HB3	8:AH:29:THR:HG23	1.82	0.61
2:Ab:322:ASP:OD2	5:Ai:59:ALA:CB	2.47	0.61
3:Ac:16:HIS:NE2	3:Ac:201:HIS:NE2	2.49	0.61
3:Ac:137:GLN:HE21	3:Ac:264:THR:HA	1.66	0.61
4:Ad:274:LEU:HD11	13:Ad:401:HEC:HMB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:131:ALA:H	4:AD:134:HIS:HB2	1.64	0.61
4:AD:201:VAL:HG22	4:AD:278:SER:OG	2.01	0.61
3:AC:137:GLN:NE2	3:AC:264:THR:HA	2.16	0.61
3:AC:260:ASN:CG	3:AC:263:ASN:H	2.08	0.61
4:AD:89:LEU:HD13	8:AH:70:PHE:HB3	1.83	0.61
5:AE:115:TYR:HB3	9:AJ:21:PHE:CE1	2.36	0.61
1:Aa:373:GLN:O	1:Aa:377:MET:HG2	2.01	0.61
2:Ab:47:LEU:HD12	2:Ab:219:ALA:HA	1.83	0.61
2:AB:100:THR:HG23	5:AI:70:LEU:HD13	1.81	0.61
4:AD:153:GLU:CG	4:AD:168:PRO:HB3	2.19	0.61
4:Ad:126:SER:HB3	4:Ad:178:PRO:HD3	1.83	0.61
4:Ad:201:VAL:HG22	4:Ad:278:SER:CB	2.31	0.60
4:Ad:315:LYS:C	6:Af:72:ARG:HH12	2.08	0.60
5:Ae:197:ASP:HB3	5:Ae:257:ASN:CG	2.25	0.60
2:AB:429:LYS:HA	2:AB:432:VAL:HG12	1.83	0.60
5:AE:93:ARG:CB	7:AG:25:ARG:HA	2.31	0.60
6:Af:92:GLU:HG2	6:Af:96:LYS:HE2	1.82	0.60
7:AG:43:ARG:O	7:AG:47:LEU:HG	2.02	0.60
1:Aa:104:ARG:HB3	1:Aa:108:ALA:CB	2.31	0.60
1:Aa:341:PHE:HE1	1:Aa:356:ALA:HB1	1.66	0.60
3:Ac:107:TYR:HB2	3:Ac:305:PRO:HG3	1.84	0.60
2:AB:45:ASN:HD21	2:AB:239:ASN:HA	1.63	0.60
3:AC:281:LEU:HD12	3:AC:290:GLY:HA3	1.82	0.60
4:AD:252:VAL:CG1	4:AD:253:LEU:N	2.64	0.60
2:Ab:138:LEU:HB3	2:Ab:237:PHE:HD2	1.66	0.60
7:Ag:46:ILE:HG21	14:Ag:103:3PE:H3H1	1.82	0.60
10:Ak:23:MET:O	10:Ak:27:VAL:HG23	2.02	0.60
3:AC:302:ALA:O	3:AC:305:PRO:HD2	2.02	0.60
2:Ab:167:GLN:CG	5:AI:43:LEU:HD13	2.32	0.60
4:Ad:126:SER:CB	4:Ad:177:LYS:HA	2.30	0.60
1:AA:168:ILE:O	1:AA:171:GLU:HG2	2.02	0.60
1:Aa:168:ILE:O	1:Aa:171:GLU:HG2	2.01	0.60
2:Ab:225:VAL:HG11	2:Ab:230:LEU:HD21	1.83	0.60
4:Ad:158:PRO:HG2	4:Ad:166:MET:H	1.66	0.60
4:Ad:158:PRO:HA	4:Ad:167:ARG:CZ	2.31	0.60
5:Ae:207:LYS:NZ	5:Ae:268:ASP:HA	2.17	0.60
5:AI:46:LYS:CG	5:AI:47:ARG:H	2.15	0.60
3:AC:63:PHE:O	3:AC:67:THR:HG23	2.02	0.60
4:AD:119:GLN:HB2	4:AD:253:LEU:HD13	1.84	0.60
5:AE:119:ALA:HA	9:AJ:25:ILE:CG1	2.31	0.60
4:Ad:288:MET:SD	16:Ad:402:3PH:H2	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:283:PRO:HB2	5:AI:42:VAL:HG12	1.83	0.60
1:AA:341:PHE:HE1	1:AA:356:ALA:HB1	1.66	0.60
12:AC:403:UQ6:H101	12:AC:403:UQ6:C13	2.31	0.60
7:AG:31:PHE:CA	7:AG:35:ILE:HD12	2.24	0.60
8:AH:42:VAL:O	8:AH:46:GLU:HG3	2.01	0.60
10:AK:23:MET:O	10:AK:27:VAL:HG23	2.01	0.60
1:Aa:103:ASN:HD21	1:Aa:104:ARG:NH1	1.99	0.60
4:Ad:223:THR:HG23	8:Ah:55:VAL:HG21	1.83	0.60
14:Ag:103:3PE:H3D1	14:Ag:103:3PE:H391	1.82	0.60
2:AB:113:THR:OG1	5:AI:65:VAL:HG11	2.02	0.60
4:AD:215:LEU:HD13	13:AD:401:HEC:HBB2	1.84	0.60
5:AE:127:TYR:O	9:AJ:33:GLU:OE1	2.20	0.60
7:AG:54:VAL:O	7:AG:58:LEU:HG	2.02	0.60
4:Ad:131:ALA:HB2	4:Ad:174:TYR:CD2	2.37	0.60
6:Af:108:TRP:HA	6:Af:111:LYS:NZ	2.17	0.60
1:Aa:402:HIS:NE2	1:Aa:403:LEU:HD12	2.17	0.59
3:Ac:345:HIS:CE1	3:Ac:346:PRO:HB3	2.37	0.59
1:AA:402:HIS:NE2	1:AA:403:LEU:HD12	2.17	0.59
3:AC:8:HIS:HE1	3:Ac:199:PHE:CZ	2.18	0.59
1:Aa:275:ILE:HD12	7:Ag:17:TYR:CE2	2.38	0.59
3:Ac:302:ALA:O	3:Ac:305:PRO:HD2	2.02	0.59
16:Ad:402:3PH:C38	5:Ae:128:ALA:HB1	2.32	0.59
16:Ad:402:3PH:H361	5:Ae:128:ALA:HB2	1.84	0.59
5:Ae:132:VAL:HA	5:Ae:135:GLN:NE2	2.17	0.59
1:AA:402:HIS:CD2	1:AA:403:LEU:HD12	2.38	0.59
3:AC:211:LEU:HD21	6:AF:37:THR:HA	1.84	0.59
3:AC:345:HIS:CE1	3:AC:346:PRO:HB3	2.38	0.59
4:AD:110:ILE:O	4:AD:273:PHE:HB2	2.03	0.59
6:AF:52:PRO:HD3	2:Ab:148:ARG:NH2	2.18	0.59
7:AG:29:SER:CB	7:AG:32:SER:HB3	2.32	0.59
2:Ab:313:VAL:HG21	2:Ab:323:VAL:HG21	1.83	0.59
4:Ad:120:VAL:HG11	4:Ad:248:ILE:HD11	1.83	0.59
7:Ag:47:LEU:HB3	14:Ag:103:3PE:O22	2.02	0.59
1:AA:111:LYS:HA	2:AB:305:THR:HG21	1.84	0.59
2:AB:138:LEU:CD2	2:AB:238:LEU:HG	2.32	0.59
3:AC:51:LEU:HD12	11:AC:401:HEM:HBA1	1.83	0.59
4:AD:215:LEU:HD23	4:AD:244:MET:HE1	1.83	0.59
7:AG:51:PRO:HB2	7:AG:52:PRO:HD3	1.82	0.59
3:Ac:215:ALA:HA	7:Ag:11:ILE:HD11	1.84	0.59
3:Ac:276:PHE:HZ	3:Ac:298:ILE:HD11	1.67	0.59
3:AC:198:LEU:HD21	3:Ac:9:PRO:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:114:PHE:HD2	4:AD:140:TYR:CZ	2.20	0.59
7:AG:68:GLU:HA	7:AG:71:LYS:HE2	1.85	0.59
4:Ad:291:LYS:HB2	16:Ad:402:3PH:H32	1.83	0.59
1:AA:190:THR:HB	1:AA:275:ILE:CD1	2.31	0.59
1:AA:403:LEU:CD1	1:AA:403:LEU:H	2.16	0.59
2:AB:286:PHE:CE1	2:AB:427:ALA:HB1	2.38	0.59
3:AC:135:TRP:CG	3:AC:135:TRP:O	2.56	0.59
8:AH:54:ARG:HA	8:AH:57:SER:HB3	1.83	0.59
1:Aa:66:HIS:HE1	1:Aa:402:HIS:HB2	1.68	0.59
2:Ab:71:TYR:O	2:Ab:212:HIS:CE1	2.56	0.59
3:Ac:137:GLN:NE2	3:Ac:141:TRP:HE1	2.01	0.59
7:Ag:19:LEU:CD2	7:Ag:24:GLN:HB3	2.30	0.59
7:AG:49:VAL:O	7:AG:52:PRO:HD2	2.03	0.59
1:Aa:186:TYR:HB3	1:Aa:275:ILE:HG21	1.84	0.59
1:Aa:402:HIS:CD2	1:Aa:403:LEU:HD12	2.38	0.59
5:Ae:143:SER:HB2	5:Ae:146:VAL:HG22	1.84	0.59
8:Ah:72:PHE:HE2	8:Ah:76:ARG:HE	1.49	0.59
1:AA:57:LEU:HD13	1:AA:229:MET:HB3	1.85	0.59
2:AB:100:THR:HG23	5:AI:70:LEU:HD11	1.84	0.59
9:AJ:33:GLU:HB2	10:AK:34:TRP:HE1	1.68	0.59
2:Ab:286:PHE:CE1	2:Ab:427:ALA:HB1	2.38	0.59
4:Ad:224:GLY:HA3	8:Ah:64:ASP:CB	2.32	0.59
3:AC:169:SER:HB3	5:Ae:172:LYS:CD	2.33	0.59
3:AC:198:LEU:HD21	3:Ac:10:LEU:CA	2.33	0.59
1:Aa:118:ALA:O	2:Ab:298:HIS:HB3	2.03	0.59
2:Ab:79:THR:HG23	2:Ab:205:LEU:HD23	1.83	0.59
4:Ad:158:PRO:HD2	4:Ad:164:MET:C	2.27	0.59
6:Af:106:GLU:O	6:Af:110:LYS:HG3	2.03	0.59
5:Ai:71:ASN:HB3	5:Ai:73:PRO:HD2	1.85	0.59
1:AA:64:SER:OG	1:AA:235:GLY:HA2	2.02	0.59
3:AC:48:GLY:HA3	11:AC:401:HEM:C2B	2.38	0.59
2:AB:45:ASN:HD22	2:AB:239:ASN:HA	1.66	0.58
3:AC:137:GLN:NE2	3:AC:141:TRP:NE1	2.51	0.58
5:AE:163:LYS:O	5:AE:177:ARG:HG3	2.03	0.58
3:Ac:312:GLN:HE21	6:Af:37:THR:CB	2.16	0.58
4:Ad:92:PRO:HD3	4:Ad:236:TYR:CE1	2.38	0.58
16:Ad:402:3PH:C36	5:Ae:128:ALA:CB	2.80	0.58
5:Ae:93:ARG:NH2	7:Ag:24:GLN:O	2.36	0.58
3:AC:65:SER:O	3:AC:69:ILE:HG13	2.03	0.58
3:AC:130:GLY:HA3	11:AC:401:HEM:C1D	2.39	0.58
3:AC:253:PRO:HB3	4:AD:202:ARG:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:75:PRO:O	7:AG:79:GLU:HB2	2.03	0.58
4:Ad:112:ARG:HD3	4:Ad:257:ASP:OD2	2.04	0.58
5:Ae:207:LYS:HD2	5:Ae:210:TRP:HD1	1.67	0.58
8:AH:67:GLU:HG3	8:AH:68:GLU:OE1	2.03	0.58
1:Aa:220:LEU:O	1:Aa:224:TYR:HB2	2.03	0.58
2:Ab:173:ILE:HG21	2:Ab:339:TYR:HE1	1.67	0.58
4:Ad:177:LYS:HD2	4:Ad:180:PRO:HA	1.85	0.58
2:AB:195:TYR:CD1	2:Ab:262:ASN:HA	2.37	0.58
1:Aa:64:SER:OG	1:Aa:235:GLY:HA2	2.03	0.58
1:Aa:98:PHE:C	1:Aa:109:LEU:HD21	2.28	0.58
1:Aa:363:MET:HA	1:Aa:464:GLN:OE1	2.03	0.58
4:Ad:299:LEU:CD1	16:Ad:402:3PH:H371	2.33	0.58
3:AC:8:HIS:NE2	3:Ac:199:PHE:CE1	2.72	0.58
4:AD:136:VAL:HA	4:AD:140:TYR:O	2.03	0.58
5:AE:239:HIS:NE2	3:Ac:278:TYR:OH	2.33	0.58
2:Ab:208:PHE:CE1	2:Ab:212:HIS:HB2	2.39	0.58
3:Ac:18:PHE:CE1	12:Ac:405:UQ6:H71	2.34	0.58
8:Ah:69:LEU:CD2	8:Ah:73:LEU:CD1	2.81	0.58
3:Ac:253:PRO:HG2	4:Ad:205:HIS:NE2	2.18	0.58
8:Ah:47:ARG:O	8:Ah:51:CYS:N	2.36	0.58
1:AA:363:MET:HA	1:AA:464:GLN:OE1	2.03	0.58
2:AB:173:ILE:CG2	2:AB:339:TYR:HE1	2.16	0.58
2:AB:177:LEU:HD21	2:AB:272:VAL:CG1	2.34	0.58
4:AD:95:PRO:HA	4:AD:99:ARG:NH2	2.18	0.58
6:AF:75:ILE:HD12	6:AF:81:TRP:CZ2	2.39	0.58
1:Aa:403:LEU:CD1	1:Aa:403:LEU:H	2.16	0.58
2:Ab:126:ILE:O	2:Ab:130:ILE:HG23	2.04	0.58
3:Ac:137:GLN:HA	3:Ac:259:ALA:HA	1.85	0.58
4:Ad:294:LEU:HB2	9:Aj:36:PHE:HZ	1.69	0.58
5:Ae:144:ALA:HA	5:Ae:147:LEU:HG	1.86	0.58
7:AG:65:GLN:O	7:AG:69:GLN:HG2	2.03	0.58
1:Aa:57:LEU:HD13	1:Aa:229:MET:HB3	1.85	0.58
1:Aa:341:PHE:HB2	1:Aa:368:MET:HE1	1.84	0.58
3:Ac:71:ARG:NE	4:Ad:199:TYR:OH	2.36	0.58
1:AA:66:HIS:HE1	1:AA:402:HIS:HB2	1.68	0.57
1:AA:70:THR:HG21	1:AA:407:THR:HA	1.85	0.57
1:AA:133:ILE:HG13	1:AA:147:LEU:HD21	1.86	0.57
2:AB:51:SER:HB2	2:AB:230:LEU:CD1	2.33	0.57
7:AG:19:LEU:HD23	7:AG:24:GLN:HB3	1.85	0.57
1:AA:402:HIS:ND1	1:AA:403:LEU:CD1	2.68	0.57
3:AC:72:ASP:O	3:AC:73:VAL:C	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:138:MET:HE1	3:AC:268:ILE:HG12	1.86	0.57
1:Aa:96:LEU:HD21	1:Aa:161:ILE:CA	2.31	0.57
3:Ac:253:PRO:CG	4:Ad:205:HIS:CD2	2.88	0.57
3:AC:198:LEU:HD11	3:Ac:9:PRO:HB2	1.85	0.57
6:AF:88:LYS:NZ	6:AF:90:TYR:HB3	2.20	0.57
3:Ac:147:THR:HG21	3:Ac:165:TRP:CD1	2.40	0.57
7:Ag:11:ILE:HG22	7:Ag:12:ARG:N	2.18	0.57
2:AB:148:ARG:NH2	6:Af:52:PRO:HD3	2.19	0.57
4:AD:94:TYR:HB2	4:AD:96:TRP:NE1	2.19	0.57
4:AD:131:ALA:HB3	4:AD:133:ARG:HG2	1.87	0.57
1:AA:310:ILE:HG22	1:AA:378:ARG:HH22	1.69	0.57
3:AC:8:HIS:HE1	3:Ac:199:PHE:HZ	1.51	0.57
3:AC:268:ILE:HD13	5:Ae:238:CYS:SG	2.42	0.57
5:AE:175:PHE:CZ	5:AE:224:PRO:HD2	2.38	0.57
7:AG:29:SER:HB3	7:AG:32:SER:HB3	1.84	0.57
2:Ab:300:LYS:HG2	2:Ab:301:ARG:HG3	1.86	0.57
7:Ag:35:ILE:HB	7:Ag:36:PRO:HD3	1.86	0.57
3:AC:18:PHE:CE1	12:AC:403:UQ6:H1M2	2.40	0.57
3:AC:168:PHE:HD2	5:Ae:170:ARG:HB3	1.70	0.57
4:AD:227:LEU:HD22	4:AD:231:LEU:HB2	1.86	0.57
11:Ac:402:HEM:O1A	11:Ac:402:HEM:HHA	2.04	0.57
4:Ad:126:SER:HB3	4:Ad:177:LYS:HA	1.85	0.57
5:Ae:207:LYS:HB3	5:Ae:209:GLU:OE1	2.05	0.57
7:Ag:27:PHE:HB3	7:Ag:30:TYR:HB2	1.87	0.57
3:Ac:150:LEU:HD13	3:Ac:164:ILE:HD12	1.86	0.57
3:Ac:171:ASP:CG	3:Ac:172:LYS:H	2.13	0.57
1:AA:87:ASN:OD1	1:AA:199:GLN:HB2	2.05	0.57
2:AB:113:THR:OG1	5:AI:65:VAL:HG12	2.04	0.57
4:AD:213:SER:HB3	4:AD:236:TYR:CD2	2.38	0.57
4:AD:311:TRP:HB3	4:AD:315:LYS:HE3	1.86	0.57
9:AJ:23:LEU:HA	10:AK:27:VAL:CG1	2.33	0.57
4:Ad:291:LYS:HE2	9:AJ:40:ALA:HB3	1.86	0.57
1:AA:74:TRP:CH2	1:AA:410:CYS:SG	2.97	0.57
1:AA:182:VAL:HG13	1:AA:186:TYR:CE2	2.40	0.57
1:AA:220:LEU:O	1:AA:224:TYR:HB2	2.03	0.57
4:AD:217:GLY:HA3	4:AD:236:TYR:HD2	1.69	0.57
4:AD:242:ILE:HG23	4:AD:243:GLY:N	2.18	0.57
8:AH:85:PHE:HA	8:AH:88:LEU:HD12	1.87	0.57
1:Aa:70:THR:HG21	1:Aa:407:THR:HA	1.85	0.57
1:Aa:402:HIS:CG	1:Aa:403:LEU:HD12	2.40	0.57
5:Ae:242:HIS:N	5:Ae:251:LYS:O	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:74:TRP:CH2	1:Aa:410:CYS:SG	2.97	0.57
1:Aa:279:ASP:OD1	7:Ag:12:ARG:NE	2.37	0.57
7:Ag:42:THR:HA	17:Ag:101:CDL:HB61	1.86	0.57
1:AA:87:ASN:HD22	1:AA:204:PRO:HD3	1.69	0.56
3:AC:171:ASP:CG	3:AC:172:LYS:H	2.13	0.56
4:Ad:159:ASN:H	4:Ad:164:MET:HB3	1.70	0.56
4:Ad:245:ALA:O	4:Ad:246:PRO:C	2.47	0.56
1:AA:375:GLN:O	1:AA:378:ARG:HB3	2.05	0.56
9:AJ:23:LEU:HA	10:AK:27:VAL:HG22	1.87	0.56
1:Aa:402:HIS:ND1	1:Aa:403:LEU:HD12	2.20	0.56
4:Ad:117:TYR:OH	4:Ad:126:SER:HA	2.04	0.56
4:Ad:227:LEU:HB2	4:Ad:231:LEU:HB2	1.86	0.56
6:Af:22:TYR:CD2	6:Af:84:TYR:HB2	2.40	0.56
6:Af:107:GLU:OE2	6:Af:111:LYS:HD3	2.05	0.56
8:Ah:45:ARG:O	8:Ah:48:LEU:HB3	2.05	0.56
1:AA:87:ASN:H	1:AA:207:ASN:HD22	1.53	0.56
4:AD:95:PRO:HG2	8:AH:85:PHE:HB2	1.86	0.56
4:AD:247:PRO:HG3	13:AD:401:HEC:CHC	2.35	0.56
1:Aa:52:ILE:HG12	1:Aa:53:LEU:H	1.69	0.56
1:Aa:87:ASN:HD21	1:Aa:199:GLN:HB2	1.69	0.56
7:Ag:33:LYS:C	7:Ag:36:PRO:HD2	2.30	0.56
1:AA:87:ASN:ND2	1:AA:204:PRO:HD3	2.20	0.56
4:AD:120:VAL:HG23	4:AD:253:LEU:CD1	2.15	0.56
8:AH:43:LYS:HA	8:AH:46:GLU:CD	2.29	0.56
8:AH:86:LYS:HG3	8:AH:87:ASN:N	2.20	0.56
5:Ae:218:THR:OG1	5:Ae:254:ALA:HB1	2.05	0.56
1:AA:402:HIS:CG	1:AA:403:LEU:HD12	2.40	0.56
4:AD:249:TYR:CE2	4:AD:252:VAL:HA	2.40	0.56
5:AE:123:VAL:HG13	9:AJ:29:ALA:CA	2.35	0.56
5:AE:218:THR:HG21	5:AE:256:LEU:C	2.30	0.56
2:Ab:146:PHE:CE1	2:Ab:206:HIS:ND1	2.73	0.56
5:Ae:155:LYS:HE2	5:Ae:157:SER:HB3	1.86	0.56
5:Ae:249:ILE:HG12	5:Ae:254:ALA:HB3	1.87	0.56
1:AA:402:HIS:ND1	1:AA:403:LEU:HD12	2.20	0.56
3:AC:97:HIS:CE1	3:AC:100:ARG:HH21	2.24	0.56
3:AC:137:GLN:HE21	3:AC:265:PRO:HD3	1.69	0.56
3:AC:375:LYS:NZ	6:AF:14:LEU:HD21	2.21	0.56
4:AD:111:ARG:HA	4:AD:140:TYR:CE1	2.40	0.56
4:AD:120:VAL:CG1	4:AD:247:PRO:HB2	2.35	0.56
4:AD:158:PRO:CB	4:AD:162:GLY:HA2	2.35	0.56
5:AE:123:VAL:HA	9:AJ:29:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:219:HIS:HB2	5:AE:254:ALA:HA	1.88	0.56
4:Ad:89:LEU:HD11	8:Ah:74:HIS:HA	1.87	0.56
5:Ae:197:ASP:HB3	5:Ae:257:ASN:ND2	2.21	0.56
2:AB:426:LYS:HA	2:AB:429:LYS:HZ3	1.70	0.56
3:AC:150:LEU:HD13	3:AC:164:ILE:HD12	1.86	0.56
4:Ad:114:PHE:CE1	4:Ad:175:PHE:HE2	2.18	0.56
4:Ad:248:ILE:HG23	4:Ad:252:VAL:HG11	1.87	0.56
5:Ae:179:ARG:NH2	5:Ae:208:PRO:HA	2.21	0.56
9:Aj:30:LEU:HA	10:Ak:34:TRP:CG	2.40	0.56
6:AF:22:TYR:CE2	6:AF:28:ASN:HB3	2.41	0.56
3:Ac:311:LYS:O	6:Af:39:HIS:N	2.31	0.56
4:Ad:237:PHE:CG	4:Ad:238:PRO:HD2	2.41	0.56
2:AB:116:ARG:HH22	2:AB:175:GLU:CD	2.14	0.56
3:AC:98:VAL:HG22	11:AC:402:HEM:CBC	2.23	0.56
1:Aa:402:HIS:ND1	1:Aa:403:LEU:CD1	2.67	0.56
4:Ad:114:PHE:HD2	4:Ad:140:TYR:CZ	2.24	0.56
3:AC:147:THR:HG21	3:AC:165:TRP:CD1	2.40	0.55
3:AC:260:ASN:O	3:AC:261:PRO:C	2.43	0.55
1:Aa:403:LEU:CD1	1:Aa:403:LEU:N	2.69	0.55
2:Ab:366:LEU:HD21	2:Ab:425:VAL:HG22	1.87	0.55
3:Ac:119:LEU:HD22	11:Ac:402:HEM:CBB	2.32	0.55
3:Ac:294:LEU:HD21	15:Ac:404:U10:H1M3	1.88	0.55
5:Ae:132:VAL:O	5:Ae:135:GLN:HG2	2.06	0.55
1:AA:118:ALA:HB2	1:AA:135:ALA:HB2	1.87	0.55
2:AB:236:GLN:HG3	2:AB:237:PHE:CD2	2.41	0.55
2:AB:366:LEU:HD21	2:AB:425:VAL:HG22	1.87	0.55
3:AC:129:MET:HB2	3:AC:182:HIS:HD1	1.71	0.55
3:AC:153:ILE:HB	3:AC:157:GLY:CA	2.36	0.55
1:Aa:120:LEU:HD23	2:Ab:299:ILE:HG12	1.88	0.55
4:Ad:224:GLY:HA3	8:Ah:64:ASP:HB3	1.87	0.55
5:Ae:159:ILE:CG2	5:Ae:163:LYS:HB2	2.35	0.55
8:Ah:42:VAL:HA	8:Ah:45:ARG:HB3	1.88	0.55
1:AA:403:LEU:CD1	1:AA:403:LEU:N	2.69	0.55
1:AA:467:ASP:OD2	3:AC:223:TYR:HE2	1.88	0.55
2:AB:60:ARG:HG3	2:AB:124:GLU:HB3	1.89	0.55
8:AH:35:CYS:O	8:AH:38:LEU:HB2	2.07	0.55
1:Aa:113:VAL:CG2	1:Aa:118:ALA:HB3	2.36	0.55
10:Ak:10:TYR:HA	10:Ak:13:LEU:HD12	1.87	0.55
1:AA:170:ARG:HG3	1:AA:171:GLU:N	2.22	0.55
4:AD:252:VAL:CG1	4:AD:253:LEU:H	2.20	0.55
8:AH:27:PRO:HB3	8:AH:87:ASN:ND2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:45:ARG:HG2	8:AH:49:GLU:HG2	1.88	0.55
1:Aa:74:TRP:CD2	1:Aa:414:GLY:HA3	2.42	0.55
2:Ab:177:LEU:HD21	2:Ab:272:VAL:CG1	2.37	0.55
16:Ad:402:3PH:C37	5:Ae:128:ALA:CB	2.84	0.55
1:AA:68:THR:OG1	2:AB:387:GLU:OE1	2.24	0.55
4:AD:219:CYS:SG	4:AD:220:GLU:N	2.79	0.55
1:Aa:87:ASN:H	1:Aa:207:ASN:HD22	1.53	0.55
1:Aa:109:LEU:CG	1:Aa:110:GLU:N	2.70	0.55
16:Ad:402:3PH:C35	5:Ae:128:ALA:CB	2.85	0.55
5:Ae:169:TRP:CD1	5:Ae:170:ARG:HG3	2.40	0.55
5:Ai:72:VAL:HG23	5:Ai:73:PRO:HD3	1.88	0.55
1:AA:182:VAL:CG1	1:AA:186:TYR:HE2	2.20	0.55
3:AC:198:LEU:CD1	3:Ac:9:PRO:HB2	2.37	0.55
8:AH:42:VAL:HG13	8:AH:45:ARG:NH2	2.20	0.55
8:AH:58:ARG:CZ	8:AH:60:GLN:HE21	2.20	0.55
1:Aa:109:LEU:HD12	1:Aa:110:GLU:HA	1.87	0.55
14:Aa:501:3PE:H112	14:Aa:501:3PE:H11	1.88	0.55
3:Ac:97:HIS:CE1	3:Ac:100:ARG:HH21	2.23	0.55
3:AC:168:PHE:CD2	5:Ae:170:ARG:HB3	2.42	0.55
5:Ae:248:ARG:HA	5:Ae:257:ASN:CG	2.32	0.55
6:Af:15:ASP:OD2	6:Af:19:LYS:NZ	2.39	0.55
5:AE:119:ALA:CA	9:AJ:25:ILE:HD11	2.29	0.55
7:AG:67:PHE:CE2	7:AG:71:LYS:HD3	2.41	0.55
7:AG:79:GLU:HG3	8:AH:58:ARG:CD	2.36	0.55
8:AH:35:CYS:SG	8:AH:80:VAL:HA	2.47	0.55
3:Ac:312:GLN:HE21	6:Af:37:THR:HB	1.72	0.55
5:Ae:244:ASP:HB3	5:Ae:250:ARG:HH11	1.71	0.55
8:Ah:73:LEU:O	8:Ah:74:HIS:C	2.50	0.55
3:AC:256:TYR:CE1	4:AD:202:ARG:HD3	2.42	0.55
6:AF:39:HIS:HD2	6:AF:41:THR:HG22	1.71	0.55
9:AJ:30:LEU:HD12	10:AK:34:TRP:HB2	1.89	0.55
1:Aa:96:LEU:HD11	1:Aa:161:ILE:HG12	1.89	0.55
2:Ab:181:ALA:O	2:Ab:254:ARG:HG2	2.07	0.55
3:Ac:30:TRP:CE2	14:Ac:403:3PE:H232	2.42	0.55
5:Ae:207:LYS:CD	5:Ae:210:TRP:HD1	2.20	0.55
1:AA:74:TRP:CD2	1:AA:414:GLY:HA3	2.42	0.55
6:AF:77:PRO:HB2	6:AF:80:GLN:HG3	1.88	0.55
7:AG:74:ASN:HB3	7:AG:77:MET:CG	2.33	0.55
2:Ab:65:VAL:HG22	2:Ab:218:MET:CG	2.35	0.55
5:Ae:192:VAL:HA	5:Ae:195:LEU:CD1	2.37	0.55
5:Ae:228:ALA:HB3	5:Ae:235:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:241:SER:OG	5:Ae:253:PRO:HD2	2.07	0.55
8:Ah:45:ARG:HD2	8:Ah:48:LEU:HD23	1.89	0.55
2:AB:85:LEU:HD21	5:AI:68:VAL:HG11	1.88	0.54
3:AC:69:ILE:HA	3:AC:73:VAL:CB	2.36	0.54
7:AG:46:ILE:HD11	7:AG:50:ALA:HB2	1.88	0.54
1:Aa:296:TRP:HH2	1:Aa:415:ARG:HH11	1.55	0.54
4:Ad:231:LEU:HD22	4:Ad:241:ALA:HB1	1.88	0.54
3:AC:8:HIS:NE2	3:Ac:199:PHE:HE1	2.05	0.54
1:Aa:139:ASP:O	1:Aa:143:VAL:HG23	2.07	0.54
2:Ab:297:PRO:CA	2:Ab:304:ASN:OD1	2.52	0.54
5:Ae:122:THR:HG21	9:Aj:25:ILE:HG21	1.89	0.54
3:AC:184:ILE:HG12	3:AC:188:ILE:HG13	1.90	0.54
2:Ab:300:LYS:HG2	2:Ab:301:ARG:CG	2.37	0.54
5:Ae:190:VAL:HG11	5:Ae:195:LEU:HD21	1.90	0.54
7:Ag:39:LEU:O	7:Ag:42:THR:HG22	2.08	0.54
8:Ah:79:CYS:O	8:Ah:82:HIS:HB3	2.07	0.54
1:AA:74:TRP:HB3	1:AA:418:LEU:HD11	1.89	0.54
1:AA:311:ILE:HD11	1:AA:379:LEU:HD11	1.88	0.54
2:AB:60:ARG:CZ	2:AB:390:GLU:HB3	2.37	0.54
2:AB:313:VAL:HG13	2:AB:350:VAL:HG13	1.89	0.54
3:AC:45:ILE:CA	11:AC:401:HEM:HAB	2.31	0.54
3:AC:319:PRO:HD2	6:AF:21:TYR:CZ	2.42	0.54
2:Ab:237:PHE:O	2:Ab:240:MET:HG2	2.08	0.54
5:Ae:195:LEU:HD11	5:Ae:248:ARG:HH11	1.72	0.54
1:AA:186:TYR:HE1	5:AE:80:HIS:O	1.91	0.54
2:Ab:159:LYS:HB2	2:Ab:197:MET:SD	2.47	0.54
3:Ac:222:PRO:HG2	3:Ac:223:TYR:CD2	2.43	0.54
1:AA:407:THR:O	1:AA:408:PRO:C	2.49	0.54
2:AB:237:PHE:O	2:AB:238:LEU:HB2	2.07	0.54
3:AC:68:HIS:ND1	3:AC:73:VAL:HG23	2.22	0.54
3:AC:260:ASN:C	3:AC:262:LEU:N	2.62	0.54
1:Aa:74:TRP:HB3	1:Aa:418:LEU:HD11	1.89	0.54
1:Aa:96:LEU:CD1	1:Aa:161:ILE:HG12	2.37	0.54
3:Ac:153:ILE:HB	3:Ac:157:GLY:CA	2.37	0.54
5:Ae:152:ILE:HD13	5:Ae:169:TRP:CD1	2.42	0.54
2:AB:171:THR:HA	5:AI:64:LEU:HD21	1.88	0.54
2:AB:339:TYR:CD2	5:AI:59:ALA:HB1	2.43	0.54
3:AC:68:HIS:O	3:AC:72:ASP:N	2.34	0.54
3:AC:222:PRO:HG2	3:AC:223:TYR:CD2	2.43	0.54
4:AD:214:LEU:HD11	4:AD:237:PHE:HD1	1.72	0.54
5:AE:127:TYR:OH	9:AJ:36:PHE:CD1	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AJ:33:GLU:CB	10:AK:34:TRP:HE1	2.20	0.54
1:Aa:170:ARG:HG3	1:Aa:171:GLU:N	2.22	0.54
3:Ac:77:TRP:HZ2	4:Ad:284:HIS:HD2	1.52	0.54
4:AD:183:GLU:HB3	4:Ad:161:ASP:HB3	1.89	0.54
4:AD:189:ASN:HB3	13:AD:401:HEC:CMD	2.29	0.54
4:AD:218:TYR:CE1	4:AD:242:ILE:HG21	2.39	0.54
4:AD:252:VAL:HG13	4:AD:253:LEU:HG	1.90	0.54
8:AH:45:ARG:O	8:AH:49:GLU:HG2	2.08	0.54
5:AI:43:LEU:O	5:AI:44:ASP:C	2.51	0.54
5:AI:72:VAL:HG23	5:AI:73:PRO:HD3	1.88	0.54
1:Aa:407:THR:O	1:Aa:408:PRO:C	2.49	0.54
4:Ad:178:PRO:HG2	4:Ad:179:TYR:H	1.72	0.54
2:AB:313:VAL:HG11	2:AB:321:PHE:CG	2.42	0.54
4:AD:255:TYR:HB3	4:AD:257:ASP:OD1	2.08	0.54
6:AF:85:GLU:H	6:AF:85:GLU:CD	2.15	0.54
7:AG:45:ARG:HG2	7:AG:48:ARG:HH22	1.71	0.54
3:Ac:377:LEU:O	3:Ac:378:LYS:HB2	2.06	0.54
5:AI:62:ARG:HB2	5:AI:78:PHE:C	2.33	0.54
3:AC:129:MET:HB3	3:AC:182:HIS:CB	2.25	0.54
3:AC:253:PRO:HB2	4:AD:203:ALA:O	2.08	0.54
5:AI:62:ARG:HB2	5:AI:78:PHE:C	2.33	0.54
5:Ae:136:PHE:O	5:Ae:137:VAL:C	2.51	0.54
1:AA:204:PRO:O	1:AA:205:SER:C	2.50	0.53
2:AB:50:ALA:HB3	2:AB:221:VAL:HG22	1.90	0.53
3:AC:148:ASN:HB2	5:Ae:220:LEU:CA	2.33	0.53
6:AF:92:GLU:O	6:AF:96:LYS:HG3	2.08	0.53
9:AJ:23:LEU:CB	10:AK:27:VAL:CG2	2.69	0.53
1:Aa:120:LEU:HD23	2:Ab:299:ILE:HG23	1.89	0.53
4:Ad:133:ARG:O	4:Ad:136:VAL:HG23	2.08	0.53
4:Ad:193:LEU:O	13:Ad:401:HEC:HAD1	2.09	0.53
5:Ae:206:LYS:HG3	5:Ae:206:LYS:O	2.07	0.53
4:AD:170:LYS:O	4:AD:173:ASP:HB3	2.07	0.53
16:Ad:402:3PH:H332	16:Ad:402:3PH:C26	2.38	0.53
5:Ae:172:LYS:HD3	5:Ae:216:VAL:HG21	1.89	0.53
5:Ae:191:GLU:H	5:Ae:191:GLU:CD	2.14	0.53
8:Ah:47:ARG:CZ	8:Ah:47:ARG:HB3	2.38	0.53
1:AA:296:TRP:HH2	1:AA:415:ARG:HH11	1.55	0.53
5:AE:222:CYS:SG	3:Ac:268:ILE:HD12	2.47	0.53
2:Ab:91:THR:HG23	2:Ab:99:ILE:HD11	1.90	0.53
5:Ae:179:ARG:HH21	5:Ae:208:PRO:HA	1.74	0.53
9:Aj:23:LEU:HA	10:Ak:27:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:148:ALA:O	1:AA:152:GLN:HG2	2.09	0.53
6:AF:29:LYS:HA	6:AF:81:TRP:CG	2.44	0.53
1:Aa:98:PHE:O	1:Aa:109:LEU:HD11	2.08	0.53
3:AC:135:TRP:O	3:AC:135:TRP:CD1	2.60	0.53
4:AD:252:VAL:HG13	4:AD:253:LEU:H	1.72	0.53
2:Ab:52:LEU:HD22	2:Ab:392:PHE:HE2	1.72	0.53
2:AB:70:ARG:NH2	2:AB:332:ASP:OD2	2.42	0.53
3:AC:122:ALA:HB1	3:AC:189:ILE:HG12	1.89	0.53
4:AD:217:GLY:O	4:AD:235:PRO:HD2	2.09	0.53
1:Aa:187:LEU:HD22	1:Aa:288:ALA:HB1	1.89	0.53
3:Ac:164:ILE:O	3:Ac:177:ARG:HD2	2.08	0.53
4:Ad:124:CYS:O	4:Ad:194:PRO:HB2	2.08	0.53
4:Ad:182:PRO:C	4:Ad:186:ARG:HH21	2.15	0.53
4:Ad:288:MET:SD	16:Ad:402:3PH:H11	2.48	0.53
9:Aj:33:GLU:O	9:Aj:34:ARG:C	2.50	0.53
4:AD:213:SER:HB3	4:AD:236:TYR:CD1	2.43	0.53
2:Ab:145:GLU:C	2:Ab:146:PHE:CD1	2.87	0.53
4:Ad:147:ALA:O	4:Ad:150:GLU:HB3	2.08	0.53
4:Ad:185:ALA:HB1	4:Ad:194:PRO:HD3	1.90	0.53
5:Ae:162:GLY:H	5:Ae:178:HIS:HD2	1.52	0.53
3:AC:131:TYR:O	3:AC:134:PRO:HD2	2.09	0.53
3:AC:145:VAL:HA	5:Ae:220:LEU:HB3	1.90	0.53
3:AC:170:VAL:HG23	3:AC:174:THR:CB	2.39	0.53
4:AD:127:MET:HE1	4:AD:197:LEU:O	2.08	0.53
3:Ac:170:VAL:HG23	3:Ac:174:THR:CB	2.39	0.53
4:Ad:111:ARG:HG3	4:Ad:140:TYR:CZ	2.43	0.53
4:Ad:202:ARG:CG	4:Ad:278:SER:HB3	2.35	0.53
4:Ad:227:LEU:HD13	4:Ad:231:LEU:O	2.08	0.53
10:Ak:6:LEU:HD12	10:Ak:11:ARG:HH12	1.72	0.53
1:AA:136:LEU:HD21	2:AB:380:ALA:HA	1.90	0.53
3:AC:164:ILE:O	3:AC:177:ARG:HD2	2.08	0.53
5:Ae:181:LYS:O	5:Ae:185:ASP:N	2.41	0.53
1:AA:158:ASP:O	1:AA:162:GLU:HG2	2.09	0.53
1:AA:207:ASN:O	1:AA:211:LEU:HG	2.10	0.53
3:AC:181:PHE:HA	3:AC:184:ILE:CG2	2.38	0.53
8:AH:35:CYS:O	8:AH:41:CYS:HB2	2.09	0.53
3:Ac:253:PRO:HG3	4:Ad:205:HIS:CD2	2.44	0.53
4:Ad:118:LYS:HZ2	4:Ad:148:LEU:HD22	1.73	0.53
4:Ad:295:MET:HB3	16:Ad:402:3PH:H361	1.91	0.53
8:Ah:32:ARG:NE	8:Ah:76:ARG:HH12	2.06	0.53
3:AC:59:THR:HG23	3:AC:172:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:128:PHE:HZ	3:AC:143:ALA:HA	1.74	0.52
4:AD:124:CYS:HA	4:AD:179:TYR:CE2	2.44	0.52
4:Ad:92:PRO:HD3	4:Ad:236:TYR:CZ	2.44	0.52
5:Ae:171:GLY:O	5:Ae:172:LYS:HE3	2.09	0.52
5:Ae:239:HIS:CG	5:Ae:239:HIS:O	2.61	0.52
6:AF:92:GLU:O	6:AF:93:PRO:C	2.48	0.52
1:Aa:207:ASN:O	1:Aa:211:LEU:HG	2.09	0.52
2:Ab:168:ASN:OD1	2:Ab:168:ASN:N	2.42	0.52
3:Ac:30:TRP:HB3	3:Ac:100:ARG:HD3	1.90	0.52
4:Ad:114:PHE:CZ	4:Ad:118:LYS:HE3	2.45	0.52
5:Ae:207:LYS:HD2	5:Ae:210:TRP:CD1	2.44	0.52
6:Af:102:ARG:HH21	6:Af:103:LYS:HE3	1.73	0.52
10:Ak:14:ALA:O	10:Ak:18:ILE:HG12	2.08	0.52
2:AB:171:THR:HG23	5:AI:64:LEU:CD2	2.39	0.52
3:AC:343:VAL:HG21	5:Ae:239:HIS:CD2	2.44	0.52
5:AE:172:LYS:HE2	5:AE:172:LYS:HA	1.90	0.52
6:AF:34:ARG:HH22	6:AF:92:GLU:CD	2.16	0.52
6:AF:101:GLU:HB3	6:AF:105:ARG:HH12	1.75	0.52
6:AF:110:LYS:HA	10:Ak:10:TYR:CE1	2.45	0.52
7:AG:69:GLN:HB3	7:AG:72:ARG:NH1	2.25	0.52
4:Ad:270:VAL:O	4:Ad:274:LEU:HG	2.09	0.52
2:AB:167:GLN:HE21	5:AI:43:LEU:HB3	1.74	0.52
3:AC:376:MET:HE3	6:AF:18:ARG:HA	1.91	0.52
4:AD:112:ARG:HD3	4:AD:257:ASP:OD2	2.09	0.52
4:AD:124:CYS:HA	4:AD:179:TYR:HE2	1.74	0.52
5:AE:107:SER:HA	5:AE:110:ARG:NE	2.25	0.52
2:Ab:234:ALA:HB1	2:Ab:238:LEU:HD12	1.91	0.52
4:Ad:321:TYR:CD2	4:Ad:323:PRO:HD3	2.44	0.52
5:Ae:263:TYR:CA	5:Ae:273:VAL:HA	2.09	0.52
1:AA:165:ARG:HD3	1:AA:209:ARG:HA	1.91	0.52
1:AA:378:ARG:HG2	1:AA:382:SER:HB2	1.90	0.52
4:AD:145:ALA:O	4:AD:149:ALA:N	2.40	0.52
4:AD:251:GLU:N	4:AD:261:ALA:O	2.37	0.52
1:Aa:74:TRP:HH2	1:Aa:410:CYS:SG	2.31	0.52
2:Ab:60:ARG:O	2:Ab:223:LEU:N	2.42	0.52
2:Ab:348:GLY:HA2	2:Ab:448:PRO:HD3	1.91	0.52
3:Ac:233:LEU:HD23	4:Ad:300:LEU:HD23	1.92	0.52
4:Ad:288:MET:SD	16:Ad:402:3PH:C2	2.98	0.52
5:Ae:164:ASN:HD21	5:Ae:175:PHE:HB3	1.74	0.52
1:AA:170:ARG:HA	1:AA:173:GLN:CD	2.34	0.52
2:AB:117:GLU:OE2	2:AB:330:TYR:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:312:SER:O	2:AB:315:LYS:HG2	2.10	0.52
2:AB:348:GLY:HA2	2:AB:448:PRO:HD3	1.91	0.52
3:AC:137:GLN:NE2	3:AC:263:ASN:O	2.39	0.52
3:AC:138:MET:CE	3:AC:268:ILE:HG23	2.40	0.52
3:AC:221:HIS:O	3:AC:225:THR:HB	2.10	0.52
4:AD:154:VAL:HG23	4:AD:176:PRO:HB3	1.92	0.52
4:AD:232:TYR:O	4:AD:242:ILE:HG22	2.09	0.52
4:AD:248:ILE:HD12	4:AD:252:VAL:HG11	1.92	0.52
4:AD:321:TYR:CD2	4:AD:323:PRO:HD3	2.44	0.52
5:AE:242:HIS:CD2	5:AE:251:LYS:HB3	2.45	0.52
2:Ab:138:LEU:HB3	2:Ab:237:PHE:CD2	2.45	0.52
2:Ab:425:VAL:HG12	2:Ab:429:LYS:HZ1	1.75	0.52
4:Ad:300:LEU:HB2	4:Ad:301:PRO:HD3	1.91	0.52
2:AB:226:SER:O	2:AB:229:VAL:HG22	2.09	0.52
4:AD:189:ASN:OD1	4:AD:194:PRO:HG3	2.09	0.52
4:AD:232:TYR:CG	4:AD:246:PRO:HD3	2.45	0.52
6:AF:41:THR:O	6:AF:42:GLU:C	2.50	0.52
3:Ac:320:ILE:HD12	3:Ac:373:GLU:HG2	1.92	0.52
10:Ak:6:LEU:HD12	10:Ak:11:ARG:NH1	2.25	0.52
1:AA:74:TRP:HH2	1:AA:410:CYS:SG	2.31	0.52
3:AC:119:LEU:HD21	3:AC:192:LEU:HB2	1.92	0.52
3:AC:120:LEU:HD23	3:AC:298:ILE:HG23	1.92	0.52
3:AC:346:PRO:O	3:AC:349:ILE:HG22	2.10	0.52
4:AD:114:PHE:CE2	4:AD:148:LEU:HD13	2.45	0.52
4:AD:242:ILE:HG12	4:AD:244:MET:HB3	1.92	0.52
4:AD:308:ARG:HD3	7:AG:27:PHE:CZ	2.44	0.52
6:AF:26:GLY:HA2	6:AF:28:ASN:OD1	2.10	0.52
7:AG:74:ASN:ND2	7:AG:76:ALA:HB3	2.25	0.52
2:Ab:235:GLU:OE1	2:Ab:235:GLU:N	2.42	0.52
5:Ae:161:GLU:O	5:Ae:163:LYS:HG2	2.10	0.52
5:Ae:249:ILE:HG12	5:Ae:254:ALA:O	2.10	0.52
1:AA:339:GLN:HB2	1:AA:359:VAL:O	2.10	0.52
1:AA:453:CYS:SG	1:AA:472:ARG:NH1	2.82	0.52
1:AA:468:TYR:O	1:AA:469:ASN:C	2.52	0.52
3:AC:107:TYR:HB2	3:AC:305:PRO:HG3	1.92	0.52
5:AE:241:SER:OG	5:AE:253:PRO:HD2	2.09	0.52
8:AH:79:CYS:O	8:AH:83:LYS:HG2	2.10	0.52
2:Ab:159:LYS:O	2:Ab:162:LYS:HG2	2.09	0.52
4:Ad:298:LEU:O	4:Ad:301:PRO:HD2	2.10	0.52
1:AA:180:GLN:HG3	1:AA:181:ASN:N	2.25	0.52
3:AC:126:THR:HB	11:AC:401:HEM:HBC2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:259:ALA:O	3:AC:261:PRO:HD3	2.09	0.52
4:AD:136:VAL:HG21	4:AD:142:GLU:HG2	1.92	0.52
4:AD:152:VAL:HG23	4:AD:156:ASP:OD2	2.09	0.52
4:AD:321:TYR:HB2	6:AF:61:PHE:CD1	2.45	0.52
5:AE:127:TYR:CZ	9:AJ:36:PHE:CD1	2.97	0.52
1:Aa:160:GLN:HA	1:Aa:163:LYS:HZ3	1.75	0.52
1:Aa:338:CYS:CB	1:Aa:368:MET:SD	2.97	0.52
2:Ab:36:GLN:NE2	2:Ab:55:TYR:HE2	2.08	0.52
3:Ac:346:PRO:O	3:Ac:349:ILE:HG22	2.10	0.52
4:Ad:157:GLY:H	4:Ad:158:PRO:HD3	1.75	0.52
2:AB:173:ILE:HD11	2:AB:439:ALA:O	2.09	0.51
2:AB:227:HIS:HD2	2:AB:231:LYS:HE2	1.75	0.51
3:AC:51:LEU:HD21	3:AC:80:ARG:HA	1.92	0.51
3:AC:198:LEU:HD21	3:Ac:10:LEU:HA	1.93	0.51
8:AH:33:GLU:O	8:AH:37:GLN:HG2	2.11	0.51
3:AC:145:VAL:CG1	5:Ae:220:LEU:CD1	2.77	0.51
5:AE:126:ALA:HB1	10:AK:34:TRP:CH2	2.45	0.51
1:Aa:98:PHE:CZ	1:Aa:122:ALA:HB2	2.46	0.51
1:Aa:170:ARG:HA	1:Aa:173:GLN:CD	2.34	0.51
1:Aa:280:ASP:OD2	7:Ag:10:ARG:HA	2.10	0.51
1:Aa:467:ASP:OD2	3:Ac:223:TYR:CE2	2.63	0.51
1:AA:172:MET:HE1	1:AA:205:SER:HA	1.92	0.51
1:AA:392:LYS:HE3	1:AA:433:ILE:O	2.11	0.51
2:AB:303:ASN:O	2:AB:304:ASN:C	2.52	0.51
3:AC:65:SER:O	3:AC:68:HIS:HB3	2.11	0.51
3:AC:70:CYS:SG	3:AC:80:ARG:NH1	2.83	0.51
4:AD:112:ARG:HE	4:AD:269:ASP:CG	2.18	0.51
4:AD:115:GLN:HG2	4:AD:140:TYR:OH	2.10	0.51
4:AD:117:TYR:CZ	4:AD:127:MET:HG2	2.46	0.51
1:Aa:339:GLN:HB2	1:Aa:359:VAL:O	2.10	0.51
3:Ac:147:THR:HG21	3:Ac:165:TRP:NE1	2.26	0.51
16:Ad:402:3PH:C36	5:Ae:128:ALA:HB2	2.39	0.51
2:AB:319:GLN:HB3	2:AB:320:PRO:HD2	1.93	0.51
3:AC:117:VAL:HG11	3:AC:302:ALA:CA	2.41	0.51
3:AC:150:LEU:HB2	3:AC:161:VAL:HG22	1.93	0.51
4:AD:318:LYS:CD	5:AE:86:PRO:HB2	2.40	0.51
1:Aa:91:TYR:CZ	1:Aa:95:HIS:CE1	2.98	0.51
4:Ad:158:PRO:HD2	4:Ad:164:MET:O	2.10	0.51
5:Ae:93:ARG:HD2	5:Ae:110:ARG:CD	2.38	0.51
7:Ag:74:ASN:HD21	7:Ag:76:ALA:HB3	1.74	0.51
3:AC:8:HIS:CE1	3:Ac:199:PHE:CE1	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:121:PHE:HZ	3:AC:299:LEU:HG	1.75	0.51
4:AD:242:ILE:CG1	4:AD:244:MET:HB3	2.39	0.51
1:Aa:92:PHE:HD1	1:Aa:168:ILE:HD12	1.75	0.51
2:Ab:69:SER:O	2:Ab:70:ARG:C	2.51	0.51
4:Ad:133:ARG:NH1	5:Ae:145:ASP:HA	2.26	0.51
2:AB:232:GLN:O	2:AB:235:GLU:HG3	2.11	0.51
3:AC:215:ALA:HB2	6:AF:60:MET:CE	2.39	0.51
4:AD:109:SER:OG	4:AD:269:ASP:HA	2.10	0.51
4:AD:215:LEU:CD1	13:AD:401:HEC:HBB2	2.39	0.51
6:AF:28:ASN:OD1	6:AF:29:LYS:N	2.43	0.51
1:Aa:113:VAL:HG23	1:Aa:118:ALA:HB3	1.92	0.51
1:Aa:392:LYS:HE3	1:Aa:433:ILE:O	2.11	0.51
2:Ab:126:ILE:HG22	2:Ab:128:SER:H	1.76	0.51
3:Ac:137:GLN:NE2	3:Ac:264:THR:HA	2.26	0.51
3:Ac:278:TYR:CZ	3:Ac:282:ARG:HD2	2.46	0.51
5:Ae:196:ARG:HD2	5:Ae:249:ILE:CG2	2.41	0.51
8:Ah:45:ARG:O	8:Ah:49:GLU:HG2	2.11	0.51
8:Ah:51:CYS:SG	8:Ah:68:GLU:HB2	2.51	0.51
2:AB:323:VAL:HA	2:AB:339:TYR:O	2.11	0.51
4:AD:235:PRO:HA	4:AD:240:GLN:HE21	1.74	0.51
5:AE:89:SER:HA	5:AE:92:ARG:CB	2.30	0.51
5:AE:130:LYS:HB2	10:AK:34:TRP:CZ2	2.45	0.51
1:Aa:148:ALA:HA	1:Aa:250:LEU:HD21	1.92	0.51
2:Ab:38:LEU:HA	2:Ab:51:SER:O	2.11	0.51
2:Ab:116:ARG:HG2	2:Ab:190:LEU:HD21	1.91	0.51
2:Ab:432:VAL:O	2:Ab:432:VAL:HG22	2.10	0.51
4:Ad:281:GLU:CD	4:Ad:281:GLU:H	2.18	0.51
8:Ah:77:ASP:O	8:Ah:78:HIS:C	2.50	0.51
1:AA:377:MET:HE2	1:AA:377:MET:HA	1.93	0.51
3:AC:107:TYR:HE1	3:AC:308:HIS:HB2	1.76	0.51
1:Aa:52:ILE:HG12	1:Aa:53:LEU:N	2.26	0.51
1:Aa:169:LEU:O	1:Aa:173:GLN:HG3	2.11	0.51
2:Ab:164:VAL:O	2:Ab:167:GLN:HG3	2.10	0.51
3:Ac:150:LEU:HB2	3:Ac:161:VAL:HG22	1.93	0.51
3:Ac:211:LEU:HD21	6:Af:37:THR:HA	1.93	0.51
3:Ac:221:HIS:O	3:Ac:225:THR:HB	2.10	0.51
1:AA:226:ALA:HB2	1:AA:253:VAL:HB	1.93	0.51
1:AA:378:ARG:CG	1:AA:382:SER:HB2	2.41	0.51
5:AE:91:TYR:O	7:AG:25:ARG:N	2.40	0.51
3:Ac:140:PHE:CE1	3:Ac:170:VAL:HG13	2.45	0.51
4:Ad:145:ALA:HA	4:Ad:148:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:243:TYR:OH	5:Ae:254:ALA:HB1	2.11	0.51
1:AA:109:LEU:O	1:AA:113:VAL:HG12	2.11	0.51
1:AA:169:LEU:O	1:AA:173:GLN:HG3	2.11	0.51
5:AE:119:ALA:HA	9:AJ:25:ILE:HG12	1.93	0.51
7:AG:9:ALA:O	7:AG:11:ILE:HD12	2.10	0.51
1:Aa:338:CYS:SG	1:Aa:339:GLN:N	2.84	0.51
3:Ac:140:PHE:HE1	3:Ac:170:VAL:HG13	1.76	0.51
4:Ad:157:GLY:N	4:Ad:158:PRO:HD3	2.26	0.51
4:Ad:220:GLU:O	4:Ad:221:PRO:C	2.52	0.51
5:Ae:195:LEU:HD11	5:Ae:248:ARG:NH1	2.26	0.51
5:Ai:46:LYS:HG2	5:Ai:47:ARG:H	1.71	0.51
3:AC:237:LEU:HD22	4:AD:300:LEU:HD11	1.93	0.50
1:Aa:113:VAL:O	1:Aa:116:ILE:HG12	2.11	0.50
1:Aa:285:ALA:O	1:Aa:359:VAL:HA	2.11	0.50
1:Aa:397:ASN:HD21	2:Ab:126:ILE:HD11	1.76	0.50
2:Ab:38:LEU:HD11	2:Ab:396:ILE:HD13	1.92	0.50
4:Ad:248:ILE:HD12	4:Ad:252:VAL:HG11	1.93	0.50
1:AA:338:CYS:SG	1:AA:339:GLN:N	2.84	0.50
3:AC:138:MET:HE1	3:AC:268:ILE:HA	1.92	0.50
7:AG:68:GLU:HA	7:AG:71:LYS:CE	2.41	0.50
4:Ad:174:TYR:O	4:Ad:175:PHE:C	2.53	0.50
8:Ah:43:LYS:HA	8:Ah:46:GLU:CD	2.36	0.50
3:AC:147:THR:HG21	3:AC:165:TRP:NE1	2.25	0.50
4:AD:140:TYR:HA	4:AD:144:GLU:CD	2.35	0.50
4:AD:218:TYR:CZ	4:AD:246:PRO:HG3	2.46	0.50
1:Aa:73:VAL:HG23	1:Aa:147:LEU:HD13	1.93	0.50
2:Ab:212:HIS:HE1	2:Ab:246:LEU:CD2	1.95	0.50
2:Ab:297:PRO:HB3	2:Ab:304:ASN:OD1	2.12	0.50
4:Ad:249:TYR:O	4:Ad:250:THR:C	2.54	0.50
10:Ak:9:ARG:NH1	10:Ak:13:LEU:HD11	2.26	0.50
1:AA:162:GLU:HA	1:AA:165:ARG:NH1	2.26	0.50
4:AD:193:LEU:O	13:AD:401:HEC:HAD2	2.11	0.50
4:AD:249:TYR:CD1	4:AD:252:VAL:HG23	2.46	0.50
4:AD:255:TYR:OH	4:AD:269:ASP:HB2	2.12	0.50
7:AG:35:ILE:HA	7:AG:38:VAL:HB	1.94	0.50
8:AH:60:GLN:H	8:AH:60:GLN:CD	2.19	0.50
2:Ab:138:LEU:HD13	2:Ab:233:VAL:O	2.11	0.50
2:Ab:218:MET:HE1	2:Ab:238:LEU:HD22	1.92	0.50
4:Ad:133:ARG:NH2	4:Ad:174:TYR:OH	2.45	0.50
5:Ae:142:ALA:C	5:Ae:147:LEU:HD23	2.36	0.50
1:AA:171:GLU:O	1:AA:175:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:397:ASN:HA	2:AB:58:LEU:HD11	1.93	0.50
2:AB:101:ARG:HB3	6:Af:108:TRP:CZ2	2.46	0.50
3:AC:117:VAL:HG11	3:AC:302:ALA:HA	1.93	0.50
3:AC:313:ARG:HB2	6:AF:39:HIS:ND1	2.27	0.50
4:AD:126:SER:HB3	4:AD:178:PRO:HD3	1.93	0.50
5:AE:165:MET:O	5:AE:176:VAL:N	2.44	0.50
6:AF:97:GLU:HA	6:AF:100:ARG:NH1	2.26	0.50
9:AJ:17:ARG:HG2	9:AJ:20:THR:H	1.77	0.50
1:Aa:180:GLN:HG3	1:Aa:181:ASN:N	2.25	0.50
3:Ac:107:TYR:HE1	3:Ac:308:HIS:HB2	1.75	0.50
4:Ad:321:TYR:HB2	6:Af:61:PHE:CE2	2.47	0.50
16:Ad:402:3PH:O31	5:Ae:131:ASN:ND2	2.43	0.50
1:AA:96:LEU:HD11	1:AA:161:ILE:HG12	1.93	0.50
1:AA:118:ALA:CB	1:AA:135:ALA:HB2	2.42	0.50
1:AA:393:ASN:HB3	2:AB:106:VAL:O	2.12	0.50
2:AB:64:PHE:HZ	2:AB:394:SER:HA	1.77	0.50
3:AC:141:TRP:CH2	5:Ae:223:VAL:CG2	2.93	0.50
3:AC:274:PHE:O	3:AC:275:LEU:C	2.55	0.50
4:AD:234:ASN:OD1	4:AD:236:TYR:HB2	2.11	0.50
5:AE:127:TYR:HB2	9:AJ:32:PHE:HD1	1.76	0.50
2:Ab:209:VAL:HA	2:Ab:213:PHE:HB2	1.94	0.50
4:Ad:186:ARG:O	4:Ad:191:GLY:N	2.45	0.50
4:Ad:291:LYS:HA	4:Ad:294:LEU:HD12	1.92	0.50
5:Ae:146:VAL:HA	5:Ae:149:MET:HE3	1.94	0.50
6:Af:97:GLU:HA	6:Af:100:ARG:HH11	1.75	0.50
2:AB:162:LYS:HE3	2:AB:166:PHE:HE2	1.76	0.50
3:AC:50:PHE:CZ	5:AE:136:PHE:CZ	2.99	0.50
3:AC:138:MET:HE1	3:AC:268:ILE:HG23	1.93	0.50
3:AC:291:VAL:O	3:AC:295:ILE:HG12	2.11	0.50
4:Ad:227:LEU:HB2	4:Ad:231:LEU:CB	2.42	0.50
4:Ad:248:ILE:HG23	4:Ad:252:VAL:CG1	2.42	0.50
4:Ad:260:PRO:HB3	8:Ah:24:LEU:CD2	2.42	0.50
1:AA:296:TRP:NE1	1:AA:347:SER:O	2.45	0.50
2:AB:177:LEU:HD21	2:AB:272:VAL:HG13	1.92	0.50
2:AB:304:ASN:CB	2:AB:307:SER:HB2	2.40	0.50
6:AF:36:ASP:OD1	6:AF:90:TYR:OH	2.23	0.50
8:AH:54:ARG:NE	8:AH:63:GLU:HB3	2.26	0.50
1:Aa:442:ARG:CZ	10:Ak:16:ASN:ND2	2.75	0.50
4:Ad:232:TYR:CG	4:Ad:245:ALA:HA	2.47	0.50
3:AC:128:PHE:HE2	3:AC:178:PHE:CE2	2.30	0.50
3:AC:182:HIS:HE1	11:AC:401:HEM:C4C	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:95:PRO:HG2	8:AH:85:PHE:CB	2.42	0.50
4:Ad:309:HIS:CE1	7:Ag:21:PRO:HB2	2.46	0.50
5:Ae:142:ALA:O	5:Ae:147:LEU:HD23	2.12	0.50
7:AG:57:TYR:CE2	7:AG:61:THR:HG21	2.47	0.49
1:Aa:272:GLY:O	7:Ag:19:LEU:HD12	2.12	0.49
4:Ad:114:PHE:HD2	4:Ad:140:TYR:CE2	2.29	0.49
4:Ad:157:GLY:O	4:Ad:158:PRO:C	2.55	0.49
5:Ae:242:HIS:CD2	5:Ae:251:LYS:HB3	2.47	0.49
1:AA:373:GLN:NE2	1:AA:471:ILE:O	2.44	0.49
3:AC:145:VAL:CA	5:Ae:220:LEU:HB3	2.41	0.49
1:Aa:113:VAL:CG1	2:Ab:299:ILE:HD11	2.43	0.49
1:Aa:171:GLU:O	1:Aa:175:ASN:N	2.45	0.49
2:Ab:45:ASN:HD22	2:Ab:239:ASN:CA	2.23	0.49
2:Ab:67:ALA:HB1	2:Ab:208:PHE:HE1	1.76	0.49
2:Ab:297:PRO:CA	2:Ab:304:ASN:CG	2.83	0.49
4:Ad:114:PHE:CD2	4:Ad:140:TYR:CE2	3.00	0.49
4:Ad:156:ASP:CB	4:Ad:167:ARG:HB3	2.38	0.49
1:AA:205:SER:O	1:AA:206:GLU:C	2.55	0.49
4:AD:129:TYR:HD2	4:AD:198:SER:CB	2.25	0.49
4:AD:158:PRO:C	4:AD:166:MET:HB2	2.37	0.49
4:AD:295:MET:HG2	9:AJ:36:PHE:CE1	2.46	0.49
4:AD:318:LYS:HD2	5:AE:86:PRO:HB2	1.94	0.49
5:AE:242:HIS:HD2	5:AE:251:LYS:HB3	1.76	0.49
9:AJ:30:LEU:HD12	10:AK:34:TRP:CB	2.42	0.49
14:Aa:501:3PE:H341	3:Ac:225:THR:HG21	1.93	0.49
2:Ab:375:LYS:NZ	2:Ab:419:VAL:O	2.36	0.49
4:Ad:131:ALA:HA	4:Ad:174:TYR:HA	1.94	0.49
4:Ad:224:GLY:HA3	8:Ah:64:ASP:CG	2.36	0.49
4:Ad:288:MET:SD	16:Ad:402:3PH:C1	3.01	0.49
5:Ae:227:ASN:N	5:Ae:233:GLY:O	2.45	0.49
5:Ae:231:PHE:CD1	5:Ae:250:ARG:HB2	2.47	0.49
5:AE:172:LYS:HE2	5:AE:173:PRO:HD3	1.93	0.49
2:Ab:145:GLU:O	2:Ab:146:PHE:C	2.55	0.49
3:Ac:361:ILE:HA	3:Ac:365:LEU:HB2	1.95	0.49
4:Ad:189:ASN:O	4:Ad:190:ASN:HB2	2.13	0.49
5:Ae:142:ALA:HB3	5:Ae:147:LEU:HD22	1.92	0.49
5:Ae:207:LYS:HZ3	5:Ae:268:ASP:HA	1.75	0.49
4:AD:189:ASN:HD22	13:AD:401:HEC:HMD2	1.78	0.49
6:AF:44:VAL:O	6:AF:48:ILE:HG13	2.12	0.49
6:AF:75:ILE:HD12	6:AF:81:TRP:HZ2	1.76	0.49
1:Aa:226:ALA:HB2	1:Aa:253:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:341:PHE:HE1	1:Aa:356:ALA:CB	2.26	0.49
2:Ab:84:ARG:CG	5:Ai:68:VAL:HG22	2.33	0.49
2:Ab:226:SER:O	2:Ab:227:HIS:C	2.56	0.49
3:Ac:218:ILE:HB	3:Ac:219:PRO:HD2	1.94	0.49
3:Ac:291:VAL:O	3:Ac:295:ILE:HG12	2.11	0.49
4:Ad:201:VAL:HG21	4:Ad:275:ARG:HD2	1.94	0.49
4:Ad:227:LEU:HD12	4:Ad:227:LEU:O	2.11	0.49
1:AA:389:THR:O	1:AA:390:ARG:C	2.55	0.49
2:AB:40:PHE:CZ	2:AB:406:TYR:HB2	2.46	0.49
2:AB:90:THR:HG23	2:AB:95:SER:HA	1.95	0.49
3:AC:199:PHE:HE1	3:Ac:8:HIS:HE2	1.42	0.49
3:Ac:136:GLY:O	3:Ac:259:ALA:HB2	2.12	0.49
3:Ac:185:LEU:HD23	3:Ac:188:ILE:HD12	1.95	0.49
3:Ac:253:PRO:HG3	4:Ad:205:HIS:CG	2.48	0.49
8:Ah:44:ALA:O	8:Ah:48:LEU:HB2	2.13	0.49
3:AC:137:GLN:HE22	3:AC:263:ASN:C	2.18	0.49
3:AC:297:SER:O	3:AC:300:ILE:HG22	2.13	0.49
4:AD:107:HIS:HA	4:AD:110:ILE:HD12	1.95	0.49
1:Aa:108:ALA:O	1:Aa:112:GLU:HG3	2.12	0.49
1:Aa:296:TRP:NE1	1:Aa:347:SER:O	2.45	0.49
3:Ac:244:LEU:HD12	4:Ad:292:MET:HE2	1.94	0.49
4:Ad:300:LEU:O	4:Ad:301:PRO:C	2.54	0.49
8:Ah:39:GLU:O	8:Ah:42:VAL:HG12	2.12	0.49
1:AA:341:PHE:HE1	1:AA:356:ALA:CB	2.26	0.49
3:AC:181:PHE:CA	3:AC:184:ILE:HG22	2.43	0.49
5:AE:92:ARG:HA	7:AG:24:GLN:HA	1.94	0.49
7:AG:67:PHE:CZ	7:AG:71:LYS:HD3	2.47	0.49
2:Ab:178:HIS:CD2	2:Ab:335:LEU:HD12	2.47	0.49
3:Ac:297:SER:O	3:Ac:300:ILE:HG22	2.13	0.49
4:Ad:175:PHE:H	4:Ad:175:PHE:HD1	1.61	0.49
4:Ad:232:TYR:CZ	4:Ad:245:ALA:HB2	2.48	0.49
4:Ad:250:THR:HA	4:Ad:263:MET:HB2	1.94	0.49
4:Ad:309:HIS:HD2	4:Ad:310:LYS:HD3	1.78	0.49
1:AA:197:LEU:HD21	1:AA:348:TYR:CD2	2.48	0.49
3:AC:361:ILE:HA	3:AC:365:LEU:HB2	1.94	0.49
5:AE:218:THR:OG1	5:AE:254:ALA:HB1	2.13	0.49
5:AE:239:HIS:CD2	3:Ac:278:TYR:OH	2.65	0.49
6:AF:83:LYS:HB2	6:AF:86:GLU:HG3	1.95	0.49
7:AG:11:ILE:HD12	7:AG:11:ILE:N	2.27	0.49
1:Aa:186:TYR:CZ	5:Ae:80:HIS:HB2	2.47	0.49
2:Ab:38:LEU:HD22	2:Ab:38:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:225:VAL:HG22	2:Ab:226:SER:H	1.78	0.49
4:Ad:249:TYR:CE2	4:Ad:252:VAL:HG23	2.48	0.49
5:Ae:159:ILE:HD11	5:Ae:165:MET:SD	2.52	0.49
3:AC:218:ILE:HB	3:AC:219:PRO:HD2	1.94	0.49
4:AD:227:LEU:HD11	4:AD:233:PHE:N	2.28	0.49
4:AD:262:THR:CB	8:AH:26:ASP:HA	2.40	0.49
5:AE:172:LYS:HD2	3:Ac:169:SER:HB3	1.94	0.49
4:Ad:132:TYR:O	4:Ad:135:LEU:HB2	2.13	0.49
5:Ae:152:ILE:HG13	5:Ae:154:ILE:CD1	2.42	0.49
5:Ae:155:LYS:CE	5:Ae:157:SER:HB3	2.42	0.49
5:Ae:163:LYS:N	5:Ae:178:HIS:HB3	2.19	0.49
5:Ae:172:LYS:HA	5:Ae:172:LYS:CE	2.43	0.49
5:Ae:179:ARG:NH1	5:Ae:184:ILE:HA	2.28	0.49
1:AA:285:ALA:O	1:AA:359:VAL:HA	2.11	0.48
2:AB:47:LEU:CD2	2:AB:234:ALA:HB1	2.43	0.48
3:AC:196:HIS:NE2	11:AC:402:HEM:ND	2.61	0.48
8:AH:49:GLU:HA	8:AH:52:ASP:OD2	2.13	0.48
3:Ac:72:ASP:HB3	5:Ae:145:ASP:HB3	1.93	0.48
4:Ad:130:VAL:O	4:Ad:175:PHE:HD1	1.95	0.48
17:Ag:102:CDL:H521	17:Ag:102:CDL:H562	1.94	0.48
1:AA:148:ALA:HA	1:AA:250:LEU:HD21	1.95	0.48
2:AB:64:PHE:CZ	2:AB:394:SER:HA	2.49	0.48
2:AB:177:LEU:HD22	2:AB:270:ALA:HB1	1.96	0.48
6:AF:101:GLU:HB3	6:AF:105:ARG:NH1	2.28	0.48
1:Aa:274:GLU:OE2	1:Aa:276:ARG:NH1	2.44	0.48
4:Ad:212:PHE:CE1	4:Ad:216:THR:HG21	2.47	0.48
5:Ae:200:HIS:O	5:Ae:201:ASP:C	2.55	0.48
1:AA:101:THR:O	1:AA:102:LYS:C	2.55	0.48
3:AC:51:LEU:HD12	11:AC:401:HEM:CBA	2.43	0.48
4:AD:237:PHE:CZ	4:AD:242:ILE:HA	2.48	0.48
5:AE:222:CYS:SG	3:Ac:268:ILE:CD1	3.01	0.48
5:AE:231:PHE:HD2	5:AE:250:ARG:NH1	2.11	0.48
7:AG:76:ALA:O	7:AG:79:GLU:HB3	2.12	0.48
2:Ab:429:LYS:HA	2:Ab:432:VAL:CG1	2.40	0.48
3:Ac:281:LEU:HD12	3:Ac:290:GLY:HA3	1.95	0.48
3:Ac:317:PHE:HB3	6:Af:27:PHE:HD2	1.78	0.48
4:Ad:181:ASN:O	4:Ad:184:ALA:N	2.46	0.48
4:Ad:321:TYR:HB2	6:Af:61:PHE:CD2	2.47	0.48
5:Ae:174:LEU:HD11	5:Ae:273:VAL:CG1	2.43	0.48
3:AC:58:ASP:O	3:AC:62:ALA:N	2.41	0.48
4:AD:214:LEU:HD11	4:AD:237:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:56:VAL:O	7:AG:57:TYR:C	2.55	0.48
9:AJ:23:LEU:HA	10:AK:27:VAL:CG2	2.44	0.48
1:Aa:160:GLN:HA	1:Aa:163:LYS:NZ	2.29	0.48
4:Ad:277:ALA:O	4:Ad:280:PRO:HD3	2.13	0.48
4:Ad:314:LEU:HB3	6:Af:71:MET:HE1	1.95	0.48
5:Ae:147:LEU:C	5:Ae:147:LEU:HD12	2.38	0.48
2:AB:195:TYR:OH	2:Ab:261:GLN:HG3	2.12	0.48
3:AC:52:ALA:N	11:AC:401:HEM:HMA2	2.27	0.48
11:AC:402:HEM:HHA	11:AC:402:HEM:O1A	2.12	0.48
4:AD:94:TYR:HD2	4:AD:209:ASP:CG	2.21	0.48
4:AD:96:TRP:CD1	4:AD:96:TRP:H	2.31	0.48
9:AJ:23:LEU:CA	10:AK:27:VAL:CG2	2.91	0.48
2:Ab:113:THR:O	2:Ab:119:MET:HG3	2.13	0.48
2:Ab:286:PHE:CZ	2:Ab:427:ALA:HB1	2.49	0.48
4:Ad:200:ILE:HG12	13:Ad:401:HEC:HMA3	1.95	0.48
5:Ai:43:LEU:O	5:Ai:44:ASP:C	2.56	0.48
2:AB:388:THR:HG23	2:AB:391:GLY:H	1.78	0.48
4:AD:159:ASN:HB3	4:AD:166:MET:HG3	1.94	0.48
1:Aa:341:PHE:HB2	1:Aa:368:MET:CE	2.43	0.48
2:Ab:81:HIS:CD2	2:Ab:158:LEU:HD12	2.48	0.48
2:Ab:159:LYS:HD2	2:Ab:197:MET:HE1	1.95	0.48
2:Ab:201:THR:OG1	2:Ab:204:GLU:HG3	2.14	0.48
2:Ab:388:THR:HG23	2:Ab:391:GLY:H	1.77	0.48
4:Ad:89:LEU:H	8:Ah:70:PHE:HE1	1.60	0.48
1:AA:341:PHE:CE1	1:AA:356:ALA:HB1	2.48	0.48
3:AC:140:PHE:CZ	3:AC:261:PRO:HA	2.48	0.48
3:AC:145:VAL:HG12	5:Ae:220:LEU:HD13	1.92	0.48
3:AC:153:ILE:HG23	3:AC:154:PRO:HD2	1.96	0.48
7:AG:50:ALA:O	7:AG:54:VAL:HG23	2.13	0.48
7:AG:69:GLN:O	7:AG:72:ARG:HB3	2.14	0.48
1:Aa:339:GLN:O	1:Aa:340:SER:C	2.56	0.48
2:Ab:91:THR:C	2:Ab:93:GLY:H	2.22	0.48
2:Ab:91:THR:C	2:Ab:93:GLY:N	2.69	0.48
3:Ac:32:ASN:ND2	3:Ac:228:ASP:OD1	2.47	0.48
4:Ad:130:VAL:HG12	4:Ad:175:PHE:CE1	2.49	0.48
4:Ad:157:GLY:N	4:Ad:158:PRO:CD	2.77	0.48
4:Ad:279:GLU:HG2	4:Ad:282:HIS:N	2.29	0.48
5:Ae:192:VAL:O	5:Ae:195:LEU:HB2	2.13	0.48
5:Ae:217:CYS:O	5:Ae:218:THR:C	2.56	0.48
10:Ak:9:ARG:O	10:Ak:10:TYR:C	2.56	0.48
2:AB:109:LYS:O	2:AB:123:VAL:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:94:TYR:HB2	4:AD:96:TRP:HE1	1.77	0.48
5:AE:108:GLU:HA	5:AE:111:LYS:HE2	1.96	0.48
8:AH:31:VAL:HG11	8:AH:84:LEU:HB2	1.95	0.48
2:Ab:231:LYS:O	2:Ab:235:GLU:HB3	2.14	0.48
4:Ad:124:CYS:O	4:Ad:125:HIS:CG	2.67	0.48
16:Ad:402:3PH:C3	5:Ae:131:ASN:ND2	2.76	0.48
7:Ag:11:ILE:CG2	7:Ag:12:ARG:N	2.77	0.48
5:AI:62:ARG:HB3	5:AI:63:PRO:HD2	1.96	0.48
1:AA:409:VAL:O	1:AA:410:CYS:C	2.55	0.48
6:AF:39:HIS:O	6:AF:44:VAL:HG21	2.14	0.48
2:Ab:163:ALA:C	5:AI:43:LEU:CD2	2.82	0.48
3:Ac:153:ILE:HG23	3:Ac:154:PRO:HD2	1.96	0.48
4:Ad:128:ASP:OD1	4:Ad:128:ASP:N	2.46	0.48
8:Ah:32:ARG:HA	8:Ah:80:VAL:HG22	1.96	0.48
8:Ah:47:ARG:HA	8:Ah:50:LEU:CG	2.44	0.48
2:AB:171:THR:HG23	5:AI:64:LEU:HD23	1.95	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:211:LEU:HD22	6:AF:37:THR:HA	1.96	0.48
3:AC:269:LYS:CE	3:AC:340:GLY:HA2	2.44	0.48
4:AD:114:PHE:CD2	4:AD:140:TYR:CE1	3.01	0.48
1:Aa:358:PHE:CD1	1:Aa:368:MET:HG2	2.48	0.48
2:Ab:158:LEU:O	2:Ab:159:LYS:C	2.53	0.48
4:Ad:124:CYS:HB2	13:Ad:401:HEC:C3C	2.44	0.48
5:Ae:196:ARG:NH1	5:Ae:252:GLY:O	2.44	0.48
7:Ag:76:ALA:O	7:Ag:77:MET:C	2.57	0.48
2:AB:170:GLN:CD	2:AB:170:GLN:H	2.21	0.47
12:AC:403:UQ6:H172	12:AC:403:UQ6:H151	1.63	0.47
5:AE:217:CYS:O	5:AE:218:THR:C	2.56	0.47
7:AG:50:ALA:N	7:AG:51:PRO:CD	2.77	0.47
1:Aa:341:PHE:CE1	1:Aa:356:ALA:HB1	2.48	0.47
1:Aa:387:GLU:HB2	1:Aa:390:ARG:HH22	1.78	0.47
3:Ac:304:MET:HA	3:Ac:307:LEU:HD12	1.96	0.47
4:Ad:89:LEU:HG	4:Ad:236:TYR:CE1	2.49	0.47
4:Ad:165:PHE:O	4:Ad:166:MET:HG3	2.13	0.47
5:Ae:166:ALA:HA	5:Ae:174:LEU:C	2.39	0.47
5:Ae:167:PHE:HB2	5:Ae:174:LEU:HD23	1.95	0.47
4:AD:122:SER:O	4:AD:178:PRO:HB3	2.14	0.47
5:AE:111:LYS:O	5:AE:115:TYR:HD1	1.97	0.47
1:Aa:137:SER:HB3	1:Aa:236:GLY:O	2.14	0.47
2:Ab:109:LYS:HD2	2:Ab:124:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:220:PHE:HE2	12:Ac:405:UQ6:H4M2	1.77	0.47
3:AC:185:LEU:O	3:AC:189:ILE:HG13	2.14	0.47
3:AC:296:LEU:O	3:AC:300:ILE:N	2.45	0.47
4:AD:127:MET:CE	4:AD:198:SER:HA	2.44	0.47
4:AD:128:ASP:N	4:AD:128:ASP:OD1	2.46	0.47
4:Ad:183:GLU:HA	4:Ad:186:ARG:HH21	1.78	0.47
1:AA:109:LEU:HD21	1:AA:120:LEU:HD21	1.95	0.47
1:AA:339:GLN:O	1:AA:340:SER:C	2.56	0.47
3:AC:141:TRP:CG	3:AC:264:THR:HG1	2.31	0.47
4:AD:98:HIS:HB3	4:AD:105:LEU:HA	1.96	0.47
5:AE:119:ALA:CA	9:AJ:25:ILE:HG12	2.44	0.47
8:AH:61:THR:HG23	8:AH:63:GLU:H	1.78	0.47
2:Ab:38:LEU:CD1	2:Ab:396:ILE:HD13	2.44	0.47
2:Ab:212:HIS:CE1	2:Ab:246:LEU:HB3	2.49	0.47
2:Ab:297:PRO:HA	2:Ab:304:ASN:ND2	2.28	0.47
5:Ae:246:SER:HB3	5:Ae:248:ARG:HE	1.79	0.47
3:AC:141:TRP:O	3:AC:145:VAL:HG23	2.14	0.47
5:AI:62:ARG:HB3	5:AI:63:PRO:HD2	1.95	0.47
5:Ae:218:THR:CG2	5:Ae:256:LEU:O	2.61	0.47
1:AA:390:ARG:HG3	2:AB:104:GLU:O	2.14	0.47
3:AC:16:HIS:NE2	3:AC:201:HIS:CD2	2.82	0.47
3:AC:44:GLN:O	3:AC:83:HIS:CE1	2.67	0.47
3:AC:141:TRP:CD1	3:AC:264:THR:HA	2.49	0.47
5:AE:130:LYS:HD2	10:AK:34:TRP:CD1	2.49	0.47
1:Aa:292:GLU:OE2	5:Ae:104:LYS:HE3	2.13	0.47
14:Aa:501:3PE:H332	3:Ac:221:HIS:HE1	1.80	0.47
3:Ac:276:PHE:CG	3:Ac:277:ALA:N	2.82	0.47
3:Ac:317:PHE:CD1	6:Af:27:PHE:HB3	2.50	0.47
4:Ad:311:TRP:CZ3	4:Ad:314:LEU:HD12	2.50	0.47
1:AA:174:GLU:C	1:AA:176:ASP:N	2.73	0.47
1:AA:183:VAL:HG21	1:AA:286:HIS:HB2	1.97	0.47
2:AB:429:LYS:O	2:AB:432:VAL:HG12	2.14	0.47
3:AC:304:MET:HA	3:AC:307:LEU:HD12	1.96	0.47
4:AD:183:GLU:CB	4:Ad:161:ASP:HB3	2.44	0.47
5:AE:231:PHE:CD2	5:AE:250:ARG:HG3	2.50	0.47
5:AE:238:CYS:SG	3:Ac:268:ILE:HD11	2.53	0.47
7:AG:31:PHE:CD1	7:AG:32:SER:N	2.83	0.47
1:Aa:92:PHE:CE2	1:Aa:161:ILE:HG23	2.49	0.47
2:Ab:72:GLU:HB3	2:Ab:76:ASN:OD1	2.15	0.47
2:Ab:109:LYS:O	2:Ab:123:VAL:HA	2.15	0.47
4:Ad:223:THR:CG2	8:Ah:55:VAL:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:159:ILE:HB	5:Ae:210:TRP:CZ3	2.49	0.47
1:AA:463:GLU:HG2	7:AG:6:GLY:H	1.78	0.47
3:AC:262:LEU:HD11	5:Ae:168:LYS:HD2	1.96	0.47
4:AD:129:TYR:HD2	4:AD:198:SER:HB2	1.80	0.47
5:AE:166:ALA:HA	5:AE:174:LEU:O	2.15	0.47
6:AF:26:GLY:C	6:AF:28:ASN:N	2.68	0.47
6:AF:72:ARG:O	6:AF:74:GLN:HG2	2.15	0.47
1:Aa:186:TYR:C	1:Aa:188:HIS:N	2.68	0.47
1:Aa:279:ASP:HA	7:Ag:12:ARG:HA	1.97	0.47
2:Ab:226:SER:O	2:Ab:229:VAL:HG22	2.15	0.47
3:Ac:141:TRP:NE1	3:Ac:263:ASN:O	2.47	0.47
4:Ad:192:ALA:HB1	13:Ad:401:HEC:CGD	2.45	0.47
5:Ae:167:PHE:O	5:Ae:168:LYS:C	2.57	0.47
3:AC:29:SER:O	3:AC:30:TRP:C	2.55	0.47
3:AC:176:THR:HB	3:Ac:53:MET:O	2.15	0.47
1:Aa:172:MET:HA	1:Aa:175:ASN:ND2	2.30	0.47
1:Aa:384:THR:HB	10:Ak:9:ARG:HG3	1.97	0.47
1:Aa:387:GLU:HB2	1:Aa:390:ARG:NH2	2.30	0.47
1:Aa:397:ASN:HA	2:Ab:58:LEU:HD11	1.95	0.47
4:Ad:318:LYS:HD2	5:Ae:86:PRO:HB2	1.96	0.47
3:Ac:16:HIS:NE2	3:Ac:201:HIS:CD2	2.82	0.47
9:Aj:42:ALA:HA	9:Aj:45:GLU:OE2	2.14	0.47
1:AA:172:MET:HA	1:AA:175:ASN:ND2	2.30	0.46
3:AC:294:LEU:O	3:AC:297:SER:HB3	2.15	0.46
4:AD:131:ALA:HB3	4:AD:134:HIS:ND1	2.30	0.46
4:AD:159:ASN:N	4:AD:166:MET:HG3	2.29	0.46
4:AD:186:ARG:NE	4:AD:193:LEU:HB2	2.30	0.46
4:AD:255:TYR:HH	4:AD:269:ASP:HB2	1.79	0.46
5:AE:79:SER:OG	5:AE:80:HIS:N	2.38	0.46
1:Aa:104:ARG:HE	1:Aa:112:GLU:CD	2.23	0.46
1:Aa:138:LYS:O	1:Aa:141:PRO:HD2	2.14	0.46
1:Aa:407:THR:HB	1:Aa:408:PRO:HD3	1.96	0.46
1:AA:274:GLU:OE2	1:AA:276:ARG:HD2	2.14	0.46
3:AC:137:GLN:NE2	3:AC:141:TRP:CD1	2.84	0.46
3:AC:137:GLN:N	3:AC:257:MET:O	2.46	0.46
3:AC:145:VAL:HG22	5:Ae:222:CYS:SG	2.54	0.46
4:AD:313:VAL:CA	7:AG:24:GLN:HE22	2.27	0.46
8:AH:76:ARG:O	8:AH:80:VAL:HG23	2.14	0.46
1:Aa:183:VAL:HG21	1:Aa:286:HIS:HB2	1.97	0.46
3:Ac:100:ARG:HH22	11:Ac:402:HEM:HBD1	1.81	0.46
4:Ad:111:ARG:HG3	4:Ad:140:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:185:ALA:HB1	4:Ad:194:PRO:CD	2.45	0.46
5:Ae:184:ILE:HD13	5:Ae:208:PRO:HB2	1.97	0.46
9:Aj:39:GLY:O	9:Aj:43:ILE:HG13	2.16	0.46
4:AD:159:ASN:OD1	4:AD:162:GLY:N	2.48	0.46
1:Aa:66:HIS:CD2	2:Ab:387:GLU:O	2.69	0.46
1:Aa:152:GLN:O	1:Aa:153:ASN:HB2	2.15	0.46
3:Ac:140:PHE:CE1	3:Ac:170:VAL:CG1	2.98	0.46
4:Ad:100:GLY:O	4:Ad:286:LYS:NZ	2.46	0.46
5:Ae:177:ARG:HG2	5:Ae:178:HIS:N	2.29	0.46
5:Ae:179:ARG:HH22	5:Ae:202:LEU:HD23	1.80	0.46
6:Af:29:LYS:HA	6:Af:81:TRP:CD1	2.49	0.46
4:AD:181:ASN:OD1	4:AD:184:ALA:N	2.49	0.46
7:AG:50:ALA:O	7:AG:51:PRO:C	2.58	0.46
2:Ab:55:TYR:HA	2:Ab:127:ARG:NH1	2.31	0.46
2:Ab:163:ALA:O	5:AI:43:LEU:HD22	2.15	0.46
3:Ac:36:LEU:HD11	17:Ag:102:CDL:H732	1.98	0.46
3:Ac:253:PRO:HG2	4:Ad:205:HIS:CD2	2.50	0.46
8:Ah:42:VAL:O	8:Ah:46:GLU:N	2.41	0.46
8:Ah:82:HIS:HD2	8:Ah:83:LYS:HE3	1.79	0.46
1:Aa:450:TYR:O	1:Aa:451:ASP:HB2	2.15	0.46
14:Ac:403:3PE:HN1	17:Ag:101:CDL:PB2	2.39	0.46
4:Ad:88:GLU:O	4:Ad:89:LEU:C	2.58	0.46
4:Ad:295:MET:HB3	16:Ad:402:3PH:C36	2.45	0.46
5:Ae:160:PRO:HD2	5:Ae:163:LYS:HG3	1.98	0.46
5:Ae:249:ILE:HD11	5:Ae:251:LYS:O	2.15	0.46
8:Ah:42:VAL:HA	8:Ah:45:ARG:CB	2.45	0.46
1:AA:74:TRP:C	1:AA:75:ILE:HG13	2.40	0.46
1:AA:287:VAL:HB	1:AA:358:PHE:CZ	2.50	0.46
1:AA:407:THR:HB	1:AA:408:PRO:HD3	1.97	0.46
4:AD:121:CYS:SG	13:AD:401:HEC:CBB	3.03	0.46
4:AD:125:HIS:HE1	4:AD:195:PRO:HD2	1.80	0.46
4:AD:126:SER:O	4:AD:196:ASP:HB3	2.16	0.46
4:AD:156:ASP:HB2	4:AD:167:ARG:O	2.16	0.46
4:AD:263:MET:HB3	8:AH:26:ASP:OD2	2.16	0.46
5:AE:122:THR:CG2	9:AJ:25:ILE:CG2	2.87	0.46
5:AE:246:SER:HB3	5:AE:248:ARG:HE	1.79	0.46
6:AF:26:GLY:O	6:AF:29:LYS:N	2.48	0.46
7:AG:50:ALA:N	7:AG:51:PRO:HD2	2.30	0.46
5:AI:43:LEU:HD12	5:AI:46:LYS:NZ	2.31	0.46
1:Aa:140:LEU:O	1:Aa:141:PRO:C	2.59	0.46
2:Ab:90:THR:HG23	2:Ab:94:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:42:MET:CE	12:Ac:405:UQ6:C19	2.94	0.46
4:Ad:267:ALA:HA	4:Ad:270:VAL:HG12	1.97	0.46
4:Ad:267:ALA:O	4:Ad:268:LYS:C	2.56	0.46
16:Ad:402:3PH:H392	5:Ae:128:ALA:HB3	1.97	0.46
6:Af:85:GLU:CD	6:Af:85:GLU:H	2.24	0.46
2:AB:225:VAL:HG22	2:AB:229:VAL:CG2	2.46	0.46
4:AD:117:TYR:OH	4:AD:126:SER:HA	2.15	0.46
5:AE:93:ARG:HB3	7:AG:24:GLN:C	2.41	0.46
6:AF:106:GLU:O	6:AF:110:LYS:HG3	2.16	0.46
1:Aa:74:TRP:HB3	1:Aa:418:LEU:CD1	2.46	0.46
1:Aa:74:TRP:C	1:Aa:75:ILE:HG13	2.40	0.46
1:Aa:409:VAL:O	1:Aa:410:CYS:C	2.55	0.46
3:Ac:294:LEU:O	3:Ac:297:SER:HB3	2.15	0.46
3:Ac:296:LEU:O	3:Ac:300:ILE:N	2.45	0.46
4:Ad:116:VAL:HG11	4:Ad:270:VAL:HB	1.98	0.46
4:Ad:201:VAL:HG22	4:Ad:278:SER:HB2	1.98	0.46
5:Ae:175:PHE:CE2	5:Ae:215:GLY:HA3	2.51	0.46
5:Ae:265:PHE:HB3	5:Ae:271:VAL:HG23	1.97	0.46
1:AA:120:LEU:HD13	1:AA:133:ILE:HG12	1.97	0.46
1:AA:286:HIS:CG	1:AA:359:VAL:HG22	2.51	0.46
2:AB:284:ASN:HB3	2:AB:419:VAL:CG2	2.45	0.46
3:AC:269:LYS:HE3	3:AC:340:GLY:HA2	1.97	0.46
4:AD:105:LEU:CB	4:AD:110:ILE:HD11	2.42	0.46
4:AD:321:TYR:HB2	6:AF:61:PHE:CE1	2.50	0.46
8:AH:51:CYS:O	8:AH:54:ARG:HB3	2.15	0.46
1:Aa:287:VAL:HB	1:Aa:358:PHE:CZ	2.50	0.46
2:Ab:284:ASN:HB3	2:Ab:419:VAL:CG2	2.45	0.46
3:Ac:146:ILE:CG1	15:Ac:404:U10:C4M	2.69	0.46
3:Ac:280:ILE:O	3:Ac:281:LEU:C	2.58	0.46
4:Ad:292:MET:SD	4:Ad:292:MET:C	2.98	0.46
4:Ad:312:SER:O	4:Ad:313:VAL:C	2.58	0.46
5:Ae:166:ALA:CA	5:Ae:175:PHE:HA	2.44	0.46
5:Ae:205:VAL:HG12	5:Ae:211:VAL:HG23	1.98	0.46
3:AC:138:MET:HB2	3:AC:254:ASP:CB	2.44	0.46
3:AC:141:TRP:CZ3	5:Ae:223:VAL:HG23	2.50	0.46
6:AF:49:ARG:HH22	6:AF:50:ARG:HE	1.62	0.46
5:AI:71:ASN:HB2	5:AI:73:PRO:HD2	1.97	0.46
2:Ab:66:LYS:HA	2:Ab:118:ASN:OD1	2.16	0.46
6:Af:83:LYS:HB3	6:Af:85:GLU:OE2	2.15	0.46
1:AA:74:TRP:HB3	1:AA:418:LEU:CD1	2.46	0.46
2:AB:425:VAL:HG12	2:AB:429:LYS:HZ1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:121:PHE:CZ	3:AC:299:LEU:HG	2.51	0.46
3:AC:152:ALA:O	3:AC:153:ILE:C	2.58	0.46
3:AC:184:ILE:HG23	3:AC:185:LEU:N	2.31	0.46
3:AC:260:ASN:O	3:AC:262:LEU:N	2.48	0.46
4:AD:218:TYR:CE1	4:AD:232:TYR:HB2	2.51	0.46
4:AD:235:PRO:HB3	8:AH:70:PHE:CE1	2.51	0.46
5:AE:131:ASN:O	5:AE:135:GLN:HG2	2.16	0.46
5:AE:231:PHE:CE2	5:AE:250:ARG:HB3	2.51	0.46
7:AG:46:ILE:C	7:AG:48:ARG:N	2.74	0.46
1:Aa:109:LEU:CD1	1:Aa:110:GLU:H	2.24	0.46
1:Aa:286:HIS:CG	1:Aa:359:VAL:HG22	2.51	0.46
3:Ac:233:LEU:HD23	4:Ad:300:LEU:HA	1.96	0.46
3:Ac:278:TYR:CE2	3:Ac:282:ARG:HD2	2.51	0.46
4:Ad:112:ARG:O	4:Ad:116:VAL:HG23	2.16	0.46
4:Ad:155:GLN:CD	4:Ad:165:PHE:HB2	2.41	0.46
4:Ad:185:ALA:O	4:Ad:189:ASN:HB2	2.16	0.46
5:Ae:217:CYS:C	5:Ae:219:HIS:N	2.72	0.46
8:Ah:47:ARG:HB3	8:Ah:47:ARG:NH1	2.30	0.46
2:AB:195:TYR:CD2	2:Ab:262:ASN:C	2.94	0.45
3:AC:51:LEU:HA	3:AC:51:LEU:HD13	1.76	0.45
8:AH:82:HIS:HB3	8:AH:83:LYS:NZ	2.29	0.45
1:Aa:294:PRO:HB3	1:Aa:448:TYR:OH	2.16	0.45
1:Aa:478:LEU:HD23	9:Aj:18:THR:CG2	2.44	0.45
2:Ab:81:HIS:HE2	2:Ab:161:ASP:HB3	1.81	0.45
4:Ad:112:ARG:HE	4:Ad:269:ASP:CG	2.24	0.45
4:Ad:158:PRO:HG3	4:Ad:167:ARG:CB	2.45	0.45
5:Ae:242:HIS:CD2	5:Ae:251:LYS:HD3	2.51	0.45
1:AA:92:PHE:HE1	1:AA:165:ARG:N	2.15	0.45
1:AA:188:HIS:NE2	1:AA:348:TYR:OH	2.47	0.45
2:AB:418:SER:O	2:AB:419:VAL:C	2.59	0.45
3:AC:48:GLY:CA	11:AC:401:HEM:C1B	2.97	0.45
3:AC:135:TRP:CH2	3:AC:140:PHE:CE1	3.04	0.45
4:AD:207:GLY:O	4:AD:208:GLU:C	2.58	0.45
4:AD:226:SER:O	4:AD:227:LEU:C	2.59	0.45
4:AD:237:PHE:CG	4:AD:238:PRO:HD2	2.51	0.45
4:AD:264:SER:CB	8:AH:28:LEU:HB2	2.34	0.45
5:AE:177:ARG:HD2	5:AE:234:TYR:CZ	2.51	0.45
6:AF:95:LEU:O	6:AF:99:ILE:HG12	2.16	0.45
4:Ad:207:GLY:O	4:Ad:208:GLU:C	2.58	0.45
5:Ae:130:LYS:HD3	9:Aj:33:GLU:OE1	2.17	0.45
1:AA:82:GLU:O	1:AA:199:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:410:CYS:O	1:AA:411:GLU:C	2.58	0.45
3:AC:202:GLU:CD	3:Ac:9:PRO:HG3	2.42	0.45
4:AD:114:PHE:HD2	4:AD:140:TYR:CE1	2.33	0.45
2:Ab:306:THR:O	2:Ab:307:SER:C	2.58	0.45
3:Ac:312:GLN:HG2	6:Af:37:THR:O	2.16	0.45
4:Ad:121:CYS:C	4:Ad:123:SER:N	2.73	0.45
4:Ad:123:SER:O	4:Ad:178:PRO:HB3	2.17	0.45
4:Ad:158:PRO:CG	4:Ad:166:MET:H	2.29	0.45
9:Aj:9:ARG:O	9:Aj:13:LEU:HD23	2.15	0.45
3:AC:170:VAL:O	3:AC:170:VAL:HG13	2.16	0.45
5:AE:217:CYS:C	5:AE:219:HIS:N	2.72	0.45
6:AF:83:LYS:HB3	6:AF:85:GLU:OE2	2.17	0.45
1:Aa:246:ALA:O	1:Aa:249:HIS:O	2.34	0.45
1:Aa:341:PHE:CZ	1:Aa:372:LEU:CD1	2.98	0.45
3:Ac:30:TRP:HZ3	3:Ac:96:LEU:HD22	1.81	0.45
3:Ac:233:LEU:CD2	4:Ad:300:LEU:HA	2.46	0.45
4:Ad:307:LYS:O	4:Ad:311:TRP:HB2	2.16	0.45
5:Ae:248:ARG:HG2	5:Ae:257:ASN:ND2	2.31	0.45
1:AA:358:PHE:CD1	1:AA:368:MET:HG2	2.52	0.45
2:AB:278:ILE:HB	2:AB:331:SER:HA	1.98	0.45
3:AC:53:MET:C	3:AC:55:TYR:N	2.74	0.45
3:AC:53:MET:HE2	3:Ac:180:ALA:HB1	1.98	0.45
3:AC:126:THR:CG2	11:AC:401:HEM:HBC2	2.45	0.45
3:AC:140:PHE:HE2	3:AC:141:TRP:CH2	2.34	0.45
4:AD:111:ARG:HA	4:AD:140:TYR:HE1	1.81	0.45
5:AE:241:SER:OG	5:AE:254:ALA:HB2	2.17	0.45
6:AF:99:ILE:O	6:AF:103:LYS:HG2	2.17	0.45
8:AH:52:ASP:HA	8:AH:55:VAL:HG23	1.98	0.45
2:Ab:297:PRO:HB3	2:Ab:304:ASN:ND2	2.26	0.45
3:Ac:170:VAL:HG13	3:Ac:170:VAL:O	2.16	0.45
3:Ac:262:LEU:HD12	3:Ac:262:LEU:N	2.32	0.45
4:Ad:159:ASN:N	4:Ad:164:MET:HB3	2.31	0.45
5:Ae:196:ARG:HH22	5:Ae:252:GLY:N	2.14	0.45
5:Ae:228:ALA:CB	5:Ae:235:TYR:HB3	2.46	0.45
5:Ae:272:VAL:HG12	5:Ae:274:GLY:N	2.32	0.45
8:Ah:47:ARG:HA	8:Ah:50:LEU:HG	1.99	0.45
1:AA:384:THR:HG23	1:AA:384:THR:O	2.15	0.45
2:AB:355:TYR:OH	2:AB:436:LYS:HE2	2.17	0.45
3:AC:48:GLY:C	11:AC:401:HEM:HMB3	2.41	0.45
3:AC:150:LEU:CD1	3:AC:164:ILE:HD12	2.46	0.45
3:AC:218:ILE:HD11	3:AC:224:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:147:ALA:O	4:AD:151:GLU:HG2	2.17	0.45
8:AH:35:CYS:HA	8:AH:38:LEU:HD13	1.98	0.45
2:Ab:278:ILE:HB	2:Ab:331:SER:HA	1.98	0.45
2:Ab:305:THR:O	2:Ab:311:GLN:HG3	2.17	0.45
4:Ad:92:PRO:HG2	4:Ad:94:TYR:CE1	2.52	0.45
4:Ad:240:GLN:HE21	8:Ah:70:PHE:HZ	1.63	0.45
5:Ae:111:LYS:HE3	9:Aj:11:TYR:CZ	2.52	0.45
5:Ae:177:ARG:HB3	5:Ae:211:VAL:HG13	1.98	0.45
1:AA:92:PHE:CZ	1:AA:161:ILE:HG23	2.52	0.45
1:AA:96:LEU:HD13	1:AA:156:LEU:HB3	1.98	0.45
3:AC:59:THR:CG2	3:AC:172:LYS:HG2	2.46	0.45
4:Ad:298:LEU:C	4:Ad:301:PRO:HD2	2.41	0.45
8:Ah:64:ASP:HB3	8:Ah:66:THR:HG23	1.98	0.45
3:AC:117:VAL:HG21	3:AC:302:ALA:HB2	1.99	0.45
3:AC:276:PHE:O	3:AC:279:ALA:HB3	2.17	0.45
4:AD:124:CYS:HB3	4:AD:194:PRO:CB	2.47	0.45
4:AD:214:LEU:HA	4:AD:234:ASN:HD21	1.81	0.45
5:AE:237:PRO:HB2	3:Ac:266:PRO:O	2.17	0.45
1:Aa:373:GLN:NE2	1:Aa:471:ILE:O	2.49	0.45
2:Ab:170:GLN:HG2	5:Ai:60:ALA:H	1.82	0.45
2:Ab:201:THR:H	2:Ab:204:GLU:CD	2.25	0.45
4:Ad:306:MET:O	4:Ad:307:LYS:C	2.60	0.45
9:Aj:11:TYR:HA	9:Aj:15:PHE:HB2	1.97	0.45
1:AA:387:GLU:HB2	1:AA:390:ARG:HH12	1.82	0.45
2:AB:47:LEU:HD11	2:AB:238:LEU:HD13	1.98	0.45
2:AB:341:ILE:HD12	5:AI:59:ALA:HB2	1.97	0.45
3:AC:223:TYR:CE1	4:AD:314:LEU:HG	2.52	0.45
4:AD:268:LYS:HD2	8:AH:88:LEU:HD13	1.97	0.45
6:AF:56:TYR:O	6:AF:60:MET:HG2	2.17	0.45
7:AG:39:LEU:HA	7:AG:42:THR:HG22	1.98	0.45
2:Ab:38:LEU:HG	2:Ab:396:ILE:HD13	1.99	0.45
2:Ab:148:ARG:HG3	2:Ab:149:TRP:N	2.32	0.45
6:Af:53:GLU:OE2	7:Ag:12:ARG:NH1	2.49	0.45
7:Ag:38:VAL:HA	7:Ag:41:ARG:HD3	1.99	0.45
1:AA:246:ALA:O	1:AA:249:HIS:O	2.34	0.45
3:AC:10:LEU:HD22	3:Ac:195:VAL:HG13	1.99	0.45
3:AC:69:ILE:HA	3:AC:73:VAL:CG2	2.47	0.45
3:AC:376:MET:CE	6:AF:18:ARG:HA	2.47	0.45
4:AD:135:LEU:HD13	4:AD:140:TYR:HB2	1.99	0.45
4:AD:310:LYS:HD2	4:AD:310:LYS:N	2.32	0.45
1:Aa:99:LYS:HE2	2:Ab:301:ARG:O	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:402:HIS:NE2	1:Aa:403:LEU:CD1	2.75	0.45
2:Ab:115:THR:HG23	2:Ab:118:ASN:N	2.27	0.45
3:Ac:150:LEU:CD1	3:Ac:164:ILE:HD12	2.46	0.45
3:Ac:280:ILE:O	3:Ac:283:SER:N	2.50	0.45
4:Ad:211:VAL:HG11	4:Ad:274:LEU:HD12	1.99	0.45
5:Ae:156:LEU:HG	5:Ae:271:VAL:CG1	2.47	0.45
8:Ah:49:GLU:O	8:Ah:50:LEU:C	2.60	0.45
1:AA:365:ILE:HG21	1:AA:465:LEU:HB2	1.98	0.44
1:AA:388:VAL:O	1:AA:392:LYS:HG3	2.17	0.44
3:AC:176:THR:O	3:AC:179:PHE:HB3	2.17	0.44
4:AD:157:GLY:N	4:AD:167:ARG:O	2.51	0.44
4:AD:279:GLU:C	4:AD:281:GLU:H	2.25	0.44
5:AE:93:ARG:HG2	7:AG:23:GLU:O	2.17	0.44
8:AH:47:ARG:HH21	8:AH:71:ASP:CB	2.24	0.44
9:AJ:27:VAL:O	9:AJ:30:LEU:HB3	2.17	0.44
1:Aa:178:SER:O	1:Aa:179:MET:C	2.60	0.44
2:Ab:170:GLN:HG3	2:Ab:339:TYR:OH	2.17	0.44
3:Ac:245:PHE:HE2	4:Ad:293:LEU:HG	1.82	0.44
3:Ac:256:TYR:HB2	4:Ad:203:ALA:HA	1.99	0.44
3:Ac:341:GLN:HE21	3:Ac:342:PRO:HD2	1.82	0.44
4:Ad:219:CYS:SG	4:Ad:220:GLU:N	2.90	0.44
5:Ae:155:LYS:NZ	5:Ae:157:SER:HB3	2.32	0.44
1:AA:165:ARG:NH2	1:AA:211:LEU:O	2.51	0.44
1:AA:463:GLU:OE2	7:AG:8:LEU:CG	2.65	0.44
3:AC:48:GLY:CA	3:AC:83:HIS:CE1	3.00	0.44
7:AG:45:ARG:O	7:AG:49:VAL:HG23	2.17	0.44
1:Aa:107:ASN:ND2	1:Aa:111:LYS:HD2	2.33	0.44
1:Aa:294:PRO:HB2	1:Aa:298:ASN:HB3	1.98	0.44
2:Ab:178:HIS:CE1	2:Ab:330:TYR:HH	2.32	0.44
3:Ac:218:ILE:HD11	3:Ac:224:TYR:CE2	2.52	0.44
3:Ac:237:LEU:HD22	4:Ad:300:LEU:HD11	1.98	0.44
4:Ad:223:THR:HG21	8:Ah:55:VAL:HB	1.98	0.44
2:AB:45:ASN:ND2	2:AB:239:ASN:CA	2.74	0.44
2:AB:255:GLY:HA3	2:AB:435:LYS:HE2	2.00	0.44
3:AC:169:SER:HB2	5:Ae:172:LYS:HZ1	1.82	0.44
4:AD:110:ILE:CG1	4:AD:272:THR:HG22	2.47	0.44
7:AG:45:ARG:HA	7:AG:48:ARG:CZ	2.48	0.44
2:Ab:142:THR:HA	2:Ab:241:ARG:HH12	1.82	0.44
3:Ac:294:LEU:HD21	15:Ac:404:U10:C1M	2.47	0.44
3:Ac:368:ILE:O	3:Ac:372:ILE:HG13	2.17	0.44
4:Ad:146:LYS:O	4:Ad:149:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ad:183:GLU:HG3	4:Ad:184:ALA:N	2.32	0.44
5:Ae:239:HIS:CE1	5:Ae:253:PRO:CG	2.87	0.44
1:AA:384:THR:HG22	1:AA:387:GLU:CB	2.45	0.44
1:AA:392:LYS:O	1:AA:396:ARG:HG3	2.17	0.44
5:AE:168:LYS:HZ3	5:AE:171:GLY:HA2	1.81	0.44
5:AE:226:ALA:HB2	5:AE:234:TYR:HE1	1.80	0.44
5:AE:239:HIS:CD2	3:Ac:278:TYR:HH	2.30	0.44
6:AF:90:TYR:O	6:AF:93:PRO:HD2	2.17	0.44
1:Aa:109:LEU:CG	1:Aa:110:GLU:H	2.31	0.44
1:Aa:389:THR:O	1:Aa:390:ARG:C	2.59	0.44
2:Ab:123:VAL:HG12	2:Ab:137:LEU:HD13	1.98	0.44
4:Ad:237:PHE:CD1	4:Ad:238:PRO:HD2	2.53	0.44
4:Ad:262:THR:HB	8:Ah:26:ASP:CB	2.47	0.44
5:Ae:263:TYR:O	5:Ae:264:GLU:C	2.59	0.44
1:AA:294:PRO:HB2	1:AA:298:ASN:HB3	1.98	0.44
1:AA:402:HIS:NE2	1:AA:403:LEU:CD1	2.75	0.44
3:AC:58:ASP:C	3:AC:60:MET:N	2.72	0.44
4:AD:230:GLY:O	4:AD:243:GLY:HA2	2.17	0.44
4:AD:244:MET:HG3	13:AD:401:HEC:NA	2.32	0.44
1:Aa:249:HIS:O	1:Aa:250:LEU:CB	2.64	0.44
1:Aa:392:LYS:O	1:Aa:396:ARG:HG3	2.17	0.44
3:Ac:152:ALA:O	3:Ac:153:ILE:C	2.58	0.44
4:Ad:291:LYS:HB3	16:Ad:402:3PH:C3	2.44	0.44
4:Ad:314:LEU:HB3	6:Af:71:MET:CE	2.47	0.44
8:Ah:34:HIS:O	8:Ah:37:GLN:HG2	2.17	0.44
2:AB:262:ASN:HA	2:Ab:195:TYR:CD1	2.53	0.44
3:AC:195:VAL:HG12	3:AC:199:PHE:HD2	1.83	0.44
3:AC:343:VAL:CG2	5:Ae:239:HIS:HD2	2.29	0.44
3:AC:376:MET:HE3	6:AF:18:ARG:HG2	1.99	0.44
4:AD:120:VAL:HG11	4:AD:247:PRO:HB2	1.98	0.44
4:AD:159:ASN:HB3	4:AD:166:MET:CG	2.47	0.44
4:AD:185:ALA:HB1	4:AD:194:PRO:HD2	2.00	0.44
4:AD:304:TYR:CE2	7:AG:27:PHE:HZ	2.35	0.44
5:AE:255:PRO:HG2	3:Ac:287:LYS:HZ1	1.81	0.44
1:Aa:384:THR:HG21	10:Ak:9:ARG:HD2	2.00	0.44
1:Aa:401:SER:O	1:Aa:404:ASP:N	2.51	0.44
2:Ab:155:ARG:HD2	2:Ab:198:GLY:H	1.82	0.44
2:Ab:160:ILE:O	2:Ab:163:ALA:HB3	2.18	0.44
2:Ab:225:VAL:HG22	2:Ab:229:VAL:CG2	2.48	0.44
4:Ad:128:ASP:O	4:Ad:174:TYR:HB3	2.17	0.44
5:Ae:152:ILE:C	5:Ae:153:GLU:CD	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:25:ARG:NH2	7:Ag:29:SER:H	2.16	0.44
2:AB:39:GLU:HG3	2:AB:227:HIS:ND1	2.32	0.44
2:AB:195:TYR:CZ	2:Ab:261:GLN:HG3	2.52	0.44
2:AB:233:VAL:HA	2:AB:236:GLN:CG	2.47	0.44
3:AC:105:GLY:HA3	3:AC:313:ARG:O	2.18	0.44
3:AC:257:MET:O	3:AC:258:PRO:C	2.60	0.44
4:AD:132:TYR:CE2	4:AD:149:ALA:HA	2.53	0.44
9:AJ:23:LEU:HD13	10:AK:27:VAL:CB	2.47	0.44
1:Aa:47:GLU:OE1	1:Aa:47:GLU:N	2.51	0.44
1:Aa:139:ASP:O	1:Aa:140:LEU:C	2.59	0.44
1:Aa:174:GLU:C	1:Aa:176:ASP:N	2.73	0.44
1:Aa:375:GLN:O	1:Aa:376:TRP:C	2.58	0.44
1:Aa:410:CYS:O	1:Aa:411:GLU:C	2.59	0.44
4:Ad:94:TYR:HB3	4:Ad:95:PRO:HD2	2.00	0.44
4:Ad:201:VAL:HG11	4:Ad:275:ARG:N	2.32	0.44
4:Ad:299:LEU:HD21	5:Ae:124:GLY:C	2.43	0.44
5:Ae:195:LEU:HD13	5:Ae:248:ARG:HD2	1.99	0.44
5:Ae:267:SER:O	5:Ae:268:ASP:C	2.61	0.44
6:Af:97:GLU:HA	6:Af:100:ARG:NH1	2.33	0.44
7:Ag:12:ARG:HB3	7:Ag:13:HIS:CD2	2.52	0.44
2:AB:63:LEU:HD12	2:AB:220:LEU:HD13	2.00	0.44
2:AB:155:ARG:HD2	2:AB:198:GLY:H	1.83	0.44
2:AB:230:LEU:O	2:AB:233:VAL:HG22	2.18	0.44
3:AC:8:HIS:HE2	3:Ac:199:PHE:HE1	1.65	0.44
3:AC:125:ALA:O	3:AC:129:MET:HG2	2.18	0.44
3:AC:148:ASN:HB2	5:Ae:220:LEU:C	2.43	0.44
4:AD:164:MET:HG3	4:AD:165:PHE:N	2.30	0.44
4:AD:213:SER:O	4:AD:217:GLY:N	2.50	0.44
4:AD:248:ILE:HA	4:AD:252:VAL:HG21	2.00	0.44
1:Aa:107:ASN:HA	1:Aa:110:GLU:HG2	2.00	0.44
1:Aa:230:VAL:HG21	1:Aa:417:LEU:HB3	2.00	0.44
4:Ad:186:ARG:HG2	4:Ad:191:GLY:O	2.17	0.44
5:Ae:142:ALA:HB1	5:Ae:147:LEU:HD23	1.95	0.44
7:Ag:19:LEU:HG	7:Ag:20:SER:N	2.33	0.44
7:Ag:74:ASN:O	7:Ag:75:PRO:C	2.60	0.44
1:AA:311:ILE:CG2	1:AA:341:PHE:CZ	3.01	0.44
2:AB:307:SER:O	2:AB:308:LEU:C	2.59	0.44
3:AC:53:MET:C	3:AC:55:TYR:H	2.26	0.44
4:AD:95:PRO:HD2	8:AH:85:PHE:CD1	2.52	0.44
7:AG:79:GLU:HA	8:AH:61:THR:HA	2.00	0.44
1:Aa:183:VAL:HG21	1:Aa:286:HIS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:142:THR:HA	2:Ab:241:ARG:HH22	1.82	0.44
2:Ab:173:ILE:O	2:Ab:174:ILE:C	2.59	0.44
2:Ab:426:LYS:HA	2:Ab:429:LYS:HZ3	1.83	0.44
4:Ad:311:TRP:HZ3	6:Af:71:MET:SD	2.41	0.44
1:Aa:78:GLY:H	1:Aa:81:TYR:HD2	1.65	0.43
2:AB:138:LEU:CD1	2:AB:233:VAL:HB	2.47	0.43
2:AB:411:THR:O	2:AB:414:GLN:HG2	2.18	0.43
3:AC:341:GLN:HE21	3:AC:342:PRO:HD2	1.82	0.43
4:AD:170:LYS:HE3	4:AD:170:LYS:HB2	1.82	0.43
4:AD:218:TYR:HA	4:AD:234:ASN:HA	2.00	0.43
1:Aa:120:LEU:HD23	2:Ab:299:ILE:CG2	2.48	0.43
2:Ab:236:GLN:HG3	2:Ab:237:PHE:N	2.33	0.43
3:Ac:146:ILE:HG12	15:Ac:404:U10:H4M3	1.94	0.43
3:Ac:253:PRO:O	4:Ad:203:ALA:HA	2.18	0.43
4:Ad:292:MET:CA	16:Ad:402:3PH:H331	2.43	0.43
5:Ae:153:GLU:C	5:Ae:154:ILE:HD12	2.43	0.43
5:Ae:225:ILE:N	5:Ae:235:TYR:O	2.51	0.43
2:AB:166:PHE:CD1	2:AB:172:ARG:HG2	2.52	0.43
3:AC:50:PHE:HB2	3:AC:79:ILE:HG21	1.99	0.43
3:AC:52:ALA:CA	11:AC:401:HEM:HMA2	2.49	0.43
3:AC:68:HIS:CD2	3:AC:72:ASP:HB2	2.53	0.43
3:AC:182:HIS:CE1	11:AC:401:HEM:C4C	3.06	0.43
3:AC:185:LEU:HA	3:AC:188:ILE:HD12	1.99	0.43
5:AE:127:TYR:CE1	9:AJ:37:ASP:OD1	2.71	0.43
5:AE:164:ASN:HB3	5:AE:226:ALA:HB2	2.00	0.43
6:AF:33:MET:HE1	6:AF:88:LYS:HG2	1.99	0.43
7:AG:33:LYS:O	7:AG:36:PRO:HD2	2.18	0.43
1:Aa:78:GLY:H	1:Aa:81:TYR:HD2	1.65	0.43
1:Aa:186:TYR:OH	5:Ae:80:HIS:CB	2.66	0.43
1:Aa:271:THR:HG22	1:Aa:273:SER:OG	2.18	0.43
2:Ab:106:VAL:CG2	2:Ab:133:LEU:HD21	2.47	0.43
2:Ab:112:VAL:HG22	2:Ab:121:TYR:CD2	2.52	0.43
2:Ab:300:LYS:HE2	2:Ab:301:ARG:HH11	1.83	0.43
2:Ab:312:SER:HA	2:Ab:315:LYS:HE3	1.99	0.43
4:Ad:223:THR:HG21	8:Ah:52:ASP:HA	1.99	0.43
2:AB:173:ILE:HD11	2:AB:439:ALA:C	2.44	0.43
3:AC:265:PRO:O	3:AC:266:PRO:C	2.62	0.43
4:AD:95:PRO:HG2	8:AH:85:PHE:CG	2.53	0.43
6:AF:22:TYR:CZ	6:AF:84:TYR:HA	2.53	0.43
7:AG:76:ALA:HA	7:AG:79:GLU:HB3	2.00	0.43
1:Aa:162:GLU:HA	1:Aa:165:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:172:MET:HE1	1:Aa:205:SER:HA	2.00	0.43
1:Aa:385:GLU:OE2	10:Ak:12:GLU:OE2	2.36	0.43
2:Ab:130:ILE:HA	2:Ab:133:LEU:HB2	2.00	0.43
2:Ab:164:VAL:N	5:Ai:43:LEU:HD22	2.33	0.43
2:Ab:411:THR:O	2:Ab:414:GLN:HG2	2.19	0.43
4:Ad:121:CYS:HB3	13:Ad:401:HEC:CHC	2.49	0.43
4:Ad:219:CYS:O	4:Ad:233:PHE:HD2	2.01	0.43
4:Ad:262:THR:O	4:Ad:263:MET:C	2.59	0.43
4:Ad:299:LEU:HD12	16:Ad:402:3PH:H372	1.98	0.43
7:Ag:29:SER:CB	7:Ag:32:SER:HB2	2.38	0.43
8:Ah:49:GLU:O	8:Ah:53:ASN:N	2.33	0.43
1:AA:183:VAL:HG21	1:AA:286:HIS:CB	2.48	0.43
2:AB:148:ARG:NH2	6:Af:50:ARG:O	2.52	0.43
3:AC:45:ILE:HG23	11:AC:401:HEM:HAB	2.00	0.43
3:AC:278:TYR:CE2	3:AC:282:ARG:HD2	2.53	0.43
5:AE:132:VAL:O	5:AE:136:PHE:HB2	2.18	0.43
5:AE:235:TYR:CE1	5:AE:240:GLY:HA2	2.53	0.43
6:AF:110:LYS:HA	10:Ak:10:TYR:HE1	1.84	0.43
7:AG:20:SER:O	7:AG:24:GLN:HG2	2.19	0.43
7:AG:29:SER:HB2	7:AG:32:SER:HB3	2.00	0.43
8:AH:58:ARG:HB3	8:AH:61:THR:HG21	2.00	0.43
1:Aa:311:ILE:CG2	1:Aa:341:PHE:CZ	3.01	0.43
2:Ab:297:PRO:CB	2:Ab:304:ASN:CG	2.91	0.43
3:Ac:138:MET:CE	3:Ac:268:ILE:HG23	2.49	0.43
4:Ad:183:GLU:N	4:Ad:186:ARG:HH21	2.17	0.43
4:Ad:302:LEU:O	4:Ad:305:ALA:HB3	2.19	0.43
2:AB:109:LYS:HD2	5:AI:71:ASN:ND2	2.31	0.43
2:AB:138:LEU:HD22	2:AB:238:LEU:HG	2.01	0.43
3:AC:269:LYS:HE3	3:AC:275:LEU:HD21	2.01	0.43
3:AC:277:ALA:HA	3:AC:280:ILE:HD12	2.00	0.43
4:AD:98:HIS:O	4:AD:286:LYS:NZ	2.52	0.43
4:AD:279:GLU:C	4:AD:281:GLU:N	2.75	0.43
1:Aa:71:VAL:HG21	1:Aa:140:LEU:CD1	2.48	0.43
1:Aa:110:GLU:HB2	2:Ab:299:ILE:CD1	2.35	0.43
2:Ab:297:PRO:HB3	2:Ab:304:ASN:CG	2.43	0.43
4:Ad:222:PRO:HB3	8:Ah:69:LEU:HD13	1.98	0.43
7:Ag:48:ARG:HH21	14:Ag:103:3PE:H322	1.83	0.43
1:AA:80:ARG:NH2	1:AA:268:CYS:SG	2.92	0.43
2:AB:130:ILE:HA	2:AB:133:LEU:HB2	2.01	0.43
2:AB:177:LEU:HD22	2:AB:270:ALA:CB	2.49	0.43
3:AC:53:MET:HG2	3:Ac:180:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:100:ARG:HH12	11:AC:402:HEM:CBD	2.30	0.43
4:AD:94:TYR:HB3	8:AH:85:PHE:CZ	2.54	0.43
4:AD:112:ARG:HB3	4:AD:255:TYR:CE1	2.53	0.43
4:AD:248:ILE:HD12	4:AD:266:VAL:HG11	2.00	0.43
4:AD:312:SER:O	4:AD:313:VAL:C	2.59	0.43
5:AE:114:SER:HB2	7:AG:22:PHE:HE2	1.83	0.43
5:AE:166:ALA:HB2	5:AE:175:PHE:HD1	1.84	0.43
1:Aa:142:LYS:HE2	1:Aa:142:LYS:HB2	1.86	0.43
2:Ab:418:SER:O	2:Ab:419:VAL:C	2.59	0.43
5:Ae:161:GLU:HA	5:Ae:178:HIS:CD2	2.54	0.43
17:Ag:101:CDL:CA5	17:Ag:101:CDL:H512	2.49	0.43
1:AA:371:PHE:O	1:AA:375:GLN:HG2	2.19	0.43
3:AC:128:PHE:CE1	3:AC:143:ALA:HA	2.52	0.43
3:AC:133:LEU:HD23	3:AC:133:LEU:HA	1.85	0.43
3:AC:264:THR:HG22	5:Ae:225:ILE:HD11	2.01	0.43
11:AC:402:HEM:HBA1	12:AC:403:UQ6:C4	2.48	0.43
4:AD:242:ILE:CG2	4:AD:243:GLY:N	2.82	0.43
4:AD:247:PRO:HB3	13:AD:401:HEC:CMC	2.33	0.43
5:AE:162:GLY:O	5:AE:227:ASN:OD1	2.36	0.43
1:Aa:74:TRP:CZ3	1:Aa:232:ALA:HB3	2.54	0.43
4:Ad:117:TYR:CD2	4:Ad:121:CYS:SG	3.11	0.43
5:Ae:122:THR:CG2	9:Aj:25:ILE:HG21	2.48	0.43
5:Ae:200:HIS:O	5:Ae:203:ASP:N	2.51	0.43
5:Ae:242:HIS:HD2	5:Ae:251:LYS:HB3	1.83	0.43
8:Ah:42:VAL:O	8:Ah:45:ARG:HB3	2.18	0.43
1:AA:96:LEU:HB3	1:AA:156:LEU:HD22	2.01	0.43
1:AA:152:GLN:O	1:AA:153:ASN:HB2	2.17	0.43
1:AA:182:VAL:HG13	1:AA:186:TYR:CZ	2.53	0.43
2:AB:332:ASP:OD1	2:AB:332:ASP:N	2.52	0.43
3:AC:193:ALA:O	3:AC:196:HIS:HB3	2.19	0.43
2:Ab:61:ILE:HG22	2:Ab:220:LEU:HD11	2.01	0.43
2:Ab:236:GLN:HG3	2:Ab:237:PHE:H	1.84	0.43
3:Ac:33:PHE:O	3:Ac:36:LEU:HB2	2.19	0.43
4:Ad:131:ALA:O	4:Ad:134:HIS:N	2.52	0.43
4:Ad:152:VAL:CG1	4:Ad:176:PRO:HG3	2.49	0.43
4:Ad:219:CYS:O	4:Ad:220:GLU:C	2.61	0.43
8:Ah:72:PHE:CE2	8:Ah:76:ARG:NE	2.85	0.43
1:AA:92:PHE:CE2	1:AA:161:ILE:HG23	2.53	0.43
1:AA:178:SER:O	1:AA:179:MET:C	2.60	0.43
3:AC:18:PHE:HE1	12:AC:403:UQ6:C8	2.32	0.43
4:AD:237:PHE:CD1	4:AD:242:ILE:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:262:THR:O	4:AD:263:MET:C	2.61	0.43
7:AG:51:PRO:O	7:AG:54:VAL:HB	2.18	0.43
8:AH:43:LYS:O	8:AH:47:ARG:HG3	2.19	0.43
5:AI:72:VAL:N	5:AI:73:PRO:HD2	2.34	0.43
1:Aa:71:VAL:HG21	1:Aa:140:LEU:HD12	2.01	0.43
3:Ac:77:TRP:CZ2	4:Ad:284:HIS:HD2	2.35	0.43
3:Ac:140:PHE:HE2	3:Ac:141:TRP:CH2	2.36	0.43
3:Ac:253:PRO:CG	4:Ad:205:HIS:CG	3.02	0.43
3:Ac:278:TYR:O	3:Ac:279:ALA:C	2.61	0.43
5:Ae:112:GLY:O	5:Ae:116:LEU:HB2	2.19	0.43
5:Ae:167:PHE:HE2	5:Ae:176:VAL:HG21	1.83	0.43
5:Ae:197:ASP:HB3	5:Ae:257:ASN:OD1	2.19	0.43
5:Ae:222:CYS:HB2	5:Ae:236:CYS:SG	2.59	0.43
5:Ae:271:VAL:HG22	5:Ae:273:VAL:HG22	2.00	0.43
2:AB:195:TYR:OH	2:Ab:261:GLN:CG	2.66	0.43
3:AC:33:PHE:O	3:AC:36:LEU:HB2	2.19	0.43
4:AD:242:ILE:HG12	4:AD:244:MET:CB	2.49	0.43
8:AH:55:VAL:CG2	8:AH:65:CYS:HB2	2.49	0.43
8:AH:85:PHE:O	8:AH:88:LEU:HB2	2.18	0.43
4:Ad:183:GLU:CA	4:Ad:186:ARG:HH21	2.32	0.43
1:AA:68:THR:HG22	1:AA:136:LEU:HD23	2.00	0.42
2:AB:286:PHE:CD1	2:AB:427:ALA:HB1	2.54	0.42
4:AD:126:SER:HB3	4:AD:177:LYS:HA	2.01	0.42
4:AD:135:LEU:CA	4:AD:276:TRP:HH2	2.20	0.42
4:AD:159:ASN:CB	4:AD:166:MET:HG3	2.48	0.42
4:AD:227:LEU:HD21	4:AD:241:ALA:HA	2.00	0.42
5:AE:249:ILE:HG12	5:AE:254:ALA:HB3	2.01	0.42
8:AH:46:GLU:O	8:AH:50:LEU:HG	2.19	0.42
1:Aa:172:MET:HA	1:Aa:175:ASN:CG	2.44	0.42
1:Aa:410:CYS:O	1:Aa:413:ILE:N	2.52	0.42
2:Ab:177:LEU:HD21	2:Ab:272:VAL:HG13	2.01	0.42
2:Ab:286:PHE:CD1	2:Ab:427:ALA:HB1	2.54	0.42
8:Ah:24:LEU:HD12	8:Ah:25:VAL:H	1.83	0.42
8:Ah:72:PHE:CE2	8:Ah:76:ARG:HD3	2.49	0.42
8:Ah:79:CYS:O	8:Ah:82:HIS:N	2.46	0.42
9:Aj:23:LEU:CD1	10:Ak:27:VAL:HG22	2.48	0.42
3:AC:113:TRP:O	3:AC:117:VAL:N	2.48	0.42
4:AD:221:PRO:HB2	4:AD:225:VAL:CG1	2.44	0.42
4:AD:221:PRO:HB3	4:AD:233:PHE:CG	2.54	0.42
4:AD:227:LEU:CD2	4:AD:241:ALA:HA	2.48	0.42
6:AF:77:PRO:O	6:AF:78:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:65:CYS:HA	8:AH:68:GLU:OE1	2.18	0.42
2:Ab:161:ASP:C	2:Ab:163:ALA:N	2.75	0.42
2:Ab:378:LEU:HD23	2:Ab:416:ILE:CG2	2.49	0.42
3:Ac:190:ALA:HB1	12:Ac:405:UQ6:C21	2.49	0.42
4:Ad:99:ARG:HA	4:Ad:99:ARG:HD3	1.94	0.42
4:Ad:186:ARG:HA	4:Ad:191:GLY:CA	2.49	0.42
4:Ad:270:VAL:HG13	4:Ad:271:ALA:N	2.34	0.42
5:Ae:205:VAL:CG1	5:Ae:211:VAL:HG23	2.49	0.42
5:Ae:243:TYR:CD2	5:Ae:258:LEU:HG	2.54	0.42
3:AC:47:THR:CB	3:AC:83:HIS:HD1	2.32	0.42
3:AC:177:ARG:NH2	5:Ae:140:MET:O	2.51	0.42
4:AD:116:VAL:HG11	4:AD:270:VAL:HB	2.02	0.42
4:AD:242:ILE:C	4:AD:244:MET:H	2.27	0.42
1:Aa:281:ALA:HA	7:Ag:10:ARG:HH12	1.84	0.42
2:Ab:346:ALA:O	2:Ab:347:ALA:C	2.62	0.42
12:Ac:405:UQ6:H151	12:Ac:405:UQ6:H172	1.79	0.42
5:Ae:122:THR:O	5:Ae:123:VAL:C	2.61	0.42
1:AA:99:LYS:HG3	1:AA:160:GLN:CG	2.48	0.42
2:AB:396:ILE:HG12	2:AB:406:TYR:HE1	1.85	0.42
3:AC:171:ASP:CG	3:AC:172:LYS:N	2.76	0.42
3:AC:208:PRO:HB2	3:AC:316:MET:HE3	2.01	0.42
3:AC:345:HIS:O	7:AG:67:PHE:HD1	2.02	0.42
3:AC:376:MET:CE	6:AF:18:ARG:HG2	2.49	0.42
4:AD:214:LEU:CD1	4:AD:237:PHE:HB2	2.49	0.42
5:Ae:271:VAL:O	5:Ae:271:VAL:HG13	2.19	0.42
1:AA:193:GLN:NE2	5:AE:85:VAL:HG11	2.34	0.42
3:AC:141:TRP:CD1	3:AC:265:PRO:CD	2.98	0.42
3:AC:256:TYR:CZ	4:AD:202:ARG:HD3	2.54	0.42
4:AD:220:GLU:O	4:AD:222:PRO:HD3	2.19	0.42
4:AD:232:TYR:HB2	4:AD:242:ILE:CG2	2.49	0.42
4:AD:247:PRO:O	4:AD:252:VAL:HG21	2.19	0.42
7:AG:46:ILE:HD12	7:AG:49:VAL:HB	2.02	0.42
2:Ab:38:LEU:CG	2:Ab:396:ILE:HD13	2.50	0.42
2:Ab:166:PHE:HE1	2:Ab:191:TYR:CD2	2.38	0.42
3:Ac:181:PHE:HA	3:Ac:184:ILE:HG22	2.00	0.42
5:Ae:115:TYR:HB3	9:Aj:21:PHE:HE1	1.85	0.42
5:Ae:271:VAL:O	5:Ae:273:VAL:HG23	2.18	0.42
1:AA:187:LEU:O	1:AA:188:HIS:C	2.62	0.42
2:AB:39:GLU:OE2	2:AB:227:HIS:HB2	2.19	0.42
2:AB:319:GLN:O	2:AB:320:PRO:C	2.62	0.42
4:AD:233:PHE:CD1	4:AD:240:GLN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:222:CYS:HB2	5:AE:236:CYS:SG	2.59	0.42
9:AJ:20:THR:O	9:AJ:24:THR:HG22	2.19	0.42
9:AJ:23:LEU:HD21	10:AK:23:MET:SD	2.52	0.42
2:Ab:61:ILE:HA	2:Ab:222:GLY:HA2	2.00	0.42
2:Ab:147:ARG:HD3	2:Ab:149:TRP:CZ2	2.54	0.42
3:Ac:215:ALA:HB2	6:Af:60:MET:HE3	2.01	0.42
4:Ad:299:LEU:HD12	16:Ad:402:3PH:H371	1.96	0.42
5:Ae:271:VAL:HG22	5:Ae:273:VAL:CG2	2.49	0.42
6:Af:102:ARG:HA	6:Af:105:ARG:CZ	2.49	0.42
8:Ah:33:GLU:O	8:Ah:34:HIS:C	2.62	0.42
9:Aj:43:ILE:O	9:Aj:47:ILE:HG13	2.20	0.42
1:AA:112:GLU:HB3	1:AA:142:LYS:NZ	2.34	0.42
3:AC:141:TRP:HA	3:AC:141:TRP:CE3	2.54	0.42
4:AD:186:ARG:HD2	4:AD:191:GLY:O	2.20	0.42
8:AH:58:ARG:HB3	8:AH:61:THR:CG2	2.48	0.42
10:AK:23:MET:HG3	10:AK:27:VAL:HG23	2.00	0.42
1:Aa:114:GLU:OE1	2:Ab:298:HIS:ND1	2.52	0.42
1:Aa:136:LEU:HD22	2:Ab:383:LEU:HD12	2.02	0.42
1:Aa:276:ARG:O	7:Ag:16:SER:N	2.53	0.42
2:Ab:103:ILE:HB	5:Ai:70:LEU:CD2	2.50	0.42
5:Ae:83:VAL:HG22	5:Ae:84:LYS:N	2.34	0.42
5:Ae:175:PHE:HE2	5:Ae:215:GLY:HA3	1.85	0.42
8:Ah:73:LEU:CD2	8:Ah:76:ARG:HH21	2.33	0.42
8:Ah:73:LEU:HD22	8:Ah:76:ARG:HH21	1.83	0.42
5:Ai:72:VAL:N	5:Ai:73:PRO:HD2	2.33	0.42
1:AA:62:GLU:CD	1:AA:423:ARG:HH12	2.23	0.42
1:AA:62:GLU:HB2	1:AA:413:ILE:HD11	2.02	0.42
1:AA:401:SER:O	1:AA:404:ASP:N	2.51	0.42
2:AB:378:LEU:HD23	2:AB:416:ILE:CG2	2.49	0.42
3:AC:195:VAL:HG12	3:AC:199:PHE:CD2	2.55	0.42
4:AD:109:SER:O	4:AD:110:ILE:C	2.62	0.42
4:AD:110:ILE:HD13	4:AD:276:TRP:HB2	2.01	0.42
4:AD:200:ILE:HG23	4:AD:201:VAL:N	2.35	0.42
4:AD:214:LEU:O	4:AD:234:ASN:ND2	2.52	0.42
10:AK:31:GLY:O	10:AK:34:TRP:HE3	2.02	0.42
2:Ab:60:ARG:CG	2:Ab:393:LEU:HD13	2.50	0.42
2:Ab:66:LYS:HB3	2:Ab:71:TYR:CE2	2.55	0.42
2:Ab:180:VAL:CG2	2:Ab:258:ILE:HG23	2.49	0.42
2:Ab:225:VAL:HG22	2:Ab:226:SER:N	2.35	0.42
3:Ac:71:ARG:NH2	4:Ad:199:TYR:CE1	2.86	0.42
9:Aj:34:ARG:CZ	9:Aj:38:GLN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:279:ASP:OD1	7:AG:12:ARG:NE	2.49	0.42
1:AA:397:ASN:ND2	2:AB:126:ILE:HD11	2.31	0.42
2:AB:163:ALA:O	2:AB:164:VAL:C	2.62	0.42
3:AC:70:CYS:SG	3:AC:80:ARG:HD3	2.59	0.42
3:AC:137:GLN:HB3	3:AC:257:MET:HE3	2.02	0.42
12:AC:403:UQ6:H1M1	12:AC:403:UQ6:H71	1.91	0.42
4:AD:159:ASN:CB	4:AD:166:MET:HE2	2.47	0.42
4:AD:189:ASN:CG	4:AD:194:PRO:HG3	2.45	0.42
8:AH:43:LYS:O	8:AH:46:GLU:HB2	2.20	0.42
2:Ab:61:ILE:CG2	2:Ab:220:LEU:HD11	2.49	0.42
2:Ab:218:MET:CE	2:Ab:238:LEU:HD22	2.50	0.42
2:Ab:396:ILE:HG12	2:Ab:406:TYR:HE1	1.85	0.42
3:Ac:171:ASP:CG	3:Ac:172:LYS:N	2.77	0.42
4:Ad:253:LEU:C	4:Ad:253:LEU:HD12	2.44	0.42
4:Ad:264:SER:O	4:Ad:267:ALA:HB3	2.20	0.42
5:Ae:249:ILE:HG22	5:Ae:257:ASN:OD1	2.20	0.42
6:Af:95:LEU:O	6:Af:96:LYS:C	2.62	0.42
9:Aj:30:LEU:CD1	10:Ak:34:TRP:HB2	2.47	0.42
1:AA:79:SER:HB3	1:AA:201:VAL:HA	2.01	0.42
3:AC:10:LEU:CA	3:Ac:198:LEU:HD21	2.49	0.42
3:AC:119:LEU:CD2	3:AC:192:LEU:HB2	2.50	0.42
3:AC:130:GLY:HA3	11:AC:401:HEM:C2D	2.55	0.42
3:AC:169:SER:O	3:AC:170:VAL:C	2.62	0.42
4:AD:249:TYR:O	4:AD:250:THR:C	2.63	0.42
5:AE:93:ARG:O	5:AE:94:ALA:C	2.62	0.42
6:AF:35:ASP:HB3	6:AF:91:LEU:HB3	2.01	0.42
6:AF:50:ARG:O	6:AF:51:LEU:C	2.63	0.42
7:AG:46:ILE:C	7:AG:48:ARG:H	2.28	0.42
8:AH:28:LEU:O	8:AH:32:ARG:HG3	2.20	0.42
1:Aa:119:HIS:ND1	2:Ab:298:HIS:HA	2.35	0.42
1:Aa:186:TYR:OH	5:Ae:80:HIS:HB2	2.19	0.42
1:Aa:397:ASN:N	1:Aa:397:ASN:HD22	2.18	0.42
2:Ab:64:PHE:CZ	2:Ab:394:SER:HA	2.55	0.42
5:Ae:159:ILE:HG21	5:Ae:178:HIS:CB	2.50	0.42
1:AA:74:TRP:CZ3	1:AA:232:ALA:HB3	2.54	0.41
1:AA:410:CYS:O	1:AA:413:ILE:N	2.52	0.41
3:AC:120:LEU:O	3:AC:121:PHE:C	2.62	0.41
4:AD:248:ILE:HG22	4:AD:263:MET:HG3	2.01	0.41
1:Aa:148:ALA:O	1:Aa:152:GLN:HG2	2.20	0.41
2:Ab:147:ARG:HD2	2:Ab:150:GLU:OE2	2.20	0.41
3:Ac:169:SER:O	3:Ac:170:VAL:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:284:ILE:HG21	3:Ac:289:GLY:HA3	2.02	0.41
4:Ad:95:PRO:HG2	8:Ah:85:PHE:HB2	2.02	0.41
4:Ad:118:LYS:HA	4:Ad:122:SER:HB2	2.01	0.41
5:Ae:196:ARG:HD2	5:Ae:249:ILE:HG23	2.01	0.41
1:AA:53:LEU:HD21	1:AA:243:LEU:CD1	2.50	0.41
1:AA:453:CYS:HB3	1:AA:468:TYR:OH	2.20	0.41
2:AB:346:ALA:O	2:AB:347:ALA:C	2.62	0.41
4:AD:106:ASP:O	4:AD:110:ILE:HG13	2.21	0.41
4:AD:242:ILE:HG12	4:AD:244:MET:N	2.31	0.41
1:Aa:174:GLU:C	1:Aa:176:ASP:H	2.27	0.41
2:Ab:126:ILE:H	2:Ab:126:ILE:CD1	2.26	0.41
14:Ac:403:3PE:H321	17:Ag:101:CDL:C12	2.50	0.41
4:Ad:123:SER:O	4:Ad:178:PRO:CB	2.68	0.41
4:Ad:292:MET:HE3	4:Ad:292:MET:HB3	1.95	0.41
4:Ad:318:LYS:CD	5:Ae:86:PRO:HB2	2.49	0.41
5:Ae:173:PRO:O	5:Ae:214:ILE:HA	2.20	0.41
5:Ae:195:LEU:CD1	5:Ae:248:ARG:HD2	2.50	0.41
9:Aj:23:LEU:HB2	10:Ak:27:VAL:HG22	2.02	0.41
10:Ak:12:GLU:HA	10:Ak:15:ARG:HD3	2.02	0.41
1:AA:230:VAL:HG21	1:AA:417:LEU:HB3	2.00	0.41
2:AB:166:PHE:CE1	2:AB:171:THR:HG22	2.56	0.41
3:AC:153:ILE:HB	3:AC:157:GLY:HA2	2.01	0.41
4:AD:157:GLY:CA	4:AD:167:ARG:HB3	2.24	0.41
4:AD:159:ASN:HB3	4:AD:166:MET:CE	2.48	0.41
4:AD:214:LEU:HG	4:AD:242:ILE:HD12	2.01	0.41
6:AF:54:ASP:OD1	6:AF:55:LEU:N	2.52	0.41
1:Aa:92:PHE:HD2	1:Aa:216:LEU:HD21	1.85	0.41
1:Aa:192:PHE:HD1	1:Aa:269:ARG:O	2.04	0.41
1:Aa:204:PRO:O	1:Aa:205:SER:C	2.63	0.41
2:Ab:92:LYS:HB2	2:Ab:143:ALA:HB1	2.02	0.41
2:Ab:212:HIS:NE2	2:Ab:246:LEU:HD23	2.21	0.41
4:Ad:181:ASN:C	4:Ad:183:GLU:N	2.76	0.41
4:Ad:294:LEU:CB	9:Aj:36:PHE:HZ	2.31	0.41
5:Ae:147:LEU:HD12	5:Ae:147:LEU:O	2.20	0.41
8:Ah:51:CYS:SG	8:Ah:69:LEU:HB2	2.60	0.41
1:AA:172:MET:HA	1:AA:175:ASN:CG	2.44	0.41
2:AB:173:ILE:CG2	2:AB:174:ILE:N	2.83	0.41
2:AB:293:LEU:HB3	2:AB:309:LEU:CG	2.48	0.41
3:AC:54:HIS:O	3:AC:65:SER:HB2	2.20	0.41
3:AC:135:TRP:CE2	3:AC:259:ALA:HB3	2.54	0.41
4:AD:216:THR:O	8:AH:32:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:245:ALA:O	4:AD:247:PRO:HD3	2.20	0.41
4:AD:259:THR:O	4:AD:260:PRO:C	2.60	0.41
5:AE:127:TYR:CG	9:AJ:32:PHE:HD1	2.37	0.41
5:AE:164:ASN:HB3	5:AE:226:ALA:CB	2.49	0.41
8:AH:65:CYS:O	8:AH:66:THR:C	2.63	0.41
1:Aa:342:GLN:HE21	1:Aa:357:HIS:CB	2.31	0.41
2:Ab:234:ALA:C	2:Ab:236:GLN:N	2.78	0.41
2:Ab:312:SER:OG	2:Ab:357:GLN:NE2	2.40	0.41
3:Ac:96:LEU:HD23	14:Ac:403:3PE:H292	2.01	0.41
3:Ac:153:ILE:HB	3:Ac:157:GLY:HA2	2.01	0.41
3:Ac:193:ALA:HB3	12:Ac:405:UQ6:H202	2.01	0.41
4:Ad:291:LYS:HD3	16:Ad:402:3PH:H31	2.01	0.41
4:Ad:317:ARG:HD2	4:Ad:319:LEU:HD21	2.02	0.41
16:Ad:402:3PH:C36	5:Ae:128:ALA:HB1	2.49	0.41
8:Ah:39:GLU:CG	8:Ah:40:LYS:H	2.31	0.41
5:Ai:71:ASN:C	5:Ai:73:PRO:HD2	2.45	0.41
1:AA:356:ALA:HB3	1:AA:372:LEU:CD2	2.50	0.41
2:AB:163:ALA:HB1	5:AI:43:LEU:HD23	2.01	0.41
2:AB:168:ASN:N	2:AB:168:ASN:OD1	2.54	0.41
3:AC:47:THR:HB	3:AC:83:HIS:HB2	2.02	0.41
12:AC:403:UQ6:H162	12:AC:403:UQ6:H121	1.80	0.41
4:AD:214:LEU:HG	4:AD:242:ILE:CD1	2.51	0.41
7:AG:45:ARG:O	7:AG:46:ILE:C	2.62	0.41
1:Aa:53:LEU:HD21	1:Aa:243:LEU:CD1	2.50	0.41
1:Aa:152:GLN:NE2	1:Aa:250:LEU:HA	2.35	0.41
2:Ab:39:GLU:O	2:Ab:50:ALA:HA	2.21	0.41
2:Ab:109:LYS:CG	2:Ab:124:GLU:HB3	2.44	0.41
4:Ad:170:LYS:O	4:Ad:173:ASP:HB3	2.20	0.41
4:Ad:306:MET:HE2	4:Ad:306:MET:HB3	1.70	0.41
5:Ae:218:THR:HG21	5:Ae:256:LEU:HB2	2.01	0.41
5:Ae:241:SER:HA	5:Ae:251:LYS:O	2.21	0.41
6:Af:86:GLU:O	6:Af:87:ASP:C	2.60	0.41
1:AA:92:PHE:HD1	1:AA:168:ILE:HD12	1.86	0.41
2:AB:100:THR:CG2	5:AI:70:LEU:HD11	2.50	0.41
2:AB:173:ILE:HG23	2:AB:174:ILE:N	2.34	0.41
2:AB:272:VAL:HA	2:AB:337:GLY:HA3	2.02	0.41
2:AB:313:VAL:HG11	2:AB:321:PHE:CD1	2.54	0.41
3:AC:100:ARG:HH12	11:AC:402:HEM:HBD1	1.86	0.41
4:AD:146:LYS:HD2	4:AD:149:ALA:HB3	2.01	0.41
4:AD:281:GLU:N	4:AD:281:GLU:OE1	2.53	0.41
7:AG:24:GLN:O	7:AG:25:ARG:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:40:ARG:NH2	7:AG:41:ARG:HB2	2.35	0.41
1:Aa:450:TYR:HD2	9:Aj:16:ARG:HH11	1.69	0.41
2:Ab:171:THR:HA	5:Ai:64:LEU:CD2	2.47	0.41
4:Ad:158:PRO:HB2	4:Ad:164:MET:CB	2.47	0.41
4:Ad:223:THR:OG1	8:Ah:55:VAL:HG11	2.21	0.41
1:AA:341:PHE:CE2	1:AA:371:PHE:HE2	2.37	0.41
1:AA:463:GLU:OE2	7:AG:6:GLY:N	2.54	0.41
2:AB:225:VAL:HG22	2:AB:229:VAL:HG21	2.02	0.41
2:AB:312:SER:HA	2:AB:315:LYS:HE3	2.02	0.41
4:AD:129:TYR:CD2	4:AD:198:SER:HB2	2.55	0.41
4:AD:179:TYR:CE1	4:AD:188:ALA:HB3	2.55	0.41
4:AD:183:GLU:H	4:AD:183:GLU:CD	2.27	0.41
2:Ab:36:GLN:OE1	2:Ab:36:GLN:N	2.53	0.41
3:Ac:119:LEU:HB3	11:Ac:402:HEM:CBB	2.51	0.41
3:Ac:364:ILE:O	3:Ac:368:ILE:HG13	2.21	0.41
4:Ad:186:ARG:HA	4:Ad:191:GLY:C	2.46	0.41
4:Ad:292:MET:HA	16:Ad:402:3PH:C33	2.44	0.41
5:Ae:235:TYR:CZ	5:Ae:240:GLY:HA2	2.55	0.41
8:Ah:31:VAL:O	8:Ah:34:HIS:HB3	2.21	0.41
9:Aj:21:PHE:O	9:Aj:24:THR:HG22	2.20	0.41
1:AA:109:LEU:HD21	1:AA:120:LEU:CD2	2.51	0.41
1:AA:115:SER:O	1:AA:116:ILE:C	2.64	0.41
1:AA:139:ASP:O	1:AA:143:VAL:HG23	2.20	0.41
1:AA:152:GLN:HE22	1:AA:250:LEU:HA	1.85	0.41
1:AA:275:ILE:HD11	5:AE:85:VAL:HG22	2.03	0.41
1:AA:397:ASN:N	1:AA:397:ASN:HD22	2.18	0.41
2:AB:407:MET:HE1	2:AB:415:GLN:CD	2.45	0.41
3:AC:140:PHE:CE2	3:AC:261:PRO:HA	2.56	0.41
3:AC:253:PRO:CB	4:AD:202:ARG:O	2.68	0.41
3:AC:256:TYR:OH	4:AD:202:ARG:NH1	2.54	0.41
3:AC:272:TRP:HA	3:AC:275:LEU:HD12	2.02	0.41
4:AD:127:MET:O	4:AD:175:PHE:HB2	2.20	0.41
4:AD:146:LYS:HB2	4:AD:171:LEU:HD21	2.03	0.41
6:AF:110:LYS:CA	10:Ak:10:TYR:HE1	2.34	0.41
5:AI:71:ASN:C	5:AI:73:PRO:HD2	2.45	0.41
1:Aa:341:PHE:O	1:Aa:341:PHE:CG	2.74	0.41
1:Aa:404:ASP:O	1:Aa:408:PRO:HG2	2.21	0.41
2:Ab:43:LEU:HB2	2:Ab:45:ASN:OD1	2.21	0.41
3:Ac:240:MET:HB3	4:Ad:292:MET:HG3	2.03	0.41
3:Ac:294:LEU:C	3:Ac:294:LEU:HD23	2.46	0.41
4:Ad:215:LEU:HD11	13:Ad:401:HEC:CMB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ae:142:ALA:CB	5:Ae:147:LEU:CD2	2.82	0.41
8:Ah:35:CYS:O	8:Ah:38:LEU:HD13	2.21	0.41
8:Ah:42:VAL:C	8:Ah:45:ARG:H	2.29	0.41
1:AA:249:HIS:O	1:AA:250:LEU:CB	2.64	0.41
1:AA:298:ASN:OD1	1:AA:299:PRO:HD2	2.21	0.41
2:AB:85:LEU:CD2	5:AI:68:VAL:HG11	2.49	0.41
3:AC:198:LEU:HD11	3:Ac:9:PRO:O	2.20	0.41
3:AC:284:ILE:HG21	3:AC:289:GLY:HA3	2.02	0.41
4:AD:133:ARG:NH2	4:AD:174:TYR:OH	2.54	0.41
4:AD:183:GLU:OE2	4:Ad:160:ASP:HB3	2.20	0.41
4:AD:317:ARG:HD2	4:AD:319:LEU:HD21	2.02	0.41
5:AE:115:TYR:O	5:AE:116:LEU:C	2.62	0.41
5:AE:127:TYR:HB2	9:AJ:32:PHE:CD1	2.56	0.41
5:AE:162:GLY:N	5:AE:178:HIS:O	2.54	0.41
5:AE:231:PHE:CD2	5:AE:250:ARG:NH1	2.88	0.41
7:AG:69:GLN:HE21	7:AG:72:ARG:CZ	2.34	0.41
5:AI:71:ASN:OD1	5:AI:71:ASN:O	2.38	0.41
1:Aa:49:GLN:CD	1:Aa:239:HIS:CD2	2.99	0.41
1:Aa:62:GLU:HB2	1:Aa:413:ILE:HD11	2.02	0.41
1:Aa:72:GLY:HA2	1:Aa:132:LEU:HA	2.03	0.41
1:Aa:74:TRP:CZ3	1:Aa:410:CYS:SG	3.13	0.41
1:Aa:95:HIS:HB3	1:Aa:164:GLU:OE1	2.21	0.41
1:Aa:298:ASN:OD1	1:Aa:299:PRO:HD2	2.20	0.41
2:Ab:38:LEU:HD22	2:Ab:38:LEU:N	2.35	0.41
2:Ab:60:ARG:HG2	2:Ab:393:LEU:HD13	2.02	0.41
2:Ab:92:LYS:HG2	2:Ab:145:GLU:HG2	2.03	0.41
2:Ab:123:VAL:HG22	2:Ab:133:LEU:HD13	2.03	0.41
2:Ab:227:HIS:CD2	2:Ab:231:LYS:HD3	2.55	0.41
2:Ab:272:VAL:HA	2:Ab:337:GLY:HA3	2.02	0.41
3:Ac:124:MET:HG2	3:Ac:274:PHE:HE1	1.85	0.41
3:Ac:208:PRO:HB2	3:Ac:316:MET:HE3	2.02	0.41
3:Ac:296:LEU:O	3:Ac:297:SER:C	2.64	0.41
4:Ad:114:PHE:CE1	4:Ad:175:PHE:CE2	3.01	0.41
5:Ae:130:LYS:HZ2	9:Aj:33:GLU:CD	2.25	0.41
5:Ae:179:ARG:HH21	5:Ae:205:VAL:HG21	1.86	0.41
5:Ae:180:THR:O	5:Ae:181:LYS:C	2.63	0.41
5:Ae:214:ILE:HB	5:Ae:259:GLU:HB3	2.03	0.41
1:AA:66:HIS:CD2	2:AB:387:GLU:O	2.73	0.41
1:AA:127:GLU:OE2	1:AA:348:TYR:HB3	2.21	0.41
1:AA:404:ASP:O	1:AA:408:PRO:HG2	2.21	0.41
2:AB:168:ASN:HB2	2:AB:170:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:44:GLN:HB3	11:AC:401:HEM:C2C	2.56	0.41
3:AC:294:LEU:HD23	3:AC:294:LEU:C	2.46	0.41
4:AD:189:ASN:O	4:AD:192:ALA:N	2.54	0.41
4:AD:237:PHE:CE1	4:AD:242:ILE:HA	2.56	0.41
5:AE:132:VAL:O	5:AE:136:PHE:CB	2.69	0.41
6:AF:34:ARG:C	6:AF:36:ASP:N	2.77	0.41
7:AG:43:ARG:HA	7:AG:46:ILE:HG22	2.02	0.41
2:Ab:91:THR:O	2:Ab:93:GLY:N	2.55	0.41
2:Ab:142:THR:CG2	2:Ab:238:LEU:HD23	2.51	0.41
3:Ac:100:ARG:N	14:Ac:403:3PE:H252	2.36	0.41
3:Ac:372:ILE:O	3:Ac:376:MET:HG2	2.21	0.41
5:Ae:172:LYS:HD3	5:Ae:216:VAL:CG2	2.51	0.41
7:Ag:26:ALA:C	7:Ag:28:PRO:HD3	2.46	0.41
3:AC:50:PHE:HZ	5:AE:136:PHE:CZ	2.38	0.40
3:AC:148:ASN:O	3:AC:149:LEU:C	2.63	0.40
3:AC:276:PHE:CG	3:AC:277:ALA:N	2.88	0.40
4:AD:155:GLN:CD	4:AD:164:MET:O	2.64	0.40
4:AD:275:ARG:HH21	4:AD:282:HIS:HD2	1.69	0.40
8:AH:80:VAL:O	8:AH:84:LEU:N	2.55	0.40
1:Aa:48:THR:HG21	1:Aa:423:ARG:CB	2.51	0.40
2:Ab:233:VAL:C	2:Ab:236:GLN:HG2	2.46	0.40
3:Ac:71:ARG:NH1	4:Ad:130:VAL:HG22	2.37	0.40
4:Ad:170:LYS:HD2	5:Ae:151:LYS:HG3	2.02	0.40
5:Ae:184:ILE:CG2	5:Ae:208:PRO:HB3	2.50	0.40
5:Ae:216:VAL:HG13	5:Ae:221:GLY:HA2	2.03	0.40
9:Aj:11:TYR:CZ	9:Aj:16:ARG:HB2	2.57	0.40
1:AA:184:PHE:O	1:AA:188:HIS:ND1	2.44	0.40
3:AC:145:VAL:O	5:Ae:220:LEU:HD22	2.21	0.40
5:AE:168:LYS:NZ	5:AE:171:GLY:HA2	2.36	0.40
8:AH:38:LEU:O	8:AH:42:VAL:N	2.42	0.40
1:Aa:111:LYS:HG3	2:Ab:305:THR:HG21	2.04	0.40
1:Aa:310:ILE:HG21	1:Aa:379:LEU:CD2	2.47	0.40
2:Ab:78:GLY:O	2:Ab:79:THR:C	2.61	0.40
5:Ae:196:ARG:HD2	5:Ae:249:ILE:HG21	2.03	0.40
6:Af:101:GLU:O	6:Af:105:ARG:HG3	2.21	0.40
1:AA:453:CYS:CB	1:AA:472:ARG:HH12	2.34	0.40
2:AB:167:GLN:NE2	5:AI:43:LEU:HB3	2.36	0.40
2:AB:339:TYR:HD2	5:AI:59:ALA:HB1	1.85	0.40
2:AB:453:LEU:O	2:AB:453:LEU:HD23	2.21	0.40
3:AC:122:ALA:CB	3:AC:189:ILE:HG12	2.52	0.40
6:AF:78:LYS:HA	6:AF:81:TRP:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:91:TYR:CE1	1:Aa:95:HIS:HE1	2.39	0.40
1:Aa:152:GLN:O	1:Aa:153:ASN:CB	2.69	0.40
1:Aa:152:GLN:HE22	1:Aa:250:LEU:HA	1.86	0.40
1:Aa:387:GLU:O	1:Aa:388:VAL:C	2.64	0.40
2:Ab:65:VAL:HG11	2:Ab:213:PHE:CD2	2.56	0.40
4:Ad:118:LYS:HZ2	4:Ad:148:LEU:HB3	1.86	0.40
4:Ad:118:LYS:NZ	4:Ad:148:LEU:HD22	2.36	0.40
5:Ae:180:THR:OG1	5:Ae:183:GLU:HG3	2.22	0.40
7:Ag:28:PRO:O	7:Ag:29:SER:C	2.64	0.40
8:Ah:43:LYS:HA	8:Ah:46:GLU:OE2	2.21	0.40
1:AA:100:GLY:HA2	1:AA:104:ARG:O	2.21	0.40
1:AA:174:GLU:C	1:AA:176:ASP:H	2.27	0.40
1:AA:383:ALA:O	1:AA:384:THR:C	2.64	0.40
2:AB:38:LEU:HD13	2:AB:52:LEU:HB2	2.02	0.40
3:AC:9:PRO:HG3	3:Ac:202:GLU:CD	2.45	0.40
3:AC:100:ARG:HH22	11:AC:402:HEM:HBD1	1.86	0.40
3:AC:220:PHE:CE2	12:AC:403:UQ6:H4M2	2.56	0.40
3:AC:280:ILE:HD13	3:AC:297:SER:HB2	2.02	0.40
3:AC:295:ILE:HG22	3:AC:299:LEU:HD12	2.03	0.40
4:AD:150:GLU:CD	4:AD:150:GLU:O	2.64	0.40
4:AD:154:VAL:C	4:AD:156:ASP:N	2.79	0.40
4:AD:195:PRO:O	4:AD:196:ASP:C	2.64	0.40
4:AD:210:TYR:O	4:AD:211:VAL:C	2.63	0.40
7:AG:35:ILE:O	7:AG:36:PRO:C	2.63	0.40
7:AG:56:VAL:O	7:AG:59:ILE:N	2.54	0.40
9:AJ:23:LEU:HD22	10:AK:23:MET:HG3	2.00	0.40
2:Ab:43:LEU:HD12	2:Ab:47:LEU:HD23	2.03	0.40
2:Ab:117:GLU:HB2	2:Ab:330:TYR:HD1	1.85	0.40
2:Ab:453:LEU:HD23	2:Ab:453:LEU:O	2.21	0.40
3:Ac:283:SER:OG	3:Ac:284:ILE:HD12	2.22	0.40
4:Ad:121:CYS:O	4:Ad:124:CYS:N	2.52	0.40
4:Ad:189:ASN:CG	13:Ad:401:HEC:HMD3	2.47	0.40
8:Ah:47:ARG:O	8:Ah:50:LEU:HB2	2.22	0.40
8:Ah:72:PHE:O	8:Ah:73:LEU:C	2.63	0.40
1:AA:86:ASN:OD1	1:AA:86:ASN:N	2.54	0.40
1:AA:361:ASP:OD1	1:AA:361:ASP:N	2.55	0.40
3:AC:296:LEU:O	3:AC:297:SER:C	2.64	0.40
4:AD:137:GLY:N	4:AD:140:TYR:O	2.51	0.40
4:AD:239:GLY:C	4:AD:241:ALA:N	2.78	0.40
5:AE:236:CYS:HA	5:AE:237:PRO:HD2	1.91	0.40
6:AF:29:LYS:HA	6:AF:81:TRP:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:47:ARG:NH1	8:AH:47:ARG:HB2	2.36	0.40
1:Aa:120:LEU:CD2	2:Ab:299:ILE:HG23	2.51	0.40
2:Ab:297:PRO:CB	2:Ab:304:ASN:OD1	2.69	0.40
2:Ab:303:ASN:O	2:Ab:304:ASN:C	2.63	0.40
2:Ab:426:LYS:HA	2:Ab:429:LYS:NZ	2.36	0.40
3:Ac:97:HIS:CE1	3:Ac:100:ARG:NH2	2.90	0.40
3:Ac:100:ARG:HH12	11:Ac:402:HEM:CBD	2.35	0.40
4:Ad:129:TYR:HD2	4:Ad:198:SER:CB	2.35	0.40
4:Ad:199:TYR:HA	4:Ad:278:SER:OG	2.21	0.40
4:Ad:228:ARG:O	4:Ad:231:LEU:HB2	2.20	0.40
4:Ad:255:TYR:CD2	4:Ad:261:ALA:HB2	2.56	0.40
4:Ad:266:VAL:O	4:Ad:270:VAL:HG12	2.21	0.40
6:Af:36:ASP:OD1	6:Af:90:TYR:OH	2.38	0.40
7:Ag:47:LEU:HD21	14:Ag:103:3PE:H3H2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	389/480 (81%)	372 (96%)	17 (4%)	0	100	100
1	Aa	386/480 (80%)	369 (96%)	17 (4%)	0	100	100
2	AB	416/453 (92%)	408 (98%)	8 (2%)	0	100	100
2	Ab	416/453 (92%)	396 (95%)	20 (5%)	0	100	100
3	AC	371/381 (97%)	361 (97%)	10 (3%)	0	100	100
3	Ac	371/381 (97%)	366 (99%)	5 (1%)	0	100	100
4	AD	234/325 (72%)	213 (91%)	21 (9%)	0	100	100
4	Ad	237/325 (73%)	224 (94%)	12 (5%)	1 (0%)	30	62
5	AE	101/274 (37%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AI	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
5	Ae	184/274 (67%)	168 (91%)	15 (8%)	1 (0%)	24	57
5	Ai	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
6	AF	95/111 (86%)	94 (99%)	1 (1%)	0	100	100
6	Af	96/111 (86%)	96 (100%)	0	0	100	100
7	AG	74/82 (90%)	70 (95%)	4 (5%)	0	100	100
7	Ag	72/82 (88%)	72 (100%)	0	0	100	100
8	AH	62/89 (70%)	61 (98%)	1 (2%)	0	100	100
8	Ah	58/89 (65%)	55 (95%)	3 (5%)	0	100	100
9	AJ	19/64 (30%)	19 (100%)	0	0	100	100
9	Aj	41/64 (64%)	40 (98%)	1 (2%)	0	100	100
10	AK	15/56 (27%)	15 (100%)	0	0	100	100
10	Ak	36/56 (64%)	34 (94%)	2 (6%)	0	100	100
All	All	3721/5178 (72%)	3572 (96%)	147 (4%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Ae	160	PRO
4	Ad	194	PRO

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	333/398 (84%)	332 (100%)	1 (0%)	86	84
1	Aa	332/398 (83%)	332 (100%)	0	100	100
2	AB	328/356 (92%)	328 (100%)	0	100	100
2	Ab	328/356 (92%)	327 (100%)	1 (0%)	86	84
3	AC	325/333 (98%)	323 (99%)	2 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
4	AD	201/260 (77%)	201 (100%)	0	100	100
4	Ad	204/260 (78%)	201 (98%)	3 (2%)	57	69
5	AE	86/224 (38%)	86 (100%)	0	100	100
5	AI	21/224 (9%)	20 (95%)	1 (5%)	23	47
5	Ae	158/224 (70%)	156 (99%)	2 (1%)	61	71
5	Ai	21/224 (9%)	20 (95%)	1 (5%)	23	47
6	AF	89/99 (90%)	89 (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	67/74 (90%)	67 (100%)	0	100	100
8	AH	61/83 (74%)	60 (98%)	1 (2%)	55	68
8	Ah	59/83 (71%)	59 (100%)	0	100	100
9	AJ	16/55 (29%)	16 (100%)	0	100	100
9	Aj	34/55 (62%)	34 (100%)	0	100	100
10	AK	10/46 (22%)	10 (100%)	0	100	100
10	Ak	29/46 (63%)	29 (100%)	0	100	100
All	All	3186/4304 (74%)	3173 (100%)	13 (0%)	81	83

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

Mol	Chain	Res	Type
1	AA	387	GLU
3	AC	51	LEU
3	AC	294	LEU
8	AH	42	VAL
5	AI	45	VAL
2	Ab	168	ASN
3	Ac	294	LEU
4	Ad	201	VAL
4	Ad	225	VAL
4	Ad	252	VAL
5	Ae	135	GLN
5	Ae	152	ILE
5	Ai	45	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	103	ASN
1	AA	119	HIS
1	AA	152	GLN
1	AA	173	GLN
1	AA	240	GLN
1	AA	249	HIS
1	AA	301	ASN
1	AA	305	GLN
1	AA	342	GLN
1	AA	345	ASN
1	AA	397	ASN
1	AA	402	HIS
2	AB	280	ASN
2	AB	284	ASN
2	AB	298	HIS
2	AB	357	GLN
2	AB	365	ASN
2	AB	415	GLN
2	AB	443	ASN
3	AC	8	HIS
3	AC	32	ASN
3	AC	312	GLN
4	AD	189	ASN
4	AD	240	GLN
5	AE	135	GLN
5	AE	227	ASN
5	AE	242	HIS
6	AF	39	HIS
6	AF	74	GLN
7	AG	7	ASN
7	AG	24	GLN
7	AG	37	ASN
7	AG	69	GLN
8	AH	37	GLN
8	AH	82	HIS
5	AI	71	ASN
1	Aa	87	ASN
1	Aa	95	HIS
1	Aa	173	GLN
1	Aa	207	ASN
1	Aa	240	GLN

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Mol	Chain	Res	Type
1	Aa	247	GLN
1	Aa	286	HIS
1	Aa	342	GLN
1	Aa	397	ASN
1	Aa	402	HIS
2	Ab	211	ASN
2	Ab	212	HIS
2	Ab	284	ASN
2	Ab	304	ASN
2	Ab	357	GLN
2	Ab	365	ASN
2	Ab	415	GLN
2	Ab	443	ASN
3	Ac	32	ASN
3	Ac	221	HIS
3	Ac	312	GLN
4	Ad	115	GLN
4	Ad	189	ASN
4	Ad	284	HIS
4	Ad	309	HIS
5	Ae	131	ASN
5	Ae	164	ASN
5	Ae	200	HIS
5	Ae	219	HIS
5	Ae	239	HIS
6	Af	80	GLN
7	Ag	69	GLN
8	Ah	82	HIS
10	Ak	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.14	3 (8%)
11	HEM	Ac	402	3	50,50,50	1.60	8 (16%)	66,82,82	1.91	15 (22%)
15	U10	Ac	404	-	23,23,63	1.25	3 (13%)	28,31,79	2.09	7 (25%)
16	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.26	4 (10%)
12	UQ6	Ac	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.51	6 (18%)
17	CDL	Ag	102	-	55,55,99	1.21	4 (7%)	61,67,111	1.24	6 (9%)
14	3PE	Aa	501	-	22,22,50	1.36	2 (9%)	25,27,55	1.20	3 (12%)
13	HEC	Ad	401	4	50,50,50	1.71	5 (10%)	68,82,82	1.35	7 (10%)
12	UQ6	AC	403	-	28,28,43	2.47	6 (21%)	33,37,55	1.67	10 (30%)
11	HEM	AC	402	3	50,50,50	1.59	8 (16%)	66,82,82	1.80	17 (25%)
17	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
11	HEM	AC	401	3	50,50,50	1.55	6 (12%)	66,82,82	1.78	12 (18%)
13	HEC	AD	401	4	50,50,50	2.80	25 (50%)	68,82,82	2.45	26 (38%)
11	HEM	Ac	401	3	50,50,50	1.31	8 (16%)	66,82,82	1.69	15 (22%)
14	3PE	Ag	103	-	37,37,50	1.06	2 (5%)	40,42,55	1.20	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	3PE	Ac	403	-	-	2/38/38/54	-
11	HEM	Ac	402	3	-	7/14/54/54	-
15	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
16	3PH	Ad	402	-	-	9/37/37/49	-
12	UQ6	Ac	405	-	-	5/21/21/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CDL	Ag	102	-	-	18/66/66/110	-
14	3PE	Aa	501	-	-	5/26/26/54	-
13	HEC	Ad	401	4	1/1/3/7	0/14/54/54	-
12	UQ6	AC	403	-	-	3/21/21/39	0/1/1/1
11	HEM	AC	402	3	-	6/14/54/54	-
17	CDL	Ag	101	-	-	11/52/52/110	-
11	HEM	AC	401	3	-	9/14/54/54	-
13	HEC	AD	401	4	1/1/3/7	8/14/54/54	-
11	HEM	Ac	401	3	-	9/14/54/54	-
14	3PE	Ag	103	-	-	8/41/41/54	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Ad	401	HEC	C3D-C2D	7.94	1.53	1.36
12	AC	403	UQ6	C5-C4	5.98	1.49	1.39
12	Ac	405	UQ6	C5-C6	5.97	1.49	1.40
12	Ac	405	UQ6	C2-C3	5.90	1.49	1.39
12	AC	403	UQ6	C2-C3	5.86	1.48	1.39
12	Ac	405	UQ6	C5-C4	5.82	1.48	1.39
12	AC	403	UQ6	C5-C6	5.79	1.48	1.40
11	AC	401	HEM	FE-NB	5.47	2.11	1.94
11	AC	402	HEM	FE-NB	5.17	2.10	1.94
12	Ac	405	UQ6	C6-C1	5.12	1.49	1.40
12	AC	403	UQ6	C6-C1	5.05	1.48	1.40
13	AD	401	HEC	C2A-C3A	4.97	1.47	1.36
11	Ac	402	HEM	FE-NB	4.94	2.10	1.94
13	AD	401	HEC	C3B-C2B	4.91	1.47	1.36
13	AD	401	HEC	FE-ND	4.89	2.10	1.94
13	AD	401	HEC	FE-NB	4.89	2.10	1.94
13	AD	401	HEC	CHA-C1A	4.79	1.47	1.38
13	AD	401	HEC	C3D-C2D	4.75	1.46	1.36
12	Ac	405	UQ6	C4-C3	4.64	1.49	1.39
13	AD	401	HEC	CHC-C4B	4.62	1.47	1.38
13	AD	401	HEC	CHB-C4A	4.59	1.47	1.38
12	AC	403	UQ6	C4-C3	4.59	1.49	1.39
13	AD	401	HEC	FE-NA	4.50	2.10	1.95
13	AD	401	HEC	FE-NC	4.46	2.10	1.95
13	AD	401	HEC	CHD-C1D	4.36	1.47	1.38
11	Ac	402	HEM	FE-NC	4.28	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Ac	405	UQ6	C2-C1	4.27	1.49	1.40
17	Ag	101	CDL	OA8-CA7	4.26	1.45	1.33
17	Ag	101	CDL	OB8-CB7	4.25	1.45	1.33
14	Aa	501	3PE	O31-C31	4.20	1.45	1.33
12	AC	403	UQ6	C2-C1	4.18	1.48	1.40
14	Ag	103	3PE	O31-C31	4.17	1.45	1.33
14	Ag	103	3PE	O21-C21	4.16	1.46	1.34
17	Ag	102	CDL	OB8-CB7	4.14	1.45	1.33
17	Ag	102	CDL	OA8-CA7	4.12	1.45	1.33
14	Ac	403	3PE	O31-C31	4.11	1.45	1.33
16	Ad	402	3PH	O21-C21	4.08	1.45	1.34
17	Ag	101	CDL	OA6-CA5	4.03	1.45	1.34
17	Ag	102	CDL	OA6-CA5	4.02	1.45	1.34
14	Aa	501	3PE	O21-C21	4.01	1.45	1.34
17	Ag	102	CDL	OB6-CB5	3.99	1.45	1.34
16	Ad	402	3PH	O31-C31	3.97	1.44	1.33
11	AC	402	HEM	FE-NC	3.93	2.08	1.95
14	Ac	403	3PE	O21-C21	3.92	1.45	1.34
17	Ag	101	CDL	OB6-CB5	3.91	1.45	1.34
13	AD	401	HEC	CHC-C1C	3.85	1.48	1.39
11	AC	402	HEM	C4D-ND	-3.83	1.33	1.40
11	AC	401	HEM	C1B-NB	-3.81	1.33	1.40
13	AD	401	HEC	CHA-C4D	3.69	1.47	1.39
13	Ad	401	HEC	FE-ND	3.68	2.06	1.94
11	Ac	401	HEM	C4D-ND	-3.67	1.34	1.40
13	Ad	401	HEC	FE-NB	3.61	2.06	1.94
13	AD	401	HEC	CHD-C4C	3.53	1.47	1.39
11	Ac	402	HEM	C4D-ND	-3.52	1.34	1.40
11	AC	402	HEM	C1B-NB	-3.37	1.34	1.40
11	Ac	402	HEM	C1B-NB	-3.35	1.34	1.40
11	AC	401	HEM	FE-NC	3.27	2.06	1.95
11	AC	401	HEM	C4D-ND	-3.18	1.34	1.40
13	AD	401	HEC	C3C-C2C	3.16	1.47	1.38
13	AD	401	HEC	C1D-ND	-3.13	1.34	1.40
13	AD	401	HEC	CHB-C1B	3.10	1.46	1.39
11	Ac	401	HEM	C1B-NB	-3.05	1.35	1.40
13	AD	401	HEC	C4B-NB	-2.98	1.35	1.40
15	Ac	404	U10	C4-C3	2.94	1.48	1.36
15	Ac	404	U10	C6-C5	-2.91	1.38	1.46
13	Ad	401	HEC	FE-NA	2.90	2.04	1.95
11	Ac	402	HEM	C1D-ND	-2.76	1.33	1.38
11	AC	401	HEM	C1C-C2C	-2.67	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Ad	401	HEC	FE-NC	2.63	2.04	1.95
13	AD	401	HEC	C1C-C2C	2.58	1.49	1.43
15	Ac	404	U10	C3-C2	-2.56	1.41	1.48
11	Ac	401	HEM	C1C-C2C	-2.55	1.40	1.45
11	AC	402	HEM	FE-ND	-2.53	1.87	1.94
11	Ac	402	HEM	C1C-C2C	-2.50	1.40	1.45
11	Ac	401	HEM	C1D-ND	-2.46	1.33	1.38
13	AD	401	HEC	C4C-NC	-2.40	1.35	1.39
13	AD	401	HEC	C4A-NA	-2.38	1.35	1.39
11	Ac	402	HEM	C1A-C2A	-2.37	1.39	1.44
11	Ac	401	HEM	FE-NB	2.35	2.02	1.94
13	AD	401	HEC	C1A-NA	-2.31	1.35	1.39
11	Ac	401	HEM	FE-ND	2.31	2.02	1.94
11	AC	402	HEM	C1C-C2C	-2.30	1.40	1.45
11	Ac	401	HEM	C3C-C4C	-2.28	1.42	1.46
13	AD	401	HEC	C4D-C3D	2.28	1.49	1.45
11	AC	401	HEM	C3C-C4C	-2.28	1.42	1.46
13	AD	401	HEC	C4B-C3B	2.24	1.48	1.45
11	Ac	402	HEM	FE-ND	-2.18	1.88	1.94
11	AC	402	HEM	C1D-ND	-2.16	1.34	1.38
11	AC	402	HEM	C3C-C4C	-2.14	1.42	1.46
13	AD	401	HEC	C1A-C2A	2.13	1.49	1.45
11	Ac	401	HEM	C4B-NB	-2.08	1.34	1.38

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Ac	404	U10	C6-C1-C2	7.78	125.33	119.18
13	Ad	401	HEC	C1D-ND-C4D	6.34	111.63	105.07
13	AD	401	HEC	C1B-C2B-C3B	-6.22	100.42	106.96
13	AD	401	HEC	C2B-C1B-NB	6.13	117.22	109.88
11	Ac	402	HEM	CHC-C4B-NB	6.08	131.03	124.42
11	AC	402	HEM	CHC-C4B-NB	5.76	130.67	124.42
11	AC	401	HEM	CHC-C4B-NB	5.12	129.98	124.42
13	AD	401	HEC	C1C-C2C-C3C	-4.91	101.08	106.83
11	AC	401	HEM	CHD-C4C-NC	4.84	129.68	124.44
11	AC	402	HEM	CHD-C1D-ND	4.80	129.63	124.42
13	AD	401	HEC	C2A-C1A-NA	4.78	114.97	110.32
13	AD	401	HEC	C2D-C1D-ND	4.77	115.50	109.84
13	AD	401	HEC	C3D-C4D-ND	4.76	114.96	110.36
11	Ac	401	HEM	CHC-C4B-NB	4.71	129.53	124.42
14	Ag	103	3PE	O21-C21-C22	4.69	121.61	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Ac	402	HEM	C4C-NC-C1C	4.42	109.67	105.35
11	Ac	401	HEM	CHD-C4C-NC	4.34	129.14	124.44
11	Ac	402	HEM	C1B-NB-C4B	4.22	109.43	105.07
11	Ac	402	HEM	CHB-C1B-NB	4.17	129.52	124.37
13	AD	401	HEC	CHB-C1B-C2B	-4.16	118.49	124.98
12	AC	403	UQ6	C10-C9-C11	4.14	122.23	115.27
15	Ac	404	U10	C1-C6-C5	-4.13	115.69	119.58
17	Ag	101	CDL	OB6-CB5-C51	4.10	120.33	111.50
16	Ad	402	3PH	O21-C21-C22	4.03	120.19	111.50
11	Ac	401	HEM	CHB-C1B-NB	4.01	129.32	124.37
11	AC	401	HEM	C1B-NB-C4B	4.00	109.20	105.07
17	Ag	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
12	Ac	405	UQ6	C7-C8-C9	-3.96	121.10	127.24
17	Ag	102	CDL	OA6-CA5-C11	3.96	120.03	111.50
11	AC	401	HEM	CHB-C1B-NB	3.94	129.24	124.37
13	AD	401	HEC	C1D-C2D-C3D	-3.91	102.84	106.96
11	AC	401	HEM	C4C-NC-C1C	3.85	109.12	105.35
11	Ac	402	HEM	CHD-C4C-NC	3.83	128.58	124.44
11	AC	402	HEM	C1B-NB-C4B	3.75	108.94	105.07
12	AC	403	UQ6	C7-C8-C9	-3.68	121.53	127.24
14	Ac	403	3PE	O21-C21-C22	3.67	119.42	111.50
11	AC	402	HEM	CHB-C1B-NB	3.60	128.82	124.37
13	AD	401	HEC	C2C-C1C-NC	3.59	115.54	110.08
13	AD	401	HEC	CBC-CAC-C3C	3.59	122.32	112.43
12	AC	403	UQ6	C6-C7-C8	-3.55	106.55	112.17
11	Ac	402	HEM	CHA-C4D-ND	3.54	128.75	124.37
13	AD	401	HEC	C3C-C4C-NC	3.46	114.01	110.15
17	Ag	101	CDL	OB8-CB7-C71	3.45	120.42	111.38
13	AD	401	HEC	CBB-CAB-C3B	3.33	121.60	112.43
11	Ac	401	HEM	C4D-ND-C1D	3.32	108.51	105.07
12	Ac	405	UQ6	C12-C13-C14	-3.31	119.68	127.66
17	Ag	101	CDL	OA6-CA5-C11	3.31	120.03	110.80
11	Ac	402	HEM	CHD-C1D-ND	3.27	127.97	124.42
15	Ac	404	U10	C4-C3-C2	-3.25	114.30	120.68
13	AD	401	HEC	C3A-C4A-NA	3.22	115.63	109.69
14	Aa	501	3PE	O21-C21-C22	3.22	119.78	110.80
13	AD	401	HEC	C1A-C2A-C3A	-3.17	102.99	107.13
11	Ac	401	HEM	C1B-NB-C4B	3.17	108.35	105.07
11	AC	402	HEM	CHA-C4D-ND	3.16	128.27	124.37
13	AD	401	HEC	CAD-C3D-C4D	3.11	130.09	124.66
11	AC	402	HEM	CHD-C4C-NC	3.10	127.79	124.44
17	Ag	101	CDL	CB4-OB6-CB5	-3.07	110.22	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AC	402	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
13	AD	401	HEC	C4A-C3A-C2A	-3.05	102.49	106.94
16	Ad	402	3PH	O31-C31-C32	2.98	121.27	111.91
11	Ac	401	HEM	CHD-C1D-ND	2.86	127.53	124.42
11	Ac	402	HEM	CHD-C1D-C2D	-2.85	120.52	124.98
17	Ag	102	CDL	CA4-OA6-CA5	-2.84	110.81	117.79
13	AD	401	HEC	CMB-C2B-C3B	2.81	133.74	126.12
13	AD	401	HEC	C4D-C3D-C2D	-2.80	102.81	106.90
13	AD	401	HEC	CAD-CBD-CGD	-2.80	107.58	113.60
11	AC	402	HEM	CBD-CAD-C3D	-2.77	104.94	112.63
12	Ac	405	UQ6	C15-C14-C16	2.77	119.92	115.27
11	Ac	402	HEM	CMA-C3A-C4A	2.75	129.55	125.37
11	Ac	402	HEM	CHA-C4D-C3D	-2.73	120.21	125.33
12	Ac	405	UQ6	C10-C9-C11	2.69	119.79	115.27
17	Ag	102	CDL	CB4-OB6-CB5	-2.67	111.21	117.79
11	Ac	402	HEM	CHA-C1A-NA	2.62	128.68	123.85
14	Ag	103	3PE	O31-C31-C32	2.61	120.10	111.91
11	AC	402	HEM	C4C-NC-C1C	2.59	107.89	105.35
15	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
12	AC	403	UQ6	C12-C13-C14	-2.59	121.42	127.66
12	AC	403	UQ6	C15-C14-C16	2.59	119.62	115.27
11	AC	401	HEM	O2A-CGA-CBA	2.58	122.31	114.03
11	AC	401	HEM	O2D-CGD-CBD	2.57	122.30	114.03
13	Ad	401	HEC	CAA-CBA-CGA	-2.56	108.09	113.60
11	Ac	401	HEM	CHA-C1A-NA	2.56	128.56	123.85
11	Ac	401	HEM	CHA-C4D-ND	2.55	127.52	124.37
15	Ac	404	U10	O4-C4-C5	-2.54	107.96	116.56
13	AD	401	HEC	CAA-C2A-C1A	2.54	129.68	124.89
11	AC	401	HEM	CHA-C1A-NA	2.53	128.50	123.85
17	Ag	102	CDL	OA8-CA7-C31	2.53	119.84	111.91
14	Ac	403	3PE	O31-C31-C32	2.52	119.83	111.91
11	Ac	402	HEM	C1A-CHA-C4D	-2.50	120.40	126.34
11	AC	402	HEM	CBA-CAA-C2A	-2.50	105.68	112.63
17	Ag	101	CDL	OA8-CA7-C31	2.47	119.65	111.91
17	Ag	101	CDL	CA4-OA6-CA5	-2.46	111.73	117.79
11	AC	401	HEM	CHD-C1D-ND	2.46	127.09	124.42
12	AC	403	UQ6	C17-C18-C19	-2.45	119.36	127.75
14	Aa	501	3PE	O31-C31-C32	2.45	119.60	111.91
11	Ac	401	HEM	C4B-C3B-C2B	-2.44	105.18	107.11
13	AD	401	HEC	CMD-C2D-C1D	2.42	128.73	125.04
13	AD	401	HEC	C3B-C4B-NB	2.42	112.86	110.17
14	Ag	103	3PE	C2-O21-C21	-2.42	111.84	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Ac	403	3PE	C2-O21-C21	-2.40	111.88	117.79
12	Ac	405	UQ6	C21-C19-C20	2.39	119.88	114.60
12	AC	403	UQ6	C21-C19-C20	2.37	119.84	114.60
11	Ac	401	HEM	C4A-NA-C1A	2.31	107.61	105.35
13	AD	401	HEC	CMC-C2C-C1C	2.28	128.85	125.37
11	Ac	402	HEM	C4C-C3C-C2C	2.28	108.63	106.75
16	Ad	402	3PH	C2-O21-C21	-2.27	112.19	117.79
11	Ac	402	HEM	CBD-CAD-C3D	-2.26	106.34	112.63
16	Ad	402	3PH	O31-C31-O32	-2.25	117.91	123.59
11	Ac	402	HEM	CHB-C1B-C2B	-2.25	120.47	126.73
14	Aa	501	3PE	C2-O21-C21	-2.24	112.27	117.79
17	Ag	101	CDL	OB6-CB5-OB7	-2.23	118.31	123.70
11	AC	402	HEM	C4D-ND-C1D	2.23	107.38	105.07
11	Ac	401	HEM	CHB-C1B-C2B	-2.22	120.56	126.73
12	Ac	405	UQ6	C17-C18-C19	-2.21	120.18	127.75
17	Ag	102	CDL	OB8-CB7-C71	2.21	118.84	111.91
11	Ac	401	HEM	C4C-NC-C1C	2.21	107.51	105.35
13	AD	401	HEC	CMA-C3A-C4A	2.20	128.59	124.71
11	AC	402	HEM	C4C-CHD-C1D	-2.19	121.33	126.06
13	Ad	401	HEC	CHA-C4D-ND	2.15	126.76	124.42
11	AC	402	HEM	C4A-NA-C1A	2.15	107.45	105.35
12	AC	403	UQ6	C4M-O4-C4	2.14	120.64	114.78
11	AC	401	HEM	CHB-C1B-C2B	-2.14	120.79	126.73
11	AC	401	HEM	C4A-NA-C1A	2.11	107.41	105.35
13	Ad	401	HEC	C4A-NA-C1A	2.09	107.40	105.35
11	Ac	401	HEM	C1C-CHC-C4B	-2.09	121.54	126.06
13	Ad	401	HEC	C2A-C1A-NA	-2.08	108.30	110.32
13	Ad	401	HEC	C3C-C4C-NC	-2.08	107.82	110.15
13	Ad	401	HEC	C4B-NB-C1B	2.07	107.21	105.07
13	AD	401	HEC	CMC-C2C-C3C	2.06	130.07	125.61
11	AC	402	HEM	CHA-C1A-NA	2.05	127.63	123.85
11	AC	402	HEM	C4A-CHB-C1B	-2.05	121.47	126.34
11	Ac	401	HEM	C4A-CHB-C1B	-2.04	121.50	126.34
15	Ac	404	U10	C3M-O3-C3	2.03	123.67	116.47
13	AD	401	HEC	CHD-C1D-C2D	-2.03	121.09	126.73
12	AC	403	UQ6	C10-C9-C8	-2.03	118.47	123.68
11	AC	402	HEM	CHB-C1B-C2B	-2.03	121.09	126.73
11	Ac	401	HEM	CAA-CBA-CGA	-2.03	109.24	113.60
15	Ac	404	U10	O4-C4-C3	2.02	131.26	123.64
12	AC	403	UQ6	C3M-O3-C3	2.01	120.28	114.78
11	AC	401	HEM	C4B-C3B-C2B	-2.00	105.53	107.11
11	AC	402	HEM	C2A-C1A-NA	-2.00	107.91	110.15

All (2) chirality outliers are listed below:

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

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	401	HEM	C2B-C3B-CAB-CBB
11	AC	401	HEM	C2C-C3C-CAC-CBC
11	AC	401	HEM	C4C-C3C-CAC-CBC
11	AC	402	HEM	C2B-C3B-CAB-CBB
11	AC	402	HEM	C2C-C3C-CAC-CBC
11	Ac	401	HEM	C2B-C3B-CAB-CBB
11	Ac	401	HEM	C2C-C3C-CAC-CBC
11	Ac	401	HEM	C4C-C3C-CAC-CBC
11	Ac	402	HEM	C2B-C3B-CAB-CBB
12	Ac	405	UQ6	C1-C6-C7-C8
12	Ac	405	UQ6	C13-C14-C16-C17
12	Ac	405	UQ6	C15-C14-C16-C17
14	Aa	501	3PE	C22-C21-O21-C2
14	Ag	103	3PE	C1-O11-P-O14
14	Ag	103	3PE	C11-O13-P-O12
14	Ag	103	3PE	C11-O13-P-O14
15	Ac	404	U10	C7-C8-C9-C10
15	Ac	404	U10	C7-C8-C9-C11
16	Ad	402	3PH	C1-O11-P-O13
16	Ad	402	3PH	O21-C2-C3-O31
17	Ag	101	CDL	CB2-OB2-PB2-OB3
17	Ag	101	CDL	CB2-OB2-PB2-OB4
17	Ag	101	CDL	CB3-OB5-PB2-OB4
17	Ag	102	CDL	C1-CB2-OB2-PB2
17	Ag	102	CDL	CB2-OB2-PB2-OB4
17	Ag	102	CDL	CB3-OB5-PB2-OB3
17	Ag	102	CDL	C51-CB5-OB6-CB4
15	Ac	404	U10	C12-C13-C14-C15
15	Ac	404	U10	C12-C13-C14-C16
13	AD	401	HEC	C2B-C3B-CAB-CBB
13	AD	401	HEC	C4B-C3B-CAB-CBB
13	AD	401	HEC	C4C-C3C-CAC-CBC
13	AD	401	HEC	C2C-C3C-CAC-CBC
14	Aa	501	3PE	O22-C21-O21-C2
17	Ag	102	CDL	OB7-CB5-OB6-CB4
12	AC	403	UQ6	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
16	Ad	402	3PH	C35-C36-C37-C38
16	Ad	402	3PH	C31-C32-C33-C34
12	AC	403	UQ6	C13-C14-C16-C17
12	Ac	405	UQ6	C5-C6-C7-C8
14	Ag	103	3PE	C1-O11-P-O13
14	Ag	103	3PE	C11-O13-P-O11
17	Ag	101	CDL	CB2-OB2-PB2-OB5
17	Ag	101	CDL	CB3-OB5-PB2-OB2
17	Ag	102	CDL	CB2-OB2-PB2-OB5
17	Ag	102	CDL	CB3-OB5-PB2-OB2
14	Aa	501	3PE	C32-C31-O31-C3
17	Ag	102	CDL	C74-C75-C76-C77
14	Aa	501	3PE	O32-C31-O31-C3
17	Ag	102	CDL	C31-CA7-OA8-CA6
17	Ag	101	CDL	C51-CB5-OB6-CB4
16	Ad	402	3PH	C22-C21-O21-C2
11	AC	401	HEM	C4B-C3B-CAB-CBB
11	AC	402	HEM	C4B-C3B-CAB-CBB
11	AC	402	HEM	C4C-C3C-CAC-CBC
11	Ac	401	HEM	C4B-C3B-CAB-CBB
11	Ac	402	HEM	C4B-C3B-CAB-CBB
17	Ag	102	CDL	OA9-CA7-OA8-CA6
16	Ad	402	3PH	O22-C21-O21-C2
17	Ag	101	CDL	OB7-CB5-OB6-CB4
16	Ad	402	3PH	C1-C2-C3-O31
16	Ad	402	3PH	C34-C35-C36-C37
16	Ad	402	3PH	C36-C37-C38-C39
14	Ac	403	3PE	C22-C21-O21-C2
14	Ag	103	3PE	C39-C3A-C3B-C3C
17	Ag	102	CDL	CB4-CB3-OB5-PB2
11	AC	401	HEM	C2A-CAA-CBA-CGA
11	Ac	401	HEM	C2A-CAA-CBA-CGA
13	AD	401	HEC	C2A-CAA-CBA-CGA
14	Ac	403	3PE	O22-C21-O21-C2
11	Ac	402	HEM	C2C-C3C-CAC-CBC
14	Ag	103	3PE	C1-O11-P-O12
17	Ag	102	CDL	CB3-OB5-PB2-OB4
17	Ag	102	CDL	C51-C52-C53-C54
17	Ag	101	CDL	C1-CA2-OA2-PA1
17	Ag	102	CDL	C1-CA2-OA2-PA1
11	Ac	402	HEM	C4C-C3C-CAC-CBC
11	AC	401	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	Ac	404	U10	C12-C11-C9-C10
11	Ac	402	HEM	CAD-CBD-CGD-O2D
17	Ag	101	CDL	C71-CB7-OB8-CB6
11	AC	402	HEM	CAD-CBD-CGD-O1D
11	AC	401	HEM	CAD-CBD-CGD-O1D
11	Ac	401	HEM	CAD-CBD-CGD-O2D
11	Ac	402	HEM	CAD-CBD-CGD-O1D
14	Aa	501	3PE	C1-C2-O21-C21
11	Ac	401	HEM	CAD-CBD-CGD-O1D
11	AC	401	HEM	CAA-CBA-CGA-O1A
11	Ac	401	HEM	CAA-CBA-CGA-O2A
11	AC	401	HEM	CAD-CBD-CGD-O2D
11	Ac	401	HEM	CAA-CBA-CGA-O1A
17	Ag	101	CDL	OB9-CB7-OB8-CB6
11	AC	402	HEM	CAD-CBD-CGD-O2D
17	Ag	102	CDL	C11-C12-C13-C14
15	Ac	404	U10	C12-C11-C9-C8
11	Ac	402	HEM	C2A-CAA-CBA-CGA
13	AD	401	HEC	CAA-CBA-CGA-O2A
17	Ag	102	CDL	OA6-CA4-CA6-OA8
17	Ag	102	CDL	C53-C54-C55-C56
12	AC	403	UQ6	C14-C16-C17-C18
14	Ag	103	3PE	O21-C21-C22-C23
17	Ag	102	CDL	C52-C53-C54-C55
13	AD	401	HEC	CAA-CBA-CGA-O1A
12	Ac	405	UQ6	C6-C7-C8-C9
17	Ag	101	CDL	C72-C71-CB7-OB8
13	AD	401	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

15 monomers are involved in 174 short contacts:

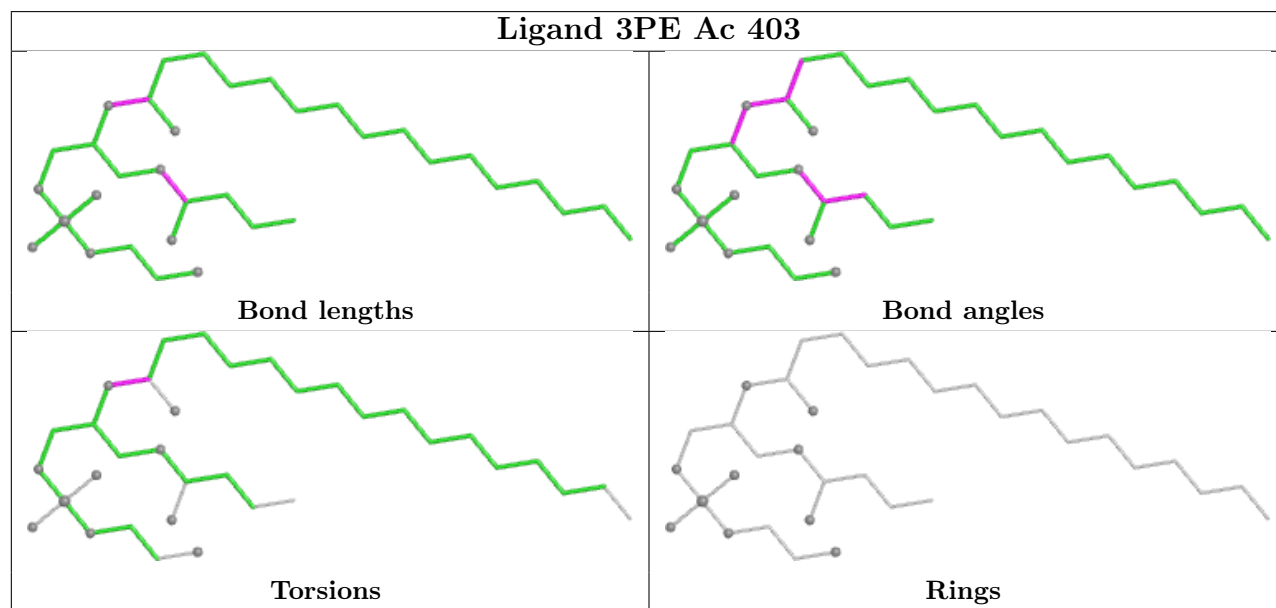
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Ac	403	3PE	7	0
11	Ac	402	HEM	10	0
15	Ac	404	U10	20	0
16	Ad	402	3PH	39	0
12	Ac	405	UQ6	15	0
17	Ag	102	CDL	4	0
14	Aa	501	3PE	3	0
13	Ad	401	HEC	12	0
12	AC	403	UQ6	11	0

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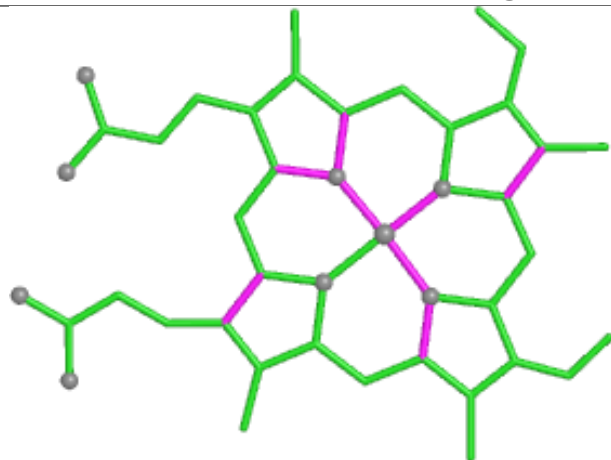
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AC	402	HEM	9	0
17	Ag	101	CDL	5	0
11	AC	401	HEM	18	0
13	AD	401	HEC	18	0
11	Ac	401	HEM	1	0
14	Ag	103	3PE	9	0

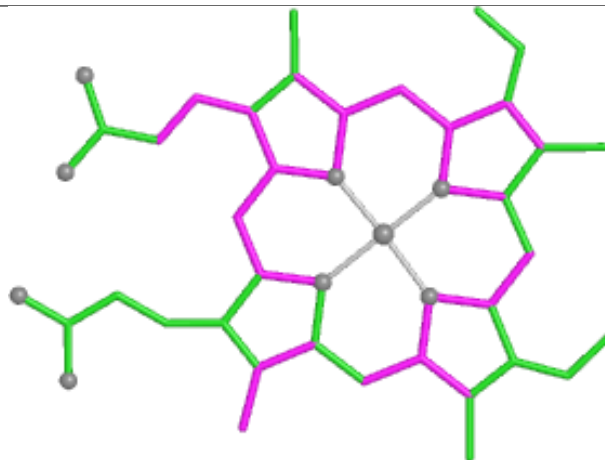
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



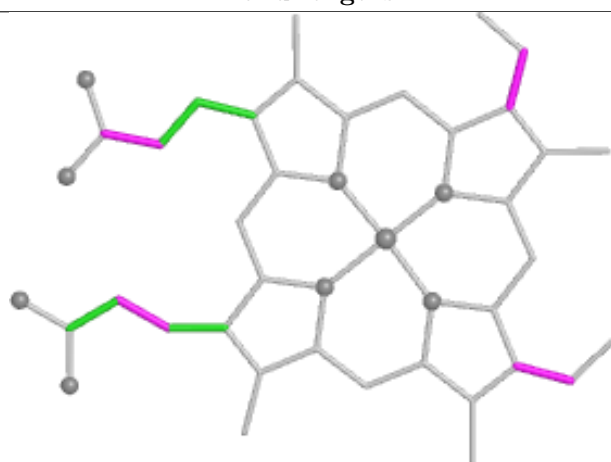
Ligand HEM Ac 402



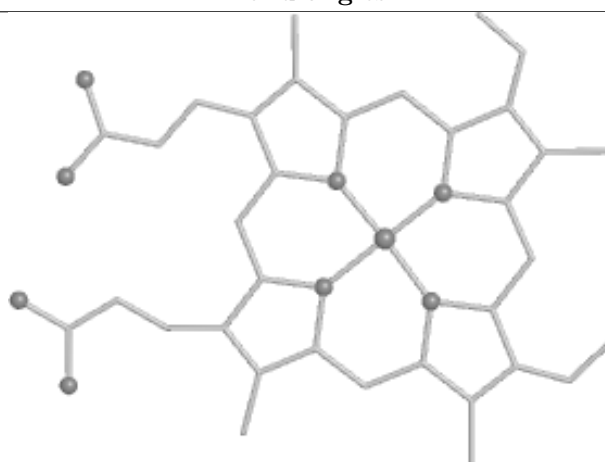
Bond lengths



Bond angles

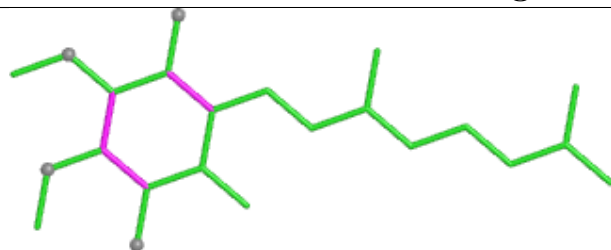


Torsions

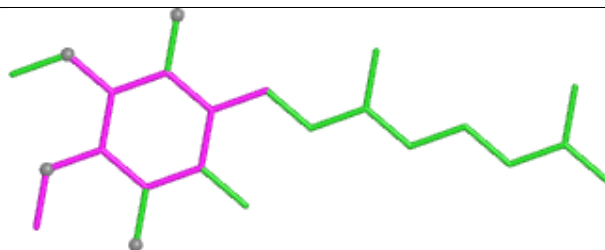


Rings

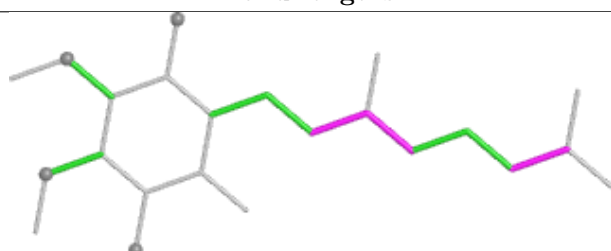
Ligand U10 Ac 404



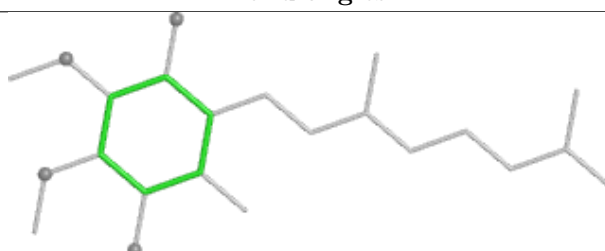
Bond lengths



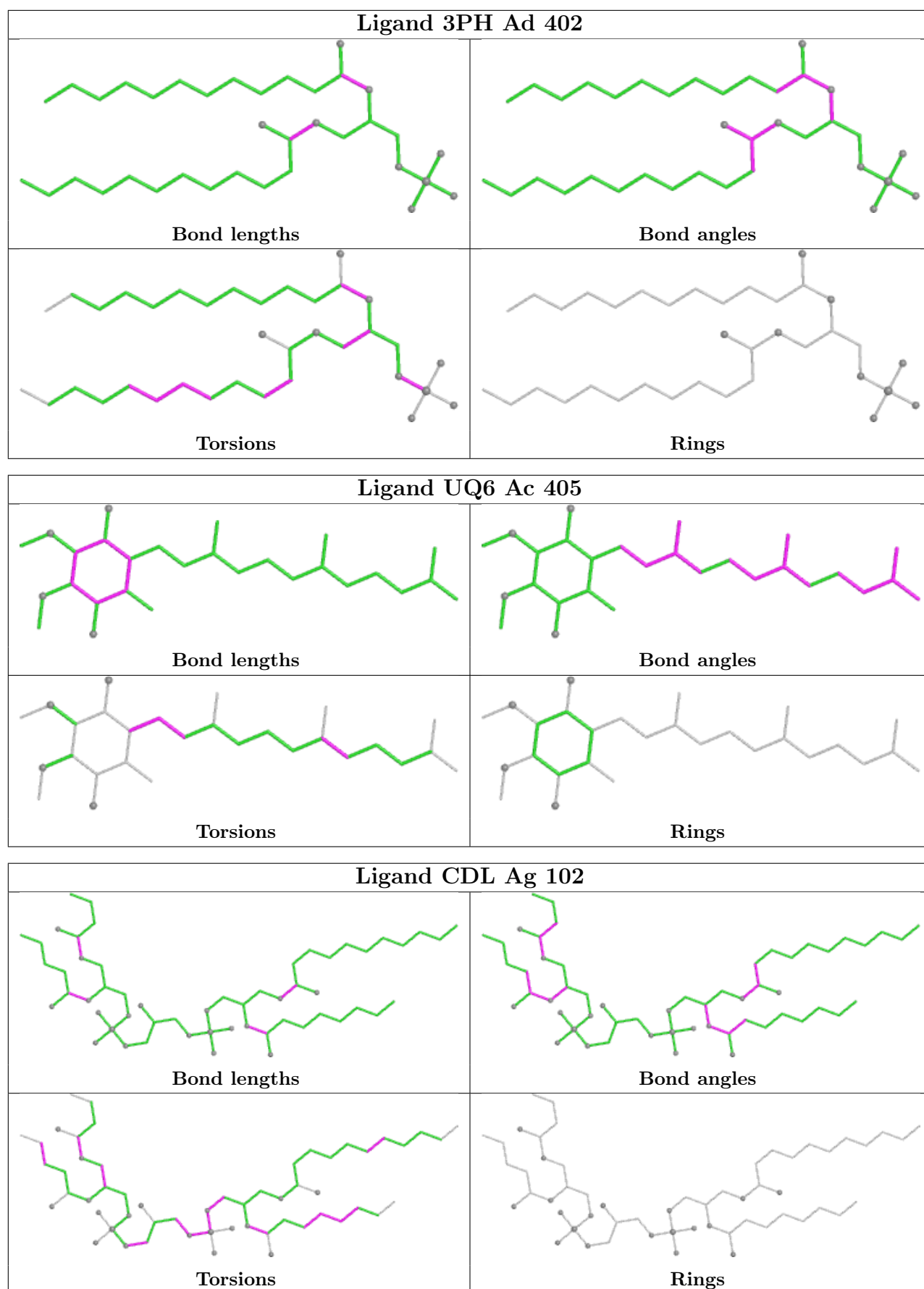
Bond angles

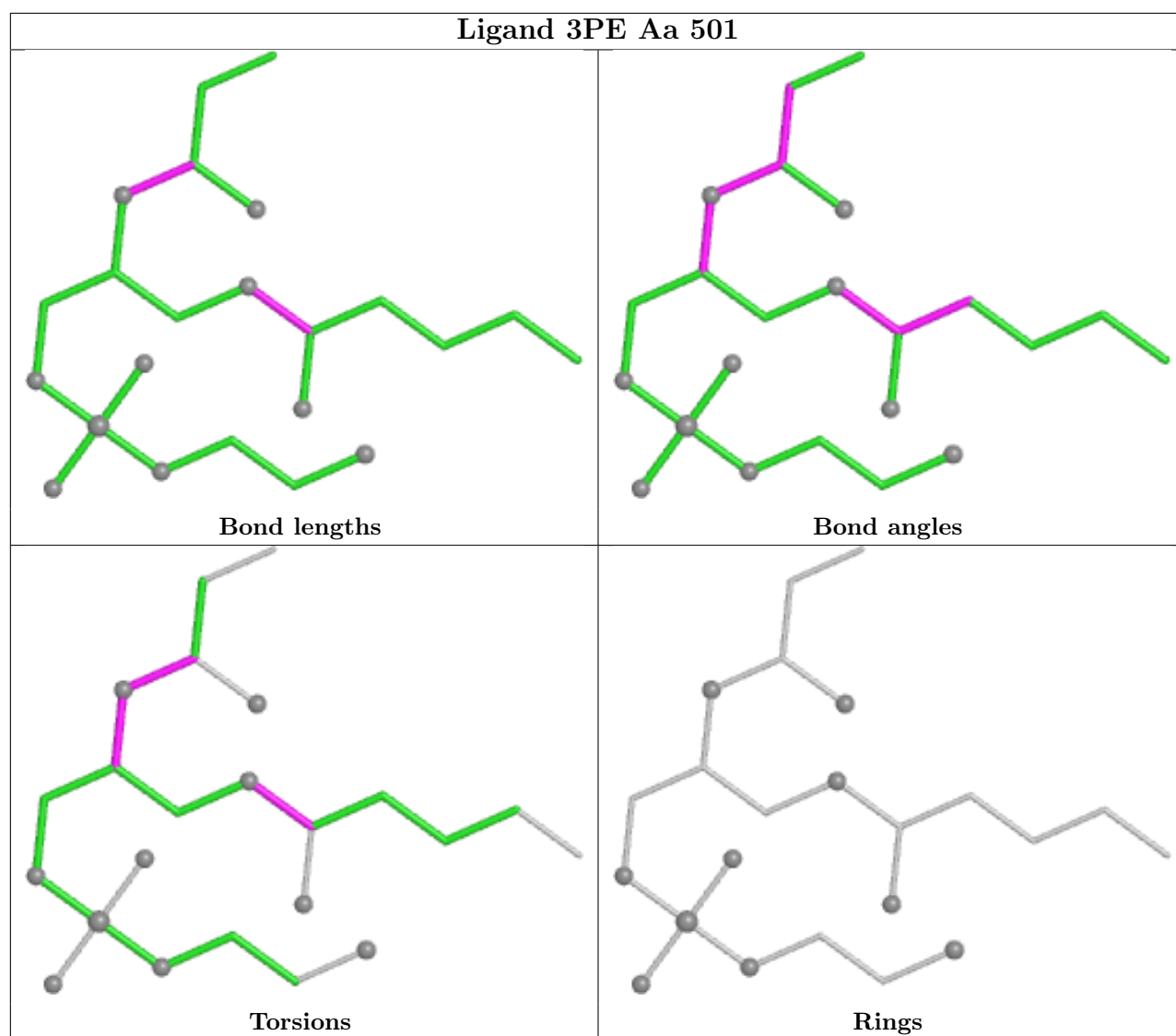


Torsions

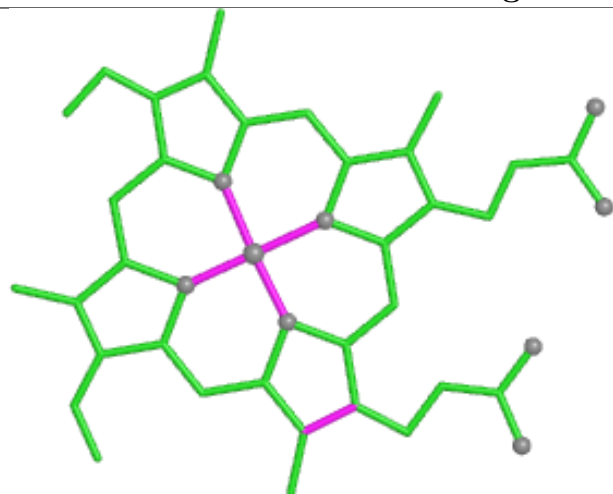


Rings

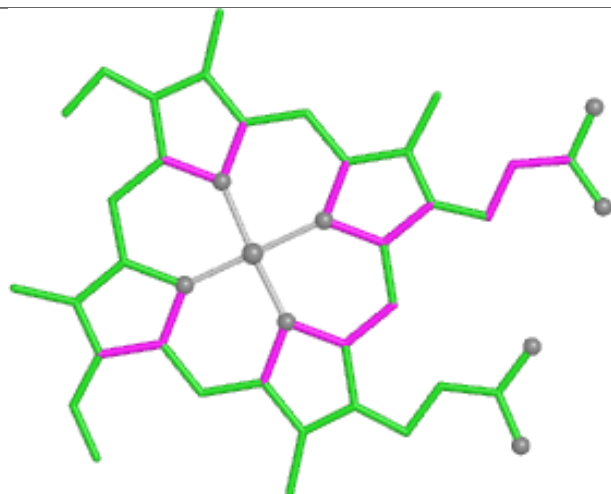




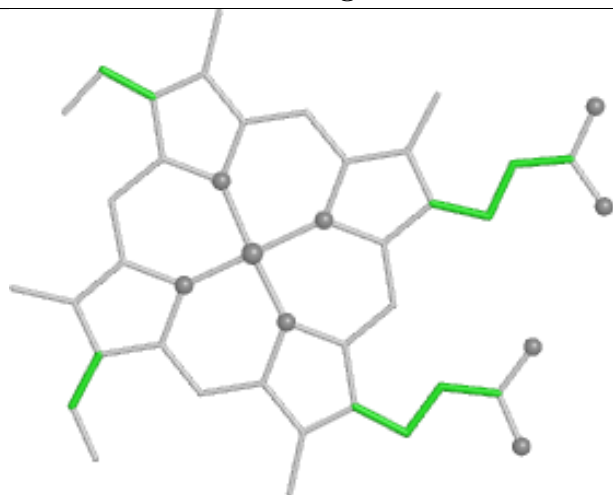
Ligand HEC Ad 401



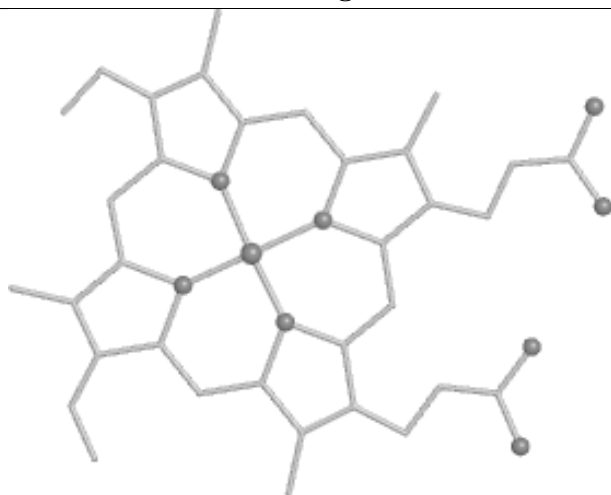
Bond lengths



Bond angles

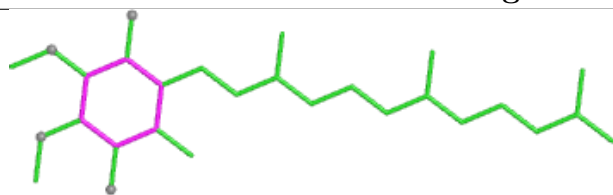


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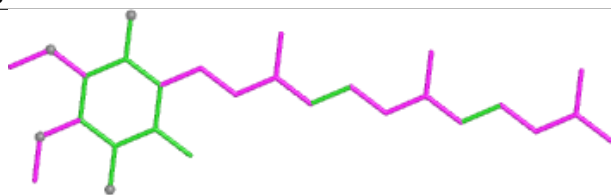


Rings

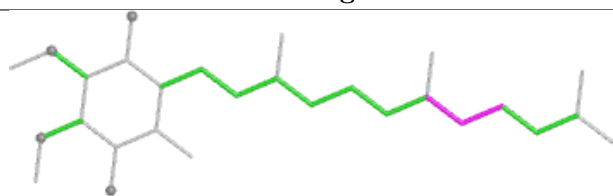
Ligand UQ6 AC 403



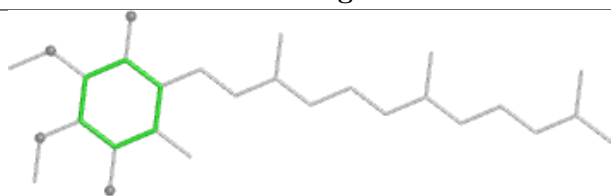
Bond lengths



Bond angles

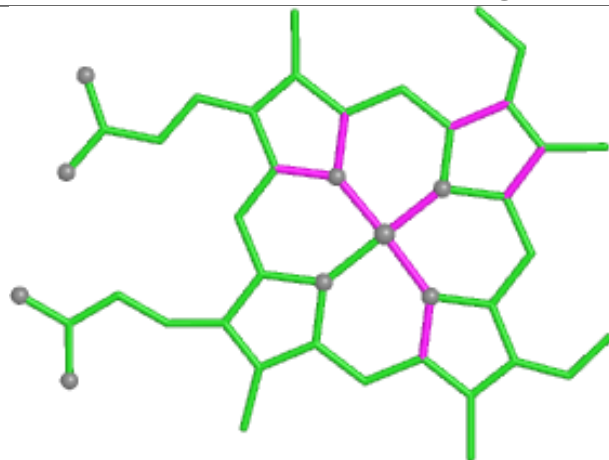


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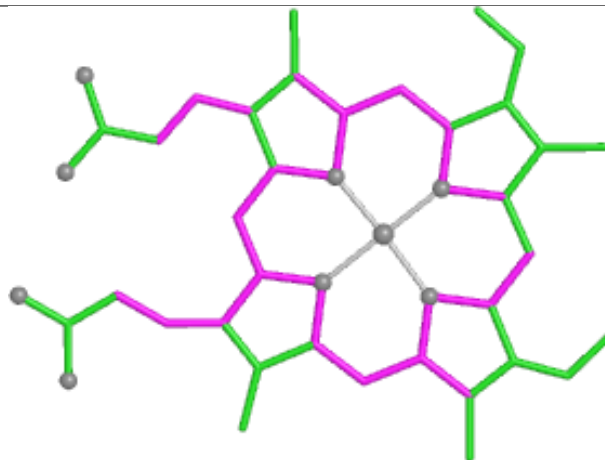


Rings

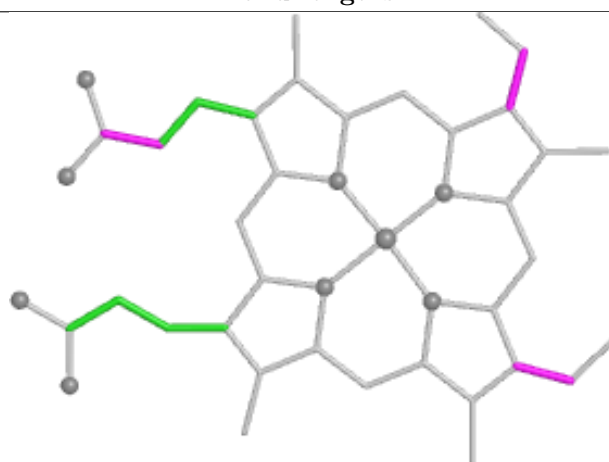
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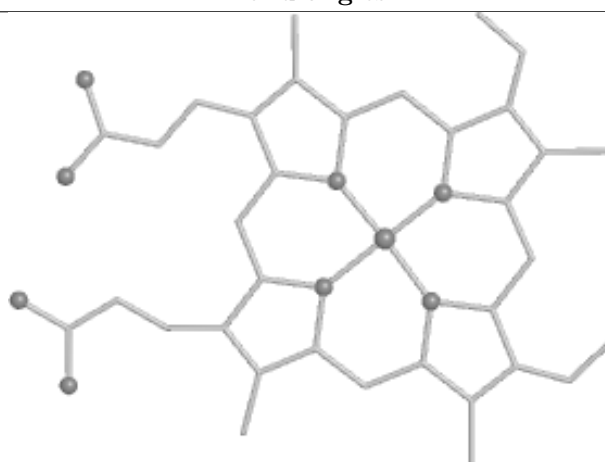
Bond lengths



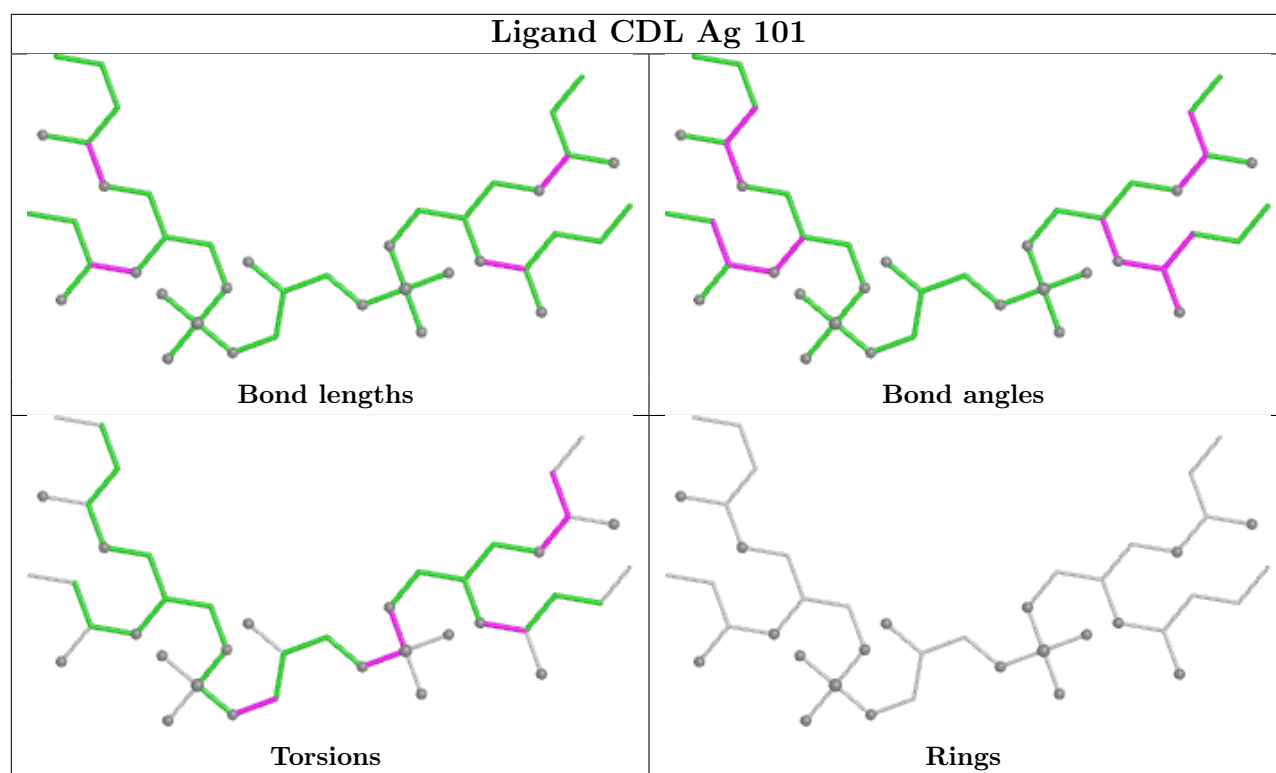
Bond angles



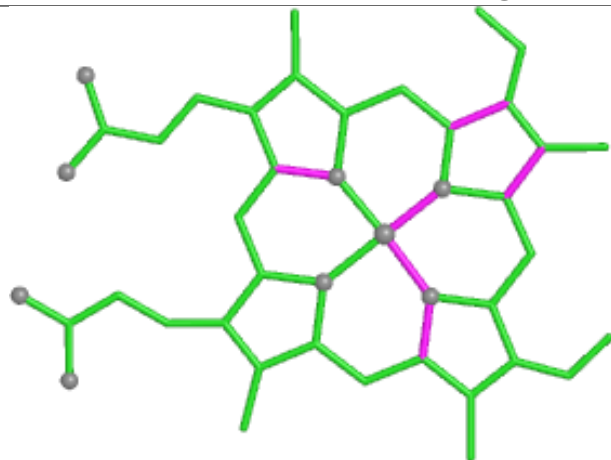
Torsions



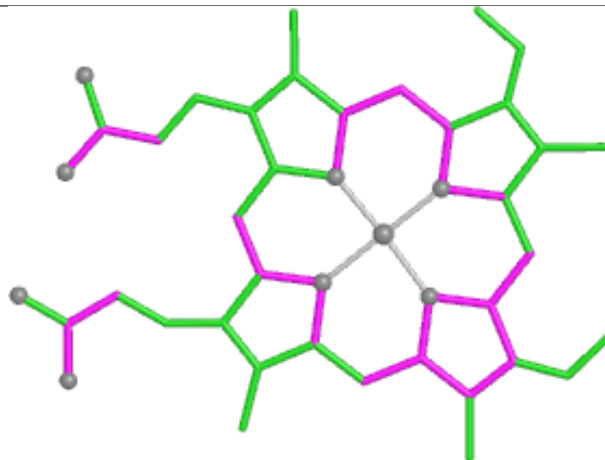
Rings



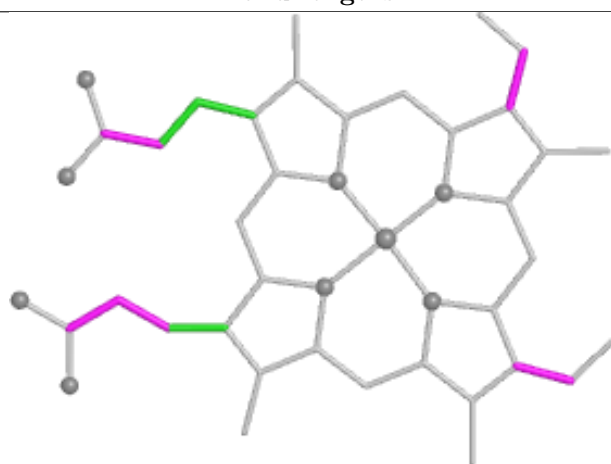
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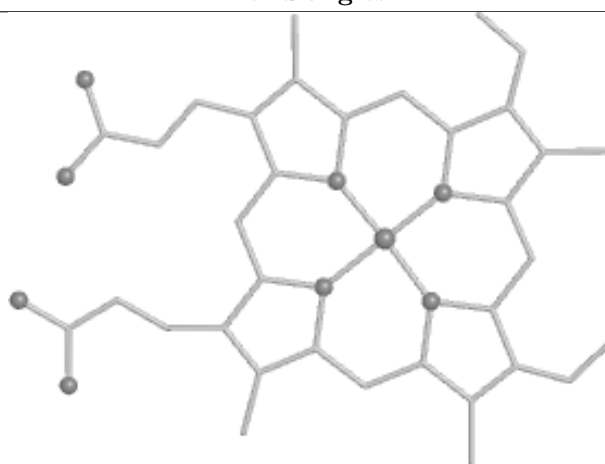
Bond lengths



Bond angles

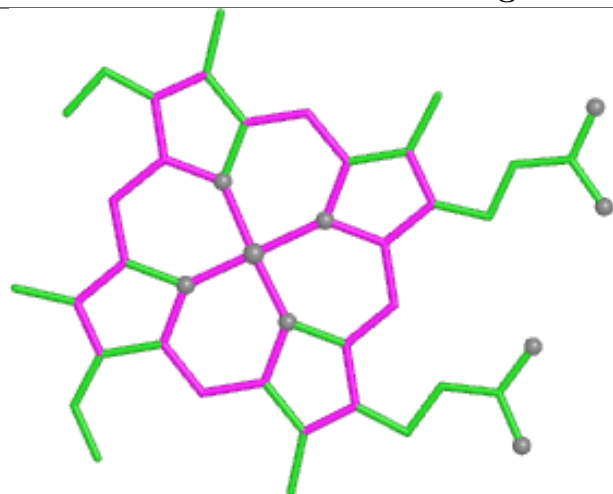


Torsions

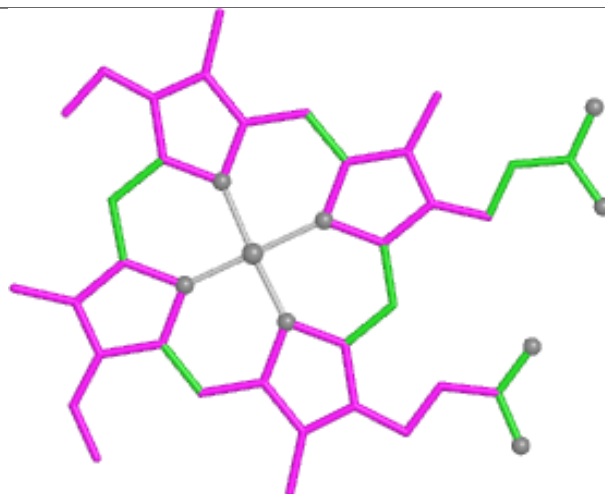


Rings

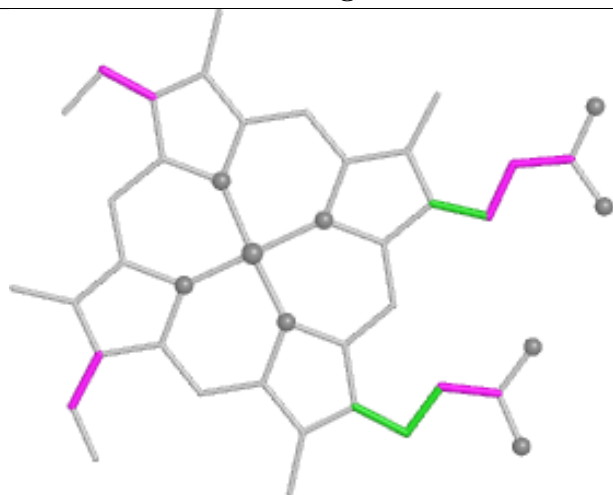
Ligand HEC AD 401



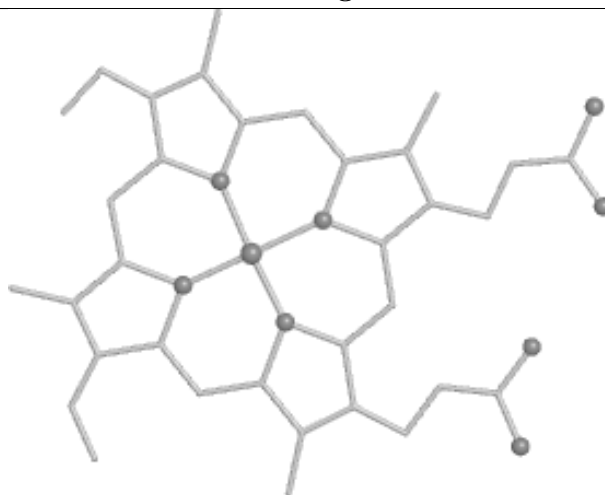
Bond lengths



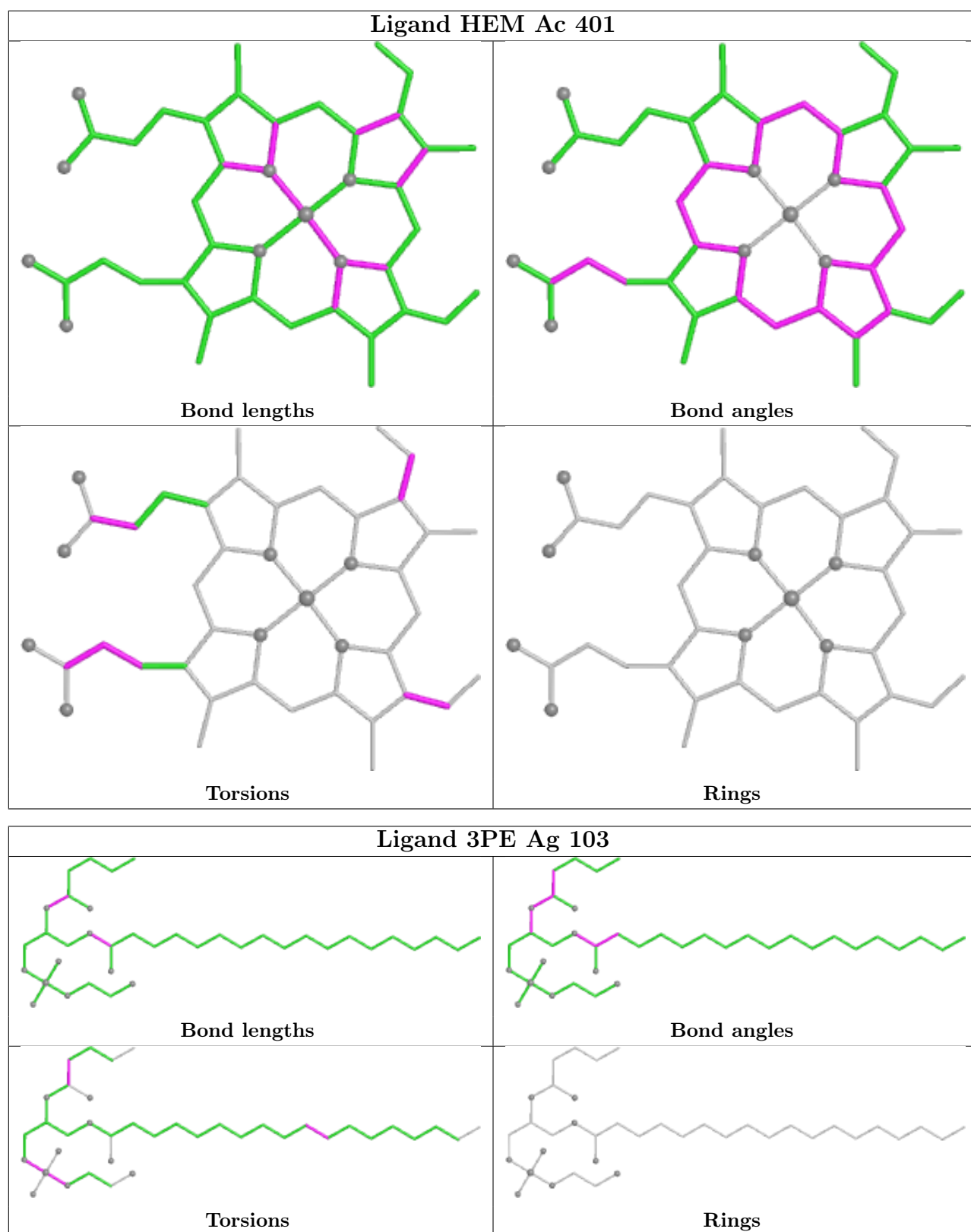
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

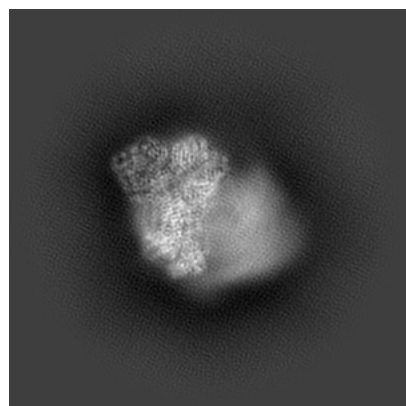
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35343. These allow visual inspection of the internal detail of the map and identification of artifacts.

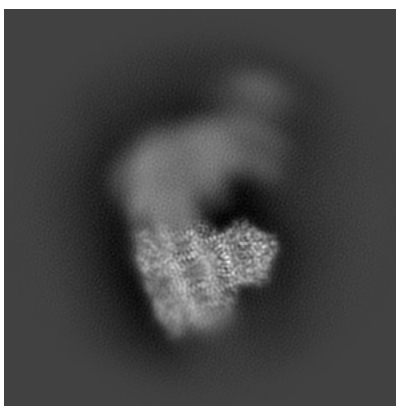
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

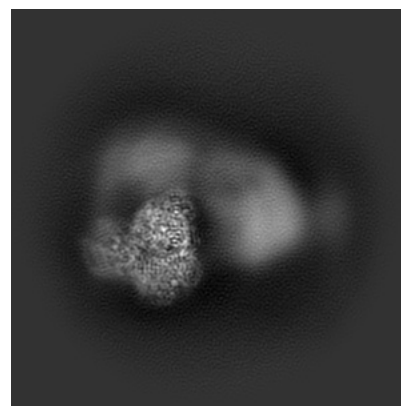
6.1.1 Primary map



X

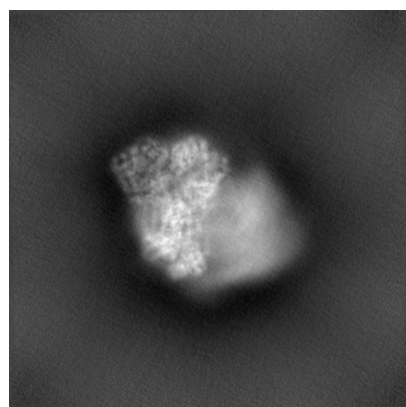


Y

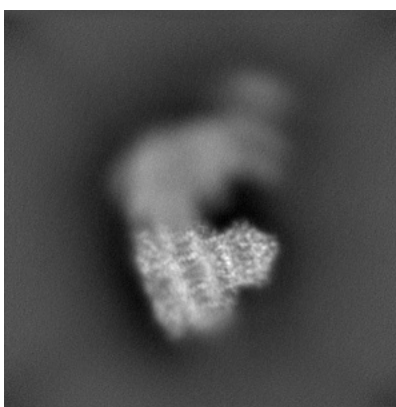


Z

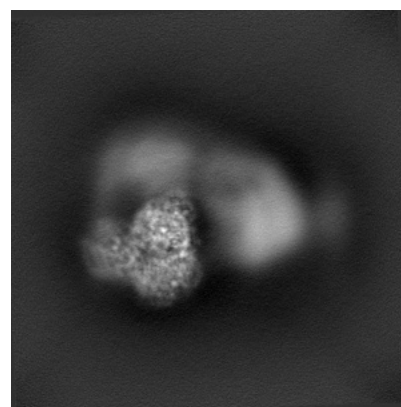
6.1.2 Raw map



X



Y

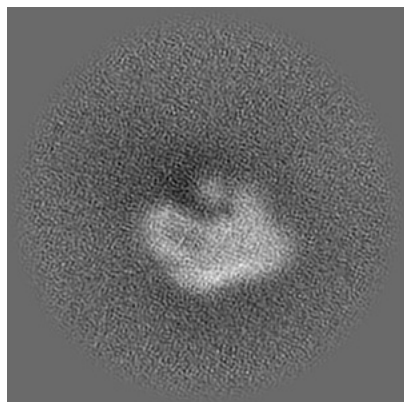


Z

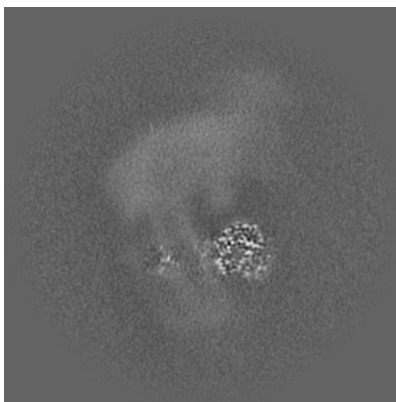
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

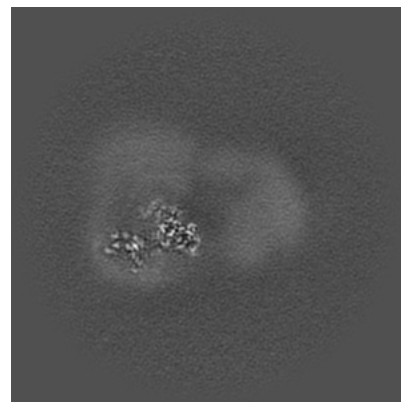
6.2.1 Primary map



X Index: 192

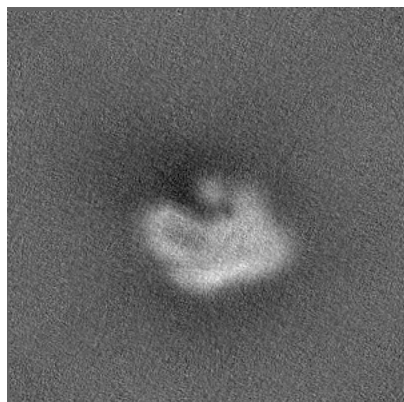


Y Index: 192

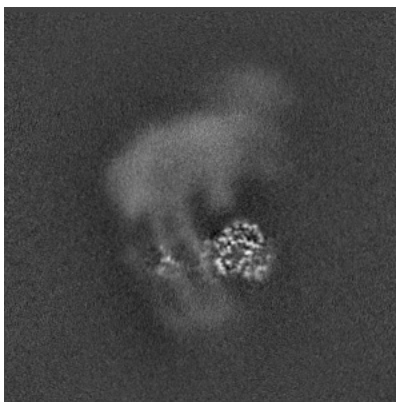


Z Index: 192

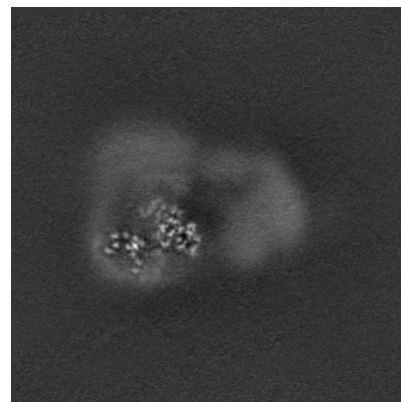
6.2.2 Raw map



X Index: 192



Y Index: 192

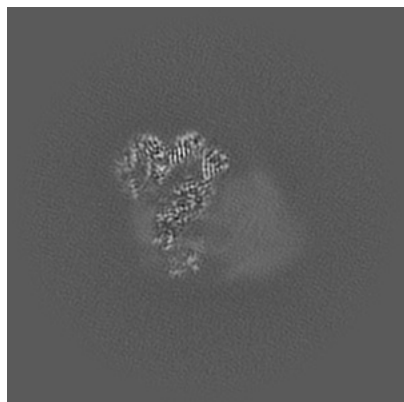


Z Index: 192

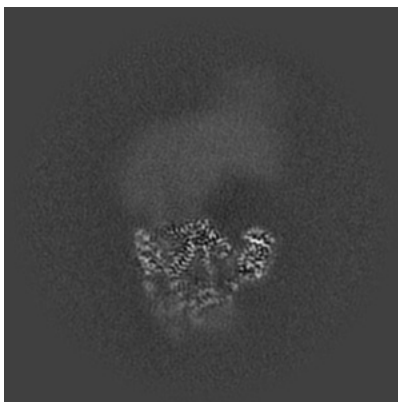
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

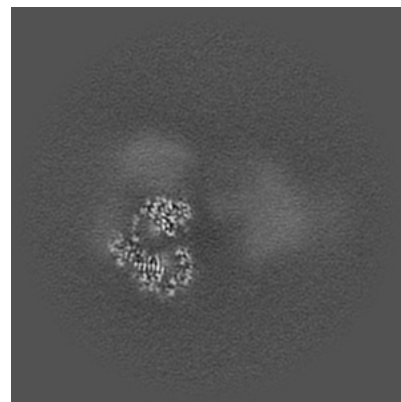
6.3.1 Primary map



X Index: 158

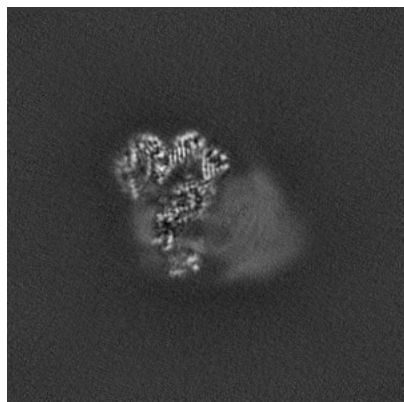


Y Index: 165

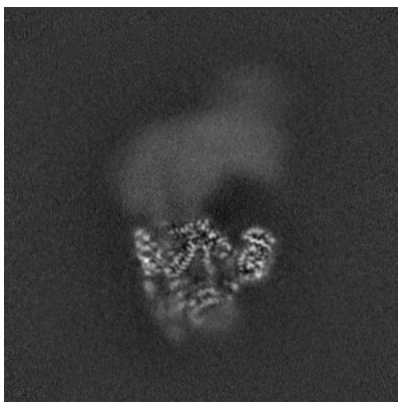


Z Index: 215

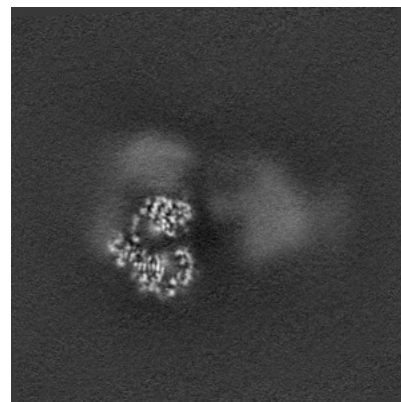
6.3.2 Raw map



X Index: 158



Y Index: 165

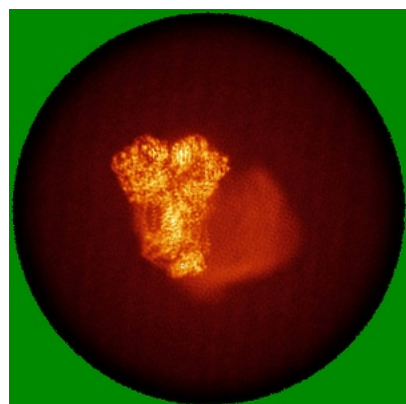


Z Index: 215

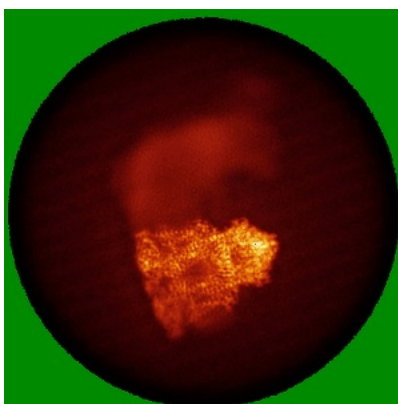
The images above show the largest variance slices of the map in three orthogonal directions.

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

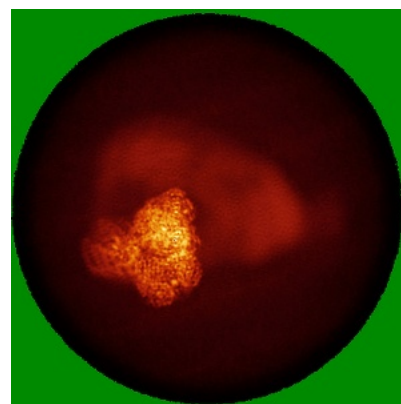
6.4.1 Primary map



X

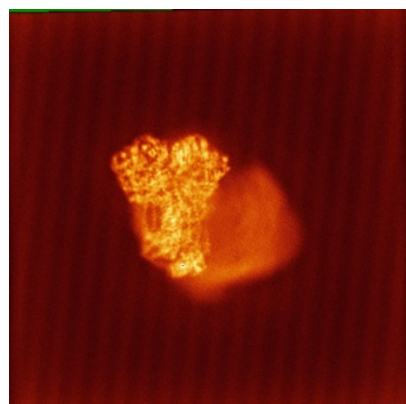


Y

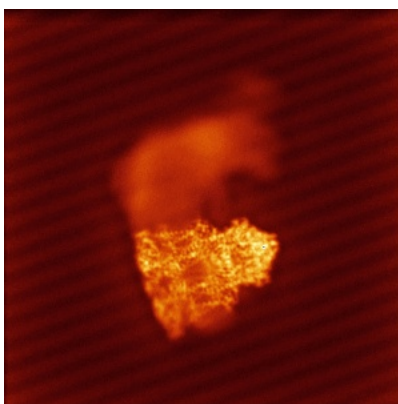


Z

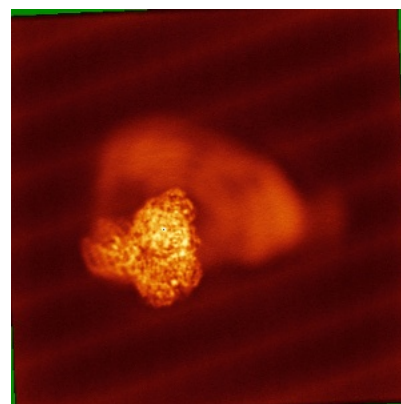
6.4.2 Raw map



X



Y

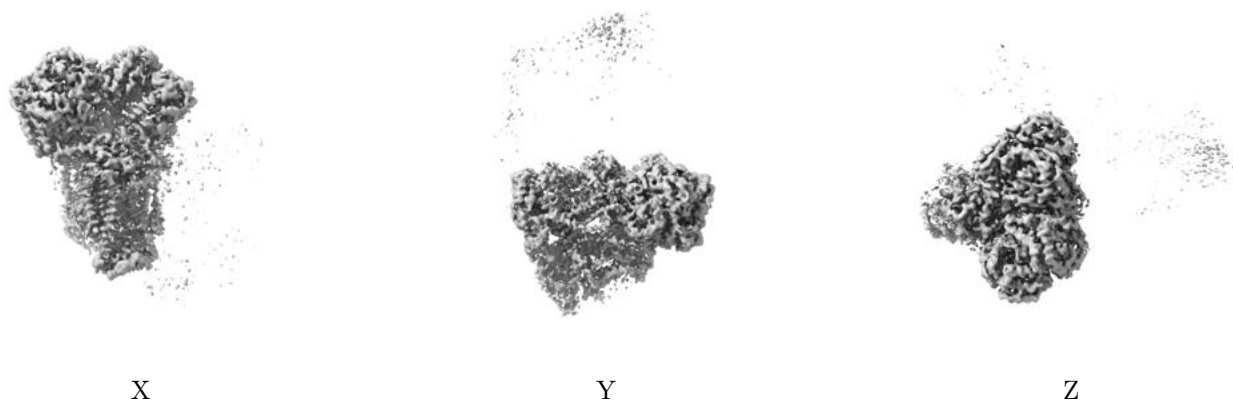


Z

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.

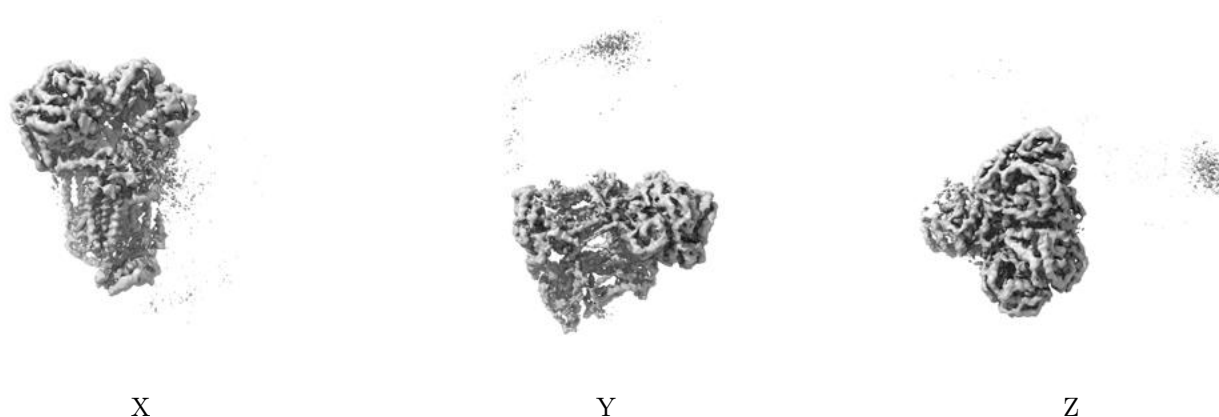
6.5 Orthogonal surface views [i](#)

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.

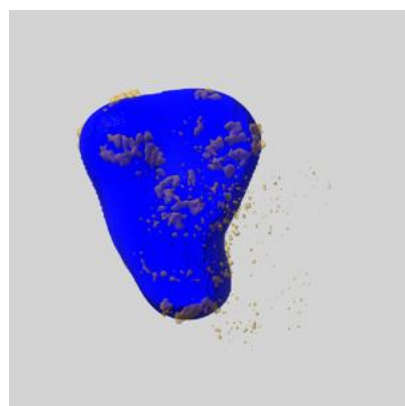
6.6 Mask visualisation [i](#)

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

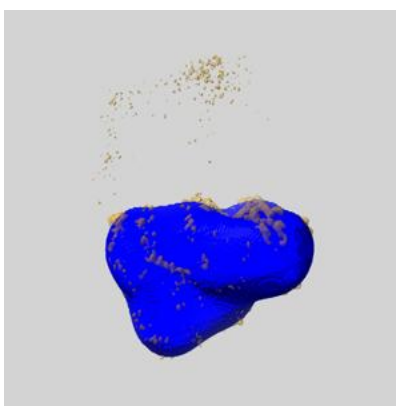
A mask typically either:

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

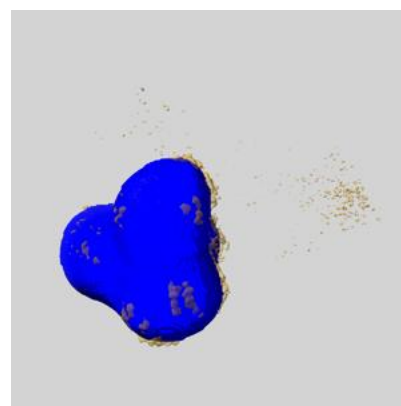
6.6.1 emd_35343_msk_1.map [i](#)



X



Y

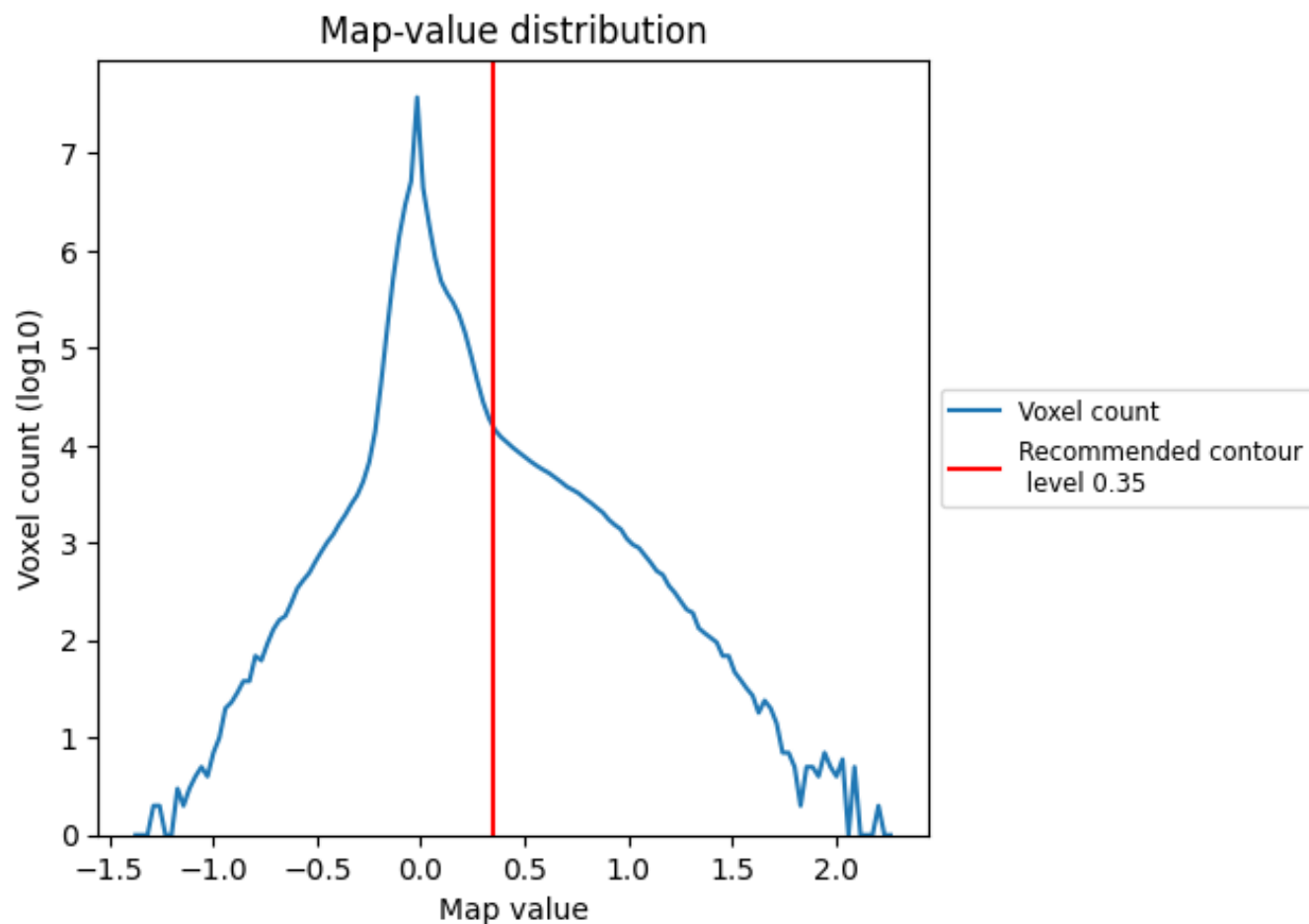


Z

7 Map analysis [i](#)

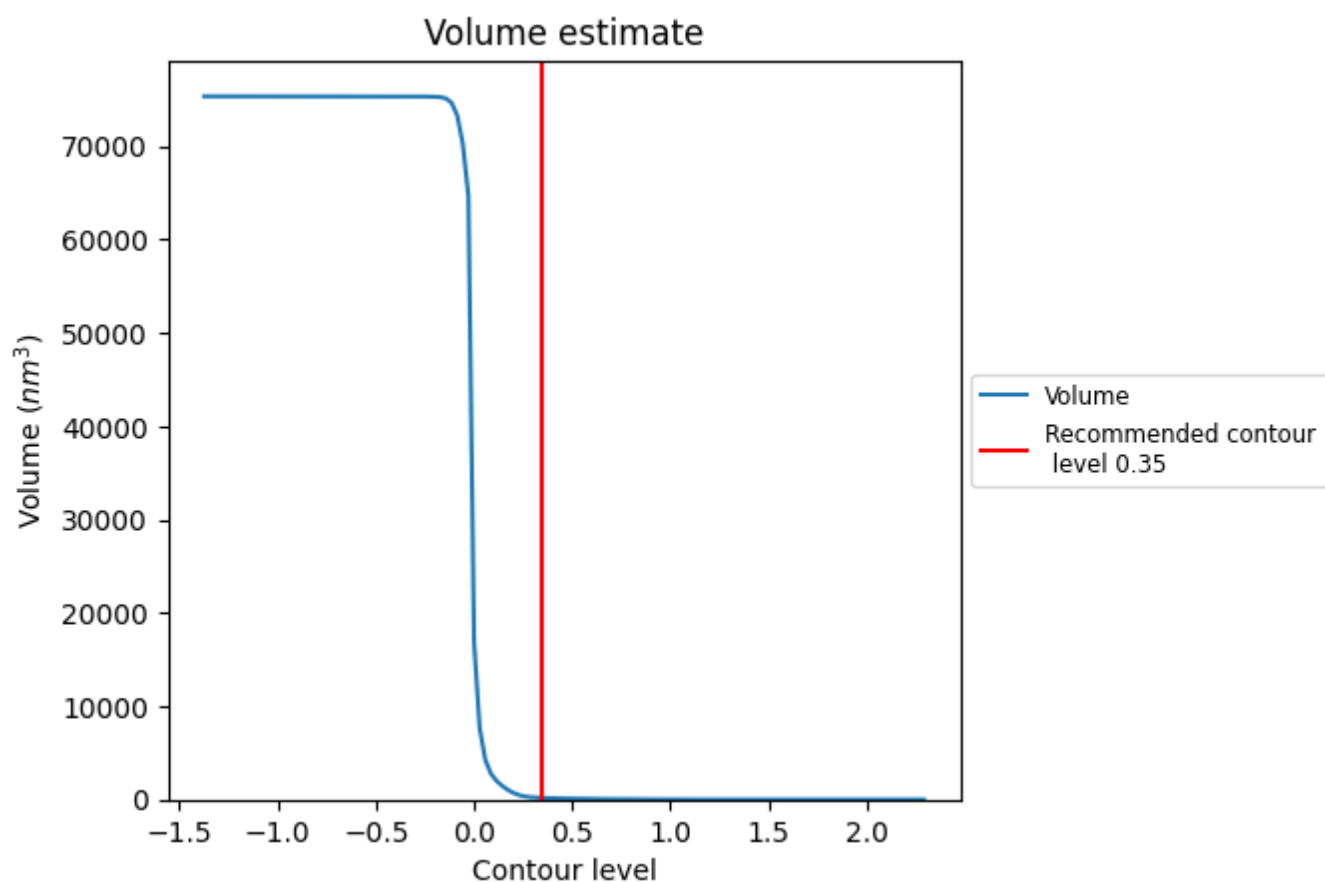
This section contains the results of statistical analysis of the map.

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.

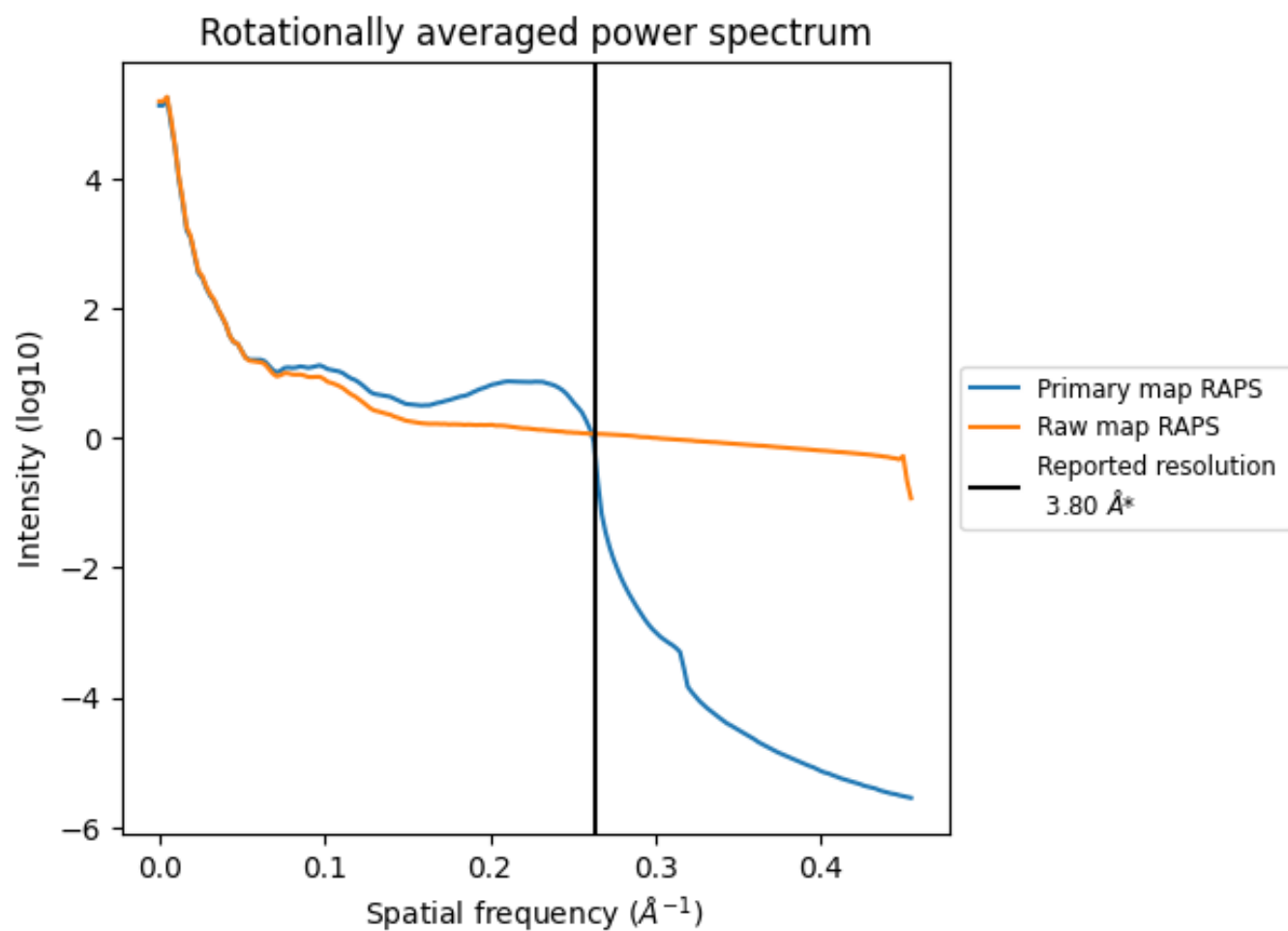
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

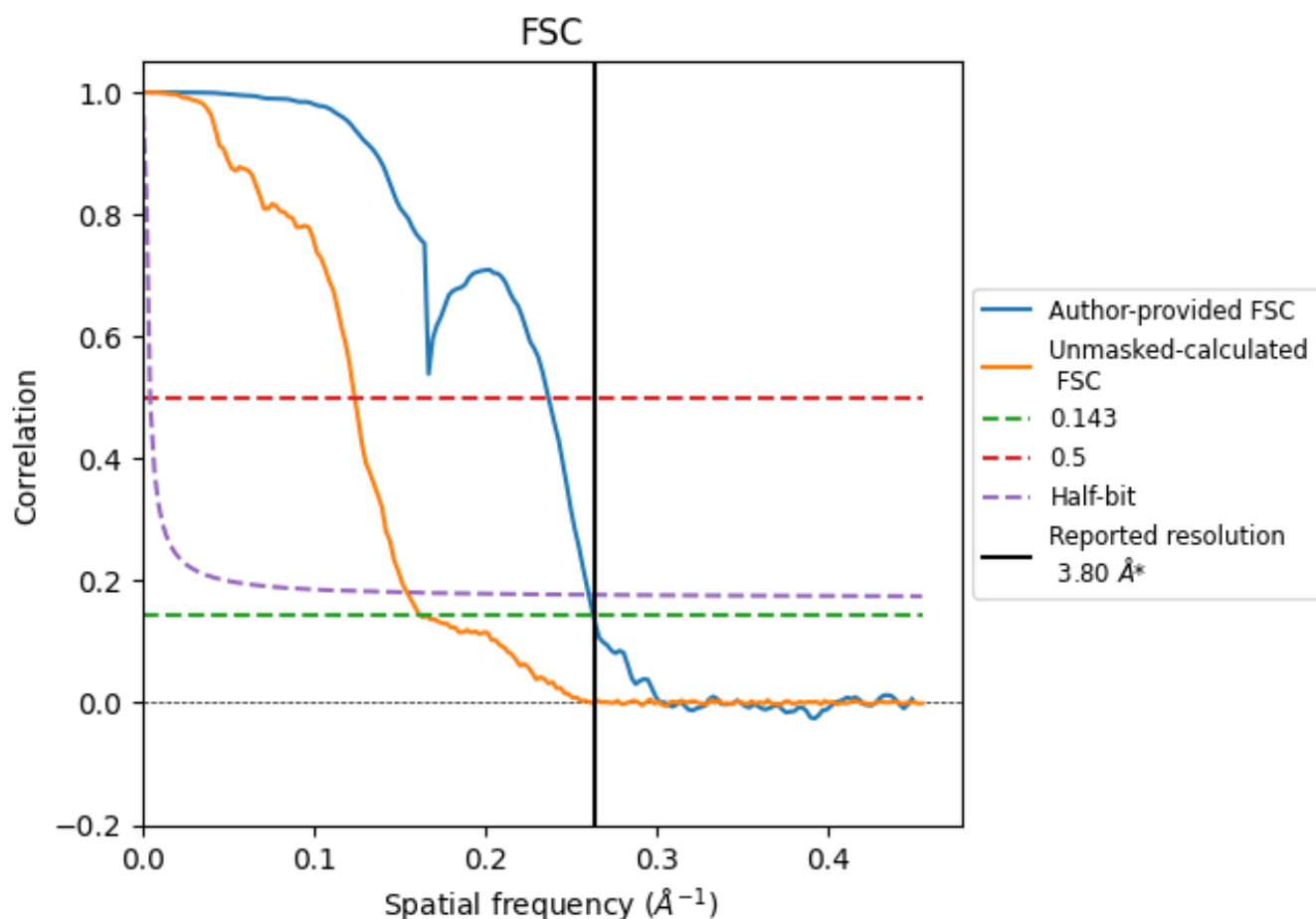


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

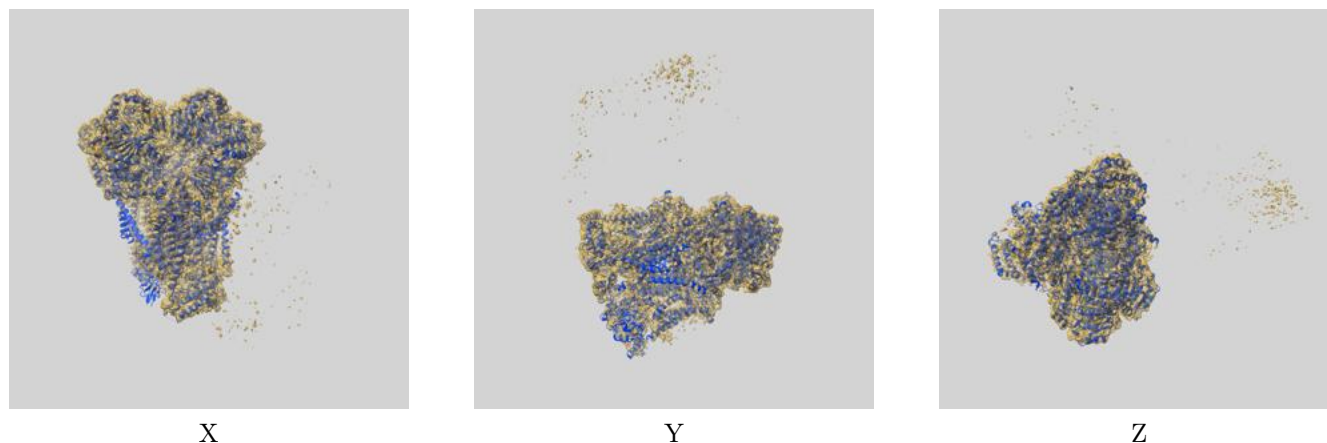
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.22	3.84
Unmasked-calculated*	6.17	8.08	6.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.17 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

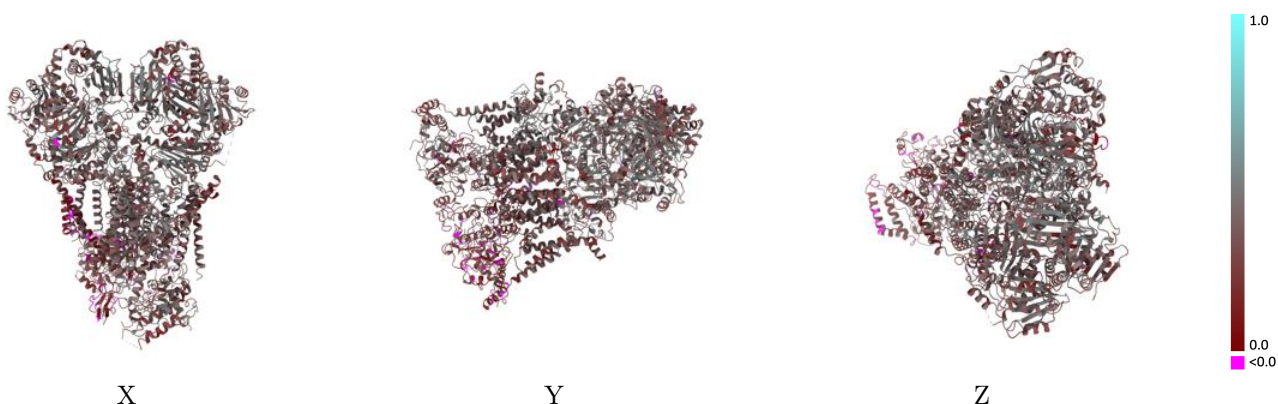
This section contains information regarding the fit between EMDB map EMD-35343 and PDB model 8IBG. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



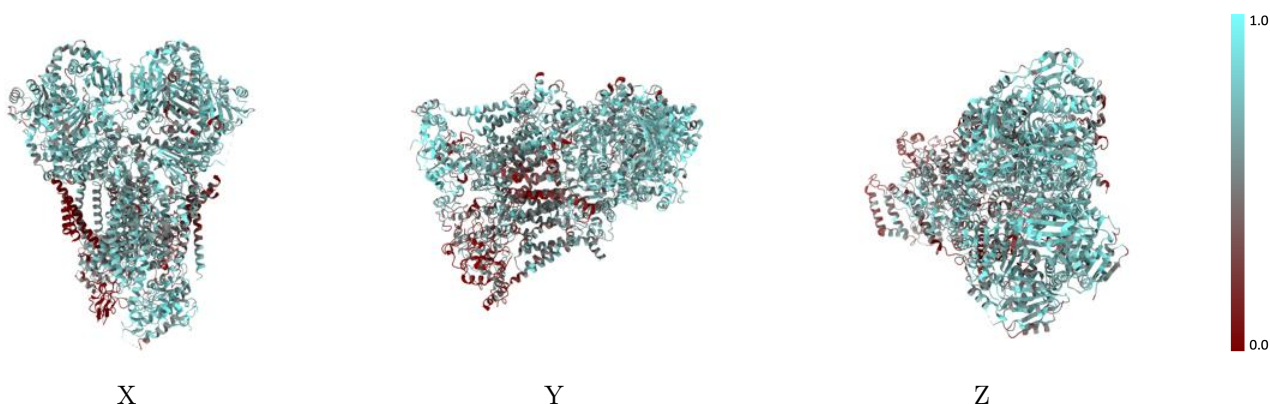
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



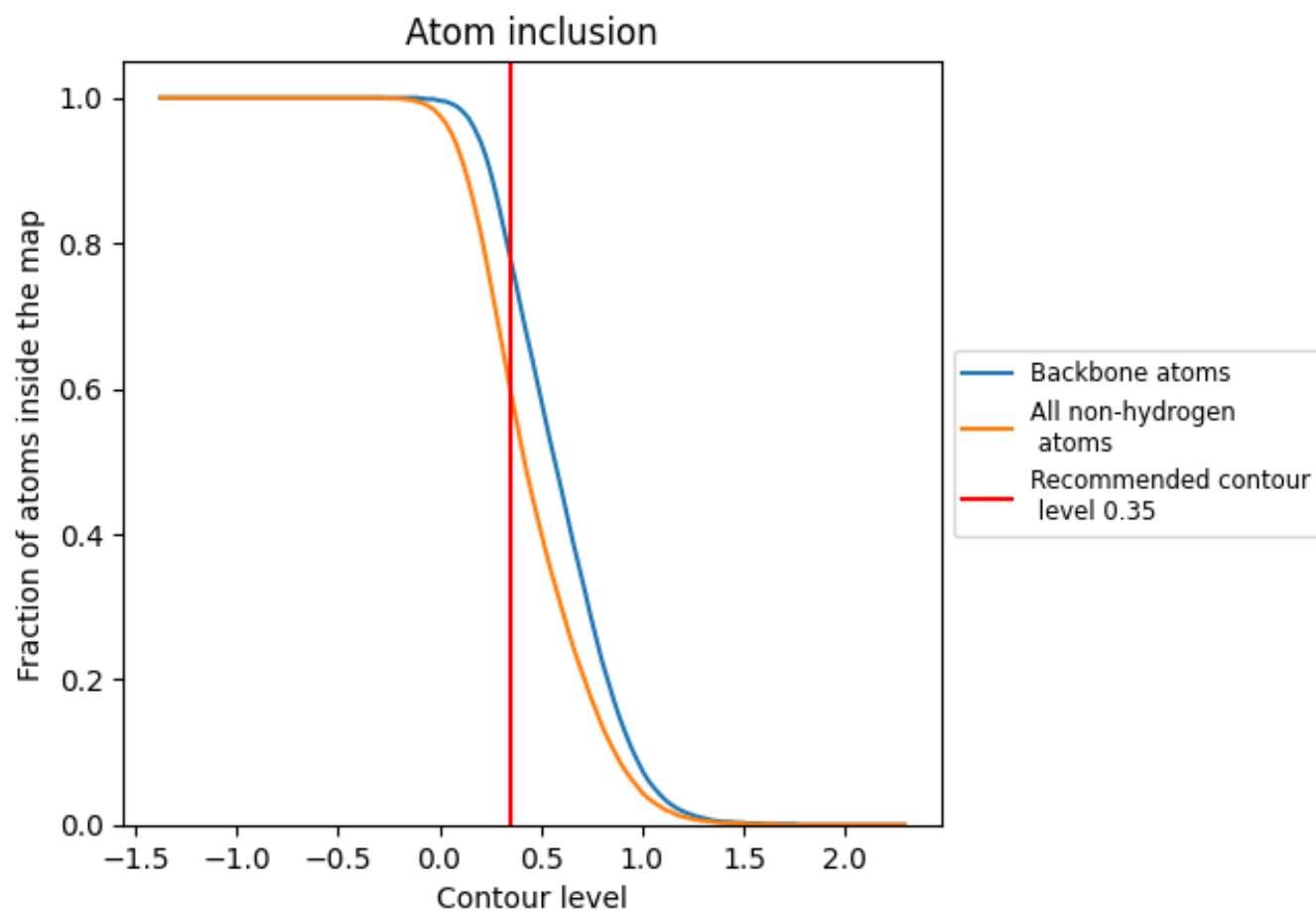
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 60% 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	 0.5980	 0.3400
AA	 0.6840	 0.3720
AB	 0.7140	 0.3880
AC	 0.5610	 0.3140
AD	 0.5090	 0.2460
AE	 0.0830	 0.1740
AF	 0.6650	 0.3680
AG	 0.4360	 0.3030
AH	 0.3090	 0.1520
AI	 0.3780	 0.2840
AJ	 0.0190	 0.1070
AK	 0.0090	 0.1800
Aa	 0.6980	 0.3920
Ab	 0.7300	 0.3910
Ac	 0.6500	 0.3660
Ad	 0.7240	 0.3610
Ae	 0.2010	 0.2350
Af	 0.6820	 0.3860
Ag	 0.6460	 0.4020
Ah	 0.6730	 0.3020
Ai	 0.3890	 0.2640
Aj	 0.4180	 0.2910
Ak	 0.1460	 0.2830

