



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:25 AM UTC

PDB ID : 8XNL / pdb_00008xnl
EMDB ID : EMD-38506
Title : Respiratory complex Peripheral Arm of CI, close form A, focus-refined map of type I, Wild type mouse under thermoneutral temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.10 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:

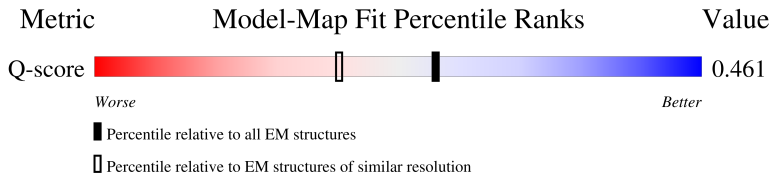
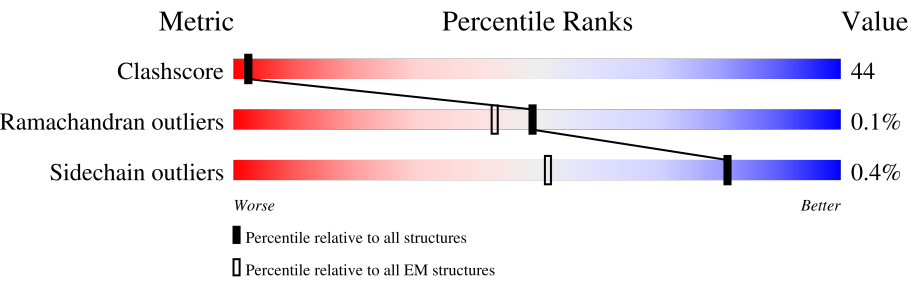
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.10 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	14724 (2.60 - 3.60)

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	A	115	12% 36% 43% 20%
2	B	224	30% 33% 6% 30%
3	C	263	35% 37% 25%
4	D	463	32% 47% 17%

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	P	377	
11	Q	175	
12	R	116	
13	S	99	
14	T	156	
15	V	116	
16	W	131	
17	X	172	
18	Z	144	
19	a	70	
20	b	84	
21	q	145	
22	r	113	
23	s	104	

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
25	SF4	B	301	-	-	X	-
25	SF4	F	502	-	-	X	-
25	SF4	G	802	-	-	X	-
25	SF4	I	302	-	-	X	-
25	SF4	I	303	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	FES	E	301	-	-	X	-
26	FES	G	803	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 34543 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	92	Total	C	N	O	S	0	0
			754	523	107	119	5		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1641	1060	279	299	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3088	1970	533	562	23		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1635	1039	275	310	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total	C	N	O	S	0	0
			3288	2073	588	605	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	315	Total	C	N	O	S	0	0
			2517	1691	381	423	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 14 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total	C	N	O	S	0	0
			1164	736	209	209	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

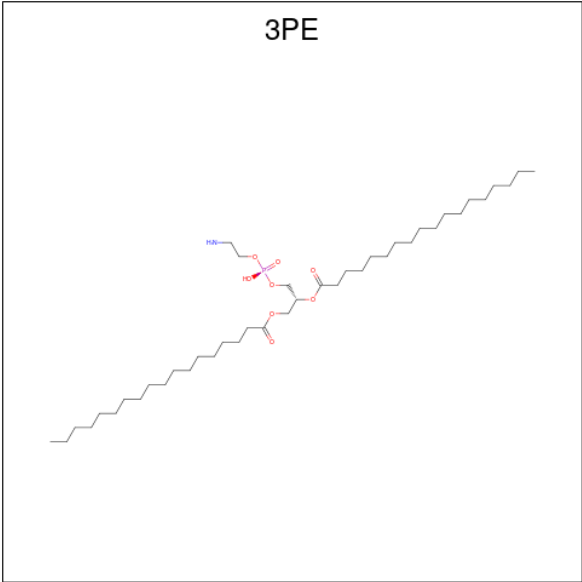
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	95	Total	C	N	O	S	0	0
			764	482	143	136	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

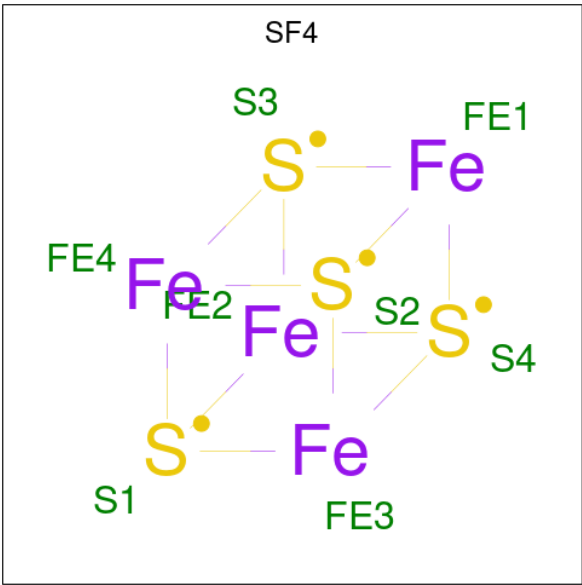
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	22	Total	C	N	O	0	0
			189	124	29	36		

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



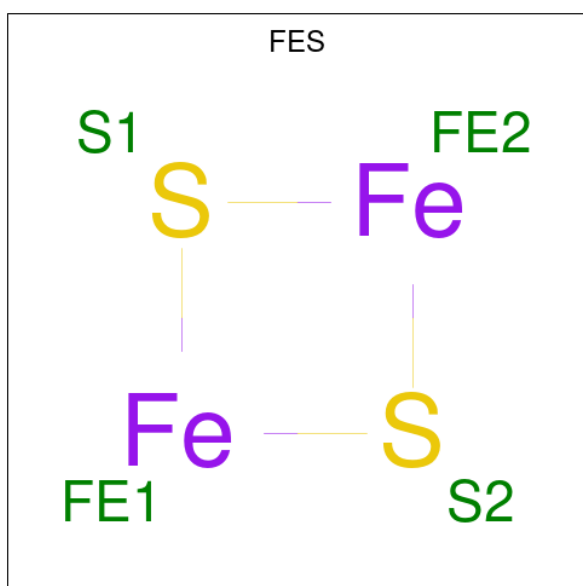
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	

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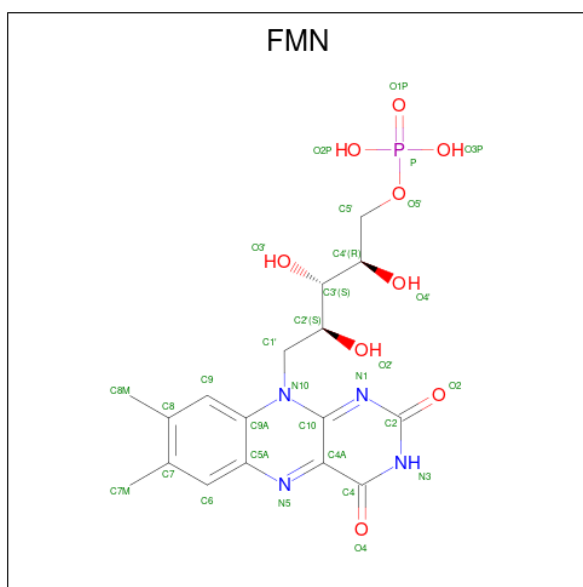
Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



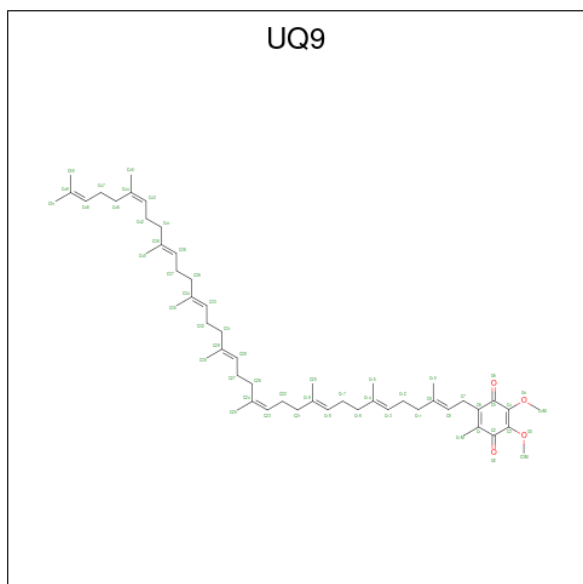
Mol	Chain	Residues	Atoms			AltConf
26	E	1	Total	Fe	S	0
			4	2	2	
26	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



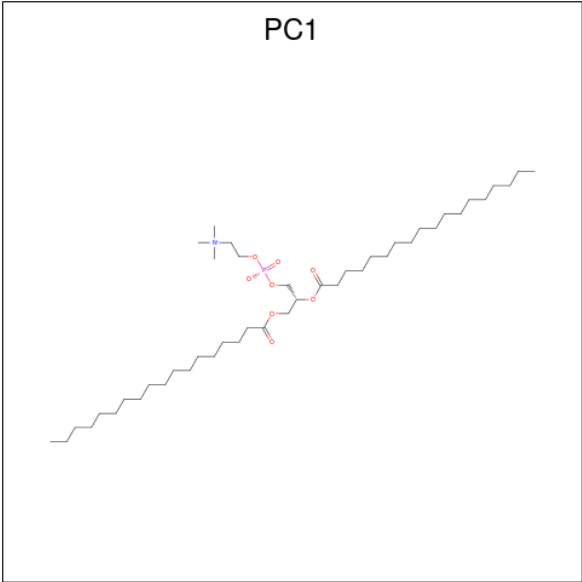
Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 28 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



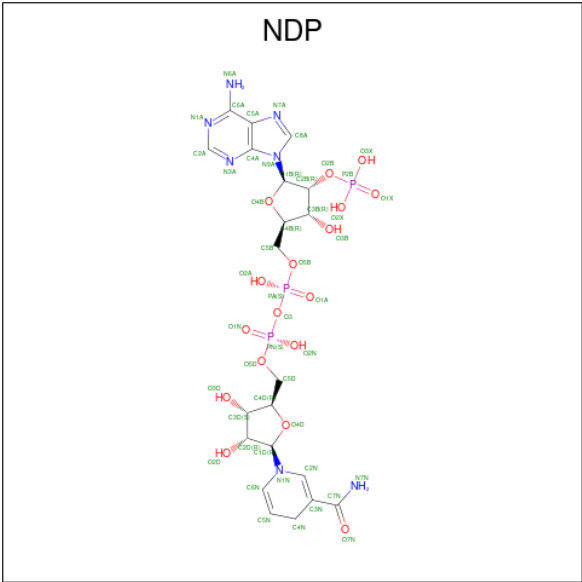
Mol	Chain	Residues	Atoms			AltConf
28	H	1	Total	C	O	0
			35	31	4	

- Molecule 29 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
29	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
29	q	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 30 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

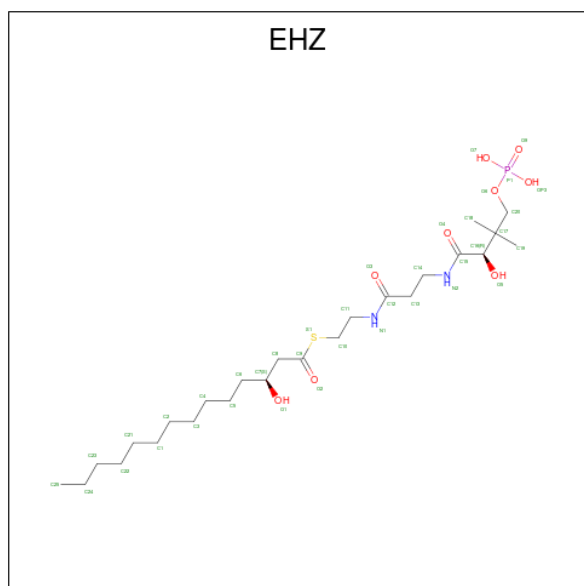


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

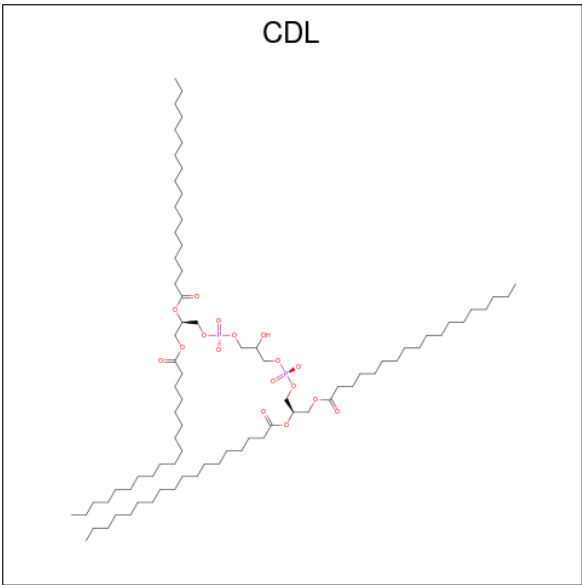
Mol	Chain	Residues	Atoms		AltConf
31	R	1	Total	Zn	0
			1	1	

- Molecule 32 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

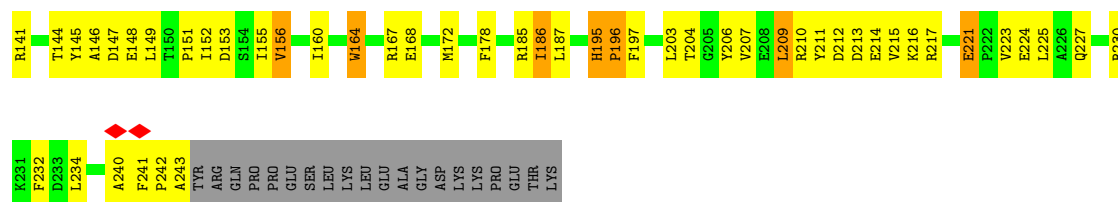


Mol	Chain	Residues	Atoms						AltConf
32	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

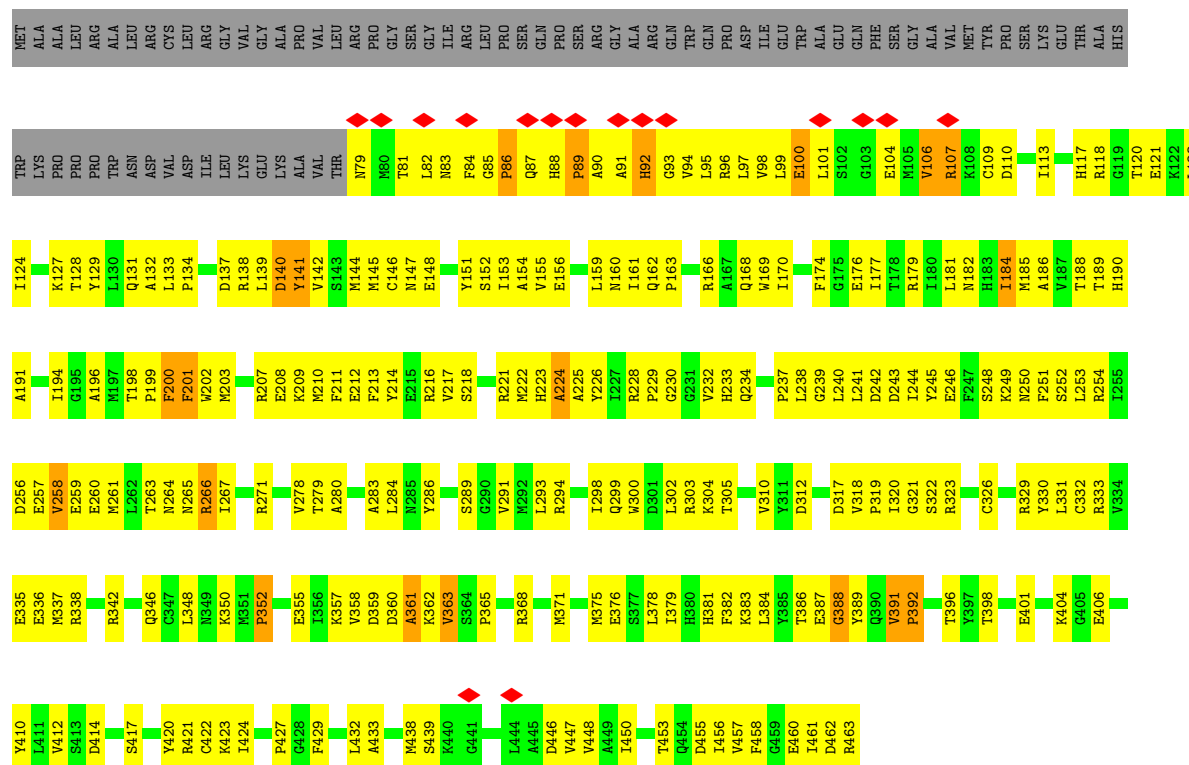
- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



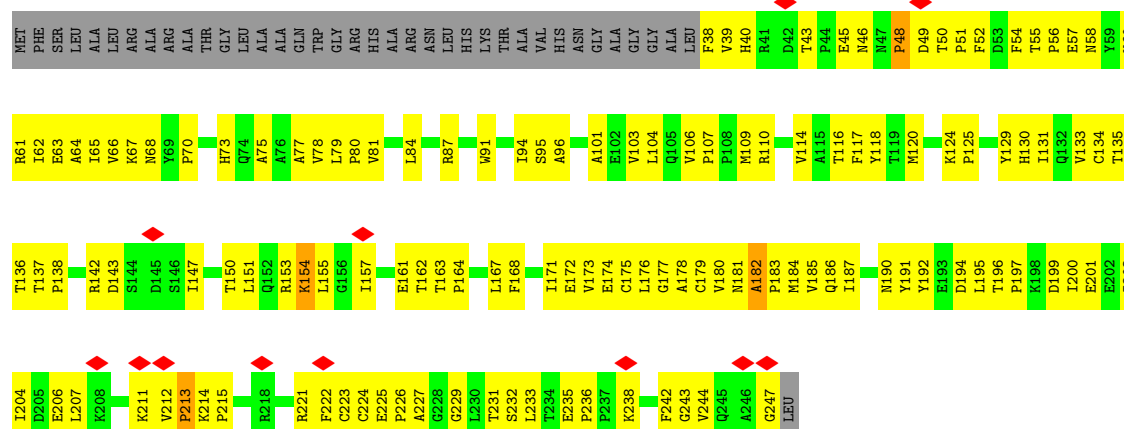
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	q	1	57	38	17	2	0



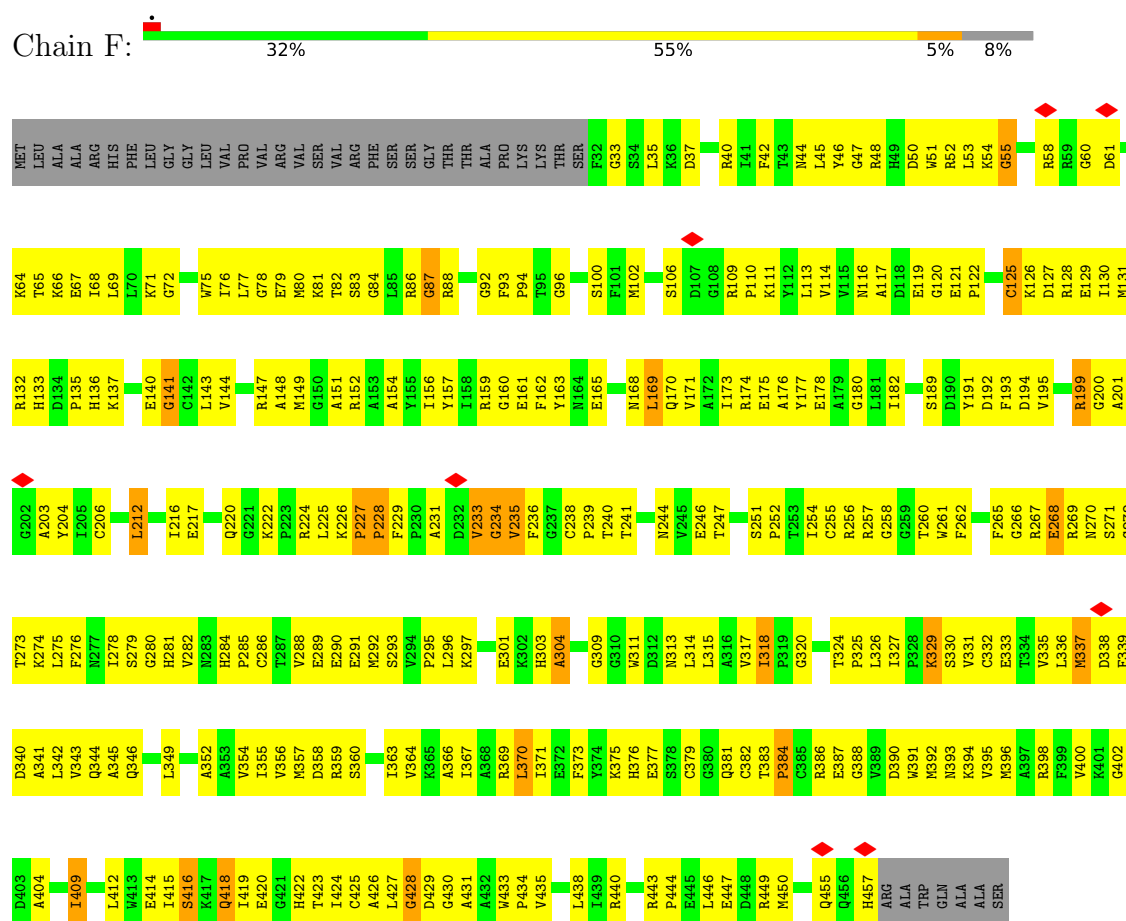
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



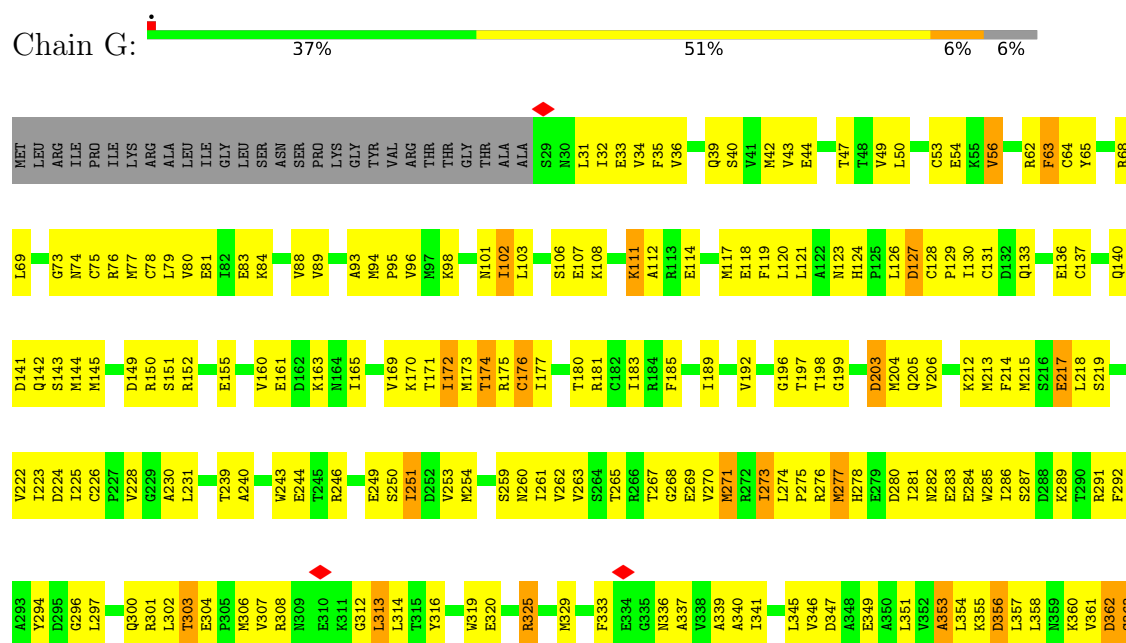
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

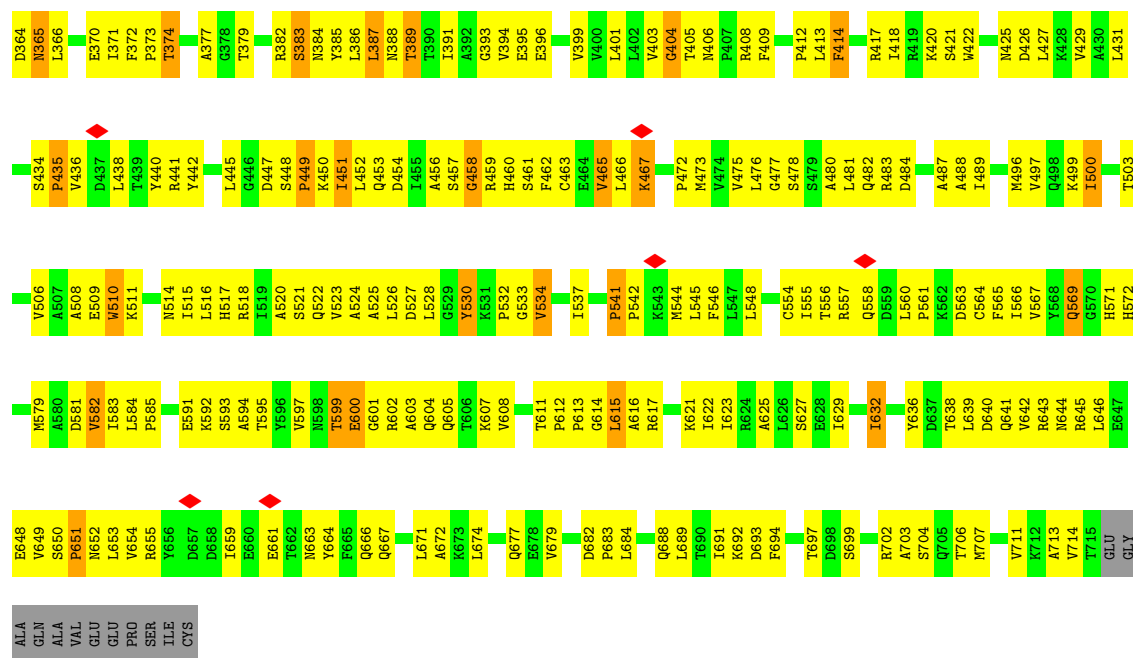


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

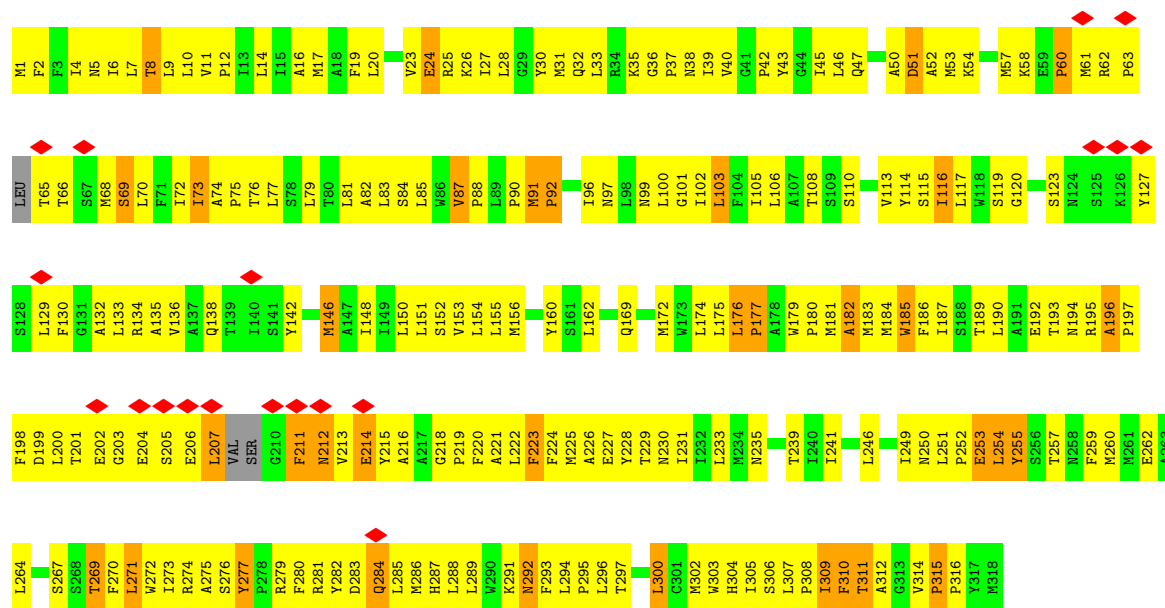


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

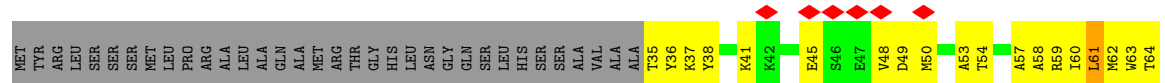


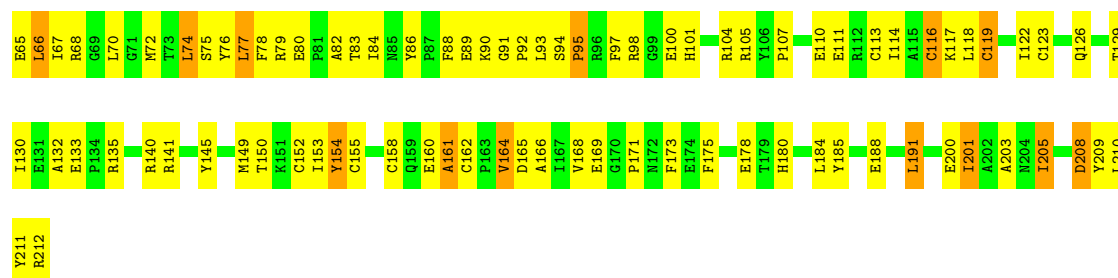


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

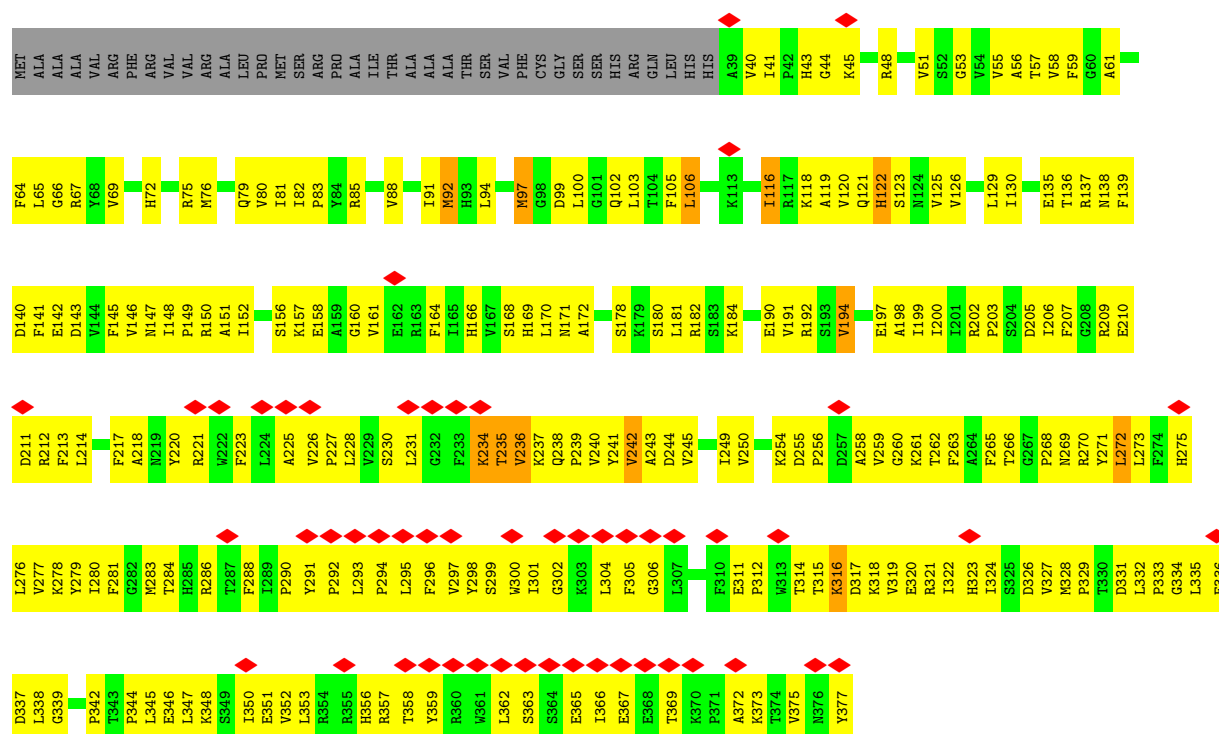


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

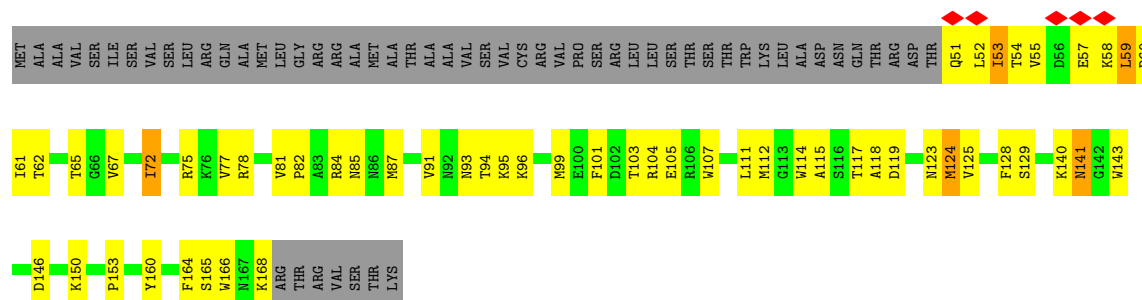




- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



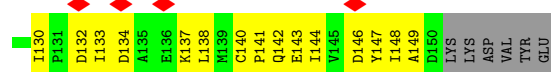
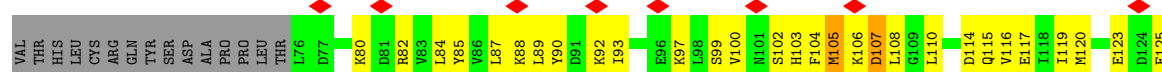
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



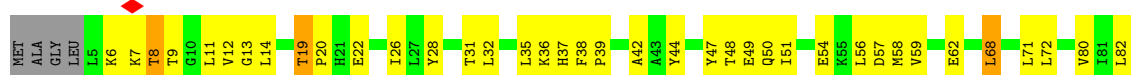
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 14: Acyl carrier protein, mitochondrial

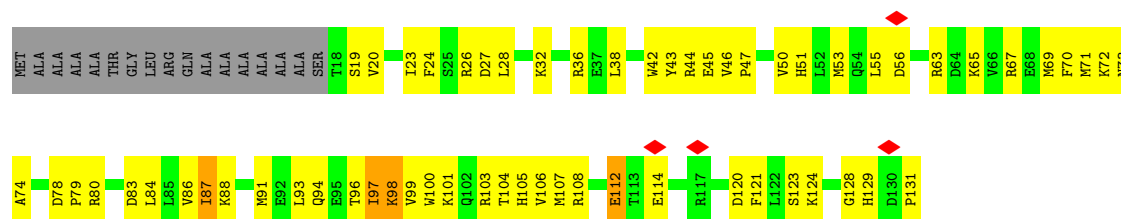


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

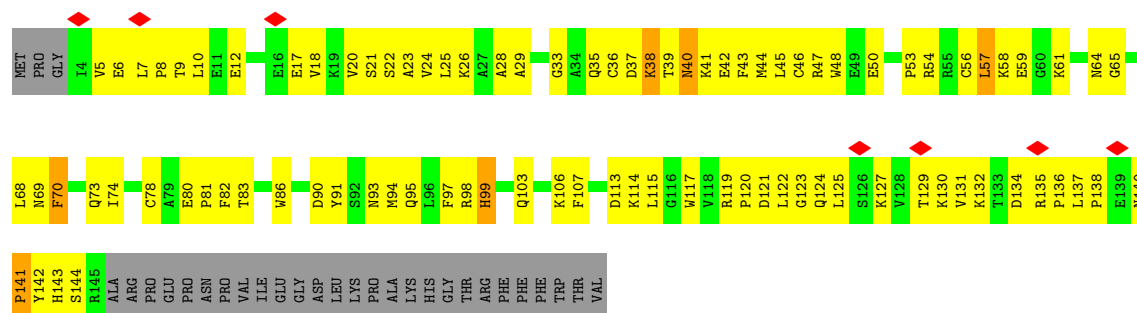


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

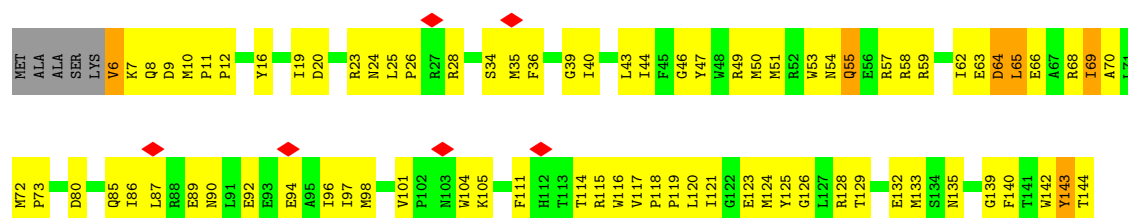




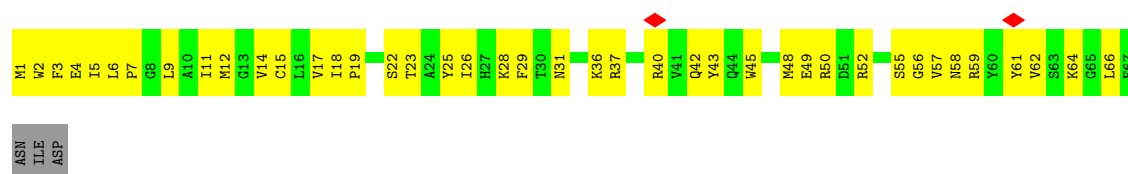
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

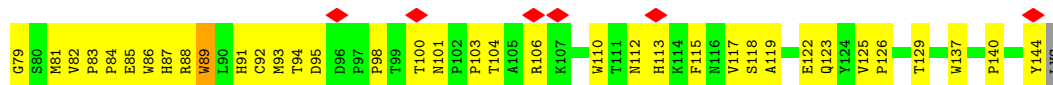
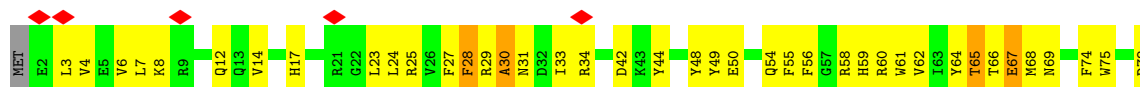


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

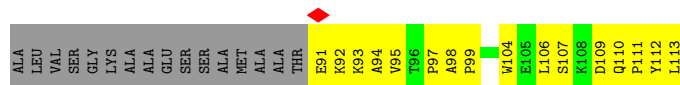
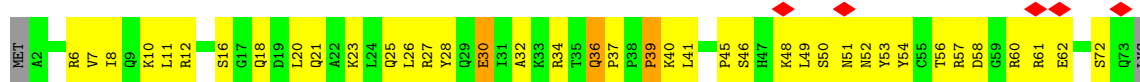




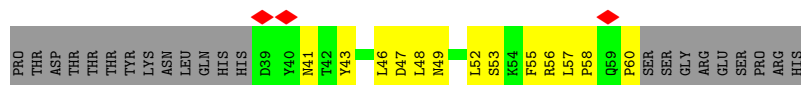
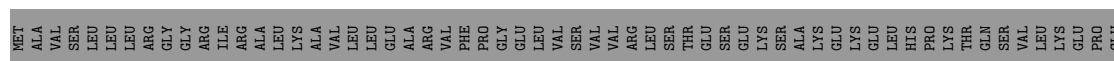
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 23: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42754	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 ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.389	Depositor
Minimum map value	-1.828	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.55	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: 3PE, UQ9, CDL, FMN, PC1, SF4, FES, ZN, NDP, EHZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	0/774	1.12	7/1056 (0.7%)
2	B	1.02	3/1289 (0.2%)	1.49	22/1744 (1.3%)
3	C	0.87	0/1687	1.26	12/2297 (0.5%)
4	D	0.95	5/3162 (0.2%)	1.35	29/4276 (0.7%)
5	E	0.71	0/1675	1.07	10/2282 (0.4%)
6	F	0.89	5/3363 (0.1%)	1.37	47/4543 (1.0%)
7	G	0.90	8/5374 (0.1%)	1.55	96/7281 (1.3%)
8	H	0.96	4/2592 (0.2%)	1.51	57/3539 (1.6%)
9	I	0.89	0/1461	1.51	20/1974 (1.0%)
10	P	0.74	1/2793 (0.0%)	1.13	18/3787 (0.5%)
11	Q	0.89	1/980 (0.1%)	1.24	8/1324 (0.6%)
12	R	0.66	0/671	0.92	2/903 (0.2%)
13	S	0.87	1/678 (0.1%)	1.37	9/915 (1.0%)
14	T	0.61	0/613	0.91	2/826 (0.2%)
15	V	0.82	0/937	1.38	12/1270 (0.9%)
16	W	0.80	1/993 (0.1%)	1.06	7/1335 (0.5%)
17	X	0.71	0/1191	1.21	13/1605 (0.8%)
18	Z	0.67	1/1183 (0.1%)	1.09	13/1597 (0.8%)
19	a	0.84	0/561	1.11	3/755 (0.4%)
20	b	0.70	0/643	1.01	3/884 (0.3%)
21	q	0.68	0/1234	1.13	10/1681 (0.6%)
22	r	0.60	0/782	1.04	6/1058 (0.6%)
23	s	0.43	0/194	0.69	0/264
All	All	0.84	30/34830 (0.1%)	1.31	406/47196 (0.9%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	234	GLY	CA-C	-10.40	1.40	1.52
6	F	227	PRO	N-CD	10.12	1.61	1.47
6	F	235	VAL	N-CA	-9.71	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	53	ILE	C-O	7.80	1.33	1.24
6	F	233	VAL	CA-C	-6.73	1.44	1.52
7	G	203	ASP	CA-C	6.72	1.62	1.52
7	G	541	PRO	N-CD	-6.72	1.38	1.47
7	G	449	PRO	N-CD	6.71	1.57	1.47
4	D	106	VAL	C-N	-6.61	1.24	1.33
7	G	600	GLU	CA-C	6.45	1.61	1.52
7	G	632	ILE	CA-C	-6.43	1.44	1.52
18	Z	63	GLU	C-N	-6.30	1.24	1.33
4	D	266	ARG	C-O	-6.25	1.16	1.24
2	B	110	PRO	C-O	-6.24	1.16	1.24
8	H	206	GLU	C-O	-6.20	1.16	1.23
7	G	127	ASP	CA-C	6.20	1.62	1.52
6	F	384	PRO	N-CD	-6.15	1.39	1.47
2	B	128	ALA	CA-C	-6.02	1.44	1.52
7	G	361	VAL	CA-C	5.87	1.60	1.52
8	H	69	SER	C-O	5.83	1.32	1.24
2	B	95	PHE	C-O	5.64	1.30	1.24
4	D	392	PRO	C-O	-5.57	1.20	1.24
4	D	107	ARG	C-N	5.51	1.40	1.33
7	G	683	PRO	N-CD	-5.51	1.40	1.47
13	S	95	LEU	CA-C	5.49	1.59	1.52
16	W	98	LYS	CA-C	-5.45	1.46	1.52
10	P	235	THR	CA-C	5.34	1.59	1.53
8	H	211	PHE	CA-C	5.31	1.59	1.52
4	D	266	ARG	CA-C	-5.28	1.45	1.52
8	H	310	PHE	CA-C	5.11	1.59	1.52

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-17.51	89.00	114.39
7	G	632	ILE	N-CA-C	-13.65	88.00	107.80
7	G	251	ILE	N-CA-C	13.30	126.79	108.17
6	F	125	CYS	N-CA-C	-12.95	93.43	113.89
7	G	500	ILE	N-CA-C	-12.47	98.81	110.53
10	P	106	LEU	N-CA-C	12.17	128.67	109.07
2	B	199	GLU	N-CA-C	-12.17	98.10	111.36
16	W	98	LYS	N-CA-C	-12.05	89.01	108.41
6	F	171	VAL	N-CA-C	-11.90	99.34	110.53
2	B	80	ASP	N-CA-C	-11.80	98.44	111.07
7	G	204	MET	N-CA-C	-11.63	91.45	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	449	ARG	N-CA-C	-11.61	98.71	111.36
7	G	599	THR	N-CA-C	11.36	126.23	112.38
11	Q	60	ASP	N-CA-C	-11.30	90.37	109.24
8	H	259	PHE	N-CA-C	-10.93	99.45	111.36
7	G	77	MET	N-CA-C	-10.82	97.38	113.61
4	D	86	PRO	N-CA-C	-10.75	100.91	114.35
2	B	105	MET	N-CA-C	-10.74	99.36	111.71
9	I	164	VAL	N-CA-C	-10.63	100.14	113.22
9	I	77	LEU	N-CA-C	-10.52	99.61	111.71
8	H	284	GLN	N-CA-C	-10.32	100.03	111.07
7	G	280	ASP	N-CA-C	10.31	122.52	111.28
4	D	337	MET	N-CA-C	-10.27	100.09	111.07
4	D	140	ASP	CB-CA-C	-10.24	98.01	111.42
7	G	414	PHE	N-CA-C	-10.11	101.45	113.88
9	I	161	ALA	N-CA-C	10.04	122.23	111.28
2	B	195	PRO	N-CA-C	-9.94	98.57	110.70
9	I	166	ALA	N-CA-C	-9.91	100.73	113.12
7	G	325	ARG	N-CA-C	-9.84	100.24	110.97
6	F	141	GLY	N-CA-C	-9.84	101.09	112.50
7	G	654	VAL	N-CA-C	9.80	123.35	111.09
6	F	178	GLU	N-CA-C	-9.79	99.36	111.11
6	F	144	VAL	N-CA-C	-9.72	101.39	110.53
6	F	418	GLN	N-CA-C	-9.63	100.74	111.14
16	W	87	ILE	N-CA-C	-9.55	101.25	110.42
7	G	337	ALA	N-CA-C	-9.55	100.85	114.12
8	H	52	ALA	N-CA-C	-9.53	100.85	111.14
17	X	70	PHE	N-CA-C	-9.49	99.72	111.11
4	D	427	PRO	N-CA-C	-9.48	95.61	110.50
21	q	123	GLN	N-CA-C	9.39	123.85	110.23
7	G	692	LYS	N-CA-C	-9.29	100.52	112.23
7	G	694	PHE	N-CA-C	9.28	121.39	111.28
18	Z	69	ILE	N-CA-C	-9.26	100.64	110.36
7	G	389	THR	N-CA-C	-9.17	96.20	109.96
8	H	91	MET	N-CA-C	-9.00	98.50	109.57
19	a	57	VAL	N-CA-C	-8.99	105.16	113.71
18	Z	143	TYR	N-CA-C	8.98	121.96	108.31
7	G	133	GLN	N-CA-CB	8.86	121.62	110.45
2	B	170	TYR	N-CA-C	-8.82	97.80	110.24
7	G	365	ASN	N-CA-C	-8.79	102.10	112.92
7	G	212	LYS	N-CA-C	-8.78	94.59	108.90
8	H	212	ASN	N-CA-C	-8.67	101.81	114.39
9	I	154	TYR	N-CA-CB	-8.67	99.22	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	62	GLU	N-CA-C	-8.59	102.78	113.18
13	S	86	GLU	N-CA-C	-8.55	102.04	111.36
17	X	99	HIS	N-CA-C	-8.41	102.19	111.36
3	C	108	LYS	N-CA-C	8.39	120.05	111.07
5	E	154	LYS	N-CA-C	-8.37	101.85	110.97
7	G	452	LEU	N-CA-C	-8.35	102.18	111.28
11	Q	54	THR	N-CA-C	8.35	123.32	109.46
7	G	558	GLN	N-CA-C	-8.30	102.19	111.07
8	H	196	ALA	N-CA-C	8.24	128.03	109.81
8	H	311	THR	N-CA-C	-8.23	102.55	112.59
7	G	691	ILE	N-CA-C	8.22	123.72	111.89
1	A	64	LEU	N-CA-C	-8.19	102.30	111.07
3	C	196	PRO	N-CA-C	8.14	124.85	113.53
7	G	484	ASP	N-CA-C	8.13	121.07	111.71
7	G	500	ILE	N-CA-CB	8.13	120.98	110.57
21	q	118	SER	N-CA-C	8.10	120.83	111.11
9	I	201	ILE	N-CA-C	-8.09	102.55	110.72
15	V	86	LYS	N-CA-C	-8.08	102.41	111.14
7	G	534	VAL	N-CA-C	-8.08	104.72	111.91
13	S	76	THR	N-CA-C	8.05	122.02	108.90
17	X	43	PHE	N-CA-C	-7.99	102.52	111.07
1	A	9	ILE	N-CA-C	-7.97	102.49	110.62
10	P	206	ILE	N-CA-C	7.96	120.98	108.87
7	G	651	PRO	CB-CA-C	-7.96	98.43	111.56
8	H	271	LEU	N-CA-C	-7.94	102.57	111.14
15	V	6	LYS	N-CA-C	-7.89	100.12	110.53
8	H	206	GLU	CA-C-O	-7.88	109.35	120.15
8	H	311	THR	N-CA-CB	7.88	123.53	110.92
9	I	160	GLU	N-CA-C	7.84	124.23	111.37
21	q	28	PHE	N-CA-C	7.84	122.61	112.89
7	G	270	VAL	N-CA-CB	-7.81	100.71	110.31
10	P	235	THR	CB-CA-C	-7.81	100.05	112.07
2	B	95	PHE	N-CA-C	-7.79	98.14	109.59
18	Z	143	TYR	CB-CA-C	-7.77	107.60	116.54
7	G	389	THR	N-CA-CB	7.76	121.42	109.85
9	I	74	LEU	N-CA-C	-7.75	102.83	111.28
21	q	89	TRP	N-CA-C	-7.71	102.82	111.14
4	D	361	ALA	N-CA-C	-7.69	103.00	112.38
8	H	253	GLU	N-CA-C	7.69	121.92	112.54
6	F	58	ARG	N-CA-C	-7.66	103.01	111.36
7	G	56	VAL	N-CA-C	-7.64	103.00	110.72
9	I	119	CYS	N-CA-C	-7.60	103.08	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	569	GLN	N-CA-C	7.59	121.99	108.24
6	F	171	VAL	N-CA-CB	7.57	120.25	110.57
8	H	223	PHE	CB-CA-C	-7.56	99.01	110.88
9	I	158	CYS	N-CA-C	-7.52	103.09	111.28
22	r	30	GLU	N-CA-C	-7.52	105.01	114.56
7	G	277	MET	N-CA-C	7.50	120.61	109.59
6	F	430	GLY	N-CA-C	7.44	121.66	112.73
7	G	467	LYS	N-CA-C	-7.43	102.34	111.33
13	S	94	VAL	N-CA-C	7.43	117.55	110.42
16	W	100	TRP	N-CA-C	-7.41	103.82	114.12
7	G	510	TRP	N-CA-CB	7.39	120.86	109.85
2	B	80	ASP	N-CA-CB	7.38	120.71	110.01
8	H	309	ILE	N-CA-C	7.37	117.44	110.30
7	G	303	THR	N-CA-C	7.33	122.93	113.18
4	D	350	LYS	CB-CA-C	-7.31	101.10	111.85
7	G	661	GLU	N-CA-C	7.28	118.90	110.97
15	V	68	LEU	N-CA-C	-7.25	103.38	111.28
3	C	195	HIS	CB-CA-C	7.24	117.34	110.17
7	G	374	THR	CB-CA-C	-7.24	99.84	111.28
7	G	384	ASN	N-CA-C	-7.23	103.43	111.82
8	H	50	ALA	N-CA-C	7.20	118.77	111.07
8	H	212	ASN	N-CA-CB	7.19	120.47	110.98
13	S	20	ARG	N-CA-C	7.17	120.67	107.99
8	H	214	GLU	N-CA-CB	-7.15	98.83	110.42
8	H	254	LEU	N-CA-C	-7.15	103.53	111.82
7	G	465	VAL	N-CA-CB	7.14	118.43	110.51
6	F	455	GLN	N-CA-C	7.12	118.69	111.07
7	G	461	SER	N-CA-C	7.12	119.95	111.33
7	G	497	VAL	N-CA-C	-7.12	103.36	110.62
9	I	45	GLU	N-CA-C	7.08	120.88	108.56
15	V	95	LEU	N-CA-C	-7.06	103.58	111.28
7	G	217	GLU	N-CA-C	-7.03	101.76	110.41
10	P	235	THR	CA-C-O	7.01	128.19	121.67
7	G	294	TYR	N-CA-C	-7.00	104.55	113.23
6	F	169	LEU	N-CA-C	6.99	118.89	111.28
6	F	418	GLN	N-CA-CB	6.99	120.20	110.07
6	F	428	GLY	N-CA-C	-6.98	103.84	112.77
8	H	176	LEU	CA-C-N	-6.98	113.61	120.52
8	H	176	LEU	C-N-CA	-6.98	113.61	120.52
8	H	70	LEU	N-CA-C	-6.95	104.93	113.41
6	F	148	ALA	N-CA-C	-6.95	103.78	111.36
6	F	246	GLU	N-CA-C	-6.95	103.71	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	292	ASN	N-CA-C	6.94	118.93	111.36
2	B	78	LEU	N-CA-C	6.94	119.87	111.82
7	G	300	GLN	N-CA-CB	6.93	122.55	112.08
16	W	99	VAL	N-CA-C	6.92	117.20	107.37
18	Z	34	SER	N-CA-C	-6.92	103.73	111.28
7	G	582	VAL	N-CA-C	6.90	118.41	108.48
12	R	108	GLY	N-CA-C	-6.89	105.97	114.92
8	H	300	LEU	N-CA-C	-6.88	104.14	112.54
7	G	362	ASP	N-CA-C	6.88	125.44	110.80
7	G	102	ILE	N-CA-C	6.87	119.68	111.09
6	F	329	LYS	N-CA-C	6.86	119.64	111.33
6	F	233	VAL	O-C-N	6.86	131.12	123.10
7	G	133	GLN	N-CA-C	-6.83	101.18	110.68
8	H	87	VAL	CA-C-N	-6.82	113.18	120.47
8	H	87	VAL	C-N-CA	-6.82	113.18	120.47
6	F	244	ASN	N-CA-C	-6.81	100.90	110.50
6	F	233	VAL	CA-C-O	-6.80	113.25	120.53
7	G	268	GLY	N-CA-C	6.79	124.73	115.30
10	P	91	ILE	CB-CA-C	-6.78	102.59	111.88
2	B	110	PRO	N-CA-C	6.77	122.78	113.65
2	B	196	PRO	N-CA-C	-6.75	100.63	111.03
8	H	305	ILE	N-CA-C	-6.74	103.48	113.39
18	Z	63	GLU	O-C-N	-6.74	114.98	122.12
4	D	141	TYR	N-CA-C	6.74	121.10	113.02
7	G	434	SER	N-CA-C	-6.74	101.00	110.29
8	H	8	THR	N-CA-C	-6.74	101.19	110.35
5	E	154	LYS	N-CA-CB	6.73	119.73	109.91
8	H	60	PRO	N-CA-C	-6.70	98.66	112.47
15	V	114	TRP	N-CA-CB	6.70	120.28	110.30
9	I	208	ASP	N-CA-C	6.69	121.60	113.17
15	V	8	THR	N-CA-C	6.67	119.00	108.79
10	P	116	ILE	N-CA-C	-6.65	104.00	110.72
15	V	86	LYS	N-CA-CB	6.63	119.68	110.07
17	X	129	THR	N-CA-C	6.63	120.84	110.17
6	F	344	GLN	N-CA-C	-6.62	103.99	111.07
3	C	125	PHE	N-CA-CB	-6.61	100.65	110.17
7	G	601	GLY	N-CA-C	6.61	124.82	115.30
6	F	228	PRO	N-CA-C	-6.60	98.87	112.47
11	Q	141	ASN	N-CA-CB	6.59	120.81	110.46
4	D	184	ILE	N-CA-C	-6.59	103.90	110.62
7	G	287	SER	N-CA-C	6.56	119.19	110.53
8	H	223	PHE	N-CA-C	-6.56	104.06	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	97	PHE	N-CA-C	6.55	118.50	111.36
2	B	79	ASP	N-CA-C	-6.55	103.63	111.69
2	B	154	GLU	CA-C-N	-6.55	112.38	119.98
2	B	154	GLU	C-N-CA	-6.55	112.38	119.98
6	F	234	GLY	CA-C-N	-6.55	111.72	120.50
6	F	234	GLY	C-N-CA	-6.55	111.72	120.50
8	H	182	ALA	N-CA-C	-6.55	104.06	111.07
18	Z	65	LEU	N-CA-C	-6.55	104.22	111.36
7	G	435	PRO	N-CA-C	-6.53	100.25	110.50
8	H	267	SER	N-CA-C	-6.52	104.25	111.36
10	P	92	MET	N-CA-C	-6.50	104.23	111.71
7	G	605	GLN	N-CA-C	6.49	119.09	108.52
9	I	66	LEU	N-CA-C	-6.49	104.29	111.36
7	G	250	SER	N-CA-C	6.48	116.83	108.34
4	D	388	GLY	N-CA-C	6.47	119.57	110.38
9	I	205	ILE	N-CA-C	-6.46	104.19	110.72
3	C	125	PHE	N-CA-C	6.44	119.58	110.50
6	F	370	LEU	N-CA-C	-6.42	104.36	111.36
6	F	178	GLU	N-CA-CB	6.42	119.50	109.94
8	H	177	PRO	N-CA-C	-6.41	101.58	111.13
8	H	255	TYR	N-CA-CB	6.40	119.28	110.01
15	V	49	GLU	N-CA-C	-6.39	104.31	111.28
17	X	98	ARG	N-CA-C	6.39	120.34	112.54
7	G	273	ILE	N-CA-C	-6.38	98.32	107.77
4	D	140	ASP	N-CA-C	-6.38	96.57	107.23
4	D	142	VAL	N-CA-C	-6.38	103.66	113.16
8	H	271	LEU	N-CA-CB	6.36	119.29	110.07
15	V	91	ALA	N-CA-C	-6.35	104.36	111.28
14	T	107	ASP	N-CA-C	6.34	122.86	110.56
11	Q	59	LEU	N-CA-C	-6.34	100.79	110.30
2	B	135	GLY	CA-C-O	-6.32	117.90	122.45
15	V	71	LEU	N-CA-C	6.31	118.16	111.28
7	G	176	CYS	N-CA-C	6.30	119.61	110.42
17	X	99	HIS	N-CA-CB	6.30	119.48	110.16
6	F	144	VAL	N-CA-CB	6.29	118.63	110.57
11	Q	141	ASN	N-CA-C	-6.29	105.60	113.28
5	E	50	THR	N-CA-CB	6.28	121.54	110.37
19	a	26	ILE	N-CA-C	-6.27	104.54	113.07
6	F	415	ILE	N-CA-C	-6.26	104.40	110.72
21	q	65	THR	N-CA-C	6.25	118.09	110.41
6	F	255	CYS	N-CA-C	-6.24	104.56	111.36
5	E	182	ALA	CA-C-N	-6.24	112.75	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	182	ALA	C-N-CA	-6.24	112.75	119.98
7	G	356	ASP	N-CA-CB	6.23	119.28	110.12
16	W	97	ILE	CB-CA-C	-6.23	104.38	111.55
10	P	118	LYS	N-CA-C	6.22	119.04	111.82
8	H	269	THR	N-CA-C	6.21	118.05	111.28
7	G	383	SER	N-CA-C	-6.21	106.93	114.75
7	G	451	ILE	N-CA-C	-6.21	104.93	113.00
8	H	52	ALA	N-CA-CB	6.20	119.06	110.07
2	B	98	ALA	N-CA-C	6.18	117.70	108.31
18	Z	69	ILE	N-CA-CB	6.18	117.37	110.51
4	D	291	VAL	N-CA-C	-6.17	103.38	111.09
7	G	420	LYS	N-CA-C	6.16	118.78	111.33
13	S	61	VAL	N-CA-C	-6.14	99.64	108.42
6	F	212	LEU	N-CA-C	-6.14	104.59	111.28
7	G	418	ILE	N-CA-C	-6.13	103.45	112.04
8	H	276	SER	N-CA-C	6.13	118.93	111.82
7	G	325	ARG	N-CA-CB	6.13	118.86	109.91
4	D	352	PRO	N-CA-C	6.12	118.17	110.70
8	H	185	TRP	N-CA-C	-6.10	103.97	112.45
4	D	92	HIS	N-CA-C	-6.09	105.10	113.56
6	F	268	GLU	CB-CA-C	-6.09	109.54	116.54
8	H	24	GLU	N-CA-C	-6.08	104.00	112.45
6	F	304	ALA	CB-CA-C	-6.08	109.55	116.54
7	G	353	ALA	N-CA-C	-6.07	104.59	112.23
1	A	101	GLY	N-CA-C	-6.06	105.47	112.50
13	S	87	VAL	N-CA-C	-6.06	104.44	110.62
21	q	104	THR	N-CA-C	6.05	118.49	109.59
8	H	7	LEU	N-CA-C	-6.05	104.32	111.03
18	Z	65	LEU	N-CA-CB	6.04	119.10	110.16
7	G	508	ALA	N-CA-C	6.01	117.83	111.28
8	H	103	LEU	N-CA-C	-5.98	104.84	111.36
4	D	90	ALA	N-CA-C	-5.97	106.60	114.31
20	b	60	ASP	N-CA-C	-5.97	105.26	112.54
7	G	387	LEU	CB-CA-C	-5.94	101.70	111.68
17	X	38	LYS	N-CA-C	-5.94	104.72	111.07
7	G	480	ALA	N-CA-C	-5.92	104.91	111.36
17	X	141	PRO	N-CA-C	-5.90	102.56	111.41
16	W	98	LYS	N-CA-CB	5.89	119.58	110.21
2	B	98	ALA	CB-CA-C	-5.87	109.79	116.54
6	F	127	ASP	N-CA-C	5.87	118.46	111.71
9	I	116	CYS	N-CA-C	-5.87	105.61	112.89
4	D	258	VAL	N-CA-C	-5.86	103.94	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	11	LEU	N-CA-C	-5.84	104.83	111.14
10	P	122	HIS	N-CA-C	5.83	120.10	112.92
13	S	86	GLU	N-CA-CB	5.81	118.76	110.16
3	C	209	LEU	N-CA-CB	-5.81	100.73	110.83
8	H	315	PRO	O-C-N	5.80	123.88	121.15
15	V	19	THR	N-CA-CB	5.79	120.69	110.37
7	G	672	ALA	N-CA-C	-5.79	104.97	111.28
10	P	97	MET	N-CA-C	-5.79	102.34	110.50
8	H	211	PHE	CA-C-O	5.78	126.95	119.95
8	H	116	ILE	N-CA-C	-5.78	104.87	110.42
7	G	289	LYS	N-CA-C	5.76	117.56	111.28
6	F	393	ASN	N-CA-C	-5.75	104.92	111.07
21	q	100	THR	N-CA-C	5.74	117.21	111.07
17	X	36	CYS	CB-CA-C	-5.74	102.62	111.74
10	P	234	LYS	CB-CA-C	-5.73	103.44	111.80
4	D	414	ASP	N-CA-C	-5.73	101.48	110.36
8	H	51	ASP	N-CA-CB	-5.72	101.41	110.28
22	r	72	SER	N-CA-C	-5.71	106.14	113.23
10	P	272	LEU	N-CA-C	-5.71	101.83	110.28
12	R	44	ARG	N-CA-C	-5.71	106.02	112.87
13	S	73	GLN	N-CA-C	-5.71	100.41	109.59
8	H	252	PRO	N-CA-CB	-5.70	98.04	103.51
10	P	119	ALA	N-CA-C	-5.69	104.99	111.14
6	F	416	SER	N-CA-C	5.68	117.93	111.11
6	F	176	ALA	N-CA-C	5.67	118.19	111.33
4	D	100	GLU	CA-C-N	-5.65	115.03	123.00
4	D	100	GLU	C-N-CA	-5.65	115.03	123.00
6	F	409	ILE	N-CA-C	5.63	116.36	110.62
2	B	95	PHE	CA-C-O	-5.63	114.05	120.58
6	F	457	HIS	N-CA-CB	-5.60	100.98	110.50
7	G	599	THR	CA-C-N	-5.60	114.21	122.83
7	G	599	THR	C-N-CA	-5.60	114.21	122.83
7	G	530	TYR	N-CA-C	-5.59	102.00	110.28
4	D	141	TYR	N-CA-CB	-5.59	102.37	110.47
9	I	191	LEU	N-CA-C	-5.58	105.28	111.36
17	X	40	ASN	N-CA-C	-5.57	104.89	110.97
19	a	25	TYR	N-CA-C	-5.57	107.73	114.75
11	Q	124	MET	CA-C-N	-5.57	115.07	122.98
11	Q	124	MET	C-N-CA	-5.57	115.07	122.98
7	G	127	ASP	CA-C-O	5.54	129.04	121.89
5	E	223	CYS	CB-CA-C	-5.53	110.18	116.54
7	G	615	LEU	N-CA-C	-5.52	106.32	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	51	ASP	CA-CB-CG	5.49	118.09	112.60
7	G	313	LEU	N-CA-C	5.46	118.46	109.72
18	Z	55	GLN	N-CA-C	-5.46	105.33	111.28
2	B	155	PRO	N-CA-C	-5.45	102.11	110.95
7	G	404	GLY	N-CA-C	5.45	121.44	113.48
17	X	113	ASP	N-CA-C	-5.45	106.57	113.43
7	G	682	ASP	CA-C-N	-5.44	114.15	119.76
7	G	682	ASP	C-N-CA	-5.44	114.15	119.76
7	G	420	LYS	N-CA-CB	-5.44	101.90	110.06
7	G	363	SER	N-CA-C	-5.44	100.32	109.07
2	B	104	MET	N-CA-C	-5.43	107.21	113.88
4	D	200	PHE	CA-CB-CG	5.43	119.23	113.80
4	D	391	VAL	CA-C-N	-5.42	115.76	119.66
4	D	391	VAL	C-N-CA	-5.42	115.76	119.66
2	B	146	ARG	N-CA-C	-5.41	105.38	111.28
7	G	510	TRP	N-CA-C	-5.41	101.85	109.96
4	D	132	ALA	N-CA-C	-5.40	106.69	113.72
21	q	30	ALA	N-CA-CB	5.38	118.54	110.53
2	B	105	MET	N-CA-CB	5.36	118.47	110.22
6	F	199	ARG	N-CA-C	5.35	117.46	109.59
4	D	201	PHE	N-CA-C	-5.35	105.53	111.36
5	E	48	PRO	N-CA-C	5.34	120.79	113.84
18	Z	50	MET	N-CA-C	-5.34	105.46	111.28
18	Z	64	ASP	N-CA-C	5.32	119.83	113.23
7	G	449	PRO	N-CA-CB	5.32	109.13	103.39
8	H	252	PRO	CA-N-CD	5.31	119.44	112.00
6	F	84	GLY	N-CA-C	-5.31	107.92	115.30
5	E	143	ASP	N-CA-C	5.29	118.42	111.28
21	q	67	GLU	N-CA-CB	-5.27	102.18	110.77
9	I	160	GLU	N-CA-CB	-5.27	100.76	109.72
7	G	111	LYS	N-CA-C	-5.26	105.60	112.23
7	G	356	ASP	N-CA-C	-5.26	105.55	111.28
11	Q	72	ILE	N-CA-C	-5.26	108.38	113.53
5	E	48	PRO	CB-CA-C	-5.26	104.39	111.85
7	G	362	ASP	CA-CB-CG	5.26	117.86	112.60
4	D	363	VAL	N-CA-C	5.25	116.32	111.81
8	H	146	MET	N-CA-C	-5.24	105.46	111.07
2	B	167	GLY	N-CA-C	-5.24	106.08	112.68
6	F	55	GLY	N-CA-C	-5.23	106.45	112.83
7	G	713	ALA	N-CA-C	-5.23	105.47	111.07
10	P	260	GLY	N-CA-C	-5.23	108.41	115.36
10	P	339	GLY	N-CA-C	5.23	122.53	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	84	ALA	N-CA-C	5.22	116.66	111.07
8	H	310	PHE	N-CA-C	5.21	119.27	113.01
18	Z	118	PRO	CA-C-N	-5.21	113.94	120.51
18	Z	118	PRO	C-N-CA	-5.21	113.94	120.51
7	G	277	MET	N-CA-CB	-5.21	101.69	109.71
7	G	556	THR	N-CA-C	-5.21	101.50	109.41
6	F	318	ILE	CA-C-N	5.21	124.83	119.05
6	F	318	ILE	C-N-CA	5.21	124.83	119.05
7	G	600	GLU	CB-CA-C	-5.20	103.00	111.06
7	G	458	GLY	N-CA-C	-5.20	108.15	115.32
8	H	46	LEU	N-CA-C	-5.19	106.72	113.16
13	S	85	ASP	N-CA-C	5.19	117.84	111.82
3	C	164	TRP	N-CA-C	5.18	117.01	111.36
8	H	277	TYR	N-CA-C	5.18	118.03	110.10
10	P	194	VAL	N-CA-CB	5.18	118.35	110.58
7	G	63	PHE	CA-C-O	-5.18	115.05	121.06
17	X	33	GLY	N-CA-C	-5.18	107.90	114.16
7	G	435	PRO	CB-CA-C	-5.17	105.93	111.56
22	r	18	GLN	N-CA-C	5.17	117.24	109.23
22	r	36	GLN	N-CA-C	-5.17	102.52	110.01
3	C	79	CYS	N-CA-C	-5.16	107.05	113.19
3	C	156	VAL	N-CA-C	-5.15	104.07	111.17
7	G	172	ILE	N-CA-C	-5.15	98.64	109.34
4	D	391	VAL	N-CA-C	5.14	113.80	109.02
8	H	196	ALA	CA-C-N	-5.14	113.51	119.47
8	H	196	ALA	C-N-CA	-5.14	113.51	119.47
1	A	2	ASN	CA-C-N	-5.14	113.00	120.29
1	A	2	ASN	C-N-CA	-5.14	113.00	120.29
20	b	82	LYS	N-CA-C	-5.14	103.75	110.53
20	b	63	MET	N-CA-C	5.12	118.87	109.10
6	F	60	GLY	N-CA-C	-5.12	105.99	114.48
1	A	73	LEU	CA-C-N	-5.11	114.44	120.12
1	A	73	LEU	C-N-CA	-5.11	114.44	120.12
10	P	198	ALA	N-CA-C	-5.11	100.18	108.52
7	G	569	GLN	CB-CA-C	-5.10	104.29	112.05
8	H	51	ASP	CB-CA-C	-5.10	100.88	110.67
7	G	387	LEU	N-CA-C	-5.10	98.40	107.98
3	C	221	GLU	N-CA-C	-5.09	102.35	108.25
6	F	337	MET	CB-CA-C	-5.09	103.02	111.41
8	H	101	GLY	N-CA-C	5.09	118.40	112.50
4	D	224	ALA	CA-C-O	-5.09	115.46	120.90
9	I	95	PRO	N-CA-C	5.08	121.18	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	61	LEU	N-CA-C	5.08	116.62	111.14
4	D	106	VAL	O-C-N	-5.07	116.75	122.94
6	F	366	ALA	N-CA-C	-5.07	105.44	110.97
7	G	203	ASP	CA-C-O	5.07	127.20	121.32
7	G	280	ASP	N-CA-CB	-5.06	102.68	110.12
8	H	214	GLU	N-CA-C	5.05	119.32	113.20
3	C	109	SER	N-CA-C	5.05	118.05	109.76
6	F	87	GLY	N-CA-C	5.05	118.36	112.50
14	T	105	MET	N-CA-C	-5.05	105.78	111.28
7	G	393	GLY	N-CA-C	-5.05	107.79	115.66
21	q	89	TRP	N-CA-CB	5.04	117.38	110.07
16	W	112	GLU	N-CA-C	5.03	116.84	111.36
9	I	90	LYS	N-CA-C	5.01	117.57	109.40
3	C	186	ILE	CB-CA-C	-5.01	107.45	111.71
5	E	213	PRO	CB-CA-C	-5.01	106.33	112.89
8	H	254	LEU	N-CA-CB	5.01	118.05	110.28
10	P	236	VAL	N-CA-C	-5.00	102.36	109.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	814	66	0
2	B	1258	0	1269	159	0
3	C	1641	0	1596	169	0
4	D	3088	0	3059	356	0
5	E	1635	0	1624	147	0
6	F	3288	0	3243	367	0
7	G	5287	0	5323	563	0
8	H	2517	0	2600	418	0
9	I	1431	0	1385	184	0
10	P	2720	0	2740	234	0
11	Q	957	0	949	73	0
12	R	660	0	639	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	S	667	0	683	70	0
14	T	604	0	596	64	0
15	V	915	0	954	101	0
16	W	970	0	991	85	0
17	X	1164	0	1154	105	0
18	Z	1152	0	1148	131	0
19	a	548	0	562	55	0
20	b	620	0	617	96	0
21	q	1192	0	1145	84	0
22	r	764	0	789	97	0
23	s	189	0	181	18	0
24	A	46	0	69	3	0
24	H	46	0	69	8	0
24	b	46	0	69	14	0
25	B	8	0	0	2	0
25	F	8	0	0	9	0
25	G	16	0	0	5	0
25	I	16	0	0	15	0
26	E	4	0	0	3	0
26	G	4	0	0	6	0
27	F	31	0	19	2	0
28	H	35	0	43	12	0
29	H	42	0	58	2	0
29	I	47	0	71	7	0
29	q	35	0	44	5	0
30	P	48	0	26	2	0
31	R	1	0	0	0	0
32	W	32	0	0	0	0
33	q	57	0	58	8	0
All	All	34543	0	34587	3039	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 44.

All (3039) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ASP:OD2	8:H:54:LYS:HD2	1.34	1.25
4:D:99:LEU:HD13	4:D:101:LEU:CD1	1.67	1.21
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.21
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.18
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.38	1.14
4:D:99:LEU:CD1	4:D:101:LEU:HD13	1.78	1.14
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.17	1.13
18:Z:144:THR:CG2	19:a:48:MET:SD	2.38	1.11
18:Z:144:THR:HG21	19:a:48:MET:SD	1.90	1.11
21:q:59:HIS:ND1	21:q:60:ARG:HG3	1.64	1.11
14:T:104:PHE:HZ	14:T:115:GLN:HG2	1.08	1.10
4:D:376:GLU:HG3	7:G:121:LEU:CD1	1.81	1.10
12:R:80:ASP:OD2	12:R:84:GLY:HA2	1.49	1.10
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.22	1.10
9:I:123:CYS:SG	25:I:302:SF4:FE1	1.42	1.09
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.32	1.09
3:C:102:HIS:HE1	15:V:48:THR:HG22	0.96	1.09
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.35	1.09
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.08
9:I:152:CYS:SG	25:I:302:SF4:FE2	1.43	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
3:C:102:HIS:CE1	15:V:48:THR:HG22	1.88	1.08
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.07
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.07
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.06
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.29	1.06
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.06
3:C:241:PHE:CD2	22:r:61:ARG:HB2	1.91	1.06
16:W:101:LYS:HG3	16:W:105:HIS:HB2	1.34	1.06
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.06
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
7:G:353:ALA:HA	7:G:636:TYR:OH	1.54	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.37	1.04
2:B:82:ILE:HG23	8:H:57:MET:SD	1.97	1.03
4:D:84:PHE:CZ	4:D:89:PRO:CB	2.40	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.03
5:E:247:GLY:HA2	6:F:64:LYS:HE2	1.36	1.03
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.39	1.02
10:P:272:LEU:HG	10:P:375:VAL:HG21	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:104:PHE:CZ	14:T:115:GLN:HG2	1.94	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.74	1.02
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.39	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.42	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.01
3:C:241:PHE:HD2	22:r:61:ARG:HB2	1.24	1.01
17:X:48:TRP:CE2	20:b:55:VAL:HG22	1.94	1.01
5:E:247:GLY:CA	6:F:64:LYS:HE2	1.89	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.87	1.00
4:D:99:LEU:HD13	4:D:101:LEU:HD13	1.03	1.00
8:H:25:ARG:HH11	28:H:401:UQ9:H10	1.25	1.00
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.24	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	1.00
3:C:48:PRO:HD3	4:D:162:GLN:OE1	1.59	0.99
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
4:D:185:MET:O	4:D:189:THR:HG22	1.63	0.99
7:G:401:LEU:HD11	7:G:462:PHE:CE2	1.98	0.99
2:B:111:ARG:HE	4:D:208:GLU:HG2	1.24	0.98
14:T:102:SER:O	14:T:141:PRO:HD3	1.62	0.98
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
9:I:113:CYS:SG	25:I:303:SF4:FE3	1.55	0.98
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.98
21:q:78:ASP:OD1	21:q:81:MET:HG3	1.61	0.97
9:I:155:CYS:SG	25:I:302:SF4:FE4	1.55	0.97
4:D:226:TYR:CZ	4:D:232:VAL:HG11	1.99	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
10:P:363:SER:HB3	16:W:51:HIS:CE1	1.98	0.97
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.04	0.97
8:H:207:LEU:CD2	8:H:279:ARG:HH12	1.78	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.44	0.96
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.63	0.96
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
6:F:318:ILE:HD11	6:F:355:ILE:HD12	1.47	0.96
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.96
21:q:59:HIS:CE1	21:q:60:ARG:HG3	2.00	0.95
4:D:84:PHE:CZ	4:D:89:PRO:HB2	2.02	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.65	0.95
17:X:132:LYS:HB3	20:b:59:ASP:HB2	1.48	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.95
2:B:126:ARG:HH12	8:H:61:MET:HG2	1.30	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.94
2:B:100:CYS:HB2	2:B:134:ALA:HB1	1.50	0.94
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
3:C:102:HIS:HE1	15:V:48:THR:CG2	1.80	0.94
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
14:T:104:PHE:HE1	14:T:115:GLN:HB2	1.32	0.94
4:D:226:TYR:CZ	4:D:232:VAL:CG1	2.51	0.93
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.93
8:H:19:PHE:CE2	19:a:11:ILE:HG21	2.03	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
4:D:79:ASN:HB2	4:D:100:GLU:HB3	1.51	0.93
2:B:89:SER:O	8:H:54:LYS:HD3	1.68	0.92
6:F:318:ILE:HG22	6:F:326:LEU:HB3	1.50	0.92
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.48	0.92
6:F:147:ARG:HD3	6:F:191:TYR:CD2	2.03	0.92
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.60	0.92
9:I:152:CYS:HG	25:I:302:SF4:FE2	0.77	0.91
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.91
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.01	0.91
21:q:25:ARG:O	21:q:29:ARG:HG2	1.69	0.91
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.36	0.91
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.85	0.91
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.91
7:G:78:CYS:SG	26:G:803:FES:FE2	1.63	0.91
10:P:363:SER:HB3	16:W:51:HIS:NE2	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
8:H:207:LEU:HD21	8:H:279:ARG:HH12	1.36	0.90
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.53	0.90
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.53	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.53	0.90
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.66	0.90
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.53	0.90
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.02	0.89
9:I:67:ILE:HG13	29:I:301:PC1:H251	1.53	0.89
18:Z:111:PHE:CZ	18:Z:117:VAL:HG21	2.06	0.89
6:F:314:LEU:HD11	6:F:317:VAL:HG23	1.55	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.08	0.89
6:F:424:ILE:HD11	7:G:73:GLY:O	1.72	0.89
4:D:280:ALA:CB	15:V:11:LEU:HG	2.03	0.89
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.21	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.03	0.89
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.08	0.89
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.53	0.89
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.89
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.55	0.88
3:C:240:ALA:HB1	22:r:61:ARG:HD2	1.56	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.55	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.88
5:E:134:CYS:HG	26:E:301:FES:FE1	0.68	0.88
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.88
6:F:266:GLY:HA3	6:F:271:SER:HA	1.54	0.88
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.74	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.08	0.87
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.56	0.87
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.55	0.87
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.08	0.87
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.88	0.87
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.57	0.87
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.04	0.87
10:P:296:PHE:CE1	10:P:297:VAL:HG23	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.40	0.86
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.57	0.86
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.61	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.57	0.86
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.10	0.86
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.38	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
7:G:607:LYS:HG3	11:Q:78:ARG:HH12	1.41	0.86
6:F:288:VAL:HG21	6:F:303:HIS:HD2	1.41	0.85
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.40	0.85
2:B:82:ILE:HG12	8:H:57:MET:CE	2.06	0.85
2:B:121:PHE:CD2	2:B:122:ARG:HG3	2.11	0.85
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.91	0.85
12:R:72:VAL:HG11	12:R:77:ILE:HD12	1.59	0.85
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.59	0.85
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.20	0.85
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.68	0.85
9:I:123:CYS:HG	25:I:302:SF4:FE1	0.57	0.85
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.84
14:T:104:PHE:CZ	14:T:115:GLN:CG	2.61	0.84
14:T:104:PHE:HD1	14:T:110:LEU:HB3	1.41	0.84
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.59	0.84
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.12	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
14:T:117:GLU:HA	14:T:120:MET:HE3	1.60	0.84
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.84
14:T:93:ILE:HD11	14:T:110:LEU:HD22	1.58	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.83
14:T:104:PHE:HZ	14:T:115:GLN:CG	1.88	0.83
9:I:162:CYS:SG	25:I:303:SF4:FE4	1.71	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
13:S:48:HIS:CE1	13:S:95:LEU:HD22	2.13	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
4:D:84:PHE:HZ	4:D:89:PRO:HB2	1.41	0.83
4:D:448:VAL:HG21	8:H:204:GLU:HG3	1.59	0.83
8:H:187:ILE:HD12	24:H:403:3PE:H251	1.60	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.82
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.41	0.82
4:D:209:LYS:HG2	22:r:27:ARG:NH2	1.94	0.82
7:G:651:PRO:HG3	13:S:57:GLU:H	1.44	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
7:G:114:GLU:OE2	22:r:53:TYR:HA	1.80	0.82
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.82
8:H:311:THR:HB	18:Z:51:MET:SD	2.19	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.82
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
9:I:162:CYS:HG	25:I:303:SF4:FE4	0.54	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
7:G:614:GLY:HA2	10:P:41:ILE:CD1	2.10	0.81
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.62	0.81
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.63	0.81
7:G:225:ILE:HD11	7:G:285:TRP:CZ3	2.16	0.81
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	1.95	0.81
5:E:84:LEU:HD12	23:s:46:LEU:HD13	1.61	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
9:I:135:ARG:HD2	12:R:61:ILE:HG12	1.61	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.63	0.81
2:B:111:ARG:HE	4:D:208:GLU:CG	1.94	0.81
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.81
2:B:127:GLN:NE2	8:H:216:ALA:HA	1.95	0.81
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.61	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
14:T:104:PHE:CD1	14:T:110:LEU:HB3	2.16	0.80
6:F:296:LEU:HB2	6:F:337:MET:HE3	1.61	0.80
7:G:607:LYS:HG3	11:Q:78:ARG:NH1	1.94	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.44	0.80
12:R:80:ASP:OD2	12:R:84:GLY:CA	2.27	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.80
20:b:20:VAL:HG13	24:b:201:3PE:H2A1	1.64	0.80
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.62	0.80
7:G:614:GLY:HA2	10:P:41:ILE:HD13	1.63	0.80
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.63	0.80
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.45	0.80
3:C:47:ARG:HB3	4:D:160:ASN:OD1	1.81	0.80
5:E:247:GLY:HA2	6:F:64:LYS:CE	2.12	0.80
8:H:116:ILE:HG21	8:H:135:ALA:HB3	1.64	0.80
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.64	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.80
14:T:108:LEU:O	14:T:108:LEU:HD23	1.82	0.80
3:C:47:ARG:HH21	4:D:156:GLU:HB3	1.47	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
16:W:96:THR:HG22	16:W:101:LYS:HD2	1.64	0.79
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.13	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
29:I:301:PC1:H2D1	29:I:301:PC1:H291	1.64	0.79
16:W:101:LYS:HG3	16:W:105:HIS:CB	2.12	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.79
4:D:376:GLU:CG	7:G:121:LEU:HD12	2.12	0.79
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.17	0.79
8:H:207:LEU:C	8:H:207:LEU:HD13	2.07	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
2:B:89:SER:O	8:H:54:LYS:CD	2.31	0.79
9:I:211:TYR:CE2	22:r:39:PRO:HG3	2.17	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.40	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
10:P:44:GLY:HA2	11:Q:107:TRP:CZ3	2.18	0.79
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:66:LYS:HZ3	6:F:189:SER:HA	1.48	0.78
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.12	0.78
4:D:362:LYS:HG3	22:r:54:TYR:CE2	2.19	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
14:T:90:TYR:HD2	14:T:93:ILE:HG12	1.48	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
2:B:129:ASP:OD2	8:H:54:LYS:CD	2.25	0.78
17:X:48:TRP:CD1	20:b:55:VAL:HG13	2.19	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.78
5:E:136:THR:HB	26:E:301:FES:S2	2.24	0.77
2:B:126:ARG:NH2	8:H:61:MET:HB3	1.98	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
18:Z:111:PHE:CZ	18:Z:117:VAL:CG2	2.66	0.77
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.09	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
13:S:19:ILE:HB	13:S:53:ILE:CD1	2.15	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
2:B:82:ILE:HA	8:H:57:MET:HE1	1.65	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.20	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.77
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.20	0.76
4:D:82:LEU:HB2	4:D:99:LEU:HD11	1.67	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.76
21:q:24:LEU:HD22	21:q:28:PHE:HE2	1.50	0.76
6:F:234:GLY:HA3	6:F:238:CYS:O	1.85	0.76
8:H:91:MET:O	8:H:92:PRO:C	2.27	0.76
10:P:231:LEU:HD13	10:P:292:PRO:HD3	1.66	0.76
20:b:20:VAL:HA	24:b:201:3PE:H282	1.67	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
8:H:39:ILE:HD11	29:q:202:PC1:H131	1.67	0.76
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	1.99	0.76
2:B:126:ARG:NH1	8:H:61:MET:HG2	2.01	0.76
3:C:88:HIS:CE1	15:V:105:GLU:HB3	2.20	0.76
7:G:225:ILE:HD11	7:G:285:TRP:HZ3	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
21:q:85:GLU:OE2	21:q:103:PRO:HD3	1.85	0.76
4:D:79:ASN:HB2	4:D:100:GLU:CB	2.15	0.76
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.16	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.76
6:F:192:ASP:HB3	23:s:57:LEU:HD11	1.67	0.76
9:I:155:CYS:HG	25:I:302:SF4:FE4	1.02	0.76
14:T:104:PHE:CE1	14:T:115:GLN:HB2	2.20	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.20	0.76
3:C:241:PHE:HD2	22:r:61:ARG:CB	1.97	0.76
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.20	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.76
5:E:75:ALA:O	5:E:78:VAL:HG23	1.85	0.75
7:G:173:MET:HE2	7:G:231:LEU:HD23	1.68	0.75
9:I:113:CYS:HG	25:I:303:SF4:FE3	0.45	0.75
16:W:97:ILE:HG13	16:W:98:LYS:N	2.02	0.75
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.21	0.75
2:B:173:TYR:O	3:C:203:LEU:HD22	1.87	0.75
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.67	0.75
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.85	0.75
5:E:120:MET:HE1	6:F:160:GLY:HA3	1.66	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.67	0.75
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.69	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
7:G:75:CYS:HG	26:G:803:FES:FE1	1.00	0.75
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.21	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.67	0.75
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.02	0.75
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.75
4:D:392:PRO:HG3	22:r:60:ARG:O	1.87	0.75
8:H:25:ARG:NH1	28:H:401:UQ9:H10	2.01	0.74
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.74
8:H:295:PRO:HB3	24:b:201:3PE:H3A1	1.69	0.74
13:S:19:ILE:HB	13:S:53:ILE:HD12	1.68	0.74
14:T:110:LEU:HG	14:T:114:ASP:CB	2.17	0.74
7:G:75:CYS:SG	26:G:803:FES:FE1	1.79	0.74
14:T:103:HIS:HB2	14:T:106:LYS:HG2	1.67	0.74
4:D:376:GLU:HG3	7:G:121:LEU:HD13	1.70	0.74
14:T:103:HIS:ND1	14:T:140:CYS:HB3	2.01	0.74
6:F:288:VAL:HG21	6:F:303:HIS:CD2	2.23	0.74
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.74
10:P:351:GLU:HB3	16:W:56:ASP:OD2	1.87	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
7:G:88:VAL:HG13	7:G:108:LYS:HE2	1.67	0.74
8:H:96:ILE:HG23	18:Z:143:TYR:OH	1.88	0.74
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.74
1:A:24:LEU:N	1:A:25:PRO:HD2	2.03	0.74
6:F:318:ILE:CG2	6:F:326:LEU:HB3	2.17	0.74
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.52	0.74
2:B:163:SER:HB2	9:I:150:THR:O	1.88	0.73
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.21	0.73
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.73
9:I:211:TYR:CZ	22:r:39:PRO:HG3	2.23	0.73
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.70	0.73
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.15	0.73
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.53	0.73
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.71	0.73
8:H:183:MET:HE2	29:I:301:PC1:H2A1	1.69	0.73
1:A:106:TRP:CE3	24:b:201:3PE:H342	2.24	0.73
10:P:293:LEU:HD12	10:P:294:PRO:HD2	1.69	0.73
19:a:7:PRO:HG3	33:q:201:CDL:H181	1.69	0.73
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.54	0.73
4:D:99:LEU:HD13	4:D:101:LEU:HD11	1.71	0.73
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.70	0.73
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.18	0.73
10:P:44:GLY:HA2	11:Q:107:TRP:CE3	2.23	0.73
10:P:94:LEU:HA	10:P:97:MET:HE2	1.68	0.73
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.70	0.73
2:B:141:MET:HE2	4:D:94:VAL:HG11	1.71	0.73
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:ASN:HD21	23:s:49:ASN:HD21	1.35	0.73
17:X:48:TRP:CZ2	20:b:55:VAL:HG22	2.23	0.73
6:F:66:LYS:NZ	6:F:189:SER:HA	2.03	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.73
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.22	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.19	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.73
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.53	0.72
14:T:140:CYS:SG	14:T:143:GLU:HB2	2.29	0.72
2:B:166:ASN:O	9:I:150:THR:HB	1.89	0.72
4:D:359:ASP:HB3	7:G:150:ARG:NH2	2.04	0.72
6:F:273:THR:HG22	6:F:291:GLU:HA	1.70	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
9:I:57:ALA:HB2	20:b:13:TRP:O	1.88	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.72	0.72
18:Z:6:VAL:CG1	22:r:40:LYS:HB3	2.19	0.72
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.24	0.72
8:H:306:SER:OG	20:b:33:PRO:HG3	1.89	0.72
20:b:23:PHE:HD2	24:b:201:3PE:H281	1.54	0.72
18:Z:6:VAL:HG13	18:Z:7:LYS:H	1.53	0.72
1:A:73:LEU:O	1:A:76:PRO:HD2	1.90	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
6:F:318:ILE:O	6:F:318:ILE:HG13	1.90	0.72
5:E:155:LEU:HB3	5:E:157:ILE:HG22	1.72	0.71
6:F:35:LEU:HD22	6:F:273:THR:HG21	1.72	0.71
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.19	0.71
9:I:64:THR:HG22	29:I:301:PC1:H222	1.72	0.71
3:C:67:ILE:HD11	15:V:47:TYR:HD2	1.55	0.71
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.71
3:C:217:ARG:NH1	16:W:112:GLU:HB2	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
6:F:110:PRO:HD2	6:F:238:CYS:SG	2.30	0.71
9:I:135:ARG:HH11	12:R:61:ILE:HG23	1.55	0.71
2:B:210:ARG:NH1	21:q:78:ASP:HB3	2.05	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
7:G:544:MET:HE3	7:G:565:PHE:HE2	1.54	0.71
8:H:310:PHE:HA	20:b:39:THR:HA	1.73	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
2:B:126:ARG:HH22	8:H:61:MET:HB3	1.54	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
18:Z:144:THR:HG22	19:a:48:MET:SD	2.30	0.71
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.88	0.71
6:F:44:ASN:ND2	6:F:133:HIS:O	2.24	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:180:PRO:CD	18:Z:43:LEU:HD21	2.19	0.71
6:F:318:ILE:HG22	6:F:326:LEU:CB	2.20	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.81	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.70
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.71	0.70
22:r:46:SER:C	22:r:52:ASN:HD21	1.99	0.70
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.70
6:F:110:PRO:O	6:F:238:CYS:HB3	1.91	0.70
9:I:188:GLU:OE1	12:R:56:ASN:N	2.24	0.70
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.25	0.70
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.39	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.56	0.70
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.55	0.70
8:H:61:MET:O	8:H:62:ARG:C	2.34	0.70
13:S:16:LEU:HD21	13:S:19:ILE:HD11	1.74	0.70
7:G:81:GLU:OE2	7:G:108:LYS:HD3	1.92	0.70
2:B:166:ASN:HB2	2:B:190:TYR:HD2	1.55	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:134:ARG:HB3	8:H:200:LEU:HD23	1.73	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.70
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.27	0.70
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.07	0.70
7:G:614:GLY:CA	10:P:41:ILE:HD13	2.22	0.70
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.57	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
10:P:365:GLU:HB2	10:P:367:GLU:OE2	1.92	0.69
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.69
2:B:116:ARG:HG2	8:H:36:GLY:O	1.92	0.69
18:Z:6:VAL:HG13	22:r:40:LYS:HB3	1.75	0.69
4:D:362:LYS:HG3	22:r:54:TYR:CZ	2.27	0.69
8:H:129:LEU:O	8:H:133:LEU:HG	1.92	0.69
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.73	0.69
22:r:98:ALA:HB1	22:r:99:PRO:HD2	1.75	0.69
2:B:121:PHE:CE2	2:B:122:ARG:NE	2.60	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
5:E:61:ARG:NE	23:s:47:ASP:OD1	2.22	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
13:S:51:LEU:HD13	13:S:95:LEU:HD12	1.75	0.69
4:D:84:PHE:CZ	4:D:89:PRO:HB3	2.26	0.69
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.74	0.69
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.74	0.69
6:F:278:ILE:HG12	6:F:304:ALA:HB2	1.73	0.69
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.69
2:B:121:PHE:CE2	2:B:122:ARG:CD	2.76	0.69
6:F:236:PHE:O	11:Q:166:TRP:HE3	1.76	0.69
7:G:117:MET:HE3	7:G:143:SER:HA	1.74	0.69
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.68
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.72	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
6:F:382:CYS:HG	25:F:502:SF4:FE3	1.10	0.68
7:G:171:THR:HB	7:G:173:MET:HG3	1.74	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:401:LEU:HD11	7:G:462:PHE:CZ	2.28	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.24	0.68
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.75	0.68
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.59	0.68
4:D:99:LEU:CD1	4:D:101:LEU:CD1	2.54	0.68
5:E:233:LEU:H	6:F:37:ASP:CG	2.02	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.68
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.75	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.68
14:T:90:TYR:HE2	14:T:110:LEU:HD11	1.58	0.68
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.39	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.29	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
22:r:112:TYR:O	22:r:113:LEU:HB2	1.93	0.68
8:H:62:ARG:O	8:H:63:PRO:C	2.37	0.68
10:P:263:PHE:HD2	10:P:333:PRO:O	1.77	0.68
14:T:104:PHE:HB2	14:T:110:LEU:HB2	1.74	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.68
6:F:147:ARG:HD3	6:F:191:TYR:CE2	2.29	0.68
7:G:78:CYS:HG	26:G:803:FES:FE2	0.46	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.28	0.68
18:Z:65:LEU:HB3	20:b:50:PRO:O	1.93	0.68
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.68
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.59	0.68
4:D:239:GLY:H	18:Z:9:ASP:CG	2.02	0.67
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
13:S:20:ARG:HB2	13:S:66:TRP:HB2	1.75	0.67
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.07	0.67
3:C:47:ARG:NH2	4:D:156:GLU:HB3	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:110:GLU:OE1	12:R:64:ILE:HB	1.94	0.67
16:W:45:GLU:CD	16:W:97:ILE:HG22	2.19	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.77	0.67
10:P:296:PHE:CZ	10:P:297:VAL:HG23	2.29	0.67
2:B:202:LEU:CD2	9:I:86:TYR:CB	2.73	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.77	0.67
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.23	0.67
8:H:300:LEU:HD23	20:b:25:VAL:HG11	1.74	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
8:H:207:LEU:CD2	8:H:279:ARG:NH1	2.55	0.67
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.76	0.67
6:F:233:VAL:HG11	11:Q:164:PHE:HB2	1.76	0.67
7:G:73:GLY:HA2	26:G:803:FES:S1	2.35	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
4:D:279:THR:HG23	15:V:13:GLY:CA	2.09	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.77	0.67
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.76	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.67
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.30	0.66
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.93	0.66
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.29	0.66
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.77	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
8:H:198:PHE:HZ	24:H:403:3PE:H231	1.59	0.66
9:I:200:GLU:OE2	21:q:93:MET:SD	2.53	0.66
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.77	0.66
17:X:130:LYS:HG2	20:b:68:SER:HA	1.77	0.66
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.24	0.66
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.13	0.66
4:D:100:GLU:C	4:D:101:LEU:HD12	2.20	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
9:I:62:MET:HE1	18:Z:36:PHE:HA	1.77	0.66
14:T:97:LYS:HZ3	14:T:108:LEU:N	1.93	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.76	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:275:LEU:HA	6:F:289:GLU:HA	1.77	0.66
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.61	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
17:X:57:LEU:HG	17:X:61:LYS:NZ	2.10	0.66
3:C:47:ARG:HG3	3:C:48:PRO:HD2	1.77	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.44	0.66
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.31	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
10:P:262:THR:H	10:P:332:LEU:HD12	1.61	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.22	0.66
8:H:69:SER:HB3	29:H:402:PC1:H221	1.77	0.66
8:H:207:LEU:HD23	8:H:279:ARG:HH12	1.59	0.66
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.66
10:P:320:GLU:O	10:P:324:ILE:HG12	1.96	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.66
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.78	0.66
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.61	0.66
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.11	0.66
17:X:48:TRP:CE2	20:b:55:VAL:CG2	2.75	0.66
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.65
8:H:310:PHE:O	20:b:38:TYR:HB2	1.95	0.65
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.79	0.65
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.65
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.65
18:Z:114:THR:O	18:Z:114:THR:HG22	1.94	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.77	0.65
18:Z:143:TYR:CD1	18:Z:144:THR:N	2.65	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
6:F:293:SER:HA	6:F:338:ASP:HB3	1.78	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.94	0.65
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.30	0.65
9:I:68:ARG:HH21	18:Z:26:PRO:HD2	1.59	0.65
13:S:16:LEU:HD11	13:S:19:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.32	0.65
4:D:226:TYR:CE2	4:D:232:VAL:CG1	2.80	0.65
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.48	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
17:X:53:PRO:HB3	18:Z:80:ASP:OD2	1.97	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.65
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.77	0.65
7:G:89:VAL:HB	7:G:94:MET:HG3	1.78	0.65
12:R:40:GLU:HA	12:R:45:ARG:NH1	2.11	0.65
2:B:81:LEU:CG	8:H:53:MET:HE1	2.27	0.65
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.96	0.65
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
2:B:141:MET:CE	4:D:94:VAL:HG11	2.27	0.64
4:D:280:ALA:CB	15:V:11:LEU:CG	2.75	0.64
7:G:226:CYS:SG	25:G:802:SF4:FE1	1.88	0.64
7:G:614:GLY:C	10:P:41:ILE:HG21	2.22	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
7:G:226:CYS:HG	25:G:802:SF4:FE1	1.14	0.64
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.64
14:T:80:LYS:HD3	14:T:100:VAL:HG11	1.79	0.64
17:X:141:PRO:O	17:X:142:TYR:HB2	1.96	0.64
4:D:81:THR:HA	4:D:99:LEU:O	1.98	0.64
4:D:84:PHE:CZ	4:D:89:PRO:CG	2.80	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.60	0.64
3:C:68:LEU:HD13	3:C:95:THR:HG23	1.80	0.64
5:E:58:ASN:HB3	5:E:84:LEU:HD21	1.80	0.64
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.27	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.64
13:S:48:HIS:CE1	13:S:95:LEU:CD2	2.80	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
1:A:7:ILE:HG21	24:A:401:3PE:H292	1.80	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.64
21:q:3:LEU:O	21:q:6:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:379:CYS:SG	25:F:502:SF4:S1	2.96	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.61	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
17:X:50:GLU:HG2	17:X:138:PRO:HG3	1.79	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.63	0.64
10:P:150:ARG:HE	10:P:190:GLU:HG2	1.62	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.23	0.64
4:D:260:GLU:CG	18:Z:25:LEU:HD22	2.27	0.64
6:F:227:PRO:HG3	7:G:94:MET:SD	2.38	0.64
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.64
7:G:557:ARG:HD3	21:q:144:TYR:CE1	2.32	0.64
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.64
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.28	0.64
10:P:296:PHE:CZ	10:P:297:VAL:CG2	2.81	0.64
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.28	0.64
3:C:241:PHE:CD2	22:r:61:ARG:CB	2.75	0.64
5:E:48:PRO:HA	5:E:95:SER:HB2	1.80	0.64
7:G:152:ARG:HD2	22:r:49:LEU:HA	1.80	0.64
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.64
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
21:q:29:ARG:O	29:q:202:PC1:C14	2.46	0.64
4:D:260:GLU:HG3	18:Z:25:LEU:CD2	2.28	0.64
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.33	0.63
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.61	0.63
10:P:299:SER:CB	10:P:316:LYS:HE3	2.22	0.63
3:C:139:ARG:NH2	4:D:406:GLU:OE2	2.31	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
4:D:279:THR:HA	15:V:12:VAL:HG13	1.78	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.63
8:H:224:PHE:CZ	28:H:401:UQ9:H7A	2.33	0.63
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.33	0.63
8:H:274:ARG:HH22	28:H:401:UQ9:C3M	2.11	0.63
13:S:20:ARG:HG2	13:S:54:LEU:HD12	1.79	0.63
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.33	0.63
4:D:260:GLU:OE2	18:Z:26:PRO:HD2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.81	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
21:q:29:ARG:O	29:q:202:PC1:H141	1.97	0.63
2:B:202:LEU:CD2	9:I:86:TYR:HB2	2.29	0.63
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.34	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
2:B:194:CYS:O	25:B:301:SF4:S4	2.56	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.81	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.79	0.63
14:T:104:PHE:CE1	14:T:115:GLN:CB	2.80	0.63
6:F:275:LEU:HG	6:F:289:GLU:HB3	1.80	0.63
6:F:425:CYS:SG	25:F:502:SF4:S4	2.96	0.63
8:H:62:ARG:HD2	8:H:68:MET:SD	2.38	0.63
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.63
10:P:365:GLU:CB	10:P:367:GLU:OE2	2.46	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.80	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
1:A:7:ILE:HG13	24:A:401:3PE:H271	1.81	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
12:R:44:ARG:HG2	12:R:47:ARG:NH1	2.14	0.63
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.79	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.63
14:T:104:PHE:HE1	14:T:115:GLN:CB	2.07	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
2:B:116:ARG:HA	8:H:37:PRO:HA	1.81	0.62
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.32	0.62
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.62
6:F:87:GLY:H	6:F:92:GLY:HA2	1.64	0.62
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.62
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.62
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.29	0.62
2:B:81:LEU:HG	8:H:53:MET:HE1	1.80	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.35	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.82	0.62
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.14	0.62
18:Z:6:VAL:HG11	22:r:40:LYS:HD3	1.80	0.62
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.81	0.62
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.79	0.62
4:D:304:LYS:HE2	9:I:35:THR:N	2.14	0.62
4:D:375:MET:HE1	7:G:126:LEU:HA	1.81	0.62
5:E:238:LYS:HE2	5:E:242:PHE:CE2	2.34	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
8:H:134:ARG:HE	8:H:200:LEU:HD21	1.65	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.40	0.62
6:F:327:ILE:HG13	6:F:331:VAL:HB	1.81	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.82	0.62
8:H:200:LEU:HD22	8:H:282:TYR:HD1	1.65	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.62
9:I:92:PRO:HG2	21:q:56:PHE:CE2	2.35	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
4:D:338:ARG:NH1	18:Z:23:ARG:HA	2.13	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.34	0.62
6:F:87:GLY:O	6:F:88:ARG:HB2	1.99	0.62
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.80	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.30	0.62
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.62
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.30	0.62
3:C:212:ASP:OD2	10:P:75:ARG:NH2	2.32	0.62
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.80	0.62
7:G:360:LYS:CE	7:G:632:ILE:HB	2.27	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.29	0.62
28:H:401:UQ9:H23	28:H:401:UQ9:H20B	1.81	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.88	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.62
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.62
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.63	0.62
2:B:108:ALA:HB1	2:B:121:PHE:HD1	1.63	0.62
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.53	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
8:H:19:PHE:CE2	19:a:11:ILE:CG2	2.81	0.62
9:I:92:PRO:HA	21:q:91:HIS:O	2.00	0.62
2:B:97:LEU:HD11	2:B:141:MET:HE2	1.82	0.61
2:B:127:GLN:HE21	8:H:216:ALA:HA	1.65	0.61
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.61
12:R:72:VAL:HG21	12:R:77:ILE:HD13	1.82	0.61
13:S:48:HIS:HE1	13:S:95:LEU:HD22	1.63	0.61
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.81	0.61
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.61
5:E:180:VAL:HG13	5:E:181:ASN:N	2.15	0.61
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.61
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.81	0.61
7:G:636:TYR:CD1	7:G:642:VAL:HG22	2.34	0.61
8:H:179:TRP:NE1	18:Z:43:LEU:HG	2.14	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
18:Z:143:TYR:HD1	18:Z:144:THR:H	1.46	0.61
21:q:84:PRO:HD2	21:q:113:HIS:CD2	2.36	0.61
33:q:201:CDL:H331	33:q:201:CDL:H722	1.83	0.61
5:E:65:ILE:HD11	23:s:46:LEU:HD22	1.83	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.28	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
17:X:18:VAL:HG11	17:X:25:LEU:HD21	1.80	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
4:D:259:GLU:HB3	18:Z:25:LEU:HD11	1.83	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
4:D:104:GLU:HG3	4:D:104:GLU:O	1.99	0.61
4:D:209:LYS:HG2	22:r:27:ARG:HH21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
7:G:372:PHE:H	7:G:532:PRO:HB2	1.66	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
17:X:46:CYS:SG	17:X:59:GLU:HG3	2.41	0.61
2:B:108:ALA:HB1	2:B:121:PHE:CD1	2.35	0.61
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.30	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.66	0.61
10:P:363:SER:CB	16:W:51:HIS:NE2	2.60	0.61
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.66	0.61
4:D:226:TYR:CE2	4:D:232:VAL:HG11	2.35	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.61
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.64	0.61
8:H:68:MET:N	29:H:402:PC1:O12	2.33	0.61
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.61
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.00	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
4:D:259:GLU:HB2	18:Z:25:LEU:HD21	1.83	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
22:r:12:ARG:HH21	22:r:20:LEU:HD11	1.65	0.60
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.31	0.60
4:D:226:TYR:CE1	4:D:232:VAL:CG1	2.85	0.60
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.36	0.60
5:E:134:CYS:SG	5:E:175:CYS:HA	2.41	0.60
6:F:69:LEU:HD11	6:F:143:LEU:CD2	2.31	0.60
6:F:318:ILE:HD11	6:F:355:ILE:CD1	2.28	0.60
8:H:19:PHE:CZ	19:a:11:ILE:HG21	2.35	0.60
8:H:306:SER:HG	8:H:310:PHE:HE2	1.31	0.60
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.66	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.82	0.60
2:B:155:PRO:HG2	8:H:58:LYS:HA	1.82	0.60
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
18:Z:144:THR:O	19:a:36:LYS:HD2	2.02	0.60
2:B:104:MET:HE1	2:B:132:ILE:HD12	1.81	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.84	0.60
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.60
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.83	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
2:B:93:MET:HB2	2:B:128:ALA:HB1	1.84	0.60
6:F:414:GLU:OE1	22:r:50:SER:HA	2.02	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.81	0.60
12:R:72:VAL:CG1	12:R:77:ILE:HD12	2.30	0.60
12:R:97:LYS:HD2	12:R:100:LYS:HB2	1.84	0.60
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.83	0.60
5:E:63:GLU:O	5:E:67:LYS:HG3	2.02	0.60
8:H:207:LEU:C	8:H:207:LEU:CD1	2.74	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.36	0.60
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.83	0.60
16:W:42:TRP:CZ2	16:W:93:LEU:HA	2.37	0.60
4:D:318:VAL:HG21	22:r:104:TRP:CH2	2.37	0.60
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.82	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.59
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.68	0.59
5:E:226:PRO:HG2	5:E:231:THR:H	1.67	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.59
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.59
7:G:617:ARG:NH1	16:W:128:GLY:C	2.59	0.59
8:H:274:ARG:NH2	28:H:401:UQ9:H3M	2.17	0.59
2:B:169:GLY:O	2:B:170:TYR:C	2.44	0.59
2:B:194:CYS:SG	4:D:138:ARG:NE	2.73	0.59
4:D:156:GLU:HG3	4:D:229:PRO:O	2.02	0.59
6:F:270:ASN:HD21	6:F:340:ASP:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:114:GLU:OE2	22:r:54:TYR:N	2.31	0.59
7:G:614:GLY:HA2	10:P:41:ILE:HD12	1.84	0.59
9:I:72:MET:HE1	22:r:16:SER:HB2	1.84	0.59
9:I:80:GLU:HG3	19:a:1:MET:SD	2.42	0.59
13:S:16:LEU:HD11	13:S:19:ILE:CD1	2.32	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
20:b:20:VAL:HG22	24:b:201:3PE:H261	1.84	0.59
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.83	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:117:MET:HE3	7:G:143:SER:CA	2.32	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.38	0.59
8:H:207:LEU:HD23	8:H:279:ARG:NH1	2.17	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
12:R:45:ARG:HA	12:R:48:PHE:HD2	1.67	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.84	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.36	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.62	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
6:F:318:ILE:CG1	6:F:355:ILE:HB	2.32	0.59
6:F:418:GLN:HE22	7:G:111:LYS:HG3	1.65	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.01	0.59
2:B:127:GLN:HE22	8:H:220:PHE:HB2	1.68	0.59
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.67	0.59
6:F:87:GLY:HA3	6:F:92:GLY:HA2	1.84	0.59
6:F:314:LEU:O	6:F:329:LYS:HB2	2.03	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
4:D:84:PHE:HD1	4:D:87:GLN:OE1	1.86	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.51	0.59
3:C:242:PRO:O	3:C:243:ALA:C	2.45	0.59
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:ASN:HD22	4:D:107:ARG:HD3	1.68	0.59
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.59
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.67	0.59
6:F:318:ILE:HG12	6:F:355:ILE:HB	1.85	0.59
8:H:172:MET:SD	18:Z:49:ARG:HB3	2.43	0.59
8:H:198:PHE:CZ	24:H:403:3PE:H231	2.38	0.59
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.59
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	1.84	0.59
12:R:32:THR:OG1	12:R:36:GLN:HB3	2.03	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
21:q:66:THR:HG22	21:q:67:GLU:OE2	2.03	0.59
2:B:126:ARG:HG3	8:H:213:VAL:O	2.02	0.58
4:D:260:GLU:OE2	18:Z:26:PRO:CD	2.51	0.58
6:F:267:ARG:HH12	6:F:340:ASP:HB3	1.68	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
22:r:20:LEU:C	22:r:20:LEU:HD12	2.27	0.58
4:D:88:HIS:N	4:D:89:PRO:HD3	2.18	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.32	0.58
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.83	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.03	0.58
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.68	0.58
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.28	0.58
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.87	0.58
6:F:270:ASN:ND2	6:F:340:ASP:H	2.00	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.19	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:119:GLU:OE1	6:F:125:CYS:HA	2.03	0.58
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.38	0.58
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.85	0.58
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.58
21:q:125:VAL:HG23	21:q:125:VAL:O	2.03	0.58
6:F:225:LEU:N	11:Q:160:TYR:HE2	1.95	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.81	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
4:D:84:PHE:C	4:D:86:PRO:HD2	2.29	0.58
6:F:51:TRP:CB	6:F:133:HIS:O	2.52	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.34	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.58
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.19	0.58
6:F:303:HIS:O	6:F:304:ALA:C	2.45	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.86	0.58
2:B:100:CYS:CB	2:B:134:ALA:HB1	2.31	0.58
4:D:159:LEU:HD22	22:r:60:ARG:HG3	1.86	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
4:D:92:HIS:HB3	4:D:456:ILE:O	2.04	0.58
6:F:297:LYS:O	6:F:301:GLU:HG2	2.03	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.04	0.58
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.66	0.58
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.39	0.58
14:T:90:TYR:CE2	14:T:110:LEU:HD11	2.39	0.58
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.69	0.57
4:D:84:PHE:CE2	4:D:89:PRO:CG	2.87	0.57
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.86	0.57
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.68	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
12:R:37:VAL:O	12:R:37:VAL:HG13	2.03	0.57
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.84	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.57
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.19	0.57
5:E:107:PRO:HB2	5:E:110:ARG:HG2	1.87	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
10:P:363:SER:O	16:W:51:HIS:CD2	2.58	0.57
12:R:52:GLN:NE2	12:R:54:GLU:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.64	0.57
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
3:C:67:ILE:HD12	15:V:44:TYR:HA	1.85	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
6:F:291:GLU:HG2	6:F:292:MET:O	2.05	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.34	0.57
2:B:126:ARG:HH22	8:H:61:MET:CG	2.17	0.57
6:F:87:GLY:N	6:F:92:GLY:HA2	2.19	0.57
7:G:632:ILE:HG13	7:G:632:ILE:O	2.04	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
20:b:23:PHE:HE1	24:b:201:3PE:H3A2	1.69	0.57
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
2:B:112:TYR:CZ	2:B:199:GLU:HG2	2.40	0.57
4:D:84:PHE:CD1	4:D:87:GLN:OE1	2.58	0.57
4:D:91:ALA:O	4:D:92:HIS:HB2	2.03	0.57
6:F:270:ASN:HD22	6:F:338:ASP:CG	2.13	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
6:F:296:LEU:O	6:F:297:LYS:C	2.47	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
2:B:127:GLN:NE2	8:H:215:TYR:O	2.38	0.57
2:B:202:LEU:HD23	9:I:86:TYR:CB	2.34	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
6:F:382:CYS:HA	7:G:74:ASN:O	2.05	0.57
18:Z:59:ARG:NH2	20:b:84:LEU:HB3	2.18	0.57
21:q:86:TRP:CG	21:q:98:PRO:HG2	2.39	0.57
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.61	0.57
3:C:123:ASN:HD22	15:V:108:PRO:HG2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.20	0.56
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.87	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.56
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.40	0.56
5:E:73:HIS:HB3	6:F:236:PHE:CE1	2.40	0.56
6:F:69:LEU:HD11	6:F:143:LEU:HD21	1.87	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.05	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.88	0.56
2:B:126:ARG:HH22	8:H:61:MET:CB	2.16	0.56
2:B:164:CYS:SG	25:B:301:SF4:S3	3.02	0.56
6:F:278:ILE:CD1	6:F:304:ALA:HB1	2.35	0.56
7:G:62:ARG:H	7:G:142:GLN:HE22	1.53	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.56
7:G:625:ALA:O	7:G:629:ILE:HG12	2.04	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
12:R:44:ARG:HG2	12:R:47:ARG:HH12	1.70	0.56
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.88	0.56
2:B:154:GLU:O	2:B:155:PRO:C	2.48	0.56
4:D:278:VAL:O	15:V:12:VAL:HG11	2.06	0.56
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.39	0.56
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
8:H:61:MET:HG3	8:H:63:PRO:HA	1.88	0.56
8:H:204:GLU:O	8:H:205:SER:C	2.49	0.56
9:I:88:PHE:CZ	21:q:30:ALA:HA	2.40	0.56
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.40	0.56
3:C:240:ALA:HB1	22:r:61:ARG:CD	2.34	0.56
8:H:200:LEU:HD22	8:H:282:TYR:CD1	2.41	0.56
17:X:103:GLN:HA	17:X:106:LYS:HD3	1.87	0.56
18:Z:8:GLN:HG3	22:r:41:LEU:HD12	1.86	0.56
20:b:67:PRO:HB3	20:b:74:LEU:HB2	1.87	0.56
21:q:59:HIS:CE1	21:q:60:ARG:CG	2.83	0.56
33:q:201:CDL:H141	33:q:201:CDL:H321	1.87	0.56
4:D:85:GLY:N	4:D:86:PRO:HD2	2.21	0.56
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.04	0.56
5:E:226:PRO:HD3	6:F:46:TYR:CE2	2.40	0.56
7:G:651:PRO:HG3	13:S:57:GLU:N	2.19	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.56
22:r:106:LEU:HD21	22:r:111:PRO:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.40	0.56
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.87	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.56
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.06	0.56
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
7:G:615:LEU:HG	10:P:41:ILE:HG23	1.86	0.56
8:H:69:SER:O	8:H:73:ILE:HB	2.06	0.56
9:I:82:ALA:HA	22:r:26:LEU:HD21	1.88	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.56
22:r:106:LEU:HD21	22:r:111:PRO:HB2	1.86	0.56
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.36	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56
10:P:375:VAL:HG12	10:P:377:TYR:HB3	1.88	0.56
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
2:B:110:PRO:HB3	8:H:33:LEU:O	2.06	0.56
4:D:245:TYR:CD1	18:Z:19:ILE:HD11	2.41	0.56
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.71	0.56
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.56
12:R:58:ASN:HB3	12:R:63:LEU:HD11	1.88	0.56
14:T:93:ILE:HA	14:T:108:LEU:HD21	1.88	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.06	0.55
17:X:47:ARG:NH2	17:X:53:PRO:HG3	2.21	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.55
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.06	0.55
2:B:126:ARG:NH2	8:H:63:PRO:HD3	2.21	0.55
3:C:151:PRO:HG2	16:W:23:ILE:HG13	1.86	0.55
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.06	0.55
5:E:231:THR:HG21	6:F:303:HIS:HA	1.88	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
13:S:27:SER:N	13:S:34:ARG:HH22	2.05	0.55
14:T:146:ASP:O	14:T:149:ALA:HB3	2.06	0.55
4:D:93:GLY:HA3	4:D:458:PHE:HD2	1.70	0.55
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.70	0.55
17:X:142:TYR:HA	18:Z:115:ARG:HD3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:69:HIS:HB3	20:b:72:ASP:OD1	2.05	0.55
3:C:62:GLU:O	3:C:66:GLU:HG3	2.06	0.55
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.20	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.45	0.55
2:B:194:CYS:HB2	9:I:153:ILE:O	2.06	0.55
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.23	0.55
4:D:226:TYR:CE2	4:D:232:VAL:HG13	2.42	0.55
6:F:51:TRP:CZ3	6:F:168:ASN:HB3	2.41	0.55
6:F:147:ARG:CD	6:F:191:TYR:CE2	2.90	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:61:MET:HG3	8:H:63:PRO:CA	2.37	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
19:a:1:MET:HB2	19:a:3:PHE:CZ	2.42	0.55
2:B:121:PHE:CE2	2:B:122:ARG:HG3	2.42	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
21:q:3:LEU:O	21:q:7:LEU:HG	2.07	0.55
21:q:56:PHE:HD2	22:r:27:ARG:HH11	1.53	0.55
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.42	0.55
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.72	0.55
5:E:247:GLY:C	6:F:64:LYS:HE2	2.30	0.55
8:H:133:LEU:HA	8:H:136:VAL:HG12	1.89	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
14:T:85:TYR:O	14:T:89:LEU:HD13	2.07	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.55
3:C:240:ALA:HB1	22:r:61:ARG:HH11	1.71	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
6:F:424:ILE:CG1	7:G:76:ARG:HD3	2.37	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:90:PRO:O	8:H:91:MET:C	2.50	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
12:R:43:TYR:O	12:R:46:VAL:HG22	2.07	0.55
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.07	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.71	0.55
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
2:B:166:ASN:O	2:B:166:ASN:OD1	2.25	0.54
3:C:98:PHE:HB2	15:V:94:MET:CE	2.37	0.54
8:H:9:LEU:HD23	8:H:91:MET:HE1	1.88	0.54
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.54
12:R:45:ARG:HA	12:R:48:PHE:CD2	2.41	0.54
2:B:161:MET:CG	2:B:196:PRO:HG2	2.37	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.15	0.54
10:P:44:GLY:H	11:Q:105:GLU:CD	2.15	0.54
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.22	0.54
21:q:50:GLU:HA	21:q:59:HIS:O	2.07	0.54
2:B:115:ASP:OD1	8:H:25:ARG:NH2	2.40	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
4:D:318:VAL:HG21	22:r:104:TRP:CZ3	2.43	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
9:I:49:ASP:O	9:I:50:MET:C	2.50	0.54
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
18:Z:40:ILE:O	18:Z:44:ILE:HG12	2.07	0.54
3:C:104:ASN:ND2	22:r:94:ALA:HB1	2.22	0.54
4:D:145:MET:O	4:D:148:GLU:N	2.39	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
7:G:655:ARG:NH1	13:S:59:SER:CB	2.70	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
11:Q:165:SER:HB2	11:Q:168:LYS:HG2	1.89	0.54
14:T:84:LEU:O	14:T:88:LYS:HG3	2.07	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
17:X:124:GLN:O	20:b:70:PRO:HB2	2.08	0.54
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.89	0.54
2:B:136:THR:OG1	4:D:118:ARG:HD3	2.08	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
18:Z:143:TYR:O	18:Z:144:THR:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
4:D:97:LEU:CD2	4:D:447:VAL:HG11	2.38	0.54
5:E:84:LEU:HD12	23:s:46:LEU:CD1	2.34	0.54
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.36	0.54
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.54
7:G:655:ARG:NH1	13:S:59:SER:HB3	2.21	0.54
8:H:116:ILE:HG21	8:H:135:ALA:CB	2.38	0.54
10:P:58:VAL:O	10:P:83:PRO:HD2	2.08	0.54
13:S:47:ALA:O	13:S:49:PRO:HD3	2.08	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.08	0.54
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.54
10:P:306:GLY:HA2	10:P:312:PRO:HB3	1.90	0.54
12:R:48:PHE:CD1	12:R:53:LYS:HB2	2.43	0.54
14:T:115:GLN:O	14:T:119:ILE:HG12	2.08	0.54
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.54
22:r:54:TYR:CZ	22:r:58:ASP:HB3	2.42	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.54
6:F:278:ILE:HG12	6:F:304:ALA:CB	2.38	0.54
6:F:286:CYS:SG	6:F:304:ALA:HA	2.47	0.54
7:G:62:ARG:H	7:G:142:GLN:NE2	2.05	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:231:LEU:HD13	10:P:292:PRO:CD	2.37	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.08	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54
1:A:69:ILE:O	1:A:73:LEU:HG	2.08	0.54
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.70	0.54
3:C:234:LEU:O	4:D:387:GLU:HG3	2.07	0.54
4:D:253:LEU:HD22	22:r:23:LYS:HD3	1.90	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.54
18:Z:120:LEU:HB2	18:Z:123:GLU:HG3	1.89	0.54
2:B:120:VAL:HG12	2:B:121:PHE:N	2.23	0.54
4:D:248:SER:OG	18:Z:19:ILE:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:ILE:HD11	5:E:84:LEU:HD22	1.90	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
8:H:116:ILE:HD13	8:H:135:ALA:HB1	1.88	0.54
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.54
6:F:119:GLU:OE1	6:F:125:CYS:CA	2.56	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.53
8:H:72:ILE:O	8:H:76:THR:HG23	2.07	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
14:T:93:ILE:HG23	14:T:108:LEU:CD1	2.38	0.53
16:W:23:ILE:HG23	16:W:24:PHE:N	2.22	0.53
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.36	0.53
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.73	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
5:E:91:TRP:CZ2	5:E:125:PRO:HD3	2.43	0.53
5:E:116:THR:O	7:G:199:GLY:HA2	2.07	0.53
6:F:102:MET:SD	6:F:149:MET:HB2	2.48	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53
8:H:74:ALA:O	8:H:75:PRO:C	2.49	0.53
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.90	0.53
21:q:49:TYR:HB2	21:q:61:TRP:CE2	2.42	0.53
22:r:36:GLN:HB3	22:r:37:PRO:HD2	1.90	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
5:E:52:PHE:CD2	5:E:96:ALA:HA	2.44	0.53
5:E:133:VAL:HA	5:E:185:VAL:HG12	1.90	0.53
6:F:87:GLY:CA	6:F:92:GLY:HA2	2.37	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.73	0.53
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.91	0.53
1:A:80:GLN:NE2	8:H:315:PRO:O	2.42	0.53
2:B:182:ASP:OD1	2:B:183:ARG:N	2.41	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.21	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
18:Z:105:LYS:HD2	18:Z:105:LYS:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:140:PHE:HD1	19:a:45:TRP:HB2	1.72	0.53
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.27	0.53
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.88	0.53
5:E:118:TYR:HE1	6:F:206:CYS:SG	2.31	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
17:X:17:GLU:HG3	17:X:64:ASN:HD22	1.73	0.53
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.08	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
7:G:617:ARG:HH12	16:W:129:HIS:N	2.06	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
2:B:94:THR:HG21	2:B:104:MET:SD	2.49	0.53
5:E:177:GLY:O	5:E:178:ALA:HB3	2.08	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.74	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
16:W:42:TRP:CD2	16:W:93:LEU:HD13	2.44	0.53
17:X:70:PHE:O	17:X:74:ILE:HG13	2.09	0.53
18:Z:59:ARG:HH21	20:b:84:LEU:HB3	1.72	0.53
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.53
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.53
21:q:31:ASN:HD21	29:q:202:PC1:H151	1.73	0.53
2:B:93:MET:HG3	2:B:125:PRO:HA	1.90	0.53
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.44	0.53
2:B:127:GLN:HE22	8:H:220:PHE:CB	2.21	0.53
6:F:86:ARG:NH1	6:F:339:PHE:HB2	2.24	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.90	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.53
10:P:363:SER:CB	16:W:51:HIS:CE1	2.84	0.53
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.53
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.53
4:D:384:LEU:CD2	7:G:144:MET:HE1	2.39	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.53
1:A:103:ALA:O	1:A:107:THR:HG23	2.09	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
2:B:199:GLU:HB2	9:I:173:PHE:HE2	1.74	0.53
3:C:63:TYR:HE1	15:V:47:TYR:CG	2.26	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
8:H:311:THR:O	18:Z:51:MET:HG3	2.08	0.53
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
3:C:51:ASP:OD1	3:C:54:HIS:HB3	2.08	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.44	0.52
4:D:381:HIS:HE1	9:I:161:ALA:O	1.93	0.52
6:F:332:CYS:HA	6:F:335:VAL:HG12	1.90	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
8:H:224:PHE:CE2	28:H:401:UQ9:H11	2.43	0.52
11:Q:53:ILE:O	16:W:20:VAL:HG22	2.09	0.52
16:W:23:ILE:HG23	16:W:24:PHE:H	1.74	0.52
21:q:44:TYR:OH	21:q:112:ASN:CG	2.52	0.52
22:r:6:ARG:O	22:r:10:LYS:HG3	2.09	0.52
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.23	0.52
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:12:PRO:O	19:a:15:CYS:HB3	2.09	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
19:a:4:GLU:O	19:a:7:PRO:HD2	2.09	0.52
2:B:163:SER:HA	2:B:166:ASN:OD1	2.09	0.52
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:338:ARG:HH12	18:Z:23:ARG:HA	1.74	0.52
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.52
7:G:161:GLU:O	7:G:163:LYS:HE3	2.10	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
12:R:40:GLU:HA	12:R:45:ARG:HH12	1.75	0.52
12:R:43:TYR:O	12:R:46:VAL:HG13	2.09	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.10	0.52
3:C:63:TYR:HB2	22:r:95:VAL:CG2	2.40	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.91	0.52
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.07	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
6:F:109:ARG:HB3	6:F:238:CYS:SG	2.50	0.52
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.42	0.52
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
20:b:23:PHE:CD2	24:b:201:3PE:H281	2.40	0.52
2:B:90:LEU:O	2:B:119:VAL:HA	2.10	0.52
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.10	0.52
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.28	0.52
4:D:348:LEU:O	18:Z:11:PRO:HB3	2.10	0.52
8:H:274:ARG:NH2	28:H:401:UQ9:C3M	2.72	0.52
14:T:130:ILE:HG23	14:T:147:TYR:HE2	1.75	0.52
4:D:361:ALA:HB3	7:G:149:ASP:HB3	1.91	0.52
8:H:172:MET:SD	18:Z:49:ARG:HG2	2.49	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
12:R:50:ASP:O	12:R:51:ARG:HG3	2.10	0.52
18:Z:126:GLY:HA2	18:Z:133:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:MET:HE2	2:B:196:PRO:HD2	1.92	0.52
2:B:199:GLU:HB2	9:I:173:PHE:CE2	2.44	0.52
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.25	0.52
4:D:159:LEU:CD2	22:r:60:ARG:HG3	2.39	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:81:GLU:O	7:G:103:LEU:HB2	2.09	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
17:X:137:LEU:HA	20:b:58:ARG:HH22	1.75	0.52
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.91	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.52
5:E:179:CYS:HA	26:E:301:FES:S1	2.50	0.52
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.91	0.52
6:F:288:VAL:HG11	6:F:303:HIS:CB	2.40	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
8:H:207:LEU:HD23	8:H:279:ARG:HH22	1.75	0.52
10:P:272:LEU:HG	10:P:375:VAL:CG2	2.26	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
2:B:101:ALA:O	2:B:104:MET:HG2	2.10	0.51
3:C:64:VAL:HG11	3:C:85:ILE:CD1	2.33	0.51
4:D:83:ASN:ND2	4:D:96:ARG:HH11	2.07	0.51
4:D:279:THR:HA	15:V:12:VAL:CG1	2.41	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.51
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.41	0.51
14:T:90:TYR:CD2	14:T:93:ILE:HG12	2.38	0.51
14:T:104:PHE:CE1	14:T:115:GLN:CG	2.94	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.51
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.45	0.51
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:288:VAL:HG11	6:F:303:HIS:HB3	1.91	0.51
8:H:195:ARG:O	8:H:199:ASP:HB2	2.10	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
21:q:101:ASN:OD1	21:q:101:ASN:O	2.28	0.51
5:E:183:PRO:HG2	5:E:194:ASP:HA	1.92	0.51
6:F:267:ARG:HD3	6:F:338:ASP:OD2	2.10	0.51
6:F:414:GLU:OE2	22:r:51:ASN:N	2.29	0.51
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.91	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.51
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.92	0.51
9:I:88:PHE:O	21:q:62:VAL:HG12	2.10	0.51
10:P:45:LYS:HB2	11:Q:118:ALA:CB	2.41	0.51
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.51
16:W:42:TRP:CE3	16:W:93:LEU:HD13	2.45	0.51
18:Z:69:ILE:CG2	20:b:54:PRO:HD3	2.40	0.51
5:E:129:TYR:HE2	5:E:167:LEU:HG	1.74	0.51
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.92	0.51
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.92	0.51
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.51
7:G:614:GLY:HA2	10:P:41:ILE:HG21	1.91	0.51
8:H:26:LYS:HB3	19:a:5:ILE:HG22	1.91	0.51
9:I:152:CYS:SG	25:I:302:SF4:S3	3.09	0.51
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.51
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.74	0.51
5:E:180:VAL:HG11	5:E:224:CYS:HB3	1.92	0.51
6:F:192:ASP:HB3	23:s:57:LEU:CD1	2.38	0.51
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.41	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.51
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.92	0.51
7:G:239:THR:HA	9:I:132:ALA:O	2.11	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.10	0.51
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:210:LEU:HD22	22:r:39:PRO:HD2	1.92	0.51
18:Z:143:TYR:HD1	18:Z:144:THR:N	2.04	0.51
21:q:8:LYS:O	21:q:12:GLN:HG2	2.10	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
2:B:95:PHE:CZ	2:B:145:LEU:HA	2.45	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
4:D:93:GLY:HA3	4:D:458:PHE:CD2	2.46	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
5:E:68:ASN:ND2	23:s:49:ASN:HD21	2.07	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.51
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.51
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.10	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
1:A:81:THR:O	20:b:46:ASN:ND2	2.44	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
8:H:316:PRO:HA	18:Z:58:ARG:NH1	2.19	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
12:R:43:TYR:C	12:R:45:ARG:N	2.69	0.51
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.51
18:Z:111:PHE:CE1	18:Z:117:VAL:HG21	2.45	0.51
21:q:65:THR:OG1	21:q:66:THR:N	2.44	0.51
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.46	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.76	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.51
2:B:121:PHE:CE2	2:B:122:ARG:HD2	2.46	0.51
6:F:42:PHE:CE2	6:F:275:LEU:HD11	2.46	0.51
6:F:280:GLY:O	6:F:356:VAL:HB	2.11	0.51
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
16:W:103:ARG:O	16:W:104:THR:C	2.54	0.51
17:X:56:CYS:HA	17:X:135:ARG:HH12	1.76	0.51
17:X:57:LEU:HG	17:X:61:LYS:HZ1	1.76	0.51
18:Z:28:ARG:HG3	18:Z:28:ARG:O	2.11	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.41	0.50
6:F:279:SER:O	6:F:355:ILE:HA	2.11	0.50
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.41	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
8:H:274:ARG:HH22	28:H:401:UQ9:H3M	1.75	0.50
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.50
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.50
18:Z:72:MET:SD	20:b:53:TYR:HB2	2.51	0.50
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.26	0.50
8:H:77:LEU:HG	8:H:81:LEU:HD11	1.93	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.12	0.50
21:q:85:GLU:CD	21:q:103:PRO:HG3	2.36	0.50
4:D:280:ALA:HB3	15:V:11:LEU:HD23	1.92	0.50
6:F:78:GLY:O	6:F:82:THR:HG23	2.12	0.50
6:F:109:ARG:HH21	6:F:239:PRO:HG3	1.75	0.50
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.50
7:G:643:ARG:O	7:G:644:ASN:C	2.55	0.50
8:H:287:HIS:HE1	24:H:403:3PE:N	2.10	0.50
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.50
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
2:B:121:PHE:CD2	2:B:122:ARG:CG	2.90	0.50
4:D:98:VAL:HG12	4:D:110:ASP:O	2.11	0.50
5:E:235:GLU:HB2	5:E:236:PRO:HD2	1.93	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:35:PHE:O	7:G:101:ASN:HA	2.10	0.50
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:277:MET:HE1	11:Q:153:PRO:HD3	1.94	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:134:ARG:NE	8:H:200:LEU:HD21	2.26	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.50
9:I:58:ALA:HB2	18:Z:36:PHE:CZ	2.45	0.50
10:P:300:TRP:O	10:P:304:LEU:HG	2.11	0.50
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
12:R:38:TYR:CE1	12:R:44:ARG:HD2	2.47	0.50
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.93	0.50
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.47	0.50
6:F:42:PHE:HE2	6:F:275:LEU:HD11	1.75	0.50
6:F:295:PRO:HA	6:F:336:LEU:HA	1.93	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.92	0.50
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.29	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.47	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.54	0.50
14:T:82:ARG:HD2	14:T:125:GLU:OE2	2.10	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.50
5:E:120:MET:HE2	6:F:201:ALA:HA	1.94	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.50
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.50
7:G:617:ARG:NH1	16:W:129:HIS:N	2.60	0.50
7:G:621:LYS:HZ3	16:W:131:PRO:HD3	1.76	0.50
8:H:292:ASN:O	20:b:18:VAL:HG11	2.11	0.50
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
22:r:48:LYS:O	22:r:49:LEU:HB2	2.12	0.50
1:A:106:TRP:HD1	1:A:111:LEU:HD12	1.76	0.50
3:C:104:ASN:O	22:r:97:PRO:HD3	2.12	0.50
3:C:210:ARG:CD	10:P:48:ARG:HD3	2.42	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
4:D:238:LEU:HD23	22:r:37:PRO:HG2	1.94	0.50
5:E:180:VAL:HG13	5:E:181:ASN:H	1.77	0.50
6:F:270:ASN:HD22	6:F:338:ASP:HB2	1.76	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
19:a:14:VAL:O	19:a:18:ILE:HG13	2.10	0.50
22:r:48:LYS:HB2	22:r:52:ASN:HD22	1.76	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.26	0.50
4:D:338:ARG:NH1	18:Z:23:ARG:CA	2.74	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.39	0.50
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.50
17:X:70:PHE:CE2	17:X:74:ILE:HD11	2.46	0.50
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.41	0.50
2:B:166:ASN:CB	2:B:190:TYR:HD2	2.24	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.50
6:F:204:TYR:CE1	27:F:501:FMN:H6	2.47	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
28:H:401:UQ9:H3MA	28:H:401:UQ9:H4MB	1.93	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.50
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
17:X:57:LEU:HD12	17:X:57:LEU:O	2.12	0.50
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.47	0.49
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.93	0.49
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.49
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:172:MET:CE	18:Z:46:GLY:HA2	2.36	0.49
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.49
14:T:97:LYS:NZ	14:T:107:ASP:C	2.69	0.49
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.11	0.49
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
5:E:247:GLY:O	6:F:64:LYS:HE2	2.12	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
9:I:36:TYR:HE2	9:I:38:TYR:CZ	2.29	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
10:P:275:HIS:CE1	10:P:373:LYS:HG2	2.47	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
10:P:375:VAL:C	10:P:377:TYR:H	2.19	0.49
15:V:12:VAL:CG1	15:V:13:GLY:H	2.23	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.49
20:b:23:PHE:CE2	24:b:201:3PE:H252	2.47	0.49
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.49
2:B:222:TYR:O	10:P:137:ARG:NH1	2.45	0.49
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.49
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.36	0.49
7:G:611:THR:CG2	11:Q:105:GLU:HA	2.22	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.49
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.94	0.49
21:q:55:PHE:CD2	22:r:26:LEU:HD22	2.47	0.49
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.94	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.42	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
9:I:54:THR:CG2	20:b:13:TRP:HE1	2.26	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.78	0.49
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.23	0.49
5:E:131:ILE:HA	5:E:187:ILE:HA	1.93	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
8:H:20:LEU:HA	19:a:12:MET:SD	2.52	0.49
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.49
2:B:95:PHE:CE2	2:B:141:MET:HE3	2.47	0.49
2:B:170:TYR:O	2:B:171:TYR:CB	2.60	0.49
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.09	0.49
3:C:97:THR:O	15:V:90:LEU:HD12	2.12	0.49
4:D:362:LYS:HG3	22:r:54:TYR:OH	2.12	0.49
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.49
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.93	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.94	0.49
6:F:278:ILE:HG22	6:F:354:VAL:HB	1.94	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.49
7:G:632:ILE:O	7:G:632:ILE:CG1	2.60	0.49
7:G:643:ARG:O	7:G:646:LEU:N	2.46	0.49
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.47	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
8:H:201:THR:HG21	8:H:211:PHE:CE2	2.48	0.49
2:B:115:ASP:O	2:B:116:ARG:C	2.54	0.49
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.49
3:C:121:ARG:NH2	15:V:114:TRP:HA	2.27	0.49
4:D:209:LYS:HG2	22:r:27:ARG:HH22	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
8:H:72:ILE:HD12	8:H:73:ILE:N	2.27	0.49
18:Z:58:ARG:CB	20:b:45:ILE:HD11	2.42	0.49
22:r:45:PRO:O	22:r:46:SER:HB2	2.13	0.49
2:B:144:ALA:O	2:B:145:LEU:C	2.55	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49
5:E:77:ALA:C	5:E:80:PRO:HD2	2.38	0.49
6:F:117:ALA:HB1	6:F:131:MET:SD	2.53	0.49
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:19:PHE:CD2	19:a:11:ILE:CG2	2.96	0.49
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.94	0.49
12:R:81:GLY:HA2	12:R:88:HIS:CD2	2.47	0.49
17:X:44:MET:O	17:X:48:TRP:CD1	2.66	0.49
21:q:74:PHE:HD2	21:q:75:TRP:CD2	2.31	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.95	0.49
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.12	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
7:G:240:ALA:HA	9:I:117:LYS:HZ3	1.78	0.49
9:I:79:ARG:CZ	22:r:20:LEU:HD22	2.43	0.49
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.47	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.13	0.49
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.94	0.49
4:D:79:ASN:OD1	4:D:79:ASN:N	2.46	0.49
4:D:253:LEU:HB2	22:r:23:LYS:HE2	1.93	0.49
4:D:335:GLU:CD	9:I:37:LYS:HZ2	2.18	0.49
7:G:240:ALA:HA	9:I:117:LYS:NZ	2.28	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.49
10:P:315:THR:HB	10:P:318:LYS:H	1.78	0.49
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.94	0.49
17:X:53:PRO:CD	18:Z:116:TRP:CD1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:7:VAL:HG13	22:r:8:ILE:N	2.28	0.49
2:B:68:ARG:NH1	2:B:70:ARG:HB3	2.28	0.48
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.94	0.48
6:F:233:VAL:CG1	11:Q:164:PHE:HB2	2.43	0.48
7:G:612:PRO:HG2	16:W:129:HIS:CD2	2.48	0.48
9:I:210:LEU:HD23	22:r:39:PRO:O	2.13	0.48
10:P:278:LYS:HB3	10:P:288:PHE:CE2	2.48	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
14:T:93:ILE:HG23	14:T:108:LEU:HD11	1.95	0.48
17:X:47:ARG:CZ	17:X:53:PRO:HG3	2.42	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.48	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.29	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
9:I:105:ARG:HH12	12:R:58:ASN:HB2	1.78	0.48
11:Q:111:LEU:HA	12:R:47:ARG:NH1	2.29	0.48
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.94	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:49:VAL:HG13	7:G:102:ILE:HD13	1.94	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
7:G:614:GLY:CA	10:P:41:ILE:HG21	2.43	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.96	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
33:q:201:CDL:OB9	33:q:201:CDL:H311	2.13	0.48
3:C:210:ARG:HD2	10:P:48:ARG:HD3	1.94	0.48
4:D:238:LEU:CD2	22:r:37:PRO:HG2	2.43	0.48
4:D:359:ASP:OD2	22:r:45:PRO:O	2.31	0.48
4:D:448:VAL:HG21	8:H:204:GLU:CG	2.37	0.48
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.48
6:F:394:LYS:HB2	7:G:155:GLU:HG2	1.95	0.48
8:H:113:VAL:HG23	8:H:136:VAL:HA	1.95	0.48
8:H:292:ASN:HD21	24:H:403:3PE:H122	1.78	0.48
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.48	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
10:P:328:MET:HE1	10:P:377:TYR:C	2.39	0.48
10:P:375:VAL:C	10:P:377:TYR:N	2.69	0.48
21:q:56:PHE:O	21:q:59:HIS:CD2	2.67	0.48
4:D:359:ASP:OD2	22:r:45:PRO:HG2	2.14	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:638:THR:O	7:G:639:LEU:C	2.56	0.48
24:H:403:3PE:H2A1	9:I:70:LEU:HD11	1.94	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
21:q:64:TYR:CD2	21:q:81:MET:HB2	2.48	0.48
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.96	0.48
2:B:112:TYR:CE1	9:I:84:ILE:HD11	2.48	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:266:ARG:NH2	9:I:59:ARG:O	2.45	0.48
4:D:280:ALA:HB1	15:V:11:LEU:CG	2.37	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
9:I:35:THR:CG2	22:r:107:SER:HA	2.44	0.48
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.48	0.48
18:Z:58:ARG:NH2	20:b:46:ASN:HA	2.29	0.48
18:Z:114:THR:O	18:Z:114:THR:CG2	2.60	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.31	0.48
2:B:170:TYR:O	2:B:171:TYR:HB2	2.14	0.48
3:C:98:PHE:HB2	15:V:94:MET:HE3	1.96	0.48
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.48	0.48
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.13	0.48
5:E:147:ILE:O	5:E:151:LEU:HD13	2.14	0.48
6:F:261:TRP:CE2	6:F:265:PHE:HE2	2.31	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.48
7:G:572:HIS:HB2	7:G:699:SER:OG	2.13	0.48
8:H:77:LEU:HG	8:H:81:LEU:CD1	2.44	0.48
9:I:72:MET:CE	22:r:16:SER:HB2	2.43	0.48
9:I:89:GLU:OE1	21:q:58:ARG:HD2	2.13	0.48
10:P:81:ILE:HD11	12:R:46:VAL:HG11	1.96	0.48
14:T:93:ILE:HD13	14:T:108:LEU:HD22	1.95	0.48
16:W:42:TRP:O	16:W:46:VAL:HG23	2.14	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
1:A:76:PRO:HA	8:H:155:LEU:HD23	1.96	0.48
5:E:142:ARG:HG3	5:E:182:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
13:S:27:SER:H	13:S:34:ARG:HH22	1.62	0.48
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.95	0.48
16:W:87:ILE:O	16:W:91:MET:HG3	2.12	0.48
17:X:80:GLU:O	17:X:81:PRO:C	2.55	0.48
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.48
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.14	0.48
6:F:50:ASP:CG	6:F:52:ARG:HB2	2.39	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:202:GLU:O	8:H:202:GLU:HG2	2.14	0.48
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.79	0.48
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.48
5:E:109:MET:HE2	7:G:196:GLY:HA3	1.96	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
8:H:180:PRO:CG	18:Z:43:LEU:HD11	2.44	0.48
9:I:123:CYS:SG	25:I:302:SF4:S3	3.12	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
12:R:60:ALA:O	12:R:61:ILE:C	2.56	0.48
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.96	0.48
18:Z:129:THR:HB	18:Z:132:GLU:CG	2.43	0.48
22:r:54:TYR:HA	22:r:57:ARG:HG2	1.96	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
7:G:140:GLN:HG3	7:G:141:ASP:N	2.28	0.47
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.47
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.47
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.47
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.47
9:I:54:THR:HA	20:b:13:TRP:HE1	1.79	0.47
22:r:32:ALA:HB1	22:r:36:GLN:HE21	1.78	0.47
2:B:131:MET:HE3	2:B:152:MET:SD	2.54	0.47
4:D:338:ARG:NH1	18:Z:23:ARG:N	2.61	0.47
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:MET:CG	6:F:149:MET:HB2	2.44	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.14	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.45	0.47
2:B:93:MET:O	2:B:131:MET:HA	2.15	0.47
2:B:111:ARG:HD2	4:D:208:GLU:OE2	2.15	0.47
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.79	0.47
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.42	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47
6:F:261:TRP:CE2	6:F:265:PHE:CE2	3.02	0.47
6:F:293:SER:CA	6:F:338:ASP:HB3	2.42	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
12:R:46:VAL:HA	12:R:49:VAL:HG23	1.96	0.47
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.47
14:T:104:PHE:CD1	14:T:110:LEU:CB	2.94	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
22:r:25:GLN:H	22:r:25:GLN:CD	2.21	0.47
1:A:106:TRP:HZ3	20:b:19:LEU:HD21	1.78	0.47
2:B:174:SER:HA	3:C:203:LEU:CD2	2.45	0.47
3:C:67:ILE:CD1	15:V:47:TYR:HD2	2.24	0.47
6:F:61:ASP:O	6:F:140:GLU:OE1	2.32	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
17:X:137:LEU:HA	20:b:58:ARG:NH2	2.30	0.47
1:A:65:PHE:CZ	8:H:294:LEU:HD21	2.49	0.47
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.95	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
9:I:107:PRO:HG3	21:q:106:ARG:NH1	2.29	0.47
10:P:272:LEU:CG	10:P:375:VAL:HG21	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.49	0.47
16:W:97:ILE:HG13	16:W:98:LYS:H	1.78	0.47
18:Z:125:TYR:HA	18:Z:128:ARG:HB2	1.95	0.47
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.47
2:B:75:VAL:HG13	2:B:218:LEU:HB3	1.95	0.47
5:E:114:VAL:HG13	5:E:118:TYR:CE2	2.50	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.95	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:150:ARG:NE	10:P:190:GLU:HG2	2.27	0.47
11:Q:129:SER:HB2	15:V:116:ILE:HD12	1.97	0.47
14:T:134:ASP:O	14:T:138:LEU:HG	2.14	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.96	0.47
3:C:66:GLU:O	3:C:69:PRO:HD3	2.14	0.47
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.14	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.47
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.48	0.47
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.45	0.47
5:E:153:ARG:NH2	5:E:154:LYS:HE2	2.29	0.47
5:E:180:VAL:CG1	5:E:181:ASN:N	2.78	0.47
5:E:190:ASN:HB3	5:E:215:PRO:HB3	1.96	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.95	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
7:G:642:VAL:O	7:G:645:ARG:HB3	2.14	0.47
8:H:19:PHE:CE1	19:a:11:ILE:CD1	2.94	0.47
9:I:54:THR:HA	20:b:13:TRP:NE1	2.30	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.02	0.47
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.36	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.29	0.47
15:V:116:ILE:HG23	15:V:116:ILE:O	2.15	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.47
17:X:25:LEU:O	17:X:29:ALA:N	2.48	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
17:X:82:PHE:HB2	17:X:107:PHE:CE1	2.50	0.47
18:Z:58:ARG:HH21	20:b:46:ASN:HA	1.78	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
1:A:65:PHE:O	1:A:69:ILE:HG13	2.14	0.47
4:D:280:ALA:HB2	15:V:11:LEU:HG	1.95	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
7:G:106:SER:O	7:G:107:GLU:C	2.57	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:19:PHE:CB	19:a:12:MET:HG3	2.45	0.47
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.47
13:S:40:ARG:HH12	13:S:84:ALA:HB1	1.79	0.47
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.15	0.47
18:Z:97:ILE:HG13	18:Z:98:MET:HE3	1.95	0.47
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.47
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.47
5:E:153:ARG:HG3	5:E:154:LYS:N	2.28	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.47
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.47
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.50	0.47
19:a:2:TRP:O	19:a:5:ILE:HG12	2.14	0.47
4:D:226:TYR:OH	4:D:232:VAL:HG11	2.12	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.47
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
7:G:544:MET:HE3	7:G:565:PHE:CE2	2.42	0.47
7:G:689:LEU:HD12	7:G:689:LEU:HA	1.79	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.47
13:S:27:SER:O	13:S:34:ARG:NH2	2.48	0.47
13:S:48:HIS:HE1	13:S:95:LEU:CD2	2.25	0.47
16:W:94:GLN:HG3	16:W:98:LYS:NZ	2.29	0.47
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.50	0.46
4:D:85:GLY:N	4:D:86:PRO:CD	2.78	0.46
4:D:420:TYR:CD2	15:V:114:TRP:HH2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.50	0.46
6:F:330:SER:O	6:F:333:GLU:HG2	2.16	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
6:F:424:ILE:HG13	7:G:76:ARG:HD3	1.97	0.46
9:I:93:LEU:O	21:q:93:MET:CG	2.63	0.46
9:I:188:GLU:OE2	12:R:33:HIS:NE2	2.47	0.46
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.46
10:P:192:ARG:HH21	10:P:200:ILE:HG12	1.80	0.46
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.46
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.44	0.46
16:W:97:ILE:CG1	16:W:98:LYS:N	2.75	0.46
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.46
21:q:117:VAL:HB	21:q:122:GLU:HB3	1.96	0.46
3:C:73:GLN:HG2	15:V:103:LEU:HD21	1.96	0.46
4:D:99:LEU:HB2	4:D:101:LEU:HD11	1.95	0.46
6:F:336:LEU:HD23	6:F:336:LEU:H	1.79	0.46
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.97	0.46
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.46
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.46
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.51	0.46
22:r:50:SER:O	22:r:51:ASN:C	2.58	0.46
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.97	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
7:G:75:CYS:SG	26:G:803:FES:S1	3.13	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
7:G:639:LEU:O	7:G:640:ASP:C	2.58	0.46
8:H:207:LEU:HD23	8:H:279:ARG:NH2	2.29	0.46
12:R:38:TYR:OH	12:R:47:ARG:NH2	2.48	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
1:A:73:LEU:O	8:H:160:TYR:OH	2.32	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:30:TYR:CE1	19:a:1:MET:C	2.94	0.46
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.51	0.46
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
12:R:38:TYR:CD2	12:R:48:PHE:HE2	2.33	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.15	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:LEU:HD23	22:r:60:ARG:CG	2.46	0.46
5:E:163:THR:HB	5:E:164:PRO:HD2	1.97	0.46
10:P:331:ASP:O	10:P:332:LEU:C	2.59	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
17:X:54:ARG:NH2	18:Z:116:TRP:HB2	2.31	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.81	0.46
3:C:70:LYS:O	15:V:104:VAL:N	2.47	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.15	0.46
6:F:270:ASN:HD21	6:F:340:ASP:N	2.13	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.51	0.46
15:V:72:LEU:C	15:V:72:LEU:CD1	2.89	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
18:Z:54:ASN:HA	18:Z:57:ARG:HD3	1.96	0.46
2:B:97:LEU:HB2	2:B:134:ALA:O	2.16	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.15	0.46
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.43	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.49	0.46
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.51	0.46
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.80	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
5:E:176:LEU:HD13	5:E:186:GLN:HB2	1.98	0.46
6:F:77:LEU:O	6:F:81:LYS:HG2	2.16	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46
9:I:155:CYS:SG	25:I:302:SF4:S2	3.14	0.46
12:R:51:ARG:HD2	21:q:125:VAL:CG1	2.46	0.46
17:X:78:CYS:SG	17:X:114:LYS:HD2	2.56	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.51	0.46
22:r:91:GLU:OE1	22:r:91:GLU:HA	2.15	0.46
1:A:73:LEU:N	1:A:74:PRO:HD2	2.31	0.46
2:B:93:MET:HE1	2:B:95:PHE:CD1	2.51	0.46
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:318:ILE:HG22	6:F:326:LEU:CA	2.45	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
7:G:643:ARG:HA	7:G:646:LEU:HD12	1.98	0.46
7:G:648:GLU:HG2	13:S:66:TRP:CZ2	2.50	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.98	0.46
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
8:H:88:PRO:CG	8:H:105:ILE:HD11	2.46	0.46
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.50	0.46
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.46
18:Z:36:PHE:O	18:Z:40:ILE:HG12	2.16	0.46
21:q:59:HIS:HE1	21:q:60:ARG:NE	2.14	0.46
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.27	0.46
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.46
6:F:88:ARG:HB2	6:F:247:THR:OG1	2.16	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:593:SER:O	7:G:643:ARG:NH2	2.46	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
12:R:104:CYS:C	12:R:106:TYR:N	2.73	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
15:V:50:GLN:HE22	22:r:93:LYS:HG3	1.80	0.46
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.46
17:X:46:CYS:HB3	17:X:56:CYS:SG	2.56	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
2:B:166:ASN:O	2:B:166:ASN:CG	2.59	0.45
4:D:209:LYS:HE3	22:r:27:ARG:HD3	1.98	0.45
6:F:93:PHE:O	6:F:94:PRO:C	2.58	0.45
6:F:120:GLY:O	6:F:121:GLU:C	2.59	0.45
7:G:301:ARG:HA	7:G:572:HIS:CD2	2.52	0.45
8:H:120:GLY:HA3	8:H:132:ALA:HB2	1.98	0.45
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.45
10:P:338:LEU:HD23	10:P:338:LEU:HA	1.83	0.45
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:131:VAL:N	20:b:59:ASP:OD1	2.49	0.45
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.16	0.45
20:b:19:LEU:HD22	24:b:201:3PE:H221	1.98	0.45
22:r:20:LEU:HD12	22:r:21:GLN:N	2.31	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
5:E:222:PHE:H	5:E:225:GLU:CD	2.23	0.45
6:F:45:LEU:O	6:F:46:TYR:HB2	2.16	0.45
7:G:165:ILE:O	7:G:213:MET:HA	2.16	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.97	0.45
12:R:101:THR:HG22	12:R:112:LYS:HB2	1.99	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
20:b:38:TYR:O	20:b:39:THR:C	2.58	0.45
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.45
2:B:120:VAL:CG1	2:B:121:PHE:N	2.80	0.45
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.45
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.82	0.45
4:D:266:ARG:HB3	9:I:66:LEU:HD21	1.97	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:73:HIS:ND1	6:F:236:PHE:CD1	2.85	0.45
6:F:261:TRP:CD2	6:F:265:PHE:HE2	2.34	0.45
7:G:43:VAL:HB	7:G:47:THR:HG21	1.99	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
8:H:127:TYR:OH	8:H:205:SER:HA	2.16	0.45
9:I:178:GLU:OE2	21:q:119:ALA:HB2	2.16	0.45
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.45
14:T:144:ILE:O	14:T:148:ILE:HG12	2.15	0.45
2:B:81:LEU:HD11	8:H:53:MET:HE1	1.98	0.45
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.98	0.45
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:252:SER:HB2	18:Z:20:ASP:O	2.16	0.45
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.16	0.45
6:F:47:GLY:O	6:F:48:ARG:HB2	2.17	0.45
6:F:270:ASN:HD22	6:F:338:ASP:CB	2.29	0.45
6:F:394:LYS:HD3	7:G:155:GLU:HB3	1.97	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
10:P:295:LEU:O	10:P:296:PHE:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:72:VAL:HG21	12:R:77:ILE:CD1	2.46	0.45
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.97	0.45
1:A:113:TRP:CH2	8:H:287:HIS:CD2	3.04	0.45
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.46	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:335:GLU:HG2	9:I:37:LYS:HD2	1.97	0.45
5:E:226:PRO:HB2	5:E:229:GLY:O	2.16	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.98	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.51	0.45
12:R:70:ASN:HB2	12:R:111:PHE:HD2	1.81	0.45
14:T:100:VAL:O	14:T:142:GLN:HB2	2.15	0.45
14:T:123:GLU:HG2	14:T:130:ILE:CD1	2.47	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
21:q:68:MET:O	21:q:69:ASN:C	2.57	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
3:C:70:LYS:O	15:V:103:LEU:HA	2.16	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:254:ARG:HE	22:r:25:GLN:HB3	1.82	0.45
4:D:375:MET:HE1	7:G:126:LEU:CA	2.46	0.45
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.85	0.45
6:F:106:SER:HB2	6:F:111:LYS:HZ2	1.81	0.45
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.81	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
15:V:99:PRO:HD2	15:V:100:TRP:CE3	2.51	0.45
2:B:121:PHE:HE2	2:B:122:ARG:HD2	1.81	0.45
2:B:197:THR:O	2:B:200:ALA:HB3	2.17	0.45
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.81	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:202:TRP:CH2	9:I:76:TYR:HE2	2.35	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
5:E:58:ASN:O	5:E:62:ILE:HG12	2.16	0.45
6:F:87:GLY:H	6:F:92:GLY:CA	2.29	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.52	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
10:P:315:THR:O	10:P:316:LYS:C	2.58	0.45
14:T:100:VAL:O	14:T:141:PRO:HD2	2.17	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
21:q:55:PHE:HD1	21:q:55:PHE:H	1.65	0.45
21:q:68:MET:HG2	21:q:115:PHE:HE2	1.82	0.45
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
2:B:82:ILE:CA	8:H:57:MET:HE1	2.42	0.45
4:D:84:PHE:CZ	4:D:89:PRO:HG3	2.52	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:72:GLY:O	6:F:76:ILE:HG13	2.17	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.45
6:F:227:PRO:HB3	7:G:95:PRO:HD2	1.98	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
7:G:649:VAL:HA	13:S:20:ARG:NE	2.31	0.45
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.45
9:I:67:ILE:HG13	29:I:301:PC1:H231	1.98	0.45
9:I:184:LEU:HD23	11:Q:114:TRP:CH2	2.51	0.45
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
16:W:23:ILE:CD1	16:W:84:LEU:HD21	2.47	0.45
16:W:67:ARG:HD2	16:W:71:MET:SD	2.57	0.45
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.31	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.16	0.45
33:q:201:CDL:H341	33:q:201:CDL:H171	1.99	0.45
2:B:81:LEU:CD1	8:H:53:MET:HE1	2.47	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.45
5:E:55:THR:O	5:E:56:PRO:C	2.59	0.45
7:G:160:VAL:O	7:G:174:THR:HG22	2.17	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
8:H:134:ARG:HB3	8:H:200:LEU:CD2	2.46	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
8:H:312:ALA:HB2	20:b:41:TYR:HB2	1.99	0.45
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.45
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:134:ASP:O	17:X:135:ARG:C	2.58	0.45
21:q:4:VAL:HA	21:q:7:LEU:HD12	1.99	0.45
2:B:95:PHE:CD1	2:B:145:LEU:HD12	2.52	0.45
4:D:85:GLY:HA3	4:D:95:LEU:O	2.17	0.45
4:D:97:LEU:O	4:D:98:VAL:C	2.60	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
6:F:61:ASP:O	6:F:256:ARG:NH2	2.50	0.45
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.93	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.45
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.45
13:S:40:ARG:HD2	13:S:88:THR:OG1	2.16	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.45
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.83	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
5:E:62:ILE:O	5:E:66:VAL:HG23	2.17	0.44
5:E:242:PHE:O	6:F:257:ARG:NH1	2.50	0.44
6:F:75:TRP:O	6:F:79:GLU:HG2	2.17	0.44
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.44
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.44
8:H:179:TRP:NE1	18:Z:39:GLY:O	2.39	0.44
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
9:I:88:PHE:CE2	21:q:30:ALA:HA	2.51	0.44
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.65	0.44
10:P:82:ILE:HD12	10:P:105:PHE:CE1	2.52	0.44
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.44
17:X:28:ALA:HB2	17:X:82:PHE:CZ	2.52	0.44
20:b:59:ASP:OD1	20:b:59:ASP:N	2.49	0.44
21:q:44:TYR:CD1	21:q:68:MET:HG3	2.52	0.44
22:r:54:TYR:CE2	22:r:58:ASP:HB3	2.51	0.44
3:C:98:PHE:HE1	15:V:44:TYR:CD1	2.34	0.44
4:D:87:GLN:OE1	8:H:127:TYR:CZ	2.71	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.44
8:H:172:MET:SD	18:Z:49:ARG:CG	3.05	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:225:ALA:HB1	10:P:291:TYR:CD1	2.52	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
19:a:1:MET:HG3	33:q:201:CDL:HB21	1.99	0.44
21:q:3:LEU:HD12	21:q:6:VAL:CG2	2.48	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
6:F:51:TRP:HB3	6:F:133:HIS:O	2.17	0.44
6:F:273:THR:HA	6:F:292:MET:H	1.82	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.98	0.44
8:H:27:ILE:O	8:H:31:MET:HG3	2.16	0.44
8:H:133:LEU:HA	8:H:136:VAL:CG1	2.48	0.44
8:H:175:LEU:HD21	29:I:301:PC1:H2C1	1.99	0.44
14:T:87:LEU:HA	14:T:87:LEU:HD23	1.72	0.44
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.66	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:243:GLY:O	6:F:257:ARG:HD2	2.18	0.44
6:F:379:CYS:SG	25:F:502:SF4:S2	3.16	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:74:ALA:HB3	8:H:75:PRO:CD	2.48	0.44
9:I:203:ALA:CB	21:q:88:ARG:NH1	2.80	0.44
10:P:59:PHE:CD1	10:P:83:PRO:HG2	2.52	0.44
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.44
21:q:23:LEU:HD11	21:q:33:ILE:HD13	1.99	0.44
21:q:44:TYR:CE1	21:q:68:MET:HE3	2.51	0.44
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.44
5:E:62:ILE:HG23	5:E:81:VAL:HG22	2.00	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
6:F:383:THR:HG23	7:G:120:LEU:HD23	1.98	0.44
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:593:SER:OG	7:G:639:LEU:HD22	2.18	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:42:VAL:O	13:S:46:LYS:HG3	2.18	0.44
17:X:137:LEU:O	17:X:138:PRO:C	2.58	0.44
21:q:86:TRP:CD2	21:q:98:PRO:HG2	2.52	0.44
2:B:97:LEU:HD23	2:B:136:THR:O	2.18	0.44
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
6:F:292:MET:O	6:F:293:SER:HB2	2.17	0.44
7:G:144:MET:HG3	7:G:144:MET:O	2.17	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
24:H:403:3PE:H372	9:I:61:LEU:O	2.18	0.44
10:P:275:HIS:CB	10:P:372:ALA:HB1	2.48	0.44
10:P:358:THR:O	10:P:359:TYR:C	2.60	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
13:S:24:CYS:SG	13:S:61:VAL:O	2.75	0.44
14:T:132:ASP:O	14:T:133:ILE:C	2.60	0.44
14:T:140:CYS:SG	14:T:143:GLU:CB	3.03	0.44
15:V:56:LEU:O	15:V:57:ASP:C	2.61	0.44
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.44
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.44
2:B:167:GLY:HA3	9:I:150:THR:HB	1.99	0.44
4:D:202:TRP:CH2	9:I:76:TYR:CE2	3.06	0.44
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.46	0.44
6:F:48:ARG:HA	6:F:48:ARG:NH1	2.29	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.31	0.44
7:G:36:VAL:HG22	7:G:102:ILE:HD12	1.98	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:621:LYS:NZ	16:W:131:PRO:HD3	2.33	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.99	0.44
9:I:79:ARG:NE	22:r:20:LEU:HD22	2.33	0.44
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
2:B:114:MET:HE3	2:B:119:VAL:HG12	2.00	0.44
2:B:202:LEU:HD21	9:I:86:TYR:HB2	1.95	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:127:ASP:OD1	7:G:127:ASP:C	2.59	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:557:ARG:HD3	21:q:144:TYR:CZ	2.53	0.44
8:H:1:MET:HE3	19:a:29:PHE:CD1	2.52	0.44
8:H:316:PRO:HG3	18:Z:57:ARG:CB	2.44	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:327:VAL:HG22	10:P:328:MET:N	2.32	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
13:S:16:LEU:HD13	13:S:69:TYR:CE1	2.52	0.44
14:T:141:PRO:O	14:T:144:ILE:HB	2.18	0.44
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	2.00	0.44
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.44
4:D:384:LEU:HD21	7:G:144:MET:HE1	2.00	0.44
5:E:117:PHE:HB2	6:F:220:GLN:HE21	1.83	0.44
6:F:67:GLU:O	6:F:71:LYS:HG2	2.18	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:68:ARG:O	7:G:189:ILE:HD11	2.18	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:339:ALA:O	7:G:545:LEU:HD12	2.18	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.44
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
13:S:19:ILE:CD1	13:S:94:VAL:HG11	2.48	0.44
13:S:51:LEU:CD1	13:S:95:LEU:HD12	2.46	0.44
17:X:58:LYS:O	17:X:59:GLU:C	2.59	0.44
17:X:140:ASN:HD21	17:X:144:SER:N	2.16	0.44
18:Z:69:ILE:CG2	20:b:54:PRO:CD	2.96	0.44
21:q:92:CYS:O	22:r:34:ARG:HG3	2.18	0.44
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
2:B:121:PHE:CE2	2:B:122:ARG:CG	3.01	0.43
2:B:170:TYR:O	2:B:171:TYR:CD2	2.71	0.43
4:D:82:LEU:HB2	4:D:99:LEU:CD1	2.41	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:231:THR:CG2	6:F:303:HIS:HA	2.47	0.43
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.43
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:196:ALA:C	8:H:198:PHE:N	2.76	0.43
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.43
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
13:S:51:LEU:HA	13:S:52:PRO:HD3	1.86	0.43
18:Z:98:MET:HB3	18:Z:104:TRP:CD1	2.53	0.43
33:q:201:CDL:HB61	33:q:201:CDL:OA9	2.18	0.43
2:B:94:THR:CG2	2:B:104:MET:SD	3.07	0.43
3:C:78:SER:C	3:C:80:LEU:H	2.26	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.43
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.43
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.99	0.43
6:F:317:VAL:HG22	6:F:356:VAL:HG22	2.00	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.43
7:G:612:PRO:HG2	16:W:129:HIS:HD2	1.83	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
17:X:37:ASP:OD2	20:b:70:PRO:HD2	2.17	0.43
1:A:72:LEU:HB3	8:H:151:LEU:CD2	2.48	0.43
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.48	0.43
2:B:112:TYR:OH	9:I:91:GLY:HA3	2.19	0.43
2:B:223:ARG:C	10:P:138:ASN:HD21	2.25	0.43
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.82	0.43
13:S:30:SER:O	13:S:31:GLN:C	2.59	0.43
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.74	0.43
1:A:10:ASN:ND2	8:H:84:SER:OG	2.51	0.43
3:C:70:LYS:HG2	15:V:104:VAL:HG23	2.01	0.43
3:C:224:GLU:OE2	10:P:45:LYS:HD3	2.18	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.40	0.43
7:G:141:ASP:O	7:G:145:MET:HG2	2.18	0.43
8:H:113:VAL:CG2	8:H:136:VAL:HA	2.49	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
12:R:104:CYS:C	12:R:106:TYR:H	2.27	0.43
18:Z:121:ILE:HA	18:Z:124:MET:HE2	1.99	0.43
20:b:82:LYS:HE2	20:b:82:LYS:HB3	1.81	0.43
22:r:54:TYR:C	22:r:56:THR:N	2.76	0.43
2:B:121:PHE:CZ	2:B:122:ARG:NE	2.86	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:104:GLU:OE1	8:H:130:PHE:HE2	2.01	0.43
5:E:232:SER:HB2	6:F:37:ASP:OD1	2.18	0.43
7:G:346:VAL:HG21	7:G:548:LEU:HD21	2.00	0.43
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
13:S:18:GLU:O	13:S:19:ILE:HD13	2.19	0.43
4:D:264:ASN:O	9:I:65:GLU:OE1	2.36	0.43
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.01	0.43
5:E:181:ASN:OD1	5:E:221:ARG:HD2	2.18	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
5:E:247:GLY:O	6:F:64:LYS:CD	2.67	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.48	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:639:LEU:HD21	7:G:643:ARG:NH2	2.34	0.43
8:H:179:TRP:HE1	18:Z:43:LEU:HG	1.81	0.43
8:H:277:TYR:CE2	24:H:403:3PE:H281	2.54	0.43
17:X:46:CYS:SG	17:X:135:ARG:HD3	2.58	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
21:q:79:GLY:O	21:q:82:VAL:HG22	2.19	0.43
1:A:72:LEU:HB3	8:H:151:LEU:HD21	2.01	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:381:GLN:HG3	7:G:74:ASN:OD1	2.19	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.34	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
28:H:401:UQ9:C9	28:H:401:UQ9:H1MB	2.48	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
12:R:40:GLU:HG3	12:R:41:LYS:HG2	2.00	0.43
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.19	0.43
18:Z:111:PHE:CE2	18:Z:117:VAL:HG21	2.52	0.43
2:B:81:LEU:HD11	29:q:202:PC1:H361	2.00	0.43
3:C:104:ASN:HD22	22:r:94:ALA:HB1	1.83	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
5:E:38:PHE:O	7:G:205:GLN:NE2	2.52	0.43
5:E:142:ARG:HG3	5:E:182:ALA:HB3	2.00	0.43
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.43
9:I:50:MET:CE	20:b:10:LYS:HG2	2.49	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.43
11:Q:52:LEU:HD23	16:W:19:SER:O	2.19	0.43
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.53	0.43
18:Z:98:MET:HE2	18:Z:98:MET:HA	2.01	0.43
1:A:109:LYS:HD2	1:A:112:GLU:HB2	2.00	0.43
2:B:172:HIS:CE1	2:B:179:ARG:HD3	2.54	0.43
3:C:70:LYS:HA	15:V:102:PRO:C	2.44	0.43
3:C:97:THR:O	15:V:90:LEU:CD1	2.67	0.43
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.54	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
17:X:120:PRO:HG3	20:b:71:GLN:NE2	2.34	0.43
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.18	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
6:F:46:TYR:O	6:F:48:ARG:HG2	2.19	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
6:F:394:LYS:CB	7:G:155:GLU:HG2	2.48	0.43
6:F:398:ARG:HH22	7:G:155:GLU:CD	2.26	0.43
7:G:31:LEU:HA	7:G:31:LEU:HD23	1.79	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:201:THR:C	8:H:203:GLY:N	2.76	0.43
8:H:295:PRO:HG3	24:b:201:3PE:H382	2.01	0.43
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.18	0.43
14:T:99:SER:O	14:T:141:PRO:HG2	2.19	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
21:q:34:ARG:HD3	21:q:54:GLN:OE1	2.18	0.43
2:B:194:CYS:HB2	9:I:153:ILE:C	2.43	0.42
4:D:159:LEU:HD23	22:r:60:ARG:HG2	2.00	0.42
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.19	0.42
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.49	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.42
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.42
8:H:272:TRP:CZ2	9:I:74:LEU:HB2	2.54	0.42
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
17:X:69:ASN:O	17:X:73:GLN:HG3	2.19	0.42
18:Z:69:ILE:HG23	20:b:54:PRO:CD	2.46	0.42
2:B:104:MET:HE3	2:B:104:MET:HB2	1.61	0.42
3:C:49:ARG:HH21	3:C:54:HIS:CG	2.37	0.42
5:E:162:THR:HG22	5:E:163:THR:N	2.34	0.42
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.54	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:409:ILE:HG12	6:F:446:LEU:HD23	1.96	0.42
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:401:LEU:HD21	7:G:466:LEU:HD11	2.01	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.42
12:R:43:TYR:C	12:R:45:ARG:H	2.27	0.42
14:T:108:LEU:HD23	14:T:108:LEU:C	2.44	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
21:q:125:VAL:O	21:q:125:VAL:CG2	2.67	0.42
4:D:101:LEU:HD12	4:D:101:LEU:N	2.33	0.42
4:D:101:LEU:HG	4:D:106:VAL:HA	2.02	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.48	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
22:r:54:TYR:HA	22:r:57:ARG:CG	2.48	0.42
1:A:65:PHE:HE2	8:H:294:LEU:HD21	1.76	0.42
2:B:100:CYS:HB2	2:B:134:ALA:CB	2.35	0.42
5:E:180:VAL:CG1	5:E:181:ASN:H	2.32	0.42
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.34	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.31	0.42
8:H:312:ALA:CB	20:b:41:TYR:HB2	2.50	0.42
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.48	0.42
29:I:301:PC1:H221	18:Z:35:MET:HE2	2.00	0.42
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.54	0.42
11:Q:51:GLN:HB3	16:W:26:ARG:HH22	1.84	0.42
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
4:D:84:PHE:C	4:D:86:PRO:CD	2.92	0.42
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.02	0.42
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.42
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.42
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
10:P:265:PHE:CD1	10:P:334:GLY:HA3	2.55	0.42
12:R:81:GLY:CA	12:R:88:HIS:CD2	3.02	0.42
13:S:16:LEU:CD1	13:S:19:ILE:HD11	2.47	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
18:Z:10:MET:HB3	18:Z:10:MET:HE2	1.75	0.42
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
3:C:85:ILE:CD1	3:C:140:ILE:HD11	2.50	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
4:D:317:ASP:HA	9:I:35:THR:O	2.19	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
5:E:114:VAL:O	5:E:118:TYR:HD2	2.02	0.42
6:F:147:ARG:HD3	6:F:191:TYR:HD2	1.71	0.42
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:360:LYS:HE3	7:G:632:ILE:CB	2.38	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
9:I:113:CYS:SG	25:I:303:SF4:S4	3.17	0.42
12:R:77:ILE:HG12	12:R:78:ALA:N	2.34	0.42
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.42
18:Z:98:MET:HA	18:Z:101:VAL:HG23	2.01	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
22:r:54:TYR:HD1	22:r:57:ARG:HG3	1.83	0.42
3:C:186:ILE:HB	4:D:113:ILE:HD11	2.02	0.42
4:D:84:PHE:CE2	4:D:89:PRO:HG3	2.53	0.42
5:E:101:ALA:HA	5:E:106:VAL:HG22	2.01	0.42
6:F:268:GLU:HG2	6:F:269:ARG:N	2.34	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.50	0.42
8:H:65:THR:O	8:H:66:THR:HG23	2.19	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.42
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42
10:P:283:MET:SD	10:P:369:THR:HG21	2.60	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
12:R:76:ILE:HD11	12:R:92:TYR:CB	2.48	0.42
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.42
18:Z:65:LEU:CB	20:b:50:PRO:O	2.63	0.42
22:r:113:LEU:HD13	22:r:113:LEU:HA	1.92	0.42
2:B:70:ARG:HG3	2:B:72:GLU:H	1.85	0.42
2:B:202:LEU:HD21	9:I:86:TYR:HB3	1.99	0.42
3:C:224:GLU:OE1	11:Q:118:ALA:HB2	2.20	0.42
5:E:110:ARG:HD3	5:E:110:ARG:HA	1.81	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:51:TRP:HB2	6:F:133:HIS:O	2.19	0.42
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.42
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.42
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.55	0.42
8:H:200:LEU:CD2	8:H:282:TYR:CD1	3.03	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:135:ARG:NH1	12:R:61:ILE:HG23	2.28	0.42
10:P:263:PHE:CD2	10:P:333:PRO:O	2.66	0.42
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.42
17:X:143:HIS:ND1	18:Z:115:ARG:HA	2.35	0.42
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.55	0.42
5:E:64:ALA:HA	5:E:67:LYS:HD3	2.02	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:360:LYS:HB3	7:G:632:ILE:HB	2.01	0.42
10:P:243:ALA:O	10:P:244:ASP:C	2.62	0.42
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.01	0.42
14:T:133:ILE:HG23	14:T:134:ASP:N	2.35	0.42
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.42
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
1:A:21:ALA:O	8:H:60:PRO:CG	2.68	0.42
2:B:126:ARG:NH2	8:H:61:MET:CB	2.74	0.42
3:C:64:VAL:HG21	3:C:85:ILE:HD11	2.01	0.42
3:C:232:PHE:CE1	7:G:244:GLU:HG3	2.55	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.55	0.42
5:E:226:PRO:HA	6:F:286:CYS:HB3	2.02	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.42
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
14:T:138:LEU:HD11	14:T:147:TYR:CD2	2.54	0.42
16:W:23:ILE:CG2	16:W:83:ASP:HB2	2.50	0.42
17:X:91:TYR:OH	19:a:28:LYS:HE2	2.19	0.42
17:X:141:PRO:C	17:X:143:HIS:H	2.27	0.42
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.42
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.83	0.41
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.41
5:E:131:ILE:HD13	5:E:151:LEU:HD21	2.02	0.41
6:F:69:LEU:CD1	6:F:143:LEU:HD21	2.49	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.41
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:79:ARG:NH2	22:r:20:LEU:HD22	2.34	0.41
10:P:99:ASP:HB3	10:P:102:GLN:CD	2.45	0.41
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.41
20:b:69:HIS:HB3	20:b:72:ASP:CG	2.45	0.41
2:B:121:PHE:HE2	2:B:122:ARG:CD	2.33	0.41
5:E:62:ILE:HD13	5:E:84:LEU:HD13	2.01	0.41
7:G:53:CYS:SG	7:G:102:ILE:HG21	2.60	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:639:LEU:C	7:G:641:GLN:N	2.77	0.41
7:G:639:LEU:O	7:G:641:GLN:N	2.54	0.41
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.63	0.41
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.41
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.41
33:q:201:CDL:H511	22:r:8:ILE:HD11	2.01	0.41
2:B:144:ALA:O	2:B:147:LYS:N	2.54	0.41
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.41
4:D:375:MET:CG	7:G:121:LEU:HD22	2.48	0.41
5:E:183:PRO:O	5:E:194:ASP:N	2.53	0.41
6:F:77:LEU:HD13	6:F:100:SER:HA	2.03	0.41
6:F:102:MET:HG3	6:F:149:MET:HB2	2.02	0.41
6:F:268:GLU:CG	6:F:269:ARG:H	2.32	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41
7:G:282:ASN:HB2	7:G:285:TRP:O	2.20	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:187:ILE:CG1	9:I:63:TRP:CH2	3.04	0.41
9:I:48:VAL:CG1	9:I:53:ALA:HB2	2.50	0.41
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.41
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.41
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.03	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:184:LEU:CD2	11:Q:114:TRP:CH2	3.03	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:283:MET:HE3	10:P:357:ARG:NH1	2.35	0.41
13:S:23:LEU:O	13:S:57:GLU:HA	2.20	0.41
14:T:93:ILE:CD1	14:T:108:LEU:HD22	2.49	0.41
14:T:133:ILE:HG13	14:T:137:LYS:NZ	2.36	0.41
16:W:86:VAL:O	16:W:87:ILE:C	2.61	0.41
17:X:48:TRP:NE1	20:b:55:VAL:HG22	2.32	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
22:r:41:LEU:N	22:r:41:LEU:HD22	2.35	0.41
1:A:104:TYR:HA	1:A:107:THR:OG1	2.21	0.41
3:C:52:VAL:O	3:C:56:GLN:HG3	2.20	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.21	0.41
6:F:54:LYS:HG3	6:F:55:GLY:H	1.85	0.41
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.36	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:384:PRO:HA	7:G:119:PHE:CD2	2.54	0.41
6:F:427:LEU:HB2	27:F:501:FMN:HM71	2.02	0.41
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:102:ILE:O	7:G:103:LEU:C	2.60	0.41
7:G:161:GLU:OE2	12:R:96:ASP:N	2.53	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.85	0.41
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.41
7:G:667:GLN:HB3	13:S:42:VAL:HG13	2.01	0.41
8:H:135:ALA:O	8:H:138:GLN:HG2	2.19	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
28:H:401:UQ9:H1MB	28:H:401:UQ9:C8	2.50	0.41
13:S:36:PHE:HZ	13:S:44:LEU:HD12	1.86	0.41
14:T:93:ILE:HG23	14:T:108:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:93:ILE:HD13	14:T:108:LEU:CD2	2.51	0.41
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.41
17:X:41:LYS:HD2	20:b:56:PRO:HG3	2.01	0.41
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.21	0.41
17:X:142:TYR:O	17:X:143:HIS:C	2.62	0.41
21:q:110:TRP:HB2	21:q:113:HIS:CE1	2.55	0.41
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.55	0.41
3:C:232:PHE:HE2	9:I:126:GLN:OE1	2.04	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
5:E:176:LEU:HB3	5:E:191:TYR:OH	2.20	0.41
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:544:MET:HE2	7:G:546:PHE:CZ	2.55	0.41
8:H:33:LEU:CD1	9:I:76:TYR:CD1	2.99	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
9:I:41:LYS:HD3	22:r:112:TYR:HE2	1.85	0.41
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.02	0.41
9:I:130:ILE:HD11	9:I:145:TYR:HE1	1.86	0.41
9:I:140:ARG:O	9:I:141:ARG:HG2	2.20	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.41
12:R:38:TYR:CD2	12:R:48:PHE:CE2	3.08	0.41
17:X:17:GLU:HG3	17:X:64:ASN:ND2	2.34	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
2:B:154:GLU:O	2:B:156:ARG:N	2.52	0.41
4:D:85:GLY:C	4:D:87:GLN:H	2.29	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.41
5:E:167:LEU:HB3	5:E:168:PHE:CD1	2.56	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:69:LEU:HD11	6:F:143:LEU:HG	2.03	0.41
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.84	0.41
9:I:82:ALA:CA	22:r:26:LEU:HD21	2.50	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:P:88:VAL:HG12	10:P:92:MET:HE2	2.02	0.41
10:P:295:LEU:O	10:P:298:TYR:N	2.53	0.41
14:T:110:LEU:HG	14:T:114:ASP:HB3	1.98	0.41
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.41
15:V:94:MET:SD	15:V:99:PRO:HG3	2.60	0.41
17:X:120:PRO:HG3	20:b:71:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:54:TYR:CD1	22:r:57:ARG:HG3	2.56	0.41
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.55	0.41
2:B:124:SER:O	2:B:125:PRO:C	2.62	0.41
2:B:166:ASN:HB2	2:B:190:TYR:CD2	2.45	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.02	0.41
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.41
4:D:271:ARG:HG2	8:H:281:ARG:CG	2.44	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.60	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.47	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
9:I:162:CYS:SG	25:I:303:SF4:S2	3.19	0.41
18:Z:142:TRP:C	18:Z:143:TYR:CD2	2.99	0.41
24:b:201:3PE:H2E1	24:b:201:3PE:H2B2	1.80	0.41
1:A:67:LEU:O	1:A:70:ALA:HB3	2.21	0.41
2:B:111:ARG:HD2	4:D:208:GLU:CD	2.46	0.41
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.42	0.41
3:C:216:LYS:HG3	10:P:209:ARG:HH11	1.85	0.41
4:D:144:MET:HE2	4:D:144:MET:HB2	1.92	0.41
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
5:E:182:ALA:O	5:E:183:PRO:C	2.59	0.41
6:F:303:HIS:O	6:F:304:ALA:HB3	2.20	0.41
6:F:309:GLY:HA3	6:F:313:ASN:HD22	1.85	0.41
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.41
7:G:127:ASP:HA	12:R:106:TYR:OH	2.20	0.41
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.41
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.41
7:G:674:LEU:HD11	13:S:46:LYS:HE2	2.03	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.41
8:H:130:PHE:HA	8:H:133:LEU:HD12	2.03	0.41
8:H:249:ILE:CD1	17:X:99:HIS:HB3	2.50	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
12:R:44:ARG:O	12:R:47:ARG:HB2	2.21	0.41
12:R:79:CYS:O	12:R:88:HIS:CE1	2.74	0.41
17:X:20:VAL:CG1	17:X:24:VAL:HB	2.51	0.41
17:X:21:SER:O	17:X:22:SER:C	2.63	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:45:LEU:HD21	20:b:58:ARG:HE	1.86	0.41
18:Z:98:MET:HB3	18:Z:104:TRP:HD1	1.86	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
20:b:23:PHE:HE2	24:b:201:3PE:H252	1.85	0.41
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.41
21:q:78:ASP:OD1	21:q:78:ASP:O	2.39	0.41
2:B:71:ALA:O	2:B:75:VAL:HG23	2.21	0.41
3:C:241:PHE:HB3	3:C:242:PRO:HD2	2.03	0.41
4:D:97:LEU:HD21	4:D:447:VAL:HG11	2.03	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:238:LEU:HD21	18:Z:7:LYS:HD3	2.01	0.41
4:D:254:ARG:NH1	22:r:23:LYS:O	2.53	0.41
6:F:418:GLN:NE2	22:r:53:TYR:OH	2.53	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:176:CYS:SG	25:G:802:SF4:S1	3.19	0.41
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
9:I:75:SER:O	22:r:12:ARG:HG2	2.21	0.41
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.51	0.41
14:T:104:PHE:CE1	14:T:105:MET:HG2	2.56	0.41
1:A:95:VAL:HG11	8:H:302:MET:CG	2.51	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
4:D:88:HIS:N	4:D:89:PRO:CD	2.84	0.40
4:D:97:LEU:O	4:D:97:LEU:HG	2.20	0.40
4:D:99:LEU:HB2	4:D:101:LEU:CD1	2.51	0.40
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.03	0.40
5:E:68:ASN:ND2	23:s:56:ARG:NH2	2.68	0.40
5:E:184:MET:HE3	5:E:184:MET:HB3	1.95	0.40
6:F:66:LYS:NZ	6:F:189:SER:CA	2.79	0.40
6:F:80:MET:O	6:F:83:SER:HB3	2.20	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.40
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.40
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.40
8:H:99:ASN:CG	19:a:40:ARG:HG3	2.46	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.40
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
10:P:203:PRO:HG2	30:P:401:NDP:C6N	2.51	0.40
10:P:265:PHE:CD1	10:P:265:PHE:N	2.87	0.40
10:P:359:TYR:HA	10:P:362:LEU:HG	2.02	0.40
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.40
13:S:17:ARG:O	13:S:52:PRO:HD2	2.21	0.40
14:T:97:LYS:NZ	14:T:108:LEU:N	2.66	0.40
17:X:25:LEU:HD11	19:a:50:ARG:NH2	2.36	0.40
21:q:17:HIS:HE1	21:q:34:ARG:N	2.19	0.40
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.91	0.40
2:B:194:CYS:SG	4:D:138:ARG:NH2	2.94	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
5:E:109:MET:HE1	7:G:198:THR:CG2	2.51	0.40
6:F:270:ASN:HD21	6:F:340:ASP:CB	2.34	0.40
6:F:276:PHE:CE2	6:F:290:GLU:HB3	2.56	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:44:GLU:O	7:G:47:THR:HG23	2.21	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.40
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.40
9:I:105:ARG:HH12	12:R:58:ASN:CB	2.35	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.21	0.40
10:P:135:GLU:HG3	10:P:140:ASP:HA	2.04	0.40
10:P:169:HIS:ND1	30:P:401:NDP:H5N	2.36	0.40
16:W:23:ILE:HG21	16:W:83:ASP:HB2	2.02	0.40
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.55	0.40
17:X:136:PRO:O	17:X:137:LEU:C	2.63	0.40
22:r:28:TYR:O	22:r:30:GLU:HG3	2.21	0.40
1:A:6:VAL:HG11	8:H:87:VAL:HG22	2.01	0.40
2:B:91:TRP:HZ2	8:H:51:ASP:OD2	2.05	0.40
2:B:92:PRO:HD3	2:B:119:VAL:HG13	2.03	0.40
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.40
3:C:68:LEU:HD13	3:C:95:THR:HA	2.03	0.40
3:C:97:THR:HG21	15:V:97:TRP:HH2	1.86	0.40
4:D:139:LEU:HD13	4:D:424:ILE:HG12	2.02	0.40
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.40
4:D:362:LYS:HD2	22:r:60:ARG:NH2	2.36	0.40
6:F:53:LEU:O	6:F:54:LYS:C	2.62	0.40
6:F:169:LEU:O	6:F:173:ILE:N	2.49	0.40
6:F:338:ASP:OD1	6:F:341:ALA:HB2	2.20	0.40
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:355:LYS:HB2	7:G:366:LEU:CD2	2.52	0.40
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.26	0.40
7:G:664:TYR:OH	13:S:23:LEU:HD21	2.21	0.40
8:H:153:VAL:O	8:H:154:LEU:C	2.65	0.40
8:H:172:MET:HB3	18:Z:49:ARG:HD2	2.01	0.40
10:P:80:VAL:HB	10:P:103:LEU:HD22	2.04	0.40
10:P:227:PRO:O	10:P:228:LEU:HD23	2.21	0.40
15:V:114:TRP:O	15:V:116:ILE:HG22	2.21	0.40
16:W:27:ASP:O	16:W:28:LEU:C	2.64	0.40
18:Z:55:GLN:O	18:Z:59:ARG:HG3	2.21	0.40
18:Z:104:TRP:O	18:Z:105:LYS:C	2.65	0.40
21:q:44:TYR:HE1	21:q:69:ASN:OD1	2.04	0.40
1:A:87:MET:HB3	1:A:87:MET:HE3	1.84	0.40
3:C:66:GLU:OE1	15:V:47:TYR:CE2	2.74	0.40
4:D:310:VAL:C	4:D:312:ASP:H	2.30	0.40
4:D:357:LYS:HE2	4:D:357:LYS:HB3	1.83	0.40
6:F:268:GLU:HG2	6:F:269:ARG:H	1.86	0.40
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.40
8:H:119:SER:OG	8:H:211:PHE:HB2	2.22	0.40
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
10:P:140:ASP:O	10:P:141:PHE:C	2.65	0.40
10:P:302:GLY:HA2	10:P:314:THR:CG2	2.50	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
24:b:201:3PE:H281	24:b:201:3PE:H252	1.72	0.40
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.89	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.40
5:E:157:ILE:HG13	5:E:161:GLU:HB2	2.03	0.40
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.57	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:281:HIS:HB2	6:F:356:VAL:O	2.21	0.40
6:F:391:TRP:CZ3	7:G:118:GLU:OE2	2.74	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
12:R:36:GLN:O	12:R:36:GLN:HG3	2.22	0.40
20:b:43:SER:O	20:b:47:LYS:HB2	2.22	0.40
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.40
22:r:8:ILE:HG22	22:r:12:ARG:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:41:ASN:HD21	23:s:43:TYR:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	83 (94%)	5 (6%)	0	100	100
2	B	155/224 (69%)	143 (92%)	10 (6%)	2 (1%)	9	35
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	383/463 (83%)	356 (93%)	26 (7%)	1 (0%)	36	67
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	634 (93%)	51 (7%)	0	100	100
8	H	309/318 (97%)	289 (94%)	19 (6%)	1 (0%)	36	67
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100	100
10	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	36	67
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	78 (96%)	3 (4%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
15	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
19	a	65/70 (93%)	62 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
21	q	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	11	39
23	s	20/104 (19%)	20 (100%)	0	0	100	100
All	All	4205/5036 (84%)	3970 (94%)	229 (5%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
10	P	329	PRO
2	B	171	TYR
4	D	89	PRO
22	r	39	PRO
2	B	195	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	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	81
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	332/395 (84%)	332 (100%)	0	100	100
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	85
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	89
8	H	277/280 (99%)	275 (99%)	2 (1%)	76	82
9	I	152/178 (85%)	152 (100%)	0	100	100
10	P	296/325 (91%)	294 (99%)	2 (1%)	76	82
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	76
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	76
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	128 (99%)	1 (1%)	73	81
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	81
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	129/131 (98%)	129 (100%)	0	100	100
22	r	85/96 (88%)	84 (99%)	1 (1%)	63	78
23	s	22/95 (23%)	22 (100%)	0	100	100
All	All	3694/4292 (86%)	3681 (100%)	13 (0%)	81	86

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

Mol	Chain	Res	Type
2	B	170	TYR
5	E	124	LYS
7	G	271	MET
8	H	73	ILE
8	H	207	LEU
10	P	242	VAL
10	P	316	LYS
11	Q	96	LYS
12	R	76	ILE
13	S	68	ARG
17	X	57	LEU
18	Z	6	VAL
22	r	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	106	HIS
2	B	127	GLN

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Mol	Chain	Res	Type
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	79	ASN
4	D	88	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	68	ASN
5	E	132	GLN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	281	HIS
6	F	303	HIS
6	F	313	ASN
6	F	346	GLN
6	F	418	GLN
7	G	74	ASN
7	G	142	GLN
7	G	205	GLN
7	G	260	ASN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	514	ASN

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Mol	Chain	Res	Type
7	G	571	HIS
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	163	GLN
8	H	169	GLN
8	H	171	HIS
8	H	212	ASN
8	H	258	ASN
8	H	287	HIS
10	P	43	HIS
10	P	79	GLN
10	P	102	GLN
10	P	154	GLN
10	P	166	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	58	ASN
13	S	25	GLN
13	S	48	HIS
16	W	54	GLN
16	W	94	GLN
16	W	105	HIS
17	X	77	HIS
17	X	140	ASN
18	Z	135	ASN
19	a	31	ASN
20	b	83	ASN
21	q	31	ASN
21	q	52	ASN
21	q	59	HIS
21	q	87	HIS

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Mol	Chain	Res	Type
21	q	91	HIS
21	q	116	ASN
22	r	21	GLN
22	r	29	GLN
22	r	52	ASN
22	r	110	GLN
23	s	59	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SF4	B	301	2	0,12,12	-	-	-		
33	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.28	6 (9%)
24	3PE	H	403	-	45,45,50	0.96	2 (4%)	48,50,55	1.13	3 (6%)
30	NDP	P	401	-	51,52,52	1.17	5 (9%)	71,80,80	1.55	11 (15%)
25	SF4	G	801	7	0,12,12	-	-	-		
29	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.22	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	FES	E	301	5	0,4,4	-	-	-		
25	SF4	G	802	7	0,12,12	-	-	-		
25	SF4	F	502	6	0,12,12	-	-	-		
26	FES	G	803	7	0,4,4	-	-	-		
29	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.11	5 (9%)
24	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.11	3 (6%)
25	SF4	I	303	9	0,12,12	-	-	-		
29	PC1	H	402	-	41,41,53	0.30	0	47,49,61	0.33	0
28	UQ9	H	401	-	35,35,58	0.84	2 (5%)	43,45,73	0.56	0
25	SF4	I	302	9	0,12,12	-	-	-		
32	EHZ	W	201	-	29,31,37	1.63	5 (17%)	37,41,47	1.63	7 (18%)
24	3PE	A	401	-	45,45,50	1.13	5 (11%)	48,50,55	1.28	3 (6%)
27	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.23	7 (14%)

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
25	SF4	B	301	2	-	-	0/6/5/5
33	CDL	q	201	-	-	14/67/67/110	-
24	3PE	H	403	-	-	13/49/49/54	-
30	NDP	P	401	-	-	2/34/77/77	0/5/5/5
25	SF4	G	801	7	-	-	0/6/5/5
29	PC1	q	202	-	-	15/38/38/57	-
26	FES	E	301	5	-	-	0/1/1/1
25	SF4	G	802	7	-	-	0/6/5/5
25	SF4	F	502	6	-	-	0/6/5/5
26	FES	G	803	7	-	-	0/1/1/1
29	PC1	I	301	-	-	11/50/50/57	-
24	3PE	b	201	-	-	10/49/49/54	-
25	SF4	I	303	9	-	-	0/6/5/5
29	PC1	H	402	-	-	7/45/45/57	-
28	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
25	SF4	I	302	9	-	-	0/6/5/5
32	EHZ	W	201	-	-	13/39/39/45	-
24	3PE	A	401	-	-	18/49/49/54	-
27	FMN	F	501	-	-	0/18/18/18	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	501	FMN	C9A-C5A	4.99	1.49	1.41
32	W	201	EHZ	C15-N2	4.82	1.44	1.33
32	W	201	EHZ	C12-N1	4.80	1.44	1.33
30	P	401	NDP	C5A-C4A	4.39	1.46	1.39
24	b	201	3PE	O31-C31	4.26	1.45	1.33
29	I	301	PC1	O31-C31	4.19	1.45	1.33
24	H	403	3PE	O31-C31	4.14	1.45	1.33
33	q	201	CDL	OB8-CB7	4.11	1.45	1.33
33	q	201	CDL	OA8-CA7	4.11	1.45	1.33
24	H	403	3PE	O21-C21	4.11	1.45	1.34
29	q	202	PC1	O31-C31	4.10	1.45	1.33
24	b	201	3PE	O21-C21	4.04	1.45	1.34
33	q	201	CDL	OA6-CA5	4.02	1.45	1.34
29	q	202	PC1	O21-C21	4.02	1.45	1.34
33	q	201	CDL	OB6-CB5	4.00	1.45	1.34
29	I	301	PC1	O21-C21	4.00	1.45	1.34
24	A	401	3PE	O21-C21	3.27	1.43	1.34
27	F	501	FMN	C8-C7	3.08	1.48	1.40
24	A	401	3PE	O31-C31	3.02	1.42	1.33
28	H	401	UQ9	C3-C2	-2.78	1.40	1.48
30	P	401	NDP	C5A-C6A	2.63	1.48	1.41
27	F	501	FMN	C4-N3	-2.60	1.34	1.38
28	H	401	UQ9	C4-C5	-2.53	1.41	1.48
32	W	201	EHZ	O4-C15	-2.52	1.18	1.23
30	P	401	NDP	C5A-N7A	-2.46	1.34	1.39
32	W	201	EHZ	O3-C12	-2.45	1.18	1.23
30	P	401	NDP	C8A-N7A	2.33	1.36	1.31
32	W	201	EHZ	C9-S1	2.20	1.81	1.76
27	F	501	FMN	C5A-N5	-2.19	1.35	1.39
24	A	401	3PE	O21-C2	-2.18	1.41	1.46
24	A	401	3PE	P-O12	-2.14	1.45	1.55
24	A	401	3PE	O31-C3	-2.07	1.40	1.45
30	P	401	NDP	C4A-N9A	-2.04	1.33	1.37
27	F	501	FMN	C2-N3	-2.02	1.34	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	201	EHZ	C8-C9-S1	5.98	121.11	113.56
30	P	401	NDP	C5A-C4A-N3A	-5.80	118.72	126.72
24	A	401	3PE	O21-C21-C22	4.70	121.65	111.48
30	P	401	NDP	N3A-C4A-N9A	4.55	134.90	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	403	3PE	O21-C21-C22	4.37	120.93	111.48
29	I	301	PC1	O21-C21-C22	4.36	120.91	111.48
33	q	201	CDL	OA6-CA5-C11	4.36	120.90	111.48
24	b	201	3PE	O21-C21-C22	4.13	120.42	111.48
29	q	202	PC1	O21-C21-C22	4.04	120.21	111.48
30	P	401	NDP	C2A-N3A-C4A	3.68	120.82	111.83
33	q	201	CDL	OB6-CB5-C51	3.61	119.29	111.48
30	P	401	NDP	C4A-C5A-N7A	-3.49	106.59	110.58
29	q	202	PC1	O31-C31-C32	3.19	121.56	111.83
30	P	401	NDP	N3A-C2A-N1A	-3.15	123.82	128.58
29	I	301	PC1	O31-C31-C32	2.94	120.79	111.83
29	I	301	PC1	C2-O21-C21	-2.89	110.87	117.80
24	A	401	3PE	O31-C31-C32	2.88	120.62	111.83
33	q	201	CDL	OB8-CB7-C71	2.84	120.49	111.83
27	F	501	FMN	C4-C4A-N5	2.81	122.09	118.21
32	W	201	EHZ	O2-C9-C8	-2.80	119.33	123.74
32	W	201	EHZ	C10-S1-C9	2.78	110.05	101.84
30	P	401	NDP	C4A-N9A-C8A	2.77	108.64	105.74
33	q	201	CDL	OA8-CA7-C31	2.73	120.15	111.83
24	b	201	3PE	O31-C31-C32	2.66	119.95	111.83
24	b	201	3PE	C2-O21-C21	-2.66	111.43	117.80
24	H	403	3PE	O31-C31-C32	2.62	119.82	111.83
30	P	401	NDP	C5A-N7A-C8A	2.56	107.47	103.45
33	q	201	CDL	CA4-OA6-CA5	-2.53	111.75	117.80
32	W	201	EHZ	O2-C9-S1	-2.46	119.56	122.68
24	A	401	3PE	O12-P-O14	-2.43	101.14	112.44
32	W	201	EHZ	C14-N2-C15	-2.40	118.23	122.55
29	q	202	PC1	C2-O21-C21	-2.38	112.09	117.80
33	q	201	CDL	CB4-OB6-CB5	-2.35	112.16	117.80
27	F	501	FMN	C4A-C10-N1	-2.34	118.85	124.59
32	W	201	EHZ	C13-C12-N1	2.31	120.56	116.34
27	F	501	FMN	C4A-C10-N10	2.21	119.65	116.48
27	F	501	FMN	O2-C2-N1	-2.20	118.14	121.80
27	F	501	FMN	O4-C4-C4A	-2.17	120.80	126.53
32	W	201	EHZ	C16-C15-N2	2.15	120.56	116.48
29	q	202	PC1	O31-C31-O32	-2.13	118.29	123.63
30	P	401	NDP	N9A-C8A-N7A	-2.12	110.92	113.94
27	F	501	FMN	C4'-C3'-C2'	-2.10	110.08	113.57
30	P	401	NDP	C6A-C5A-N7A	2.09	136.12	132.09
30	P	401	NDP	C3D-C2D-C1D	2.06	105.36	101.46
29	I	301	PC1	O31-C31-O32	-2.04	118.53	123.63
29	I	301	PC1	O21-C21-O22	-2.03	118.96	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	403	3PE	C2-O21-C21	-2.02	112.97	117.80
30	P	401	NDP	C6N-N1N-C2N	2.01	121.47	119.32
27	F	501	FMN	C4A-C4-N3	2.00	118.35	113.25

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	O22-C21-O21-C2
24	H	403	3PE	C1-O11-P-O12
24	H	403	3PE	C1-O11-P-O13
24	b	201	3PE	C1-O11-P-O14
24	b	201	3PE	O22-C21-O21-C2
29	H	402	PC1	C1-O11-P-O14
29	H	402	PC1	C2-C1-O11-P
29	H	402	PC1	O22-C21-O21-C2
29	I	301	PC1	C11-O13-P-O12
29	I	301	PC1	C11-O13-P-O14
29	I	301	PC1	C11-O13-P-O11
29	q	202	PC1	C11-O13-P-O14
29	q	202	PC1	C1-O11-P-O12
29	q	202	PC1	C1-O11-P-O14
29	q	202	PC1	C1-O11-P-O13
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C6-C7-C8-C9
32	W	201	EHZ	C16-C17-C20-O6
32	W	201	EHZ	C18-C17-C20-O6
32	W	201	EHZ	C19-C17-C20-O6
32	W	201	EHZ	O2-C9-S1-C10
32	W	201	EHZ	C8-C9-S1-C10
33	q	201	CDL	CA3-OA5-PA1-OA2
33	q	201	CDL	CA3-OA5-PA1-OA3
33	q	201	CDL	CA3-OA5-PA1-OA4
24	b	201	3PE	C32-C31-O31-C3
24	H	403	3PE	O32-C31-O31-C3
24	b	201	3PE	O32-C31-O31-C3
24	A	401	3PE	C22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
29	H	402	PC1	C22-C21-O21-C2
24	H	403	3PE	C32-C31-O31-C3
29	I	301	PC1	C32-C31-O31-C3
28	H	401	UQ9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
28	H	401	UQ9	C13-C14-C16-C17
29	I	301	PC1	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3
28	H	401	UQ9	C9-C11-C12-C13
29	q	202	PC1	C2-C1-O11-P
24	H	403	3PE	C21-C22-C23-C24
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C3-C2-O21-C21
33	q	201	CDL	C12-C13-C14-C15
24	H	403	3PE	C22-C21-O21-C2
24	H	403	3PE	O22-C21-O21-C2
32	W	201	EHZ	C5-C6-C7-O1
24	H	403	3PE	C35-C36-C37-C38
33	q	201	CDL	C11-CA5-OA6-CA4
32	W	201	EHZ	C5-C6-C7-C8
28	H	401	UQ9	C7-C8-C9-C10
33	q	201	CDL	C31-CA7-OA8-CA6
32	W	201	EHZ	C3-C4-C5-C6
24	A	401	3PE	O21-C2-C3-O31
29	q	202	PC1	C32-C31-O31-C3
24	A	401	3PE	C27-C28-C29-C2A
30	P	401	NDP	O4D-C1D-N1N-C6N
29	H	402	PC1	C23-C24-C25-C26
33	q	201	CDL	OB6-CB4-CB6-OB8
24	H	403	3PE	C22-C23-C24-C25
24	A	401	3PE	C37-C38-C39-C3A
33	q	201	CDL	OA9-CA7-OA8-CA6
29	I	301	PC1	C11-C12-N-C13
29	I	301	PC1	C11-C12-N-C15
29	q	202	PC1	O32-C31-O31-C3
24	A	401	3PE	C2B-C2C-C2D-C2E
33	q	201	CDL	OA7-CA5-OA6-CA4
28	H	401	UQ9	C5-C6-C7-C8
29	H	402	PC1	O13-C11-C12-N
29	q	202	PC1	O13-C11-C12-N
29	q	202	PC1	C32-C33-C34-C35
32	W	201	EHZ	O4-C15-C16-O5
24	A	401	3PE	C22-C23-C24-C25
33	q	201	CDL	CB3-CB4-CB6-OB8
24	A	401	3PE	C1-O11-P-O14
24	A	401	3PE	O13-C11-C12-N
24	b	201	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
24	b	201	3PE	C1-O11-P-O13
29	I	301	PC1	C11-C12-N-C14
29	q	202	PC1	C11-O13-P-O12
29	q	202	PC1	C11-O13-P-O11
33	q	201	CDL	CA4-CA3-OA5-PA1
32	W	201	EHZ	C2-C3-C4-C5
24	A	401	3PE	O11-C1-C2-O21
29	H	402	PC1	C24-C25-C26-C27
24	A	401	3PE	C1-C2-C3-O31
30	P	401	NDP	PN-O3-PA-O2A
28	H	401	UQ9	C1-C6-C7-C8
24	A	401	3PE	C25-C26-C27-C28
33	q	201	CDL	C1-CA2-OA2-PA1
33	q	201	CDL	C1-CB2-OB2-PB2
24	H	403	3PE	C24-C25-C26-C27
24	b	201	3PE	C25-C26-C27-C28
29	q	202	PC1	O11-C1-C2-C3
28	H	401	UQ9	C12-C11-C9-C10
24	H	403	3PE	C2D-C2E-C2F-C2G
29	q	202	PC1	C34-C35-C36-C37
24	b	201	3PE	C2B-C2C-C2D-C2E
24	A	401	3PE	C21-C22-C23-C24
24	A	401	3PE	C39-C3A-C3B-C3C
24	A	401	3PE	O11-C1-C2-C3
29	q	202	PC1	C11-C12-N-C15
24	H	403	3PE	C23-C24-C25-C26
24	b	201	3PE	C37-C38-C39-C3A
28	H	401	UQ9	C12-C11-C9-C8
28	H	401	UQ9	C16-C17-C18-C19
29	I	301	PC1	C2C-C2D-C2E-C2F
29	q	202	PC1	C11-C12-N-C14
24	H	403	3PE	O31-C31-C32-C33
32	W	201	EHZ	N2-C15-C16-O5
33	q	201	CDL	C18-C19-C20-C21
29	I	301	PC1	C2E-C2F-C2G-C2H
29	I	301	PC1	C25-C26-C27-C28

There are no ring outliers.

17 monomers are involved in 103 short contacts:

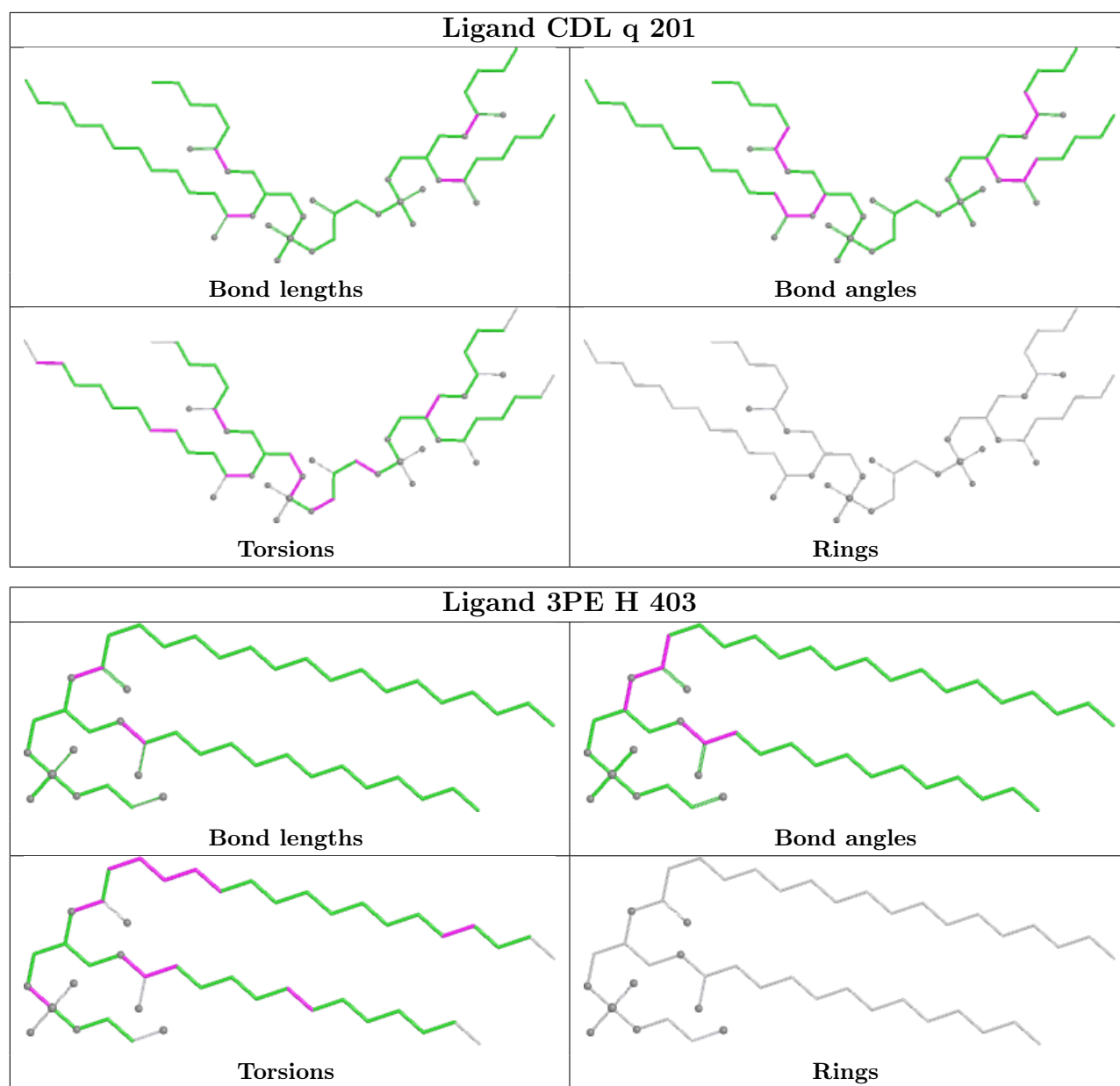
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	301	SF4	2	0

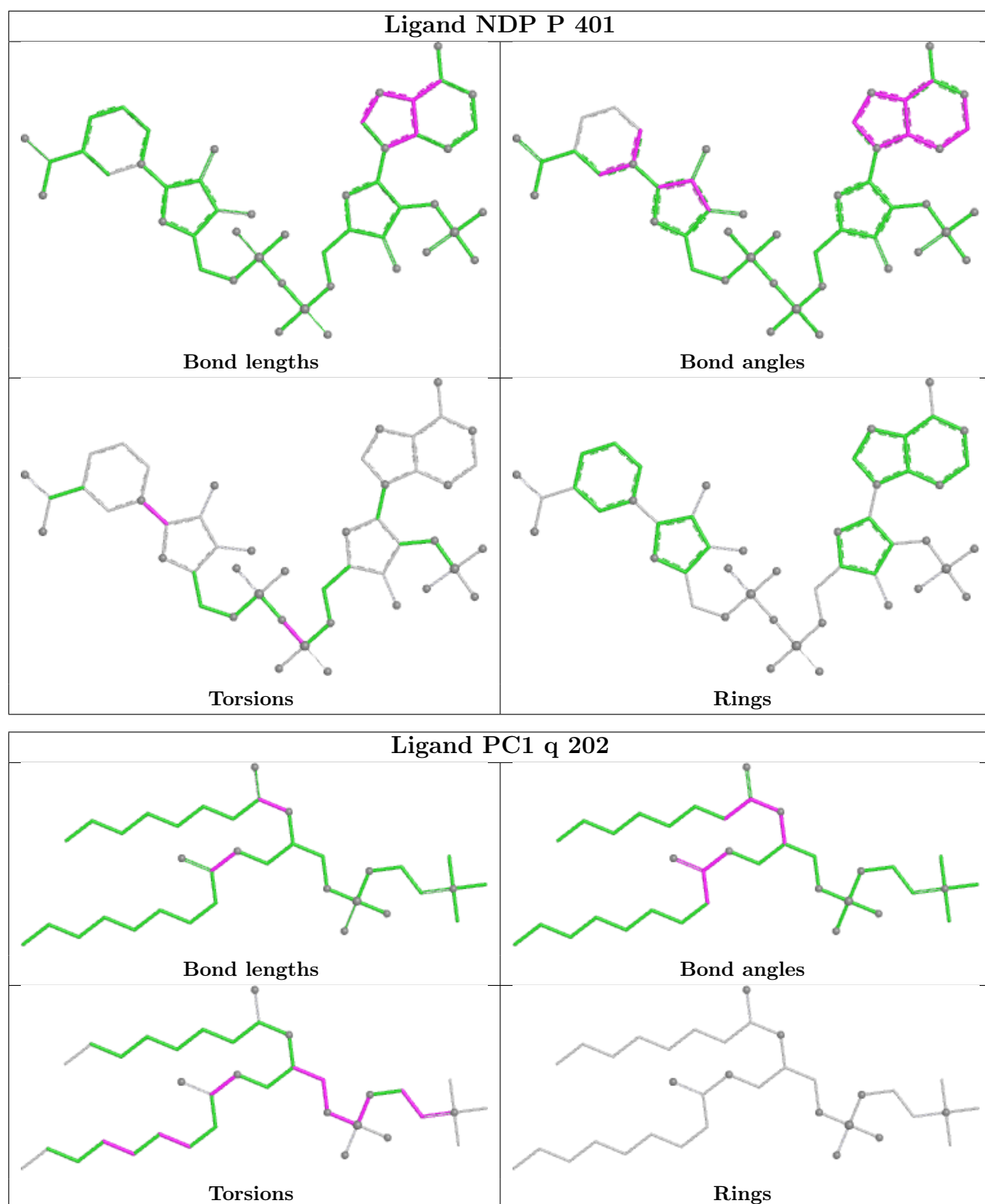
Continued on next page...

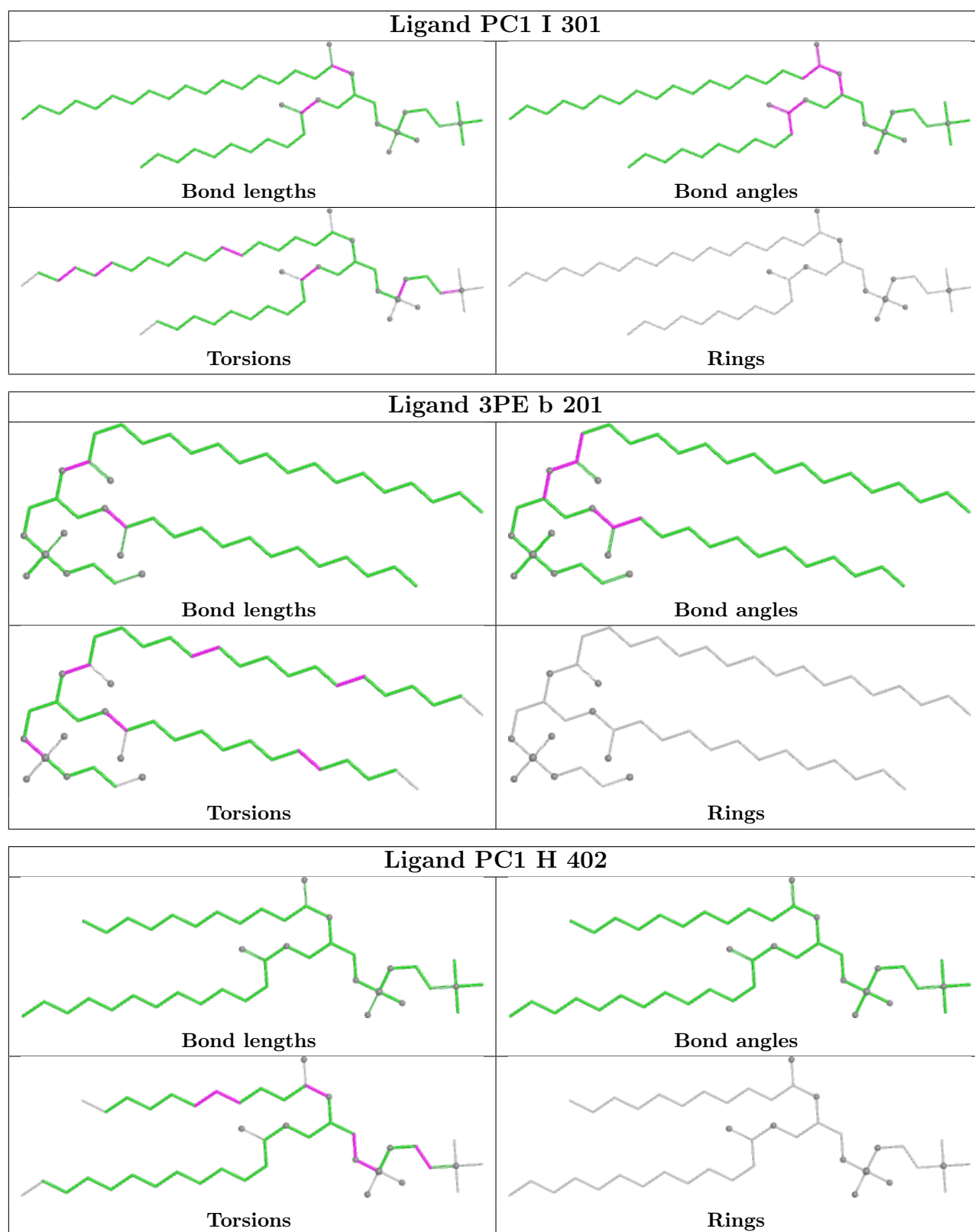
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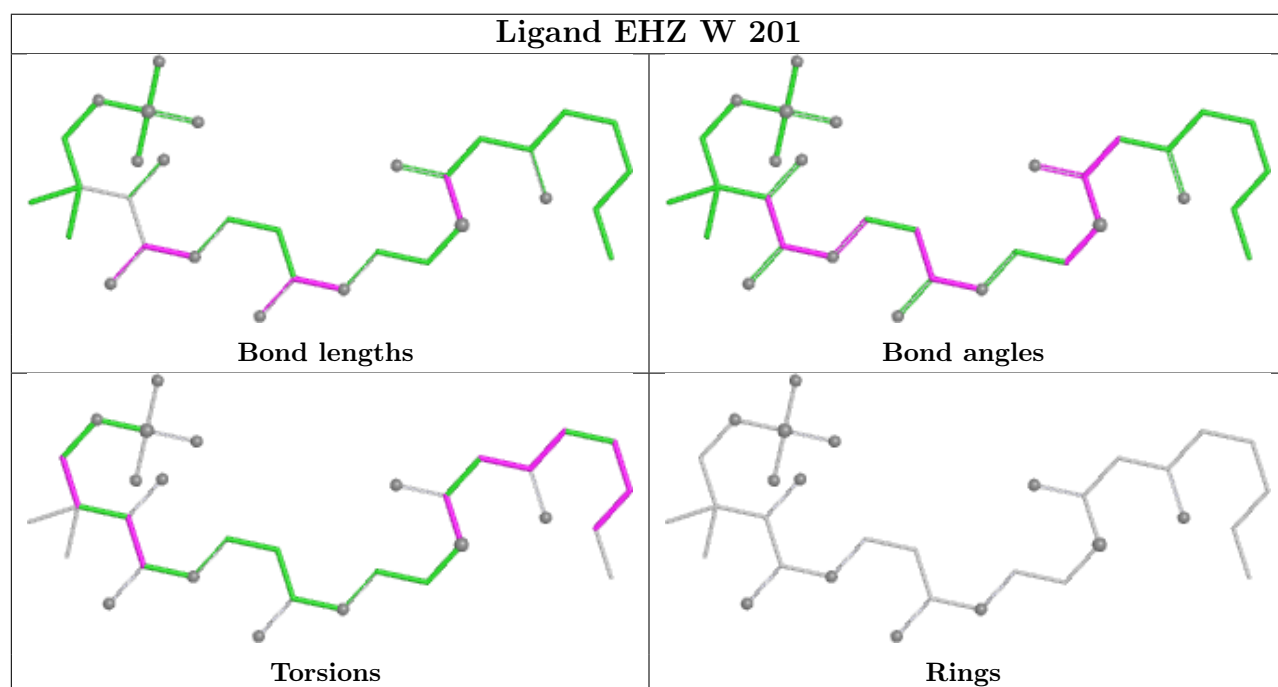
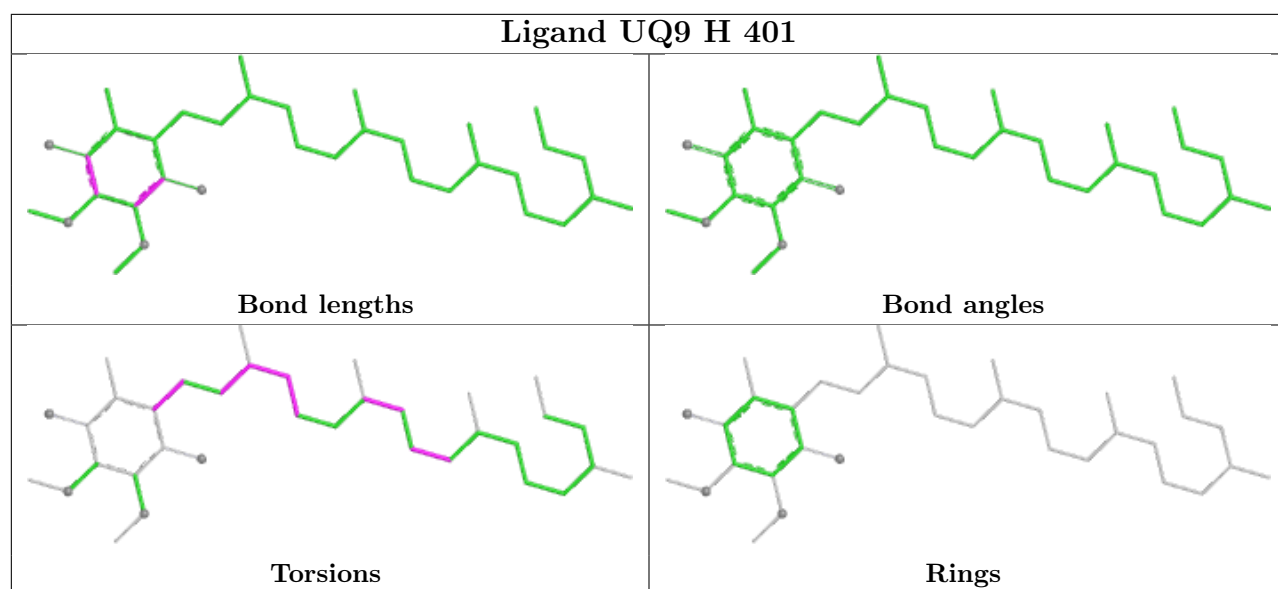
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	q	201	CDL	8	0
24	H	403	3PE	8	0
30	P	401	NDP	2	0
29	q	202	PC1	5	0
26	E	301	FES	3	0
25	G	802	SF4	5	0
25	F	502	SF4	9	0
26	G	803	FES	6	0
29	I	301	PC1	7	0
24	b	201	3PE	14	0
25	I	303	SF4	6	0
29	H	402	PC1	2	0
28	H	401	UQ9	12	0
25	I	302	SF4	9	0
24	A	401	3PE	3	0
27	F	501	FMN	2	0

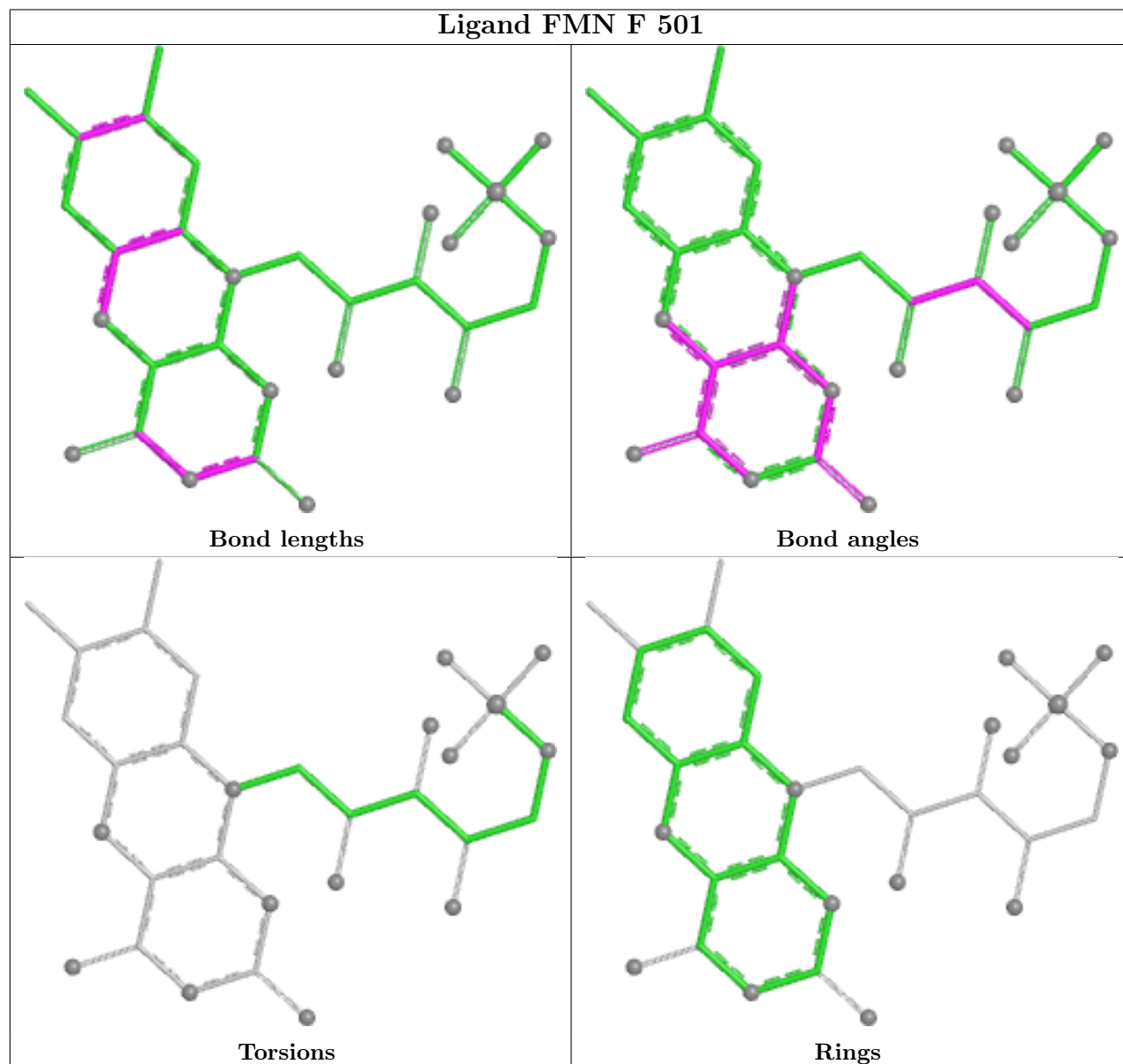
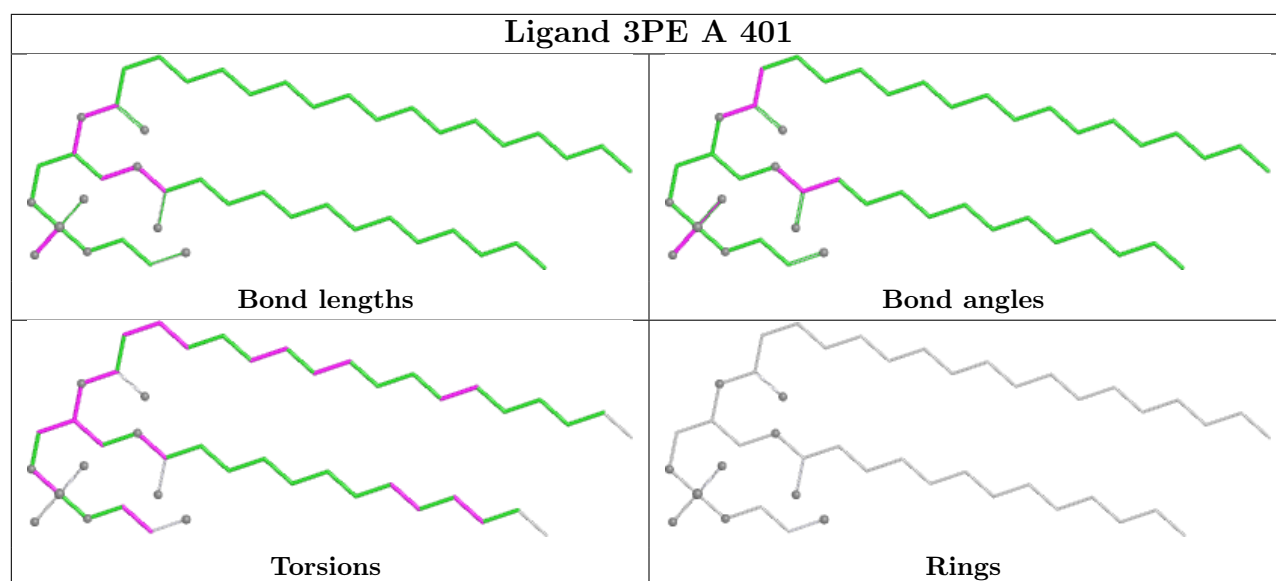
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

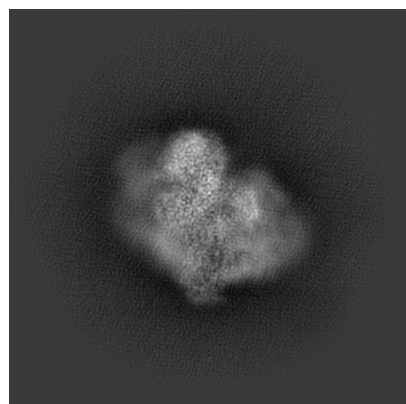
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38506. These allow visual inspection of the internal detail of the map and identification of artifacts.

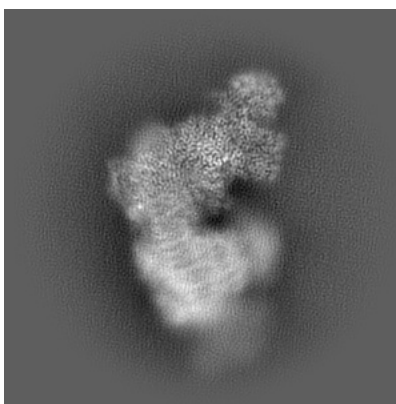
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

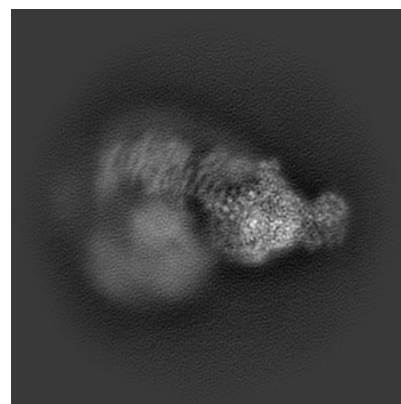
6.1.1 Primary map



X

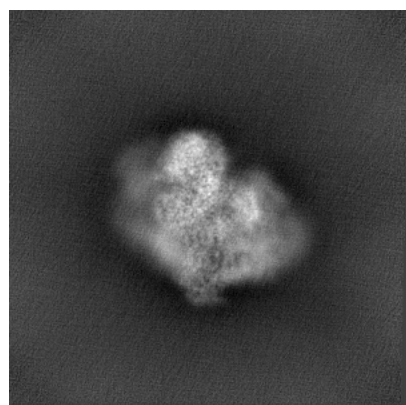


Y

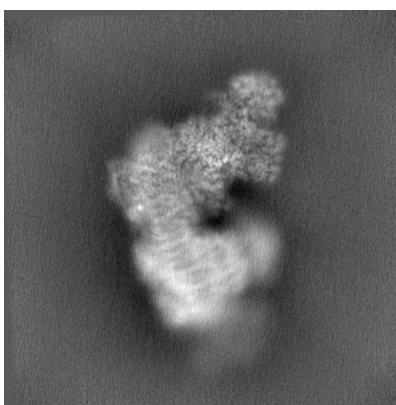


Z

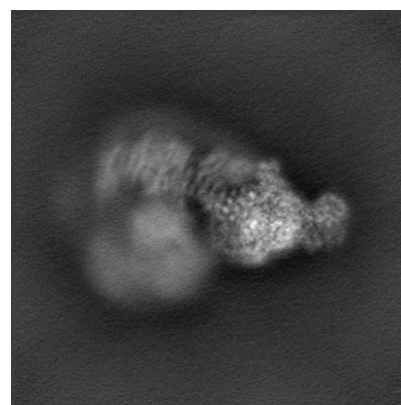
6.1.2 Raw map



X



Y

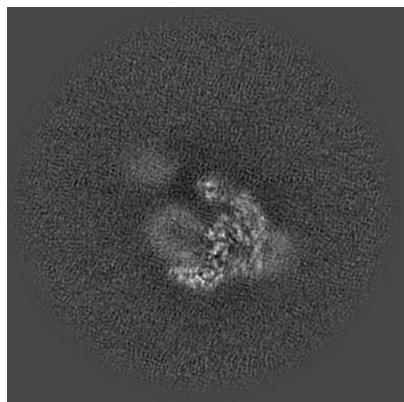


Z

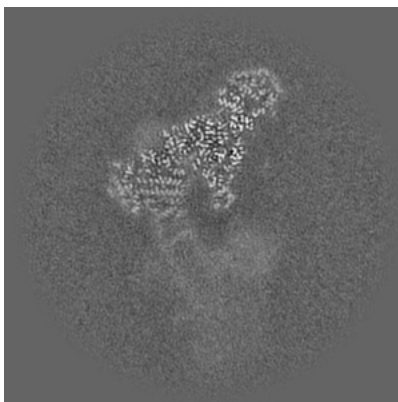
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

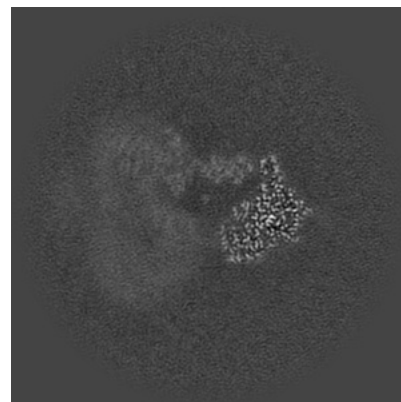
6.2.1 Primary map



X Index: 192

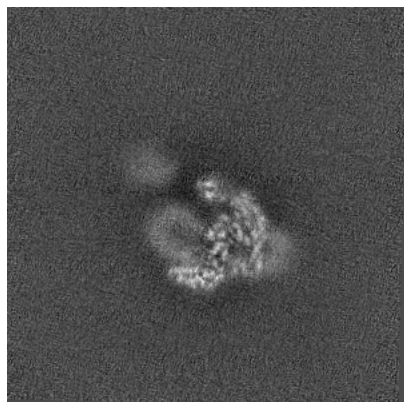


Y Index: 192

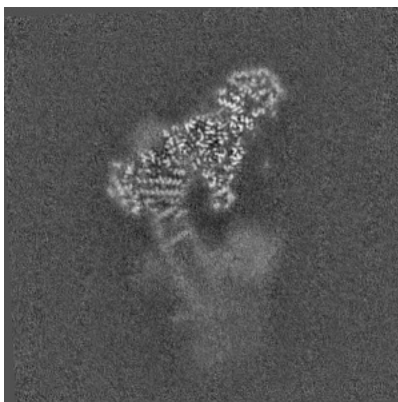


Z Index: 192

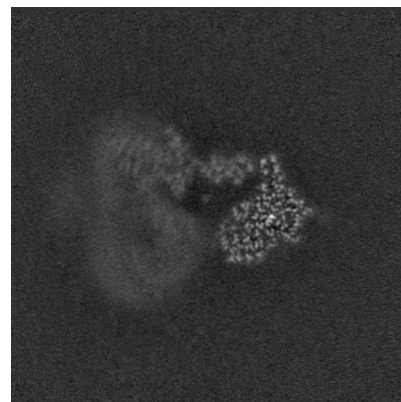
6.2.2 Raw map



X Index: 192



Y Index: 192

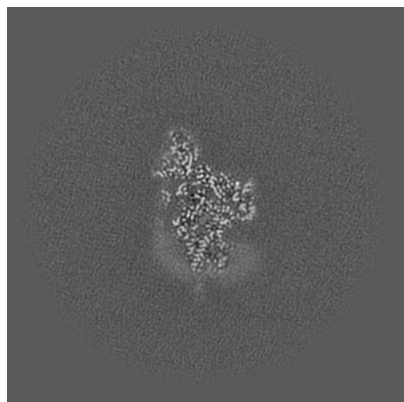


Z Index: 192

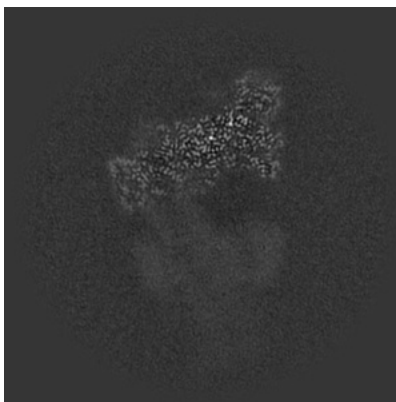
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

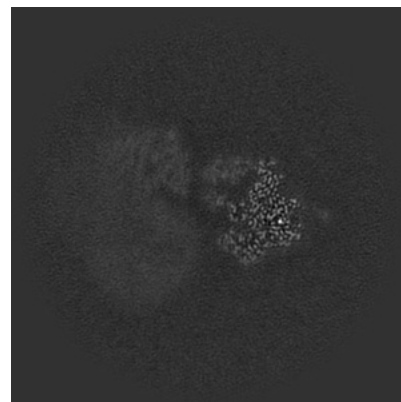
6.3.1 Primary map



X Index: 244

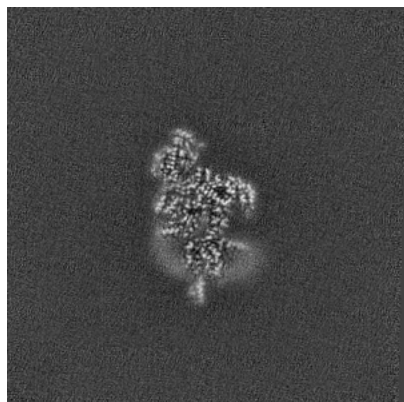


Y Index: 178

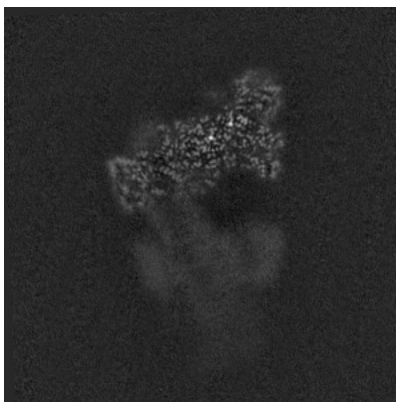


Z Index: 198

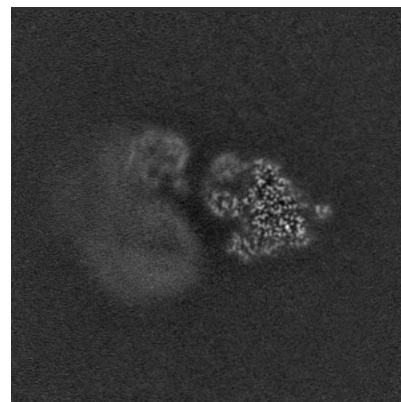
6.3.2 Raw map



X Index: 239



Y Index: 178

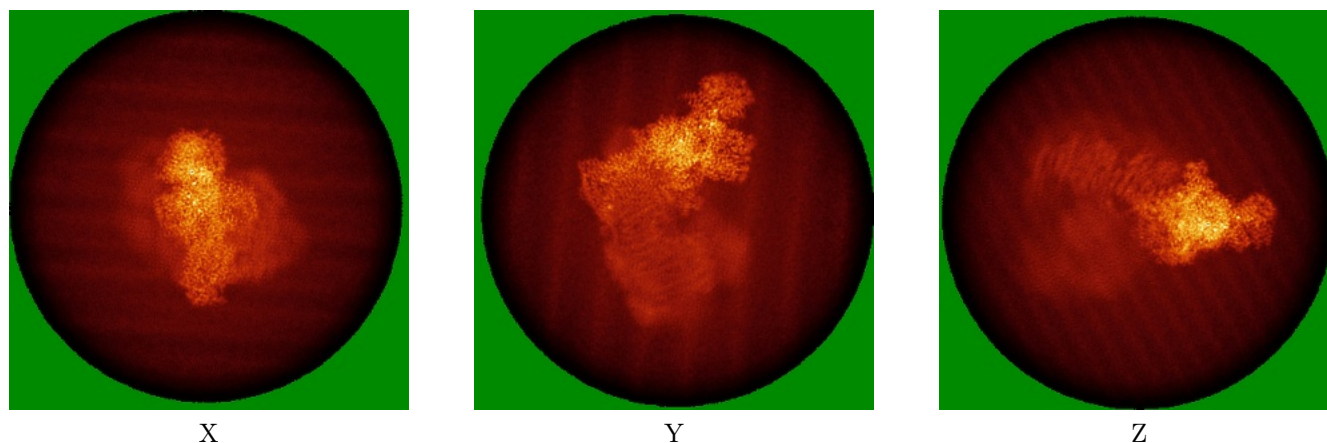


Z Index: 206

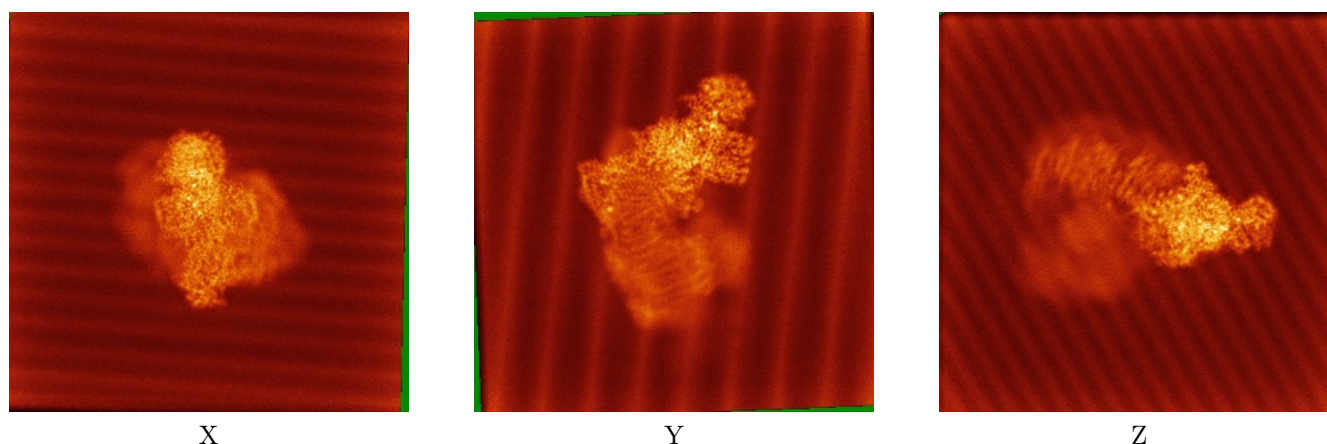
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

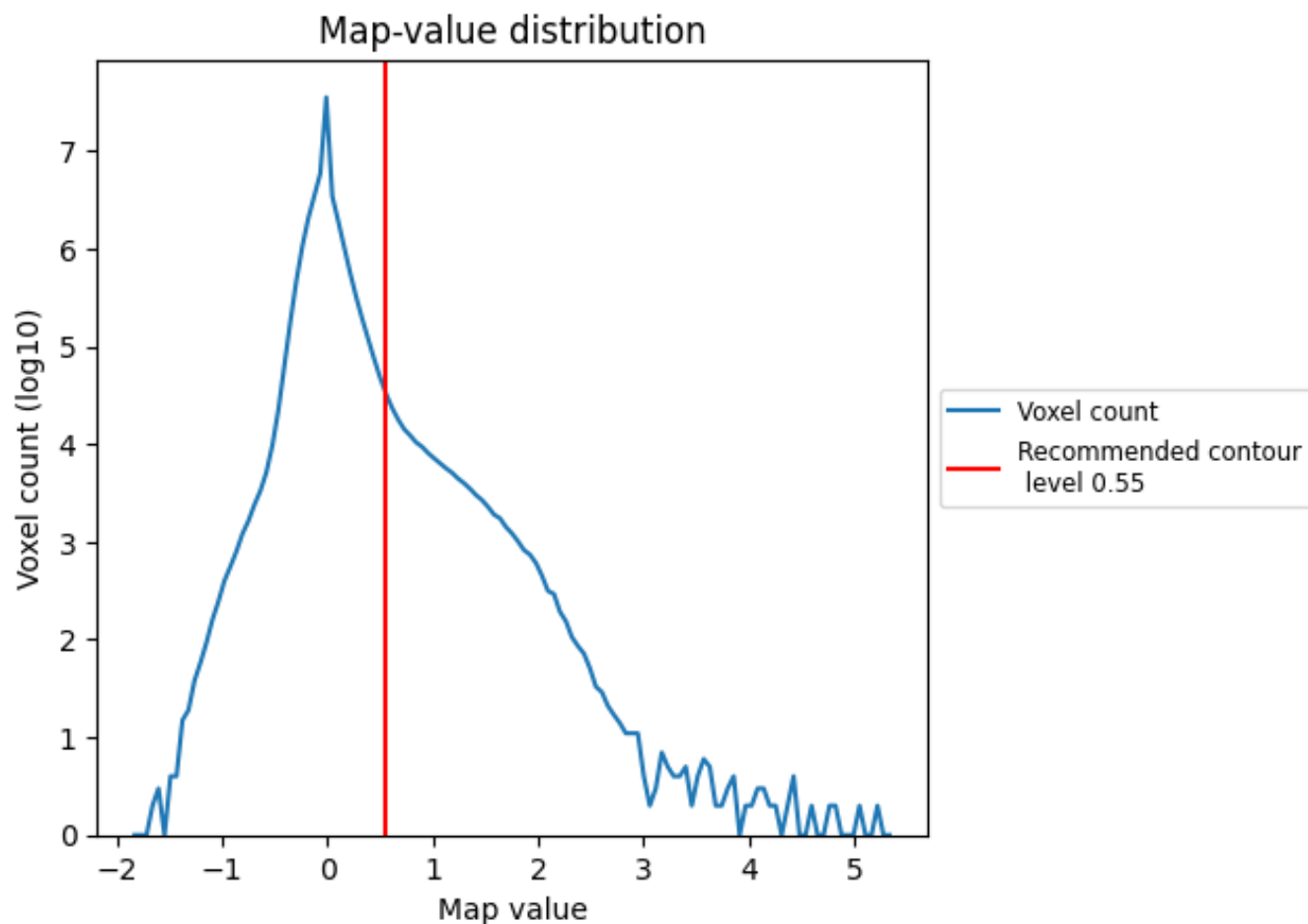
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

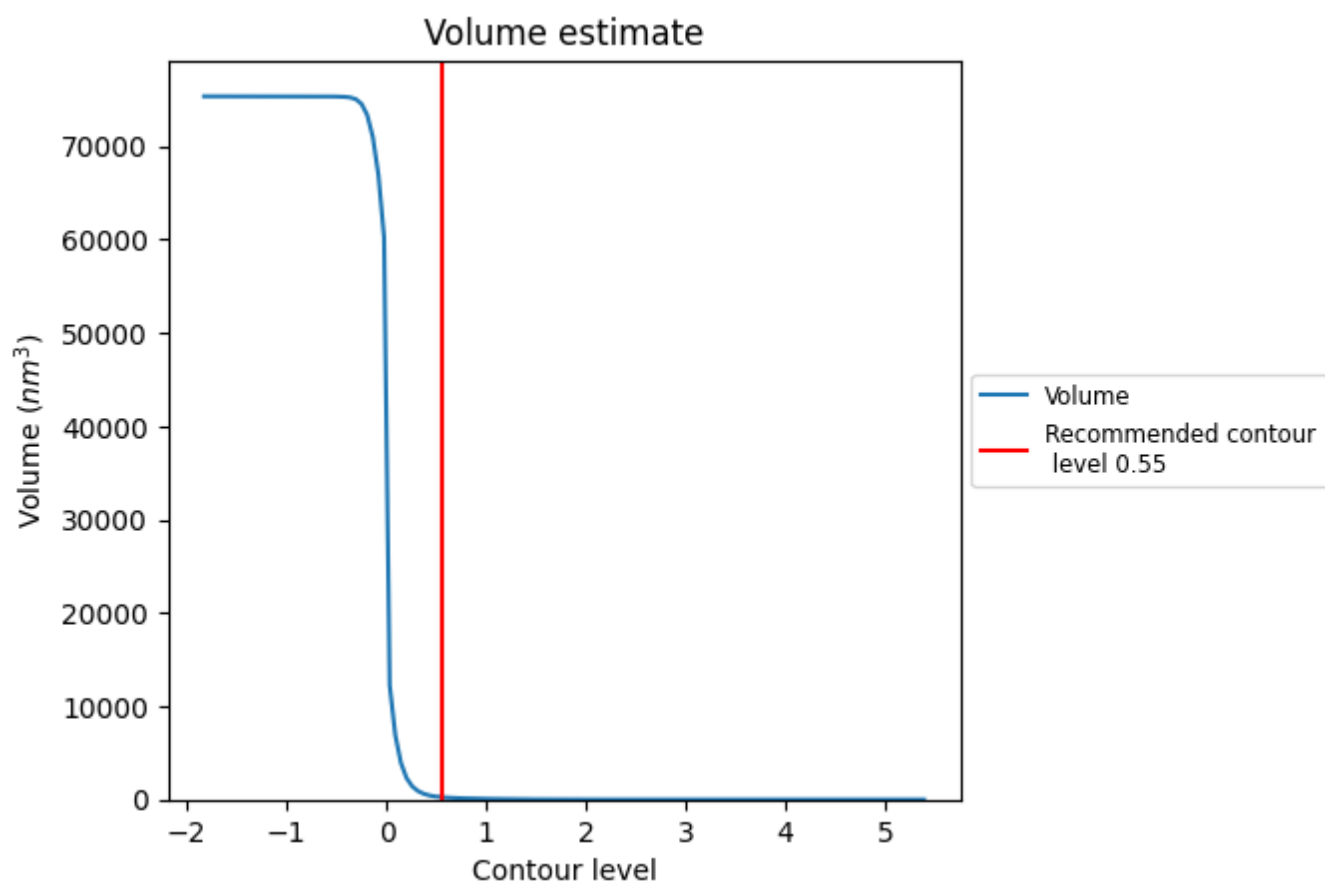
This section contains the results of statistical analysis of the map.

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.

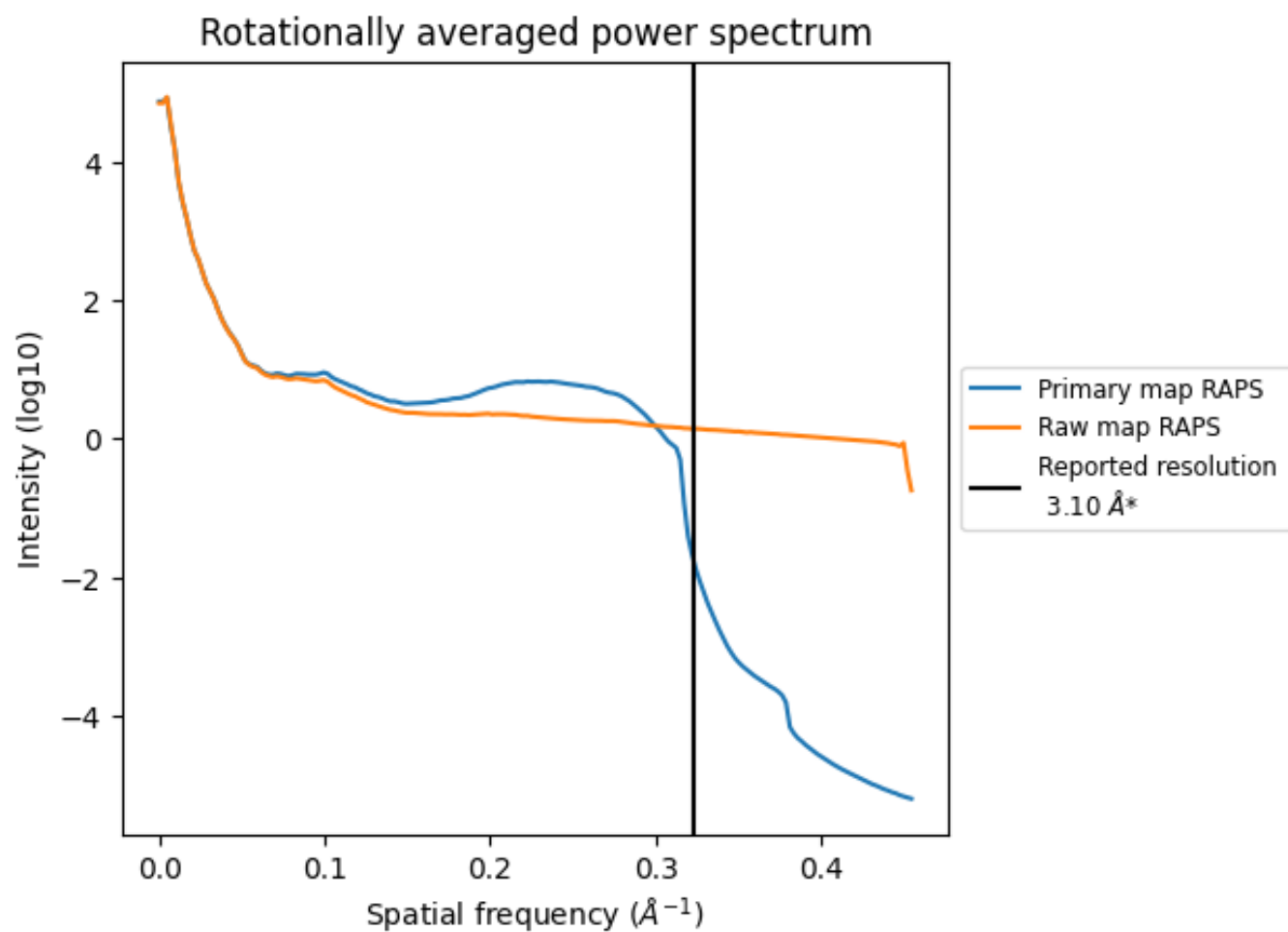
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm^3 ; this corresponds to an approximate mass of 229 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 ⓘ

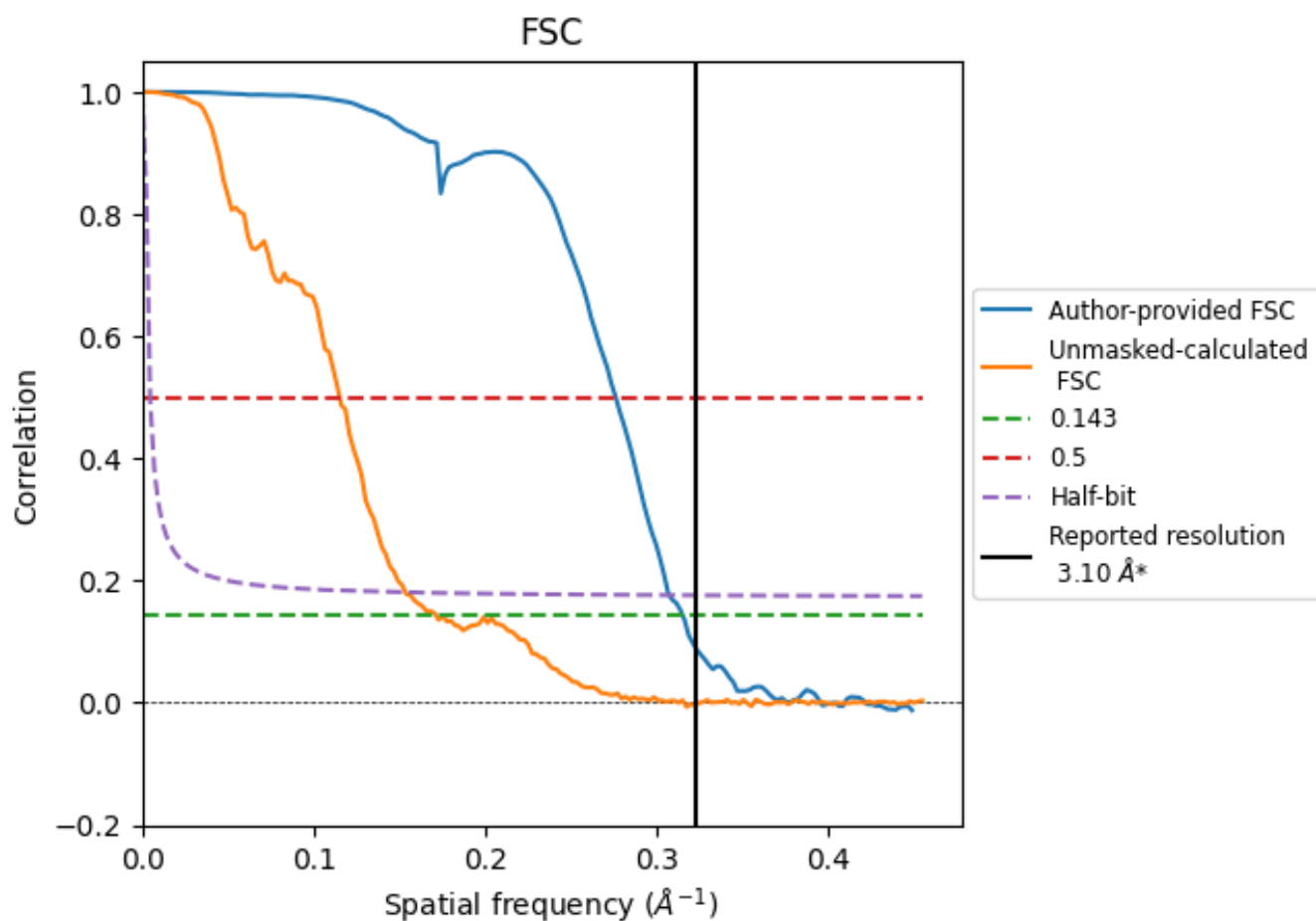


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

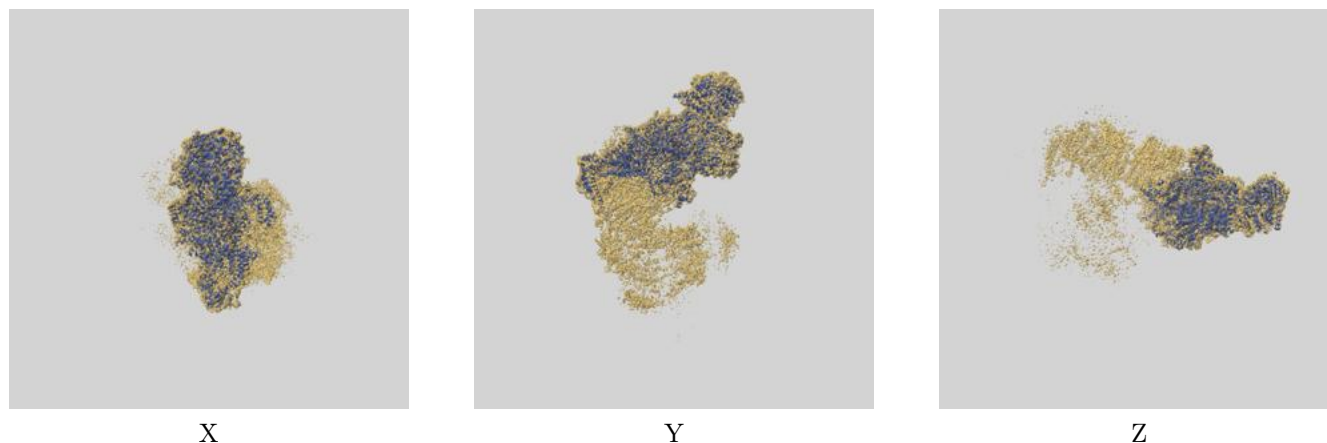
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.18	3.62	3.26
Unmasked-calculated*	5.84	8.70	6.52

*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 5.84 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

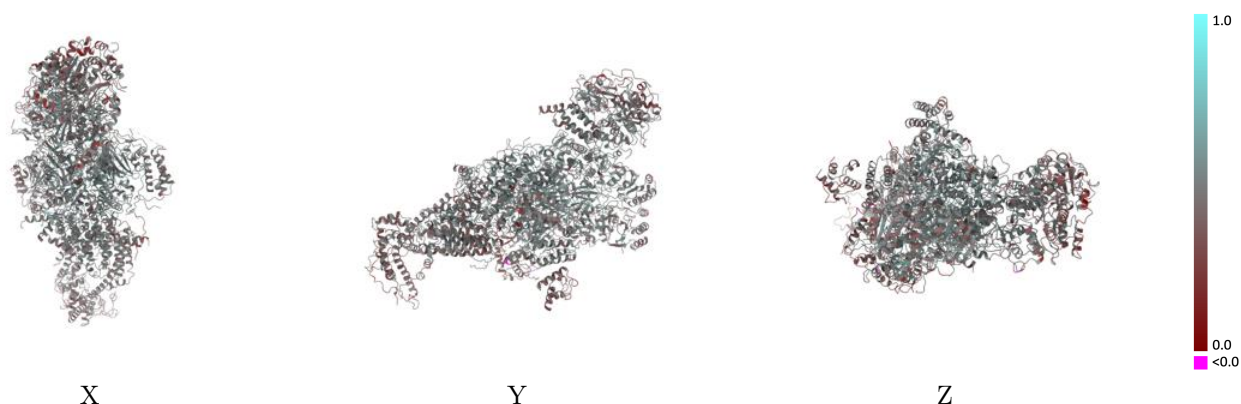
This section contains information regarding the fit between EMDB map EMD-38506 and PDB model 8XNL. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.55 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](#)

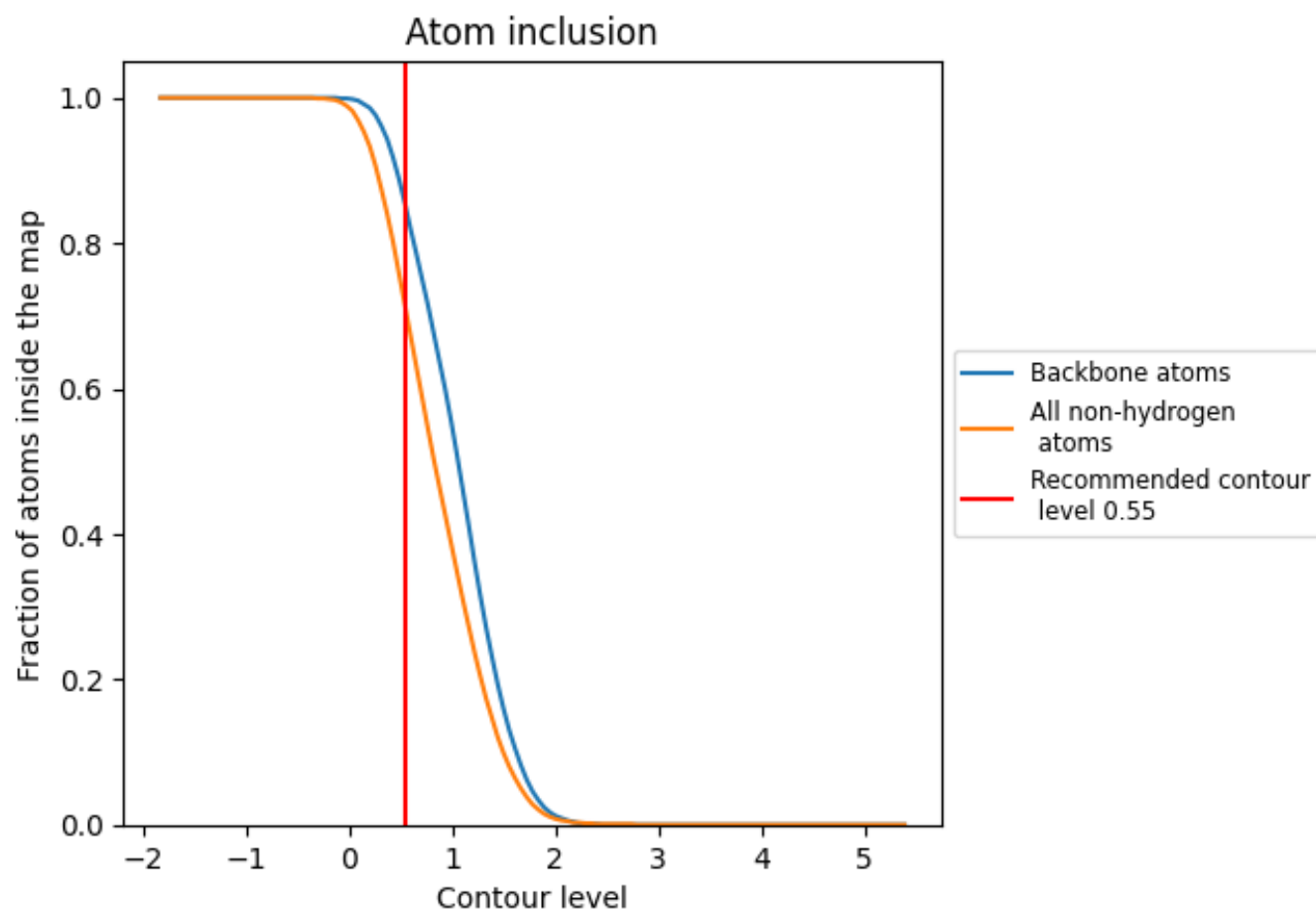


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.4610
A	 0.5400	 0.4330
B	 0.7610	 0.5150
C	 0.7960	 0.5260
D	 0.7750	 0.5120
E	 0.7000	 0.4270
F	 0.7280	 0.4370
G	 0.7610	 0.4790
H	 0.6480	 0.4690
I	 0.7520	 0.4940
P	 0.6160	 0.4200
Q	 0.7260	 0.4870
R	 0.6710	 0.4700
S	 0.7440	 0.4430
T	 0.5630	 0.3630
V	 0.7330	 0.4490
W	 0.7020	 0.4710
X	 0.6810	 0.3800
Z	 0.6970	 0.4170
a	 0.7450	 0.4570
b	 0.6310	 0.4120
q	 0.6590	 0.4700
r	 0.6500	 0.4800
s	 0.5620	 0.3690

