



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:21 PM UTC

PDB ID : 8XNP / pdb_00008xnp
EMDB ID : EMD-38510
Title : Respiratory complex Peripheral Arm of CI, close form B, focus-refined map of type IA, Wild type mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.50 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:

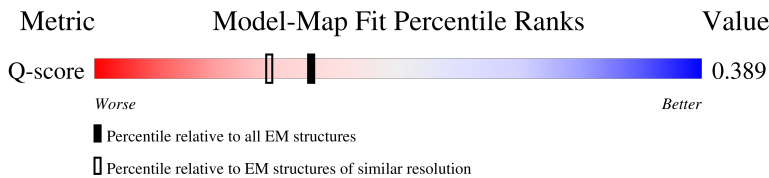
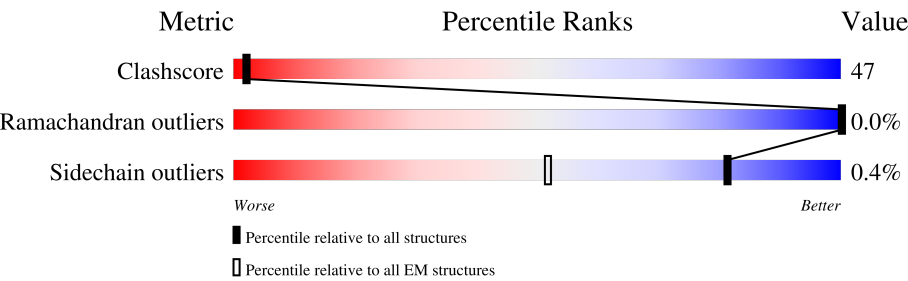
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	34% 21% 72% ...
2	B	224	6% 30% 35% 5% 30%
3	C	263	8% 38% 36% • 25%
4	D	463	5% 34% 45% • 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
24	SF4	B	301	-	-	X	-
24	SF4	F	502	-	-	X	-
24	SF4	G	802	-	-	X	-
24	SF4	I	303	-	-	X	-
24	SF4	I	304	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	FES	E	301	-	-	X	-
27	FES	G	803	-	-	X	-
33	CDL	a	101	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 34048 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	113	Total	C	N	O	S	0	0
			915	623	131	154	7		

- 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	318	Total	C	N	O	S	0	0
			2538	1705	384	427	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	174	Total	C	N	O	S	0	0
			1398	880	240	266	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	340	Total	C	N	O	S	0	0
			2730	1765	479	479	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	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	120	Total	C	N	O	S	0	0
			1004	645	178	177	4		

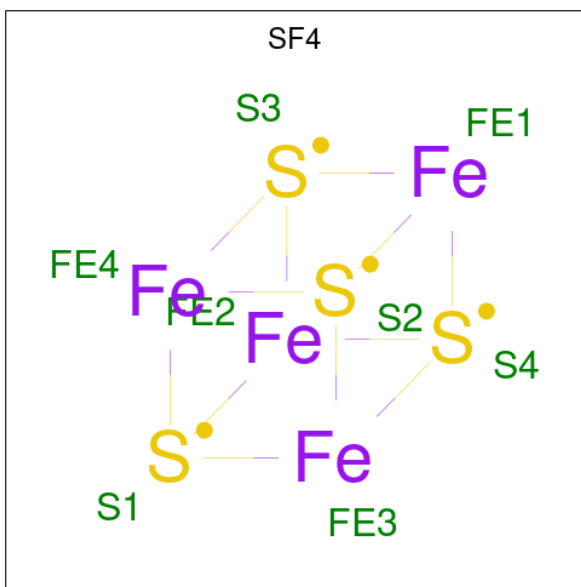
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

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

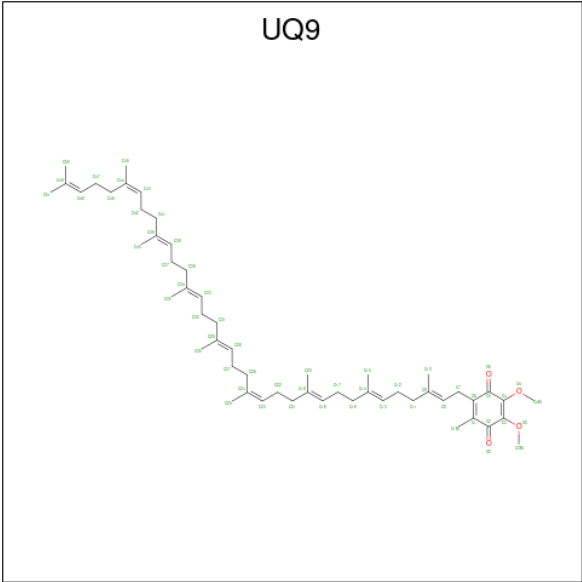
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	13	Total	C	N	O	0	0
			107	69	15	23		

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



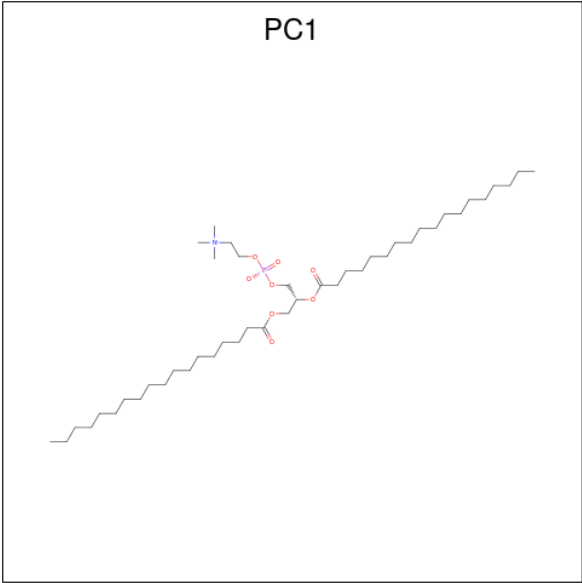
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	Fe	S	0
			8	4	4	
24	F	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 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
25	B	1	Total	C	O	0
			30	26	4	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



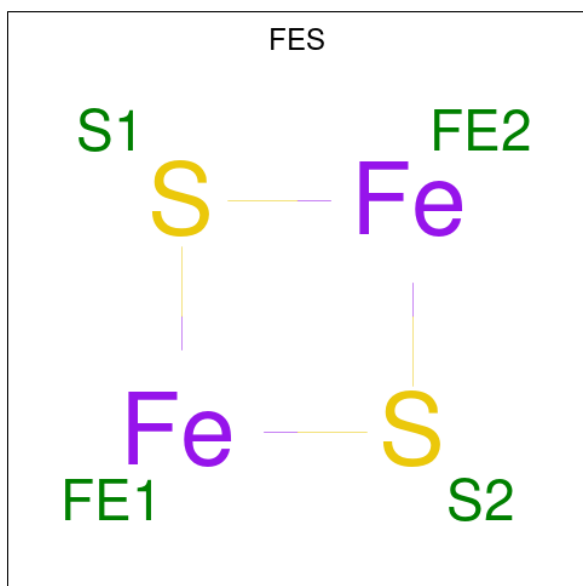
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
26	H	1	Total	C	N	O	P	0
			42	32	1	8	1	

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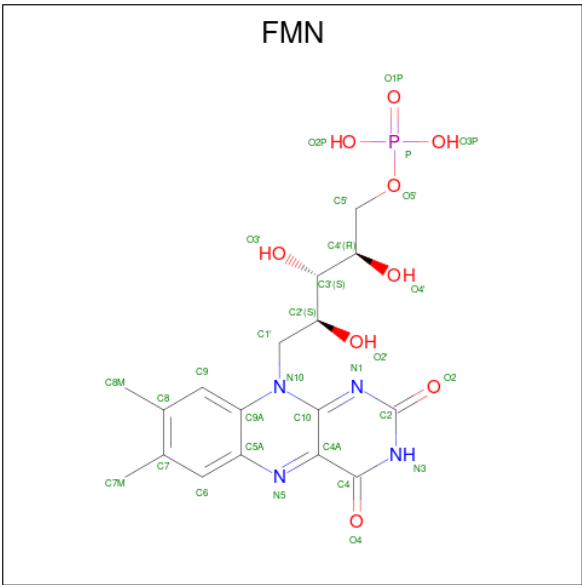
Mol	Chain	Residues	Atoms					AltConf
26	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

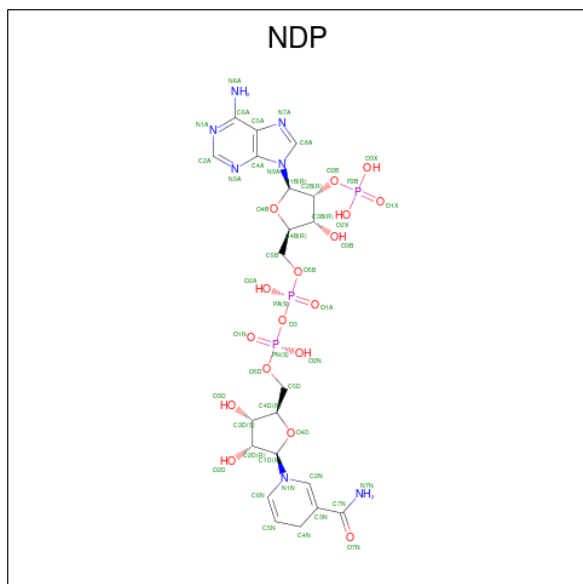


Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	Fe	S	0
			4	2	2	
27	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 28 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).



- 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).

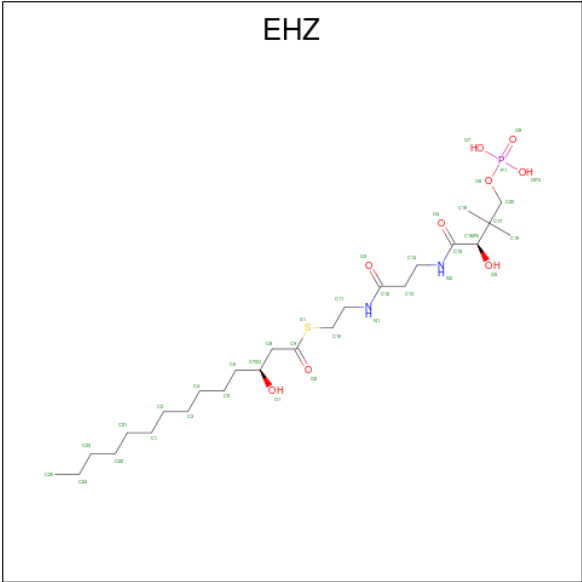


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

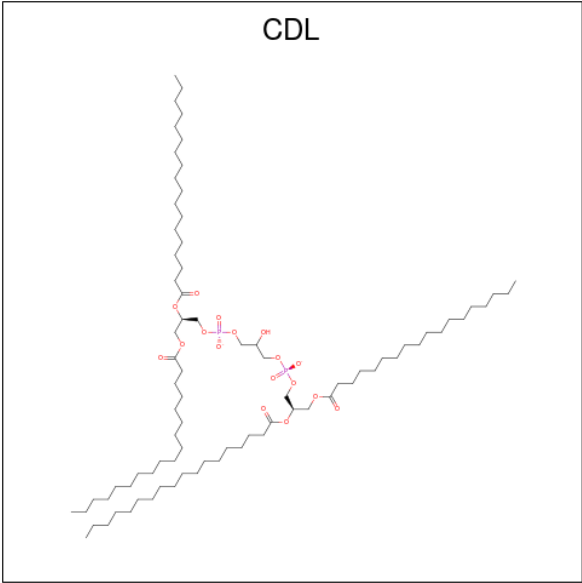
Mol	Chain	Residues	Atoms		AltConf
31	R	1	Total	Zn	0
			1	1	

- 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: $C_{25}H_{49}N_2O_9PS$) (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: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

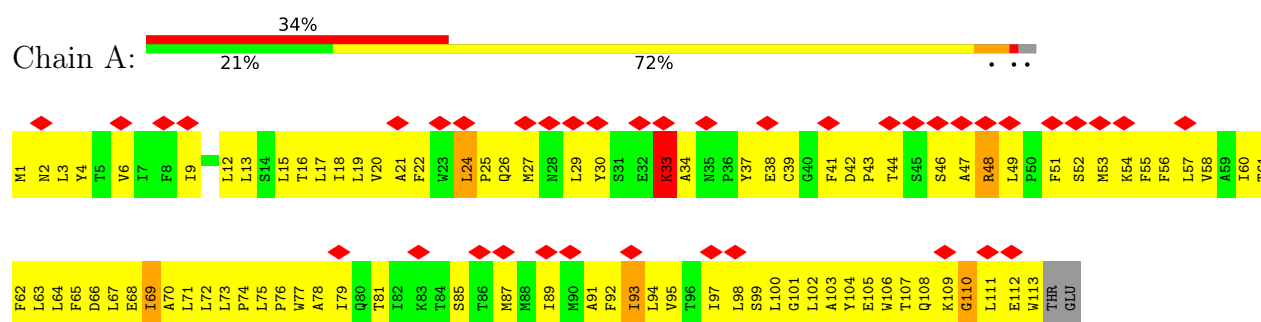


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	a	1	57	38	17	2	0

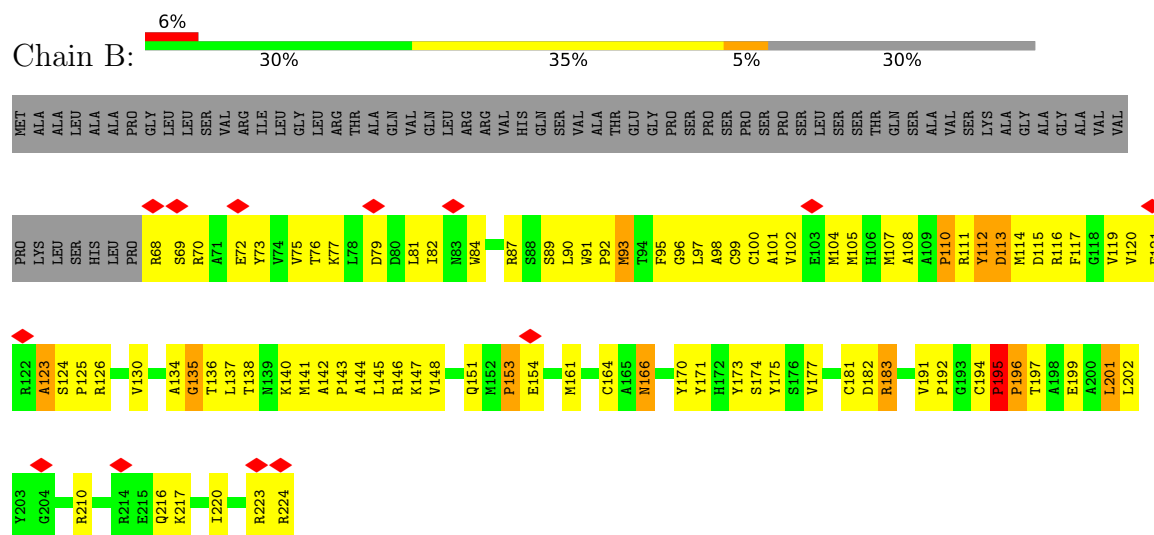
3 Residue-property plots

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

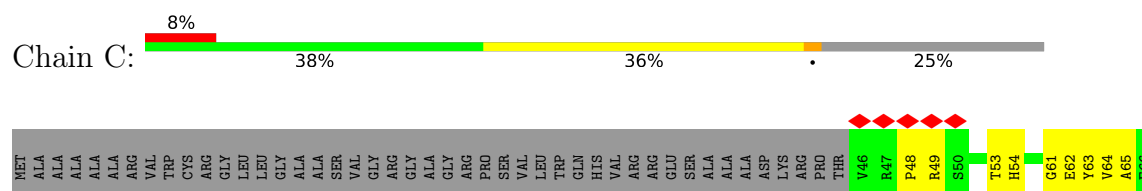
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

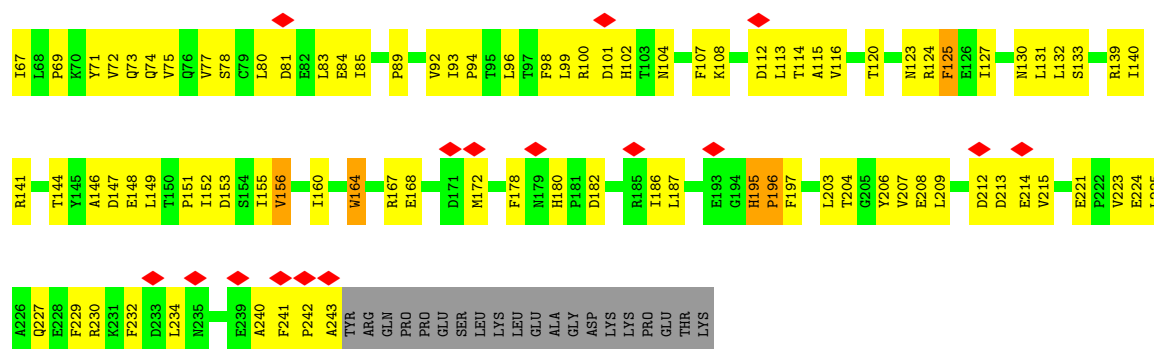


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

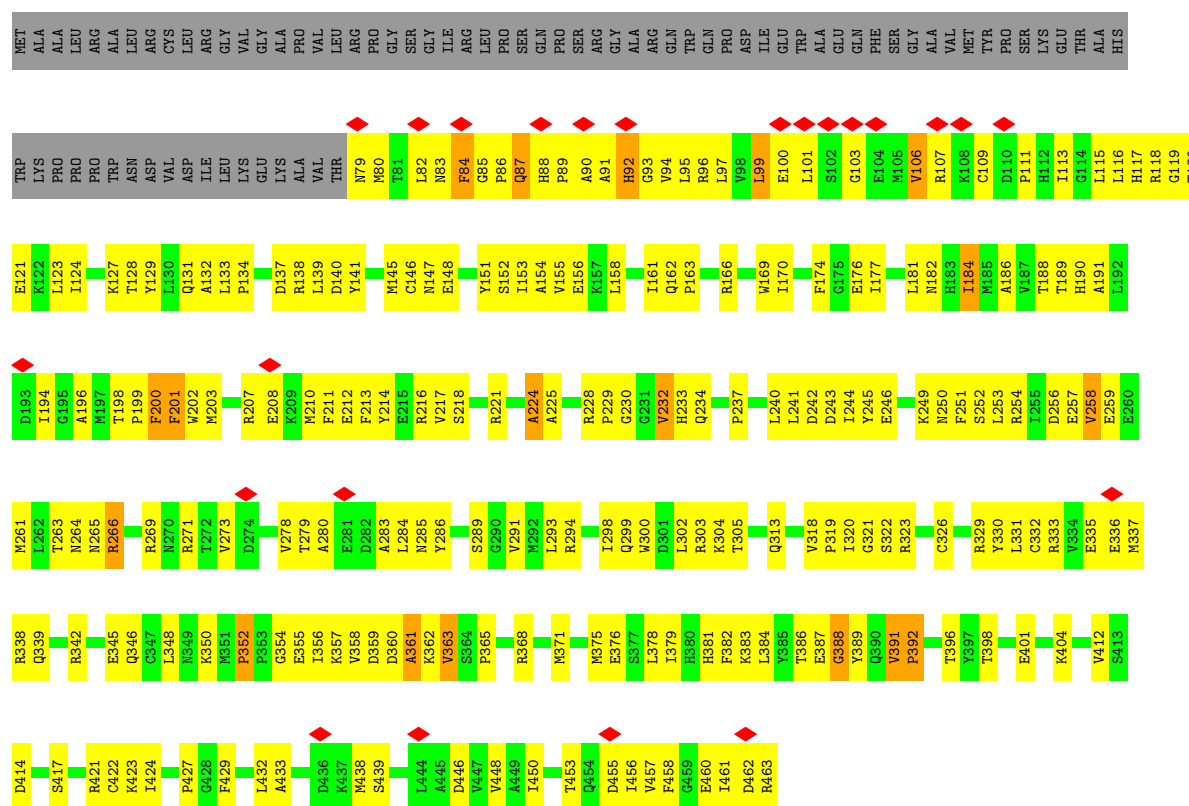


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

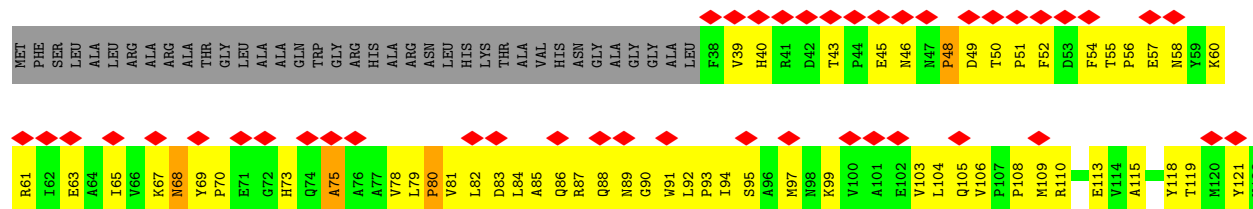


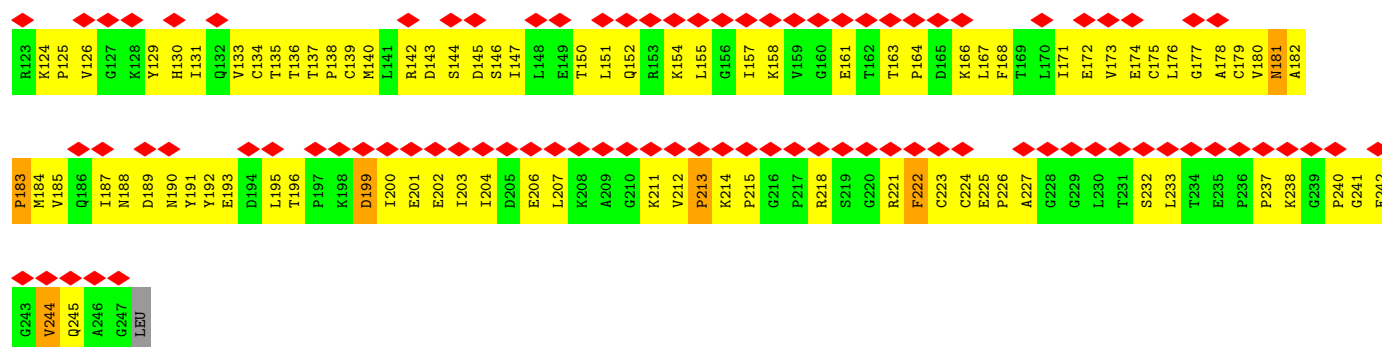


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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

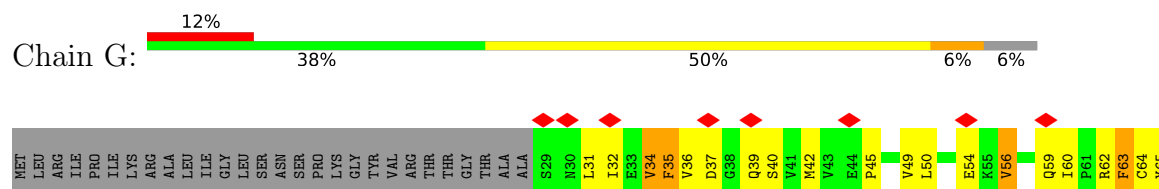


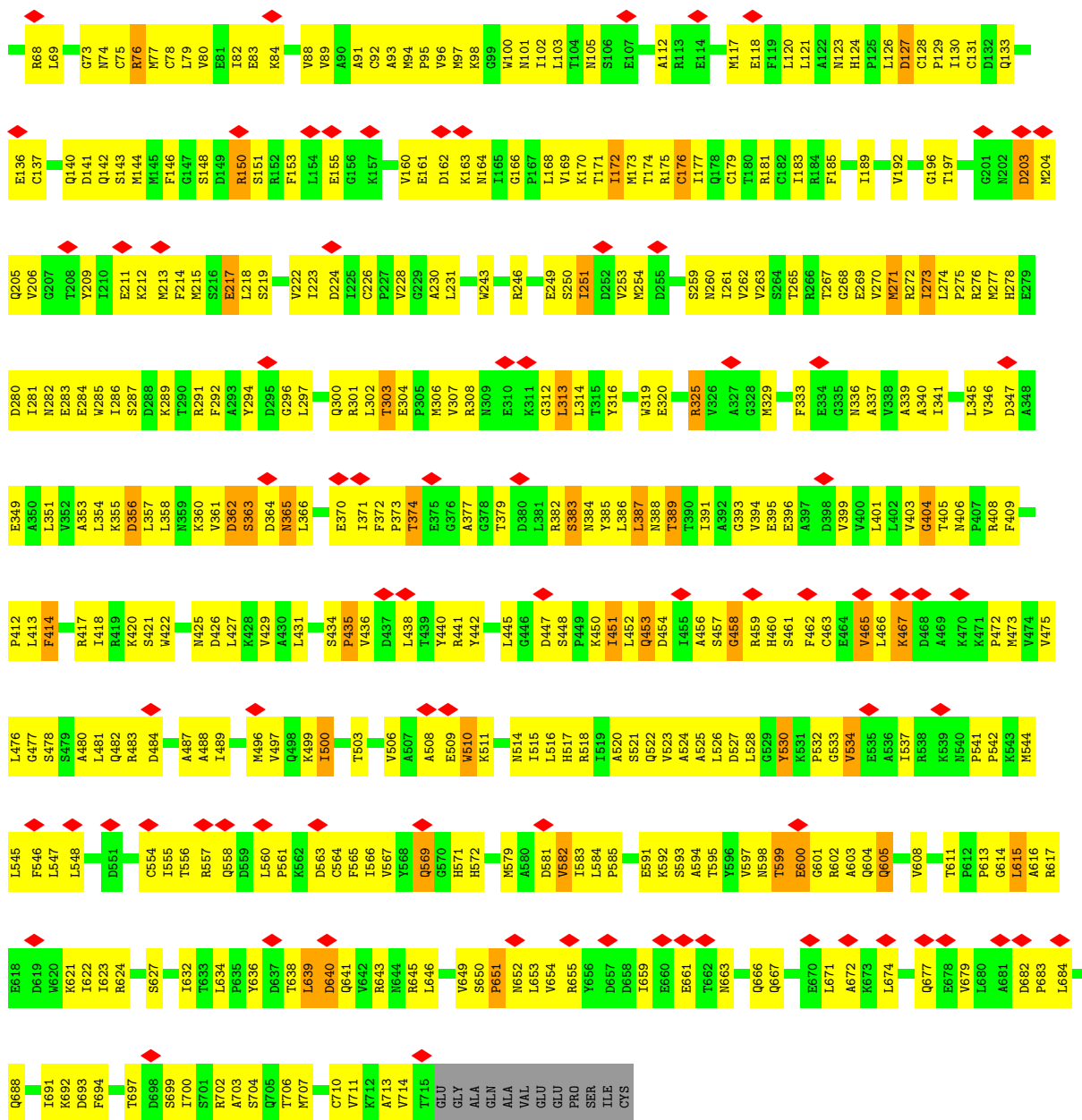


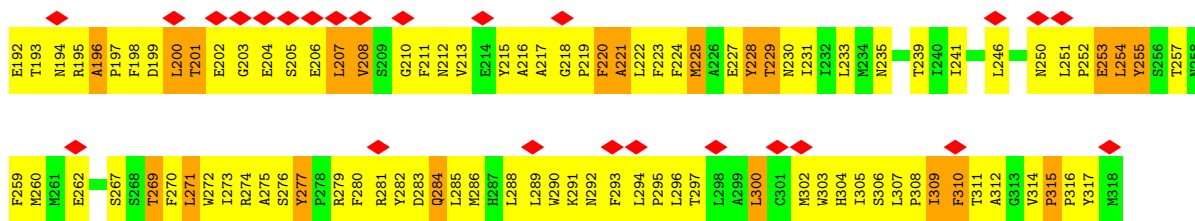
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



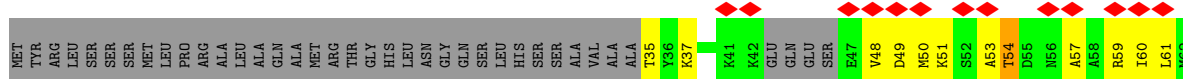
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



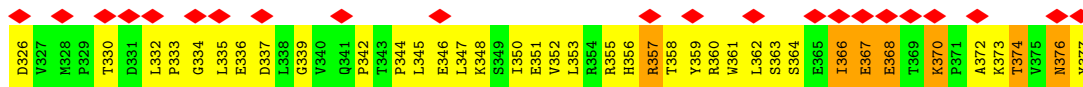
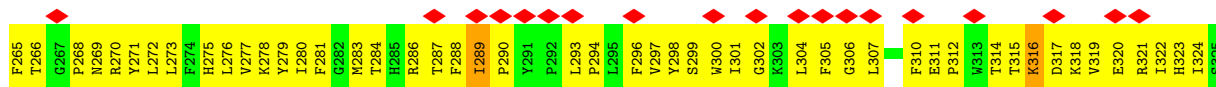
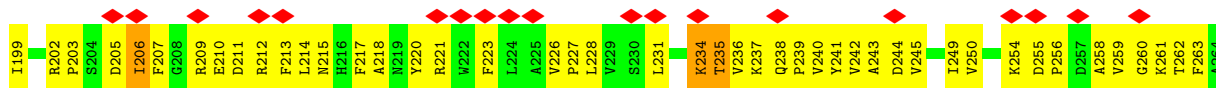
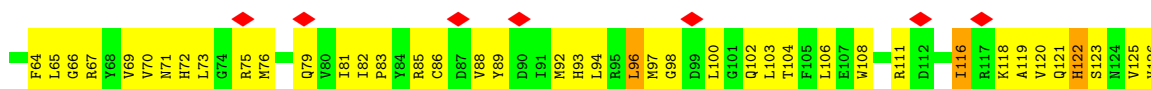
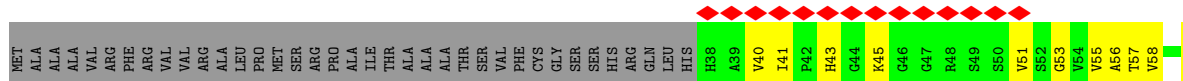




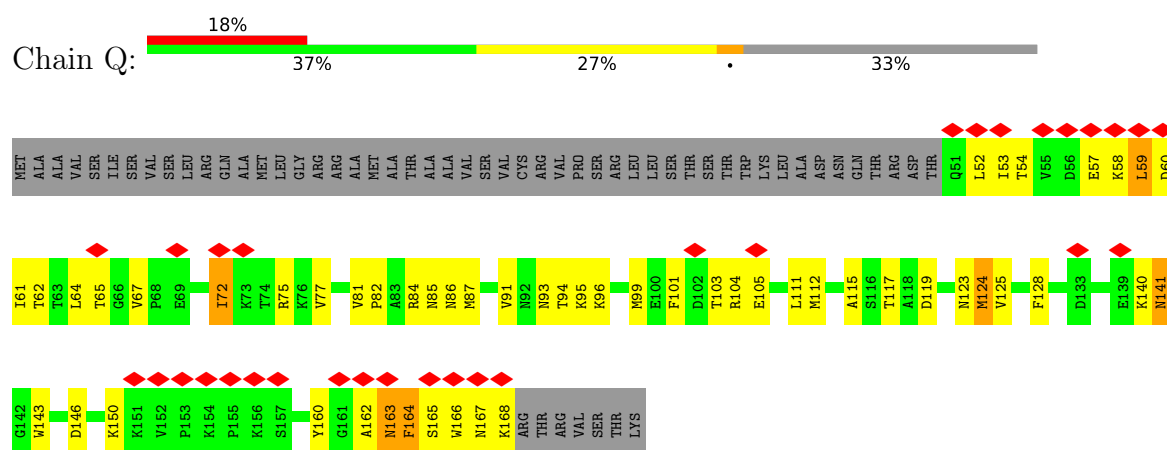
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



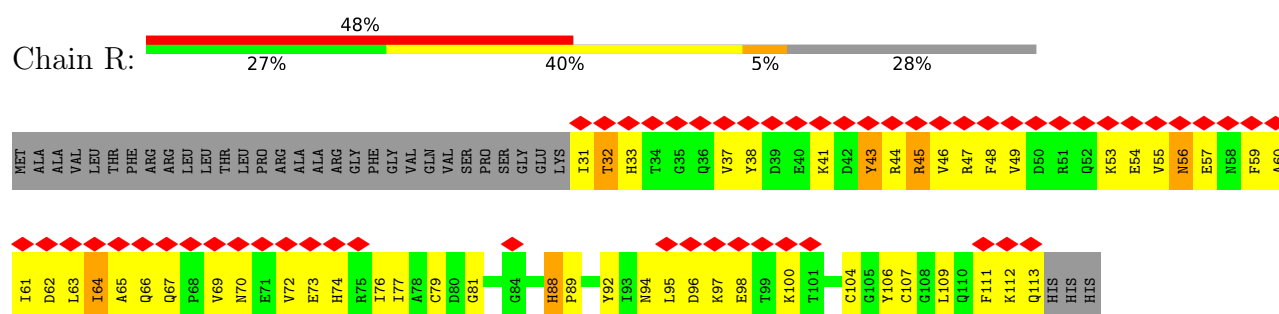
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



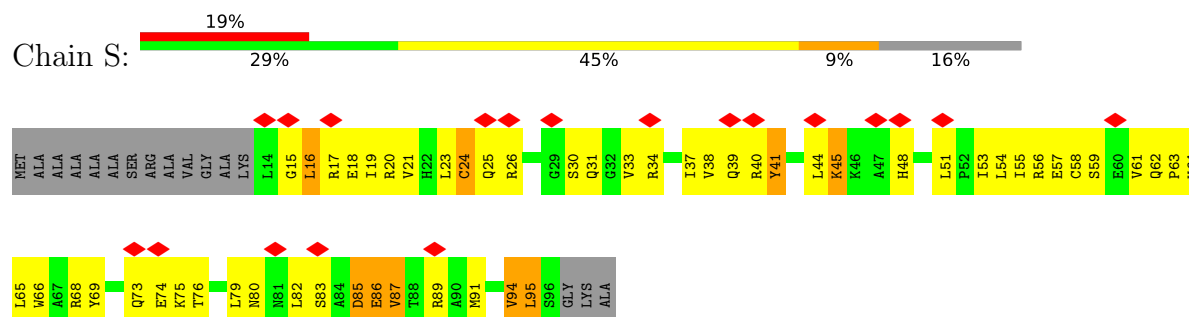
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



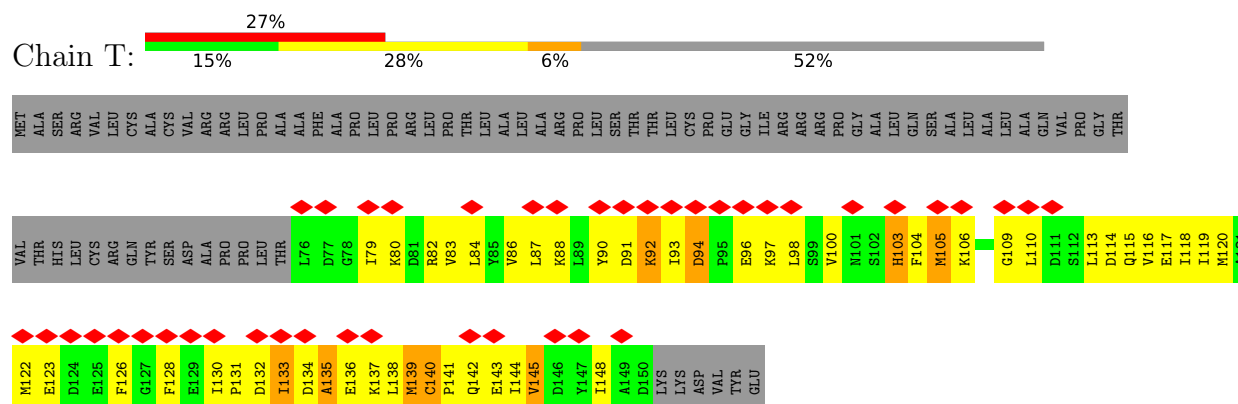
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



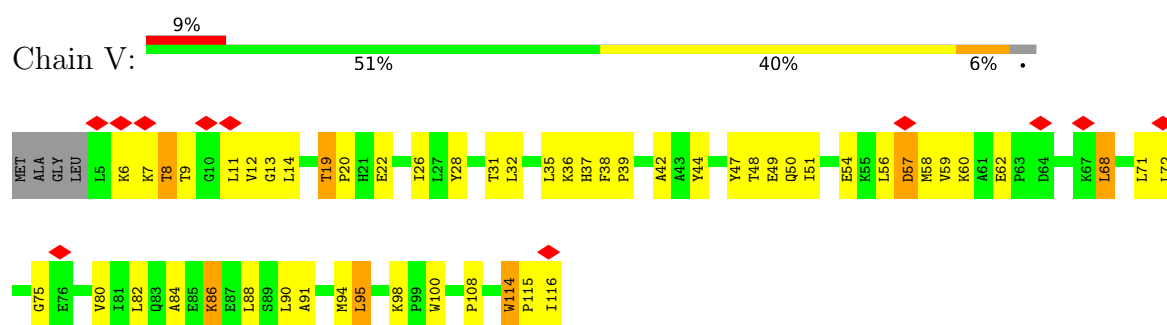
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



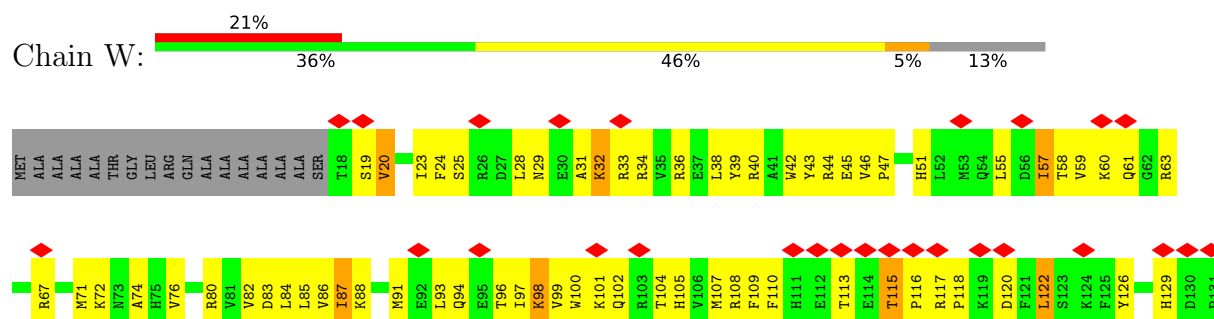
- Molecule 14: Acyl carrier protein, mitochondrial



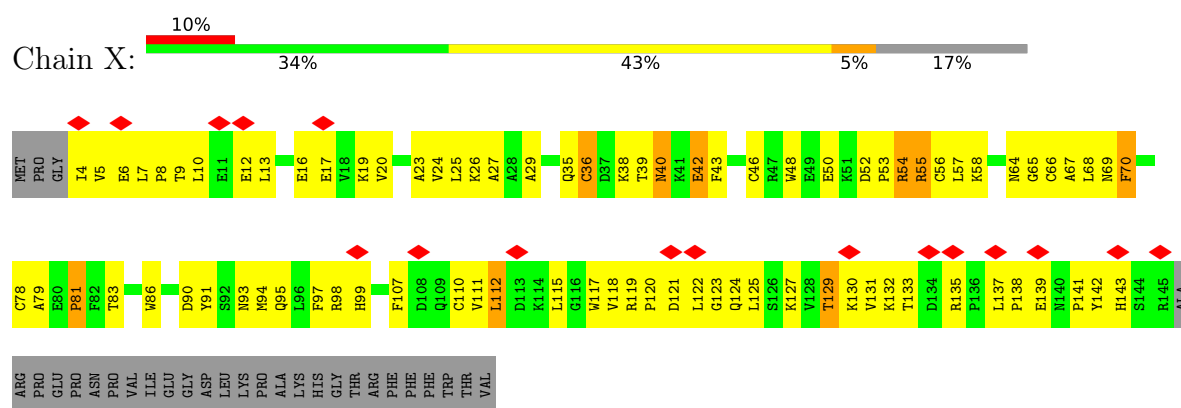
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



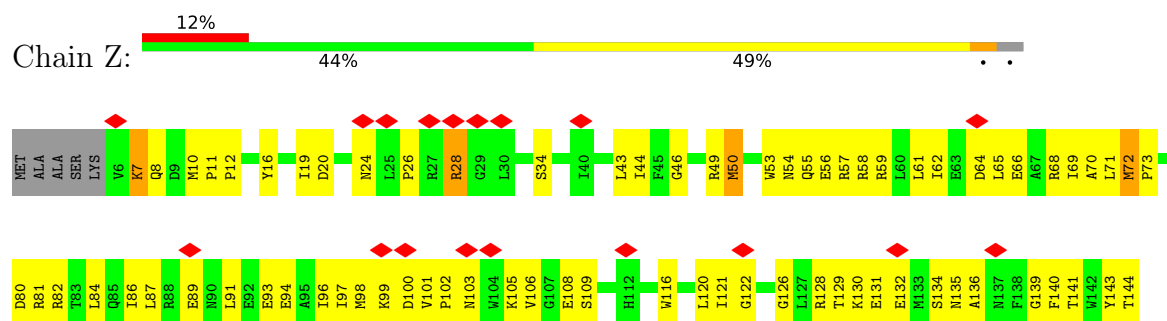
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

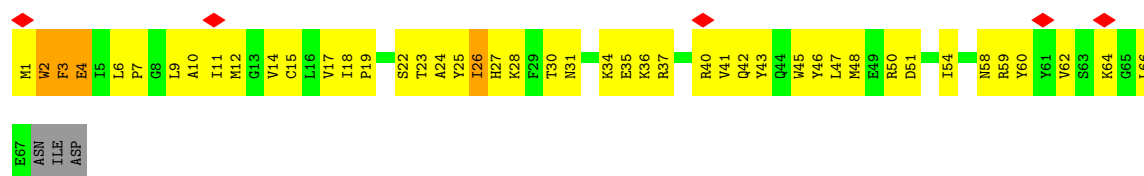


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

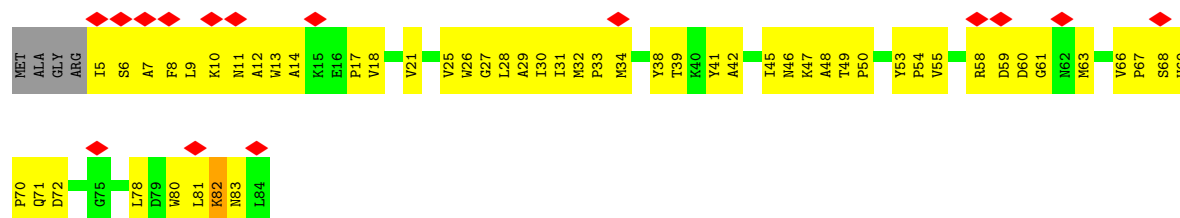


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1





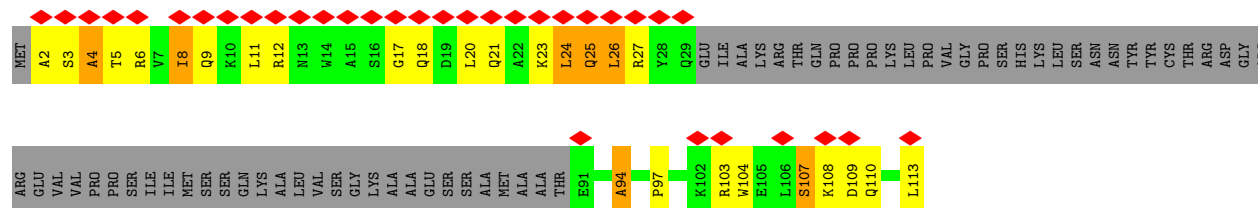
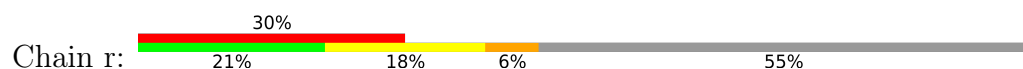
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



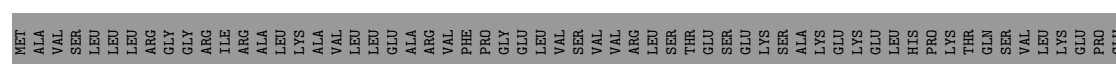
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



PRO	THR	ASP	THR	THR	THR	TYR	LYS	ASN	LEU	GLN	HIS	HIS	ASP	TYR																																																																																																																																																																																																																																																																																																																																																																																																																								
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.385	Depositor
Minimum map value	-1.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.083	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: ZN, FMN, UQ9, FES, SF4, CDL, NDP, 3PE, EHZ, PC1

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	0.99	0/941	1.24	10/1285 (0.8%)
2	B	1.00	1/1289 (0.1%)	1.36	11/1744 (0.6%)
3	C	0.87	1/1687 (0.1%)	1.31	14/2297 (0.6%)
4	D	0.94	5/3162 (0.2%)	1.31	22/4276 (0.5%)
5	E	0.81	2/1675 (0.1%)	1.25	15/2282 (0.7%)
6	F	0.88	1/3363 (0.0%)	1.44	54/4543 (1.2%)
7	G	0.89	6/5374 (0.1%)	1.59	104/7281 (1.4%)
8	H	0.97	2/2615 (0.1%)	1.55	60/3574 (1.7%)
9	I	0.90	0/1427	1.54	19/1927 (1.0%)
10	P	0.79	1/2804 (0.0%)	1.26	34/3802 (0.9%)
11	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	0.63	0/671	1.19	9/903 (1.0%)
13	S	0.93	1/678 (0.1%)	1.65	17/915 (1.9%)
14	T	0.91	0/613	1.51	9/826 (1.1%)
15	V	0.87	0/937	1.47	14/1270 (1.1%)
16	W	0.80	0/993	1.33	15/1335 (1.1%)
17	X	0.84	1/1191 (0.1%)	1.44	21/1605 (1.3%)
18	Z	0.76	0/1183	1.10	7/1597 (0.4%)
19	a	0.82	0/561	1.36	5/755 (0.7%)
20	b	0.70	0/651	0.91	1/895 (0.1%)
21	q	0.96	2/1037 (0.2%)	1.44	15/1408 (1.1%)
22	r	0.98	1/426 (0.2%)	1.57	9/573 (1.6%)
23	s	0.76	0/108	1.08	0/147
All	All	0.88	25/34366 (0.1%)	1.41	477/46564 (1.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	60	PRO	N-CD	13.80	1.67	1.47
6	F	235	VAL	N-CA	-9.28	1.34	1.46
11	Q	53	ILE	C-O	7.78	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	203	ASP	CA-C	6.75	1.62	1.52
4	D	106	VAL	C-N	-6.55	1.24	1.33
7	G	600	GLU	CA-C	6.44	1.61	1.52
2	B	110	PRO	C-O	-6.29	1.16	1.24
4	D	266	ARG	C-O	-6.28	1.16	1.24
7	G	127	ASP	CA-C	6.27	1.62	1.52
7	G	76	ARG	CA-C	6.12	1.61	1.53
5	E	93	PRO	N-CD	-5.94	1.39	1.47
17	X	54	ARG	CA-C	5.92	1.60	1.52
7	G	361	VAL	CA-C	5.87	1.60	1.52
22	r	25	GLN	CA-C	5.80	1.60	1.52
5	E	80	PRO	N-CD	5.64	1.55	1.47
4	D	392	PRO	C-O	-5.57	1.20	1.24
13	S	95	LEU	CA-C	5.54	1.59	1.52
4	D	107	ARG	C-N	5.49	1.40	1.33
7	G	683	PRO	N-CD	-5.47	1.40	1.47
21	q	126	PRO	N-CD	5.41	1.55	1.47
10	P	235	THR	CA-C	5.28	1.59	1.53
4	D	266	ARG	CA-C	-5.26	1.45	1.52
8	H	310	PHE	CA-C	5.07	1.59	1.52
3	C	61	GLY	C-N	-5.04	1.27	1.33
21	q	69	ASN	CA-C	5.00	1.60	1.52

All (477) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-16.80	89.10	114.64
8	H	208	VAL	N-CA-C	-13.66	100.83	111.62
7	G	251	ILE	N-CA-C	13.31	126.81	108.17
7	G	77	MET	N-CA-C	-13.09	97.28	113.38
9	I	164	VAL	N-CA-C	-12.87	100.09	112.83
7	G	500	ILE	N-CA-C	-12.57	98.72	110.53
6	F	171	VAL	N-CA-C	-11.82	99.42	110.53
7	G	204	MET	N-CA-C	-11.62	91.47	109.25
6	F	449	ARG	N-CA-C	-11.60	98.72	111.36
7	G	599	THR	N-CA-C	11.38	126.26	112.38
11	Q	60	ASP	N-CA-C	-11.35	90.29	109.24
13	S	39	GLN	N-CA-C	11.17	125.43	111.69
16	W	87	ILE	N-CA-C	-11.08	99.78	110.42
15	V	57	ASP	N-CA-C	-11.04	99.26	111.07
8	H	259	PHE	N-CA-C	-11.00	99.37	111.36
17	X	70	PHE	N-CA-C	-10.62	99.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	77	LEU	N-CA-C	-10.47	99.66	111.71
14	T	139	MET	N-CA-C	-10.43	97.41	113.89
16	W	59	VAL	N-CA-C	-10.33	100.50	110.42
8	H	284	GLN	N-CA-C	-10.33	100.02	111.07
2	B	195	PRO	N-CA-C	-10.32	98.11	110.70
5	E	68	ASN	N-CA-C	-10.32	100.03	111.07
7	G	280	ASP	N-CA-C	10.29	122.50	111.28
4	D	337	MET	N-CA-C	-10.26	100.10	111.07
19	a	4	GLU	N-CA-C	10.25	124.89	112.38
10	P	366	ILE	N-CA-C	10.24	121.07	110.62
9	I	161	ALA	N-CA-C	10.06	122.25	111.28
7	G	414	PHE	N-CA-C	-10.04	101.53	113.88
14	T	135	ALA	N-CA-C	-10.03	100.35	111.28
9	I	166	ALA	N-CA-C	-9.89	100.76	113.12
6	F	178	GLU	N-CA-C	-9.88	99.26	111.11
7	G	325	ARG	N-CA-C	-9.86	100.23	110.97
6	F	103	ASN	N-CA-C	-9.82	100.98	113.16
7	G	654	VAL	N-CA-C	9.77	123.30	111.09
6	F	144	VAL	N-CA-C	-9.77	101.35	110.53
6	F	141	GLY	N-CA-C	-9.76	101.18	112.50
7	G	35	PHE	N-CA-C	9.64	124.29	108.96
7	G	337	ALA	N-CA-C	-9.61	100.77	114.12
8	H	52	ALA	N-CA-C	-9.55	100.85	111.07
6	F	418	GLN	N-CA-C	-9.54	100.84	111.14
4	D	427	PRO	N-CA-C	-9.48	95.62	110.50
8	H	200	LEU	N-CA-C	-9.44	100.99	111.28
19	a	2	TRP	N-CA-C	-9.43	101.69	113.01
14	T	133	ILE	N-CA-C	9.38	119.92	110.82
7	G	692	LYS	N-CA-C	-9.33	100.47	112.23
7	G	694	PHE	N-CA-C	9.33	121.45	111.28
10	P	367	GLU	N-CA-C	9.28	122.58	111.82
7	G	640	ASP	N-CA-C	-9.19	101.34	111.36
5	E	85	ALA	N-CA-C	-9.17	101.36	111.36
10	P	157	LYS	N-CA-C	-9.11	101.43	111.36
7	G	389	THR	N-CA-C	-9.10	96.31	109.96
17	X	55	ARG	N-CA-C	9.02	130.02	110.80
7	G	365	ASN	N-CA-C	-8.77	102.14	112.92
7	G	133	GLN	N-CA-CB	8.73	121.46	110.45
7	G	212	LYS	N-CA-C	-8.72	94.69	108.90
9	I	154	TYR	N-CA-CB	-8.69	99.19	111.62
10	P	96	LEU	N-CA-C	8.68	121.70	111.71
16	W	20	VAL	N-CA-C	8.67	120.77	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	207	LEU	N-CA-C	-8.62	92.43	110.80
10	P	373	LYS	N-CA-C	8.52	121.94	110.35
13	S	86	GLU	N-CA-C	-8.50	102.09	111.36
13	S	18	GLU	N-CA-C	8.47	123.21	109.40
12	R	57	GLU	N-CA-C	-8.46	98.32	110.59
16	W	100	TRP	N-CA-C	-8.44	99.88	112.04
17	X	99	HIS	N-CA-C	-8.43	102.18	111.36
7	G	452	LEU	N-CA-C	-8.35	102.18	111.28
3	C	108	LYS	N-CA-C	8.35	120.00	111.07
8	H	141	SER	N-CA-C	-8.33	102.16	111.07
16	W	57	ILE	N-CA-C	8.32	121.99	109.17
11	Q	54	THR	N-CA-C	8.32	123.27	109.46
8	H	311	THR	N-CA-C	-8.27	102.50	112.59
7	G	558	GLN	N-CA-C	-8.26	102.23	111.07
8	H	196	ALA	N-CA-C	8.23	128.00	109.81
3	C	196	PRO	N-CA-C	8.19	124.91	113.53
7	G	691	ILE	N-CA-C	8.15	123.63	111.89
7	G	484	ASP	N-CA-C	8.14	121.08	111.71
15	V	86	LYS	N-CA-C	-8.14	102.35	111.14
16	W	96	THR	N-CA-C	-8.12	102.37	111.14
6	F	298	GLU	N-CA-C	8.12	120.13	111.28
6	F	191	TYR	N-CA-C	8.11	121.67	110.24
2	B	110	PRO	N-CA-C	8.09	124.58	113.65
7	G	500	ILE	N-CA-CB	8.05	120.88	110.57
7	G	534	VAL	N-CA-C	-8.02	104.77	111.91
17	X	43	PHE	N-CA-C	-8.00	102.50	111.14
13	S	76	THR	N-CA-C	7.99	121.92	108.90
16	W	98	LYS	N-CA-C	-7.99	101.58	113.72
8	H	271	LEU	N-CA-C	-7.98	102.53	111.14
17	X	112	LEU	N-CA-C	-7.96	102.54	111.14
7	G	651	PRO	CB-CA-C	-7.95	98.44	111.56
21	q	67	GLU	CB-CA-C	-7.94	99.59	112.06
10	P	206	ILE	N-CA-C	7.93	120.92	108.87
9	I	201	ILE	N-CA-C	-7.93	102.71	110.72
8	H	311	THR	N-CA-CB	7.91	123.58	110.92
17	X	46	CYS	N-CA-C	-7.91	102.74	111.36
15	V	6	LYS	N-CA-C	-7.88	100.13	110.53
17	X	55	ARG	N-CA-CB	-7.85	97.23	110.49
7	G	270	VAL	N-CA-CB	-7.83	100.67	110.31
9	I	160	GLU	N-CA-C	7.79	124.15	111.37
7	G	389	THR	N-CA-CB	7.79	121.46	109.85
10	P	235	THR	CB-CA-C	-7.77	100.10	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	58	LYS	N-CA-C	-7.77	102.76	111.07
4	D	84	PHE	N-CA-C	-7.75	98.00	109.62
8	H	201	THR	N-CA-C	-7.74	99.83	110.35
9	I	74	LEU	N-CA-C	-7.70	102.89	111.28
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
21	q	44	TYR	N-CA-C	-7.67	98.93	110.28
6	F	58	ARG	N-CA-C	-7.66	103.01	111.36
6	F	171	VAL	N-CA-CB	7.66	120.37	110.57
12	R	32	THR	N-CA-C	7.65	119.68	110.19
21	q	89	TRP	N-CA-C	-7.61	102.92	111.14
7	G	569	GLN	N-CA-C	7.61	122.00	108.24
7	G	56	VAL	N-CA-C	-7.60	103.04	110.72
5	E	68	ASN	N-CA-CB	7.55	120.96	110.01
7	G	467	LYS	N-CA-C	-7.52	102.23	111.33
12	R	74	HIS	N-CA-C	7.52	121.10	110.50
9	I	119	CYS	N-CA-C	-7.51	103.17	111.36
7	G	277	MET	N-CA-C	7.47	120.57	109.59
7	G	303	THR	N-CA-C	7.47	123.12	113.18
9	I	158	CYS	N-CA-C	-7.46	103.15	111.28
6	F	430	GLY	N-CA-C	7.45	121.67	112.73
4	D	99	LEU	N-CA-C	7.43	121.03	109.07
7	G	510	TRP	N-CA-CB	7.40	120.88	109.85
15	V	57	ASP	N-CA-CB	7.38	120.71	110.01
2	B	183	ARG	N-CA-C	-7.38	104.53	113.97
4	D	350	LYS	CB-CA-C	-7.37	101.02	111.85
21	q	24	LEU	N-CA-C	-7.30	103.33	111.28
13	S	94	VAL	N-CA-C	7.28	117.41	110.42
8	H	309	ILE	N-CA-C	7.27	117.35	110.30
1	A	93	ILE	N-CA-C	-7.26	102.74	110.36
3	C	195	HIS	CB-CA-C	7.25	117.35	110.17
7	G	384	ASN	N-CA-C	-7.25	103.41	111.82
7	G	374	THR	CB-CA-C	-7.24	99.84	111.28
7	G	497	VAL	N-CA-C	-7.24	103.24	110.62
7	G	465	VAL	N-CA-CB	7.22	118.53	110.51
15	V	68	LEU	N-CA-C	-7.22	103.41	111.28
14	T	105	MET	N-CA-C	7.22	119.23	111.36
8	H	50	ALA	N-CA-C	7.20	118.78	111.07
8	H	139	THR	N-CA-CB	7.20	120.45	110.01
6	F	73	PRO	N-CA-C	-7.18	103.78	113.40
10	P	370	LYS	N-CA-C	7.18	119.22	109.24
7	G	217	GLU	N-CA-C	-7.17	101.59	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	81	LYS	N-CA-C	-7.17	103.55	111.36
7	G	661	GLU	N-CA-C	7.16	118.78	110.97
7	G	461	SER	N-CA-C	7.11	119.93	111.33
15	V	95	LEU	N-CA-C	-7.09	103.56	111.28
6	F	78	GLY	N-CA-C	-7.08	104.23	112.73
8	H	254	LEU	N-CA-C	-7.07	103.62	111.82
11	Q	162	ALA	N-CA-C	7.05	118.96	111.28
21	q	77	VAL	N-CA-C	-7.02	99.67	109.21
7	G	148	SER	N-CA-C	7.01	120.83	109.40
2	B	166	ASN	N-CA-C	-6.99	103.35	110.97
7	G	150	ARG	N-CA-C	6.99	119.55	109.14
6	F	246	GLU	N-CA-C	-6.97	103.68	111.28
6	F	418	GLN	N-CA-CB	6.97	120.18	110.07
6	F	169	LEU	N-CA-C	6.97	118.88	111.28
6	F	455	GLN	N-CA-C	6.97	118.53	111.07
8	H	176	LEU	CA-C-N	-6.96	113.63	120.52
8	H	176	LEU	C-N-CA	-6.96	113.63	120.52
7	G	294	TYR	N-CA-C	-6.96	104.60	113.23
6	F	103	ASN	N-CA-CB	6.95	121.08	110.44
7	G	582	VAL	N-CA-C	6.95	118.48	108.48
8	H	292	ASN	N-CA-C	6.95	118.93	111.36
7	G	300	GLN	N-CA-CB	6.93	122.55	112.08
6	F	428	GLY	N-CA-C	-6.92	103.91	112.77
16	W	87	ILE	N-CA-CB	6.92	118.65	110.55
10	P	235	THR	CA-C-O	6.92	128.10	121.67
6	F	148	ALA	N-CA-C	-6.91	103.83	111.36
8	H	300	LEU	N-CA-C	-6.91	104.11	112.54
3	C	69	PRO	N-CA-C	-6.90	104.34	113.65
5	E	152	GLN	N-CA-C	-6.89	103.70	111.07
7	G	362	ASP	N-CA-C	6.87	125.43	110.80
14	T	145	VAL	N-CA-C	-6.86	103.79	110.72
1	A	9	ILE	N-CA-C	-6.84	102.50	111.05
18	Z	28	ARG	N-CA-C	6.83	119.66	108.52
18	Z	34	SER	N-CA-C	-6.83	103.76	111.07
8	H	305	ILE	N-CA-C	-6.81	103.38	113.39
7	G	268	GLY	N-CA-C	6.80	124.76	115.30
6	F	244	ASN	N-CA-C	-6.80	100.91	110.50
12	R	56	ASN	N-CA-C	6.80	119.98	108.90
7	G	133	GLN	N-CA-C	-6.78	101.25	110.68
7	G	434	SER	N-CA-C	-6.74	100.98	110.29
22	r	11	LEU	N-CA-C	-6.71	104.04	111.36
15	V	8	THR	N-CA-C	6.71	119.06	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	97	PHE	N-CA-C	6.69	118.66	111.36
7	G	601	GLY	N-CA-C	6.68	124.92	115.30
8	H	8	THR	N-CA-C	-6.67	101.27	110.35
5	E	199	ASP	N-CA-C	-6.67	103.70	110.97
17	X	129	THR	N-CA-C	6.67	120.91	110.17
8	H	220	PHE	N-CA-C	-6.67	103.94	111.07
1	A	24	LEU	CA-C-N	-6.66	113.86	120.98
1	A	24	LEU	C-N-CA	-6.66	113.86	120.98
9	I	208	ASP	N-CA-C	6.66	121.56	113.17
16	W	105	HIS	N-CA-C	-6.66	104.98	113.23
6	F	344	GLN	N-CA-C	-6.65	103.95	111.07
7	G	640	ASP	N-CA-CB	6.64	119.98	110.16
15	V	114	TRP	N-CA-CB	6.63	120.19	110.30
3	C	125	PHE	N-CA-CB	-6.62	100.63	110.17
15	V	86	LYS	N-CA-CB	6.61	119.65	110.07
7	G	287	SER	N-CA-C	6.61	119.25	110.53
2	B	123	ALA	N-CA-C	6.61	118.28	111.14
6	F	228	PRO	N-CA-C	-6.61	98.86	112.47
8	H	182	ALA	N-CA-C	-6.60	104.00	111.07
6	F	336	LEU	N-CA-CB	-6.60	100.94	111.43
10	P	116	ILE	N-CA-C	-6.60	104.06	110.72
1	A	33	LYS	N-CA-C	-6.58	104.48	113.30
7	G	435	PRO	N-CA-C	-6.57	100.19	110.50
13	S	40	ARG	N-CA-C	6.56	122.80	113.02
8	H	93	HIS	CB-CA-C	6.55	117.73	108.76
4	D	184	ILE	N-CA-C	-6.54	103.95	110.62
11	Q	141	ASN	N-CA-CB	6.53	120.71	110.46
7	G	605	GLN	N-CA-C	6.52	119.15	108.52
13	S	16	LEU	N-CA-C	-6.50	98.30	108.90
22	r	24	LEU	N-CA-C	6.49	119.65	110.50
17	X	81	PRO	N-CA-C	-6.46	104.23	113.47
17	X	98	ARG	N-CA-C	6.46	120.42	112.54
7	G	250	SER	N-CA-C	6.46	116.81	108.34
4	D	388	GLY	N-CA-C	6.45	119.55	110.38
15	V	49	GLU	N-CA-C	-6.45	104.25	111.28
12	R	81	GLY	N-CA-C	-6.45	106.82	115.21
3	C	125	PHE	N-CA-C	6.45	119.59	110.50
21	q	75	TRP	N-CA-C	6.45	121.41	112.45
8	H	267	SER	N-CA-C	-6.44	104.34	111.36
9	I	205	ILE	N-CA-C	-6.42	104.24	110.72
6	F	178	GLU	N-CA-CB	6.41	119.49	109.94
8	H	177	PRO	N-CA-C	-6.41	101.58	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	125	CYS	N-CA-C	-6.40	105.45	113.20
8	H	255	TYR	N-CA-CB	6.40	119.29	110.01
7	G	273	ILE	N-CA-C	-6.40	98.30	107.77
12	R	43	TYR	N-CA-C	-6.40	99.81	109.79
9	I	66	LEU	N-CA-C	-6.38	104.40	111.36
8	H	271	LEU	N-CA-CB	6.38	119.31	110.07
11	Q	59	LEU	N-CA-C	-6.37	100.74	110.30
7	G	95	PRO	N-CA-C	-6.37	101.18	110.80
6	F	370	LEU	N-CA-C	-6.37	104.42	111.36
6	F	144	VAL	N-CA-CB	6.34	118.69	110.57
15	V	91	ALA	N-CA-C	-6.33	104.38	111.28
22	r	8	ILE	N-CA-C	-6.30	104.35	110.72
6	F	415	ILE	N-CA-C	-6.30	104.36	110.72
19	a	26	ILE	N-CA-C	-6.29	104.51	113.07
21	q	28	PHE	N-CA-C	6.29	117.81	111.07
17	X	99	HIS	N-CA-CB	6.28	119.45	110.16
7	G	176	CYS	N-CA-C	6.28	119.58	110.42
6	F	255	CYS	N-CA-C	-6.26	104.53	111.36
7	G	383	SER	N-CA-C	-6.26	106.86	114.75
21	q	69	ASN	N-CA-CB	6.26	121.42	111.66
7	G	356	ASP	N-CA-CB	6.25	119.31	110.12
6	F	101	PHE	N-CA-C	6.25	118.89	111.33
11	Q	141	ASN	N-CA-C	-6.24	105.67	113.28
15	V	71	LEU	N-CA-C	6.23	118.07	111.28
8	H	67	SER	N-CA-C	-6.23	102.14	110.55
2	B	113	ASP	N-CA-CB	6.23	119.49	109.28
8	H	269	THR	N-CA-C	6.21	118.05	111.28
5	E	50	THR	N-CA-CB	6.20	121.41	110.37
10	P	118	LYS	N-CA-C	6.20	119.02	111.82
8	H	52	ALA	N-CA-CB	6.20	119.00	110.01
7	G	451	ILE	N-CA-C	-6.19	104.95	113.00
10	P	368	GLU	N-CA-CB	6.18	119.82	110.30
6	F	192	ASP	N-CA-C	6.18	119.02	109.07
17	X	36	CYS	CB-CA-C	-6.18	97.29	110.76
4	D	291	VAL	N-CA-C	-6.18	103.37	111.09
6	F	212	LEU	N-CA-C	-6.17	104.55	111.28
22	r	26	LEU	N-CA-CB	-6.17	101.15	110.35
18	Z	44	ILE	N-CA-C	-6.15	104.75	110.53
7	G	418	ILE	N-CA-C	-6.14	103.45	112.04
7	G	420	LYS	N-CA-C	6.12	118.74	111.33
8	H	276	SER	N-CA-C	6.12	118.92	111.82
13	S	40	ARG	N-CA-CB	-6.12	101.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	325	ARG	N-CA-CB	6.08	118.79	109.91
8	H	185	TRP	N-CA-C	-6.07	104.02	112.45
7	G	508	ALA	N-CA-C	6.04	117.87	111.28
13	S	87	VAL	N-CA-C	-6.04	104.46	110.62
7	G	353	ALA	N-CA-C	-6.02	104.64	112.23
7	G	638	THR	N-CA-C	-6.00	100.18	109.24
22	r	108	LYS	N-CA-C	6.00	117.90	111.36
8	H	24	GLU	N-CA-C	-6.00	104.11	112.45
8	H	103	LEU	N-CA-C	-6.00	104.82	111.36
13	S	61	VAL	N-CA-C	-5.99	99.61	107.88
17	X	40	ASN	N-CA-C	-5.98	104.67	111.07
8	H	7	LEU	N-CA-C	-5.98	104.39	111.03
8	H	315	PRO	O-C-N	5.97	123.96	121.15
2	B	196	PRO	N-CA-C	-5.96	101.84	111.03
6	F	291	GLU	N-CA-C	5.95	118.22	110.43
9	I	116	CYS	N-CA-C	-5.94	105.52	112.89
14	T	94	ASP	N-CA-CB	-5.92	105.09	111.66
13	S	30	SER	N-CA-C	-5.91	106.11	113.38
7	G	387	LEU	CB-CA-C	-5.91	101.75	111.68
8	H	228	TYR	CB-CA-C	5.88	120.01	110.96
4	D	258	VAL	N-CA-C	-5.86	103.94	110.62
7	G	480	ALA	N-CA-C	-5.85	104.98	111.36
21	q	5	GLU	N-CA-C	-5.85	104.98	111.36
21	q	65	THR	N-CA-C	5.85	119.21	110.14
4	D	352	PRO	N-CA-C	5.84	117.83	110.70
3	C	209	LEU	N-CA-CB	-5.83	100.68	110.83
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
15	V	19	THR	N-CA-CB	5.83	120.75	110.37
3	C	71	TYR	N-CA-C	5.83	120.20	113.38
13	S	86	GLU	N-CA-CB	5.82	118.78	110.16
2	B	135	GLY	CA-C-O	-5.82	117.92	122.52
7	G	34	VAL	N-CA-C	5.81	116.24	108.11
6	F	226	LYS	CA-C-N	-5.80	114.40	120.38
6	F	226	LYS	C-N-CA	-5.80	114.40	120.38
10	P	367	GLU	CB-CA-C	-5.79	99.55	110.67
10	P	157	LYS	N-CA-CB	5.79	118.72	110.16
8	H	116	ILE	N-CA-C	-5.78	104.87	110.42
10	P	234	LYS	CB-CA-C	-5.78	103.37	111.80
10	P	122	HIS	N-CA-C	5.78	120.02	112.92
7	G	672	ALA	N-CA-C	-5.77	104.99	111.28
6	F	299	LEU	N-CA-C	5.77	118.52	111.82
11	Q	164	PHE	N-CA-CB	5.77	119.77	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	289	LYS	N-CA-C	5.77	117.57	111.28
12	R	45	ARG	N-CA-C	-5.77	104.96	113.61
6	F	102	MET	CB-CA-C	-5.76	101.43	110.94
4	D	414	ASP	N-CA-C	-5.76	101.44	110.36
10	P	272	LEU	N-CA-C	-5.75	101.76	110.28
21	q	140	PRO	N-CA-C	-5.72	102.16	110.80
13	S	73	GLN	N-CA-C	-5.71	100.39	109.59
17	X	65	GLY	N-CA-C	-5.70	105.88	112.50
6	F	393	ASN	N-CA-C	-5.70	104.98	111.07
5	E	119	THR	N-CA-C	-5.69	105.83	112.89
10	P	119	ALA	N-CA-C	-5.69	105.00	111.14
8	H	252	PRO	N-CA-CB	-5.69	98.05	103.51
18	Z	72	MET	CA-C-N	-5.67	113.34	119.24
18	Z	72	MET	C-N-CA	-5.67	113.34	119.24
6	F	41	ILE	N-CA-C	5.67	115.75	110.42
8	H	221	ALA	CA-C-N	-5.66	112.25	120.29
8	H	221	ALA	C-N-CA	-5.66	112.25	120.29
6	F	457	HIS	N-CA-CB	-5.66	100.88	110.50
17	X	79	ALA	N-CA-C	5.66	117.12	111.07
2	B	112	TYR	N-CA-C	5.65	122.84	110.80
17	X	56	CYS	N-CA-C	5.65	119.87	112.92
6	F	304	ALA	CB-CA-C	-5.64	110.05	116.54
7	G	59	GLN	N-CA-C	5.64	117.97	107.99
8	H	126	LYS	N-CA-C	5.63	117.42	111.28
11	Q	124	MET	CA-C-N	-5.63	114.99	122.98
11	Q	124	MET	C-N-CA	-5.63	114.99	122.98
2	B	201	LEU	N-CA-C	-5.62	105.16	111.28
9	I	191	LEU	N-CA-C	-5.61	105.25	111.36
7	G	530	TYR	N-CA-C	-5.61	101.98	110.28
7	G	599	THR	CA-C-N	-5.60	114.20	122.83
7	G	599	THR	C-N-CA	-5.60	114.20	122.83
7	G	615	LEU	N-CA-C	-5.60	106.22	113.16
6	F	416	SER	N-CA-C	5.60	117.83	111.11
6	F	176	ALA	N-CA-C	5.59	118.10	111.33
8	H	76	THR	N-CA-C	-5.59	104.56	111.33
21	q	142	THR	N-CA-CB	5.57	119.87	109.68
4	D	92	HIS	N-CA-C	-5.56	105.57	112.47
5	E	183	PRO	N-CA-C	-5.55	102.22	111.26
14	T	135	ALA	N-CA-CB	5.54	118.27	110.12
6	F	294	VAL	CA-C-N	-5.54	114.05	119.76
6	F	294	VAL	C-N-CA	-5.54	114.05	119.76
10	P	130	ILE	N-CA-C	5.54	115.23	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	363	SER	N-CA-C	-5.53	100.17	109.07
21	q	68	MET	N-CA-C	5.53	119.28	112.54
5	E	222	PHE	CB-CA-C	-5.52	100.64	109.75
7	G	127	ASP	CA-C-O	5.52	129.01	121.89
17	X	54	ARG	CB-CA-C	5.50	119.43	110.96
21	q	71	LYS	N-CA-C	5.50	119.97	113.16
6	F	118	ASP	N-CA-C	-5.49	102.15	110.28
8	H	141	SER	N-CA-CB	5.49	117.97	110.01
22	r	94	ALA	N-CA-C	-5.48	101.74	109.96
3	C	71	TYR	CB-CA-C	-5.48	102.30	111.23
7	G	313	LEU	N-CA-C	5.47	118.48	109.72
10	P	86	CYS	N-CA-C	-5.46	103.18	110.55
4	D	132	ALA	N-CA-C	-5.46	106.62	113.72
7	G	682	ASP	CA-C-N	-5.45	114.14	119.76
7	G	682	ASP	C-N-CA	-5.45	114.14	119.76
7	G	404	GLY	N-CA-C	5.45	121.43	113.48
4	D	200	PHE	CA-CB-CG	5.43	119.23	113.80
19	a	25	TYR	N-CA-C	-5.43	107.91	114.75
7	G	150	ARG	N-CA-CB	-5.42	102.83	111.62
14	T	92	LYS	N-CA-C	-5.42	106.25	112.92
12	R	88	HIS	CB-CA-C	5.41	117.36	109.08
10	P	357	ARG	N-CA-C	5.41	117.51	110.43
3	C	81	ASP	N-CA-C	-5.40	104.45	111.74
7	G	420	LYS	N-CA-CB	-5.40	101.96	110.06
13	S	41	TYR	N-CA-C	-5.39	105.48	111.36
10	P	374	THR	N-CA-C	5.39	117.51	108.73
17	X	27	ALA	N-CA-C	-5.39	105.06	111.69
5	E	48	PRO	N-CA-C	5.38	120.84	113.84
1	A	110	GLY	N-CA-C	-5.38	104.37	112.60
4	D	391	VAL	CA-C-N	-5.38	115.79	119.66
4	D	391	VAL	C-N-CA	-5.38	115.79	119.66
4	D	201	PHE	N-CA-C	-5.37	105.51	111.36
6	F	199	ARG	N-CA-C	5.36	117.46	109.59
10	P	339	GLY	N-CA-C	5.35	122.71	115.00
11	Q	164	PHE	N-CA-C	-5.35	106.72	113.20
7	G	510	TRP	N-CA-C	-5.35	101.94	109.96
18	Z	55	GLN	N-CA-C	-5.34	105.46	111.28
8	H	94	PRO	N-CA-C	5.34	118.70	111.22
13	S	24	CYS	N-CA-C	-5.33	103.35	110.55
11	Q	163	ASN	CB-CA-C	-5.33	99.35	109.95
16	W	32	LYS	N-CA-C	-5.33	104.88	111.33
7	G	356	ASP	N-CA-C	-5.33	105.47	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	252	PRO	CA-N-CD	5.33	119.45	112.00
5	E	222	PHE	N-CA-C	5.32	117.91	109.24
1	A	101	GLY	N-CA-C	-5.32	106.33	112.50
5	E	48	PRO	CB-CA-C	-5.30	104.32	111.85
9	I	54	THR	N-CA-C	-5.30	104.92	111.33
18	Z	50	MET	N-CA-C	-5.30	105.50	111.28
10	P	137	ARG	N-CA-C	5.30	122.08	110.80
7	G	435	PRO	CB-CA-C	-5.28	105.80	111.56
8	H	146	MET	N-CA-C	-5.27	105.43	111.07
10	P	330	THR	N-CA-C	-5.27	106.75	114.39
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
11	Q	72	ILE	N-CA-C	-5.26	108.37	113.53
16	W	122	LEU	N-CA-C	-5.26	105.55	111.28
4	D	363	VAL	N-CA-C	5.25	116.33	111.81
8	H	46	LEU	N-CA-C	-5.25	106.64	113.16
2	B	153	PRO	N-CA-C	5.25	118.83	111.33
8	H	310	PHE	N-CA-C	5.24	119.29	113.01
16	W	120	ASP	N-CA-C	-5.24	102.53	110.28
7	G	277	MET	N-CA-CB	-5.23	101.65	109.71
6	F	300	ILE	N-CA-CB	5.23	119.29	110.56
7	G	362	ASP	CA-CB-CG	5.22	117.82	112.60
10	P	260	GLY	N-CA-C	-5.22	108.42	115.36
7	G	600	GLU	CB-CA-C	-5.20	103.00	111.06
3	C	164	TRP	N-CA-C	5.20	117.02	111.36
22	r	107	SER	N-CA-C	-5.18	102.19	109.96
7	G	556	THR	N-CA-C	-5.18	101.54	109.41
10	P	194	VAL	N-CA-CB	5.18	118.35	110.58
10	P	192	ARG	N-CA-C	-5.18	105.64	111.28
7	G	713	ALA	N-CA-C	-5.18	105.53	111.07
8	H	90	PRO	CA-C-O	-5.17	117.39	121.38
10	P	198	ALA	N-CA-C	-5.17	100.09	108.52
6	F	337	MET	CB-CA-C	-5.17	102.99	111.68
8	H	277	TYR	N-CA-C	5.17	118.00	110.10
7	G	172	ILE	N-CA-C	-5.16	98.60	109.34
7	G	63	PHE	CA-C-O	-5.16	115.08	121.06
7	G	569	GLN	CB-CA-C	-5.15	104.22	112.05
22	r	25	GLN	N-CA-C	5.15	118.82	112.54
13	S	85	ASP	N-CA-C	5.15	117.79	111.82
4	D	391	VAL	N-CA-C	5.14	113.80	109.02
19	a	3	PHE	CB-CA-C	-5.14	102.59	110.81
7	G	387	LEU	N-CA-C	-5.13	98.33	107.98
8	H	196	ALA	CA-C-N	-5.13	113.52	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	196	ALA	C-N-CA	-5.13	113.52	119.47
20	b	82	LYS	N-CA-C	-5.12	103.77	110.53
16	W	115	THR	CA-C-N	-5.12	113.44	119.84
16	W	115	THR	C-N-CA	-5.12	113.44	119.84
6	F	60	GLY	N-CA-C	-5.12	105.99	114.48
1	A	48	ARG	N-CA-C	-5.11	106.59	114.16
5	E	181	ASN	N-CA-C	-5.11	99.46	108.20
9	I	95	PRO	N-CA-C	5.09	121.20	113.81
16	W	91	MET	N-CA-C	-5.09	105.92	111.82
7	G	458	GLY	N-CA-C	-5.08	108.30	115.32
15	V	84	ALA	N-CA-C	5.08	116.51	111.07
12	R	65	ALA	N-CA-C	-5.08	105.87	111.71
10	P	356	HIS	N-CA-C	-5.08	105.87	111.71
13	S	45	LYS	N-CA-C	-5.07	105.84	111.36
10	P	170	LEU	N-CA-C	5.07	117.07	110.43
7	G	203	ASP	CA-C-O	5.06	127.19	121.32
10	P	376	ASN	CB-CA-C	-5.06	102.25	110.85
17	X	42	GLU	N-CA-C	-5.06	105.84	111.36
3	C	156	VAL	N-CA-C	-5.06	104.19	111.17
4	D	106	VAL	O-C-N	-5.06	116.77	122.94
8	H	101	GLY	N-CA-C	5.06	118.36	112.50
5	E	75	ALA	N-CA-C	5.05	117.45	111.33
3	C	208	GLU	CA-C-O	-5.05	115.69	121.40
1	A	66	ASP	N-CA-C	-5.05	105.69	111.14
22	r	4	ALA	N-CA-C	-5.04	105.87	112.23
4	D	224	ALA	CA-C-O	-5.04	115.51	120.90
7	G	393	GLY	N-CA-C	-5.04	107.80	115.66
6	F	366	ALA	N-CA-C	-5.04	105.48	110.97
21	q	13	GLN	N-CA-C	-5.04	105.68	111.07
7	G	280	ASP	N-CA-CB	-5.03	102.72	110.12
10	P	289	ILE	CA-C-N	-5.03	114.39	119.83
10	P	289	ILE	C-N-CA	-5.03	114.39	119.83
1	A	69	ILE	N-CA-C	-5.03	105.08	110.36
8	H	225	MET	N-CA-C	-5.03	105.47	112.45
3	C	221	GLU	N-CA-C	-5.02	102.42	108.25
5	E	213	PRO	CB-CA-C	-5.02	106.31	112.89
8	H	221	ALA	N-CA-C	-5.02	106.25	112.38
14	T	140	CYS	CB-CA-C	-5.02	104.13	109.85
7	G	453	GLN	N-CA-C	-5.01	105.90	111.36
8	H	254	LEU	N-CA-CB	5.01	118.04	110.28
9	I	160	GLU	CB-CA-C	5.01	119.15	110.84

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	915	0	957	189	0
2	B	1258	0	1270	164	0
3	C	1641	0	1596	131	0
4	D	3088	0	3059	305	0
5	E	1635	0	1626	181	0
6	F	3288	0	3243	348	0
7	G	5287	0	5323	554	0
8	H	2538	0	2627	496	0
9	I	1398	0	1359	205	0
10	P	2730	0	2747	245	0
11	Q	957	0	949	73	0
12	R	660	0	639	74	0
13	S	667	0	685	72	0
14	T	604	0	596	88	0
15	V	915	0	954	76	0
16	W	970	0	991	89	0
17	X	1164	0	1150	83	0
18	Z	1152	0	1148	104	0
19	a	548	0	562	96	0
20	b	628	0	628	136	0
21	q	1004	0	962	83	0
22	r	418	0	434	46	0
23	s	107	0	100	9	0
24	B	8	0	0	6	0
24	F	8	0	0	10	0
24	G	16	0	0	7	0
24	I	16	0	0	16	0
25	B	30	0	35	17	0
26	B	35	0	44	6	0
26	H	42	0	58	13	0
26	I	47	0	71	6	0
27	E	4	0	0	5	0
27	G	4	0	0	5	0
28	F	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	I	51	0	82	17	0
29	Z	46	0	69	6	0
30	P	48	0	26	7	0
31	R	1	0	0	0	0
32	W	32	0	0	7	0
33	a	57	0	58	28	0
All	All	34048	0	34067	3219	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 47.

All (3219) 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)
8:H:127:TYR:CE1	8:H:208:VAL:HG23	1.47	1.48
1:A:51:PHE:HD1	4:D:80:MET:SD	1.36	1.47
9:I:53:ALA:CB	20:b:14:ALA:HB2	1.48	1.42
1:A:51:PHE:CE1	4:D:80:MET:HE1	1.55	1.42
9:I:50:MET:SD	20:b:10:LYS:HG2	1.61	1.39
1:A:51:PHE:CD1	4:D:80:MET:SD	2.26	1.28
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.26
1:A:33:LYS:HG2	8:H:61:MET:CE	1.68	1.22
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.22
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.38	1.21
7:G:126:LEU:HD12	7:G:126:LEU:O	1.37	1.21
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
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.17
1:A:51:PHE:HZ	8:H:130:PHE:CE1	1.62	1.17
1:A:33:LYS:CG	8:H:61:MET:HE2	1.74	1.16
10:P:156:SER:HB2	10:P:161:VAL:CG2	1.75	1.16
6:F:392:MET:CE	6:F:419:ILE:HD12	1.76	1.16
1:A:51:PHE:CZ	8:H:130:PHE:CE1	2.33	1.15
9:I:57:ALA:HB1	20:b:17:PRO:CB	1.75	1.15
9:I:57:ALA:HA	20:b:17:PRO:HG3	1.27	1.15
25:B:302:UQ9:C4M	4:D:189:THR:HG23	1.75	1.14
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.63	1.14
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.13
6:F:392:MET:HE3	6:F:419:ILE:CD1	1.78	1.13
7:G:126:LEU:CD1	12:R:89:PRO:HB2	1.77	1.13
9:I:123:CYS:SG	24:I:303:SF4:FE1	1.40	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.13
8:H:63:PRO:HB2	8:H:66:THR:OG1	1.47	1.13
6:F:382:CYS:SG	24:F:502:SF4:FE3	1.38	1.12
9:I:61:LEU:HD11	20:b:17:PRO:O	1.47	1.12
8:H:134:ARG:NH2	8:H:200:LEU:HD23	1.65	1.12
8:H:127:TYR:CE1	8:H:208:VAL:CG2	2.31	1.11
9:I:57:ALA:CB	20:b:17:PRO:HB3	1.81	1.11
9:I:53:ALA:CA	20:b:14:ALA:HB2	1.80	1.10
25:B:302:UQ9:H4M	4:D:189:THR:HG23	1.12	1.10
10:P:40:VAL:HG22	12:R:43:TYR:CE2	1.86	1.09
8:H:1:MET:HB2	19:a:30:THR:HG21	1.23	1.09
9:I:53:ALA:HB2	20:b:14:ALA:HB2	1.27	1.09
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.23	1.09
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.10	1.09
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
6:F:379:CYS:SG	24:F:502:SF4:FE4	1.43	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
1:A:27:MET:CG	8:H:59:GLU:HG3	1.83	1.08
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.08
8:H:127:TYR:CD1	8:H:208:VAL:HG23	1.88	1.08
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.20	1.07
8:H:127:TYR:CZ	8:H:208:VAL:CG2	2.37	1.07
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.07
9:I:53:ALA:HA	20:b:14:ALA:CB	1.83	1.07
9:I:57:ALA:HB1	20:b:17:PRO:HB2	1.29	1.07
9:I:57:ALA:HB2	20:b:13:TRP:O	1.54	1.07
9:I:152:CYS:SG	24:I:303:SF4:FE2	1.46	1.07
8:H:66:THR:HG23	8:H:122:ALA:O	1.54	1.07
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.07
22:r:2:ALA:N	22:r:26:LEU:HD12	1.69	1.06
10:P:156:SER:HB2	10:P:161:VAL:HG22	1.34	1.06
8:H:127:TYR:CZ	8:H:208:VAL:HG23	1.90	1.05
1:A:62:PHE:CE1	8:H:144:VAL:CG2	2.39	1.05
8:H:1:MET:HG3	19:a:30:THR:HG22	1.38	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.05
4:D:99:LEU:HD13	4:D:101:LEU:HD13	1.38	1.05
2:B:100:CYS:SG	24:B:301:SF4:FE4	1.48	1.05
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.36	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.04
9:I:53:ALA:CB	20:b:14:ALA:CB	2.33	1.04
9:I:57:ALA:CB	20:b:17:PRO:CB	2.35	1.04
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.04
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.03
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.23	1.03
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.03
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.03
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.33	1.03
8:H:200:LEU:HD13	8:H:282:TYR:HA	1.39	1.03
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.36	1.02
1:A:51:PHE:CE1	4:D:80:MET:CE	2.42	1.02
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.02
5:E:179:CYS:SG	27:E:301:FES:FE2	1.50	1.02
9:I:54:THR:HG22	20:b:13:TRP:NE1	1.75	1.02
8:H:1:MET:HE3	19:a:26:ILE:HG23	1.42	1.02
1:A:27:MET:HG2	8:H:59:GLU:CG	1.89	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.02
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	1.01
6:F:199:ARG:HD3	23:s:80:PHE:CE2	1.95	1.01
6:F:300:ILE:HG23	6:F:305:GLY:O	1.59	1.01
8:H:1:MET:CB	19:a:30:THR:HG21	1.89	1.01
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.01
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.41	1.01
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	1.01
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.01
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.00
9:I:155:CYS:SG	24:I:303:SF4:FE4	1.51	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.87	1.00
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	1.00
8:H:200:LEU:HD13	8:H:282:TYR:CA	1.92	1.00
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.42	1.00
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.99
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.99
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.98
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.44	0.98
8:H:1:MET:HG3	19:a:30:THR:CG2	1.92	0.98
8:H:203:GLY:HA3	8:H:206:GLU:HB3	1.43	0.97
1:A:15:LEU:O	1:A:18:ILE:HG22	1.63	0.97
3:C:168:GLU:CB	3:C:186:ILE:HD11	1.92	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.97
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
9:I:53:ALA:HB1	20:b:14:ALA:N	1.78	0.96
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.96
8:H:172:MET:HE1	18:Z:46:GLY:CA	1.95	0.96
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.96
1:A:62:PHE:CD1	8:H:144:VAL:HG21	2.01	0.96
7:G:92:CYS:SG	27:G:803:FES:S1	2.63	0.96
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.96
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.96
1:A:62:PHE:CD1	8:H:144:VAL:CG2	2.48	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
10:P:40:VAL:HG22	12:R:43:TYR:CD2	2.00	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.96
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.46	0.96
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.95
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.95
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.49	0.95
19:a:1:MET:HG3	33:a:101:CDL:HB21	1.46	0.95
10:P:215:ASN:ND2	10:P:355:ARG:HH11	1.65	0.95
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.49	0.95
8:H:134:ARG:CZ	8:H:200:LEU:CD2	2.44	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
1:A:27:MET:HG2	8:H:59:GLU:HG3	0.96	0.94
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
9:I:50:MET:SD	20:b:10:LYS:CG	2.55	0.94
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
8:H:134:ARG:CZ	8:H:200:LEU:HD21	1.97	0.94
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.94
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.94
33:a:101:CDL:HB4	21:q:3:LEU:HD13	1.49	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
7:G:179:CYS:HG	24:G:802:SF4:FE3	0.80	0.93
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.50	0.93
6:F:382:CYS:HG	24:F:502:SF4:FE3	0.63	0.93
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.93
1:A:51:PHE:CZ	8:H:130:PHE:CD1	2.57	0.93
8:H:99:ASN:CG	19:a:40:ARG:HG3	1.94	0.93
9:I:152:CYS:HG	24:I:303:SF4:FE2	0.69	0.93
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.49	0.93
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.92
6:F:425:CYS:HG	24:F:502:SF4:FE1	0.62	0.92
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.51	0.92
9:I:113:CYS:SG	24:I:304:SF4:FE3	1.59	0.92
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.92
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.51	0.92
6:F:379:CYS:HG	24:F:502:SF4:FE4	0.75	0.91
8:H:1:MET:CG	19:a:30:THR:HG22	1.99	0.91
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.91
9:I:57:ALA:HB2	20:b:17:PRO:HB3	1.51	0.91
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.91
1:A:51:PHE:CD1	4:D:80:MET:CE	2.52	0.91
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.62	0.91
1:A:25:PRO:HB3	8:H:57:MET:O	1.69	0.91
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.36	0.91
8:H:1:MET:CB	19:a:30:THR:CG2	2.49	0.91
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.53	0.90
8:H:134:ARG:NH2	8:H:200:LEU:CD2	2.34	0.90
1:A:22:PHE:HA	8:H:60:PRO:HG3	1.50	0.90
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.90
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.90
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
1:A:51:PHE:CZ	8:H:130:PHE:HE1	1.81	0.90
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.90
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.52	0.90
5:E:179:CYS:HG	27:E:301:FES:FE2	0.64	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
9:I:50:MET:HG2	20:b:10:LYS:HE2	1.54	0.89
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.89
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.73	0.89
8:H:1:MET:HB2	19:a:30:THR:CG2	2.01	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.54	0.89
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
1:A:51:PHE:CD1	4:D:80:MET:HE1	2.08	0.89
1:A:51:PHE:HZ	8:H:130:PHE:HE1	0.95	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
8:H:1:MET:CG	19:a:30:THR:CG2	2.51	0.89
2:B:81:LEU:HG	26:B:303:PC1:H261	1.52	0.88
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.88
1:A:52:SER:O	4:D:103:GLY:HA3	1.72	0.88
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.37	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.88
8:H:96:ILE:HG12	18:Z:143:TYR:OH	1.73	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.88
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.88
1:A:51:PHE:HE1	4:D:80:MET:HE1	0.93	0.87
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
1:A:62:PHE:HD1	8:H:144:VAL:HG21	1.35	0.87
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
2:B:73:TYR:CE1	2:B:77:LYS:HE2	2.10	0.87
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.05	0.86
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.55	0.86
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
3:C:168:GLU:HB2	3:C:186:ILE:CD1	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.86
8:H:59:GLU:CD	8:H:61:MET:SD	2.58	0.86
9:I:53:ALA:HB1	20:b:14:ALA:CA	2.06	0.86
2:B:95:PHE:CZ	2:B:141:MET:HE2	2.09	0.85
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.90	0.85
9:I:162:CYS:HG	24:I:304:SF4:FE4	0.54	0.85
9:I:162:CYS:SG	24:I:304:SF4:FE4	1.68	0.85
2:B:95:PHE:HZ	2:B:141:MET:HE2	1.39	0.85
7:G:78:CYS:SG	27:G:803:FES:FE2	1.68	0.85
10:P:132:ARG:HG2	30:P:401:NDP:H8A	1.56	0.85
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.85
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
8:H:303:TRP:HE3	20:b:29:ALA:HB2	1.38	0.85
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.39	0.85
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.85
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.42	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.85
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.85
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.85
8:H:200:LEU:CD1	8:H:282:TYR:N	2.40	0.85
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.76	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.84
8:H:96:ILE:HG23	18:Z:143:TYR:CE1	2.12	0.84
3:C:80:LEU:CD1	4:D:396:THR:HG22	2.07	0.84
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
1:A:62:PHE:HE1	8:H:144:VAL:CG2	1.87	0.84
4:D:99:LEU:HD12	4:D:99:LEU:O	1.78	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.84
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.08	0.84
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.84
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.96	0.84
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
9:I:49:ASP:HA	20:b:10:LYS:NZ	1.93	0.83
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.83
7:G:78:CYS:HG	27:G:803:FES:FE2	0.53	0.83
8:H:66:THR:HG22	8:H:67:SER:O	1.79	0.83
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.43	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.12	0.83
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.83
9:I:57:ALA:HA	20:b:17:PRO:CG	2.08	0.83
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.19	0.82
8:H:200:LEU:CD1	8:H:282:TYR:CA	2.56	0.82
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.82
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.82
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.82
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.11	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
1:A:62:PHE:CE1	8:H:144:VAL:HG23	2.14	0.82
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.94	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.61	0.82
9:I:155:CYS:HG	24:I:303:SF4:FE4	0.94	0.82
1:A:69:ILE:HD11	8:H:144:VAL:HG13	1.60	0.81
2:B:112:TYR:OH	9:I:91:GLY:CA	2.27	0.81
3:C:186:ILE:CD1	4:D:429:PHE:HZ	1.93	0.81
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.81
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.81
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.81
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
8:H:203:GLY:CA	8:H:206:GLU:HB3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:2:TRP:HH2	33:a:101:CDL:H522	1.46	0.80
33:a:101:CDL:HB4	21:q:3:LEU:CD1	2.11	0.80
1:A:62:PHE:HA	8:H:290:TRP:HH2	1.46	0.80
8:H:63:PRO:CB	8:H:66:THR:OG1	2.30	0.80
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.80
7:G:73:GLY:HA2	27:G:803:FES:S1	2.21	0.80
8:H:171:HIS:HB3	18:Z:49:ARG:HD3	1.63	0.80
1:A:41:PHE:HB3	16:W:102:GLN:NE2	1.96	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.80
18:Z:58:ARG:NH2	20:b:49:THR:HG21	1.95	0.80
19:a:2:TRP:CH2	33:a:101:CDL:H522	2.17	0.80
19:a:2:TRP:HZ2	33:a:101:CDL:OB6	1.65	0.80
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.80
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.79
9:I:53:ALA:CA	20:b:14:ALA:CB	2.46	0.79
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	2.16	0.79
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.12	0.79
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.61	0.79
17:X:4:ILE:HG22	17:X:5:VAL:H	1.48	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
8:H:306:SER:HG	8:H:310:PHE:HE2	1.27	0.79
9:I:54:THR:HG22	20:b:13:TRP:CD1	2.18	0.79
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
6:F:109:ARG:HD2	6:F:237:GLY:O	1.82	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.79
9:I:113:CYS:HG	24:I:304:SF4:FE3	0.49	0.79
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.64	0.78
10:P:142:GLU:O	10:P:146:VAL:HG12	1.84	0.78
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.65	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.97	0.78
9:I:54:THR:HA	20:b:13:TRP:NE1	1.98	0.78
8:H:66:THR:CG2	8:H:122:ALA:O	2.30	0.78
8:H:99:ASN:OD1	19:a:40:ARG:HG3	1.82	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.23	0.78
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.78
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.78
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.19	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.78
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.78
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.99	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
16:W:47:PRO:HG3	16:W:63:ARG:HH21	1.49	0.77
3:C:80:LEU:CD1	4:D:396:THR:CG2	2.63	0.77
25:B:302:UQ9:O3	4:D:92:HIS:HA	1.85	0.77
10:P:40:VAL:CG2	12:R:43:TYR:CE2	2.66	0.77
2:B:73:TYR:CE1	2:B:77:LYS:CE	2.68	0.77
1:A:27:MET:SD	8:H:60:PRO:HD2	2.24	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.77
1:A:51:PHE:CE1	4:D:103:GLY:HA2	2.20	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.66	0.77
21:q:96:ASP:OD1	21:q:97:PRO:HD2	1.85	0.77
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.15	0.77
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.76
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.31	0.76
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.76
9:I:123:CYS:HG	24:I:303:SF4:FE1	0.47	0.76
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.24	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
8:H:69:SER:CB	26:H:401:PC1:H221	2.16	0.76
8:H:183:MET:HE2	26:I:302:PC1:H2A1	1.68	0.76
8:H:134:ARG:NH1	8:H:200:LEU:HD21	1.99	0.76
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.20	0.76
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.76
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.76
1:A:62:PHE:CE1	8:H:144:VAL:HG22	2.19	0.76
2:B:73:TYR:CZ	2:B:77:LYS:HE3	2.22	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.75
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.75
5:E:183:PRO:HB2	5:E:195:LEU:H	1.50	0.75
1:A:25:PRO:HG2	8:H:60:PRO:HD3	1.67	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.67	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.16	0.75
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.75
8:H:65:THR:O	8:H:124:ASN:HB3	1.87	0.75
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.87	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
6:F:425:CYS:SG	24:F:502:SF4:FE1	1.78	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.21	0.74
2:B:89:SER:O	8:H:54:LYS:HE2	1.87	0.74
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.69	0.74
3:C:99:LEU:HD13	3:C:140:ILE:HD11	1.70	0.74
25:B:302:UQ9:C4M	4:D:189:THR:CG2	2.61	0.74
5:E:139:CYS:SG	27:E:301:FES:FE1	1.78	0.74
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.74
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.48	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.67	0.74
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.68	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.70	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
5:E:192:TYR:CE1	5:E:215:PRO:HA	2.23	0.74
10:P:40:VAL:CG2	12:R:43:TYR:CD2	2.71	0.74
13:S:51:LEU:CD1	13:S:95:LEU:HD21	2.12	0.74
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.73
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.73
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.52	0.73
8:H:272:TRP:HH2	26:I:302:PC1:H381	1.52	0.73
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.73
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.73
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.69	0.73
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
14:T:117:GLU:HA	14:T:120:MET:HE3	1.67	0.73
10:P:203:PRO:HG2	30:P:401:NDP:H6N	1.69	0.73
16:W:110:PHE:HZ	32:W:201:EHZ:C2	2.00	0.73
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.73
33:a:101:CDL:HA32	21:q:13:GLN:HE22	1.54	0.73
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.73
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
9:I:61:LEU:CD1	20:b:17:PRO:O	2.31	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
19:a:1:MET:HG3	33:a:101:CDL:CB2	2.19	0.73
3:C:102:HIS:HE1	15:V:48:THR:CG2	2.01	0.73
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.73
8:H:218:GLY:O	8:H:222:LEU:HD13	1.88	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.69	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.73
1:A:41:PHE:HD2	16:W:102:GLN:NE2	1.86	0.72
1:A:68:GLU:CD	1:A:98:LEU:HG	2.13	0.72
5:E:43:THR:HG23	5:E:46:ASN:H	1.52	0.72
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.53	0.72
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.72
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.72
7:G:226:CYS:HG	24:G:802:SF4:FE1	1.05	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
1:A:62:PHE:HE1	8:H:144:VAL:HG23	1.50	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
7:G:126:LEU:HD13	12:R:89:PRO:HB2	1.68	0.72
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.71	0.72
18:Z:98:MET:HE3	18:Z:101:VAL:HG21	1.70	0.72
1:A:17:LEU:HD21	8:H:56:PHE:CZ	2.24	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.72
9:I:110:GLU:OE2	12:R:64:ILE:HB	1.88	0.72
4:D:280:ALA:CB	15:V:11:LEU:HG	2.19	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
8:H:200:LEU:CD1	8:H:282:TYR:HB2	2.19	0.72
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.72
6:F:236:PHE:HA	11:Q:166:TRP:CD1	2.25	0.72
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.72	0.72
5:E:163:THR:CG2	5:E:168:PHE:HB2	2.19	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.72
8:H:172:MET:CE	18:Z:46:GLY:HA2	2.20	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.72
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.70	0.72
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
1:A:41:PHE:CD2	16:W:102:GLN:NE2	2.58	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.71
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.73	0.71
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.71	0.71
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.71
8:H:99:ASN:HD21	19:a:40:ARG:HA	1.54	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.71
25:B:302:UQ9:C3M	4:D:92:HIS:HA	2.20	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
9:I:53:ALA:HB1	20:b:14:ALA:CB	2.15	0.71
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.72	0.71
26:I:302:PC1:H2D1	26:I:302:PC1:H291	1.73	0.71
10:P:262:THR:H	10:P:332:LEU:HD12	1.54	0.71
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.71
7:G:226:CYS:SG	24:G:802:SF4:FE1	1.82	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
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.70
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.26	0.70
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.70
3:C:84:GLU:HG2	3:C:141:ARG:HH11	1.56	0.70
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.73	0.70
8:H:96:ILE:HG23	18:Z:143:TYR:CZ	2.25	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
1:A:41:PHE:HB3	16:W:102:GLN:HE21	1.55	0.70
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.70
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.70
2:B:95:PHE:CE1	2:B:97:LEU:HG	2.27	0.70
13:S:48:HIS:ND1	13:S:95:LEU:HD23	2.05	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.72	0.70
1:A:33:LYS:HG2	8:H:61:MET:HE2	0.83	0.70
1:A:113:TRP:HZ2	8:H:286:MET:HB2	1.57	0.70
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.70
9:I:54:THR:CG2	20:b:13:TRP:HE1	2.05	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
8:H:1:MET:HB3	19:a:26:ILE:CG2	2.22	0.70
13:S:51:LEU:HD13	13:S:95:LEU:CD2	2.11	0.70
4:D:99:LEU:CD1	4:D:101:LEU:HD13	2.19	0.70
6:F:329:LYS:HA	6:F:332:CYS:SG	2.31	0.70
16:W:110:PHE:CZ	32:W:201:EHZ:C2	2.75	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.70
19:a:2:TRP:CH2	33:a:101:CDL:OB8	2.44	0.70
8:H:187:ILE:HD12	29:I:301:3PE:H242	1.72	0.70
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
8:H:12:PRO:O	19:a:15:CYS:HB3	1.91	0.69
16:W:58:THR:HB	16:W:61:GLN:CB	2.22	0.69
19:a:37:ARG:CB	19:a:48:MET:HE2	2.22	0.69
4:D:99:LEU:HD13	4:D:101:LEU:CD1	2.20	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69
18:Z:141:THR:O	29:Z:401:3PE:H11	1.93	0.69
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
7:G:64:CYS:SG	27:G:803:FES:FE1	1.83	0.69
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
9:I:93:LEU:O	21:q:93:MET:HG2	1.93	0.69
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.57	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.23	0.69
1:A:41:PHE:HE1	4:D:86:PRO:HG2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.69
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.74	0.69
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.69
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.69
13:S:23:LEU:HD12	13:S:23:LEU:O	1.93	0.69
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.72	0.69
1:A:41:PHE:CB	16:W:102:GLN:NE2	2.56	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.92	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69
16:W:84:LEU:HD21	16:W:88:LYS:HE3	1.75	0.69
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.69
8:H:63:PRO:HB2	8:H:66:THR:CB	2.22	0.69
8:H:227:GLU:O	8:H:231:ILE:HG13	1.92	0.69
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.69
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.28	0.68
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.91	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
9:I:200:GLU:OE2	21:q:93:MET:SD	2.51	0.68
33:a:101:CDL:H341	33:a:101:CDL:H171	1.74	0.68
6:F:126:LYS:O	6:F:129:GLU:HG2	1.93	0.68
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.29	0.68
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
2:B:114:MET:HB2	2:B:119:VAL:HG23	1.76	0.68
8:H:203:GLY:HA3	8:H:206:GLU:CB	2.20	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
3:C:186:ILE:HB	4:D:113:ILE:HD11	1.75	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.24	0.68
8:H:127:TYR:CZ	8:H:208:VAL:HG22	2.27	0.68
9:I:49:ASP:HA	20:b:10:LYS:HZ1	1.59	0.68
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.75	0.68
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.68
19:a:7:PRO:HD3	33:a:101:CDL:H181	1.76	0.68
2:B:95:PHE:HE1	2:B:97:LEU:HG	1.58	0.67
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.76	0.67
5:E:78:VAL:HG12	5:E:104:LEU:HD13	1.76	0.67
5:E:190:ASN:HB3	5:E:192:TYR:CE2	2.28	0.67
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.22	0.67
17:X:64:ASN:O	17:X:68:LEU:HG	1.94	0.67
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.22	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
17:X:78:CYS:SG	17:X:111:VAL:HG13	2.35	0.67
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.24	0.67
19:a:60:TYR:O	19:a:62:VAL:HG13	1.95	0.67
1:A:113:TRP:HZ2	8:H:286:MET:CB	2.07	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:CB	2.24	0.67
1:A:105:GLU:HG3	1:A:110:GLY:HA3	1.76	0.67
2:B:93:MET:HE2	4:D:87:GLN:CD	2.19	0.67
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.60	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
1:A:113:TRP:CZ2	8:H:286:MET:HB2	2.29	0.67
8:H:176:LEU:O	18:Z:43:LEU:HD23	1.95	0.67
25:B:302:UQ9:H4MB	4:D:189:THR:HG23	1.76	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:HB1	1.77	0.67
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.30	0.67
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.67
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.67
17:X:124:GLN:O	20:b:70:PRO:HB2	1.95	0.67
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.67
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.67
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.10	0.67
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.38	0.67
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.67
9:I:53:ALA:HA	20:b:14:ALA:HB1	1.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
10:P:180:SER:O	10:P:184:LYS:HG3	1.95	0.67
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.67
1:A:61:THR:O	1:A:62:PHE:C	2.35	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.25	0.66
1:A:51:PHE:CZ	4:D:103:GLY:HA2	2.30	0.66
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
10:P:320:GLU:O	10:P:324:ILE:HG12	1.96	0.66
23:s:78:TYR:HA	23:s:81:LEU:HD12	1.76	0.66
2:B:82:ILE:HA	8:H:57:MET:HE1	1.77	0.66
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
16:W:24:PHE:HB2	16:W:83:ASP:CG	2.20	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.58	0.66
6:F:383:THR:N	6:F:384:PRO:HD2	2.10	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.95	0.66
9:I:67:ILE:HG13	26:I:302:PC1:H251	1.77	0.66
5:E:240:PRO:HG3	6:F:57:LEU:O	1.94	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.66
9:I:92:PRO:HA	21:q:91:HIS:O	1.96	0.66
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.30	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.77	0.66
2:B:125:PRO:HG3	2:B:148:VAL:HG13	1.77	0.66
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.25	0.66
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.66
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.66
1:A:41:PHE:HA	16:W:102:GLN:HE22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.21	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.66
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.66
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.66
1:A:106:TRP:CD1	8:H:291:LYS:HD3	2.31	0.66
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.49	0.66
10:P:169:HIS:H	10:P:184:LYS:HE3	1.61	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
1:A:27:MET:HE3	8:H:59:GLU:HG2	1.78	0.65
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.57	0.65
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.65
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.65
13:S:24:CYS:HA	13:S:58:CYS:O	1.96	0.65
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.11	0.65
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.65
8:H:200:LEU:HD13	8:H:282:TYR:CB	2.26	0.65
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.65
18:Z:98:MET:CE	18:Z:101:VAL:HG21	2.26	0.65
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.76	0.65
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.61	0.65
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.65
1:A:73:LEU:N	1:A:74:PRO:HD2	2.11	0.65
3:C:99:LEU:HD13	3:C:140:ILE:CD1	2.27	0.65
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.26	0.65
10:P:299:SER:CB	10:P:316:LYS:HE3	2.23	0.65
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.65
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.65
5:E:81:VAL:HB	5:E:104:LEU:HD11	1.79	0.65
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.65
8:H:310:PHE:CB	20:b:33:PRO:HA	2.24	0.65
10:P:263:PHE:HD2	10:P:333:PRO:O	1.79	0.65
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.64
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.62	0.64
5:E:163:THR:HG21	5:E:168:PHE:HB2	1.79	0.64
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.78	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
1:A:44:THR:HG22	16:W:99:VAL:HG13	1.79	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.32	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
7:G:651:PRO:HG3	13:S:57:GLU:H	1.60	0.64
8:H:67:SER:HA	26:H:401:PC1:H153	1.78	0.64
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.62	0.64
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.79	0.64
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.60	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.64
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.64
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.64
25:B:302:UQ9:H3M	4:D:92:HIS:HA	1.80	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.79	0.64
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
12:R:38:TYR:HB2	12:R:45:ARG:HD3	1.79	0.64
4:D:79:ASN:HB2	4:D:100:GLU:HB3	1.80	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
4:D:137:ASP:OD1	4:D:148:GLU:HG3	1.97	0.64
8:H:68:MET:H	26:H:401:PC1:H121	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:TYR:OH	2:B:77:LYS:HE3	1.98	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.64
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.64
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.79	0.64
8:H:131:GLY:CA	8:H:207:LEU:HD11	2.28	0.64
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.64
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.80	0.64
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.64
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.34	0.63
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.63
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.78	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
10:P:156:SER:CB	10:P:161:VAL:HG22	2.20	0.63
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.62	0.63
5:E:87:ARG:HD2	23:s:77:THR:HG22	1.80	0.63
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.63
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.63
19:a:2:TRP:CZ2	33:a:101:CDL:OB6	2.49	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
16:W:115:THR:O	16:W:116:PRO:C	2.39	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.63
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.63
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.79	0.63
4:D:354:GLY:O	18:Z:8:GLN:NE2	2.22	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.63
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.63
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.63
1:A:38:GLU:HG2	4:D:83:ASN:OD1	1.99	0.63
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.63
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.63
8:H:1:MET:HB3	19:a:26:ILE:HG23	1.80	0.63
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.63
21:q:137:TRP:CZ2	21:q:140:PRO:HD3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:CE2	29:Z:401:3PE:H231	2.34	0.63
2:B:105:MET:HE2	25:B:302:UQ9:C6	2.28	0.63
2:B:105:MET:HG2	25:B:302:UQ9:H10	1.81	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.63
10:P:363:SER:HB3	16:W:51:HIS:CD2	2.32	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.63
1:A:29:LEU:CD2	8:H:59:GLU:OE2	2.47	0.63
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	0.63
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.66	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.64	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.63
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.63
10:P:132:ARG:HG2	30:P:401:NDP:C8A	2.29	0.63
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.63
17:X:53:PRO:O	17:X:57:LEU:HG	1.99	0.63
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.34	0.62
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.62
1:A:3:LEU:HD23	29:Z:401:3PE:H251	1.80	0.62
4:D:375:MET:HE1	7:G:126:LEU:HA	1.80	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.62
8:H:221:ALA:O	8:H:225:MET:HB2	2.00	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.62
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.78	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.62
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.62
2:B:95:PHE:HE1	2:B:97:LEU:CG	2.12	0.62
6:F:426:ALA:HB3	28:F:501:FMN:HM81	1.80	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:5:ASN:ND2	19:a:23:THR:HA	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:61:LEU:CD2	20:b:18:VAL:HG22	2.29	0.62
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.62
8:H:69:SER:HB3	26:H:401:PC1:H221	1.80	0.62
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
1:A:27:MET:HE3	8:H:59:GLU:CG	2.29	0.62
1:A:58:VAL:HG22	1:A:111:LEU:HD23	1.80	0.62
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.35	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.62
6:F:226:LYS:O	6:F:227:PRO:C	2.42	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
33:a:101:CDL:H311	21:q:7:LEU:HD23	1.82	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.48	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.81	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.62
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
9:I:53:ALA:CB	20:b:14:ALA:CA	2.73	0.62
16:W:32:LYS:NZ	32:W:201:EHZ:C19	2.63	0.62
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.62
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.82	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
8:H:228:TYR:O	8:H:229:THR:C	2.41	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.29	0.62
1:A:34:ALA:O	8:H:64:LEU:N	2.22	0.61
1:A:112:GLU:O	1:A:113:TRP:HB2	1.99	0.61
2:B:99:CYS:HB3	4:D:141:TYR:CB	2.30	0.61
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:MET:H	20:b:10:LYS:NZ	1.98	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
16:W:24:PHE:HB2	16:W:83:ASP:HB3	1.82	0.61
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.99	0.61
8:H:218:GLY:O	8:H:222:LEU:CD1	2.47	0.61
10:P:179:LYS:HA	10:P:182:ARG:HG2	1.82	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.80	0.61
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.30	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
13:S:19:ILE:CG1	13:S:95:LEU:HD11	2.26	0.61
13:S:31:GLN:HA	13:S:34:ARG:HE	1.65	0.61
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.61
1:A:51:PHE:CE1	8:H:130:PHE:CD1	2.88	0.61
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.30	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.61
16:W:25:SER:HB2	16:W:31:ALA:HB2	1.83	0.61
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.82	0.61
33:a:101:CDL:H1	22:r:3:SER:HB2	1.82	0.61
1:A:39:CYS:SG	8:H:208:VAL:CG2	2.89	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
8:H:69:SER:N	26:H:401:PC1:O12	2.33	0.61
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.61
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.61
20:b:8:PHE:C	20:b:9:LEU:HD12	2.26	0.61
1:A:75:LEU:HB2	8:H:155:LEU:HD21	1.81	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
8:H:94:PRO:O	19:a:27:HIS:HE1	1.84	0.61
33:a:101:CDL:HA21	21:q:6:VAL:HG13	1.82	0.61
1:A:15:LEU:HA	1:A:18:ILE:HG22	1.82	0.61
1:A:65:PHE:O	1:A:69:ILE:HG13	2.00	0.61
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.83	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.61
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.49	0.61
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
10:P:169:HIS:H	10:P:184:LYS:CE	2.13	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.82	0.61
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:183:MET:HE2	26:I:302:PC1:H271	1.83	0.61
9:I:54:THR:CG2	20:b:13:TRP:NE1	2.57	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.49	0.61
1:A:15:LEU:C	1:A:18:ILE:HG22	2.26	0.61
5:E:233:LEU:HD22	6:F:43:THR:HA	1.83	0.61
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.33	0.61
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.61
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.89	0.61
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.01	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
3:C:186:ILE:HG13	3:C:187:LEU:HG	1.83	0.60
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.60
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.60
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.60
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.82	0.60
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.82	0.60
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.83	0.60
5:E:190:ASN:HB3	5:E:192:TYR:CD2	2.36	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.60
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.60
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.60
16:W:58:THR:HB	16:W:61:GLN:HB2	1.83	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.15	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.63	0.60
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.60
16:W:122:LEU:HD11	16:W:126:TYR:CZ	2.37	0.60
1:A:51:PHE:HE1	4:D:80:MET:CE	1.87	0.60
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.83	0.60
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
10:P:156:SER:CB	10:P:161:VAL:CG2	2.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:215:ASN:ND2	10:P:355:ARG:NH1	2.44	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
8:H:127:TYR:HE1	8:H:207:LEU:C	2.09	0.60
8:H:200:LEU:CD1	8:H:282:TYR:CB	2.79	0.60
1:A:55:PHE:HB3	1:A:113:TRP:CD1	2.36	0.60
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.60
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.60
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.31	0.60
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.60
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.60
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.83	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.84	0.60
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.60
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.60
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.27	0.60
1:A:29:LEU:HD23	8:H:59:GLU:OE2	2.02	0.60
2:B:114:MET:HB2	2:B:119:VAL:CG2	2.32	0.60
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.60
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.84	0.60
1:A:44:THR:HA	16:W:99:VAL:HG11	1.84	0.60
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.01	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.01	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.10	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.37	0.60
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.59
18:Z:61:LEU:HA	18:Z:64:ASP:OD2	2.02	0.59
2:B:73:TYR:CZ	2:B:77:LYS:CE	2.85	0.59
8:H:200:LEU:HD11	8:H:282:TYR:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.59
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
29:Z:401:3PE:H2E1	29:Z:401:3PE:H2I2	1.83	0.59
2:B:100:CYS:SG	24:B:301:SF4:S2	2.99	0.59
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
8:H:172:MET:CE	18:Z:46:GLY:CA	2.74	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.59
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.67	0.59
1:A:12:LEU:O	1:A:13:LEU:C	2.44	0.59
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.06	0.59
5:E:222:PHE:H	5:E:225:GLU:CD	2.10	0.59
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.59
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.59
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.83	0.59
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.38	0.59
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
16:W:32:LYS:HZ2	32:W:201:EHZ:C19	2.15	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.59
4:D:388:GLY:HA3	4:D:417:SER:OG	2.02	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.32	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.67	0.59
10:P:215:ASN:HD22	10:P:355:ARG:HH11	1.44	0.59
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.99	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.03	0.59
1:A:52:SER:O	4:D:103:GLY:CA	2.49	0.59
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.59
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.37	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
6:F:199:ARG:CD	23:s:80:PHE:CE2	2.79	0.59
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.85	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
9:I:54:THR:HA	20:b:13:TRP:CD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:25:GLN:HG3	13:S:26:ARG:N	2.17	0.59
21:q:85:GLU:HG2	21:q:98:PRO:CB	2.31	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.17	0.59
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.32	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
8:H:93:HIS:CE1	19:a:24:ALA:HB1	2.38	0.59
9:I:63:TRP:CZ2	29:I:301:3PE:H331	2.37	0.59
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.34	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.58
8:H:127:TYR:CE1	8:H:207:LEU:C	2.82	0.58
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.80	0.58
9:I:54:THR:CB	20:b:13:TRP:HE1	2.15	0.58
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.58
18:Z:82:ARG:O	18:Z:86:ILE:HG13	2.03	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
9:I:53:ALA:HA	20:b:14:ALA:HB2	1.50	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
16:W:42:TRP:CZ2	32:W:201:EHZ:O1	2.56	0.58
2:B:154:GLU:O	10:P:89:TYR:OH	2.20	0.58
4:D:95:LEU:HD13	4:D:458:PHE:CE1	2.38	0.58
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.18	0.58
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.02	0.58
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.84	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.34	0.58
8:H:69:SER:HB2	26:H:401:PC1:O12	2.04	0.58
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.58
1:A:106:TRP:CD1	8:H:291:LYS:CD	2.87	0.58
6:F:382:CYS:SG	24:F:502:SF4:S1	3.02	0.58
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.86	0.58
17:X:52:ASP:HA	18:Z:116:TRP:CD1	2.39	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:CYS:HB3	4:D:141:TYR:HB3	1.86	0.58
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.58
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.84	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.39	0.58
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.84	0.58
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.58
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.27	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.58
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.85	0.58
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
2:B:202:LEU:HD13	2:B:202:LEU:C	2.28	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
4:D:95:LEU:HD22	4:D:458:PHE:HZ	1.69	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.85	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.58
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.58
9:I:54:THR:CG2	20:b:13:TRP:CD1	2.86	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.58
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.58
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.57
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.57
7:G:179:CYS:SG	24:G:802:SF4:FE3	1.88	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.57
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.57
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.86	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.57
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.57
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
8:H:175:LEU:HD21	26:I:302:PC1:H2C1	1.84	0.57
8:H:200:LEU:HD13	8:H:282:TYR:HB2	1.85	0.57
10:P:81:ILE:CD1	12:R:46:VAL:HG11	2.34	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
17:X:48:TRP:CD1	20:b:55:VAL:HG13	2.39	0.57
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.57
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.51	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.57
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.57
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
19:a:43:TYR:CZ	19:a:47:LEU:HD11	2.40	0.57
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.35	0.57
5:E:187:ILE:O	5:E:188:ASN:C	2.48	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
16:W:25:SER:CB	16:W:31:ALA:HB2	2.34	0.57
16:W:67:ARG:HD3	16:W:71:MET:HG2	1.85	0.57
1:A:15:LEU:HD23	8:H:76:THR:HG21	1.86	0.57
1:A:92:PHE:O	1:A:93:ILE:C	2.46	0.57
2:B:68:ARG:HG2	2:B:70:ARG:H	1.68	0.57
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.52	0.57
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.70	0.57
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
19:a:36:LYS:HA	19:a:59:ARG:NH2	2.19	0.57
1:A:18:ILE:CD1	8:H:72:ILE:HB	2.34	0.57
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.57
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.04	0.57
8:H:69:SER:OG	26:H:401:PC1:H221	2.05	0.57
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.05	0.57
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.69	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
5:E:163:THR:HG23	5:E:168:PHE:HB2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.87	0.57
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.57
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.57
25:B:302:UQ9:H16	4:D:201:PHE:HZ	1.69	0.57
8:H:316:PRO:HB3	18:Z:58:ARG:HD2	1.86	0.57
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.57
1:A:1:MET:O	1:A:4:TYR:N	2.38	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.04	0.57
2:B:124:SER:O	2:B:125:PRO:C	2.43	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
8:H:171:HIS:CB	18:Z:49:ARG:HD3	2.34	0.57
13:S:23:LEU:HD12	13:S:23:LEU:C	2.29	0.57
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.57
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.04	0.57
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.57
1:A:39:CYS:SG	8:H:208:VAL:HG21	2.45	0.56
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.56
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
18:Z:131:GLU:O	18:Z:132:GLU:C	2.49	0.56
3:C:167:ARG:HB3	3:C:186:ILE:HG23	1.86	0.56
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.56
1:A:110:GLY:O	1:A:111:LEU:C	2.48	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
25:B:302:UQ9:H4MB	4:D:189:THR:CG2	2.32	0.56
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.06	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.56
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
19:a:50:ARG:NH1	19:a:54:ILE:HD11	2.20	0.56
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.56
1:A:41:PHE:CB	16:W:102:GLN:HE22	2.18	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:372:PHE:H	7:G:532:PRO:HB2	1.70	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
7:G:655:ARG:HH12	13:S:59:SER:N	2.03	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.89	0.56
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.56
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
19:a:2:TRP:CZ2	33:a:101:CDL:CB6	2.88	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
2:B:173:TYR:O	3:C:203:LEU:HD22	2.05	0.56
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.30	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
8:H:5:ASN:CG	19:a:23:THR:HA	2.30	0.56
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.40	0.56
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
18:Z:122:GLY:O	18:Z:126:GLY:N	2.36	0.56
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.40	0.56
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.70	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.87	0.56
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.56
1:A:26:GLN:O	2:B:154:GLU:HG2	2.05	0.56
1:A:102:LEU:HD22	8:H:294:LEU:HD23	1.86	0.56
2:B:114:MET:HE1	2:B:121:PHE:CZ	2.41	0.56
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.88	0.56
4:D:90:ALA:HB1	4:D:448:VAL:HG13	1.88	0.56
6:F:392:MET:HE1	6:F:419:ILE:HD12	1.80	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
12:R:38:TYR:OH	21:q:127:TYR:HB2	2.06	0.56
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.41	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:ASN:HD21	19:a:23:THR:HA	1.71	0.56
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
33:a:101:CDL:OB7	21:q:3:LEU:HD13	2.06	0.56
2:B:81:LEU:HD22	26:B:303:PC1:H352	1.87	0.56
26:B:303:PC1:H131	8:H:39:ILE:HD11	1.87	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.56
10:P:358:THR:HG22	10:P:359:TYR:CD1	2.41	0.56
12:R:41:LYS:H	12:R:41:LYS:HD2	1.71	0.56
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.86	0.56
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.56
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.56
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.56
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.56
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.56
2:B:115:ASP:O	2:B:116:ARG:C	2.44	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
16:W:58:THR:HG22	16:W:60:LYS:N	2.21	0.55
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.55
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.36	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
9:I:61:LEU:HD21	20:b:18:VAL:HG22	1.88	0.55
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.55
1:A:69:ILE:HG22	1:A:73:LEU:HD21	1.88	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.86	0.55
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.55
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.55
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.42	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
8:H:203:GLY:C	8:H:206:GLU:HB3	2.31	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:24:PHE:HB2	16:W:83:ASP:CB	2.37	0.55
1:A:68:GLU:HG3	1:A:69:ILE:N	2.21	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
6:F:382:CYS:SG	24:F:502:SF4:S4	3.05	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.07	0.55
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.88	0.55
17:X:55:ARG:HB3	17:X:135:ARG:HH22	1.72	0.55
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.55
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.88	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.71	0.55
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.07	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
1:A:94:LEU:O	1:A:97:ILE:HG12	2.07	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
10:P:104:THR:HG22	10:P:106:LEU:CD1	2.37	0.55
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.55
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	0.55
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.55
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.88	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.55
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.43	0.54
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.54
1:A:111:LEU:HB2	8:H:291:LYS:NZ	2.22	0.54
3:C:186:ILE:O	4:D:113:ILE:HG13	2.07	0.54
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.90	0.54
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:655:ARG:HH12	13:S:59:SER:H	1.56	0.54
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:156:SER:CB	10:P:161:VAL:HG21	2.30	0.54
1:A:41:PHE:CA	16:W:102:GLN:HE22	2.18	0.54
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.89	0.54
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.54
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.08	0.54
9:I:54:THR:HA	20:b:13:TRP:HE1	1.68	0.54
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.38	0.54
1:A:39:CYS:SG	8:H:208:VAL:HG22	2.47	0.54
2:B:114:MET:SD	2:B:121:PHE:CE1	3.01	0.54
5:E:178:ALA:HA	6:F:125:CYS:SG	2.46	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
8:H:93:HIS:CE1	19:a:24:ALA:CB	2.90	0.54
8:H:131:GLY:HA3	8:H:207:LEU:HD11	1.90	0.54
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.54
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	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:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.37	0.54
7:G:36:VAL:O	7:G:39:GLN:HG2	2.07	0.54
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:21:THR:HG22	8:H:228:TYR:CE2	2.43	0.54
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.54
13:S:44:LEU:HD13	13:S:91:MET:HG2	1.88	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
1:A:15:LEU:CA	1:A:18:ILE:HG22	2.38	0.54
6:F:382:CYS:C	6:F:384:PRO:HD2	2.32	0.54
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
26:H:401:PC1:H281	26:H:401:PC1:H3B1	1.90	0.54
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.54
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:VAL:O	2:B:76:THR:C	2.50	0.54
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.54
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.54
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.48	0.54
6:F:80:MET:HE2	6:F:95:THR:HG21	1.90	0.54
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.54
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.54
8:H:9:LEU:HA	19:a:19:PRO:HB3	1.90	0.54
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
12:R:32:THR:OG1	12:R:33:HIS:N	2.39	0.54
16:W:23:ILE:HG22	16:W:24:PHE:CD1	2.42	0.54
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.54
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.54
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.54
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.90	0.54
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.71	0.54
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.54
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
10:P:206:ILE:HG13	30:P:401:NDP:H42N	1.89	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.54
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.54
16:W:58:THR:HG22	16:W:60:LYS:H	1.72	0.54
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.54
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.54
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	1.89	0.54
5:E:131:ILE:HG13	5:E:187:ILE:HG12	1.89	0.54
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:VAL:HG11	20:b:11:ASN:HB3	1.90	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.08	0.54
10:P:203:PRO:HG2	30:P:401:NDP:C6N	2.37	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
19:a:2:TRP:CZ2	33:a:101:CDL:HB62	2.42	0.54
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.53
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.53
4:D:84:PHE:HZ	4:D:90:ALA:HB3	1.73	0.53
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.53
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.53
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.53
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
6:F:199:ARG:HD3	23:s:80:PHE:CD2	2.41	0.53
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.27	0.53
8:H:206:GLU:O	8:H:207:LEU:C	2.49	0.53
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.73	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
1:A:65:PHE:O	1:A:68:GLU:HG2	2.08	0.53
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.53
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.53
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.53
9:I:123:CYS:SG	24:I:303:SF4:S3	3.06	0.53
13:S:16:LEU:O	13:S:16:LEU:CD1	2.52	0.53
29:Z:401:3PE:H322	29:Z:401:3PE:H262	1.88	0.53
19:a:1:MET:HB2	19:a:3:PHE:CE2	2.43	0.53
2:B:114:MET:HE1	2:B:121:PHE:CE1	2.43	0.53
2:B:138:THR:HG21	4:D:116:LEU:HA	1.91	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.38	0.53
8:H:206:GLU:O	8:H:208:VAL:N	2.41	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
9:I:57:ALA:CA	20:b:17:PRO:CB	2.87	0.53
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
1:A:19:LEU:O	1:A:20:VAL:C	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
6:F:392:MET:CE	6:F:419:ILE:CD1	2.60	0.53
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53
9:I:106:TYR:O	9:I:107:PRO:C	2.49	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.90	0.53
1:A:61:THR:O	1:A:64:LEU:N	2.41	0.53
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.53
4:D:88:HIS:NE2	8:H:207:LEU:O	2.40	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
8:H:5:ASN:OD1	19:a:23:THR:HA	2.09	0.53
8:H:75:PRO:HB2	8:H:222:LEU:CD2	2.37	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.53
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.53
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
18:Z:58:ARG:NH2	20:b:49:THR:CG2	2.68	0.53
1:A:15:LEU:O	1:A:18:ILE:CG2	2.48	0.53
5:E:81:VAL:CB	5:E:104:LEU:HD11	2.38	0.53
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.53
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
10:P:357:ARG:HB2	10:P:362:LEU:HD23	1.89	0.53
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.53
3:C:104:ASN:O	22:r:97:PRO:HD3	2.09	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53
4:D:95:LEU:HD12	4:D:96:ARG:H	1.74	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.53
10:P:85:ARG:HE	30:P:401:NDP:C2A	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.53
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.53
19:a:1:MET:CG	33:a:101:CDL:HB21	2.30	0.53
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.74	0.53
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.53
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.53
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.53
10:P:122:HIS:CB	12:R:46:VAL:HG22	2.39	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.53
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.53
10:P:153:ALA:CB	10:P:191:VAL:HG23	2.39	0.53
1:A:49:LEU:HD23	1:A:49:LEU:H	1.72	0.53
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.24	0.53
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.91	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
2:B:194:CYS:O	24:B:301:SF4:S2	2.67	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.52
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.52
18:Z:65:LEU:O	18:Z:69:ILE:HG12	2.09	0.52
19:a:51:ASP:HA	19:a:54:ILE:HD12	1.91	0.52
1:A:53:MET:HE3	1:A:55:PHE:CE1	2.44	0.52
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.52
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.52
1:A:15:LEU:O	1:A:16:THR:C	2.51	0.52
1:A:75:LEU:O	1:A:79:ILE:HG12	2.09	0.52
5:E:63:GLU:O	5:E:67:LYS:HD3	2.09	0.52
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.44	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.52
8:H:131:GLY:HA2	8:H:207:LEU:HD11	1.89	0.52
9:I:53:ALA:HB2	20:b:14:ALA:CB	2.18	0.52
12:R:69:VAL:HG12	12:R:112:LYS:N	2.25	0.52
17:X:35:GLN:HB2	17:X:70:PHE:CE1	2.44	0.52
17:X:91:TYR:OH	19:a:28:LYS:HE2	2.10	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.52
2:B:73:TYR:CE1	2:B:77:LYS:HE3	2.44	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.52
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.52
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.52
10:P:179:LYS:O	10:P:182:ARG:HG2	2.10	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.75	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
5:E:196:THR:O	5:E:200:ILE:HD12	2.10	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
8:H:15:ILE:HG22	19:a:15:CYS:SG	2.49	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
18:Z:68:ARG:O	18:Z:69:ILE:C	2.49	0.52
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.52
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.32	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	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:51:ASP:OD1	8:H:51:ASP:C	2.52	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52
16:W:71:MET:O	16:W:72:LYS:C	2.51	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:364:ASP:C	7:G:364:ASP:OD1	2.51	0.52
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.92	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.52
18:Z:94:GLU:HA	18:Z:97:ILE:CG1	2.39	0.52
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.44	0.52
1:A:73:LEU:N	1:A:74:PRO:CD	2.73	0.52
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.52
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.34	0.52
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.52
12:R:45:ARG:HD2	12:R:48:PHE:CD1	2.44	0.52
16:W:101:LYS:HZ1	16:W:109:PHE:HE2	1.58	0.52
25:B:302:UQ9:H16	4:D:201:PHE:CZ	2.44	0.52
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.90	0.52
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.52
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.52
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.52
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.52
20:b:7:ALA:C	20:b:9:LEU:N	2.68	0.52
21:q:66:THR:HG22	21:q:74:PHE:CB	2.28	0.52
2:B:170:TYR:OH	4:D:131:GLN:O	2.28	0.52
4:D:89:PRO:HB2	8:H:205:SER:OG	2.09	0.52
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.52
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.53	0.52
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.52
17:X:54:ARG:NH2	18:Z:116:TRP:N	2.58	0.52
18:Z:99:LYS:HG3	18:Z:100:ASP:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:O	1:A:76:PRO:HD2	2.10	0.51
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
6:F:227:PRO:HG3	7:G:94:MET:SD	2.50	0.51
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.51
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.51
18:Z:69:ILE:HD12	20:b:53:TYR:HA	1.92	0.51
4:D:279:THR:HA	15:V:12:VAL:HG13	1.93	0.51
5:E:87:ARG:HD2	23:s:77:THR:CG2	2.40	0.51
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.51
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.75	0.51
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
2:B:92:PRO:HG2	2:B:121:PHE:CD1	2.46	0.51
2:B:93:MET:HE2	4:D:87:GLN:OE1	2.11	0.51
2:B:95:PHE:HE1	2:B:97:LEU:CD1	2.23	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.51
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.92	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.51
8:H:216:ALA:O	8:H:217:ALA:C	2.53	0.51
9:I:53:ALA:CA	20:b:14:ALA:CA	2.88	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.51
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.51
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.51
10:P:172:ALA:H	10:P:202:ARG:NH2	2.08	0.51
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.51
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.51
16:W:28:LEU:HG	16:W:32:LYS:HE2	1.93	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
3:C:84:GLU:CG	3:C:141:ARG:HH11	2.23	0.51
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.29	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
8:H:179:TRP:CD1	18:Z:43:LEU:CD2	2.93	0.51
8:H:195:ARG:O	8:H:199:ASP:HB2	2.10	0.51
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
13:S:54:LEU:HD22	13:S:56:ARG:NH1	2.25	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.40	0.51
18:Z:81:ARG:HG3	18:Z:82:ARG:N	2.25	0.51
18:Z:121:ILE:HG23	18:Z:122:GLY:N	2.25	0.51
2:B:87:ARG:HH11	26:B:303:PC1:P	2.34	0.51
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.43	0.51
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.51
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
18:Z:80:ASP:O	18:Z:84:LEU:HG	2.11	0.51
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.51
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
18:Z:130:LYS:O	18:Z:131:GLU:C	2.52	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.51
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.93	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
9:I:53:ALA:CB	20:b:10:LYS:O	2.58	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
9:I:155:CYS:SG	24:I:303:SF4:S2	3.08	0.51
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.51
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.51
1:A:68:GLU:O	1:A:69:ILE:C	2.53	0.51
2:B:105:MET:HE2	25:B:302:UQ9:C5	2.41	0.51
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.45	0.51
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.38	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.51
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.51
8:H:16:ALA:HB2	19:a:15:CYS:CB	2.41	0.51
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.51
14:T:100:VAL:O	14:T:141:PRO:HD2	2.10	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
17:X:141:PRO:HG2	17:X:142:TYR:HD1	1.75	0.51
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
7:G:401:LEU:HD23	7:G:496:MET:HE1	1.92	0.51
26:H:401:PC1:H151	10:P:359:TYR:CD1	2.46	0.51
9:I:61:LEU:HD23	20:b:18:VAL:HG22	1.93	0.51
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.51
13:S:16:LEU:HD21	13:S:95:LEU:CD1	2.41	0.51
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.51
18:Z:93:GLU:O	18:Z:97:ILE:HG12	2.11	0.51
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:31:LEU:HB3	7:G:42:MET:HE2	1.93	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
19:a:1:MET:HE2	33:a:101:CDL:HB22	1.93	0.50
2:B:126:ARG:HD3	2:B:151:GLN:O	2.11	0.50
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.50
5:E:199:ASP:O	5:E:202:GLU:HB3	2.11	0.50
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.50
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.50
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.50
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
8:H:71:PHE:CE1	8:H:215:TYR:CE1	2.99	0.50
8:H:273:ILE:HD11	29:I:301:3PE:H2A1	1.93	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
1:A:49:LEU:HD11	4:D:80:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:19:PHE:CE2	19:a:11:ILE:HG21	2.46	0.50
9:I:50:MET:N	20:b:10:LYS:NZ	2.60	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
13:S:21:VAL:CG2	13:S:91:MET:HE1	2.41	0.50
19:a:37:ARG:CB	19:a:48:MET:CE	2.90	0.50
1:A:42:ASP:OD1	1:A:42:ASP:N	2.45	0.50
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.18	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.50
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.46	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
8:H:69:SER:C	8:H:71:PHE:N	2.68	0.50
8:H:135:ALA:HA	8:H:201:THR:OG1	2.12	0.50
10:P:215:ASN:HD22	10:P:355:ARG:NH1	2.06	0.50
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.50
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.50
8:H:75:PRO:HB2	8:H:222:LEU:CB	2.42	0.50
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.50
11:Q:64:LEU:HG	16:W:84:LEU:HD22	1.94	0.50
12:R:32:THR:HA	12:R:59:PHE:CZ	2.46	0.50
18:Z:102:PRO:O	18:Z:103:ASN:C	2.53	0.50
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.26	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.50
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.47	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
6:F:300:ILE:CG2	6:F:305:GLY:O	2.45	0.50
8:H:67:SER:HB3	8:H:122:ALA:HA	1.94	0.50
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.50
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.50
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.76	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:ILE:HG13	3:C:187:LEU:N	2.27	0.50
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.12	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.50
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
5:E:129:TYR:HD2	5:E:167:LEU:O	1.94	0.50
6:F:126:LYS:CD	6:F:275:LEU:HB2	2.42	0.50
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.50
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.50
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.10	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
1:A:2:ASN:HB2	18:Z:143:TYR:CZ	2.46	0.49
1:A:104:TYR:CE2	1:A:108:GLN:HG3	2.47	0.49
2:B:164:CYS:SG	24:B:301:SF4:S4	3.10	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.49
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.12	0.49
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
3:C:241:PHE:H	7:G:146:PHE:HE1	1.59	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.49
8:H:187:ILE:CD1	29:I:301:3PE:H242	2.41	0.49
9:I:57:ALA:CB	20:b:13:TRP:O	2.43	0.49
10:P:262:THR:N	10:P:332:LEU:HD12	2.24	0.49
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.49
18:Z:26:PRO:HG3	22:r:17:GLY:O	2.13	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.55	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.12	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.49
4:D:304:LYS:HE2	9:I:35:THR:N	2.26	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.42	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.49
8:H:303:TRP:CE3	20:b:29:ALA:HB2	2.31	0.49
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.13	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.94	0.49
18:Z:62:ILE:HG12	20:b:49:THR:HG22	1.94	0.49
19:a:51:ASP:O	19:a:54:ILE:HB	2.11	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.27	0.49
5:E:75:ALA:O	5:E:78:VAL:HG22	2.11	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
8:H:75:PRO:HB2	8:H:222:LEU:HD22	1.95	0.49
9:I:61:LEU:HD21	20:b:17:PRO:O	2.13	0.49
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.49
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.12	0.49
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.49
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.49
8:H:212:ASN:O	8:H:213:VAL:C	2.55	0.49
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
16:W:42:TRP:O	16:W:43:TYR:C	2.55	0.49
5:E:78:VAL:CG1	5:E:104:LEU:HD13	2.42	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.47	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.49
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.49
3:C:107:PHE:CE2	3:C:140:ILE:HD13	2.48	0.49
4:D:166:ARG:CZ	18:Z:8:GLN:HG2	2.42	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.49
6:F:163:TYR:CE1	23:s:80:PHE:HB3	2.48	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
8:H:15:ILE:CG2	19:a:15:CYS:SG	3.00	0.49
8:H:200:LEU:HD11	8:H:282:TYR:N	2.25	0.49
10:P:360:ARG:O	10:P:361:TRP:HB2	2.13	0.49
12:R:32:THR:HA	12:R:59:PHE:HZ	1.78	0.49
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.49
16:W:122:LEU:HD11	16:W:126:TYR:CE2	2.47	0.49
2:B:68:ARG:HG2	2:B:69:SER:N	2.28	0.49
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.49
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.94	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
6:F:379:CYS:SG	24:F:502:SF4:S1	3.11	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.95	0.49
8:H:312:ALA:CB	20:b:38:TYR:HB3	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
1:A:18:ILE:HD13	8:H:72:ILE:HB	1.95	0.49
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.48	0.49
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.49
4:D:79:ASN:O	4:D:80:MET:C	2.55	0.49
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.49
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.49
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.49
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
10:P:122:HIS:HB2	12:R:46:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.49
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.49
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.49
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.49
19:a:2:TRP:O	19:a:3:PHE:C	2.56	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.76	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
8:H:127:TYR:CE2	8:H:208:VAL:CG2	2.94	0.48
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	0.48
4:D:91:ALA:C	4:D:93:GLY:N	2.67	0.48
6:F:46:TYR:O	6:F:48:ARG:HG2	2.13	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.48
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.48
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.76	0.48
8:H:220:PHE:O	8:H:221:ALA:C	2.54	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
9:I:48:VAL:HG11	20:b:11:ASN:CA	2.43	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.48
18:Z:72:MET:O	18:Z:73:PRO:C	2.56	0.48
18:Z:89:GLU:HG2	18:Z:128:ARG:NH1	2.28	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.48	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.48
16:W:32:LYS:HG2	32:W:201:EHZ:C19	2.44	0.48
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.48
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.29	0.48
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.73	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
5:E:137:THR:HG22	6:F:370:LEU:HD21	1.95	0.48
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:53:ALA:HA	20:b:14:ALA:CA	2.41	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
12:R:31:ILE:HD11	12:R:37:VAL:HG23	1.95	0.48
17:X:53:PRO:HD3	18:Z:116:TRP:NE1	2.28	0.48
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.48	0.48
25:B:302:UQ9:H4MB	25:B:302:UQ9:H3MA	1.95	0.48
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
7:G:117:MET:HE3	7:G:142:GLN:C	2.39	0.48
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:59:GLU:OE2	8:H:61:MET:SD	2.71	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.48
1:A:41:PHE:HD2	16:W:102:GLN:CD	2.22	0.48
2:B:91:TRP:CD1	8:H:54:LYS:HE2	2.48	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.48
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.79	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.29	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:401:LEU:HD23	7:G:496:MET:CE	2.43	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:96:ILE:HG12	18:Z:143:TYR:HH	1.76	0.48
13:S:25:GLN:O	13:S:26:ARG:C	2.55	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.96	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.48	0.48
9:I:57:ALA:CA	20:b:17:PRO:CG	2.87	0.48
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.96	0.48
4:D:84:PHE:CZ	4:D:90:ALA:HB3	2.49	0.48
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
5:E:129:TYR:CD2	5:E:167:LEU:O	2.66	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
6:F:333:GLU:OE2	6:F:334:THR:HG23	2.13	0.48
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.48
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.48
14:T:82:ARG:NH1	14:T:126:PHE:HA	2.29	0.48
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.95	0.48
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.44	0.48
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.48
1:A:54:LYS:O	1:A:113:TRP:HA	2.13	0.48
2:B:126:ARG:HB2	8:H:213:VAL:O	2.14	0.48
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.48
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.48
6:F:127:ASP:O	6:F:131:MET:HG3	2.14	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
8:H:68:MET:O	8:H:71:PHE:HB2	2.14	0.48
8:H:71:PHE:CZ	8:H:215:TYR:CE1	3.01	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
10:P:358:THR:HG22	10:P:359:TYR:H	1.79	0.48
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.48
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.48
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.28	0.48
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.48
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.79	0.48
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.48
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.48
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.48	0.47
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.49	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:108:TRP:CZ2	30:P:401:NDP:H2A	2.49	0.47
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:32:THR:O	12:R:33:HIS:C	2.57	0.47
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.47
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.47
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.47
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.47
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.47
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.12	0.47
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.47
7:G:557:ARG:CG	7:G:579:MET:HE3	2.33	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
10:P:315:THR:O	10:P:316:LYS:C	2.57	0.47
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.47
2:B:91:TRP:CD1	2:B:91:TRP:N	2.80	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.47
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.47
6:F:166:ALA:HB1	23:s:80:PHE:CD1	2.50	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:410:ASP:O	6:F:413:TRP:HB3	2.14	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.47
8:H:5:ASN:CB	19:a:26:ILE:HD12	2.44	0.47
8:H:131:GLY:HA3	8:H:207:LEU:CD1	2.43	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
8:H:296:LEU:HD21	29:I:301:3PE:H351	1.95	0.47
9:I:50:MET:H	20:b:10:LYS:HZ1	1.61	0.47
12:R:43:TYR:CD1	12:R:44:ARG:HB2	2.49	0.47
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.48	0.47
21:q:68:MET:SD	21:q:81:MET:HG2	2.55	0.47
3:C:131:LEU:O	3:C:139:ARG:HG3	2.12	0.47
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.49	0.47
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.47
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.47
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.28	0.47
9:I:107:PRO:O	9:I:108:SER:C	2.57	0.47
14:T:132:ASP:HB3	16:W:40:ARG:HH12	1.78	0.47
29:Z:401:3PE:H262	29:Z:401:3PE:C32	2.45	0.47
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:CE1	4:D:86:PRO:HG2	2.43	0.47
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.47
2:B:140:LYS:O	2:B:143:PRO:HD2	2.15	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
8:H:140:ILE:HG13	8:H:141:SER:N	2.29	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
10:P:111:ARG:NH1	10:P:138:ASN:O	2.44	0.47
16:W:113:THR:O	16:W:113:THR:HG22	2.15	0.47
17:X:36:CYS:O	17:X:39:THR:HG22	2.15	0.47
17:X:52:ASP:HB3	18:Z:116:TRP:HB3	1.96	0.47
19:a:3:PHE:O	19:a:6:LEU:HG	2.15	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.48	0.47
1:A:47:ALA:HB1	8:H:126:LYS:N	2.30	0.47
3:C:73:GLN:O	3:C:74:GLN:C	2.57	0.47
4:D:86:PRO:HG3	4:D:115:LEU:CD2	2.44	0.47
4:D:94:VAL:HG21	4:D:116:LEU:HB2	1.96	0.47
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.47
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.47
4:D:375:MET:HE1	7:G:126:LEU:CA	2.43	0.47
4:D:381:HIS:HE1	9:I:161:ALA:O	1.98	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.50	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.47
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.47
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.15	0.47
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.95	0.47
16:W:71:MET:O	16:W:74:ALA:N	2.43	0.47
17:X:69:ASN:OD1	17:X:70:PHE:N	2.47	0.47
17:X:133:THR:HG23	20:b:58:ARG:NH1	2.30	0.47
17:X:139:GLU:CD	17:X:139:GLU:H	2.22	0.47
33:a:101:CDL:H141	33:a:101:CDL:H321	1.97	0.47
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
2:B:135:GLY:HA2	24:B:301:SF4:S3	2.54	0.47
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.47
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.96	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
1:A:102:LEU:CD2	8:H:295:PRO:HG3	2.45	0.47
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.50	0.47
5:E:164:PRO:C	5:E:166:LYS:H	2.21	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
19:a:43:TYR:CE1	19:a:47:LEU:HD11	2.50	0.47
1:A:24:LEU:N	1:A:25:PRO:CD	2.78	0.47
1:A:48:ARG:HG3	1:A:48:ARG:O	2.14	0.47
2:B:96:GLY:HA3	25:B:302:UQ9:H1M	1.97	0.47
4:D:88:HIS:CD2	8:H:208:VAL:HA	2.50	0.47
4:D:145:MET:O	4:D:146:CYS:C	2.58	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.47
8:H:5:ASN:HA	19:a:26:ILE:HD12	1.96	0.47
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.47
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.47
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.46
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:82:LEU:HG	4:D:83:ASN:N	2.30	0.46
4:D:94:VAL:O	4:D:94:VAL:HG22	2.14	0.46
5:E:191:TYR:O	5:E:192:TYR:C	2.58	0.46
6:F:240:THR:HG22	6:F:241:THR:N	2.30	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
9:I:50:MET:N	20:b:10:LYS:HZ3	2.13	0.46
9:I:53:ALA:O	20:b:14:ALA:HA	2.15	0.46
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.46
9:I:123:CYS:SG	24:I:303:SF4:S4	3.13	0.46
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.46
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.46
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
15:V:50:GLN:HE22	22:r:94:ALA:H	1.63	0.46
17:X:4:ILE:HG22	17:X:5:VAL:N	2.25	0.46
17:X:120:PRO:CB	17:X:125:LEU:CD1	2.91	0.46
18:Z:65:LEU:HB3	20:b:50:PRO:O	2.15	0.46
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.80	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.46
5:E:70:PRO:HG2	6:F:236:PHE:CE2	2.50	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.46
29:I:301:3PE:H3C2	20:b:21:VAL:CG1	2.45	0.46
12:R:47:ARG:HG3	12:R:48:PHE:CD1	2.50	0.46
13:S:16:LEU:HD21	13:S:95:LEU:HD12	1.97	0.46
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.46
17:X:29:ALA:HA	18:Z:71:LEU:HD21	1.97	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:68:MET:O	8:H:71:PHE:CB	2.63	0.46
8:H:116:ILE:HG23	8:H:211:PHE:CZ	2.50	0.46
12:R:54:GLU:HB2	21:q:124:TYR:CD1	2.51	0.46
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:29:ASN:O	16:W:29:ASN:OD1	2.33	0.46
17:X:130:LYS:HG2	20:b:67:PRO:CA	2.46	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.51	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
5:E:78:VAL:HG12	5:E:104:LEU:CD1	2.44	0.46
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.46
6:F:425:CYS:SG	24:F:502:SF4:S4	3.13	0.46
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.46
8:H:93:HIS:CE1	19:a:24:ALA:CA	2.99	0.46
13:S:34:ARG:O	13:S:38:VAL:HG23	2.16	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
16:W:58:THR:HB	16:W:61:GLN:HB3	1.94	0.46
17:X:35:GLN:O	17:X:36:CYS:CB	2.64	0.46
33:a:101:CDL:HA21	21:q:6:VAL:CG1	2.45	0.46
23:s:76:ASN:HB3	23:s:79:THR:HB	1.96	0.46
5:E:179:CYS:H	6:F:125:CYS:HB2	1.79	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.46
8:H:200:LEU:HD12	8:H:282:TYR:N	2.25	0.46
9:I:61:LEU:O	29:I:301:3PE:H332	2.15	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.46
5:E:69:TYR:HE2	5:E:80:PRO:HG2	1.80	0.46
5:E:164:PRO:C	5:E:166:LYS:N	2.72	0.46
5:E:245:GLN:HB3	6:F:256:ARG:O	2.16	0.46
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.46
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:66:THR:HG23	8:H:122:ALA:C	2.34	0.46
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.46
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.14	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.46
1:A:72:LEU:C	1:A:74:PRO:HD2	2.40	0.46
5:E:73:HIS:ND1	11:Q:166:TRP:CE3	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:THR:HB	27:E:301:FES:S2	2.56	0.46
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.98	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.46
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.46
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.46
8:H:316:PRO:HA	18:Z:58:ARG:NH1	2.23	0.46
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.79	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.46
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.51	0.46
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.46
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.46
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.46
2:B:174:SER:HA	3:C:203:LEU:CD2	2.46	0.46
3:C:78:SER:C	3:C:80:LEU:H	2.24	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
6:F:225:LEU:N	11:Q:160:TYR:HE2	2.07	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.46
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.46
8:H:69:SER:HB3	26:H:401:PC1:C22	2.46	0.46
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.46
17:X:107:PHE:O	17:X:110:CYS:SG	2.73	0.46
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.46	0.46
19:a:45:TRP:O	19:a:46:TYR:C	2.58	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
1:A:48:ARG:HH11	8:H:124:ASN:HA	1.81	0.46
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.80	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:133:VAL:HG22	5:E:185:VAL:CG1	2.45	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.46
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
9:I:60:ILE:CG2	29:I:301:3PE:H111	2.46	0.46
29:I:301:3PE:H3C2	20:b:21:VAL:HG11	1.97	0.46
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.46
4:D:85:GLY:HA2	4:D:96:ARG:HA	1.98	0.46
4:D:140:ASP:HB3	4:D:147:ASN:ND2	2.17	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.98	0.46
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.46
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.46
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.46
8:H:168:THR:HG23	18:Z:50:MET:HE1	1.98	0.46
29:I:301:3PE:H241	29:I:301:3PE:H272	1.60	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.51	0.46
4:D:359:ASP:O	7:G:150:ARG:NH2	2.48	0.45
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.45
9:I:53:ALA:CA	20:b:14:ALA:HA	2.46	0.45
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
7:G:176:CYS:SG	24:G:802:SF4:S1	3.14	0.45
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
7:G:655:ARG:NH1	13:S:59:SER:H	2.14	0.45
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.98	0.45
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.45
26:H:401:PC1:C21	26:H:401:PC1:H252	2.46	0.45
12:R:54:GLU:HB2	21:q:124:TYR:HD1	1.81	0.45
13:S:44:LEU:CD1	13:S:91:MET:HG2	2.45	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.45
1:A:51:PHE:CE1	8:H:130:PHE:CE1	2.97	0.45
1:A:62:PHE:CD1	8:H:144:VAL:HG23	2.43	0.45
1:A:73:LEU:HA	8:H:151:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD23	8:H:295:PRO:HG3	1.97	0.45
3:C:133:SER:O	3:C:133:SER:OG	2.32	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.47	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
8:H:69:SER:O	8:H:70:LEU:C	2.57	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:153:ALA:HB3	10:P:194:VAL:CG2	2.46	0.45
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.45
1:A:37:TYR:HE2	8:H:208:VAL:HG11	1.82	0.45
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.96	0.45
2:B:114:MET:O	2:B:119:VAL:HG22	2.16	0.45
2:B:117:PHE:CD2	2:B:202:LEU:HD21	2.51	0.45
2:B:117:PHE:CE2	2:B:202:LEU:HD21	2.52	0.45
2:B:125:PRO:O	2:B:126:ARG:C	2.58	0.45
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.52	0.45
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	3.05	0.45
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.45
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.45
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.45
9:I:50:MET:O	9:I:54:THR:N	2.37	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.45
1:A:37:TYR:CE1	2:B:125:PRO:HD2	2.52	0.45
1:A:56:PHE:O	1:A:57:LEU:C	2.58	0.45
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.64	0.45
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.16	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.97	0.45
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.45
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.51	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	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
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.45
17:X:130:LYS:HG2	20:b:67:PRO:HA	1.99	0.45
19:a:45:TRP:O	19:a:48:MET:N	2.50	0.45
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.45
1:A:73:LEU:O	8:H:160:TYR:OH	2.35	0.45
5:E:60:LYS:O	5:E:61:ARG:C	2.57	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.45
9:I:57:ALA:HA	20:b:17:PRO:CB	2.46	0.45
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.45
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.45
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
33:a:101:CDL:CA2	21:q:6:VAL:HG13	2.47	0.45
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.45
7:G:32:ILE:HD11	7:G:45:PRO:HG3	1.98	0.45
8:H:220:PHE:O	8:H:223:PHE:N	2.49	0.45
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.45
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.45
2:B:99:CYS:CB	4:D:141:TYR:CB	2.94	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.45
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
8:H:203:GLY:O	8:H:206:GLU:HB3	2.17	0.45
9:I:57:ALA:CA	20:b:17:PRO:HG3	2.19	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
18:Z:62:ILE:O	18:Z:66:GLU:HG3	2.16	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.45
8:H:202:GLU:HA	8:H:210:GLY:CA	2.47	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.45
8:H:293:PHE:CE1	29:I:301:3PE:H32	2.52	0.45
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.45
17:X:137:LEU:HA	17:X:138:PRO:HD3	1.85	0.45
1:A:97:ILE:HG13	1:A:98:LEU:N	2.32	0.45
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.45
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.52	0.45
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.98	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.45
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.45
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.45
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.45
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.45
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:127:TYR:HD1	8:H:207:LEU:HB3	1.82	0.45
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
17:X:48:TRP:NE1	20:b:55:VAL:HG22	2.32	0.45
18:Z:94:GLU:HA	18:Z:97:ILE:HG12	1.99	0.45
1:A:30:TYR:HD2	1:A:33:LYS:NZ	2.15	0.44
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.44
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.44
6:F:333:GLU:H	6:F:333:GLU:CD	2.25	0.44
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.44
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.44
26:H:401:PC1:H251	26:H:401:PC1:H342	1.99	0.44
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.44
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.98	0.44
1:A:2:ASN:HB3	18:Z:143:TYR:OH	2.17	0.44
1:A:53:MET:HE3	1:A:55:PHE:CD1	2.52	0.44
4:D:139:LEU:HD13	4:D:424:ILE:HG21	1.98	0.44
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.44
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:300:ILE:CG2	6:F:306:GLY:C	2.90	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.44
33:a:101:CDL:H321	33:a:101:CDL:C14	2.46	0.44
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.44
21:q:98:PRO:O	21:q:99:THR:C	2.59	0.44
1:A:33:LYS:HE2	8:H:61:MET:HE1	1.98	0.44
1:A:60:ILE:O	1:A:61:THR:C	2.57	0.44
1:A:62:PHE:HE1	8:H:144:VAL:HG22	1.65	0.44
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.35	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
4:D:376:GLU:HG2	7:G:121:LEU:HD12	1.98	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.98	0.44
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.44
6:F:383:THR:N	6:F:384:PRO:CD	2.79	0.44
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.44
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.44
7:G:450:LYS:HG3	7:G:450:LYS:O	2.17	0.44
9:I:54:THR:CA	20:b:13:TRP:HE1	2.30	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
16:W:58:THR:HB	16:W:61:GLN:H	1.82	0.44
19:a:43:TYR:O	19:a:47:LEU:HD13	2.18	0.44
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.44
1:A:53:MET:HE2	1:A:56:PHE:N	2.32	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.18	0.44
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ASN:ND2	3:C:141:ARG:HE	2.13	0.44
3:C:149:LEU:O	16:W:23:ILE:HD11	2.17	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.31	0.44
5:E:177:GLY:O	27:E:301:FES:S1	2.75	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.44
8:H:216:ALA:HA	8:H:220:PHE:HB2	1.99	0.44
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.98	0.44
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.44
10:P:357:ARG:NH2	10:P:364:SER:O	2.46	0.44
18:Z:131:GLU:O	18:Z:134:SER:N	2.51	0.44
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.36	0.44
1:A:91:ALA:O	1:A:94:LEU:HB3	2.17	0.44
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.44
7:G:450:LYS:CD	7:G:453:GLN:HG3	2.31	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.44
8:H:202:GLU:HA	8:H:210:GLY:HA3	2.00	0.44
8:H:277:TYR:CE2	29:I:301:3PE:H271	2.53	0.44
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.47	0.44
1:A:38:GLU:CD	1:A:43:PRO:HA	2.42	0.44
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.98	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.52	0.44
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.32	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.44
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.44
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:93:HIS:HE1	19:a:24:ALA:HB1	1.82	0.44
9:I:54:THR:CA	20:b:13:TRP:NE1	2.76	0.44
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:81:ILE:HG23	10:P:106:LEU:HD13	2.00	0.44
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.44
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.44
10:P:361:TRP:O	10:P:364:SER:HB3	2.17	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
1:A:93:ILE:O	1:A:97:ILE:HG23	2.18	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.44
6:F:299:LEU:C	6:F:299:LEU:CD1	2.91	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.98	0.44
8:H:186:PHE:CE2	29:I:301:3PE:H2B1	2.52	0.44
9:I:61:LEU:HD21	20:b:18:VAL:HA	2.00	0.44
10:P:140:ASP:O	10:P:143:ASP:N	2.51	0.44
10:P:310:PHE:O	10:P:311:GLU:C	2.59	0.44
13:S:25:GLN:HG3	13:S:26:ARG:H	1.80	0.44
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.29	0.44
19:a:62:VAL:HG23	19:a:62:VAL:O	2.18	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
1:A:67:LEU:O	1:A:70:ALA:HB3	2.18	0.44
4:D:266:ARG:NH2	9:I:59:ARG:O	2.50	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.82	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:228:TYR:O	8:H:231:ILE:N	2.50	0.44
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.44
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.99	0.44
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.99	0.44
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.44
2:B:93:MET:HE3	2:B:93:MET:HB2	1.88	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.44
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:220:PHE:C	8:H:222:LEU:N	2.74	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
1:A:108:GLN:O	1:A:109:LYS:C	2.60	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.47	0.43
5:E:233:LEU:CD2	6:F:43:THR:HA	2.48	0.43
7:G:32:ILE:CG2	7:G:98:LYS:HD2	2.47	0.43
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.43
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.17	0.43
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.43
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.43
16:W:36:ARG:O	16:W:39:TYR:N	2.51	0.43
17:X:35:GLN:HB2	17:X:70:PHE:CD1	2.53	0.43
18:Z:68:ARG:HG3	18:Z:69:ILE:N	2.33	0.43
19:a:50:ARG:O	19:a:54:ILE:HG13	2.18	0.43
1:A:15:LEU:O	1:A:18:ILE:N	2.51	0.43
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.43
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.37	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.43
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.43
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.84	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
8:H:56:PHE:HE1	8:H:221:ALA:HB3	1.82	0.43
8:H:227:GLU:O	8:H:228:TYR:C	2.60	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.43
1:A:97:ILE:O	1:A:98:LEU:C	2.57	0.43
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.64	0.43
4:D:95:LEU:HG	4:D:96:ARG:N	2.32	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)
5:E:140:MET:HE1	6:F:366:ALA:HA	2.00	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:297:LYS:HB2	6:F:333:GLU:HB2	2.00	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.43
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.43
8:H:127:TYR:HE1	8:H:207:LEU:O	2.00	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
9:I:60:ILE:HG23	29:I:301:3PE:H111	1.99	0.43
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.43
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.43
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.43
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.43
16:W:57:ILE:HG23	16:W:107:MET:HE1	2.00	0.43
17:X:50:GLU:OE1	17:X:55:ARG:HB3	2.18	0.43
17:X:66:CYS:O	17:X:67:ALA:C	2.62	0.43
18:Z:140:PHE:CD2	19:a:42:GLN:NE2	2.86	0.43
2:B:90:LEU:HD22	2:B:130:VAL:HG21	1.99	0.43
25:B:302:UQ9:O5	25:B:302:UQ9:C8	2.66	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.43
6:F:127:ASP:HB3	6:F:245:VAL:HG21	2.00	0.43
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.43
8:H:12:PRO:HB2	19:a:19:PRO:HG3	2.01	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.43
1:A:37:TYR:CE1	2:B:125:PRO:CD	3.02	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.43
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	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
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.43
9:I:162:CYS:SG	24:I:304:SF4:S2	3.17	0.43
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	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
2:B:116:ARG:NH2	9:I:86:TYR:H	2.17	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:17:MET:HE3	8:H:225:MET:HG2	2.01	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
17:X:39:THR:HG23	17:X:40:ASN:N	2.33	0.43
18:Z:99:LYS:HB2	18:Z:99:LYS:HE3	1.77	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.43
1:A:65:PHE:CD2	8:H:294:LEU:HD21	2.53	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
3:C:180:HIS:CD2	3:C:182:ASP:H	2.37	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
8:H:196:ALA:C	8:H:198:PHE:N	2.76	0.43
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.43
13:S:58:CYS:SG	13:S:59:SER:N	2.92	0.43
13:S:85:ASP:O	13:S:89:ARG:N	2.42	0.43
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.53	0.43
20:b:53:TYR:HA	20:b:54:PRO:HD3	1.92	0.43
2:B:123:ALA:O	2:B:124:SER:C	2.61	0.43
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.53	0.43
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
7:G:651:PRO:HB3	13:S:58:CYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.75	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:228:TYR:N	8:H:228:TYR:CD1	2.87	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:153:ALA:HB2	10:P:191:VAL:HG23	2.01	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
16:W:25:SER:OG	16:W:34:ARG:NH2	2.52	0.43
17:X:129:THR:HA	20:b:66:VAL:O	2.19	0.43
3:C:149:LEU:HD21	11:Q:59:LEU:HD22	2.00	0.43
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.43
4:D:280:ALA:CB	15:V:11:LEU:CG	2.95	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.43
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.43
8:H:5:ASN:CA	19:a:26:ILE:HD12	2.49	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
10:P:81:ILE:HD11	12:R:46:VAL:HG11	2.00	0.43
10:P:156:SER:O	10:P:160:GLY:N	2.45	0.43
10:P:231:LEU:CD1	10:P:290:PRO:HB2	2.49	0.43
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.00	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
13:S:16:LEU:HD21	13:S:95:LEU:HG	2.00	0.43
14:T:113:LEU:HD22	16:W:71:MET:HE2	2.01	0.43
19:a:37:ARG:H	19:a:59:ARG:NH2	2.17	0.43
2:B:194:CYS:SG	4:D:138:ARG:NE	2.91	0.43
3:C:167:ARG:CZ	3:C:186:ILE:HG22	2.49	0.43
3:C:168:GLU:HA	3:C:186:ILE:HD11	2.00	0.43
4:D:279:THR:HA	15:V:12:VAL:CG1	2.49	0.43
5:E:70:PRO:HG2	6:F:236:PHE:CD2	2.54	0.43
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.43
6:F:44:ASN:HB2	6:F:59:ARG:HD3	1.99	0.43
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.43
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.43
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.43
29:I:301:3PE:H3I2	20:b:28:LEU:CD2	2.49	0.43
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.43
16:W:45:GLU:O	16:W:46:VAL:C	2.62	0.43
17:X:10:LEU:HD12	17:X:13:LEU:HD12	2.01	0.43
20:b:6:SER:OG	20:b:10:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:O	1:A:43:PRO:C	2.61	0.42
2:B:81:LEU:CD2	26:B:303:PC1:H352	2.48	0.42
4:D:140:ASP:CB	4:D:147:ASN:HD21	2.20	0.42
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.44	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:283:GLU:O	7:G:283:GLU:CG	2.51	0.42
10:P:169:HIS:CD2	10:P:181:LEU:HD11	2.49	0.42
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.42
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.42
13:S:25:GLN:CG	13:S:26:ARG:N	2.82	0.42
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.42
33:a:101:CDL:H311	21:q:7:LEU:CD2	2.49	0.42
1:A:27:MET:HE1	8:H:60:PRO:O	2.19	0.42
1:A:71:LEU:HB2	1:A:94:LEU:HD21	2.01	0.42
1:A:74:PRO:C	1:A:76:PRO:HD2	2.44	0.42
4:D:91:ALA:HB1	4:D:95:LEU:HB3	2.01	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.42
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
9:I:54:THR:CA	20:b:13:TRP:CD1	3.01	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
2:B:99:CYS:HB2	4:D:141:TYR:HB2	2.01	0.42
3:C:78:SER:C	3:C:80:LEU:N	2.76	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
5:E:136:THR:HG21	6:F:122:PRO:HG3	2.01	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
9:I:152:CYS:SG	24:I:303:SF4:S1	3.17	0.42
10:P:81:ILE:HD13	12:R:46:VAL:HG11	2.00	0.42
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.42
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.42
10:P:324:ILE:HD13	10:P:324:ILE:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:358:THR:O	10:P:362:LEU:HG	2.19	0.42
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.52	0.42
18:Z:121:ILE:HD11	18:Z:136:ALA:HB3	1.98	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
8:H:23:VAL:HG11	19:a:9:LEU:HD21	2.00	0.42
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:140:ASP:O	10:P:141:PHE:C	2.61	0.42
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.54	0.42
1:A:30:TYR:HD2	1:A:33:LYS:HZ1	1.68	0.42
2:B:112:TYR:HE1	9:I:84:ILE:HD11	1.72	0.42
4:D:264:ASN:O	9:I:65:GLU:OE1	2.38	0.42
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.01	0.42
5:E:196:THR:O	5:E:199:ASP:HB2	2.19	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.42
8:H:204:GLU:O	8:H:205:SER:HB2	2.19	0.42
26:H:401:PC1:H133	26:H:401:PC1:H111	1.73	0.42
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.01	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.42
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.42
16:W:23:ILE:HG22	16:W:24:PHE:HD1	1.81	0.42
16:W:55:LEU:HB3	16:W:57:ILE:HG12	2.01	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
1:A:3:LEU:CA	8:H:96:ILE:HD13	2.45	0.42
1:A:108:GLN:OE1	1:A:108:GLN:HA	2.19	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.50	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.42
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.42
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.42
8:H:200:LEU:HD11	8:H:282:TYR:CB	2.47	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	2.01	0.42
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:48:TRP:HD1	20:b:55:VAL:HG13	1.83	0.42
22:r:20:LEU:C	22:r:20:LEU:CD1	2.89	0.42
1:A:113:TRP:HZ2	8:H:286:MET:HB3	1.82	0.42
3:C:168:GLU:CA	3:C:186:ILE:CD1	2.97	0.42
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.82	0.42
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.42
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.35	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:317:TYR:CZ	19:a:40:ARG:NH1	2.67	0.42
10:P:104:THR:HG22	10:P:106:LEU:HD12	2.00	0.42
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
18:Z:129:THR:O	18:Z:130:LYS:C	2.62	0.42
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.42
1:A:18:ILE:HG23	1:A:19:LEU:N	2.34	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
4:D:166:ARG:CD	18:Z:8:GLN:NE2	2.82	0.42
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.51	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.35	0.42
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
16:W:38:LEU:O	16:W:39:TYR:C	2.62	0.42
17:X:38:LYS:O	17:X:42:GLU:HG3	2.20	0.42
18:Z:94:GLU:HA	18:Z:97:ILE:HD11	2.01	0.42
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.42
20:b:5:ILE:HD12	20:b:6:SER:N	2.34	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.42
2:B:95:PHE:HE1	2:B:97:LEU:HD11	1.84	0.42
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.42
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.42
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.42
6:F:70:LEU:O	6:F:71:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:113:LEU:HD13	6:F:149:MET:SD	2.60	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.42
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.42
21:q:56:PHE:HD2	22:r:27:ARG:HH22	1.68	0.42
1:A:49:LEU:HD23	1:A:49:LEU:N	2.34	0.42
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.42
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.42
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.42
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.02	0.42
5:E:65:ILE:HG21	5:E:80:PRO:HB2	2.01	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
6:F:300:ILE:CG2	6:F:306:GLY:CA	2.95	0.42
6:F:315:LEU:HD23	6:F:315:LEU:O	2.20	0.42
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.02	0.42
8:H:20:LEU:CD2	8:H:228:TYR:CD2	3.02	0.42
8:H:59:GLU:OE1	8:H:61:MET:SD	2.78	0.42
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.42
9:I:50:MET:SD	20:b:10:LYS:HA	2.60	0.42
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.42
11:Q:167:ASN:C	11:Q:168:LYS:CG	2.93	0.42
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.42
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.42
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.42
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.42
18:Z:72:MET:N	18:Z:73:PRO:CD	2.83	0.42
18:Z:91:LEU:HD13	18:Z:91:LEU:C	2.45	0.42
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:H	1:A:25:PRO:HD3	1.84	0.41
1:A:46:SER:O	1:A:47:ALA:HB3	2.20	0.41
1:A:75:LEU:N	1:A:76:PRO:CD	2.83	0.41
1:A:93:ILE:O	1:A:97:ILE:HG12	2.20	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
2:B:210:ARG:NE	21:q:78:ASP:OD1	2.53	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
5:E:67:LYS:O	5:E:68:ASN:C	2.64	0.41
5:E:78:VAL:O	5:E:82:LEU:HB2	2.20	0.41
5:E:181:ASN:HB3	5:E:193:GLU:HB2	2.01	0.41
6:F:126:LYS:HG3	6:F:275:LEU:HD22	2.01	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.41
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.50	0.41
8:H:167:THR:O	18:Z:53:TRP:NE1	2.49	0.41
8:H:203:GLY:O	8:H:206:GLU:N	2.50	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
11:Q:52:LEU:HD23	16:W:19:SER:O	2.20	0.41
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.81	0.41
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
20:b:7:ALA:C	20:b:9:LEU:H	2.27	0.41
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.41
20:b:59:ASP:HA	20:b:63:MET:CE	2.50	0.41
1:A:57:LEU:O	1:A:58:VAL:C	2.62	0.41
1:A:99:SER:O	1:A:100:LEU:C	2.63	0.41
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.41
5:E:241:GLY:HA3	6:F:63:TYR:CZ	2.56	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.50	0.41
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.41
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.41
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.41
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.01	0.41
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.97	0.41
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.41
14:T:132:ASP:O	16:W:40:ARG:NH2	2.53	0.41
2:B:72:GLU:O	2:B:76:THR:HG23	2.20	0.41
2:B:100:CYS:SG	24:B:301:SF4:S3	3.19	0.41
2:B:114:MET:O	2:B:115:ASP:C	2.62	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	2.02	0.41
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
1:A:37:TYR:CE1	2:B:125:PRO:CG	3.04	0.41
1:A:61:THR:C	1:A:63:LEU:N	2.75	0.41
1:A:61:THR:OG1	1:A:62:PHE:N	2.52	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.36	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.02	0.41
4:D:348:LEU:O	18:Z:11:PRO:HB3	2.20	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
6:F:363:ILE:O	6:F:364:VAL:C	2.64	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.20	0.41
8:H:1:MET:HG3	19:a:30:THR:HG23	1.94	0.41
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.35	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.55	0.41
10:P:315:THR:HG22	10:P:317:ASP:N	2.35	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
16:W:47:PRO:HG3	16:W:63:ARG:NH2	2.26	0.41
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.41
17:X:130:LYS:CG	20:b:67:PRO:HB3	2.50	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
3:C:229:PHE:O	11:Q:123:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.03	0.41
13:S:33:VAL:O	13:S:34:ARG:C	2.63	0.41
17:X:112:LEU:HD13	17:X:118:VAL:HG22	2.03	0.41
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.20	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
21:q:5:GLU:HG2	21:q:9:ARG:HE	1.85	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.28	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.41
10:P:172:ALA:H	10:P:202:ARG:HH21	1.67	0.41
12:R:48:PHE:CE2	12:R:53:LYS:HB2	2.56	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
1:A:38:GLU:HG2	4:D:83:ASN:CG	2.45	0.41
1:A:57:LEU:C	1:A:57:LEU:HD23	2.46	0.41
2:B:121:PHE:CD1	2:B:121:PHE:N	2.88	0.41
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.41
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.56	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.02	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.41
8:H:20:LEU:HA	19:a:12:MET:SD	2.61	0.41
8:H:296:LEU:CD2	29:I:301:3PE:H351	2.50	0.41
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.86	0.41
10:P:56:ALA:HA	10:P:125:VAL:O	2.21	0.41
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.41
10:P:231:LEU:HD12	10:P:231:LEU:HA	1.95	0.41
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.41
16:W:24:PHE:HB2	16:W:83:ASP:OD2	2.20	0.41
16:W:44:ARG:O	16:W:47:PRO:HG2	2.20	0.41
18:Z:96:ILE:H	18:Z:96:ILE:HG13	1.72	0.41
19:a:2:TRP:CZ2	33:a:101:CDL:H522	2.55	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
21:q:138:VAL:O	21:q:139:PRO:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:O	1:A:73:LEU:HG	2.20	0.41
1:A:106:TRP:CE3	1:A:107:THR:HG22	2.56	0.41
2:B:115:ASP:OD1	2:B:120:VAL:HG22	2.21	0.41
3:C:224:GLU:OE2	10:P:45:LYS:HE2	2.21	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.20	0.41
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.85	0.41
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.94	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:339:ALA:CB	7:G:537:ILE:CD1	2.96	0.41
8:H:124:ASN:O	8:H:124:ASN:CG	2.62	0.41
8:H:224:PHE:CE1	8:H:228:TYR:CE1	3.09	0.41
29:I:301:3PE:H3H2	29:I:301:3PE:H3E1	1.90	0.41
10:P:179:LYS:O	10:P:180:SER:C	2.63	0.41
10:P:227:PRO:O	10:P:228:LEU:HD23	2.21	0.41
12:R:38:TYR:HE2	12:R:44:ARG:HE	1.69	0.41
13:S:21:VAL:HG23	13:S:91:MET:HE1	2.02	0.41
16:W:32:LYS:HZ3	32:W:201:EHZ:C19	2.33	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
1:A:33:LYS:CG	8:H:61:MET:CE	2.59	0.41
1:A:33:LYS:CB	8:H:61:MET:HE2	2.45	0.41
4:D:158:LEU:O	4:D:392:PRO:HG2	2.21	0.41
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.41
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:61:ASP:O	6:F:256:ARG:NH2	2.54	0.41
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.41
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.56	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.41
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.41
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.41
8:H:1:MET:CE	19:a:26:ILE:HG23	2.30	0.41
8:H:63:PRO:O	8:H:66:THR:HB	2.21	0.41
8:H:135:ALA:HB2	8:H:201:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:152:CYS:SG	24:I:303:SF4:S3	3.17	0.41
10:P:75:ARG:HH21	16:W:113:THR:HG23	1.86	0.41
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.85	0.41
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.41
11:Q:166:TRP:O	11:Q:167:ASN:C	2.64	0.41
14:T:82:ARG:O	14:T:86:VAL:HG23	2.20	0.41
16:W:117:ARG:HA	16:W:118:PRO:HD3	1.94	0.41
21:q:89:TRP:HB2	21:q:98:PRO:HD3	2.03	0.41
1:A:103:ALA:O	1:A:106:TRP:HB3	2.20	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.41
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.41
8:H:65:THR:HB	8:H:124:ASN:ND2	2.36	0.41
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:61:LEU:CG	20:b:17:PRO:O	2.68	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
13:S:26:ARG:HG3	13:S:26:ARG:O	2.21	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
17:X:38:LYS:HD2	17:X:131:VAL:HG12	2.02	0.41
33:a:101:CDL:HA62	21:q:6:VAL:O	2.21	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.40
2:B:153:PRO:HG3	8:H:58:LYS:HD2	2.02	0.40
25:B:302:UQ9:O5	25:B:302:UQ9:H4MA	2.21	0.40
3:C:243:ALA:C	7:G:105:ASN:ND2	2.80	0.40
5:E:78:VAL:CA	5:E:104:LEU:HD13	2.46	0.40
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	0.40
6:F:45:LEU:O	6:F:46:TYR:HB2	2.21	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.02	0.40
6:F:427:LEU:HB2	28:F:501:FMN:HM73	2.03	0.40
7:G:49:VAL:HB	7:G:91:ALA:HA	2.03	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.40
7:G:355:LYS:NZ	7:G:528:LEU:O	2.47	0.40
7:G:655:ARG:NH1	13:S:59:SER:N	2.69	0.40
8:H:5:ASN:ND2	19:a:23:THR:HG23	2.28	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
10:P:96:LEU:HD12	10:P:97:MET:CA	2.51	0.40
10:P:177:SER:O	10:P:182:ARG:NH2	2.53	0.40
10:P:315:THR:H	10:P:318:LYS:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
16:W:32:LYS:O	16:W:33:ARG:C	2.65	0.40
17:X:143:HIS:CG	17:X:143:HIS:O	2.73	0.40
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.40
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.40
4:D:116:LEU:O	4:D:118:ARG:HG3	2.22	0.40
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.40
5:E:223:CYS:CB	6:F:133:HIS:CE1	3.04	0.40
6:F:128:ARG:HA	6:F:131:MET:CE	2.37	0.40
6:F:294:VAL:HG12	6:F:337:MET:HB2	2.03	0.40
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.40
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
10:P:180:SER:HB2	10:P:321:ARG:HH21	1.87	0.40
10:P:221:ARG:CG	10:P:286:ARG:HD3	2.52	0.40
17:X:127:LYS:HD2	20:b:70:PRO:O	2.20	0.40
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.40
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.40
1:A:49:LEU:H	1:A:49:LEU:CD2	2.34	0.40
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.84	0.40
3:C:77:VAL:HG22	3:C:83:LEU:HD13	2.03	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.52	0.40
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.40
4:D:313:GLN:HE21	4:D:313:GLN:HB2	1.67	0.40
6:F:177:TYR:O	6:F:178:GLU:C	2.64	0.40
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.52	0.40
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.52	0.40
7:G:356:ASP:OD2	7:G:645:ARG:NE	2.51	0.40
7:G:404:GLY:HA3	7:G:684:LEU:CD1	2.34	0.40
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.40
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.87	0.40
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.40
8:H:199:ASP:C	8:H:201:THR:O	2.65	0.40
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.40
10:P:40:VAL:HG13	12:R:43:TYR:CZ	2.57	0.40
10:P:40:VAL:HG13	12:R:43:TYR:OH	2.22	0.40
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.40
2:B:84:TRP:CZ3	26:B:303:PC1:H351	2.56	0.40
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:213:PHE:O	4:D:214:TYR:C	2.65	0.40
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
8:H:206:GLU:O	8:H:207:LEU:HB2	2.21	0.40
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.40
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.40
10:P:300:TRP:CE2	10:P:304:LEU:HD21	2.57	0.40
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.40
14:T:118:ILE:CG2	14:T:122:MET:HE3	2.47	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
19:a:58:ASN:ND2	19:a:60:TYR:OH	2.55	0.40
33:a:101:CDL:CA3	21:q:13:GLN:HE22	2.28	0.40
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.40
4:D:362:LYS:O	4:D:384:LEU:HD21	2.22	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.51	0.40
6:F:349:LEU:HA	6:F:349:LEU:HD12	1.91	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.10	0.40
7:G:598:ASN:ND2	7:G:600:GLU:OE2	2.51	0.40
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.40
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.40
8:H:145:THR:HG22	8:H:289:LEU:HD11	2.03	0.40
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.43	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.40
9:I:50:MET:O	9:I:54:THR:HG23	2.22	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
10:P:123:SER:O	10:P:161:VAL:HG12	2.22	0.40
10:P:359:TYR:CG	10:P:360:ARG:N	2.89	0.40
11:Q:85:ASN:O	11:Q:86:ASN:C	2.64	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	111/115 (96%)	100 (90%)	11 (10%)	0	100	100
2	B	155/224 (69%)	144 (93%)	10 (6%)	1 (1%)	21	54
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	383/463 (83%)	357 (93%)	26 (7%)	0	100	100
5	E	208/248 (84%)	188 (90%)	20 (10%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	627 (92%)	58 (8%)	0	100	100
8	H	316/318 (99%)	296 (94%)	19 (6%)	1 (0%)	36	67
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	316 (94%)	22 (6%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	76 (94%)	5 (6%)	0	100	100
13	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
19	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
20	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
21	q	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	11/104 (11%)	11 (100%)	0	0	100	100
All	All	4153/5036 (82%)	3891 (94%)	260 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	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	102/104 (98%)	101 (99%)	1 (1%)	68	75
2	B	133/185 (72%)	131 (98%)	2 (2%)	57	71
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	332/395 (84%)	330 (99%)	2 (1%)	78	79
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	80
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	280/280 (100%)	279 (100%)	1 (0%)	84	81
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	296 (100%)	1 (0%)	86	83
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
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%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	71/73 (97%)	71 (100%)	0	100	100
21	q	108/131 (82%)	107 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	13/95 (14%)	13 (100%)	0	100	100
All	All	3642/4292 (85%)	3627 (100%)	15 (0%)	81	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
2	B	93	MET
2	B	104	MET
4	D	87	GLN
4	D	232	VAL
5	E	244	VAL
7	G	271	MET
8	H	229	THR
10	P	316	LYS
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS
21	q	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	83	ASN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	117	HIS

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Mol	Chain	Res	Type
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	116	ASN
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
6	F	393	ASN
7	G	59	GLN
7	G	74	ASN
7	G	101	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	495	ASN
7	G	498	GLN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	32	GLN
8	H	47	GLN
8	H	93	HIS
8	H	97	ASN
8	H	99	ASN

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Mol	Chain	Res	Type
8	H	124	ASN
8	H	169	GLN
8	H	171	HIS
8	H	212	ASN
8	H	258	ASN
8	H	292	ASN
9	I	126	GLN
10	P	43	HIS
10	P	71	ASN
10	P	79	GLN
10	P	169	HIS
10	P	215	ASN
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
11	Q	51	GLN
11	Q	88	GLN
15	V	41	HIS
15	V	50	GLN
16	W	29	ASN
16	W	54	GLN
16	W	102	GLN
17	X	30	HIS
17	X	77	HIS
19	a	27	HIS
19	a	58	ASN
20	b	69	HIS
20	b	83	ASN
21	q	13	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	21	GLN
22	r	110	GLN
23	s	84	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z > 2$
33	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.31	8 (12%)
24	SF4	I	304	9	0,12,12	-	-	-		
28	FMN	F	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.22	6 (12%)
29	3PE	Z	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.02	2 (4%)
30	NDP	P	401	-	51,52,52	1.18	5 (9%)	71,80,80	1.56	10 (14%)
27	FES	G	803	7	0,4,4	-	-	-		
26	PC1	B	303	-	34,34,53	1.16	2 (5%)	40,42,61	1.17	3 (7%)
24	SF4	I	303	9	0,12,12	-	-	-		
26	PC1	I	302	-	46,46,53	1.00	2 (4%)	52,54,61	1.09	3 (5%)
24	SF4	B	301	2	0,12,12	-	-	-		
26	PC1	H	401	-	41,41,53	1.05	2 (4%)	47,49,61	1.07	4 (8%)
24	SF4	F	502	6	0,12,12	-	-	-		
27	FES	E	301	5	0,4,4	-	-	-		
24	SF4	G	801	7	0,12,12	-	-	-		
25	UQ9	B	302	-	30,30,58	1.05	3 (10%)	37,39,73	0.90	2 (5%)
29	3PE	I	301	-	50,50,50	0.90	2 (4%)	53,55,55	1.04	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	EHZ	W	201	-	29,31,37	1.79	7 (24%)	37,41,47	1.94	11 (29%)
24	SF4	G	802	7	0,12,12	-	-	-		

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
33	CDL	a	101	-	-	12/67/67/110	-
24	SF4	I	304	9	-	-	0/6/5/5
28	FMN	F	501	-	-	4/18/18/18	0/3/3/3
29	3PE	Z	401	-	-	13/49/49/54	-
30	NDP	P	401	-	-	6/34/77/77	0/5/5/5
24	SF4	F	502	6	-	-	0/6/5/5
27	FES	G	803	7	-	-	0/1/1/1
26	PC1	B	303	-	-	11/38/38/57	-
24	SF4	I	303	9	-	-	0/6/5/5
26	PC1	I	302	-	-	12/50/50/57	-
29	3PE	I	301	-	-	17/54/54/54	-
26	PC1	H	401	-	-	16/45/45/57	-
32	EHZ	W	201	-	-	21/39/39/45	-
24	SF4	B	301	2	-	-	0/6/5/5
24	SF4	G	801	7	-	-	0/6/5/5
25	UQ9	B	302	-	-	14/24/48/81	0/1/1/1
27	FES	E	301	5	-	-	0/1/1/1
24	SF4	G	802	7	-	-	0/6/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.00	1.45	1.33
28	F	501	FMN	C9A-C5A	4.96	1.49	1.41
32	W	201	EHZ	C12-N1	4.92	1.45	1.33
30	P	401	NDP	C5A-C4A	4.39	1.46	1.39
26	I	302	PC1	O31-C31	4.20	1.45	1.33
26	B	303	PC1	O31-C31	4.18	1.45	1.33
33	a	101	CDL	OB8-CB7	4.18	1.45	1.33
26	H	401	PC1	O31-C31	4.15	1.45	1.33
29	I	301	3PE	O31-C31	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I	302	PC1	O21-C21	4.12	1.45	1.34
33	a	101	CDL	OA8-CA7	4.10	1.45	1.33
33	a	101	CDL	OA6-CA5	4.09	1.45	1.34
33	a	101	CDL	OB6-CB5	4.09	1.45	1.34
29	Z	401	3PE	O31-C31	4.08	1.45	1.33
26	B	303	PC1	O21-C21	4.05	1.45	1.34
26	H	401	PC1	O21-C21	3.99	1.45	1.34
29	I	301	3PE	O21-C21	3.98	1.45	1.34
29	Z	401	3PE	O21-C21	3.95	1.45	1.34
28	F	501	FMN	C8-C7	3.26	1.48	1.40
25	B	302	UQ9	O4-C4M	-3.02	1.38	1.45
25	B	302	UQ9	C3-C2	-2.82	1.40	1.48
28	F	501	FMN	C4-N3	-2.73	1.33	1.38
32	W	201	EHZ	P1-O7	2.65	1.64	1.54
30	P	401	NDP	C5A-C6A	2.56	1.48	1.41
32	W	201	EHZ	O4-C15	-2.55	1.18	1.23
28	F	501	FMN	C5A-N5	-2.49	1.34	1.39
30	P	401	NDP	C5A-N7A	-2.47	1.34	1.39
32	W	201	EHZ	O3-C12	-2.44	1.18	1.23
32	W	201	EHZ	C9-S1	2.40	1.81	1.76
30	P	401	NDP	C8A-N7A	2.31	1.36	1.31
32	W	201	EHZ	P1-OP3	-2.29	1.46	1.54
25	B	302	UQ9	C4-C5	-2.25	1.42	1.48
30	P	401	NDP	C4A-N9A	-2.09	1.33	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	201	EHZ	C8-C9-S1	6.20	121.39	113.56
30	P	401	NDP	C5A-C4A-N3A	-5.69	118.88	126.72
30	P	401	NDP	N3A-C4A-N9A	4.53	134.87	127.17
33	a	101	CDL	OA6-CA5-C11	4.36	120.91	111.48
26	I	302	PC1	O21-C21-C22	4.21	120.59	111.48
33	a	101	CDL	OB6-CB5-C51	4.11	120.37	111.48
29	Z	401	3PE	O21-C21-C22	3.76	119.61	111.48
26	B	303	PC1	O21-C21-C22	3.74	119.58	111.48
26	H	401	PC1	O21-C21-C22	3.72	119.54	111.48
29	I	301	3PE	O21-C21-C22	3.69	119.46	111.48
30	P	401	NDP	C2A-N3A-C4A	3.63	120.69	111.83
30	P	401	NDP	C4A-C5A-N7A	-3.46	106.63	110.58
32	W	201	EHZ	O2-C9-C8	-3.22	118.67	123.74
30	P	401	NDP	N3A-C2A-N1A	-3.16	123.81	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	302	UQ9	C4M-O4-C4	-3.11	105.54	116.47
32	W	201	EHZ	C14-C13-C12	-3.07	107.28	112.39
32	W	201	EHZ	OP3-P1-O9	-2.96	99.31	110.83
32	W	201	EHZ	C7-C8-C9	-2.95	107.27	113.86
26	I	302	PC1	C2-O21-C21	-2.93	110.79	117.80
30	P	401	NDP	C4A-N9A-C8A	2.93	108.81	105.74
26	B	303	PC1	O31-C31-C32	2.88	120.63	111.83
32	W	201	EHZ	C13-C12-N1	2.87	121.58	116.34
33	a	101	CDL	OA8-CA7-C31	2.86	120.54	111.83
33	a	101	CDL	CA4-OA6-CA5	-2.79	111.12	117.80
26	B	303	PC1	C2-O21-C21	-2.78	111.13	117.80
29	I	301	3PE	O31-C31-C32	2.76	120.24	111.83
26	H	401	PC1	O31-C31-C32	2.71	120.09	111.83
25	B	302	UQ9	C7-C6-C1	-2.69	120.27	124.89
26	I	302	PC1	O31-C31-C32	2.68	120.02	111.83
29	Z	401	3PE	O31-C31-C32	2.67	119.98	111.83
30	P	401	NDP	C5A-N7A-C8A	2.54	107.44	103.45
28	F	501	FMN	O4-C4-C4A	-2.52	119.89	126.53
33	a	101	CDL	OB8-CB7-C71	2.51	119.49	111.83
32	W	201	EHZ	C5-C6-C7	-2.45	107.93	114.68
30	P	401	NDP	C3D-C2D-C1D	2.45	106.10	101.46
28	F	501	FMN	C4A-C10-N1	-2.43	118.64	124.59
32	W	201	EHZ	C10-S1-C9	2.38	108.88	101.84
28	F	501	FMN	C4-C4A-N5	2.30	121.38	118.21
33	a	101	CDL	CB4-OB6-CB5	-2.28	112.33	117.80
26	H	401	PC1	C2-O21-C21	-2.23	112.47	117.80
32	W	201	EHZ	C11-N1-C12	-2.22	118.70	122.82
32	W	201	EHZ	O6-P1-O9	2.18	112.32	106.44
30	P	401	NDP	N9A-C8A-N7A	-2.16	110.87	113.94
32	W	201	EHZ	O2-C9-S1	-2.15	119.94	122.68
28	F	501	FMN	C4A-C10-N10	2.15	119.56	116.48
26	H	401	PC1	C11-C12-N	-2.15	108.93	115.82
30	P	401	NDP	C6A-C5A-N7A	2.08	136.10	132.09
28	F	501	FMN	O2-C2-N1	-2.08	118.35	121.80
29	I	301	3PE	O31-C31-O32	-2.07	118.45	123.63
29	I	301	3PE	C2-O21-C21	-2.06	112.88	117.80
28	F	501	FMN	C4-N3-C2	-2.03	122.04	125.64
33	a	101	CDL	OA8-CA7-OA9	-2.02	118.56	123.63
33	a	101	CDL	OA6-CA5-OA7	-2.02	118.99	123.70

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	302	UQ9	C12-C13-C14-C16
25	B	302	UQ9	C12-C13-C14-C15
25	B	302	UQ9	C1-C6-C7-C8
25	B	302	UQ9	C5-C6-C7-C8
26	B	303	PC1	C1-O11-P-O12
26	B	303	PC1	C1-O11-P-O14
26	B	303	PC1	C1-O11-P-O13
26	B	303	PC1	C22-C21-O21-C2
26	H	401	PC1	C11-O13-P-O12
26	H	401	PC1	C11-O13-P-O14
26	H	401	PC1	C11-O13-P-O11
26	H	401	PC1	C12-C11-O13-P
26	H	401	PC1	O32-C31-O31-C3
26	I	302	PC1	C11-O13-P-O12
26	I	302	PC1	C11-O13-P-O14
26	I	302	PC1	C11-O13-P-O11
26	I	302	PC1	C1-O11-P-O12
26	I	302	PC1	C1-O11-P-O13
28	F	501	FMN	N10-C1'-C2'-O2'
28	F	501	FMN	C5'-O5'-P-O1P
28	F	501	FMN	C5'-O5'-P-O3P
29	I	301	3PE	C11-O13-P-O11
29	I	301	3PE	C11-O13-P-O12
29	Z	401	3PE	C11-O13-P-O11
29	Z	401	3PE	C12-C11-O13-P
29	Z	401	3PE	O32-C31-O31-C3
29	Z	401	3PE	C32-C31-O31-C3
30	P	401	NDP	C2N-C3N-C7N-N7N
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C6-C7-C8-C9
32	W	201	EHZ	S1-C10-C11-N1
32	W	201	EHZ	C16-C17-C20-O6
32	W	201	EHZ	C20-O6-P1-O7
32	W	201	EHZ	C20-O6-P1-O9
32	W	201	EHZ	C20-O6-P1-OP3
33	a	101	CDL	CA3-OA5-PA1-OA2
33	a	101	CDL	CA3-OA5-PA1-OA3
33	a	101	CDL	CA3-OA5-PA1-OA4
26	I	302	PC1	O32-C31-O31-C3
26	I	302	PC1	C32-C31-O31-C3
26	B	303	PC1	O22-C21-O21-C2
26	H	401	PC1	C32-C31-O31-C3
25	B	302	UQ9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
25	B	302	UQ9	C12-C11-C9-C10
25	B	302	UQ9	C18-C19-C21-C22
25	B	302	UQ9	C12-C11-C9-C8
25	B	302	UQ9	C17-C18-C19-C21
29	I	301	3PE	C32-C31-O31-C3
29	Z	401	3PE	C22-C21-O21-C2
29	I	301	3PE	O32-C31-O31-C3
33	a	101	CDL	C12-C13-C14-C15
29	Z	401	3PE	O22-C21-O21-C2
25	B	302	UQ9	C17-C18-C19-C20
33	a	101	CDL	C31-CA7-OA8-CA6
26	I	302	PC1	C11-C12-N-C15
26	H	401	PC1	C24-C25-C26-C27
33	a	101	CDL	OA9-CA7-OA8-CA6
26	I	302	PC1	C11-C12-N-C13
33	a	101	CDL	C51-CB5-OB6-CB4
26	I	302	PC1	C11-C12-N-C14
33	a	101	CDL	OB7-CB5-OB6-CB4
29	I	301	3PE	C22-C21-O21-C2
29	Z	401	3PE	C31-C32-C33-C34
25	B	302	UQ9	C19-C21-C22-C23
29	I	301	3PE	C24-C25-C26-C27
26	B	303	PC1	C2-C1-O11-P
32	W	201	EHZ	N2-C15-C16-C17
26	B	303	PC1	C32-C31-O31-C3
29	I	301	3PE	O22-C21-O21-C2
26	B	303	PC1	C32-C33-C34-C35
32	W	201	EHZ	C3-C4-C5-C6
29	Z	401	3PE	C3-C2-O21-C21
26	B	303	PC1	O32-C31-O31-C3
26	H	401	PC1	C22-C23-C24-C25
26	B	303	PC1	O13-C11-C12-N
26	H	401	PC1	O13-C11-C12-N
32	W	201	EHZ	O4-C15-C16-O5
29	Z	401	3PE	O11-C1-C2-C3
26	H	401	PC1	O22-C21-O21-C2
32	W	201	EHZ	C18-C17-C20-O6
32	W	201	EHZ	C19-C17-C20-O6
29	Z	401	3PE	C2E-C2F-C2G-C2H
32	W	201	EHZ	C11-C10-S1-C9
29	Z	401	3PE	O11-C1-C2-O21
26	H	401	PC1	C22-C21-O21-C2

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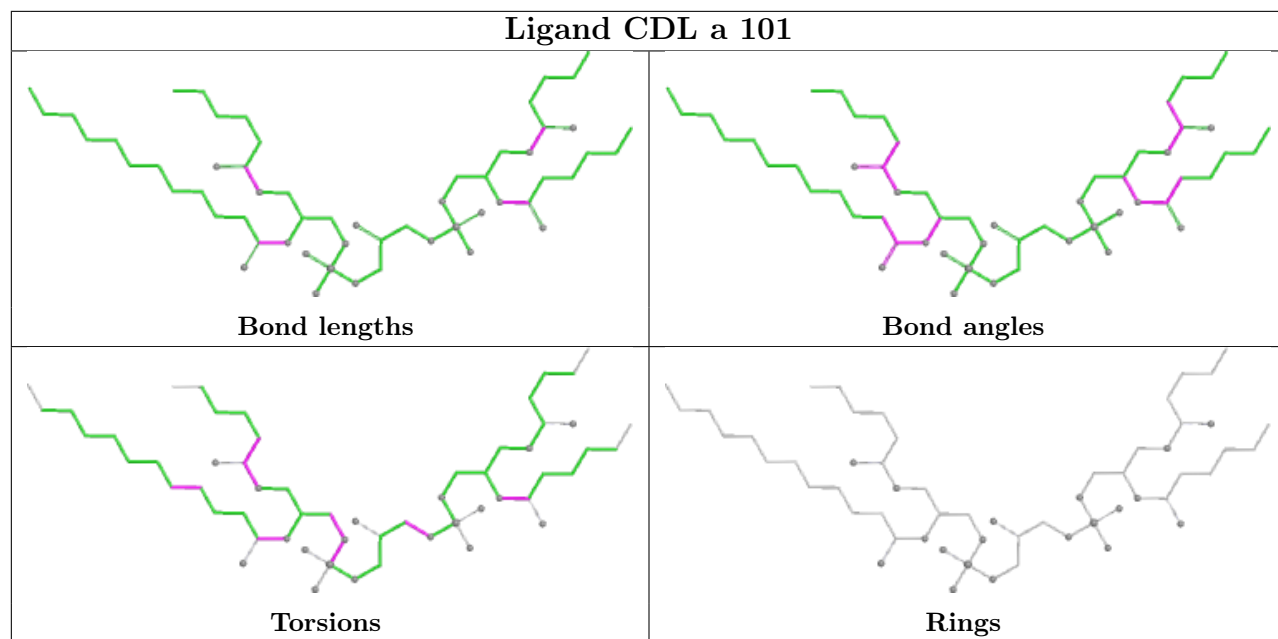
Mol	Chain	Res	Type	Atoms
29	I	301	3PE	O21-C2-C3-O31
26	H	401	PC1	C27-C28-C29-C2A
26	H	401	PC1	C1-O11-P-O14
29	I	301	3PE	C1-O11-P-O12
29	I	301	3PE	C1-O11-P-O13
29	I	301	3PE	C1-O11-P-O14
29	I	301	3PE	C11-O13-P-O14
29	Z	401	3PE	C11-O13-P-O14
29	Z	401	3PE	C2-C1-O11-P
33	a	101	CDL	CA4-CA3-OA5-PA1
32	W	201	EHZ	C5-C6-C7-O1
25	B	302	UQ9	C15-C14-C16-C17
25	B	302	UQ9	C13-C14-C16-C17
26	B	303	PC1	C34-C35-C36-C37
32	W	201	EHZ	C2-C3-C4-C5
32	W	201	EHZ	N2-C15-C16-O5
29	I	301	3PE	C37-C38-C39-C3A
32	W	201	EHZ	O2-C9-S1-C10
30	P	401	NDP	O4D-C1D-N1N-C6N
30	P	401	NDP	PN-O3-PA-O2A
26	I	302	PC1	C2E-C2F-C2G-C2H
33	a	101	CDL	C1-CB2-OB2-PB2
29	I	301	3PE	C35-C36-C37-C38
29	I	301	3PE	C33-C34-C35-C36
30	P	401	NDP	C2D-C1D-N1N-C6N
28	F	501	FMN	C5'-O5'-P-O2P
32	W	201	EHZ	C15-C16-C17-C18
26	H	401	PC1	C11-C12-N-C13
32	W	201	EHZ	O5-C16-C17-C18
32	W	201	EHZ	O4-C15-C16-C17
32	W	201	EHZ	C15-C16-C17-C20
33	a	101	CDL	C32-C31-CA7-OA8
26	H	401	PC1	C35-C36-C37-C38
26	H	401	PC1	C11-C12-N-C14
30	P	401	NDP	C2N-C3N-C7N-O7N
26	I	302	PC1	C2C-C2D-C2E-C2F
29	I	301	3PE	C1-C2-C3-O31
29	I	301	3PE	C2-C1-O11-P
25	B	302	UQ9	C2-C3-O3-C3M
33	a	101	CDL	C11-CA5-OA6-CA4
30	P	401	NDP	PN-O3-PA-O1A

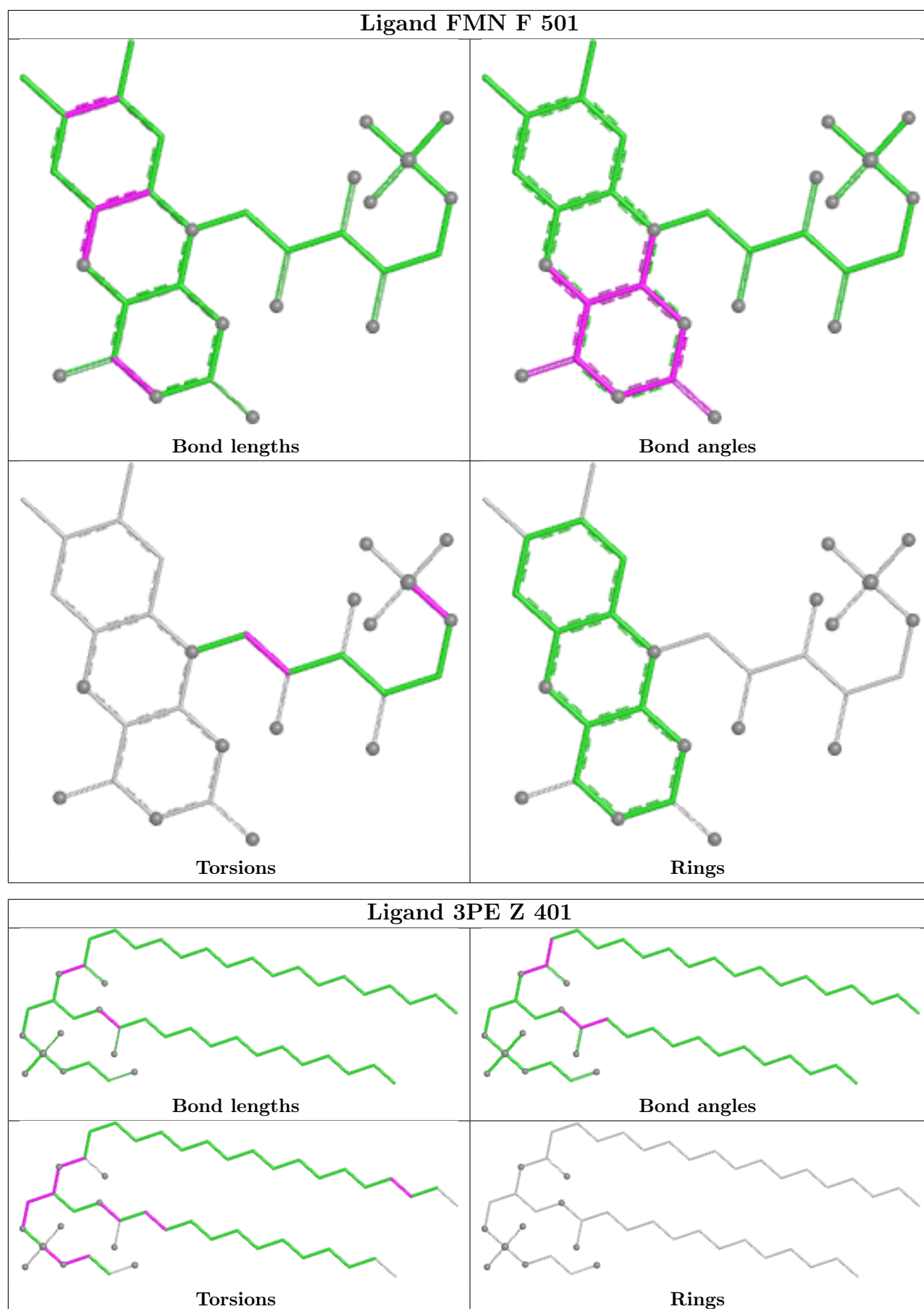
There are no ring outliers.

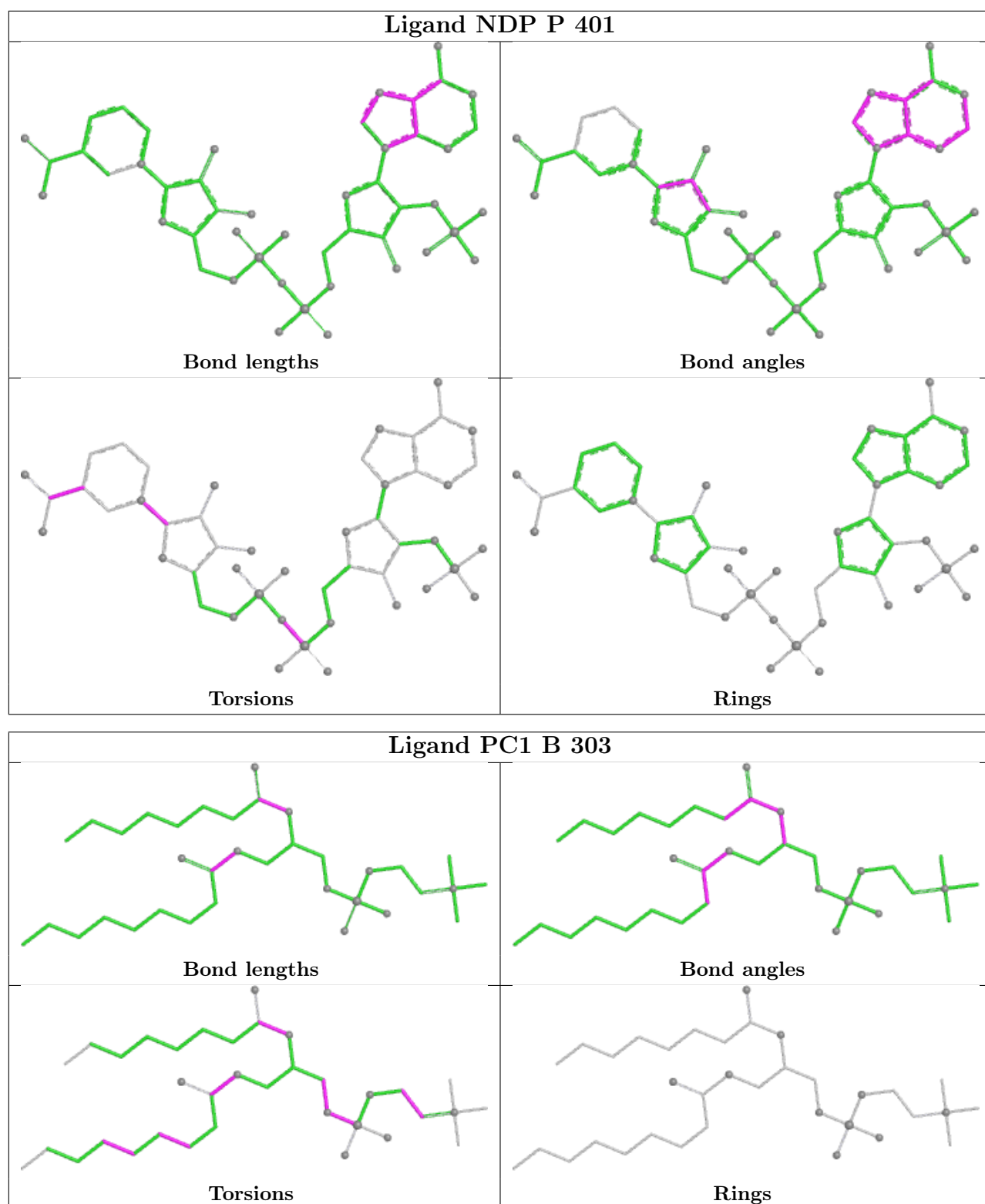
17 monomers are involved in 158 short contacts:

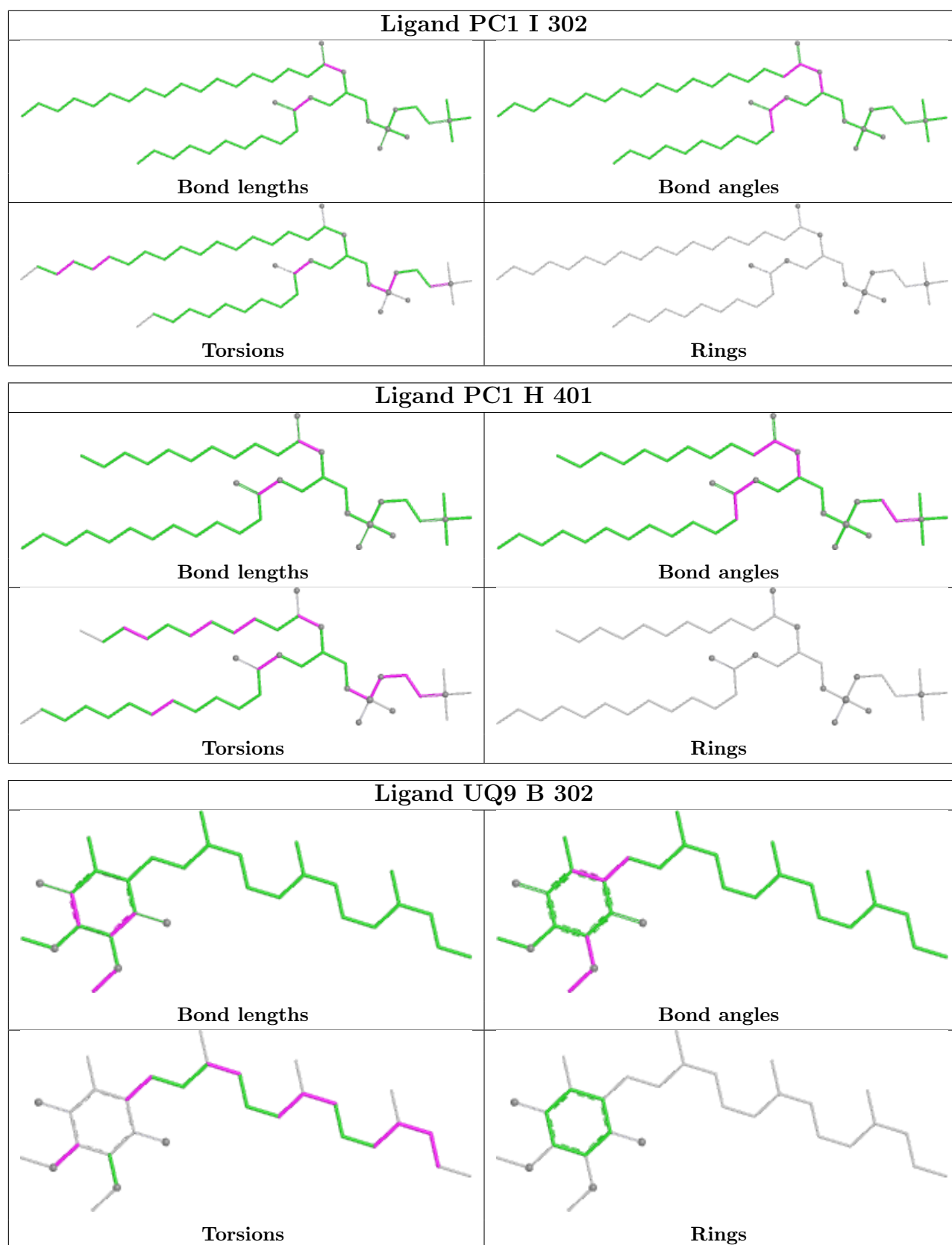
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	101	CDL	28	0
24	I	304	SF4	5	0
28	F	501	FMN	2	0
29	Z	401	3PE	6	0
30	P	401	NDP	7	0
27	G	803	FES	5	0
26	B	303	PC1	6	0
24	I	303	SF4	11	0
26	I	302	PC1	6	0
24	B	301	SF4	6	0
26	H	401	PC1	13	0
24	F	502	SF4	10	0
27	E	301	FES	5	0
25	B	302	UQ9	17	0
29	I	301	3PE	17	0
32	W	201	EHZ	7	0
24	G	802	SF4	7	0

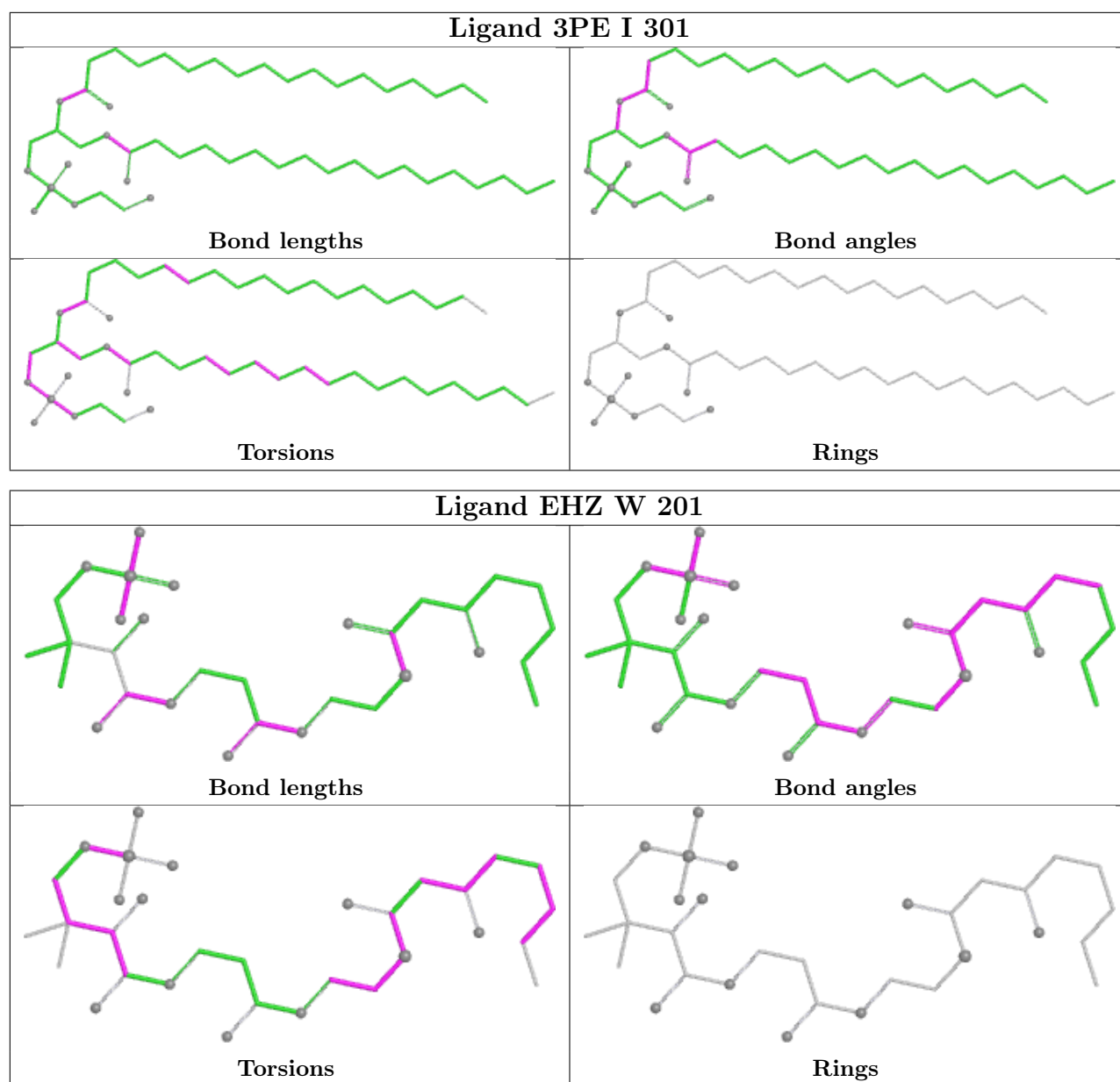
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

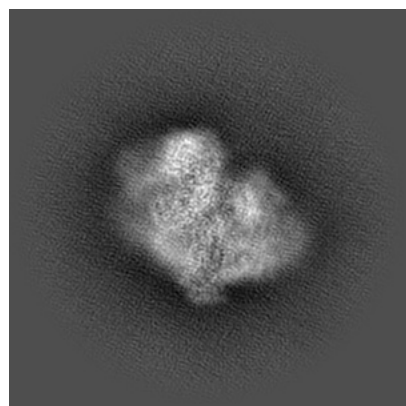
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38510. These allow visual inspection of the internal detail of the map and identification of artifacts.

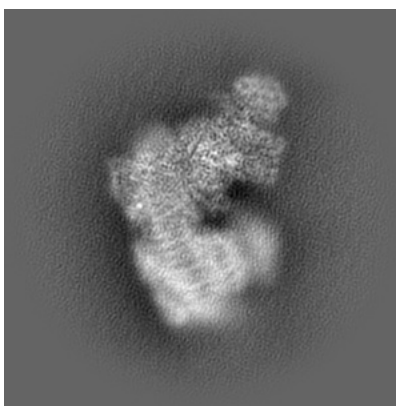
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

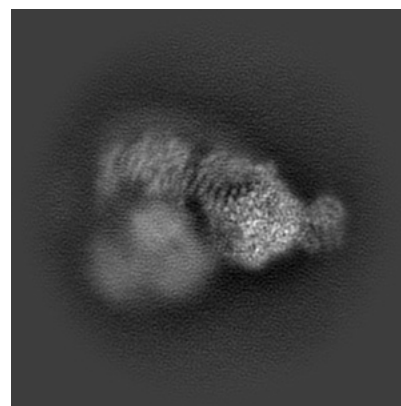
6.1.1 Primary map



X

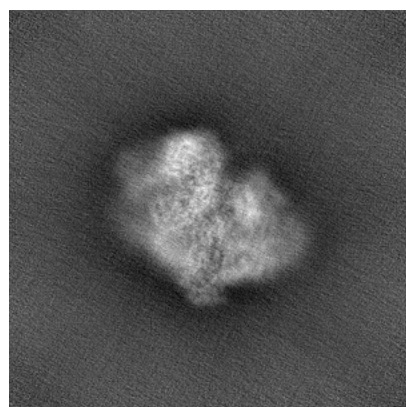


Y

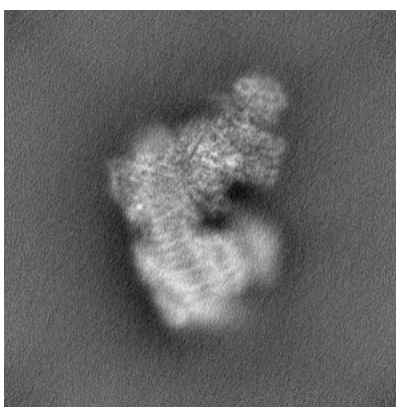


Z

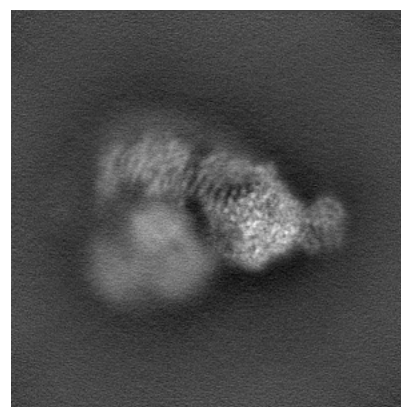
6.1.2 Raw map



X



Y

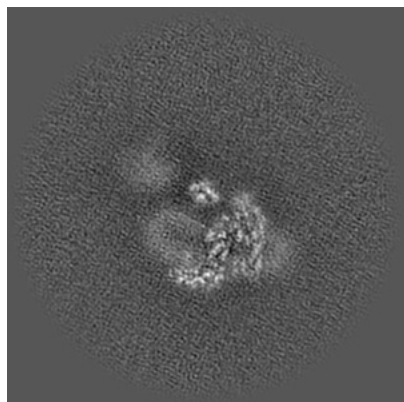


Z

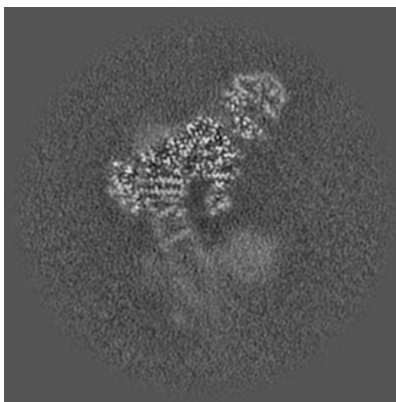
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

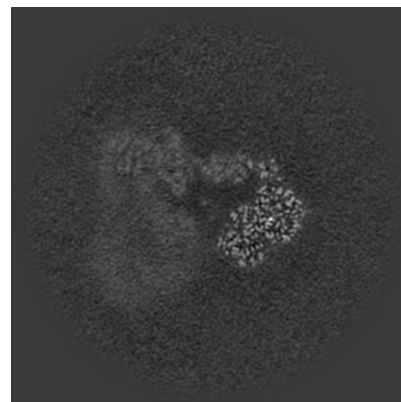
6.2.1 Primary map



X Index: 192

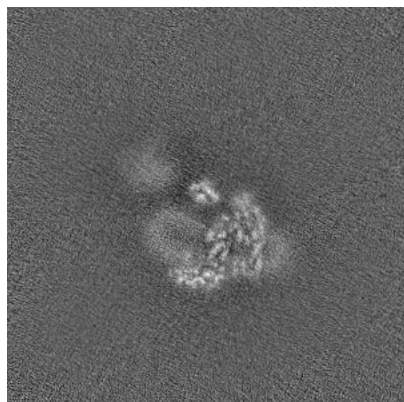


Y Index: 192

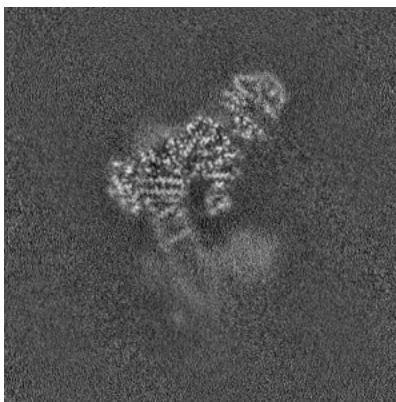


Z Index: 192

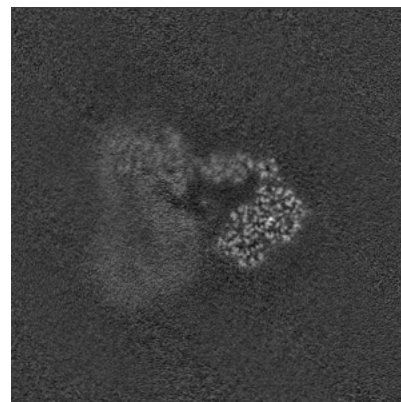
6.2.2 Raw map



X Index: 192



Y Index: 192

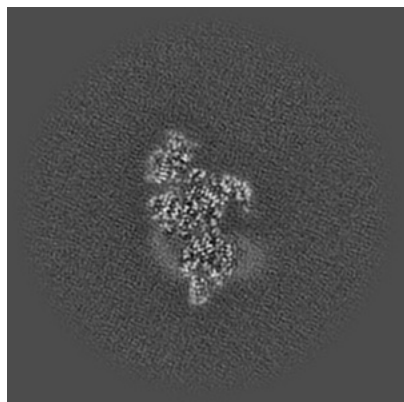


Z Index: 192

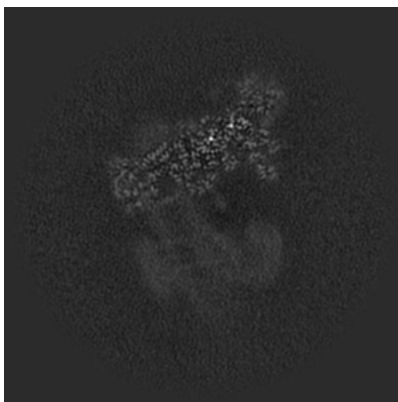
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

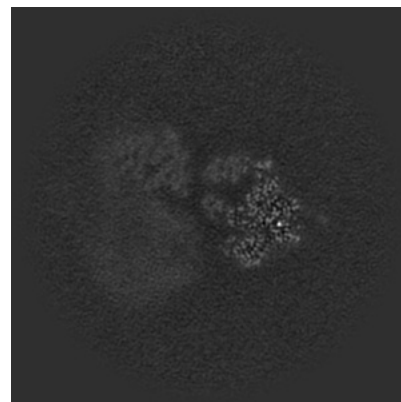
6.3.1 Primary map



X Index: 235

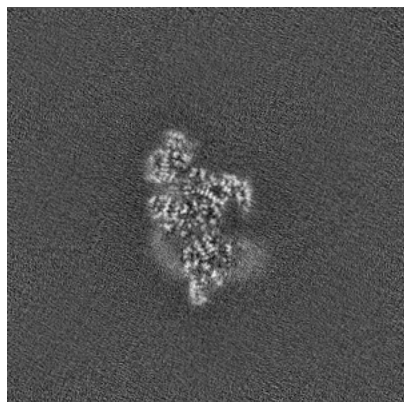


Y Index: 175

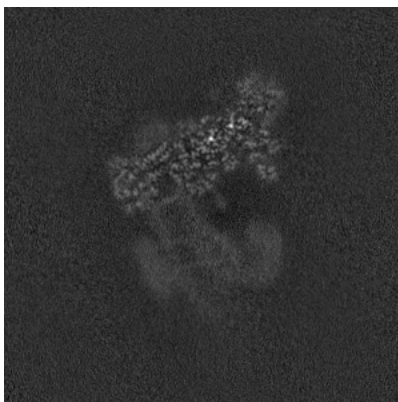


Z Index: 198

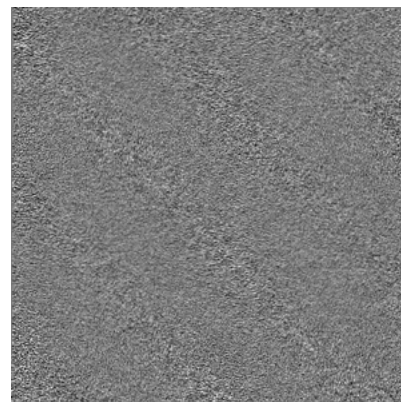
6.3.2 Raw map



X Index: 236



Y Index: 175

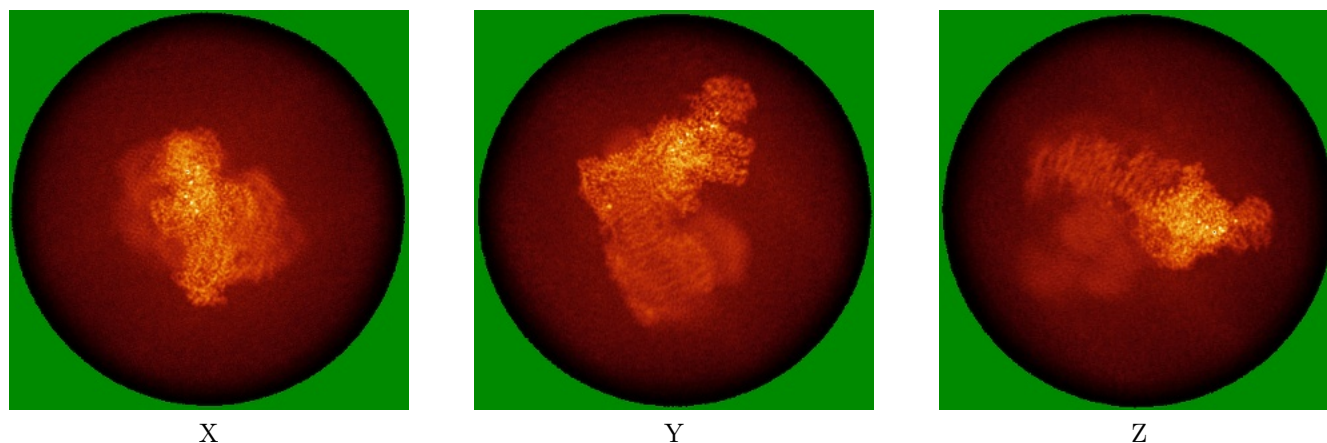


Z Index: 3

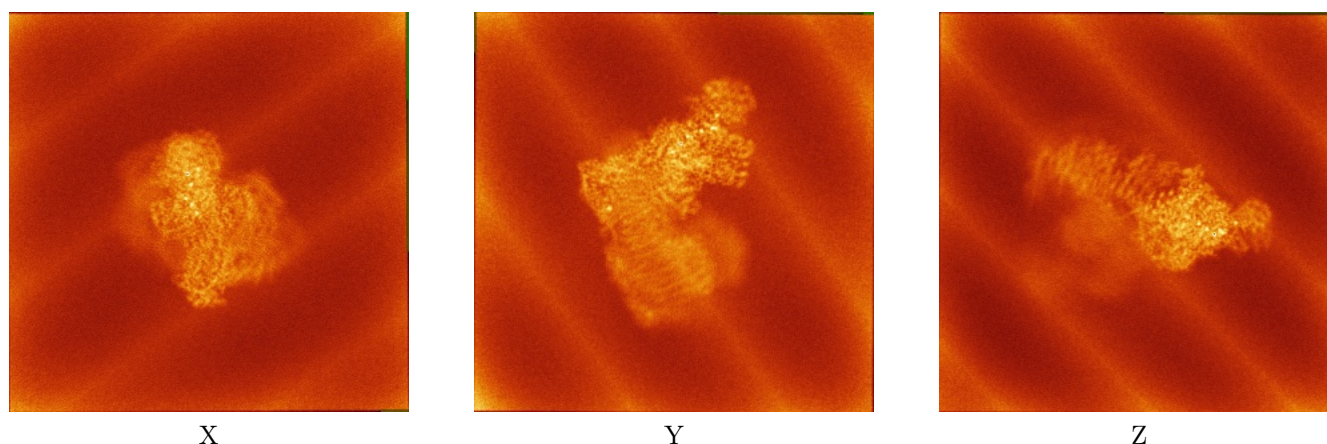
The images above show the largest variance slices of the map in three orthogonal directions.

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.

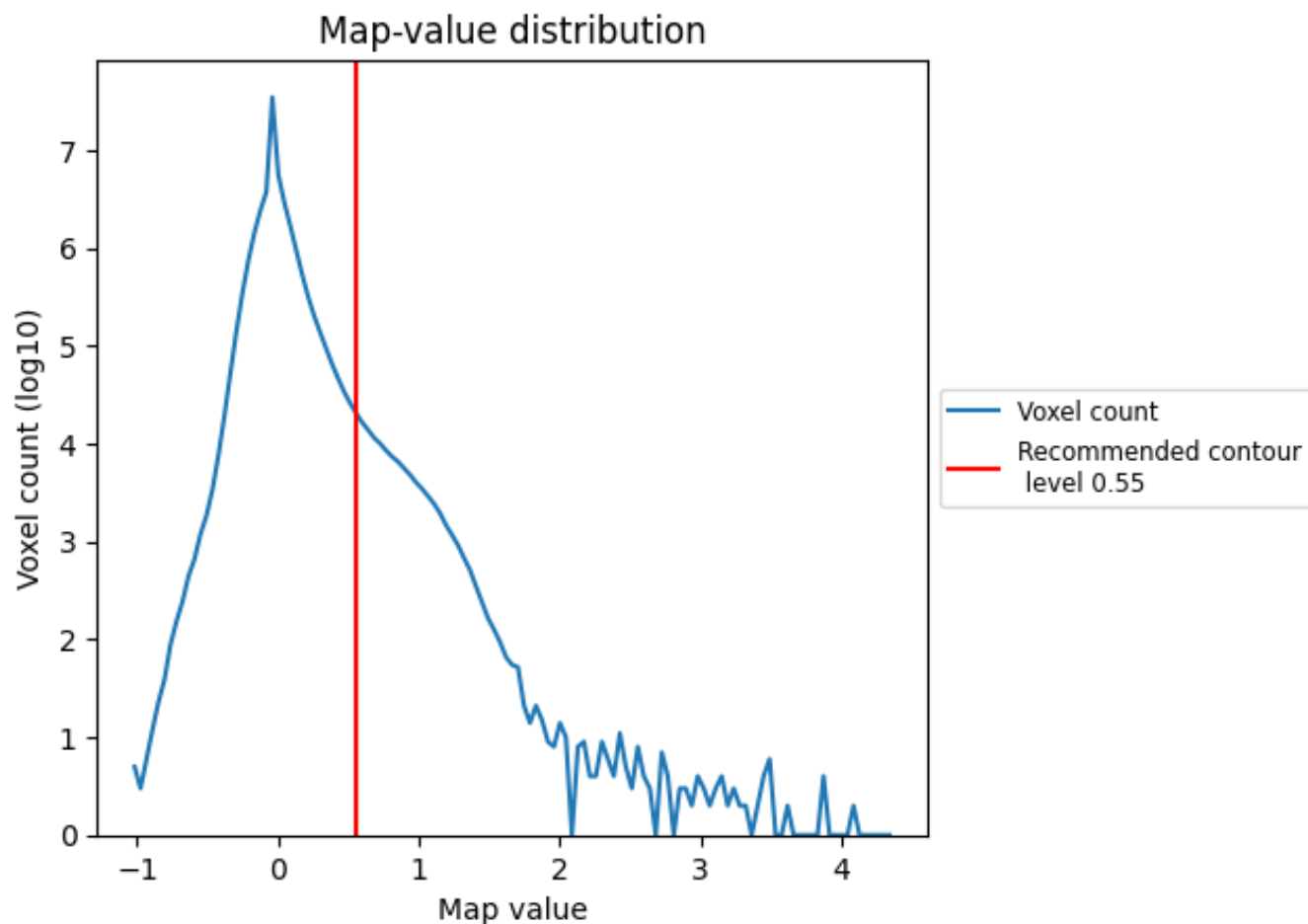
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

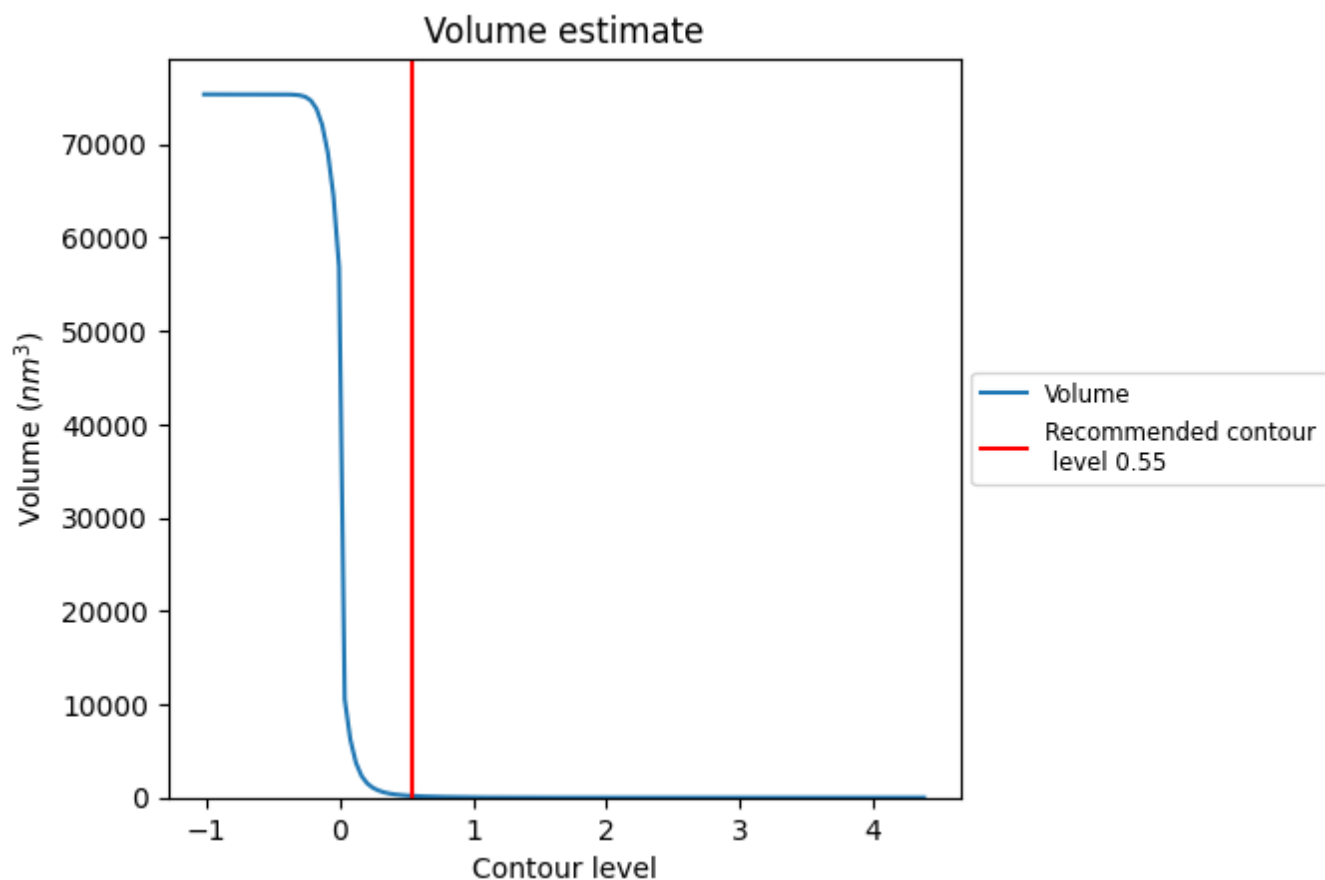
This section contains the results of statistical analysis of the map.

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.

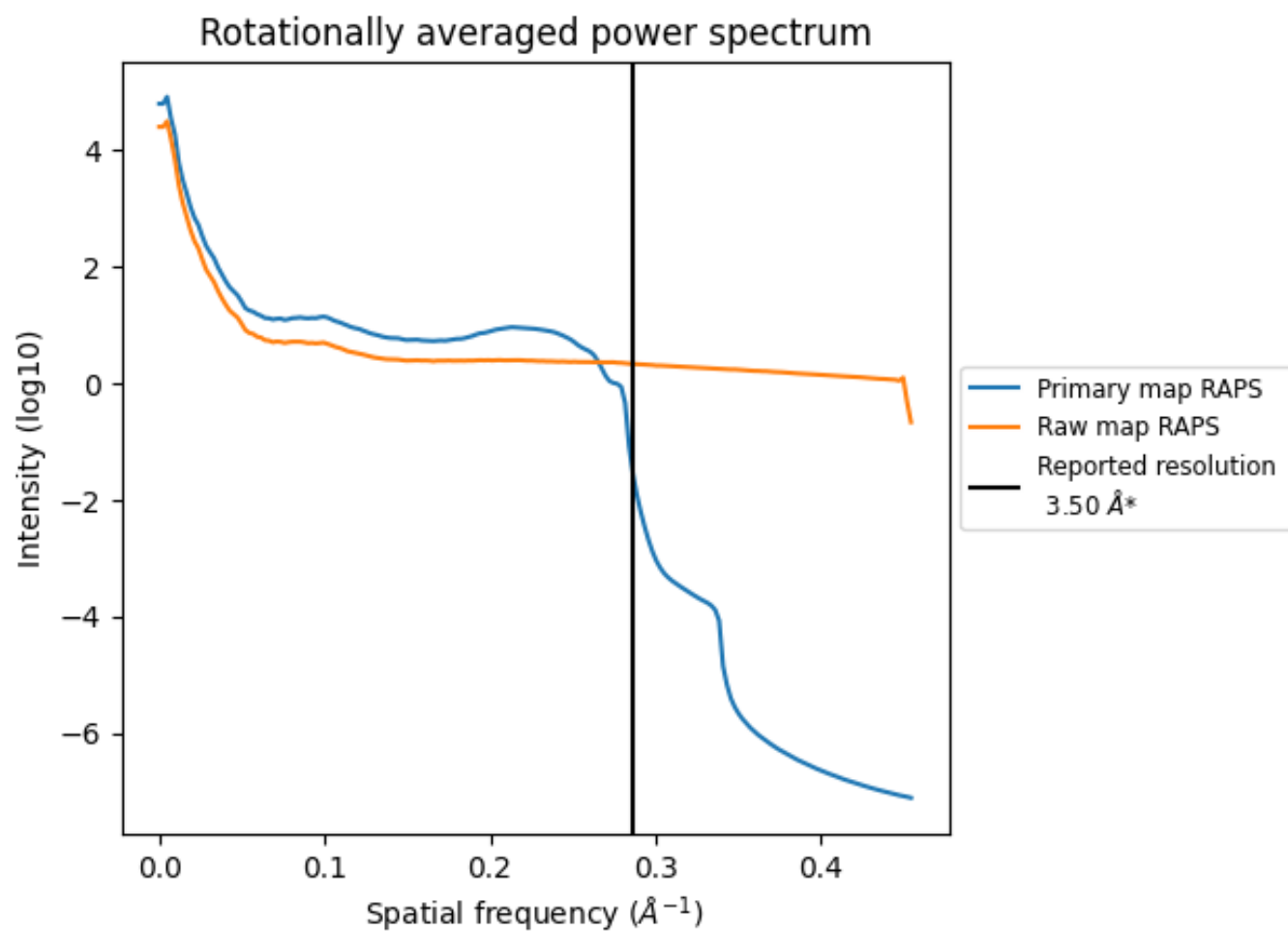
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 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 ⓘ

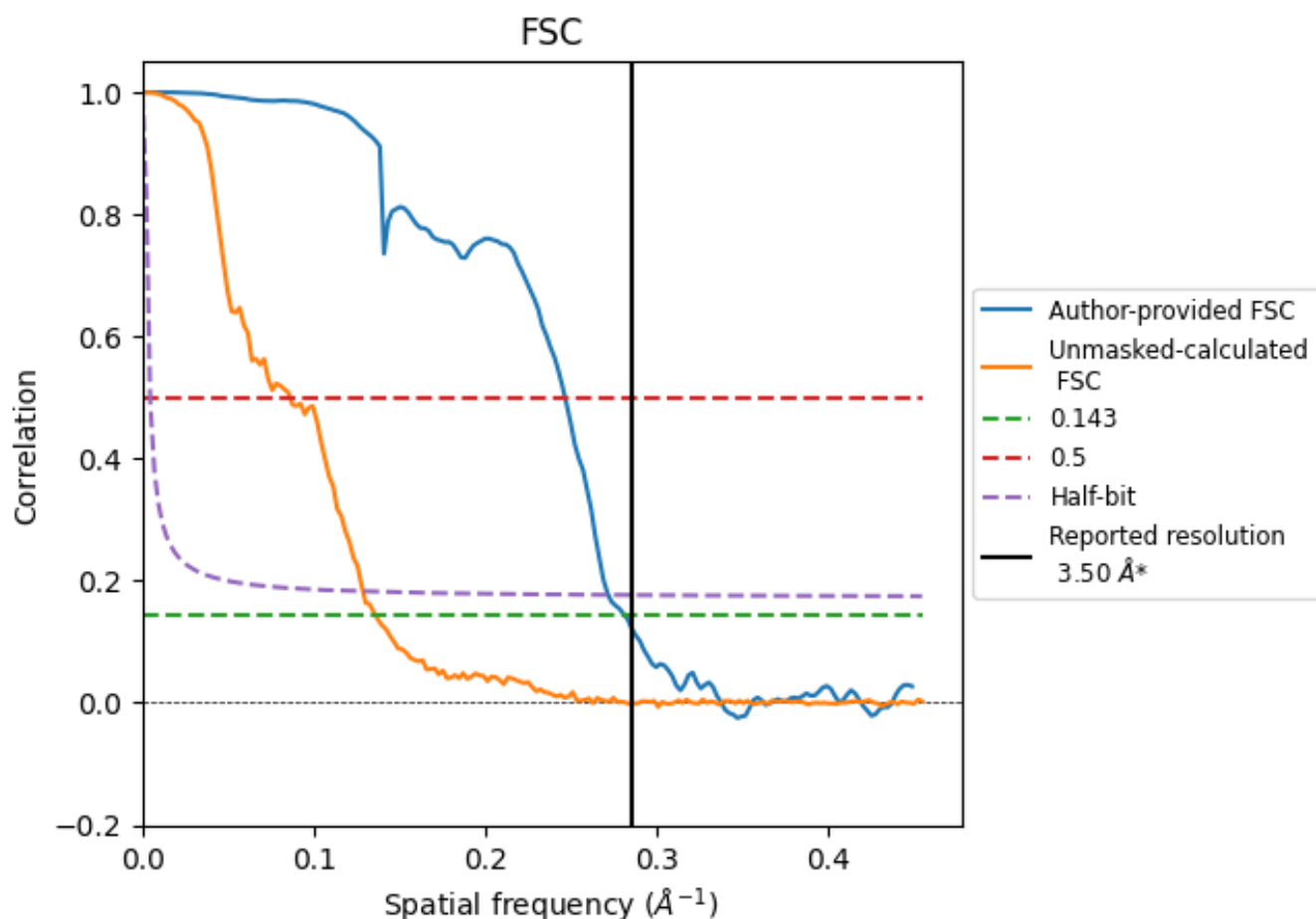


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

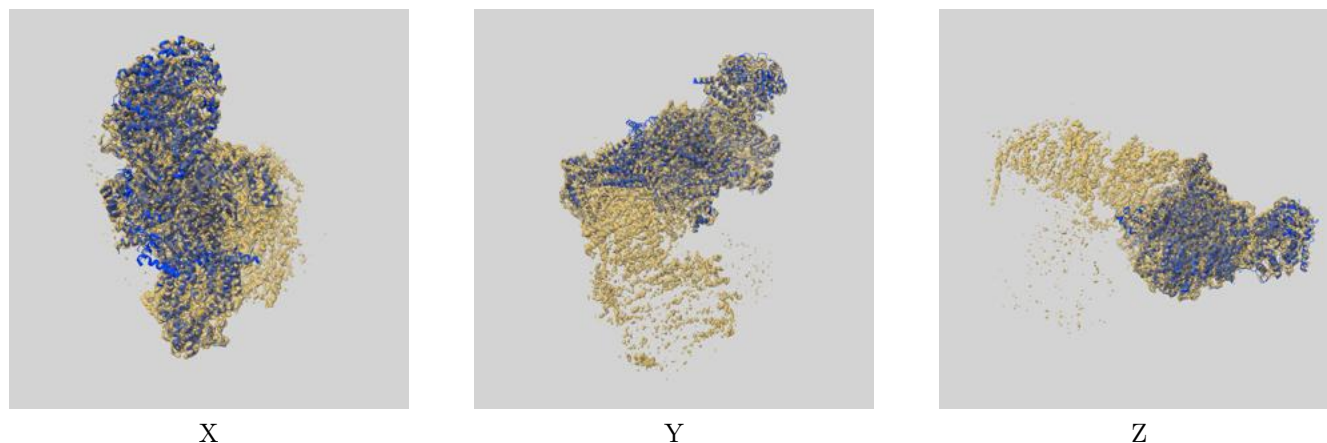
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.56	4.06	3.68
Unmasked-calculated*	7.35	11.60	7.77

*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 7.35 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

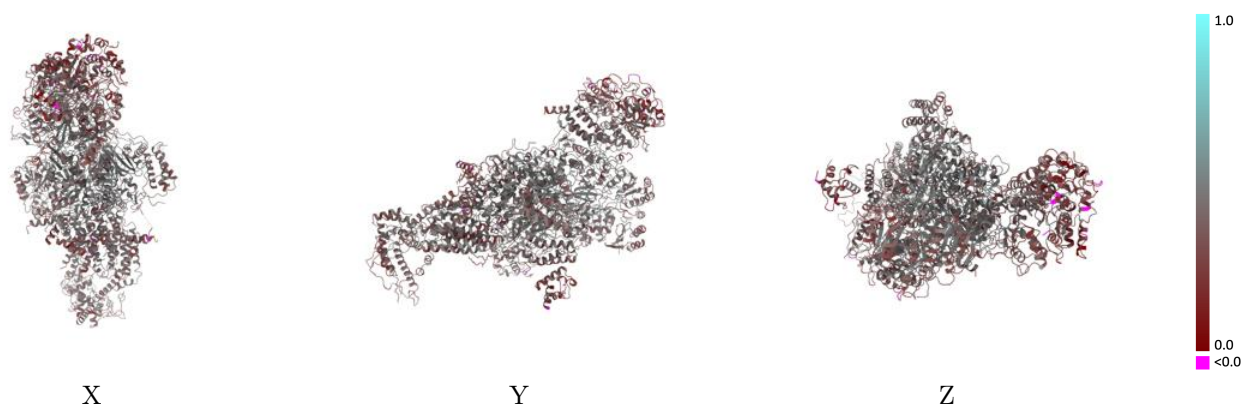
This section contains information regarding the fit between EMDB map EMD-38510 and PDB model 8XNP. Per-residue inclusion information can be found in section 3 on page 15.

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](#)

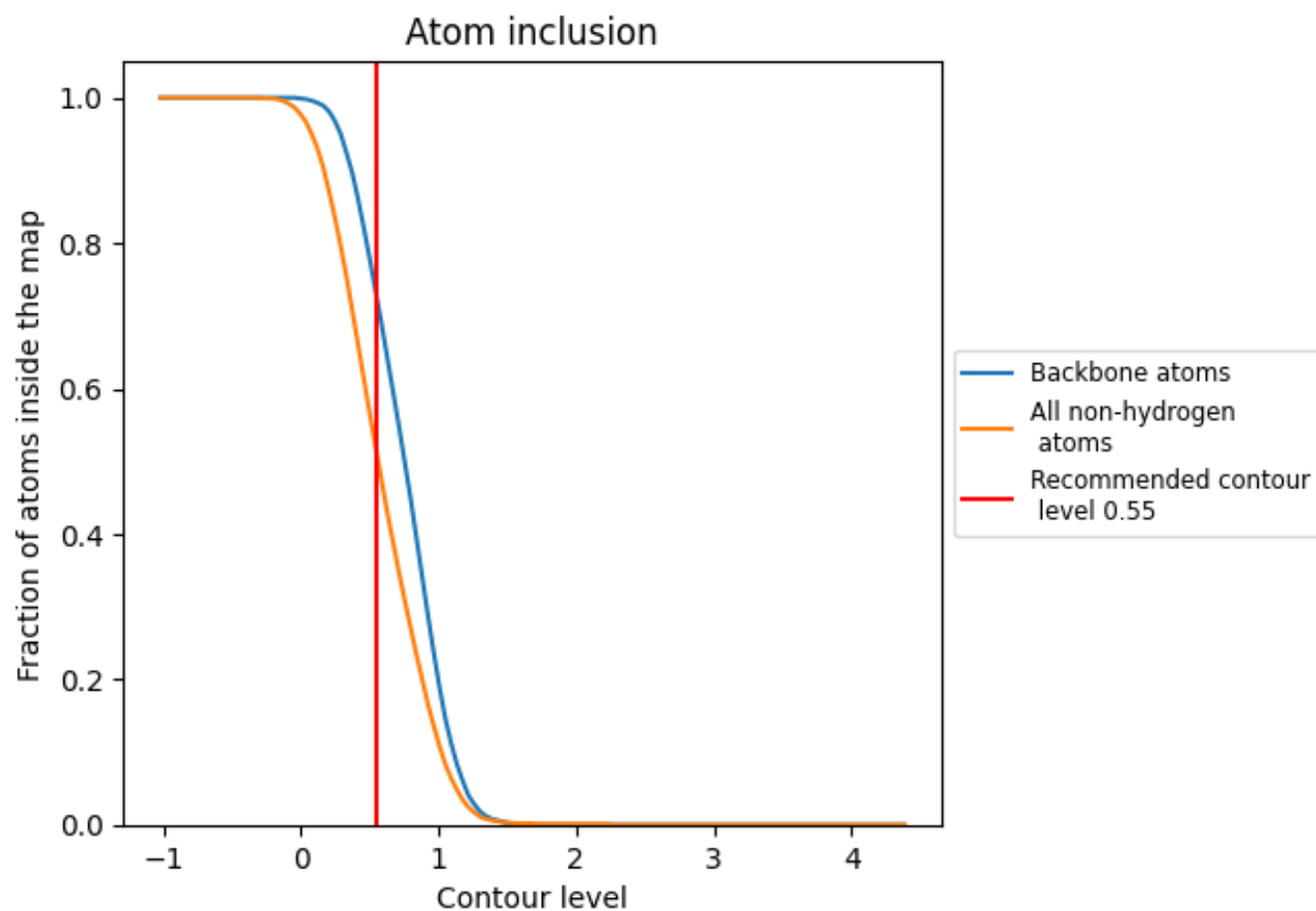


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 73% of all backbone atoms, 51% 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	 0.5130	 0.3890
A	 0.4770	 0.4190
B	 0.5980	 0.4540
C	 0.6130	 0.4550
D	 0.6340	 0.4570
E	 0.3230	 0.3040
F	 0.3990	 0.3280
G	 0.5880	 0.4140
H	 0.5230	 0.3910
I	 0.6130	 0.4340
P	 0.5230	 0.3740
Q	 0.4870	 0.4230
R	 0.2260	 0.3350
S	 0.5490	 0.3490
T	 0.3420	 0.2640
V	 0.5820	 0.3960
W	 0.5120	 0.4000
X	 0.6020	 0.3660
Z	 0.5710	 0.3710
a	 0.5580	 0.3970
b	 0.5610	 0.3770
q	 0.1460	 0.3440
r	 0.2560	 0.3110
s	 0.0660	 0.2200

